Full wwPDB X-ray Structure Validation Report ⓘ

Jun 18, 2024 – 08:21 PM EDT

PDB ID	:	4AH4
Title	:	Crystal Structure of Fucose binding lectin from Aspergillus Fumigatus (AFL) in complex with BGA Oligosaccharide.
Authors	:	Houser, J.; Komarek, J.; Kostlanova, N.; Lahmann, M.; Cioci, G.; Varrot, A.; Imberty, A.; Wimmerova, M.
Deposited on	:	2012-02-03
Resolution	:	1.75 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

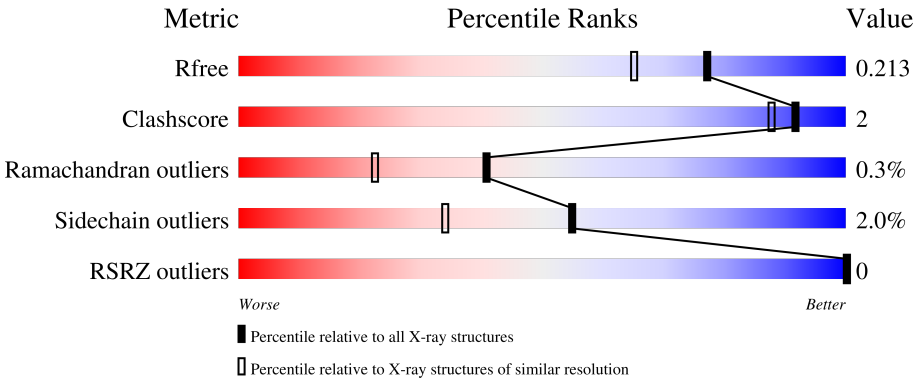
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 1.75 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	2340 (1.76-1.76)
Clashscore	141614	2466 (1.76-1.76)
Ramachandran outliers	138981	2437 (1.76-1.76)
Sidechain outliers	138945	2437 (1.76-1.76)
RSRZ outliers	127900	2298 (1.76-1.76)

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 >=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	315	95% .
1	B	315	95% . .
2	C	3	33% 67%
2	D	3	33% 67%
2	E	3	100%

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Mol	Chain	Length	Quality of chain
2	F	3	67% 33%
2	G	3	67% 33%
2	H	3	67% 33%
2	I	3	67% 33%
2	J	3	100%
2	K	3	33% 67%

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	GAL	E	1	X	-	-	-
2	GAL	F	1	X	-	-	-
2	GAL	H	1	X	-	-	-
2	GAL	I	1	X	-	-	-
2	GAL	J	1	X	-	-	-
2	GAL	K	1	X	-	-	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 5813 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.

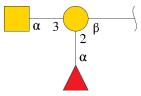
- Molecule 1 is a protein called FUCOSE-SPECIFIC LECTIN FLEA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	314	Total	C	N	O	S	0	2	0
			2454	1562	423	464	5			
1	B	314	Total	C	N	O	S	0	0	0
			2445	1557	422	462	4			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	20	SER	LEU	conflict	UNP Q4WW81
A	111	CYS	ARG	conflict	UNP Q4WW81
B	20	SER	LEU	conflict	UNP Q4WW81
B	111	CYS	ARG	conflict	UNP Q4WW81

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	3	Total	C	N	O	0	0	0
			36	20	1	15			
2	D	3	Total	C	N	O	0	0	0
			36	20	1	15			
2	E	3	Total	C	N	O	0	0	0
			36	20	1	15			
2	F	3	Total	C	N	O	0	0	0
			36	20	1	15			
2	G	3	Total	C	N	O	0	0	0
			36	20	1	15			

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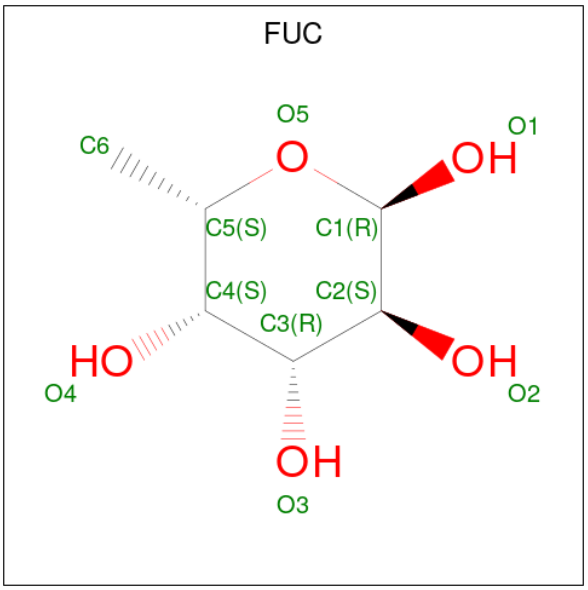
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
2	H	3	Total C N O 36 20 1 15	0	0	0
2	I	3	Total C N O 36 20 1 15	0	0	0
2	J	3	Total C N O 36 20 1 15	0	0	0
2	K	3	Total C N O 36 20 1 15	0	0	0

- Molecule 3 is alpha-L-fucopyranose (three-letter code: FUC) (formula: $C_6H_{12}O_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 11 6 5	0	0
3	B	1	Total C O 11 6 5	0	0
3	B	1	Total C O 11 6 5	0	0

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Cl 1 1	0	0

- Molecule 5 is water.

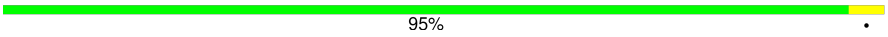
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	291	Total O 291 291	0	0
5	B	265	Total O 265 265	0	0

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.

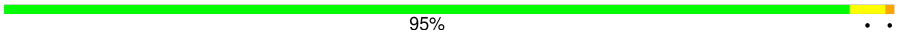
• Molecule 1: FUCOSE-SPECIFIC LECTIN FLEA

Chain A:



• Molecule 1: FUCOSE-SPECIFIC LECTIN FLEA

Chain B:



• Molecule 2: alpha-L-fucopyranose-(1-2)-[2-acetamido-2-deoxy-alpha-D-galactopyranose-(1-3)]beta-D-galactopyranose

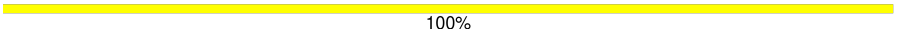
Chain C:

• Molecule 2: alpha-L-fucopyranose-(1-2)-[2-acetamido-2-deoxy-alpha-D-galactopyranose-(1-3)]beta-D-galactopyranose

Chain D:

• Molecule 2: alpha-L-fucopyranose-(1-2)-[2-acetamido-2-deoxy-alpha-D-galactopyranose-(1-3)]beta-D-galactopyranose

Chain E:



• Molecule 2: alpha-L-fucopyranose-(1-2)-[2-acetamido-2-deoxy-alpha-D-galactopyranose-(1-3)]beta-D-galactopyranose

Chain F:

• Molecule 2: alpha-L-fucopyranose-(1-2)-[2-acetamido-2-deoxy-alpha-D-galactopyranose-(1-3)]beta-D-galactopyranose

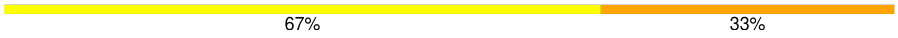
Chain G:

• Molecule 2: alpha-L-fucopyranose-(1-2)-[2-acetamido-2-deoxy-alpha-D-galactopyranose-(1-3)]beta-D-galactopyranose

Chain H:

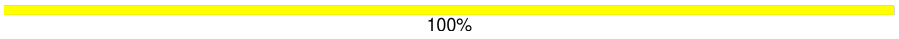
• Molecule 2: alpha-L-fucopyranose-(1-2)-[2-acetamido-2-deoxy-alpha-D-galactopyranose-(1-3)]beta-D-galactopyranose

Chain I:



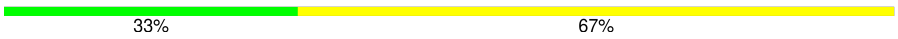
• Molecule 2: alpha-L-fucopyranose-(1-2)-[2-acetamido-2-deoxy-alpha-D-galactopyranose-(1-3)]beta-D-galactopyranose

Chain J:



• Molecule 2: alpha-L-fucopyranose-(1-2)-[2-acetamido-2-deoxy-alpha-D-galactopyranose-(1-3)]beta-D-galactopyranose

Chain K:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	46.42Å 47.44Å 80.09Å 103.61° 91.96° 113.08°	Depositor
Resolution (Å)	77.15 – 1.75 42.02 – 1.75	Depositor EDS
% Data completeness (in resolution range)	94.1 (77.15-1.75) 94.1 (42.02-1.75)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.50 (at 1.75Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.168 , 0.211 0.172 , 0.213	Depositor DCC
R_{free} test set	2897 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	15.8	Xtriage
Anisotropy	0.611	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 37.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	5813	wwPDB-VP
Average B, all atoms (Å^2)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.82% 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: FUC, A2G, GAL, CL, CSD

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	0.83	3/2520 (0.1%)	0.80	1/3435 (0.0%)
1	B	0.82	1/2508 (0.0%)	0.82	0/3419
All	All	0.82	4/5028 (0.1%)	0.81	1/6854 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	271	TRP	CD2-CE2	6.53	1.49	1.41
1	A	141	TRP	CD2-CE2	5.35	1.47	1.41
1	B	179	TRP	CD2-CE2	5.25	1.47	1.41
1	A	241	TRP	CD2-CE2	5.17	1.47	1.41

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	39	LEU	CA-CB-CG	5.73	128.48	115.30

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	2454	0	2336	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2445	0	2327	5	0
2	C	36	0	32	1	0
2	D	36	0	32	1	0
2	E	36	0	32	1	0
2	F	36	0	32	0	0
2	G	36	0	32	1	0
2	H	36	0	32	0	0
2	I	36	0	32	1	0
2	J	36	0	32	0	0
2	K	36	0	32	0	0
3	A	11	0	12	0	0
3	B	22	0	24	0	0
4	A	1	0	0	1	0
5	A	291	0	0	5	0
5	B	265	0	0	2	0
All	All	5813	0	4987	16	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 2.

