



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 2, 2024 – 08:06 pm GMT

PDB ID : 5FX8  
Title : Complete structure of manganese lipoxygenase of *Gaeumannomyces graminis* and partial structure of zonadhesin of *Komagataella pastoris*  
Authors : Chen, Y.; Wennman, A.; Karkehanadi, S.; Engstrom, A.; Oliw, E.H.  
Deposited on : 2016-02-25  
Resolution : 2.60 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 : 1.8.4, 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

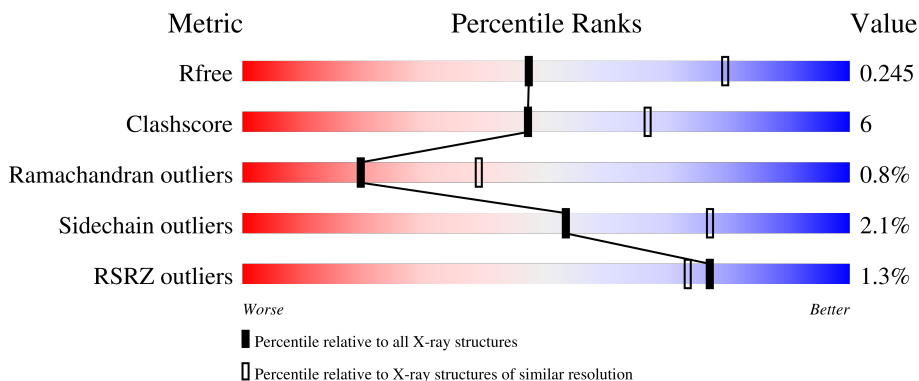
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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.




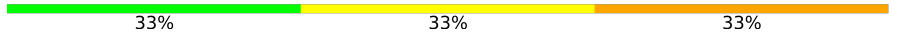

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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	618	81% 9% . 9%
1	B	618	76% 13% . 10%
2	U	320	4% 79% 15% . .
3	C	2	100%
3	E	2	100%

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Mol	Chain	Length	Quality of chain
3	F	2	 50% 50%
4	D	3	 33% 33% 33%
5	G	2	 50% 50%

## 2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 11543 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 LINOLEATE 11-LIPOXYGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	563	Total	C	N	O	S	0	0	0
			4397	2807	780	799	11			
1	B	556	Total	C	N	O	S	0	0	0
			4353	2783	772	787	11			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	52	ASN	LYS	conflict	UNP Q8X151
A	158	CYS	TYR	conflict	UNP Q8X151
B	52	ASN	LYS	conflict	UNP Q8X151
B	158	CYS	TYR	conflict	UNP Q8X151

- Molecule 2 is a protein called ZONADHESIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	U	309	Total	C	N	O	S	0	0	0
			2344	1491	351	500	2			

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



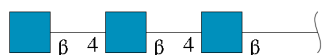
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	C	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	E	2	Total	C	N	O	0	0	0
			28	16	2	10			

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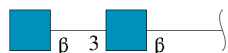
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	F	2	28	16	2	10	0	0	0

- Molecule 4 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(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	D	3	42	24	3	15	0	0	0

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



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

- Molecule 6 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Mn	0	0
			1	1		
6	B	1	Total	Mn	0	0
			1	1		

- Molecule 7 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>).

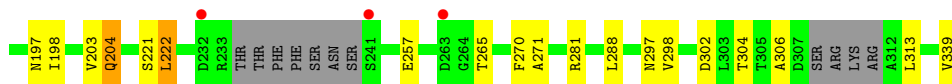


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
7	A	1	14	8	1	5	0	0
7	A	1	14	8	1	5	0	0
7	B	1	14	8	1	5	0	0
7	B	1	14	8	1	5	0	0
7	B	1	14	8	1	5	0	0

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
8	A	125	125	125	0	0
8	B	72	72	72	0	0
8	U	26	26	26	0	0





- 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 E: 100%

MAG1  
MAG2

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

Chain F: 50% 50%

MAG1  
MAG2

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

Chain D: 33% 33% 33%

MAG1  
MAG2  
MAG3

- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G: 50% 50%

MAG1  
MAG2



## 4 Data and refinement statistics i

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	226.31Å 50.47Å 177.62Å 90.00° 91.28° 90.00°	Depositor
Resolution (Å)	43.16 – 2.60 43.16 – 2.60	Depositor EDS
% Data completeness (in resolution range)	96.0 (43.16-2.60) 96.0 (43.16-2.60)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.33 (at 2.61Å)	Xtrriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, $R_{free}$	0.195 , 0.245 0.195 , 0.245	Depositor DCC
$R_{free}$ test set	3049 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	27.5	Xtrriage
Anisotropy	0.529	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 40.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.014 for -h,-k,l	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	11543	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	23.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.46% 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: NAG, MN

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	2/4513 (0.0%)	0.70	2/6132 (0.0%)
1	B	0.58	0/4469	0.64	1/6072 (0.0%)
2	U	0.59	0/2397	0.64	0/3283
All	All	0.62	2/11379 (0.0%)	0.66	3/15487 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	451	ASP	C-N	-6.29	1.19	1.34
1	A	174	TYR	CD1-CE1	-5.53	1.31	1.39

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	229	ARG	NE-CZ-NH1	6.52	123.56	120.30
1	B	143	LYS	CD-CE-NZ	-6.33	97.15	111.70
1	A	322	MET	CG-SD-CE	-5.07	92.10	100.20

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	4397	0	4296	46	0
1	B	4353	0	4266	55	0
2	U	2344	0	2176	36	0
3	C	28	0	25	0	0
3	E	28	0	25	0	0
3	F	28	0	25	1	0
4	D	42	0	37	1	0
5	G	28	0	25	2	0
6	A	1	0	0	0	0
6	B	1	0	0	1	0
7	A	28	0	26	1	0
7	B	42	0	39	0	0
8	A	125	0	0	6	0
8	B	72	0	0	5	0
8	U	26	0	0	0	0
All	All	11543	0	10940	139	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 6.

