



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 1, 2024 – 07:14 PM JST

PDB ID : 5YOT  
Title : Isoprimeverose-producing enzyme from *Aspergillus oryzae* in complex with isoprimeverose  
Authors : Matsuzawa, T.; Watanabe, M.; Nakamichi, Y.; Yaoi, K.  
Deposited on : 2017-10-31  
Resolution : 1.98 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

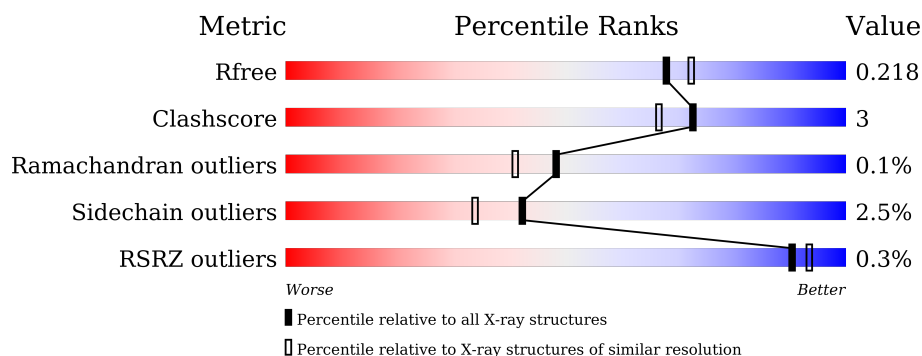
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.98 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.



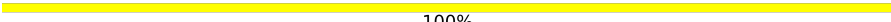
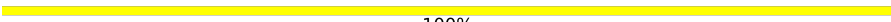

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	164625	1356 (1.98-1.98)
Clashscore	180529	1437 (1.98-1.98)
Ramachandran outliers	177936	1426 (1.98-1.98)
Sidechain outliers	177891	1426 (1.98-1.98)
RSRZ outliers	164620	1356 (1.98-1.98)

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	765	<div> <div>90%</div> <div>8%</div> </div>
1	B	765	<div> <div>90%</div> <div>8%</div> </div>
2	C	2	<div> <div>100%</div> </div>
2	D	2	<div> <div>50%</div> <div>50%</div> </div>
2	E	2	<div> <div>100%</div> </div>
2	F	2	<div> <div>50%</div> <div>50%</div> </div>

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Mol	Chain	Length	Quality of chain
2	G	2	 100%
2	H	2	 100%
2	I	2	 100%

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	GOL	B	816	-	-	X	-

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 12902 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 Isoprimeverose-producing enzyme.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	754	Total	C	N	O	S	0	3	0
			5852	3728	974	1131	19			
1	B	754	Total	C	N	O	S	0	3	0
			5850	3728	973	1130	19			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	780	VAL	-	expression tag	UNP Q2U8V9
A	781	ASP	-	expression tag	UNP Q2U8V9
A	782	HIS	-	expression tag	UNP Q2U8V9
A	783	HIS	-	expression tag	UNP Q2U8V9
A	784	HIS	-	expression tag	UNP Q2U8V9
A	785	HIS	-	expression tag	UNP Q2U8V9
A	786	HIS	-	expression tag	UNP Q2U8V9
A	787	HIS	-	expression tag	UNP Q2U8V9
B	780	VAL	-	expression tag	UNP Q2U8V9
B	781	ASP	-	expression tag	UNP Q2U8V9
B	782	HIS	-	expression tag	UNP Q2U8V9
B	783	HIS	-	expression tag	UNP Q2U8V9
B	784	HIS	-	expression tag	UNP Q2U8V9
B	785	HIS	-	expression tag	UNP Q2U8V9
B	786	HIS	-	expression tag	UNP Q2U8V9
B	787	HIS	-	expression tag	UNP Q2U8V9

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

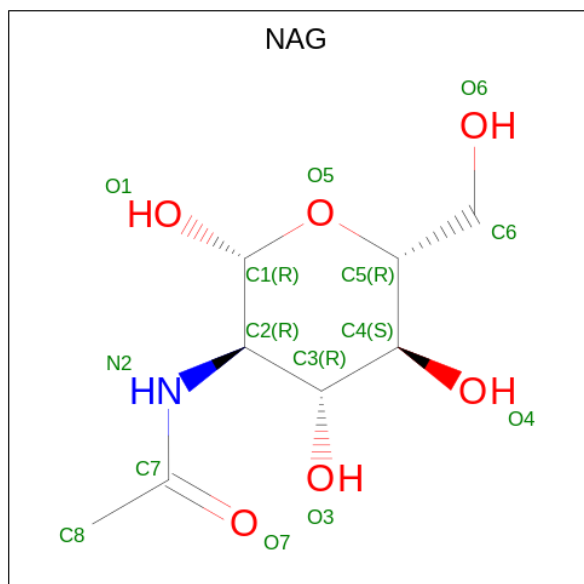


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	D	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	E	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	F	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	G	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	H	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	I	2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

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

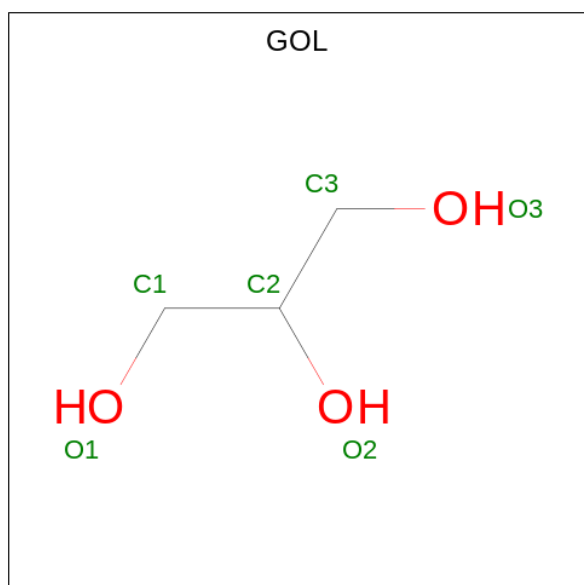
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Ca	0	0
			1	1		
3	B	1	Total	Ca	0	0
			1	1		

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



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

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



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

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

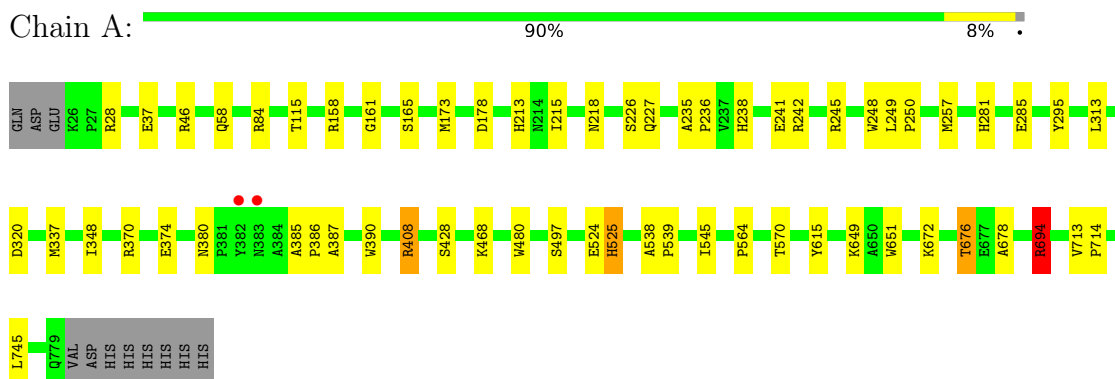
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	412	Total 412	O 412	0	0
6	B	402	Total 402	O 402	0	0

### 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: Isoprimeverose-producing enzyme







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

Chain E:  100%



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

Chain F:  50% 50%



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

Chain G:  100%



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

Chain H:  100%



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

Chain I:  100%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	70.14Å 130.45Å 94.84Å 90.00° 94.46° 90.00°	Depositor
Resolution (Å)	30.00 – 1.98 30.00 – 1.98	Depositor EDS
% Data completeness (in resolution range)	92.7 (30.00-1.98) 92.7 (30.00-1.98)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.08 (at 1.98Å)	Xtriage
Refinement program	REFMAC 5.8.0222	Depositor
R, $R_{free}$	0.167 , 0.211 0.178 , 0.218	Depositor DCC
$R_{free}$ test set	5877 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	25.2	Xtriage
Anisotropy	0.067	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 35.1	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	12902	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.65% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, NAG, GOL

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	0.68	0/5992	0.77	1/8156 (0.0%)
1	B	0.67	0/5994	0.77	1/8161 (0.0%)
All	All	0.67	0/11986	0.77	2/16317 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	6
1	B	0	3
All	All	0	9

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	370	ARG	NE-CZ-NH1	7.05	123.82	120.30
1	B	453	ARG	NE-CZ-NH2	-5.67	117.46	120.30

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	158	ARG	Sidechain
1	A	242	ARG	Sidechain
1	A	245	ARG	Sidechain
1	A	408	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	A	46	ARG	Sidechain
1	A	694	ARG	Sidechain
1	B	187	ARG	Sidechain
1	B	242	ARG	Sidechain
1	B	245	ARG	Sidechain

