Full wwPDB X-ray Structure Validation Report ⓘ

Sep 24, 2023 – 09:09 PM EDT

PDB ID	:	5UTF
Title	:	Crystal Structure of a Stabilized DS-SOSIP.6mut BG505 gp140 HIV-1 Env Trimer, Containing Mutations I201C-P433C (DS), L154M, Y177W, N300M, N302M, T320L, I420M in Complex with Human Antibodies PGT122 and 35O22 at 4.3 A
Authors	:	Pancera, M.; Chuang, G.-Y.; Xu, K.; Kwong, P.D.
Deposited on	:	2017-02-14
Resolution	:	3.50 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

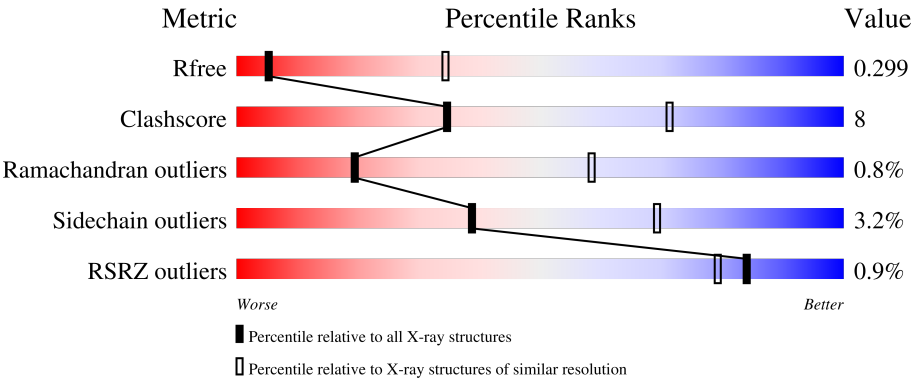
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 3.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1659 (3.60-3.40)
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (3.60-3.40)

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

Mol	Chain	Length	Quality of chain
1	G	481	68% 22% • 9%
2	B	153	% 53% 24% • 20%
3	L	213	79% 18% •
4	H	235	82% 14% • •

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	D	243	2% 80% 19%
6	E	216	2% 78% 20%
7	A	10	10% 40% 50%
8	C	3	67% 33%
9	F	2	100%
9	J	2	100%
9	K	2	100%
9	M	2	50% 50%
9	N	2	50% 50%
9	P	2	50% 50%
9	Q	2	100%
9	R	2	100%
9	S	2	100%
10	I	6	33% 67%
11	O	5	60% 40%
12	T	10	10% 70% 20%

2 Entry composition (i)

There are 13 unique types of molecules in this entry. The entry contains 11964 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 Envelope glycoprotein gp120.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	G	439	Total	C	N	O	S	0	0	0
			3464	2179	609	642	34			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	154	MET	LEU	engineered mutation	UNP Q2N0S6
G	177	TRP	TYR	engineered mutation	UNP Q2N0S6
G	201	CYS	ILE	engineered mutation	UNP Q2N0S6
G	300	MET	ASN	engineered mutation	UNP Q2N0S6
G	302	MET	ASN	engineered mutation	UNP Q2N0S6
G	320	LEU	THR	engineered mutation	UNP Q2N0S6
G	332	ASN	THR	engineered mutation	UNP Q2N0S6
G	420	MET	ILE	engineered mutation	UNP Q2N0S6
G	433	CYS	ALA	engineered mutation	UNP Q2N0S6
G	501	CYS	ALA	engineered mutation	UNP Q2N0S6
G	509	ARG	GLU	engineered mutation	UNP Q2N0S6
G	510	ARG	LYS	engineered mutation	UNP Q2N0S6
G	512	ARG	ALA	engineered mutation	UNP Q2N0S6
G	513	ARG	VAL	engineered mutation	UNP Q2N0S6

- Molecule 2 is a protein called Envelope glycoprotein gp41.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	123	Total	C	N	O	S	0	0	0
			980	620	169	185	6			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	559	PRO	ILE	engineered mutation	UNP Q2N0S6
B	605	CYS	THR	engineered mutation	UNP Q2N0S6

- Molecule 3 is a protein called PGT122 Light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	208	Total	C	N	O	S	0	0	0
			1577	990	265	318	4			

- Molecule 4 is a protein called PGT122 Heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	228	Total	C	N	O	S	0	0	0
			1742	1109	295	333	5			

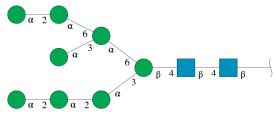
- Molecule 5 is a protein called 35022 Heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	D	242	Total	C	N	O	S	0	0	0
			1832	1165	306	353	8			

- Molecule 6 is a protein called 35022 Light Chain.

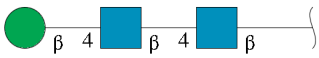
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	E	213	Total	C	N	O	S	0	0	0
			1615	1012	267	328	8			

- Molecule 7 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[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
7	A	10	Total	C	N	O	0	0	0
			116	64	2	50			

- Molecule 8 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.

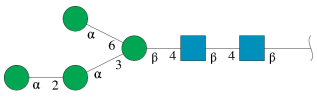


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
8	C	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 9 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

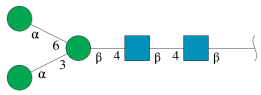
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	F	2	Total	C	N	O	0	0	0
			28	16	2	10			
9	J	2	Total	C	N	O	0	0	0
			28	16	2	10			
9	K	2	Total	C	N	O	0	0	0
			28	16	2	10			
9	M	2	Total	C	N	O	0	0	0
			28	16	2	10			
9	N	2	Total	C	N	O	0	0	0
			28	16	2	10			
9	P	2	Total	C	N	O	0	0	0
			28	16	2	10			
9	Q	2	Total	C	N	O	0	0	0
			28	16	2	10			
9	R	2	Total	C	N	O	0	0	0
			28	16	2	10			
9	S	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 10 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-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.



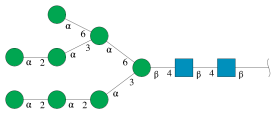
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	I	6	Total	C	N	O	0	0	0
			72	40	2	30			

- Molecule 11 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.



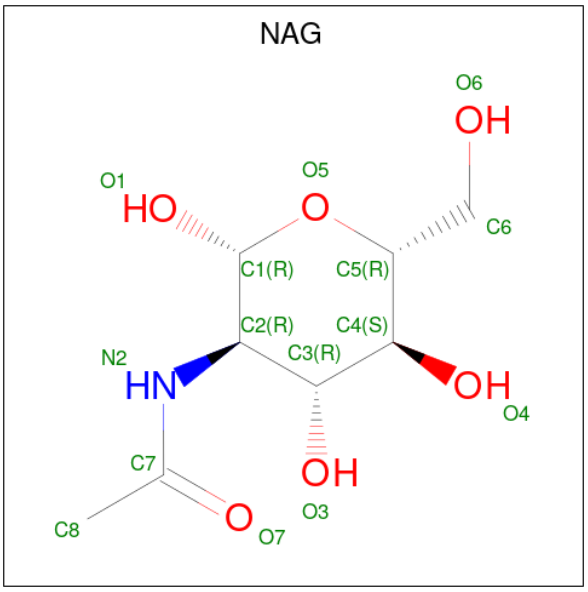
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
11	O	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 12 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]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
12	T	10	Total	C	N	O	0	0	0
			116	64	2	50			

