Full wwPDB X-ray Structure Validation Report ⓘ

Aug 6, 2020 – 08:47 PM BST

PDB ID	:	2A0Z
Title	:	The molecular structure of toll-like receptor 3 ligand binding domain
Authors	:	Bell, J.K.; Botos, I.; Hall, P.R.; Askins, J.; Shiloach, J.; Segal, D.M.; Davies, D.R.
Deposited on	:	2005-06-17
Resolution	:	2.40 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 ①) were used in the production of this report:

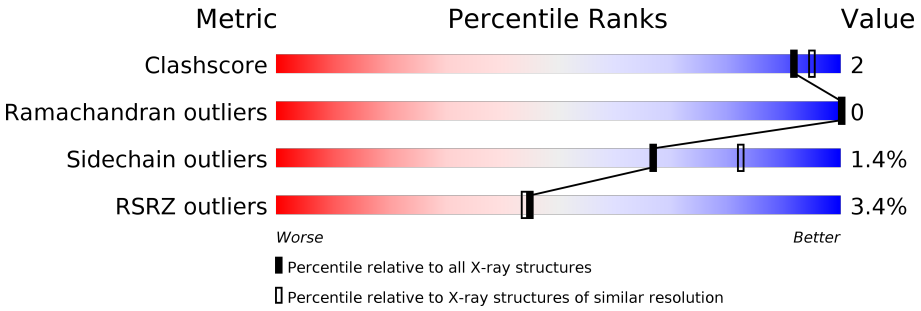
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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 2.40 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))
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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	705	3%, 92%, 5%
2	B	2	100%
2	C	2	50%, 50%
2	D	2	50%, 50%
2	F	2	100%
2	G	2	100%
3	E	3	100%

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Mol	Chain	Length	Quality of chain
4	H	3	33% 33% 33%
4	J	3	33% 67%
5	I	5	100%
6	K	2	50% 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	NAG	B	2	-	-	-	X
2	NAG	C	2	-	-	-	X
2	NAG	G	2	-	-	-	X

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 6183 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 Toll-like receptor 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	671	Total	C	N	O	S	0	6	0
			5420	3459	919	1023	19			

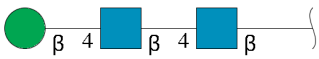
There are 23 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	704	GLU	-	SEE REMARK 999	UNP O15455
A	705	ASN	-	SEE REMARK 999	UNP O15455
A	706	LEU	-	SEE REMARK 999	UNP O15455
A	707	TYR	-	SEE REMARK 999	UNP O15455
A	708	PHE	-	SEE REMARK 999	UNP O15455
A	709	GLN	-	SEE REMARK 999	UNP O15455
A	710	GLY	-	SEE REMARK 999	UNP O15455
A	711	ASP	-	SEE REMARK 999	UNP O15455
A	712	TYR	-	SEE REMARK 999	UNP O15455
A	713	LYS	-	SEE REMARK 999	UNP O15455
A	714	ASP	-	SEE REMARK 999	UNP O15455
A	715	ASP	-	SEE REMARK 999	UNP O15455
A	716	ASP	-	SEE REMARK 999	UNP O15455
A	717	ASP	-	SEE REMARK 999	UNP O15455
A	718	LYS	-	SEE REMARK 999	UNP O15455
A	719	GLY	-	expression tag	UNP O15455
A	720	SER	-	expression tag	UNP O15455
A	721	HIS	-	expression tag	UNP O15455
A	722	HIS	-	expression tag	UNP O15455
A	723	HIS	-	expression tag	UNP O15455
A	724	HIS	-	expression tag	UNP O15455
A	725	HIS	-	expression tag	UNP O15455
A	726	HIS	-	expression tag	UNP O15455

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

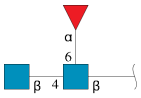
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	C	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	D	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	F	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	G	2	Total	C	N	O	0	0	0
			28	16	2	10			

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



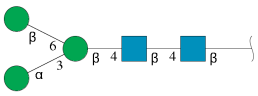
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	E	3	Total	C	N	O	0	0	0
			39	22	2	15			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	H	3	Total	C	N	O	0	0	0
			37	22	2	13			
4	J	3	Total	C	N	O	0	0	0
			38	22	2	14			

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

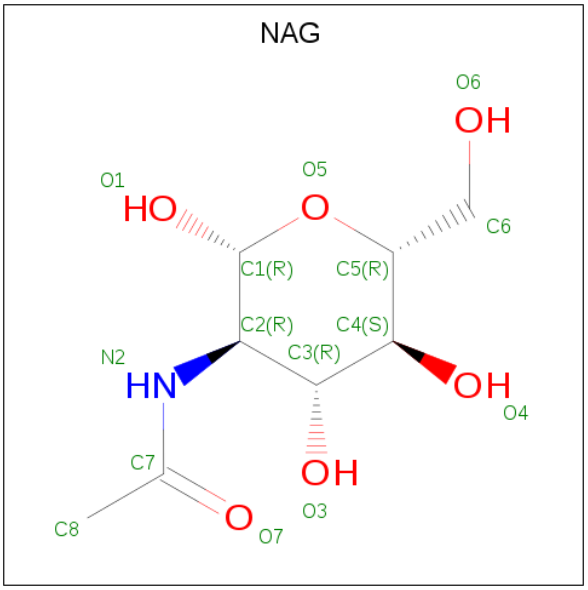


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
5	I	5	61	34	2	25	0	0	0

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

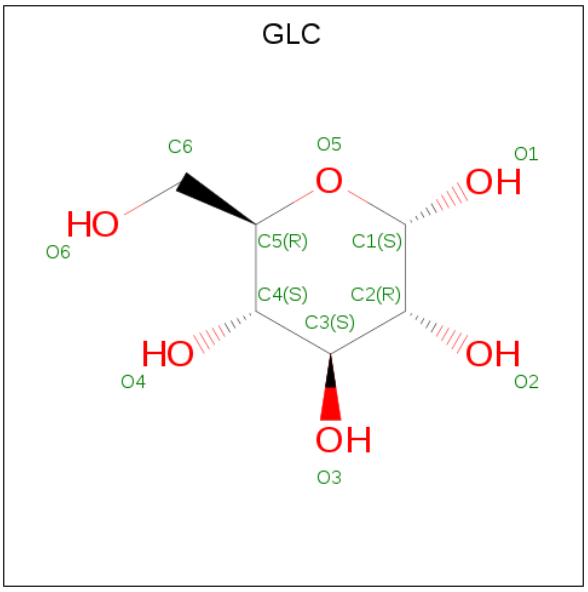
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
6	K	2	28	16	2	10	0	0	0

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



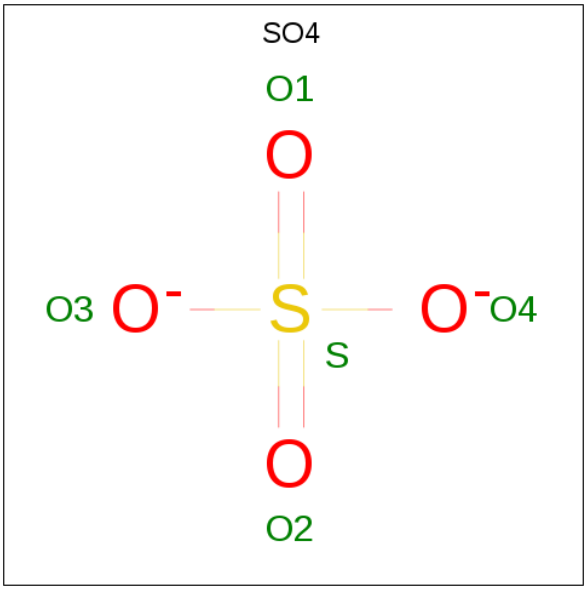
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
7	A	1	14	8	1	5	0	0

- Molecule 8 is alpha-D-glucopyranose (three-letter code: GLC) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C O 12 6 6	0	0
8	A	1	Total C O 12 6 6	0	0

- Molecule 9 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	1	Total O S 5 4 1	0	0
9	A	1	Total O S 5 4 1	0	0

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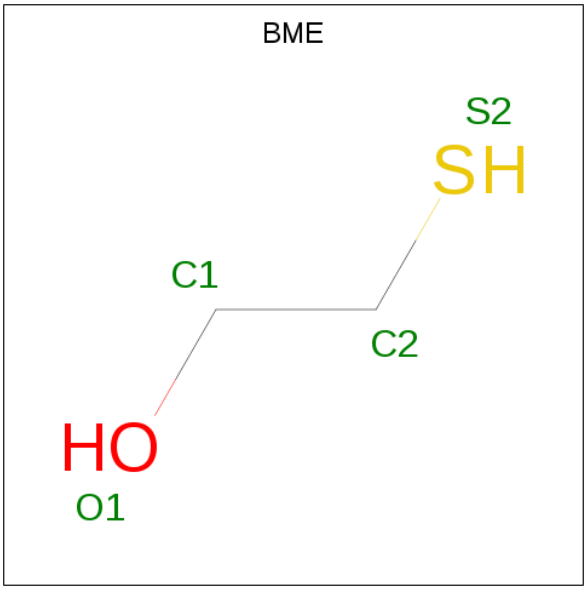
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	1	Total O S 5 4 1	0	0

- Molecule 10 is BETA-MERCAPTOETHANOL (three-letter code: BME) (formula: C_2H_6OS).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	1	Total C O S 4 2 1 1	0	0

- Molecule 11 is water.

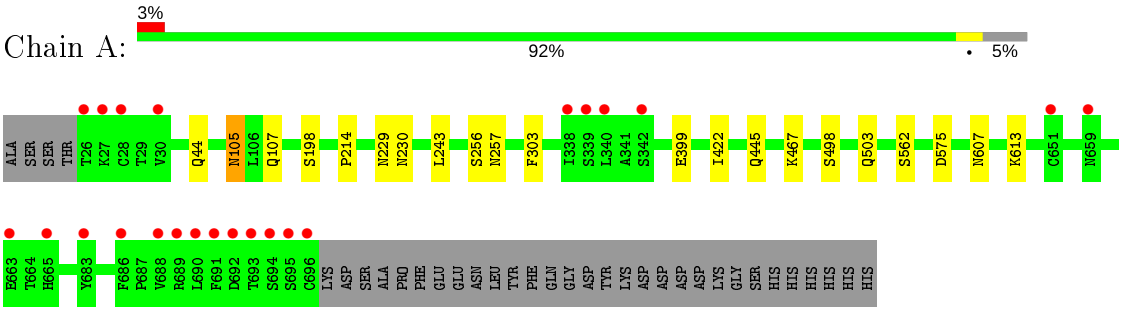
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	363	Total O 363 363	0	0

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.

