Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2020 – 12:05 PM BST

PDB ID	:	4MC5
Title	:	Crystal structure of a subtype H18 hemagglutinin homologue from A/flat-faced bat/Peru/033/2010 (H18N11)
Authors	:	Yang, H.; Carney, P.J.; Chang, J.C.; Guo, Z.; Stevens, J.
Deposited on	:	2013-08-21
Resolution	:	2.24 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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

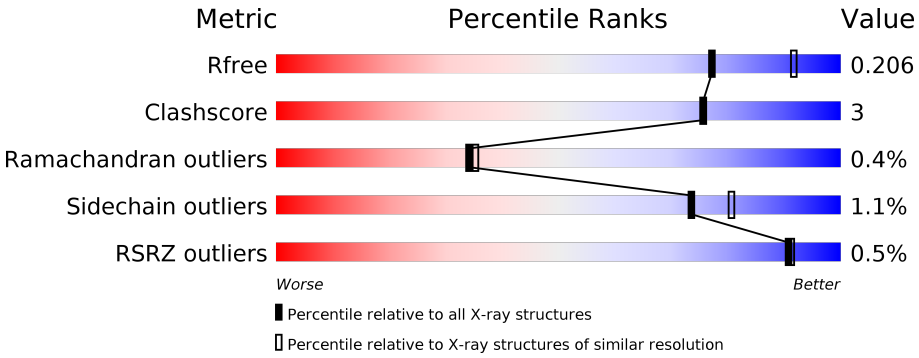
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

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 2.24 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	2391 (2.26-2.22)
Clashscore	141614	2539 (2.26-2.22)
Ramachandran outliers	138981	2489 (2.26-2.22)
Sidechain outliers	138945	2490 (2.26-2.22)
RSRZ outliers	127900	2353 (2.26-2.22)

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 on the lower bar indicate the fraction of residues that contain outliers for >=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 <=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	510	% 91% 5% ·
1	B	510	90% 6% ·
1	C	510	91% 6% ·
2	D	4	25% 75%
3	E	7	29% 29% 43%
3	G	7	29% 43% 29%

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Mol	Chain	Length	Quality of chain
4	F	2	100%
4	H	2	50% 50%
4	J	2	50% 50%
5	I	4	25% 25% 50%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	MAN	D	4	-	-	-	X
3	MAN	G	4	-	-	-	X
7	NAG	A	616	X	-	-	-
7	NAG	B	612	X	-	-	-
7	NAG	C	610	X	-	-	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 13219 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.

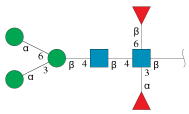
- Molecule 1 is a protein called Hemagglutinin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	494	Total	C	N	O	S	0	0	0
			3914	2459	660	777	18			
1	B	494	Total	C	N	O	S	0	0	0
			3914	2459	660	777	18			
1	C	497	Total	C	N	O	S	0	0	0
			3938	2476	664	780	18			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	D	4	Total	C	N	O	0	0	0
			50	28	2	20			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	E	7	Total	C	N	O	0	0	0
			81	46	2	33			

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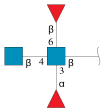
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	G	7	Total	C	N	O	0	0	0
			81	46	2	33			

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

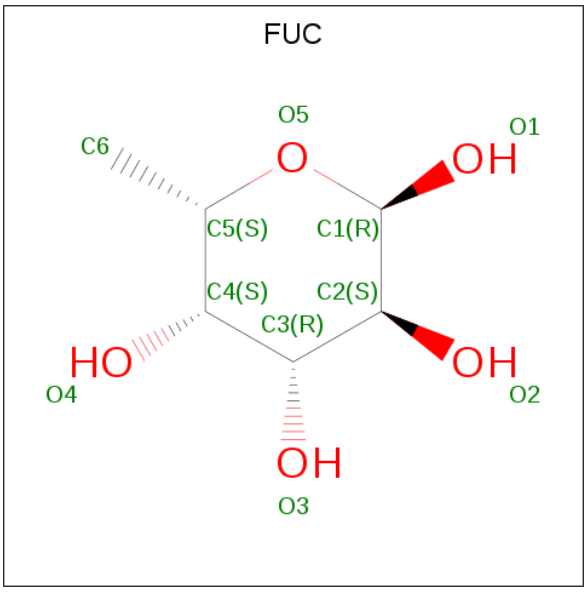
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	F	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	H	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	J	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 5 is an oligosaccharide called alpha-L-fucopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)][beta-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



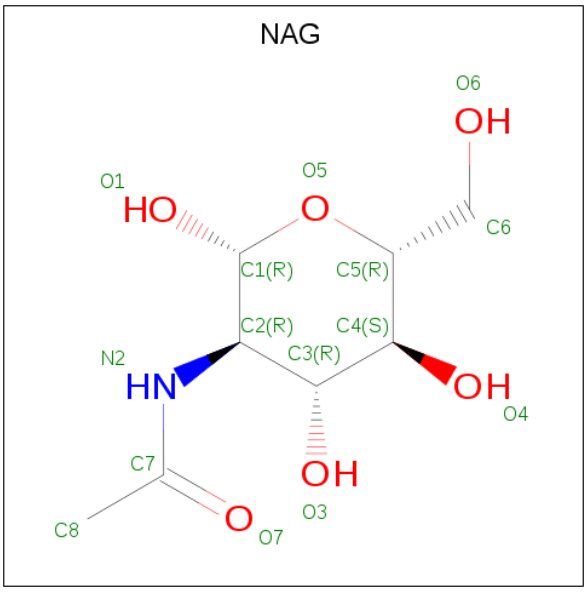
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	I	4	Total	C	N	O	0	0	0
			48	28	2	18			

- Molecule 6 is alpha-L-fucopyranose (three-letter code: FUC) (formula: $C_6H_{12}O_5$).



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

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 8 is water.

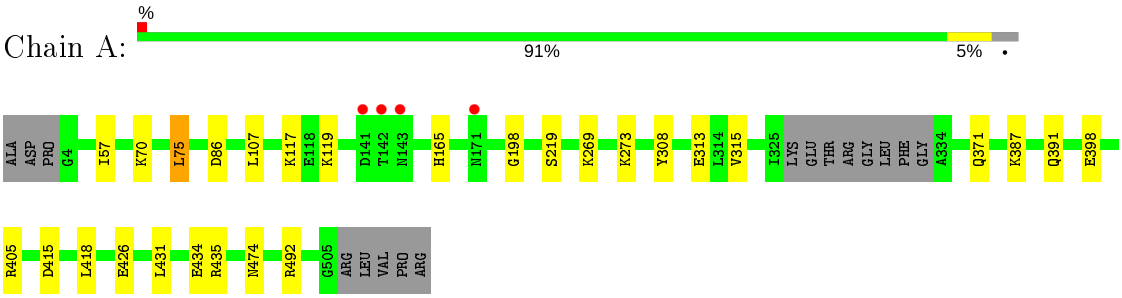
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	292	Total O 292 292	0	0
8	B	343	Total O 343 343	0	0
8	C	332	Total O 332 332	0	0

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.

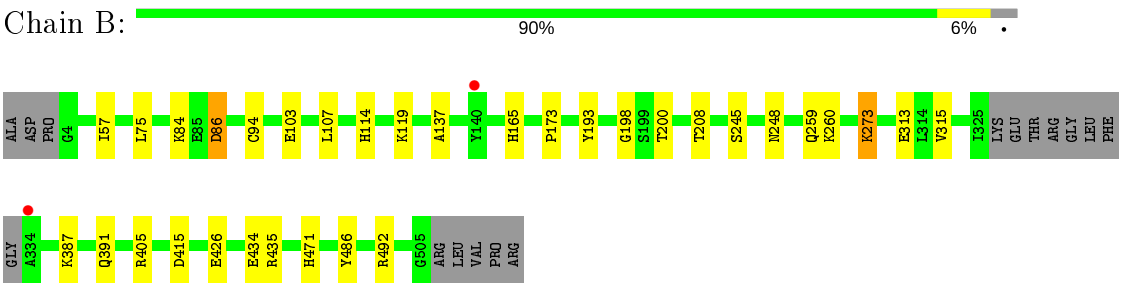
- Molecule 1: Hemagglutinin

Chain A:



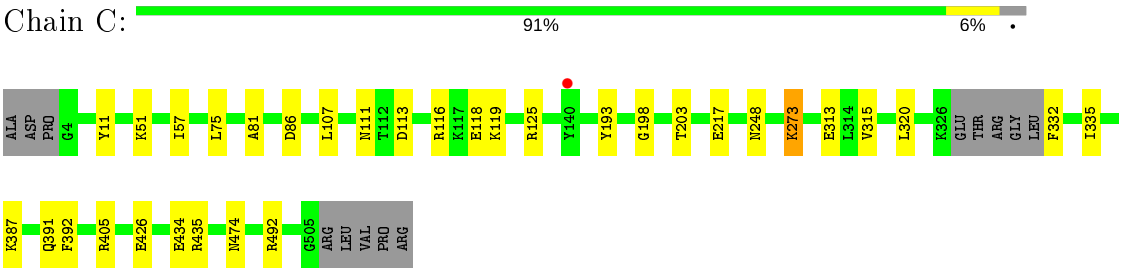
- Molecule 1: Hemagglutinin

Chain B:



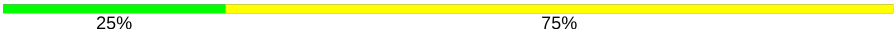
- Molecule 1: Hemagglutinin

Chain C:



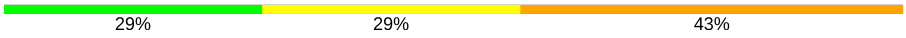
- Molecule 2: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

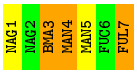
Chain D:



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

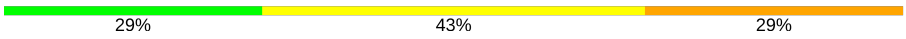
Chain E:

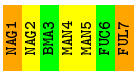




• Molecule 3: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-3)][beta-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

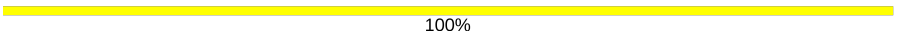
Chain G:





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

Chain F:



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

Chain H:

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

Chain J:

• Molecule 5: alpha-L-fucopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)][beta-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, α, β, γ	239.09Å 239.09Å 161.23Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.02 – 2.24 48.02 – 2.24	Depositor EDS
% Data completeness (in resolution range)	99.8 (48.02-2.24) 95.7 (48.02-2.24)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.32 (at 2.24Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.175 , 0.204 0.177 , 0.206	Depositor DCC
R_{free} test set	5563 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	32.1	Xtriage
Anisotropy	0.171	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 47.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	13219	wwPDB-VP
Average B, all atoms (Å^2)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.47% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: MAN, FUL, BMA, NAG, FUC