All (139) 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)
2:U:61:GLY:O	2:U:63:ALA:N	1.87	1.06
1:A:263:THR:HG22	1:A:265:LEU:H	1.34	0.90
8:A:2079:HOH:O	1:B:101:ARG:NH2	2.13	0.80
1:A:577:GLU:OE1	8:A:2119:HOH:O	1.99	0.79
1:A:519:LEU:HD13	1:A:520:LEU:N	2.00	0.77
2:U:194:ASP:OD1	2:U:306:ALA:N	2.18	0.76
1:B:454:ALA:O	8:B:2062:HOH:O	2.04	0.75
2:U:60:ALA:HB3	2:U:120:ILE:HD13	1.67	0.75
1:A:519:LEU:HD12	1:A:521:ALA:H	1.50	0.74
1:B:81:THR:CG2	1:B:299:ILE:HB	2.19	0.73
1:B:574:ARG:NH1	1:B:578:ASP:OD1	2.22	0.72
1:A:81:THR:CG2	1:A:299:ILE:HB	2.18	0.72
2:U:203:VAL:HG12	2:U:265:THR:HG22	1.73	0.70
2:U:60:ALA:HA	2:U:61:GLY:O	1.92	0.69
1:A:423:ASP:OD1	1:A:423:ASP:O	2.11	0.68
1:B:618:VAL:N	8:B:2013:HOH:O	2.15	0.68
1:B:166:MET:HB3	1:B:600:MET:HE2	1.76	0.68
2:U:203:VAL:HG22	2:U:298:VAL:CG1	2.26	0.66
1:A:81:THR:HG21	1:A:299:ILE:HB	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:194:VAL:HG13	1:B:265:LEU:HD12	1.77	0.65
2:U:221:SER:OG	2:U:222:LEU:N	2.29	0.65
1:B:140:GLY:C	1:B:143:LYS:HZ1	2.00	0.65
1:B:618:VAL:O	8:B:2043:HOH:O	2.15	0.64
1:B:486:PRO:HA	1:B:490:SER:HB2	1.80	0.64
5:G:1:NAG:H83	5:G:1:NAG:H3	1.79	0.64
1:A:519:LEU:CD1	1:A:521:ALA:H	2.11	0.62
1:B:81:THR:HG21	1:B:299:ILE:HB	1.79	0.62
1:B:178:ARG:NH2	1:B:390:PRO:O	2.33	0.62
1:B:218:SER:HA	1:B:233:ALA:HB1	1.82	0.62
6:B:1000:MN:MN	8:B:2043:HOH:O	1.56	0.61
4:D:3:NAG:H3	4:D:3:NAG:H83	1.83	0.61
2:U:193:GLY:HA2	2:U:194:ASP:HB3	1.83	0.61
2:U:203:VAL:HG22	2:U:298:VAL:HG12	1.84	0.60
1:A:424:ASP:C	1:A:460:ARG:HD2	2.22	0.60
1:A:396:PRO:HG2	1:A:600:MET:HE3	1.84	0.59
1:B:298:GLU:OE1	1:B:329:ARG:NH2	2.34	0.59
2:U:193:GLY:CA	2:U:194:ASP:HB3	2.32	0.59
1:B:165:SER:HB3	1:B:249:PRO:HD3	1.83	0.59
1:B:166:MET:HB3	1:B:600:MET:CE	2.32	0.58
1:A:550:THR:HG23	1:A:609:PRO:O	2.03	0.58
2:U:204:GLN:HE21	2:U:297:ASN:HD22	1.51	0.58
1:B:110:THR:O	1:B:114:GLU:HG3	2.04	0.58
1:A:452:PHE:CG	1:A:453:PRO:HD2	2.38	0.58
1:B:81:THR:HG23	1:B:299:ILE:HB	1.86	0.58
1:B:483:GLN:NE2	1:B:617:SER:O	2.32	0.57
1:A:151:SER:HB3	1:A:154:MET:HB2	1.86	0.57
1:A:81:THR:HG23	1:A:299:ILE:HB	1.86	0.57
1:A:80:THR:OG1	1:A:81:THR:N	2.38	0.56
1:A:581:ARG:HH12	2:U:194:ASP:H	1.54	0.56
2:U:60:ALA:CB	2:U:120:ILE:HD13	2.36	0.56
1:B:543:GLN:HG3	5:G:1:NAG:C7	2.35	0.56
2:U:184:TRP:HE1	2:U:204:GLN:HE22	1.52	0.55
1:A:519:LEU:HD13	1:A:520:LEU:H	1.71	0.55
2:U:21:PHE:CE1	2:U:56:ASP:HB2	2.42	0.54
1:B:360:SER:O	1:B:364:GLN:HG3	2.09	0.53
1:B:409:ARG:NH1	1:B:465:ASP:OD1	2.35	0.53
2:U:43:TRP:CE2	2:U:132:LYS:HE3	2.44	0.52
1:A:107:GLN:HB2	1:A:543:GLN:HE22	1.75	0.52
2:U:58:THR:C	2:U:60:ALA:H	2.14	0.52
2:U:21:PHE:CZ	2:U:56:ASP:HB2	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:166:MET:HB3	1:A:600:MET:CE	2.42	0.51
1:A:377:ASP:OD1	8:A:2087:HOH:O	2.19	0.50
2:U:135:GLU:O	2:U:139:GLU:HG2	2.12	0.50
1:A:422:ALA:HB3	1:A:460:ARG:NH2	2.26	0.50
2:U:58:THR:O	2:U:60:ALA:N	2.45	0.49
2:U:187:ASP:OD2	2:U:281:ARG:NH2	2.39	0.49
1:B:253:LYS:HE3	1:B:259:ASP:OD1	2.12	0.49
1:B:374:LEU:HD22	1:B:405:ILE:HD12	1.95	0.49
1:B:113:ARG:HG3	1:B:114:GLU:N	2.28	0.49
1:A:486:PRO:HA	1:A:490:SER:HB2	1.95	0.49
1:B:83:TYR:CG	1:B:84:PRO:HD2	2.49	0.48
1:B:526:GLU:O	1:B:530:VAL:HG23	2.14	0.48
1:A:253:LYS:HE2	1:A:259:ASP:OD1	2.13	0.48
1:A:83:TYR:HH	1:A:93:SER:HG	1.44	0.48
1:B:187:PRO:HB2	1:B:188:PHE:CD2	2.49	0.48
1:B:375:GLU:O	1:B:379:ARG:HG2	2.14	0.48
1:B:56:GLN:HG2	3:F:1:NAG:HN2	1.78	0.47
1:A:374:LEU:HD22	1:A:405:ILE:HD12	1.97	0.47
1:A:108:THR:HG23	1:A:538:ARG:HD3	1.97	0.46
1:A:417:ASP:OD1	1:A:460:ARG:NH1	2.48	0.46
1:A:452:PHE:CD1	1:A:453:PRO:HD2	2.50	0.46
1:B:495:LEU:HD23	1:B:495:LEU:HA	1.78	0.46
1:B:158:CYS:O	1:B:495:LEU:HD11	2.16	0.46
1:A:166:MET:O	1:A:600:MET:HE1	2.16	0.46
1:A:51:ASN:OD1	1:A:51:ASN:N	2.50	0.45
1:A:417:ASP:HA	1:A:460:ARG:HH12	1.80	0.45
1:B:502:ALA:HB3	1:B:522:TRP:CD1	2.51	0.45
1:A:424:ASP:HA	8:A:2096:HOH:O	2.17	0.45
1:B:264:PRO:HG3	1:B:271:TRP:CZ2	2.52	0.45
1:B:168:ARG:HD3	8:B:2024:HOH:O	2.16	0.45
2:U:197:ASN:HB2	2:U:304:THR:HB	1.97	0.45
1:B:298:GLU:OE1	1:B:329:ARG:NE	2.46	0.45
1:B:552:ARG:HG2	1:B:579:THR:OG1	2.16	0.45
1:B:572:ASN:O	1:B:576:VAL:HG23	2.17	0.44
1:A:550:THR:HG22	1:A:552:ARG:H	1.83	0.44
1:A:81:THR:HB	1:A:295:THR:HB	1.99	0.44
1:A:436:LEU:HD12	1:A:439:TRP:HE3	1.82	0.44
1:B:177:LYS:HE2	1:B:381:ARG:HG2	1.99	0.44
1:A:396:PRO:HG2	1:A:600:MET:CE	2.45	0.44
2:U:198:ILE:HB	2:U:270:PHE:HB2	2.00	0.44
1:A:479:HIS:CD2	1:A:612:ASN:HB3	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:355:ILE:HD13	1:B:355:ILE:HA	1.86	0.44
2:U:182:VAL:CG2	2:U:288:LEU:HD11	2.48	0.44
1:A:232:ALA:HA	1:A:256:VAL:HG21	1.99	0.44
1:B:294:HIS:CE1	1:B:328:ILE:HG12	2.53	0.44
1:B:478:HIS:CE1	1:B:482:ASN:HB3	2.53	0.44
1:B:201:THR:OG1	1:B:202:THR:N	2.51	0.43
1:A:91:ASN:HD22	7:A:1006:NAG:H83	1.82	0.43
1:B:417:ASP:HA	1:B:460:ARG:HH12	1.81	0.43
2:U:143:PRO:HA	2:U:144:GLY:HA2	1.75	0.43
2:U:57:GLU:H	2:U:57:GLU:HG3	1.66	0.43
2:U:64:THR:HA	2:U:111:PHE:O	2.19	0.43
2:U:123:LEU:HD23	2:U:123:LEU:HA	1.93	0.43
1:B:122:ILE:HD11	1:B:137:LEU:HA	1.99	0.43
1:B:173:PRO:HG3	1:B:397:PHE:CG	2.54	0.43
2:U:194:ASP:OD1	2:U:194:ASP:O	2.37	0.43
1:B:48:THR:O	1:B:59:ARG:NH2	2.46	0.42
2:U:30:SER:HB2	2:U:38:ALA:HB2	2.00	0.42
2:U:302:ASP:HB3	2:U:313:LEU:HD21	2.00	0.42
2:U:257:GLU:CD	2:U:271:ALA:HB2	2.40	0.42
1:A:409:ARG:NH1	1:A:465:ASP:OD1	2.47	0.42
1:B:48:THR:HG22	1:B:59:ARG:HH12	1.85	0.42
2:U:118:GLN:NE2	2:U:339:VAL:O	2.53	0.42
1:A:194:VAL:HG13	1:A:265:LEU:HD12	2.02	0.42
1:B:479:HIS:CD2	1:B:612:ASN:HB3	2.55	0.42
1:B:140:GLY:CA	1:B:143:LYS:HZ1	2.32	0.42
1:A:170:SER:HB3	1:A:600:MET:HE3	2.02	0.41
1:B:338:ASN:OD1	1:B:338:ASN:N	2.49	0.41
1:A:284:PHE:CE2	1:A:349:LEU:HD12	2.55	0.41
1:B:140:GLY:HA2	1:B:143:LYS:HZ1	1.86	0.41
1:B:226:GLN:NE2	1:B:347:PHE:O	2.54	0.41
2:U:116:PRO:O	2:U:117:GLY:C	2.59	0.41
1:B:166:MET:O	1:B:600:MET:HE3	2.21	0.40
1:B:273:LEU:O	1:B:277:MET:HG3	2.21	0.40
2:U:20:ALA:N	2:U:154:ASP:OD1	2.53	0.40
1:A:167:GLU:OE1	1:A:168:ARG:NH2	2.54	0.40
1:A:531:GLU:OE2	8:A:2112:HOH:O	2.22	0.40
1:A:391:ARG:NH1	8:A:2090:HOH:O	2.23	0.40
2:U:148:PHE:O	2:U:158:SER:HA	2.21	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	557/618 (90%)	533 (96%)	22 (4%)	2 (0%)	34	57
1	B	550/618 (89%)	523 (95%)	26 (5%)	1 (0%)	47	71
2	U	303/320 (95%)	282 (93%)	13 (4%)	8 (3%)	5	9
All	All	1410/1556 (91%)	1338 (95%)	61 (4%)	11 (1%)	19	39

