Full wwPDB X-ray Structure Validation Report ⓘ

Aug 7, 2020 – 09:29 AM BST

PDB ID	:	4GWM
Title	:	Crystal structure of human promeprin beta
Authors	:	Arolas, J.L.; Broder, C.; Jefferson, T.; Guevara, T.; Sterchi, E.E.; Bode, W.; Stocker, W.; Becker-Pauly, C.; Gomis-Ruth, F.X.
Deposited on	:	2012-09-03
Resolution	:	1.85 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

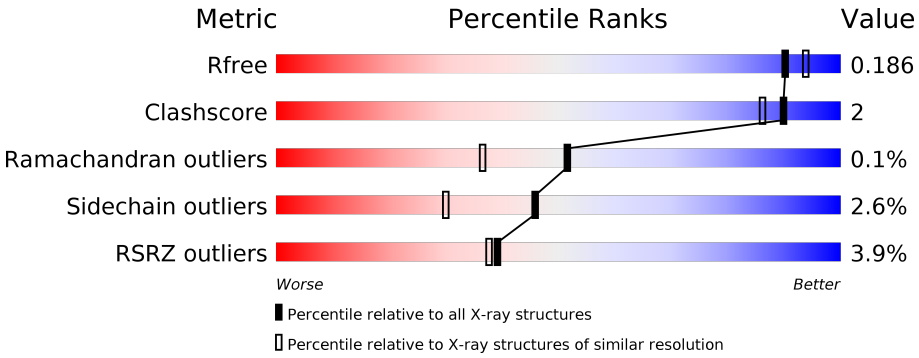
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.85 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	2469 (1.86-1.86)
Clashscore	141614	2625 (1.86-1.86)
Ramachandran outliers	138981	2592 (1.86-1.86)
Sidechain outliers	138945	2592 (1.86-1.86)
RSRZ outliers	127900	2436 (1.86-1.86)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	592	3% 90% 5% • 5%
1	B	592	4% 86% 7% 6%
2	C	3	33% 67%
2	G	3	100%
3	D	7	43% 57%
4	E	2	50% 50%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	L	2	100%
5	F	9	44% 56%
5	K	9	33% 67%
6	H	2	50% 50%
7	I	6	50% 50%
8	J	4	50% 50%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	MAN	I	4	-	-	-	X

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 10380 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.

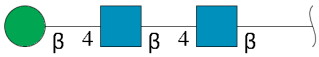
- Molecule 1 is a protein called Meprin A subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	561	Total	C	N	O	S	0	0	0
			4508	2834	782	872	20			
1	B	554	Total	C	N	O	S	0	0	0
			4458	2810	774	854	20			

There are 4 discrepancies between the modelled and reference sequences:

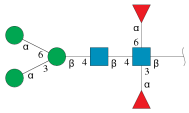
Chain	Residue	Modelled	Actual	Comment	Reference
A	23	PRO	THR	engineered mutation	UNP Q16820
A	24	TRP	PRO	engineered mutation	UNP Q16820
B	23	PRO	THR	engineered mutation	UNP Q16820
B	24	TRP	PRO	engineered mutation	UNP Q16820

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



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

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

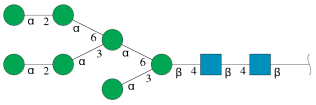


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
3	D	7	Total C N O 81 46 2 33	0	0	0

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

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

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

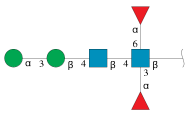


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
5	F	9	Total C N O 105 58 2 45	0	0	0
5	K	9	Total C N O 105 58 2 45	0	0	0

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

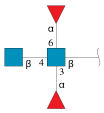
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
6	H	2	Total C N O 28 16 2 10	0	0	0

- Molecule 7 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-3)][alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
7	I	6	Total C N O 70 40 2 28	0	0	0

- Molecule 8 is an oligosaccharide called alpha-L-fucopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)][alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



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

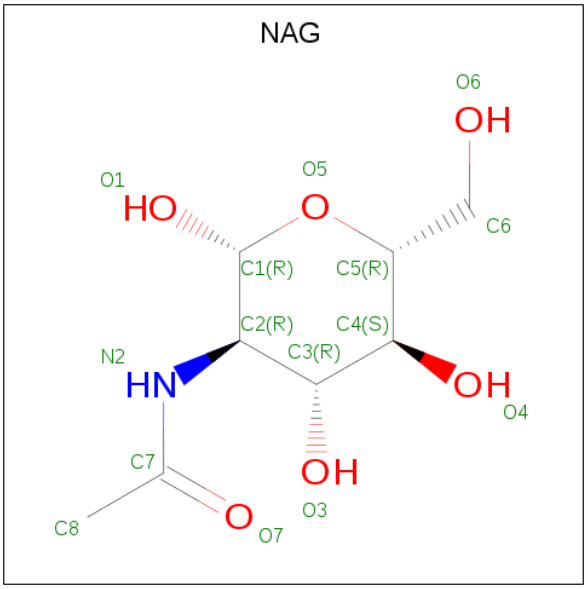
- Molecule 9 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	B	1	Total Zn 1 1	0	0
9	A	1	Total Zn 1 1	0	0

- Molecule 10 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	B	1	Total Na 1 1	0	0
10	A	1	Total Na 1 1	0	0

- Molecule 11 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).

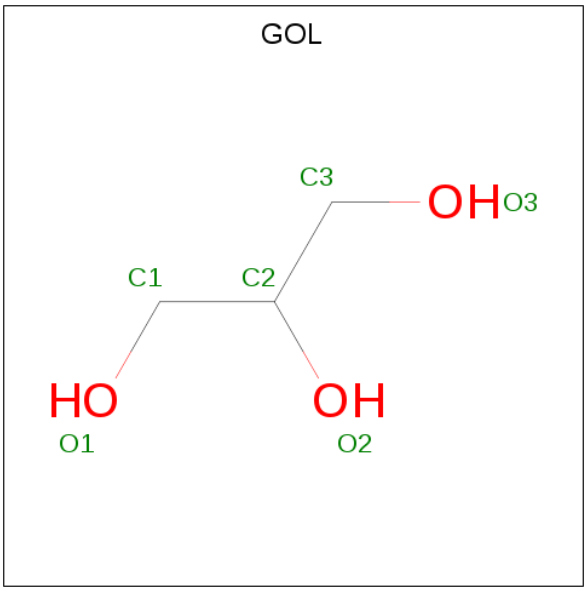


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	1	Total C N O 14 8 1 5	0	0
11	B	1	Total C N O 14 8 1 5	0	0

- Molecule 12 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	B	3	Total Cl 3 3	0	0
12	A	2	Total Cl 2 2	0	0

- Molecule 13 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	A	1	Total C O 6 3 3	0	0

- Molecule 14 is water.

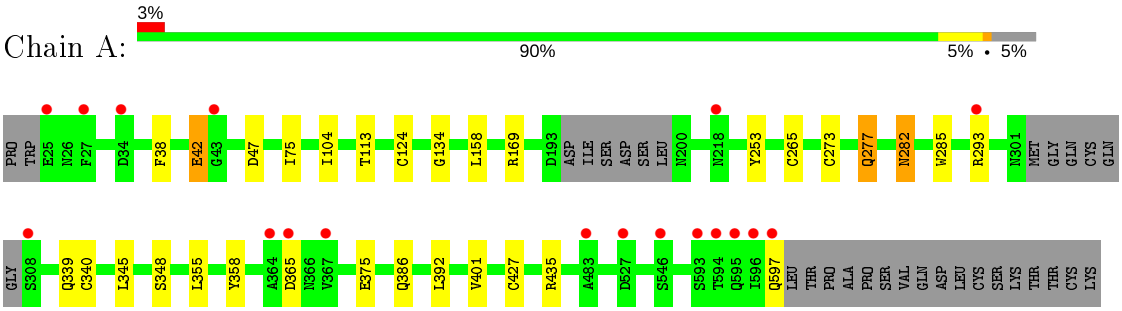
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	A	352	Total O 352 352	0	0
14	B	456	Total O 456 456	0	0

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.

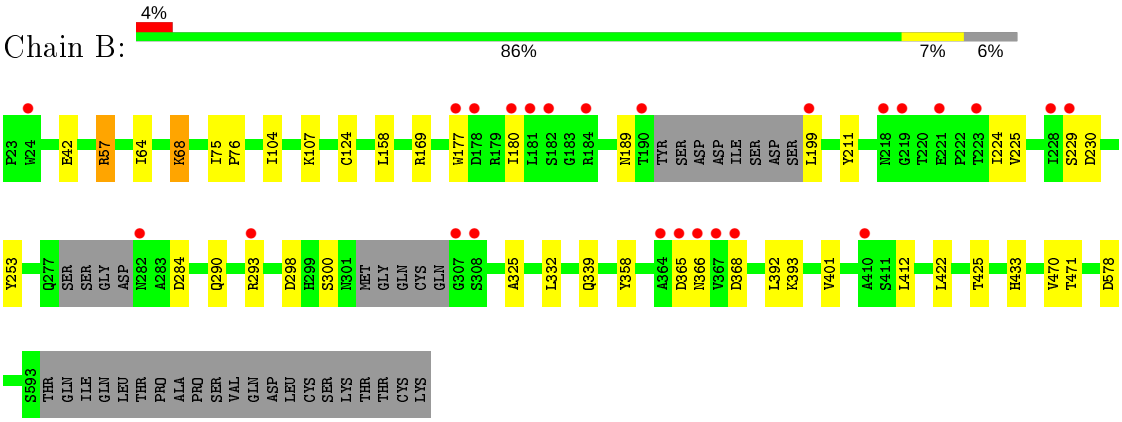
• Molecule 1: Meprin A subunit beta

Chain A:



• Molecule 1: Meprin A subunit beta

Chain B:

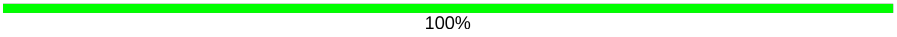


• Molecule 2: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C:

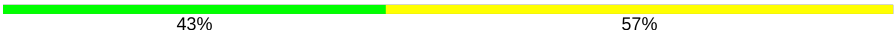
• Molecule 2: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

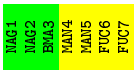
Chain G:



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

Chain D:



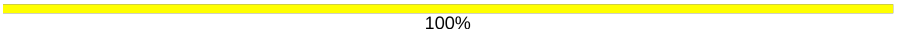


• Molecule 4: alpha-L-fucopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:

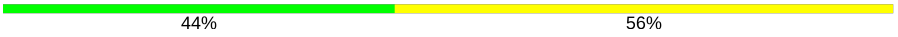
• Molecule 4: alpha-L-fucopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain L:



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

Chain F:



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

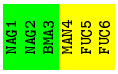
Chain K:

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

Chain H:

• Molecule 7: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-3)][alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I: 



• Molecule 8: alpha-L-fucopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)][alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J: 

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	69.62Å 71.12Å 85.74Å 74.87° 80.08° 65.13°	Depositor
Resolution (Å)	48.45 – 1.85 48.44 – 1.85	Depositor EDS
% Data completeness (in resolution range)	96.6 (48.45-1.85) 96.6 (48.44-1.85)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.95 (at 1.86Å)	Xtriage
Refinement program	BUSTER 2.11.2	Depositor
R, R_{free}	0.168 , 0.188 0.173 , 0.186	Depositor DCC
R_{free} test set	1124 reflections (0.95%)	wwPDB-VP
Wilson B-factor (Å^2)	25.4	Xtriage
Anisotropy	0.128	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 52.8	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	0.97	EDS
Total number of atoms	10380	wwPDB-VP
Average B, all atoms (Å^2)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.40% 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: GOL, ZN, BMA, NAG, CL, NA, FUC, MAN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.51	0/4617	0.62	0/6252
1	B	0.58	0/4568	0.63	0/6185
All	All	0.54	0/9185	0.62	0/12437