All (16) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:111[B]:CYS:SG	5:A:2134:HOH:O	2.22	0.96
5:A:2173:HOH:O	2:E:1:GAL:H1	1.95	0.66
1:B:49:GLU:CD	1:B:49:GLU:H	2.04	0.59
5:A:2013:HOH:O	2:G:1:GAL:H2	2.02	0.58
1:A:49:GLU:HG2	5:A:2071:HOH:O	2.05	0.56
1:A:39:LEU:HD21	2:C:3:A2G:H8B	1.89	0.53
5:B:2261:HOH:O	2:I:3:A2G:C1	2.61	0.49
1:B:200:PRO:HD2	5:B:2169:HOH:O	2.12	0.49
1:A:119:GLY:HA3	1:A:167:ARG:HD3	2.01	0.43
1:B:39:LEU:C	1:B:39:LEU:HD12	2.39	0.43
1:B:242:GLN:O	1:B:254:LYS:HA	2.19	0.43
1:A:111[B]:CYS:SG	5:A:2135:HOH:O	2.24	0.43
1:A:50:LYS:HE3	4:A:1000:CL:CL	2.57	0.42
1:B:156:LEU:CD1	1:B:185:LEU:HD23	2.51	0.41
1:A:87:ALA:O	1:A:94:TRP:HA	2.21	0.40
2:D:1:GAL:O4	2:D:3:A2G:N2	2.53	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	313/315 (99%)	306 (98%)	6 (2%)	1 (0%)	41 22
1	B	311/315 (99%)	305 (98%)	5 (2%)	1 (0%)	41 22
All	All	624/630 (99%)	611 (98%)	11 (2%)	2 (0%)	41 22

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	46	ASN
1	A	46	ASN

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	250/249 (100%)	246 (98%)	4 (2%)	62 45
1	B	248/249 (100%)	242 (98%)	6 (2%)	49 26
All	All	498/498 (100%)	488 (98%)	10 (2%)	55 34

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	LEU
1	A	50	LYS
1	A	254	LYS
1	A	280	ASP

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Mol	Chain	Res	Type
1	B	39	LEU
1	B	49	GLU
1	B	140	MET
1	B	195	HIS
1	B	280	ASP
1	B	310	SER

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

Mol	Chain	Res	Type
1	A	105	GLN
1	A	303	HIS
1	B	105	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)

2 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
1	CSD	B	244	1	4,7,8	2.93	2 (50%)	1,8,10	1.38	0
1	CSD	A	244	1	4,7,8	4.68	2 (50%)	1,8,10	2.03	1 (100%)

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
1	CSD	B	244	1	-	0/2/6/8	-
1	CSD	A	244	1	-	0/2/6/8	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	244	CSD	OD1-SG	9.11	1.55	1.47
1	B	244	CSD	OD1-SG	5.30	1.52	1.47
1	B	244	CSD	CB-SG	-2.04	1.67	1.79
1	A	244	CSD	CB-SG	-2.01	1.67	1.79

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	244	CSD	OD1-SG-CB	2.03	109.35	105.60

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

27 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	GAL	C	1	2	12,12,12	0.62	0	17,17,17	1.42	2 (11%)
2	FUC	C	2	2	10,10,11	0.68	0	14,14,16	0.86	0
2	A2G	C	3	2	14,14,15	0.48	0	17,19,21	0.95	0
2	GAL	D	1	2	12,12,12	0.68	0	17,17,17	2.14	7 (41%)
2	FUC	D	2	2	10,10,11	0.54	0	14,14,16	1.04	0
2	A2G	D	3	2	14,14,15	0.61	0	17,19,21	1.78	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	GAL	E	1	2	12,12,12	0.65	0	17,17,17	0.90	0
2	FUC	E	2	2	10,10,11	1.06	0	14,14,16	0.78	1 (7%)
2	A2G	E	3	2	14,14,15	0.34	0	17,19,21	1.05	1 (5%)
2	GAL	F	1	2	12,12,12	0.61	0	17,17,17	1.27	2 (11%)
2	FUC	F	2	2	10,10,11	0.73	0	14,14,16	1.00	0
2	A2G	F	3	2	14,14,15	0.65	0	17,19,21	0.90	0
2	GAL	G	1	2	12,12,12	0.85	0	17,17,17	2.30	7 (41%)
2	FUC	G	2	2	10,10,11	0.91	1 (10%)	14,14,16	1.27	3 (21%)
2	A2G	G	3	2	14,14,15	0.78	1 (7%)	17,19,21	1.25	1 (5%)
2	GAL	H	1	2	12,12,12	0.71	0	17,17,17	1.06	0
2	FUC	H	2	2	10,10,11	0.79	0	14,14,16	1.32	1 (7%)
2	A2G	H	3	2	14,14,15	0.46	0	17,19,21	0.85	0
2	GAL	I	1	2	12,12,12	0.67	0	17,17,17	1.19	3 (17%)
2	FUC	I	2	2	10,10,11	0.82	0	14,14,16	1.43	3 (21%)
2	A2G	I	3	2	14,14,15	0.44	0	17,19,21	1.12	1 (5%)
2	GAL	J	1	2	12,12,12	0.50	0	17,17,17	0.95	1 (5%)
2	FUC	J	2	2	10,10,11	0.77	0	14,14,16	1.05	1 (7%)
2	A2G	J	3	2	14,14,15	0.66	0	17,19,21	1.43	3 (17%)
2	GAL	K	1	2	12,12,12	0.67	0	17,17,17	1.24	1 (5%)
2	FUC	K	2	2	10,10,11	0.65	0	14,14,16	0.59	0
2	A2G	K	3	2	14,14,15	0.39	0	17,19,21	1.01	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
2	GAL	C	1	2	-	0/2/22/22	0/1/1/1
2	FUC	C	2	2	-	-	0/1/1/1
2	A2G	C	3	2	-	0/6/23/26	0/1/1/1
2	GAL	D	1	2	-	2/2/22/22	0/1/1/1
2	FUC	D	2	2	-	-	0/1/1/1
2	A2G	D	3	2	-	0/6/23/26	0/1/1/1
2	GAL	E	1	2	1/1/5/5	2/2/22/22	0/1/1/1
2	FUC	E	2	2	-	-	0/1/1/1
2	A2G	E	3	2	-	4/6/23/26	0/1/1/1
2	GAL	F	1	2	1/1/5/5	2/2/22/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FUC	F	2	2	-	-	0/1/1/1
2	A2G	F	3	2	-	0/6/23/26	0/1/1/1
2	GAL	G	1	2	-	2/2/22/22	0/1/1/1
2	FUC	G	2	2	-	-	0/1/1/1
2	A2G	G	3	2	-	4/6/23/26	0/1/1/1
2	GAL	H	1	2	1/1/5/5	0/2/22/22	0/1/1/1
2	FUC	H	2	2	-	-	0/1/1/1
2	A2G	H	3	2	-	0/6/23/26	0/1/1/1
2	GAL	I	1	2	1/1/5/5	0/2/22/22	0/1/1/1
2	FUC	I	2	2	-	-	0/1/1/1
2	A2G	I	3	2	-	2/6/23/26	0/1/1/1
2	GAL	J	1	2	1/1/5/5	0/2/22/22	0/1/1/1
2	FUC	J	2	2	-	-	0/1/1/1
2	A2G	J	3	2	-	2/6/23/26	0/1/1/1
2	GAL	K	1	2	1/1/5/5	2/2/22/22	0/1/1/1
2	FUC	K	2	2	-	-	0/1/1/1
2	A2G	K	3	2	-	0/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	2	FUC	O5-C1	-2.20	1.40	1.43
2	G	3	A2G	C1-C2	2.07	1.55	1.52

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	G	1	GAL	O3-C3-C4	-5.36	97.75	110.38
2	D	3	A2G	C1-O5-C5	-4.81	105.74	112.19
2	J	3	A2G	C1-C2-N2	-4.20	103.81	110.43
2	D	1	GAL	O3-C3-C4	-4.02	100.89	110.38
2	G	1	GAL	C4-C3-C2	3.90	117.67	110.83
2	C	1	GAL	C1-C2-C3	-3.90	102.40	110.36
2	D	1	GAL	O2-C2-C1	3.48	117.29	109.25
2	I	2	FUC	C3-C4-C5	-3.39	104.67	109.81
2	D	3	A2G	C6-C5-C4	3.35	121.24	113.02
2	G	3	A2G	O5-C5-C6	3.04	113.58	107.66
2	G	1	GAL	O5-C5-C4	-3.02	104.26	109.70
2	D	1	GAL	O1-C1-O5	-2.86	101.93	110.41
2	F	1	GAL	C1-C2-C3	-2.84	104.55	110.36
2	J	1	GAL	O5-C5-C6	2.71	113.16	106.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	1	GAL	O1-C1-C2	2.66	116.70	108.98
2	G	1	GAL	O5-C5-C6	2.65	113.02	106.44
2	I	2	FUC	C6-C5-C4	-2.60	108.33	113.08
2	D	1	GAL	O5-C1-C2	-2.59	105.74	110.30
2	G	1	GAL	O2-C2-C3	-2.59	104.27	110.38
2	F	1	GAL	O5-C5-C6	2.55	112.77	106.44
2	I	2	FUC	O2-C2-C3	2.55	115.43	110.15
2	K	1	GAL	O2-C2-C1	2.52	115.07	109.25
2	E	3	A2G	O5-C5-C6	2.49	112.51	107.66
2	G	2	FUC	C3-C4-C5	-2.45	106.09	109.81
2	D	1	GAL	O5-C5-C4	-2.43	105.32	109.70
2	K	3	A2G	C1-O5-C5	2.42	115.43	112.19
2	H	2	FUC	O3-C3-C4	2.41	116.05	110.38
2	I	1	GAL	O3-C3-C4	-2.41	104.70	110.38
2	D	1	GAL	O5-C5-C6	2.38	112.33	106.44
2	J	3	A2G	C2-N2-C7	2.35	126.06	122.90
2	I	1	GAL	O5-C1-C2	-2.35	106.17	110.30
2	I	1	GAL	O4-C4-C5	2.32	115.03	109.32
2	C	1	GAL	O6-C6-C5	-2.28	103.56	111.33
2	G	1	GAL	C6-C5-C4	-2.25	107.49	113.02
2	G	1	GAL	O5-C1-C2	2.23	114.22	110.30
2	I	3	A2G	C1-C2-N2	-2.18	106.99	110.43
2	G	2	FUC	C1-C2-C3	2.17	112.81	109.64
2	J	3	A2G	C1-O5-C5	2.15	115.06	112.19
2	G	2	FUC	O3-C3-C4	2.08	115.28	110.38
2	J	2	FUC	C1-C2-C3	2.08	112.67	109.64
2	E	2	FUC	O2-C2-C1	2.04	113.89	109.22

All (6) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	E	1	GAL	C1
2	F	1	GAL	C1
2	H	1	GAL	C1
2	I	1	GAL	C1
2	J	1	GAL	C1
2	K	1	GAL	C1

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	3	A2G	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	G	3	A2G	O5-C5-C6-O6
2	K	1	GAL	C4-C5-C6-O6
2	K	1	GAL	O5-C5-C6-O6
2	I	3	A2G	O7-C7-N2-C2
2	I	3	A2G	C8-C7-N2-C2
2	G	3	A2G	C4-C5-C6-O6
2	E	3	A2G	O7-C7-N2-C2
2	E	3	A2G	C8-C7-N2-C2
2	G	3	A2G	O7-C7-N2-C2
2	G	3	A2G	C8-C7-N2-C2
2	J	3	A2G	O7-C7-N2-C2
2	J	3	A2G	C8-C7-N2-C2
2	E	1	GAL	C4-C5-C6-O6
2	F	1	GAL	C4-C5-C6-O6
2	D	1	GAL	O5-C5-C6-O6
2	E	3	A2G	C4-C5-C6-O6
2	F	1	GAL	O5-C5-C6-O6
2	E	1	GAL	O5-C5-C6-O6
2	D	1	GAL	C4-C5-C6-O6
2	G	1	GAL	O5-C5-C6-O6
2	G	1	GAL	C4-C5-C6-O6

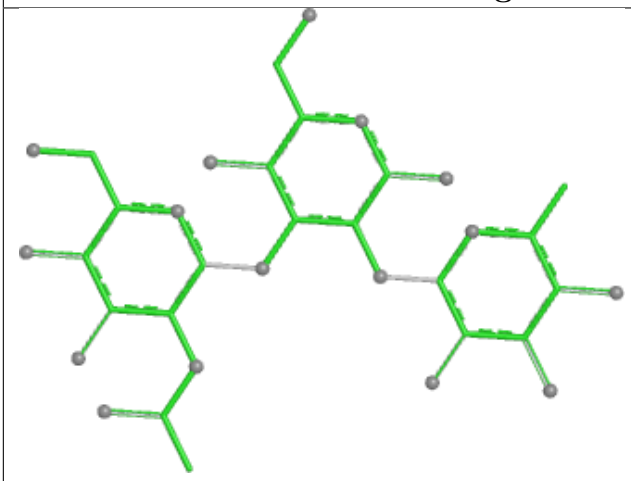
There are no ring outliers.

