wwPDB X-ray Structure Validation Summary Report (i)

Oct 26, 2023 – 12:50 AM EDT

PDB ID	:	2ZMK
Title	:	Crystl structure of Basic Winged bean lectin in complex with Gal-alpha-1,4-Gal-Beta-Ethylene
Authors	:	Kulkarni, K.A.; Katiyar, S.; Surolia, A.; Vijayan, M.
Deposited on	:	2008-04-19
Resolution	:	2.50 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i) 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 (i)) were used in the production of this report:

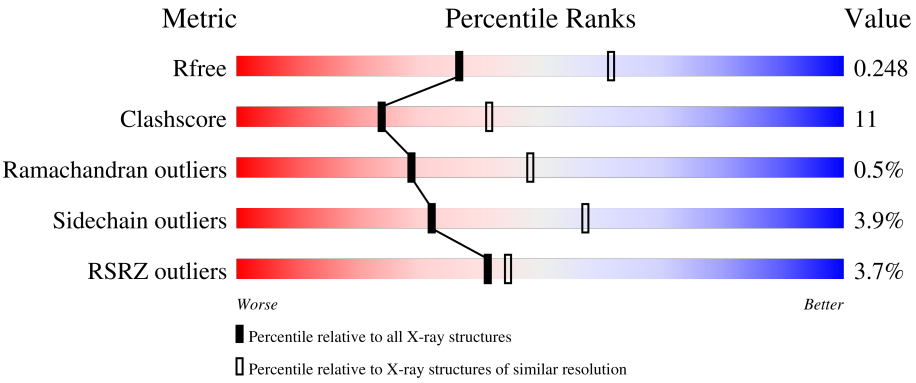
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	241	4% 73% 22%
1	B	241	% 75% 21%
1	C	241	2% 78% 18%
1	D	241	7% 75% 22%
2	E	2	50% 50%

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Mol	Chain	Length	Quality of chain
2	H	2	50% 50%
2	L	2	100%
2	M	2	50% 50%
3	F	3	67% 33%
3	N	3	100%
4	G	2	50% 50%
4	J	2	50% 50%
4	K	2	100%
4	O	2	50% 50%
5	I	2	50% 50%

2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 7739 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.

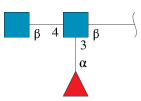
- Molecule 1 is a protein called Basic agglutinin.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	237	Total	C	N	O	0	0	0
			1825	1174	304	347			
1	B	237	Total	C	N	O	0	0	0
			1811	1167	300	344			
1	C	237	Total	C	N	O	0	0	0
			1811	1165	301	345			
1	D	237	Total	C	N	O	0	0	0
			1788	1150	294	344			

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

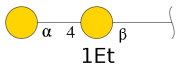
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	2	Total	C	N	O	0	0	0
			24	14	1	9			
2	H	2	Total	C	N	O	0	0	0
			24	14	1	9			
2	L	2	Total	C	N	O	0	0	0
			24	14	1	9			
2	M	2	Total	C	N	O	0	0	0
			24	14	1	9			

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



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
3	F	3	Total C N O 38 22 2 14	0	0	0
3	N	3	Total C N O 38 22 2 14	0	0	0

- Molecule 4 is an oligosaccharide called alpha-D-galactopyranose-(1-4)-ethyl beta-D-galactopyranoside.



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
4	G	2	Total C O 25 14 11	0	0	0
4	J	2	Total C O 25 14 11	0	0	0
4	K	2	Total C O 25 14 11	0	0	0
4	O	2	Total C O 25 14 11	0	0	0

- Molecule 5 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
5	I	2	Total C N O 28 16 2 10	0	0	0

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

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

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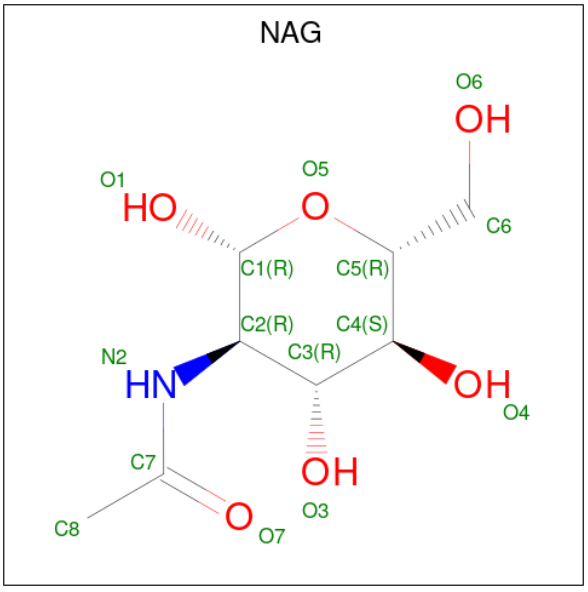
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	D	1	Total Mn 1 1	0	0

- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca).

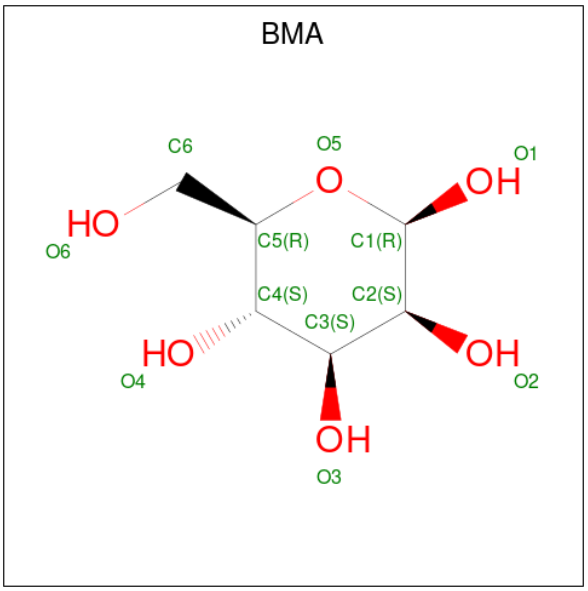
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total Ca 1 1	0	0
7	B	1	Total Ca 1 1	0	0
7	C	1	Total Ca 1 1	0	0
7	D	1	Total Ca 1 1	0	0

- Molecule 8 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 9 is beta-D-mannopyranose (three-letter code: BMA) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	C	1	Total C O 11 6 5	0	0

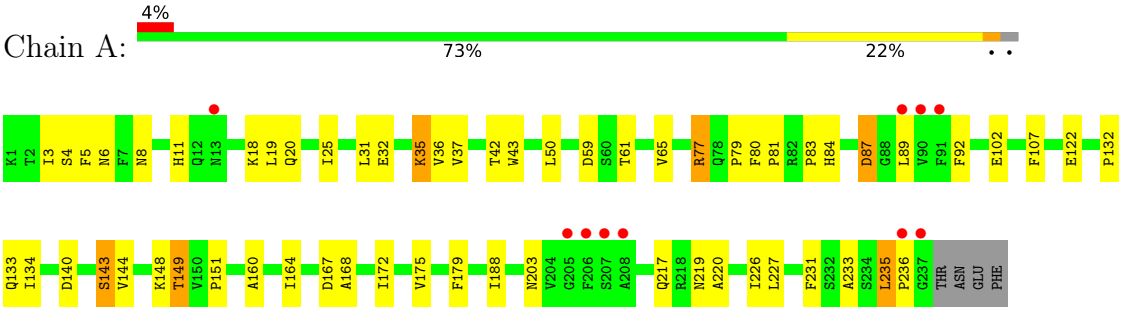
- Molecule 10 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	56	Total O 56 56	0	0
10	B	38	Total O 38 38	0	0
10	C	45	Total O 45 45	0	0
10	D	32	Total O 32 32	0	0

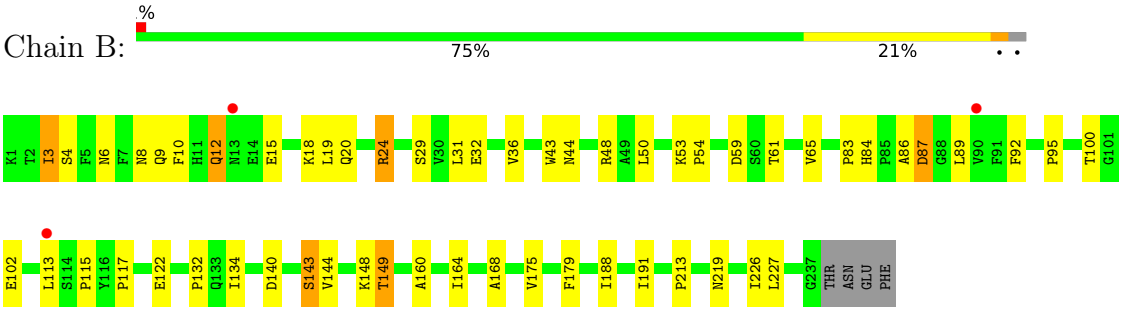
3 Residue-property plots (i)

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.

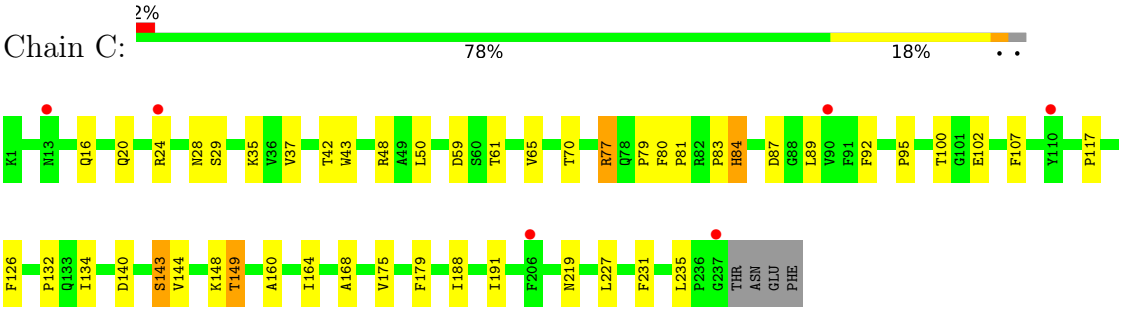
• Molecule 1: Basic agglutinin



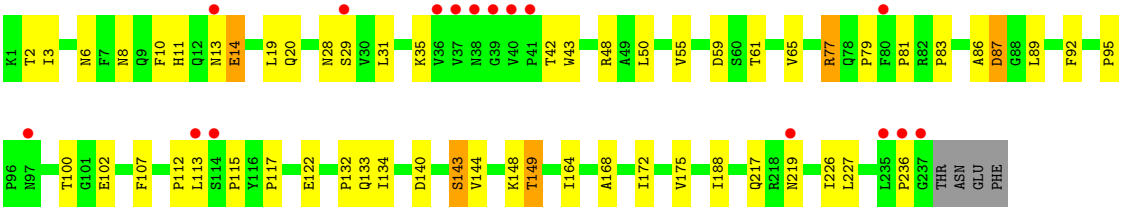
• Molecule 1: Basic agglutinin



• Molecule 1: Basic agglutinin



• Molecule 1: Basic agglutinin



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

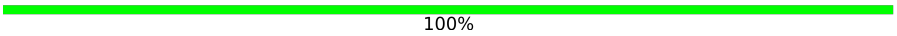
Chain E:

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

Chain H:

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

Chain L:

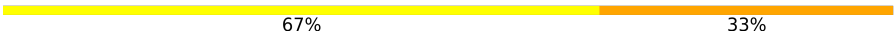


• Molecule 2: alpha-L-fucopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:

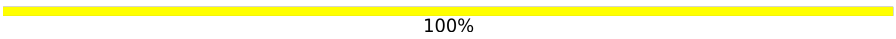
• Molecule 3: alpha-L-fucopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:



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

Chain N:



• Molecule 4: alpha-D-galactopyranose-(1-4)-ethyl beta-D-galactopyranoside

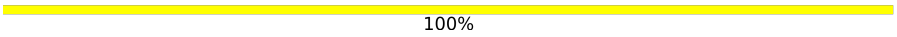
Chain G:

• Molecule 4: alpha-D-galactopyranose-(1-4)-ethyl beta-D-galactopyranoside

Chain J:

• Molecule 4: alpha-D-galactopyranose-(1-4)-ethyl beta-D-galactopyranoside

Chain K:



• Molecule 4: alpha-D-galactopyranose-(1-4)-ethyl beta-D-galactopyranoside

Chain O:

• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	156.92Å 89.96Å 73.32Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.63 – 2.50 29.63 – 2.48	Depositor EDS
% Data completeness (in resolution range)	98.4 (29.63-2.50) 97.3 (29.63-2.48)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	0.13	Depositor
$< I/\sigma(I) >$ [1]	1.83 (at 2.48Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.217 , 0.256 0.210 , 0.248	Depositor DCC
R_{free} test set	1696 reflections (4.65%)	wwPDB-VP
Wilson B-factor (Å^2)	41.5	Xtriage
Anisotropy	0.845	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 43.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	7739	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 3.50% 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: CA, NAG, EGA, FUC, GLA, BMA, MN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.40	0/1878	0.70	2/2573 (0.1%)
1	B	0.39	0/1864	0.66	0/2556
1	C	0.38	0/1864	0.69	2/2558 (0.1%)
1	D	0.38	0/1840	0.70	2/2526 (0.1%)
All	All	0.39	0/7446	0.69	6/10213 (0.1%)

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	77	ARG	NE-CZ-NH2	-7.96	116.32	120.30
1	D	77	ARG	NE-CZ-NH2	-7.61	116.50	120.30
1	C	77	ARG	NE-CZ-NH2	-7.40	116.60	120.30
1	C	77	ARG	NE-CZ-NH1	6.94	123.77	120.30
1	D	77	ARG	NE-CZ-NH1	6.87	123.73	120.30

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	1825	0	1759	45	0
1	B	1811	0	1734	42	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1811	0	1731	35	0
1	D	1788	0	1683	38	0
2	E	24	0	22	1	0
2	H	24	0	22	3	0
2	L	24	0	22	0	0
2	M	24	0	22	1	0
3	F	38	0	34	2	0
3	N	38	0	34	2	0
4	G	25	0	25	0	0
4	J	25	0	25	0	0
4	K	25	0	25	1	0
4	O	25	0	25	0	0
5	I	28	0	25	2	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
7	D	1	0	0	0	0
8	C	14	0	13	0	0
9	C	11	0	10	0	0
10	A	56	0	0	2	0
10	B	38	0	0	1	0
10	C	45	0	0	0	0
10	D	32	0	0	1	0
All	All	7739	0	7211	164	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 11.