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4508	0	4255	15	0
1	B	4458	0	4217	16	0
2	C	39	0	34	0	0
2	G	39	0	34	0	0
3	D	81	0	70	0	0
4	E	24	0	22	0	0
4	L	24	0	22	0	0
5	F	105	0	88	0	0
5	K	105	0	88	0	0
6	H	28	0	25	0	0
7	I	70	0	61	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	J	48	0	43	0	0
9	A	1	0	0	0	0
9	B	1	0	0	0	0
10	A	1	0	0	0	0
10	B	1	0	0	0	0
11	A	14	0	13	0	0
11	B	14	0	13	0	0
12	A	2	0	0	0	0
12	B	3	0	0	0	0
13	A	6	0	8	0	0
14	A	352	0	0	0	0
14	B	456	0	0	2	0
All	All	10380	0	8993	31	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (31) 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:340:CYS:HG	1:A:427:CYS:HG	1.12	0.89
1:B:433:HIS:HE1	1:B:578:ASP:HB3	1.62	0.63
1:A:277:GLN:HG3	1:A:285:TRP:H	1.66	0.59
1:A:265:CYS:HG	1:A:273:CYS:HG	1.48	0.56
1:A:75:ILE:HD11	1:A:158:LEU:HD21	1.88	0.55
1:A:345:LEU:HD11	1:A:355:LEU:HD22	1.89	0.54
1:B:75:ILE:HD11	1:B:158:LEU:HD21	1.89	0.54
1:B:225:VAL:HA	14:B:1136:HOH:O	2.07	0.53
1:A:358:TYR:HB2	1:A:401:VAL:HB	1.92	0.52
1:B:358:TYR:HB2	1:B:401:VAL:HB	1.92	0.50
1:B:339:GLN:HB2	1:B:392:LEU:HB2	1.95	0.48
1:A:265:CYS:SG	1:A:273:CYS:SG	3.05	0.47
1:B:332:LEU:HD13	1:B:422:LEU:HD23	1.96	0.47
1:A:293:ARG:HD2	1:A:348:SER:HB2	1.96	0.47
1:B:284:ASP:HB3	1:B:325:ALA:CB	2.45	0.47
1:B:470:VAL:HG13	1:B:471:THR:HG23	1.96	0.47
1:A:339:GLN:HB2	1:A:392:LEU:HB2	1.97	0.46
1:B:433:HIS:CE1	1:B:578:ASP:HB3	2.48	0.45
1:A:340:CYS:CB	1:A:427:CYS:HG	2.28	0.45
1:A:104:ILE:HD11	1:A:253:TYR:CD1	2.52	0.44
1:B:293:ARG:HG3	1:B:412:LEU:O	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:113:THR:O	1:A:134:GLY:HA2	2.18	0.43
1:B:76:PRO:HA	1:B:107:LYS:O	2.18	0.43
1:B:177:TRP:HA	1:B:180:ILE:HD12	2.01	0.43
1:B:211:TYR:HD2	1:B:224:ILE:HD11	1.84	0.42
1:B:425:THR:HG21	14:B:1106:HOH:O	2.18	0.42
1:B:68:LYS:H	1:B:68:LYS:HD3	1.84	0.42
1:A:282:ASN:HD22	1:A:282:ASN:HA	1.77	0.42
1:A:38:PHE:O	1:A:42:GLU:HB2	2.20	0.41
1:B:104:ILE:HD11	1:B:253:TYR:CD1	2.56	0.41
1:A:386:GLN:OE1	1:A:435:ARG:NH2	2.54	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	555/592 (94%)	543 (98%)	12 (2%)	0	100	100
1	B	546/592 (92%)	534 (98%)	11 (2%)	1 (0%)	47	33
All	All	1101/1184 (93%)	1077 (98%)	23 (2%)	1 (0%)	51	36

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	57	ARG

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	497/525 (95%)	488 (98%)	9 (2%)	59 45
1	B	490/525 (93%)	473 (96%)	17 (4%)	36 18
All	All	987/1050 (94%)	961 (97%)	26 (3%)	46 30

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	42	GLU
1	A	47	ASP
1	A	124	CYS
1	A	169	ARG
1	A	277	GLN
1	A	282	ASN
1	A	365	ASP
1	A	375	GLU
1	A	597	GLN
1	B	42	GLU
1	B	57	ARG
1	B	64	ILE
1	B	68	LYS
1	B	124	CYS
1	B	169	ARG
1	B	189	ASN
1	B	199	LEU
1	B	229	SER
1	B	230	ASP
1	B	290	GLN
1	B	298	ASP
1	B	300	SER
1	B	365	ASP
1	B	366	ASN
1	B	368	ASP
1	B	393	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	282	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	528	ASN
1	A	530	ASN
1	A	597	GLN
1	B	433	HIS
1	B	487	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

47 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	0.27	0	17,19,21	0.69	0
2	NAG	C	2	2	14,14,15	0.34	0	17,19,21	0.97	1 (5%)
2	BMA	C	3	2	11,11,12	0.32	0	15,15,17	0.68	1 (6%)
3	NAG	D	1	1,3	14,14,15	0.30	0	17,19,21	0.47	0
3	NAG	D	2	3	14,14,15	0.27	0	17,19,21	0.50	0
3	BMA	D	3	3	11,11,12	0.30	0	15,15,17	0.47	0
3	MAN	D	4	3	11,11,12	0.42	0	15,15,17	2.60	3 (20%)
3	MAN	D	5	3	11,11,12	0.41	0	15,15,17	0.81	1 (6%)
3	FUC	D	6	3	10,10,11	0.46	0	14,14,16	0.82	1 (7%)
3	FUC	D	7	3	10,10,11	0.48	0	14,14,16	0.95	1 (7%)
4	NAG	E	1	1,4	14,14,15	0.30	0	17,19,21	0.72	0
4	FUC	E	2	4	10,10,11	0.47	0	14,14,16	0.84	1 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	NAG	F	1	1,5	14,14,15	0.28	0	17,19,21	0.42	0
5	NAG	F	2	5	14,14,15	0.28	0	17,19,21	0.57	0
5	BMA	F	3	5	11,11,12	0.31	0	15,15,17	0.65	0
5	MAN	F	4	5	11,11,12	0.35	0	15,15,17	0.80	1 (6%)
5	MAN	F	5	5	11,11,12	0.33	0	15,15,17	0.81	1 (6%)
5	MAN	F	6	5	11,11,12	0.32	0	15,15,17	0.73	1 (6%)
5	MAN	F	7	5	11,11,12	0.34	0	15,15,17	0.68	1 (6%)
5	MAN	F	8	5	11,11,12	0.35	0	15,15,17	0.83	1 (6%)
5	MAN	F	9	5	11,11,12	0.34	0	15,15,17	0.65	0
2	NAG	G	1	1,2	14,14,15	0.27	0	17,19,21	0.71	0
2	NAG	G	2	2	14,14,15	0.27	0	17,19,21	0.47	0
2	BMA	G	3	2	11,11,12	0.28	0	15,15,17	0.49	0
6	NAG	H	1	1,6	14,14,15	0.26	0	17,19,21	0.81	1 (5%)
6	NAG	H	2	6	14,14,15	0.28	0	17,19,21	0.72	0
7	NAG	I	1	1,7	14,14,15	0.30	0	17,19,21	0.52	0
7	NAG	I	2	7	14,14,15	0.27	0	17,19,21	0.58	0
7	BMA	I	3	7	11,11,12	0.34	0	15,15,17	0.62	0
7	MAN	I	4	7	11,11,12	0.59	0	15,15,17	2.36	2 (13%)
7	FUC	I	5	7	10,10,11	0.39	0	14,14,16	0.89	1 (7%)
7	FUC	I	6	7	10,10,11	0.47	0	14,14,16	0.95	1 (7%)
8	NAG	J	1	1,8	14,14,15	0.29	0	17,19,21	0.73	0
8	FUC	J	2	8	10,10,11	0.50	0	14,14,16	0.88	1 (7%)
8	NAG	J	3	8	14,14,15	0.26	0	17,19,21	0.41	0
8	FUC	J	4	8	10,10,11	0.46	0	14,14,16	0.83	1 (7%)
5	NAG	K	1	1,5	14,14,15	0.24	0	17,19,21	0.37	0
5	NAG	K	2	5	14,14,15	0.27	0	17,19,21	0.55	0
5	BMA	K	3	5	11,11,12	0.30	0	15,15,17	0.54	0
5	MAN	K	4	5	11,11,12	0.38	0	15,15,17	0.72	1 (6%)
5	MAN	K	5	5	11,11,12	0.30	0	15,15,17	0.84	1 (6%)
5	MAN	K	6	5	11,11,12	0.34	0	15,15,17	0.72	1 (6%)
5	MAN	K	7	5	11,11,12	0.34	0	15,15,17	0.95	1 (6%)
5	MAN	K	8	5	11,11,12	0.31	0	15,15,17	0.83	1 (6%)
5	MAN	K	9	5	11,11,12	0.36	0	15,15,17	0.83	1 (6%)
4	NAG	L	1	1,4	14,14,15	0.28	0	17,19,21	0.63	1 (5%)
4	FUC	L	2	4	10,10,11	0.47	0	14,14,16	0.85	1 (7%)

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	-	0/6/23/26	0/1/1/1
2	NAG	C	2	2	-	0/6/23/26	0/1/1/1
2	BMA	C	3	2	-	0/2/19/22	0/1/1/1
3	NAG	D	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	D	2	3	-	0/6/23/26	0/1/1/1
3	BMA	D	3	3	-	0/2/19/22	0/1/1/1
3	MAN	D	4	3	-	0/2/19/22	0/1/1/1
3	MAN	D	5	3	-	0/2/19/22	0/1/1/1
3	FUC	D	6	3	-	-	0/1/1/1
3	FUC	D	7	3	-	-	0/1/1/1
4	NAG	E	1	1,4	-	0/6/23/26	0/1/1/1
4	FUC	E	2	4	-	-	0/1/1/1
5	NAG	F	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	F	2	5	-	0/6/23/26	0/1/1/1
5	BMA	F	3	5	-	0/2/19/22	0/1/1/1
5	MAN	F	4	5	-	0/2/19/22	0/1/1/1
5	MAN	F	5	5	-	0/2/19/22	0/1/1/1
5	MAN	F	6	5	-	0/2/19/22	0/1/1/1
5	MAN	F	7	5	-	0/2/19/22	0/1/1/1
5	MAN	F	8	5	-	0/2/19/22	0/1/1/1
5	MAN	F	9	5	-	1/2/19/22	0/1/1/1
2	NAG	G	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	G	2	2	-	1/6/23/26	0/1/1/1
2	BMA	G	3	2	-	0/2/19/22	0/1/1/1
6	NAG	H	1	1,6	-	0/6/23/26	0/1/1/1
6	NAG	H	2	6	-	0/6/23/26	0/1/1/1
7	NAG	I	1	1,7	-	0/6/23/26	0/1/1/1
7	NAG	I	2	7	-	0/6/23/26	0/1/1/1
7	BMA	I	3	7	-	0/2/19/22	0/1/1/1
7	MAN	I	4	7	-	0/2/19/22	0/1/1/1
7	FUC	I	5	7	-	-	0/1/1/1
7	FUC	I	6	7	-	-	0/1/1/1
8	NAG	J	1	1,8	-	0/6/23/26	0/1/1/1
8	FUC	J	2	8	-	-	0/1/1/1
8	NAG	J	3	8	-	2/6/23/26	0/1/1/1
8	FUC	J	4	8	-	-	0/1/1/1
5	NAG	K	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	K	2	5	-	0/6/23/26	0/1/1/1
5	BMA	K	3	5	-	0/2/19/22	0/1/1/1
5	MAN	K	4	5	-	0/2/19/22	0/1/1/1
5	MAN	K	5	5	-	2/2/19/22	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	MAN	K	6	5	-	1/2/19/22	0/1/1/1
5	MAN	K	7	5	-	2/2/19/22	0/1/1/1
5	MAN	K	8	5	-	0/2/19/22	0/1/1/1
5	MAN	K	9	5	-	2/2/19/22	0/1/1/1
4	NAG	L	1	1,4	-	0/6/23/26	0/1/1/1
4	FUC	L	2	4	-	-	0/1/1/1

There are no bond length outliers.

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	4	MAN	C1-O5-C5	8.62	123.88	112.19
7	I	4	MAN	C1-O5-C5	8.54	123.76	112.19
3	D	4	MAN	C1-C2-C3	3.63	114.13	109.67
5	K	7	MAN	C1-O5-C5	3.53	116.97	112.19
3	D	4	MAN	O5-C1-C2	3.25	115.80	110.77
7	I	6	FUC	C1-O5-C5	3.05	119.70	112.78
5	K	5	MAN	C1-O5-C5	2.90	116.12	112.19
3	D	7	FUC	C1-O5-C5	2.89	119.32	112.78
7	I	5	FUC	C1-O5-C5	2.66	118.81	112.78
5	K	9	MAN	C1-O5-C5	2.61	115.72	112.19
5	F	8	MAN	C1-O5-C5	2.60	115.71	112.19
5	K	8	MAN	C1-O5-C5	2.59	115.71	112.19
3	D	6	FUC	C1-O5-C5	2.46	118.35	112.78
5	F	4	MAN	C1-O5-C5	2.43	115.49	112.19
4	L	2	FUC	C1-O5-C5	2.42	118.27	112.78
4	E	2	FUC	C1-O5-C5	2.42	118.25	112.78
5	K	6	MAN	C1-O5-C5	2.40	115.44	112.19
8	J	2	FUC	C1-O5-C5	2.39	118.19	112.78
5	F	5	MAN	C1-O5-C5	2.37	115.40	112.19
5	F	6	MAN	C1-O5-C5	2.32	115.33	112.19
5	F	7	MAN	C1-O5-C5	2.31	115.32	112.19
8	J	4	FUC	C1-O5-C5	2.26	117.89	112.78
3	D	5	MAN	C1-O5-C5	2.15	115.10	112.19
2	C	3	BMA	C1-O5-C5	2.10	115.04	112.19
5	K	4	MAN	C1-O5-C5	2.08	115.01	112.19
7	I	4	MAN	C1-C2-C3	2.08	112.22	109.67
6	H	1	NAG	C1-O5-C5	2.07	115.00	112.19
4	L	1	NAG	C1-O5-C5	2.05	114.97	112.19
2	C	2	NAG	O5-C1-C2	-2.04	108.07	111.29

There are no chirality outliers.