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	U	58	THR
2	U	62	ASP
2	U	61	GLY
2	U	117	GLY
1	A	476	GLY
2	U	179	THR
1	A	422	ALA
1	B	476	GLY
2	U	222	LEU
2	U	181	GLY
2	U	59	ILE

### 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	451/491 (92%)	445 (99%)	6 (1%)	69	86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	448/491 (91%)	437 (98%)	11 (2%)	47	73
2	U	265/277 (96%)	258 (97%)	7 (3%)	46	72
All	All	1164/1259 (92%)	1140 (98%)	24 (2%)	53	77

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	51	ASN
1	A	168	ARG
1	A	391	ARG
1	A	395	PHE
1	A	531	GLU
1	A	550	THR
1	B	48	THR
1	B	98	LEU
1	B	113	ARG
1	B	148	GLU
1	B	290	HIS
1	B	379	ARG
1	B	395	PHE
1	B	482	ASN
1	B	574	ARG
1	B	600	MET
1	B	617	SER
2	U	56	ASP
2	U	57	GLU
2	U	115	ASP
2	U	123	LEU
2	U	160	SER
2	U	166	LEU
2	U	204	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	U	204	GLN

### 5.3.3 RNA

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](#)

11 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
3	NAG	C	1	1,3	14,14,15	0.58	0	17,19,21	0.40	0
3	NAG	C	2	3	14,14,15	0.39	0	17,19,21	0.65	0
4	NAG	D	1	1,4	14,14,15	0.60	0	17,19,21	0.55	0
4	NAG	D	2	4	14,14,15	0.56	0	17,19,21	1.02	1 (5%)
4	NAG	D	3	4	14,14,15	1.31	1 (7%)	17,19,21	2.14	4 (23%)
3	NAG	E	1	1,3	14,14,15	0.21	0	17,19,21	0.53	0
3	NAG	E	2	3	14,14,15	0.28	0	17,19,21	0.53	0
3	NAG	F	1	1,3	14,14,15	0.98	1 (7%)	17,19,21	1.98	2 (11%)
3	NAG	F	2	3	14,14,15	1.46	1 (7%)	17,19,21	0.75	0
5	NAG	G	1	5,1	14,14,15	0.55	0	17,19,21	1.49	2 (11%)
5	NAG	G	2	5	14,14,15	0.31	0	17,19,21	0.68	1 (5%)

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
3	NAG	C	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	C	2	3	-	2/6/23/26	0/1/1/1
4	NAG	D	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	D	2	4	-	0/6/23/26	0/1/1/1
4	NAG	D	3	4	-	5/6/23/26	0/1/1/1
3	NAG	E	1	1,3	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	E	2	3	-	2/6/23/26	0/1/1/1
3	NAG	F	1	1,3	-	1/6/23/26	0/1/1/1
3	NAG	F	2	3	-	4/6/23/26	0/1/1/1
5	NAG	G	1	5,1	-	4/6/23/26	0/1/1/1
5	NAG	G	2	5	-	2/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	2	NAG	O5-C1	-5.00	1.35	1.43
4	D	3	NAG	O5-C1	4.58	1.51	1.43
3	F	1	NAG	O5-C1	3.04	1.48	1.43

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	3	NAG	C1-O5-C5	5.95	120.25	112.19
3	F	1	NAG	C1-O5-C5	5.48	119.61	112.19
3	F	1	NAG	O4-C4-C5	5.13	122.03	109.30
4	D	3	NAG	C2-N2-C7	4.23	128.93	122.90
5	G	1	NAG	C2-N2-C7	4.21	128.90	122.90
5	G	1	NAG	C1-C2-N2	2.80	115.28	110.49
4	D	3	NAG	C1-C2-N2	2.75	115.18	110.49
4	D	2	NAG	C1-O5-C5	2.49	115.57	112.19
4	D	3	NAG	O3-C3-C4	2.30	115.66	110.35
5	G	2	NAG	C1-O5-C5	2.04	114.96	112.19

There are no chirality outliers.

