



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 2, 2023 – 03:35 PM EDT

PDB ID : 3W82  
Title : Human alpha-L-iduronidase in complex with iduronic acid  
Authors : Maita, N.; Tsukimura, T.; Taniguchi, T.; Saito, S.; Ohno, K.; Taniguchi, H.; Sakuraba, H.  
Deposited on : 2013-03-11  
Resolution : 2.76 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 : 2.36  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

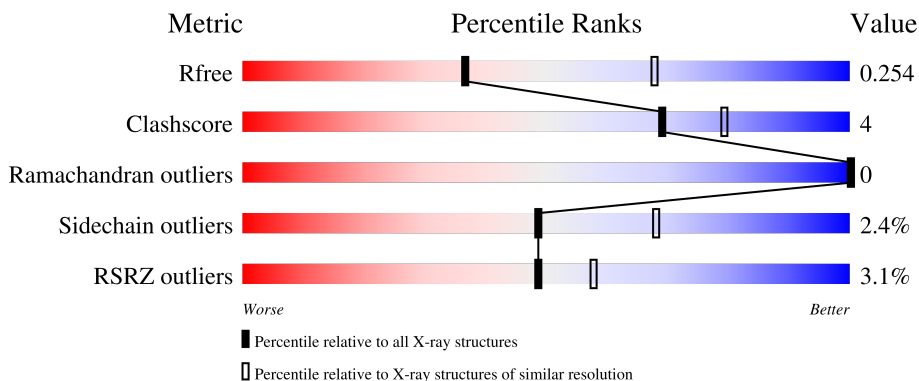
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.76 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



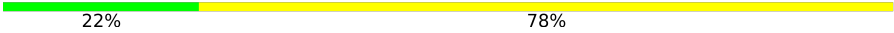

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1235 (2.78-2.74)
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)
RSRZ outliers	127900	1207 (2.78-2.74)

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	627	 3% 88% 10%
1	B	627	 3% 88% 9%
2	C	10	 30% 70%
3	D	2	 50% 50%
3	G	2	 100%

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Mol	Chain	Length	Quality of chain
4	E	9	 22% 78%
5	F	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
4	MAN	E	9	-	-	-	X
5	NAG	F	1	-	-	-	X
8	PO4	A	715	-	-	-	X
9	CL	A	716	-	-	X	-

## 2 Entry composition i

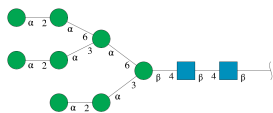
There are 12 unique types of molecules in this entry. The entry contains 10232 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Alpha-L-iduronidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	616	4885	3119	885	869	12	0	0	0
1	B	616	4885	3119	885	869	12	0	0	0

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



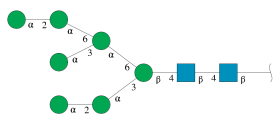
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	C	10	116	64	2	50	0	0	0

- 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
			Total	C	N	O			
3	D	2	28	16	2	10	0	0	0
3	G	2	28	16	2	10	0	0	0

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



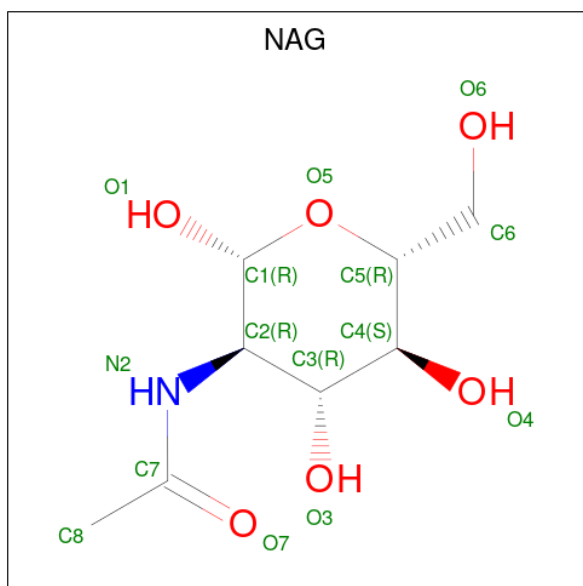
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
4	E	9	105	58	2	45	0	0	0

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



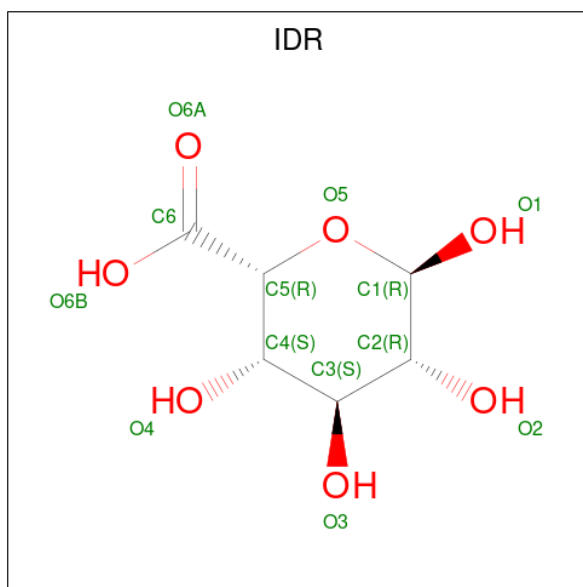
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
5	F	2	24	14	1	9	0	0	0

- Molecule 6 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
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 7 is alpha-L-idopyranuronic acid (three-letter code: IDR) (formula: C<sub>6</sub>H<sub>10</sub>O<sub>7</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			13	6	7		
7	B	1	Total	C	O	0	0
			13	6	7		

- Molecule 8 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).

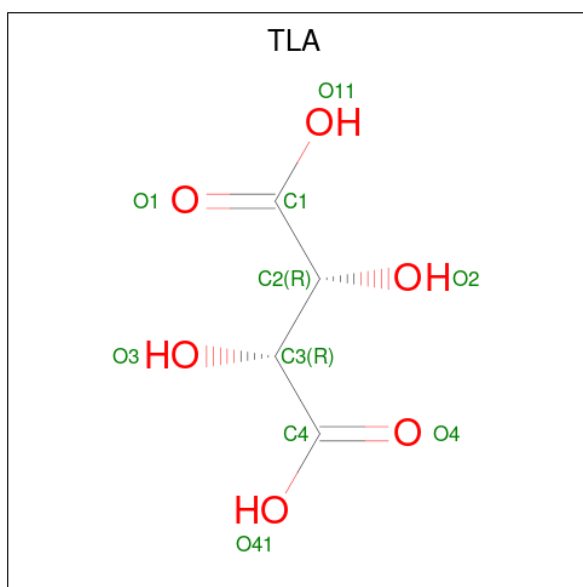


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total O P 5 4 1	0	0
8	B	1	Total O P 5 4 1	0	0

- Molecule 9 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

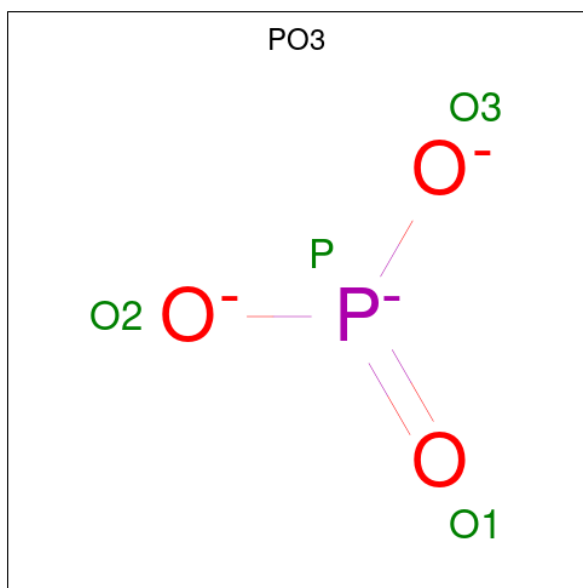
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	1	Total Cl 1 1	0	0
9	B	1	Total Cl 1 1	0	0

- Molecule 10 is L(+)-TARTARIC ACID (three-letter code: TLA) (formula: C<sub>4</sub>H<sub>6</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	B	1	Total C O 10 4 6	0	0

- Molecule 11 is PHOSPHITE ION (three-letter code: PO3) (formula: O<sub>3</sub>P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	B	1	Total O P 4 3 1	0	0

- Molecule 12 is water.

