Full wwPDB X-ray Structure Validation Report (i)

Jun 19, 2024 – 01:04 AM EDT

PDB ID	:	4G1M
Title	:	Re-refinement of alpha V beta 3 structure
Authors	:	Springer, T.A.; Mi, L.; Zhu, J.
Deposited on	:	2012-07-10
Resolution	:	2.90 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 (1)) were used in the production of this report:

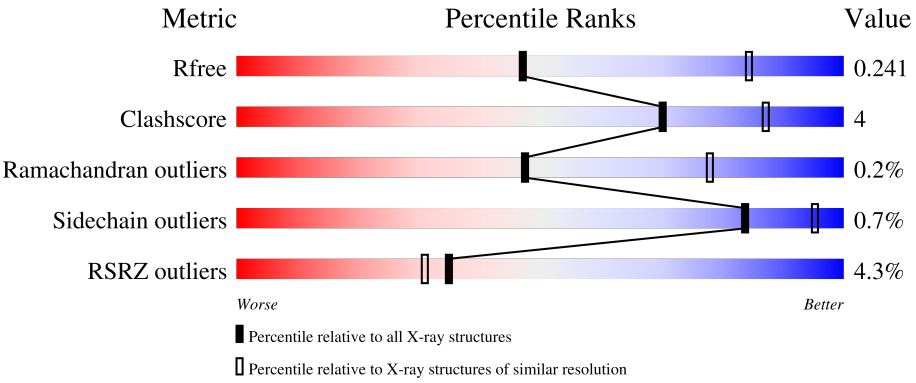
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA,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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.90 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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	959	3% 86% 11% .
2	B	692	6% 91% 9%
3	C	5	40% 60%
4	D	2	100%
4	F	2	100%

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Mol	Chain	Length	Quality of chain
4	G	2	100%
4	H	2	100%
4	I	2	100%
4	J	2	100%
4	K	2	50% 50%
4	L	2	50% 50%
4	M	2	100%
5	E	7	57% 43%
6	N	3	67% 33%

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
4	NAG	G	2	-	-	-	X

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 13132 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.

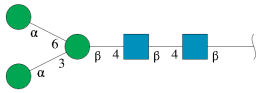
- Molecule 1 is a protein called Integrin alpha-V.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	929	7215	4568	1226	1386	35	0	0	2

- Molecule 2 is a protein called Integrin beta-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	692	5312	3261	907	1074	70	0	1	1

- 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)-2-acetamido-2-deoxy-beta-D-glucopyranose.



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

- Molecule 4 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			
4	D	2	28	16	2	10	0	0	0

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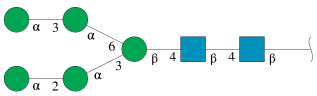
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	F	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	G	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	H	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	I	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	J	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	K	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	L	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	M	2	Total	C	N	O	0	0	0
			28	16	2	10			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	7	Total	C	N	O	0	0	0
			83	46	2	35			

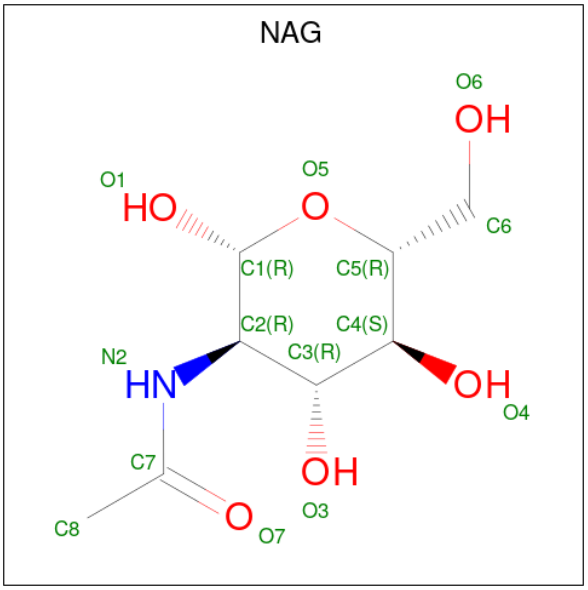
- Molecule 6 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

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

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	5	Total Ca 5 5	0	0
7	B	2	Total Ca 2 2	0	0

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



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

- Molecule 9 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	1	Total Na 1 1	0	0

- Molecule 10 is water.

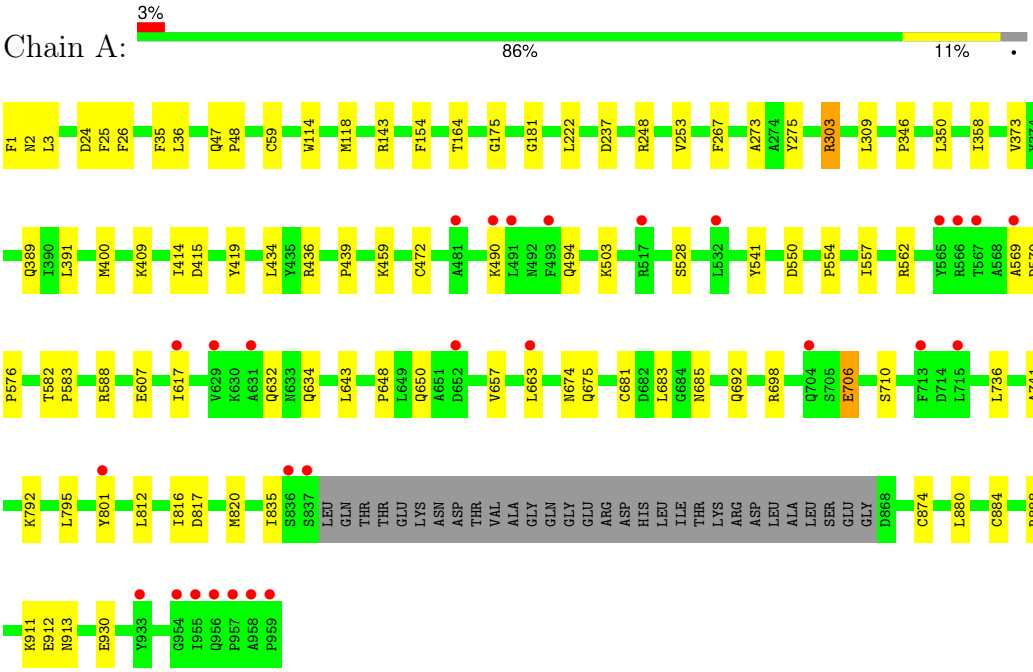
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	66	Total O 66 66	0	0
10	B	40	Total O 40 40	0	0

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.

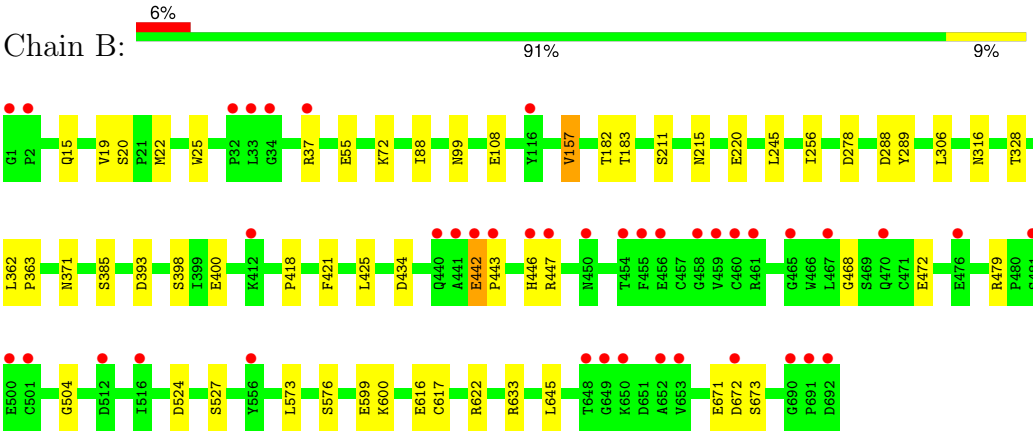
• Molecule 1: Integrin alpha-V

Chain A:



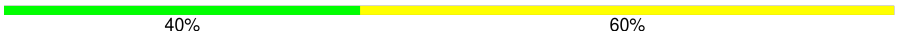
• Molecule 2: Integrin beta-3

Chain B:



• 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)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C:

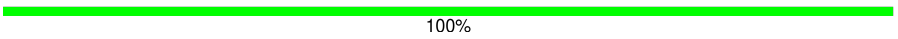


• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:

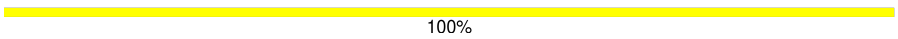
• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:



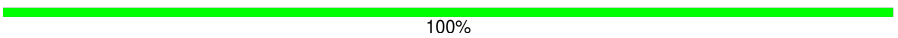
• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:



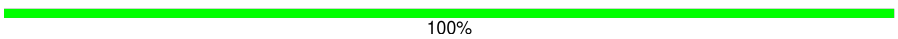
• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:



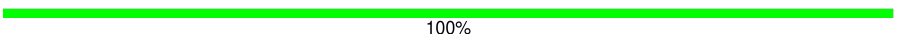
• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:



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

Chain J:



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

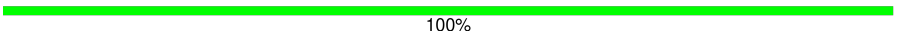
Chain K:

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

Chain L:

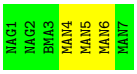
• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:



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

Chain E:



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

Chain N:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	129.87Å 129.87Å 305.90Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	65.00 – 2.90 64.94 – 2.90	Depositor EDS
% Data completeness (in resolution range)	92.7 (65.00-2.90) 92.7 (64.94-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.16 (at 2.91Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_276), CNS	Depositor
R, R_{free}	0.179 , 0.233 0.186 , 0.241	Depositor DCC
R_{free} test set	2924 reflections (4.70%)	wwPDB-VP
Wilson B-factor (Å^2)	82.4	Xtriage
Anisotropy	0.191	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 67.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.020 for -h,-k,l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	13132	wwPDB-VP
Average B, all atoms (Å^2)	97.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.04% 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: NAG, BMA, NA, MAN, CA

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	0.24	0/7372	0.42	0/9996
2	B	0.23	0/5409	0.41	0/7316
All	All	0.23	0/12781	0.41	0/17312

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	7215	0	7028	60	0
2	B	5312	0	5036	33	0
3	C	61	0	52	0	0
4	D	28	0	25	0	0
4	F	28	0	25	0	0
4	G	28	0	25	0	0
4	H	28	0	25	0	0
4	I	28	0	25	0	0
4	J	28	0	25	0	0
4	K	28	0	25	0	0
4	L	28	0	25	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	M	28	0	25	0	0
5	E	83	0	70	0	0
6	N	39	0	34	0	0
7	A	5	0	0	0	0
7	B	2	0	0	0	0
8	A	28	0	26	0	0
8	B	28	0	26	0	0
9	A	1	0	0	0	0
10	A	66	0	0	0	0
10	B	40	0	0	0	0
All	All	13132	0	12497	92	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 4.