All (22) torsion outliers are listed below:

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

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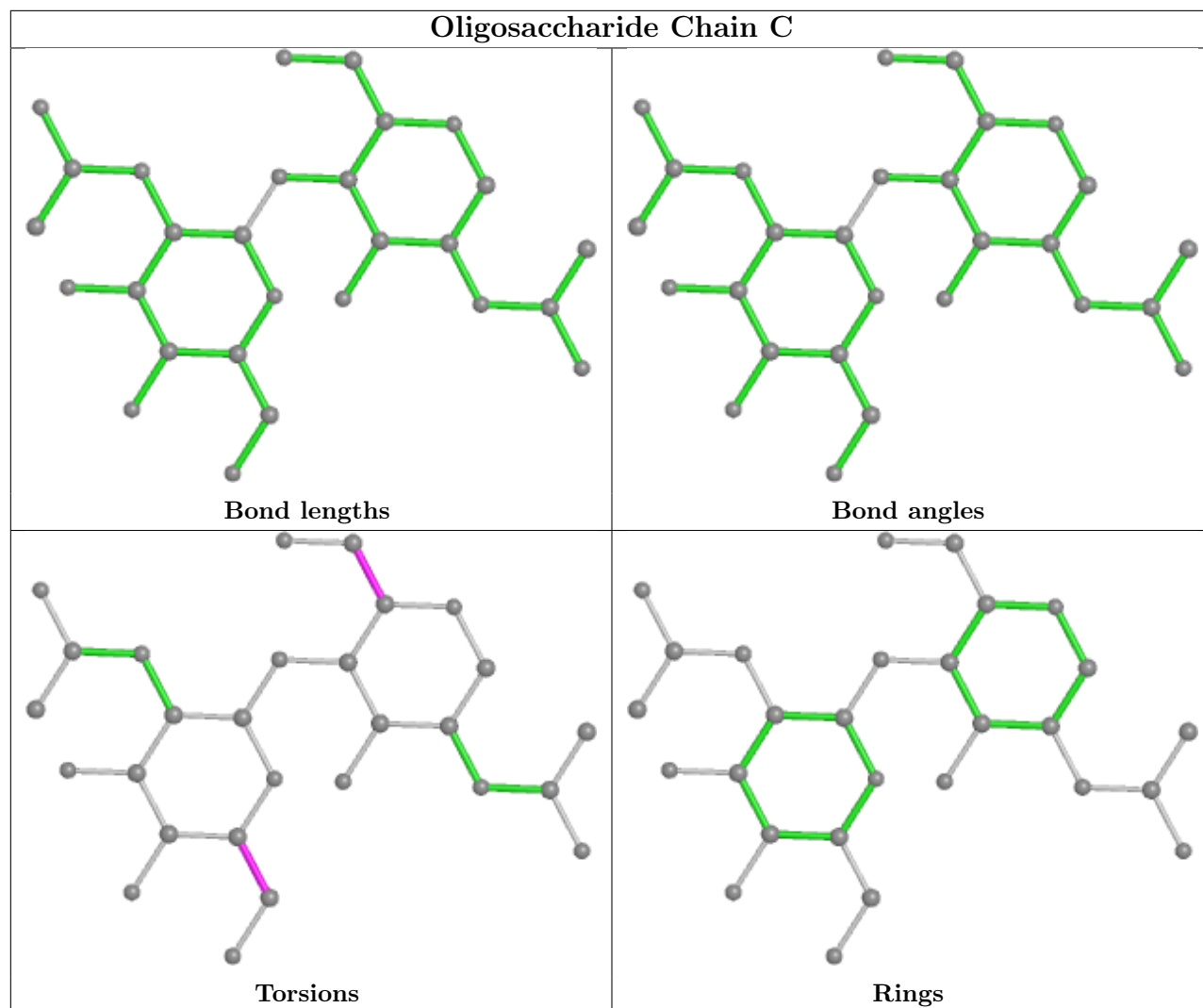
Mol	Chain	Res	Type	Atoms
4	D	3	NAG	O7-C7-N2-C2
5	G	1	NAG	C8-C7-N2-C2
5	G	1	NAG	O7-C7-N2-C2
4	D	3	NAG	C4-C5-C6-O6
3	F	2	NAG	O5-C5-C6-O6
5	G	2	NAG	C4-C5-C6-O6
3	C	1	NAG	O5-C5-C6-O6
3	C	1	NAG	C4-C5-C6-O6
5	G	2	NAG	O5-C5-C6-O6
5	G	1	NAG	O5-C5-C6-O6
4	D	3	NAG	C3-C2-N2-C7
5	G	1	NAG	C3-C2-N2-C7
3	F	1	NAG	C4-C5-C6-O6

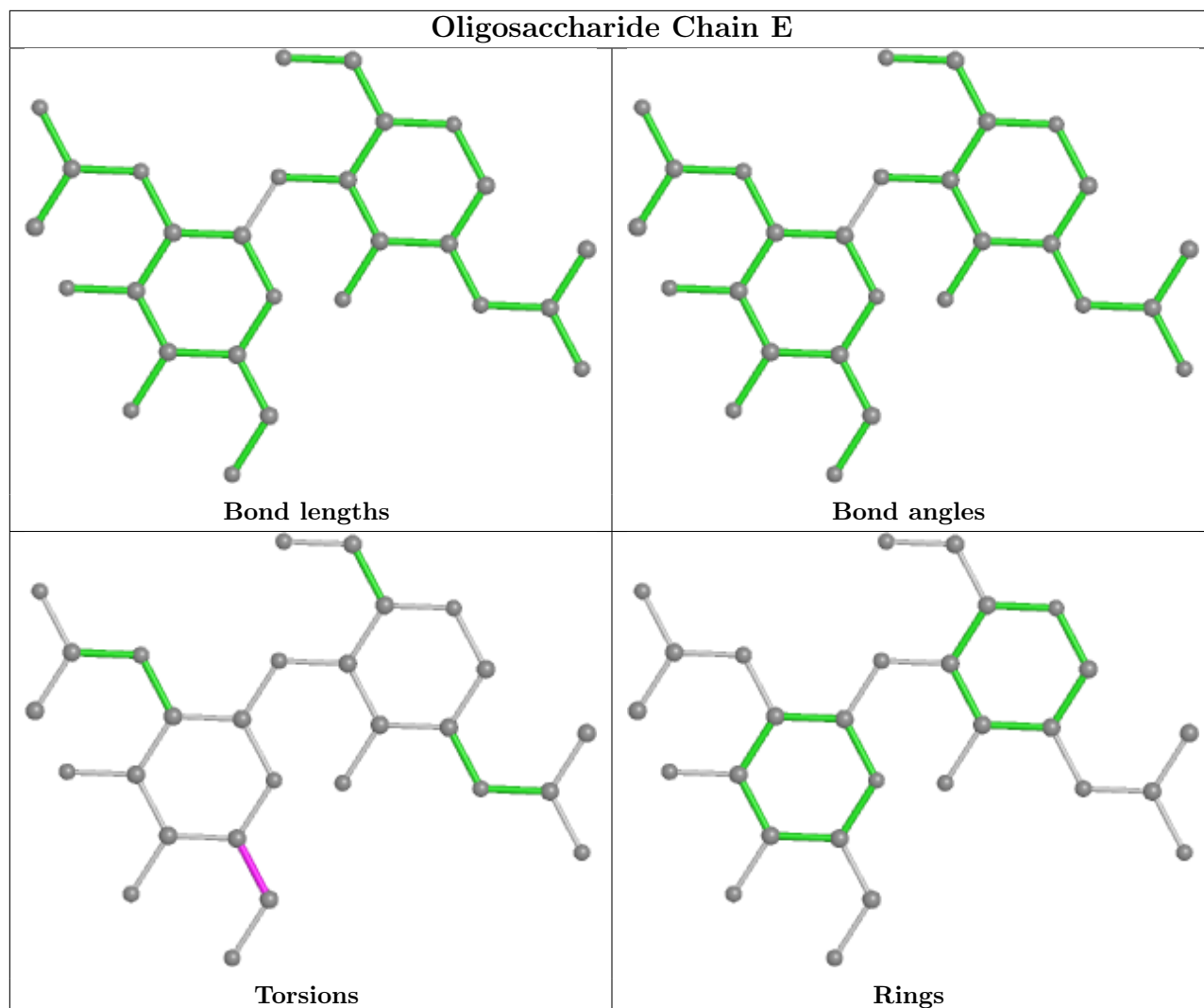
There are no ring outliers.