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	0.30	0/3998	0.46	0/5425
1	B	0.31	0/3998	0.47	0/5425
1	C	0.30	0/4023	0.46	0/5457
All	All	0.30	0/12019	0.46	0/16307

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	3914	0	3734	27	0
1	B	3914	0	3733	26	1
1	C	3938	0	3758	26	0
2	D	50	0	43	0	0
3	E	81	0	70	2	1
3	G	81	0	70	2	1
4	F	28	0	25	0	0
4	H	28	0	25	0	0
4	J	28	0	25	3	0
5	I	48	0	43	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	10	0	10	2	0
6	B	10	0	10	1	0
6	C	10	0	10	3	0
7	A	28	0	26	0	0
7	B	42	0	39	1	0
7	C	42	0	39	0	0
8	A	292	0	0	12	0
8	B	343	0	0	7	1
8	C	332	0	0	12	0
All	All	13219	0	11660	74	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

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)
1:C:125:ARG:NH2	8:C:980:HOH:O	2.01	0.91
8:C:997:HOH:O	4:J:2:NAG:O4	1.91	0.87
1:C:113:ASP:OD2	8:C:927:HOH:O	1.96	0.82
1:C:474:ASN:OD1	8:C:811:HOH:O	1.99	0.80
1:A:474:ASN:OD1	8:A:812:HOH:O	2.01	0.78
1:B:119:LYS:NZ	8:B:811:HOH:O	2.15	0.77
1:C:217:GLU:OE1	8:C:897:HOH:O	2.04	0.76
1:C:111:ASN:ND2	8:C:903:HOH:O	2.17	0.75
1:A:371:GLN:OE1	8:A:899:HOH:O	2.04	0.75
1:B:208:THR:OG1	8:B:770:HOH:O	2.06	0.73
1:A:119:LYS:NZ	8:A:712:HOH:O	2.22	0.73
1:A:391:GLN:HB3	6:A:614:FUC:H61	1.70	0.73
8:A:896:HOH:O	3:E:3:BMA:O2	2.07	0.72
8:C:981:HOH:O	4:J:1:NAG:O3	2.07	0.71
1:C:203:THR:OG1	8:C:784:HOH:O	2.10	0.68
1:B:260:LYS:NZ	8:B:1024:HOH:O	2.26	0.67
1:B:391:GLN:HB3	6:B:610:FUC:H61	1.77	0.67
1:A:435:ARG:HH22	1:B:434:GLU:CD	1.98	0.67
1:A:434:GLU:CD	1:C:435:ARG:HH22	1.97	0.67
1:A:426:GLU:HG2	1:C:387:LYS:HD2	1.79	0.65
1:B:86:ASP:OD2	8:B:785:HOH:O	2.15	0.65
1:B:435:ARG:HH22	1:C:434:GLU:CD	2.00	0.65
1:B:313:GLU:HG3	1:B:315:VAL:HG23	1.79	0.65
1:A:387:LYS:HD2	1:B:426:GLU:HG2	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:119:LYS:NZ	8:C:736:HOH:O	2.19	0.64
1:C:313:GLU:HG3	1:C:315:VAL:HG23	1.78	0.64
1:B:387:LYS:HD2	1:C:426:GLU:HG2	1.77	0.64
1:C:273:LYS:NZ	8:C:970:HOH:O	2.31	0.64
1:A:313:GLU:HG3	1:A:315:VAL:HG23	1.78	0.64
1:A:398:GLU:HG3	8:A:931:HOH:O	1.99	0.60
1:C:391:GLN:HB3	6:C:608:FUC:H61	1.83	0.60
1:A:117:LYS:NZ	8:A:807:HOH:O	2.18	0.57
1:A:165:HIS:HD2	8:A:922:HOH:O	1.88	0.56
1:A:165:HIS:CG	3:E:7:FUL:H5	2.41	0.55
1:B:103:GLU:OE2	8:B:842:HOH:O	2.18	0.55
1:A:70:LYS:NZ	8:A:945:HOH:O	2.41	0.53
1:B:165:HIS:CG	3:G:7:FUL:H5	2.43	0.53
1:B:165:HIS:CD2	3:G:7:FUL:H5	2.44	0.53
1:C:11:TYR:HB2	1:C:320:LEU:HD22	1.95	0.48
1:B:471:HIS:HE2	1:B:486:TYR:HH	1.62	0.48
1:C:313:GLU:CG	1:C:315:VAL:HG23	2.44	0.47
8:C:850:HOH:O	4:J:2:NAG:O3	2.18	0.47
7:B:611:NAG:O4	8:B:851:HOH:O	2.21	0.46
1:B:107:LEU:HD11	1:C:405:ARG:HA	1.98	0.46
1:A:405:ARG:HA	1:C:107:LEU:HD11	1.98	0.45
1:A:431:LEU:O	1:A:435:ARG:HG3	2.16	0.45
1:B:173:PRO:HG3	1:B:260:LYS:HE3	1.98	0.45
1:B:313:GLU:CG	1:B:315:VAL:HG23	2.46	0.44
1:B:387:LYS:CD	1:C:426:GLU:HG2	2.47	0.44
1:C:193:TYR:CZ	1:C:248:ASN:HA	2.52	0.44
1:A:435:ARG:NH2	8:A:834:HOH:O	2.41	0.44
1:A:308:TYR:CD2	1:A:418:LEU:HD13	2.53	0.44
1:A:107:LEU:HD11	1:B:405:ARG:HA	2.00	0.44
1:A:219:SER:OG	8:A:856:HOH:O	2.09	0.43
1:A:313:GLU:CG	1:A:315:VAL:HG23	2.46	0.43
1:A:435:ARG:NE	8:A:834:HOH:O	2.48	0.42
1:C:113:ASP:O	8:C:941:HOH:O	2.21	0.42
1:A:269:LYS:HE2	8:A:818:HOH:O	2.19	0.42
1:B:84:LYS:NZ	8:B:718:HOH:O	2.28	0.42
6:A:614:FUC:H62	1:B:415:ASP:OD2	2.20	0.42
1:B:193:TYR:CZ	1:B:248:ASN:HA	2.54	0.42
1:C:273:LYS:HA	1:C:273:LYS:HE3	2.01	0.42
1:C:474:ASN:OD1	1:C:474:ASN:N	2.52	0.41
5:I:2:FUC:H3	5:I:3:NAG:O5	2.19	0.41
1:A:474:ASN:OD1	1:A:474:ASN:N	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:94:CYS:HB2	1:B:137:ALA:O	2.20	0.41
1:A:75:LEU:HA	1:A:75:LEU:HD12	1.92	0.41
1:C:116:ARG:NH1	1:C:118:GLU:OE1	2.47	0.41
1:B:200:THR:HG23	1:B:245:SER:HB2	2.03	0.41
1:A:387:LYS:CD	1:B:426:GLU:HG2	2.48	0.41
1:B:114:HIS:ND1	1:B:259:GLN:OE1	2.54	0.40
1:A:415:ASP:OD2	6:C:608:FUC:H62	2.20	0.40
1:C:392:PHE:HB3	6:C:608:FUC:H63	2.03	0.40
1:C:51:LYS:HB3	1:C:81:ALA:HB2	2.02	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:4:MAN:O4	3:G:1:NAG:O7[3_755]	2.16	0.04
1:B:273:LYS:NZ	8:B:969:HOH:O[6_575]	2.18	0.02

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	490/510 (96%)	480 (98%)	8 (2%)	2 (0%)	34	35
1	B	490/510 (96%)	479 (98%)	9 (2%)	2 (0%)	34	35
1	C	493/510 (97%)	482 (98%)	9 (2%)	2 (0%)	34	35
All	All	1473/1530 (96%)	1441 (98%)	26 (2%)	6 (0%)	34	35

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	57	ILE
1	A	198	GLY

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Mol	Chain	Res	Type
1	B	57	ILE
1	C	57	ILE
1	C	198	GLY
1	B	198	GLY

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	437/450 (97%)	433 (99%)	4 (1%)	78	84
1	B	437/450 (97%)	433 (99%)	4 (1%)	78	84
1	C	439/450 (98%)	433 (99%)	6 (1%)	67	74
All	All	1313/1350 (97%)	1299 (99%)	14 (1%)	73	80

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	75	LEU
1	A	86	ASP
1	A	273	LYS
1	A	492	ARG
1	B	75	LEU
1	B	86	ASP
1	B	273	LYS
1	B	492	ARG
1	C	75	LEU
1	C	86	ASP
1	C	273	LYS
1	C	332	PHE
1	C	335	ILE
1	C	492	ARG

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

Mol	Chain	Res	Type
1	B	165	HIS
1	C	133	ASN
1	C	161	GLN

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)

28 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	D	1	1,2	14,14,15	0.48	0	17,19,21	1.56	2 (11%)
2	NAG	D	2	2	14,14,15	0.57	0	17,19,21	0.96	0
2	BMA	D	3	2	11,11,12	0.63	0	15,15,17	1.00	1 (6%)
2	MAN	D	4	2	11,11,12	0.54	0	15,15,17	0.83	1 (6%)
3	NAG	E	1	1,3	14,14,15	0.56	0	17,19,21	1.00	1 (5%)
3	NAG	E	2	3	14,14,15	0.49	0	17,19,21	0.81	0
3	BMA	E	3	3	11,11,12	0.60	0	15,15,17	1.18	1 (6%)
3	MAN	E	4	3	11,11,12	0.61	0	15,15,17	0.99	1 (6%)
3	MAN	E	5	3	11,11,12	0.54	0	15,15,17	1.28	2 (13%)
3	FUC	E	6	3	10,10,11	0.85	0	14,14,16	0.73	0
3	FUL	E	7	3	10,10,11	1.10	1 (10%)	14,14,16	1.16	2 (14%)
4	NAG	F	1	1,4	14,14,15	0.45	0	17,19,21	1.20	2 (11%)
4	NAG	F	2	4	14,14,15	0.52	0	17,19,21	1.87	3 (17%)
3	NAG	G	1	1,3	14,14,15	0.55	0	17,19,21	1.32	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	NAG	G	2	3	14,14,15	0.54	0	17,19,21	0.96	1 (5%)
3	BMA	G	3	3	11,11,12	0.64	0	15,15,17	1.02	0
3	MAN	G	4	3	11,11,12	0.49	0	15,15,17	2.13	2 (13%)
3	MAN	G	5	3	11,11,12	0.58	0	15,15,17	1.76	3 (20%)
3	FUC	G	6	3	10,10,11	0.92	0	14,14,16	0.66	0
3	FUL	G	7	3	10,10,11	1.11	1 (10%)	14,14,16	1.24	2 (14%)
4	NAG	H	1	1,4	14,14,15	0.54	0	17,19,21	0.99	0
4	NAG	H	2	4	14,14,15	0.45	0	17,19,21	2.32	4 (23%)
5	NAG	I	1	1,5	14,14,15	0.41	0	17,19,21	1.30	2 (11%)
5	FUC	I	2	5	10,10,11	1.20	2 (20%)	14,14,16	1.34	2 (14%)
5	NAG	I	3	5	14,14,15	0.58	0	17,19,21	1.24	2 (11%)
5	FUL	I	4	5	10,10,11	1.08	0	14,14,16	0.93	0
4	NAG	J	1	1,4	14,14,15	0.46	0	17,19,21	0.96	1 (5%)
4	NAG	J	2	4	14,14,15	0.57	0	17,19,21	0.90	0