All (92) 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)
2:B:484:ASP:HB2	2:B:504:GLY:HA2	1.80	0.64
2:B:616[A]:GLU:HG3	2:B:622:ARG:HG3	1.80	0.63
1:A:741:ALA:H	1:A:786:GLY:HA3	1.66	0.59
1:A:490:LYS:NZ	1:A:528:SER:HB2	2.18	0.58
1:A:1:PHE:HA	1:A:389:GLN:HB2	1.85	0.58
1:A:24:ASP:OD2	1:A:25:PHE:N	2.37	0.56
2:B:362:LEU:HD12	2:B:363:PRO:HD2	1.88	0.56
2:B:15:GLN:O	2:B:19:VAL:HG23	2.08	0.54
1:A:607:GLU:HG3	1:A:632:GLN:HG3	1.91	0.53
2:B:72:LYS:NZ	2:B:108:GLU:HG2	2.24	0.52
1:A:26:PHE:HB3	1:A:35:PHE:HB2	1.90	0.52
1:A:24:ASP:HA	1:A:409:LYS:HG2	1.93	0.51
1:A:181:GLY:HA3	1:A:222:LEU:HB3	1.93	0.51
1:A:494:GLN:HB3	1:A:562:ARG:HB3	1.92	0.51
2:B:88:ILE:HG13	2:B:425:LEU:HD11	1.92	0.50
1:A:472:CYS:HA	1:A:541:TYR:HA	1.93	0.50
1:A:817:ASP:HB2	1:A:898:TYR:HE1	1.76	0.50
1:A:118:MET:SD	1:A:118:MET:N	2.85	0.49
2:B:288:ASP:OD1	2:B:289:TYR:N	2.44	0.49
1:A:648:PRO:HB2	1:A:650:GLN:OE1	2.12	0.49
2:B:316:ASN:HB2	4:L:1:NAG:H82	1.94	0.49
1:A:911:LYS:O	1:A:913:ASN:N	2.47	0.48
1:A:769:GLU:HG2	1:A:812:LEU:HD11	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:570:ASP:OD1	1:A:574:LEU:N	2.29	0.47
1:A:632:GLN:OE1	1:A:634:GLN:NE2	2.47	0.47
2:B:182:THR:OG1	2:B:183:THR:N	2.47	0.47
2:B:356:GLU:HG3	2:B:385:SER:HB3	1.97	0.47
1:A:503:LYS:HE3	1:A:550:ASP:OD2	2.14	0.47
1:A:248:ARG:HD2	4:L:1:NAG:C7	2.45	0.47
1:A:36:LEU:HB2	1:A:59:CYS:HB2	1.97	0.47
1:A:569:ALA:HB2	1:A:575:GLN:HG2	1.97	0.47
1:A:801:TYR:HB2	1:A:880:LEU:HB2	1.96	0.46
1:A:795:LEU:HB3	1:A:884:CYS:HB2	1.98	0.46
1:A:414:ILE:HG21	1:A:434:LEU:HD21	1.98	0.46
2:B:157:VAL:O	2:B:220:GLU:HB3	2.17	0.45
2:B:215:ASN:OD1	2:B:215:ASN:N	2.49	0.45
1:A:554:PRO:HG3	1:A:685:ASN:ND2	2.31	0.45
1:A:490:LYS:HZ3	1:A:528:SER:HB2	1.81	0.45
1:A:273:ALA:HA	2:B:256:ILE:HD12	1.98	0.45
2:B:468:GLY:HA3	2:B:472:GLU:HB2	1.98	0.45
1:A:154:PHE:O	1:A:175:GLY:HA3	2.17	0.45
2:B:446:HIS:ND1	2:B:447:ARG:HG3	2.32	0.44
1:A:114:TRP:CE3	1:A:143:ARG:HD2	2.53	0.44
1:A:582:THR:HA	1:A:583:PRO:HD3	1.83	0.44
2:B:371:ASN:HB2	2:B:398:SER:HB3	2.00	0.44
1:A:253:VAL:HB	1:A:267:PHE:HB2	2.00	0.43
1:A:164:THR:HB	1:A:237:ASP:HB2	1.99	0.43
1:A:3:LEU:HD21	1:A:350:LEU:HD11	2.00	0.43
1:A:47:GLN:HA	1:A:48:PRO:HD3	1.83	0.43
2:B:393:ASP:OD1	2:B:633:ARG:NH2	2.52	0.43
1:A:373:VAL:HB	1:A:391:LEU:HB2	2.01	0.43
1:A:643:LEU:HB2	1:A:683:LEU:HD11	2.01	0.43
1:A:792:LYS:HB2	1:A:930:GLU:HB2	2.01	0.43
1:A:816:ILE:HG21	1:A:820:MET:O	2.19	0.43
2:B:306:LEU:HB3	2:B:328:THR:HG23	2.01	0.43
1:A:2:ASN:OD1	1:A:2:ASN:N	2.52	0.43
1:A:617:ILE:HB	1:A:736:LEU:HD23	2.01	0.43
1:A:643:LEU:HB3	1:A:681:CYS:HB2	2.01	0.42
2:B:573:LEU:HB3	2:B:576:SER:O	2.19	0.42
2:B:599:GLU:HG2	2:B:600:LYS:HG3	1.99	0.42
1:A:376:PHE:HB3	1:A:383:LEU:HD11	2.01	0.42
1:A:657:VAL:HG12	1:A:698:ARG:HG3	2.01	0.42
2:B:20:SER:OG	2:B:22:MET:HG2	2.19	0.42
1:A:490:LYS:HZ2	1:A:528:SER:HB2	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:37:ARG:HD2	2:B:37:ARG:HA	1.92	0.42
1:A:632:GLN:HB3	1:A:692:GLN:HG2	2.02	0.42
1:A:769:GLU:HG2	1:A:902:LEU:HD11	2.01	0.42
2:B:72:LYS:HZ2	2:B:108:GLU:HG2	1.84	0.42
1:A:706:GLU:OE1	1:A:888:ARG:NH2	2.50	0.42
2:B:418:PRO:HG2	2:B:421:PHE:HB2	2.01	0.42
1:A:303:ARG:NH1	1:A:309:LEU:HD21	2.35	0.42
1:A:459:LYS:H	1:A:459:LYS:HG2	1.62	0.41
1:A:663:LEU:HD12	1:A:663:LEU:HA	1.86	0.41
2:B:99:ASN:HA	2:B:400:GLU:HA	2.03	0.41
2:B:245:LEU:HD11	2:B:348:TYR:HD1	1.84	0.41
2:B:25:TRP:HB3	2:B:55:GLU:HB2	2.01	0.41
1:A:575:GLN:HA	1:A:576:PRO:HD3	1.92	0.41
1:A:346:PRO:HA	1:A:358:ILE:HG13	2.01	0.41
1:A:419:TYR:CE1	1:A:439:PRO:HA	2.56	0.41
1:A:674:ASN:HB3	1:A:675:GLN:H	1.76	0.41
2:B:524:ASP:CG	2:B:527:SER:HB3	2.42	0.41
2:B:645:LEU:HD23	2:B:645:LEU:HA	1.81	0.41
2:B:671:GLU:O	2:B:673:SER:N	2.49	0.41
1:A:375:ILE:HD13	1:A:391:LEU:HD13	2.01	0.41
1:A:557:ILE:N	1:A:588:ARG:O	2.53	0.41
1:A:835:ILE:HD12	1:A:835:ILE:HA	1.99	0.41
1:A:415:ASP:OD2	1:A:436:ARG:HD2	2.21	0.40
2:B:278:ASP:OD1	2:B:278:ASP:N	2.55	0.40
2:B:468:GLY:HA3	2:B:472:GLU:H	1.86	0.40
1:A:710:SER:HA	1:A:736:LEU:HG	2.02	0.40
1:A:911:LYS:HA	1:A:911:LYS:HD2	1.83	0.40
2:B:442:GLU:HA	2:B:443:PRO:HD3	1.93	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	925/959 (96%)	862 (93%)	62 (7%)	1 (0%)	51 82
2	B	691/692 (100%)	630 (91%)	58 (8%)	3 (0%)	34 66
All	All	1616/1651 (98%)	1492 (92%)	120 (7%)	4 (0%)	47 78

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	912	GLU
2	B	672	ASP
2	B	479	ARG
2	B	157	VAL

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	785/813 (97%)	779 (99%)	6 (1%)	81 94
2	B	614/614 (100%)	610 (99%)	4 (1%)	84 95
All	All	1399/1427 (98%)	1389 (99%)	10 (1%)	84 95

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

Mol	Chain	Res	Type
1	A	275	TYR
1	A	303	ARG
1	A	400	MET
1	A	571	THR
1	A	706	GLU
1	A	874	CYS
2	B	211	SER
2	B	434	ASP
2	B	442	GLU
2	B	617	CYS

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

sidechains are listed below:

Mol	Chain	Res	Type
1	A	632	GLN
1	A	634	GLN
1	A	692	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

33 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	$\#\|Z\| > 2$
3	NAG	C	1	1,3	14,14,15	0.50	0	17,19,21	1.09	1 (5%)
3	NAG	C	2	3	14,14,15	0.54	0	17,19,21	0.83	0
3	BMA	C	3	3	11,11,12	0.62	0	15,15,17	1.03	1 (6%)
3	MAN	C	4	3	11,11,12	0.49	0	15,15,17	1.51	1 (6%)
3	MAN	C	5	3	11,11,12	0.60	0	15,15,17	0.64	0
4	NAG	D	1	1,4	14,14,15	0.59	0	17,19,21	0.61	0
4	NAG	D	2	4	14,14,15	0.61	0	17,19,21	0.80	0
5	NAG	E	1	1,5	14,14,15	0.58	0	17,19,21	0.80	0
5	NAG	E	2	5	14,14,15	0.54	0	17,19,21	0.75	0
5	BMA	E	3	5	11,11,12	0.71	0	15,15,17	0.57	0
5	MAN	E	4	5	11,11,12	0.51	0	15,15,17	1.34	3 (20%)
5	MAN	E	5	5	11,11,12	0.66	0	15,15,17	0.86	1 (6%)
5	MAN	E	6	5	11,11,12	0.70	0	15,15,17	1.03	1 (6%)
5	MAN	E	7	5	11,11,12	0.64	0	15,15,17	0.45	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	NAG	F	1	1,4	14,14,15	0.55	0	17,19,21	0.78	0
4	NAG	F	2	4	14,14,15	0.50	0	17,19,21	0.67	0
4	NAG	G	1	1,4	14,14,15	0.60	0	17,19,21	0.85	1 (5%)
4	NAG	G	2	4	14,14,15	0.56	0	17,19,21	1.93	2 (11%)
4	NAG	H	1	1,4	14,14,15	0.48	0	17,19,21	0.64	0
4	NAG	H	2	4	14,14,15	0.57	0	17,19,21	0.75	0
4	NAG	I	1	1,4	14,14,15	0.52	0	17,19,21	0.89	0
4	NAG	I	2	4	14,14,15	0.53	0	17,19,21	0.70	0
4	NAG	J	1	1,4	14,14,15	0.54	0	17,19,21	0.63	0
4	NAG	J	2	4	14,14,15	0.54	0	17,19,21	0.61	0
4	NAG	K	1	1,4	14,14,15	0.50	0	17,19,21	0.81	1 (5%)
4	NAG	K	2	4	14,14,15	0.60	0	17,19,21	0.74	0
4	NAG	L	1	4,2	14,14,15	0.57	0	17,19,21	0.61	0
4	NAG	L	2	4	14,14,15	0.52	0	17,19,21	0.58	0
4	NAG	M	1	4,2	14,14,15	0.52	0	17,19,21	0.86	0
4	NAG	M	2	4	14,14,15	0.57	0	17,19,21	0.91	0
6	NAG	N	1	6,2	14,14,15	0.49	0	17,19,21	0.74	0
6	NAG	N	2	6	14,14,15	0.57	0	17,19,21	0.91	1 (5%)
6	BMA	N	3	6	11,11,12	0.65	0	15,15,17	0.56	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	C	1	1,3	-	1/6/23/26	0/1/1/1
3	NAG	C	2	3	-	1/6/23/26	0/1/1/1
3	BMA	C	3	3	-	0/2/19/22	0/1/1/1
3	MAN	C	4	3	-	0/2/19/22	0/1/1/1
3	MAN	C	5	3	-	1/2/19/22	0/1/1/1
4	NAG	D	1	1,4	-	1/6/23/26	0/1/1/1
4	NAG	D	2	4	-	0/6/23/26	0/1/1/1
5	NAG	E	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	E	2	5	-	0/6/23/26	0/1/1/1
5	BMA	E	3	5	-	2/2/19/22	0/1/1/1
5	MAN	E	4	5	-	0/2/19/22	0/1/1/1
5	MAN	E	5	5	-	0/2/19/22	0/1/1/1
5	MAN	E	6	5	-	0/2/19/22	0/1/1/1
5	MAN	E	7	5	-	0/2/19/22	0/1/1/1
4	NAG	F	1	1,4	-	3/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	F	2	4	-	1/6/23/26	0/1/1/1
4	NAG	G	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	G	2	4	-	2/6/23/26	0/1/1/1
4	NAG	H	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	H	2	4	-	0/6/23/26	0/1/1/1
4	NAG	I	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	I	2	4	-	2/6/23/26	0/1/1/1
4	NAG	J	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	J	2	4	-	2/6/23/26	0/1/1/1
4	NAG	K	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	K	2	4	-	0/6/23/26	0/1/1/1
4	NAG	L	1	4,2	-	0/6/23/26	0/1/1/1
4	NAG	L	2	4	-	3/6/23/26	0/1/1/1
4	NAG	M	1	4,2	-	0/6/23/26	0/1/1/1
4	NAG	M	2	4	-	0/6/23/26	0/1/1/1
6	NAG	N	1	6,2	-	2/6/23/26	0/1/1/1
6	NAG	N	2	6	-	3/6/23/26	0/1/1/1
6	BMA	N	3	6	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	G	2	NAG	C1-O5-C5	6.14	120.41	112.19
3	C	4	MAN	C1-O5-C5	4.97	118.85	112.19
4	G	2	NAG	O5-C1-C2	4.27	117.90	111.29
5	E	4	MAN	C1-C2-C3	-3.06	105.19	109.64
3	C	1	NAG	C1-O5-C5	2.58	115.65	112.19
4	G	1	NAG	C4-C3-C2	2.35	114.46	111.02
3	C	3	BMA	C3-C4-C5	2.32	114.43	110.23
5	E	4	MAN	O2-C2-C3	2.15	114.60	110.15
5	E	5	MAN	C1-C2-C3	2.14	112.75	109.64
5	E	4	MAN	C1-O5-C5	2.09	114.98	112.19
6	N	2	NAG	C4-C3-C2	2.08	114.07	111.02
4	K	1	NAG	C2-N2-C7	-2.07	120.13	122.90
5	E	6	MAN	O3-C3-C2	-2.01	105.96	110.05

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	N	1	NAG	O7-C7-N2-C2
6	N	2	NAG	C8-C7-N2-C2
6	N	2	NAG	O7-C7-N2-C2
6	N	1	NAG	C8-C7-N2-C2
5	E	3	BMA	O5-C5-C6-O6
4	I	2	NAG	O5-C5-C6-O6
5	E	3	BMA	C4-C5-C6-O6
4	J	2	NAG	C8-C7-N2-C2
4	J	2	NAG	O7-C7-N2-C2
4	L	2	NAG	C8-C7-N2-C2
4	L	2	NAG	O7-C7-N2-C2
4	I	2	NAG	C4-C5-C6-O6
4	F	1	NAG	C8-C7-N2-C2
6	N	2	NAG	O5-C5-C6-O6
3	C	5	MAN	O5-C5-C6-O6
4	G	2	NAG	C8-C7-N2-C2
4	F	2	NAG	O5-C5-C6-O6
4	F	1	NAG	O7-C7-N2-C2
3	C	2	NAG	O5-C5-C6-O6
4	G	2	NAG	O7-C7-N2-C2
3	C	1	NAG	C1-C2-N2-C7
4	F	1	NAG	C1-C2-N2-C7
4	L	2	NAG	C1-C2-N2-C7
4	D	1	NAG	O5-C5-C6-O6

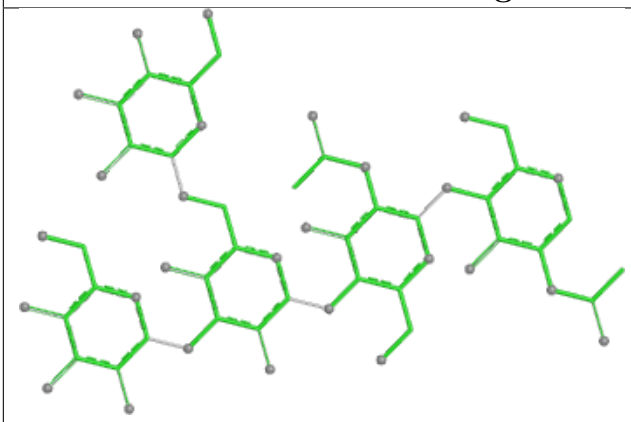
There are no ring outliers.