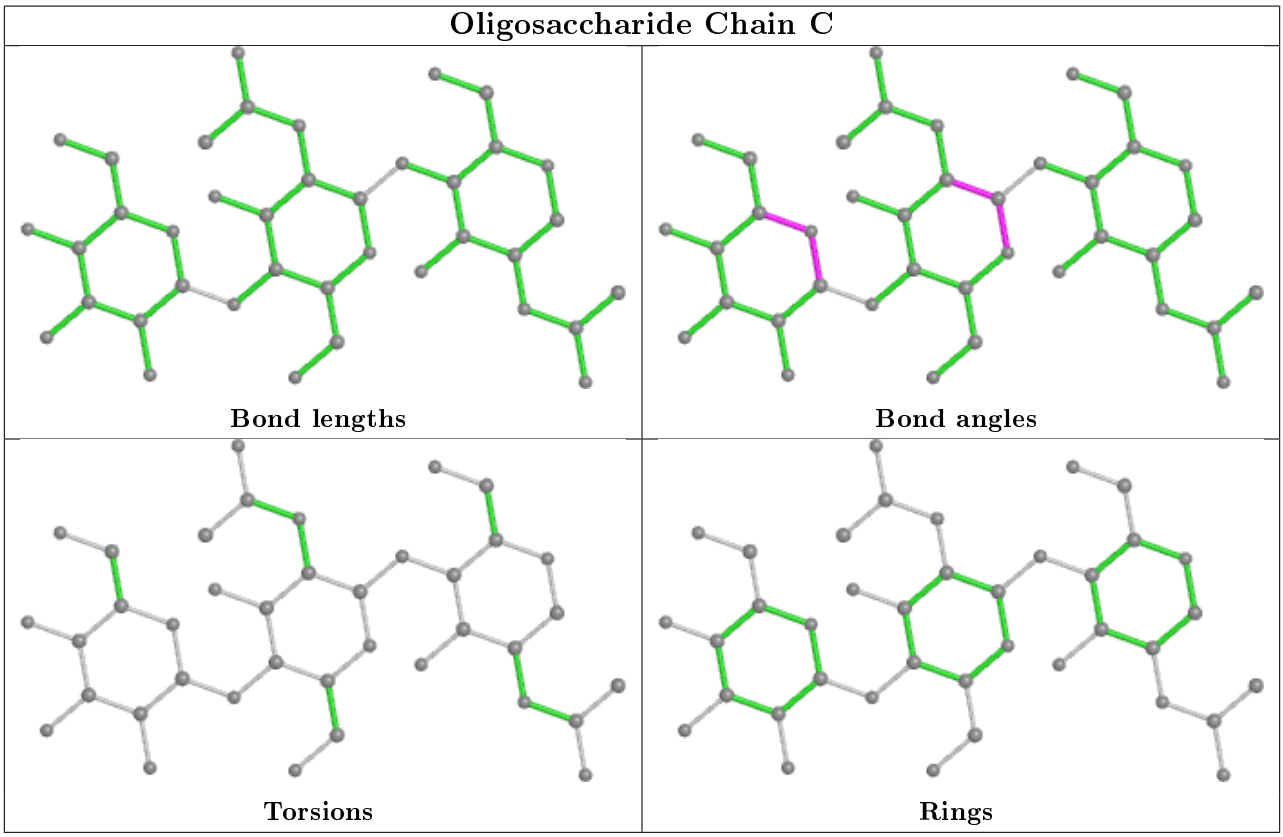
All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	K	9	MAN	O5-C5-C6-O6
5	K	6	MAN	O5-C5-C6-O6
5	K	7	MAN	O5-C5-C6-O6
2	G	2	NAG	O5-C5-C6-O6
5	F	9	MAN	C4-C5-C6-O6
8	J	3	NAG	C4-C5-C6-O6
5	K	9	MAN	C4-C5-C6-O6
5	K	5	MAN	C4-C5-C6-O6
8	J	3	NAG	O5-C5-C6-O6
5	K	5	MAN	O5-C5-C6-O6
5	K	7	MAN	C4-C5-C6-O6

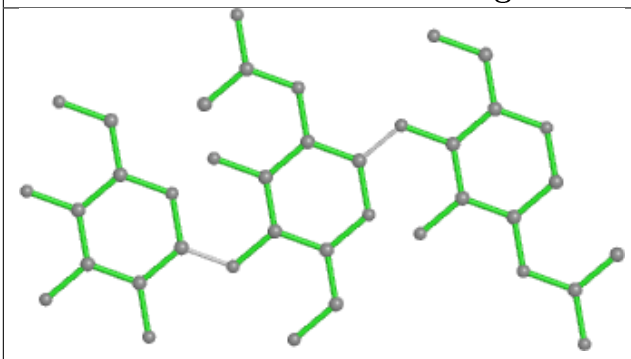
There are no ring outliers.

No monomer is involved in short contacts.

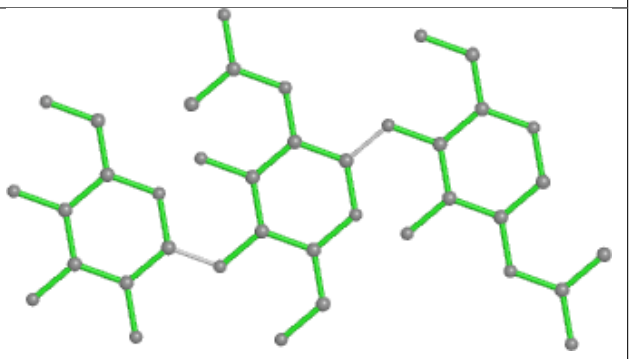
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