- Molecule 13 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



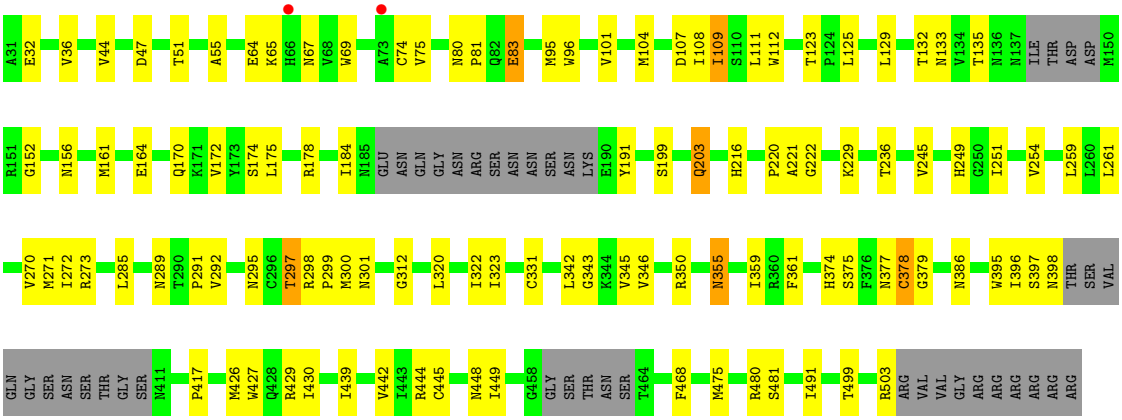
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	G	1	Total C N O 14 8 1 5	0	0
13	G	1	Total C N O 14 8 1 5	0	0
13	G	1	Total C N O 14 8 1 5	0	0
13	G	1	Total C N O 14 8 1 5	0	0
13	B	1	Total C N O 14 8 1 5	0	0
13	B	1	Total C N O 14 8 1 5	0	0
13	B	1	Total C N O 14 8 1 5	0	0

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.

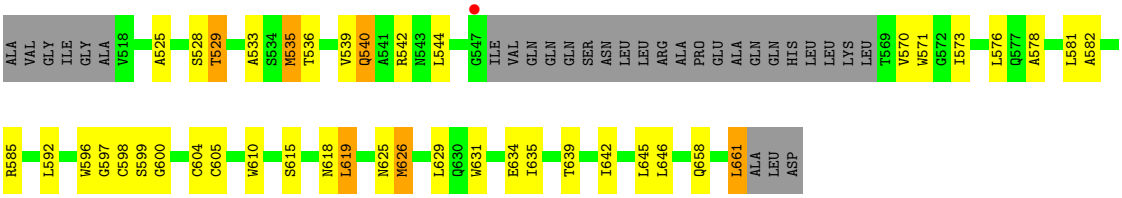
• Molecule 1: Envelope glycoprotein gp120

Chain G:



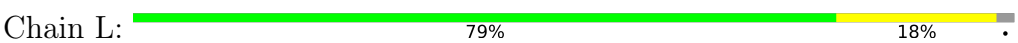
• Molecule 2: Envelope glycoprotein gp41

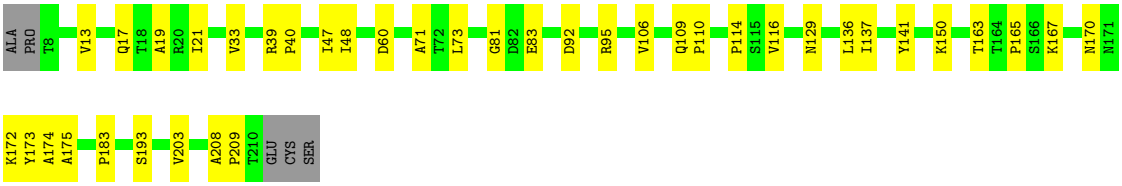
Chain B:



• Molecule 3: PGT122 Light chain

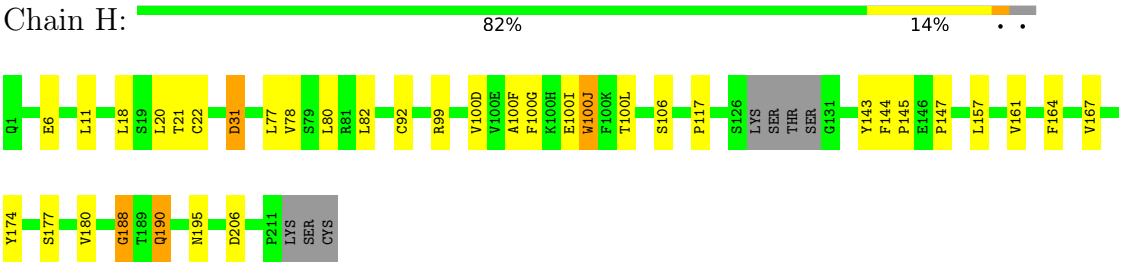
Chain L:





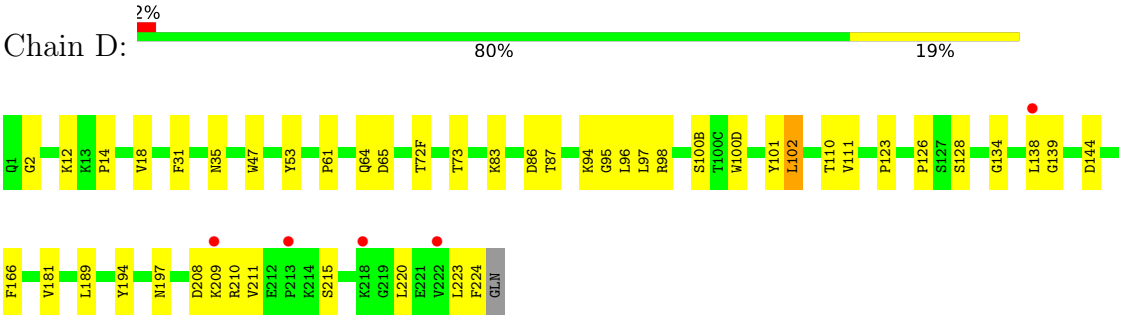
• Molecule 4: PGT122 Heavy chain

Chain H:



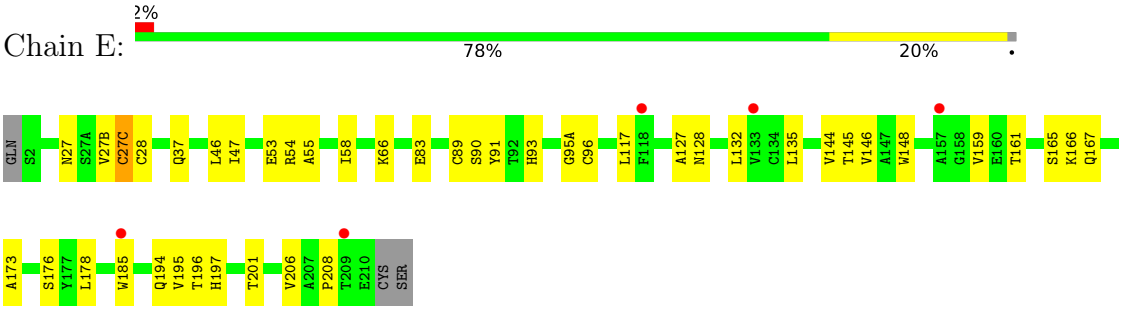
• Molecule 5: 35022 Heavy chain

Chain D:



• Molecule 6: 35022 Light Chain

Chain E:



• Molecule 7: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[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

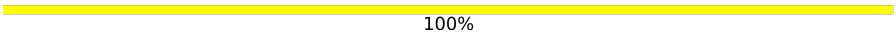
Chain A:

• Molecule 8: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C:

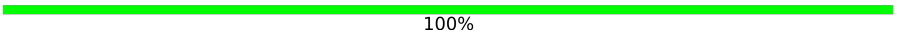
• Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:



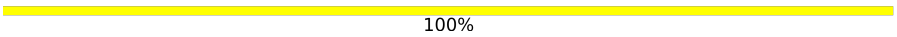
• Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:



• Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:



• Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:

• Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

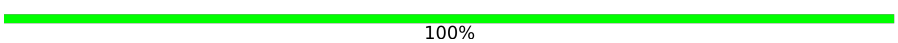
Chain N:

• Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain P:

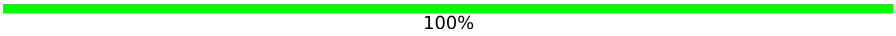
• Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Q:



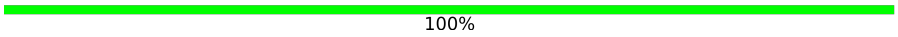
• Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain R:



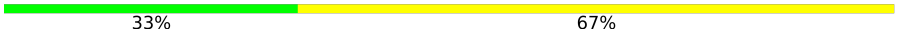
• Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain S:



• Molecule 10: alpha-D-mannopyranose-(1-2)-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 I:

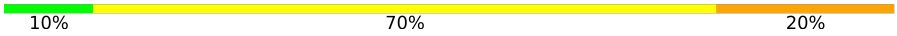


• Molecule 11: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O:

• Molecule 12: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]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 T:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α, β, γ	128.38Å 128.38Å 313.13Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	38.98 – 3.50 38.98 – 3.50	Depositor EDS
% Data completeness (in resolution range)	50.8 (38.98-3.50) 50.8 (38.98-3.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.41 (at 3.48Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.215 , 0.299 0.215 , 0.299	Depositor DCC
R_{free} test set	951 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å^2)	73.7	Xtriage
Anisotropy	0.036	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.24 , 12.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.41$, $< L^2 > = 0.23$	Xtriage
Estimated twinning fraction	0.156 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.86	EDS
Total number of atoms	11964	wwPDB-VP
Average B, all atoms (Å^2)	113.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.87% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, MAN, NAG

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	G	0.28	0/3537	0.47	0/4796
2	B	0.26	0/998	0.45	0/1353
3	L	0.27	0/1619	0.47	0/2217
4	H	0.26	0/1789	0.47	0/2443
5	D	0.25	0/1880	0.46	0/2560
6	E	0.25	0/1659	0.45	0/2269
All	All	0.26	0/11482	0.46	0/15638

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	G	3464	0	3394	68	0
2	B	980	0	955	27	0
3	L	1577	0	1518	25	0
4	H	1742	0	1716	26	0
5	D	1832	0	1806	30	0
6	E	1615	0	1542	31	0
7	A	116	0	97	6	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	C	39	0	34	0	0
9	F	28	0	25	1	0
9	J	28	0	25	0	0
9	K	28	0	25	1	0
9	M	28	0	25	1	0
9	N	28	0	25	2	0
9	P	28	0	25	1	0
9	Q	28	0	25	0	0
9	R	28	0	25	0	0
9	S	28	0	25	0	0
10	I	72	0	61	2	0
11	O	61	0	52	0	0
12	T	116	0	97	2	0
13	B	42	0	39	3	0
13	G	56	0	52	2	0
All	All	11964	0	11588	195	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 8.

