



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 23, 2025 – 01:26 am BST

PDB ID : 9GTD / pdb\_00009gtd  
Title : Crystal structure of human lysosomal acid-alpha-glucosidase, GAA, in complex with iminosugar compound 4i  
Authors : Sulzenbacher, G.; Roig-Zamboni, V.; Moracci, M.; Parenti, G.; Py, S.  
Deposited on : 2024-09-17  
Resolution : 2.25 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.46

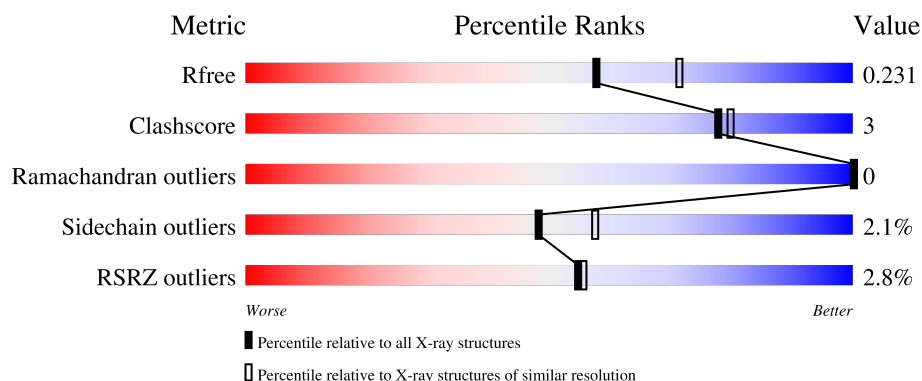
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.25 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.



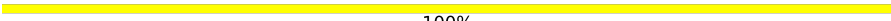
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	164625	1763 (2.26-2.26)
Clashscore	180529	1919 (2.26-2.26)
Ramachandran outliers	177936	1884 (2.26-2.26)
Sidechain outliers	177891	1885 (2.26-2.26)
RSRZ outliers	164620	1763 (2.26-2.26)

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	952	
2	B	3	
2	F	3	
3	C	2	
3	D	2	

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Mol	Chain	Length	Quality of chain
4	E	3	 100%

## 2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 7433 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.

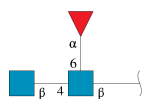
- Molecule 1 is a protein called Lysosomal alpha-glucosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	845	Total	C	N	O	S	0	3	0
			6668	4279	1122	1235	32			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	199	ARG	HIS	variant	UNP P10253
A	223	HIS	ARG	variant	UNP P10253
A	780	ILE	VAL	variant	UNP P10253

- Molecule 2 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
2	B	3	Total	C	N	O	0	0	0
			38	22	2	14			
2	F	3	Total	C	N	O	0	0	0
			38	22	2	14			

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



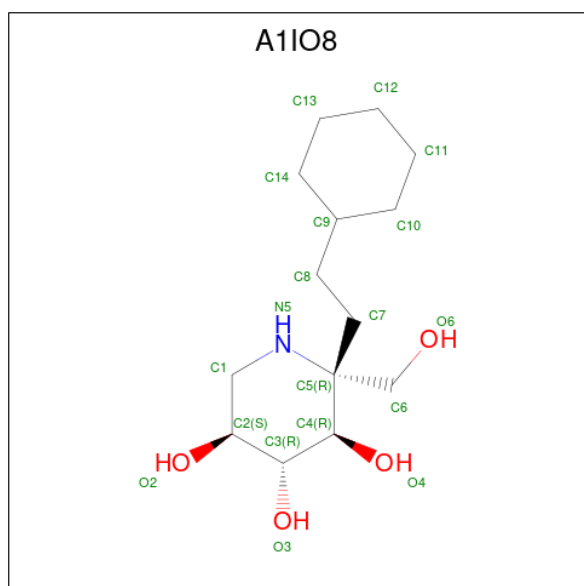
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	D	2	Total	C	N	O	0	0	0
			28	16	2	10			

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



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

- Molecule 5 is (2 {R},3 {R},4 {R},5 {S})-2-(2-cyclohexylethyl)-2-(hydroxymethyl)piperidine-3,4,5-triol (CCD ID: A1IO8) (formula: C<sub>14</sub>H<sub>27</sub>NO<sub>4</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			19	14	1	4		

- Molecule 6 is SULFATE ION (CCD ID: SO4) (formula: O<sub>4</sub>S).



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

- Molecule 7 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

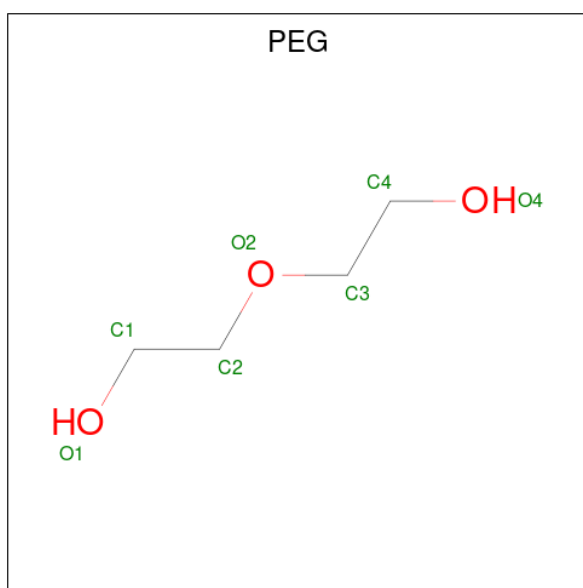
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	3	Total	Cl	0	0
			3	3		

- Molecule 8 is GLYCEROL (CCD ID: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			6	3	3		
8	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 9 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula:  $C_4H_{10}O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	C	O	0	0
			7	4	3		

- Molecule 10 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula:  $C_2H_6O_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	A	1	Total	C	O	0	0
			4	2	2		
10	A	1	Total	C	O	0	0
			4	2	2		
10	A	1	Total	C	O	0	0
			4	2	2		
10	A	1	Total	C	O	0	0
			4	2	2		
10	A	1	Total	C	O	0	0
			4	2	2		
10	A	1	Total	C	O	0	0
			4	2	2		
10	A	1	Total	C	O	0	0
			4	2	2		
10	A	1	Total	C	O	0	0
			4	2	2		
10	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 11 is water.

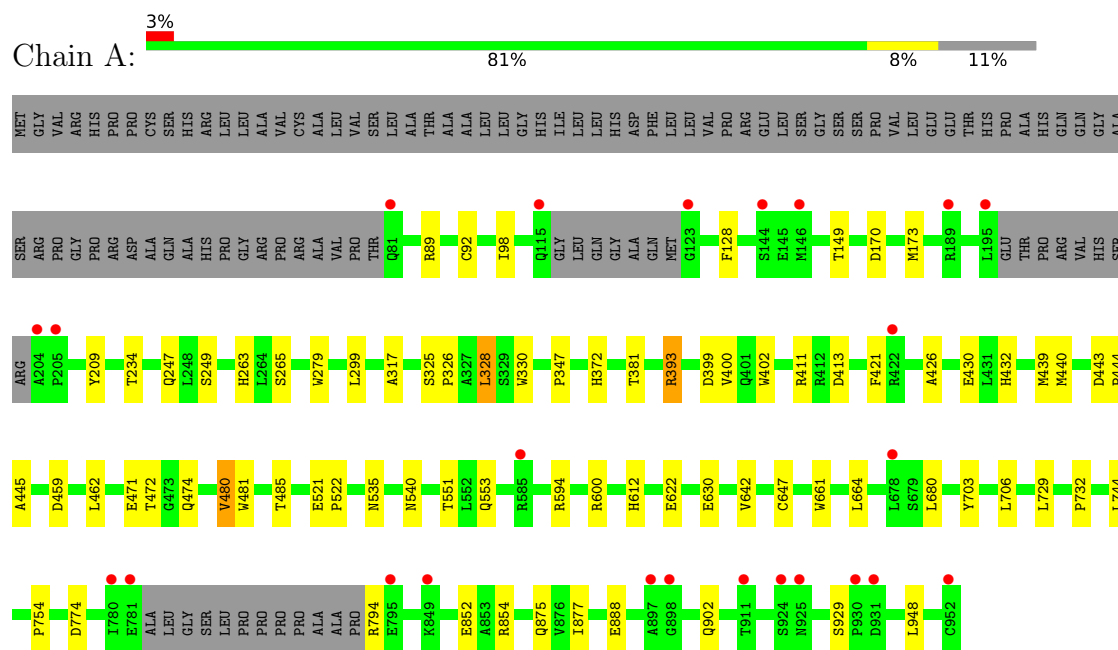
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	484	Total	O	0	0
			484	484		



### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

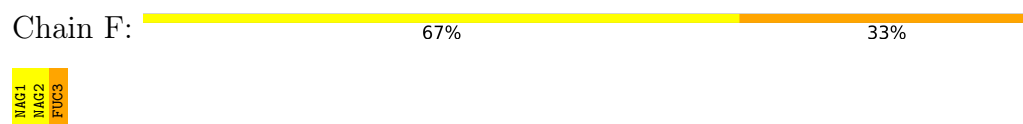
- Molecule 1: Lysosomal alpha-glucosidase



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



- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]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 C:  100%


MAG1  
MAG2

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

Chain D:  100%

MAG1  
MAG2

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

Chain E:  100%

MAG1  
MAG2  
BMA3

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	97.42Å 102.94Å 129.67Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.88 – 2.25 47.88 – 2.25	Depositor EDS
% Data completeness (in resolution range)	99.7 (47.88-2.25) 99.7 (47.88-2.25)	Depositor EDS
$R_{merge}$	0.33	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.13 (at 2.24Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, $R_{free}$	0.172 , 0.220 0.181 , 0.231	Depositor DCC
$R_{free}$ test set	3118 reflections (1.86%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	30.7	Xtriage
Anisotropy	0.233	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 44.2	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	0.95	EDS
Total number of atoms	7433	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.71% 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, PEG, GOL, BMA, EDO, A1IO8, SO4, CL, 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	0.64	1/6876 (0.0%)	1.08	7/9395 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	263	HIS	CE1-NE2	5.45	1.38	1.32

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	888	GLU	CB-CA-C	6.02	120.60	109.70
1	A	902	GLN	CB-CA-C	5.79	119.27	109.55
1	A	622	GLU	CB-CA-C	5.54	120.27	110.85
1	A	594	ARG	CG-CD-NE	-5.43	100.04	112.00
1	A	630	GLU	CB-CG-CD	5.33	121.66	112.60
1	A	393	ARG	CB-CA-C	5.25	120.34	110.63
1	A	459	ASP	CA-CB-CG	5.22	117.82	112.60

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	6668	0	6444	35	0
2	B	38	0	34	0	0
2	F	38	0	34	1	0
3	C	28	0	25	0	0
3	D	28	0	25	1	0
4	E	39	0	34	0	0
5	A	19	0	0	0	0
6	A	25	0	0	0	0
7	A	3	0	0	1	0
8	A	12	0	16	0	0
9	A	7	0	10	0	0
10	A	44	0	66	1	0
11	A	484	0	0	4	0
All	All	7433	0	6688	37	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 3.

All (37) 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)
7:A:1008:CL:CL	11:A:1539:HOH:O	2.37	0.78
1:A:521:GLU:N	1:A:522:PRO:HA	2.16	0.60
1:A:444:PRO:HD2	11:A:1481:HOH:O	2.01	0.60
1:A:664:LEU:HD13	1:A:754:PRO:HG3	1.83	0.59
1:A:443:ASP:HB3	11:A:1481:HOH:O	2.05	0.55
1:A:325:SER:N	1:A:326:PRO:HA	2.21	0.55
1:A:647:CYS:H	1:A:661:TRP:CG	2.27	0.53
1:A:234:THR:HA	1:A:249:SER:O	2.08	0.52
3:D:1:NAG:H61	3:D:2:NAG:H82	1.92	0.52
1:A:299:LEU:C	1:A:299:LEU:HD23	2.35	0.51
1:A:328:LEU:C	1:A:328:LEU:HD23	2.35	0.51
1:A:612:HIS:O	1:A:642:VAL:HA	2.11	0.51
1:A:680:LEU:HD11	2:F:3:FUC:H5	1.92	0.50
1:A:426:ALA:O	1:A:430:GLU:HG3	2.14	0.48
1:A:445:ALA:HB1	1:A:485:THR:HB	1.95	0.48
1:A:472:THR:OG1	1:A:474:GLN:OE1	2.28	0.48
1:A:279:TRP:CE3	1:A:317:ALA:HB2	2.49	0.48
1:A:402:TRP:HA	1:A:439:MET:O	2.14	0.47
1:A:600:ARG:O	1:A:612:HIS:CE1	2.68	0.47
1:A:774:ASP:OD2	1:A:794:ARG:NH1	2.45	0.46
1:A:247:GLN:HA	1:A:330:TRP:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:381:THR:HG23	1:A:421:PHE:HA	1.97	0.45
1:A:89:ARG:HG2	1:A:128:PHE:CD2	2.52	0.45
1:A:703:TYR:HA	1:A:706:LEU:HG	1.99	0.44
1:A:92:CYS:O	1:A:92:CYS:SG	2.76	0.43
1:A:471:GLU:HB2	11:A:1432:HOH:O	2.18	0.43
1:A:149:THR:HG22	1:A:170:ASP:OD1	2.20	0.42
1:A:535:ASN:ND2	1:A:540:ASN:OD1	2.52	0.42
1:A:347:PRO:HG2	1:A:732:PRO:HB3	2.02	0.42
1:A:462:LEU:HD23	1:A:462:LEU:HA	1.86	0.42
1:A:854[B]:ARG:NH2	1:A:877:ILE:HD13	2.35	0.42
1:A:173:MET:HG2	1:A:209:TYR:HE1	1.85	0.41
1:A:413:ASP:OD2	1:A:443:ASP:O	2.39	0.41
1:A:372:HIS:CE1	1:A:400:VAL:HG21	2.54	0.41
1:A:480:VAL:HG12	1:A:481:TRP:H	1.86	0.41
1:A:744:LEU:HD23	1:A:744:LEU:N	2.35	0.41
1:A:432:HIS:HA	10:A:1022:EDO:H21	2.04	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	840/952 (88%)	813 (97%)	27 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	725/806 (90%)	710 (98%)	15 (2%)	48 57

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	98	ILE
1	A	265	SER
1	A	328	LEU
1	A	393	ARG
1	A	399	ASP
1	A	411	ARG
1	A	440	MET
1	A	480	VAL
1	A	551	THR
1	A	553	GLN
1	A	729	LEU
1	A	852	GLU
1	A	875	GLN
1	A	929	SER
1	A	948	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	352	GLN
1	A	401	GLN
1	A	535	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 ⓘ

13 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	0.59	0	17,19,21	1.09	2 (11%)
2	NAG	B	2	2	14,14,15	0.84	0	17,19,21	1.73	3 (17%)
2	FUC	B	3	2	10,10,11	0.74	0	14,14,16	1.15	2 (14%)
3	NAG	C	1	3,1	14,14,15	0.44	0	17,19,21	1.72	4 (23%)
3	NAG	C	2	3	14,14,15	0.84	0	17,19,21	1.76	4 (23%)
3	NAG	D	1	3,1	14,14,15	0.72	0	17,19,21	1.29	3 (17%)
3	NAG	D	2	3	14,14,15	0.73	0	17,19,21	1.68	3 (17%)
4	NAG	E	1	4,1	14,14,15	0.66	0	17,19,21	1.68	4 (23%)
4	NAG	E	2	4	14,14,15	0.68	0	17,19,21	1.48	4 (23%)
4	BMA	E	3	4	11,11,12	0.67	0	15,15,17	1.60	2 (13%)
2	NAG	F	1	2,1	14,14,15	0.72	0	17,19,21	1.22	1 (5%)
2	NAG	F	2	2	14,14,15	0.64	0	17,19,21	1.47	2 (11%)
2	FUC	F	3	2	10,10,11	1.16	0	14,14,16	1.81	4 (28%)

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	-	1/6/23/26	0/1/1/1
2	NAG	B	2	2	-	2/6/23/26	0/1/1/1
2	FUC	B	3	2	-	-	0/1/1/1
3	NAG	C	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	C	2	3	-	2/6/23/26	0/1/1/1
3	NAG	D	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	D	2	3	-	4/6/23/26	0/1/1/1
4	NAG	E	1	4,1	-	0/6/23/26	0/1/1/1

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

There are no bond length outliers.