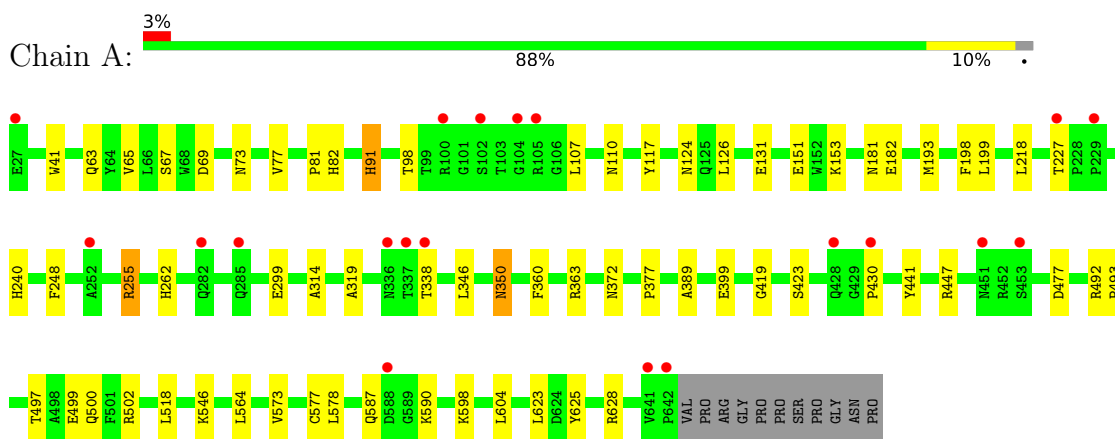


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	46	Total 46	O 46	0	0
12	B	35	Total 35	O 35	0	0

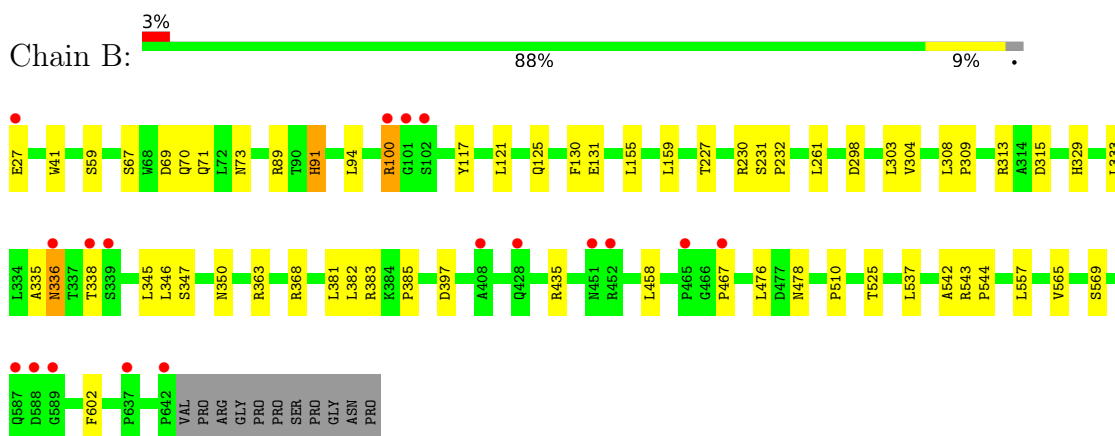
### 3 Residue-property plots [i](#)

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

- Molecule 1: Alpha-L-iduronidase



- Molecule 1: Alpha-L-iduronidase



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

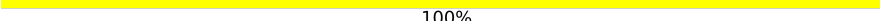


- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:  50% 50%

MAG1  
MAG2

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

Chain G:  100%

MAG1  
MAG2

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

Chain E:  22% 78%

MAG1  
MAG2  
MAN3  
MAN4  
MAN5  
MAN6  
MAN7  
MAN8  
MAN9

- Molecule 5: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:  100%

MAG1  
FUC2

## 4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	259.98Å 259.98Å 65.30Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	37.55 – 2.76 37.52 – 2.76	Depositor EDS
% Data completeness (in resolution range)	95.7 (37.55-2.76) 95.8 (37.52-2.76)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.40 (at 2.77Å)	Xtrriage
Refinement program	REFMAC 5.7.0029	Depositor
R, $R_{free}$	0.195 , 0.254 0.199 , 0.254	Depositor DCC
$R_{free}$ test set	2042 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	29.6	Xtrriage
Anisotropy	0.194	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 31.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	0.024 for h,-h-k,-l	Xtrriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	10232	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.33% 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: FUC, BMA, IDR, PO4, NAG, TLA, CL, PO3, 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	0.37	0/5037	0.54	0/6884
1	B	0.37	0/5037	0.54	0/6884
All	All	0.37	0/10074	0.54	0/13768

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

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	4885	0	4779	38	0
1	B	4885	0	4778	33	0
2	C	116	0	97	0	0
3	D	28	0	25	1	0
3	G	28	0	25	0	0
4	E	105	0	88	1	0
5	F	24	0	22	1	0
6	A	14	0	13	0	0
6	B	14	0	13	1	0
7	A	13	0	9	2	0
7	B	13	0	9	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	A	5	0	0	0	0
8	B	5	0	0	0	0
9	A	1	0	0	2	0
9	B	1	0	0	1	0
10	B	10	0	4	0	0
11	B	4	0	0	0	0
12	A	46	0	0	1	0
12	B	35	0	0	0	0
All	All	10232	0	9862	74	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 4.