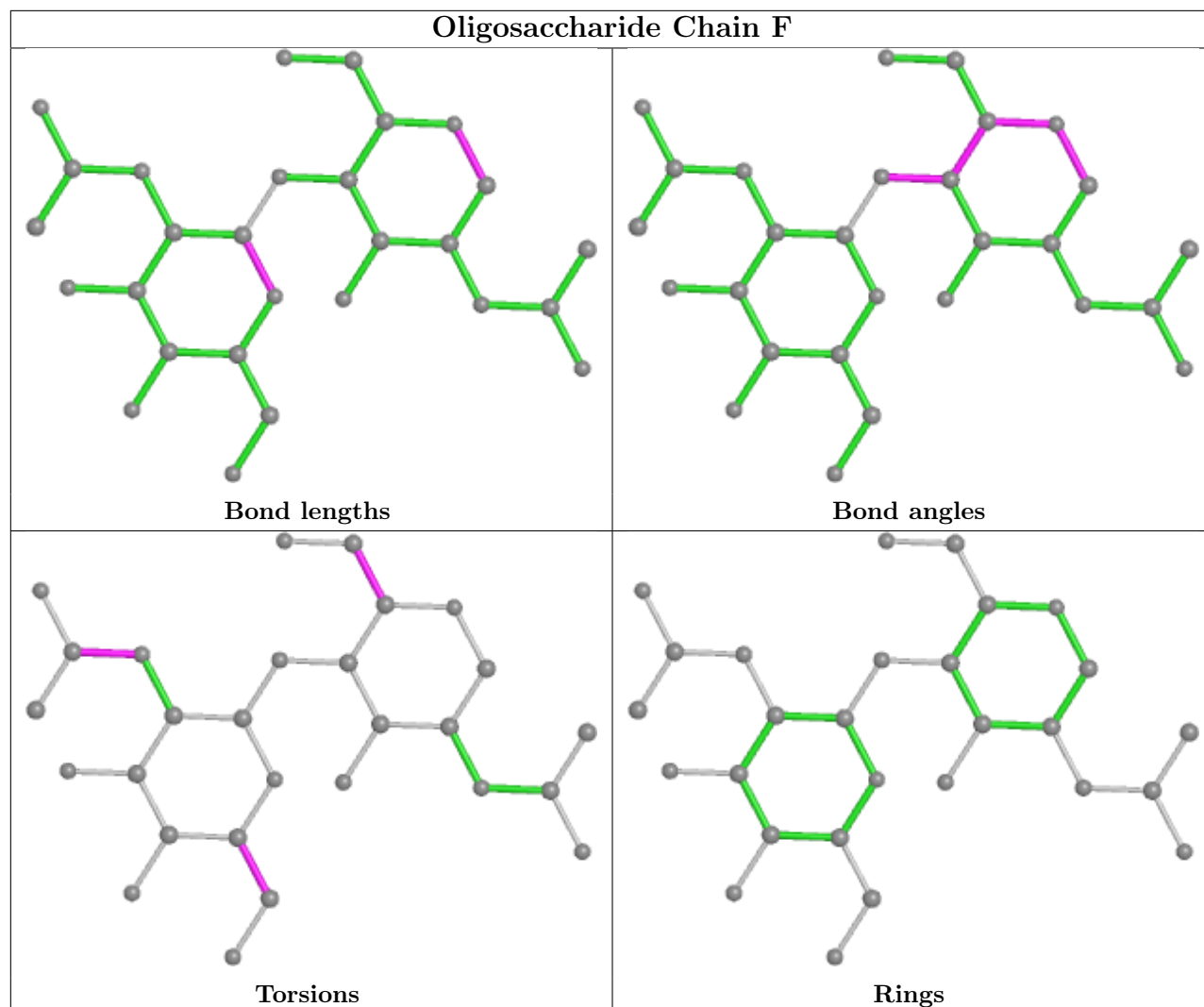
3 monomers are involved in 4 short contacts:

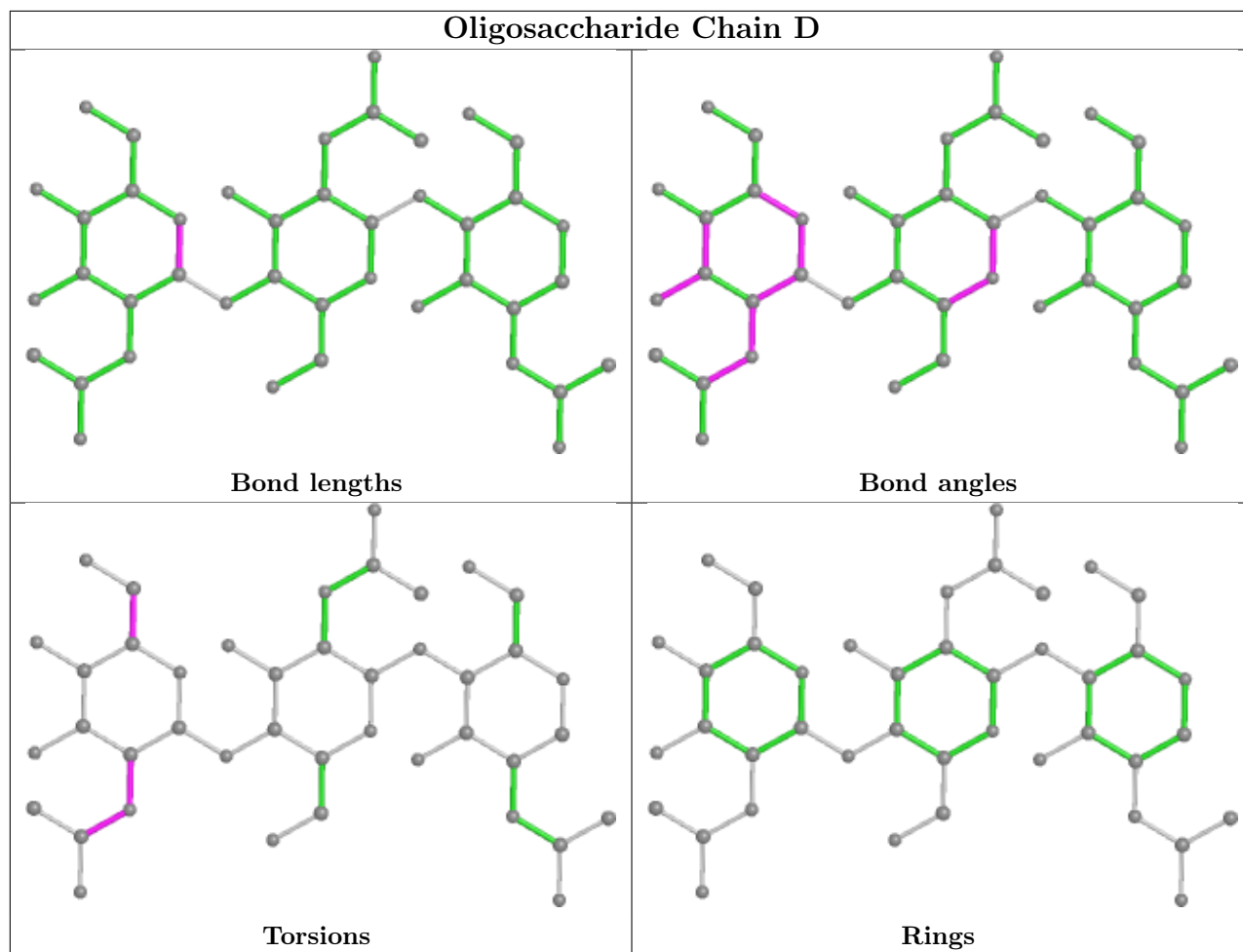
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	G	1	NAG	2	0
3	F	1	NAG	1	0
4	D	3	NAG	1	0