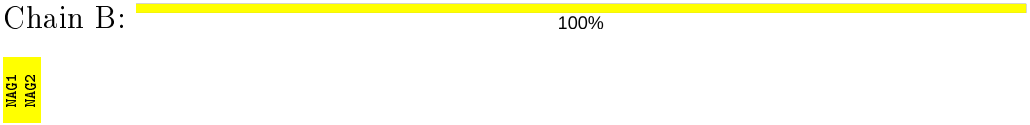
• Molecule 1: Toll-like receptor 3

Chain A:



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

Chain B:



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

Chain C:

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

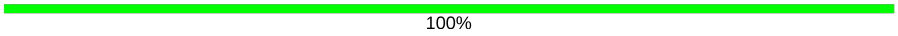
Chain D:

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

Chain F:

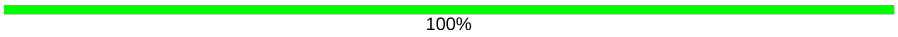
• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:



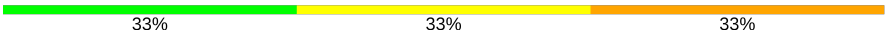
• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:



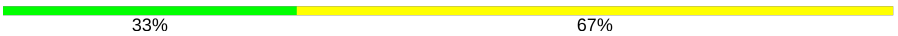
• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:



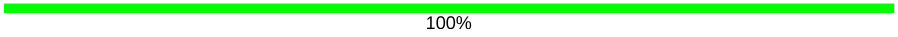
• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:



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

Chain I:



• Molecule 6: 2-acetamido-2-deoxy-alpha-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	141.60Å 160.79Å 122.54Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.40 48.75 – 2.42	Depositor EDS
% Data completeness (in resolution range)	91.1 (50.00-2.40) 93.6 (48.75-2.42)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.29 (at 2.42Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.206 , 0.232 0.202 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	38.7	Xtriage
Anisotropy	0.385	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 51.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	6183	wwPDB-VP
Average B, all atoms (Å^2)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.44% 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: BMA, NAG, BME, GLC, NDG, FUC, SO4, MAN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.71	1/5533 (0.0%)	0.73	0/7511

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	198	SER	CB-OG	7.28	1.51	1.42

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	5420	0	5399	15	1
2	B	28	0	25	1	0
2	C	28	0	25	1	0
2	D	28	0	25	1	0
2	F	28	0	25	0	0
2	G	28	0	25	0	0
3	E	39	0	34	0	0
4	H	37	0	32	1	0
4	J	38	0	34	2	0
5	I	61	0	52	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	K	28	0	24	0	0
7	A	14	0	13	0	0
8	A	24	0	24	0	0
9	A	15	0	0	0	0
10	A	4	0	5	0	0
11	A	363	0	0	1	0
All	All	6183	0	5742	19	1

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 (19) 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:422:ILE:H	1:A:445:GLN:HE22	1.23	0.86
4:J:1:NAG:H61	4:J:2:NAG:H82	1.72	0.70
1:A:230[A]:ASN:ND2	1:A:257:ASN:HD22	1.95	0.64
1:A:422:ILE:N	1:A:445:GLN:HE22	1.98	0.56
1:A:230[A]:ASN:HD22	1:A:257:ASN:HD22	1.52	0.55
1:A:230[A]:ASN:HD22	1:A:257:ASN:ND2	2.06	0.54
1:A:399:GLU:OE2	4:H:1:NAG:H83	2.08	0.52
1:A:422:ILE:H	1:A:445:GLN:NE2	2.02	0.52
1:A:229[A]:ASN:HD22	1:A:256:SER:H	1.57	0.51
1:A:562:SER:HB3	11:A:6550:HOH:O	2.11	0.51
1:A:229[A]:ASN:ND2	1:A:256:SER:H	2.09	0.51
4:J:1:NAG:H61	4:J:2:NAG:C8	2.42	0.47
1:A:44:GLN:OE1	2:C:2:NAG:H62	2.16	0.46
2:D:1:NAG:H82	2:D:1:NAG:H3	1.99	0.45
1:A:105:ASN:HD22	1:A:107:GLN:H	1.65	0.44
1:A:105:ASN:ND2	1:A:107:GLN:H	2.16	0.43
2:B:1:NAG:H61	2:B:2:NAG:N2	2.33	0.42
1:A:105:ASN:HD22	1:A:105:ASN:C	2.23	0.42
1:A:105:ASN:HD21	1:A:107:GLN:HG2	1.86	0.41

All (1) 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)
1:A:575:ASP:OD2	1:A:575:ASP:OD2[4_555]	2.15	0.05

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	674/705 (96%)	634 (94%)	40 (6%)	0	100 100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	631/656 (96%)	622 (99%)	9 (1%)	67 82

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	105	ASN
1	A	214	PRO
1	A	243	LEU
1	A	303	PHE
1	A	467	LYS
1	A	498	SER
1	A	503	GLN
1	A	607	ASN
1	A	613	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	62	GLN
1	A	105	ASN
1	A	107	GLN
1	A	229[A]	ASN
1	A	309	ASN
1	A	311	GLN
1	A	445	GLN
1	A	494	ASN
1	A	659	ASN
1	A	678	ASN

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)

26 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	B	1	1,2	14,14,15	0.69	0	17,19,21	0.53	0
2	NAG	B	2	2	14,14,15	0.56	0	17,19,21	0.67	0
2	NAG	C	1	1,2	14,14,15	0.56	0	17,19,21	0.64	0
2	NAG	C	2	2	14,14,15	0.66	0	17,19,21	0.48	0
2	NAG	D	1	1,2	14,14,15	0.59	0	17,19,21	0.56	0
2	NAG	D	2	2	14,14,15	0.58	0	17,19,21	0.63	0
3	NAG	E	1	1,3	14,14,15	0.47	0	17,19,21	0.67	0
3	NAG	E	2	3	14,14,15	0.52	0	17,19,21	0.67	0
3	BMA	E	3	3	11,11,12	0.56	0	15,15,17	0.23	0
2	NAG	F	1	1,2	14,14,15	0.59	0	17,19,21	0.64	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	NAG	F	2	2	14,14,15	0.59	0	17,19,21	0.65	0
2	NAG	G	1	1,2	14,14,15	0.52	0	17,19,21	0.60	0
2	NAG	G	2	2	14,14,15	0.57	0	17,19,21	0.57	0
4	NAG	H	1	1,9,4	13,13,15	1.11	1 (7%)	16,17,21	0.92	0
4	NAG	H	2	4	14,14,15	0.58	0	17,19,21	0.69	1 (5%)
4	FUC	H	3	4	10,10,11	0.64	0	14,14,16	0.35	0
5	NAG	I	1	1,5	14,14,15	0.51	0	17,19,21	0.63	0
5	NAG	I	2	5	14,14,15	0.55	0	17,19,21	0.63	0
5	BMA	I	3	5	11,11,12	0.64	0	15,15,17	0.50	0
5	MAN	I	4	5	11,11,12	0.70	0	15,15,17	0.59	0
5	BMA	I	5	5	11,11,12	0.66	0	15,15,17	0.45	0
4	NAG	J	1	1,4	14,14,15	0.60	0	17,19,21	0.74	0
4	NAG	J	2	4	14,14,15	0.70	0	17,19,21	0.78	0
4	FUC	J	3	4	10,10,11	0.69	0	14,14,16	0.40	0
6	NAG	K	1	1,6	14,14,15	1.04	1 (7%)	17,19,21	0.69	0
6	NDG	K	2	6	14,14,15	0.66	0	17,19,21	0.65	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	B	1	1,2	-	3/6/23/26	0/1/1/1
2	NAG	B	2	2	-	4/6/23/26	0/1/1/1
2	NAG	C	1	1,2	-	4/6/23/26	0/1/1/1
2	NAG	C	2	2	-	3/6/23/26	0/1/1/1
2	NAG	D	1	1,2	-	5/6/23/26	0/1/1/1
2	NAG	D	2	2	-	4/6/23/26	0/1/1/1
3	NAG	E	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	E	2	3	-	2/6/23/26	0/1/1/1
3	BMA	E	3	3	-	0/2/19/22	0/1/1/1
2	NAG	F	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	F	2	2	-	4/6/23/26	0/1/1/1
2	NAG	G	1	1,2	-	4/6/23/26	0/1/1/1
2	NAG	G	2	2	-	3/6/23/26	0/1/1/1
4	NAG	H	1	1,9,4	-	2/6/19/26	0/1/1/1
4	NAG	H	2	4	-	2/6/23/26	0/1/1/1
4	FUC	H	3	4	-	-	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	I	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	I	2	5	-	0/6/23/26	0/1/1/1
5	BMA	I	3	5	-	2/2/19/22	0/1/1/1
5	MAN	I	4	5	-	2/2/19/22	1/1/1/1
5	BMA	I	5	5	-	0/2/19/22	0/1/1/1
4	NAG	J	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	J	2	4	-	4/6/23/26	0/1/1/1
4	FUC	J	3	4	-	-	0/1/1/1
6	NAG	K	1	1,6	-	3/6/23/26	0/1/1/1
6	NDG	K	2	6	-	4/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	1	NAG	C1-C2	3.34	1.55	1.51
6	K	1	NAG	C1-C2	2.03	1.55	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	H	2	NAG	C2-N2-C7	-2.07	119.95	122.90

There are no chirality outliers.

All (61) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	2	NAG	C8-C7-N2-C2
2	B	2	NAG	O7-C7-N2-C2
3	E	2	NAG	C8-C7-N2-C2
3	E	2	NAG	O7-C7-N2-C2
2	C	2	NAG	C3-C2-N2-C7
2	C	2	NAG	C8-C7-N2-C2
2	C	2	NAG	O7-C7-N2-C2
4	H	2	NAG	C8-C7-N2-C2
4	H	2	NAG	O7-C7-N2-C2
3	E	1	NAG	C8-C7-N2-C2
3	E	1	NAG	O7-C7-N2-C2
2	G	1	NAG	C8-C7-N2-C2
2	G	1	NAG	O7-C7-N2-C2
2	G	2	NAG	C8-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
2	G	2	NAG	O7-C7-N2-C2
2	C	1	NAG	C8-C7-N2-C2
2	C	1	NAG	O7-C7-N2-C2
2	D	1	NAG	C8-C7-N2-C2
2	D	1	NAG	O7-C7-N2-C2
2	B	1	NAG	C3-C2-N2-C7
2	B	1	NAG	C8-C7-N2-C2
2	B	1	NAG	O7-C7-N2-C2
6	K	2	NDG	C8-C7-N2-C2
6	K	2	NDG	O7-C7-N2-C2
6	K	1	NAG	C3-C2-N2-C7
6	K	1	NAG	C8-C7-N2-C2
6	K	1	NAG	O7-C7-N2-C2
2	F	2	NAG	C8-C7-N2-C2
2	F	2	NAG	O7-C7-N2-C2
2	D	2	NAG	C8-C7-N2-C2
2	D	2	NAG	O7-C7-N2-C2
4	H	1	NAG	C8-C7-N2-C2
4	H	1	NAG	O7-C7-N2-C2
4	J	1	NAG	C8-C7-N2-C2
2	G	1	NAG	O5-C5-C6-O6
5	I	3	BMA	O5-C5-C6-O6
4	J	2	NAG	C8-C7-N2-C2
2	G	1	NAG	C4-C5-C6-O6
2	D	1	NAG	O5-C5-C6-O6
2	D	2	NAG	O5-C5-C6-O6
5	I	3	BMA	C4-C5-C6-O6
4	J	2	NAG	O7-C7-N2-C2
4	J	1	NAG	O7-C7-N2-C2
2	B	2	NAG	C4-C5-C6-O6
3	E	1	NAG	C4-C5-C6-O6
2	B	2	NAG	O5-C5-C6-O6
2	D	2	NAG	C4-C5-C6-O6
2	D	1	NAG	C4-C5-C6-O6
3	E	1	NAG	O5-C5-C6-O6
5	I	4	MAN	C4-C5-C6-O6
2	F	2	NAG	C4-C5-C6-O6
2	C	1	NAG	C4-C5-C6-O6
6	K	2	NDG	C4-C5-C6-O6
2	F	2	NAG	O5-C5-C6-O6
6	K	2	NDG	O5-C5-C6-O6
4	J	2	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	C	1	NAG	O5-C5-C6-O6
2	D	1	NAG	C3-C2-N2-C7
5	I	4	MAN	O5-C5-C6-O6
2	G	2	NAG	O5-C5-C6-O6
4	J	2	NAG	O5-C5-C6-O6

All (1) ring outliers are listed below:

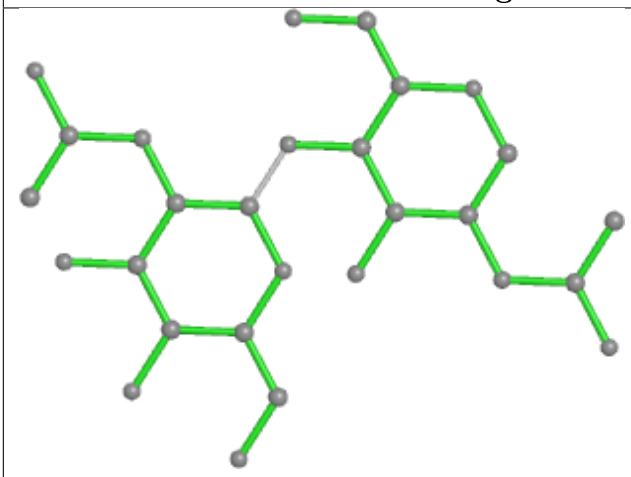
Mol	Chain	Res	Type	Atoms
5	I	4	MAN	C1-C2-C3-C4-C5-O5

7 monomers are involved in 6 short contacts:

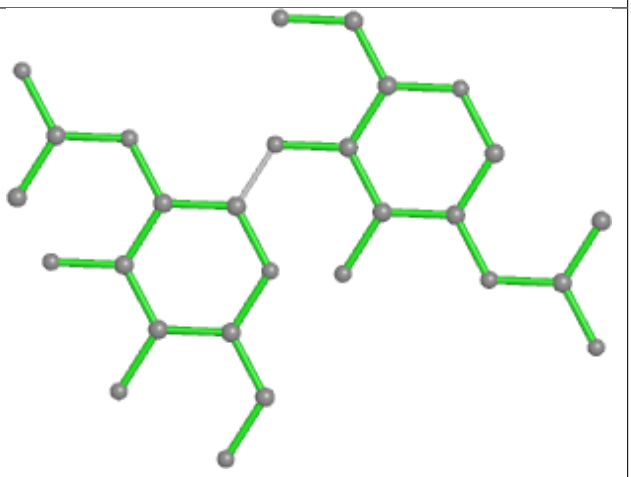
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	2	NAG	1	0
2	C	2	NAG	1	0
4	J	2	NAG	2	0
2	D	1	NAG	1	0
2	B	1	NAG	1	0
4	J	1	NAG	2	0
4	H	1	NAG	1	0

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

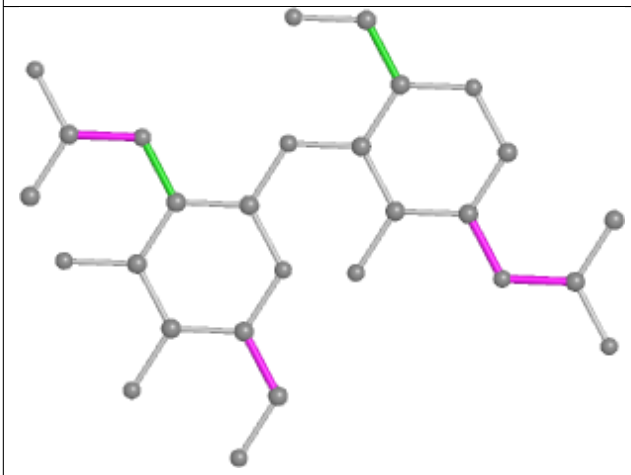
Oligosaccharide Chain B



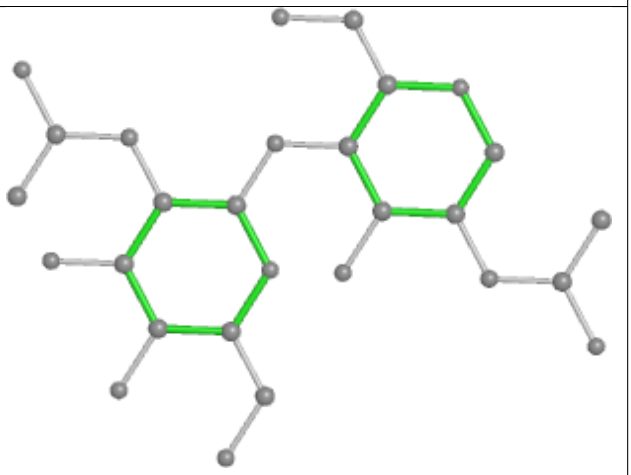
Bond lengths



Bond angles

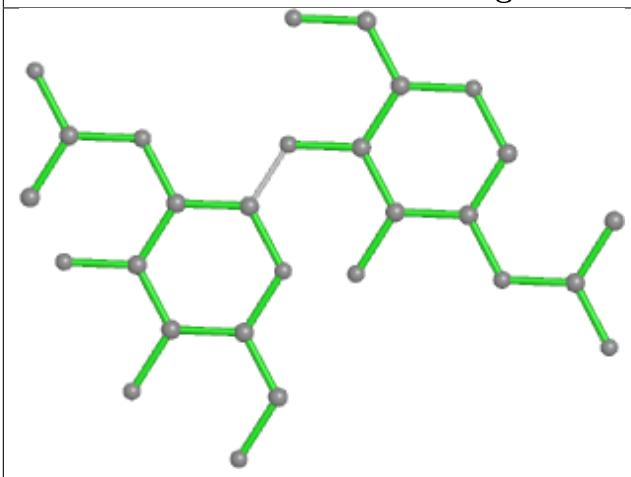


Torsions

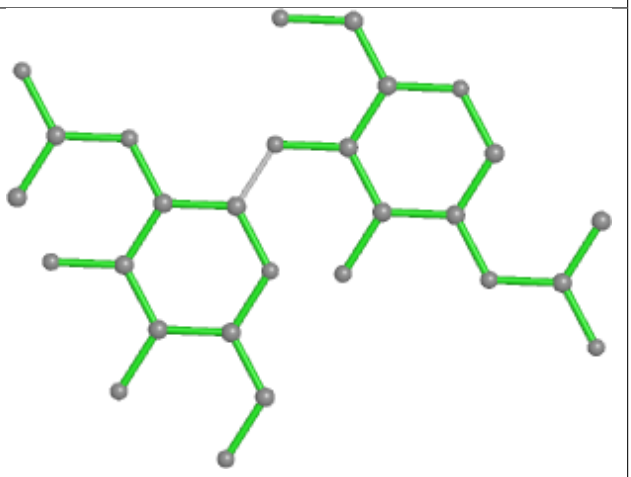


Rings

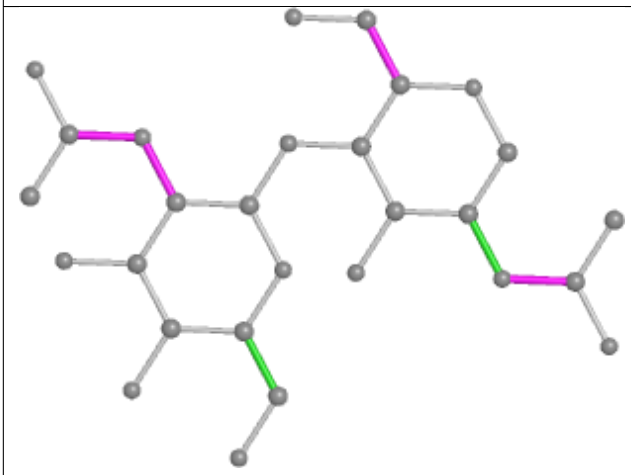
Oligosaccharide Chain C



Bond lengths



Bond angles



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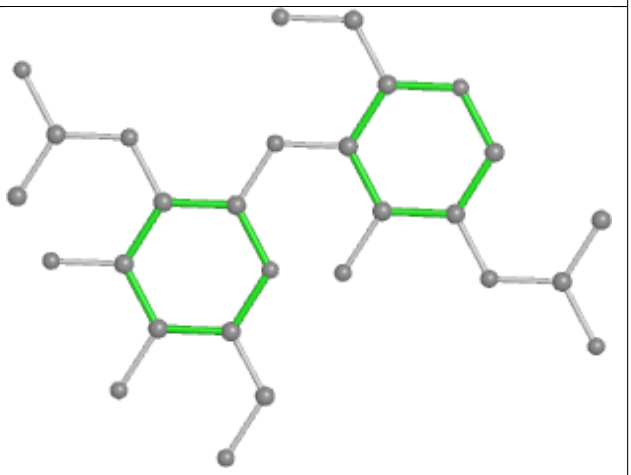
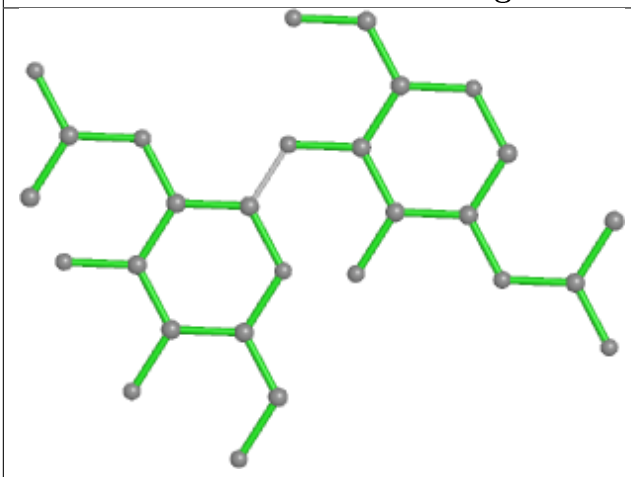
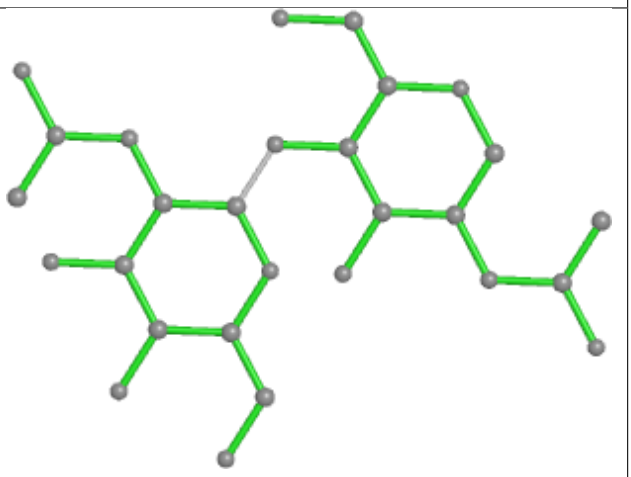