1 monomer is involved in 2 short contacts:

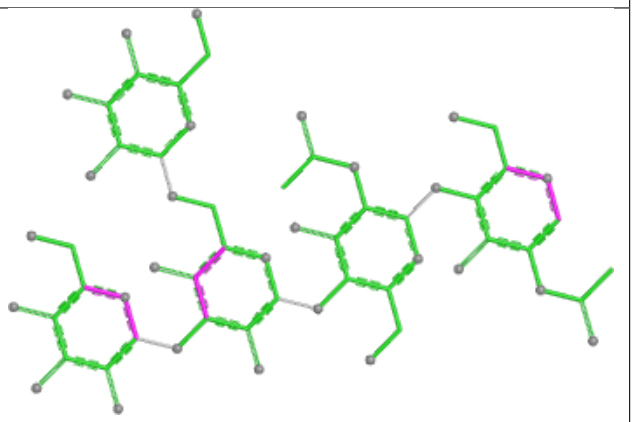
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	L	1	NAG	2	0

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

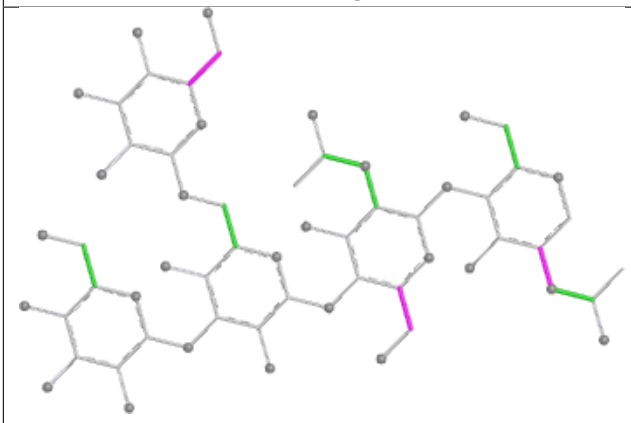
Oligosaccharide Chain C



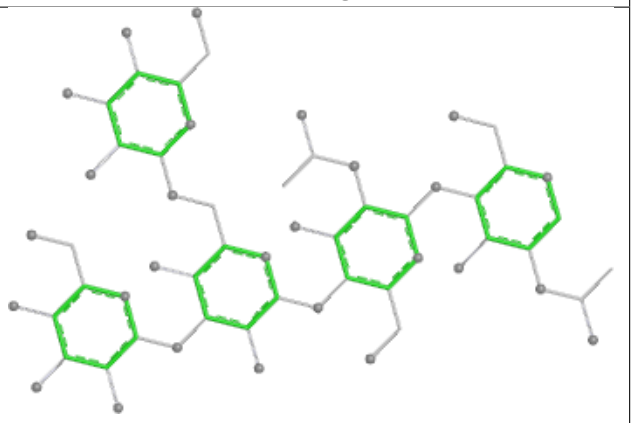
Bond lengths



Bond angles

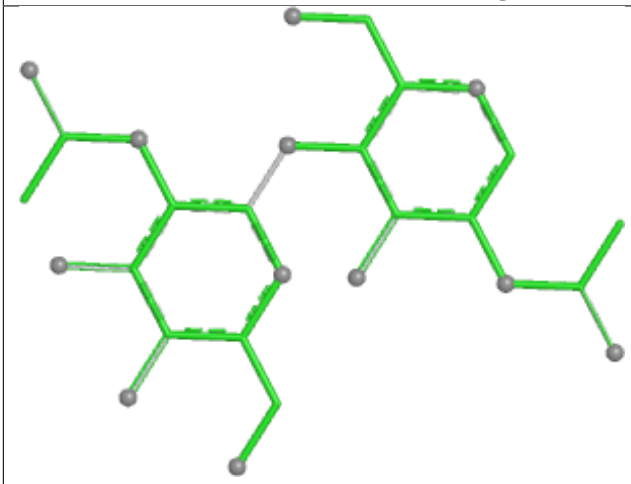


Torsions

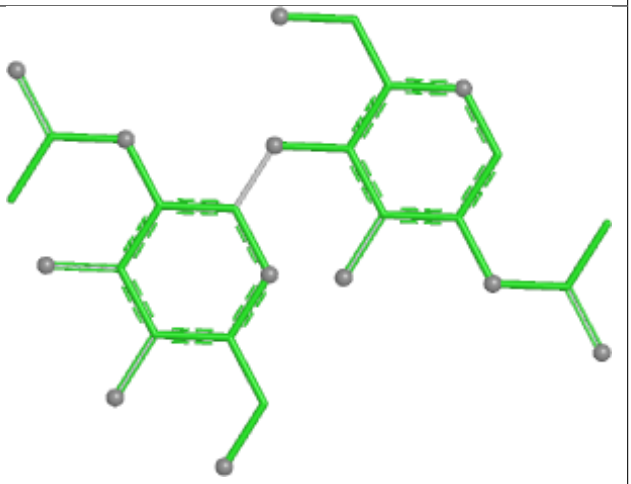


Rings

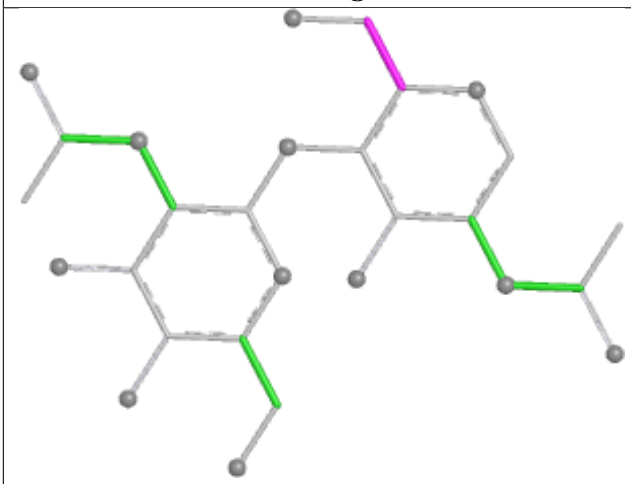
Oligosaccharide Chain D



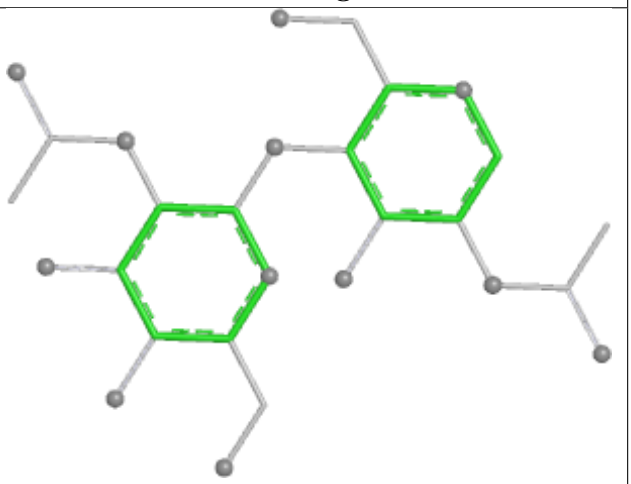
Bond lengths



Bond angles

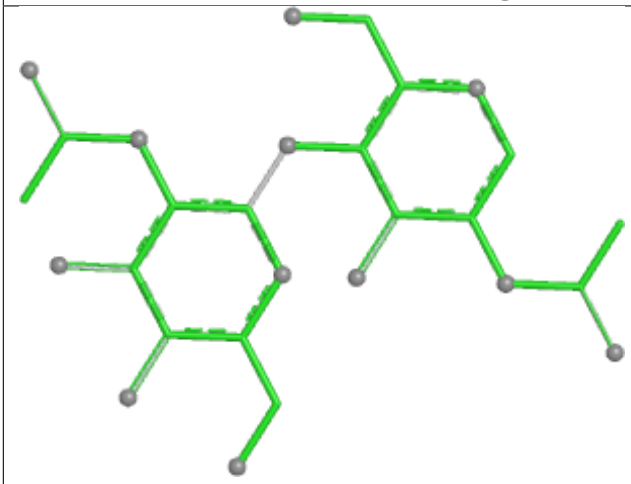


Torsions

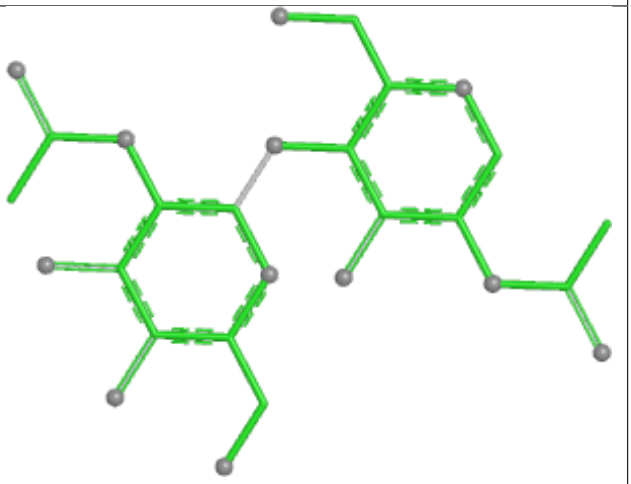


Rings

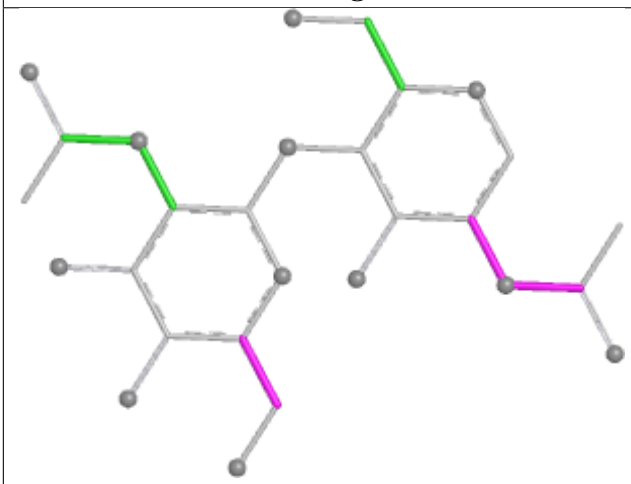
Oligosaccharide Chain F



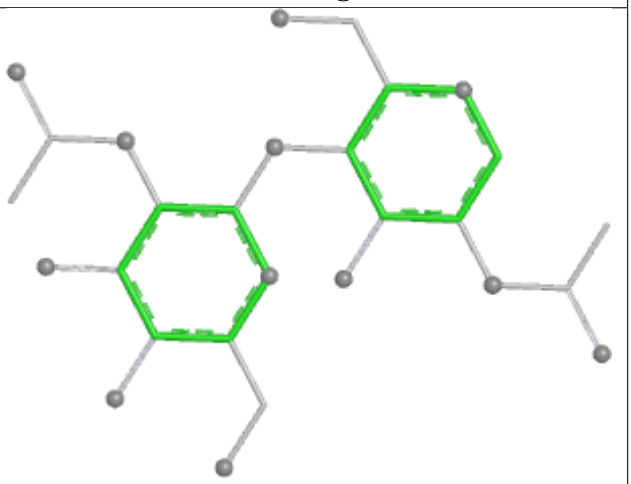
Bond lengths



Bond angles

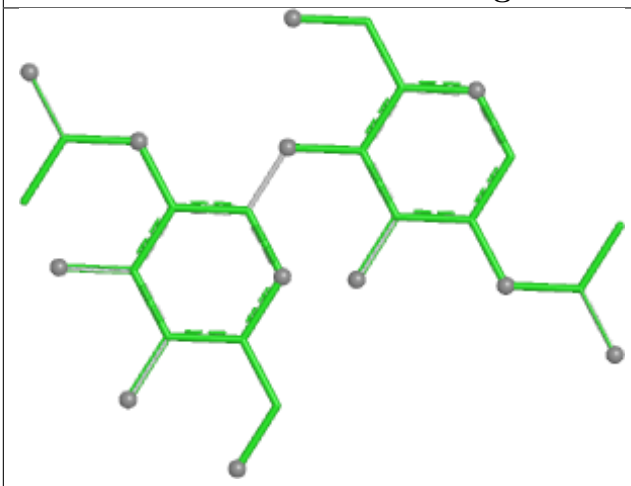


Torsions

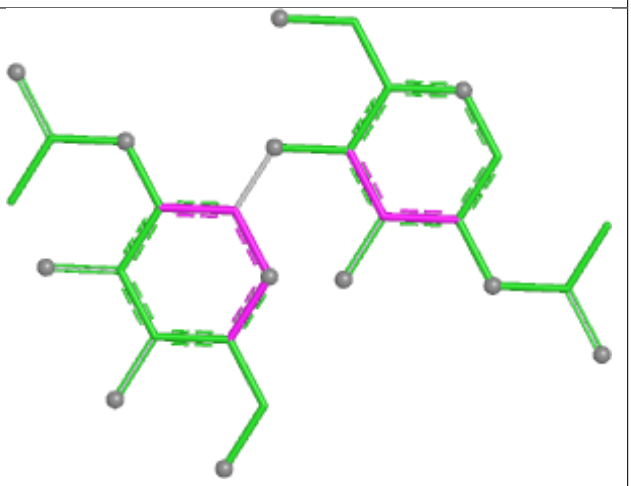


Rings

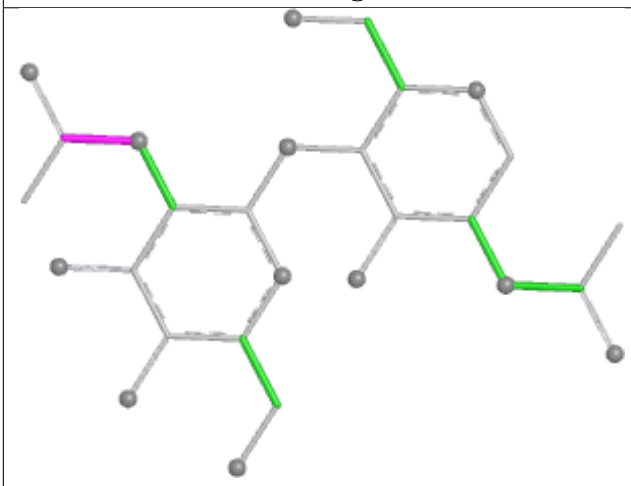
Oligosaccharide Chain G



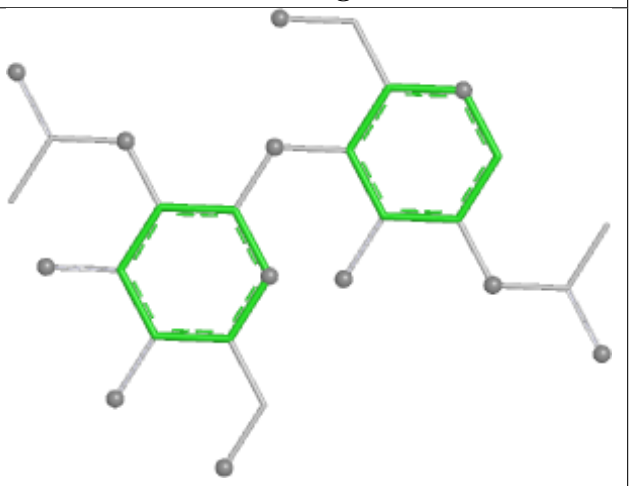
Bond lengths



Bond angles

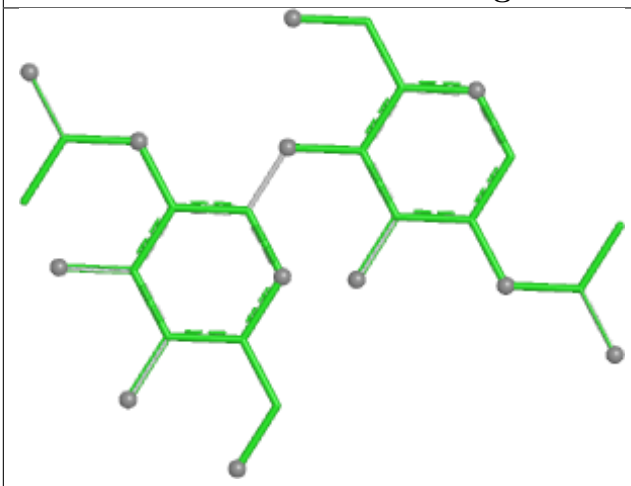


Torsions

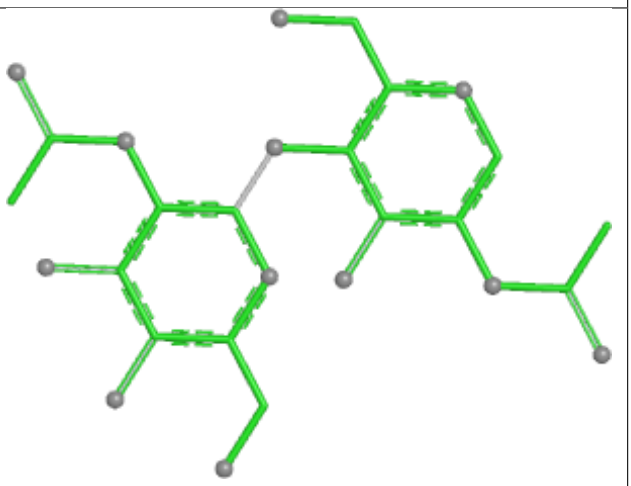


Rings

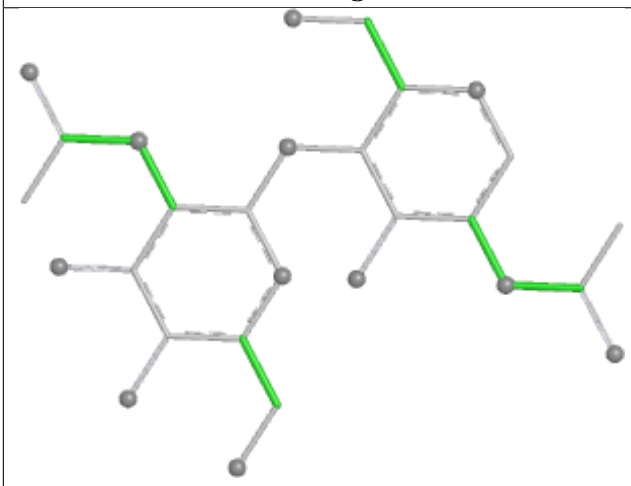
Oligosaccharide Chain H



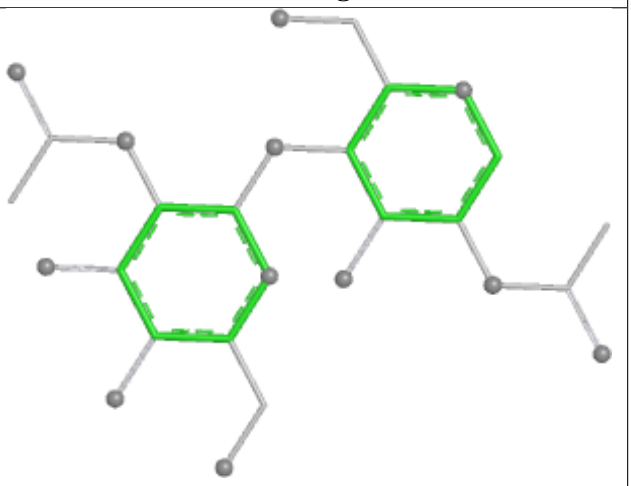
Bond lengths



Bond angles

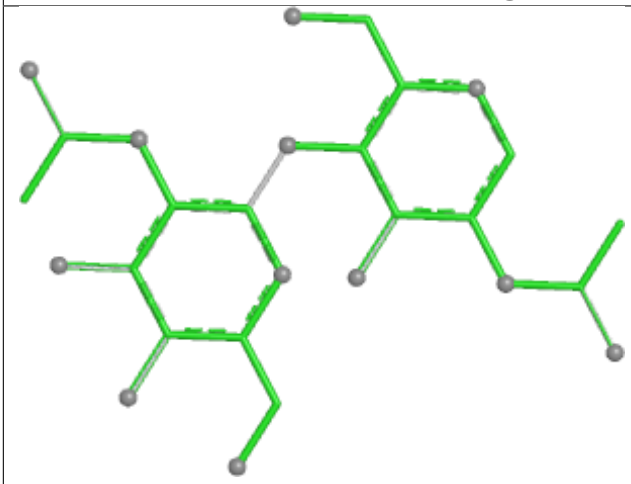


Torsions

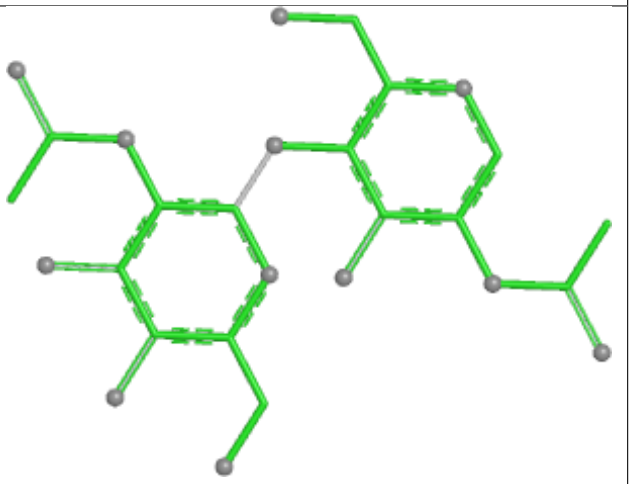


Rings

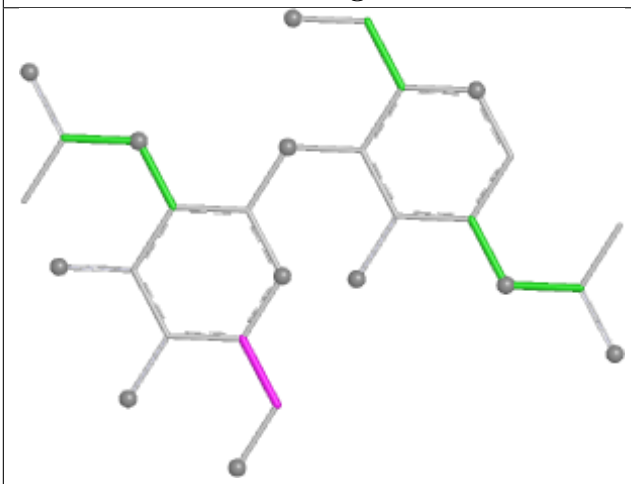
Oligosaccharide Chain I



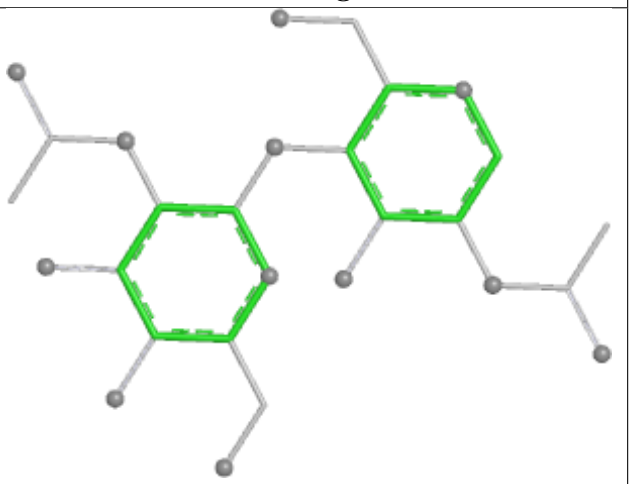
Bond lengths



Bond angles

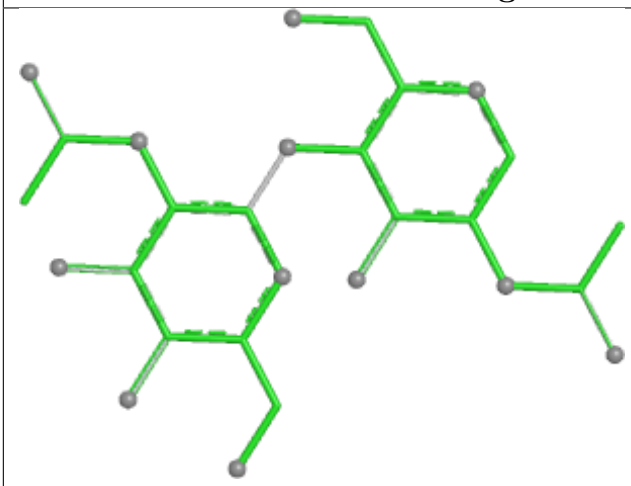


Torsions

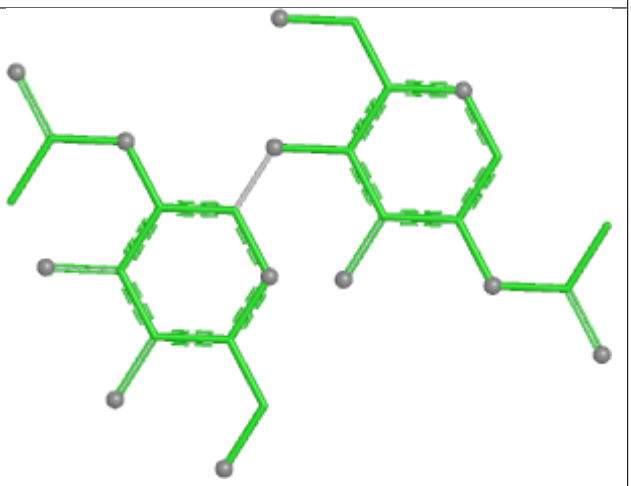


Rings

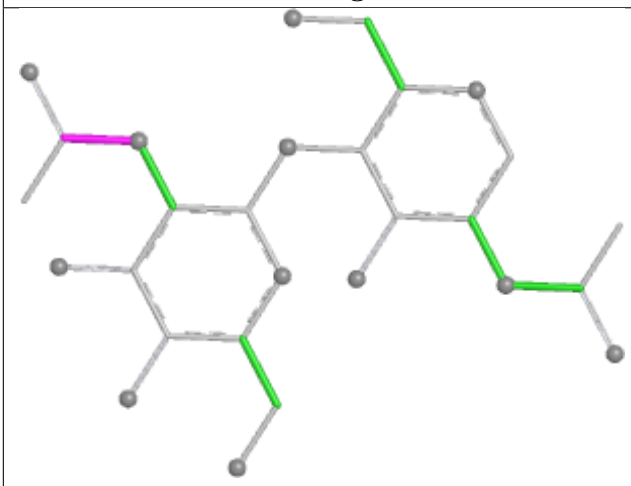
