Full wwPDB X-ray Structure Validation Report (i)

Jun 24, 2024 – 11:53 PM EDT

PDB ID	:	5YQS
Title	:	Isoprimeverose-producing enzyme from Aspergillus oryzae in complex with isoprimeverose
Authors	:	Yaoi, K.; Matsuzawa, T.; Watanabe, M.; Nakamichi, Y.
Deposited on	:	2017-11-07
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 (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:

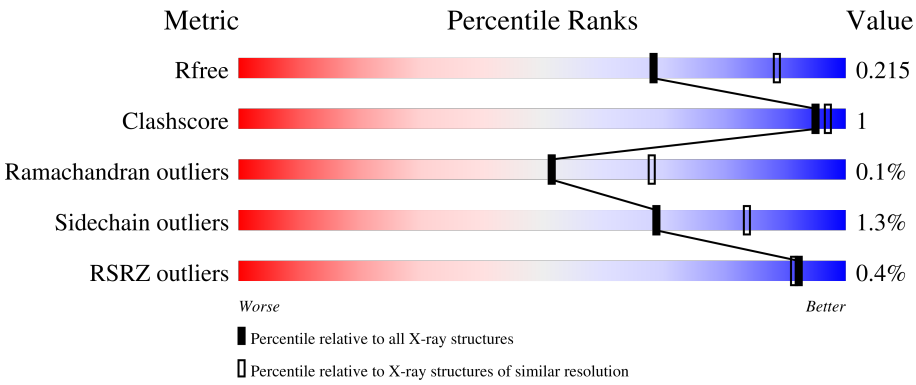
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 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))
R_{free}	130704	3907 (2.40-2.40)
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 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	765	94%
1	B	765	% 95%
2	C	2	100%
2	D	2	50% 50%
2	E	2	100%

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

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	J	2	-	-	-	X
3	XYS	H	2	-	-	-	X
3	XYS	N	2	-	-	-	X

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 12656 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 Isoprimeverose-producing enzyme.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	754	5835	3719	972	1125	19	0	1	0
1	B	754	5835	3719	972	1125	19	0	1	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	780	VAL	-	expression tag	UNP Q2U8V9
A	781	ASP	-	expression tag	UNP Q2U8V9
A	782	HIS	-	expression tag	UNP Q2U8V9
A	783	HIS	-	expression tag	UNP Q2U8V9
A	784	HIS	-	expression tag	UNP Q2U8V9
A	785	HIS	-	expression tag	UNP Q2U8V9
A	786	HIS	-	expression tag	UNP Q2U8V9
A	787	HIS	-	expression tag	UNP Q2U8V9
B	780	VAL	-	expression tag	UNP Q2U8V9
B	781	ASP	-	expression tag	UNP Q2U8V9
B	782	HIS	-	expression tag	UNP Q2U8V9
B	783	HIS	-	expression tag	UNP Q2U8V9
B	784	HIS	-	expression tag	UNP Q2U8V9
B	785	HIS	-	expression tag	UNP Q2U8V9
B	786	HIS	-	expression tag	UNP Q2U8V9
B	787	HIS	-	expression tag	UNP Q2U8V9

- 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
			Total	C	N	O			
2	C	2	28	16	2	10	0	0	0
2	D	2	28	16	2	10	0	0	0
2	E	2	28	16	2	10	0	0	0
2	I	2	28	16	2	10	0	0	0
2	J	2	28	16	2	10	0	0	0
2	K	2	28	16	2	10	0	0	0

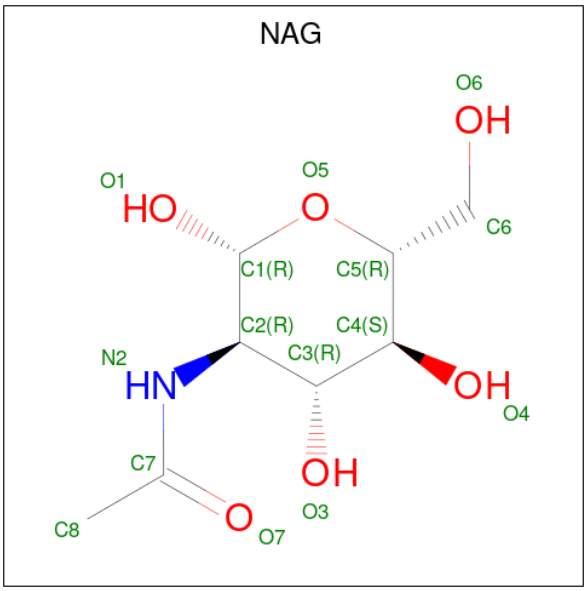
- Molecule 3 is an oligosaccharide called alpha-D-xylopyranose-(1-6)-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
			Total	C	O			
3	F	2	21	11	10	0	0	0
3	H	2	21	11	10	0	0	0
3	L	2	21	11	10	0	0	0
3	N	2	21	11	10	0	0	0

- Molecule 4 is an oligosaccharide called alpha-D-xylopyranose-(1-6)-alpha-D-glucopyranose.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
			Total	C	O			
4	G	2	21	11	10	0	0	0
4	M	2	21	11	10	0	0	0

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).

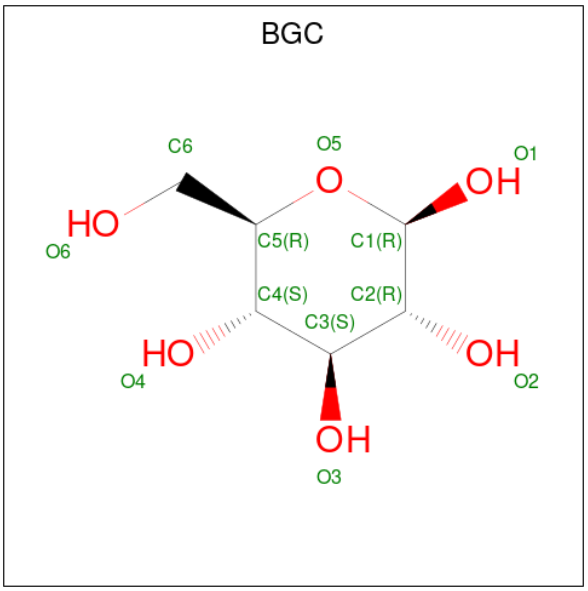


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
5	A	1	14	8	1	5	0	0
			Total	C	N	O		
5	A	1	14	8	1	5	0	0
			Total	C	N	O		
5	A	1	14	8	1	5	0	0
			Total	C	N	O		
5	A	1	14	8	1	5	0	0
			Total	C	N	O		
5	A	1	14	8	1	5	0	0
			Total	C	N	O		
5	B	1	14	8	1	5	0	0
			Total	C	N	O		
5	B	1	14	8	1	5	0	0
			Total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

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 7 is beta-D-glucopyranose (three-letter code: BGC) (formula: $C_6H_{12}O_6$).



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

- Molecule 8 is water.

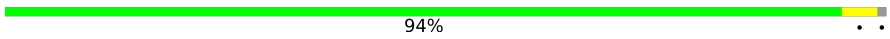
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
8	A	285	285	285	0	0
			Total	O		
8	B	267	267	267	0	0

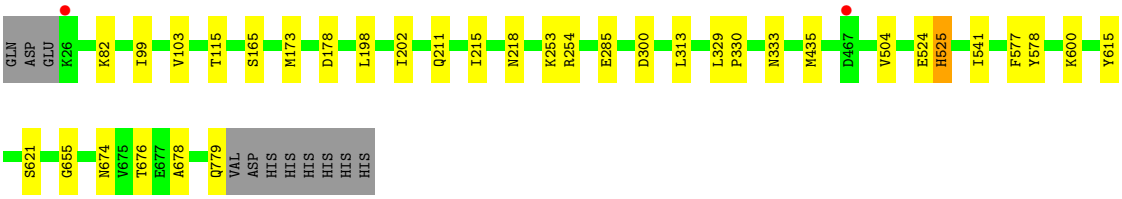
3 Residue-property plots (i)

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: Isoprimeverose-producing enzyme

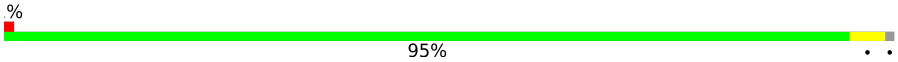
Chain A:

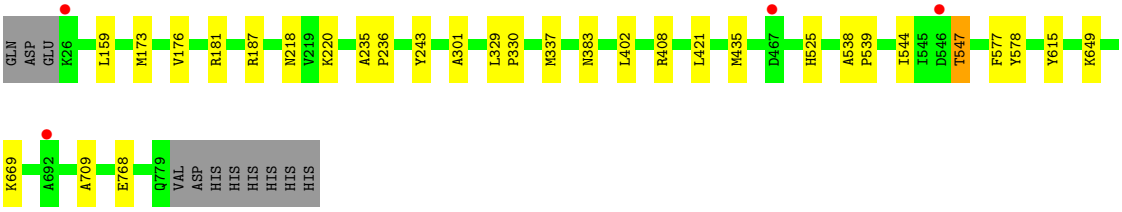




• Molecule 1: Isoprimeverose-producing enzyme

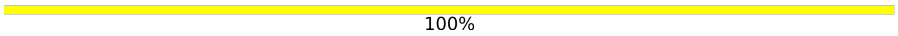
Chain B:





• 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 E: 100%

NAG1
NAG2

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

Chain I: 100%

NAG1
NAG2

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

Chain J: 100%

NAG1
NAG2

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

Chain K: 100%

NAG1
NAG2

• Molecule 3: alpha-D-xylopyranose-(1-6)-beta-D-glucopyranose

Chain F: 50% 50%

BGC1
XYS2

• Molecule 3: alpha-D-xylopyranose-(1-6)-beta-D-glucopyranose

Chain H: 100%

BGC1
XYS2

• Molecule 3: alpha-D-xylopyranose-(1-6)-beta-D-glucopyranose

Chain L: 100%

BGC1
XYS2

• Molecule 3: alpha-D-xylopyranose-(1-6)-beta-D-glucopyranose

Chain N: 50% 50%

BGC1 XYS2

- Molecule 4: alpha-D-xylopyranose-(1-6)-alpha-D-glucopyranose

Chain G: 100%

GLC1 XYS2

- Molecule 4: alpha-D-xylopyranose-(1-6)-alpha-D-glucopyranose

Chain M: 100%

GLC1 XYS2

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	69.79Å 129.91Å 95.16Å 90.00° 94.44° 90.00°	Depositor
Resolution (Å)	30.00 – 2.40 29.78 – 2.40	Depositor EDS
% Data completeness (in resolution range)	90.6 (30.00-2.40) 90.6 (29.78-2.40)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	8.91 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.8.0222	Depositor
R, R_{free}	0.153 , 0.208 0.162 , 0.215	Depositor DCC
R_{free} test set	3061 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å^2)	22.8	Xtriage
Anisotropy	0.019	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 41.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	12656	wwPDB-VP
Average B, all atoms (Å^2)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.64% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: BGC, GLC, CA, NAG, XYS

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	0.61	0/5976	0.77	2/8137 (0.0%)
1	B	0.60	0/5976	0.78	2/8137 (0.0%)
All	All	0.60	0/11952	0.77	4/16274 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	254	ARG	NE-CZ-NH1	6.16	123.38	120.30
1	B	187	ARG	NE-CZ-NH2	-5.46	117.57	120.30
1	B	187	ARG	NE-CZ-NH1	5.24	122.92	120.30
1	A	178	ASP	CB-CG-OD2	-5.18	113.64	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5835	0	5690	18	0
1	B	5835	0	5691	11	0
2	C	28	0	25	0	0
2	D	28	0	25	0	0
2	E	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	I	28	0	25	0	0
2	J	28	0	25	0	0
2	K	28	0	25	0	0
3	F	21	0	19	1	0
3	H	21	0	19	0	0
3	L	21	0	19	0	0
3	N	21	0	19	0	0
4	G	21	0	19	0	0
4	M	21	0	19	0	0
5	A	70	0	65	0	0
5	B	56	0	52	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
7	A	12	0	12	0	0
8	A	285	0	0	2	0
8	B	267	0	0	0	0
All	All	12656	0	11774	28	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 1.