Rings

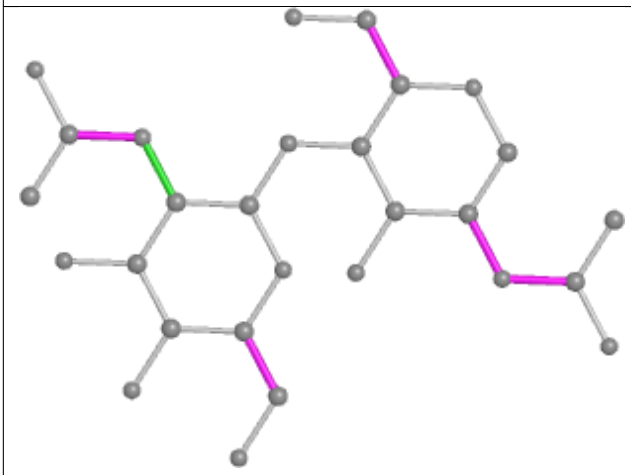
Oligosaccharide Chain D



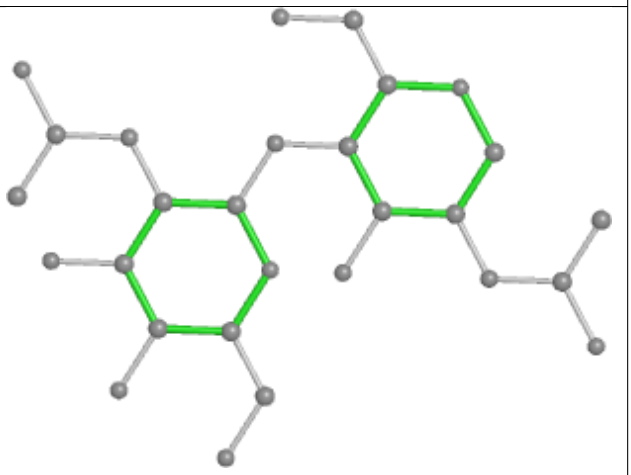
Bond lengths



Bond angles

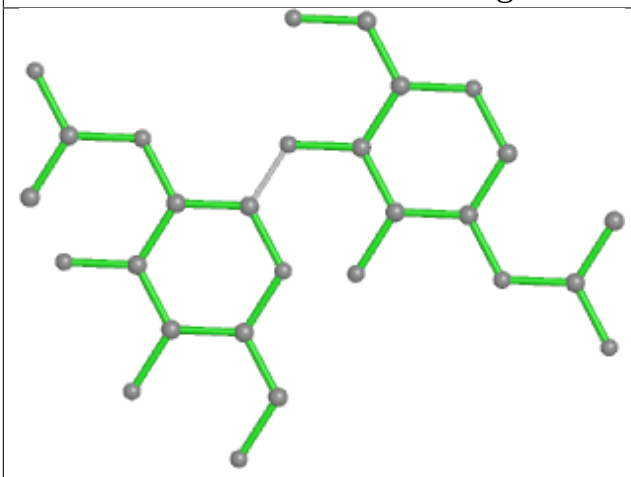


Torsions

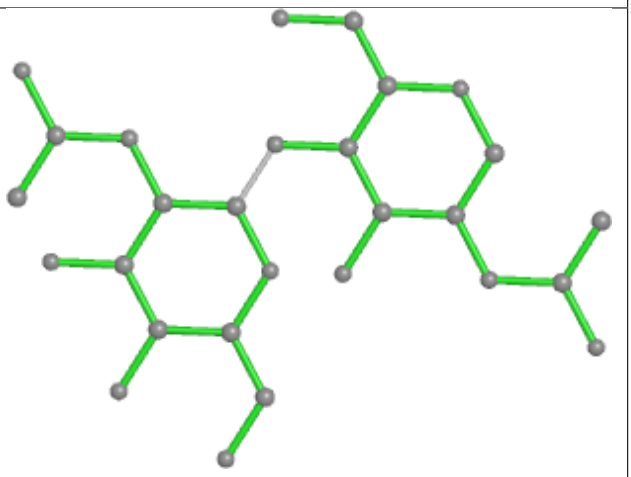


Rings

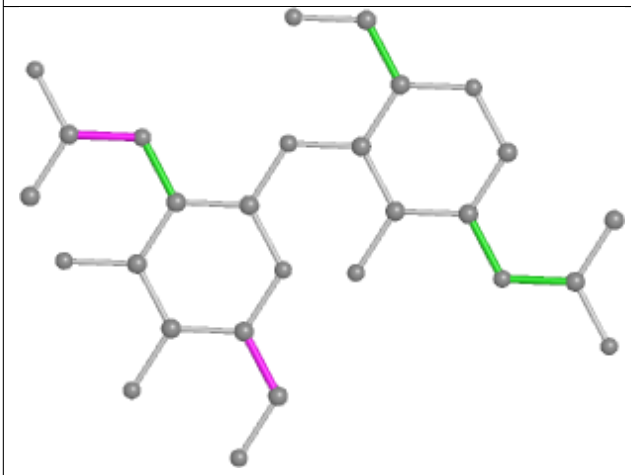
Oligosaccharide Chain F



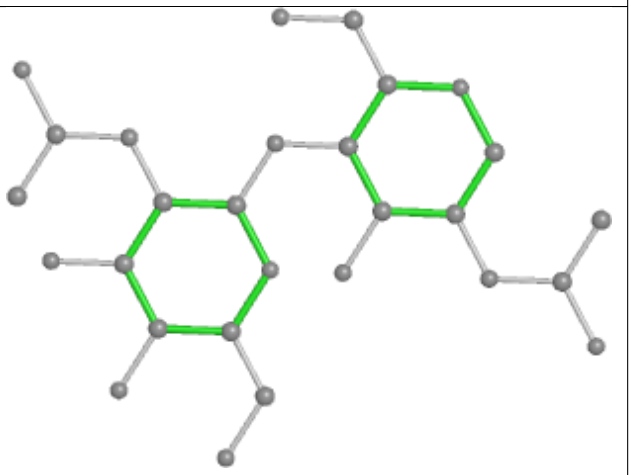
Bond lengths



Bond angles

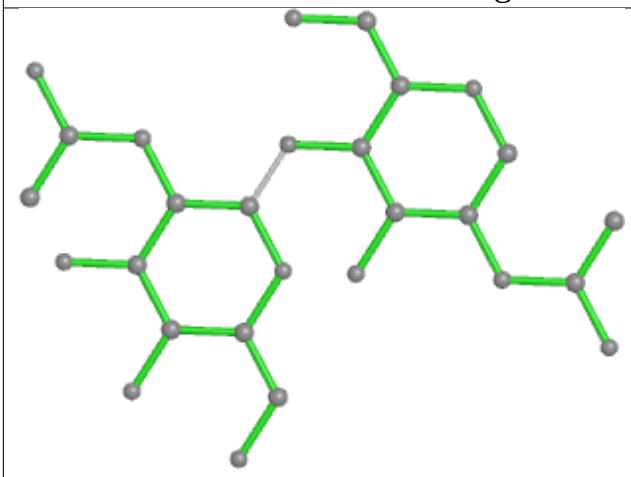


Torsions

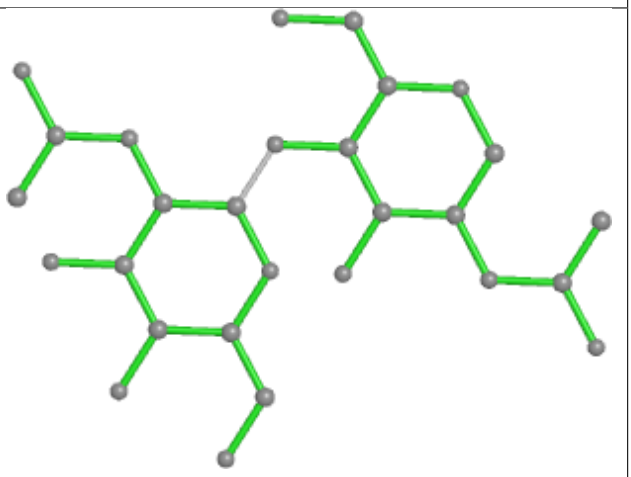


Rings

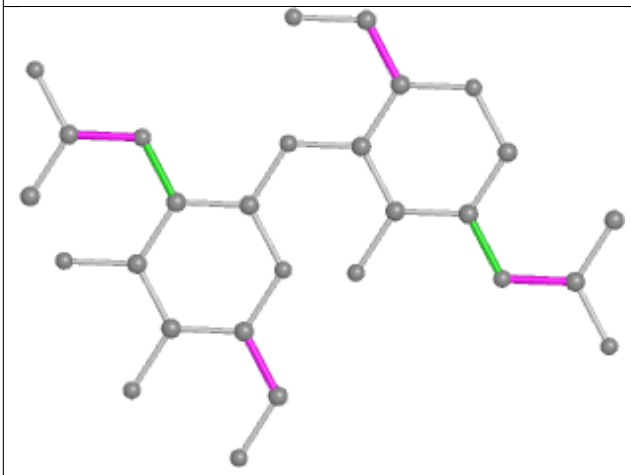
Oligosaccharide Chain G



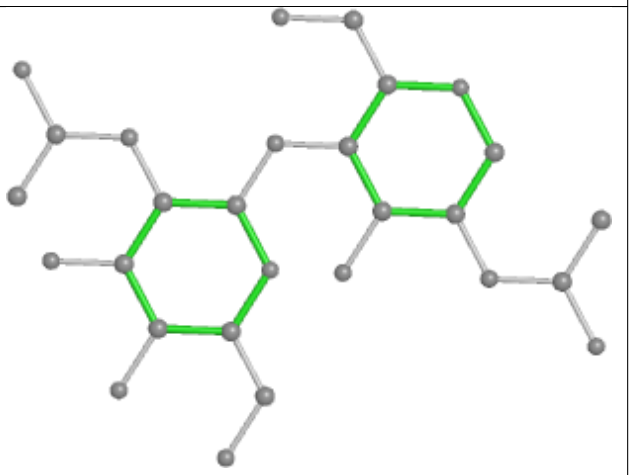
Bond lengths



Bond angles

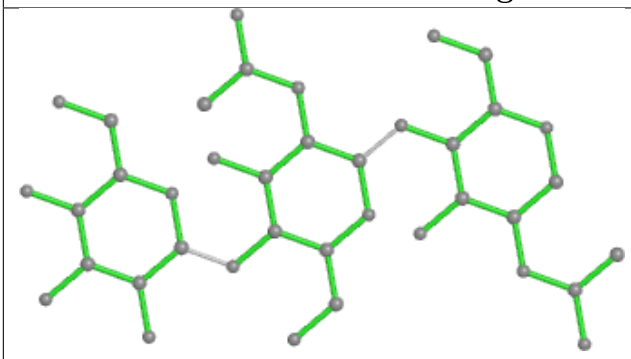


Torsions

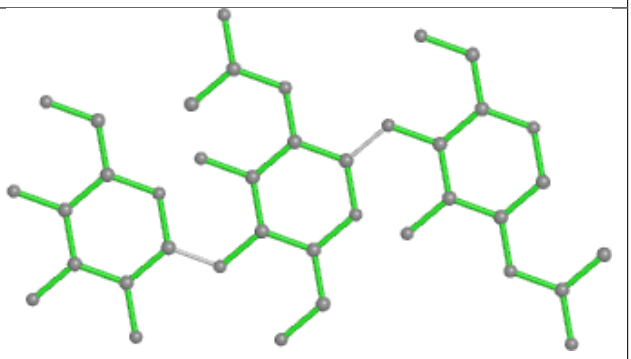


Rings

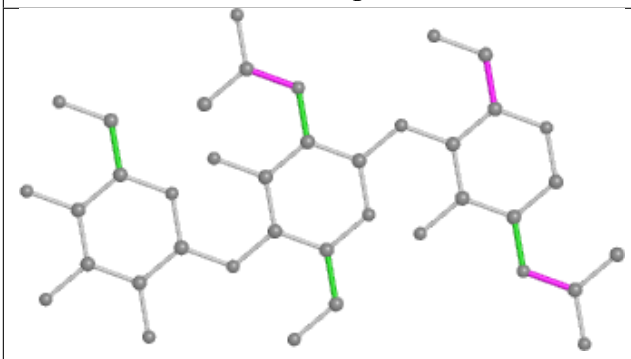
Oligosaccharide Chain E



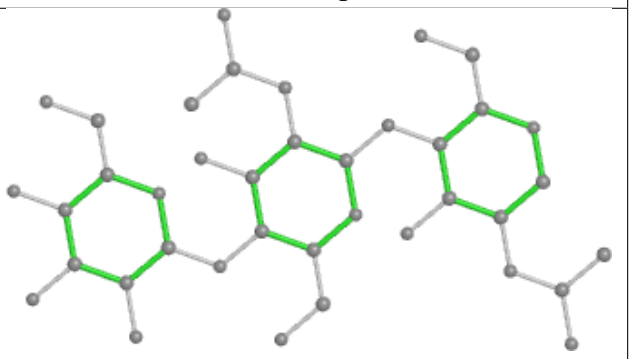
Bond lengths



Bond angles

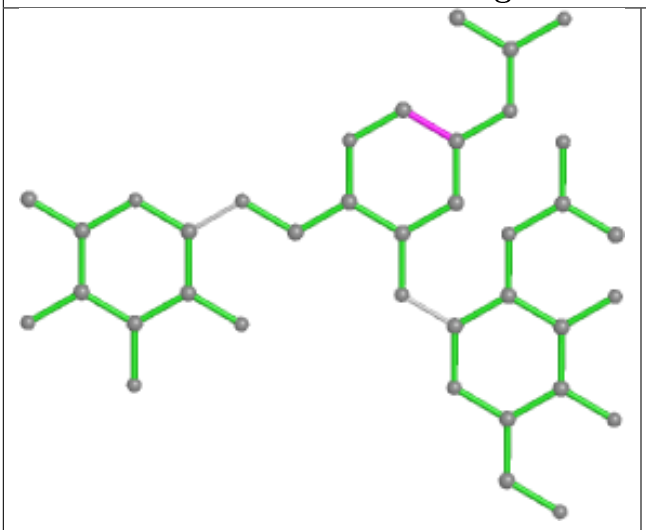


Torsions

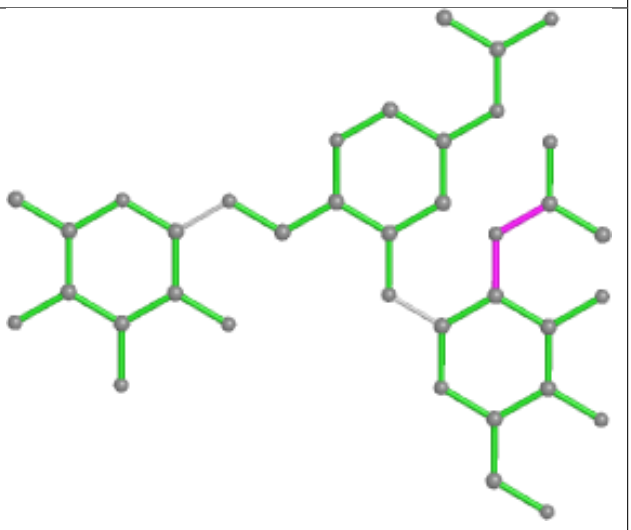


Rings

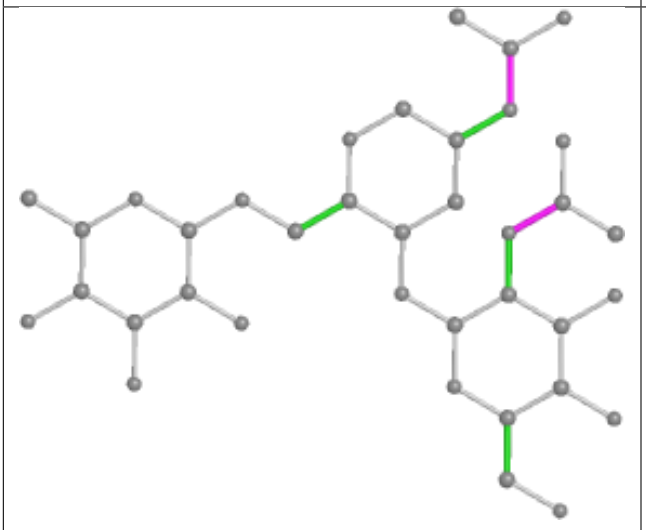
Oligosaccharide Chain H



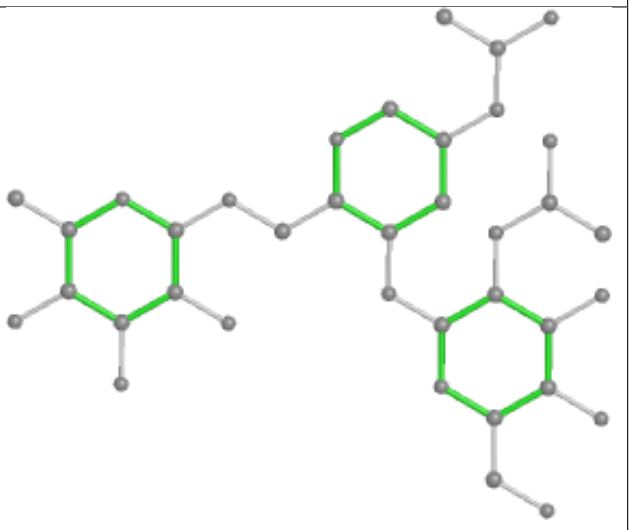
Bond lengths



Bond angles

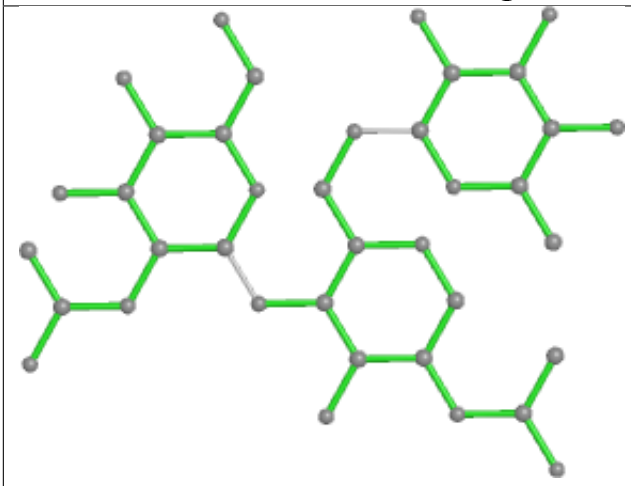


Torsions

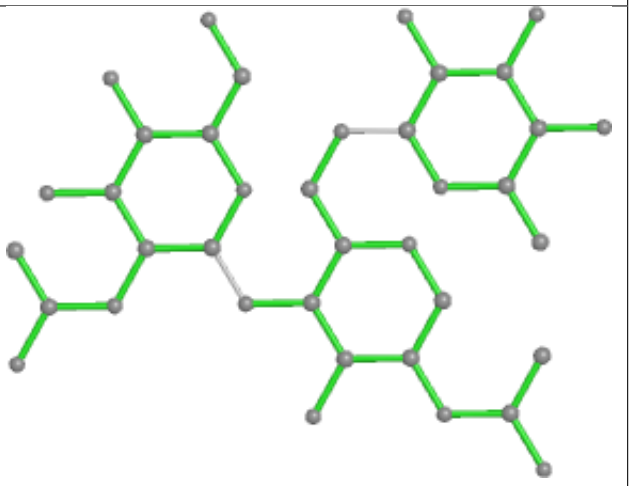


Rings

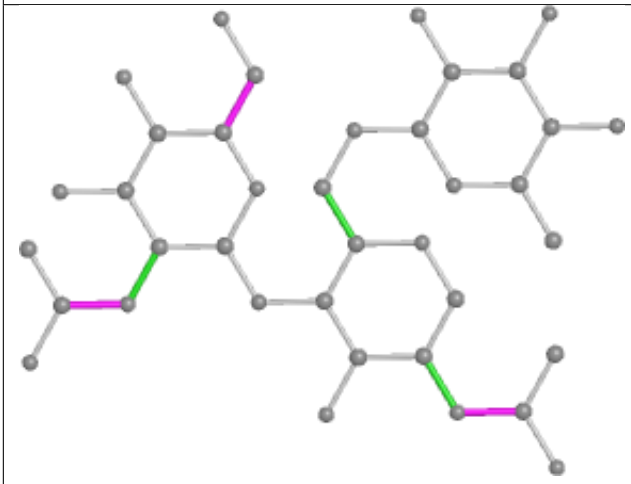
Oligosaccharide Chain J



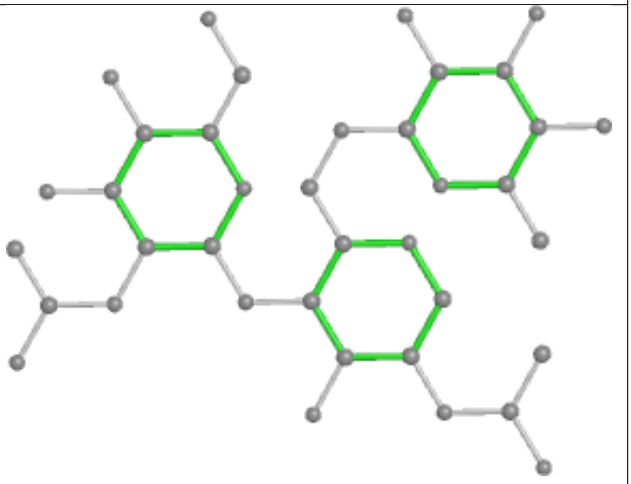
Bond lengths



Bond angles

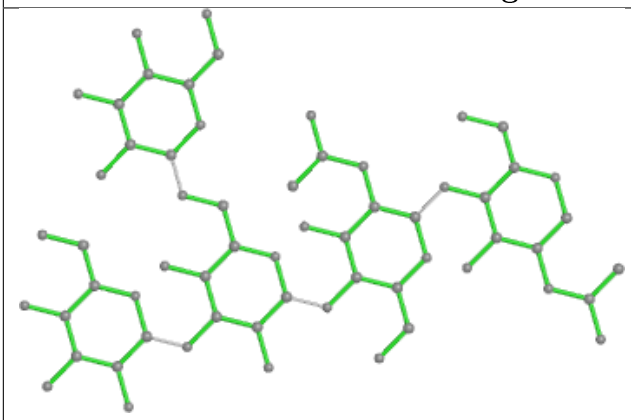


Torsions

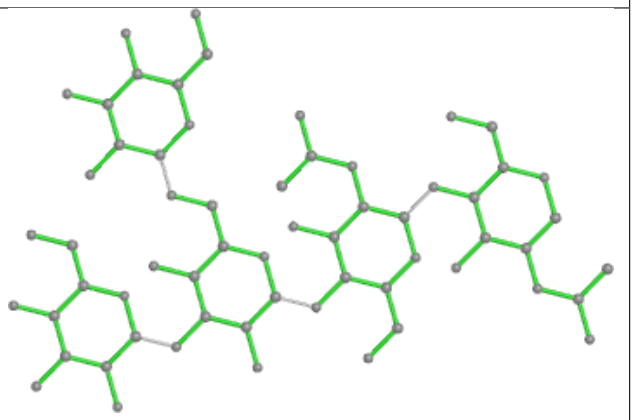


Rings

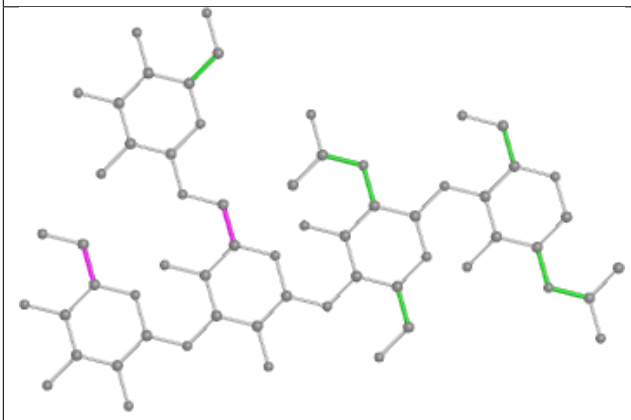
Oligosaccharide Chain I



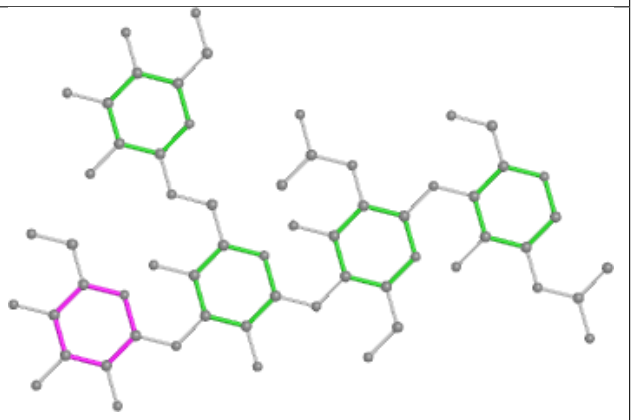
Bond lengths



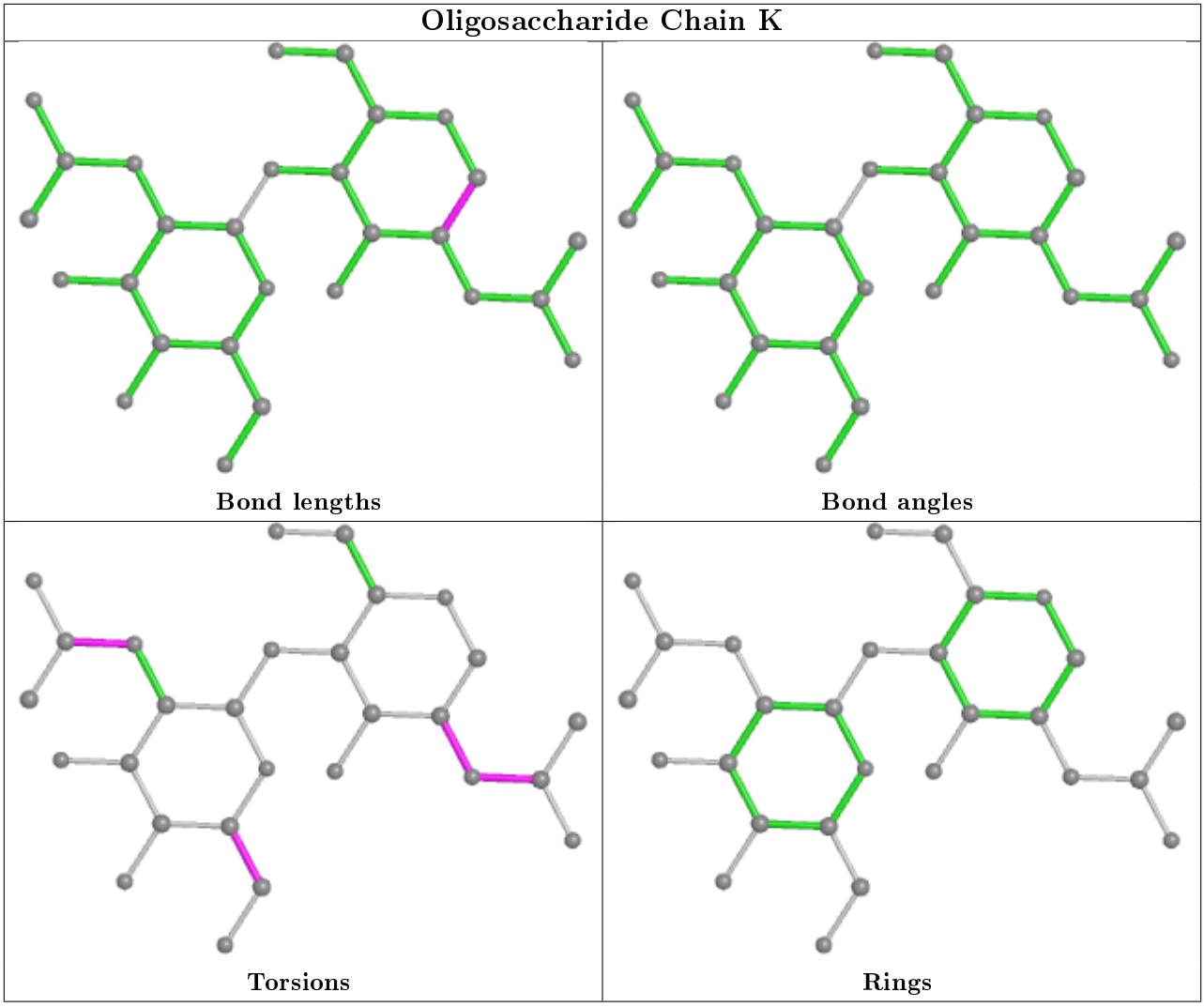
Bond angles



Torsions



Rings



5.6 Ligand geometry

7 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	$\#\|Z\| > 2$