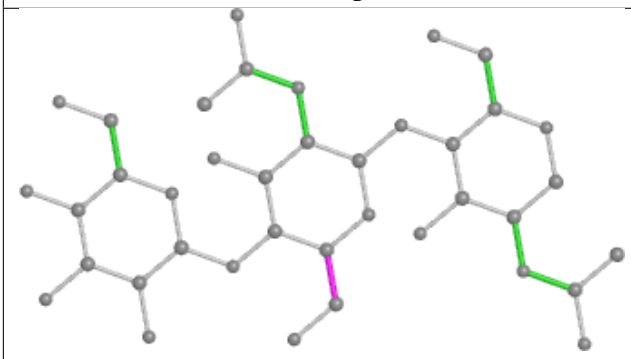
Oligosaccharide Chain G



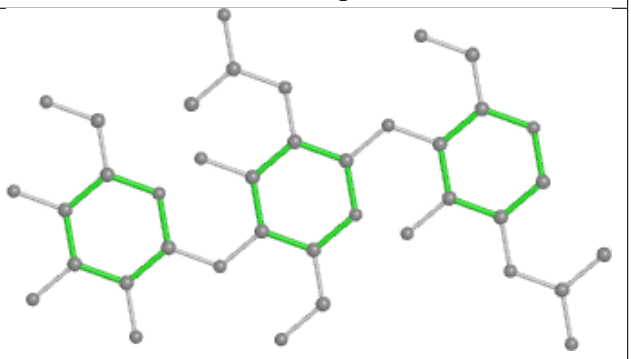
Bond lengths



Bond angles

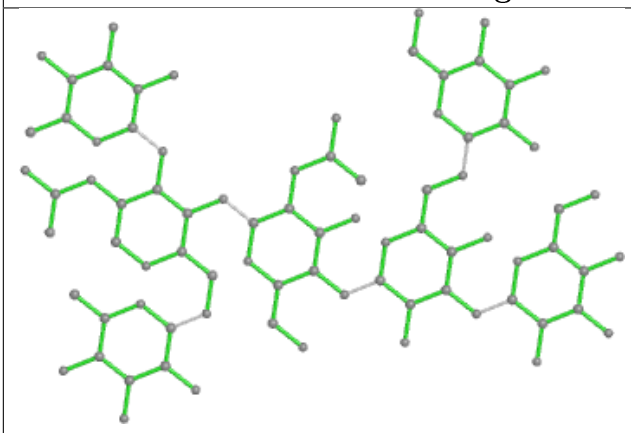


Torsions

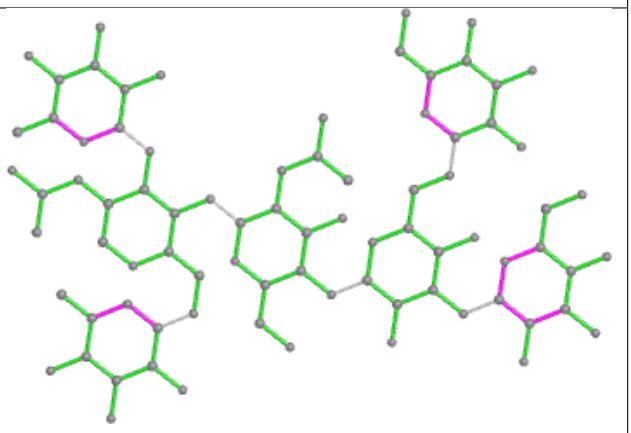


Rings

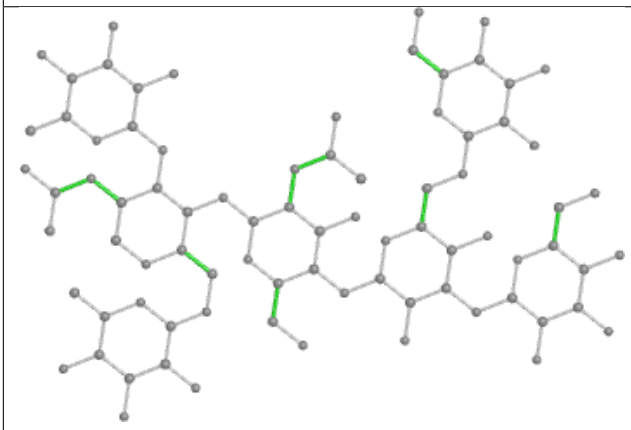
Oligosaccharide Chain D



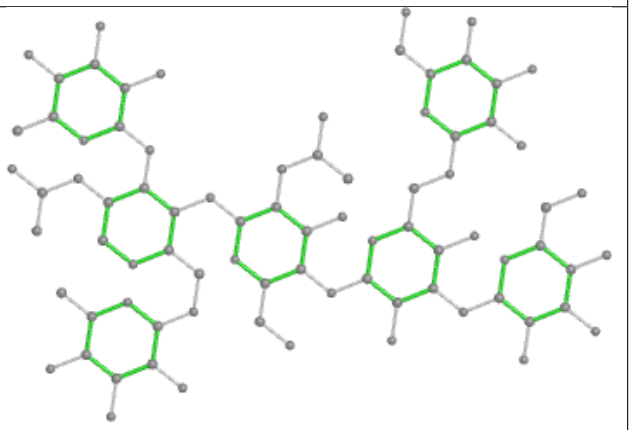
Bond lengths



Bond angles

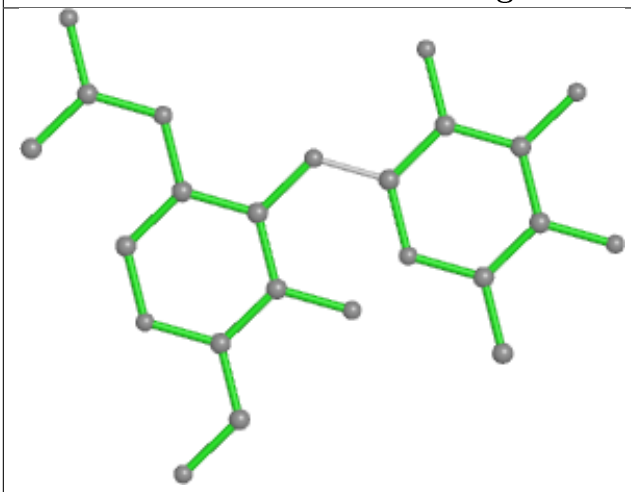


Torsions

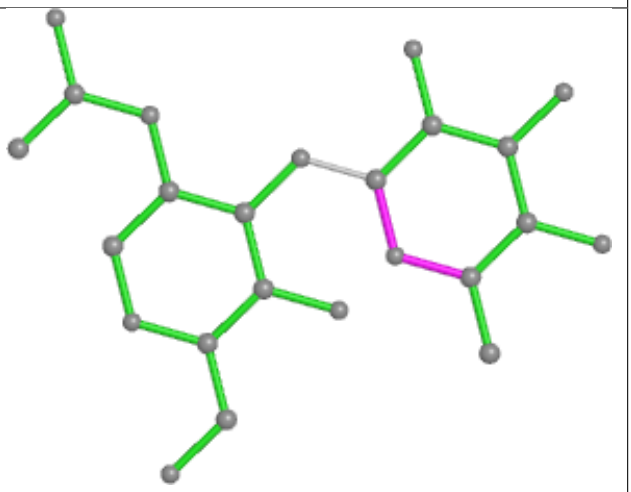


Rings

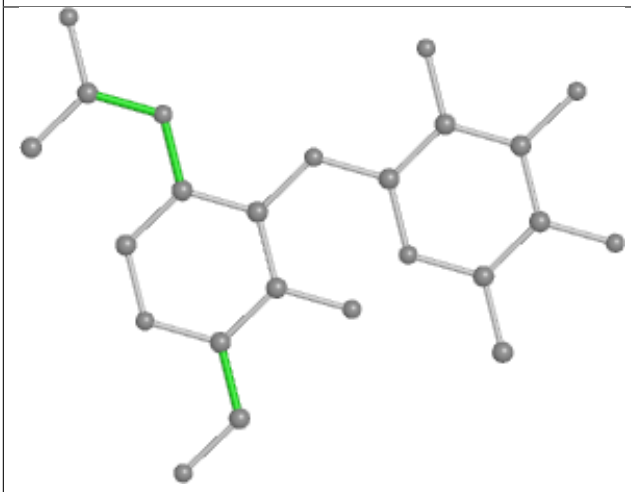
Oligosaccharide Chain E



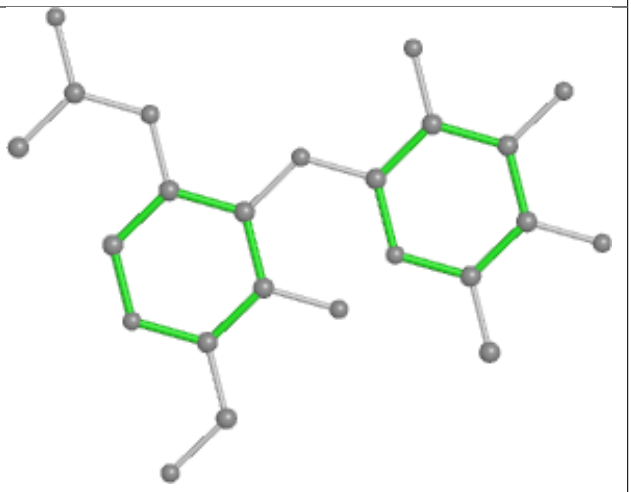
Bond lengths



Bond angles

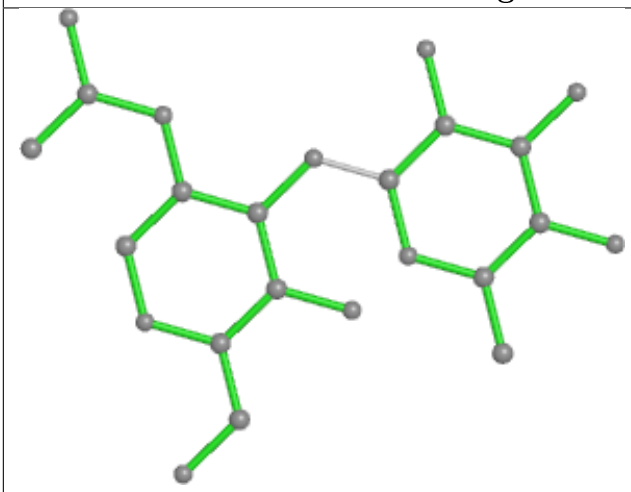


Torsions

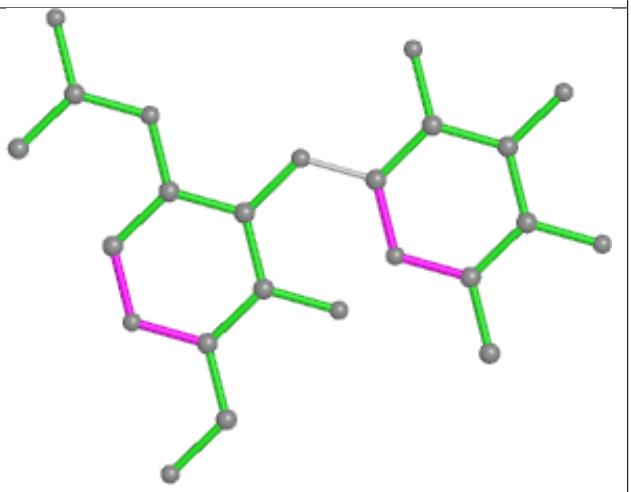


Rings

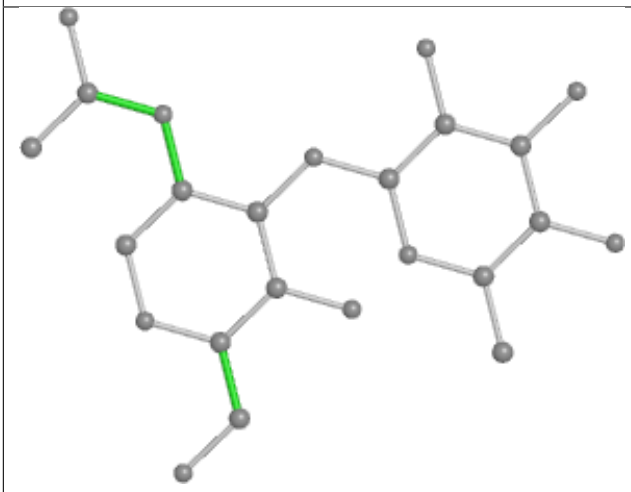
Oligosaccharide Chain L



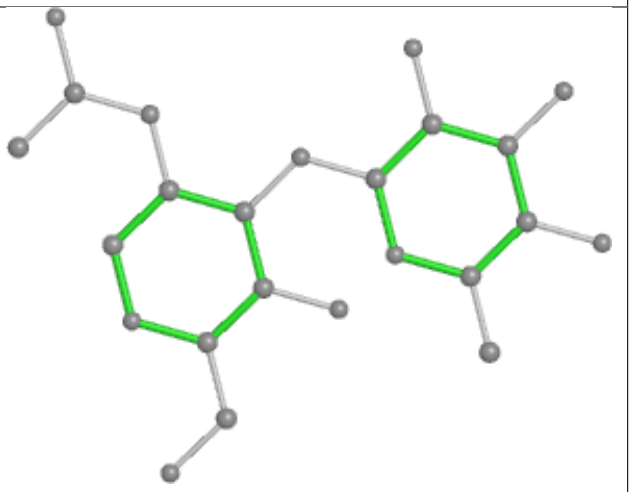
Bond lengths



Bond angles

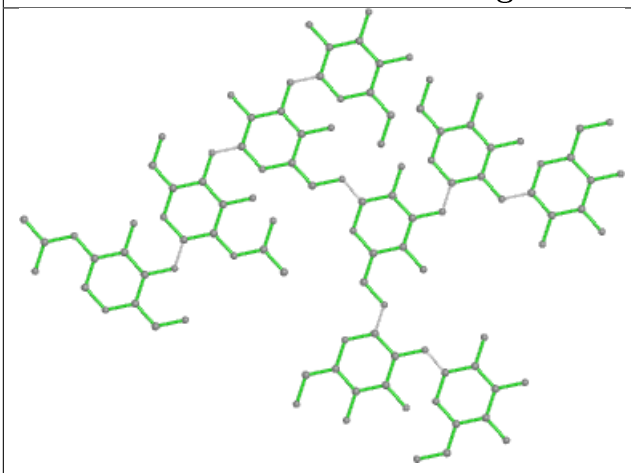


Torsions

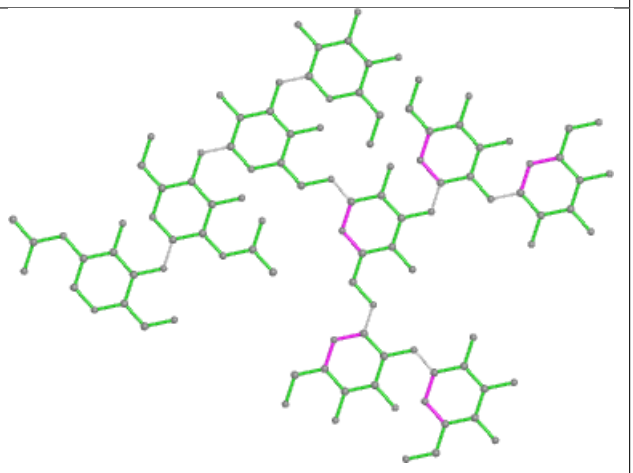


Rings

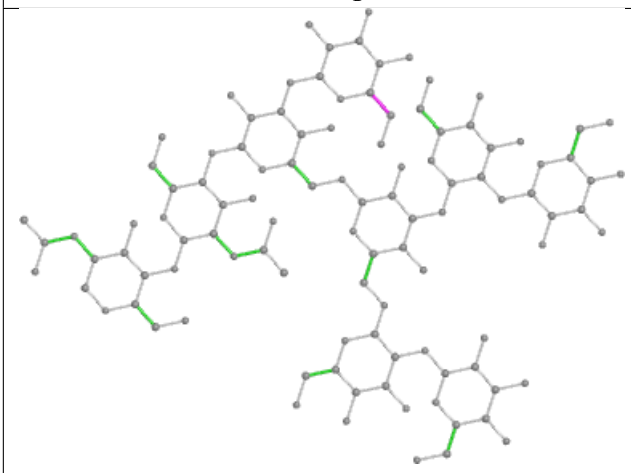
Oligosaccharide Chain F



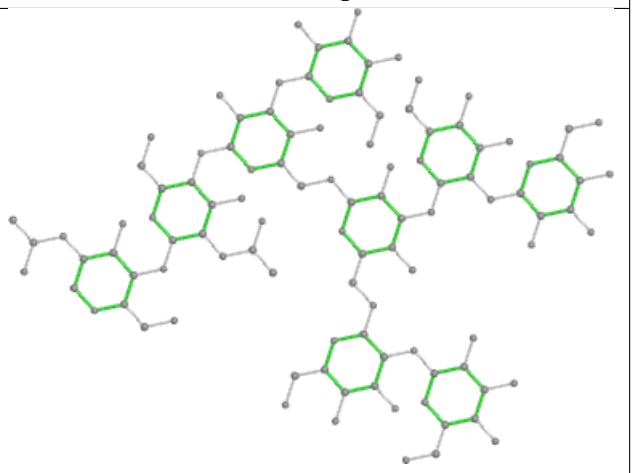
Bond lengths



Bond angles

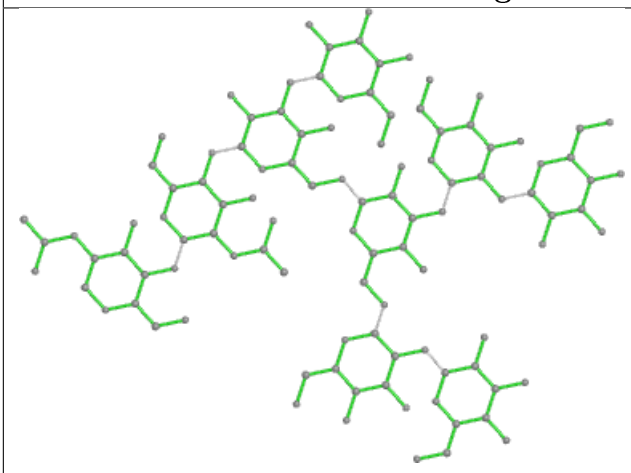


Torsions

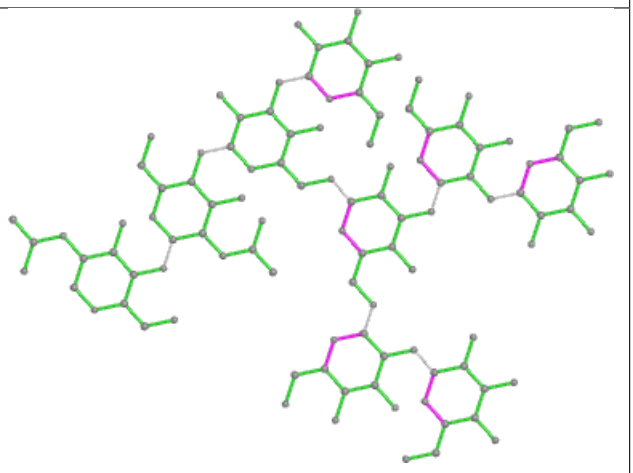


Rings

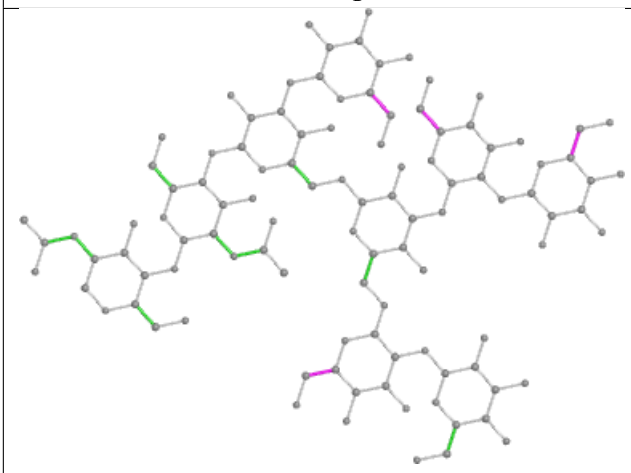