All (74) 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)
3:D:1:NAG:O3	3:D:2:NAG:H61	1.89	0.73
1:A:447:ARG:NH1	12:A:842:HOH:O	2.23	0.72
1:A:497:THR:OG1	1:A:500:GLN:HG3	1.90	0.70
1:A:363:ARG:HD3	9:A:716:CL:CL	2.28	0.70
1:B:335:ALA:O	1:B:336:ASN:C	2.34	0.65
1:A:65:VAL:HG13	1:A:117:TYR:CD2	2.32	0.64
1:B:397:ASP:OD1	1:B:435:ARG:NH1	2.33	0.62
1:B:363:ARG:HD3	9:B:719:CL:CL	2.38	0.60
1:B:298:ASP:HA	1:B:347:SER:HB3	1.84	0.60
1:B:303:LEU:HB3	1:B:313:ARG:HH21	1.68	0.58
1:B:125:GLN:NE2	1:B:569:SER:OG	2.37	0.57
1:A:363:ARG:CD	9:A:716:CL:CL	2.91	0.56
1:B:94:LEU:HD21	1:B:159:LEU:HD11	1.89	0.54
1:B:155:LEU:O	1:B:159:LEU:HB2	2.08	0.53
1:A:363:ARG:NH2	7:A:714:IDR:O4	2.41	0.53
1:A:573:VAL:HG11	1:A:578:LEU:HD11	1.91	0.53
1:B:100:ARG:NH2	6:B:710:NAG:O7	2.42	0.52
1:A:65:VAL:CG1	1:A:117:TYR:CD2	2.93	0.51
1:A:372:ASN:HA	1:A:377:PRO:HB3	1.93	0.50
1:A:181:ASN:O	1:A:182:GLU:C	2.49	0.50
5:F:1:NAG:H4	5:F:2:FUC:O5	2.12	0.50
1:B:346:LEU:C	1:B:346:LEU:HD23	2.32	0.49
1:B:91:HIS:ND1	1:B:131:GLU:OE1	2.44	0.49
1:B:117:TYR:CE1	1:B:121:LEU:HD11	2.47	0.49
1:A:218:LEU:HB3	1:A:255:ARG:HD3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:70:GLN:HE22	1:B:73:ASN:HD22	1.60	0.49
1:A:430:PRO:HB2	1:A:546:LYS:HD3	1.94	0.48
1:A:350:ASN:N	1:A:350:ASN:HD22	2.11	0.48
1:A:98:THR:OG1	1:A:110:ASN:HB3	2.14	0.48
1:A:81:PRO:HB2	1:A:82:HIS:CD2	2.48	0.47
1:A:587:GLN:O	1:A:590:LYS:HG2	2.14	0.47
1:A:199:LEU:HB3	1:A:240:HIS:CD2	2.49	0.47
1:A:314:ALA:HB1	1:A:360:PHE:HB3	1.94	0.47
1:B:363:ARG:NH2	7:B:715:IDR:O4	2.47	0.47
1:A:350:ASN:HD22	1:A:350:ASN:H	1.61	0.47
1:B:345:LEU:HD13	1:B:346:LEU:N	2.29	0.46
1:B:308:LEU:HD12	1:B:309:PRO:HD2	1.98	0.46
1:A:73:ASN:O	1:A:77:VAL:HG23	2.16	0.46
1:A:604:LEU:C	1:A:604:LEU:HD23	2.36	0.46
1:B:231:SER:N	1:B:232:PRO:CD	2.80	0.45
1:A:91:HIS:ND1	1:A:131:GLU:OE1	2.49	0.45
1:B:303:LEU:O	1:B:363:ARG:NH1	2.50	0.45
1:B:557:LEU:HB2	1:B:565:VAL:HB	1.99	0.45
1:B:315:ASP:HB2	1:B:478:ASN:OD1	2.17	0.45
1:A:193:MET:SD	1:A:198:PHE:HA	2.57	0.44
1:B:368:ARG:HA	1:B:381:LEU:HD23	2.00	0.44
1:A:63:GLN:O	1:A:67:SER:HB3	2.17	0.44
1:A:153:LYS:HD3	1:A:248:PHE:CE1	2.52	0.44
1:A:299:GLU:OE1	7:A:714:IDR:H1	2.18	0.44
1:B:329:HIS:O	1:B:333:LEU:HB3	2.18	0.44
1:A:499:GLU:HA	1:A:502:ARG:NH1	2.33	0.43
1:B:130:PHE:CZ	1:B:159:LEU:HD21	2.54	0.43
1:A:564:LEU:C	1:A:564:LEU:HD12	2.39	0.43
1:B:467:PRO:HB2	1:B:543:ARG:HB3	1.99	0.43
1:B:476:LEU:HG	1:B:510:PRO:HB3	2.01	0.43
7:B:715:IDR:H2	4:E:6:MAN:O3	2.18	0.43
1:A:124:ASN:O	1:A:126:LEU:HG	2.18	0.43
1:A:107:LEU:HD22	1:A:151:GLU:OE2	2.19	0.42
1:B:383:ARG:HD3	1:B:602:PHE:CZ	2.54	0.42
1:B:315:ASP:HA	1:B:385:PRO:HG2	2.01	0.42
1:A:419:GLY:HA3	1:A:441:TYR:CZ	2.55	0.42
1:A:492:ARG:N	1:A:493:PRO:CD	2.83	0.42
1:B:261:LEU:C	1:B:261:LEU:HD12	2.40	0.42
1:A:262:HIS:CE1	1:A:299:GLU:OE2	2.73	0.42
1:A:577:CYS:HB3	1:A:625:TYR:CD2	2.56	0.41
1:B:303:LEU:HB3	1:B:313:ARG:NH2	2.33	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:67:SER:O	1:B:71:GLN:HG3	2.20	0.41
1:A:477:ASP:OD2	1:A:477:ASP:C	2.59	0.41
1:B:542:ALA:O	1:B:544:PRO:HD3	2.20	0.41
1:A:346:LEU:C	1:A:346:LEU:HD23	2.40	0.41
1:B:89:ARG:CZ	1:B:131:GLU:OE2	2.69	0.41
1:A:399:GLU:O	1:A:423:SER:HA	2.22	0.40
1:B:458:LEU:O	1:B:525:THR:HA	2.22	0.40
1:A:319:ALA:HB1	1:A:389:ALA:HB2	2.02	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	614/627 (98%)	584 (95%)	30 (5%)	0	100	100
1	B	614/627 (98%)	585 (95%)	29 (5%)	0	100	100
All	All	1228/1254 (98%)	1169 (95%)	59 (5%)	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	518/527 (98%)	507 (98%)	11 (2%)	53	71

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	518/527 (98%)	504 (97%)	14 (3%)	44 65
All	All	1036/1054 (98%)	1011 (98%)	25 (2%)	49 68

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	TRP
1	A	69	ASP
1	A	91	HIS
1	A	227	THR
1	A	255	ARG
1	A	338	THR
1	A	350	ASN
1	A	518	LEU
1	A	598	LYS
1	A	623	LEU
1	A	628	ARG
1	B	27	GLU
1	B	41	TRP
1	B	59	SER
1	B	69	ASP
1	B	91	HIS
1	B	100	ARG
1	B	227	THR
1	B	230	ARG
1	B	304	VAL
1	B	336	ASN
1	B	338	THR
1	B	350	ASN
1	B	382	LEU
1	B	537	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	73	ASN
1	A	176	ASN
1	A	240	HIS
1	A	336	ASN
1	A	350	ASN
1	A	356	HIS

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Mol	Chain	Res	Type
1	B	70	GLN
1	B	82	HIS
1	B	125	GLN
1	B	147	GLN
1	B	196	GLN
1	B	350	ASN
1	B	358	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

25 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	NAG	C	1	2,1	14,14,15	0.70	0	17,19,21	1.36	3 (17%)
2	MAN	C	10	2	11,11,12	0.66	0	15,15,17	0.84	0
2	NAG	C	2	2	14,14,15	0.64	0	17,19,21	1.23	2 (11%)
2	BMA	C	3	2	11,11,12	0.28	0	15,15,17	1.14	1 (6%)
2	MAN	C	4	2	11,11,12	0.96	0	15,15,17	1.11	1 (6%)
2	MAN	C	5	2	11,11,12	0.73	0	15,15,17	0.86	0
2	MAN	C	6	2	11,11,12	0.62	0	15,15,17	0.56	0
2	MAN	C	7	2	11,11,12	0.59	0	15,15,17	1.34	2 (13%)
2	MAN	C	8	2	11,11,12	0.65	0	15,15,17	1.08	1 (6%)
2	MAN	C	9	2	11,11,12	0.56	0	15,15,17	1.34	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	NAG	D	1	3,1	14,14,15	0.65	0	17,19,21	0.80	0
3	NAG	D	2	3	14,14,15	0.47	0	17,19,21	1.96	2 (11%)
4	NAG	E	1	4,1	14,14,15	0.74	0	17,19,21	1.21	1 (5%)
4	NAG	E	2	4	14,14,15	0.60	0	17,19,21	0.88	1 (5%)
4	BMA	E	3	4	11,11,12	0.26	0	15,15,17	0.71	0
4	MAN	E	4	4	11,11,12	0.91	1 (9%)	15,15,17	1.09	0
4	MAN	E	5	4	11,11,12	0.60	0	15,15,17	0.90	1 (6%)
4	MAN	E	6	4	11,11,12	0.64	0	15,15,17	0.74	0
4	MAN	E	7	4	11,11,12	0.65	0	15,15,17	0.79	0
4	MAN	E	8	4	11,11,12	0.64	0	15,15,17	1.04	1 (6%)
4	MAN	E	9	4	11,11,12	0.71	0	15,15,17	0.95	1 (6%)
5	NAG	F	1	5,1	14,14,15	0.52	0	17,19,21	1.53	2 (11%)
5	FUC	F	2	5	10,10,11	0.54	0	14,14,16	1.60	2 (14%)
3	NAG	G	1	3,1	14,14,15	0.71	0	17,19,21	1.80	4 (23%)
3	NAG	G	2	3	14,14,15	0.39	0	17,19,21	1.30	2 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	C	1	2,1	-	1/6/23/26	0/1/1/1
2	MAN	C	10	2	-	2/2/19/22	0/1/1/1
2	NAG	C	2	2	-	1/6/23/26	0/1/1/1
2	BMA	C	3	2	-	0/2/19/22	0/1/1/1
2	MAN	C	4	2	-	0/2/19/22	0/1/1/1
2	MAN	C	5	2	-	0/2/19/22	0/1/1/1
2	MAN	C	6	2	-	2/2/19/22	0/1/1/1
2	MAN	C	7	2	-	2/2/19/22	0/1/1/1
2	MAN	C	8	2	-	2/2/19/22	0/1/1/1
2	MAN	C	9	2	-	2/2/19/22	0/1/1/1
3	NAG	D	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	D	2	3	-	2/6/23/26	0/1/1/1
4	NAG	E	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	E	2	4	-	0/6/23/26	0/1/1/1
4	BMA	E	3	4	-	0/2/19/22	0/1/1/1
4	MAN	E	4	4	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	MAN	E	5	4	-	0/2/19/22	0/1/1/1
4	MAN	E	6	4	-	2/2/19/22	0/1/1/1
4	MAN	E	7	4	-	1/2/19/22	0/1/1/1
4	MAN	E	8	4	-	2/2/19/22	0/1/1/1
4	MAN	E	9	4	-	0/2/19/22	0/1/1/1
5	NAG	F	1	5,1	-	2/6/23/26	0/1/1/1
5	FUC	F	2	5	-	-	0/1/1/1
3	NAG	G	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	G	2	3	-	1/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	4	MAN	O5-C1	-2.10	1.40	1.43