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

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	FUC	G	6	3	-	-	0/1/1/1
3	FUL	G	7	3	-	-	0/1/1/1
4	NAG	H	1	1,4	-	4/6/23/26	0/1/1/1
4	NAG	H	2	4	-	2/6/23/26	0/1/1/1
5	NAG	I	1	1,5	-	4/6/23/26	0/1/1/1
5	FUC	I	2	5	-	-	0/1/1/1
5	NAG	I	3	5	-	2/6/23/26	0/1/1/1
5	FUL	I	4	5	-	-	0/1/1/1
4	NAG	J	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	J	2	4	-	3/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	7	FUL	O5-C1	-2.28	1.40	1.43
3	E	7	FUL	C4-C5	2.18	1.57	1.52
5	I	2	FUC	C4-C5	2.16	1.57	1.52
5	I	2	FUC	O5-C5	2.08	1.48	1.43

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	G	4	MAN	C1-O5-C5	7.31	122.09	112.19
4	H	2	NAG	C1-O5-C5	7.17	121.91	112.19
4	F	2	NAG	C1-O5-C5	5.33	119.41	112.19
2	D	1	NAG	C1-O5-C5	4.94	118.88	112.19
3	G	5	MAN	C1-O5-C5	4.47	118.25	112.19
4	H	2	NAG	C4-C3-C2	-3.73	105.56	111.02
4	F	2	NAG	C3-C4-C5	3.43	116.36	110.24
3	G	1	NAG	C2-N2-C7	-3.29	118.22	122.90
5	I	2	FUC	O5-C5-C4	3.22	115.29	109.52
3	E	5	MAN	C1-C2-C3	-3.21	105.72	109.67
4	H	2	NAG	O5-C5-C4	3.20	118.62	110.83
5	I	1	NAG	O5-C5-C6	3.16	112.16	107.20
5	I	3	NAG	O5-C1-C2	-3.09	106.41	111.29
3	E	3	BMA	C6-C5-C4	-2.99	106.01	113.00
2	D	3	BMA	C1-C2-C3	2.97	113.32	109.67
4	F	2	NAG	O5-C5-C4	2.93	117.97	110.83
3	G	5	MAN	C3-C4-C5	2.86	115.33	110.24
3	G	1	NAG	O5-C5-C6	2.84	111.65	107.20
4	F	1	NAG	O5-C1-C2	-2.81	106.85	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	H	2	NAG	C2-N2-C7	-2.77	118.96	122.90
3	E	4	MAN	C1-O5-C5	2.71	115.86	112.19
3	G	7	FUL	O5-C5-C4	2.63	114.23	109.52
4	F	1	NAG	C2-N2-C7	-2.57	119.25	122.90
3	E	1	NAG	O5-C5-C6	2.52	111.16	107.20
3	G	4	MAN	C2-C3-C4	-2.49	106.58	110.89
4	J	1	NAG	C1-O5-C5	2.46	115.53	112.19
5	I	3	NAG	C3-C4-C5	2.44	114.60	110.24
5	I	2	FUC	C1-O5-C5	2.44	118.31	112.78
3	G	2	NAG	C2-N2-C7	-2.29	119.64	122.90
2	D	1	NAG	O4-C4-C3	-2.25	105.14	110.35
3	E	7	FUL	O5-C5-C4	2.24	113.54	109.52
3	E	7	FUL	O2-C2-C1	2.23	113.72	109.15
3	G	5	MAN	O5-C5-C4	2.19	116.16	110.83
3	G	7	FUL	O2-C2-C1	2.16	113.58	109.15
5	I	1	NAG	O3-C3-C2	2.13	113.87	109.47
3	E	5	MAN	O5-C5-C6	2.10	110.50	107.20
2	D	4	MAN	O5-C1-C2	-2.02	107.65	110.77

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	I	3	NAG	C8-C7-N2-C2
5	I	3	NAG	O7-C7-N2-C2
4	F	2	NAG	O5-C5-C6-O6
5	I	1	NAG	C8-C7-N2-C2
4	H	2	NAG	O5-C5-C6-O6
4	J	1	NAG	O5-C5-C6-O6
4	H	1	NAG	O5-C5-C6-O6
4	F	1	NAG	O5-C5-C6-O6
5	I	1	NAG	O7-C7-N2-C2
4	F	2	NAG	C4-C5-C6-O6
3	E	4	MAN	O5-C5-C6-O6
4	F	1	NAG	C4-C5-C6-O6
4	H	1	NAG	C4-C5-C6-O6
4	H	1	NAG	C8-C7-N2-C2
4	H	2	NAG	C4-C5-C6-O6
4	J	2	NAG	C8-C7-N2-C2
3	G	5	MAN	O5-C5-C6-O6
4	J	2	NAG	O7-C7-N2-C2
4	J	1	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	H	1	NAG	O7-C7-N2-C2
3	E	5	MAN	C4-C5-C6-O6
4	J	2	NAG	O5-C5-C6-O6
3	E	4	MAN	C4-C5-C6-O6
5	I	1	NAG	O5-C5-C6-O6
3	E	1	NAG	O5-C5-C6-O6
3	E	1	NAG	C4-C5-C6-O6
5	I	1	NAG	C4-C5-C6-O6
2	D	4	MAN	O5-C5-C6-O6
3	E	5	MAN	O5-C5-C6-O6

All (1) ring outliers are listed below:

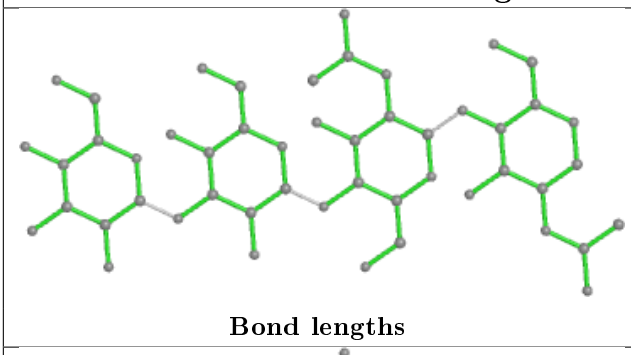
Mol	Chain	Res	Type	Atoms
3	E	4	MAN	C1-C2-C3-C4-C5-O5

9 monomers are involved in 9 short contacts:

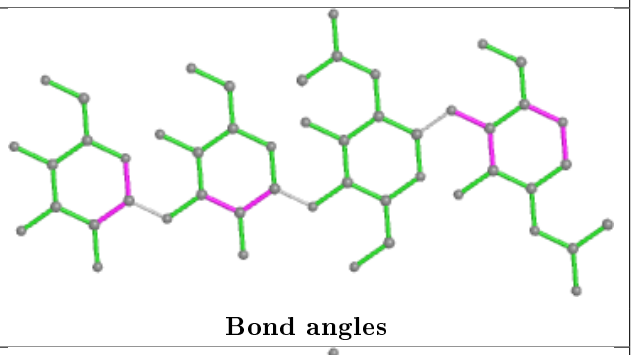
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	J	1	NAG	1	0
3	G	1	NAG	0	1
3	G	7	FUL	2	0
5	I	2	FUC	1	0
3	E	4	MAN	0	1
3	E	3	BMA	1	0
3	E	7	FUL	1	0
5	I	3	NAG	1	0
4	J	2	NAG	2	0