## 5.2 Too-close contacts ⓘ

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	5852	0	5696	32	0
1	B	5850	0	5701	38	0
2	C	28	0	25	0	0
2	D	28	0	25	0	0
2	E	28	0	25	0	0
2	F	28	0	25	1	0
2	G	28	0	25	0	0
2	H	28	0	25	0	0
2	I	28	0	25	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	84	0	78	0	0
4	B	56	0	52	1	0
5	A	24	0	32	4	0
5	B	24	0	32	9	0
6	A	412	0	0	7	0
6	B	402	0	0	6	0
All	All	12902	0	11766	73	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 (73) 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:480:TRP:CA	1:A:480:TRP:CG	2.55	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:814:GOL:H11	1:B:612:LEU:HB2	1.63	0.81
1:B:544:ILE:O	1:B:547:THR:HB	1.90	0.72
1:A:285[B]:GLU:CD	6:A:928:HOH:O	2.29	0.70
1:B:547:THR:HG22	1:B:549:VAL:H	1.59	0.67
1:B:178:ASP:OD2	1:B:221:HIS:HD2	1.81	0.63
1:A:337[B]:MET:HE1	6:A:955:HOH:O	1.98	0.63
1:A:676:THR:HG23	1:A:678:ALA:H	1.65	0.62
5:B:814:GOL:O2	6:B:901:HOH:O	1.86	0.62
1:B:384:ALA:HB3	5:B:816:GOL:H12	1.80	0.62
1:B:706:ASP:HB2	5:B:814:GOL:H32	1.82	0.60
1:A:58:GLN:OE1	5:A:815:GOL:H11	2.02	0.60
1:A:694:ARG:HD3	6:A:946:HOH:O	2.02	0.58
1:B:384:ALA:CB	5:B:816:GOL:H12	2.34	0.58
1:A:538:ALA:HB3	1:A:539:PRO:HD3	1.85	0.57
1:B:538:ALA:HB3	1:B:539:PRO:HD3	1.88	0.56
1:B:329:LEU:HB3	1:B:330:PRO:HD3	1.87	0.56
1:A:28:ARG:NH1	6:A:909:HOH:O	2.39	0.55
1:B:220:LYS:HD3	1:B:221:HIS:CE1	2.42	0.55
1:B:176:VAL:HG22	1:B:220:LYS:HD2	1.89	0.54
1:A:281:HIS:O	1:A:285[B]:GLU:HB2	2.08	0.54
1:B:337[A]:MET:HE1	6:B:964:HOH:O	2.09	0.53
1:B:104:LYS:HB2	5:B:816:GOL:H32	1.91	0.53
1:B:547:THR:HG23	1:B:549:VAL:HG23	1.89	0.53
1:B:462:LYS:NZ	6:B:909:HOH:O	2.42	0.52
1:A:676:THR:CG2	1:A:678:ALA:H	2.23	0.51
1:B:73:ASN:HD22	2:F:1:NAG:H83	1.76	0.50
1:B:220:LYS:HB3	1:B:265:MET:HB3	1.95	0.48
1:B:58:GLN:OE1	5:B:815:GOL:H11	2.12	0.48
1:B:774:ALA:HB1	6:B:1153:HOH:O	2.14	0.48
1:B:104:LYS:HB2	5:B:816:GOL:H11	1.95	0.47
5:B:814:GOL:H12	6:B:1008:HOH:O	2.14	0.47
1:B:547:THR:CG2	1:B:549:VAL:HG23	2.44	0.47
1:A:428:SER:OG	1:A:497:SER:HA	2.14	0.47
1:B:446:VAL:HG13	1:B:450:SER:HB2	1.96	0.47
5:A:814:GOL:C1	1:B:612:LEU:HB2	2.39	0.46
1:A:227:GLN:HE21	1:A:248:TRP:HZ2	1.62	0.46
1:B:159:LEU:HD13	1:B:399:ALA:HA	1.98	0.46
1:A:161:GLY:O	1:A:165:SER:HB2	2.16	0.46
1:A:524:GLU:O	1:A:525:HIS:HD2	1.98	0.46
1:A:238:HIS:HD2	6:A:1084:HOH:O	2.00	0.45
1:A:173:MET:HA	1:A:218:ASN:HB3	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:713:VAL:HB	1:A:714:PRO:HD2	1.98	0.45
1:B:221:HIS:HE1	6:B:1078:HOH:O	1.99	0.44
1:B:385:ALA:HB1	1:B:386:PRO:HD2	1.99	0.44
1:B:235:ALA:HB1	1:B:236:PRO:HD2	2.00	0.44
1:A:295:TYR:OH	1:A:374:GLU:OE1	2.30	0.43
1:B:626:GLY:HA3	1:B:642:GLN:OE1	2.18	0.43
1:A:235:ALA:HB1	1:A:236:PRO:HD2	1.99	0.43
1:B:173:MET:HA	1:B:218:ASN:HB3	1.99	0.43
1:B:173:MET:HE1	1:B:337[A]:MET:HE3	2.00	0.43
1:B:432:ILE:HA	1:B:474:ALA:O	2.18	0.43
1:A:337[B]:MET:HE2	5:A:815:GOL:H2	2.01	0.42
1:B:391:ASN:HD22	1:B:391:ASN:HA	1.69	0.42
1:A:672:LYS:NZ	6:A:926:HOH:O	2.51	0.42
1:B:264:ILE:HD12	1:B:293:TYR:CE2	2.55	0.42
1:A:385:ALA:HB1	1:A:386:PRO:HD2	2.00	0.42
1:B:332:GLY:HA2	5:B:817:GOL:H31	2.02	0.42
1:A:178:ASP:HB3	1:A:226:SER:OG	2.19	0.42
1:A:249:LEU:N	1:A:250:PRO:CD	2.83	0.42
1:A:745:LEU:C	1:A:745:LEU:HD12	2.40	0.42
1:A:524:GLU:O	1:A:525:HIS:CD2	2.72	0.41
1:B:58:GLN:OE1	1:B:337[B]:MET:HG3	2.20	0.41
1:A:58:GLN:OE1	1:A:337[A]:MET:HG3	2.20	0.41
1:A:213:HIS:HB2	1:A:215:ILE:HD12	2.03	0.41
1:B:370:ARG:O	1:B:374:GLU:HG2	2.19	0.41
1:A:564:PRO:HA	1:A:651:TRP:CZ2	2.56	0.41
1:B:131:LEU:HG	1:B:447:VAL:HG12	2.03	0.41
1:A:320:ASP:OD2	6:A:901:HOH:O	2.21	0.41
1:A:545:ILE:HD11	1:A:570:THR:HG22	2.02	0.41
1:B:126:SER:O	1:B:127:LEU:C	2.60	0.41
1:A:387:ALA:HA	1:A:390:TRP:CD2	2.56	0.40
4:B:812:NAG:H82	4:B:812:NAG:H2	1.97	0.40

There are no symmetry-related clashes.

## 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	755/765 (99%)	735 (97%)	20 (3%)	0	100	100
1	B	755/765 (99%)	733 (97%)	21 (3%)	1 (0%)	48	41
All	All	1510/1530 (99%)	1468 (97%)	41 (3%)	1 (0%)	48	41

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	621	SER

### 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	622/631 (99%)	607 (98%)	15 (2%)	44	36
1	B	623/631 (99%)	607 (97%)	16 (3%)	41	32
All	All	1245/1262 (99%)	1214 (98%)	31 (2%)	42	34

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	GLU
1	A	84	ARG
1	A	115	THR
1	A	241	GLU
1	A	257	MET
1	A	313	LEU
1	A	348	ILE
1	A	380	ASN
1	A	408	ARG
1	A	468	LYS
1	A	525	HIS
1	A	615	TYR

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Mol	Chain	Res	Type
1	A	649	LYS
1	A	676	THR
1	A	694	ARG
1	B	26	LYS
1	B	84	ARG
1	B	115	THR
1	B	220	LYS
1	B	314	CYS
1	B	355	LYS
1	B	383	ASN
1	B	392	LYS
1	B	421	LEU
1	B	446	VAL
1	B	468	LYS
1	B	525	HIS
1	B	547	THR
1	B	615	TYR
1	B	672	LYS
1	B	768	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	227	GLN
1	A	238	HIS
1	A	391	ASN
1	A	525	HIS
1	B	218	ASN
1	B	221	HIS
1	B	227	GLN
1	B	391	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 ⓘ

14 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	NAG	C	1	2,1	14,14,15	0.67	0	17,19,21	2.57	4 (23%)
2	NAG	C	2	2	14,14,15	0.88	0	17,19,21	1.90	4 (23%)
2	NAG	D	1	2,1	14,14,15	0.80	0	17,19,21	0.87	0
2	NAG	D	2	2	14,14,15	1.08	2 (14%)	17,19,21	2.15	5 (29%)
2	NAG	E	1	2,1	14,14,15	0.92	0	17,19,21	2.36	2 (11%)
2	NAG	E	2	2	14,14,15	1.74	4 (28%)	17,19,21	2.23	4 (23%)
2	NAG	F	1	2,1	14,14,15	1.34	1 (7%)	17,19,21	2.49	7 (41%)
2	NAG	F	2	2	14,14,15	0.66	0	17,19,21	1.96	5 (29%)
2	NAG	G	1	2,1	14,14,15	0.87	0	17,19,21	1.51	3 (17%)
2	NAG	G	2	2	14,14,15	0.83	1 (7%)	17,19,21	1.85	3 (17%)
2	NAG	H	1	2,1	14,14,15	0.54	0	17,19,21	1.43	4 (23%)
2	NAG	H	2	2	14,14,15	1.12	2 (14%)	17,19,21	2.36	5 (29%)
2	NAG	I	1	2,1	14,14,15	0.61	0	17,19,21	1.29	2 (11%)
2	NAG	I	2	2	14,14,15	0.93	1 (7%)	17,19,21	1.74	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
2	NAG	C	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	C	2	2	-	2/6/23/26	0/1/1/1
2	NAG	D	1	2,1	-	1/6/23/26	0/1/1/1
2	NAG	D	2	2	-	1/6/23/26	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
2	NAG	F	1	2,1	-	4/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	F	2	2	-	4/6/23/26	0/1/1/1
2	NAG	G	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	G	2	2	-	1/6/23/26	0/1/1/1
2	NAG	H	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	H	2	2	-	0/6/23/26	0/1/1/1
2	NAG	I	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	I	2	2	-	2/6/23/26	0/1/1/1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	1	NAG	O5-C1	-4.07	1.37	1.43
2	E	2	NAG	O5-C5	-3.87	1.35	1.43
2	E	2	NAG	C1-C2	-2.76	1.48	1.52
2	E	2	NAG	O4-C4	2.54	1.49	1.43
2	H	2	NAG	O5-C1	-2.48	1.39	1.43
2	I	2	NAG	C2-N2	-2.26	1.42	1.46
2	D	2	NAG	O5-C5	2.21	1.47	1.43
2	E	2	NAG	O5-C1	-2.20	1.40	1.43
2	D	2	NAG	O4-C4	2.18	1.48	1.43
2	G	2	NAG	O4-C4	2.08	1.47	1.43
2	H	2	NAG	C2-N2	-2.06	1.42	1.46