All (28) 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:674:ASN:HB3	1:A:779:GLN:HE22	1.21	1.01
1:A:674:ASN:HB3	1:A:779:GLN:NE2	1.77	1.00
1:B:301:ALA:HB2	1:B:337[B]:MET:HE2	1.85	0.57
1:B:176:VAL:HG22	1:B:220:LYS:HD2	1.87	0.56
1:B:329:LEU:HB3	1:B:330:PRO:HD3	1.88	0.55
1:A:676:THR:HG22	1:A:678:ALA:H	1.74	0.53
1:B:173:MET:HA	1:B:218:ASN:HB3	1.94	0.49
1:B:544:ILE:O	1:B:547:THR:HG22	2.11	0.49
1:A:285:GLU:HB3	8:A:951:HOH:O	2.13	0.48
1:A:173:MET:HA	1:A:218:ASN:HB3	1.96	0.48
1:A:300:ASP:OD1	3:F:1:BGC:H1	2.13	0.48
1:A:165:SER:HB2	1:A:215:ILE:HD11	1.97	0.47
1:B:235:ALA:HB1	1:B:236:PRO:HD2	1.98	0.45
1:A:198:LEU:HD11	1:A:202:ILE:HD11	1.99	0.44
1:A:253:LYS:NZ	8:A:915:HOH:O	2.51	0.44
1:A:674:ASN:CB	1:A:779:GLN:NE2	2.64	0.44
1:B:577:PHE:O	1:B:578:TYR:C	2.57	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:159:LEU:HD12	1:B:402:LEU:HD23	2.01	0.43
1:A:600:LYS:HD2	1:A:655:GLY:O	2.19	0.43
1:A:329:LEU:HB3	1:A:330:PRO:HD3	1.99	0.43
1:A:504:VAL:HG21	1:A:541:ILE:HD11	2.00	0.43
1:B:538:ALA:HB3	1:B:539:PRO:HD3	2.00	0.43
1:A:211:GLN:HG2	1:A:215:ILE:O	2.19	0.42
1:A:99:ILE:O	1:A:103:VAL:HG23	2.21	0.41
1:A:577:PHE:O	1:A:578:TYR:C	2.59	0.41
1:A:313:LEU:HA	1:B:709:ALA:O	2.21	0.40
1:A:524:GLU:O	1:A:525:HIS:HD2	2.05	0.40
1:B:181:ARG:HE	1:B:243:TYR:HH	1.69	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	753/765 (98%)	727 (96%)	25 (3%)	1 (0%)	51 68
1	B	753/765 (98%)	734 (98%)	19 (2%)	0	100 100
All	All	1506/1530 (98%)	1461 (97%)	44 (3%)	1 (0%)	51 68

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	621	SER

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	621/631 (98%)	615 (99%)	6 (1%)	76	88
1	B	621/631 (98%)	611 (98%)	10 (2%)	62	79
All	All	1242/1262 (98%)	1226 (99%)	16 (1%)	69	84

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	82	LYS
1	A	115	THR
1	A	333	ASN
1	A	435	MET
1	A	525	HIS
1	A	615	TYR
1	B	383	ASN
1	B	408	ARG
1	B	421	LEU
1	B	435	MET
1	B	525	HIS
1	B	547	THR
1	B	615	TYR
1	B	649	LYS
1	B	669	LYS
1	B	768	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	218	ASN
1	A	227	GLN
1	A	238	HIS
1	A	525	HIS
1	A	779	GLN
1	B	218	ASN
1	B	221	HIS
1	B	227	GLN
1	B	391	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	C	1	1,2	14,14,15	0.78	1 (7%)	17,19,21	1.75	4 (23%)
2	NAG	C	2	2	14,14,15	0.82	0	17,19,21	1.32	3 (17%)
2	NAG	D	1	1,2	14,14,15	0.57	0	17,19,21	1.36	3 (17%)
2	NAG	D	2	2	14,14,15	0.61	0	17,19,21	1.16	0
2	NAG	E	1	1,2	14,14,15	0.55	0	17,19,21	1.63	1 (5%)
2	NAG	E	2	2	14,14,15	0.57	0	17,19,21	1.54	4 (23%)
3	BGC	F	1	3	12,12,12	0.82	0	17,17,17	1.19	1 (5%)
3	XYS	F	2	3	9,9,10	0.98	0	10,12,14	1.45	2 (20%)
4	GLC	G	1	4	12,12,12	0.68	0	17,17,17	1.19	1 (5%)
4	XYS	G	2	4	9,9,10	1.34	2 (22%)	10,12,14	1.63	3 (30%)
3	BGC	H	1	3	12,12,12	0.86	0	17,17,17	1.01	1 (5%)
3	XYS	H	2	3	9,9,10	0.77	0	10,12,14	1.77	1 (10%)
2	NAG	I	1	1,2	14,14,15	0.87	1 (7%)	17,19,21	1.88	4 (23%)
2	NAG	I	2	2	14,14,15	0.82	0	17,19,21	1.37	3 (17%)
2	NAG	J	1	1,2	14,14,15	0.70	0	17,19,21	1.17	2 (11%)
2	NAG	J	2	2	14,14,15	0.97	0	17,19,21	1.75	2 (11%)
2	NAG	K	1	1,2	14,14,15	0.62	0	17,19,21	1.25	3 (17%)
2	NAG	K	2	2	14,14,15	0.58	0	17,19,21	1.41	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	BGC	L	1	3	12,12,12	0.82	0	17,17,17	0.98	1 (5%)
3	XYS	L	2	3	9,9,10	1.11	0	10,12,14	2.03	2 (20%)
4	GLC	M	1	4	12,12,12	0.87	0	17,17,17	1.52	4 (23%)
4	XYS	M	2	4	9,9,10	0.89	0	10,12,14	1.75	4 (40%)
3	BGC	N	1	3	12,12,12	0.56	0	17,17,17	0.81	0
3	XYS	N	2	3	9,9,10	0.88	0	10,12,14	1.80	3 (30%)

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	C	1	1,2	-	1/6/23/26	0/1/1/1
2	NAG	C	2	2	-	2/6/23/26	0/1/1/1
2	NAG	D	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	D	2	2	-	0/6/23/26	0/1/1/1
2	NAG	E	1	1,2	-	1/6/23/26	0/1/1/1
2	NAG	E	2	2	-	0/6/23/26	0/1/1/1
3	BGC	F	1	3	-	0/2/22/22	0/1/1/1
3	XYS	F	2	3	-	-	0/1/1/1
4	GLC	G	1	4	-	0/2/22/22	0/1/1/1
4	XYS	G	2	4	-	-	0/1/1/1
3	BGC	H	1	3	-	0/2/22/22	0/1/1/1
3	XYS	H	2	3	-	-	0/1/1/1
2	NAG	I	1	1,2	-	4/6/23/26	0/1/1/1
2	NAG	I	2	2	-	2/6/23/26	0/1/1/1
2	NAG	J	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	J	2	2	-	2/6/23/26	0/1/1/1
2	NAG	K	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	K	2	2	-	1/6/23/26	0/1/1/1
3	BGC	L	1	3	-	0/2/22/22	0/1/1/1
3	XYS	L	2	3	-	-	0/1/1/1
4	GLC	M	1	4	-	0/2/22/22	0/1/1/1
4	XYS	M	2	4	-	-	0/1/1/1
3	BGC	N	1	3	-	0/2/22/22	0/1/1/1
3	XYS	N	2	3	-	-	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	2	XYS	C4-C3	2.98	1.56	1.52
2	I	1	NAG	C1-C2	2.46	1.56	1.52
4	G	2	XYS	O5-C1	2.14	1.47	1.42
2	C	1	NAG	C1-C2	2.11	1.55	1.52

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	J	2	NAG	O5-C5-C6	5.58	115.96	107.20
2	E	1	NAG	C1-O5-C5	5.48	119.62	112.19
3	H	2	XYS	C5-C4-C3	5.12	115.96	109.67
3	L	2	XYS	C5-O5-C1	4.76	118.84	111.52
2	C	1	NAG	C1-O5-C5	4.46	118.23	112.19
3	N	2	XYS	C5-O5-C1	4.21	118.00	111.52
2	E	2	NAG	C1-O5-C5	4.07	117.70	112.19
2	I	1	NAG	C8-C7-N2	4.05	122.96	116.10
2	K	2	NAG	C1-O5-C5	3.63	117.11	112.19
3	L	2	XYS	O2-C2-C1	3.33	115.96	109.15
2	I	1	NAG	C2-N2-C7	3.32	127.63	122.90
4	M	1	GLC	C1-C2-C3	3.05	116.63	110.31
2	D	1	NAG	C1-C2-N2	-2.88	105.57	110.49
2	I	1	NAG	O5-C1-C2	-2.85	106.79	111.29
3	F	2	XYS	O2-C2-C1	2.77	114.82	109.15
2	J	1	NAG	O5-C1-C2	-2.73	106.97	111.29
4	M	2	XYS	O2-C2-C3	-2.73	104.66	110.14
2	K	1	NAG	O5-C5-C6	2.73	111.49	107.20
4	G	2	XYS	C5-C4-C3	2.67	112.94	109.67
2	D	1	NAG	C3-C4-C5	2.66	114.98	110.24
4	M	1	GLC	O4-C4-C5	2.65	115.87	109.30
2	D	1	NAG	C1-O5-C5	2.64	115.77	112.19
2	K	1	NAG	O5-C1-C2	-2.63	107.13	111.29
3	F	2	XYS	C5-O5-C1	2.62	115.56	111.52
2	I	2	NAG	C1-O5-C5	2.59	115.71	112.19
4	M	1	GLC	O5-C1-C2	2.59	114.91	110.28
4	G	1	GLC	C1-O5-C5	2.59	118.55	113.66
4	M	2	XYS	O2-C2-C1	2.54	114.36	109.15
2	J	2	NAG	C1-O5-C5	2.47	115.54	112.19
3	N	2	XYS	C5-C4-C3	2.46	112.69	109.67
4	M	2	XYS	C5-C4-C3	2.43	112.65	109.67
2	C	1	NAG	C2-N2-C7	2.42	126.34	122.90
3	F	1	BGC	O4-C4-C5	2.40	115.25	109.30
2	E	2	NAG	O5-C1-C2	-2.37	107.54	111.29
2	C	2	NAG	C1-C2-N2	2.36	114.52	110.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	2	NAG	C3-C4-C5	-2.35	106.05	110.24
3	L	1	BGC	O4-C4-C5	2.34	115.10	109.30
2	I	2	NAG	C1-C2-N2	2.33	114.47	110.49
2	C	1	NAG	C6-C5-C4	-2.32	107.57	113.00
2	K	1	NAG	C1-C2-N2	2.31	114.44	110.49
3	H	1	BGC	O5-C5-C6	2.30	112.15	106.44
4	M	1	GLC	C4-C3-C2	2.26	114.78	110.82
2	C	2	NAG	O5-C5-C6	2.25	110.73	107.20
4	M	2	XYS	C5-O5-C1	2.20	114.90	111.52
2	I	1	NAG	C1-O5-C5	2.19	115.16	112.19
2	E	2	NAG	O4-C4-C5	2.18	114.70	109.30
2	C	1	NAG	O5-C5-C4	2.16	116.08	110.83
4	G	2	XYS	O2-C2-C1	2.15	113.55	109.15
2	J	1	NAG	O4-C4-C5	2.14	114.61	109.30
4	G	2	XYS	O2-C2-C3	-2.12	105.89	110.14
3	N	2	XYS	C4-C3-C2	-2.07	108.47	110.92
2	I	2	NAG	O5-C1-C2	-2.05	108.05	111.29
2	C	2	NAG	O3-C3-C2	2.02	113.66	109.47

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	2	NAG	O5-C5-C6-O6
2	I	1	NAG	O5-C5-C6-O6
2	I	1	NAG	C4-C5-C6-O6
2	I	2	NAG	O5-C5-C6-O6
2	J	2	NAG	O5-C5-C6-O6
2	I	2	NAG	C4-C5-C6-O6
2	I	1	NAG	C8-C7-N2-C2
2	I	1	NAG	O7-C7-N2-C2
2	J	2	NAG	C4-C5-C6-O6
2	C	2	NAG	C4-C5-C6-O6
2	C	1	NAG	C4-C5-C6-O6
2	K	2	NAG	C4-C5-C6-O6
2	E	1	NAG	C4-C5-C6-O6