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	3	BMA	O5-C5-C6	4.43	114.15	107.20
3	D	2	NAG	C4-C3-C2	4.37	117.42	111.02
2	B	2	NAG	C4-C3-C2	4.02	116.91	111.02
3	C	2	NAG	C1-O5-C5	3.87	117.44	112.19
4	E	1	NAG	O5-C5-C6	3.63	112.89	107.20
3	C	1	NAG	C4-C3-C2	3.52	116.18	111.02
4	E	2	NAG	C1-O5-C5	3.46	116.88	112.19
4	E	1	NAG	C1-O5-C5	3.44	116.85	112.19
2	B	2	NAG	C1-O5-C5	-3.43	107.54	112.19
2	F	2	NAG	C2-N2-C7	3.43	127.79	122.90
2	F	1	NAG	C1-O5-C5	3.31	116.67	112.19
3	D	2	NAG	C1-O5-C5	3.29	116.66	112.19
3	C	2	NAG	O5-C5-C6	-3.06	102.41	107.20
2	B	2	NAG	O5-C5-C6	3.05	111.98	107.20
2	F	3	FUC	O5-C1-C2	-3.04	106.07	110.77
3	C	2	NAG	C3-C4-C5	2.98	115.55	110.24
3	C	1	NAG	C2-N2-C7	-2.94	118.72	122.90
3	C	1	NAG	O5-C5-C6	2.82	111.63	107.20
2	F	3	FUC	O2-C2-C1	2.82	114.92	109.15
4	E	2	NAG	O7-C7-N2	-2.71	116.97	121.95
2	F	3	FUC	O5-C5-C4	2.70	114.36	109.52
3	C	1	NAG	O5-C1-C2	-2.63	107.14	111.29
3	D	2	NAG	C3-C4-C5	2.58	114.84	110.24
2	B	1	NAG	O5-C1-C2	-2.58	107.22	111.29
4	E	1	NAG	C2-N2-C7	-2.57	119.24	122.90
2	B	3	FUC	O3-C3-C4	2.41	115.92	110.35
2	B	1	NAG	C4-C3-C2	2.33	114.44	111.02
2	F	2	NAG	C1-O5-C5	2.22	115.20	112.19
4	E	1	NAG	O6-C6-C5	-2.14	103.94	111.29
2	F	3	FUC	C1-C2-C3	-2.13	107.04	109.67
4	E	2	NAG	C6-C5-C4	-2.09	108.10	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	3	FUC	O2-C2-C3	-2.08	105.98	110.14
3	D	1	NAG	C1-O5-C5	2.03	114.94	112.19
4	E	2	NAG	C8-C7-N2	2.02	119.52	116.10
3	D	1	NAG	O5-C1-C2	-2.02	108.10	111.29
3	D	1	NAG	C4-C3-C2	2.01	113.97	111.02
4	E	3	BMA	O2-C2-C3	2.01	114.16	110.14
3	C	2	NAG	O5-C1-C2	-2.00	108.13	111.29

There are no chirality outliers.

All (13) torsion outliers are listed below:

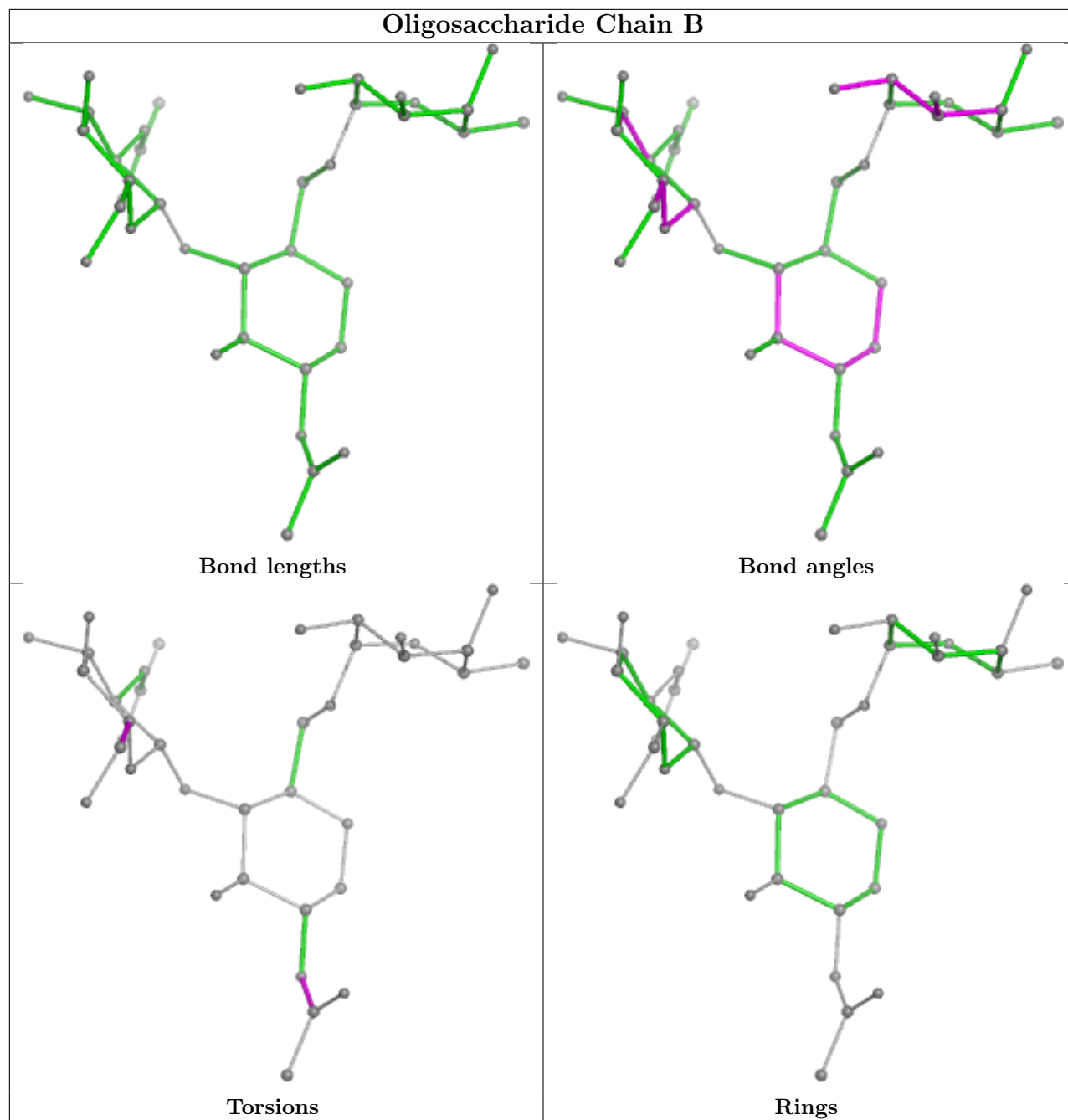
Mol	Chain	Res	Type	Atoms
2	F	2	NAG	C8-C7-N2-C2
2	F	2	NAG	O7-C7-N2-C2
3	D	2	NAG	O5-C5-C6-O6
3	D	2	NAG	C4-C5-C6-O6
2	B	2	NAG	C4-C5-C6-O6
2	B	2	NAG	O5-C5-C6-O6
3	C	2	NAG	O5-C5-C6-O6
3	D	2	NAG	C8-C7-N2-C2
3	C	2	NAG	C4-C5-C6-O6
4	E	3	BMA	C4-C5-C6-O6
4	E	3	BMA	O5-C5-C6-O6
3	D	2	NAG	O7-C7-N2-C2
2	B	1	NAG	C8-C7-N2-C2