All (195) 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)
3:L:163:THR:HG22	4:H:167:VAL:HB	1.58	0.84
4:H:100(D):VAL:HA	12:T:2:NAG:H2	1.59	0.82
1:G:350:ARG:NH2	1:G:396:ILE:O	2.13	0.81
13:B:702:NAG:H83	6:E:54:ARG:HH21	1.52	0.73
2:B:536:THR:O	2:B:540:GLN:NE2	2.23	0.72
1:G:221:ALA:HB3	2:B:582:ALA:HB1	1.73	0.71
1:G:291:PRO:HG3	9:N:1:NAG:H61	1.73	0.70
3:L:47:ILE:HG22	3:L:48:ILE:HG13	1.75	0.67
1:G:36:VAL:HG12	2:B:610:TRP:HE3	1.58	0.67
3:L:137:ILE:HB	3:L:175:ALA:HB3	1.78	0.66
6:E:37:GLN:HB2	6:E:47:ILE:HD11	1.77	0.65
5:D:123:PRO:HD3	5:D:209:LYS:HE2	1.77	0.65
3:L:39:ARG:NH1	3:L:81:GLY:O	2.30	0.65
1:G:298:ARG:NH2	1:G:439:ILE:O	2.30	0.65
3:L:116:VAL:HG12	3:L:137:ILE:HG23	1.80	0.64
1:G:175:LEU:HB3	1:G:320:LEU:HB2	1.80	0.63
5:D:12:LYS:HG3	5:D:18:VAL:HB	1.80	0.63
5:D:72(F):THR:HG1	5:D:73:THR:HG1	1.47	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:539:VAL:HG13	2:B:542:ARG:HH22	1.63	0.63
3:L:170:ASN:HB3	3:L:172:LYS:H	1.63	0.63
4:H:11:LEU:HB2	4:H:145:PRO:HG3	1.83	0.61
5:D:72(F):THR:OG1	5:D:73:THR:OG1	2.20	0.59
2:B:625:ASN:HB2	5:D:97:LEU:HD22	1.84	0.59
4:H:100(D):VAL:O	4:H:100(F):ALA:N	2.34	0.58
1:G:426:MET:HB3	1:G:427:TRP:CE3	2.39	0.58
7:A:2:NAG:H3	7:A:2:NAG:H83	1.86	0.58
1:G:109:ILE:HG12	1:G:430:ILE:HG21	1.85	0.58
2:B:525:ALA:HB1	2:B:528:SER:HB2	1.86	0.58
13:G:622:NAG:H83	13:G:622:NAG:H3	1.86	0.57
5:D:35:ASN:HD21	5:D:100(D):TRP:HE3	1.50	0.57
1:G:292:VAL:HB	1:G:449:ILE:HB	1.86	0.57
1:G:261:LEU:HD11	1:G:374:HIS:CE1	2.39	0.56
9:P:2:NAG:H83	9:P:2:NAG:H3	1.87	0.56
3:L:13:VAL:HG21	3:L:19:ALA:HA	1.88	0.56
1:G:261:LEU:HD11	1:G:374:HIS:HE1	1.71	0.55
6:E:165:SER:O	6:E:173:ALA:N	2.37	0.55
1:G:379:GLY:N	10:I:2:NAG:O6	2.39	0.55
4:H:188:GLY:HA3	4:H:190:GLN:N	2.21	0.55
5:D:128:SER:HB2	5:D:220:LEU:HB2	1.89	0.55
5:D:126:PRO:HB2	5:D:215:SER:HB2	1.89	0.54
1:G:83:GLU:HG2	1:G:245:VAL:HG22	1.90	0.54
1:G:297:THR:HG23	1:G:444:ARG:HG3	1.88	0.54
3:L:33:VAL:HG11	3:L:71:ALA:HB1	1.90	0.54
2:B:598:CYS:O	2:B:600:GLY:N	2.40	0.54
1:G:132:THR:HA	13:G:633:NAG:H82	1.89	0.54
1:G:108:ILE:HD13	1:G:111:LEU:HD12	1.90	0.54
1:G:503:ARG:HD2	2:B:605:CYS:O	2.07	0.54
6:E:93:HIS:NE2	7:A:6:MAN:H5	2.23	0.54
6:E:145:THR:OG1	6:E:196:THR:HB	2.08	0.54
4:H:20:LEU:HB2	4:H:80:LEU:HB3	1.89	0.53
1:G:503:ARG:NH1	2:B:597:GLY:HA3	2.23	0.53
4:H:99:ARG:HD3	4:H:100(J):TRP:CZ3	2.43	0.53
1:G:270:VAL:HG12	1:G:289:ASN:H	1.74	0.53
4:H:21:THR:HG23	4:H:77:LEU:HD13	1.90	0.53
3:L:92:ASP:HB3	3:L:95:ARG:HB2	1.90	0.53
1:G:396:ILE:HG22	1:G:397:SER:H	1.73	0.53
4:H:157:LEU:HD21	4:H:180:VAL:HG11	1.90	0.53
6:E:127:ALA:N	6:E:128:ASN:HA	2.24	0.53
4:H:22:CYS:HB3	4:H:78:VAL:HB	1.91	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:55:ALA:HB3	1:G:216:HIS:HB2	1.91	0.52
1:G:96:TRP:HH2	1:G:285:LEU:HG	1.74	0.52
3:L:150:LYS:HB2	3:L:193:SER:HB2	1.90	0.52
1:G:386:ASN:HB3	1:G:417:PRO:HD2	1.92	0.52
2:B:634:GLU:HA	13:B:703:NAG:H82	1.91	0.51
3:L:39:ARG:HG3	3:L:40:PRO:HD2	1.91	0.51
13:B:702:NAG:H62	6:E:53:GLU:HG2	1.93	0.51
6:E:54:ARG:HD2	6:E:58:ILE:HG22	1.93	0.51
4:H:117:PRO:HB3	4:H:143:TYR:HB3	1.92	0.51
1:G:272:ILE:HD11	1:G:345:VAL:HG13	1.92	0.51
4:H:31:ASP:N	4:H:31:ASP:OD1	2.43	0.51
5:D:2:GLY:H	5:D:102:LEU:HD11	1.76	0.51
5:D:96:LEU:HD13	5:D:101:TYR:HB2	1.94	0.50
1:G:295:ASN:O	1:G:331:CYS:HA	2.11	0.50
1:G:222:GLY:HA3	2:B:585:ARG:HD3	1.94	0.50
6:E:144:VAL:HG12	6:E:197:HIS:HB2	1.92	0.50
4:H:161:VAL:HG22	4:H:180:VAL:HG22	1.93	0.49
6:E:185:TRP:CZ3	6:E:208:PRO:HG3	2.47	0.49
1:G:448:ASN:HD22	9:N:1:NAG:H83	1.76	0.49
5:D:134:GLY:HA2	5:D:223:LEU:HD13	1.94	0.49
2:B:529:THR:O	2:B:533:ALA:N	2.40	0.49
1:G:174:SER:OG	1:G:175:LEU:N	2.46	0.48
6:E:46:LEU:HG	6:E:55:ALA:HB2	1.96	0.48
1:G:254:VAL:HG11	1:G:261:LEU:HB2	1.95	0.48
1:G:350:ARG:HD3	1:G:355:ASN:O	2.14	0.47
6:E:93:HIS:CG	7:A:4:MAN:H2	2.49	0.47
6:E:27(C):CYS:HA	6:E:28:CYS:HA	1.65	0.47
1:G:95:MET:SD	1:G:273:ARG:HD3	2.53	0.47
3:L:167:LYS:HB3	3:L:173:TYR:CZ	2.49	0.47
2:B:618:ASN:OD1	2:B:619:LEU:N	2.44	0.47
4:H:106:SER:HB3	4:H:147:PRO:HD3	1.96	0.47
3:L:21:ILE:HB	3:L:73:LEU:HB3	1.96	0.47
4:H:6:GLU:N	4:H:6:GLU:OE1	2.47	0.47
5:D:31:PHE:HA	7:A:1:NAG:O6	2.15	0.46
5:D:47:TRP:CZ3	6:E:95(A):GLY:HA3	2.50	0.46
1:G:51:THR:HB	2:B:578:ALA:HB2	1.97	0.46
4:H:100(D):VAL:HG21	4:H:100(G):PHE:HD2	1.80	0.46
2:B:529:THR:HG22	2:B:626:MET:H	1.79	0.46
6:E:132:LEU:HD12	6:E:178:LEU:HD23	1.96	0.46
3:L:129:ASN:HA	3:L:183:PRO:HG2	1.98	0.46
6:E:27(B):VAL:O	6:E:90:SER:OG	2.19	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:165:SER:N	6:E:173:ALA:O	2.33	0.46