The worst 5 of 164 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:D:3:ILE:HD13	1:D:55:VAL:HG12	1.61	0.80
1:A:6:ASN:HD21	1:A:8:ASN:ND2	1.78	0.80
1:D:65:VAL:HG13	1:D:168:ALA:HB1	1.66	0.76
1:C:65:VAL:HG13	1:C:168:ALA:HB1	1.67	0.75
1:A:65:VAL:HG13	1:A:168:ALA:HB1	1.67	0.75

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	235/241 (98%)	224 (95%)	10 (4%)	1 (0%)	34 54
1	B	235/241 (98%)	224 (95%)	11 (5%)	0	100 100
1	C	235/241 (98%)	222 (94%)	12 (5%)	1 (0%)	34 54
1	D	235/241 (98%)	221 (94%)	11 (5%)	3 (1%)	12 21
All	All	940/964 (98%)	891 (95%)	44 (5%)	5 (0%)	29 48

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	14	GLU
1	D	107	PHE
1	A	107	PHE
1	C	107	PHE
1	D	236	PRO

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	201/210 (96%)	193 (96%)	8 (4%)	31 56
1	B	197/210 (94%)	187 (95%)	10 (5%)	24 45
1	C	198/210 (94%)	191 (96%)	7 (4%)	36 62

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	D	192/210 (91%)	186 (97%)	6 (3%)	40 67
All	All	788/840 (94%)	757 (96%)	31 (4%)	32 57

5 of 31 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	87	ASP
1	D	102	GLU
1	B	149	THR
1	D	143	SER
1	C	235	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 31 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	196	GLN
1	D	97	ASN
1	C	38	ASN
1	D	196	GLN
1	D	8	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)

24 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	E	1	2,1	14,14,15	0.54	0	17,19,21	0.70	1 (5%)
2	FUC	E	2	2	10,10,11	0.61	0	14,14,16	0.35	0
3	NAG	F	1	3,1	14,14,15	0.73	0	17,19,21	0.78	0
3	FUC	F	2	3	10,10,11	0.56	0	14,14,16	0.33	0
3	NAG	F	3	3	14,14,15	0.56	0	17,19,21	0.78	1 (5%)
4	EGA	G	1	4	14,14,14	0.56	0	19,19,19	1.06	1 (5%)
4	GLA	G	2	4	11,11,12	0.56	0	15,15,17	0.51	0
2	NAG	H	1	2,1	14,14,15	0.66	0	17,19,21	0.79	1 (5%)
2	FUC	H	2	2	10,10,11	0.51	0	14,14,16	0.42	0
5	NAG	I	1	5,1	14,14,15	0.88	0	17,19,21	0.95	1 (5%)
5	NAG	I	2	5	14,14,15	0.69	0	17,19,21	0.64	0
4	EGA	J	1	4	14,14,14	0.53	0	19,19,19	1.01	1 (5%)
4	GLA	J	2	4	11,11,12	0.79	0	15,15,17	0.58	0
4	EGA	K	1	4	14,14,14	0.56	0	19,19,19	1.06	1 (5%)
4	GLA	K	2	4	11,11,12	0.51	0	15,15,17	0.63	0
2	NAG	L	1	2,1	14,14,15	0.79	0	17,19,21	0.64	0
2	FUC	L	2	2	10,10,11	0.60	0	14,14,16	0.35	0
2	NAG	M	1	2,1	14,14,15	0.79	0	17,19,21	0.79	0
2	FUC	M	2	2	10,10,11	0.57	0	14,14,16	0.44	0
3	NAG	N	1	3,1	14,14,15	0.70	0	17,19,21	0.68	0
3	FUC	N	2	3	10,10,11	0.48	0	14,14,16	0.43	0
3	NAG	N	3	3	14,14,15	0.67	0	17,19,21	0.82	0
4	EGA	O	1	4	14,14,14	0.57	0	19,19,19	1.02	1 (5%)
4	GLA	O	2	4	11,11,12	0.56	0	15,15,17	0.55	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	E	1	2,1	-	2/6/23/26	0/1/1/1
2	FUC	E	2	2	-	-	0/1/1/1
3	NAG	F	1	3,1	-	4/6/23/26	0/1/1/1
3	FUC	F	2	3	-	-	0/1/1/1
3	NAG	F	3	3	-	2/6/23/26	0/1/1/1
4	EGA	G	1	4	-	3/5/25/25	0/1/1/1
4	GLA	G	2	4	-	0/2/19/22	0/1/1/1
2	NAG	H	1	2,1	-	2/6/23/26	0/1/1/1
2	FUC	H	2	2	-	-	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	I	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	I	2	5	-	6/6/23/26	0/1/1/1
4	EGA	J	1	4	-	2/5/25/25	0/1/1/1
4	GLA	J	2	4	-	2/2/19/22	0/1/1/1
4	EGA	K	1	4	-	5/5/25/25	0/1/1/1
4	GLA	K	2	4	-	0/2/19/22	0/1/1/1
2	NAG	L	1	2,1	-	2/6/23/26	0/1/1/1
2	FUC	L	2	2	-	-	0/1/1/1
2	NAG	M	1	2,1	-	5/6/23/26	0/1/1/1
2	FUC	M	2	2	-	-	0/1/1/1
3	NAG	N	1	3,1	-	4/6/23/26	0/1/1/1
3	FUC	N	2	3	-	-	0/1/1/1
3	NAG	N	3	3	-	4/6/23/26	0/1/1/1
4	EGA	O	1	4	-	4/5/25/25	0/1/1/1
4	GLA	O	2	4	-	1/2/19/22	0/1/1/1

There are no bond length outliers.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	O	1	EGA	C7-O1-C1	4.18	123.35	113.92
4	K	1	EGA	C7-O1-C1	4.17	123.32	113.92
4	G	1	EGA	C7-O1-C1	4.06	123.09	113.92
4	J	1	EGA	C7-O1-C1	3.88	122.67	113.92
3	F	3	NAG	C2-N2-C7	-2.41	119.47	122.90

There are no chirality outliers.

5 of 50 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	1	NAG	O7-C7-N2-C2
2	H	1	NAG	C8-C7-N2-C2
2	H	1	NAG	O7-C7-N2-C2
2	M	1	NAG	C8-C7-N2-C2
2	M	1	NAG	O7-C7-N2-C2

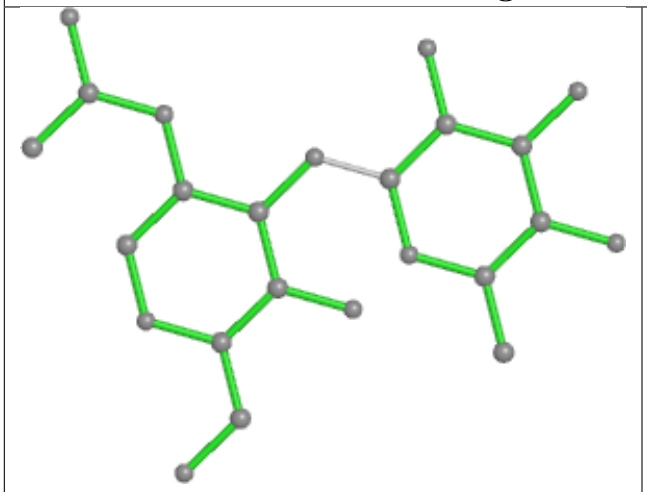
There are no ring outliers.

12 monomers are involved in 12 short contacts:

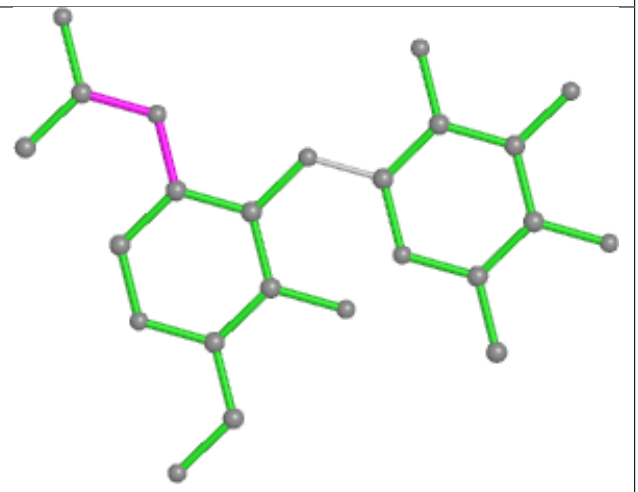
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	K	2	GLA	1	0
3	N	2	FUC	1	0
3	F	3	NAG	1	0
2	E	1	NAG	1	0
3	F	2	FUC	1	0
3	N	1	NAG	2	0
3	F	1	NAG	2	0
2	M	1	NAG	1	0
3	N	3	NAG	1	0
2	H	1	NAG	3	0
5	I	2	NAG	2	0
5	I	1	NAG	1	0