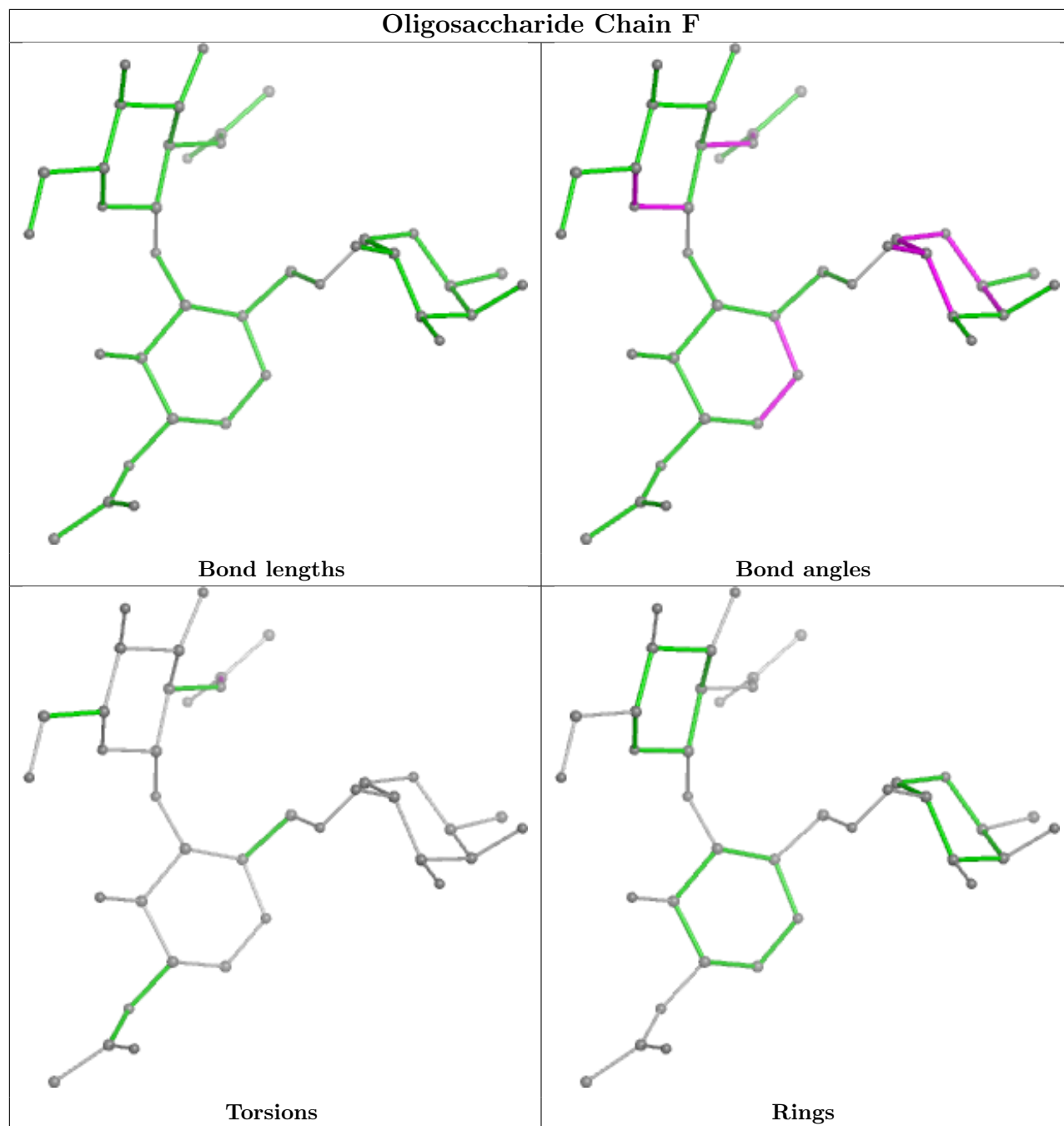
There are no ring outliers.

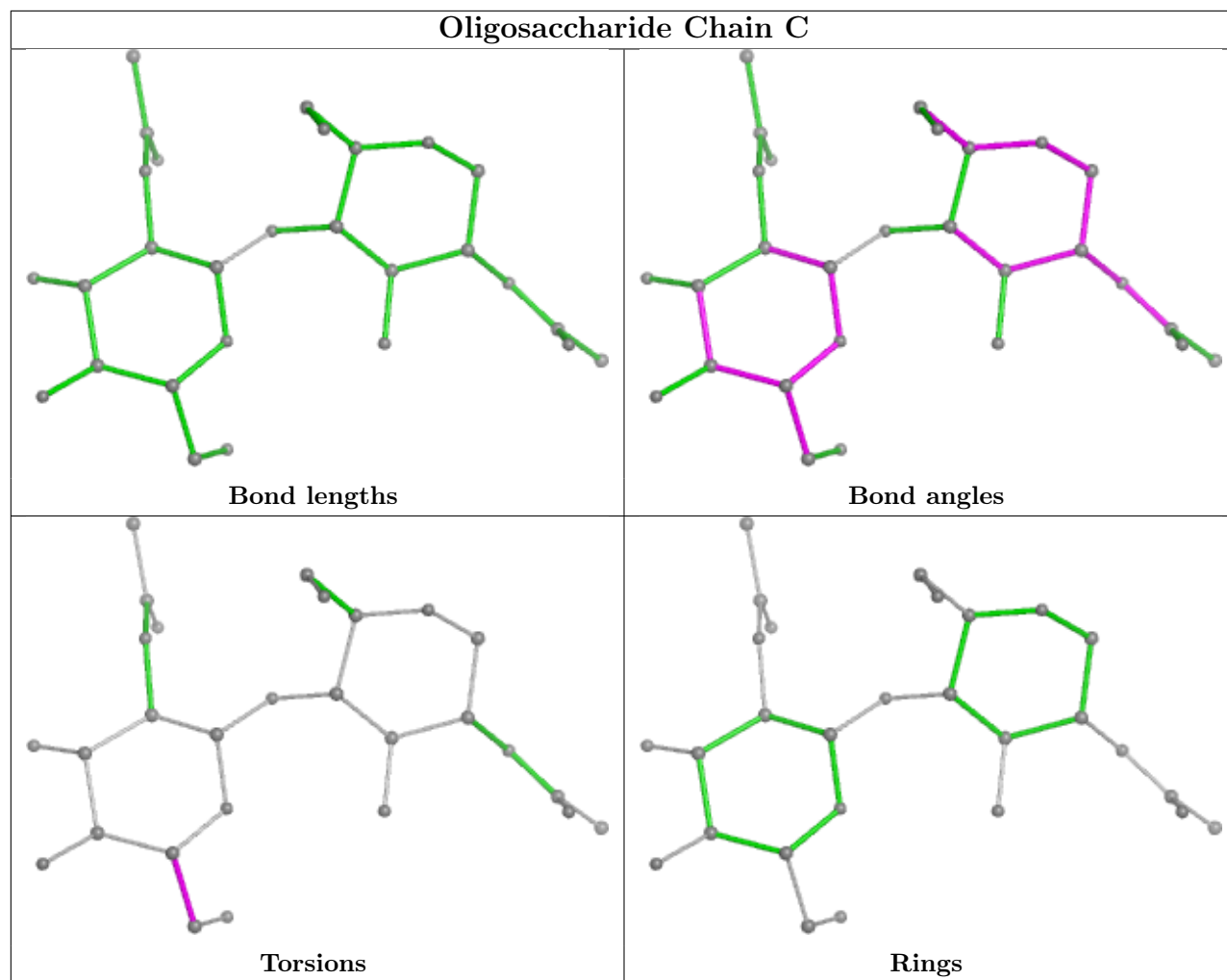
3 monomers are involved in 2 short contacts:

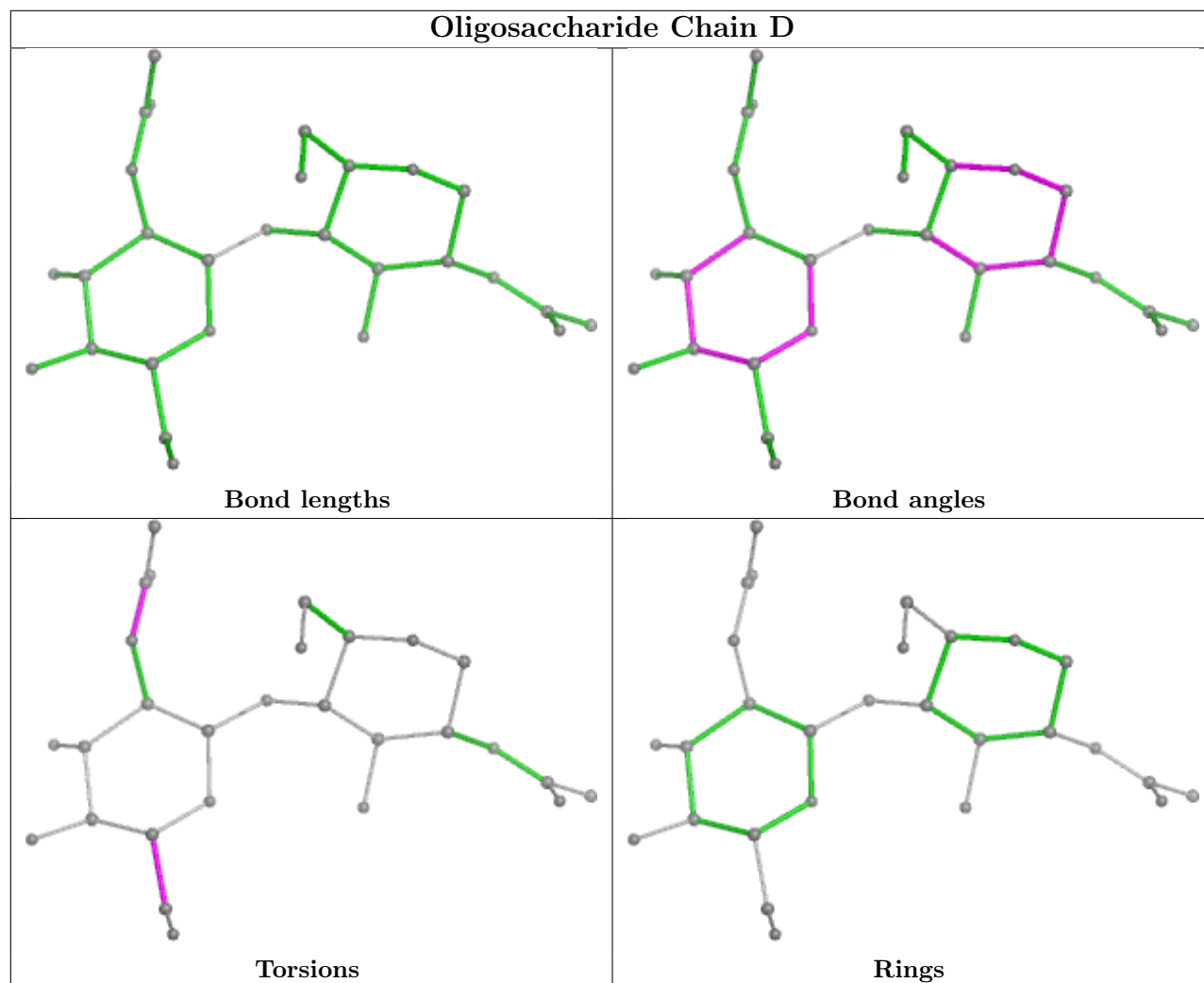
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	3	FUC	1	0
3	D	2	NAG	1	0
3	D	1	NAG	1	0

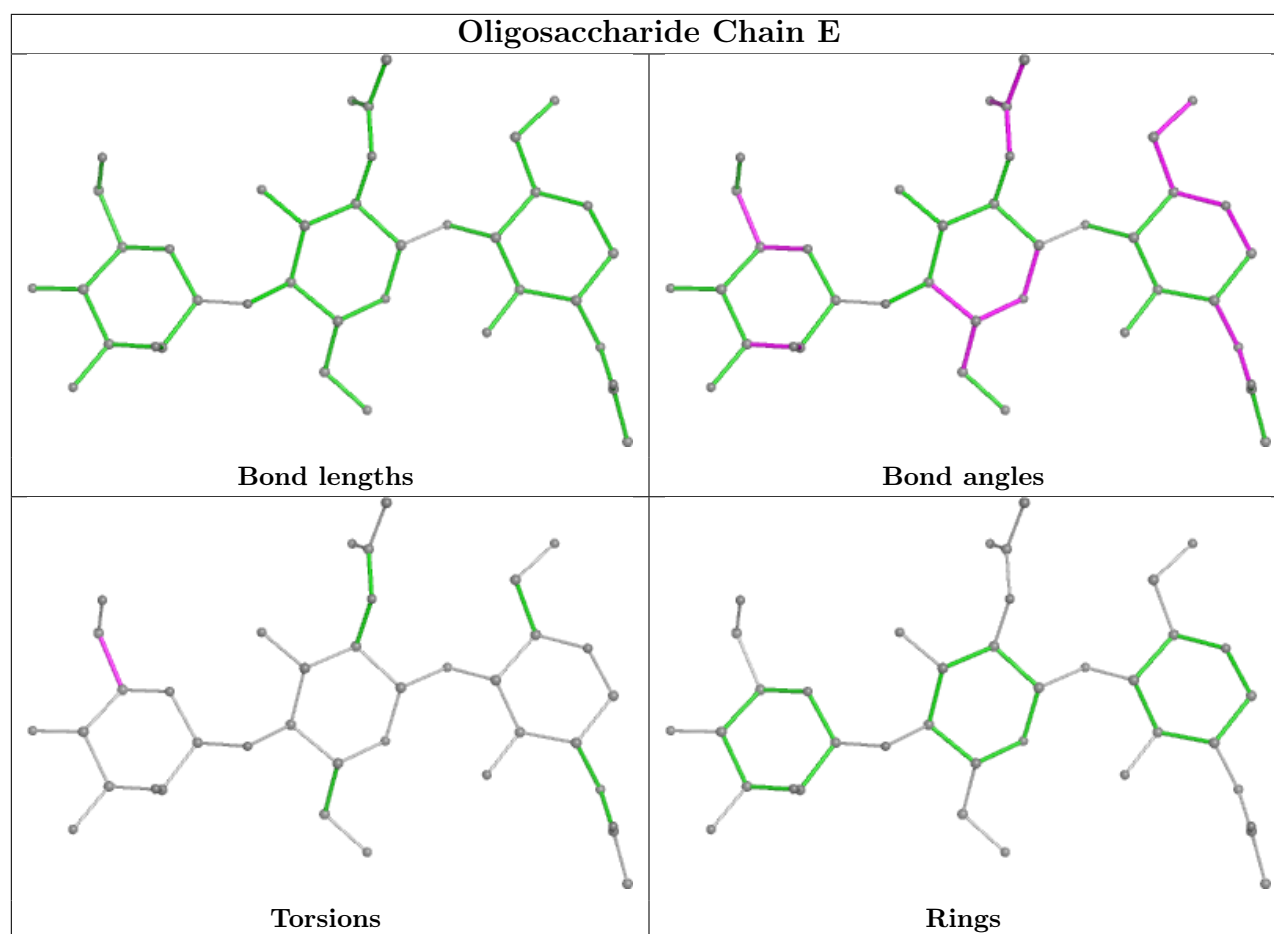
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.











## 5.6 Ligand geometry [i](#)

Of 23 ligands modelled in this entry, 3 are monoatomic - leaving 20 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	$\# Z  > 2$
10	EDO	A	1017	-	3,3,3	0.26	0	2,2,2	0.70	0
8	GOL	A	1010	-	5,5,5	0.11	0	5,5,5	0.29	0
10	EDO	A	1023	-	3,3,3	0.38	0	2,2,2	0.73	0
10	EDO	A	1015	-	3,3,3	0.24	0	2,2,2	0.19	0
10	EDO	A	1020	-	3,3,3	0.14	0	2,2,2	0.37	0
10	EDO	A	1021	-	3,3,3	0.30	0	2,2,2	0.62	0
6	SO4	A	1006	-	4,4,4	0.23	0	6,6,6	0.09	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
10	EDO	A	1022	-	3,3,3	0.22	0	2,2,2	0.92	0
6	SO4	A	1004	-	4,4,4	0.23	0	6,6,6	0.06	0
10	EDO	A	1019	-	3,3,3	0.39	0	2,2,2	0.29	0
10	EDO	A	1016	-	3,3,3	0.30	0	2,2,2	0.37	0
10	EDO	A	1013	-	3,3,3	0.90	0	2,2,2	0.33	0
6	SO4	A	1002	-	4,4,4	0.27	0	6,6,6	0.21	0
6	SO4	A	1003	-	4,4,4	0.41	0	6,6,6	0.15	0
8	GOL	A	1011	-	5,5,5	0.33	0	5,5,5	0.92	0
5	A1IO8	A	1001	-	16,20,20	0.73	1 (6%)	21,28,28	1.45	4 (19%)
9	PEG	A	1012	-	6,6,6	0.63	0	5,5,5	0.37	0
10	EDO	A	1018	-	3,3,3	0.42	0	2,2,2	0.46	0
6	SO4	A	1005	-	4,4,4	0.29	0	6,6,6	0.23	0
10	EDO	A	1014	-	3,3,3	0.26	0	2,2,2	0.03	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	EDO	A	1021	-	-	0/1/1/1	-
10	EDO	A	1016	-	-	0/1/1/1	-
8	GOL	A	1011	-	-	2/4/4/4	-
5	A1IO8	A	1001	-	-	2/9/37/37	0/2/2/2
9	PEG	A	1012	-	-	1/4/4/4	-
10	EDO	A	1022	-	-	1/1/1/1	-
10	EDO	A	1017	-	-	1/1/1/1	-
8	GOL	A	1010	-	-	0/4/4/4	-
10	EDO	A	1023	-	-	0/1/1/1	-
10	EDO	A	1018	-	-	1/1/1/1	-
10	EDO	A	1019	-	-	1/1/1/1	-
10	EDO	A	1015	-	-	1/1/1/1	-
10	EDO	A	1013	-	-	1/1/1/1	-
10	EDO	A	1020	-	-	1/1/1/1	-
10	EDO	A	1014	-	-	1/1/1/1	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1001	A1IO8	C2-C3	2.50	1.56	1.52

All (4) bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1001	A1IO8	C12-C11-C10	2.69	116.91	111.42
5	A	1001	A1IO8	C2-C1-N5	-2.39	106.13	111.08
5	A	1001	A1IO8	C7-C8-C9	2.19	119.75	113.95
5	A	1001	A1IO8	C11-C10-C9	2.16	116.23	112.15

There are no chirality outliers.