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1	NAG	C1-O5-C5	8.58	123.82	112.19
2	E	1	NAG	C1-O5-C5	7.93	122.93	112.19
2	E	2	NAG	C1-O5-C5	-6.72	103.08	112.19
2	H	2	NAG	C1-O5-C5	-6.61	103.23	112.19
2	D	2	NAG	C1-O5-C5	6.23	120.63	112.19
2	F	1	NAG	C1-O5-C5	5.56	119.73	112.19
2	F	2	NAG	O5-C5-C6	4.97	114.99	107.20
2	G	2	NAG	O5-C5-C6	4.72	114.61	107.20
2	C	2	NAG	C2-N2-C7	-4.61	116.34	122.90
2	C	2	NAG	O5-C5-C6	4.17	113.74	107.20
2	H	2	NAG	C2-N2-C7	-4.03	117.16	122.90
2	G	2	NAG	C3-C4-C5	-3.94	103.21	110.24
2	G	1	NAG	C1-O5-C5	3.89	117.46	112.19
2	F	1	NAG	C6-C5-C4	-3.84	104.00	113.00
2	F	2	NAG	O5-C1-C2	-3.79	105.30	111.29
2	I	2	NAG	C1-O5-C5	-3.74	107.13	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	2	NAG	C3-C4-C5	-3.47	104.05	110.24
2	F	1	NAG	C4-C3-C2	-3.47	105.94	111.02
2	E	2	NAG	C1-C2-N2	-3.37	104.73	110.49
2	F	1	NAG	C8-C7-N2	3.36	121.80	116.10
2	H	2	NAG	O5-C5-C6	3.28	112.35	107.20
2	C	1	NAG	C6-C5-C4	-3.17	105.58	113.00
2	D	2	NAG	O4-C4-C5	3.13	117.07	109.30
2	H	1	NAG	C1-C2-N2	2.98	115.58	110.49
2	D	2	NAG	O5-C5-C4	2.90	117.88	110.83
2	I	1	NAG	O5-C1-C2	-2.86	106.78	111.29
2	F	2	NAG	C2-N2-C7	-2.74	119.00	122.90
2	H	1	NAG	O4-C4-C3	-2.71	104.09	110.35
2	I	2	NAG	O4-C4-C5	2.67	115.92	109.30
2	H	1	NAG	C1-O5-C5	2.64	115.76	112.19
2	C	1	NAG	O6-C6-C5	-2.63	102.26	111.29
2	E	1	NAG	O3-C3-C2	-2.61	104.07	109.47
2	D	2	NAG	C6-C5-C4	-2.60	106.90	113.00
2	G	1	NAG	C1-C2-N2	-2.57	106.10	110.49
2	C	2	NAG	O5-C1-C2	-2.56	107.25	111.29
2	C	1	NAG	O5-C1-C2	-2.48	107.37	111.29
2	F	1	NAG	O5-C5-C4	2.35	116.54	110.83
2	E	2	NAG	O4-C4-C3	2.34	115.75	110.35
2	G	2	NAG	O4-C4-C5	2.34	115.10	109.30
2	C	2	NAG	O4-C4-C3	-2.33	104.97	110.35
2	F	1	NAG	C2-N2-C7	2.32	126.21	122.90
2	F	1	NAG	O6-C6-C5	-2.29	103.43	111.29
2	G	1	NAG	C3-C4-C5	-2.22	106.27	110.24
2	D	2	NAG	C4-C3-C2	2.17	114.19	111.02
2	I	1	NAG	C1-O5-C5	2.16	115.12	112.19
2	E	2	NAG	C6-C5-C4	-2.16	107.95	113.00
2	H	1	NAG	C3-C4-C5	-2.15	106.41	110.24
2	F	2	NAG	C1-C2-N2	2.13	114.13	110.49
2	F	2	NAG	C1-O5-C5	-2.12	109.31	112.19
2	I	2	NAG	O5-C5-C6	2.10	110.49	107.20
2	H	2	NAG	C3-C4-C5	-2.06	106.56	110.24
2	H	2	NAG	O5-C5-C4	-2.01	105.94	110.83

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	F	1	NAG	C8-C7-N2-C2

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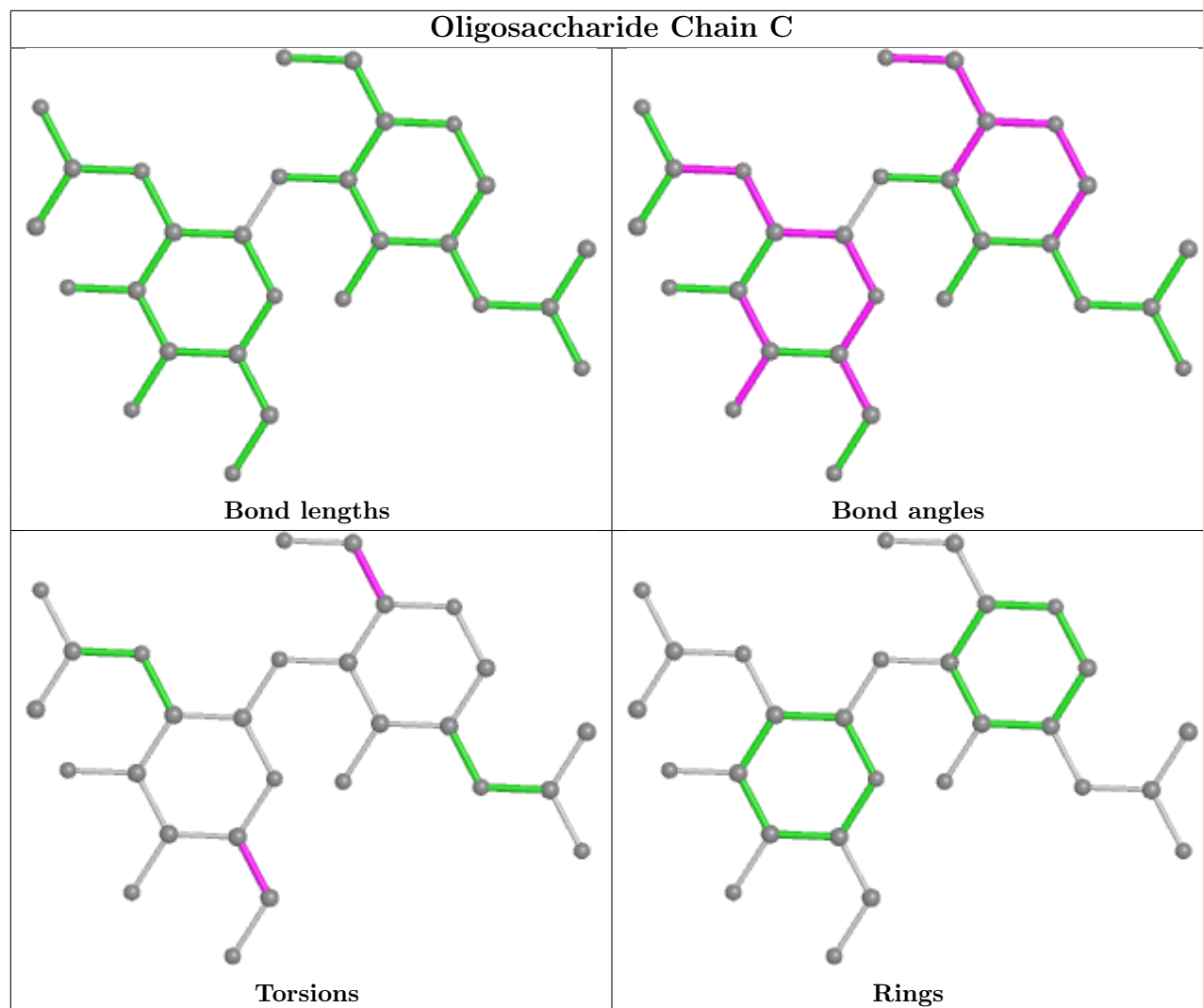
Mol	Chain	Res	Type	Atoms
2	C	2	NAG	O5-C5-C6-O6
2	I	2	NAG	O5-C5-C6-O6
2	F	2	NAG	O5-C5-C6-O6
2	F	1	NAG	O7-C7-N2-C2
2	F	2	NAG	C4-C5-C6-O6
2	F	1	NAG	C4-C5-C6-O6
2	C	1	NAG	O5-C5-C6-O6
2	E	2	NAG	O5-C5-C6-O6
2	F	1	NAG	O5-C5-C6-O6
2	E	2	NAG	C4-C5-C6-O6
2	I	2	NAG	C4-C5-C6-O6
2	C	2	NAG	C4-C5-C6-O6
2	C	1	NAG	C4-C5-C6-O6
2	F	2	NAG	C8-C7-N2-C2
2	G	2	NAG	O5-C5-C6-O6
2	D	2	NAG	C4-C5-C6-O6
2	F	2	NAG	O7-C7-N2-C2
2	D	1	NAG	C4-C5-C6-O6