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	2	NAG	C1-O5-C5	6.80	121.41	112.19
5	F	1	NAG	C1-O5-C5	4.56	118.38	112.19
3	G	2	NAG	C1-O5-C5	4.01	117.62	112.19
5	F	2	FUC	C1-C2-C3	3.84	114.39	109.67
3	G	1	NAG	C1-O5-C5	3.78	117.31	112.19
5	F	2	FUC	C1-O5-C5	3.64	121.02	112.78
3	G	1	NAG	O5-C5-C6	-3.46	101.78	107.20
2	C	9	MAN	O2-C2-C1	3.32	115.95	109.15
2	C	8	MAN	C1-O5-C5	3.01	116.27	112.19
2	C	2	NAG	O5-C5-C6	2.83	111.64	107.20
4	E	1	NAG	O5-C1-C2	-2.76	106.94	111.29
2	C	7	MAN	O2-C2-C3	-2.70	104.73	110.14
5	F	1	NAG	O5-C5-C6	2.69	111.42	107.20
2	C	1	NAG	C1-O5-C5	2.65	115.79	112.19
3	G	1	NAG	O5-C1-C2	-2.62	107.15	111.29
2	C	7	MAN	O5-C5-C6	2.38	110.93	107.20
4	E	8	MAN	C1-C2-C3	2.37	112.58	109.67
2	C	3	BMA	O3-C3-C2	-2.35	105.50	109.99
2	C	4	MAN	O5-C1-C2	-2.30	107.21	110.77
3	G	2	NAG	O5-C5-C6	2.25	110.73	107.20
3	D	2	NAG	C1-C2-N2	-2.23	106.67	110.49
2	C	1	NAG	C6-C5-C4	-2.22	107.80	113.00
4	E	5	MAN	O2-C2-C3	-2.22	105.70	110.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1	NAG	O3-C3-C2	-2.20	104.92	109.47
3	G	1	NAG	O4-C4-C3	-2.18	105.31	110.35
2	C	9	MAN	C3-C4-C5	2.16	114.09	110.24
2	C	2	NAG	C6-C5-C4	-2.14	108.00	113.00
4	E	2	NAG	O5-C1-C2	-2.03	108.08	111.29
4	E	9	MAN	C2-C3-C4	2.02	114.39	110.89

There are no chirality outliers.

All (26) torsion outliers are listed below:

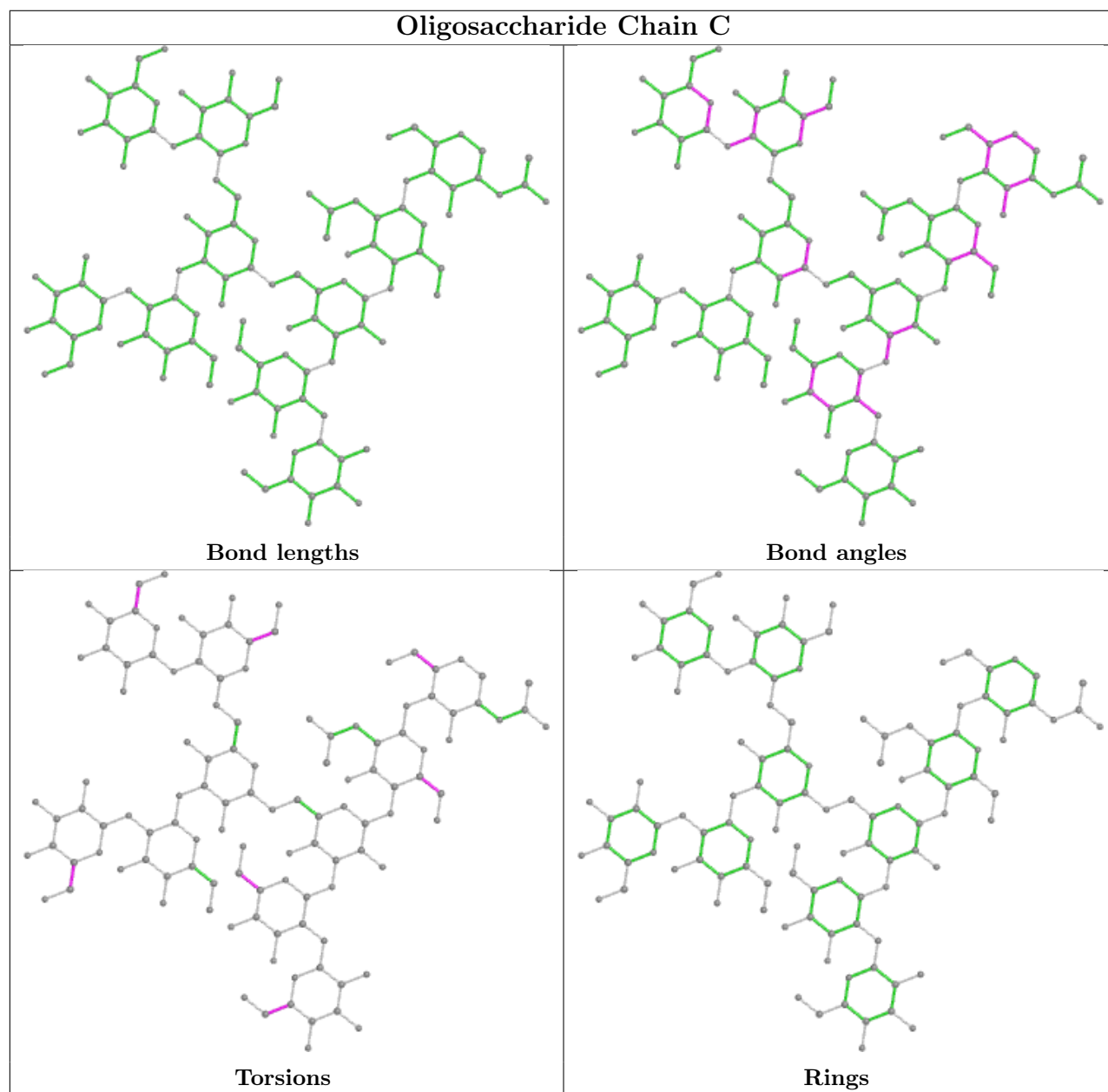
Mol	Chain	Res	Type	Atoms
2	C	7	MAN	O5-C5-C6-O6
2	C	8	MAN	O5-C5-C6-O6
3	D	2	NAG	O5-C5-C6-O6
2	C	7	MAN	C4-C5-C6-O6
2	C	9	MAN	C4-C5-C6-O6
2	C	8	MAN	C4-C5-C6-O6
2	C	9	MAN	O5-C5-C6-O6
4	E	8	MAN	C4-C5-C6-O6
3	G	1	NAG	C4-C5-C6-O6
4	E	6	MAN	C4-C5-C6-O6
4	E	8	MAN	O5-C5-C6-O6
5	F	1	NAG	O5-C5-C6-O6
5	F	1	NAG	C4-C5-C6-O6
2	C	6	MAN	C4-C5-C6-O6
3	G	1	NAG	O5-C5-C6-O6
4	E	6	MAN	O5-C5-C6-O6
4	E	7	MAN	O5-C5-C6-O6
3	D	2	NAG	C4-C5-C6-O6
2	C	6	MAN	O5-C5-C6-O6
2	C	10	MAN	C4-C5-C6-O6
2	C	1	NAG	C4-C5-C6-O6
2	C	10	MAN	O5-C5-C6-O6
2	C	2	NAG	O5-C5-C6-O6
3	D	1	NAG	C4-C5-C6-O6
3	G	2	NAG	O5-C5-C6-O6
3	D	1	NAG	O5-C5-C6-O6