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

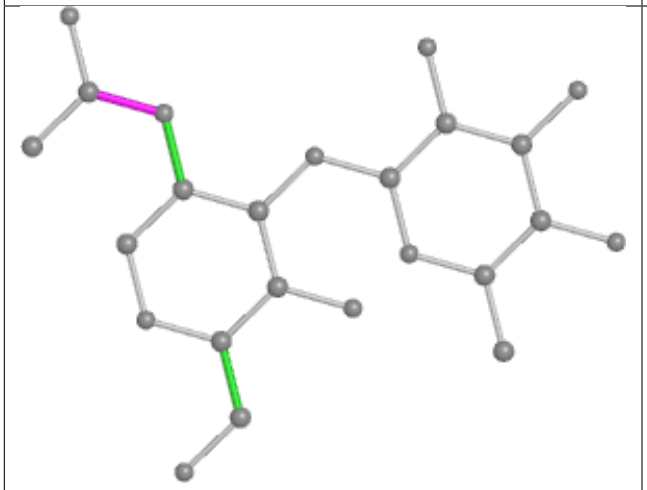
Oligosaccharide Chain E



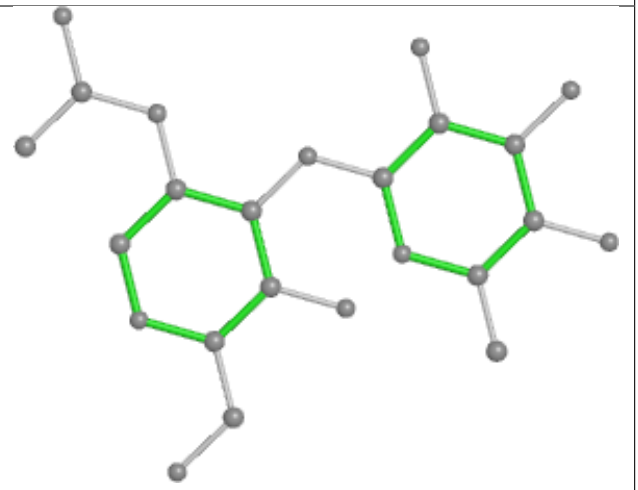
Bond lengths



Bond angles

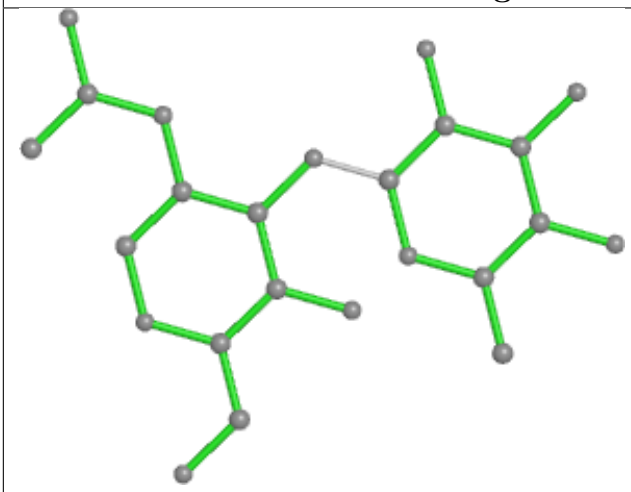


Torsions

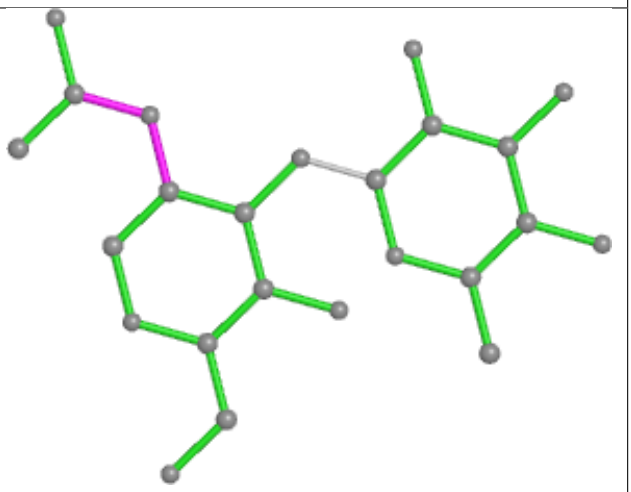


Rings

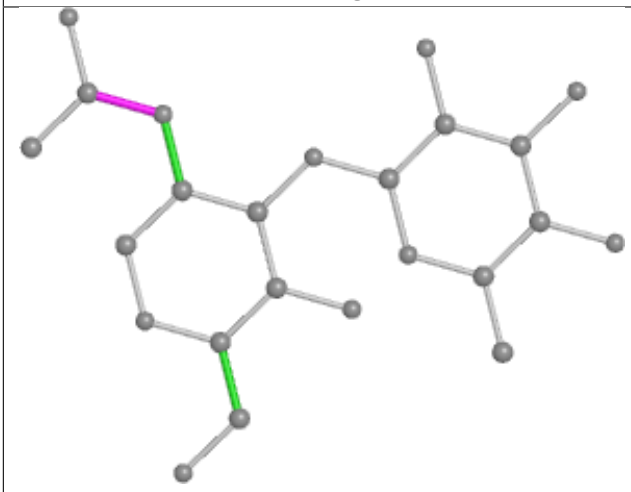
Oligosaccharide Chain H



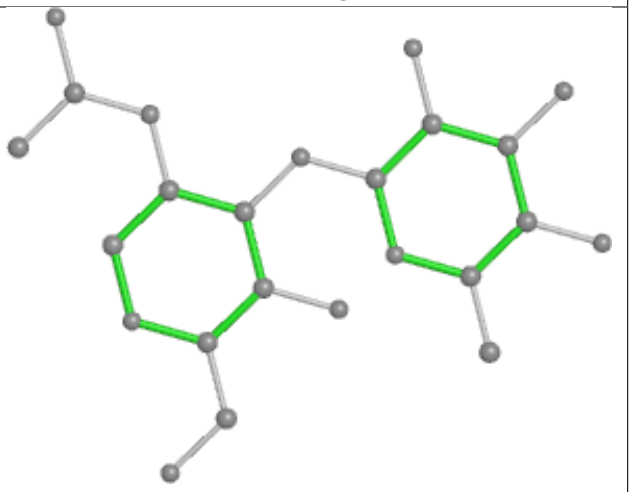
Bond lengths



Bond angles

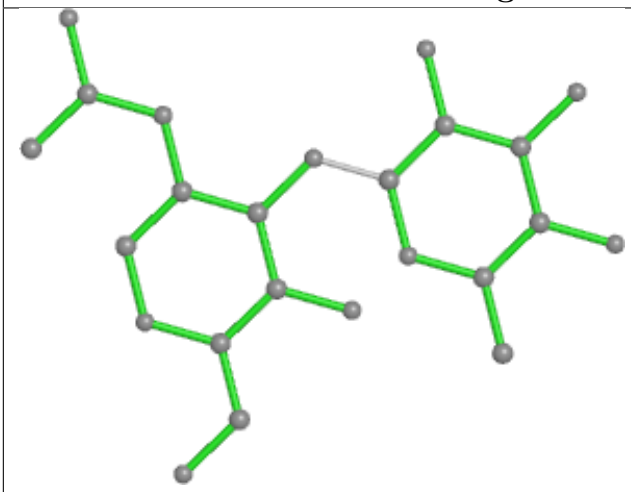


Torsions

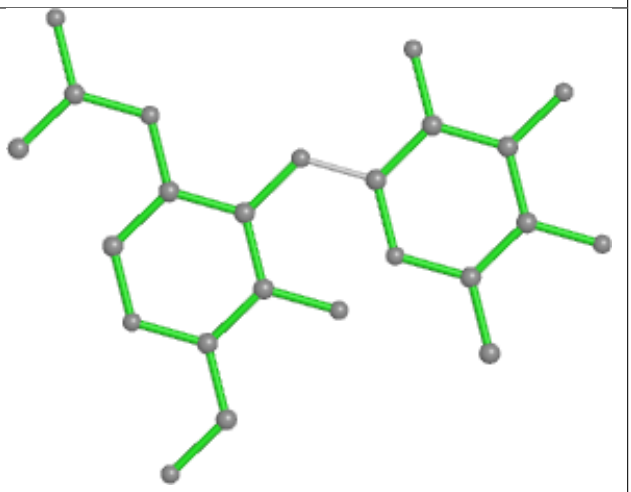


Rings

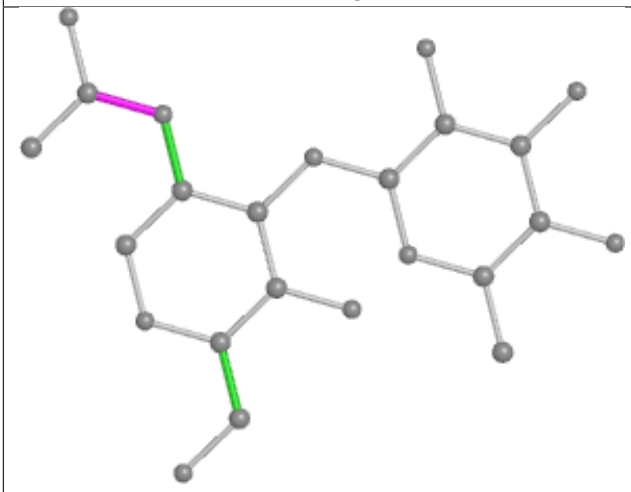
Oligosaccharide Chain L



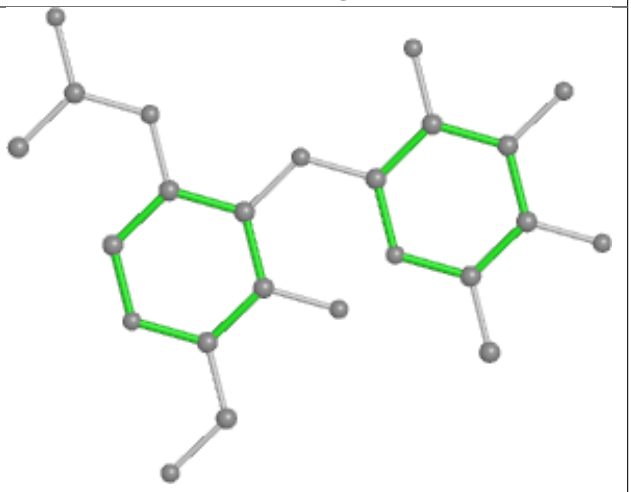
Bond lengths



Bond angles

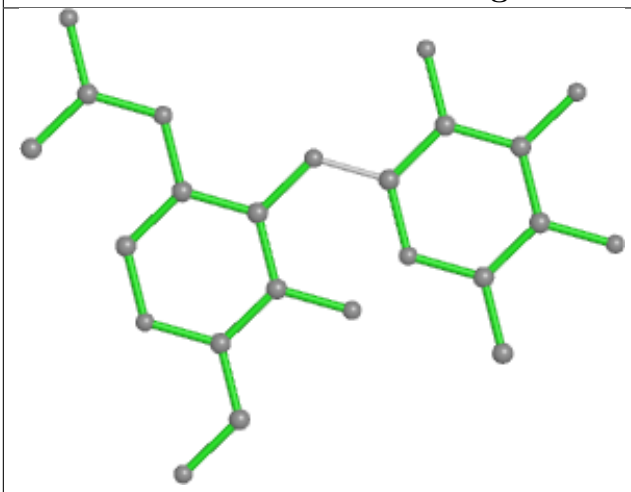


Torsions

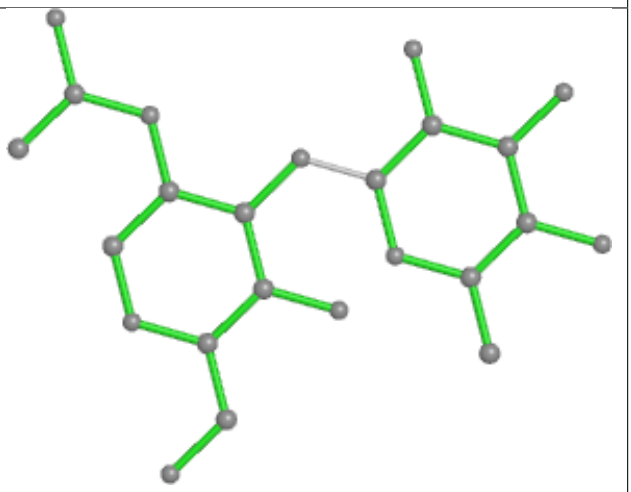


Rings

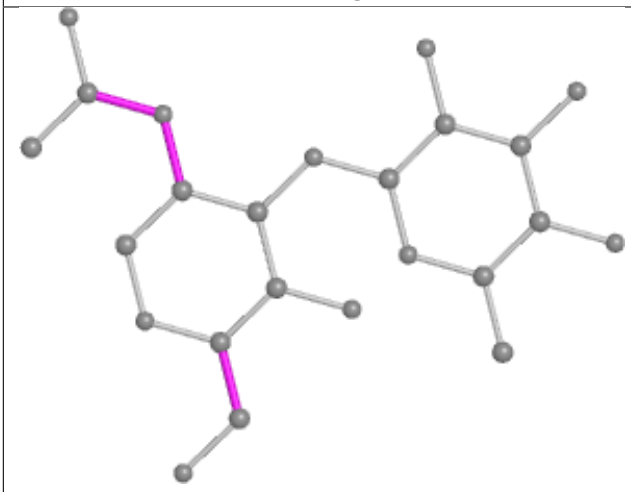
Oligosaccharide Chain M



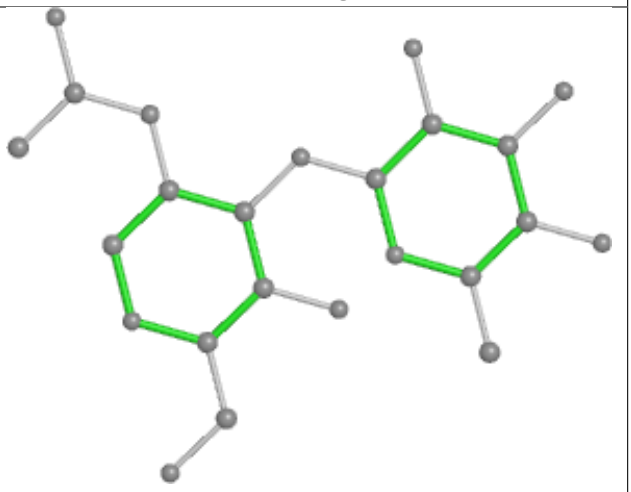
Bond lengths



Bond angles

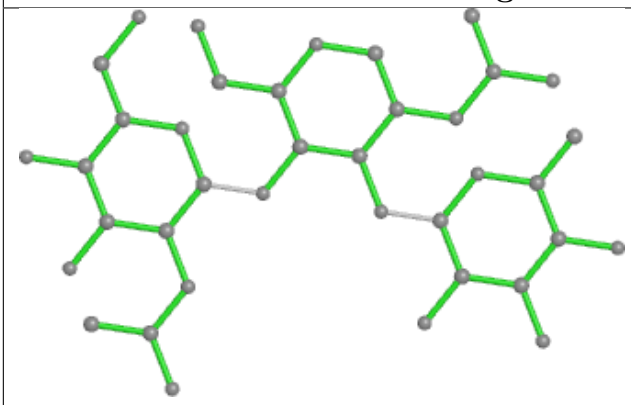


Torsions

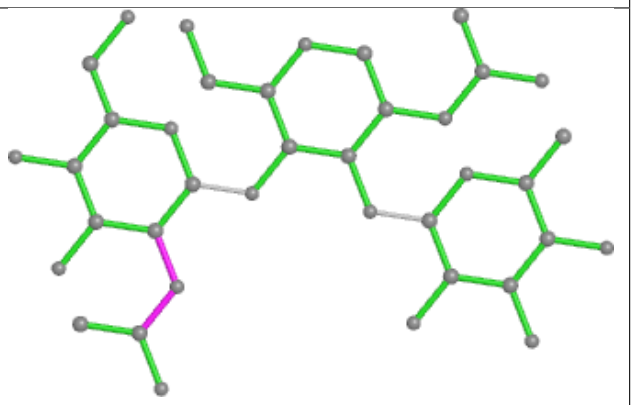


Rings

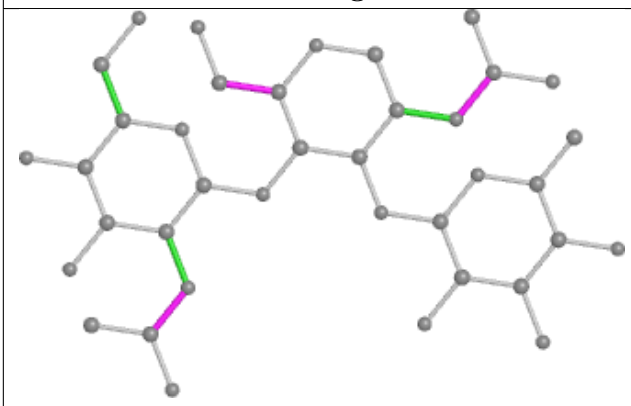