6 monomers are involved in 5 short contacts:

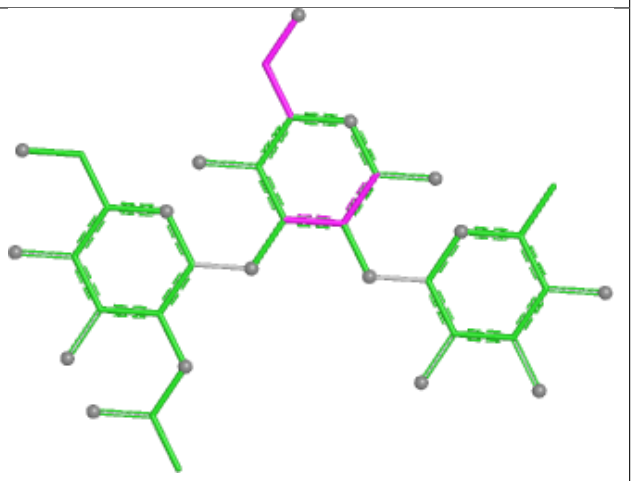
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	3	A2G	1	0
2	E	1	GAL	1	0
2	C	3	A2G	1	0
2	D	1	GAL	1	0
2	G	1	GAL	1	0
2	I	3	A2G	1	0