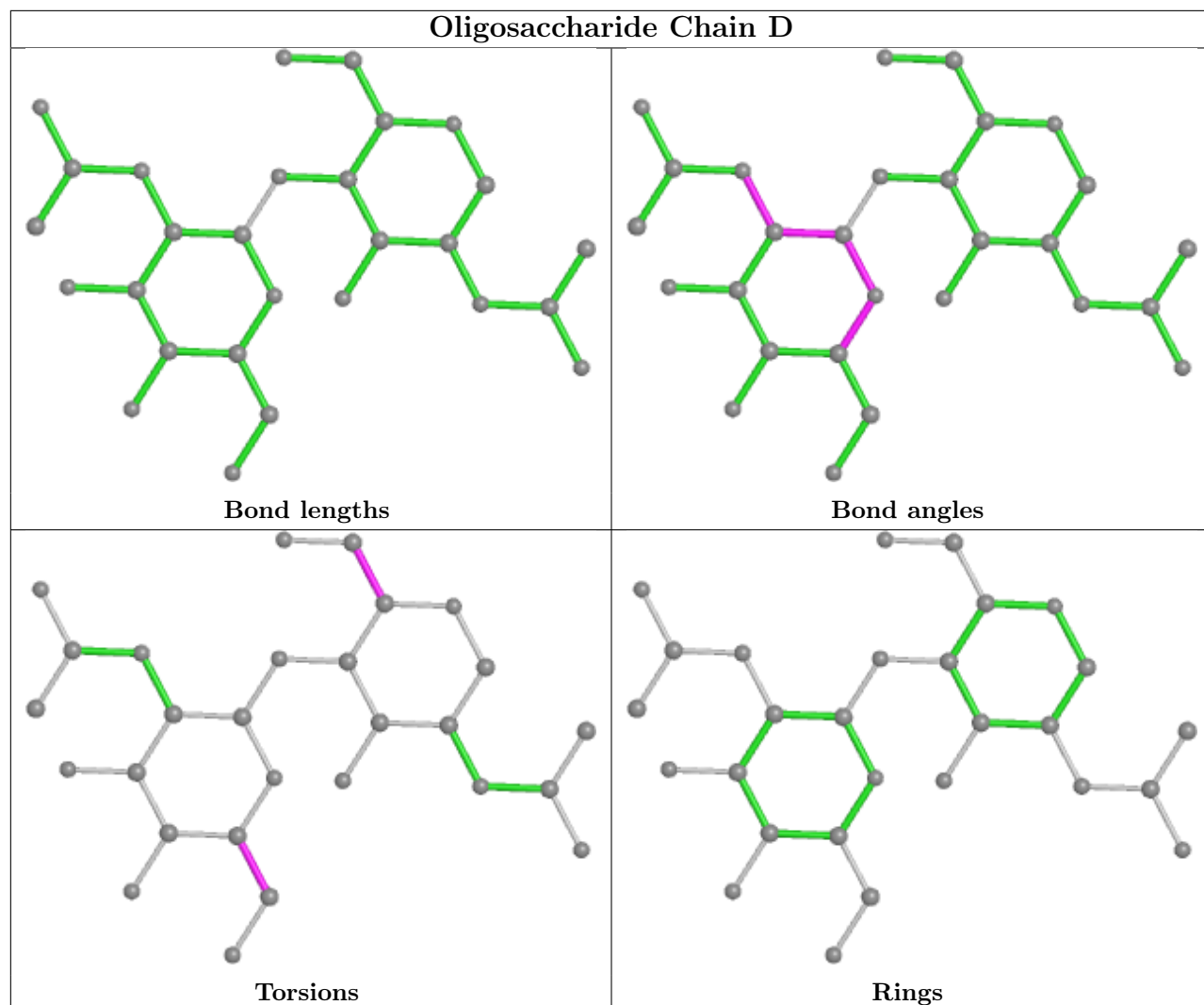
There are no ring outliers.

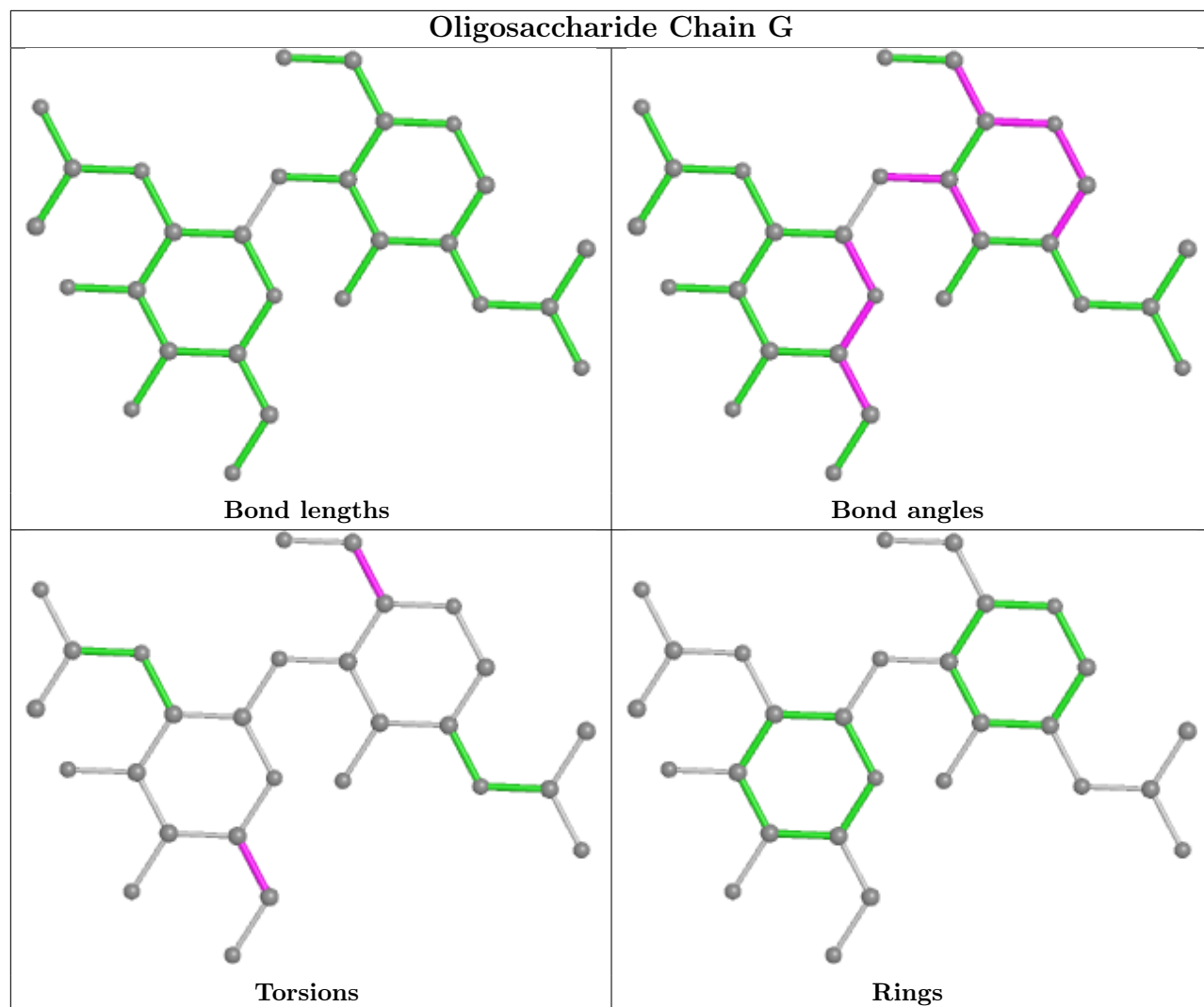
5 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	6	MAN	1	0
5	F	1	NAG	1	0
3	D	1	NAG	1	0
3	D	2	NAG	1	0
5	F	2	FUC	1	0