1:G:361:PHE:HE2	1:G:395:TRP:CD1	2.33	0.46
1:G:152:GLY:C	1:G:178:ARG:HH21	2.19	0.45
1:G:271:MET:HG2	1:G:273:ARG:CZ	2.46	0.45
1:G:427:TRP:CD1	1:G:475:MET:HG3	2.51	0.45
1:G:36:VAL:HG12	2:B:610:TRP:CE3	2.45	0.45
5:D:138:LEU:HD13	5:D:211:VAL:HG11	1.97	0.45
1:G:164:GLU:HG3	1:G:312:GLY:HA3	1.99	0.45
1:G:270:VAL:HG12	1:G:289:ASN:N	2.31	0.45
5:D:61:PRO:HA	5:D:64:GLN:HB2	1.97	0.45
5:D:194:TYR:O	5:D:210:ARG:HD2	2.16	0.45
1:G:74:CYS:SG	1:G:75:VAL:N	2.90	0.45
3:L:167:LYS:HB3	3:L:173:TYR:CE2	2.52	0.45
9:F:1:NAG:H62	9:F:2:NAG:C7	2.47	0.45
1:G:377:ASN:OD1	1:G:378:CYS:N	2.50	0.45
3:L:60:ASP:OD1	3:L:60:ASP:N	2.50	0.45
3:L:165:PRO:HA	3:L:174:ALA:O	2.17	0.45
6:E:196:THR:HA	6:E:201:THR:HA	1.98	0.45
1:G:161:MET:HB3	1:G:170:GLN:HB3	2.00	0.44
4:H:195:ASN:ND2	4:H:206:ASP:OD1	2.48	0.44
5:D:14:PRO:HG3	5:D:111:VAL:HG12	2.00	0.44
4:H:157:LEU:O	4:H:161:VAL:HG21	2.18	0.44
2:B:642:ILE:O	2:B:646:LEU:HD12	2.18	0.44
5:D:100(B):SER:OG	6:E:91:TYR:OH	2.28	0.44
5:D:139:GLY:HA3	5:D:181:VAL:HA	1.98	0.44
6:E:117:LEU:HD23	6:E:206:VAL:HG13	1.99	0.44
1:G:132:THR:OG1	1:G:133:ASN:N	2.51	0.44
2:B:570:VAL:HG12	2:B:571:TRP:H	1.83	0.44
2:B:631:TRP:CE2	2:B:635:ILE:HG13	2.53	0.44
7:A:3:BMA:H61	7:A:7:MAN:H2	1.42	0.44
1:G:343:GLY:HA2	1:G:346:VAL:HG12	1.99	0.43
6:E:83:GLU:O	6:E:166:LYS:NZ	2.40	0.43
6:E:148:TRP:CD1	6:E:159:VAL:HG13	2.53	0.43
1:G:156:ASN:HA	1:G:175:LEU:HD12	2.00	0.43
1:G:299:PRO:HA	1:G:442:VAL:HG22	2.00	0.43
1:G:491:ILE:O	2:B:585:ARG:NH2	2.43	0.43
3:L:109:GLN:HG3	3:L:141:TYR:CZ	2.52	0.43
1:G:259:LEU:HD12	1:G:374:HIS:CD2	2.54	0.43
4:H:18:LEU:HB3	4:H:82:LEU:HB3	2.00	0.43
4:H:188:GLY:HA3	4:H:190:GLN:H	1.83	0.43
5:D:100(D):TRP:CZ2	6:E:91:TYR:HB2	2.54	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:27:ASN:HA	6:E:27(C):CYS:O	2.19	0.43
1:G:44:VAL:HA	2:B:629:LEU:HD23	2.00	0.42
1:G:359:ILE:HD12	1:G:468:PHE:HE2	1.84	0.42
1:G:203:GLN:HE21	1:G:203:GLN:HB3	1.59	0.42
3:L:174:ALA:HB1	4:H:164:PHE:CD2	2.54	0.42
12:T:8:MAN:H2	12:T:9:MAN:H2	1.71	0.42
2:B:529:THR:HG23	5:D:98:ARG:HD2	2.00	0.42
6:E:167:GLN:OE1	6:E:173:ALA:HB2	2.19	0.42
3:L:114:PRO:HG2	3:L:203:VAL:HG21	2.02	0.42
4:H:6:GLU:OE2	4:H:92:CYS:N	2.51	0.42
5:D:94:LYS:HD3	5:D:102:LEU:HB2	2.02	0.42
9:K:1:NAG:H61	9:K:2:NAG:N2	2.35	0.42
1:G:107:ASP:O	1:G:111:LEU:HG	2.20	0.42
5:D:87:THR:HG23	5:D:110:THR:HA	2.02	0.42
5:D:220:LEU:HD12	5:D:223:LEU:HD12	2.02	0.42
1:G:221:ALA:HB1	2:B:544:LEU:O	2.20	0.42
3:L:95:ARG:HD3	3:L:95:ARG:HA	1.77	0.42
6:E:146:VAL:HG22	6:E:195:VAL:HG22	2.01	0.42
1:G:300:MET:HE2	1:G:322:ILE:HG21	2.02	0.41
1:G:503:ARG:HH12	2:B:597:GLY:HA3	1.84	0.41
3:L:208:ALA:HA	3:L:209:PRO:HD3	1.94	0.41
6:E:146:VAL:HA	6:E:194:GLN:O	2.20	0.41
1:G:301:ASN:HB3	1:G:323:ILE:O	2.19	0.41
4:H:144:PHE:HA	4:H:145:PRO:HA	1.86	0.41
3:L:83:GLU:HB2	3:L:106:VAL:HG23	2.01	0.41
5:D:166:PHE:CZ	6:E:135:LEU:HB3	2.55	0.41
5:D:197:ASN:ND2	5:D:208:ASP:OD1	2.50	0.41
6:E:161:THR:HG23	6:E:176:SER:HB2	2.01	0.41
1:G:109:ILE:HG23	1:G:430:ILE:HG12	2.03	0.41
1:G:261:LEU:HA	1:G:448:ASN:O	2.20	0.41
9:M:1:NAG:H4	9:M:2:NAG:N2	2.35	0.41
1:G:64:GLU:HG3	1:G:65:LYS:H	1.86	0.41
2:B:535:MET:H	2:B:535:MET:HG2	1.65	0.41
2:B:592:LEU:HD22	2:B:596:TRP:CZ2	2.55	0.41
1:G:108:ILE:HG22	1:G:427:TRP:CZ2	2.55	0.41
1:G:112:TRP:CG	1:G:427:TRP:HZ3	2.38	0.41
5:D:83:LYS:N	5:D:86:ASP:OD2	2.52	0.41
1:G:104:MET:O	1:G:108:ILE:HG12	2.21	0.41
1:G:129:LEU:O	1:G:191:TYR:N	2.51	0.41
1:G:170:GLN:HG2	1:G:172:VAL:HG13	2.03	0.41
1:G:249:HIS:O	1:G:251:ILE:HG13	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:100(D):VAL:HG22	4:H:100(I):GLU:OE1	2.20	0.41
4:H:167:VAL:O	4:H:174:TYR:HA	2.21	0.41
5:D:189:LEU:HD21	5:D:224:PHE:HE1	1.86	0.41
6:E:28:CYS:HB3	6:E:66:LYS:HD2	2.03	0.41
1:G:83:GLU:OE1	1:G:229:LYS:HD3	2.20	0.41
1:G:101:VAL:HG21	1:G:480:ARG:HG2	2.03	0.41
5:D:53:TYR:CD2	7:A:1:NAG:H5	2.56	0.41
2:B:661:LEU:HA	2:B:661:LEU:HD13	1.82	0.40
3:L:13:VAL:HG13	3:L:17:GLN:HB2	2.03	0.40
5:D:94:LYS:HG2	5:D:95:GLY:O	2.21	0.40
6:E:161:THR:HA	6:E:176:SER:HA	2.03	0.40
1:G:445:CYS:HB3	10:I:2:NAG:H61	2.03	0.40
3:L:136:LEU:HD11	4:H:177:SER:HB2	2.02	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	G	429/481 (89%)	371 (86%)	52 (12%)	6 (1%)	11 46
2	B	119/153 (78%)	105 (88%)	12 (10%)	2 (2%)	9 42
3	L	206/213 (97%)	187 (91%)	18 (9%)	1 (0%)	29 68
4	H	224/235 (95%)	207 (92%)	15 (7%)	2 (1%)	17 56
5	D	240/243 (99%)	223 (93%)	16 (7%)	1 (0%)	34 72
6	E	211/216 (98%)	191 (90%)	20 (10%)	0	100 100
All	All	1429/1541 (93%)	1284 (90%)	133 (9%)	12 (1%)	19 58