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

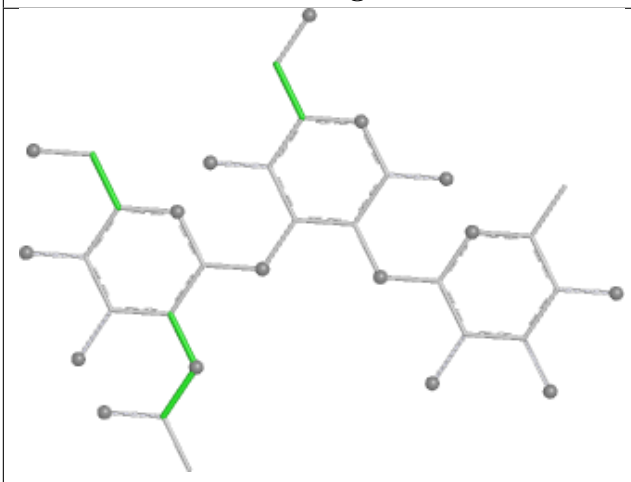
Oligosaccharide Chain C



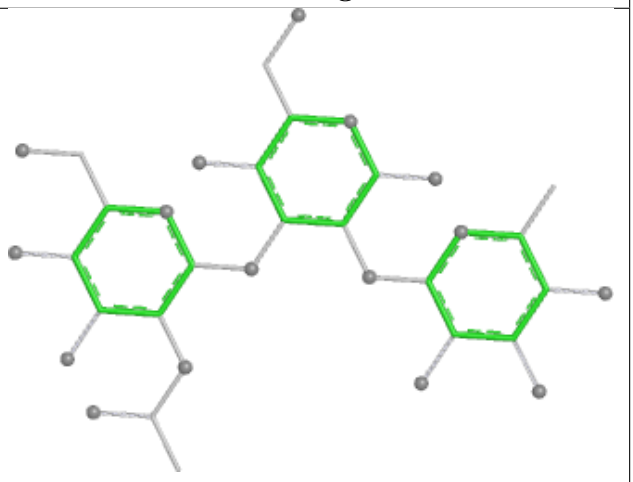
Bond lengths



Bond angles

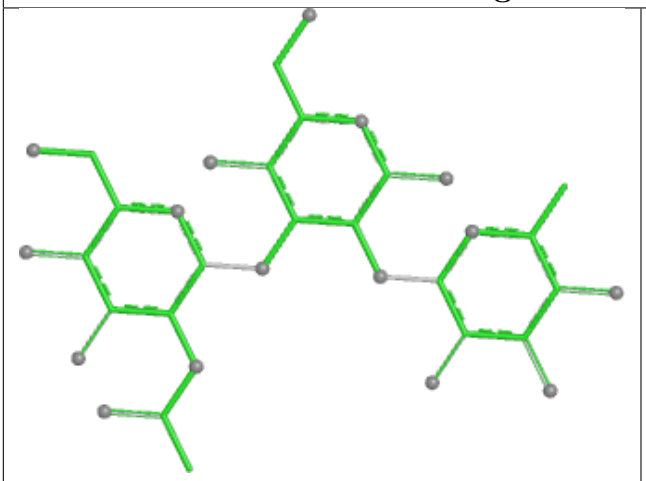


Torsions

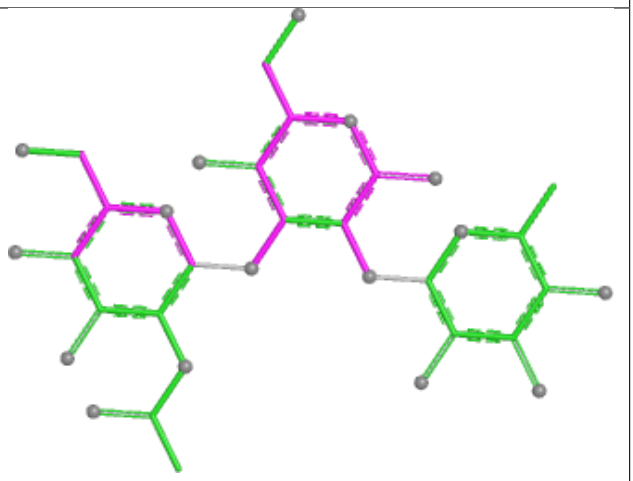


Rings

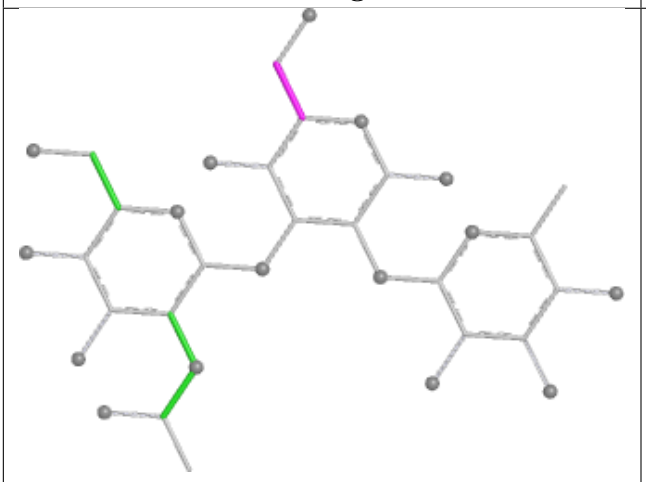
Oligosaccharide Chain D



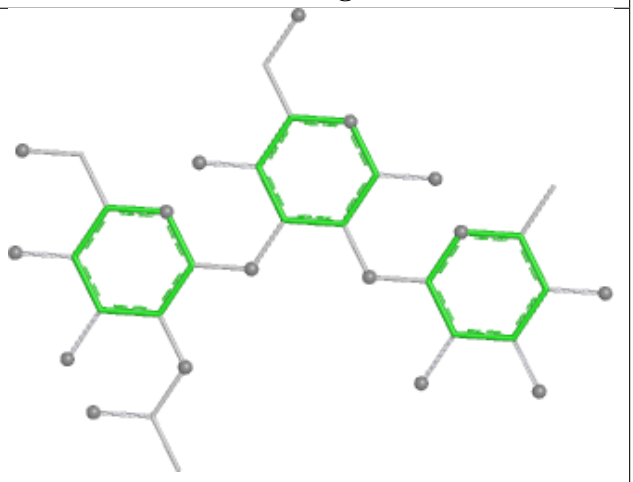
Bond lengths



Bond angles

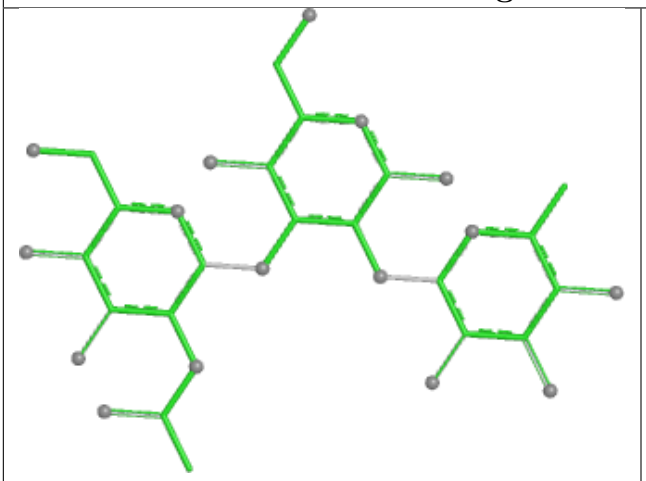


Torsions

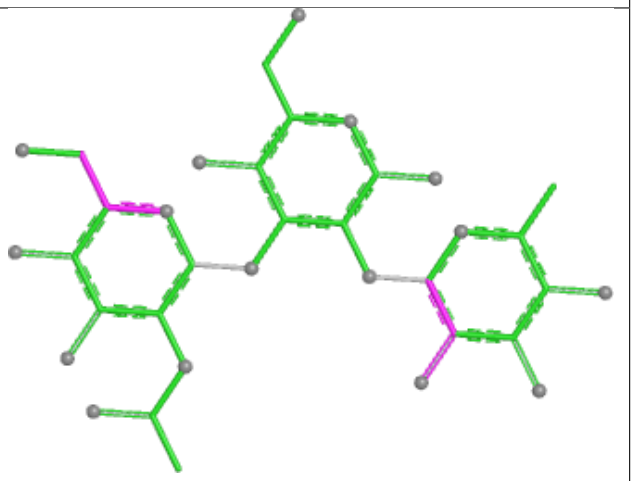


Rings

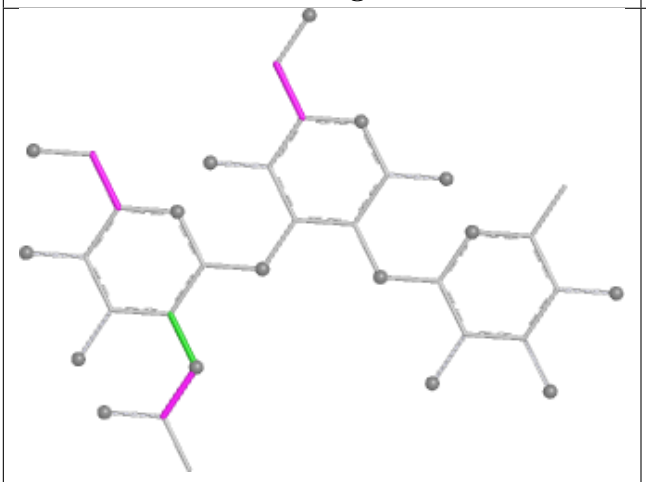
Oligosaccharide Chain E



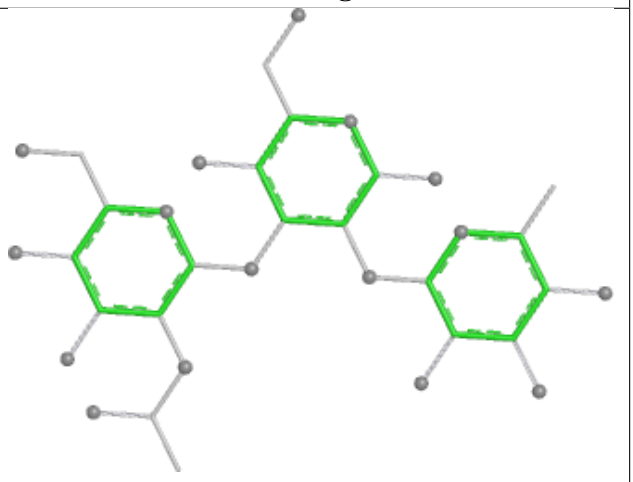
Bond lengths



Bond angles

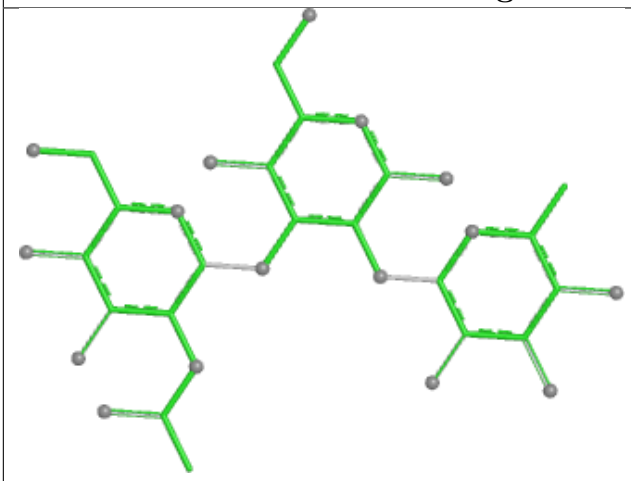


Torsions

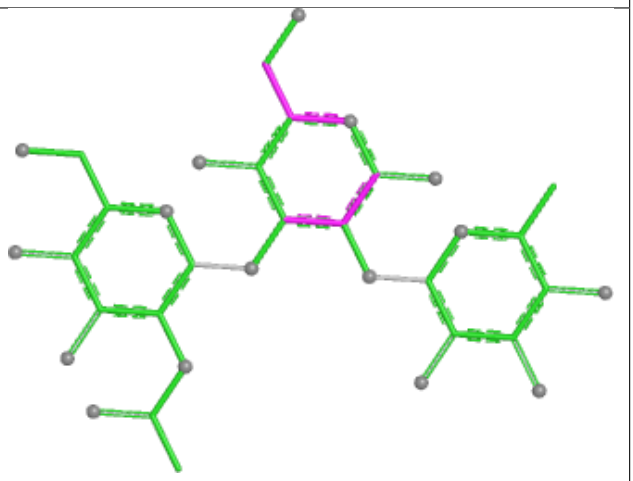


Rings

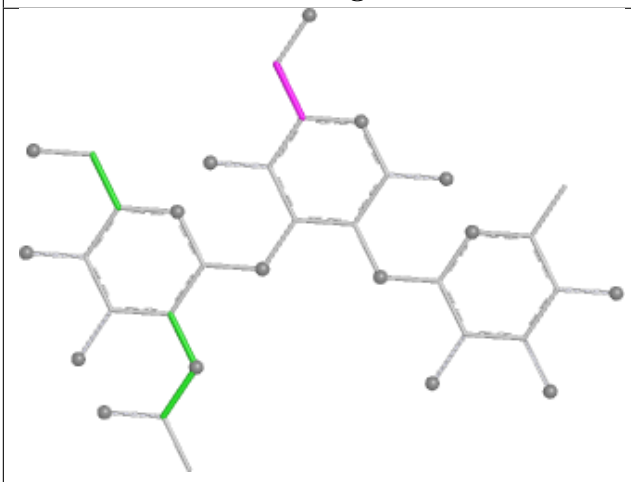
Oligosaccharide Chain F



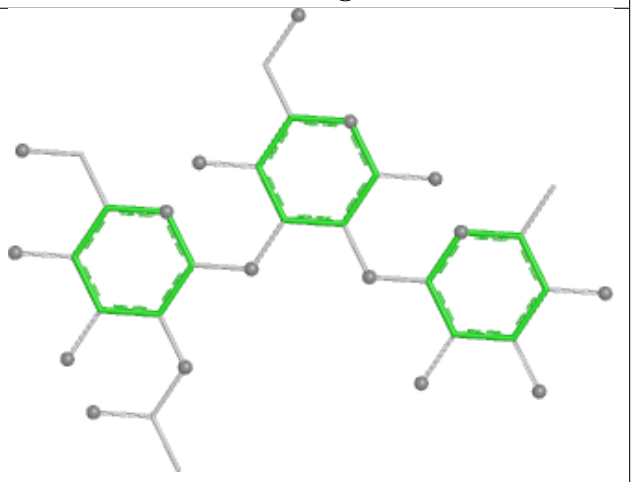
Bond lengths



Bond angles

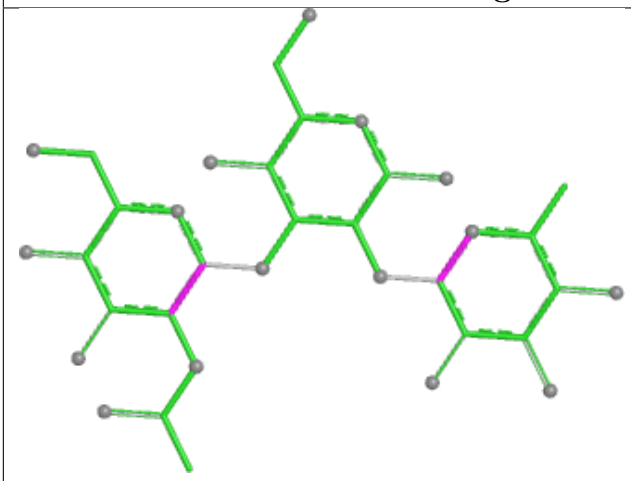


Torsions

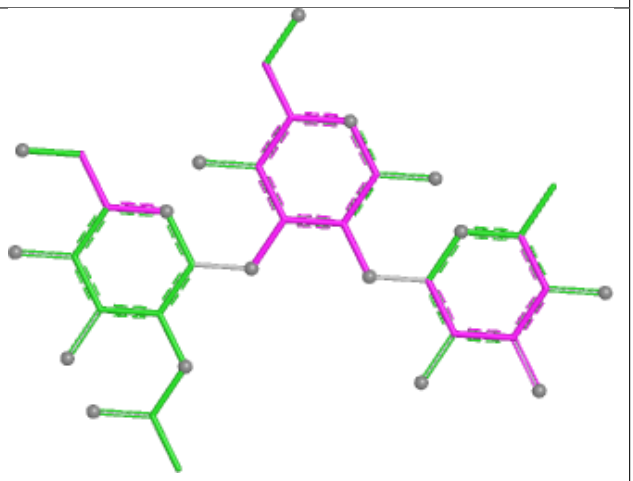


Rings

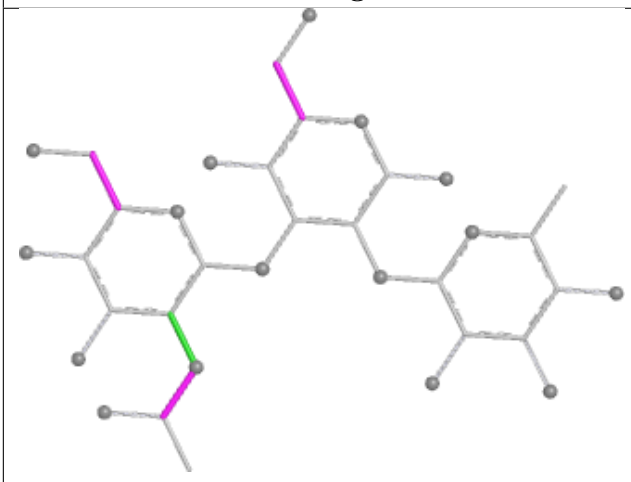
Oligosaccharide Chain G



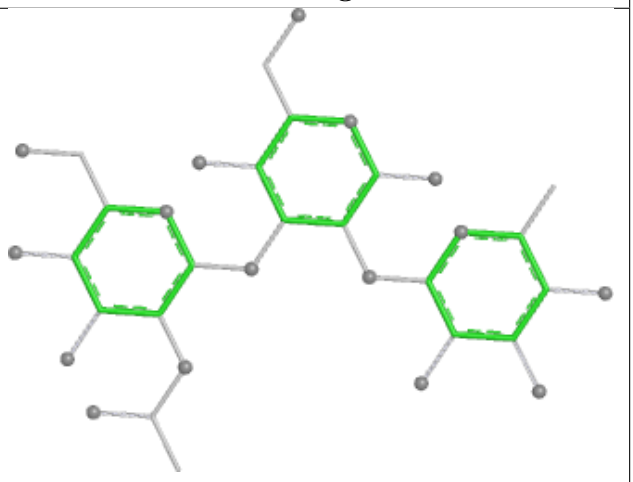
Bond lengths



Bond angles

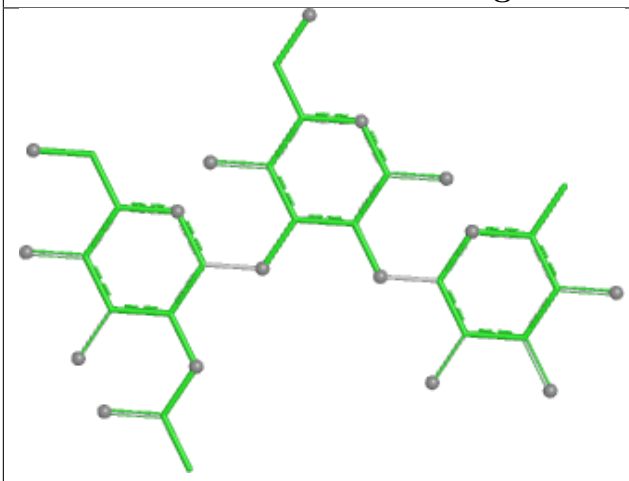


Torsions

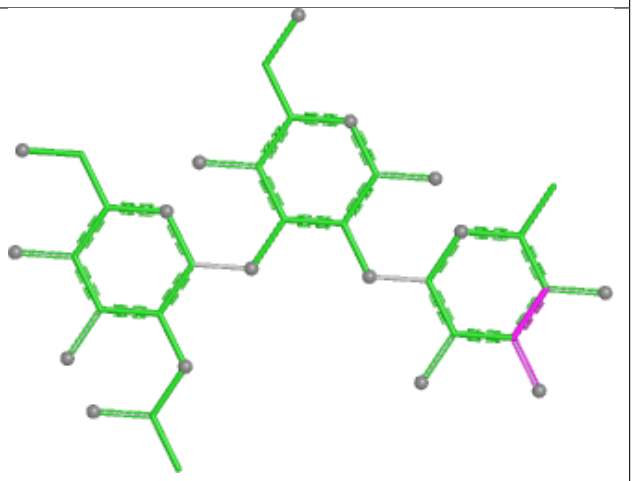


Rings