Oligosaccharide Chain K



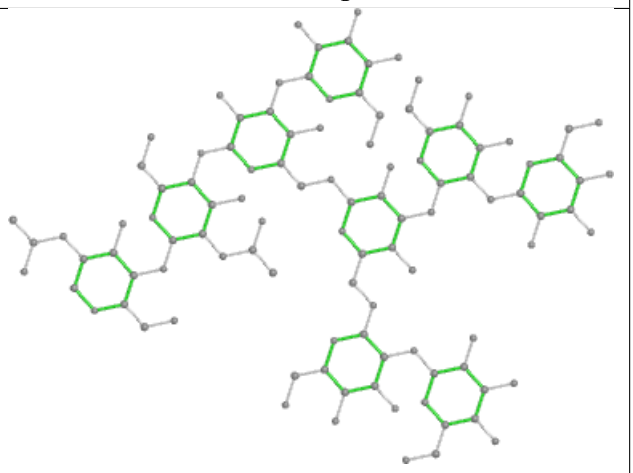
Bond lengths



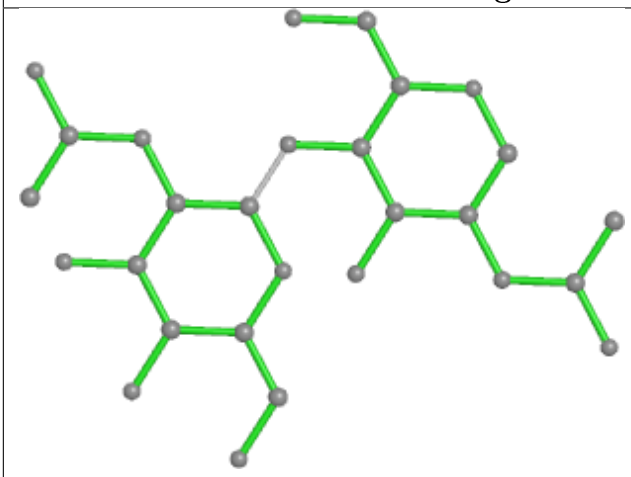
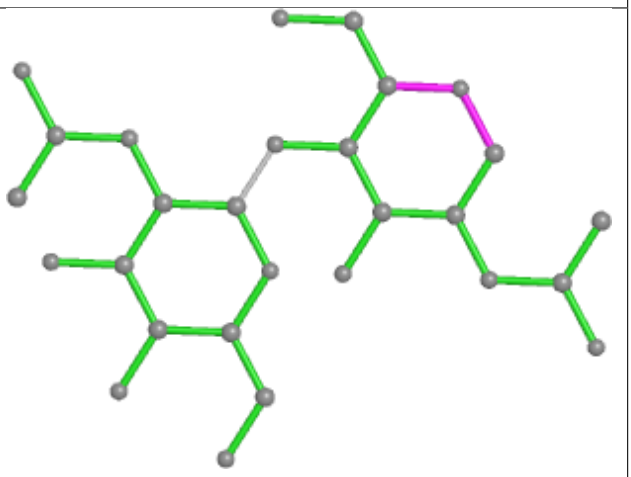
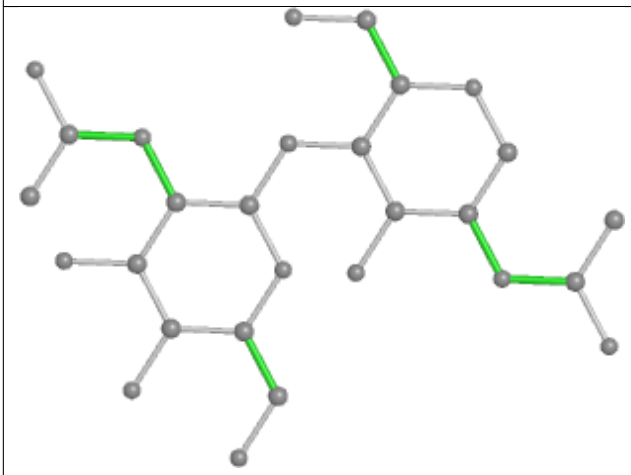
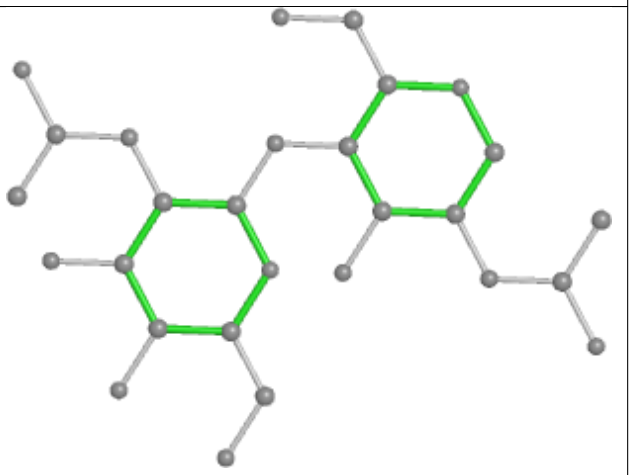
Bond angles



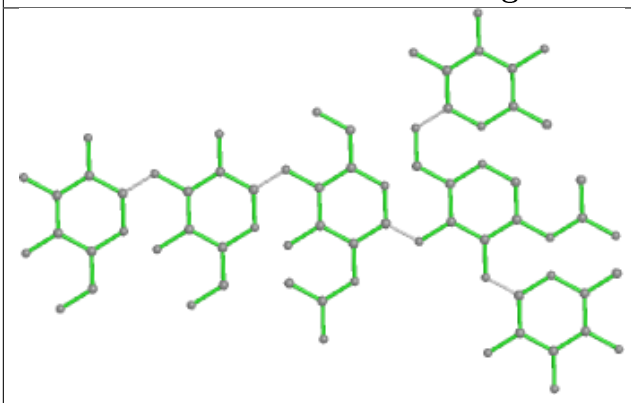
Torsions



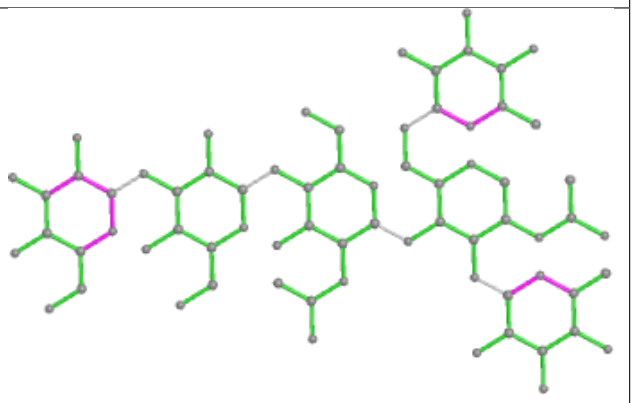
Rings

Oligosaccharide Chain H	
 Bond lengths	 Bond angles
 Torsions	 Rings

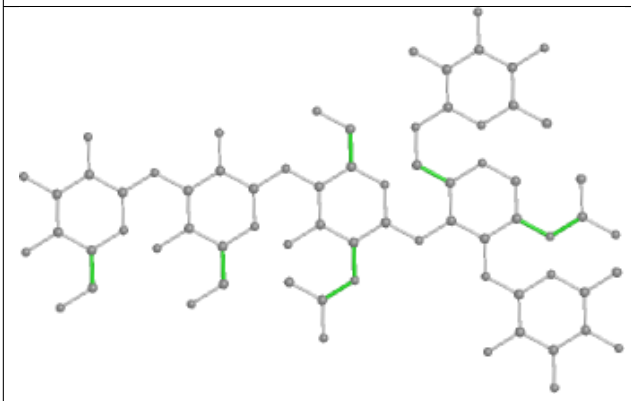
Oligosaccharide Chain I



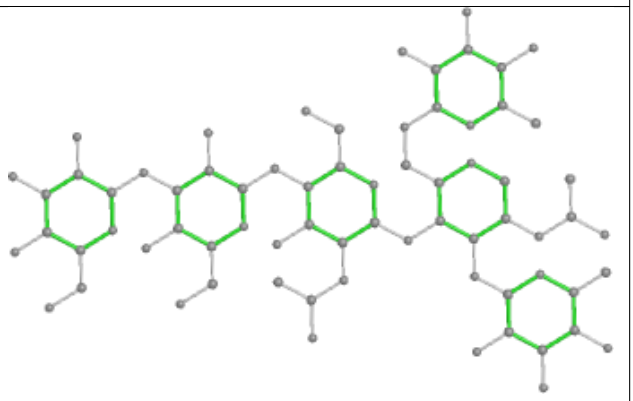
Bond lengths



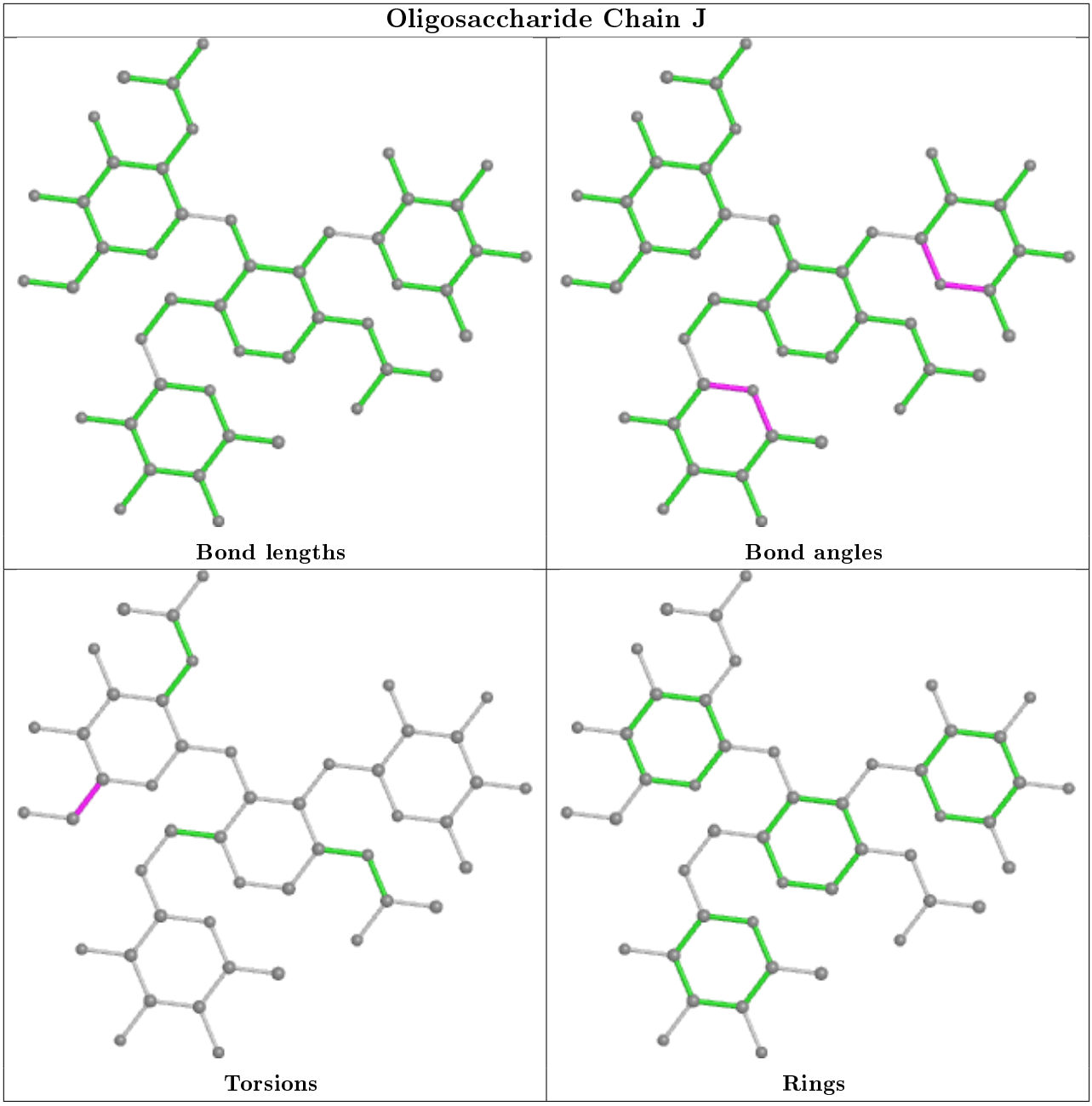
Bond angles



Torsions



Rings



5.6 Ligand geometry (i)

Of 12 ligands modelled in this entry, 9 are monoatomic - leaving 3 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
11	NAG	A	727	1	14,14,15	0.28	0	17,19,21	0.72	1 (5%)
11	NAG	B	724	1	14,14,15	0.29	0	17,19,21	0.67	1 (5%)
13	GOL	A	730	-	5,5,5	0.09	0	5,5,5	0.20	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
11	NAG	A	727	1	-	0/6/23/26	0/1/1/1
11	NAG	B	724	1	-	0/6/23/26	0/1/1/1
13	GOL	A	730	-	-	2/4/4/4	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	A	727	NAG	C1-O5-C5	2.34	115.37	112.19
11	B	724	NAG	C1-O5-C5	2.12	115.07	112.19