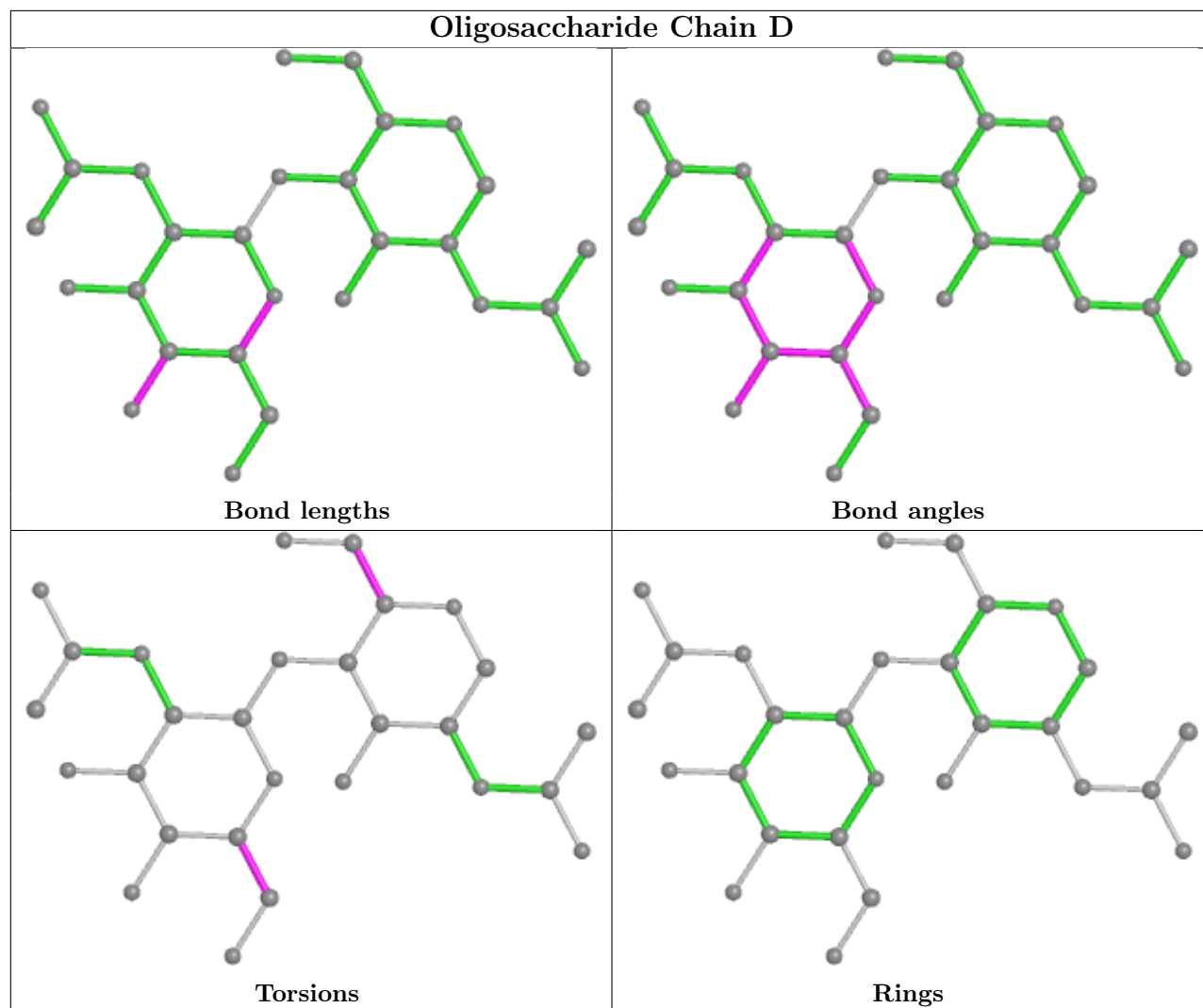
There are no ring outliers.

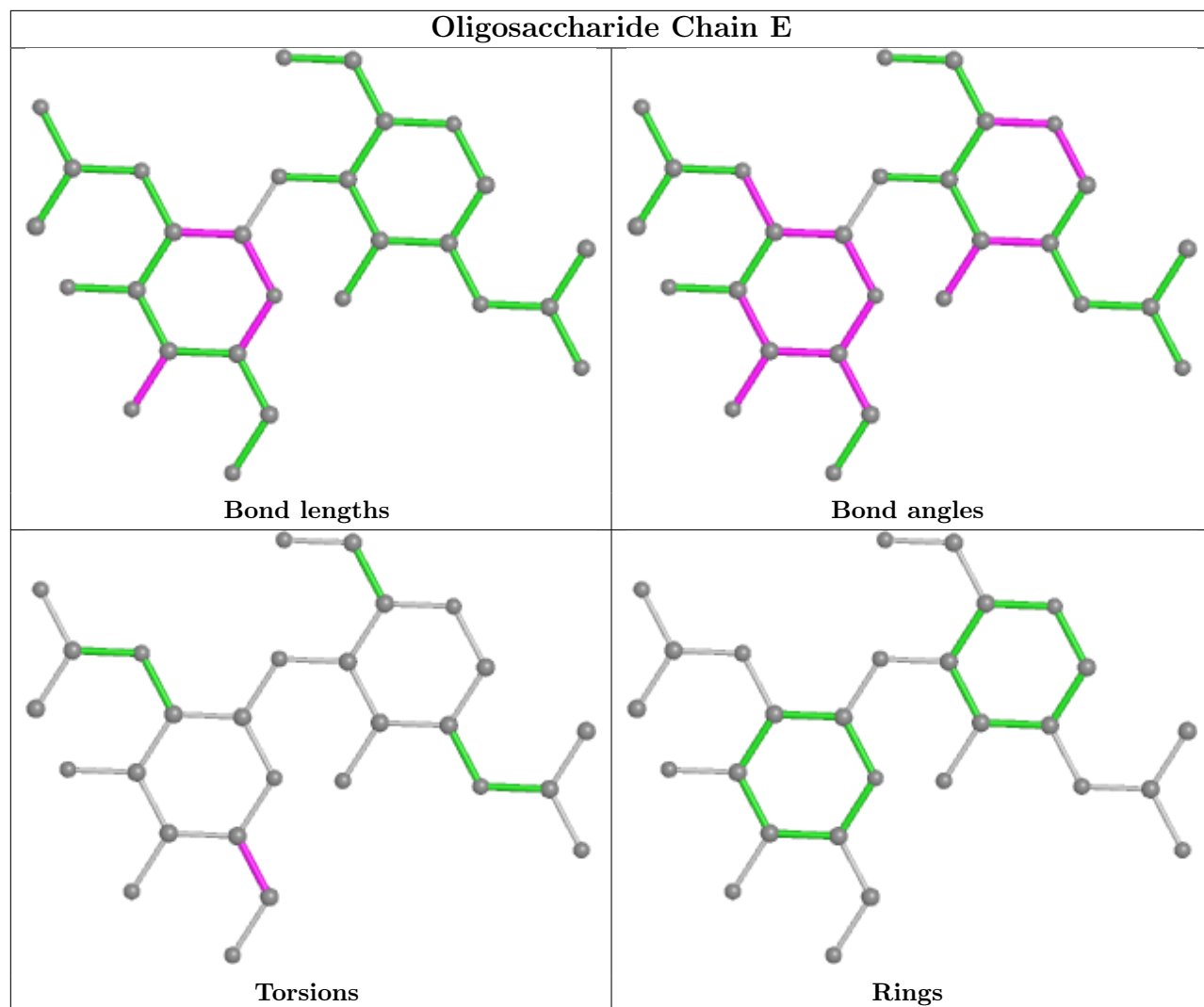
1 monomer is involved in 1 short contact:

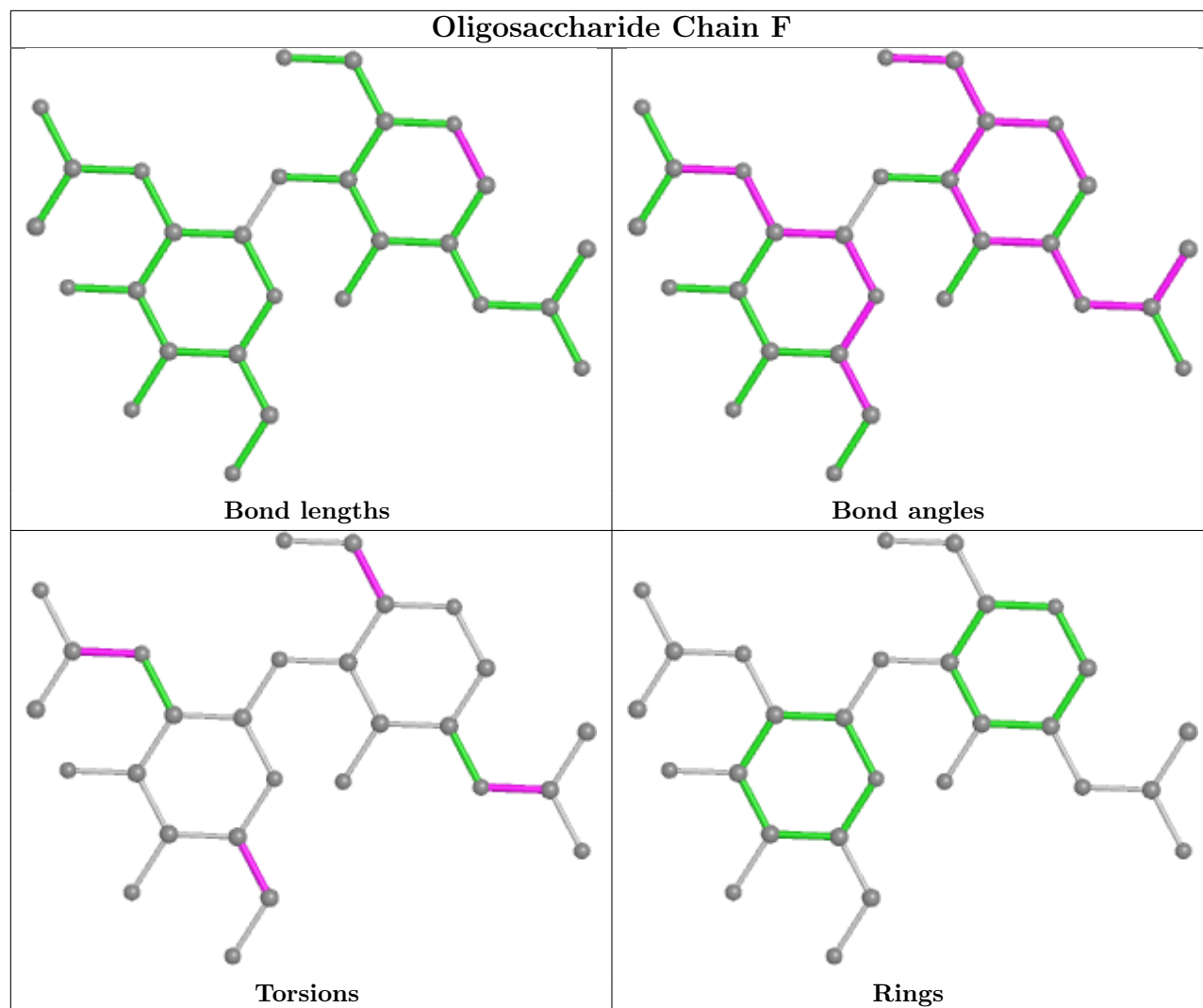
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	1	NAG	1	0