Oligosaccharide Chain F



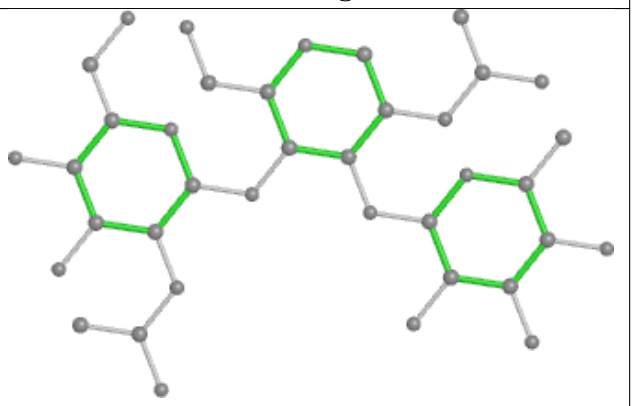
Bond lengths



Bond angles

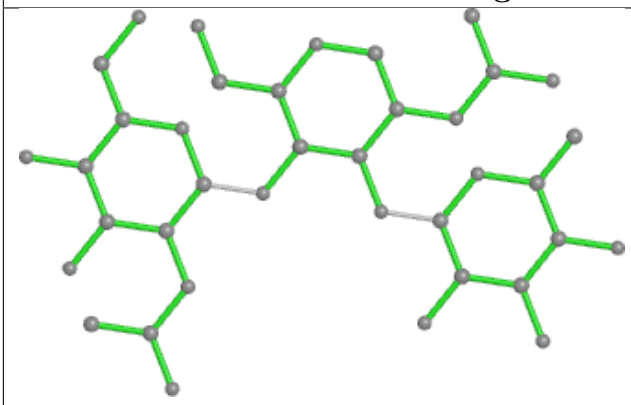


Torsions

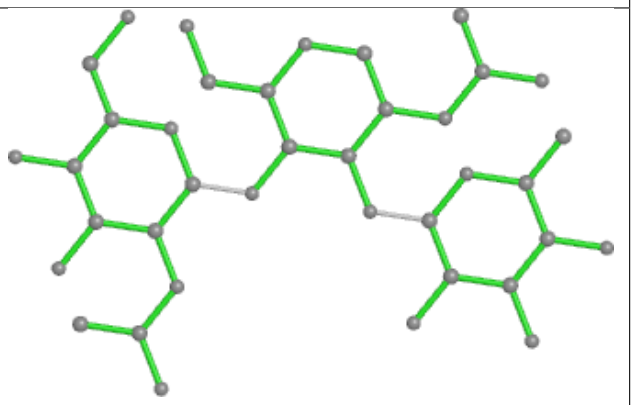


Rings

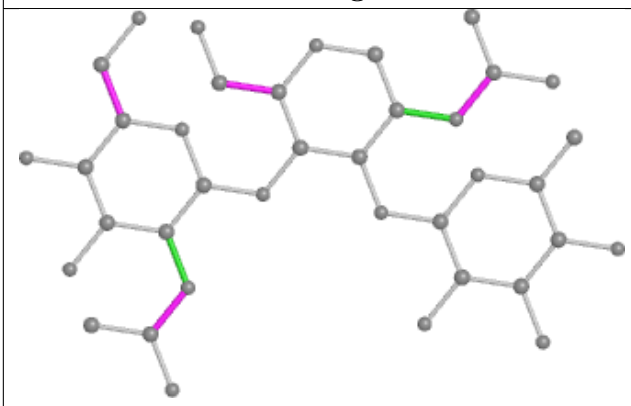
Oligosaccharide Chain N



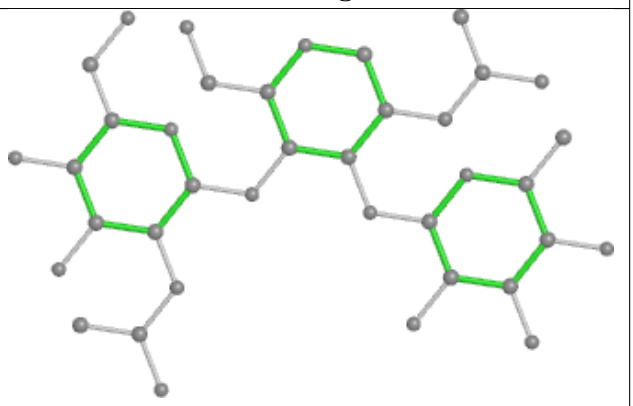
Bond lengths



Bond angles

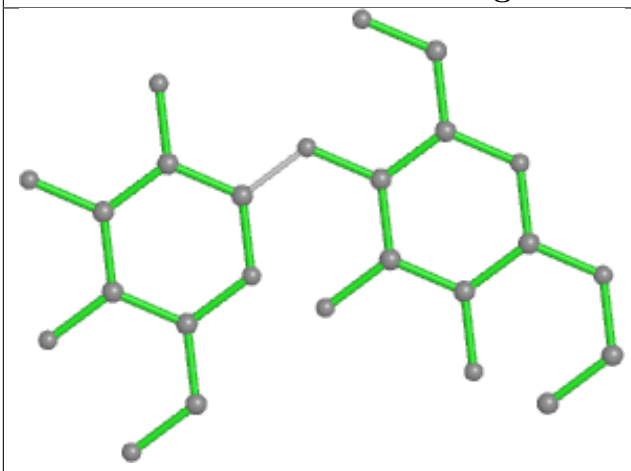


Torsions

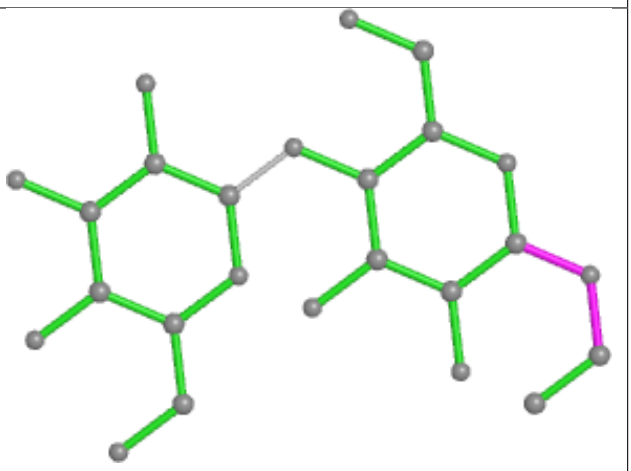


Rings

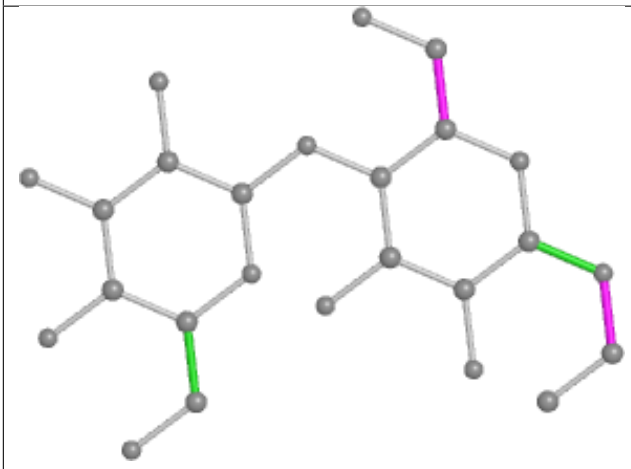
Oligosaccharide Chain G



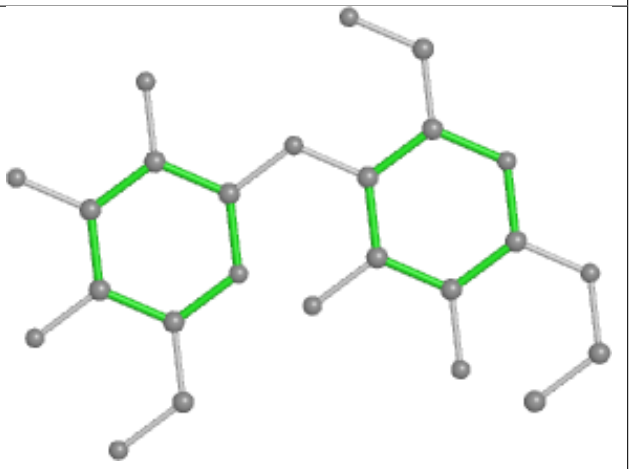
Bond lengths



Bond angles

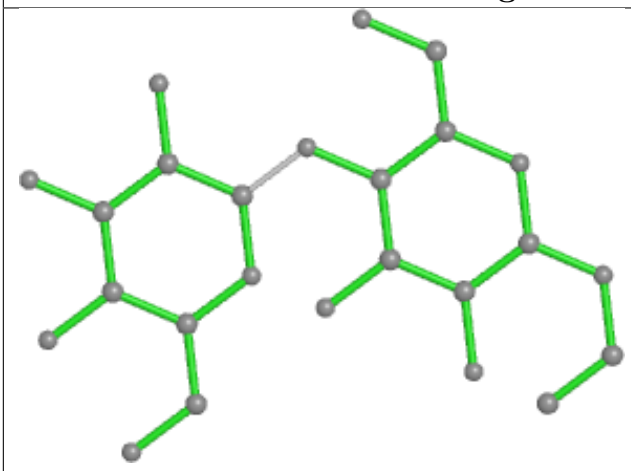


Torsions

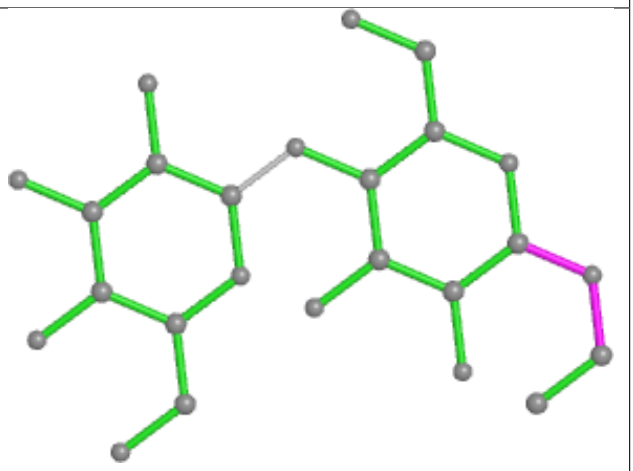


Rings

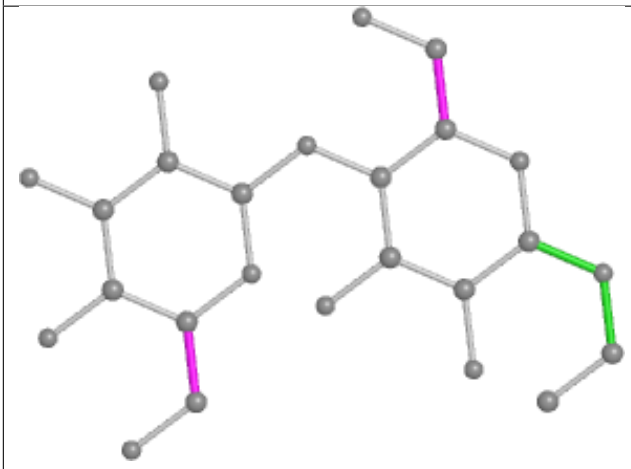
Oligosaccharide Chain J



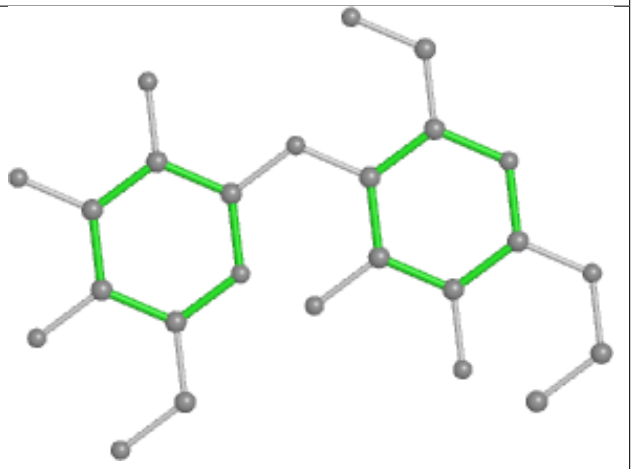
Bond lengths



Bond angles

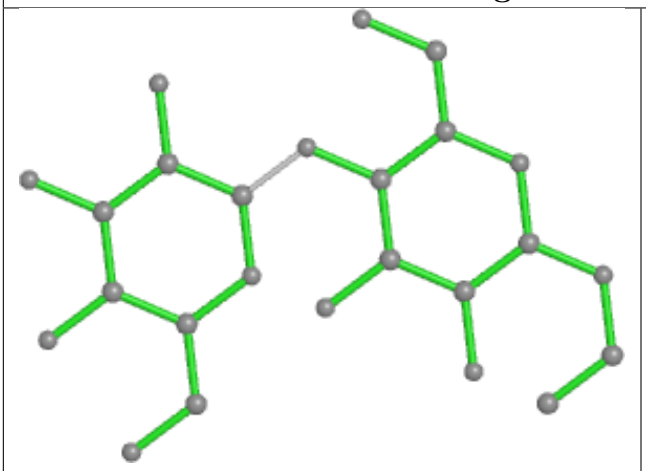


Torsions

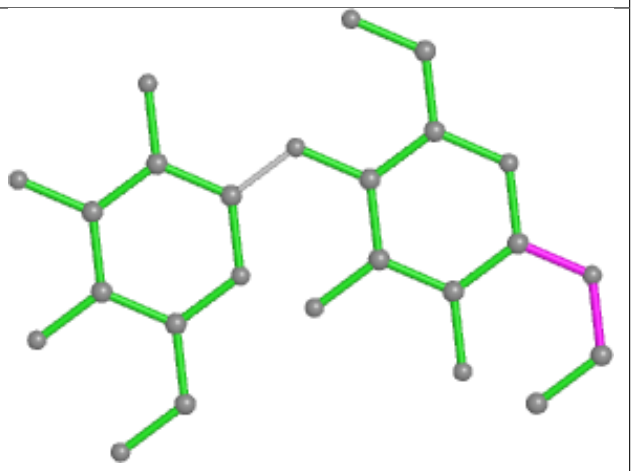


Rings

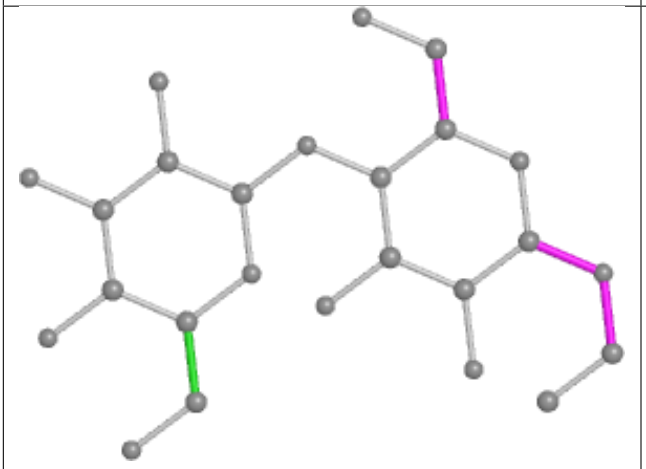
Oligosaccharide Chain K



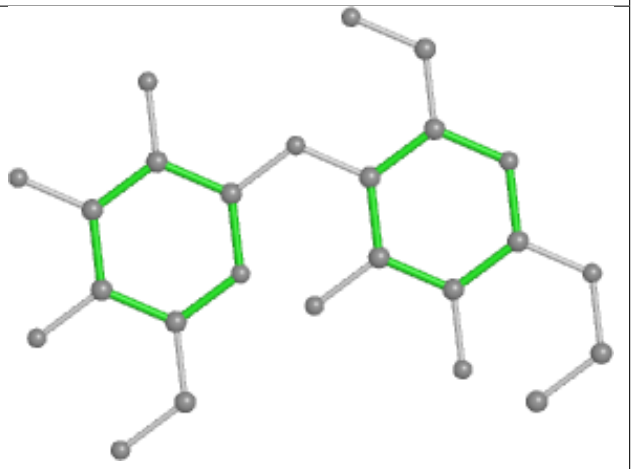