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	81	PRO
2	B	599	SER
3	L	110	PRO
4	H	190	GLN
1	G	67	ASN
1	G	69	TRP
2	B	615	SER
1	G	80	ASN
1	G	135	THR
4	H	188	GLY
5	D	144	ASP
1	G	220	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	G	392/429 (91%)	373 (95%)	19 (5%)	25 60
2	B	106/129 (82%)	93 (88%)	13 (12%)	4 23
3	L	177/181 (98%)	177 (100%)	0	100 100
4	H	198/205 (97%)	195 (98%)	3 (2%)	65 84
5	D	205/206 (100%)	203 (99%)	2 (1%)	76 88
6	E	186/189 (98%)	183 (98%)	3 (2%)	62 83
All	All	1264/1339 (94%)	1224 (97%)	40 (3%)	39 69

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	32	GLU
1	G	47	ASP
1	G	83	GLU
1	G	109	ILE
1	G	123	THR
1	G	125	LEU
1	G	184	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	199	SER
1	G	203	GLN
1	G	236	THR
1	G	297	THR
1	G	342	LEU
1	G	355	ASN
1	G	375	SER
1	G	378	CYS
1	G	398	ASN
1	G	429	ARG
1	G	481	SER
1	G	499	THR
2	B	529	THR
2	B	535	MET
2	B	540	GLN
2	B	573	ILE
2	B	576	LEU
2	B	581	LEU
2	B	604	CYS
2	B	619	LEU
2	B	626	MET
2	B	639	THR
2	B	645	LEU
2	B	658	GLN
2	B	661	LEU
4	H	31	ASP
4	H	100(J)	TRP
4	H	100(L)	THR
5	D	65	ASP
5	D	102	LEU
6	E	27(C)	CYS
6	E	89	CYS
6	E	96	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	G	203	GLN
1	G	374	HIS
2	B	540	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)

52 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	$\#\|Z\| > 2$
7	NAG	A	1	7,1	14,14,15	0.17	0	17,19,21	0.73	1 (5%)
7	MAN	A	10	7	11,11,12	0.74	0	15,15,17	1.33	2 (13%)
7	NAG	A	2	7	14,14,15	0.45	0	17,19,21	1.36	3 (17%)
7	BMA	A	3	7	11,11,12	0.79	0	15,15,17	1.01	0
7	MAN	A	4	7	11,11,12	0.74	0	15,15,17	1.17	2 (13%)
7	MAN	A	5	7	11,11,12	0.74	0	15,15,17	0.92	0
7	MAN	A	6	7	11,11,12	0.72	0	15,15,17	1.43	2 (13%)
7	MAN	A	7	7	11,11,12	1.36	1 (9%)	15,15,17	1.91	4 (26%)
7	MAN	A	8	7	11,11,12	0.88	0	15,15,17	1.28	1 (6%)
7	MAN	A	9	7	11,11,12	1.02	0	15,15,17	1.23	2 (13%)
8	NAG	C	1	8,1	14,14,15	0.47	0	17,19,21	0.45	0
8	NAG	C	2	8	14,14,15	0.38	0	17,19,21	0.39	0
8	BMA	C	3	8	11,11,12	0.52	0	15,15,17	0.93	1 (6%)
9	NAG	F	1	9,1	14,14,15	0.30	0	17,19,21	0.44	0
9	NAG	F	2	9	14,14,15	0.34	0	17,19,21	0.54	0
10	NAG	I	1	10,1	14,14,15	0.31	0	17,19,21	0.52	0
10	NAG	I	2	10	14,14,15	0.43	0	17,19,21	0.43	0
10	BMA	I	3	10	11,11,12	0.95	0	15,15,17	0.90	0
10	MAN	I	4	10	11,11,12	0.98	0	15,15,17	0.95	1 (6%)
10	MAN	I	5	10	11,11,12	0.92	1 (9%)	15,15,17	1.28	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
10	MAN	I	6	10	11,11,12	0.79	0	15,15,17	1.05	2 (13%)
9	NAG	J	1	9,1	14,14,15	0.39	0	17,19,21	0.50	0
9	NAG	J	2	9	14,14,15	0.16	0	17,19,21	0.56	0
9	NAG	K	1	9,1	14,14,15	0.35	0	17,19,21	0.55	0
9	NAG	K	2	9	14,14,15	0.42	0	17,19,21	0.58	0
9	NAG	M	1	9,1	14,14,15	0.24	0	17,19,21	0.56	0
9	NAG	M	2	9	14,14,15	0.72	0	17,19,21	0.69	1 (5%)
9	NAG	N	1	9,1	14,14,15	0.18	0	17,19,21	0.55	0
9	NAG	N	2	9	14,14,15	0.21	0	17,19,21	0.44	0
11	NAG	O	1	11,1	14,14,15	0.23	0	17,19,21	0.52	0
11	NAG	O	2	11	14,14,15	0.26	0	17,19,21	0.46	0
11	BMA	O	3	11	11,11,12	0.75	0	15,15,17	0.75	0
11	MAN	O	4	11	11,11,12	0.81	0	15,15,17	1.26	2 (13%)
11	MAN	O	5	11	11,11,12	0.67	0	15,15,17	1.55	3 (20%)
9	NAG	P	1	9,1	14,14,15	0.26	0	17,19,21	0.51	0
9	NAG	P	2	9	14,14,15	0.59	0	17,19,21	1.33	2 (11%)
9	NAG	Q	1	9,1	14,14,15	0.18	0	17,19,21	0.41	0
9	NAG	Q	2	9	14,14,15	0.32	0	17,19,21	0.48	0
9	NAG	R	1	9,1	14,14,15	0.32	0	17,19,21	0.52	0
9	NAG	R	2	9	14,14,15	0.21	0	17,19,21	0.41	0
9	NAG	S	1	9,1	14,14,15	0.39	0	17,19,21	0.31	0
9	NAG	S	2	9	14,14,15	0.16	0	17,19,21	0.51	0
12	NAG	T	1	12,1	14,14,15	0.40	0	17,19,21	0.40	0
12	MAN	T	10	12	11,11,12	0.78	0	15,15,17	0.96	2 (13%)
12	NAG	T	2	12	14,14,15	0.31	0	17,19,21	0.72	0
12	BMA	T	3	12	11,11,12	1.04	0	15,15,17	1.34	3 (20%)
12	MAN	T	4	12	11,11,12	0.88	0	15,15,17	1.15	2 (13%)
12	MAN	T	5	12	11,11,12	0.78	0	15,15,17	1.28	2 (13%)
12	MAN	T	6	12	11,11,12	0.60	0	15,15,17	1.32	1 (6%)
12	MAN	T	7	12	11,11,12	1.10	1 (9%)	15,15,17	0.81	1 (6%)
12	MAN	T	8	12	11,11,12	0.76	0	15,15,17	1.03	1 (6%)
12	MAN	T	9	12	11,11,12	0.93	0	15,15,17	1.18	2 (13%)