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

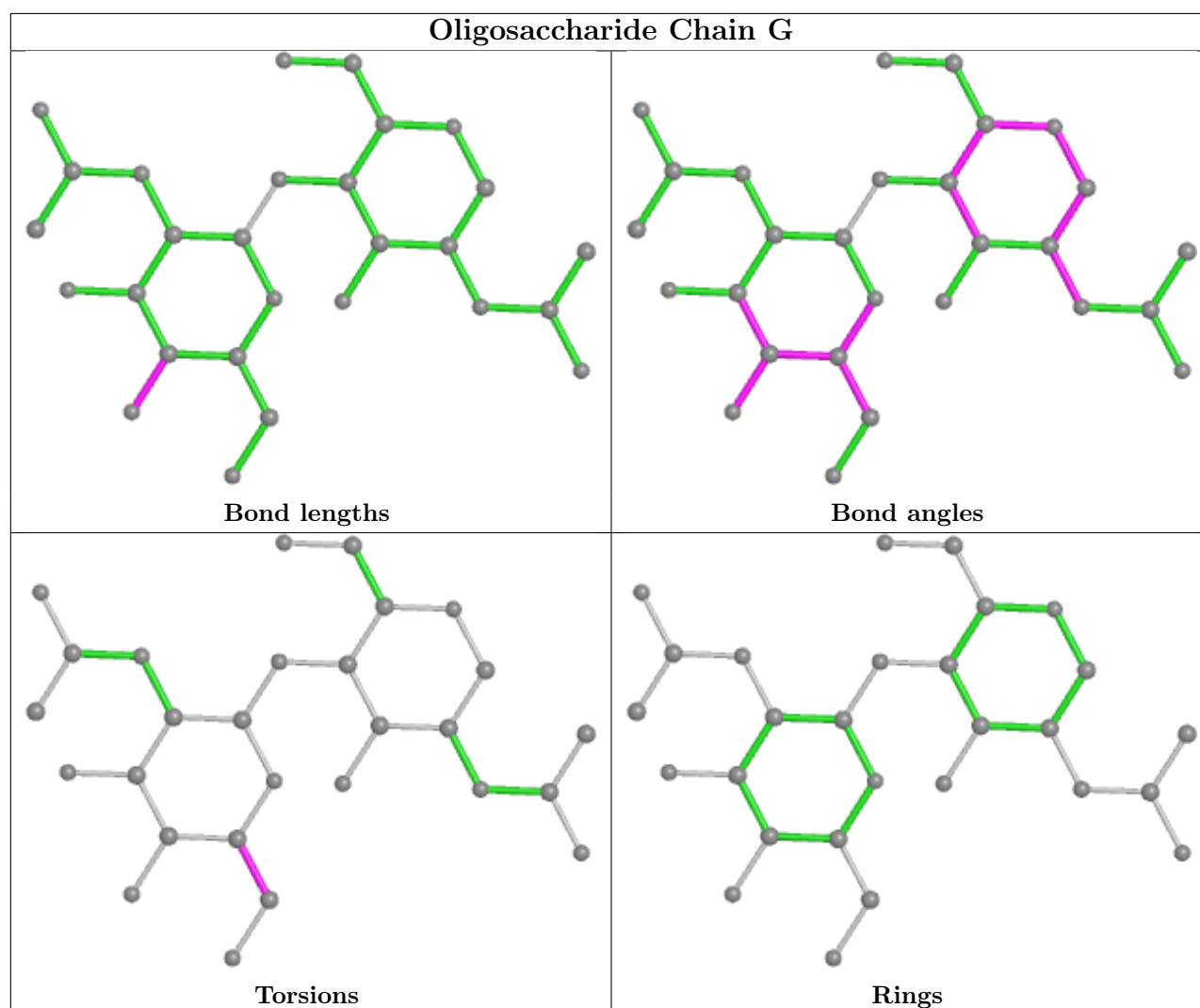


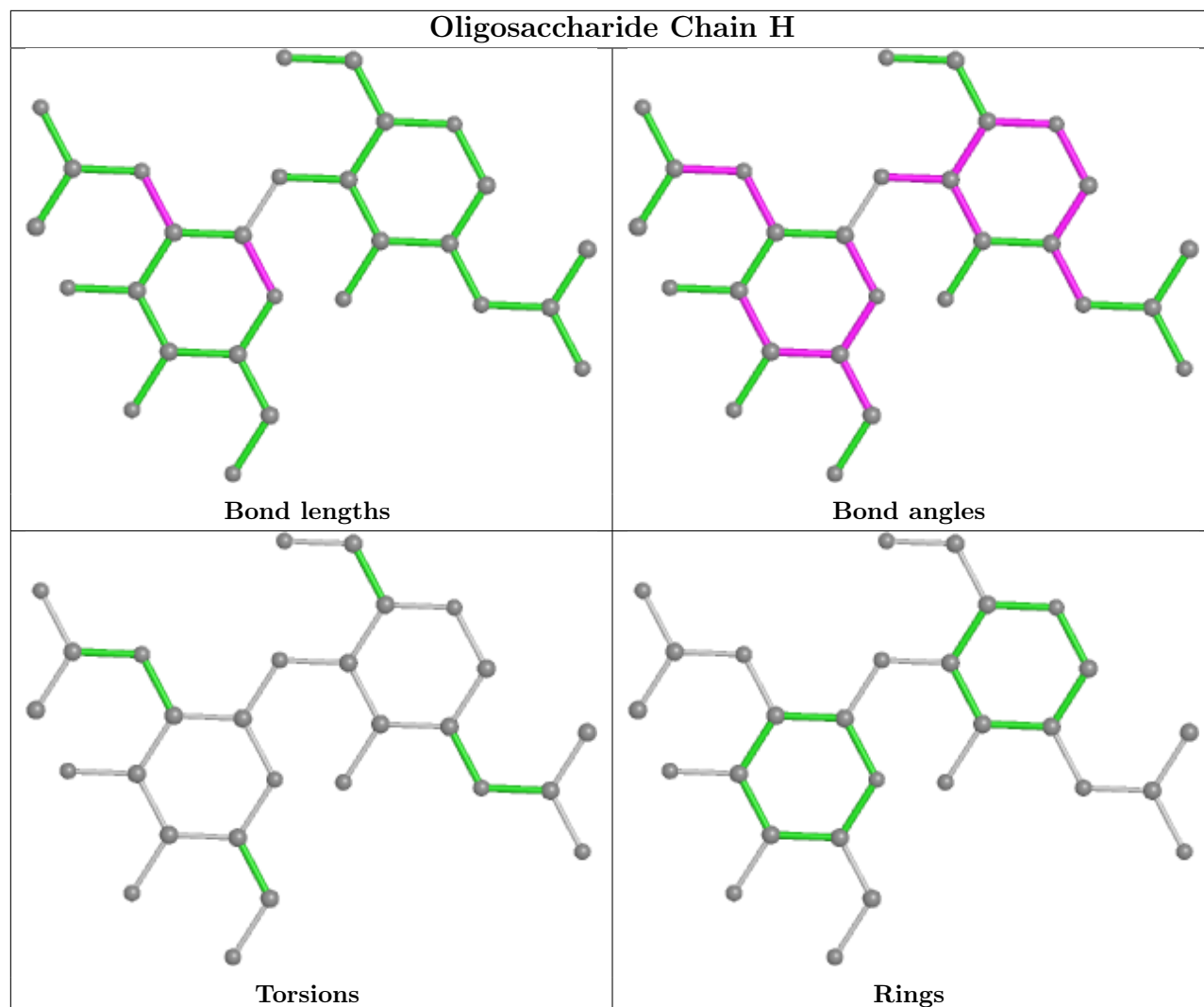


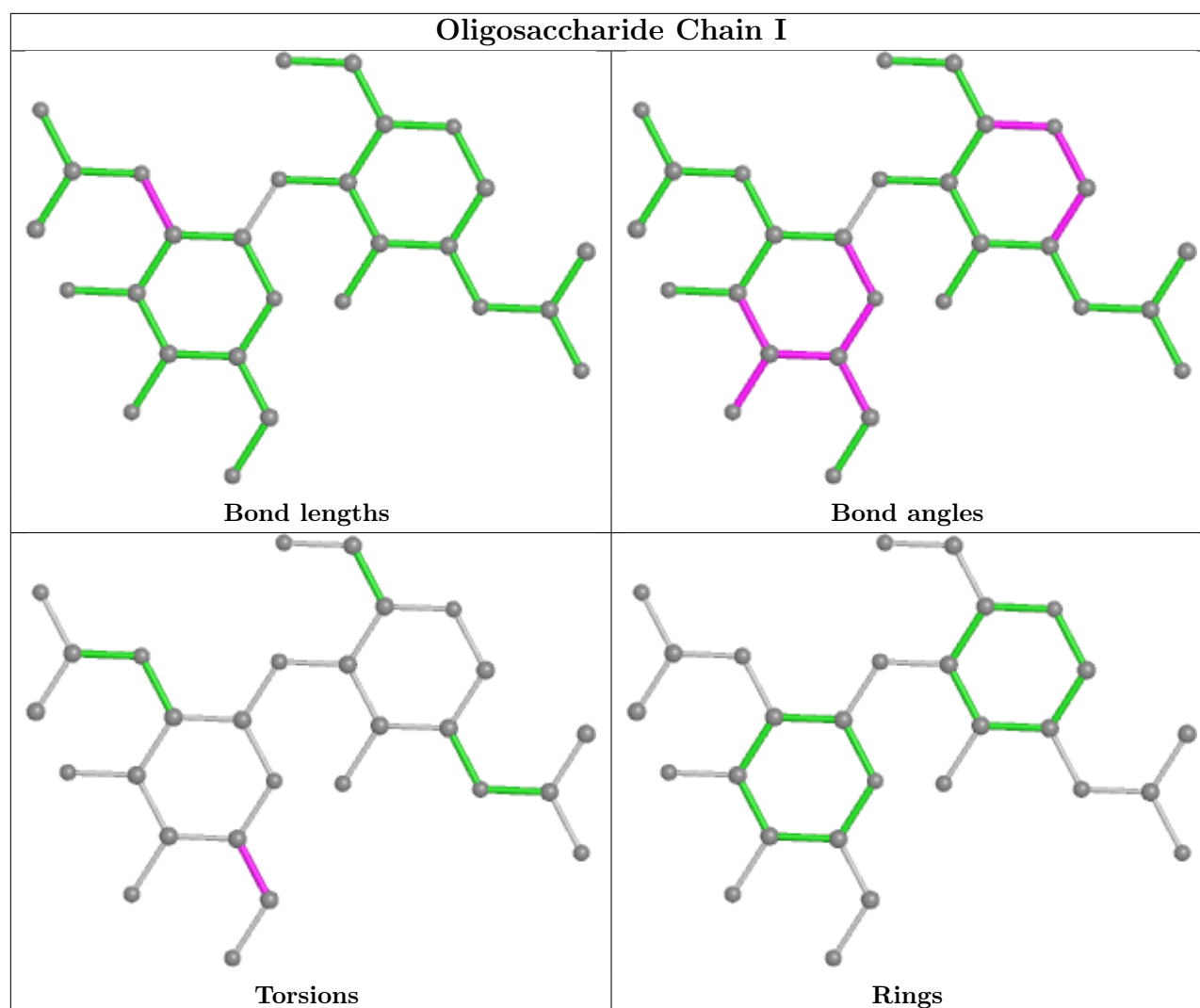












## 5.6 Ligand geometry [i](#)

Of 20 ligands modelled in this entry, 2 are monoatomic - leaving 18 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	$\# Z  > 2$
4	NAG	A	809	1	14,14,15	0.82	0	17,19,21	2.51	7 (41%)
5	GOL	B	817	-	5,5,5	0.40	0	5,5,5	1.06	0
5	GOL	A	815	-	5,5,5	0.94	0	5,5,5	1.17	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	NAG	A	811	1	14,14,15	1.10	2 (14%)	17,19,21	1.73	4 (23%)
5	GOL	B	815	-	5,5,5	1.00	0	5,5,5	1.00	0
4	NAG	B	810	1	14,14,15	0.74	1 (7%)	17,19,21	1.41	3 (17%)
4	NAG	A	812	1	14,14,15	0.97	2 (14%)	17,19,21	1.71	4 (23%)
5	GOL	A	816	-	5,5,5	0.34	0	5,5,5	0.45	0
5	GOL	A	817	-	5,5,5	0.36	0	5,5,5	0.49	0
4	NAG	B	813	1	14,14,15	0.87	1 (7%)	17,19,21	1.37	1 (5%)
5	GOL	A	814	-	5,5,5	0.43	0	5,5,5	1.11	0
4	NAG	A	810	1	14,14,15	1.17	0	17,19,21	1.93	6 (35%)
4	NAG	B	811	1	14,14,15	0.61	0	17,19,21	1.37	3 (17%)
5	GOL	B	816	-	5,5,5	0.63	0	5,5,5	1.59	2 (40%)
5	GOL	B	814	-	5,5,5	0.93	0	5,5,5	1.94	2 (40%)
4	NAG	A	813	1	14,14,15	1.04	1 (7%)	17,19,21	2.19	2 (11%)
4	NAG	B	812	1	14,14,15	1.53	3 (21%)	17,19,21	2.71	5 (29%)
4	NAG	A	808	1	14,14,15	1.25	2 (14%)	17,19,21	2.54	5 (29%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	809	1	-	0/6/23/26	0/1/1/1
5	GOL	B	817	-	-	4/4/4/4	-
5	GOL	A	815	-	-	2/4/4/4	-
4	NAG	A	811	1	-	2/6/23/26	0/1/1/1
5	GOL	B	815	-	-	4/4/4/4	-
4	NAG	B	810	1	-	2/6/23/26	0/1/1/1
4	NAG	A	812	1	-	1/6/23/26	0/1/1/1
5	GOL	A	816	-	-	1/4/4/4	-
5	GOL	A	817	-	-	2/4/4/4	-
4	NAG	B	813	1	-	2/6/23/26	0/1/1/1
5	GOL	A	814	-	-	4/4/4/4	-
4	NAG	A	810	1	-	0/6/23/26	0/1/1/1
4	NAG	B	811	1	-	0/6/23/26	0/1/1/1
5	GOL	B	816	-	-	0/4/4/4	-
5	GOL	B	814	-	-	0/4/4/4	-
4	NAG	A	813	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	B	812	1	-	4/6/23/26	0/1/1/1
4	NAG	A	808	1	-	2/6/23/26	0/1/1/1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	812	NAG	O5-C1	-3.34	1.38	1.43
4	B	812	NAG	C1-C2	-3.17	1.47	1.52
4	A	808	NAG	C1-C2	3.13	1.57	1.52
4	A	813	NAG	C1-C2	3.06	1.56	1.52
4	A	811	NAG	O5-C1	-2.57	1.39	1.43
4	A	808	NAG	C2-N2	2.48	1.50	1.46
4	A	812	NAG	O5-C1	-2.22	1.40	1.43
4	A	812	NAG	O5-C5	-2.22	1.39	1.43
4	B	812	NAG	C2-N2	-2.15	1.42	1.46
4	A	811	NAG	C1-C2	2.12	1.55	1.52
4	B	810	NAG	O5-C1	2.12	1.47	1.43
4	B	813	NAG	C1-C2	2.05	1.55	1.52

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	813	NAG	C1-O5-C5	7.82	122.79	112.19
4	A	808	NAG	O5-C5-C6	5.95	116.52	107.20
4	A	809	NAG	C6-C5-C4	-5.90	99.19	113.00