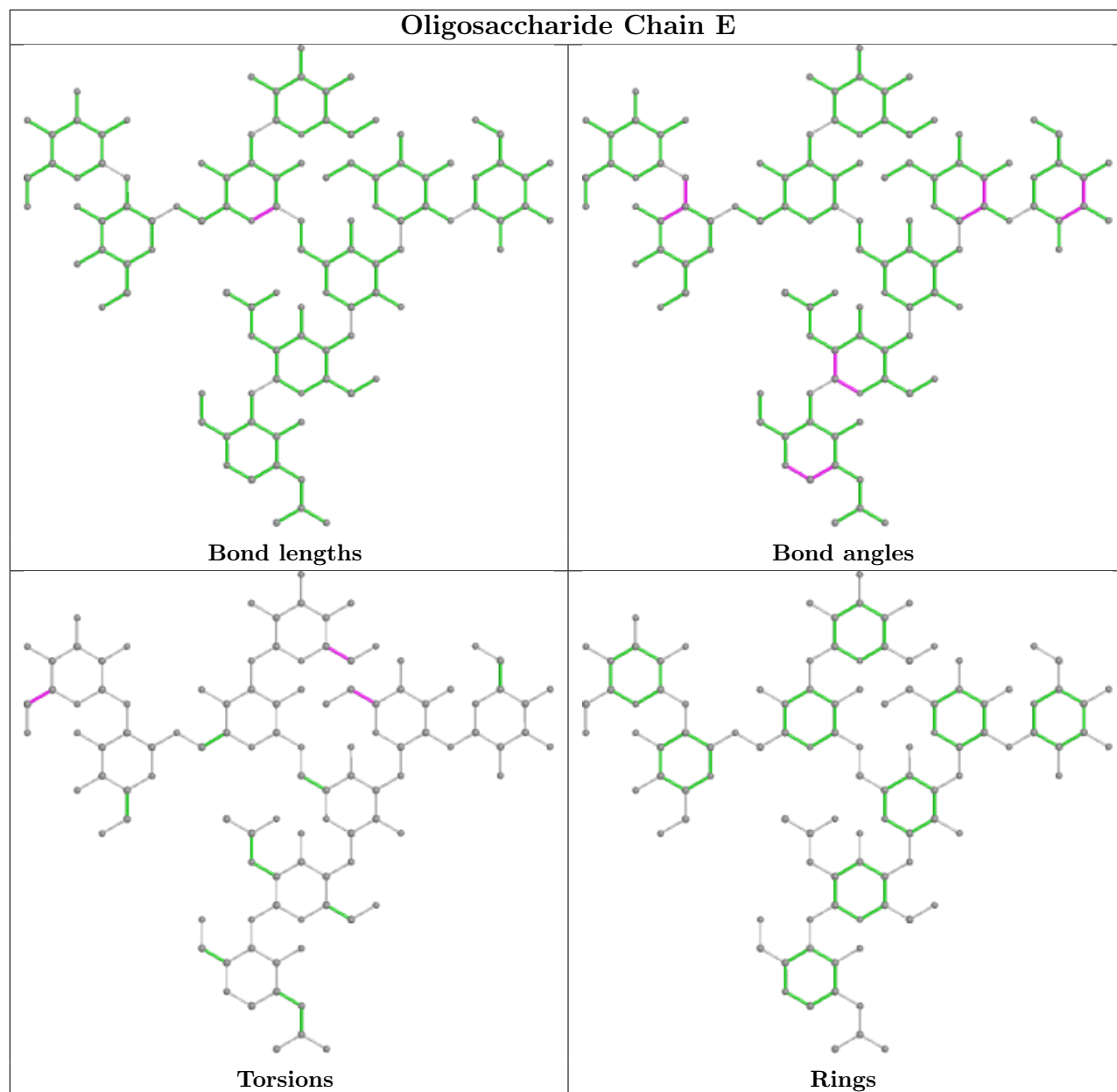
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

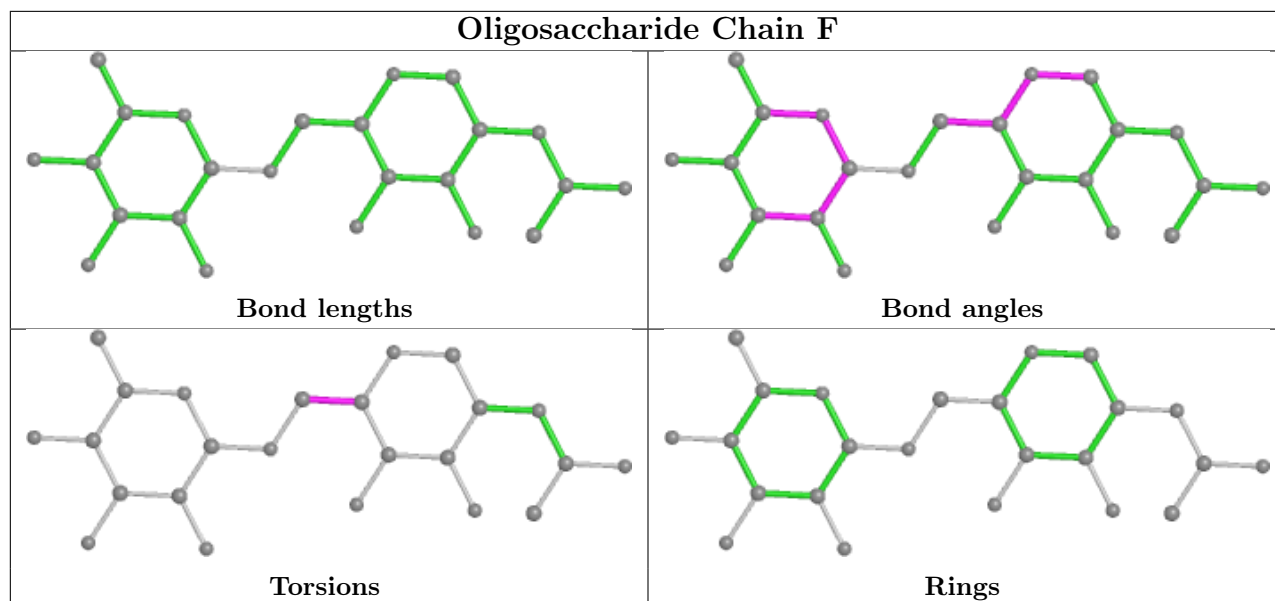












## 5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 2 are monoatomic - leaving 8 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
8	PO4	A	715	-	4,4,4	0.84	0	6,6,6	0.40	0
6	NAG	A	711	1	14,14,15	0.49	0	17,19,21	0.92	1 (5%)
7	IDR	B	715	-	13,13,13	0.90	0	18,19,19	0.63	0
8	PO4	B	718	-	4,4,4	0.80	0	6,6,6	0.42	0
10	TLA	B	716	-	9,9,9	1.17	1 (11%)	12,12,12	1.40	2 (16%)
6	NAG	B	710	1	14,14,15	0.52	0	17,19,21	1.40	2 (11%)
11	PO3	B	717	-	0,3,3	-	-	0,3,3	-	-
7	IDR	A	714	-	13,13,13	1.06	0	18,19,19	0.83	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
6	NAG	A	711	1	-	0/6/23/26	0/1/1/1
7	IDR	B	715	-	-	1/4/24/24	0/1/1/1
10	TLA	B	716	-	-	0/12/12/12	-
6	NAG	B	710	1	-	1/6/23/26	0/1/1/1
7	IDR	A	714	-	-	0/4/24/24	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	716	TLA	C2-C1	-2.08	1.49	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	710	NAG	C1-O5-C5	3.91	117.49	112.19
10	B	716	TLA	O41-C4-C3	2.78	120.78	113.27
10	B	716	TLA	O2-C2-C1	-2.24	105.97	110.66
6	B	710	NAG	O7-C7-C8	-2.19	117.99	122.06
6	A	711	NAG	C1-O5-C5	2.15	115.11	112.19

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	710	NAG	O5-C5-C6-O6
7	B	715	IDR	O5-C5-C6-O6B

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	715	IDR	2	0
6	B	710	NAG	1	0
7	A	714	IDR	2	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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	616/627 (98%)	-0.07	20 (3%) 47 56	15, 24, 48, 75	0
1	B	616/627 (98%)	-0.10	18 (2%) 51 61	15, 26, 51, 76	0
All	All	1232/1254 (98%)	-0.09	38 (3%) 49 58	15, 25, 48, 76	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	338	THR	4.6
1	B	27	GLU	4.4
1	B	451	ASN	4.0
1	B	588	ASP	3.5
1	A	100	ARG	3.5
1	A	641	VAL	3.4
1	A	642	PRO	3.3
1	A	588	ASP	3.3
1	B	465	PRO	3.3
1	B	642	PRO	3.2
1	B	336	ASN	3.1
1	B	467	PRO	3.1
1	A	27	GLU	3.1
1	A	451	ASN	2.9
1	A	337	THR	2.8
1	B	589	GLY	2.8
1	B	339	SER	2.7
1	A	285	GLN	2.7
1	A	428	GLN	2.6
1	B	452	ARG	2.6
1	A	338	THR	2.5
1	A	282	GLN	2.4
1	B	637	PRO	2.4
1	A	104	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	101	GLY	2.4
1	A	453	SER	2.4
1	B	428	GLN	2.4
1	A	336	ASN	2.2
1	B	408	ALA	2.2
1	A	105	ARG	2.2
1	A	252	ALA	2.1
1	B	100	ARG	2.1
1	B	102	SER	2.1
1	A	227	THR	2.1
1	A	102	SER	2.1
1	A	229	PRO	2.1
1	A	430	PRO	2.1
1	B	587	GLN	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.