9	SO4	A	750	-	4,4,4	0.23	0	6,6,6	0.10	0
7	NAG	A	1961	1	14,14,15	0.67	0	17,19,21	0.66	1 (5%)
10	BME	A	1270	1	3,3,3	0.43	0	1,2,2	0.20	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
9	SO4	A	752	4	4,4,4	0.35	0	6,6,6	0.23	0
8	GLC	A	753	-	12,12,12	1.68	2 (16%)	17,17,17	1.63	4 (23%)
9	SO4	A	751	-	4,4,4	0.24	0	6,6,6	0.06	0
8	GLC	A	754	-	12,12,12	1.59	1 (8%)	17,17,17	1.57	3 (17%)

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
10	BME	A	1270	1	-	0/1/1/1	-
8	GLC	A	753	-	-	2/2/22/22	0/1/1/1
7	NAG	A	1961	1	-	2/6/23/26	0/1/1/1
8	GLC	A	754	-	-	2/2/22/22	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	753	GLC	O5-C1	4.57	1.54	1.42
8	A	754	GLC	O5-C1	4.52	1.54	1.42
8	A	753	GLC	C4-C5	2.15	1.57	1.53

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	A	753	GLC	C6-C5-C4	-3.49	104.83	113.00
8	A	754	GLC	O5-C5-C6	3.47	115.06	106.44
8	A	754	GLC	C6-C5-C4	-3.44	104.95	113.00
8	A	753	GLC	O5-C5-C6	3.38	114.83	106.44
8	A	753	GLC	O6-C6-C5	-2.38	103.13	111.29
8	A	754	GLC	O6-C6-C5	-2.15	103.92	111.29
8	A	753	GLC	O1-C1-C2	2.13	115.04	109.03
7	A	1961	NAG	C2-N2-C7	-2.03	120.01	122.90

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	1961	NAG	C8-C7-N2-C2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
7	A	1961	NAG	O7-C7-N2-C2
8	A	754	GLC	O5-C5-C6-O6
8	A	753	GLC	O5-C5-C6-O6
8	A	754	GLC	C4-C5-C6-O6
8	A	753	GLC	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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	671/705 (95%)	-0.09	23 (3%) 45 44	22, 39, 76, 95	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	26	THR	8.3
1	A	693	THR	5.1
1	A	696	CYS	4.9
1	A	694	SER	4.8
1	A	692	ASP	4.6
1	A	690	LEU	4.6
1	A	695	SER	4.2
1	A	688	VAL	3.7
1	A	339	SER	3.3
1	A	338	ILE	3.2
1	A	27	LYS	3.2
1	A	691	PHE	3.2
1	A	686	PHE	3.1
1	A	663	GLU	3.0
1	A	342	SER	3.0
1	A	340	LEU	2.8