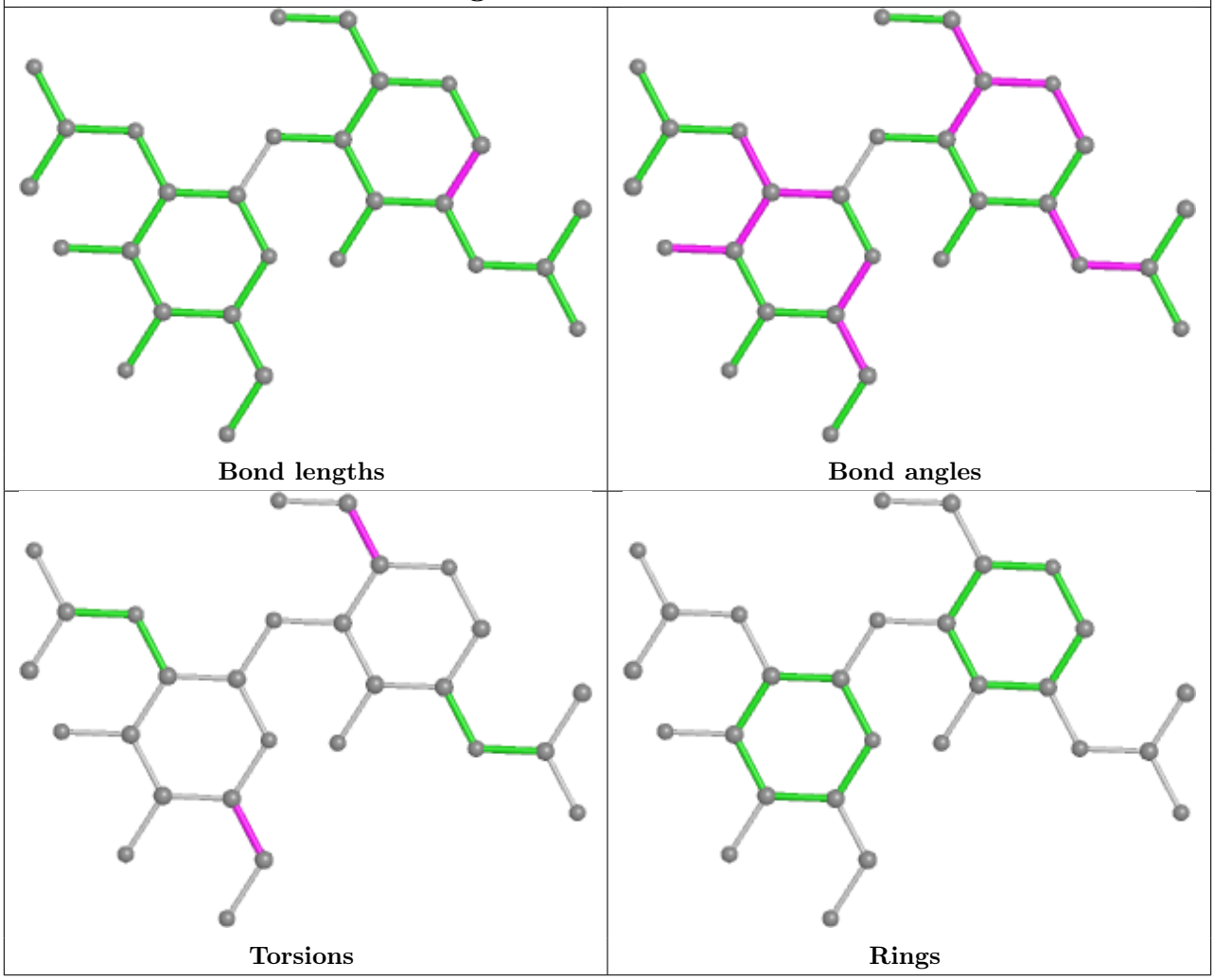
There are no ring outliers.

1 monomer is involved in 1 short contact:

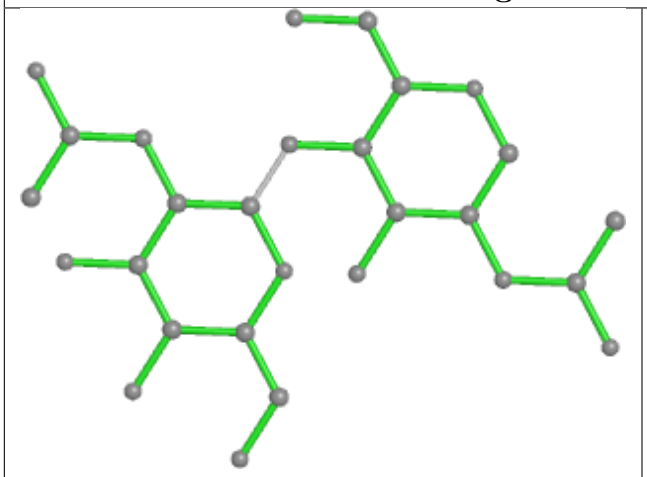
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	1	BGC	1	0