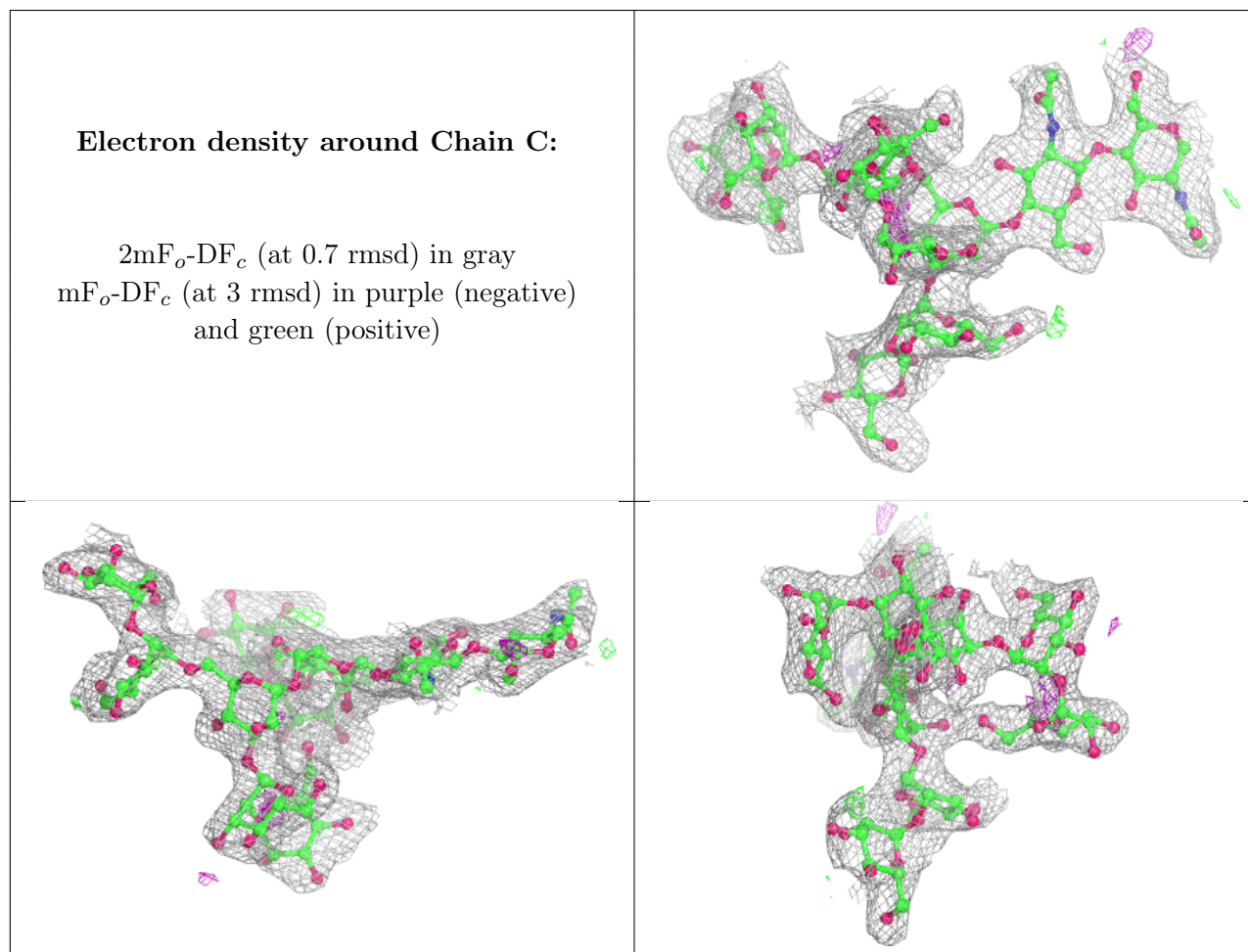
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
5	NAG	F	1	14/15	0.68	0.42	60,72,83,84	0
4	MAN	E	5	11/12	0.78	0.30	52,58,61,63	0
4	MAN	E	9	11/12	0.80	0.41	61,65,69,69	0
3	NAG	D	2	14/15	0.80	0.36	69,74,83,85	0
5	FUC	F	2	10/11	0.80	0.50	83,87,91,91	0
4	MAN	E	8	11/12	0.81	0.35	54,55,61,62	0
2	MAN	C	10	11/12	0.83	0.24	50,55,58,59	0
4	MAN	E	6	11/12	0.85	0.30	62,66,67,68	0
4	MAN	E	7	11/12	0.86	0.28	50,53,56,57	0
3	NAG	G	2	14/15	0.89	0.38	61,65,67,68	0
3	NAG	D	1	14/15	0.90	0.22	41,44,51,62	0
2	MAN	C	6	11/12	0.91	0.25	26,28,29,30	0
4	BMA	E	3	11/12	0.92	0.21	39,40,43,49	0
2	MAN	C	9	11/12	0.92	0.15	38,41,43,46	0

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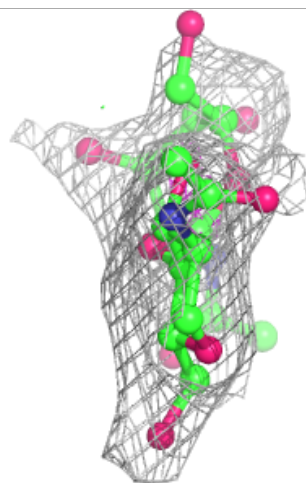
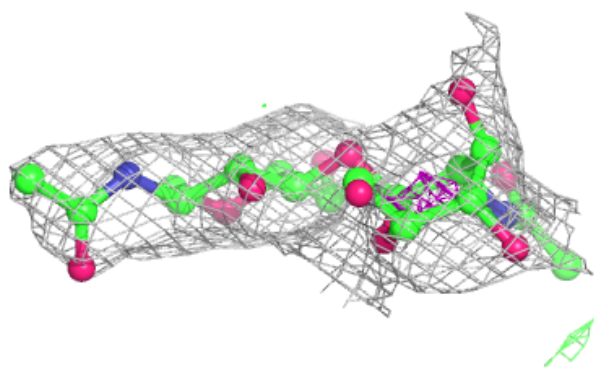
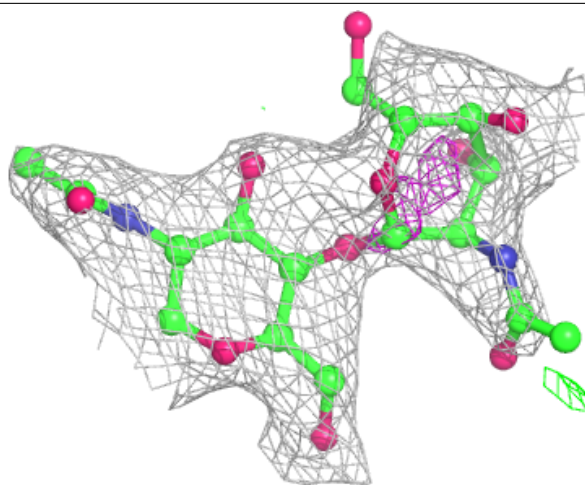
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	MAN	E	4	11/12	0.93	0.22	44,49,52,59	0
2	MAN	C	5	11/12	0.93	0.19	25,26,28,28	0
4	NAG	E	2	14/15	0.94	0.20	31,33,35,38	0
2	MAN	C	8	11/12	0.94	0.15	24,25,26,27	0
3	NAG	G	1	14/15	0.94	0.20	35,41,46,53	0
2	MAN	C	7	11/12	0.94	0.14	26,27,27,28	0
4	NAG	E	1	14/15	0.94	0.18	28,30,32,34	0
2	MAN	C	4	11/12	0.95	0.14	23,25,27,27	0
2	BMA	C	3	11/12	0.95	0.12	24,26,27,33	0
2	NAG	C	2	14/15	0.96	0.13	19,20,21,22	0
2	NAG	C	1	14/15	0.97	0.13	16,17,18,19	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:**