All (13) torsion outliers are listed below:

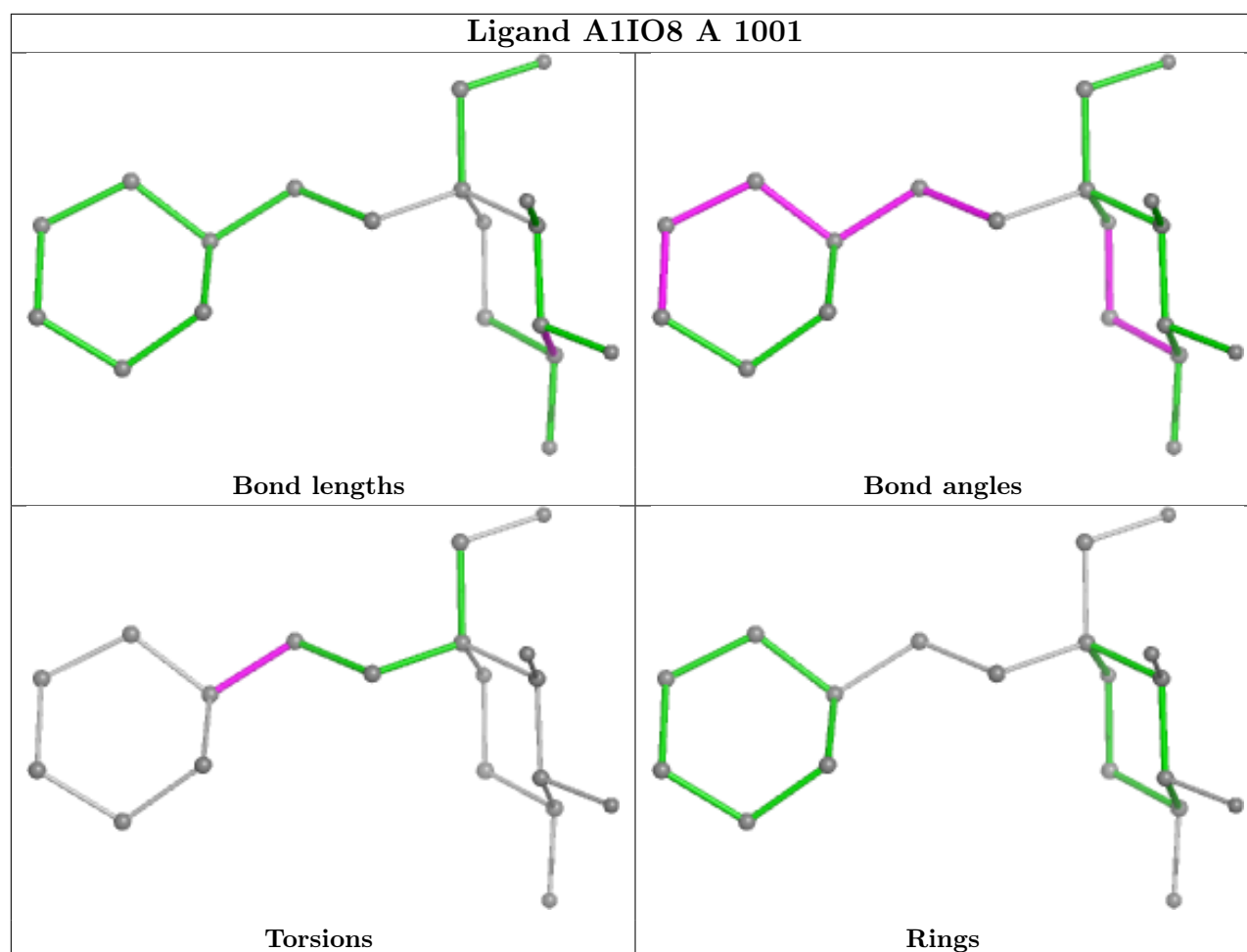
Mol	Chain	Res	Type	Atoms
8	A	1011	GOL	O1-C1-C2-C3
5	A	1001	A1IO8	C7-C8-C9-C14
10	A	1017	EDO	O1-C1-C2-O2
5	A	1001	A1IO8	C7-C8-C9-C10
8	A	1011	GOL	O1-C1-C2-O2
10	A	1014	EDO	O1-C1-C2-O2
10	A	1015	EDO	O1-C1-C2-O2
10	A	1019	EDO	O1-C1-C2-O2
10	A	1018	EDO	O1-C1-C2-O2
10	A	1020	EDO	O1-C1-C2-O2
10	A	1013	EDO	O1-C1-C2-O2
10	A	1022	EDO	O1-C1-C2-O2
9	A	1012	PEG	C1-C2-O2-C3

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	A	1022	EDO	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	845/952 (88%)	-0.11	24 (2%) 55 55	29, 50, 71, 119	3 (0%)

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	195	LEU	5.1
1	A	204	ALA	4.9
1	A	781	GLU	4.8
1	A	144	SER	3.9
1	A	146	MET	3.9
1	A	81	GLN	3.7
1	A	911	THR	3.3
1	A	925	ASN	3.2
1	A	897	ALA	3.1
1	A	115	GLN	3.0
1	A	678	LEU	3.0
1	A	205	PRO	3.0
1	A	931	ASP	2.7
1	A	795	GLU	2.7
1	A	780	ILE	2.5
1	A	123	GLY	2.4
1	A	898	GLY	2.4
1	A	930	PRO	2.2
1	A	189	ARG	2.2
1	A	422	ARG	2.1
1	A	924	SER	2.1
1	A	952	CYS	2.1
1	A	849	LYS	2.1
1	A	585	ARG	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 6.3 Carbohydrates ⓘ