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

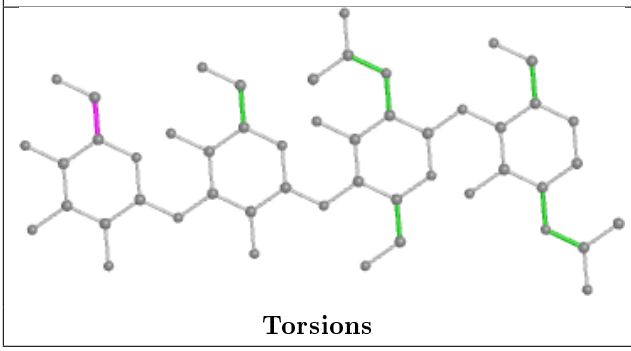
Oligosaccharide Chain D



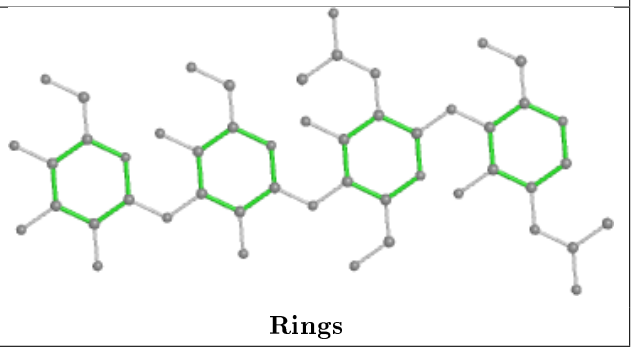
Bond lengths



Bond angles

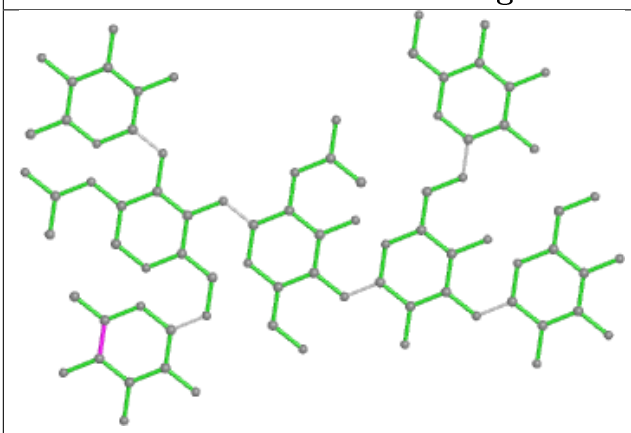


Torsions

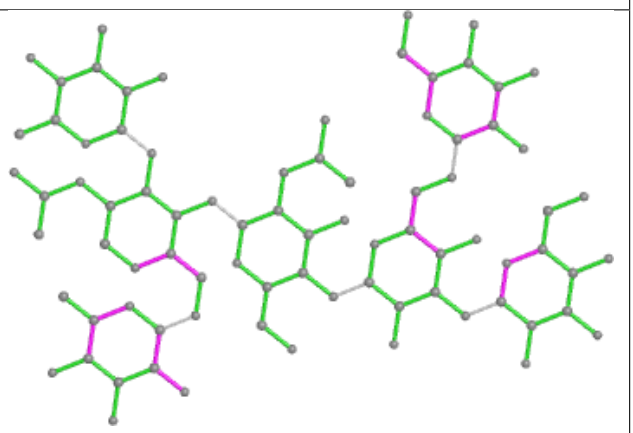


Rings

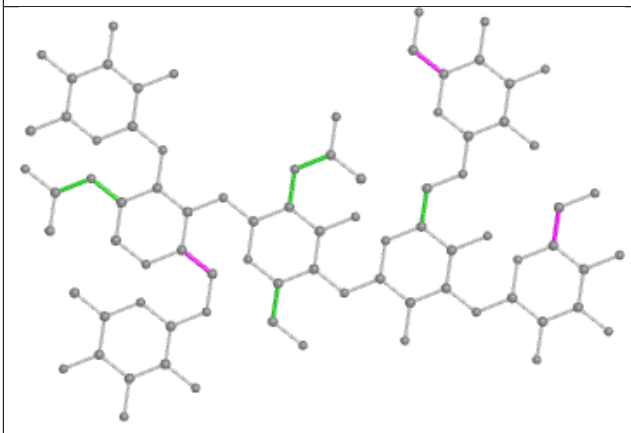
Oligosaccharide Chain E



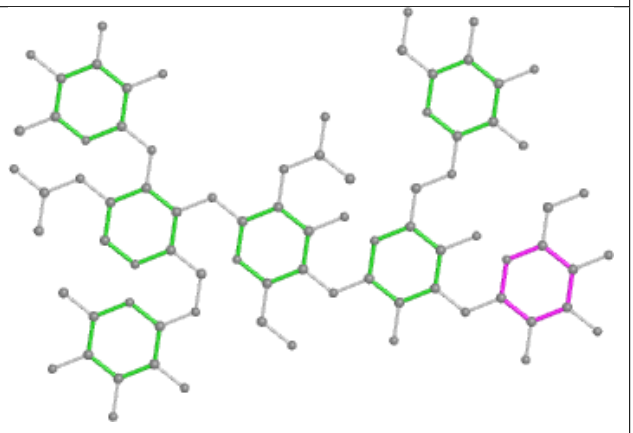
Bond lengths



Bond angles

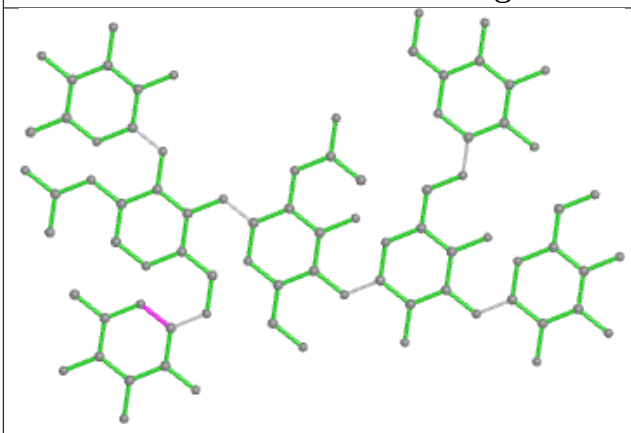


Torsions

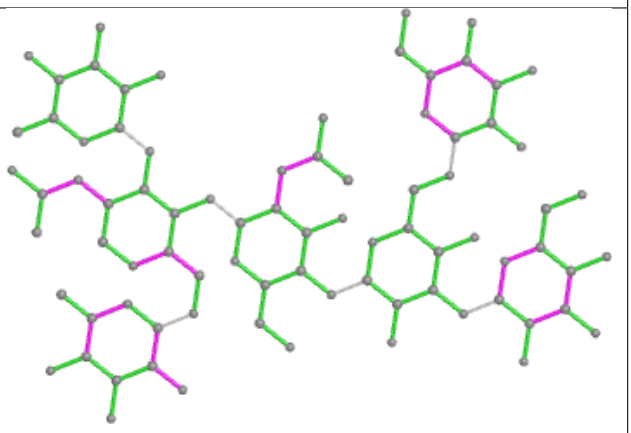


Rings

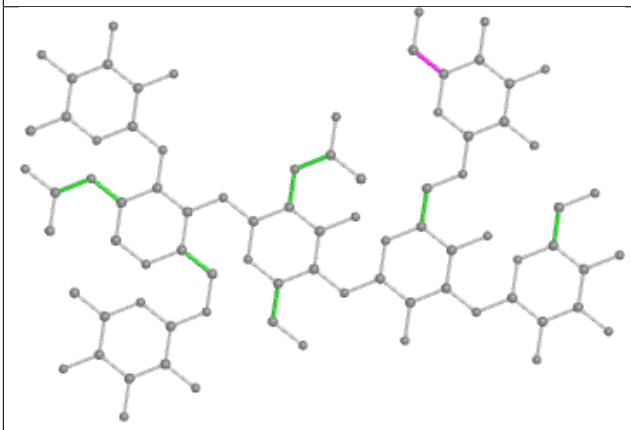
Oligosaccharide Chain G



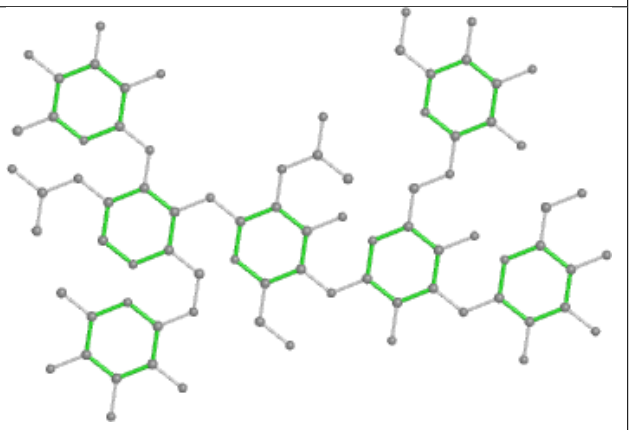
Bond lengths



Bond angles

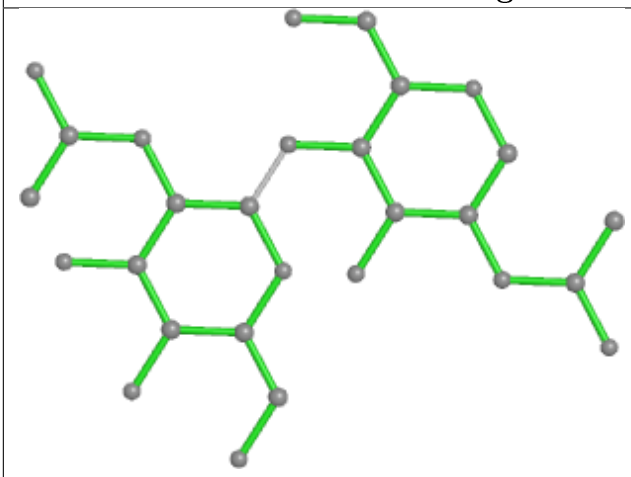


Torsions

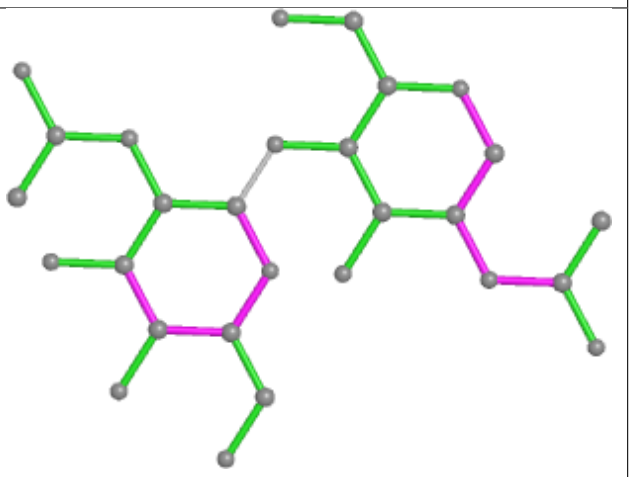


Rings

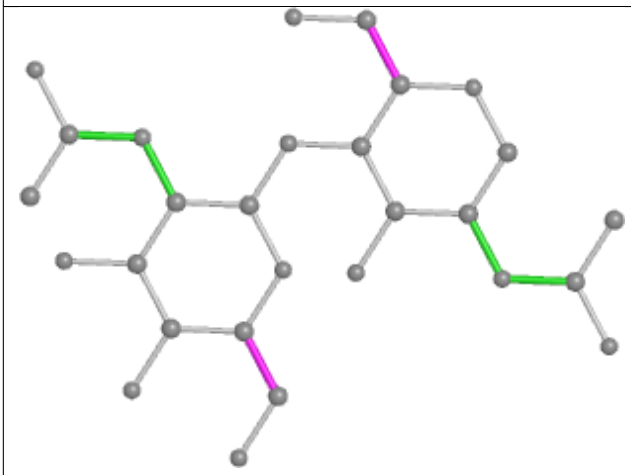
Oligosaccharide Chain F



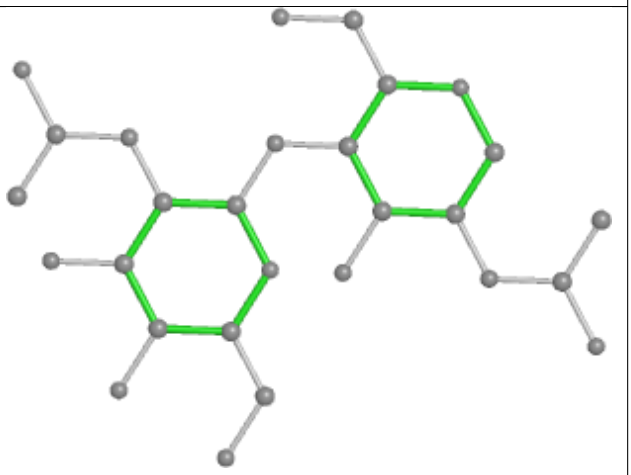
Bond lengths



Bond angles

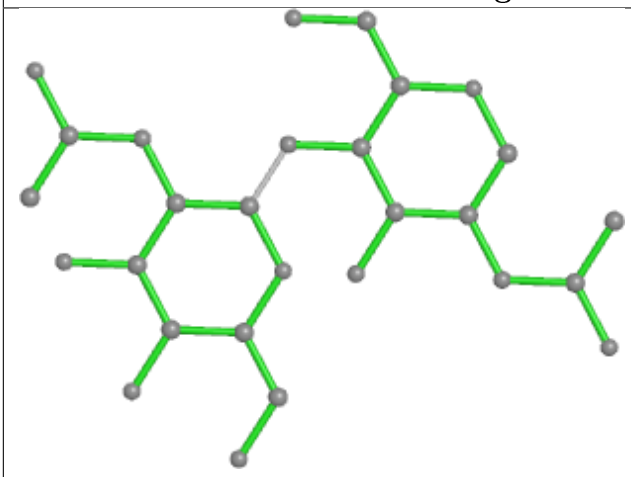


Torsions

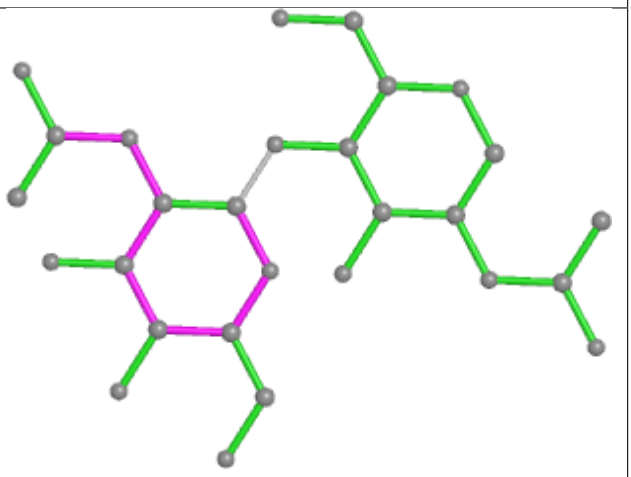


Rings

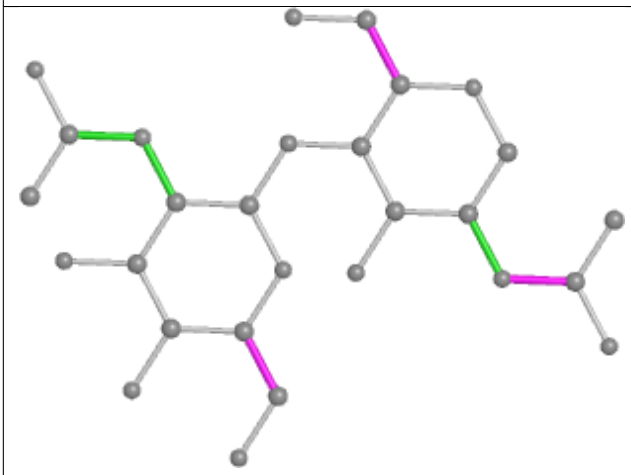