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	A	730	GOL	O1-C1-C2-C3
13	A	730	GOL	O1-C1-C2-O2

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	561/592 (94%)	-0.07	18 (3%)	47	45	21, 36, 66, 128	0
1	B	554/592 (93%)	-0.04	25 (4%)	33	32	16, 30, 63, 90	0
All	All	1115/1184 (94%)	-0.05	43 (3%)	39	38	16, 34, 65, 128	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	596	ILE	7.1
1	B	199	LEU	6.1
1	B	364	ALA	5.7
1	B	307	GLY	5.5
1	B	181	LEU	5.2
1	A	597	GLN	4.9
1	B	178	ASP	4.4
1	B	182	SER	4.4
1	B	365	ASP	4.2
1	B	368	ASP	4.2
1	B	190	THR	3.9
1	A	43	GLY	3.8
1	B	308	SER	3.8
1	B	366	ASN	3.7
1	A	293	ARG	3.6
1	B	24	TRP	3.4
1	A	527	ASP	3.4
1	A	365	ASP	3.2
1	A	308	SER	3.2
1	B	223	THR	3.2
1	B	367	VAL	3.0
1	A	367	VAL	2.9
1	B	177	TRP	2.9
1	B	184	ARG	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	218	ASN	2.8
1	A	483	ALA	2.7
1	B	180	ILE	2.6
1	B	410	ALA	2.6
1	A	364	ALA	2.5
1	B	282	ASN	2.5
1	A	595	GLN	2.4
1	A	25	GLU	2.4
1	A	218	ASN	2.2
1	A	27	PHE	2.2
1	A	593	SER	2.2
1	B	293	ARG	2.2
1	A	546	SER	2.1
1	A	34	ASP	2.1
1	B	229	SER	2.1
1	B	221	GLU	2.1
1	A	594	THR	2.0
1	B	219	GLY	2.0
1	B	228	ILE	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, 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	BMA	G	3	11/12	0.48	0.40	99,102,105,106	0
2	BMA	C	3	11/12	0.72	0.38	92,101,105,107	0
7	MAN	I	4	11/12	0.74	0.52	114,116,117,118	0
7	BMA	I	3	11/12	0.75	0.38	95,106,109,110	0
5	MAN	K	6	11/12	0.75	0.38	91,97,99,100	0
4	FUC	L	2	10/11	0.77	0.36	84,86,88,89	0
3	MAN	D	4	11/12	0.79	0.24	93,98,100,101	0
3	MAN	D	5	11/12	0.80	0.15	80,83,87,89	0
4	NAG	L	1	14/15	0.82	0.23	70,74,83,88	0

Continued on next page...

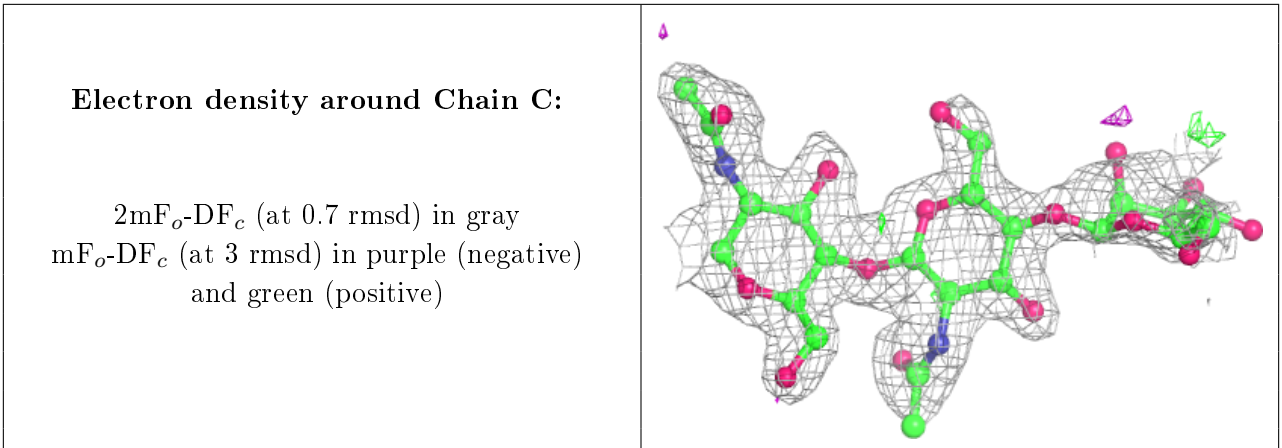
Continued from previous page...

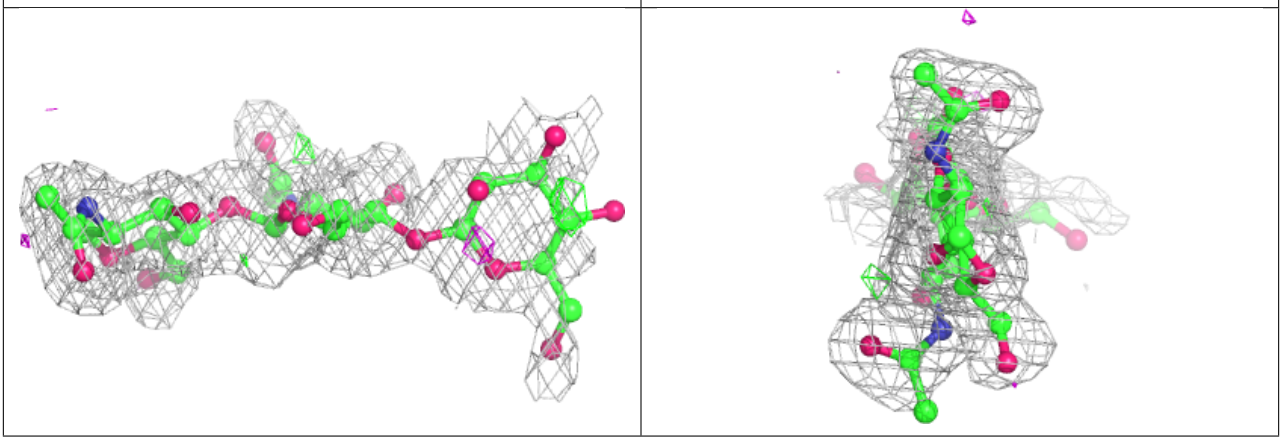
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NAG	G	2	14/15	0.83	0.36	83,89,97,98	0
5	MAN	F	6	11/12	0.83	0.23	97,102,103,103	0
4	FUC	E	2	10/11	0.83	0.30	97,102,103,103	0
3	FUC	D	6	10/11	0.83	0.19	62,67,70,73	0
5	MAN	K	9	11/12	0.84	0.17	80,86,90,91	0
3	BMA	D	3	11/12	0.84	0.15	73,80,84,87	0
2	NAG	G	1	14/15	0.87	0.20	70,73,79,81	0
5	MAN	F	9	11/12	0.88	0.36	90,95,98,99	0
8	FUC	J	2	10/11	0.88	0.29	62,72,79,79	0
8	NAG	J	3	14/15	0.89	0.23	48,53,61,66	0
2	NAG	C	2	14/15	0.89	0.22	50,59,69,82	0
6	NAG	H	2	14/15	0.90	0.23	51,55,59,61	0
5	BMA	F	3	11/12	0.91	0.17	62,67,74,82	0
5	MAN	F	5	11/12	0.91	0.15	81,84,90,91	0
5	BMA	K	3	11/12	0.91	0.08	47,55,62,70	0
4	NAG	E	1	14/15	0.92	0.27	80,85,91,93	0
7	NAG	I	1	14/15	0.92	0.16	43,57,64,66	0
5	MAN	F	4	11/12	0.92	0.08	59,66,69,74	0
5	MAN	K	7	11/12	0.93	0.13	47,50,59,64	0
5	MAN	F	7	11/12	0.93	0.13	64,68,74,76	0
7	NAG	I	2	14/15	0.93	0.18	61,70,75,83	0
5	MAN	F	8	11/12	0.93	0.12	66,69,73,75	0
3	NAG	D	2	14/15	0.94	0.10	48,56,62,66	0
5	MAN	K	5	11/12	0.94	0.12	68,74,79,84	0
3	NAG	D	1	14/15	0.94	0.07	36,43,56,59	0
8	FUC	J	4	10/11	0.94	0.17	42,47,49,51	0
5	MAN	K	8	11/12	0.95	0.20	51,54,56,59	0
2	NAG	C	1	14/15	0.95	0.10	35,43,48,50	0
7	FUC	I	5	10/11	0.95	0.16	59,62,69,70	0
3	FUC	D	7	10/11	0.95	0.07	36,38,41,48	0
5	NAG	K	1	14/15	0.95	0.11	41,46,60,62	0
5	NAG	F	1	14/15	0.96	0.16	52,56,64,65	0
7	FUC	I	6	10/11	0.96	0.10	39,42,46,49	0
5	NAG	K	2	14/15	0.96	0.08	30,41,53,55	0
6	NAG	H	1	14/15	0.96	0.08	33,39,45,46	0
5	NAG	F	2	14/15	0.96	0.15	48,52,58,61	0
5	MAN	K	4	11/12	0.97	0.06	42,45,49,56	0
8	NAG	J	1	14/15	0.97	0.09	33,38,45,50	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:

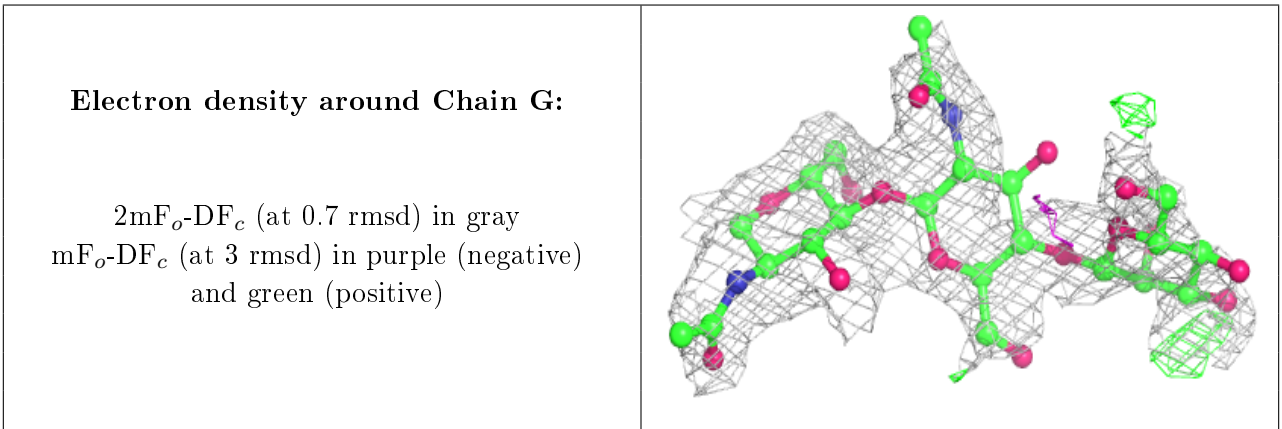
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

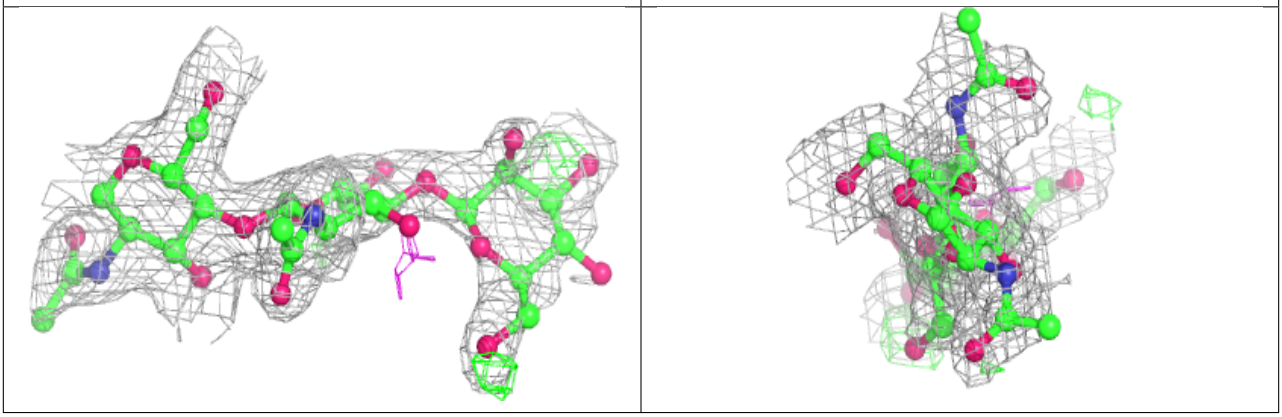




Electron density around Chain G:

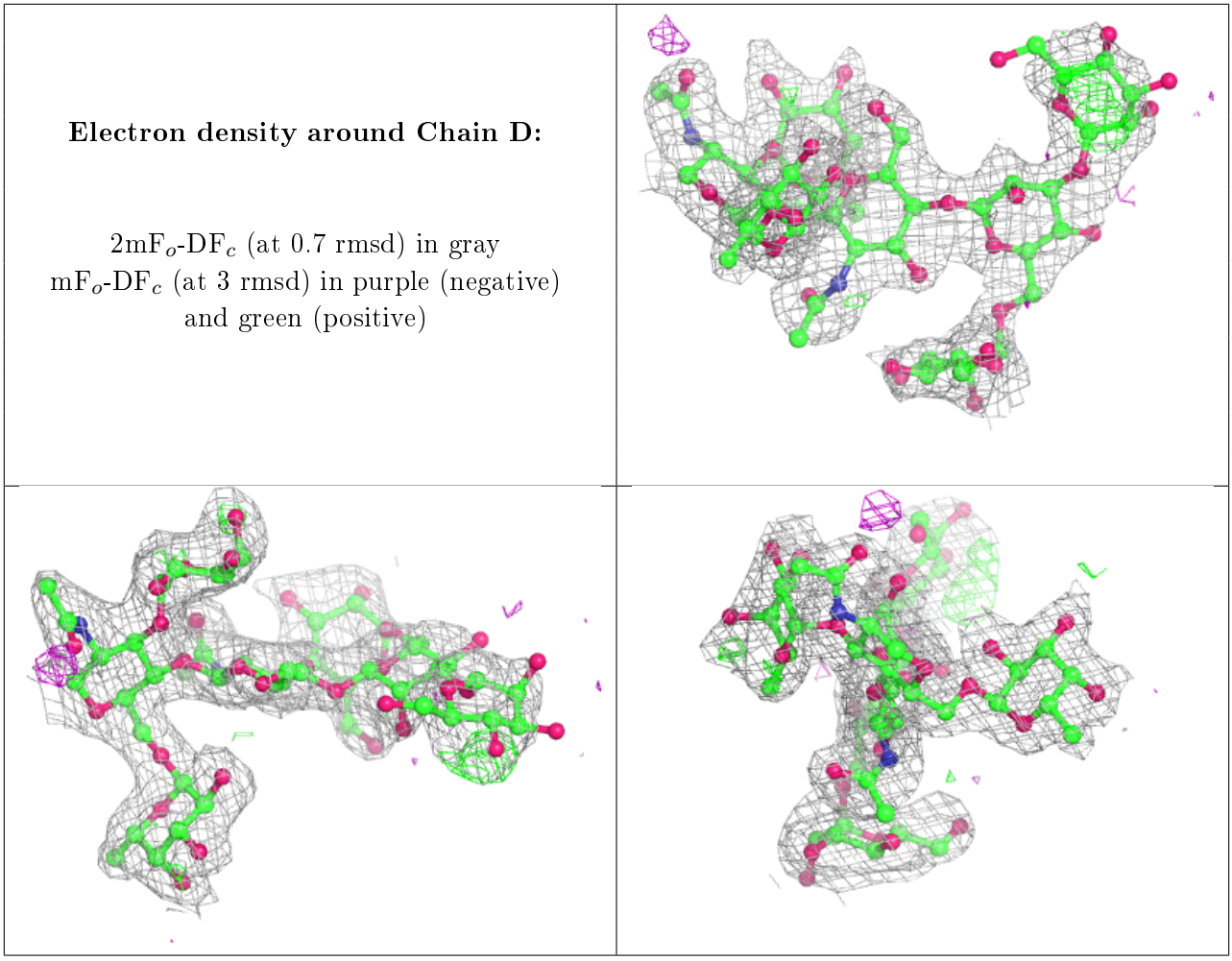
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





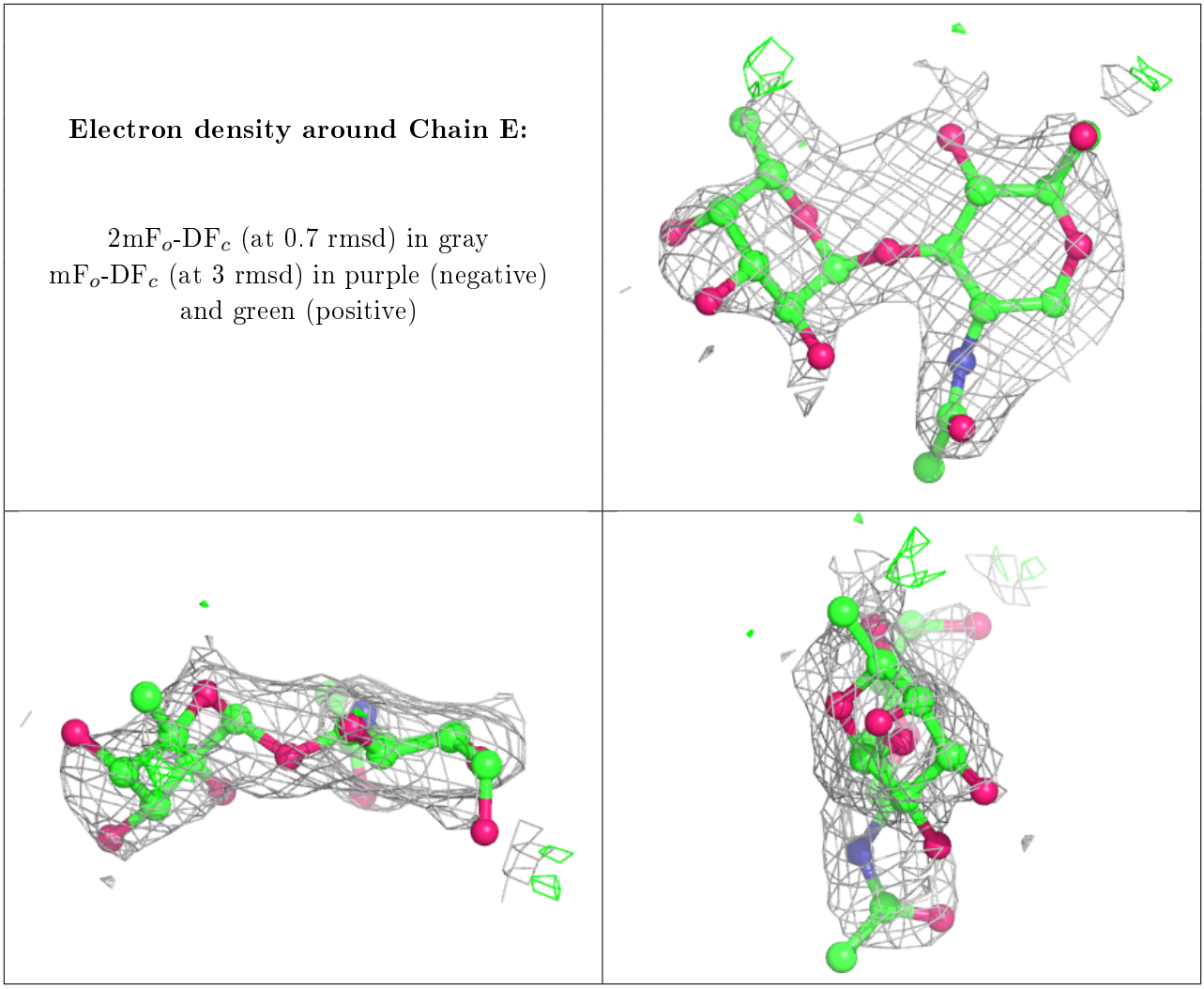
Electron density around Chain D:

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



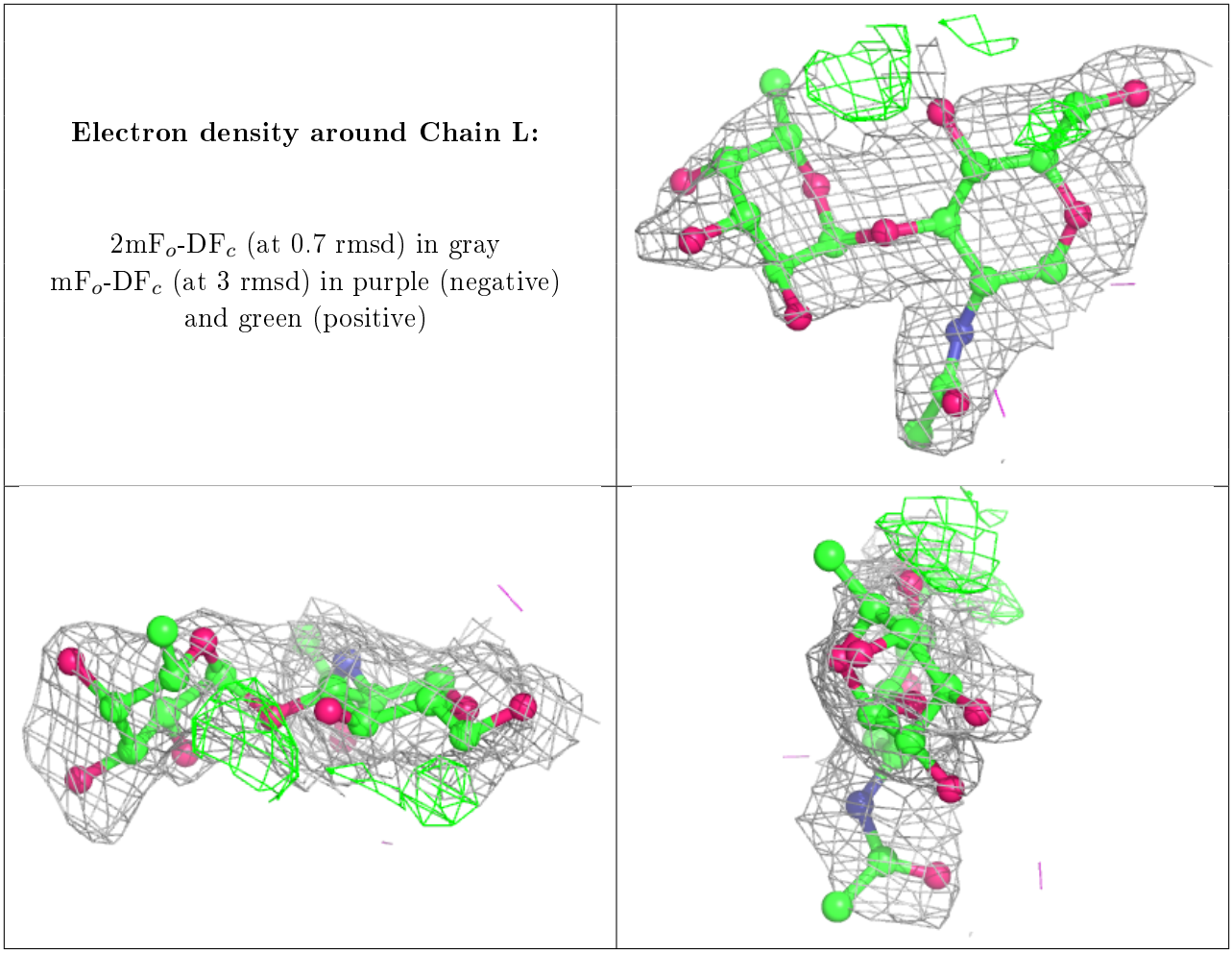
Electron density around Chain E:

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



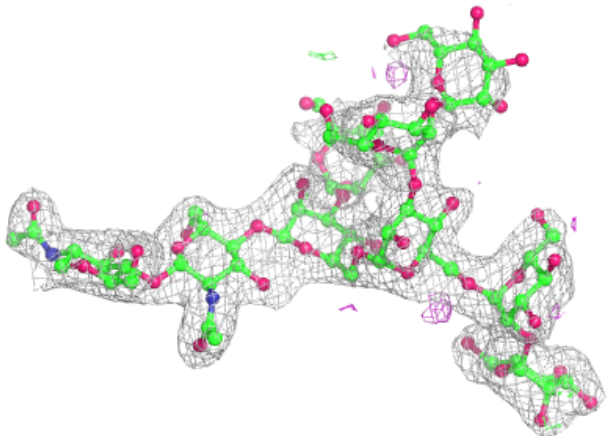
Electron density around Chain L:

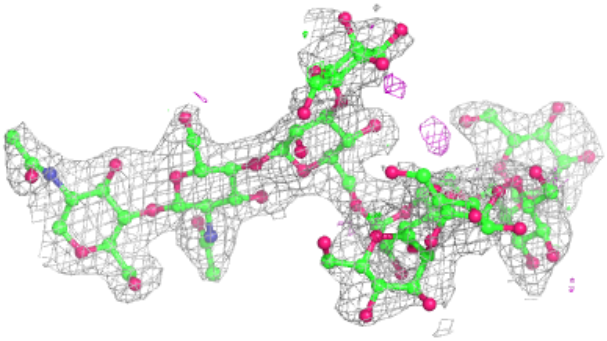
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