Oligosaccharide Chain J



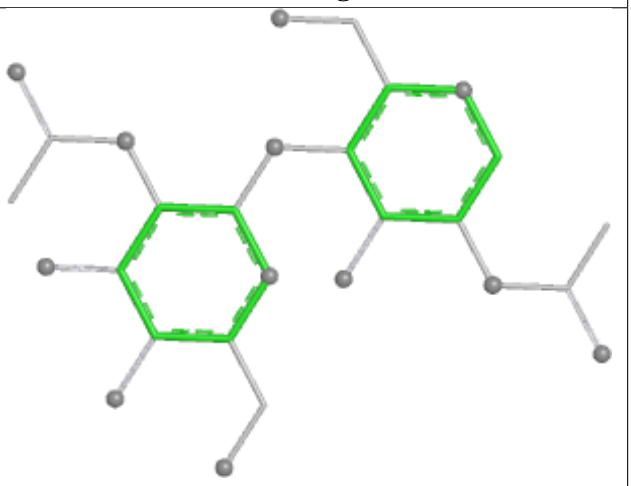
Bond lengths



Bond angles

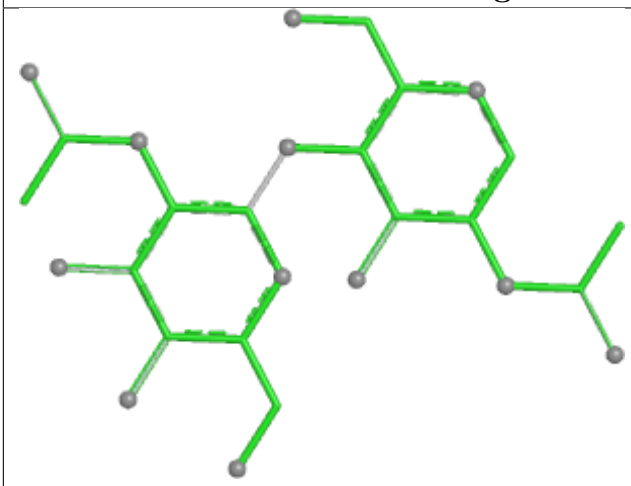


Torsions

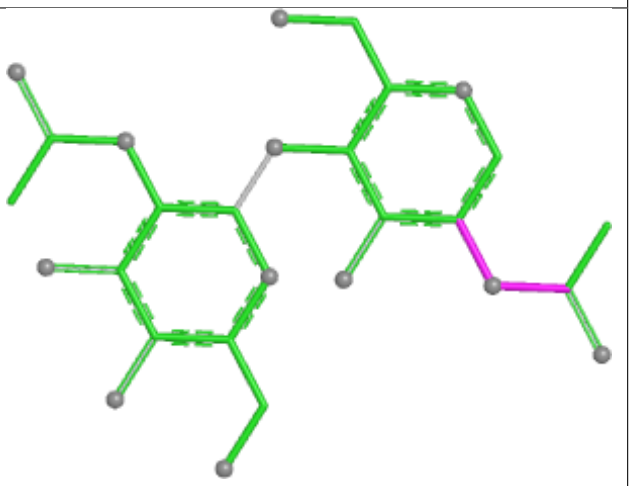


Rings

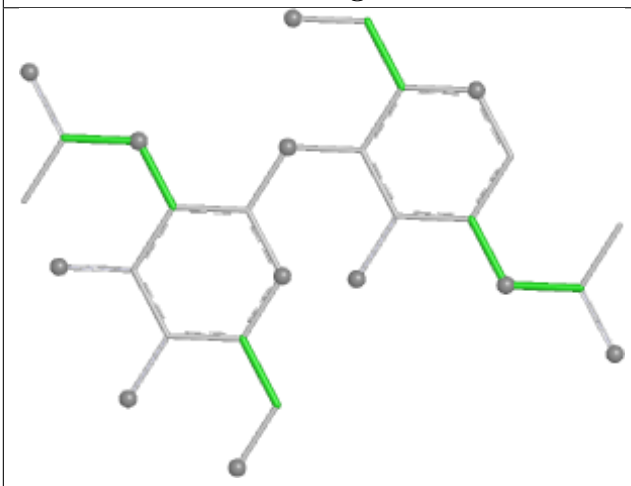
Oligosaccharide Chain K



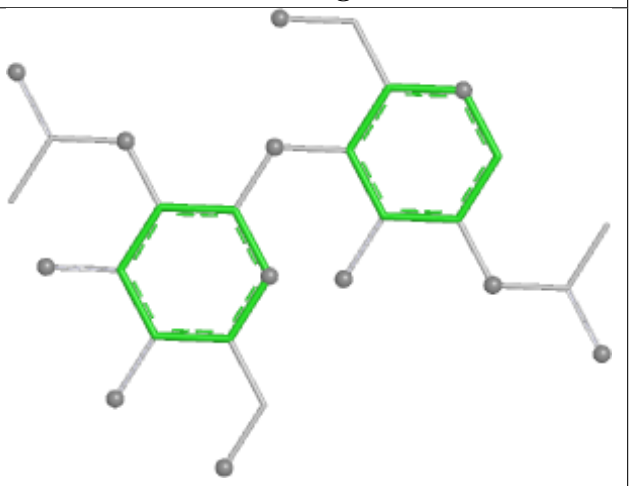
Bond lengths



Bond angles

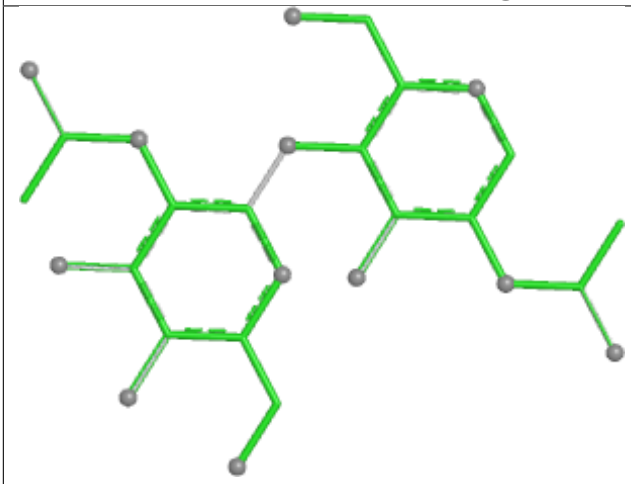


Torsions

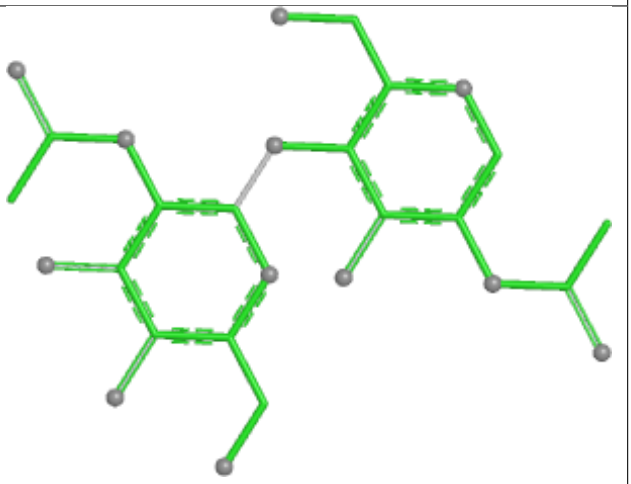


Rings

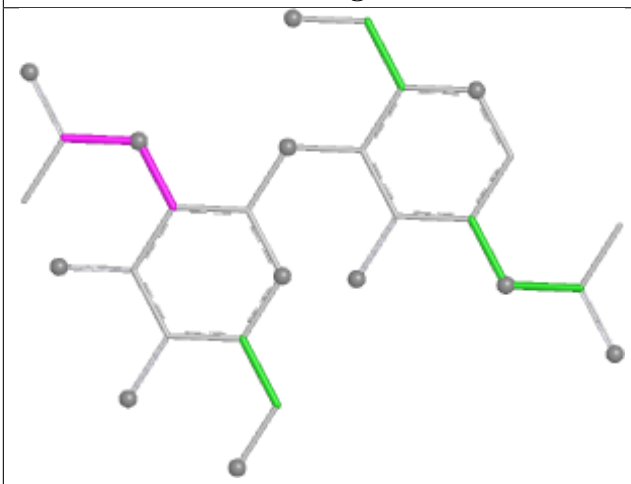
Oligosaccharide Chain L



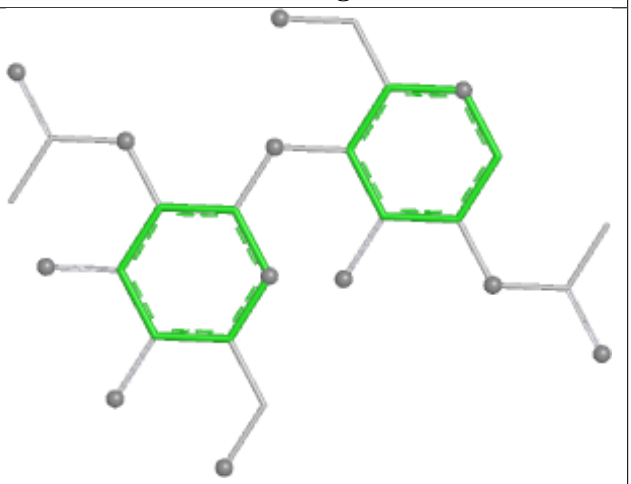
Bond lengths



Bond angles

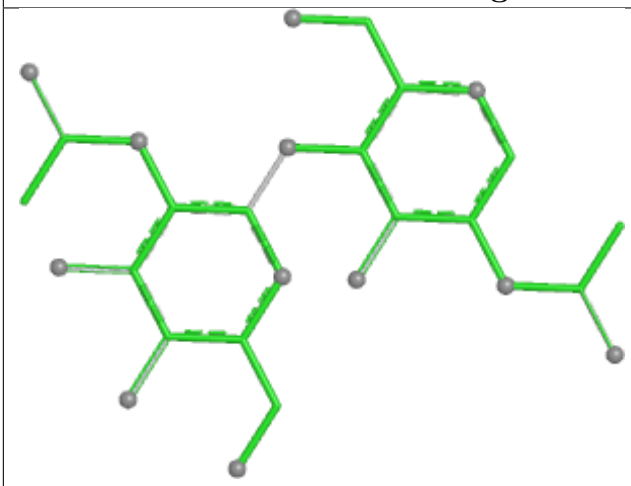


Torsions

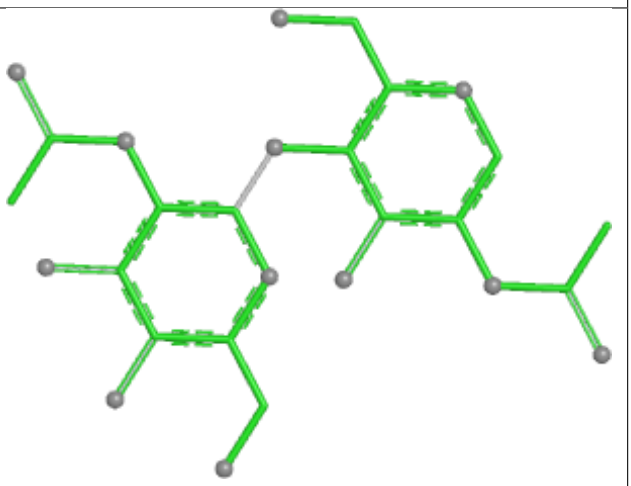


Rings

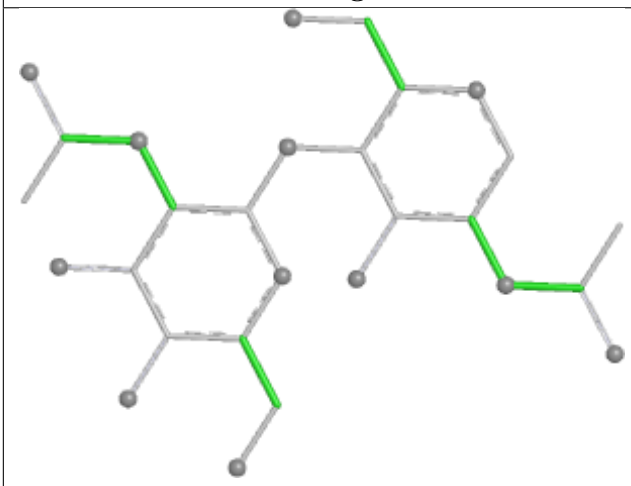
Oligosaccharide Chain M



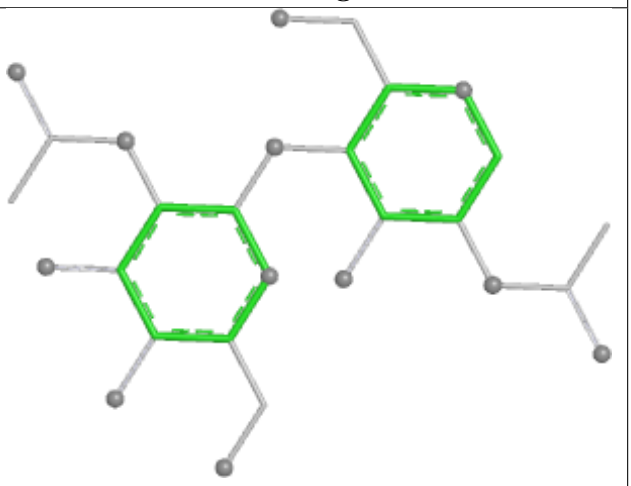
Bond lengths



Bond angles

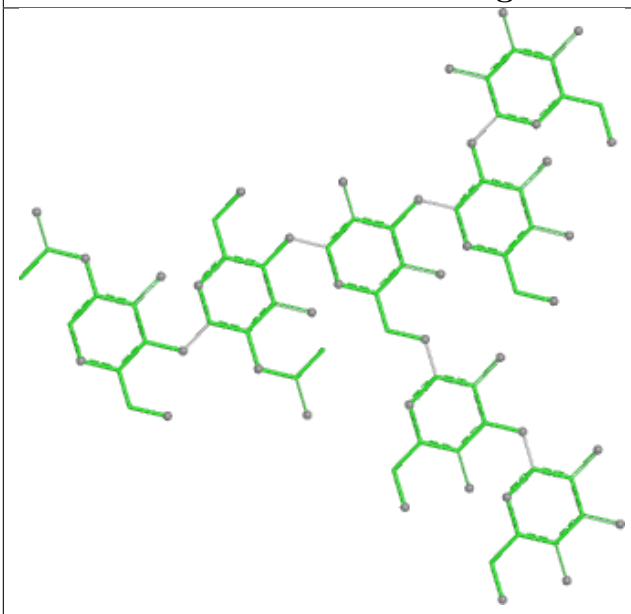


Torsions

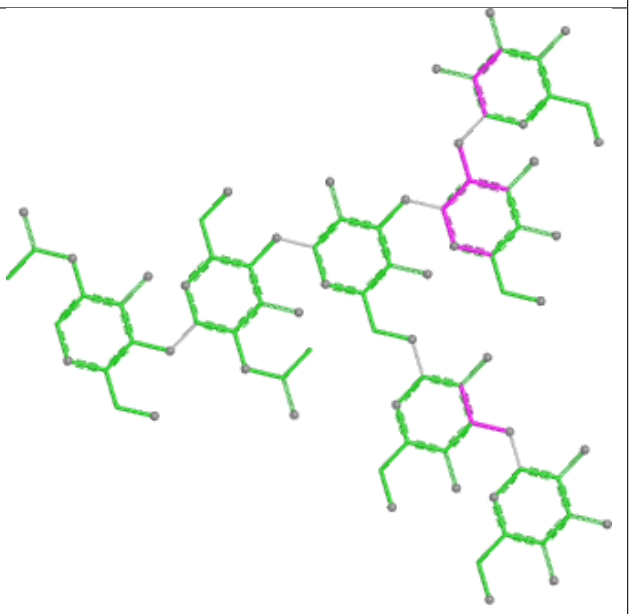


Rings

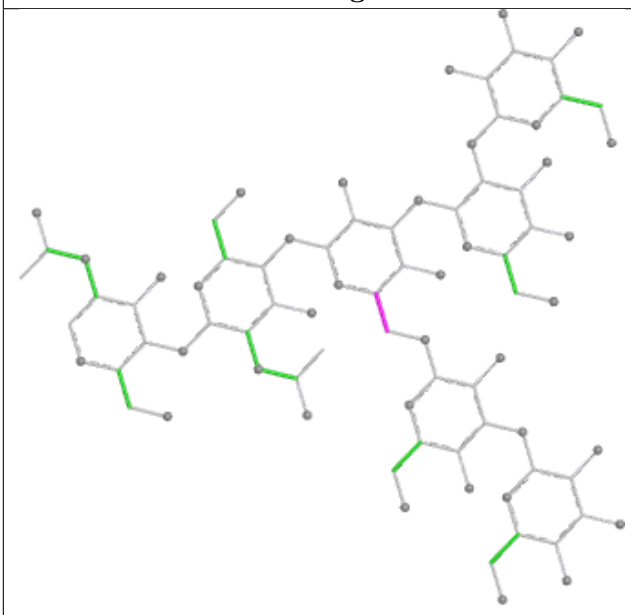
Oligosaccharide Chain E



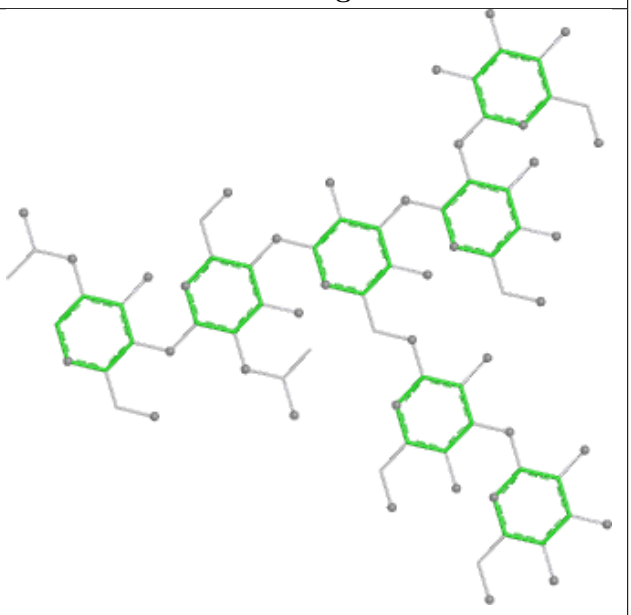
Bond lengths



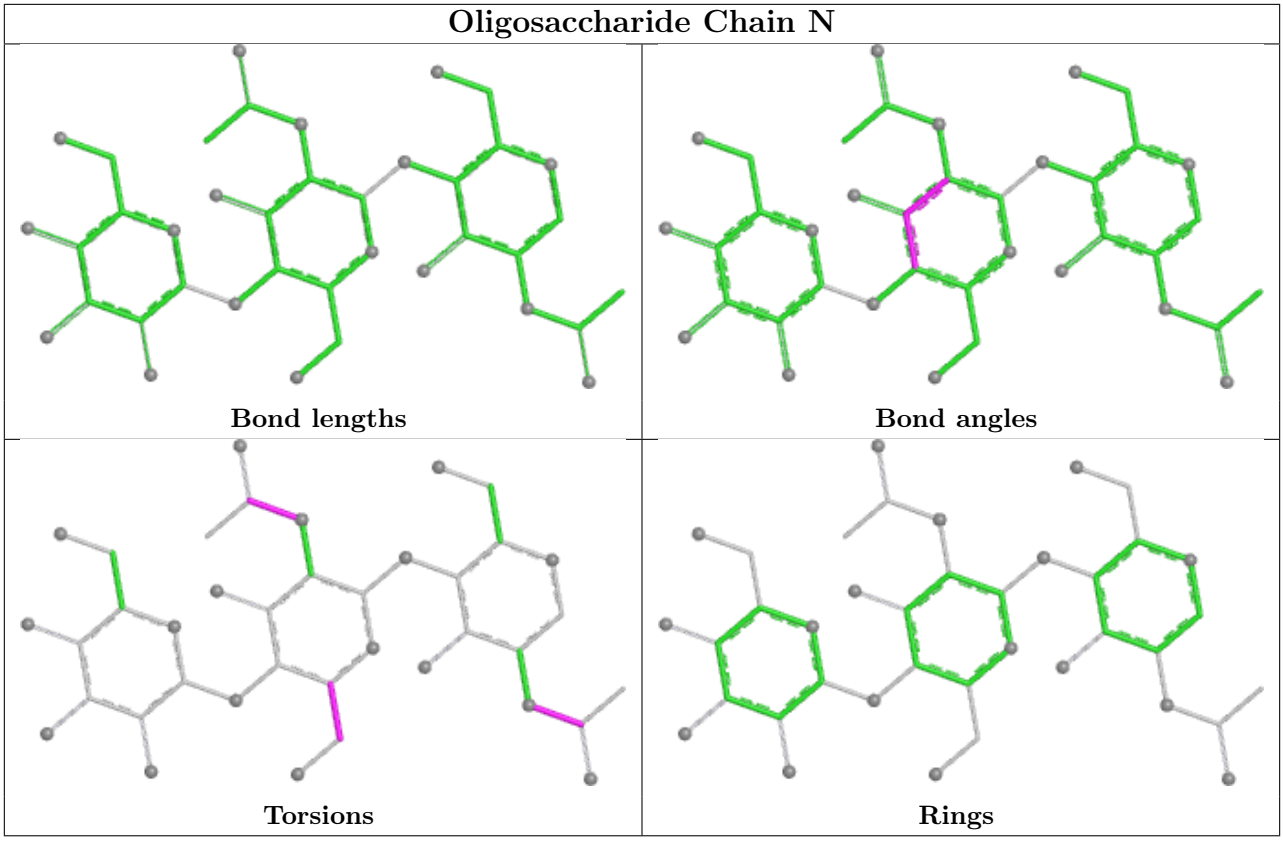
Bond angles



Torsions



Rings



5.6 Ligand geometry (i)

Of 12 ligands modelled in this entry, 8 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
8	NAG	B	3099	2	14,14,15	0.62	0	17,19,21	0.93	2 (11%)
8	NAG	A	3674	1	14,14,15	0.51	0	17,19,21	0.75	0
8	NAG	B	3452	2	14,14,15	0.50	0	17,19,21	0.92	1 (5%)
8	NAG	A	3805	1	14,14,15	0.56	0	17,19,21	0.71	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
8	NAG	B	3099	2	-	2/6/23/26	0/1/1/1
8	NAG	A	3674	1	-	0/6/23/26	0/1/1/1
8	NAG	B	3452	2	-	0/6/23/26	0/1/1/1
8	NAG	A	3805	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	B	3099	NAG	C2-N2-C7	-2.48	119.58	122.90