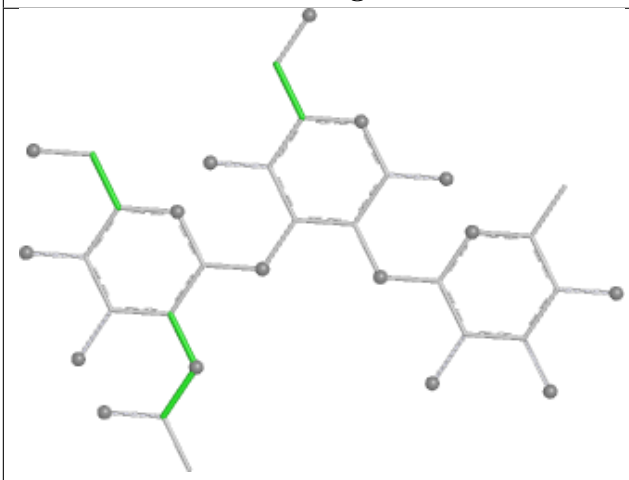
Oligosaccharide Chain H



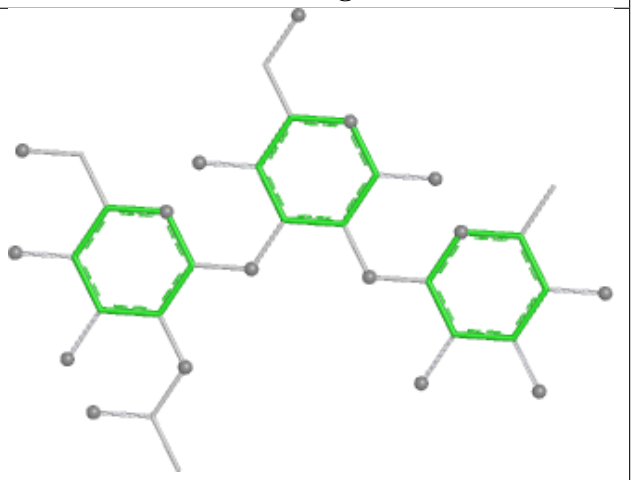
Bond lengths



Bond angles

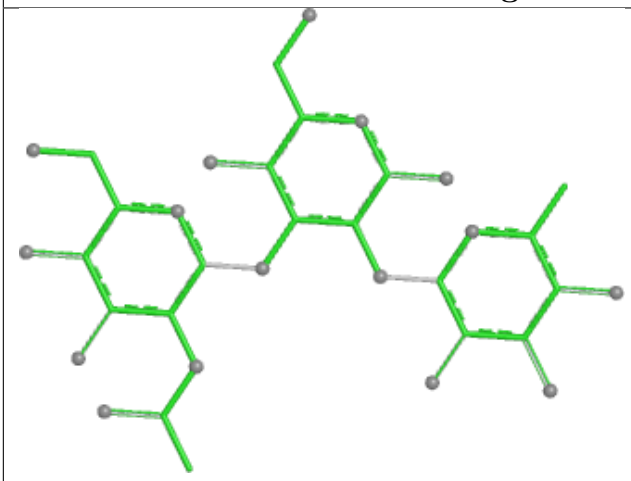


Torsions

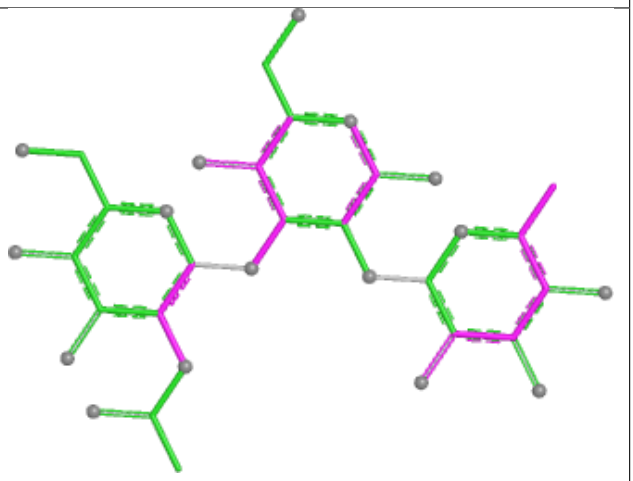


Rings

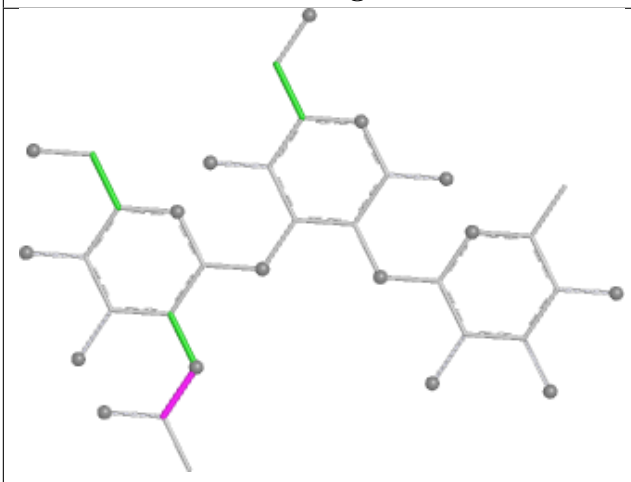
Oligosaccharide Chain I



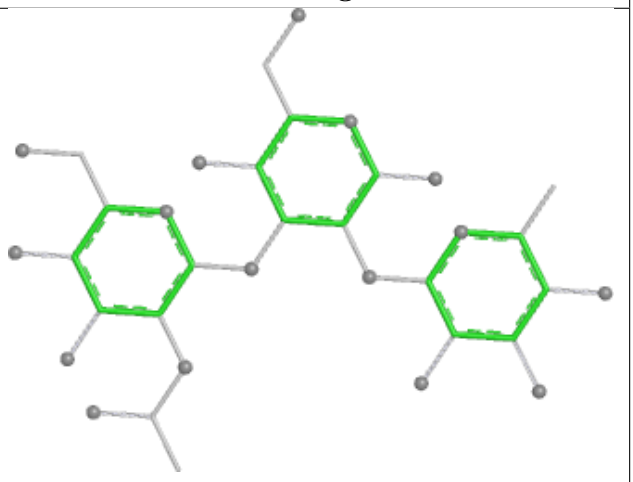
Bond lengths



Bond angles

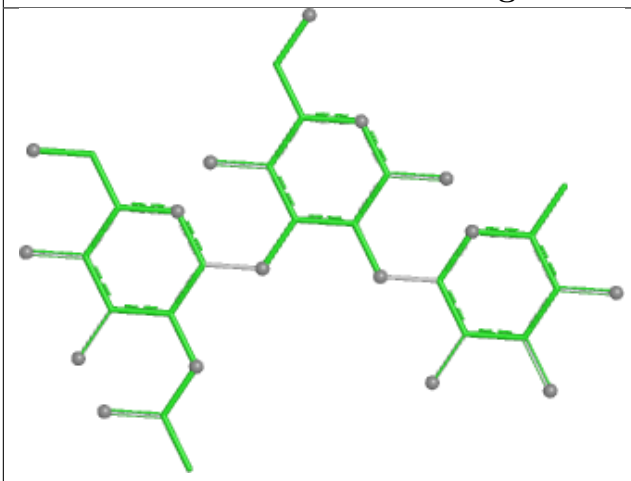


Torsions

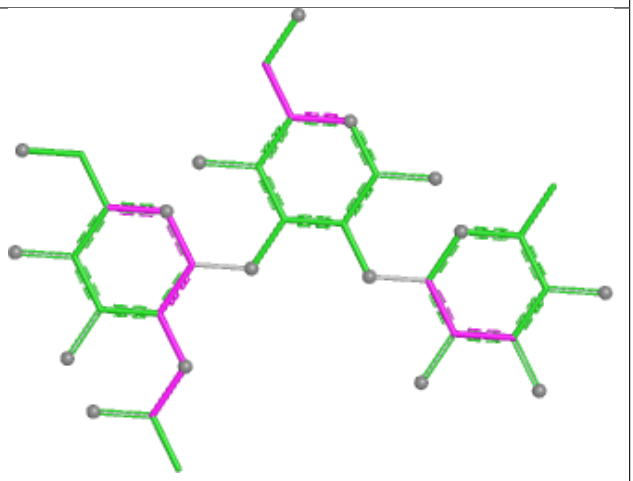


Rings

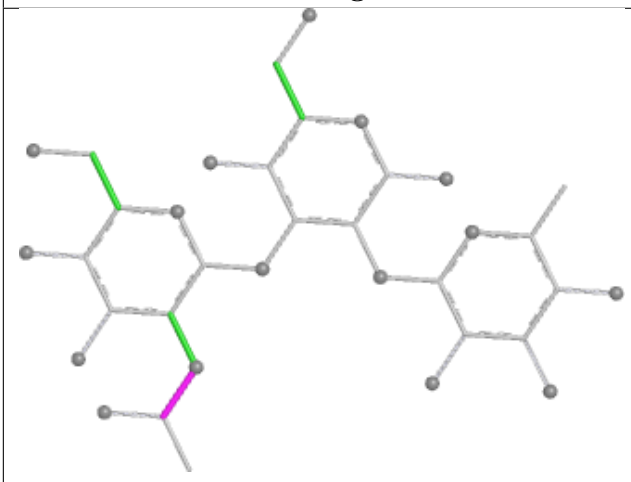
Oligosaccharide Chain J



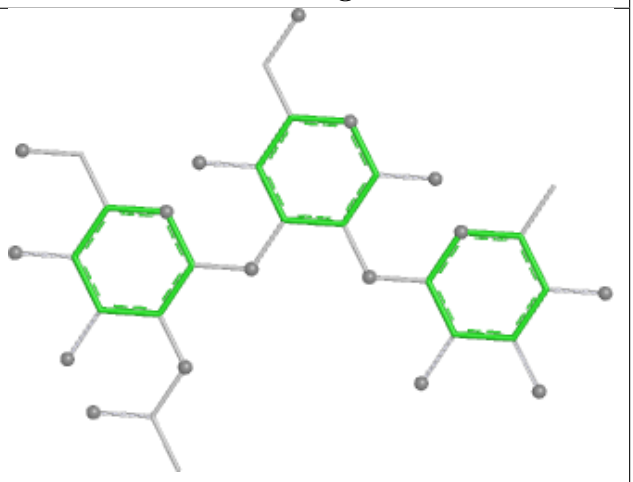
Bond lengths



Bond angles

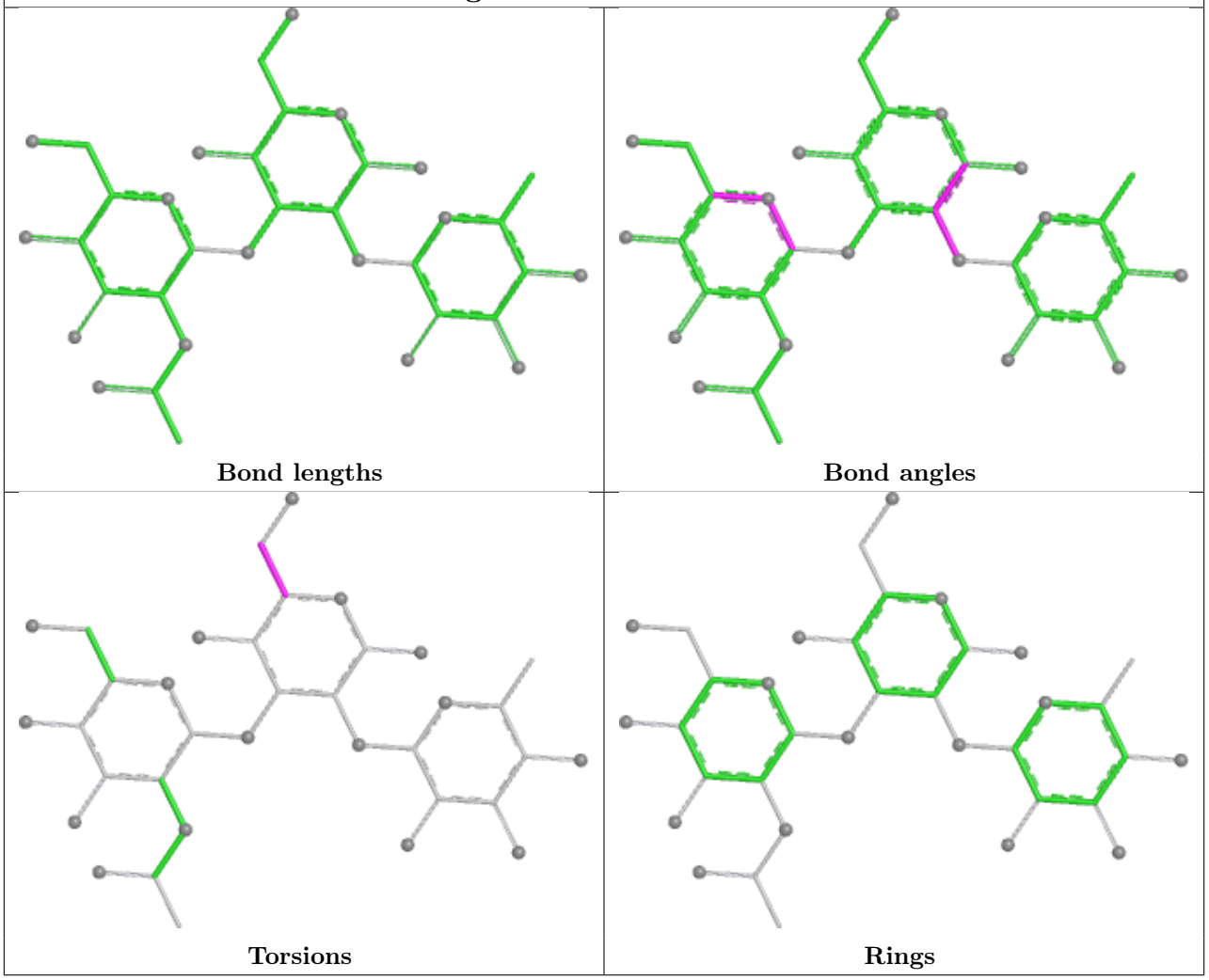


Torsions



Rings

Oligosaccharide Chain K



5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 1 is monoatomic - leaving 3 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	$\#\|Z\| > 2$
3	FUC	B	930	-	11,11,11	0.56	0	16,16,16	0.93	0
3	FUC	B	920	-	11,11,11	0.63	0	16,16,16	1.08	2 (12%)
3	FUC	A	930	-	11,11,11	0.63	0	16,16,16	0.99	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
3	FUC	B	930	-	-	-	0/1/1/1
3	FUC	B	920	-	-	-	0/1/1/1
3	FUC	A	930	-	-	-	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	920	FUC	C1-O5-C5	2.48	118.23	114.37
3	B	920	FUC	O5-C5-C6	2.07	111.33	106.74