4	B	812	NAG	O7-C7-N2	-5.81	111.27	121.95
4	A	808	NAG	C1-C2-N2	5.54	119.96	110.49
4	B	812	NAG	C2-N2-C7	-5.37	115.25	122.90
4	A	812	NAG	C1-O5-C5	-5.09	105.29	112.19
4	B	812	NAG	O5-C1-C2	-4.76	103.77	111.29
4	A	808	NAG	C1-O5-C5	4.50	118.29	112.19
4	A	809	NAG	C1-O5-C5	4.05	117.68	112.19
4	A	811	NAG	O4-C4-C5	3.67	118.40	109.30
4	B	812	NAG	C8-C7-N2	3.60	122.20	116.10
4	B	813	NAG	C3-C4-C5	3.49	116.46	110.24
4	A	811	NAG	O5-C5-C6	-3.44	101.81	107.20
4	A	809	NAG	O5-C5-C6	3.42	112.57	107.20
4	B	810	NAG	O5-C1-C2	-3.40	105.93	111.29
4	A	809	NAG	C4-C3-C2	-3.33	106.14	111.02
4	A	810	NAG	O4-C4-C5	3.31	117.52	109.30
4	A	809	NAG	C3-C4-C5	3.10	115.77	110.24
4	B	812	NAG	C4-C3-C2	-3.07	106.52	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	810	NAG	O3-C3-C2	-3.05	103.16	109.47
4	A	808	NAG	C6-C5-C4	-2.96	106.07	113.00
4	A	812	NAG	O5-C1-C2	-2.87	106.75	111.29
4	A	809	NAG	O3-C3-C4	-2.79	103.89	110.35
4	A	810	NAG	C2-N2-C7	2.75	126.82	122.90
4	A	813	NAG	C6-C5-C4	-2.72	106.63	113.00
4	B	811	NAG	C3-C4-C5	-2.59	105.62	110.24
5	B	814	GOL	O1-C1-C2	2.53	122.34	110.20
4	A	810	NAG	C6-C5-C4	2.49	118.84	113.00
5	B	814	GOL	O3-C3-C2	2.49	122.13	110.20
4	A	811	NAG	C3-C4-C5	-2.46	105.86	110.24
4	A	812	NAG	C3-C4-C5	2.44	114.59	110.24
4	A	810	NAG	C1-O5-C5	2.41	115.45	112.19
4	A	810	NAG	C4-C3-C2	2.27	114.35	111.02
4	A	812	NAG	C6-C5-C4	-2.27	107.69	113.00
4	A	809	NAG	O6-C6-C5	-2.25	103.56	111.29
5	B	816	GOL	C3-C2-C1	-2.17	103.29	111.70
4	B	810	NAG	O7-C7-C8	-2.16	118.04	122.06
5	B	816	GOL	O2-C2-C1	2.16	118.64	109.12
4	B	810	NAG	C2-N2-C7	-2.14	119.86	122.90
4	A	811	NAG	O7-C7-N2	-2.11	118.08	121.95
4	A	808	NAG	O7-C7-C8	-2.09	118.17	122.06
4	B	811	NAG	O3-C3-C4	-2.08	105.55	110.35
4	B	811	NAG	O5-C5-C6	2.07	110.46	107.20

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	812	NAG	C8-C7-N2-C2
4	B	812	NAG	O7-C7-N2-C2
5	A	815	GOL	O1-C1-C2-C3
5	A	817	GOL	O1-C1-C2-O2
5	A	817	GOL	O1-C1-C2-C3
5	B	817	GOL	O1-C1-C2-C3
4	A	808	NAG	O5-C5-C6-O6
4	B	812	NAG	O5-C5-C6-O6
4	B	812	NAG	C4-C5-C6-O6
4	A	808	NAG	C4-C5-C6-O6
4	A	811	NAG	C4-C5-C6-O6
4	B	813	NAG	C4-C5-C6-O6
4	A	811	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
5	A	814	GOL	O1-C1-C2-C3
5	A	814	GOL	C1-C2-C3-O3
5	B	815	GOL	O1-C1-C2-C3
5	B	815	GOL	C1-C2-C3-O3
5	B	817	GOL	C1-C2-C3-O3
5	A	814	GOL	O1-C1-C2-O2
5	A	814	GOL	O2-C2-C3-O3
5	B	817	GOL	O1-C1-C2-O2
4	B	813	NAG	O5-C5-C6-O6
4	A	812	NAG	O5-C5-C6-O6
5	A	815	GOL	O1-C1-C2-O2
5	B	815	GOL	O1-C1-C2-O2
5	B	817	GOL	O2-C2-C3-O3
4	B	810	NAG	C4-C5-C6-O6
5	B	815	GOL	O2-C2-C3-O3
5	A	816	GOL	O1-C1-C2-C3
4	B	810	NAG	O5-C5-C6-O6

There are no ring outliers.