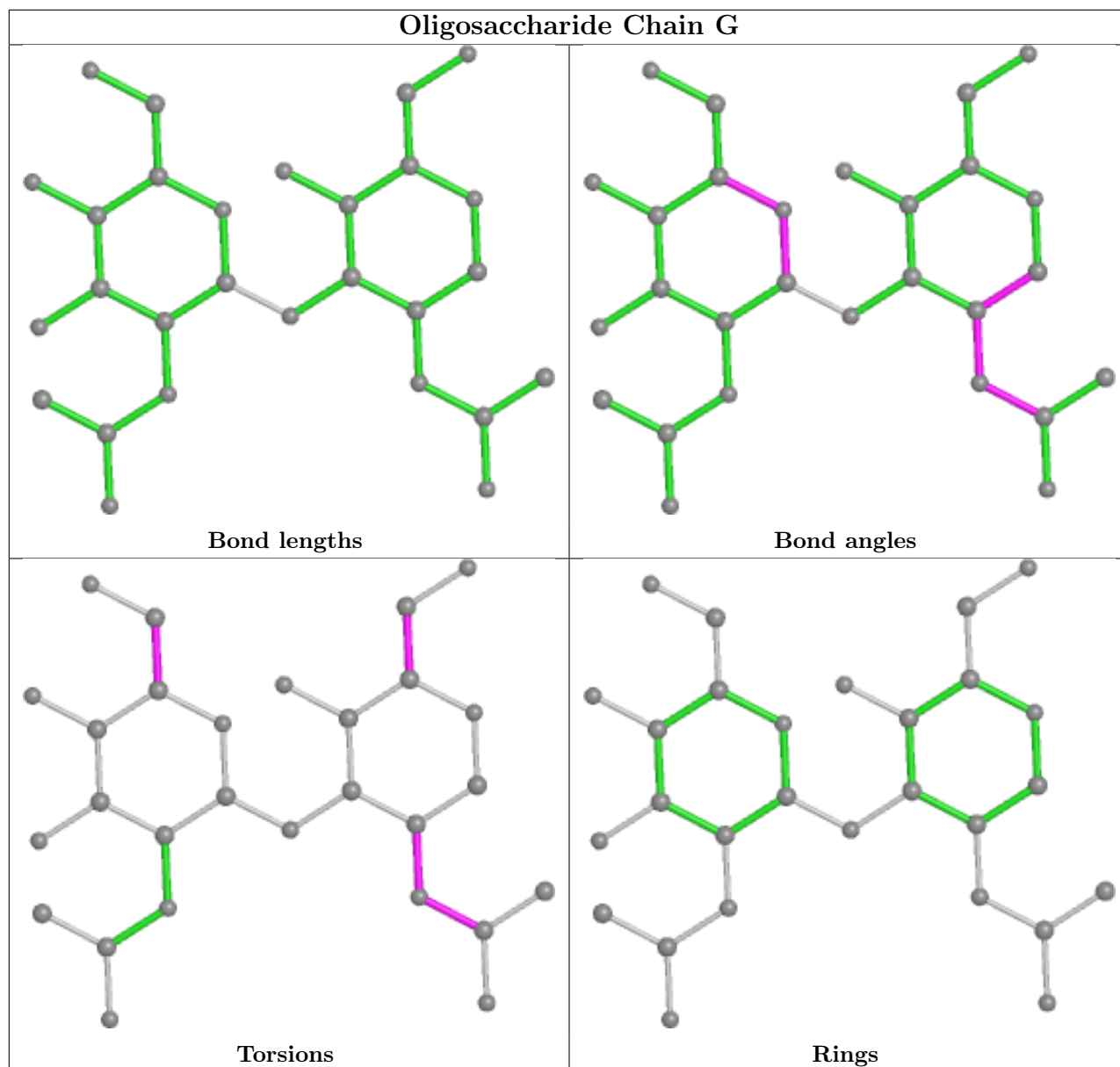
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.











## 5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 2 are monoatomic - leaving 5 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
7	NAG	A	1009	1	14,14,15	0.74	1 (7%)	17,19,21	0.74	0
7	NAG	B	1006	1	14,14,15	0.49	0	17,19,21	0.91	1 (5%)
7	NAG	B	1003	1	14,14,15	0.26	0	17,19,21	0.70	1 (5%)
7	NAG	A	1006	1	14,14,15	0.45	0	17,19,21	0.63	0
7	NAG	B	1007	1	14,14,15	0.40	0	17,19,21	0.38	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
7	NAG	A	1009	1	-	0/6/23/26	0/1/1/1
7	NAG	B	1006	1	-	2/6/23/26	0/1/1/1
7	NAG	B	1003	1	-	0/6/23/26	0/1/1/1
7	NAG	A	1006	1	-	3/6/23/26	0/1/1/1
7	NAG	B	1007	1	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	1009	NAG	O5-C1	-2.21	1.40	1.43

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	1006	NAG	C1-O5-C5	2.80	115.98	112.19
7	B	1003	NAG	C1-O5-C5	2.30	115.31	112.19

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	1006	NAG	C8-C7-N2-C2
7	A	1006	NAG	O7-C7-N2-C2
7	B	1006	NAG	O5-C5-C6-O6
7	B	1006	NAG	C4-C5-C6-O6
7	B	1007	NAG	C4-C5-C6-O6
7	B	1007	NAG	O5-C5-C6-O6
7	A	1006	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
7	A	1006	NAG	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	451:ASP	C	452:PHE	N	1.19

## 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	563/618 (91%)	-0.54	2 (0%) 92 91	6, 14, 31, 69	0
1	B	556/618 (89%)	-0.37	2 (0%) 92 91	11, 23, 42, 73	0
2	U	309/320 (96%)	-0.03	14 (4%) 33 26	15, 29, 74, 105	0
All	All	1428/1556 (91%)	-0.36	18 (1%) 77 73	6, 21, 43, 105	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	U	59	ILE	4.8
2	U	62	ASP	3.7
2	U	118	GLN	3.5
2	U	117	GLY	3.4
2	U	241	SER	3.4
2	U	60	ALA	3.1
1	B	386	GLU	3.0
1	A	388	SER	2.7
2	U	57	GLU	2.7
2	U	115	ASP	2.6
2	U	116	PRO	2.5
2	U	61	GLY	2.4
2	U	263	ASP	2.3
2	U	194	ASP	2.3
2	U	193	GLY	2.3
2	U	232	ASP	2.2
1	B	459	ARG	2.1
1	A	423	ASP	2.0