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
7	NAG	A	1	7,1	-	2/6/23/26	0/1/1/1
7	MAN	A	10	7	-	0/2/19/22	0/1/1/1
7	NAG	A	2	7	-	3/6/23/26	0/1/1/1
7	BMA	A	3	7	-	2/2/19/22	0/1/1/1
7	MAN	A	4	7	-	1/2/19/22	0/1/1/1
7	MAN	A	5	7	-	0/2/19/22	0/1/1/1
7	MAN	A	6	7	-	1/2/19/22	0/1/1/1
7	MAN	A	7	7	-	0/2/19/22	0/1/1/1
7	MAN	A	8	7	-	1/2/19/22	0/1/1/1
7	MAN	A	9	7	-	2/2/19/22	0/1/1/1
8	NAG	C	1	8,1	-	1/6/23/26	0/1/1/1
8	NAG	C	2	8	-	0/6/23/26	0/1/1/1
8	BMA	C	3	8	-	2/2/19/22	0/1/1/1
9	NAG	F	1	9,1	-	0/6/23/26	0/1/1/1
9	NAG	F	2	9	-	0/6/23/26	0/1/1/1
10	NAG	I	1	10,1	-	0/6/23/26	0/1/1/1
10	NAG	I	2	10	-	3/6/23/26	0/1/1/1
10	BMA	I	3	10	-	0/2/19/22	0/1/1/1
10	MAN	I	4	10	-	2/2/19/22	0/1/1/1
10	MAN	I	5	10	-	2/2/19/22	1/1/1/1
10	MAN	I	6	10	-	2/2/19/22	0/1/1/1
9	NAG	J	1	9,1	-	0/6/23/26	0/1/1/1
9	NAG	J	2	9	-	2/6/23/26	0/1/1/1
9	NAG	K	1	9,1	-	3/6/23/26	0/1/1/1
9	NAG	K	2	9	-	2/6/23/26	0/1/1/1
9	NAG	M	1	9,1	-	2/6/23/26	0/1/1/1
9	NAG	M	2	9	-	2/6/23/26	0/1/1/1
9	NAG	N	1	9,1	-	4/6/23/26	0/1/1/1
9	NAG	N	2	9	-	2/6/23/26	0/1/1/1
11	NAG	O	1	11,1	-	2/6/23/26	0/1/1/1
11	NAG	O	2	11	-	2/6/23/26	0/1/1/1
11	BMA	O	3	11	-	2/2/19/22	0/1/1/1
11	MAN	O	4	11	-	1/2/19/22	0/1/1/1
11	MAN	O	5	11	-	2/2/19/22	0/1/1/1
9	NAG	P	1	9,1	-	4/6/23/26	0/1/1/1
9	NAG	P	2	9	-	5/6/23/26	0/1/1/1
9	NAG	Q	1	9,1	-	3/6/23/26	0/1/1/1
9	NAG	Q	2	9	-	2/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	NAG	R	1	9,1	-	2/6/23/26	0/1/1/1
9	NAG	R	2	9	-	0/6/23/26	0/1/1/1
9	NAG	S	1	9,1	-	0/6/23/26	0/1/1/1
9	NAG	S	2	9	-	2/6/23/26	0/1/1/1
12	NAG	T	1	12,1	-	0/6/23/26	0/1/1/1
12	MAN	T	10	12	-	0/2/19/22	0/1/1/1
12	NAG	T	2	12	-	3/6/23/26	0/1/1/1
12	BMA	T	3	12	-	0/2/19/22	0/1/1/1
12	MAN	T	4	12	-	2/2/19/22	0/1/1/1
12	MAN	T	5	12	-	0/2/19/22	0/1/1/1
12	MAN	T	6	12	-	2/2/19/22	0/1/1/1
12	MAN	T	7	12	-	2/2/19/22	0/1/1/1
12	MAN	T	8	12	-	0/2/19/22	0/1/1/1
12	MAN	T	9	12	-	0/2/19/22	1/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	7	MAN	C1-C2	3.94	1.61	1.52
12	T	7	MAN	O5-C1	-3.05	1.38	1.43
10	I	5	MAN	O5-C5	2.10	1.47	1.43

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	P	2	NAG	C2-N2-C7	4.42	129.20	122.90
7	A	2	NAG	C2-N2-C7	4.38	129.15	122.90
7	A	6	MAN	C1-O5-C5	4.31	118.03	112.19
11	O	5	MAN	C1-O5-C5	3.96	117.56	112.19
12	T	6	MAN	C1-O5-C5	3.86	117.43	112.19
7	A	10	MAN	C1-O5-C5	3.86	117.43	112.19
7	A	7	MAN	C1-O5-C5	3.59	117.05	112.19
7	A	7	MAN	C1-C2-C3	3.54	114.02	109.67
7	A	8	MAN	C1-O5-C5	3.48	116.91	112.19
7	A	7	MAN	O5-C1-C2	3.43	116.07	110.77
10	I	5	MAN	C1-O5-C5	3.41	116.81	112.19
7	A	9	MAN	C1-O5-C5	3.23	116.57	112.19
12	T	9	MAN	C1-O5-C5	3.11	116.40	112.19
12	T	5	MAN	C1-O5-C5	2.95	116.19	112.19
11	O	4	MAN	C1-O5-C5	2.87	116.08	112.19
7	A	4	MAN	C1-O5-C5	2.85	116.05	112.19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	O	5	MAN	O5-C1-C2	2.82	115.12	110.77
12	T	4	MAN	C1-O5-C5	2.69	115.84	112.19
12	T	8	MAN	C1-O5-C5	2.65	115.78	112.19
12	T	3	BMA	O5-C1-C2	2.61	114.80	110.77
7	A	4	MAN	O2-C2-C3	-2.59	104.94	110.14
7	A	7	MAN	O2-C2-C3	-2.54	105.06	110.14
9	M	2	NAG	C1-O5-C5	2.47	115.54	112.19
10	I	5	MAN	O2-C2-C3	-2.47	105.20	110.14
7	A	1	NAG	C1-O5-C5	2.39	115.42	112.19
8	C	3	BMA	C1-O5-C5	2.36	115.39	112.19
12	T	3	BMA	C1-C2-C3	2.32	112.52	109.67
10	I	6	MAN	C1-O5-C5	2.32	115.33	112.19
7	A	10	MAN	O2-C2-C3	-2.30	105.53	110.14
12	T	10	MAN	O2-C2-C3	-2.28	105.57	110.14
12	T	10	MAN	C1-O5-C5	2.23	115.21	112.19
12	T	9	MAN	O2-C2-C3	-2.23	105.67	110.14
7	A	6	MAN	O2-C2-C3	-2.22	105.70	110.14
12	T	4	MAN	O5-C1-C2	2.19	114.15	110.77
12	T	5	MAN	O3-C3-C2	2.18	114.16	109.99
12	T	7	MAN	O2-C2-C3	-2.16	105.82	110.14
11	O	5	MAN	O2-C2-C3	-2.13	105.88	110.14
10	I	4	MAN	C1-O5-C5	2.12	115.07	112.19
9	P	2	NAG	C1-C2-N2	2.11	114.10	110.49
11	O	4	MAN	O5-C1-C2	2.11	114.03	110.77
7	A	9	MAN	O2-C2-C3	-2.10	105.93	110.14
12	T	3	BMA	C1-O5-C5	2.10	115.03	112.19
10	I	6	MAN	O2-C2-C3	-2.08	105.96	110.14
7	A	2	NAG	C1-C2-N2	2.06	114.02	110.49
7	A	2	NAG	C1-O5-C5	2.04	114.96	112.19

There are no chirality outliers.