7 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	817	GOL	1	0
5	A	815	GOL	2	0
5	B	815	GOL	1	0
5	A	814	GOL	2	0
5	B	816	GOL	4	0
5	B	814	GOL	3	0
4	B	812	NAG	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	754/765 (98%)	-0.26	2 (0%) 90 93	11, 25, 40, 65	3 (0%)
1	B	754/765 (98%)	-0.22	2 (0%) 90 93	13, 26, 41, 73	3 (0%)
All	All	1508/1530 (98%)	-0.24	4 (0%) 90 93	11, 26, 40, 73	6 (0%)

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	382	TYR	3.3
1	B	383	ASN	2.6
1	A	382	TYR	2.5
1	A	383	ASN	2.4

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

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

### 6.3 Carbohydrates [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	NAG	I	2	14/15	0.64	0.14	68,73,76,77	0
2	NAG	H	2	14/15	0.65	0.15	50,59,65,68	0
2	NAG	E	2	14/15	0.70	0.12	55,63,75,80	0
2	NAG	G	2	14/15	0.70	0.13	58,62,65,69	0
2	NAG	D	2	14/15	0.76	0.13	41,46,52,58	0

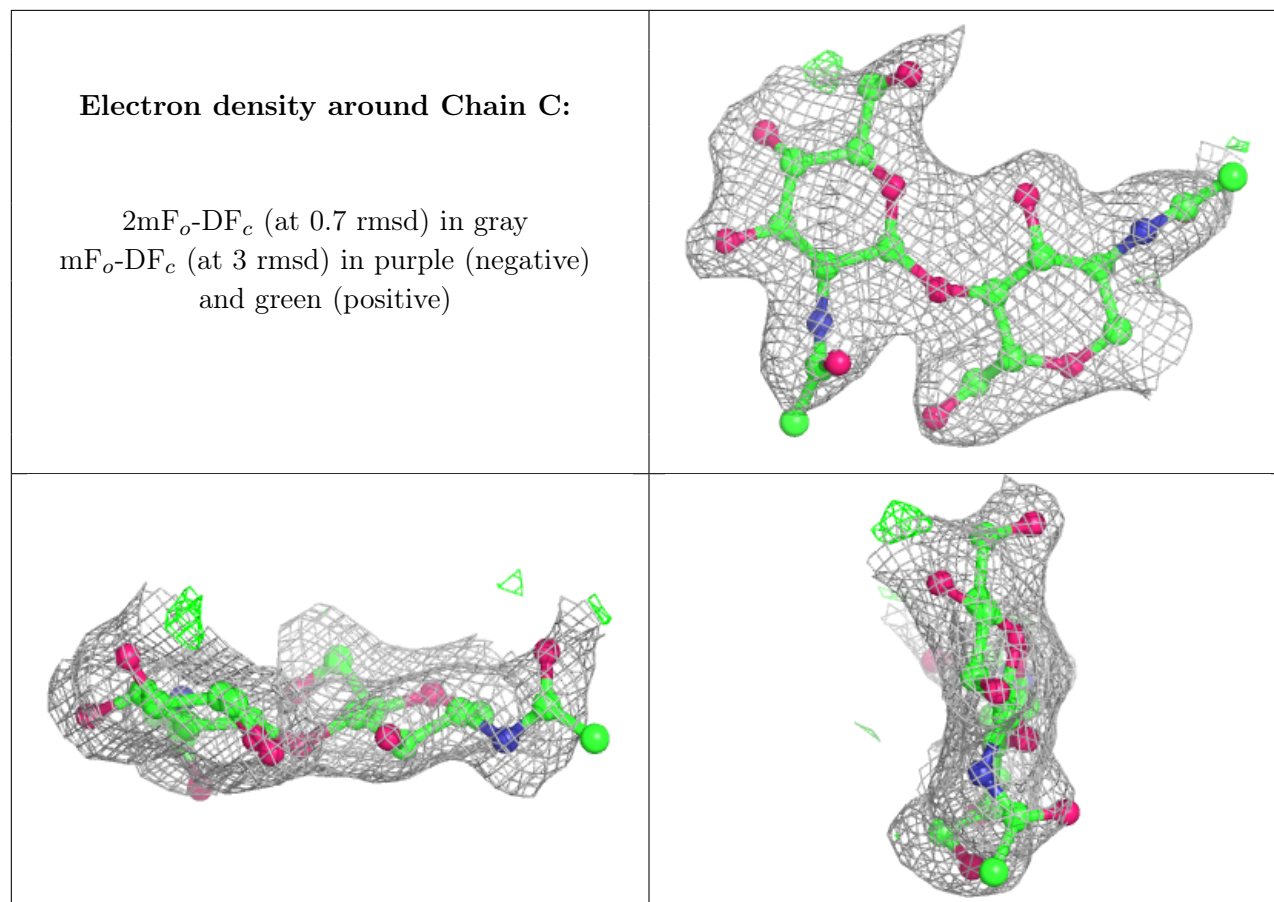
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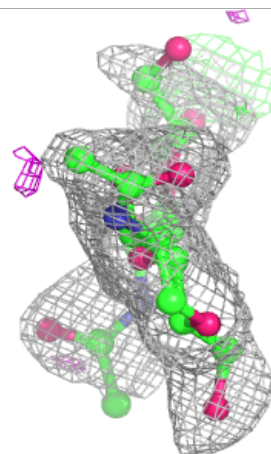
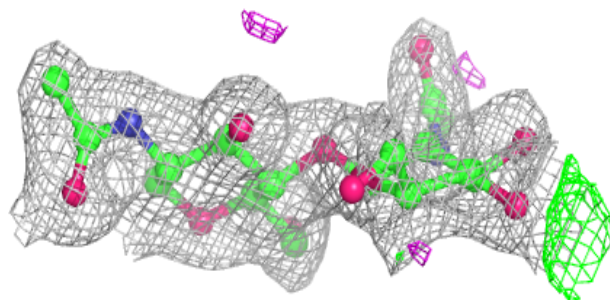
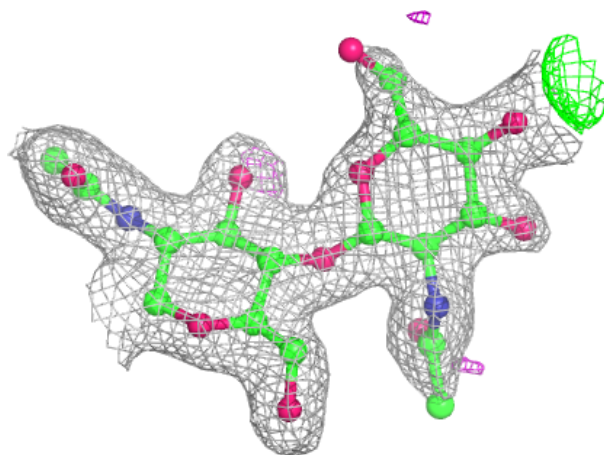
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	NAG	F	2	14/15	0.77	0.13	60,63,68,73	0
2	NAG	F	1	14/15	0.83	0.14	47,54,61,70	0
2	NAG	C	2	14/15	0.84	0.11	55,60,65,69	0
2	NAG	G	1	14/15	0.86	0.10	37,40,47,57	0
2	NAG	E	1	14/15	0.87	0.09	32,36,44,51	0
2	NAG	I	1	14/15	0.87	0.09	37,40,51,58	0
2	NAG	C	1	14/15	0.87	0.11	42,48,55,62	0
2	NAG	H	1	14/15	0.91	0.08	30,36,41,45	0
2	NAG	D	1	14/15	0.95	0.07	26,28,32,34	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.



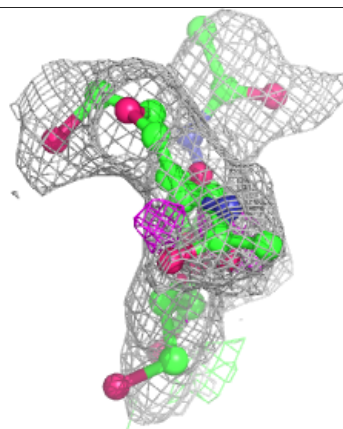
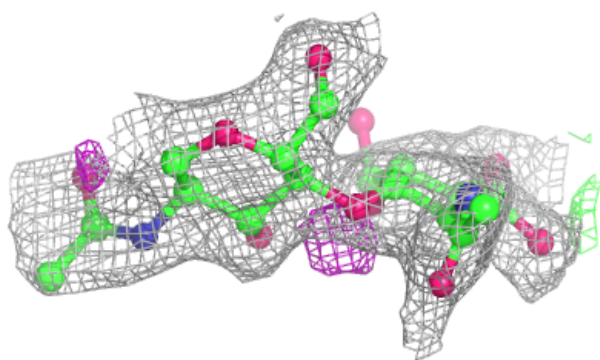
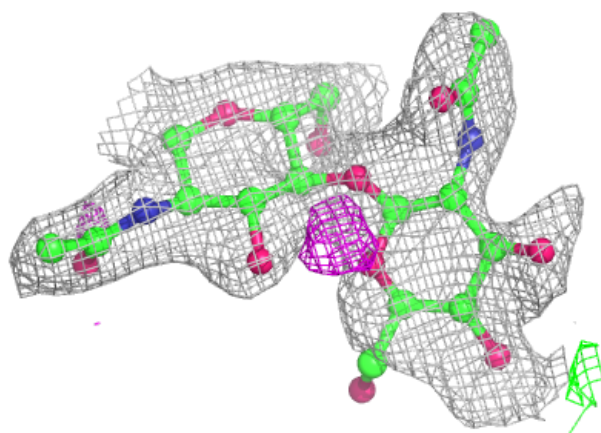
**Electron density around Chain D:**

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



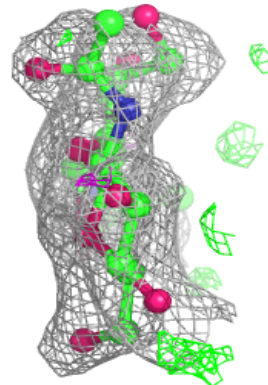
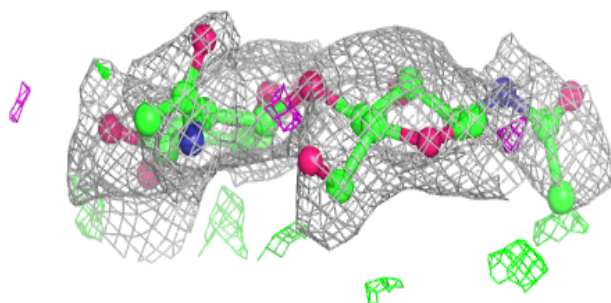
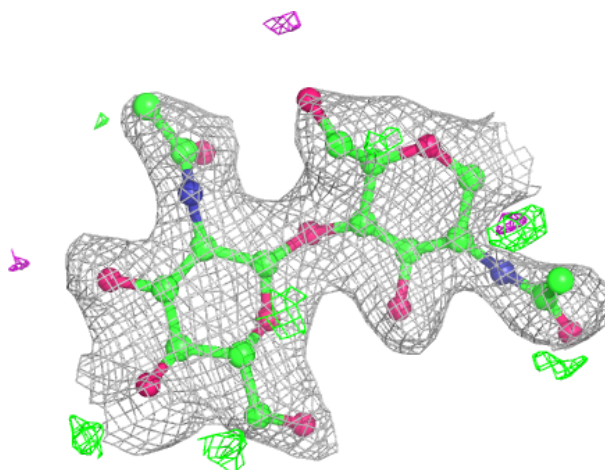
**Electron density around Chain E:**