Oligosaccharide Chain H



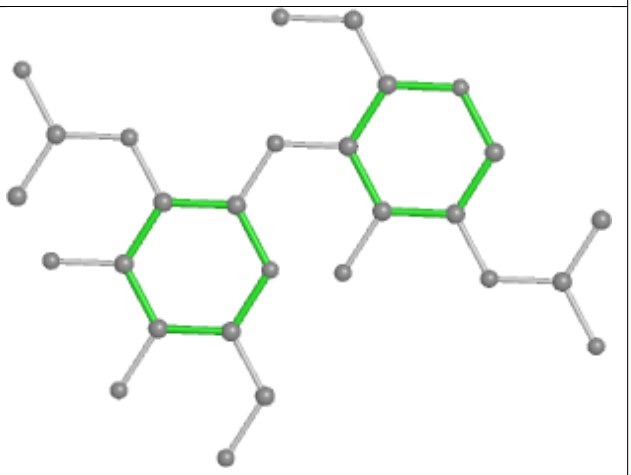
Bond lengths



Bond angles

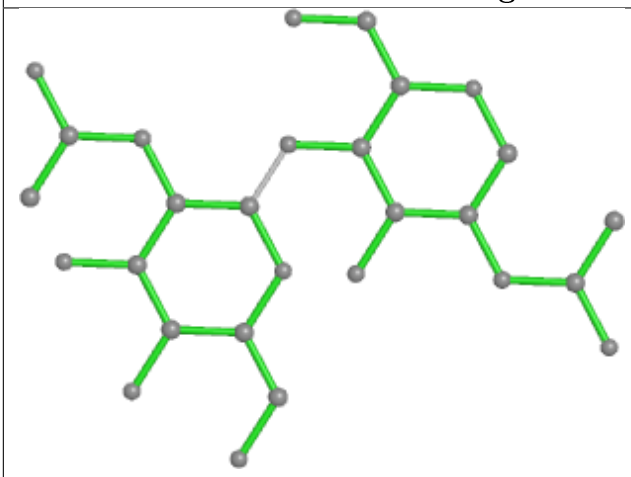


Torsions

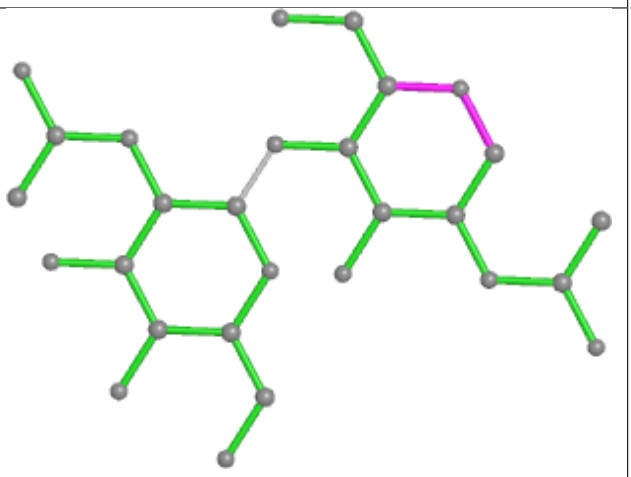


Rings

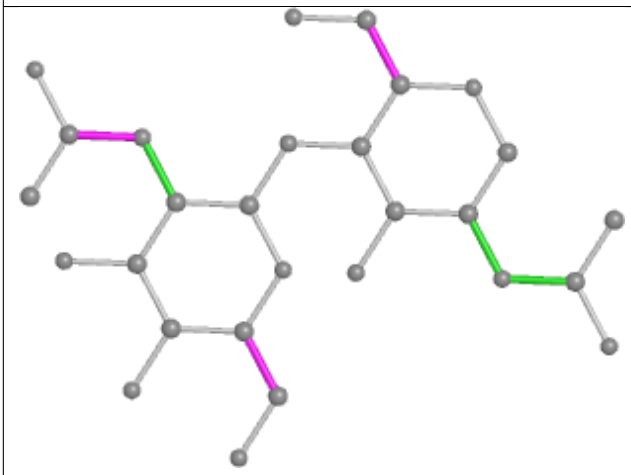
Oligosaccharide Chain J



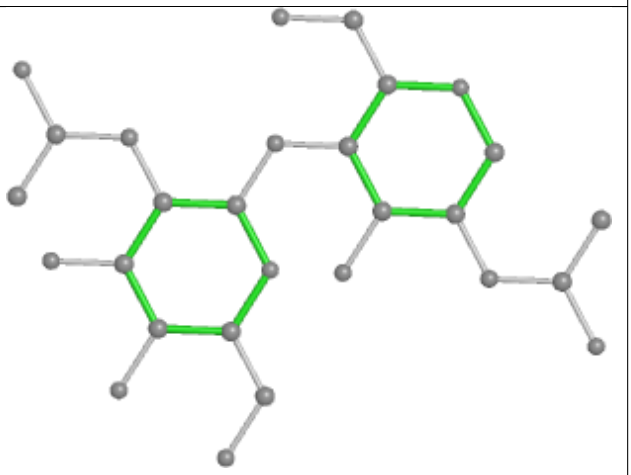
Bond lengths



Bond angles

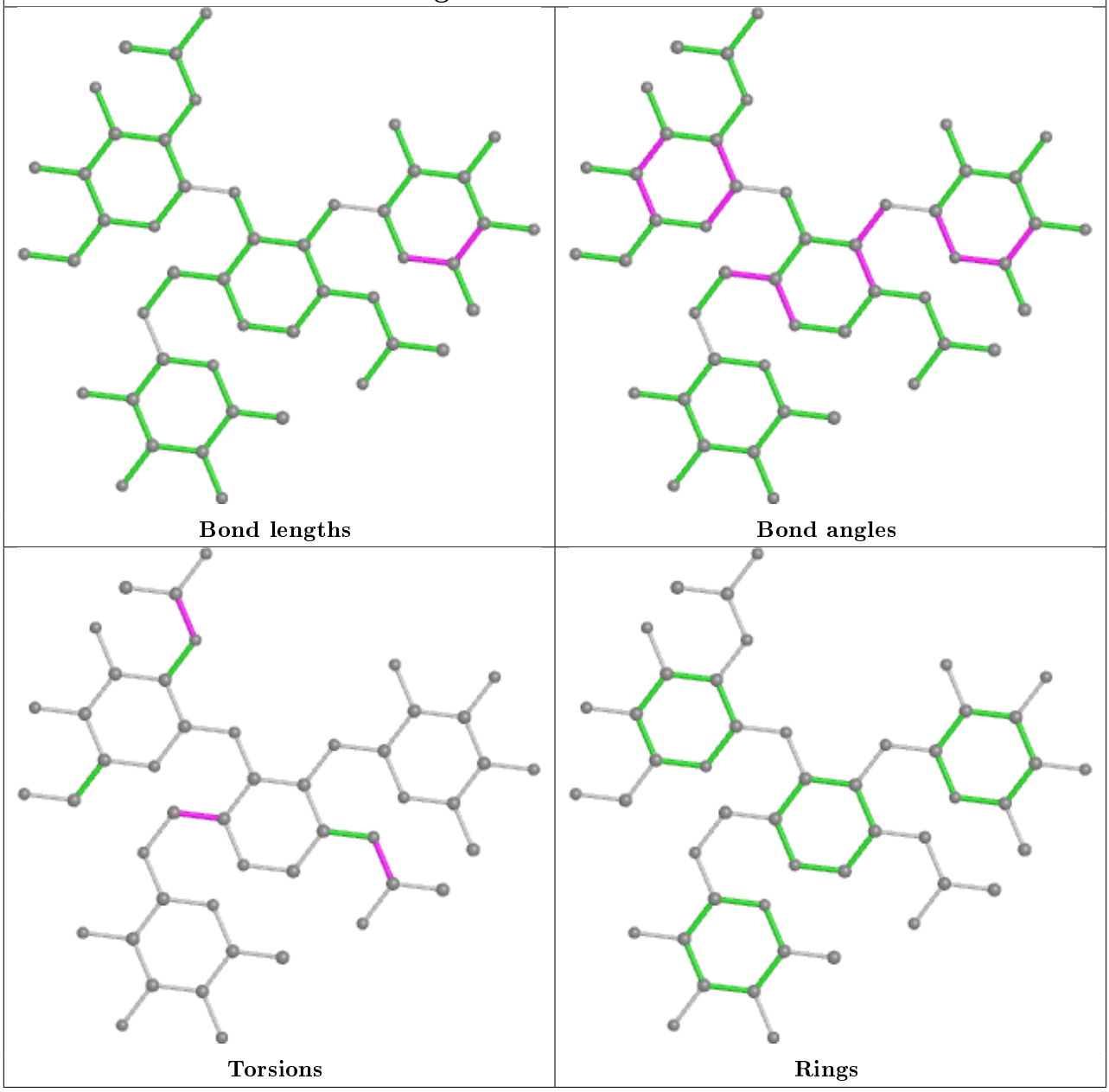


Torsions



Rings

Oligosaccharide Chain I



5.6 Ligand geometry (i)

11 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
7	NAG	B	613	1	14,14,15	0.47	0	17,19,21	1.01	1 (5%)
7	NAG	C	610	1	14,14,15	0.56	0	17,19,21	0.95	1 (5%)
7	NAG	C	609	1	14,14,15	0.57	0	17,19,21	0.73	0
6	FUC	B	610	-	10,10,11	1.02	1 (10%)	14,14,16	2.15	4 (28%)
7	NAG	B	611	1	14,14,15	0.56	0	17,19,21	0.87	0
7	NAG	A	615	1	14,14,15	0.55	0	17,19,21	0.89	1 (5%)
7	NAG	B	612	1	14,14,15	0.47	0	17,19,21	0.95	1 (5%)
7	NAG	C	601	1	14,14,15	0.38	0	17,19,21	2.10	4 (23%)
7	NAG	A	616	1	14,14,15	0.50	0	17,19,21	1.01	2 (11%)
6	FUC	C	608	-	10,10,11	0.92	1 (10%)	14,14,16	2.36	4 (28%)
6	FUC	A	614	-	10,10,11	1.04	1 (10%)	14,14,16	2.17	3 (21%)