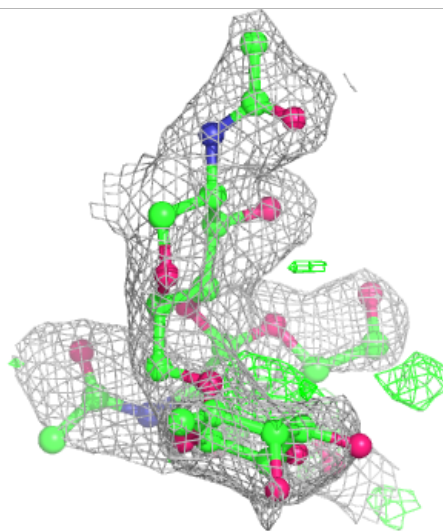
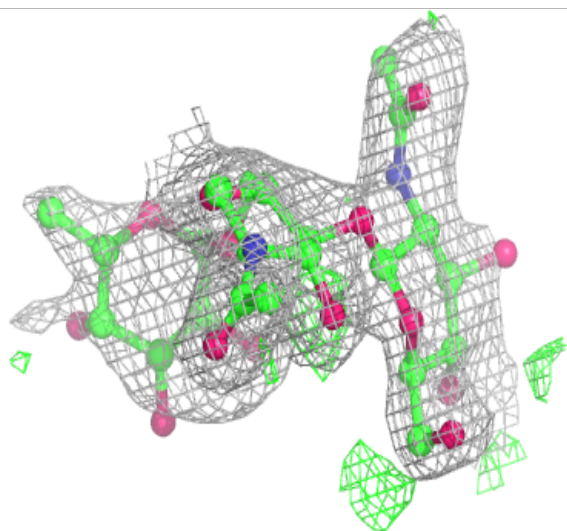
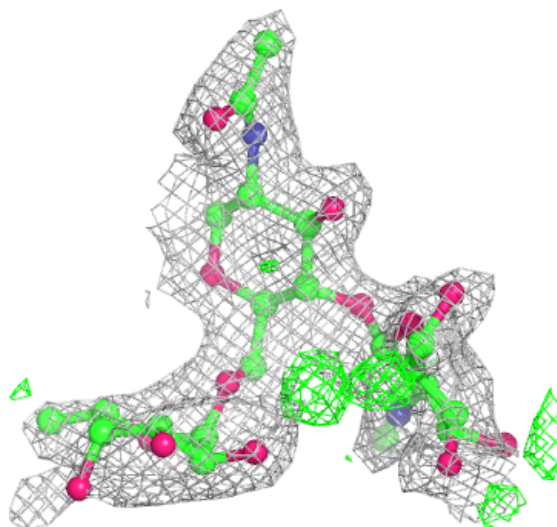
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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	F	2	14/15	0.57	0.23	96,132,146,149	0
4	BMA	E	3	11/12	0.67	0.19	84,96,104,116	0
3	NAG	D	2	14/15	0.69	0.20	75,110,136,150	0
2	NAG	B	2	14/15	0.70	0.20	78,94,113,113	0
2	FUC	F	3	10/11	0.71	0.25	84,104,115,125	0
2	FUC	B	3	10/11	0.73	0.21	87,97,104,109	0
3	NAG	C	2	14/15	0.74	0.20	68,86,96,96	0
2	NAG	F	1	14/15	0.86	0.16	68,89,100,117	0
3	NAG	D	1	14/15	0.92	0.12	50,63,77,86	0
3	NAG	C	1	14/15	0.93	0.10	50,60,67,75	0
4	NAG	E	2	14/15	0.94	0.10	43,61,65,79	0
2	NAG	B	1	14/15	0.95	0.10	58,66,74,84	0
4	NAG	E	1	14/15	0.98	0.07	49,52,57,59	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.

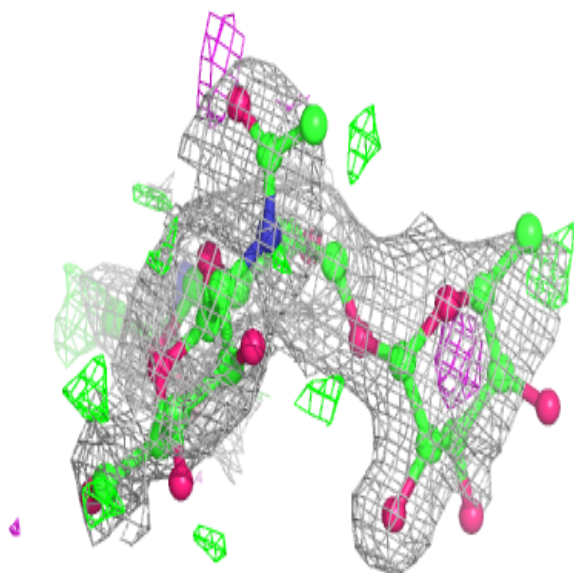
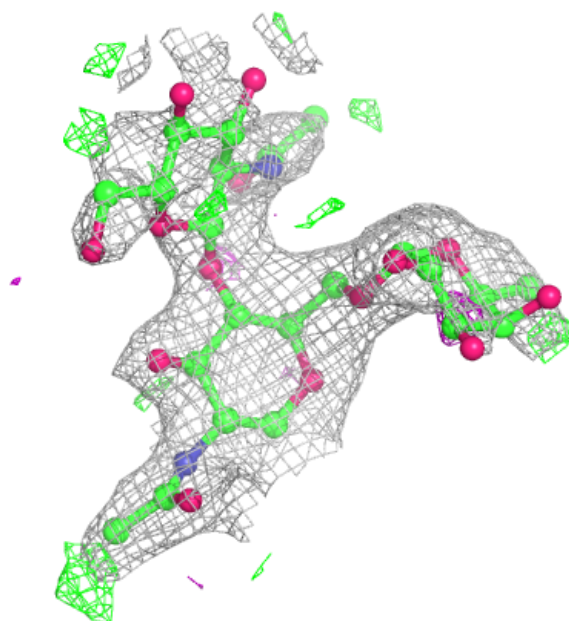
**Electron density around Chain B:**

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



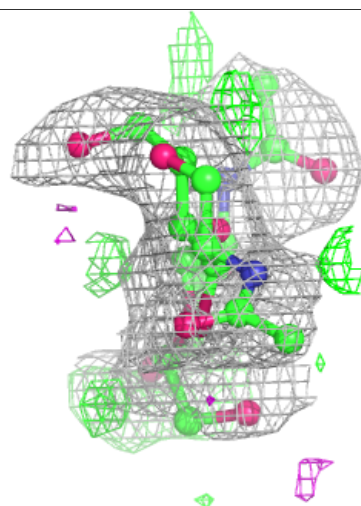
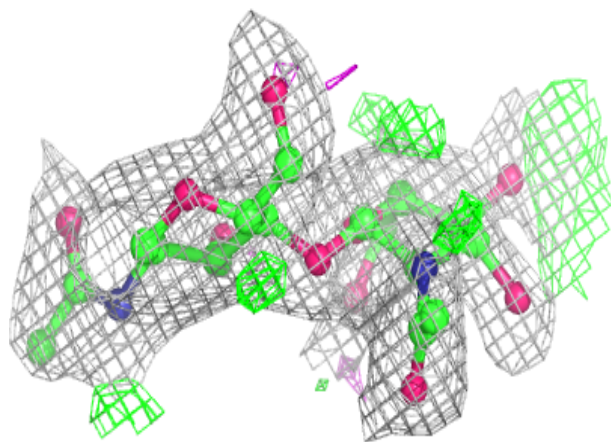
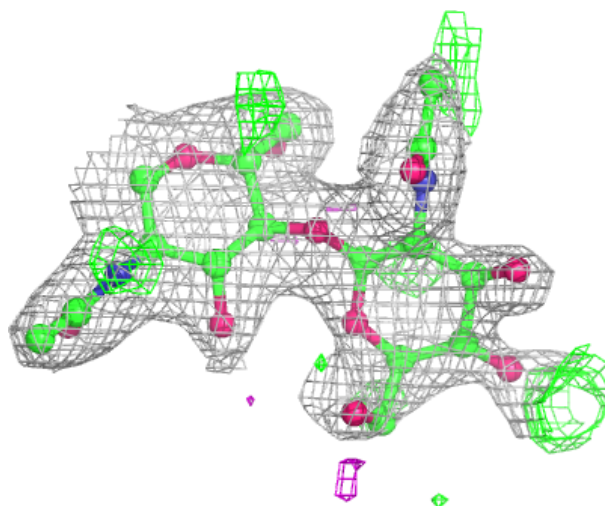
**Electron density around Chain F:**

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



**Electron density around Chain C:**

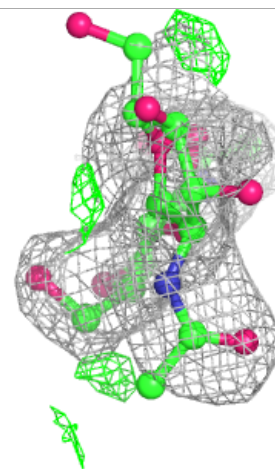
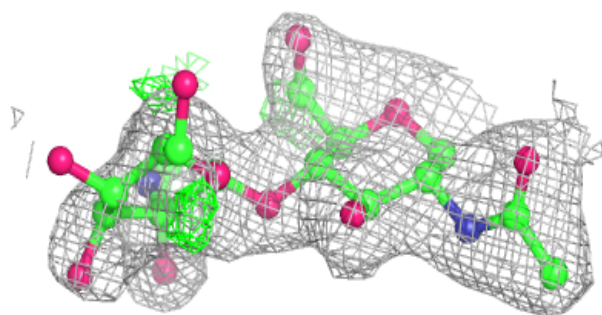
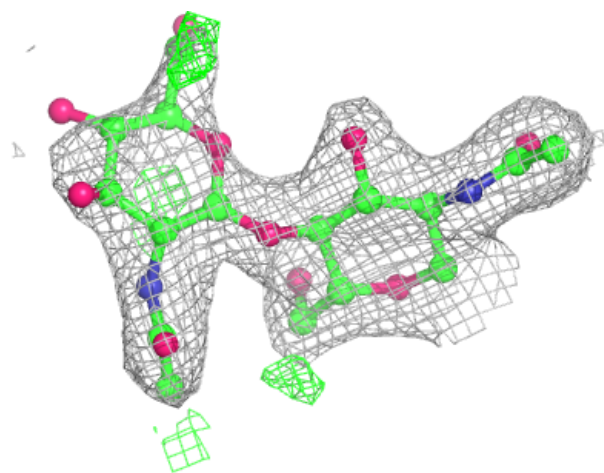
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