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



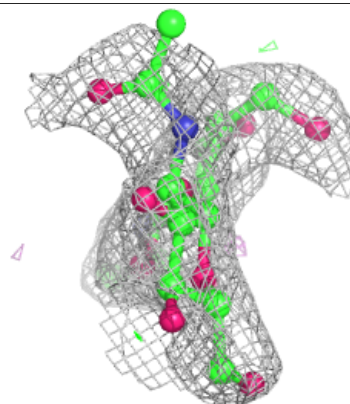
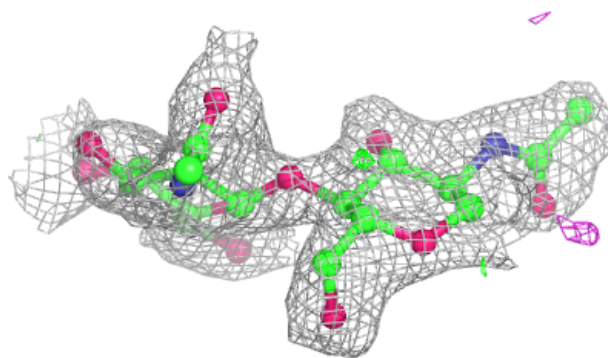
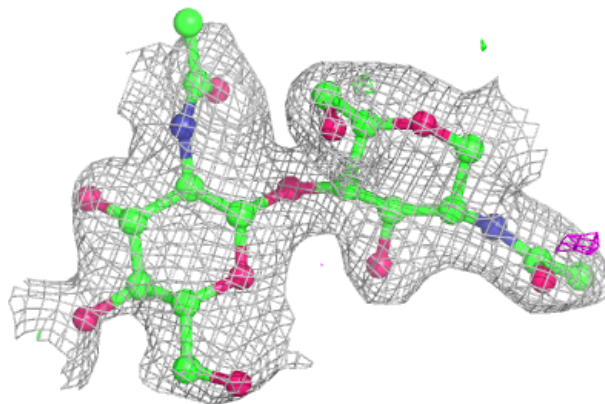
**Electron density around Chain F:**

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



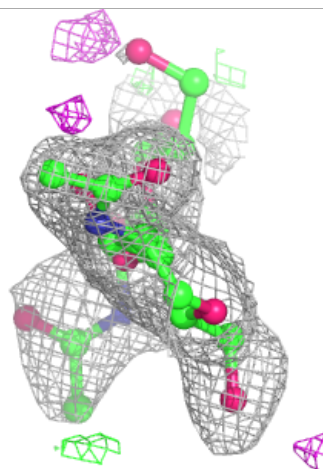
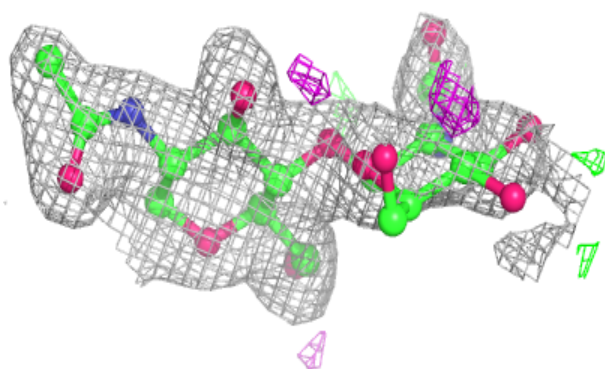
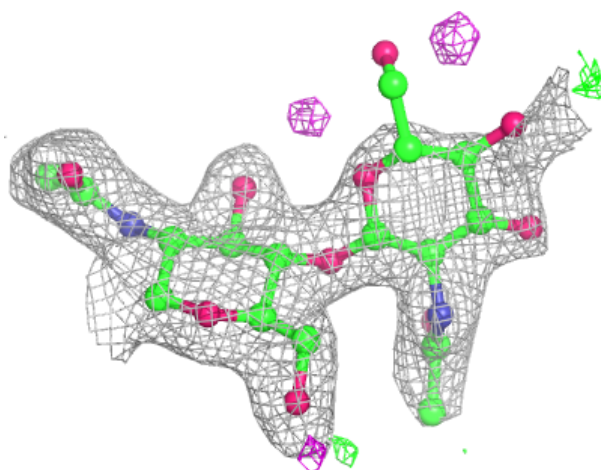
**Electron density around Chain G:**

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

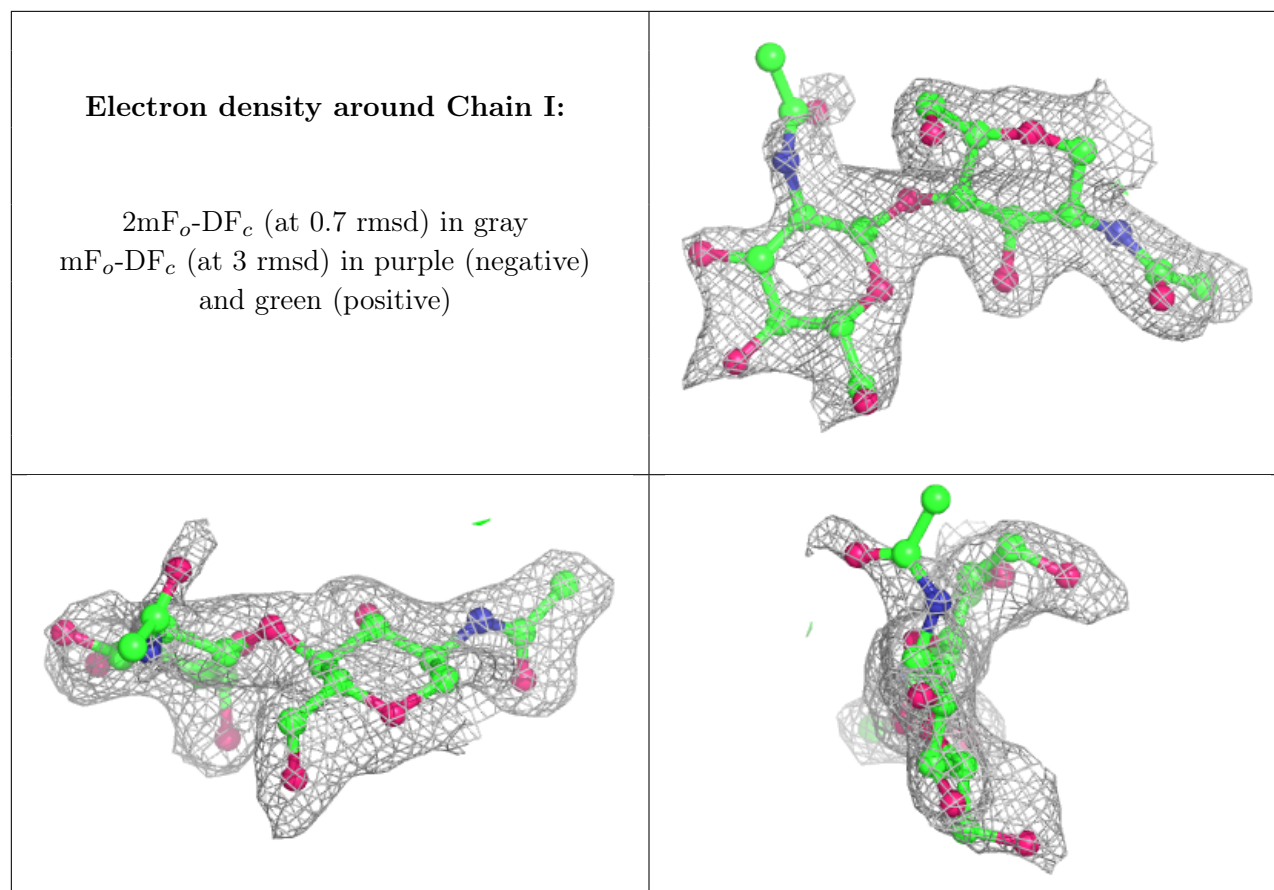


**Electron density around Chain H:**

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







## 6.4 Ligands [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
4	NAG	B	813	14/15	0.65	0.14	55,65,79,80	0
4	NAG	A	812	14/15	0.68	0.14	49,68,73,74	0
5	GOL	A	816	6/6	0.70	0.16	55,57,63,65	0
4	NAG	B	810	14/15	0.74	0.15	55,60,67,70	0
4	NAG	A	808	14/15	0.75	0.14	59,64,71,79	0
5	GOL	B	816	6/6	0.77	0.15	47,47,49,52	0
4	NAG	B	812	14/15	0.78	0.13	45,54,62,73	0
4	NAG	A	813	14/15	0.78	0.12	54,62,68,69	0
5	GOL	A	817	6/6	0.81	0.15	54,59,63,66	0
5	GOL	A	815	6/6	0.84	0.15	29,34,43,49	0
4	NAG	A	811	14/15	0.84	0.13	44,51,62,64	0
5	GOL	B	815	6/6	0.86	0.12	32,33,39,48	0
4	NAG	A	810	14/15	0.86	0.09	35,39,48,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	NAG	A	809	14/15	0.87	0.09	28,31,35,43	0
5	GOL	B	814	6/6	0.91	0.23	26,28,34,45	0
4	NAG	B	811	14/15	0.92	0.08	30,34,38,41	0
5	GOL	A	814	6/6	0.92	0.12	31,36,38,44	0
5	GOL	B	817	6/6	0.93	0.13	31,38,46,47	0
3	CA	A	801	1/1	0.99	0.02	25,25,25,25	0
3	CA	B	801	1/1	1.00	0.03	26,26,26,26	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.