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

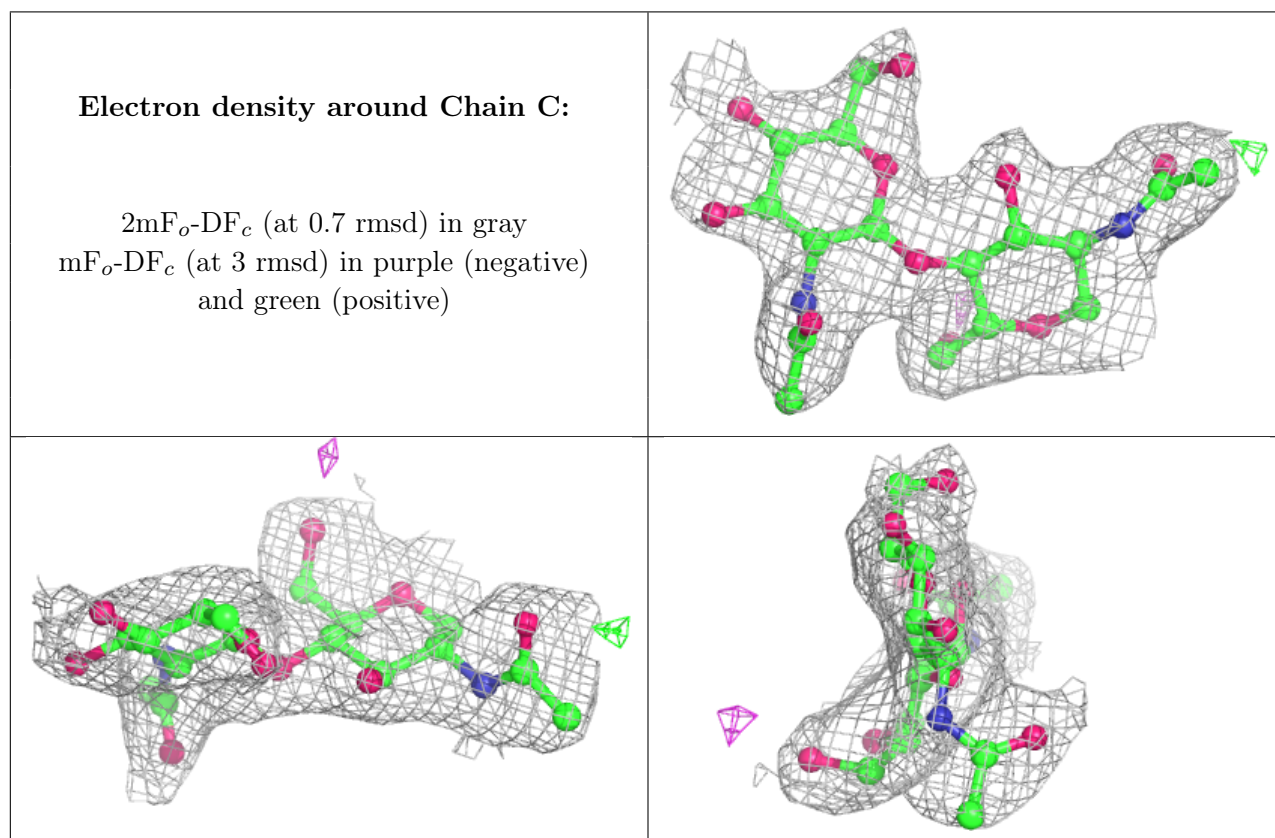
There are no non-standard protein/DNA/RNA residues in this entry.

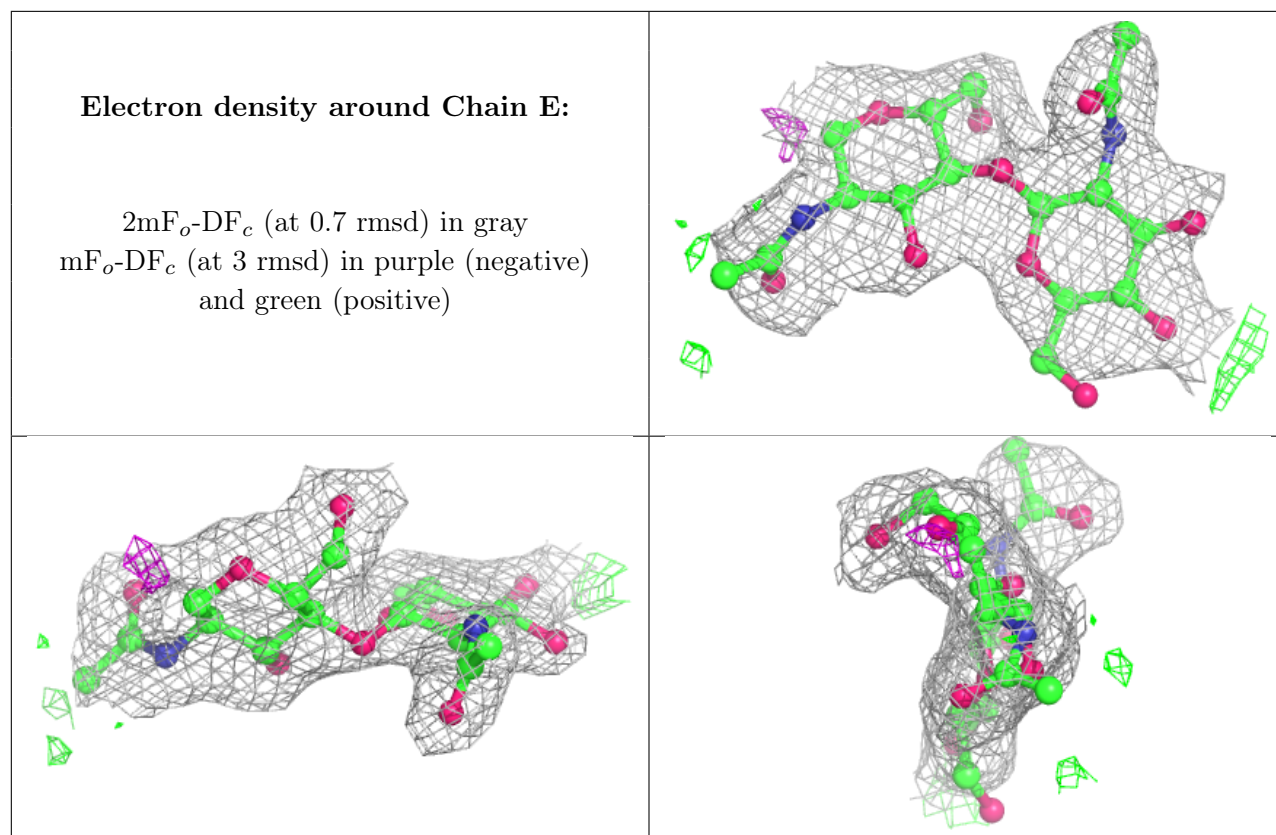
### 6.3 Carbohydrates [i](#)

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	G	1	14/15	0.84	0.32	41,47,52,63	0
4	NAG	D	3	14/15	0.85	0.20	24,27,39,40	0
5	NAG	G	2	14/15	0.85	0.26	49,52,56,57	0
3	NAG	C	2	14/15	0.86	0.27	40,48,54,55	0
3	NAG	F	2	14/15	0.87	0.24	43,48,55,62	0
3	NAG	E	2	14/15	0.91	0.24	32,38,48,58	0
3	NAG	E	1	14/15	0.92	0.15	24,31,35,42	0
3	NAG	F	1	14/15	0.93	0.17	28,34,41,42	0
3	NAG	C	1	14/15	0.95	0.12	18,26,32,35	0
4	NAG	D	2	14/15	0.97	0.13	15,19,23,24	0
4	NAG	D	1	14/15	0.97	0.11	11,12,15,18	0