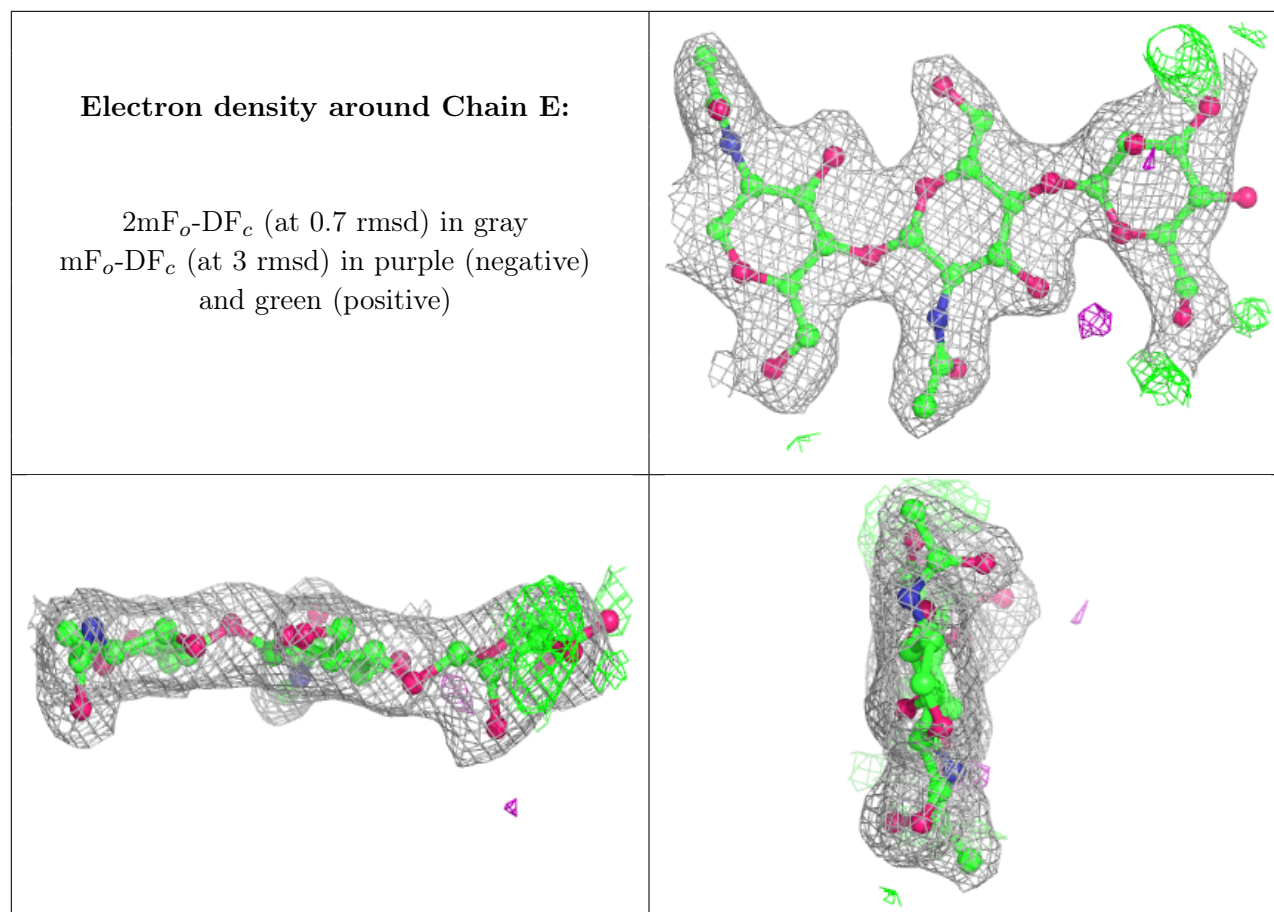


**Electron density around Chain D:**

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







## 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
6	SO4	A	1004	5/5	0.75	0.16	90,92,101,107	0
10	EDO	A	1019	4/4	0.75	0.30	88,92,93,95	0
6	SO4	A	1006	5/5	0.78	0.14	84,97,117,119	0
10	EDO	A	1014	4/4	0.79	0.22	74,76,78,82	0
10	EDO	A	1020	4/4	0.81	0.20	67,74,76,80	0
10	EDO	A	1015	4/4	0.82	0.24	71,73,83,84	0
10	EDO	A	1016	4/4	0.83	0.25	57,80,82,88	0
10	EDO	A	1018	4/4	0.83	0.27	89,94,105,105	0
9	PEG	A	1012	7/7	0.84	0.23	72,74,83,86	0
10	EDO	A	1013	4/4	0.84	0.29	96,99,111,113	0
6	SO4	A	1005	5/5	0.85	0.13	71,83,94,96	0
10	EDO	A	1021	4/4	0.86	0.26	74,82,84,84	0

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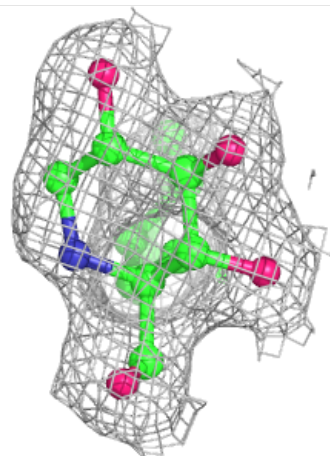
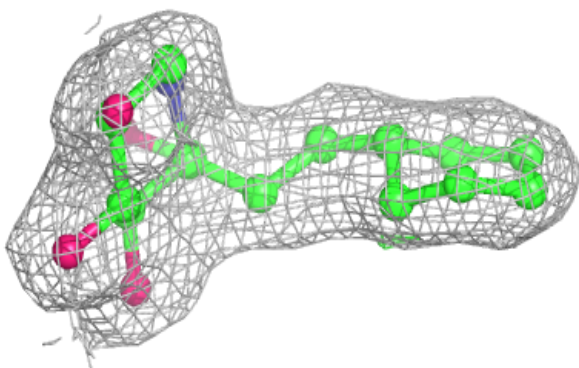
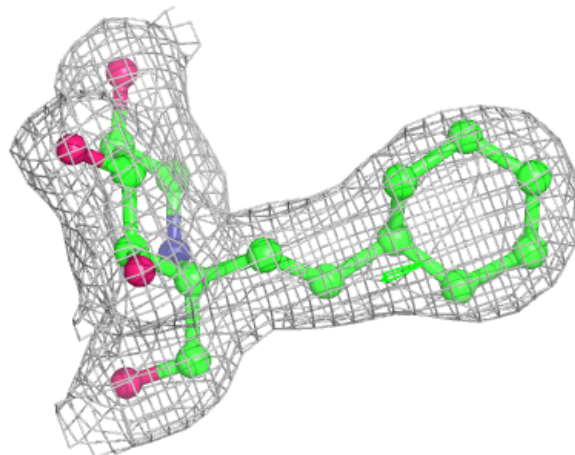
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
10	EDO	A	1023	4/4	0.90	0.20	75,80,85,87	0
10	EDO	A	1017	4/4	0.92	0.16	74,75,83,85	0
8	GOL	A	1011	6/6	0.92	0.15	46,60,68,73	0
7	CL	A	1007	1/1	0.92	0.20	82,82,82,82	0
10	EDO	A	1022	4/4	0.94	0.13	62,63,69,72	0
7	CL	A	1008	1/1	0.95	0.13	87,87,87,87	0
7	CL	A	1009	1/1	0.95	0.17	84,84,84,84	0
6	SO4	A	1002	5/5	0.95	0.16	60,67,68,70	0
8	GOL	A	1010	6/6	0.96	0.09	57,61,66,74	0
5	A1IO8	A	1001	19/19	0.97	0.09	40,45,62,64	0
6	SO4	A	1003	5/5	0.98	0.10	64,67,67,69	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 A1IO8 A 1001:**

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.