Bond lengths



Bond angles

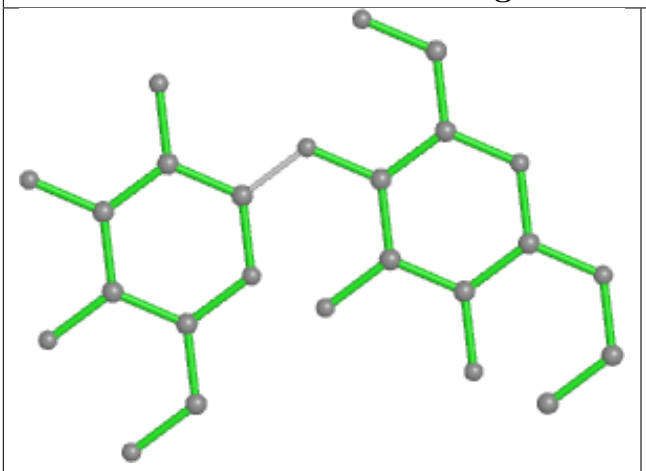


Torsions

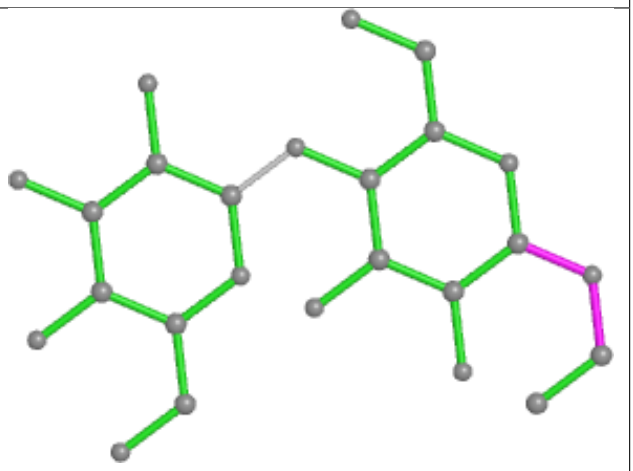


Rings

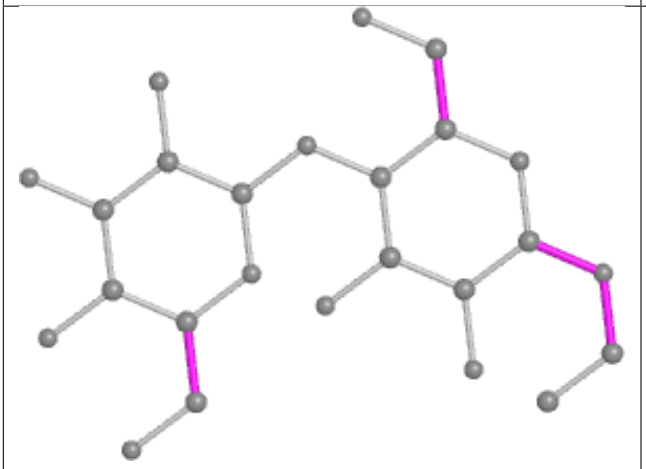
Oligosaccharide Chain O



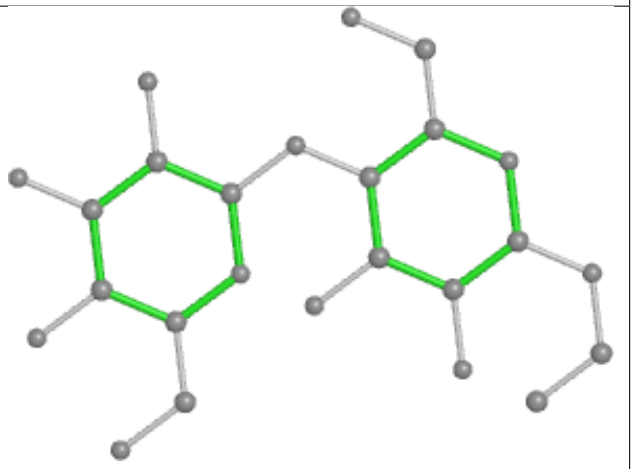
Bond lengths



Bond angles

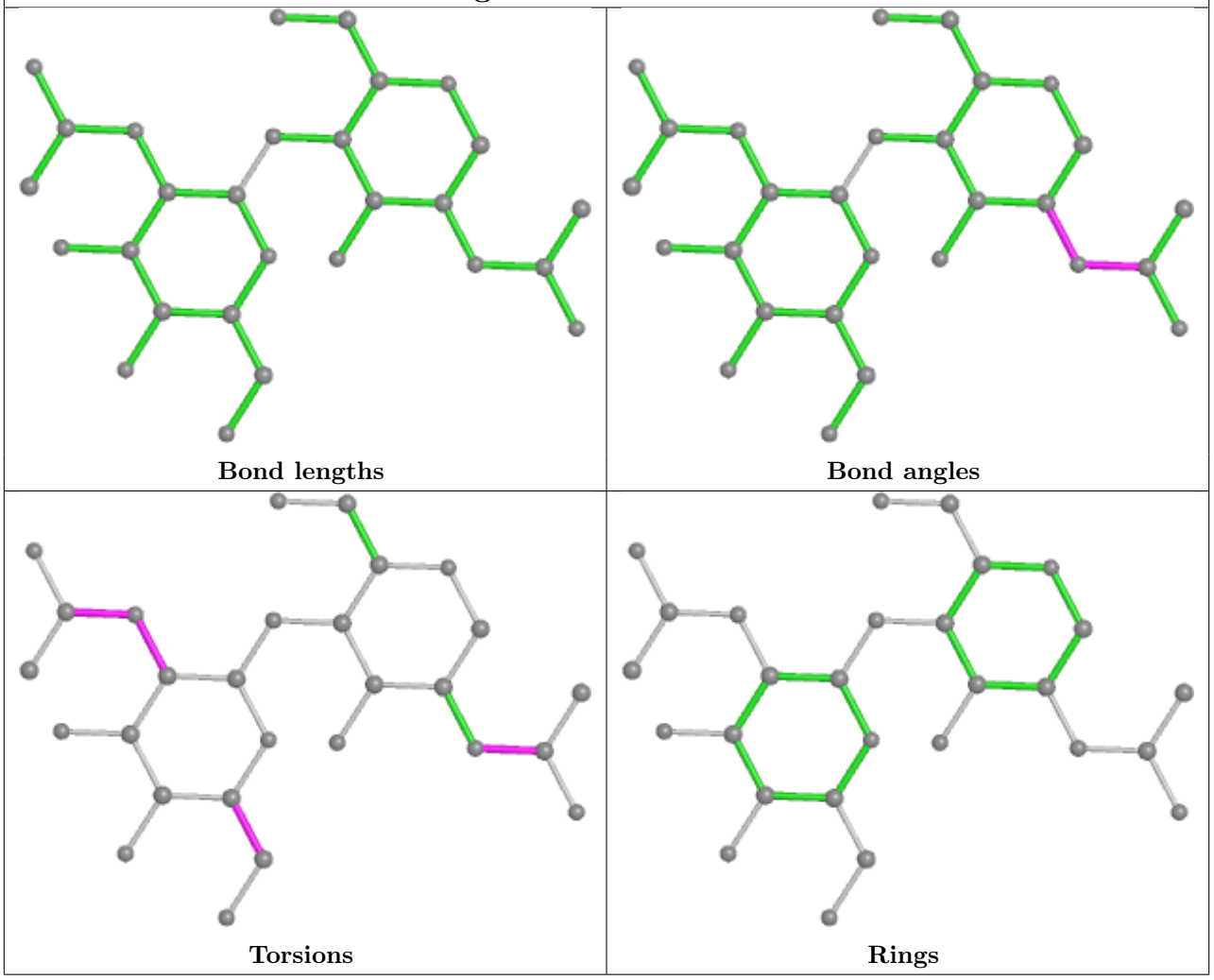


Torsions



Rings

Oligosaccharide Chain I



5.6 Ligand geometry (i)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
8	NAG	C	305	1	14,14,15	0.77	0	17,19,21	1.07	1 (5%)
9	BMA	C	306	-	11,11,12	0.77	0	15,15,17	0.75	1 (6%)

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
8	NAG	C	305	1	-	4/6/23/26	0/1/1/1
9	BMA	C	306	-	-	2/2/19/22	1/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	C	306	BMA	C1-O5-C5	2.28	115.28	112.19
8	C	305	NAG	C2-N2-C7	-2.13	119.87	122.90

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	C	306	BMA	O5-C5-C6-O6
8	C	305	NAG	C8-C7-N2-C2
8	C	305	NAG	O7-C7-N2-C2
8	C	305	NAG	O5-C5-C6-O6
9	C	306	BMA	C4-C5-C6-O6

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	C	306	BMA	C1-C2-C3-C4-C5-O5