8	B	3452	NAG	C1-O5-C5	2.22	115.16	112.19
8	B	3099	NAG	O5-C5-C6	2.01	111.57	107.66

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	B	3099	NAG	C8-C7-N2-C2
8	B	3099	NAG	O7-C7-N2-C2

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	929/959 (96%)	0.26	28 (3%)	50	45	47, 81, 146, 235	0
2	B	692/692 (100%)	0.30	42 (6%)	21	17	50, 93, 187, 244	0
All	All	1621/1651 (98%)	0.28	70 (4%)	35	31	47, 86, 169, 244	0

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	837	SER	18.4
2	B	649	GLY	8.5
2	B	692	ASP	7.2
2	B	648	THR	6.8
1	A	569	ALA	6.0
1	A	565	TYR	5.7
2	B	447	ARG	5.4
1	A	704	GLN	5.4
2	B	1	GLY	5.2
2	B	460	CYS	5.1
2	B	441	ALA	4.8
2	B	461	ARG	4.8
1	A	959	PRO	4.7
2	B	467	LEU	4.6
2	B	481	SER	4.5
1	A	567	THR	4.5
1	A	836	SER	4.1
2	B	691	PRO	4.0
2	B	446	HIS	4.0
2	B	650	LYS	3.8
1	A	566	ARG	3.7
2	B	652	ALA	3.6
2	B	440	GLN	3.6
1	A	957	PRO	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	958	ALA	3.4
1	A	491	LEU	3.3
2	B	34	GLY	3.2
2	B	455	PHE	3.1
2	B	37	ARG	3.1
2	B	501	CYS	3.0
1	A	617	ILE	3.0
2	B	459	VAL	2.9
2	B	33	LEU	2.9
1	A	490	LYS	2.8
1	A	955	ILE	2.7
2	B	672	ASP	2.7
2	B	470	GLN	2.7
2	B	2	PRO	2.7
2	B	454	THR	2.6
2	B	556	TYR	2.6
1	A	532	LEU	2.6
2	B	443	PRO	2.6
2	B	450	ASN	2.6
1	A	631	ALA	2.5
1	A	801	TYR	2.5
1	A	933	TYR	2.5
2	B	32	PRO	2.5
1	A	956	GLN	2.4
2	B	465	GLY	2.4
2	B	442	GLU	2.4
1	A	715	LEU	2.4
2	B	458	GLY	2.4
2	B	456	GLU	2.4
1	A	713	PHE	2.4
1	A	663	LEU	2.4
2	B	476	GLU	2.3
1	A	629	VAL	2.3
2	B	482	GLN	2.3
2	B	412	LYS	2.3
1	A	652	ASP	2.2
1	A	954	GLY	2.2
2	B	653	VAL	2.2
2	B	690	GLY	2.2
2	B	500	GLU	2.1
2	B	116	TYR	2.1
1	A	481	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	516	ILE	2.1
1	A	517	ARG	2.1
2	B	512	ASP	2.0