1	A	659	ASN	2.8
1	A	30	VAL	2.7
1	A	651	CYS	2.5
1	A	665	HIS	2.5
1	A	683	TYR	2.5
1	A	28	CYS	2.5
1	A	689	ARG	2.4

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

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

6.3 Carbohydrates (i)

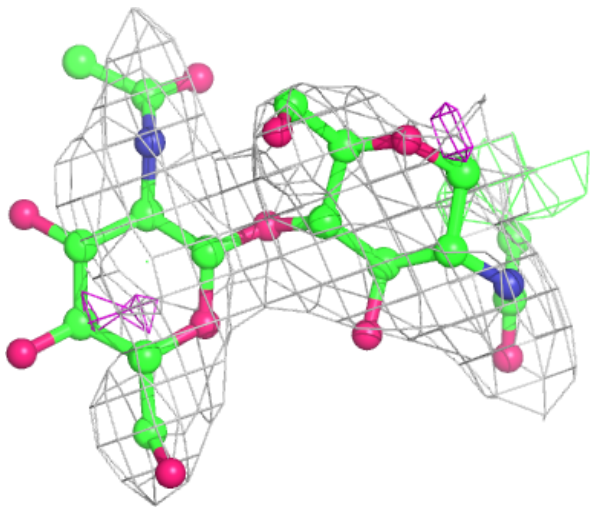
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

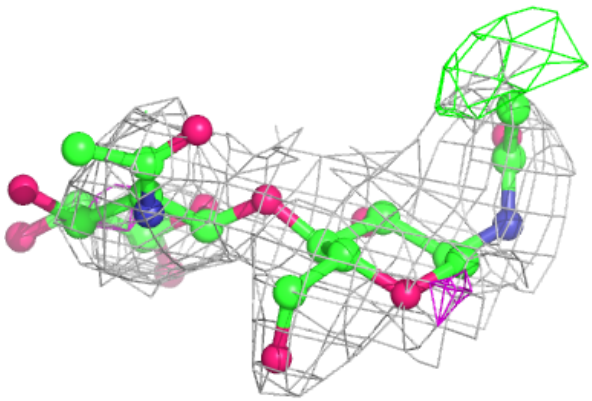
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	NAG	K	1	14/15	0.64	0.29	79,85,87,91	0
5	BMA	I	5	11/12	0.65	0.36	99,99,100,100	0
2	NAG	G	2	14/15	0.66	0.43	88,90,92,92	0
2	NAG	C	2	14/15	0.75	0.51	97,99,100,100	0
3	BMA	E	3	11/12	0.76	0.27	91,92,93,93	0
2	NAG	B	1	14/15	0.77	0.29	88,90,92,95	0
5	MAN	I	4	11/12	0.77	0.33	97,99,100,100	0
2	NAG	C	1	14/15	0.78	0.38	81,85,89,93	0
2	NAG	B	2	14/15	0.78	0.43	98,99,100,100	0
4	FUC	H	3	10/11	0.78	0.35	84,85,86,87	0
2	NAG	F	2	14/15	0.78	0.29	80,84,85,86	0
3	NAG	E	2	14/15	0.81	0.19	84,86,88,90	0
2	NAG	D	2	14/15	0.81	0.24	76,79,80,81	0
6	NDG	K	2	14/15	0.82	0.35	95,97,98,98	0
2	NAG	D	1	14/15	0.82	0.17	59,65,68,72	0
4	NAG	H	2	14/15	0.83	0.33	89,91,92,92	0
4	FUC	J	3	10/11	0.84	0.23	73,76,77,77	0
4	NAG	H	1	13/15	0.85	0.18	72,75,83,86	0
4	NAG	J	2	14/15	0.86	0.23	73,77,79,80	0
2	NAG	G	1	14/15	0.86	0.20	68,73,76,83	0
5	BMA	I	3	11/12	0.86	0.26	84,91,94,97	0
2	NAG	F	1	14/15	0.88	0.16	59,63,69,75	0
5	NAG	I	2	14/15	0.91	0.14	55,59,67,77	0
3	NAG	E	1	14/15	0.91	0.15	68,74,76,80	0
4	NAG	J	1	14/15	0.95	0.12	37,53,66,68	0
5	NAG	I	1	14/15	0.98	0.14	32,35,39,45	0

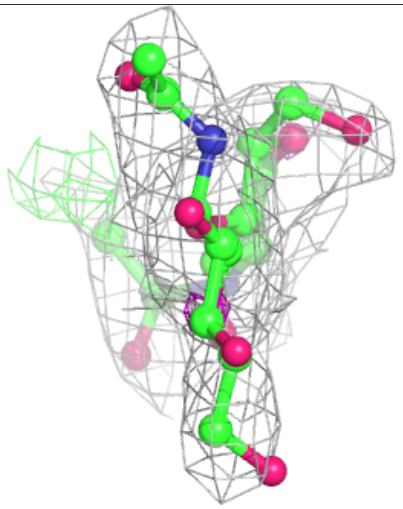
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain B:

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

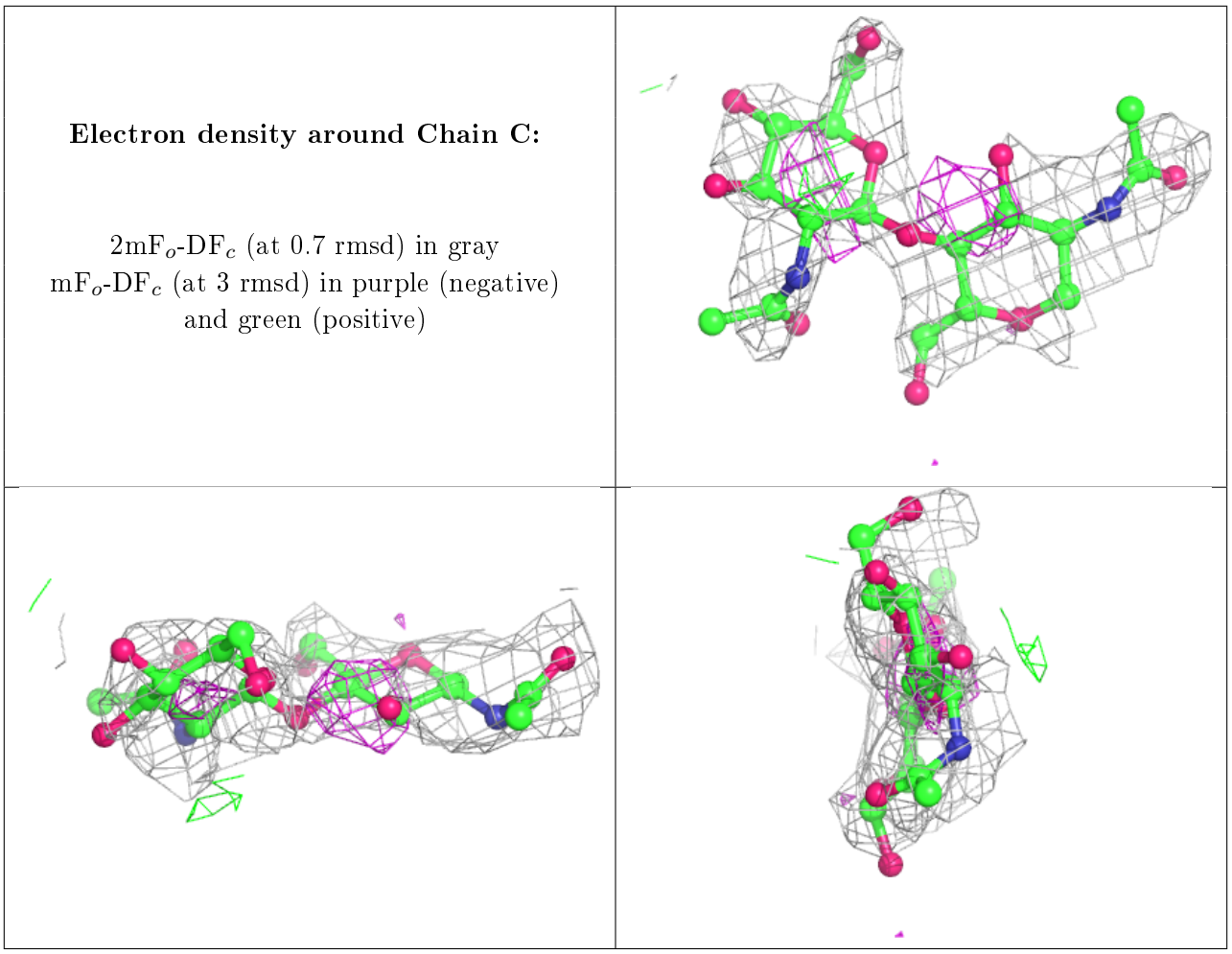






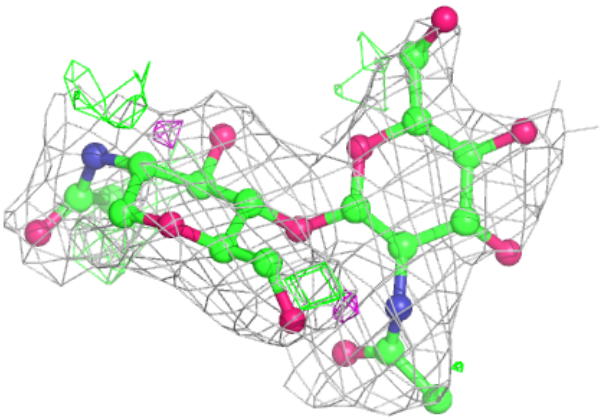
Electron density around Chain C:

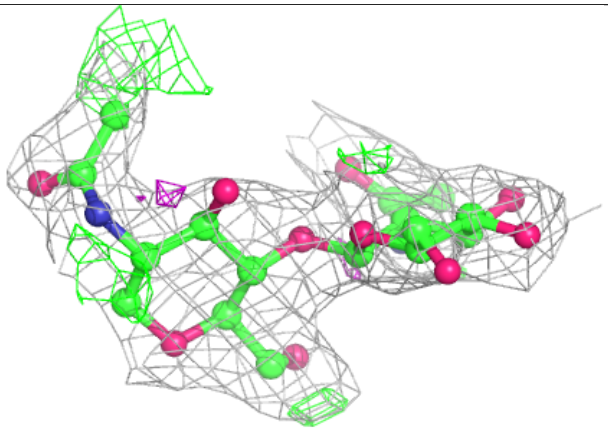
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

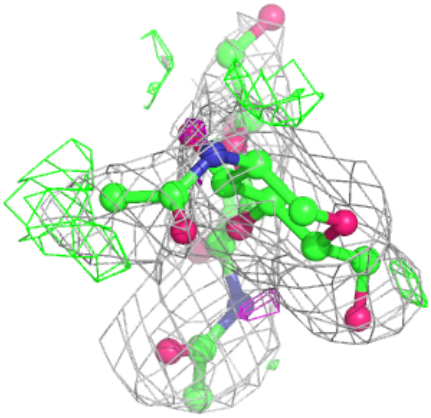


Electron density around Chain D:

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

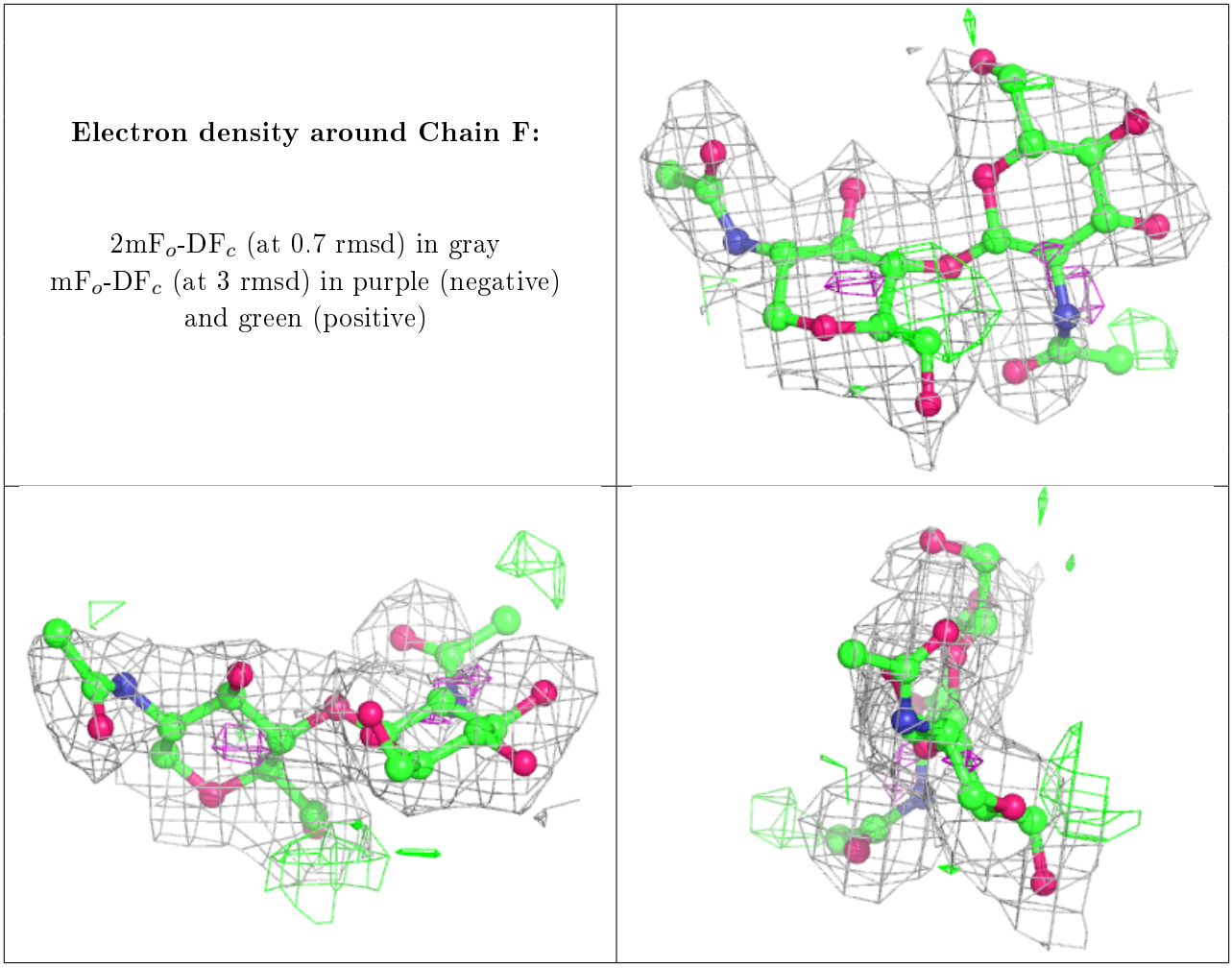






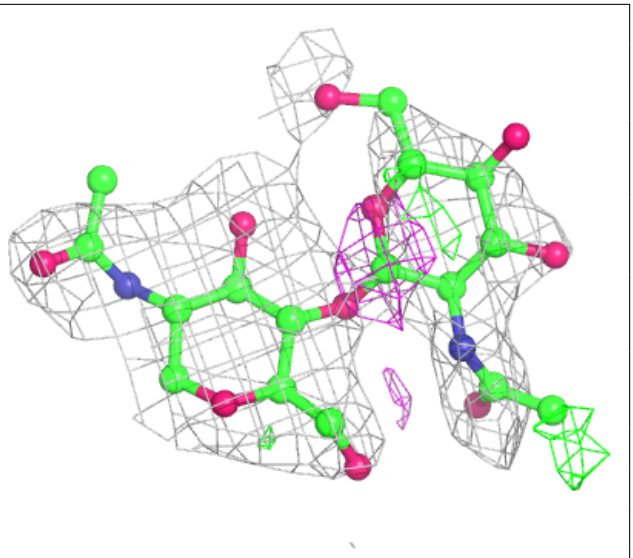
Electron density around Chain F:

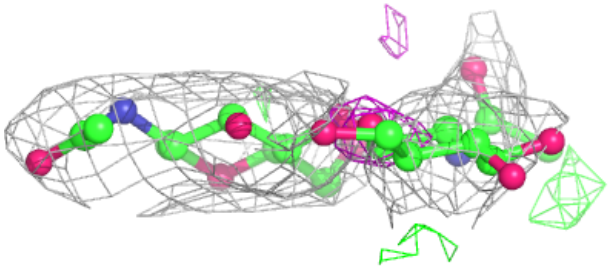
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

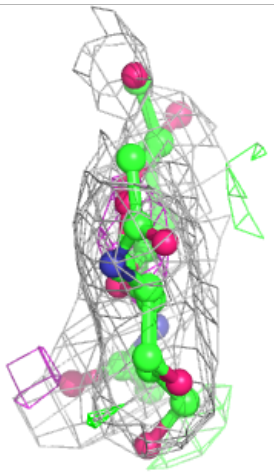


Electron density around Chain G:

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

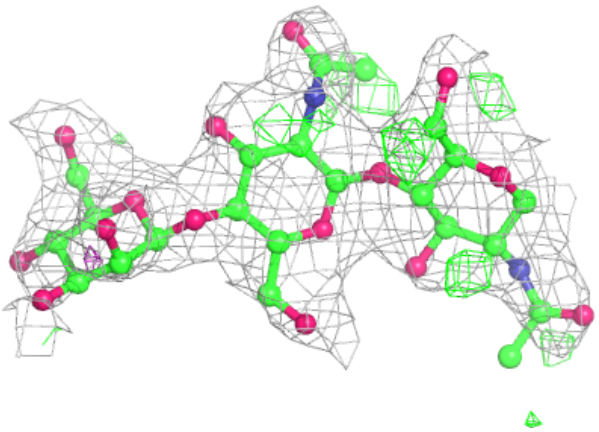


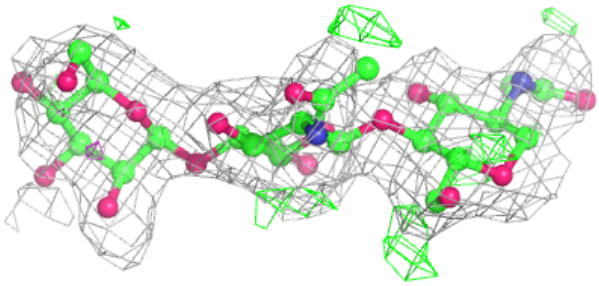


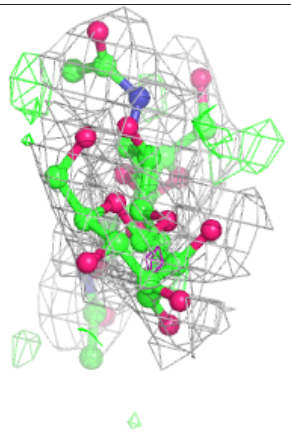


Electron density around Chain E:

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

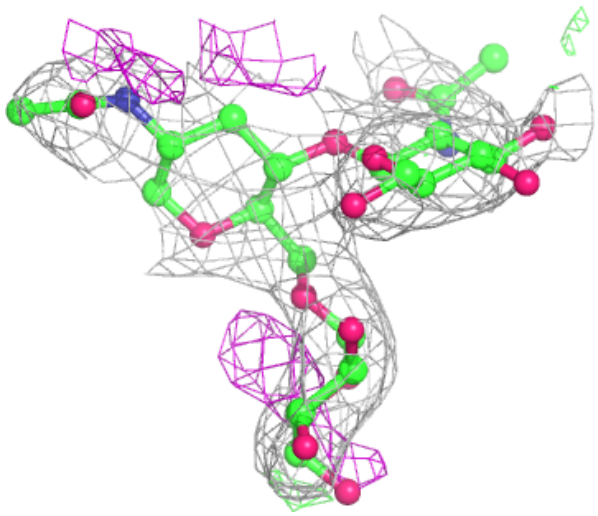


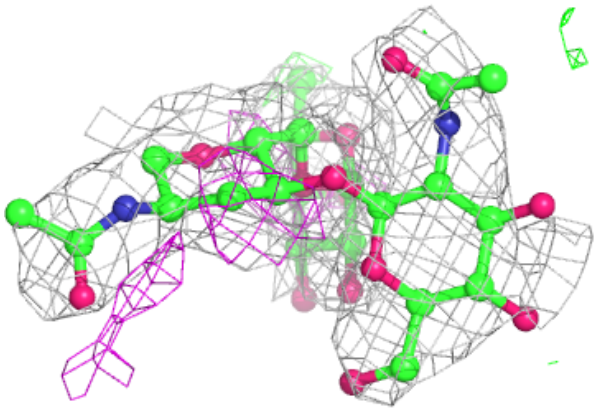


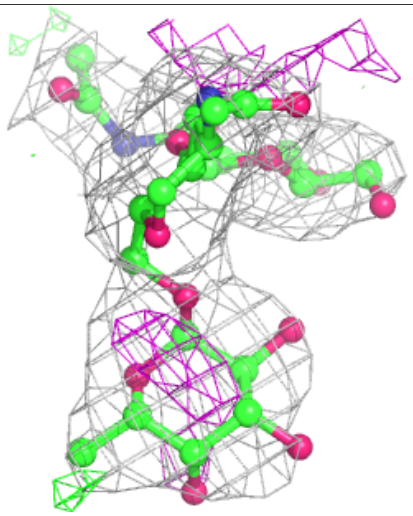


Electron density around Chain H:

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

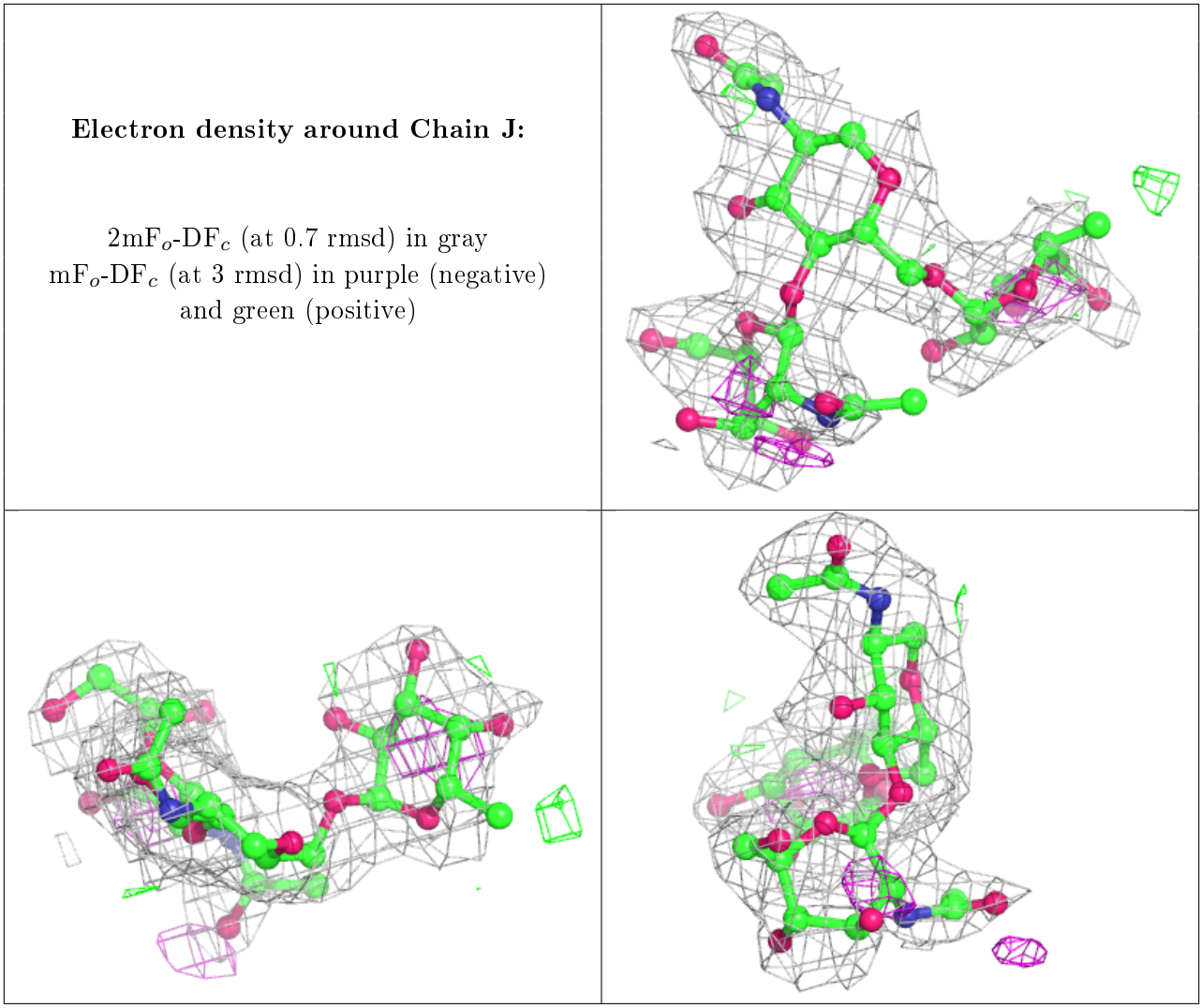






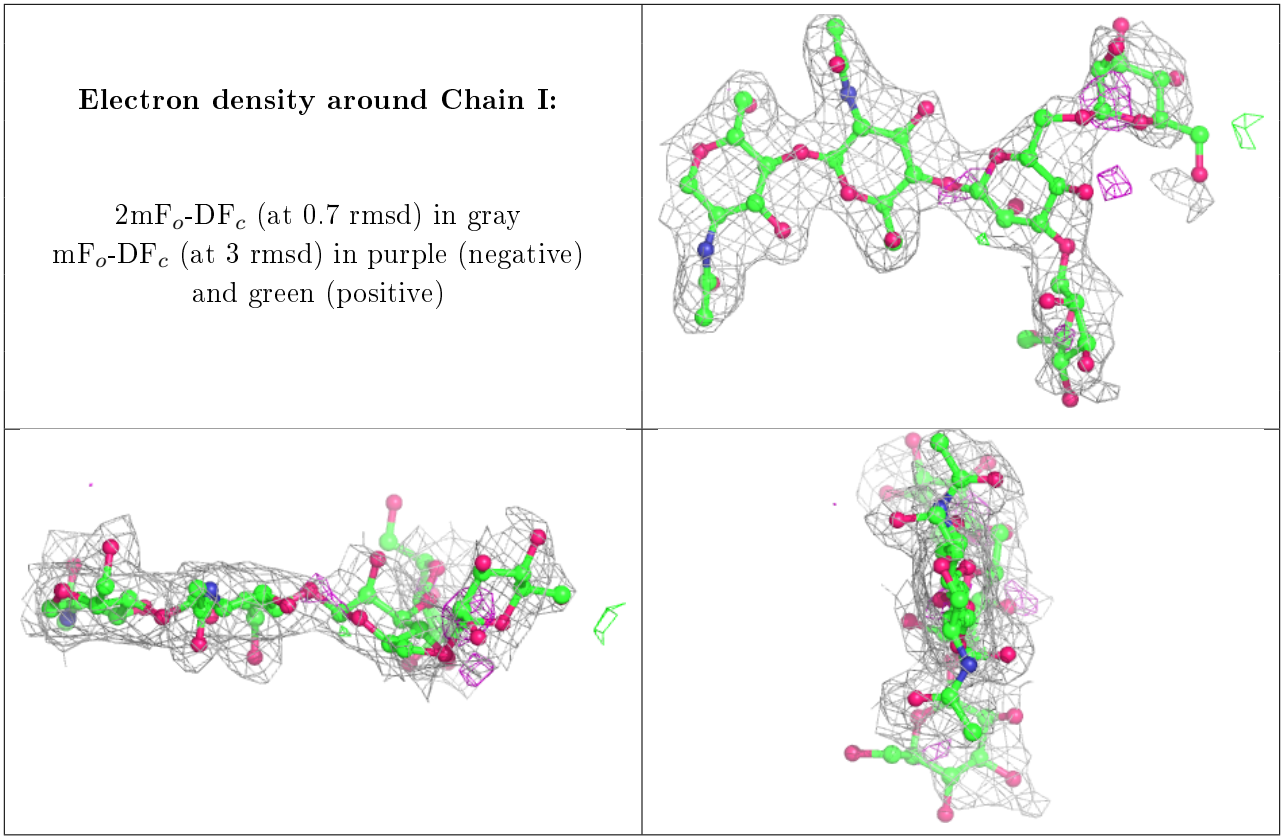
Electron density around Chain J:

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



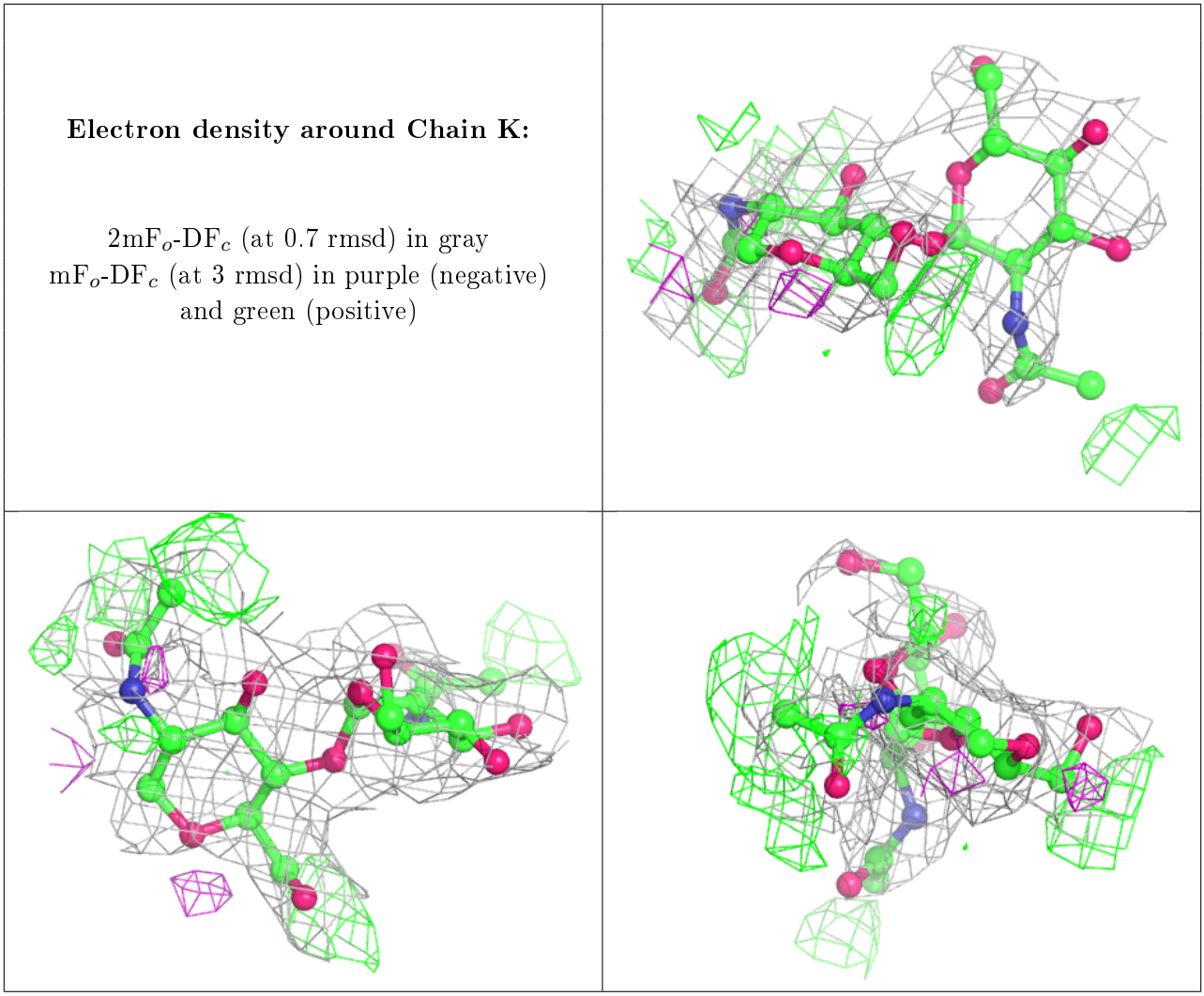
Electron density around Chain I:

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



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
8	GLC	A	754	12/12	0.66	0.25	99,100,100,100	0
8	GLC	A	753	12/12	0.73	0.23	54,59,62,67	0
7	NAG	A	1961	14/15	0.74	0.23	74,78,79,81	0
9	SO4	A	752	5/5	0.76	0.31	88,92,92,93	0
10	BME	A	1270	4/4	0.94	0.26	57,57,61,64	0
9	SO4	A	751	5/5	0.97	0.12	67,69,69,70	0
9	SO4	A	750	5/5	0.99	0.12	43,44,46,48	0

6.5 Other polymers (i)

There are no such residues in this entry.