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{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	313/315 (99%)	-0.44	0	100	100	9, 16, 28, 35	0
1	B	313/315 (99%)	-0.45	0	100	100	10, 16, 28, 37	0
All	All	626/630 (99%)	-0.44	0	100	100	9, 16, 28, 37	0

There are no RSRZ outliers to report.

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

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
1	CSD	B	244	8/9	0.95	0.07	17,18,23,29	0
1	CSD	A	244	8/9	0.96	0.07	16,17,21,28	0

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
2	A2G	F	3	14/15	0.65	0.39	41,53,60,61	0
2	A2G	H	3	14/15	0.75	0.22	42,49,53,53	0
2	GAL	E	1	12/12	0.77	0.21	30,40,42,44	0
2	A2G	K	3	14/15	0.78	0.18	42,52,57,57	0
2	GAL	G	1	12/12	0.80	0.20	27,45,48,55	0

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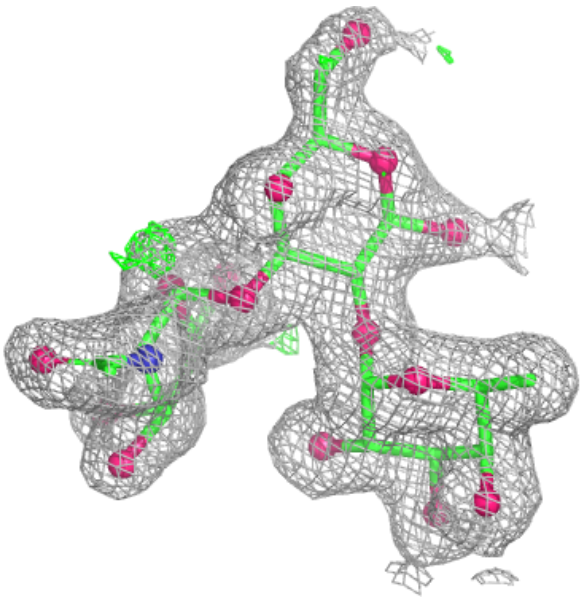
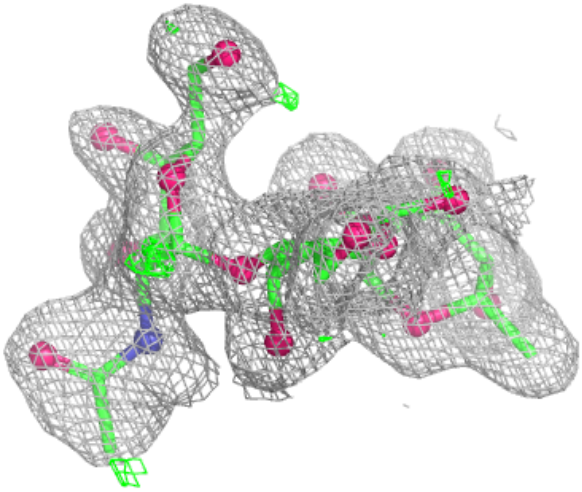
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	A2G	I	3	14/15	0.81	0.22	41,45,55,59	0
2	A2G	C	3	14/15	0.81	0.19	34,37,40,43	0
2	GAL	F	1	12/12	0.82	0.25	28,41,46,46	0
2	GAL	D	1	12/12	0.83	0.19	22,36,42,44	0
2	A2G	E	3	14/15	0.83	0.26	42,47,52,53	0
2	GAL	K	1	12/12	0.84	0.18	30,48,52,53	0
2	GAL	J	1	12/12	0.84	0.22	24,37,44,44	0
2	A2G	J	3	14/15	0.85	0.25	41,43,45,45	0
2	A2G	G	3	14/15	0.85	0.14	32,38,43,45	0
2	A2G	D	3	14/15	0.85	0.18	40,42,48,50	0
2	GAL	I	1	12/12	0.88	0.15	27,32,34,35	0
2	GAL	H	1	12/12	0.88	0.12	30,35,41,45	0
2	GAL	C	1	12/12	0.90	0.16	22,34,37,38	0
2	FUC	E	2	10/11	0.91	0.11	18,21,24,24	0
2	FUC	I	2	10/11	0.92	0.08	17,20,23,24	0
2	FUC	J	2	10/11	0.94	0.09	15,17,21,22	0
2	FUC	K	2	10/11	0.94	0.07	16,19,24,26	0
2	FUC	H	2	10/11	0.94	0.08	20,21,24,24	0
2	FUC	G	2	10/11	0.96	0.08	15,16,20,20	0
2	FUC	D	2	10/11	0.96	0.06	15,17,18,19	0
2	FUC	C	2	10/11	0.97	0.06	14,16,17,17	0
2	FUC	F	2	10/11	0.97	0.08	15,17,21,22	0

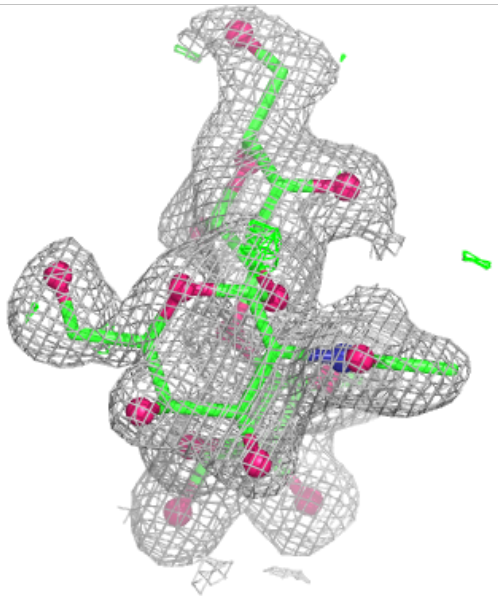
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain C:

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

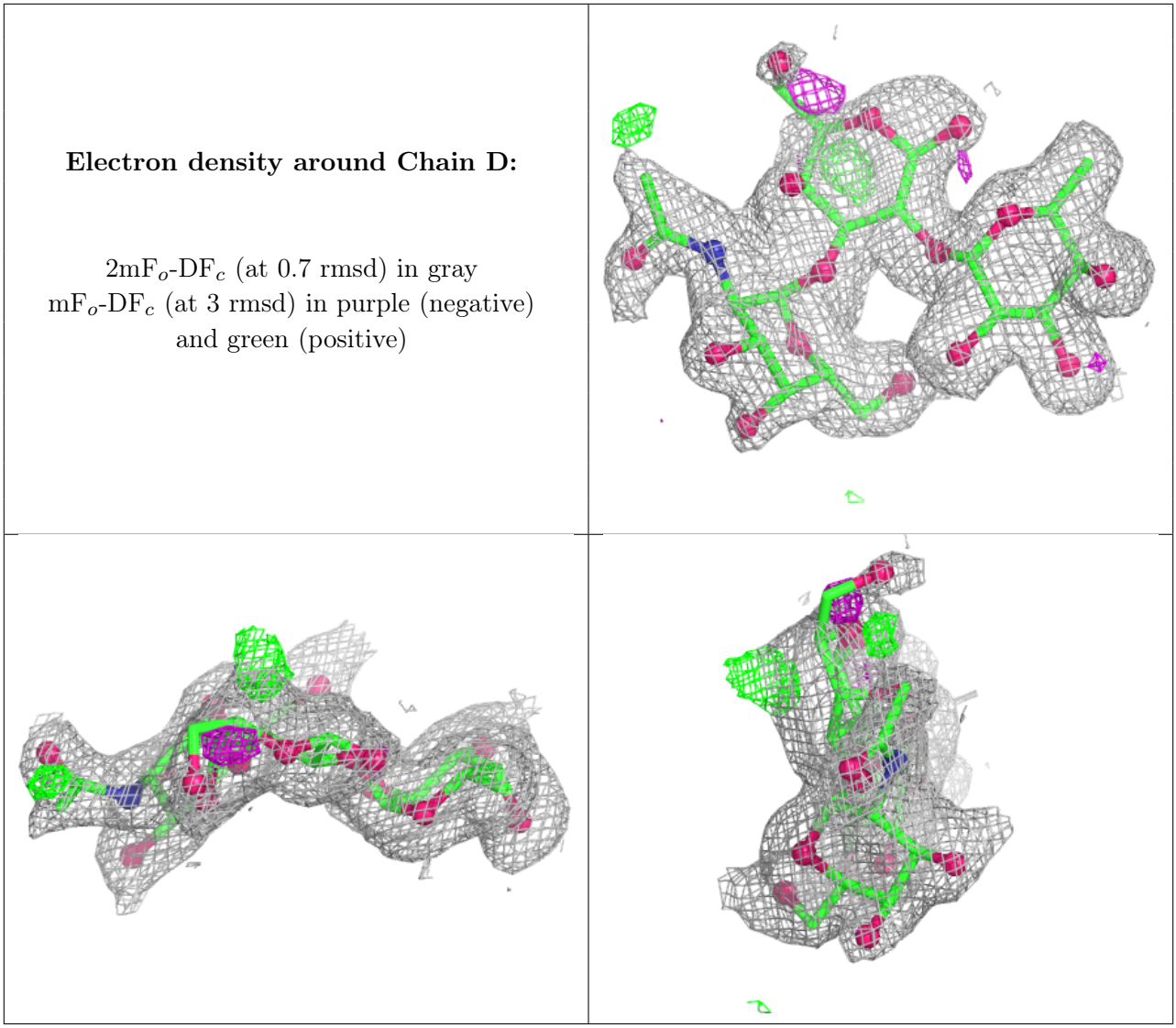






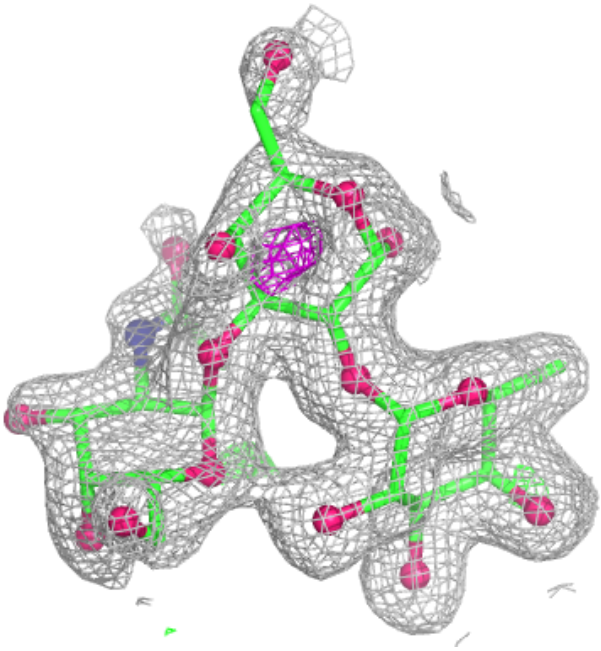
Electron density around Chain D:

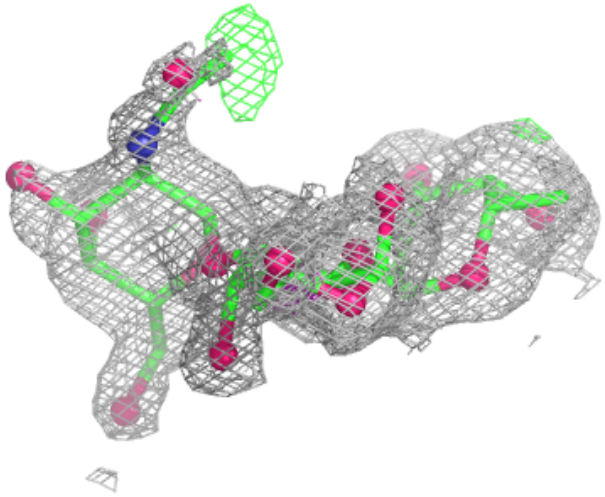
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

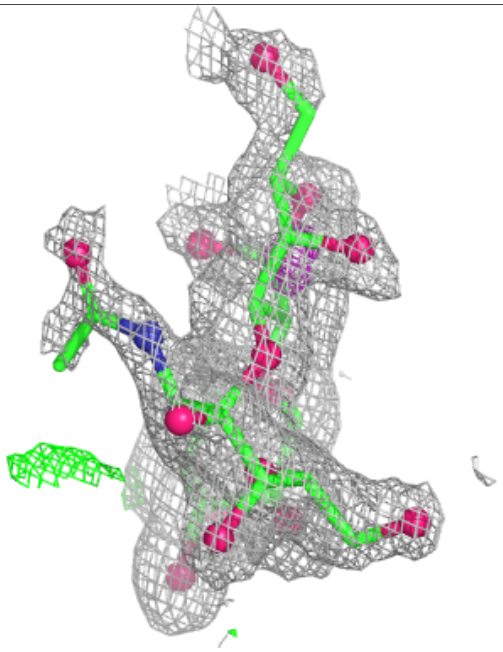


Electron density around Chain E:

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

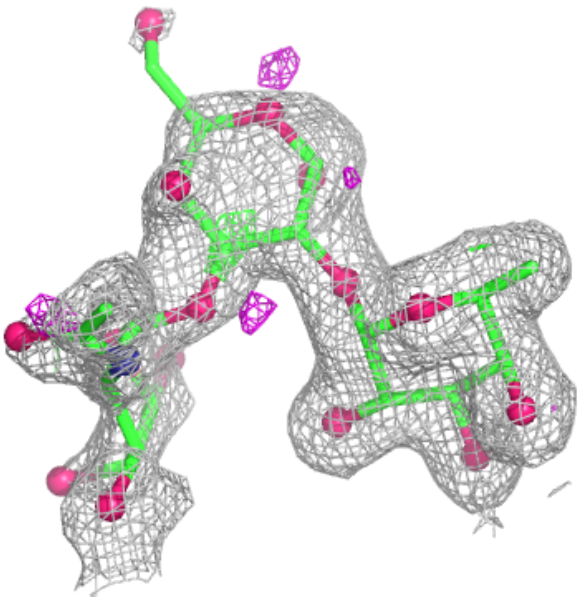


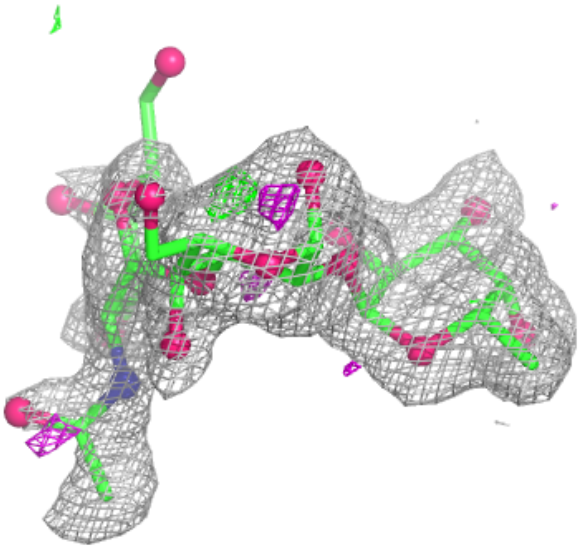


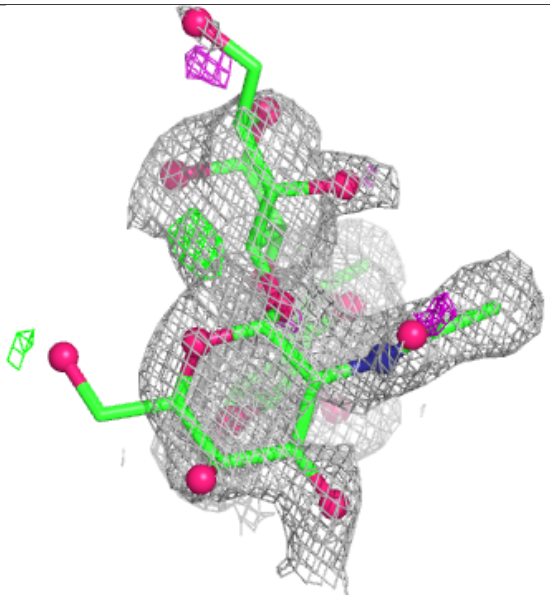


Electron density around Chain F:

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

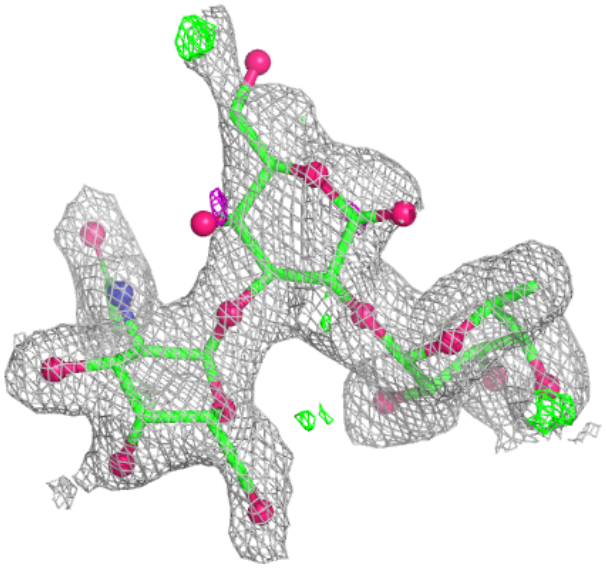


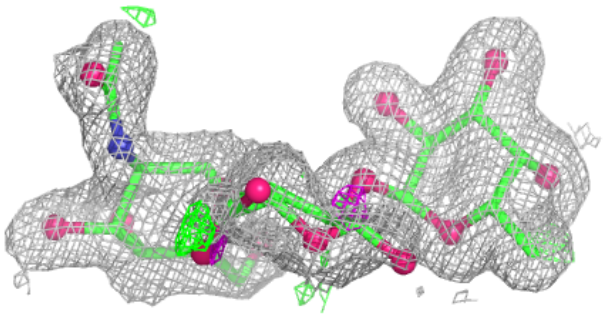


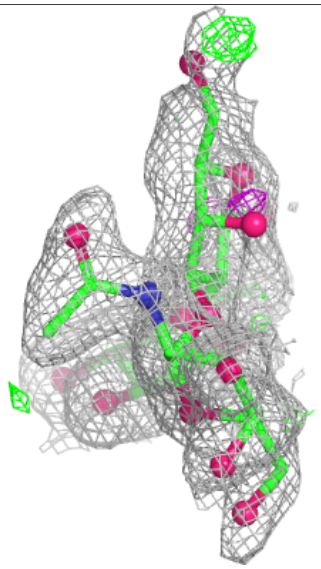


Electron density around Chain G:

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

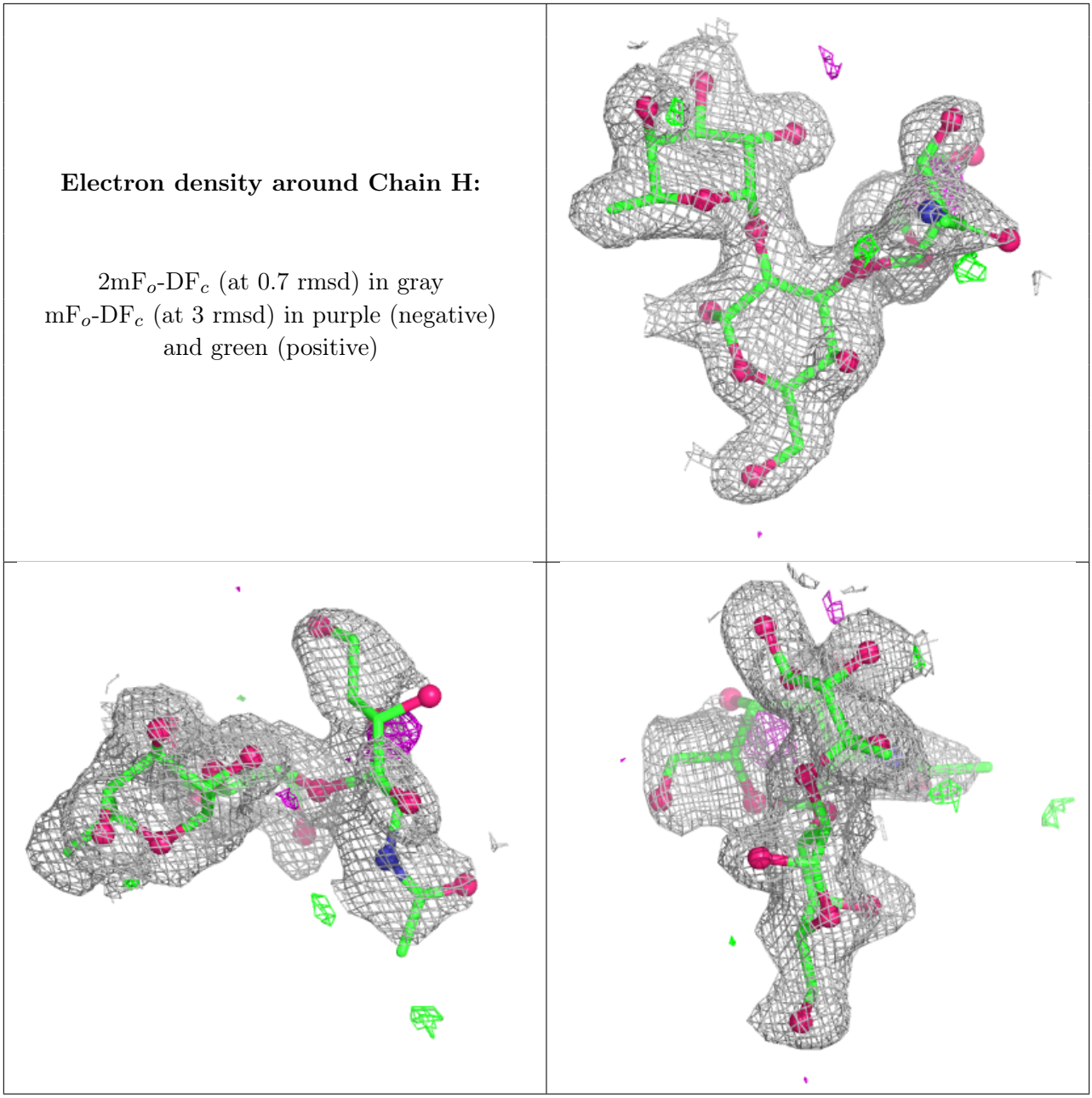






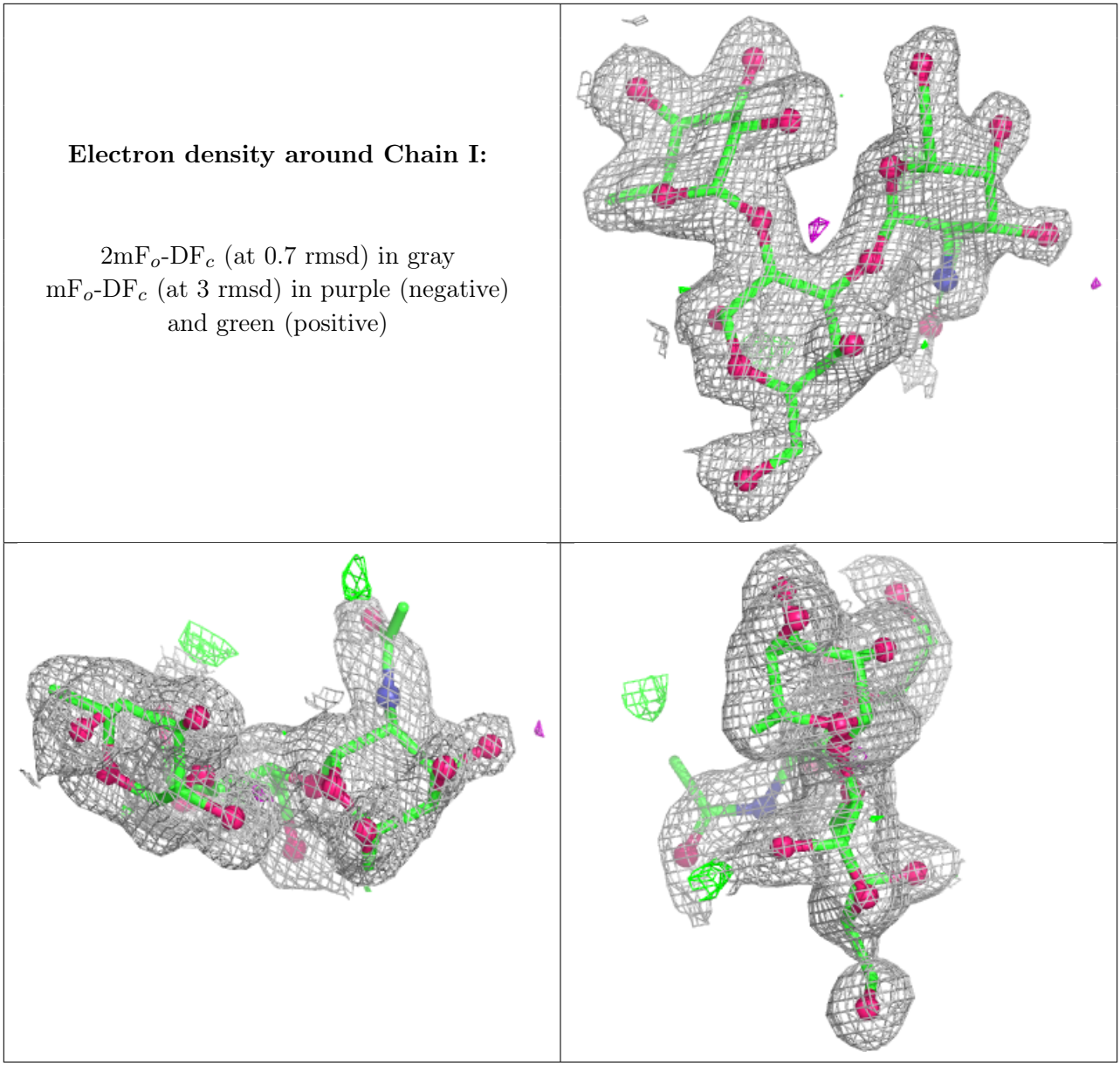
Electron density around Chain H:

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



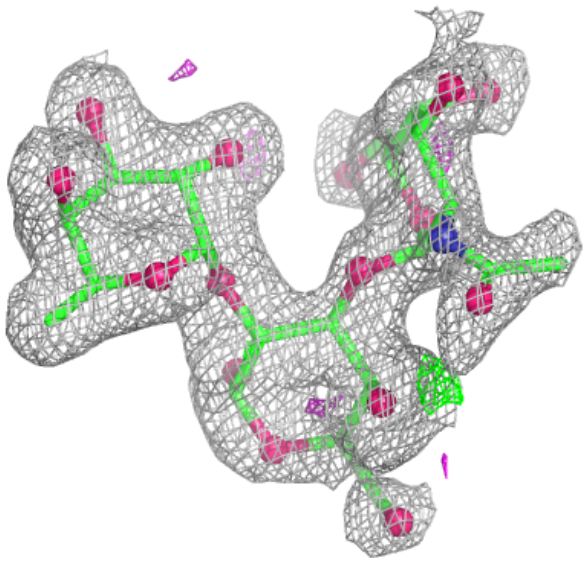
Electron density around Chain I:

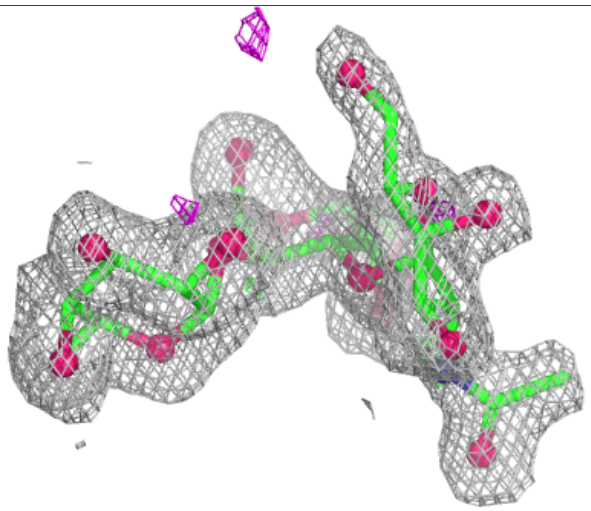
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

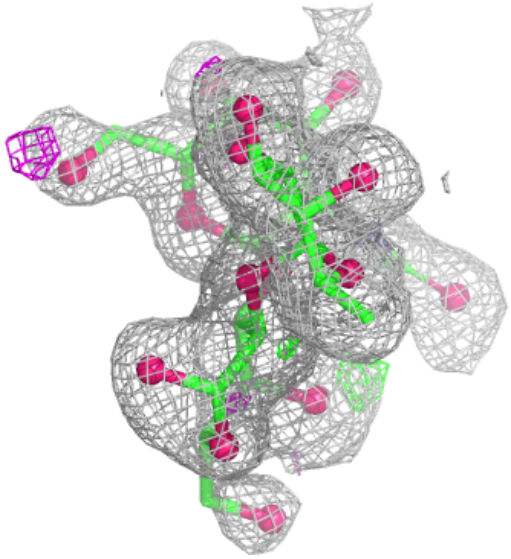


Electron density around Chain J:

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

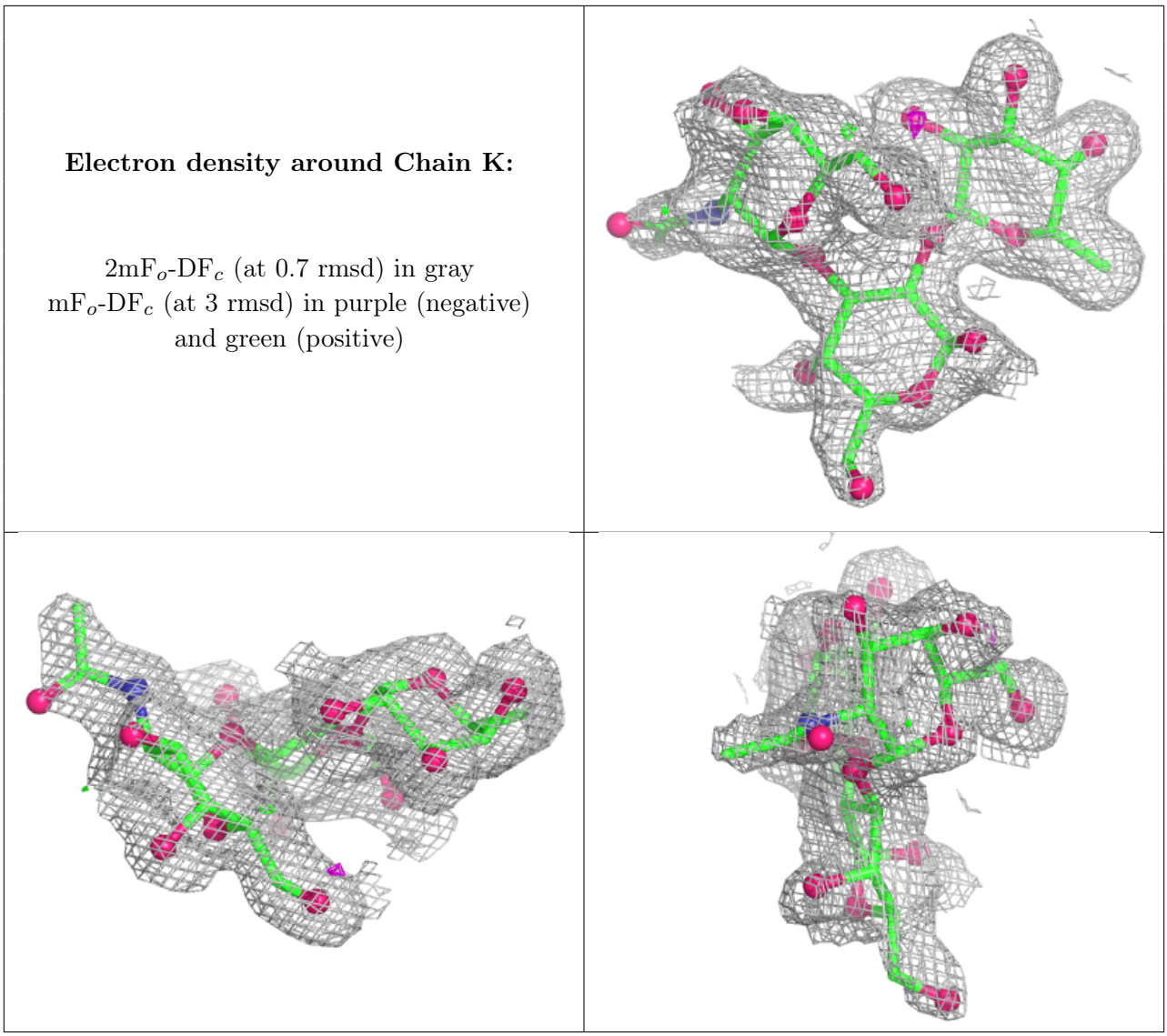






Electron density around Chain K:

$2mF_o$-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
3	FUC	B	930	11/11	0.95	0.06	13,16,18,19	0
3	FUC	A	930	11/11	0.96	0.07	14,16,18,20	0
3	FUC	B	920	11/11	0.97	0.07	17,18,19,20	0
4	CL	A	1000	1/1	0.98	0.07	35,35,35,35	0

6.5 Other polymers (i)

There are no such residues in this entry.