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	237/241 (98%)	0.08	10 (4%)	36	39	26, 40, 62, 74	0
1	B	237/241 (98%)	0.04	3 (1%)	77	79	27, 41, 63, 70	0
1	C	237/241 (98%)	0.07	6 (2%)	57	61	29, 41, 64, 87	0
1	D	237/241 (98%)	0.19	16 (6%)	17	17	29, 43, 66, 80	0
All	All	948/964 (98%)	0.09	35 (3%)	41	45	26, 42, 64, 87	0

The worst 5 of 35 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	237	GLY	5.8
1	D	40	VAL	4.5
1	D	114	SER	4.5
1	C	13	ASN	4.3
1	D	36	VAL	4.1

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

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

6.3 Carbohydrates

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NAG	M	1	14/15	0.62	0.33	87,93,96,100	0
3	NAG	N	3	14/15	0.69	0.32	92,94,94,96	0

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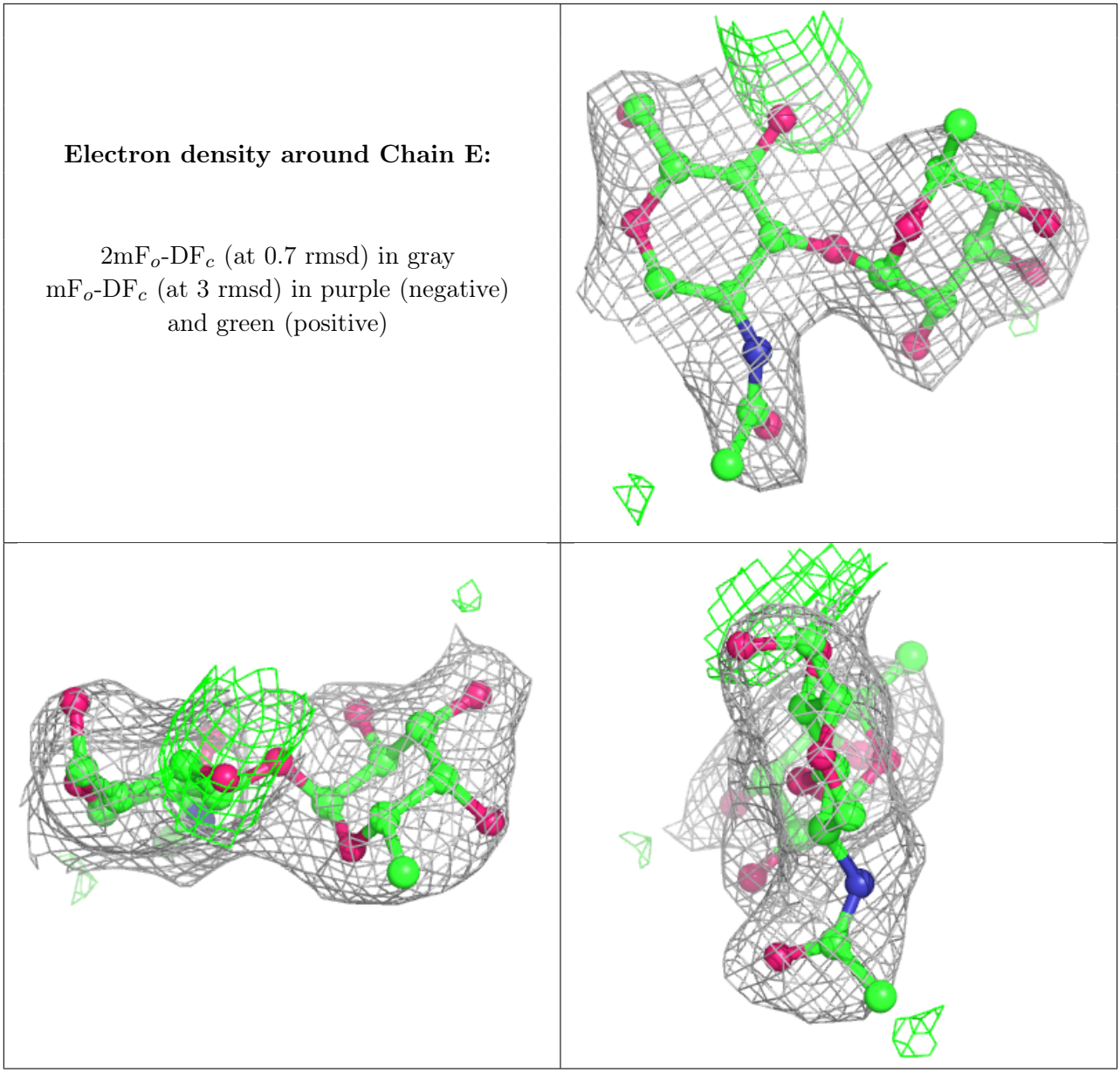
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	FUC	M	2	10/11	0.71	0.33	98,99,99,100	0
4	GLA	O	2	11/12	0.76	0.28	80,82,84,87	0
3	FUC	F	2	10/11	0.77	0.27	84,86,87,88	0
5	NAG	I	2	14/15	0.78	0.38	87,91,92,93	0
3	FUC	N	2	10/11	0.80	0.31	93,95,95,96	0
3	NAG	F	3	14/15	0.81	0.25	87,89,90,92	0
4	EGA	O	1	14/14	0.82	0.26	82,84,86,89	0
2	NAG	E	1	14/15	0.83	0.17	63,64,68,73	0
5	NAG	I	1	14/15	0.85	0.27	61,71,79,82	0
2	NAG	L	1	14/15	0.85	0.18	67,70,73,77	0
2	FUC	H	2	10/11	0.86	0.26	82,83,85,86	0
2	NAG	H	1	14/15	0.86	0.25	73,76,81,82	0
2	FUC	L	2	10/11	0.89	0.25	80,82,83,84	0
4	EGA	K	1	14/14	0.90	0.19	60,61,61,62	0
3	NAG	N	1	14/15	0.91	0.20	77,81,89,89	0
4	GLA	K	2	11/12	0.91	0.19	58,59,62,62	0
3	NAG	F	1	14/15	0.92	0.18	70,73,81,83	0
4	EGA	G	1	14/14	0.92	0.21	53,57,59,60	0
4	EGA	J	1	14/14	0.93	0.16	46,50,52,52	0
4	GLA	G	2	11/12	0.94	0.13	50,52,56,58	0
2	FUC	E	2	10/11	0.94	0.18	67,69,69,70	0
4	GLA	J	2	11/12	0.94	0.13	43,45,48,51	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.

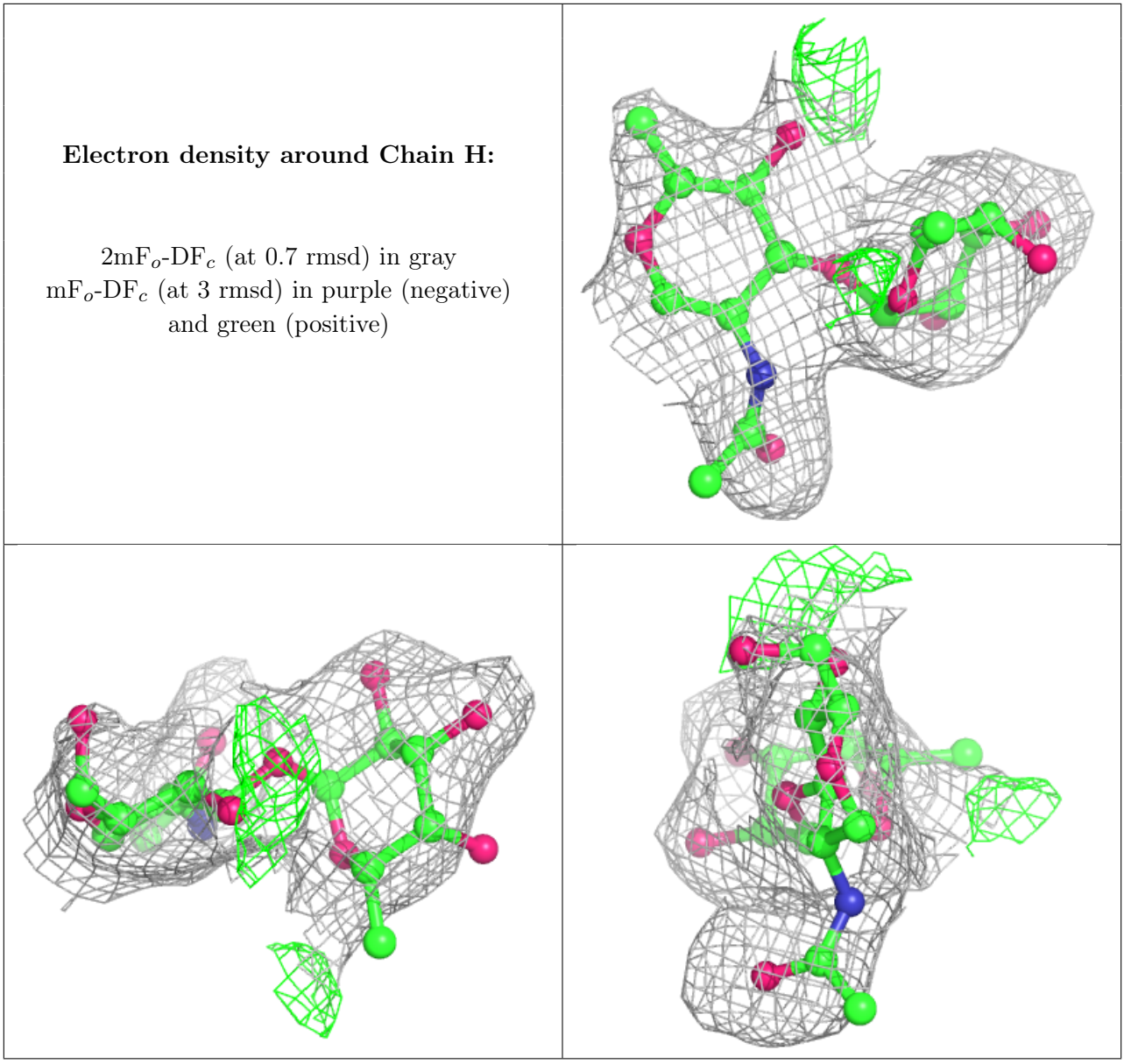
Electron density around Chain E:

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



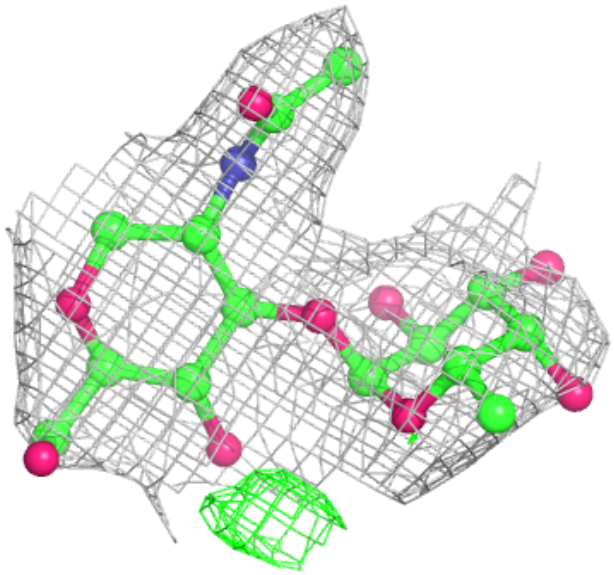
Electron density around Chain H:

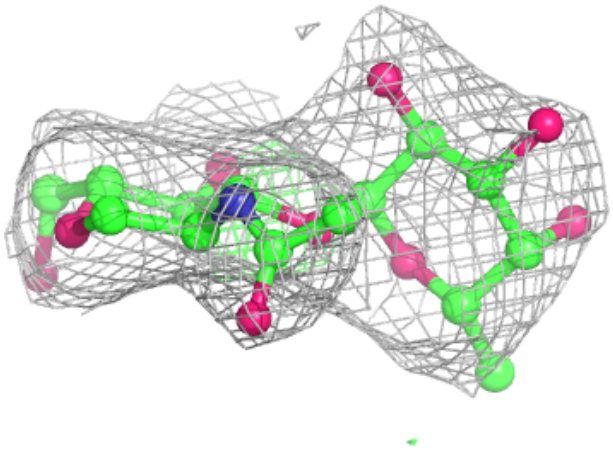
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

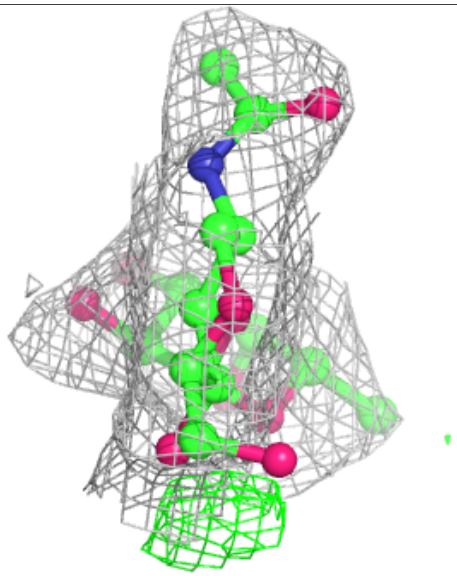


Electron density around Chain L:

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

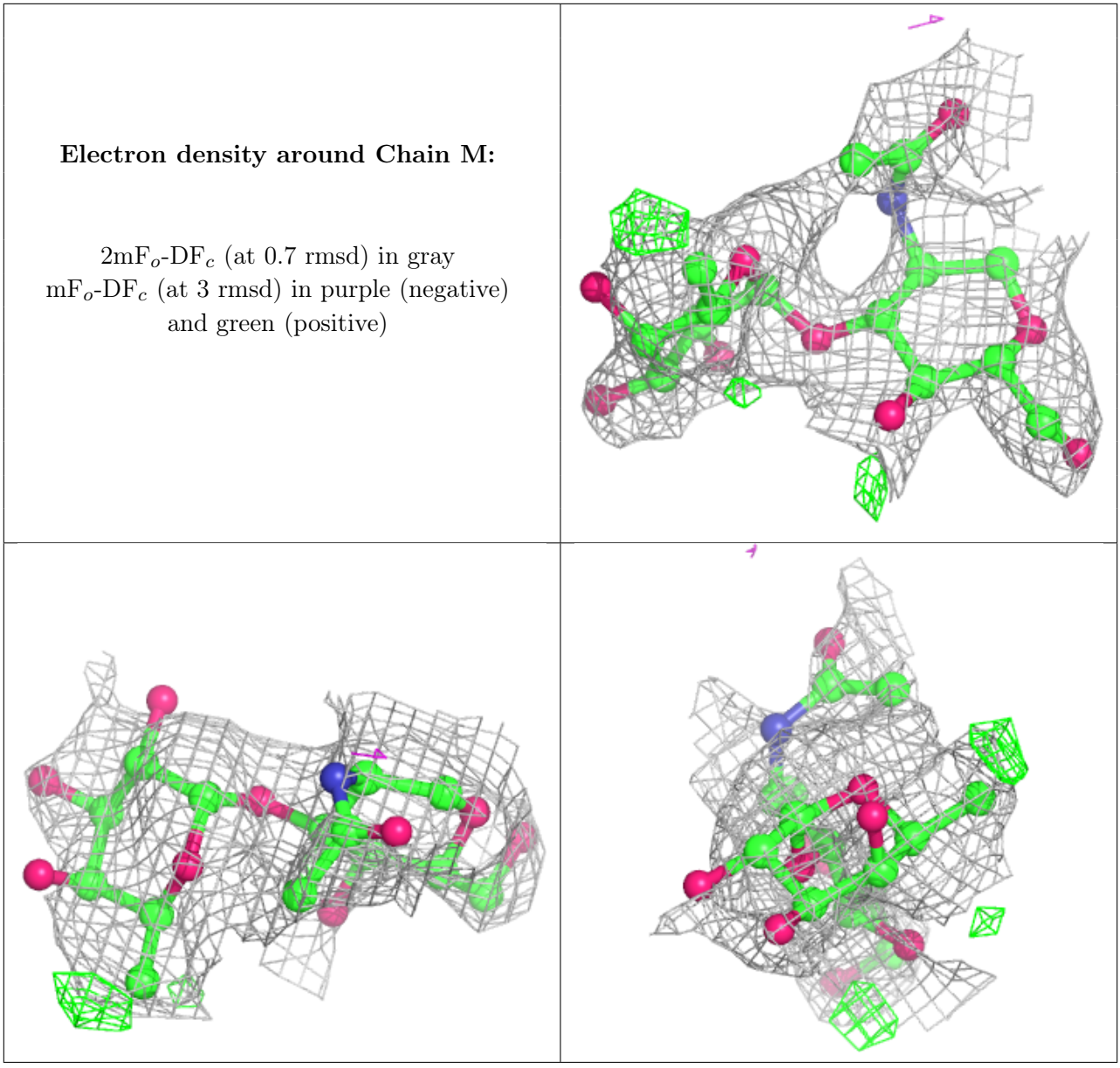






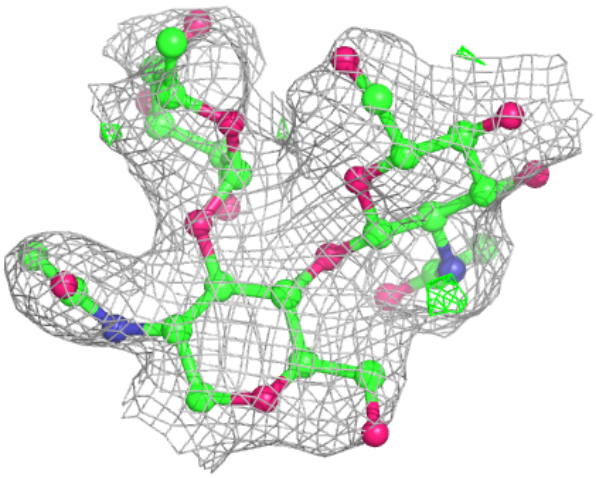
Electron density around Chain M:

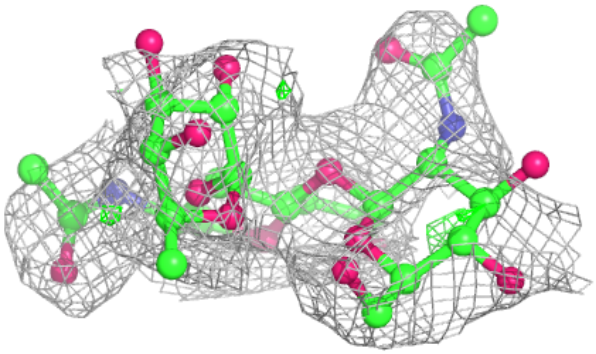
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

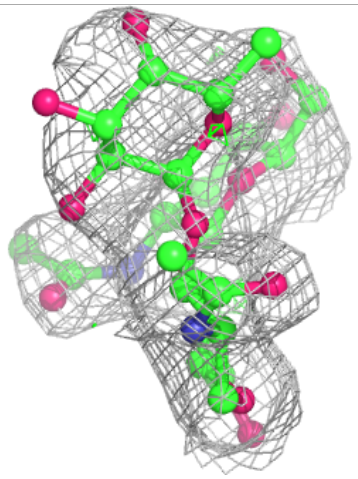


Electron density around Chain F:

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

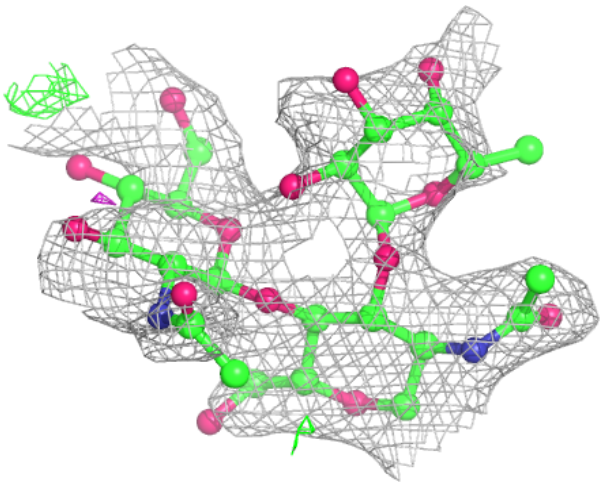


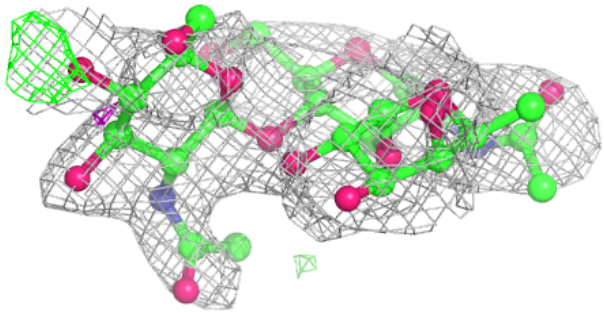


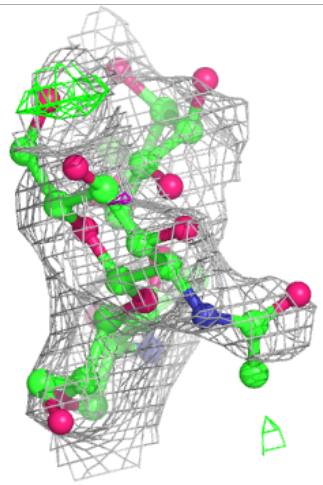


Electron density around Chain N:

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

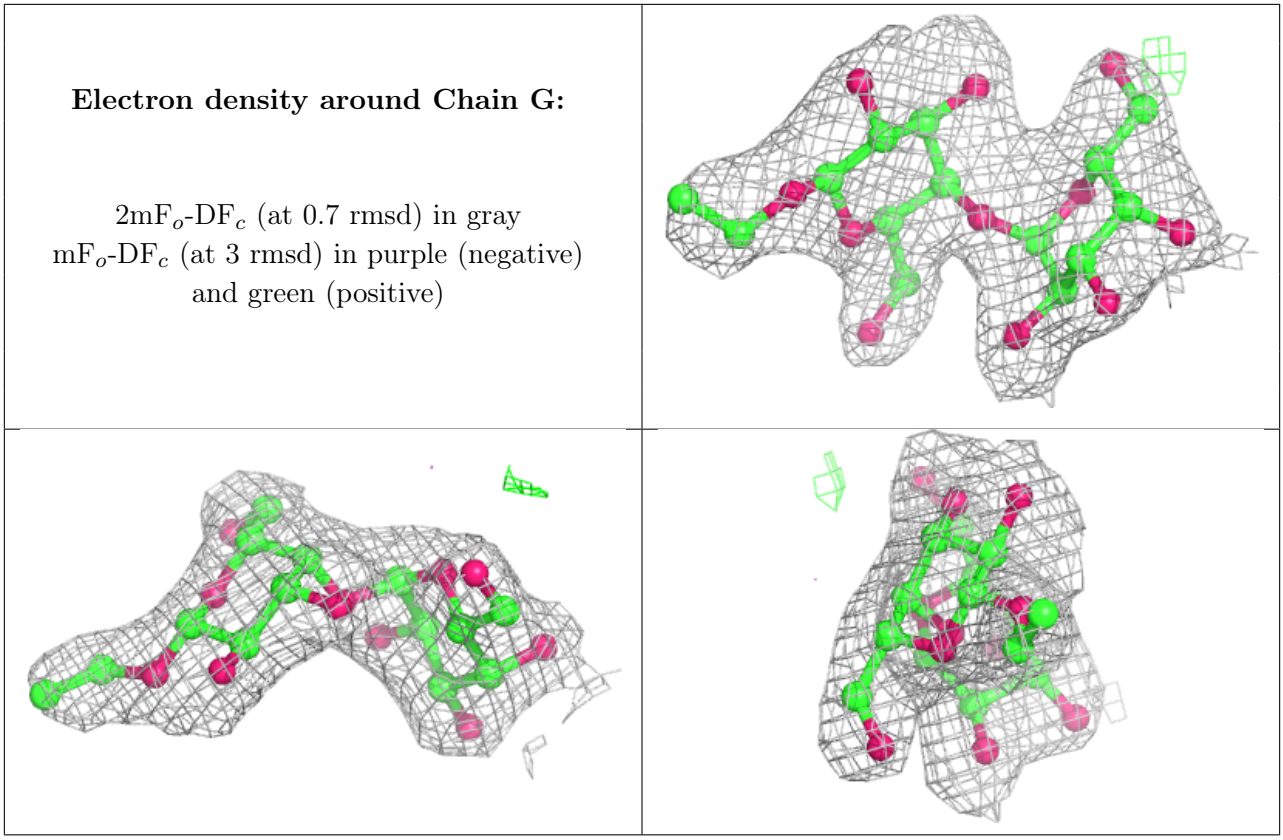






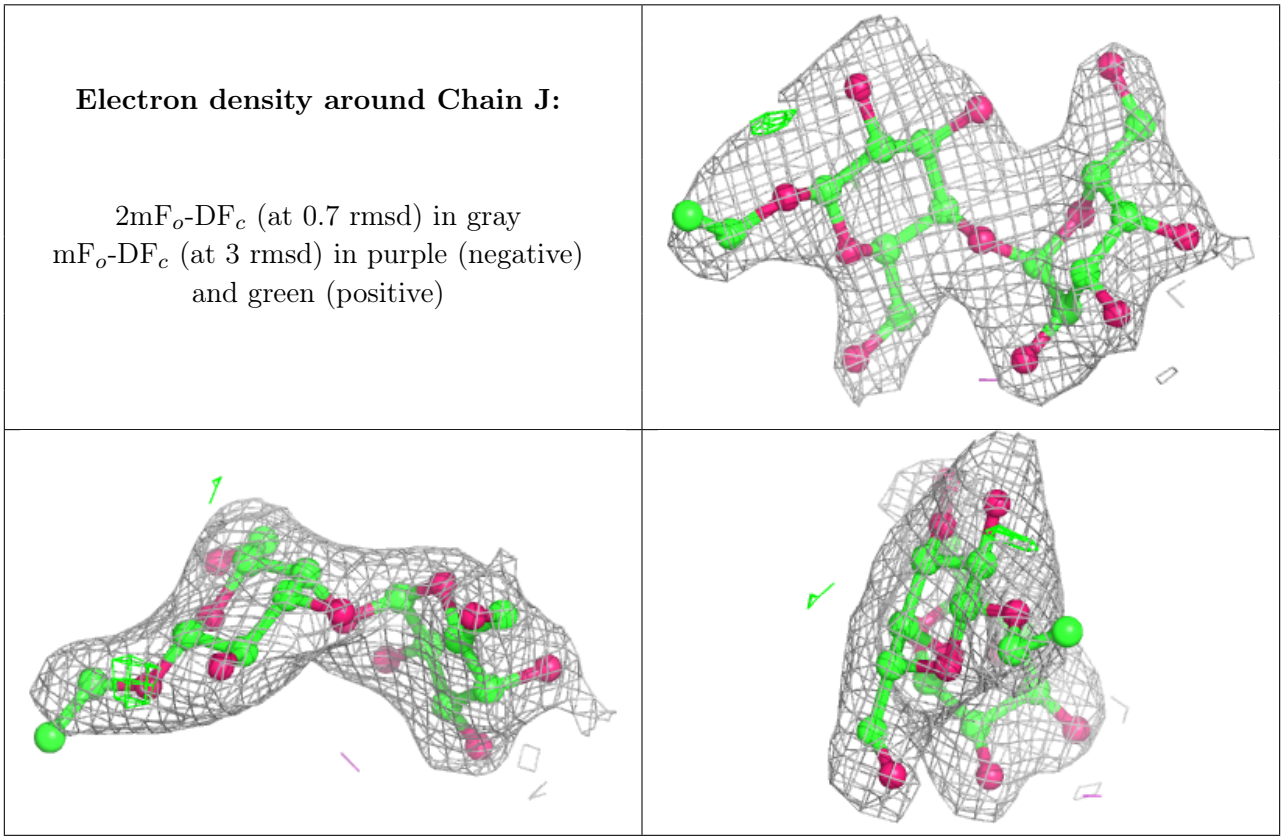
Electron density around Chain G:

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



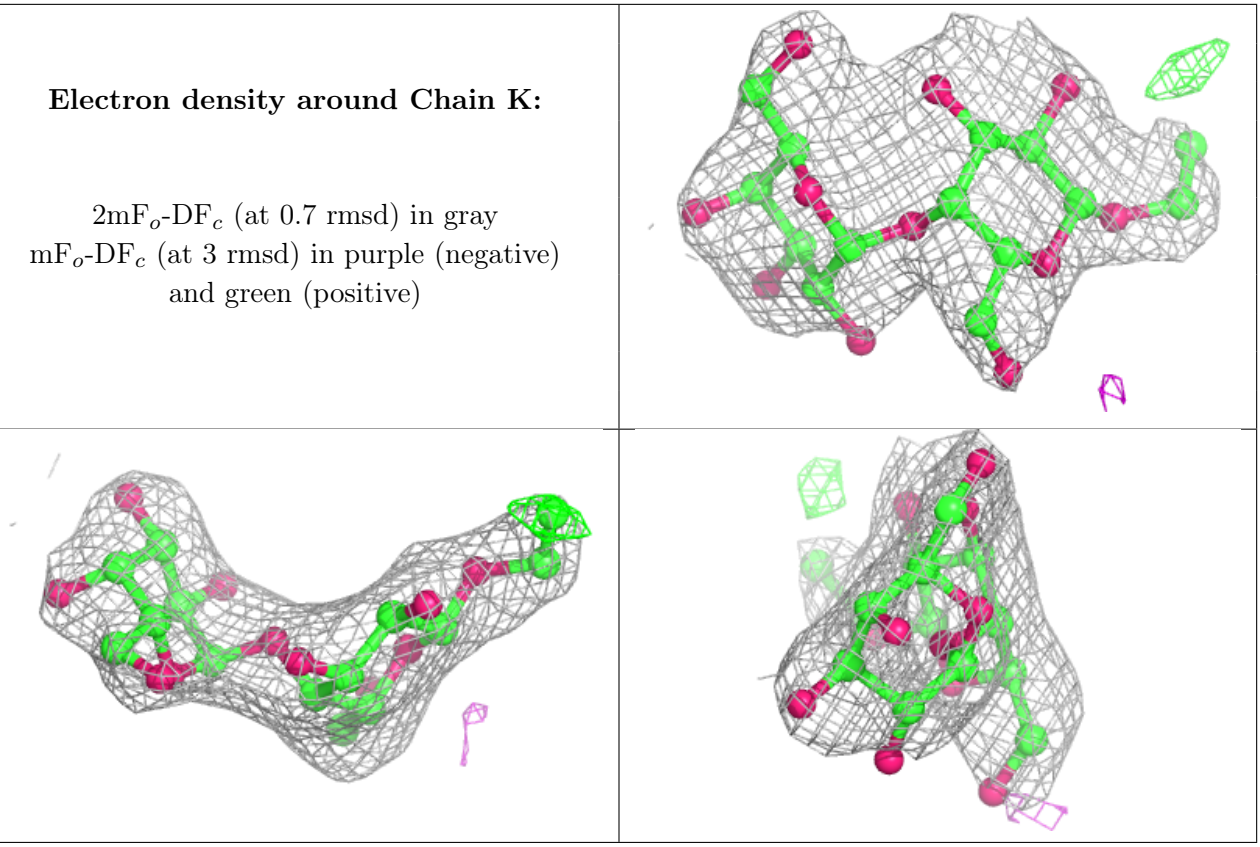
Electron density around Chain J:

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



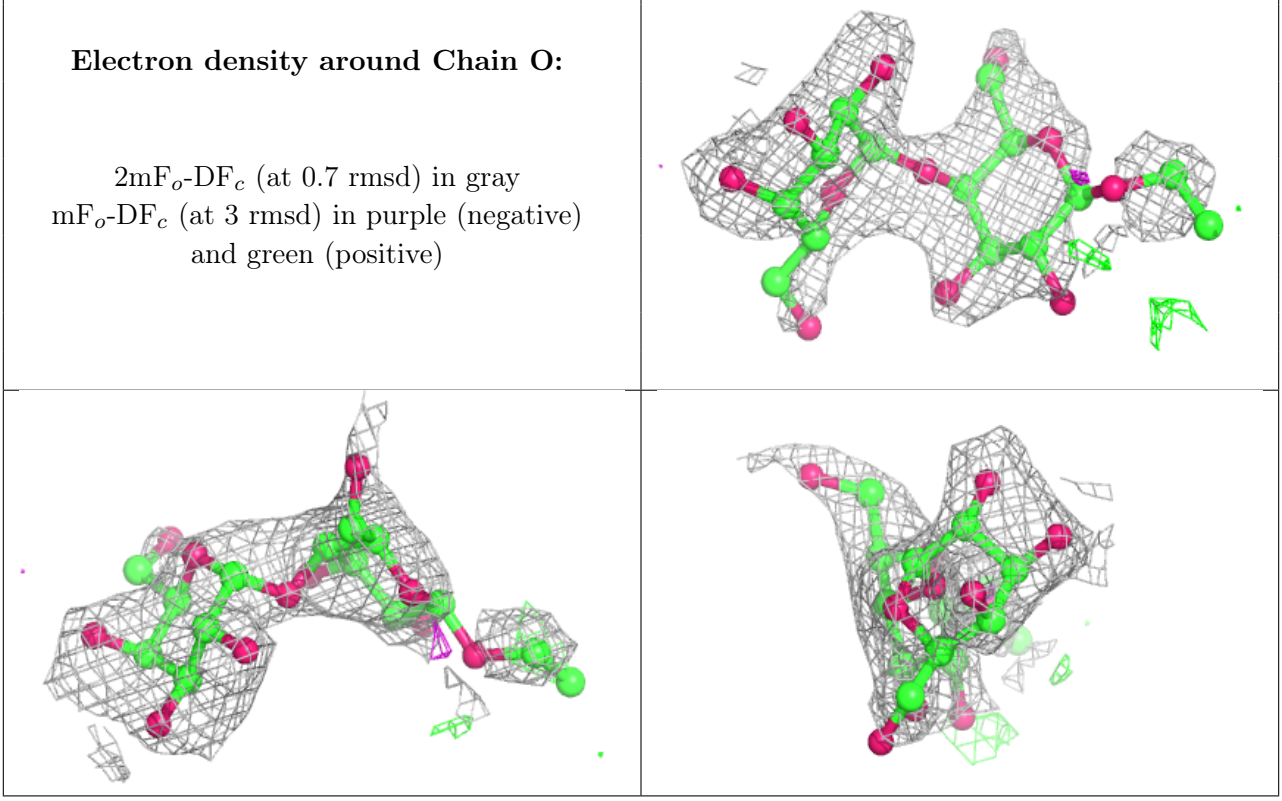
Electron density around Chain K:

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



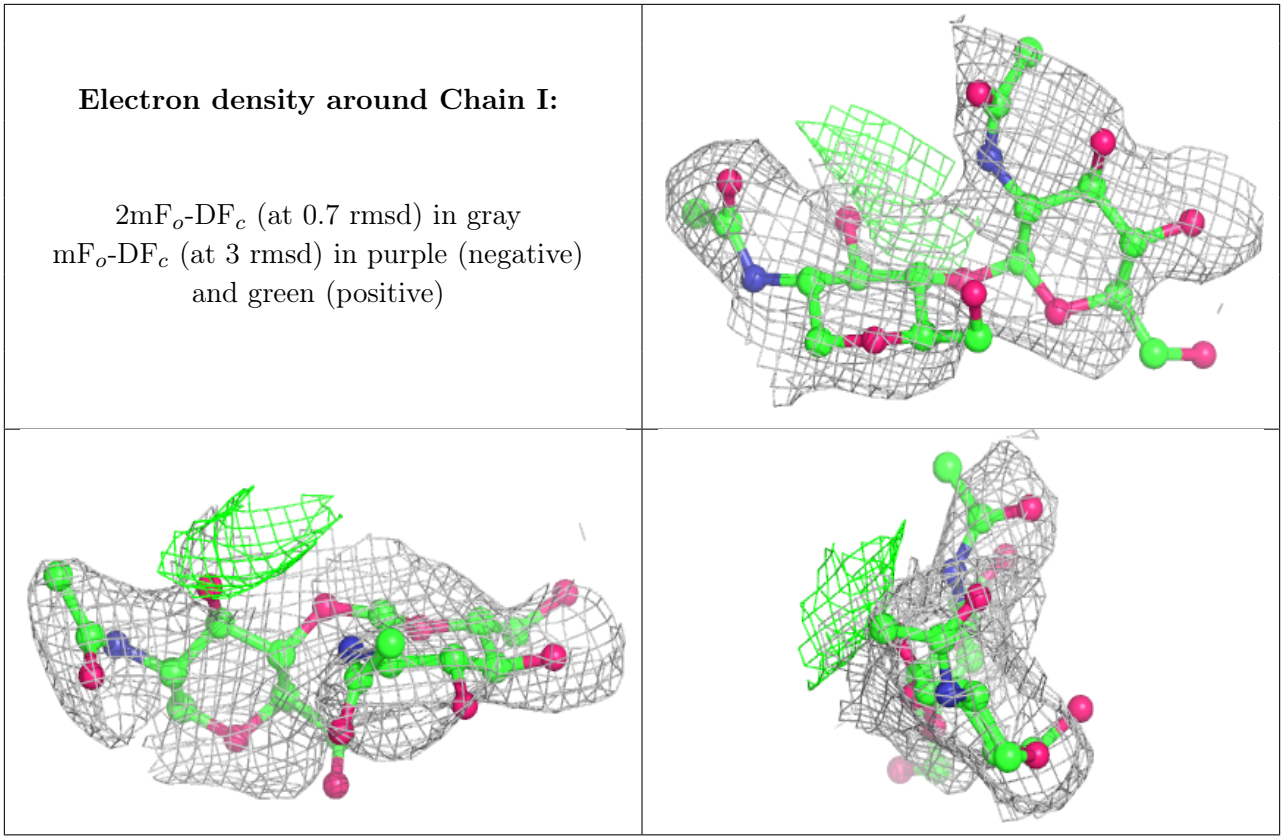
Electron density around Chain O:

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



Electron density around Chain I:

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



6.4 Ligands

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
8	NAG	C	305	14/15	0.71	0.24	69,71,76,78	0
9	BMA	C	306	11/12	0.74	0.22	86,86,87,88	0
7	CA	D	302	1/1	0.93	0.18	44,44,44,44	0
7	CA	A	302	1/1	0.97	0.15	34,34,34,34	0
7	CA	C	302	1/1	0.98	0.17	40,40,40,40	0
7	CA	B	302	1/1	0.98	0.19	39,39,39,39	0
6	MN	C	301	1/1	0.99	0.11	50,50,50,50	0
6	MN	D	301	1/1	0.99	0.04	44,44,44,44	0
6	MN	A	301	1/1	0.99	0.06	48,48,48,48	0
6	MN	B	301	1/1	0.99	0.06	40,40,40,40	0

6.5 Other polymers

There are no such residues in this entry.