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

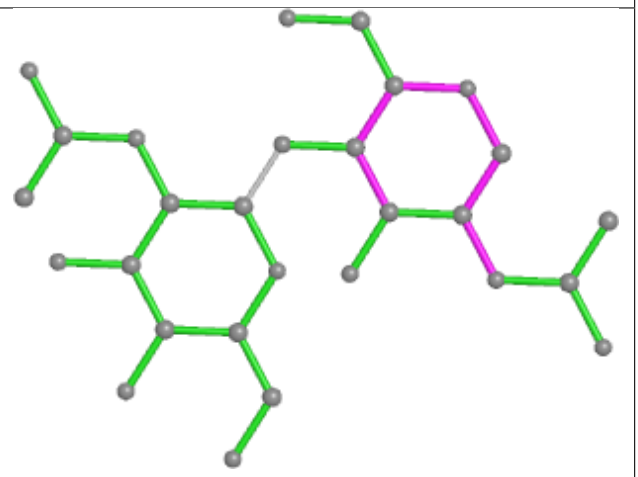
Oligosaccharide Chain C



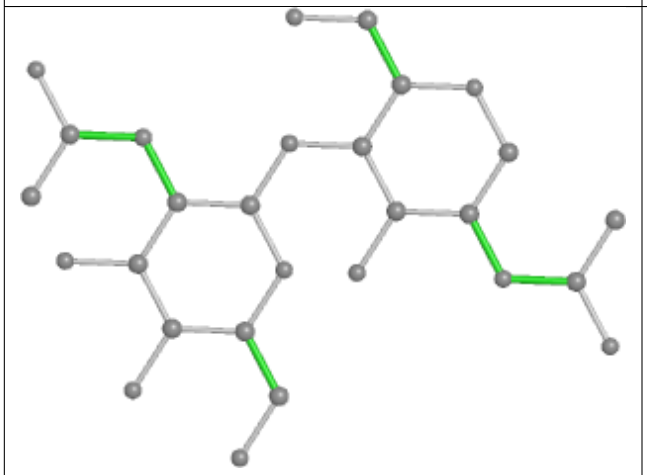
Oligosaccharide Chain D



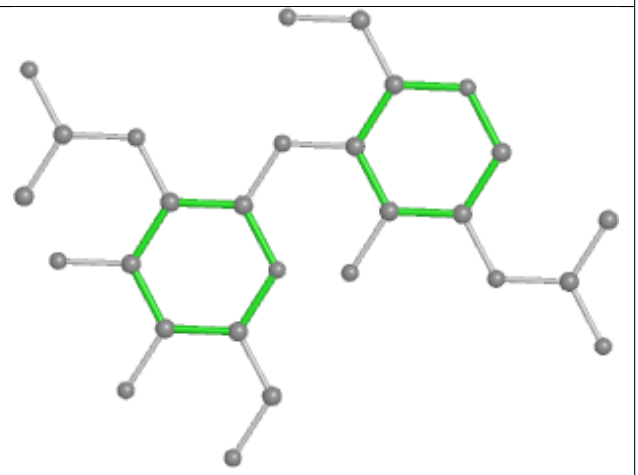
Bond lengths



Bond angles

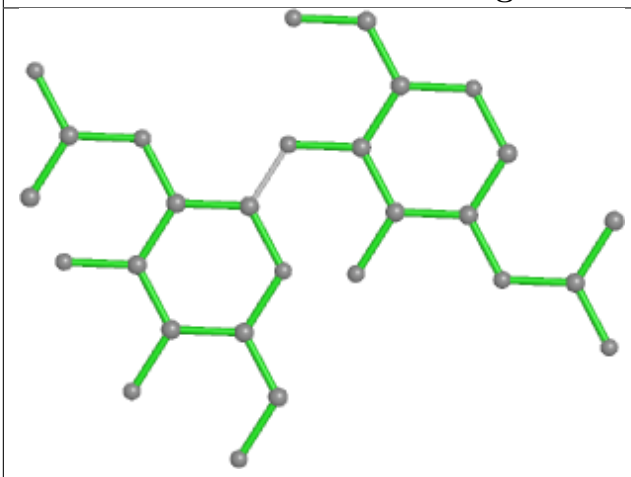


Torsions

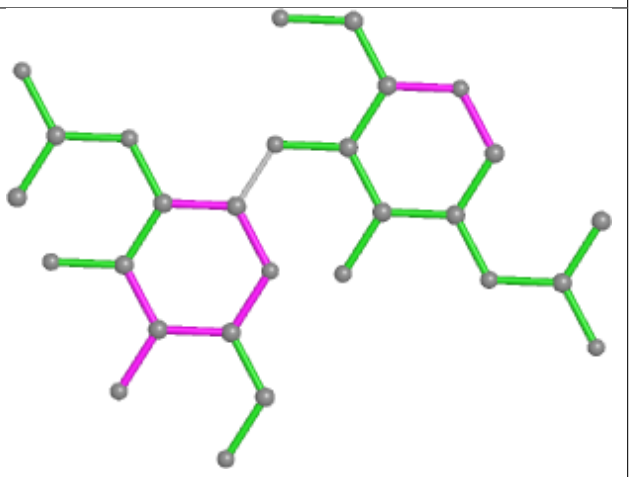


Rings

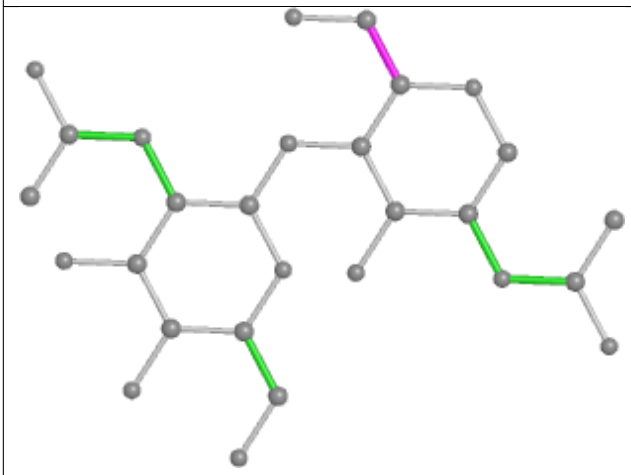
Oligosaccharide Chain E



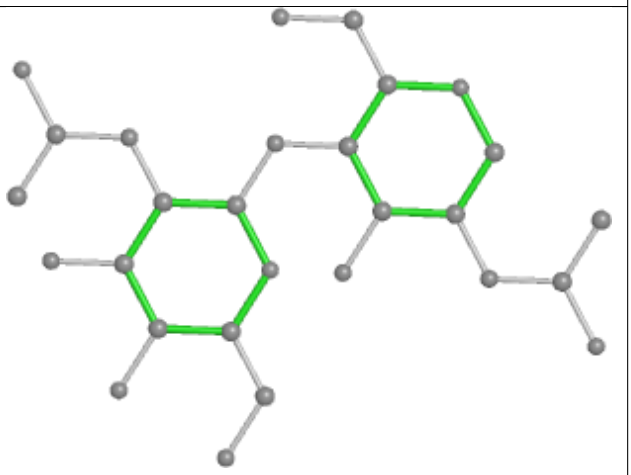
Bond lengths



Bond angles

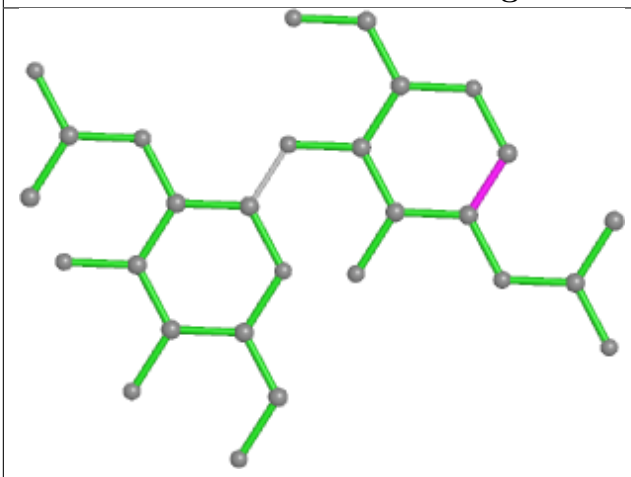


Torsions

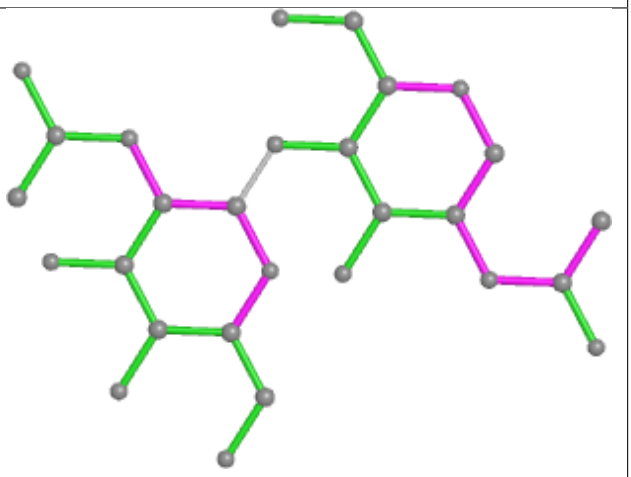


Rings

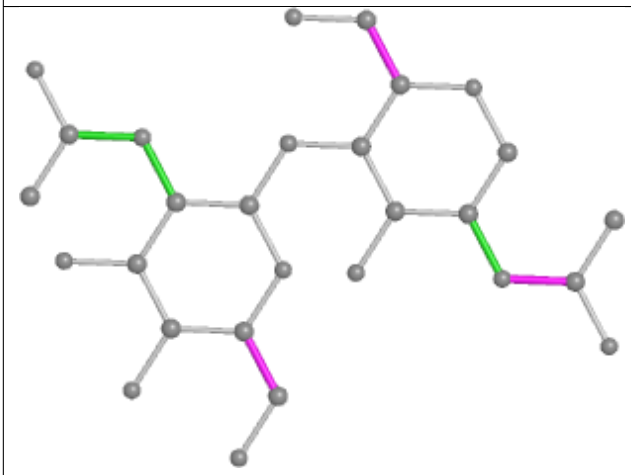
Oligosaccharide Chain I



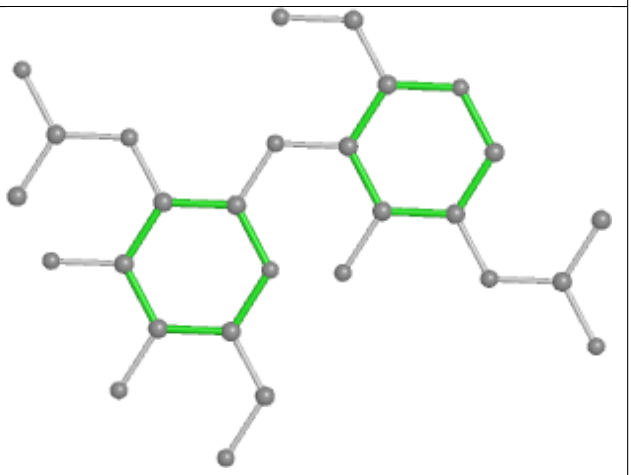
Bond lengths



Bond angles

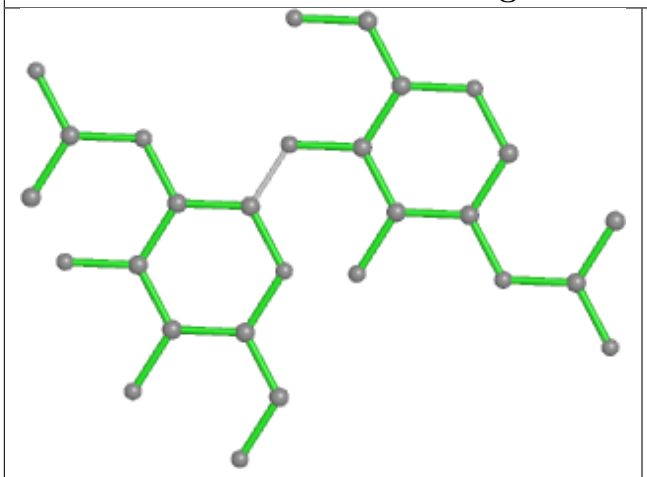


Torsions

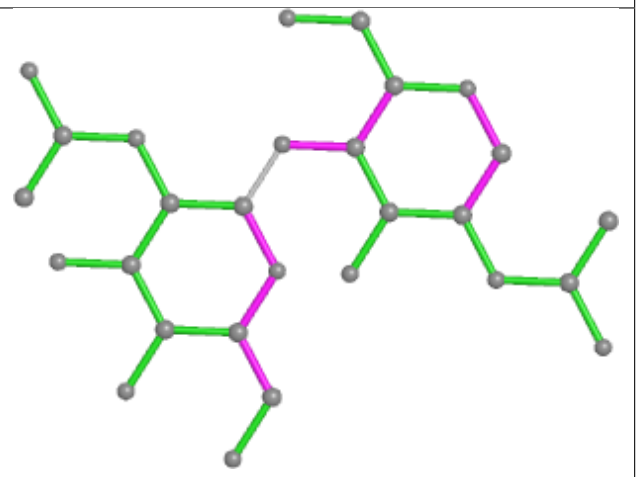


Rings

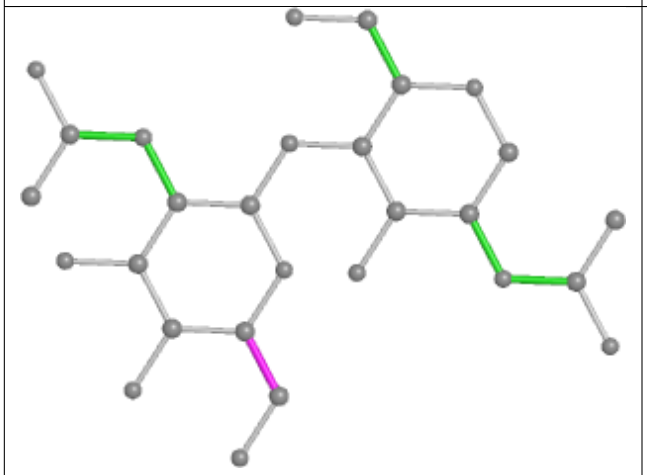
Oligosaccharide Chain J



Bond lengths



Bond angles



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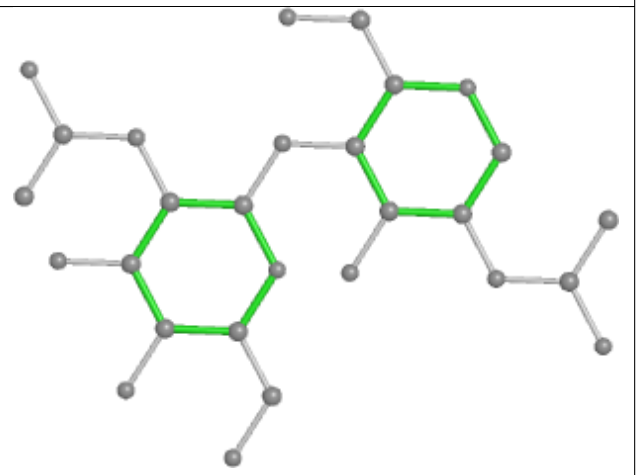
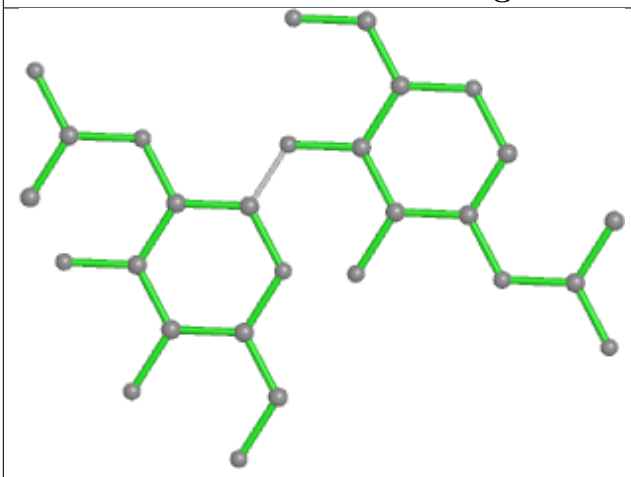
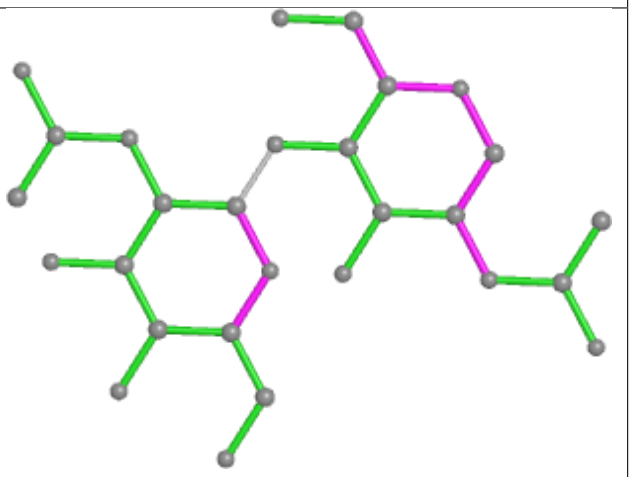


Rings

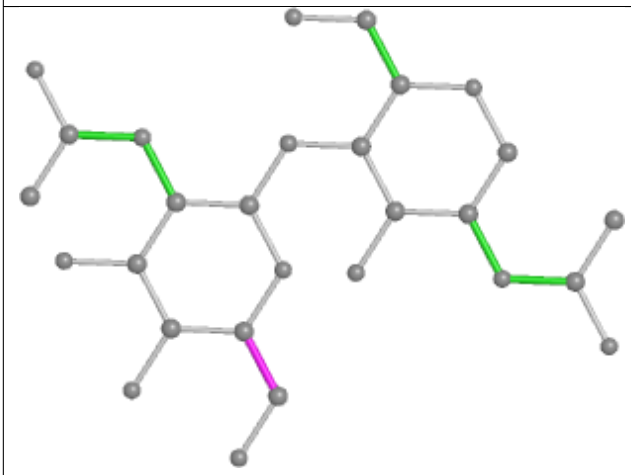
Oligosaccharide Chain K



Bond lengths



Bond angles



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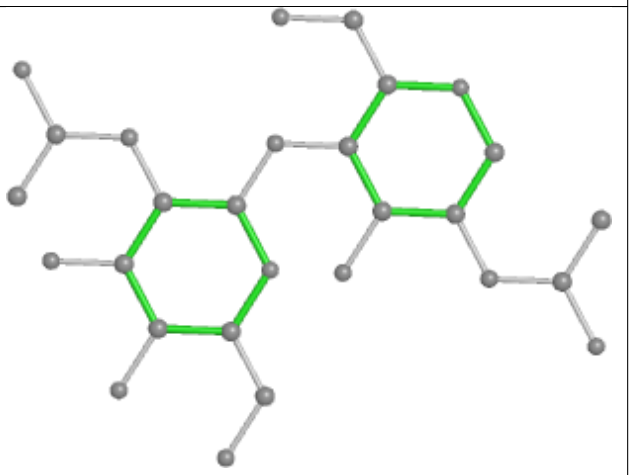
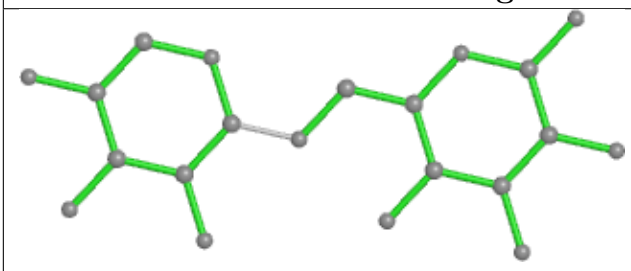
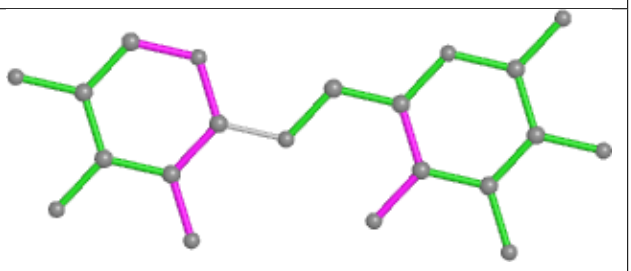