1	A	493	PHE	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
4	NAG	G	2	14/15	0.69	0.44	178,200,206,207	0
4	NAG	D	2	14/15	0.76	0.18	152,165,185,193	0
4	NAG	L	2	14/15	0.76	0.29	140,161,168,170	0
3	MAN	C	5	11/12	0.77	0.34	200,205,209,212	0
4	NAG	J	2	14/15	0.78	0.33	149,179,195,197	0
4	NAG	H	2	14/15	0.79	0.24	147,170,190,195	0
4	NAG	I	2	14/15	0.81	0.34	146,159,168,169	0
4	NAG	G	1	14/15	0.82	0.21	158,176,190,201	0
3	MAN	C	4	11/12	0.84	0.17	174,188,196,197	0
3	BMA	C	3	11/12	0.85	0.18	170,180,188,189	0
4	NAG	M	2	14/15	0.86	0.15	90,151,161,163	0
5	MAN	E	7	11/12	0.86	0.23	98,126,134,136	0
5	MAN	E	5	11/12	0.87	0.25	139,156,169,170	0
4	NAG	F	1	14/15	0.87	0.19	92,109,143,146	0
4	NAG	I	1	14/15	0.88	0.18	92,108,114,142	0
4	NAG	L	1	14/15	0.88	0.22	93,124,141,164	0
4	NAG	F	2	14/15	0.89	0.26	133,148,154,160	0
4	NAG	J	1	14/15	0.89	0.19	99,126,141,168	0
4	NAG	K	2	14/15	0.90	0.30	141,156,164,168	0
5	MAN	E	6	11/12	0.91	0.13	134,144,168,172	0
4	NAG	H	1	14/15	0.91	0.11	132,146,157,161	0
6	BMA	N	3	11/12	0.91	0.10	134,139,142,142	0
4	NAG	M	1	14/15	0.92	0.20	101,135,148,152	0
5	BMA	E	3	11/12	0.92	0.10	111,116,127,141	0

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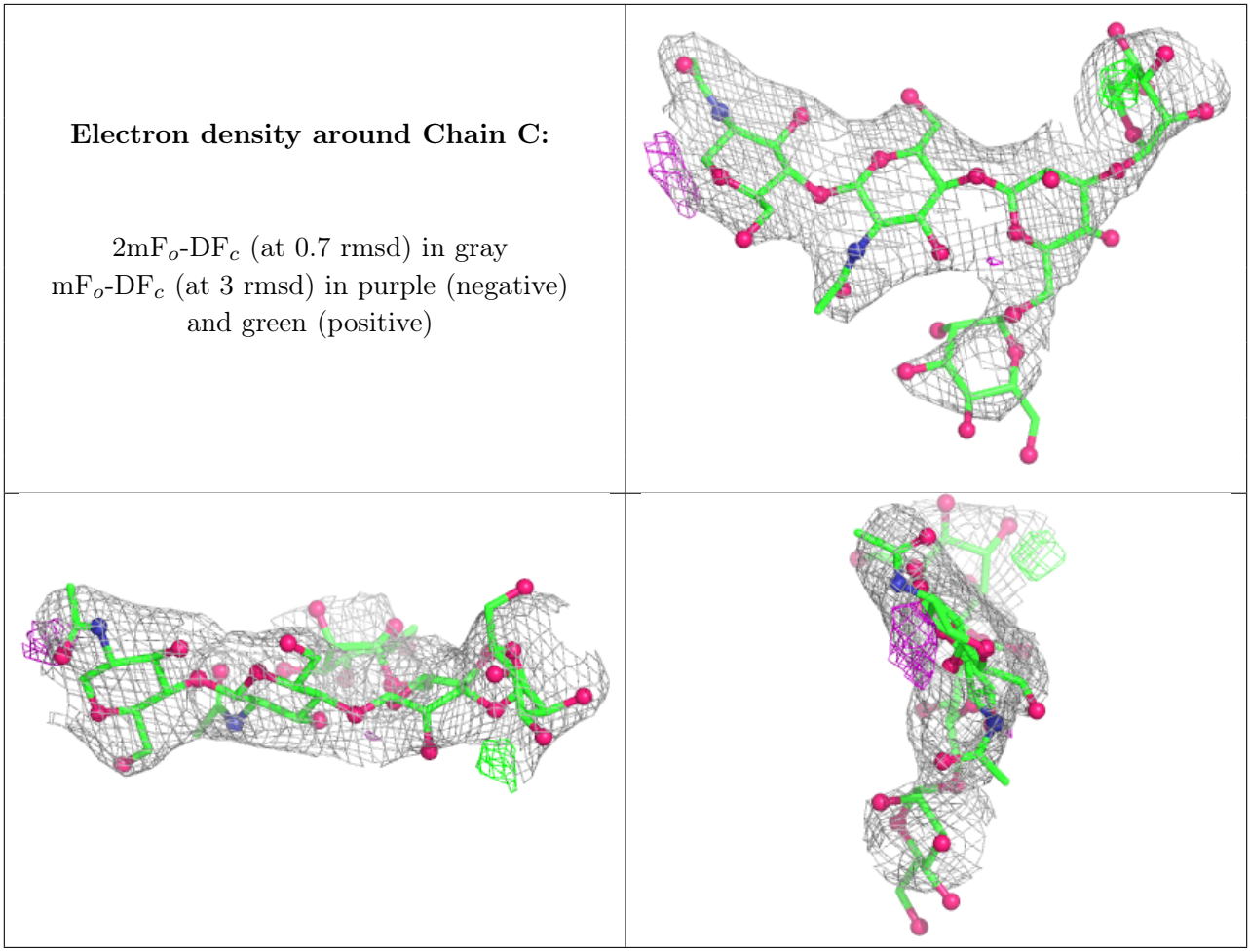
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	NAG	D	1	14/15	0.93	0.14	97,119,152,155	0
5	MAN	E	4	11/12	0.93	0.17	116,132,152,164	0
6	NAG	N	2	14/15	0.94	0.14	103,117,142,151	0
6	NAG	N	1	14/15	0.94	0.15	84,99,109,109	0
3	NAG	C	2	14/15	0.95	0.18	97,125,132,151	0
4	NAG	K	1	14/15	0.96	0.16	80,101,119,123	0
5	NAG	E	2	14/15	0.97	0.12	52,76,96,103	0
3	NAG	C	1	14/15	0.97	0.18	56,68,92,99	0
5	NAG	E	1	14/15	0.97	0.15	56,64,79,86	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.