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	B	613	1	-	2/6/23/26	0/1/1/1
7	NAG	C	610	1	1/1/5/7	4/6/23/26	0/1/1/1
6	FUC	A	614	-	-	-	0/1/1/1
7	NAG	B	611	1	-	3/6/23/26	0/1/1/1
7	NAG	A	615	1	-	2/6/23/26	0/1/1/1
7	NAG	B	612	1	1/1/5/7	0/6/23/26	0/1/1/1
7	NAG	C	601	1	-	2/6/23/26	0/1/1/1
6	FUC	B	610	-	-	-	0/1/1/1
7	NAG	A	616	1	1/1/5/7	2/6/23/26	0/1/1/1
6	FUC	C	608	-	-	-	0/1/1/1
7	NAG	C	609	1	-	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)
6	B	610	FUC	O5-C5	3.00	1.50	1.43
6	A	614	FUC	O5-C5	2.91	1.49	1.43
6	C	608	FUC	O5-C5	2.67	1.49	1.43

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	C	608	FUC	O5-C1-C2	6.98	121.54	110.77
7	C	601	NAG	C1-O5-C5	6.70	121.27	112.19
6	A	614	FUC	O5-C1-C2	6.33	120.53	110.77
6	B	610	FUC	O5-C1-C2	6.28	120.46	110.77
7	C	601	NAG	C4-C3-C2	-3.66	105.66	111.02
6	A	614	FUC	O5-C5-C4	3.27	115.39	109.52
7	B	613	NAG	C1-O5-C5	3.17	116.48	112.19
6	C	608	FUC	C1-O5-C5	3.06	119.71	112.78
6	C	608	FUC	O5-C5-C4	2.97	114.85	109.52
6	B	610	FUC	O5-C5-C4	2.88	114.68	109.52
7	B	612	NAG	C1-O5-C5	2.79	115.97	112.19
6	A	614	FUC	C1-O5-C5	2.64	118.75	112.78
6	B	610	FUC	C1-O5-C5	2.61	118.69	112.78
7	A	616	NAG	C1-O5-C5	2.23	115.22	112.19
7	C	601	NAG	O5-C1-C2	2.21	114.77	111.29
6	C	608	FUC	C1-C2-C3	2.14	112.29	109.67
7	A	615	NAG	C1-O5-C5	2.06	114.98	112.19
6	B	610	FUC	C2-C3-C4	-2.05	107.34	110.89
7	C	610	NAG	O5-C5-C6	2.04	110.41	107.20
7	A	616	NAG	O5-C5-C6	2.03	110.38	107.20
7	C	601	NAG	C2-N2-C7	-2.03	120.02	122.90

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	C	610	NAG	C1
7	B	612	NAG	C1
7	A	616	NAG	C1

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	C	610	NAG	C4-C5-C6-O6
7	C	610	NAG	C8-C7-N2-C2
7	C	609	NAG	C8-C7-N2-C2
7	B	611	NAG	C8-C7-N2-C2
7	B	613	NAG	O5-C5-C6-O6
7	C	610	NAG	O5-C5-C6-O6
7	C	601	NAG	O5-C5-C6-O6
7	C	610	NAG	O7-C7-N2-C2
7	C	609	NAG	O7-C7-N2-C2
7	B	611	NAG	O7-C7-N2-C2
7	C	601	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
7	B	613	NAG	C4-C5-C6-O6
7	A	615	NAG	C8-C7-N2-C2
7	A	615	NAG	O7-C7-N2-C2
7	A	616	NAG	C4-C5-C6-O6
7	A	616	NAG	O5-C5-C6-O6
7	B	611	NAG	C4-C5-C6-O6

There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	610	FUC	1	0
7	B	611	NAG	1	0
6	C	608	FUC	3	0
6	A	614	FUC	2	0

5.7 Other polymers

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^{th} 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^2)	Q<0.9
1	A	494/510 (96%)	-0.32	4 (0%)	86	86	23, 39, 59, 110	0
1	B	494/510 (96%)	-0.49	2 (0%)	92	93	21, 34, 56, 86	0
1	C	497/510 (97%)	-0.51	1 (0%)	95	96	22, 36, 56, 82	0
All	All	1485/1530 (97%)	-0.44	7 (0%)	91	91	21, 37, 57, 110	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	143	ASN	7.2
1	A	142	THR	7.1
1	A	171	ASN	2.8
1	B	334	ALA	2.5
1	B	140	TYR	2.4
1	A	141	ASP	2.1
1	C	140	TYR	2.1

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

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

6.3 Carbohydrates

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} 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^2)	Q<0.9
5	NAG	I	3	14/15	0.58	0.33	104,114,120,120	0

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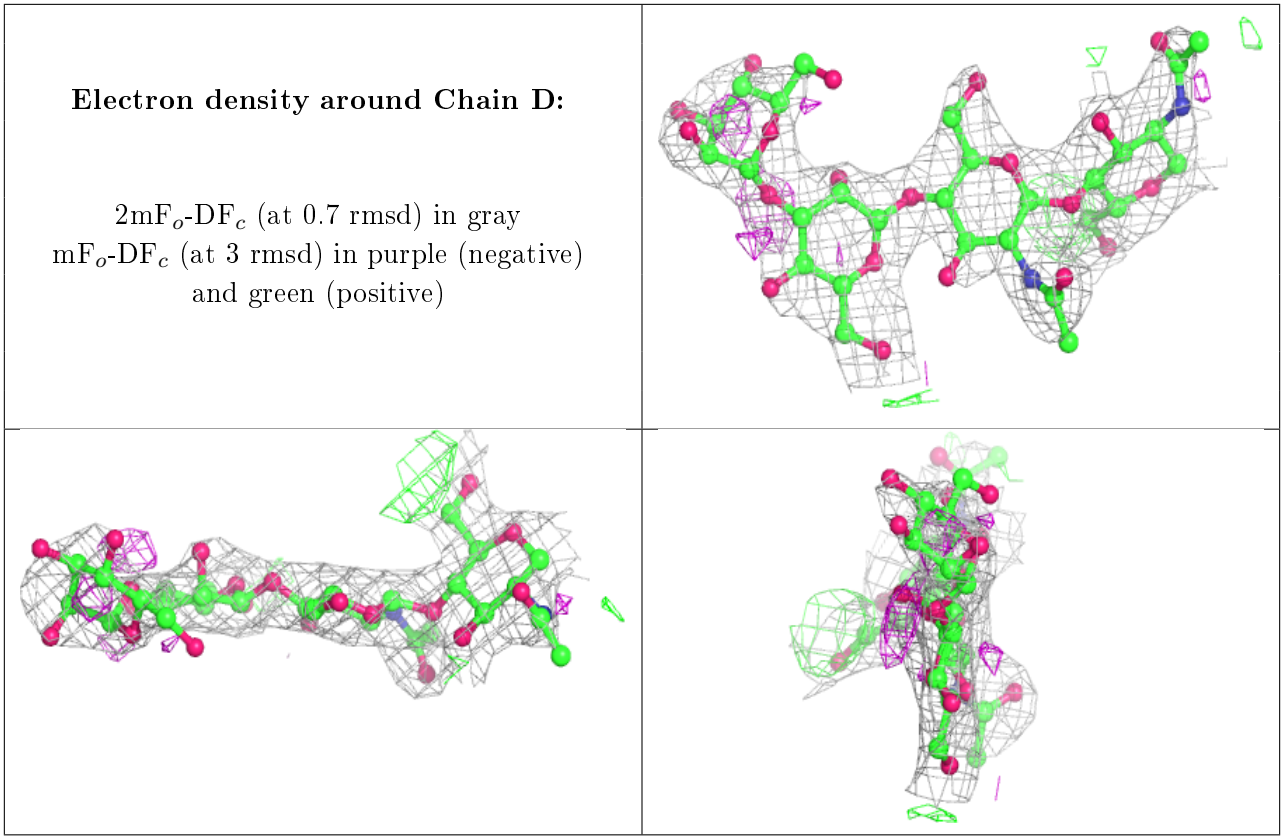
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	MAN	G	4	11/12	0.60	0.44	103,109,114,114	0
5	FUL	I	4	10/11	0.64	0.34	93,106,135,135	0
4	NAG	J	2	14/15	0.71	0.34	73,84,90,90	0
3	BMA	G	3	11/12	0.73	0.20	74,82,89,92	0
2	BMA	D	3	11/12	0.76	0.31	66,72,77,80	0
2	MAN	D	4	11/12	0.76	0.48	82,87,91,91	0
3	MAN	E	5	11/12	0.76	0.24	67,76,86,87	0
4	NAG	H	2	14/15	0.78	0.21	66,73,86,86	0
3	MAN	G	5	11/12	0.79	0.25	84,90,96,96	0
3	FUL	G	7	10/11	0.81	0.17	63,73,84,85	0
3	FUL	E	7	10/11	0.82	0.21	58,68,71,72	0
4	NAG	F	2	14/15	0.82	0.19	72,74,80,81	0
2	NAG	D	1	14/15	0.82	0.28	73,79,85,85	0
4	NAG	F	1	14/15	0.82	0.24	61,69,75,81	0
5	NAG	I	1	14/15	0.83	0.23	80,87,100,108	0
3	MAN	E	4	11/12	0.83	0.23	82,88,94,94	0
5	FUC	I	2	10/11	0.85	0.43	102,104,105,106	0
3	BMA	E	3	11/12	0.88	0.17	65,69,75,75	0
4	NAG	J	1	14/15	0.89	0.28	55,64,76,79	0
4	NAG	H	1	14/15	0.90	0.14	57,65,76,82	0
2	NAG	D	2	14/15	0.90	0.30	78,80,82,83	0
3	NAG	E	2	14/15	0.92	0.19	53,58,63,65	0
3	NAG	G	2	14/15	0.93	0.11	52,59,63,63	0
3	FUC	E	6	10/11	0.94	0.13	52,58,63,65	0
3	NAG	E	1	14/15	0.94	0.16	42,52,62,69	0
3	NAG	G	1	14/15	0.94	0.10	37,47,57,66	0
3	FUC	G	6	10/11	0.96	0.14	52,55,59,60	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.