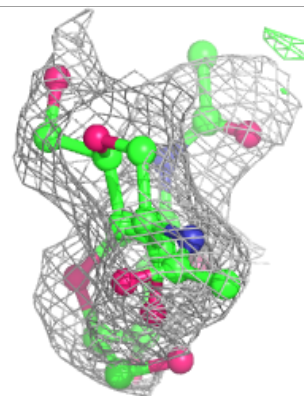
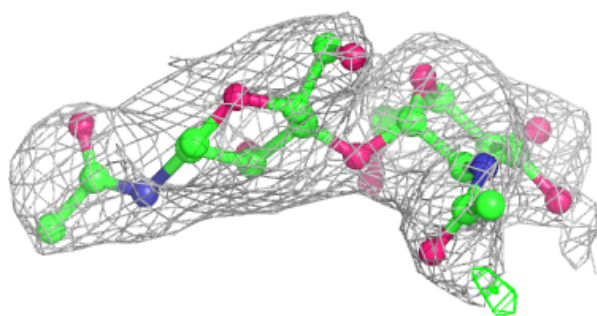
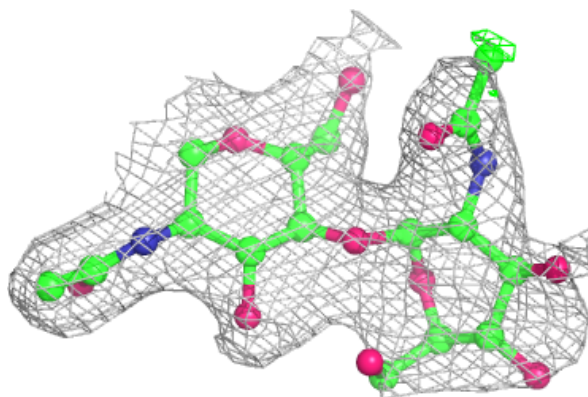
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



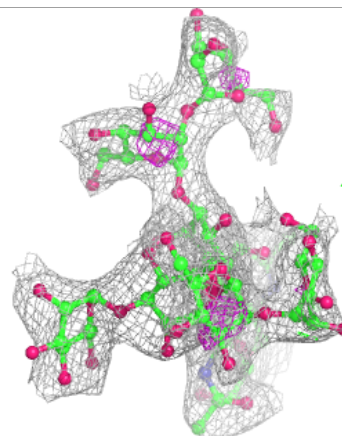
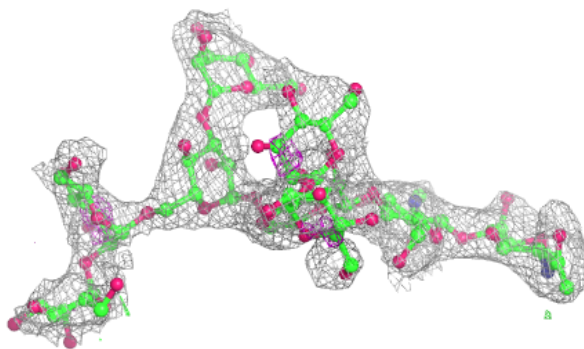
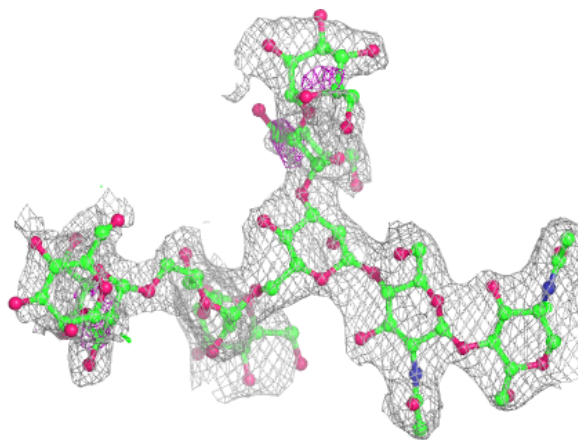


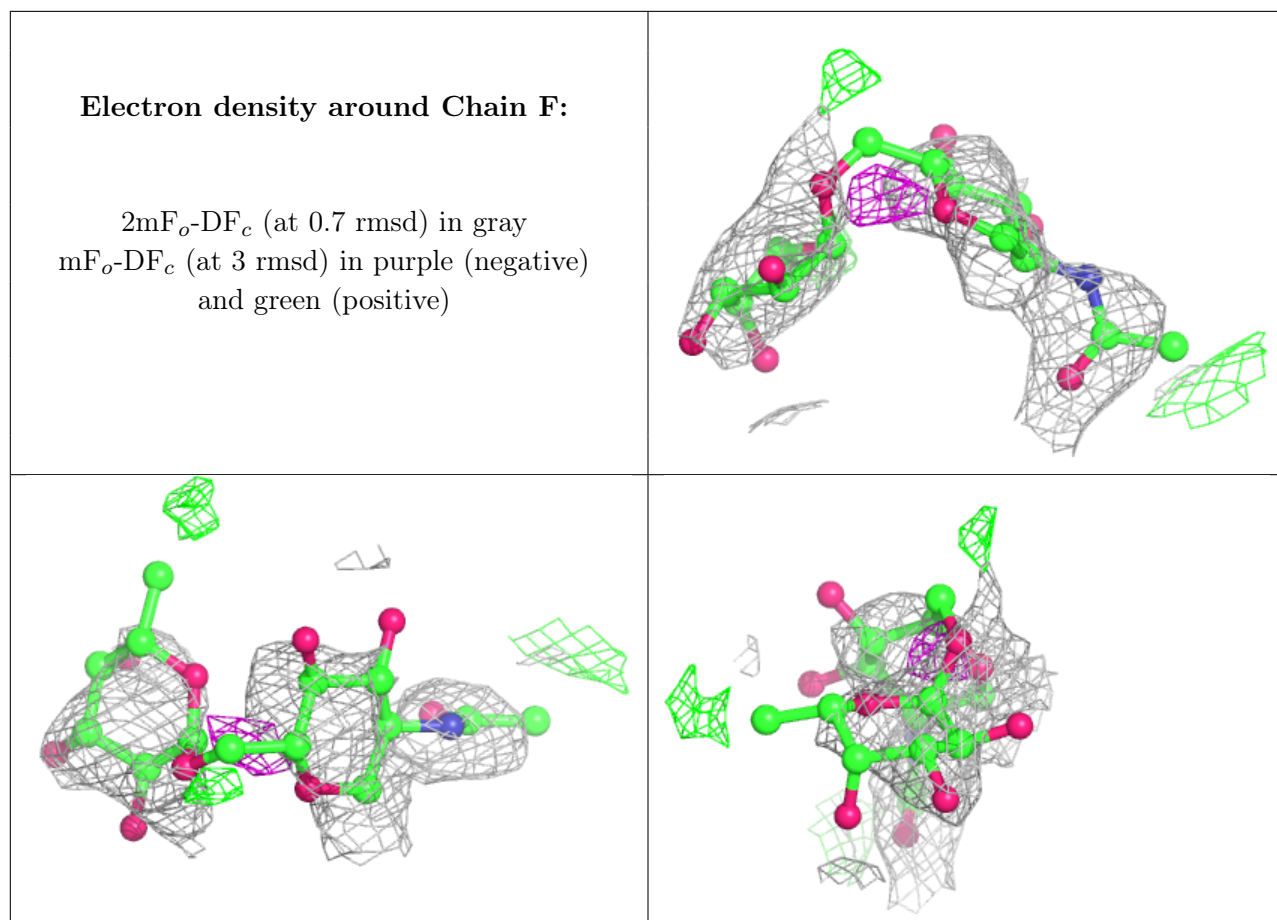
**Electron density around Chain G:**

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

**Electron density around Chain E:**

$2mF_o-DF_c$  (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
8	PO4	A	715	5/5	0.68	0.47	95,95,99,100	0
6	NAG	B	710	14/15	0.87	0.31	30,34,39,39	0
11	PO3	B	717	4/4	0.88	0.20	45,45,49,50	0
6	NAG	A	711	14/15	0.90	0.23	38,40,44,45	0
7	IDR	B	715	13/13	0.90	0.20	30,35,37,38	0
10	TLA	B	716	10/10	0.92	0.17	36,38,38,39	0
8	PO4	B	718	5/5	0.93	0.30	54,55,57,58	0
7	IDR	A	714	13/13	0.95	0.13	21,22,23,23	0
9	CL	A	716	1/1	0.99	0.12	18,18,18,18	0
9	CL	B	719	1/1	0.99	0.07	15,15,15,15	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.