Rings

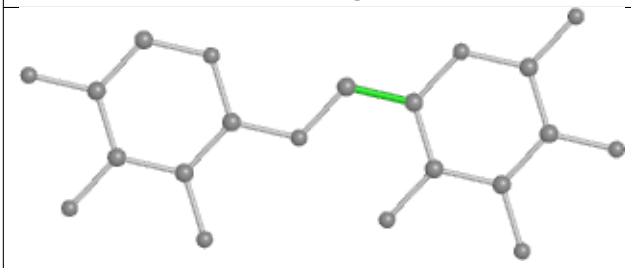
Oligosaccharide Chain F



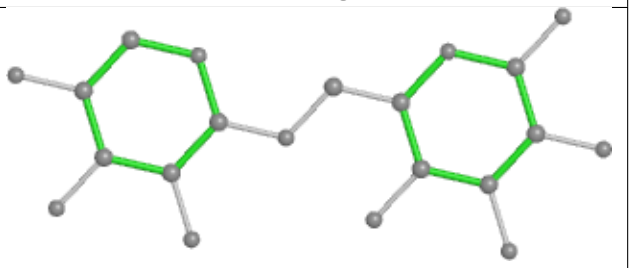
Bond lengths



Bond angles

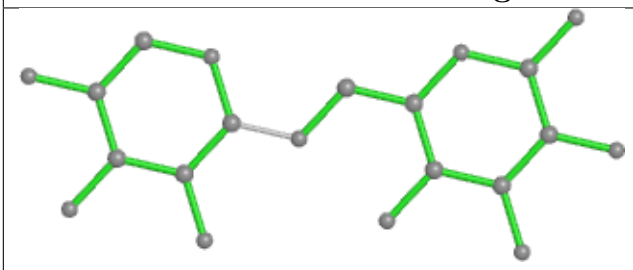


Torsions

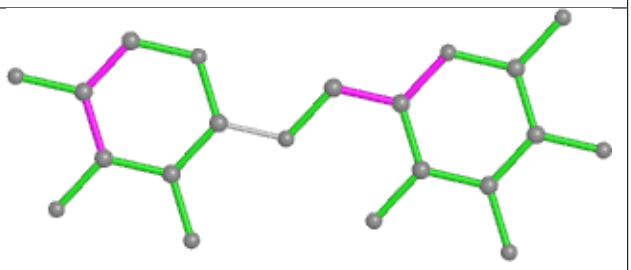


Rings

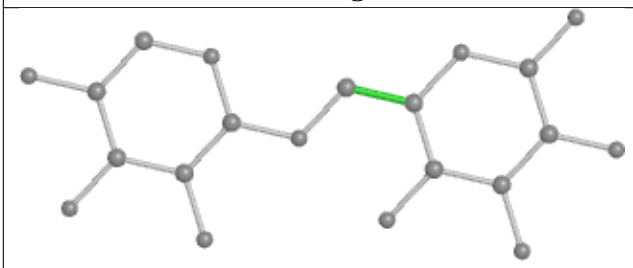
Oligosaccharide Chain H



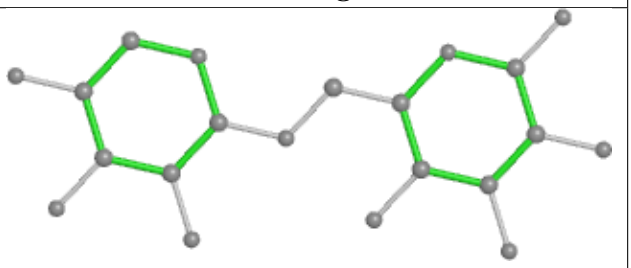
Bond lengths



Bond angles

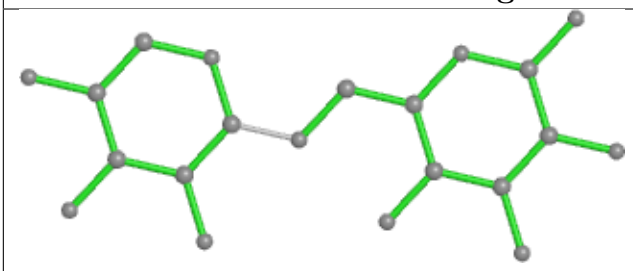


Torsions

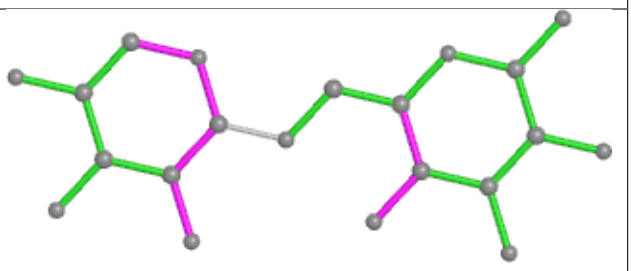


Rings

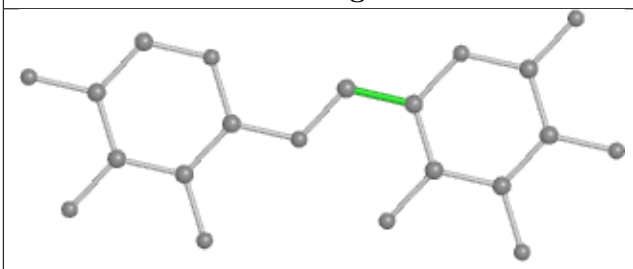
Oligosaccharide Chain L



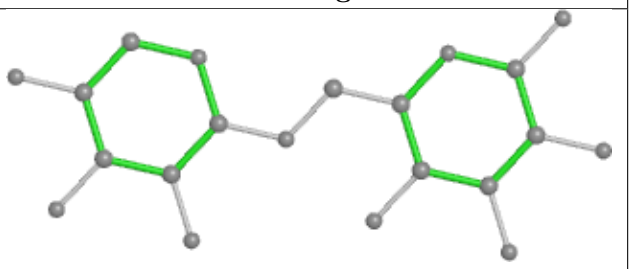
Bond lengths



Bond angles

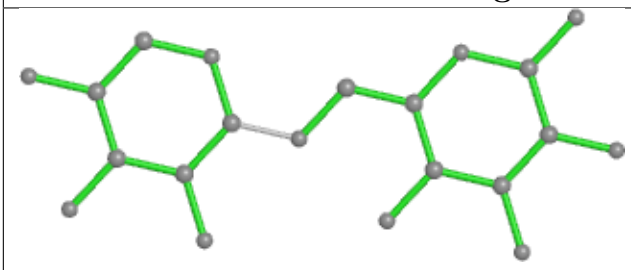


Torsions

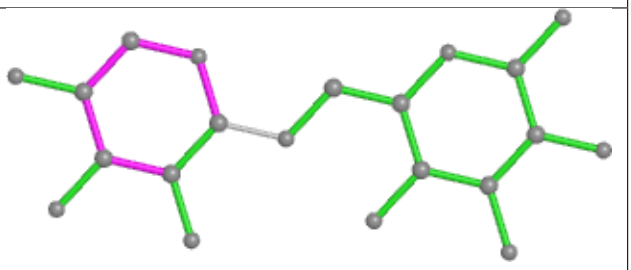


Rings

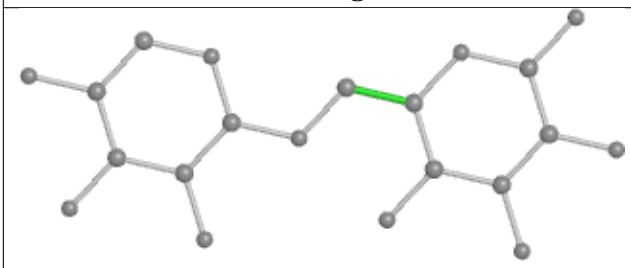
Oligosaccharide Chain N



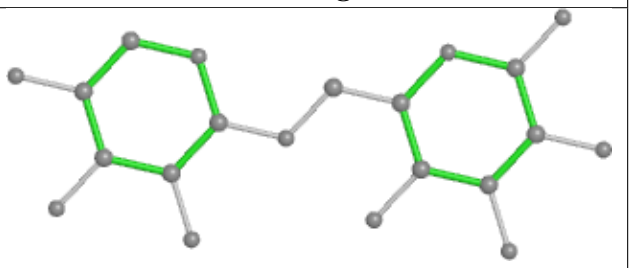
Bond lengths



Bond angles

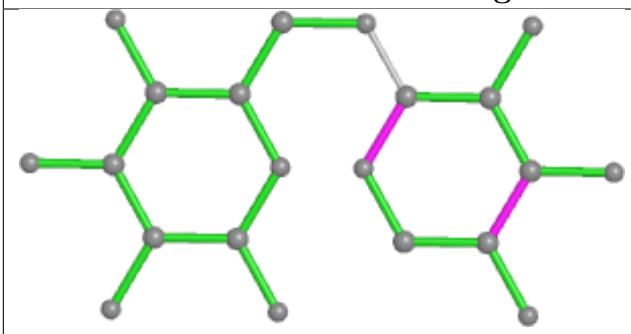


Torsions

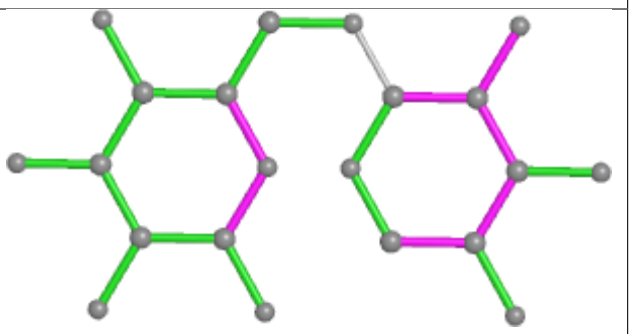


Rings

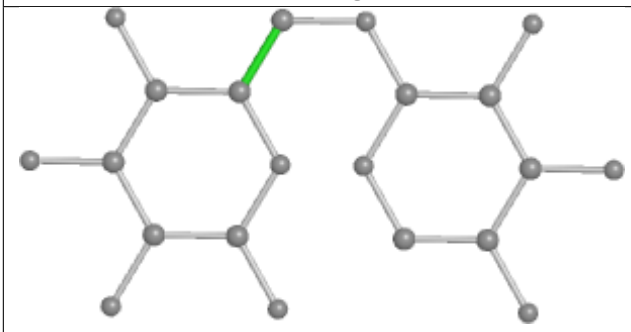
Oligosaccharide Chain G



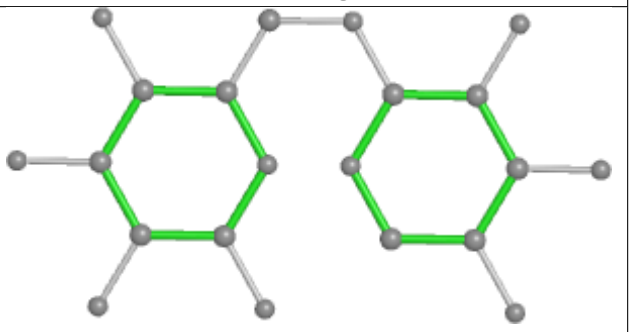
Bond lengths



Bond angles

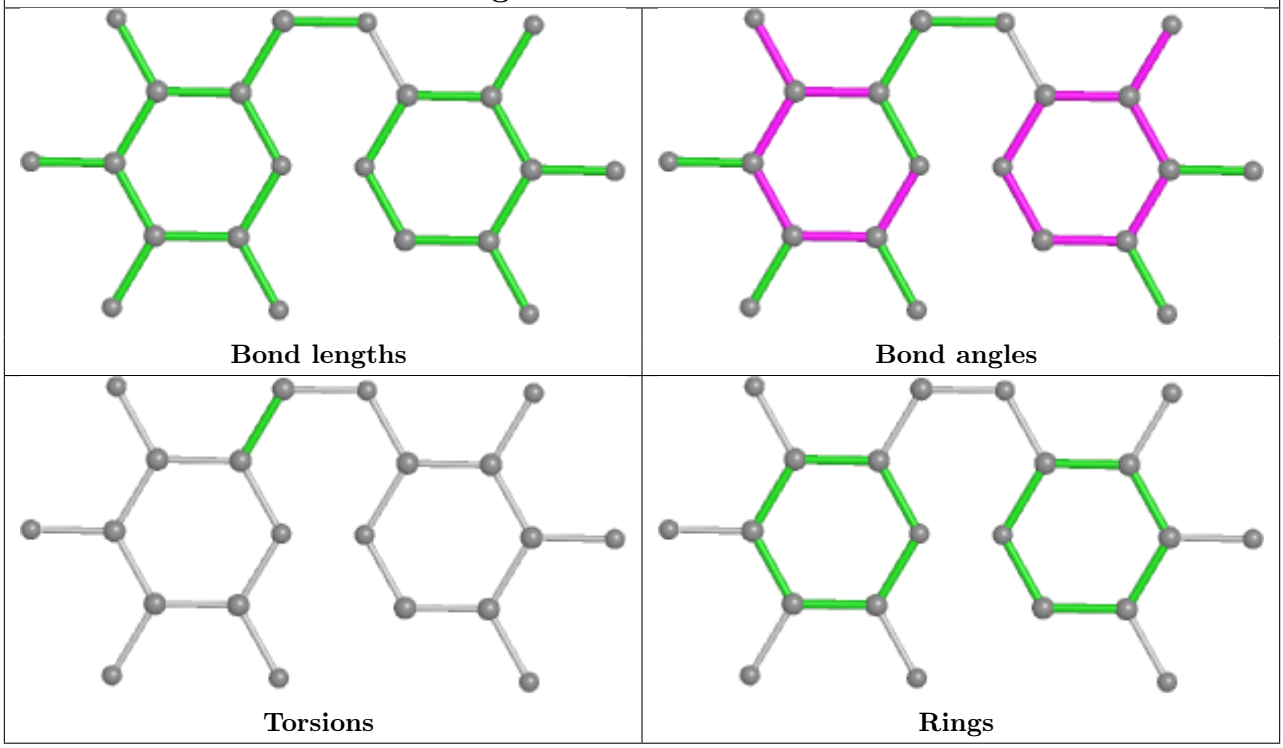


Torsions



Rings

Oligosaccharide Chain M



5.6 Ligand geometry (i)

Of 12 ligands modelled in this entry, 2 are monoatomic - leaving 10 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	$\#\|Z\| > 2$
5	NAG	B	809	1	14,14,15	0.68	0	17,19,21	1.49	2 (11%)
5	NAG	B	804	1	14,14,15	0.50	0	17,19,21	1.85	4 (23%)
5	NAG	A	811	1	14,14,15	0.63	0	17,19,21	1.37	3 (17%)
5	NAG	A	810	1	14,14,15	0.99	0	17,19,21	1.77	5 (29%)
5	NAG	B	801	1	14,14,15	0.57	0	17,19,21	1.35	2 (11%)
5	NAG	A	804	1	14,14,15	0.49	0	17,19,21	1.49	3 (17%)
7	BGC	A	815	-	12,12,12	0.73	0	17,17,17	1.30	3 (17%)
5	NAG	A	801	1	14,14,15	0.67	0	17,19,21	2.03	7 (41%)
5	NAG	B	810	1	14,14,15	0.64	0	17,19,21	1.39	4 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	NAG	A	809	1	14,14,15	0.64	0	17,19,21	1.39	2 (11%)