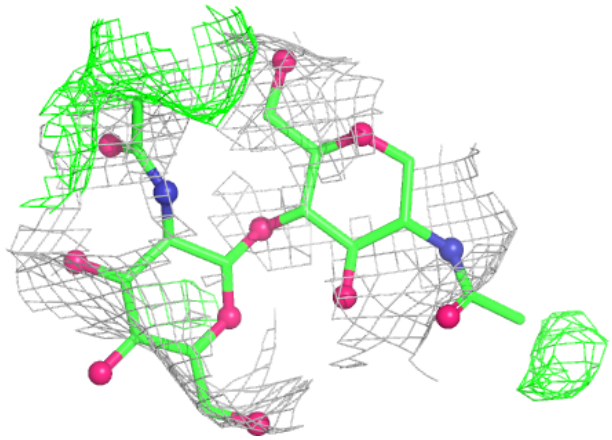
Electron density around Chain C:

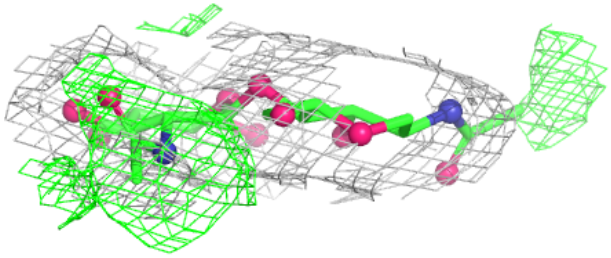
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

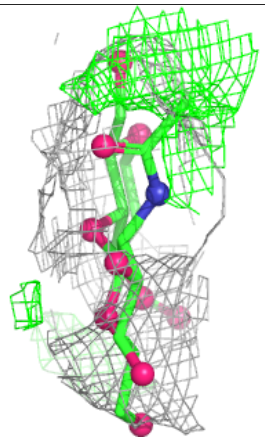


Electron density around Chain D:

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

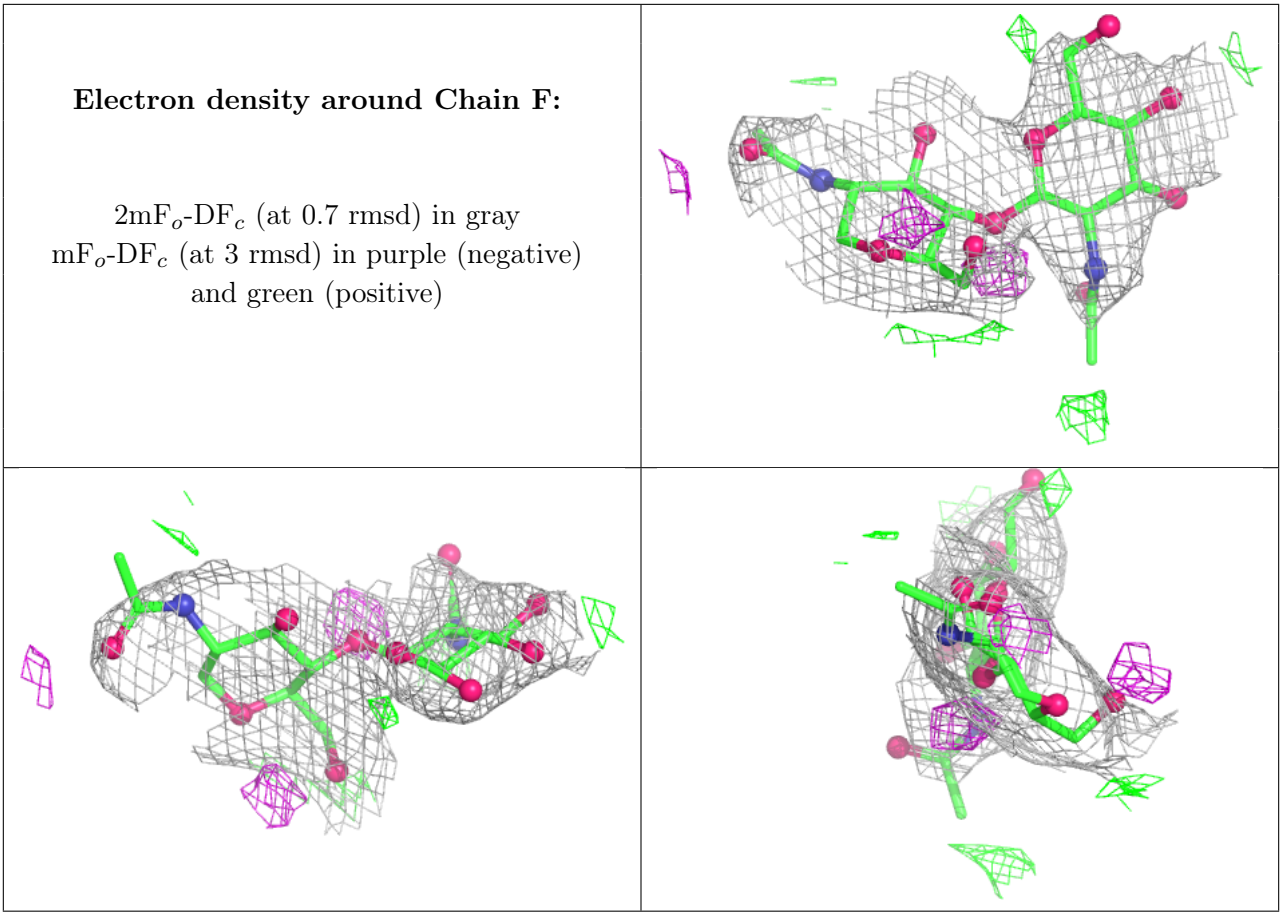






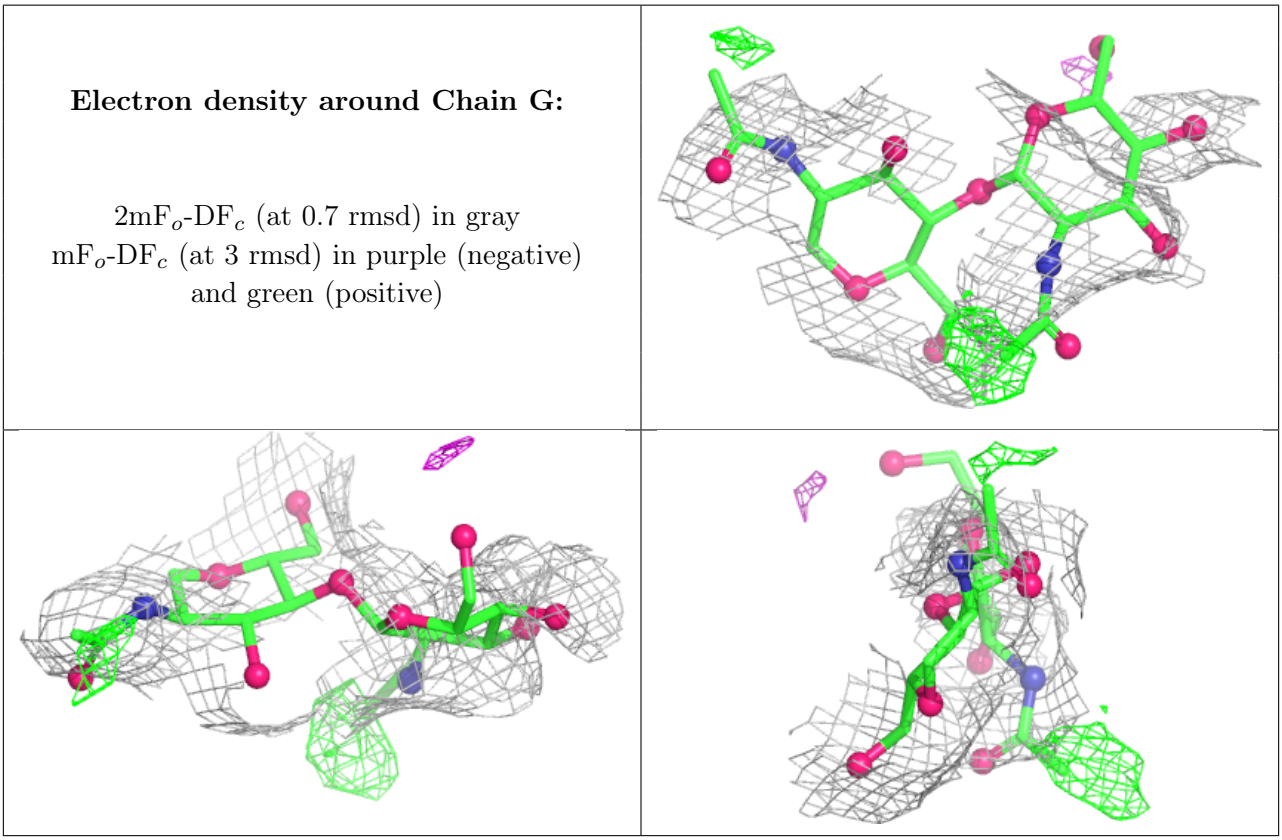
Electron density around Chain F:

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



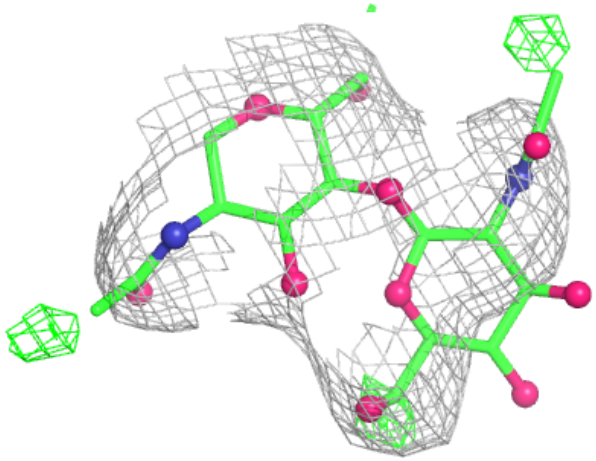
Electron density around Chain G:

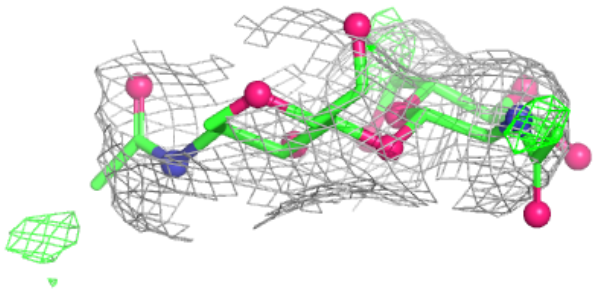
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

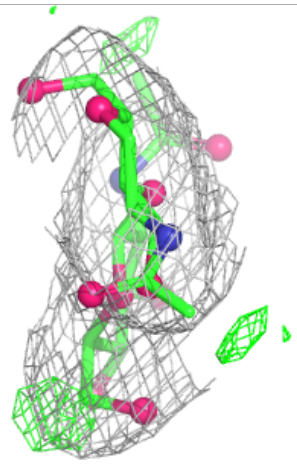


Electron density around Chain H:

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

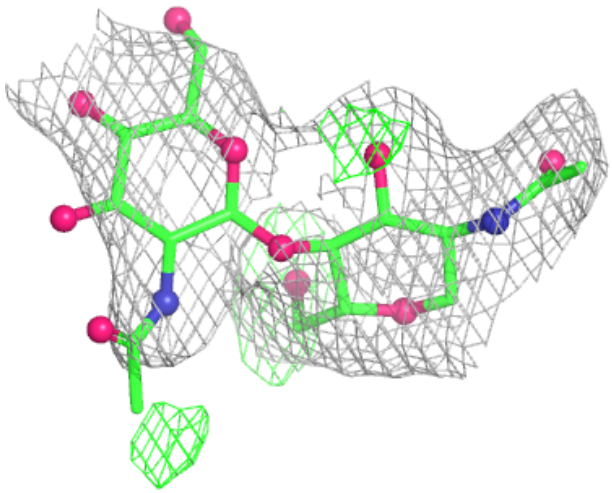


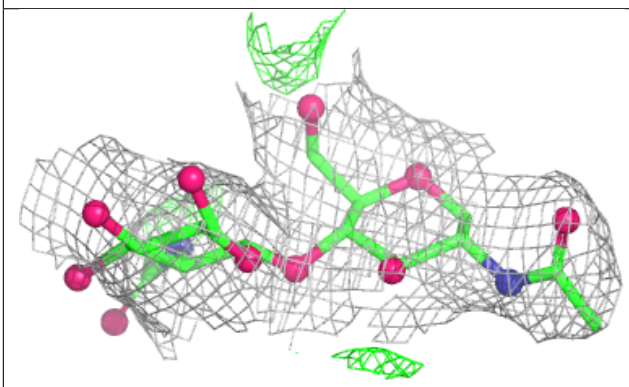


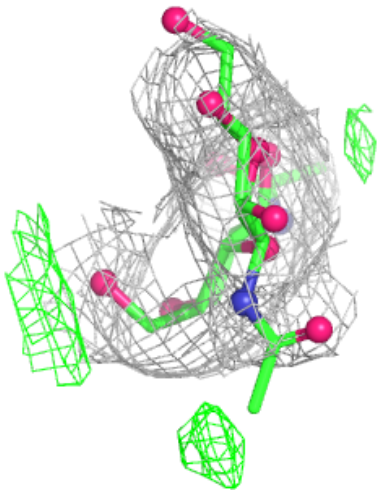


Electron density around Chain I:

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

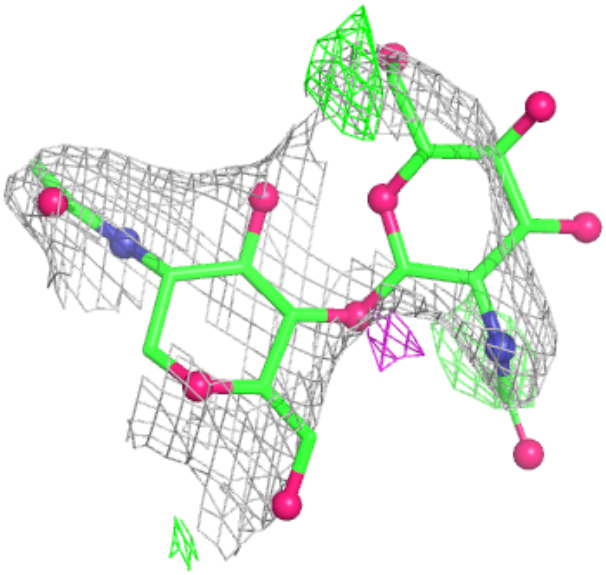


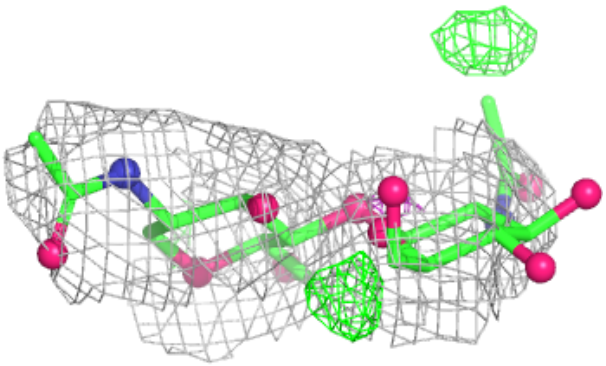


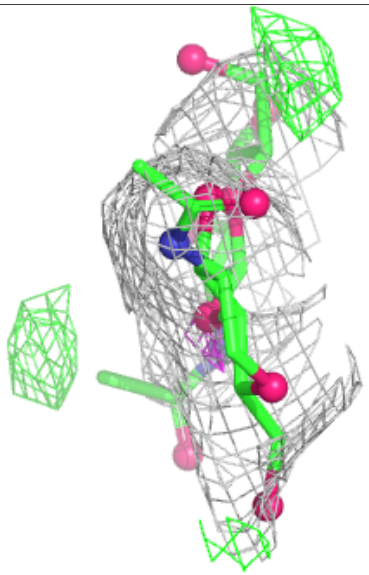


Electron density around Chain J:

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

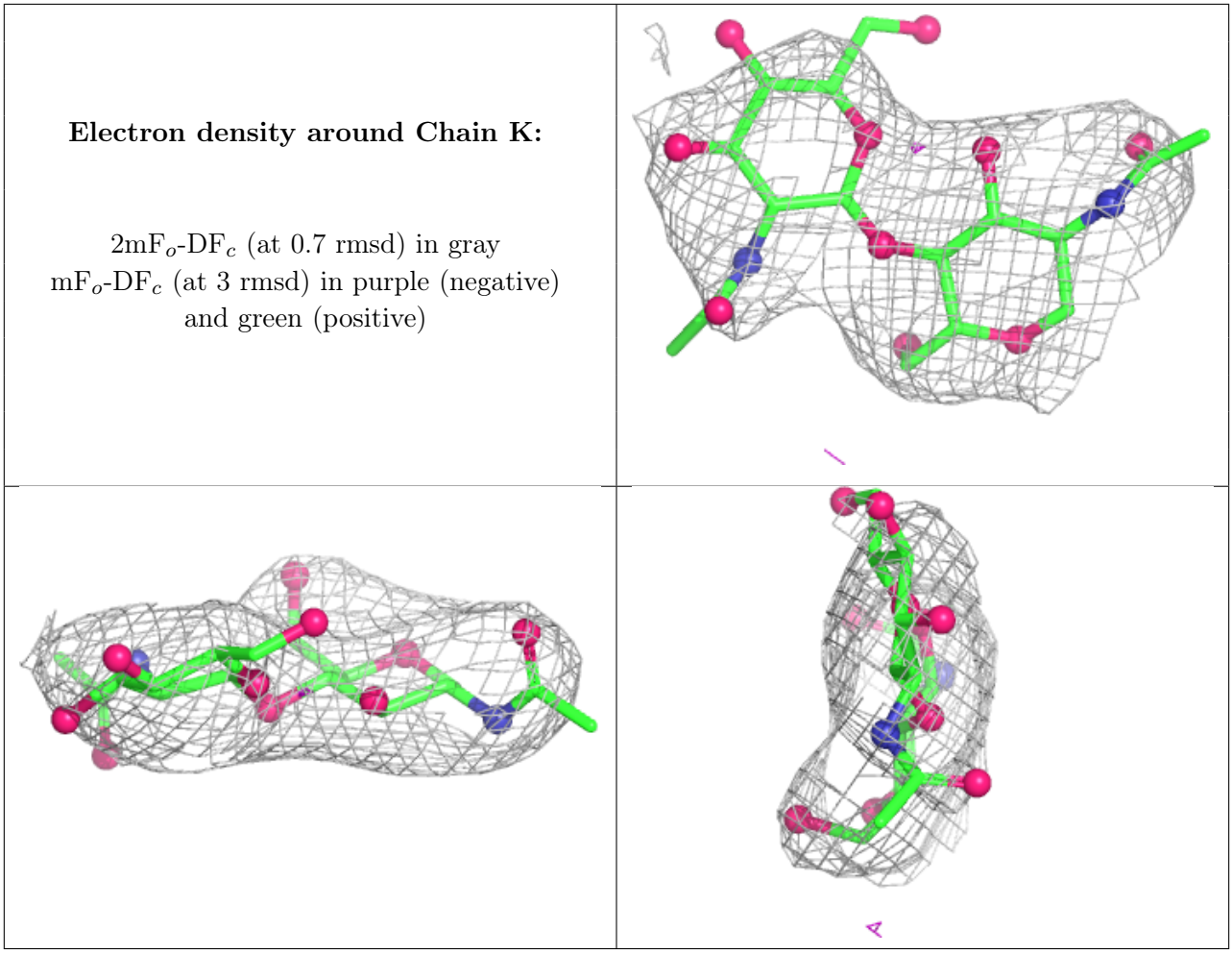






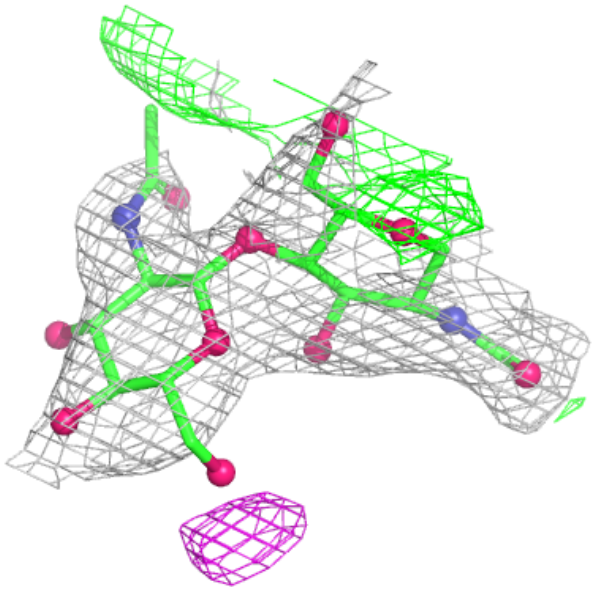
Electron density around Chain K:

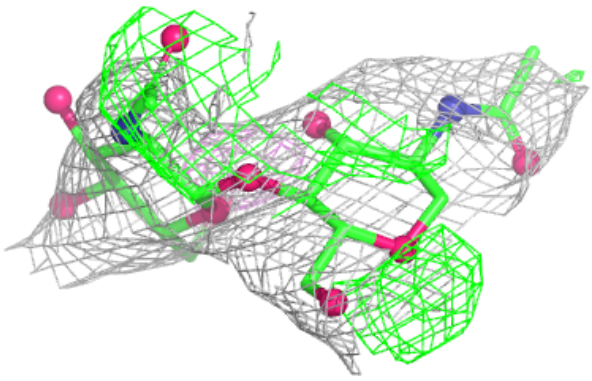
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

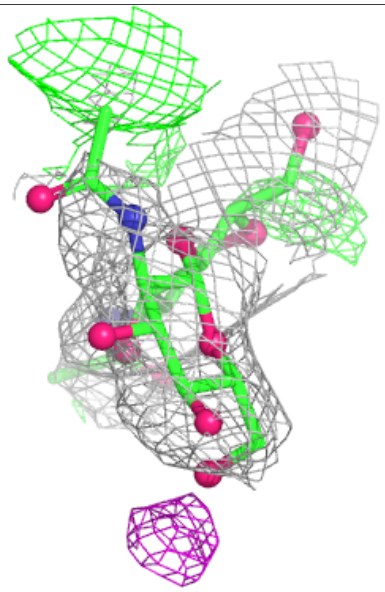


Electron density around Chain L:

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

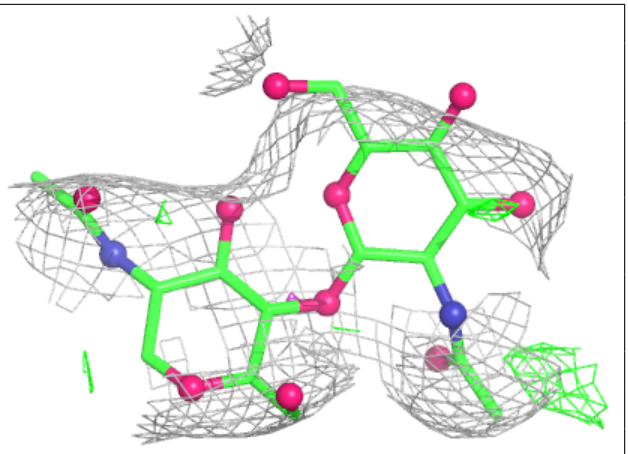


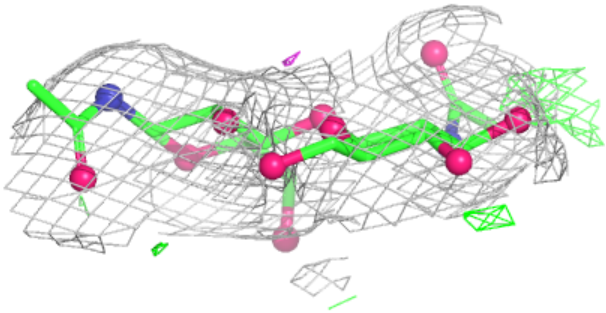


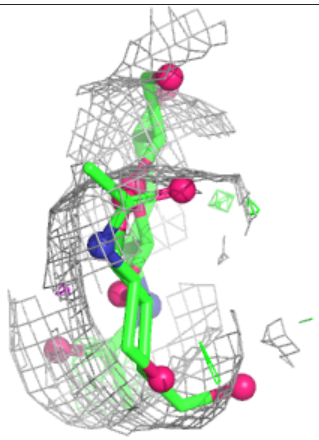


Electron density around Chain M:

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

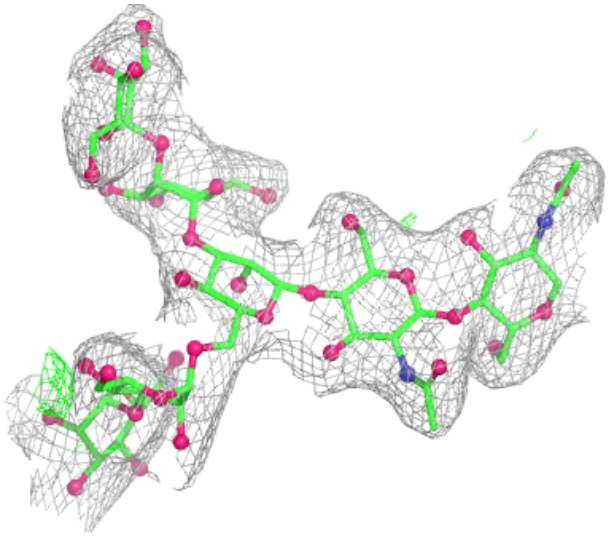


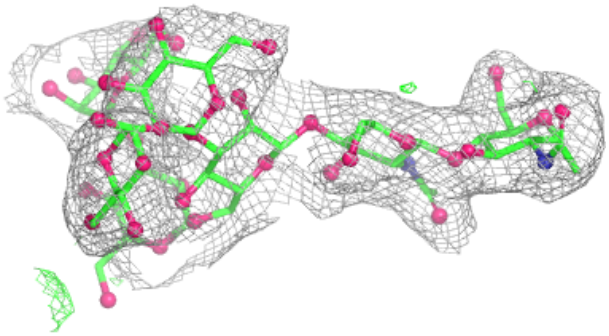


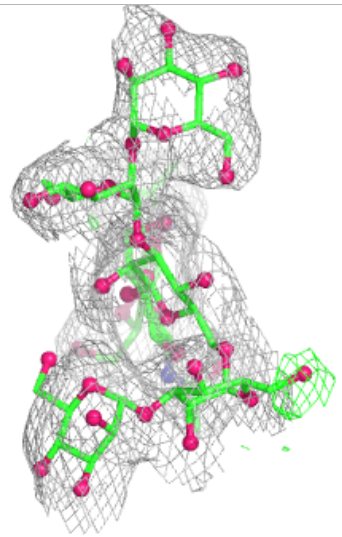


Electron density around Chain E:

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

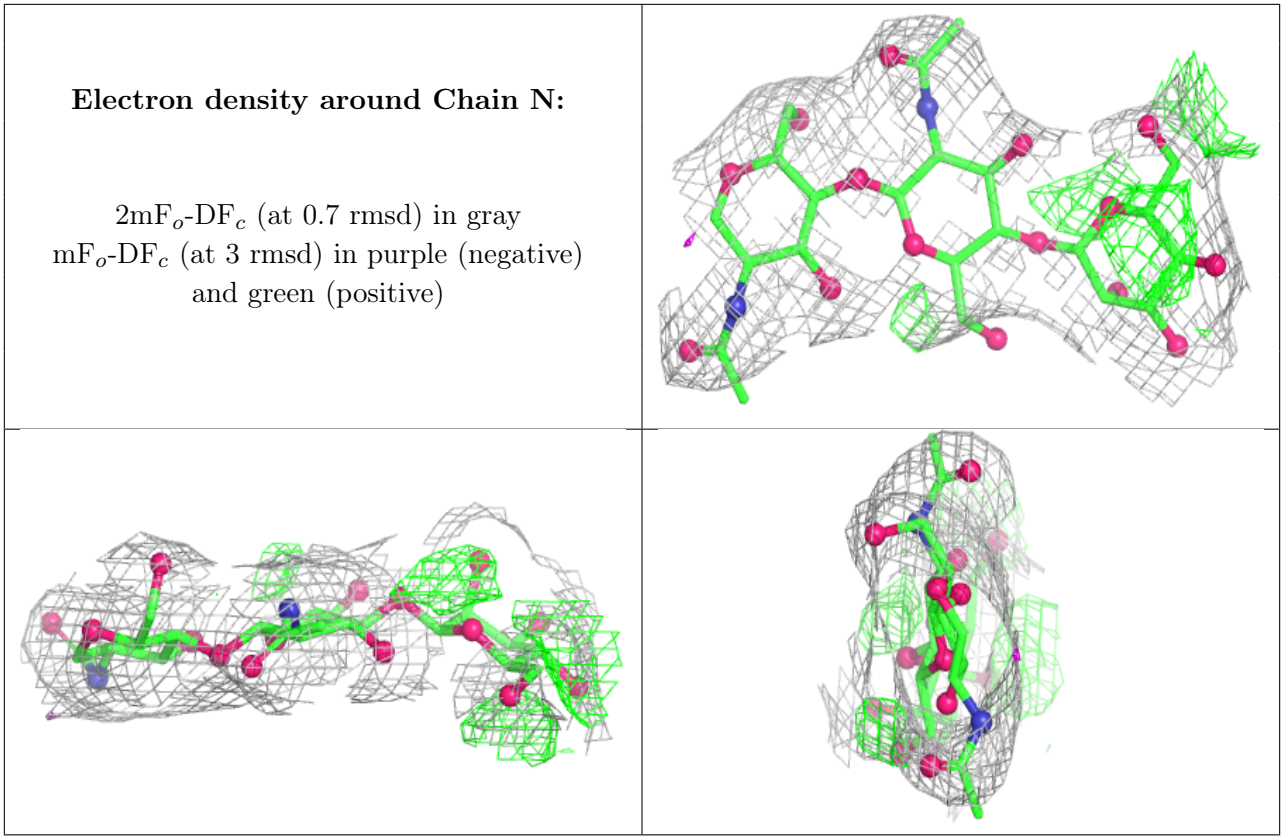






Electron density around Chain N:

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



6.4 Ligands

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
8	NAG	A	3674	14/15	0.64	0.37	181,199,203,206	0
8	NAG	A	3805	14/15	0.67	0.29	158,176,182,183	0
8	NAG	B	3452	14/15	0.68	0.25	162,188,190,191	0
9	NA	A	3000	1/1	0.79	0.19	127,127,127,127	0
7	CA	B	2001	1/1	0.88	0.16	121,121,121,121	0
8	NAG	B	3099	14/15	0.88	0.21	138,164,185,190	0
7	CA	A	2005	1/1	0.91	0.20	80,80,80,80	0
7	CA	A	2004	1/1	0.93	0.14	82,82,82,82	0
7	CA	B	2002	1/1	0.96	0.12	86,86,86,86	0
7	CA	A	2008	1/1	0.98	0.16	90,90,90,90	0
7	CA	A	2007	1/1	0.98	0.21	78,78,78,78	0
7	CA	A	2006	1/1	0.99	0.16	80,80,80,80	0

6.5 Other polymers (i)

There are no such residues in this entry.