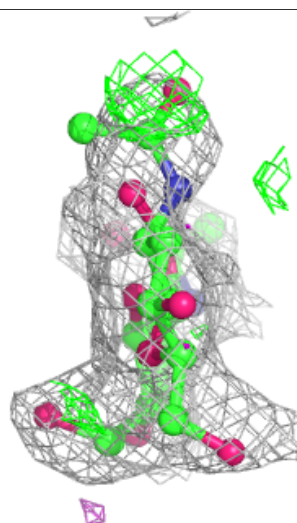
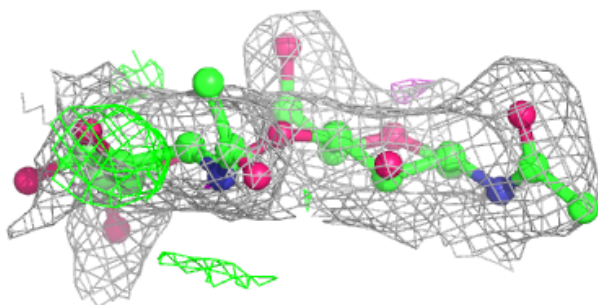
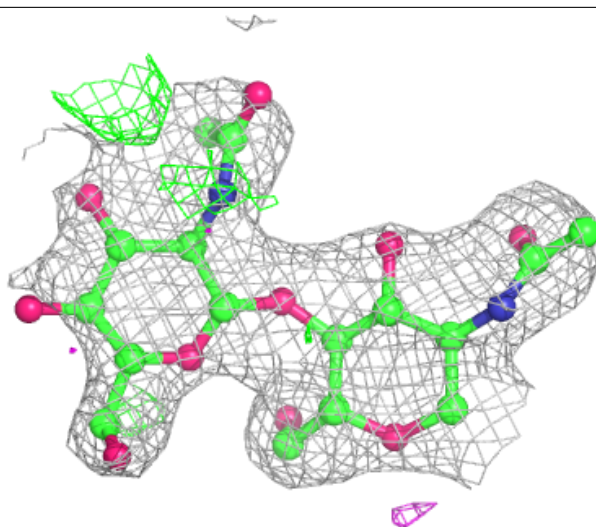
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.





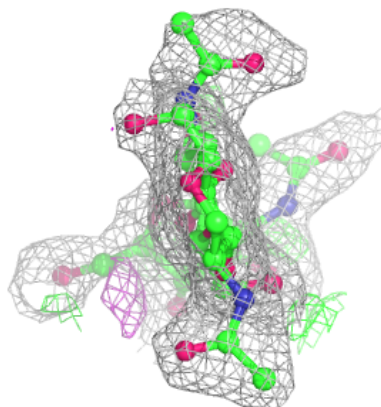
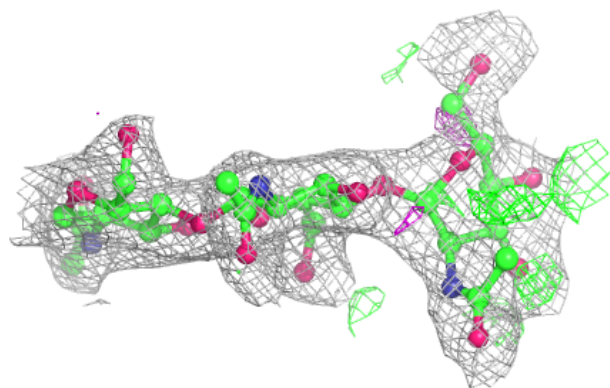
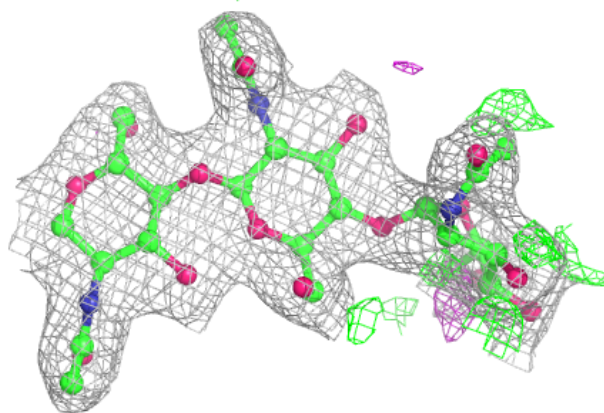
**Electron density around Chain F:**

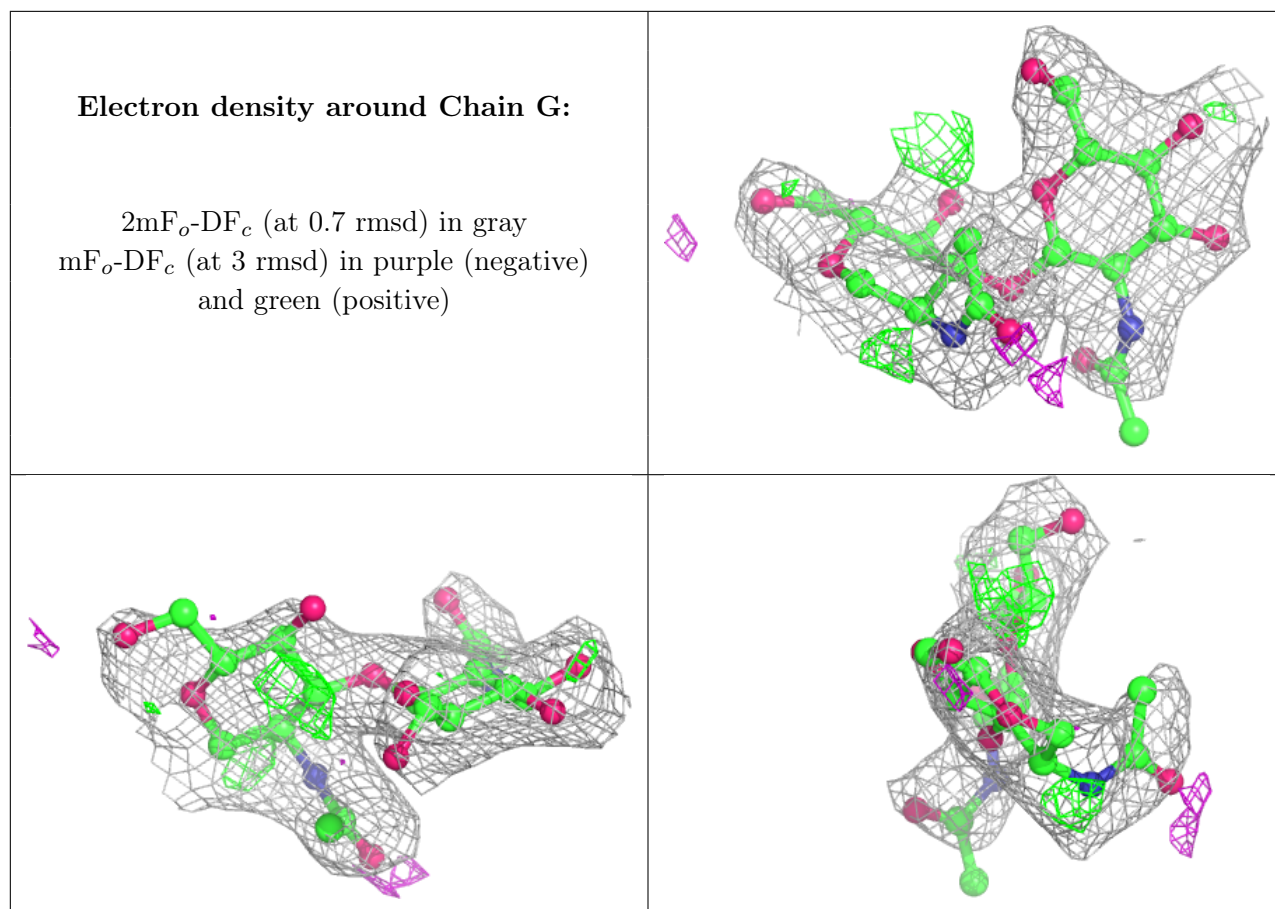
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around Chain 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
7	NAG	B	1006	14/15	0.76	0.31	47,59,66,73	0
7	NAG	A	1006	14/15	0.83	0.35	32,46,59,63	0
7	NAG	B	1003	14/15	0.86	0.36	45,63,71,76	0
7	NAG	B	1007	14/15	0.90	0.15	32,35,39,40	0
6	MN	B	1000	1/1	0.95	0.28	56,56,56,56	0
7	NAG	A	1009	14/15	0.97	0.15	14,17,21,24	0
6	MN	A	1000	1/1	0.99	0.12	8,8,8,8	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.