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
5	NAG	B	809	1	-	0/6/23/26	0/1/1/1
5	NAG	B	804	1	-	1/6/23/26	0/1/1/1
5	NAG	A	811	1	-	1/6/23/26	0/1/1/1
5	NAG	A	810	1	-	2/6/23/26	0/1/1/1
5	NAG	B	801	1	-	2/6/23/26	0/1/1/1
5	NAG	A	804	1	-	2/6/23/26	0/1/1/1
7	BGC	A	815	-	-	0/2/22/22	0/1/1/1
5	NAG	A	801	1	-	1/6/23/26	0/1/1/1
5	NAG	B	810	1	-	2/6/23/26	0/1/1/1
5	NAG	A	809	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	801	NAG	C1-C2-N2	5.18	119.33	110.49
5	B	804	NAG	C1-O5-C5	4.22	117.91	112.19
5	A	810	NAG	C1-O5-C5	3.52	116.96	112.19
5	B	801	NAG	O5-C5-C6	3.50	112.69	107.20
5	B	809	NAG	O4-C4-C5	3.27	117.43	109.30
5	B	809	NAG	C3-C4-C5	-3.02	104.84	110.24
5	A	809	NAG	O5-C5-C6	3.00	111.91	107.20
5	A	810	NAG	C1-C2-N2	-2.94	105.46	110.49
5	A	801	NAG	C4-C3-C2	-2.90	106.76	111.02
5	B	804	NAG	C6-C5-C4	-2.88	106.25	113.00
5	A	804	NAG	C6-C5-C4	-2.80	106.44	113.00
7	A	815	BGC	C4-C3-C2	-2.68	106.14	110.82
5	A	804	NAG	C1-O5-C5	2.68	115.82	112.19
5	A	810	NAG	O5-C5-C4	2.64	117.26	110.83
7	A	815	BGC	C1-O5-C5	2.61	118.58	113.66
5	B	810	NAG	C2-N2-C7	2.60	126.60	122.90
5	A	811	NAG	C1-O5-C5	2.54	115.63	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	804	NAG	O6-C6-C5	-2.53	102.61	111.29
5	A	801	NAG	C3-C4-C5	2.52	114.73	110.24
5	A	801	NAG	O5-C5-C6	2.52	111.15	107.20
5	A	811	NAG	O5-C1-C2	-2.44	107.44	111.29
5	A	811	NAG	C4-C3-C2	2.42	114.56	111.02
5	B	810	NAG	O4-C4-C5	2.35	115.13	109.30
5	A	809	NAG	C1-C2-N2	2.31	114.43	110.49
5	A	804	NAG	O7-C7-N2	2.30	126.18	121.95
5	B	804	NAG	O7-C7-N2	2.29	126.16	121.95
5	A	810	NAG	C3-C4-C5	2.28	114.31	110.24
5	B	810	NAG	O4-C4-C3	-2.23	105.20	110.35
5	B	801	NAG	C1-O5-C5	2.18	115.14	112.19
5	A	801	NAG	O7-C7-C8	-2.17	118.03	122.06
7	A	815	BGC	O3-C3-C4	2.16	115.34	110.35
5	A	801	NAG	C6-C5-C4	-2.15	107.97	113.00
5	A	801	NAG	O7-C7-N2	2.12	125.85	121.95
5	A	810	NAG	C4-C3-C2	2.11	114.11	111.02
5	B	810	NAG	O3-C3-C2	2.08	113.76	109.47

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	801	NAG	O5-C5-C6-O6
5	B	801	NAG	C4-C5-C6-O6
5	A	804	NAG	C4-C5-C6-O6
5	A	810	NAG	O5-C5-C6-O6
5	A	809	NAG	O5-C5-C6-O6
5	A	801	NAG	O5-C5-C6-O6
5	A	809	NAG	C4-C5-C6-O6
5	B	810	NAG	C1-C2-N2-C7
5	A	811	NAG	O5-C5-C6-O6
5	B	810	NAG	O5-C5-C6-O6
5	A	804	NAG	O5-C5-C6-O6
5	A	810	NAG	C4-C5-C6-O6
5	B	804	NAG	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th 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	754/765 (98%)	-0.52	2 (0%)	94	93	14, 23, 38, 64	0
1	B	754/765 (98%)	-0.43	4 (0%)	91	89	15, 26, 41, 72	0
All	All	1508/1530 (98%)	-0.48	6 (0%)	92	91	14, 24, 40, 72	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	26	LYS	3.2
1	B	467	ASP	2.7
1	A	26	LYS	2.6
1	B	546	ASP	2.5
1	A	467	ASP	2.4
1	B	692	ALA	2.0

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

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

6.3 Carbohydrates (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	XYS	N	2	9/10	0.59	0.55	79,97,109,109	0
3	XYS	H	2	9/10	0.62	0.64	105,109,117,119	0
2	NAG	I	2	14/15	0.72	0.32	61,73,77,83	0

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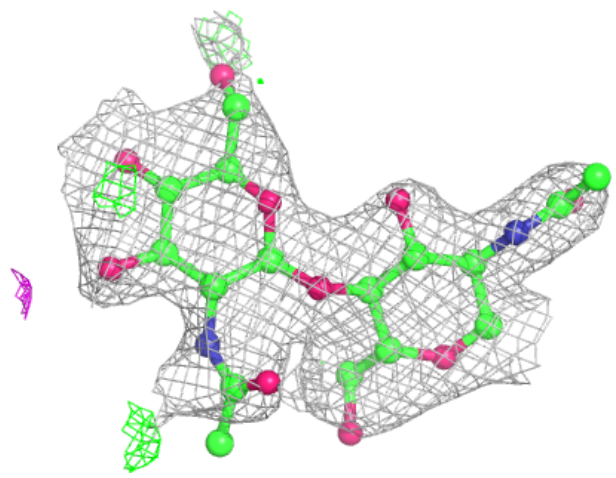
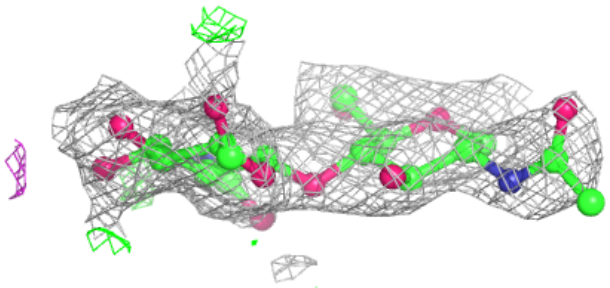
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	BGC	H	1	12/12	0.77	0.28	58,66,71,78	0
2	NAG	J	2	14/15	0.79	0.40	52,60,69,72	0
2	NAG	C	2	14/15	0.83	0.25	58,70,72,73	0
3	BGC	N	1	12/12	0.84	0.26	53,68,75,87	0
2	NAG	K	2	14/15	0.84	0.39	51,55,58,60	0
2	NAG	D	2	14/15	0.86	0.36	52,60,65,65	0
2	NAG	I	1	14/15	0.87	0.25	52,61,68,68	0
2	NAG	C	1	14/15	0.89	0.24	51,53,56,57	0
2	NAG	E	2	14/15	0.89	0.31	44,51,54,55	0
2	NAG	J	1	14/15	0.89	0.33	37,40,45,58	0
4	GLC	G	1	12/12	0.89	0.18	33,42,46,46	0
4	XYS	G	2	9/10	0.89	0.20	32,37,39,40	0
2	NAG	D	1	14/15	0.90	0.26	38,41,45,49	0
4	GLC	M	1	12/12	0.90	0.14	43,50,52,52	0
2	NAG	K	1	14/15	0.92	0.16	30,36,40,48	0
4	XYS	M	2	9/10	0.94	0.16	38,43,45,47	0
2	NAG	E	1	14/15	0.96	0.13	25,27,29,31	0
3	XYS	F	2	9/10	0.96	0.09	21,23,25,26	0
3	XYS	L	2	9/10	0.96	0.09	22,25,25,30	0
3	BGC	L	1	12/12	0.97	0.09	19,24,26,26	0
3	BGC	F	1	12/12	0.97	0.08	17,19,21,24	0

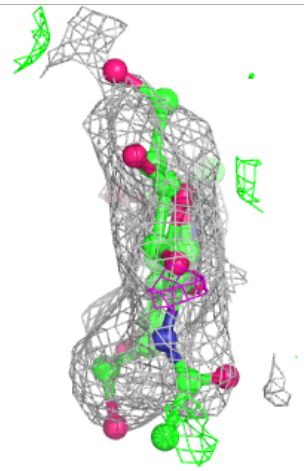
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain C:

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

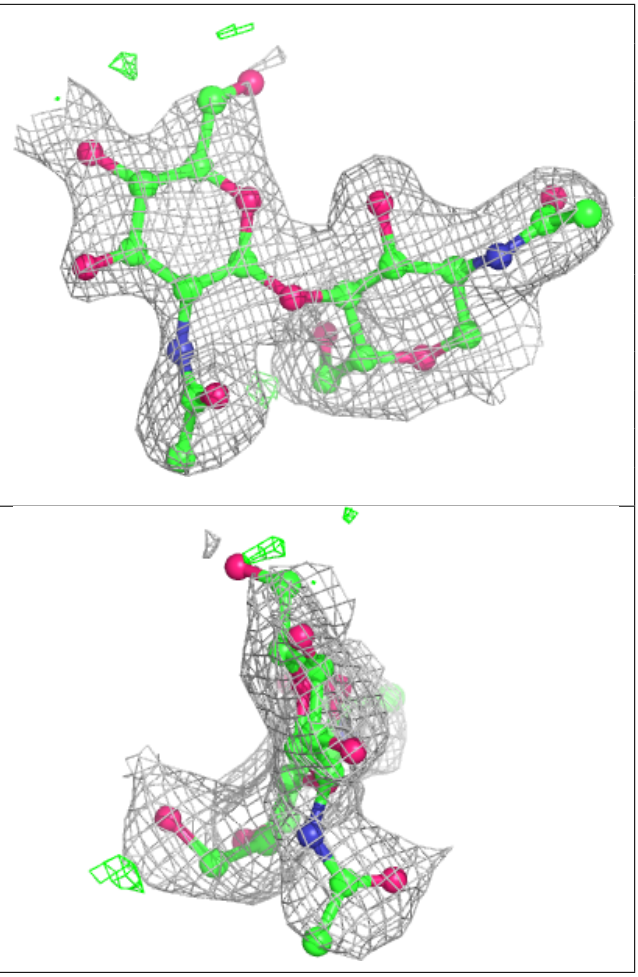






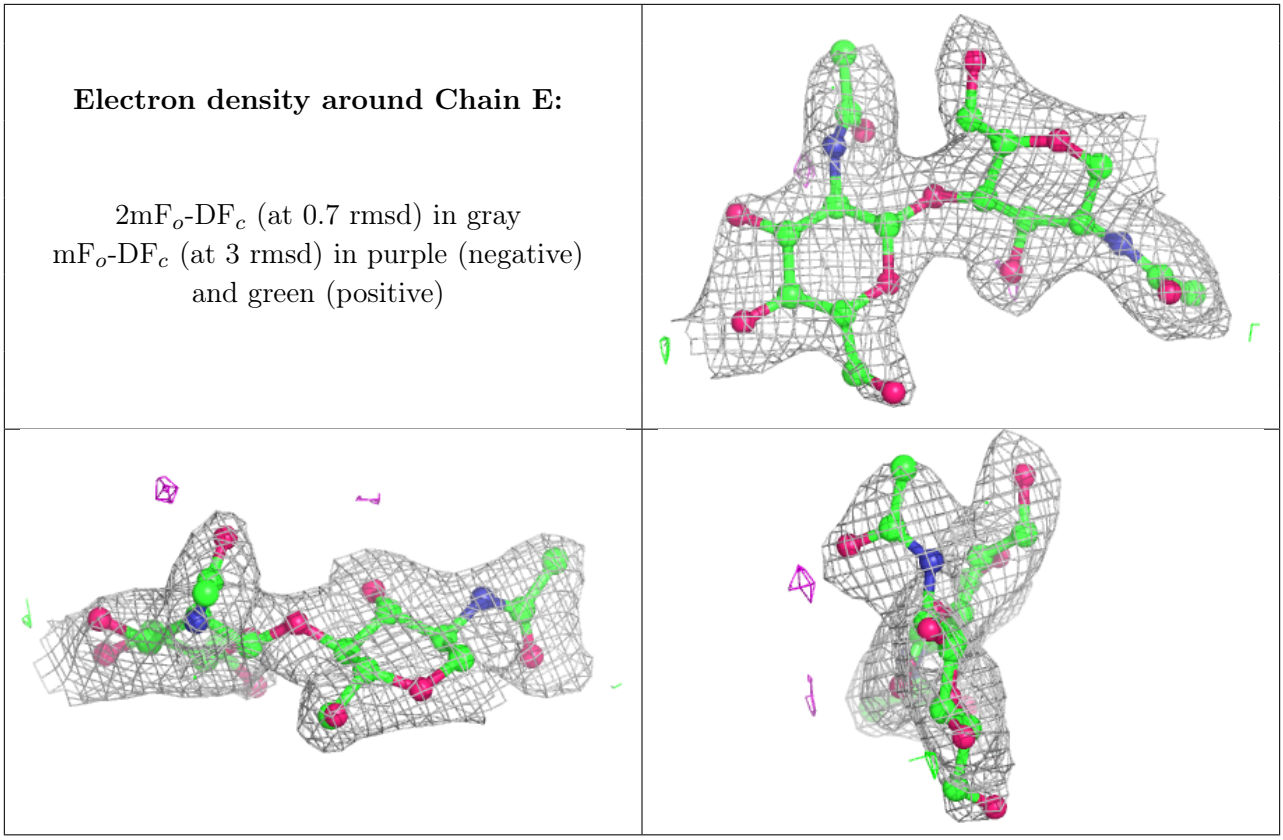
Electron density around Chain D:

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



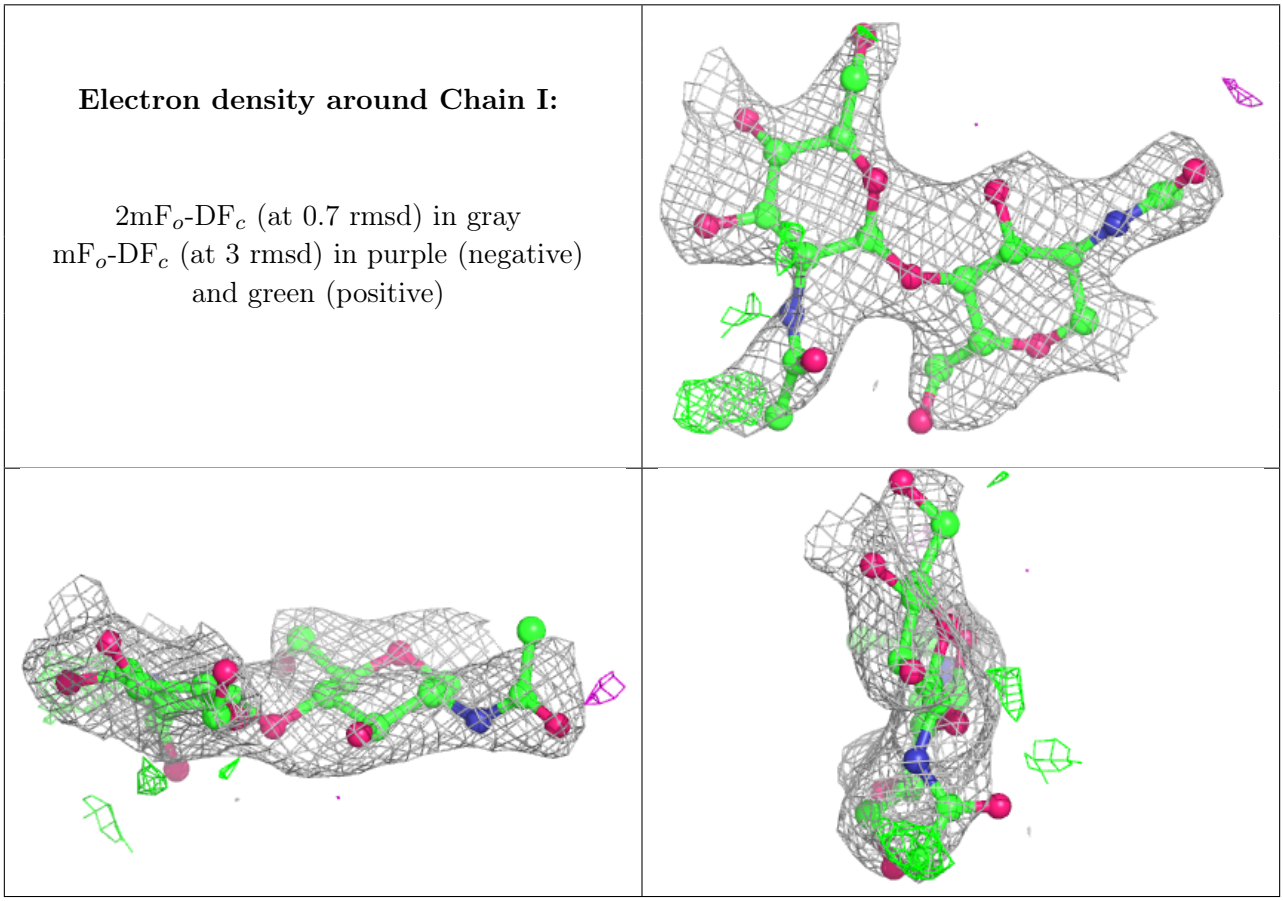
Electron density around Chain E:

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



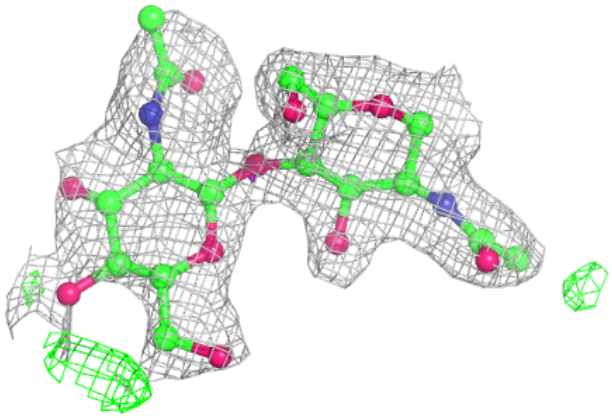
Electron density around Chain I:

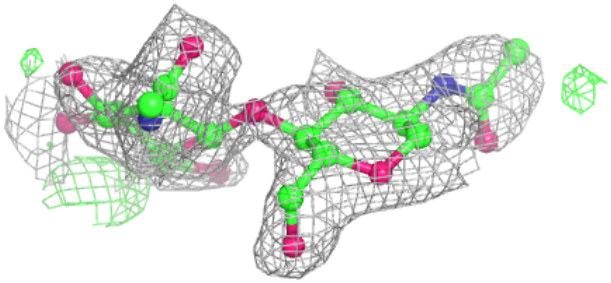
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

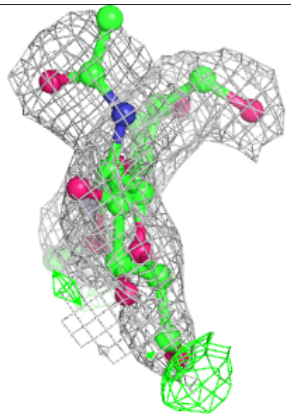


Electron density around Chain J:

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

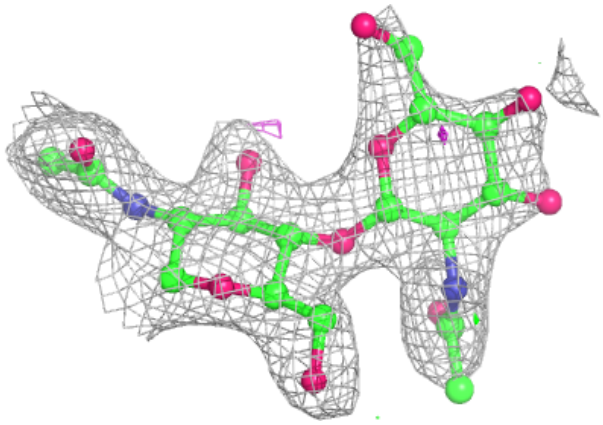


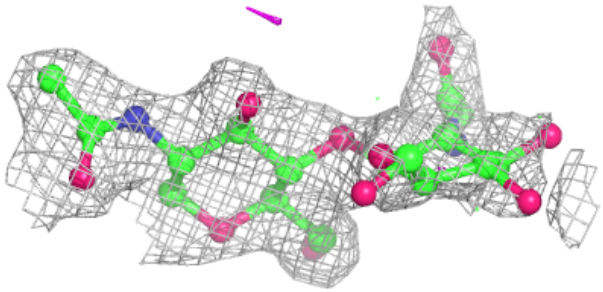


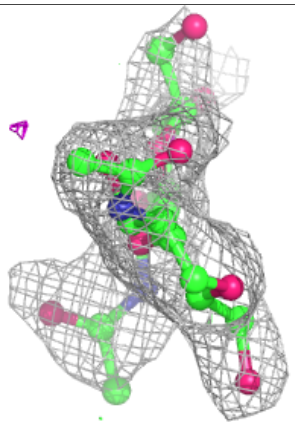


Electron density around Chain K:

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

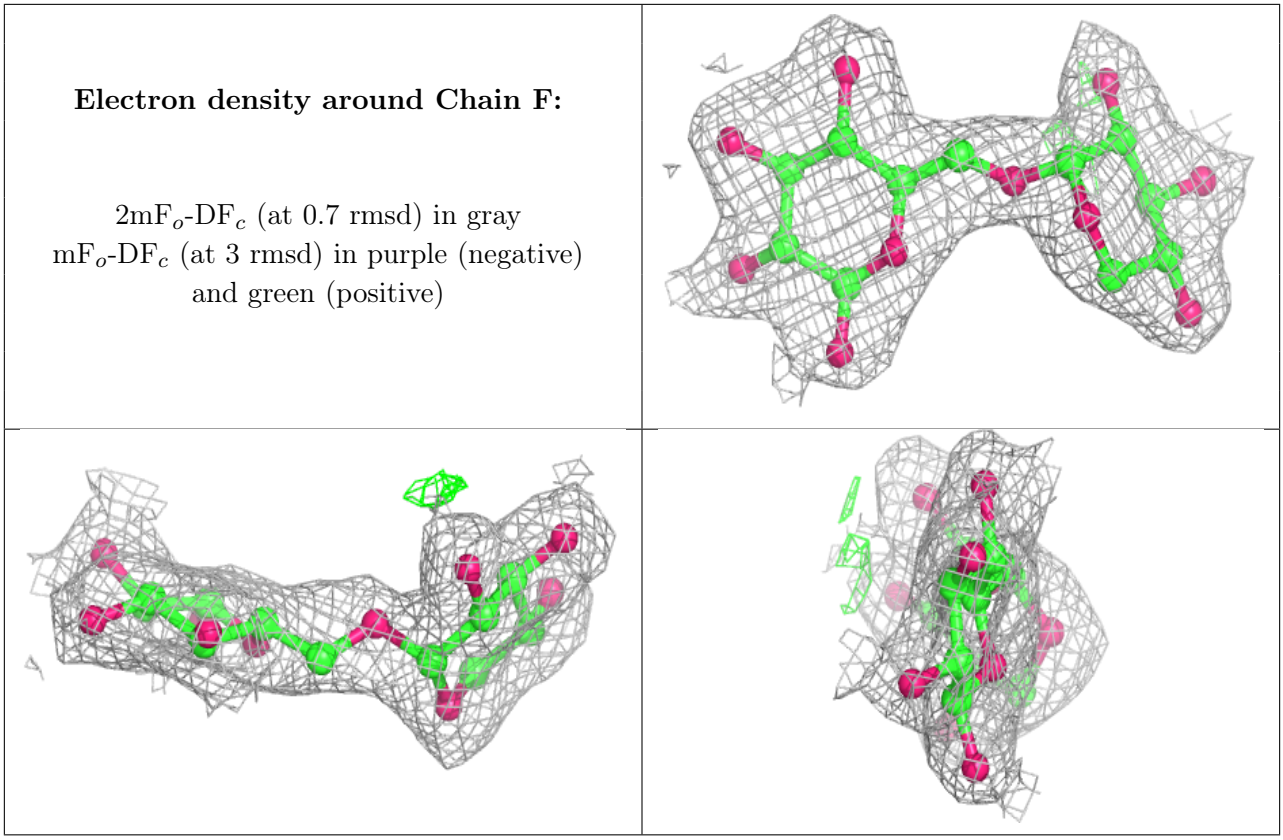






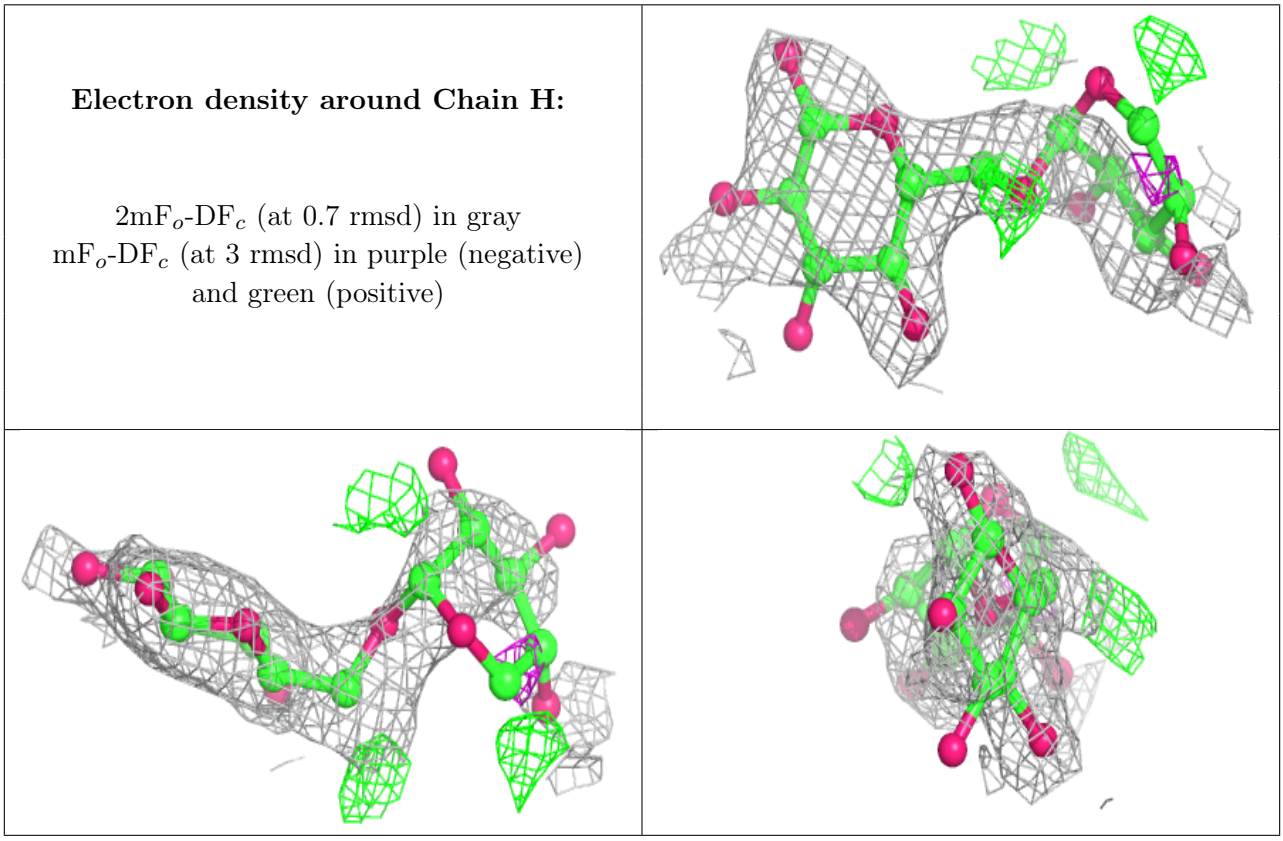
Electron density around Chain F:

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



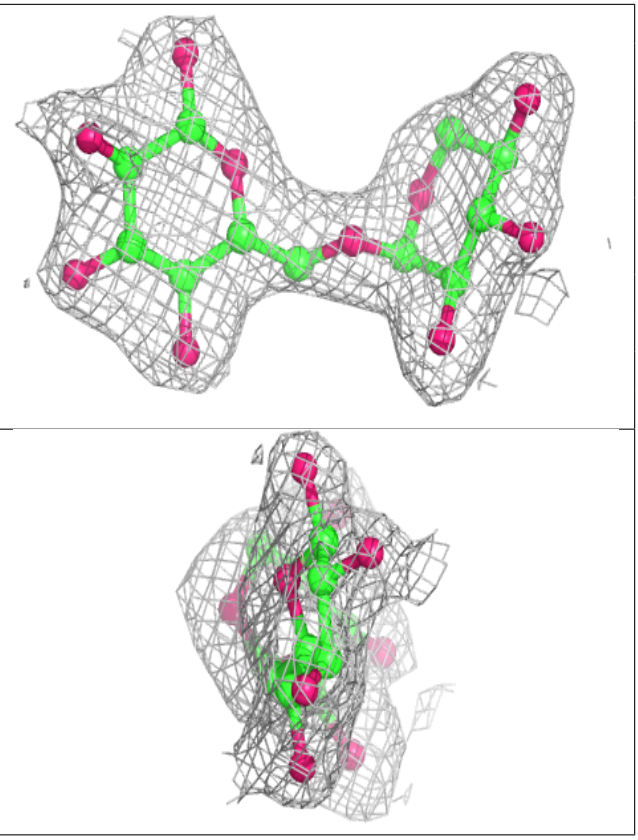
Electron density around Chain H:

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



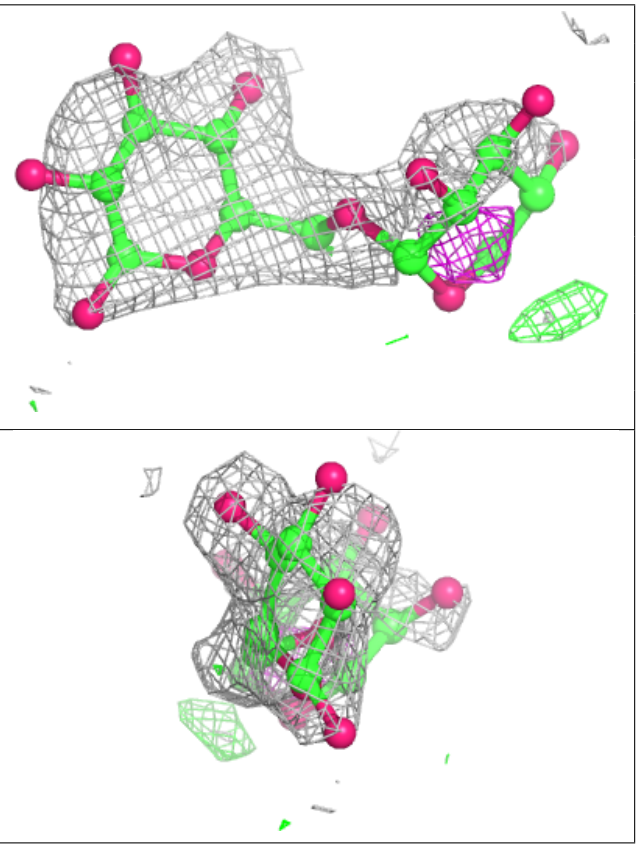
Electron density around Chain L:

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



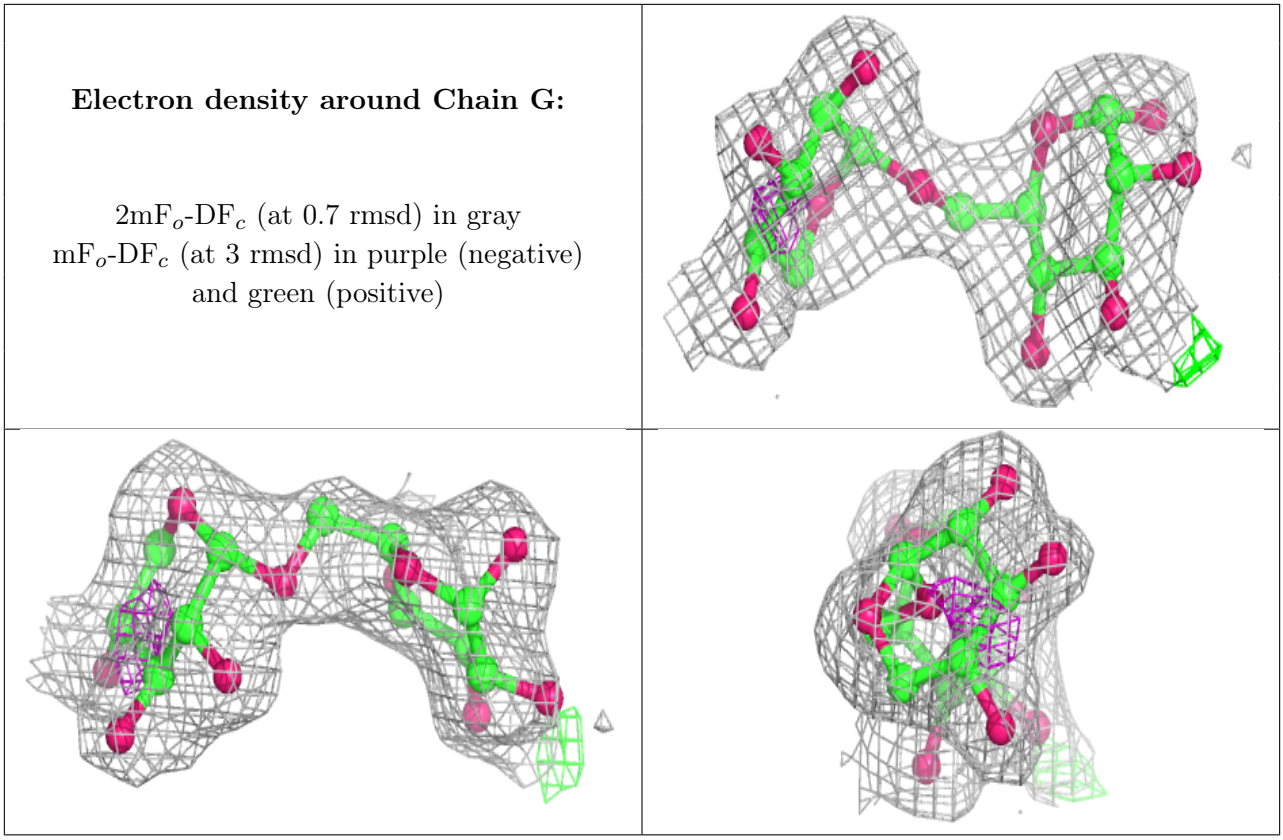
Electron density around Chain N:

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



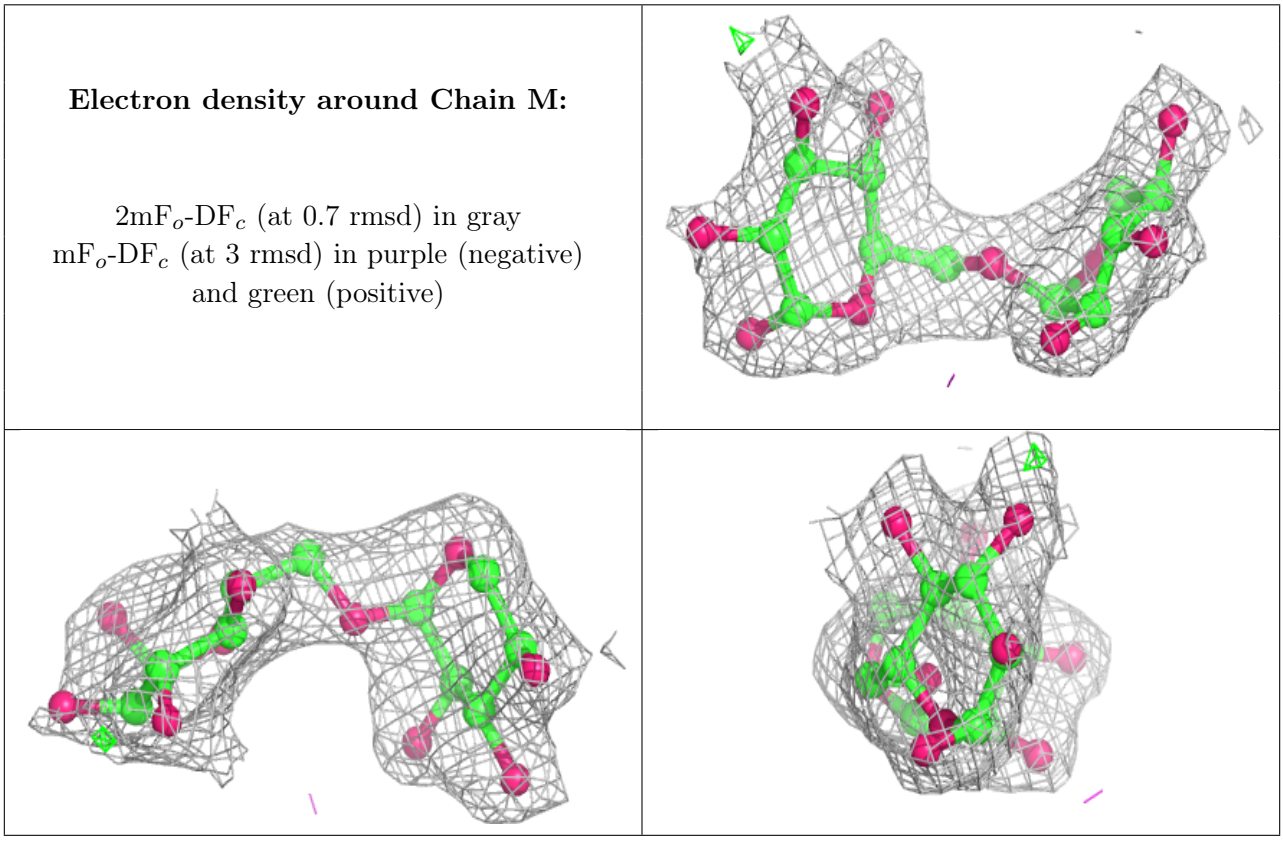
Electron density around Chain G:

$2mF_o$-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 M:

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



6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th 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
7	BGC	A	815	12/12	0.77	0.30	54,61,66,72	0
5	NAG	A	811	14/15	0.83	0.37	59,69,71,79	0
5	NAG	B	810	14/15	0.85	0.33	54,58,69,70	0
5	NAG	B	809	14/15	0.88	0.31	39,46,51,54	0
5	NAG	A	810	14/15	0.88	0.27	42,51,55,63	0
5	NAG	A	801	14/15	0.88	0.27	48,53,64,65	0
5	NAG	A	809	14/15	0.89	0.32	39,49,53,54	0
5	NAG	B	801	14/15	0.92	0.29	51,58,64,64	0
5	NAG	B	804	14/15	0.93	0.15	25,27,32,36	0
5	NAG	A	804	14/15	0.93	0.16	28,33,35,37	0
6	CA	B	811	1/1	0.99	0.03	22,22,22,22	0
6	CA	A	812	1/1	0.99	0.04	22,22,22,22	0

6.5 Other polymers (i)

There are no such residues in this entry.