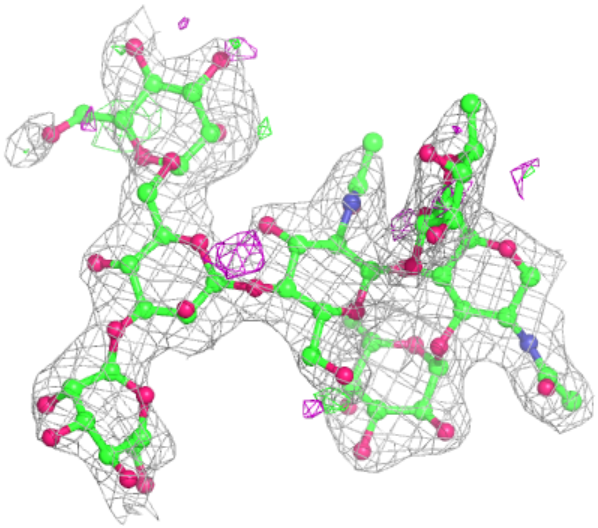
Electron density around Chain D:

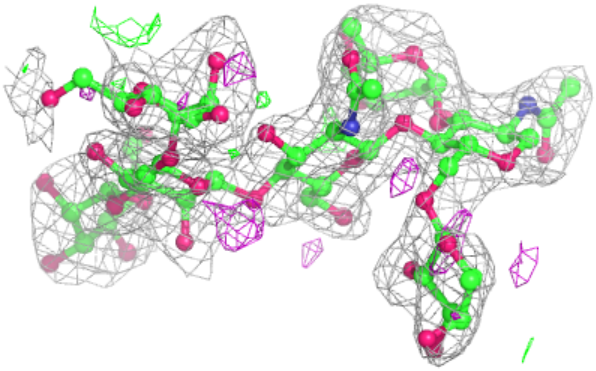
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

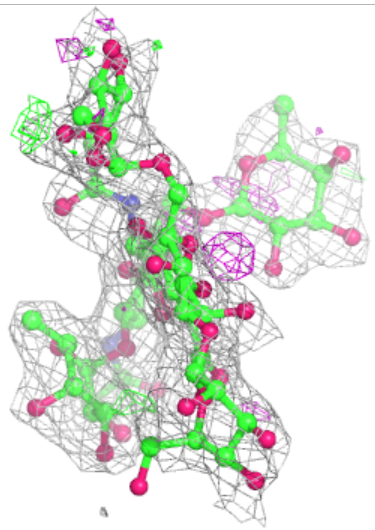


Electron density around Chain E:

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

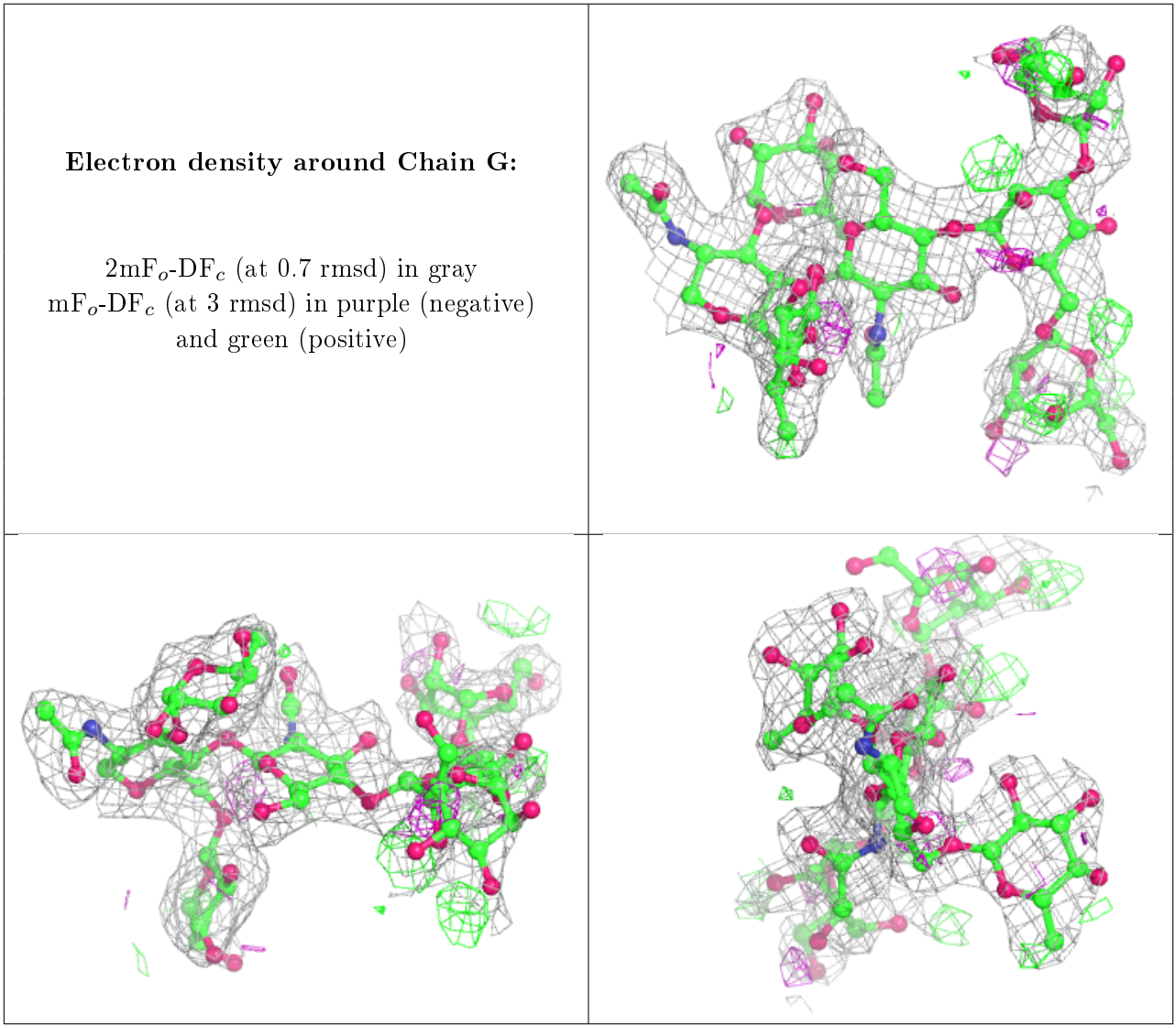






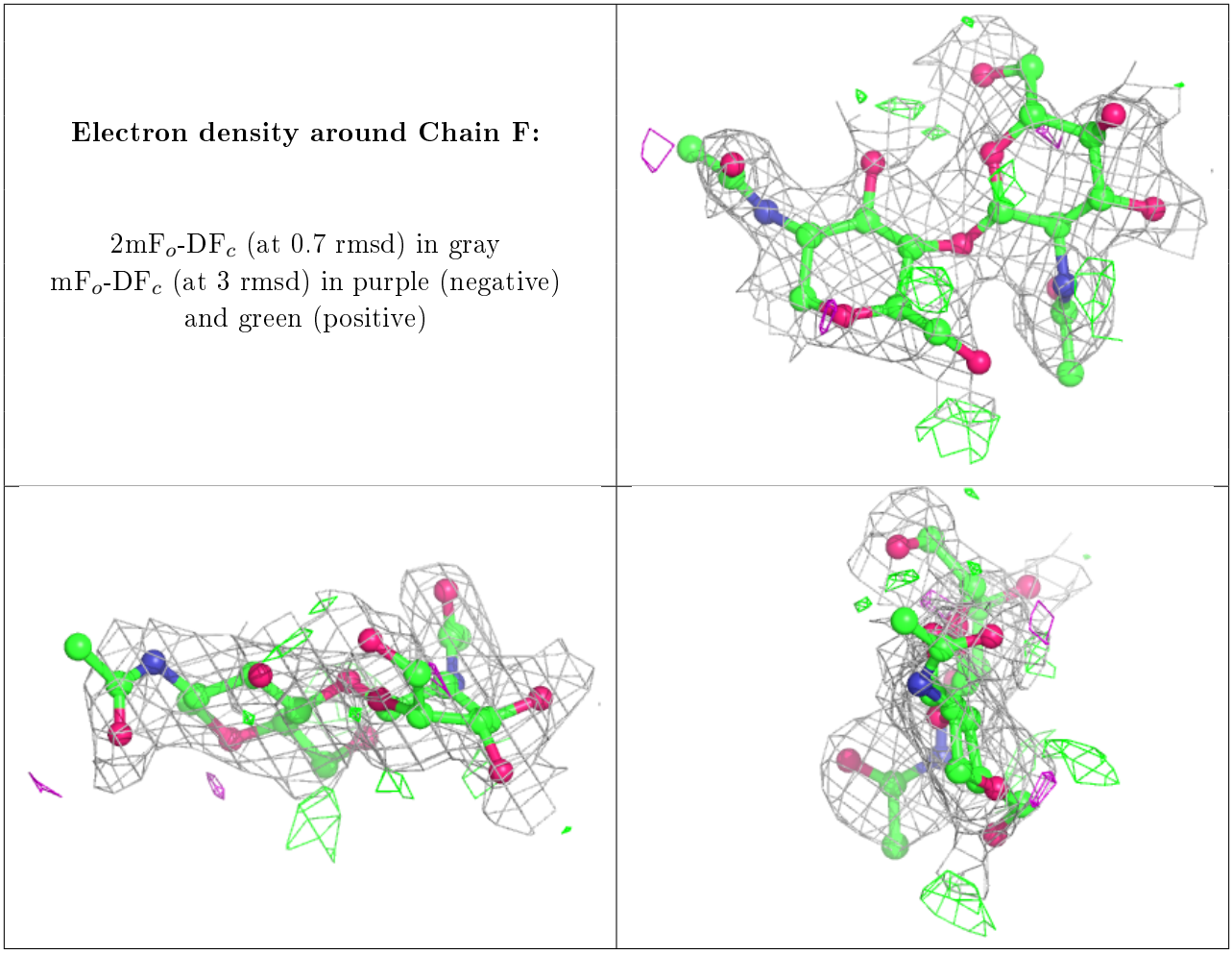
Electron density around Chain G:

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



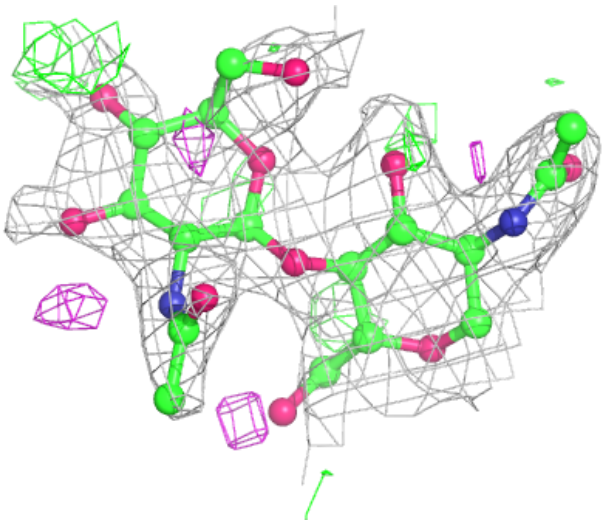
Electron density around Chain F:

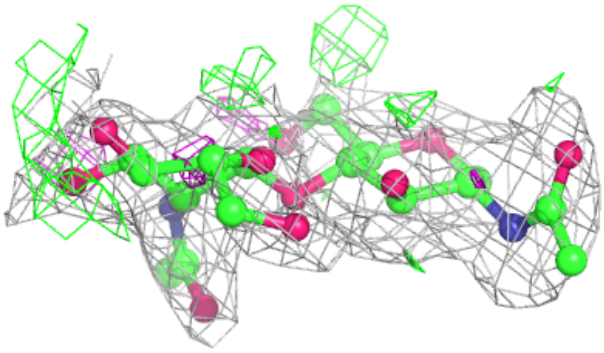
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

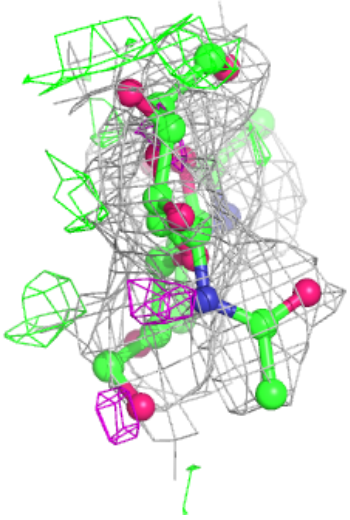


Electron density around Chain H:

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

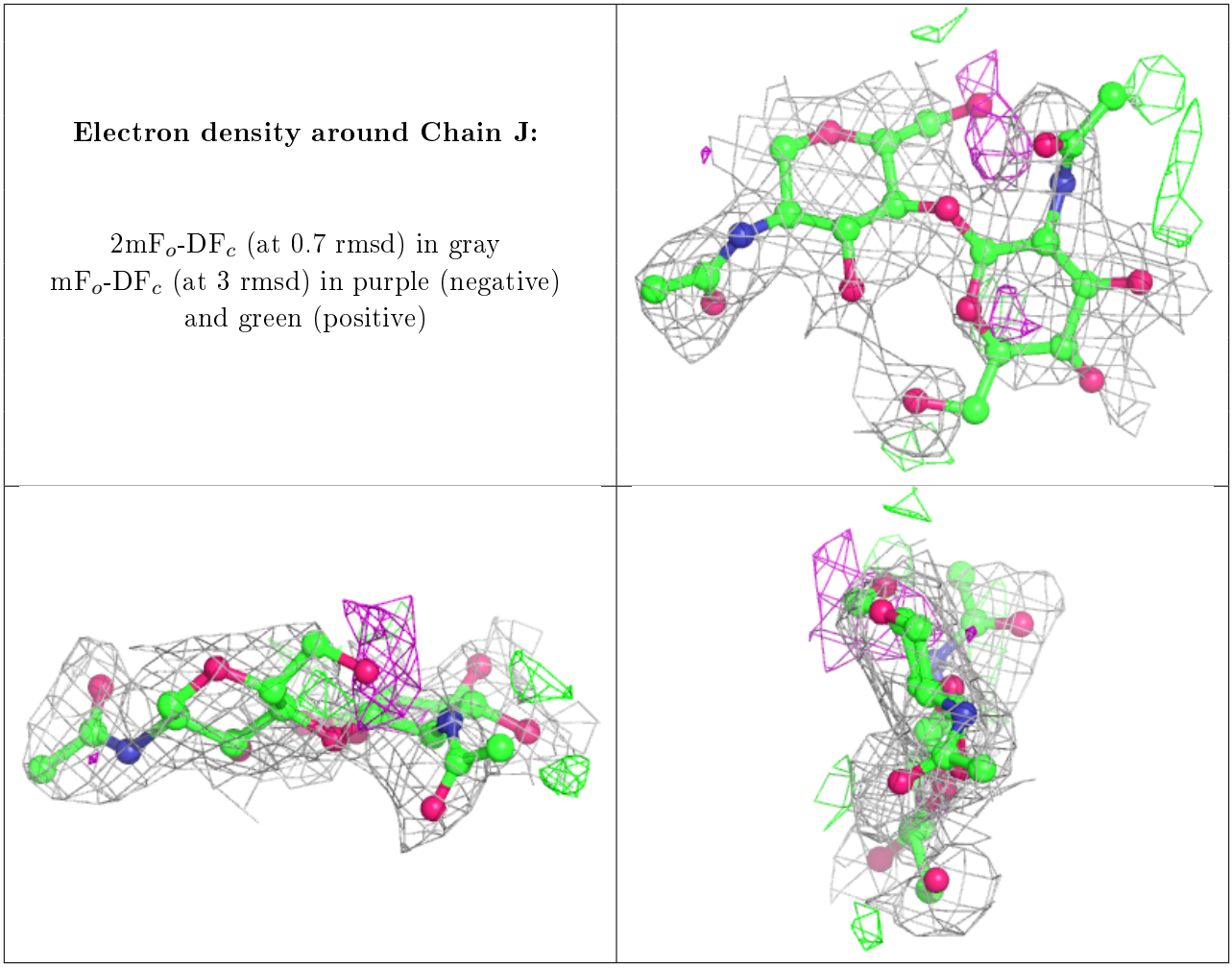






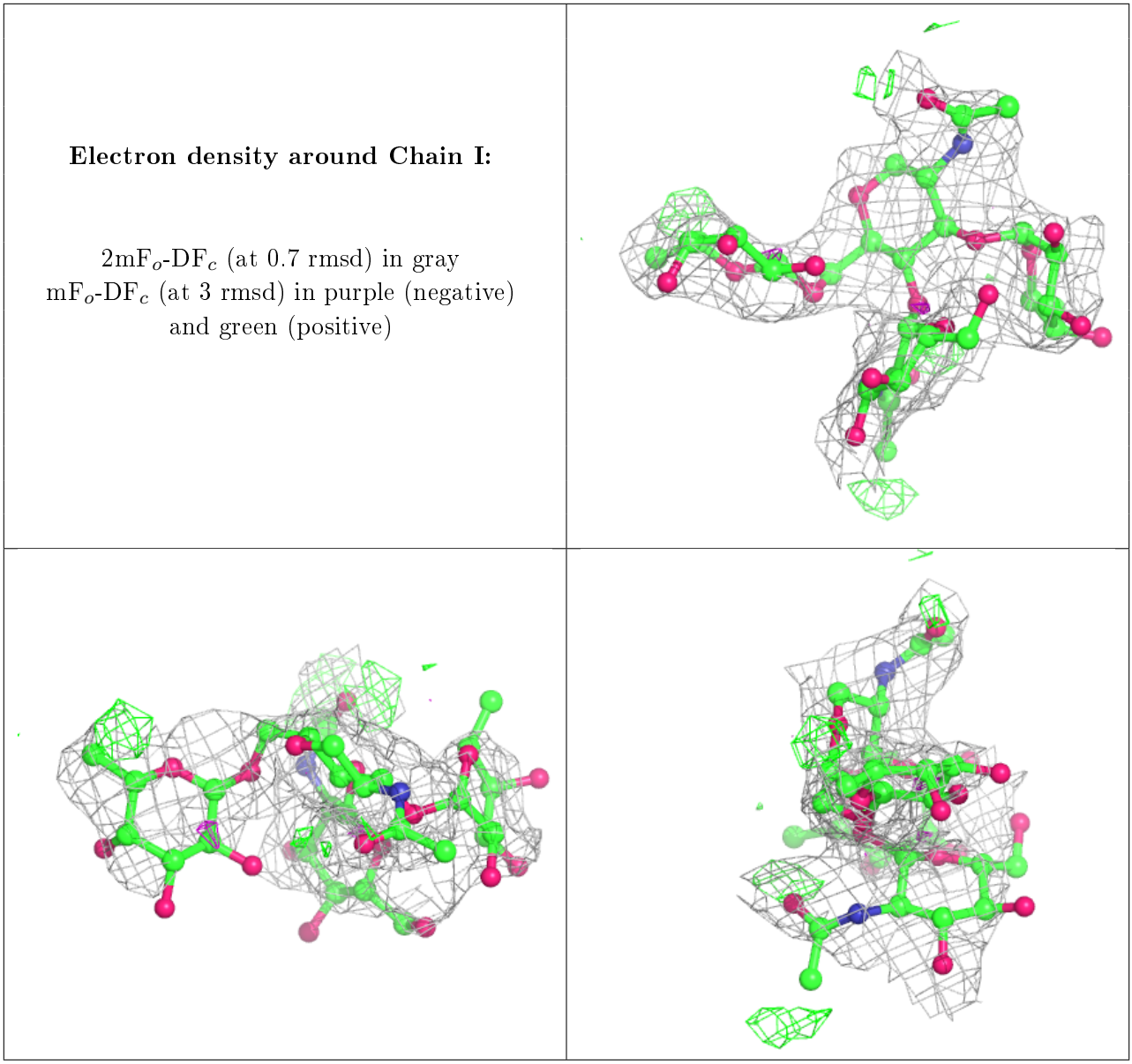
Electron density around Chain J:

$2mF_o$-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 I:

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



6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} 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^2)	Q<0.9
6	FUC	C	608	10/11	0.56	0.32	86,89,92,94	0
6	FUC	B	610	10/11	0.60	0.39	81,86,87,87	0
6	FUC	A	614	10/11	0.64	0.24	75,83,85,86	0
7	NAG	B	613	14/15	0.76	0.39	85,90,93,95	0
7	NAG	C	601	14/15	0.79	0.20	95,103,107,108	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	NAG	C	610	14/15	0.82	0.22	81,88,89,90	0
7	NAG	C	609	14/15	0.83	0.22	58,68,71,73	0
7	NAG	A	615	14/15	0.84	0.15	64,73,75,76	0
7	NAG	B	611	14/15	0.85	0.19	63,68,73,75	0
7	NAG	A	616	14/15	0.87	0.23	82,89,91,92	0
7	NAG	B	612	14/15	0.88	0.18	83,91,92,93	0

6.5 Other polymers

There are no such residues in this entry.