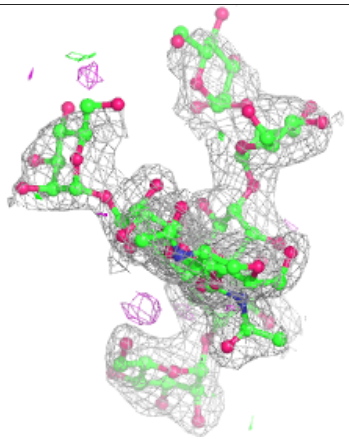


Electron density around Chain F:

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

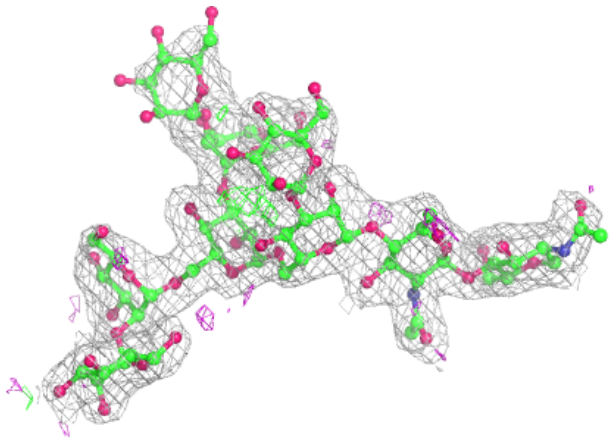


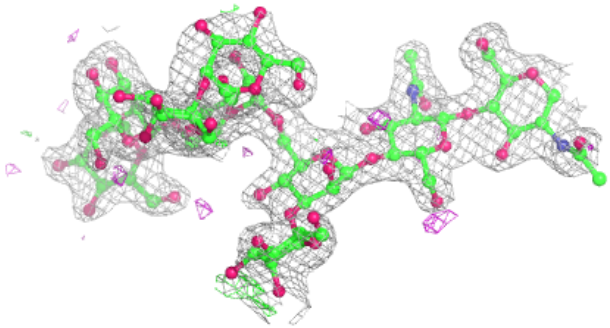


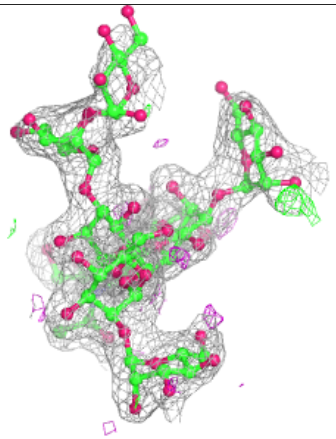


Electron density around Chain K:

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

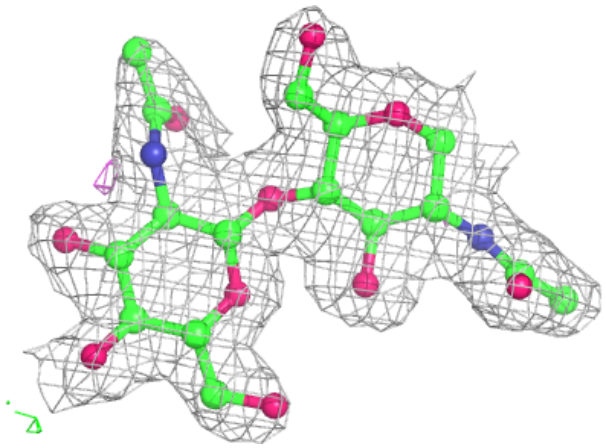


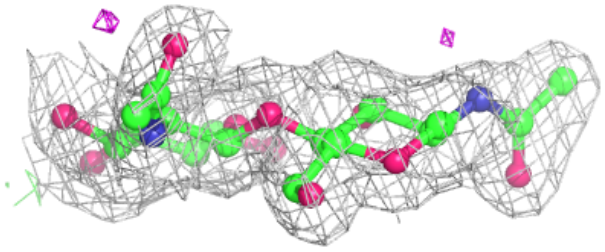


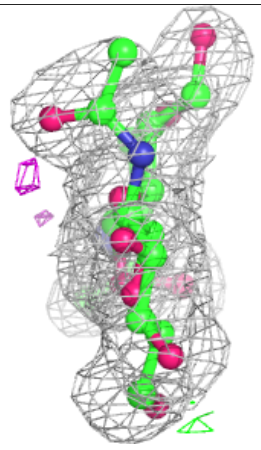


Electron density around Chain H:

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

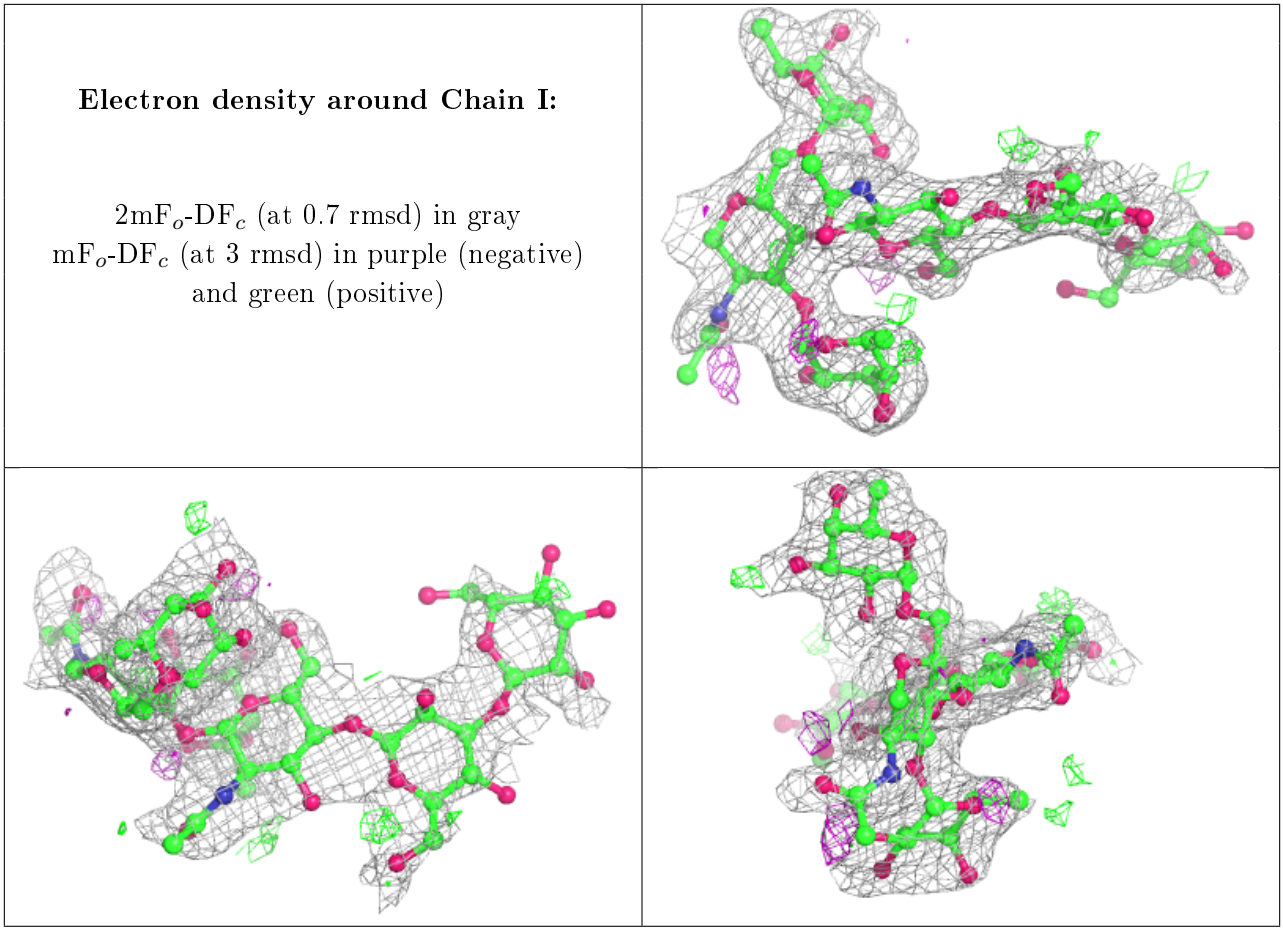






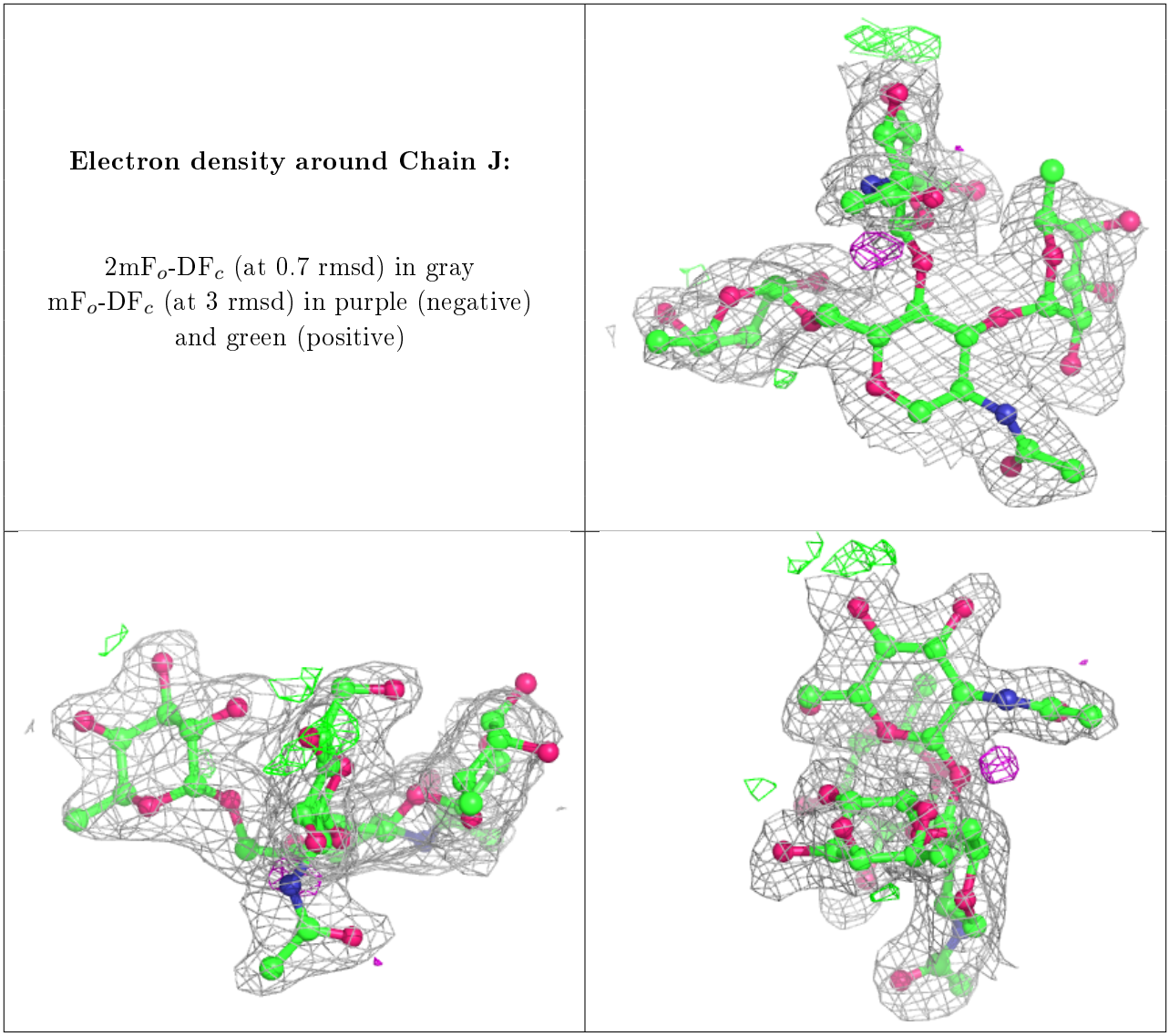
Electron density around Chain I:

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



Electron density around Chain J:

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



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
11	NAG	A	727	14/15	0.77	0.31	81,85,90,92	0
11	NAG	B	724	14/15	0.80	0.29	84,89,92,94	0
13	GOL	A	730	6/6	0.89	0.17	53,54,55,59	0
10	NA	B	702	1/1	0.98	0.09	27,27,27,27	0
12	CL	B	729	1/1	0.99	0.09	20,20,20,20	1
12	CL	B	728	1/1	0.99	0.08	32,32,32,32	1
12	CL	A	728	1/1	0.99	0.08	28,28,28,28	1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
10	NA	A	702	1/1	0.99	0.05	31,31,31,31	0
12	CL	B	727	1/1	1.00	0.10	18,18,18,18	0
12	CL	A	729	1/1	1.00	0.10	28,28,28,28	0
9	ZN	A	701	1/1	1.00	0.09	25,25,25,25	0
9	ZN	B	701	1/1	1.00	0.10	20,20,20,20	0

6.5 Other polymers

There are no such residues in this entry.