All (77) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	J	2	NAG	O5-C5-C6-O6
9	K	2	NAG	O5-C5-C6-O6
9	R	1	NAG	O5-C5-C6-O6
10	I	4	MAN	O5-C5-C6-O6
10	I	6	MAN	O5-C5-C6-O6
12	T	2	NAG	O5-C5-C6-O6
9	S	2	NAG	O5-C5-C6-O6
9	J	2	NAG	C4-C5-C6-O6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
9	K	1	NAG	O5-C5-C6-O6
12	T	4	MAN	O5-C5-C6-O6
7	A	3	BMA	C4-C5-C6-O6
9	K	2	NAG	C4-C5-C6-O6
10	I	6	MAN	C4-C5-C6-O6
11	O	2	NAG	O5-C5-C6-O6
9	R	1	NAG	C4-C5-C6-O6
9	N	1	NAG	O5-C5-C6-O6
11	O	1	NAG	O5-C5-C6-O6
9	S	2	NAG	C4-C5-C6-O6
12	T	6	MAN	O5-C5-C6-O6
9	N	2	NAG	O5-C5-C6-O6
11	O	5	MAN	C4-C5-C6-O6
9	Q	2	NAG	O5-C5-C6-O6
12	T	4	MAN	C4-C5-C6-O6
12	T	7	MAN	O5-C5-C6-O6
9	K	1	NAG	C4-C5-C6-O6
11	O	1	NAG	C4-C5-C6-O6
12	T	2	NAG	C4-C5-C6-O6
7	A	1	NAG	O5-C5-C6-O6
9	M	2	NAG	O5-C5-C6-O6
10	I	4	MAN	C4-C5-C6-O6
7	A	2	NAG	C8-C7-N2-C2
7	A	2	NAG	O7-C7-N2-C2
9	N	1	NAG	C8-C7-N2-C2
9	N	1	NAG	O7-C7-N2-C2
9	P	1	NAG	C8-C7-N2-C2
9	P	1	NAG	O7-C7-N2-C2
9	P	2	NAG	C8-C7-N2-C2
9	P	2	NAG	O7-C7-N2-C2
9	Q	1	NAG	C8-C7-N2-C2
9	Q	1	NAG	O7-C7-N2-C2
7	A	1	NAG	C4-C5-C6-O6
11	O	3	BMA	C4-C5-C6-O6
12	T	7	MAN	C4-C5-C6-O6
9	N	1	NAG	C4-C5-C6-O6
10	I	2	NAG	C4-C5-C6-O6
11	O	2	NAG	C4-C5-C6-O6
9	P	2	NAG	O5-C5-C6-O6
7	A	3	BMA	O5-C5-C6-O6
9	M	1	NAG	O5-C5-C6-O6
11	O	5	MAN	O5-C5-C6-O6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
9	N	2	NAG	C4-C5-C6-O6
9	M	2	NAG	C4-C5-C6-O6
10	I	2	NAG	O5-C5-C6-O6
11	O	3	BMA	O5-C5-C6-O6
7	A	9	MAN	C4-C5-C6-O6
10	I	5	MAN	C4-C5-C6-O6
11	O	4	MAN	O5-C5-C6-O6
7	A	6	MAN	O5-C5-C6-O6
9	P	2	NAG	C4-C5-C6-O6
9	Q	2	NAG	C4-C5-C6-O6
9	P	1	NAG	C4-C5-C6-O6
9	M	1	NAG	C4-C5-C6-O6
7	A	8	MAN	C4-C5-C6-O6
7	A	4	MAN	O5-C5-C6-O6
8	C	3	BMA	C4-C5-C6-O6
7	A	9	MAN	O5-C5-C6-O6
12	T	6	MAN	C4-C5-C6-O6
7	A	2	NAG	C3-C2-N2-C7
9	K	1	NAG	C3-C2-N2-C7
12	T	2	NAG	C3-C2-N2-C7
10	I	5	MAN	O5-C5-C6-O6
9	P	1	NAG	O5-C5-C6-O6
8	C	3	BMA	O5-C5-C6-O6
10	I	2	NAG	C1-C2-N2-C7
9	Q	1	NAG	C4-C5-C6-O6
8	C	1	NAG	C3-C2-N2-C7
9	P	2	NAG	C3-C2-N2-C7

All (2) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	T	9	MAN	C1-C2-C3-C4-C5-O5
10	I	5	MAN	C1-C2-C3-C4-C5-O5

18 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	2	NAG	1	0
12	T	8	MAN	1	0
9	N	1	NAG	2	0
9	M	2	NAG	1	0
12	T	2	NAG	1	0

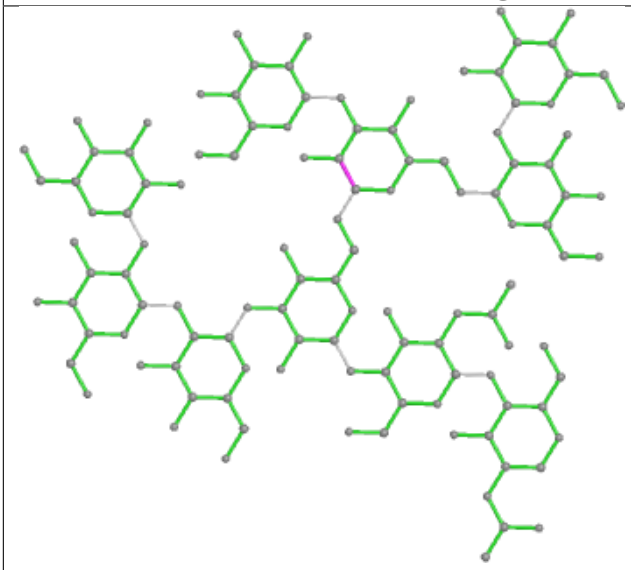
Continued on next page...

Continued from previous page...

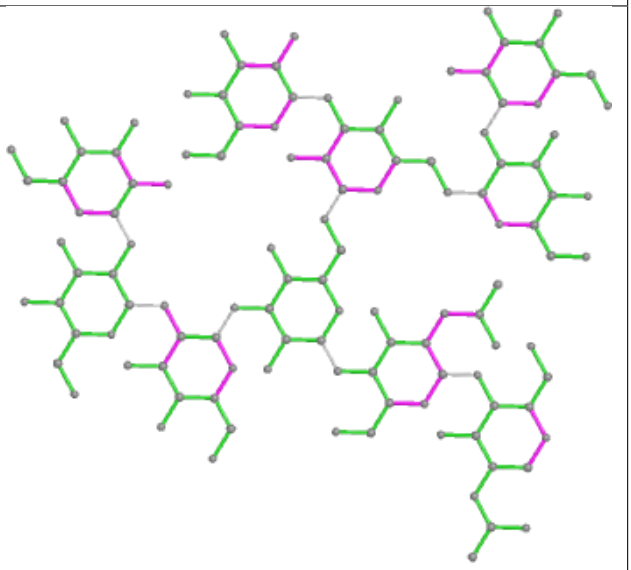
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	3	BMA	1	0
7	A	4	MAN	1	0
7	A	1	NAG	2	0
9	K	2	NAG	1	0
12	T	9	MAN	1	0
10	I	2	NAG	2	0
9	M	1	NAG	1	0
9	F	1	NAG	1	0
9	P	2	NAG	1	0
9	K	1	NAG	1	0
7	A	7	MAN	1	0
7	A	6	MAN	1	0
9	F	2	NAG	1	0

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

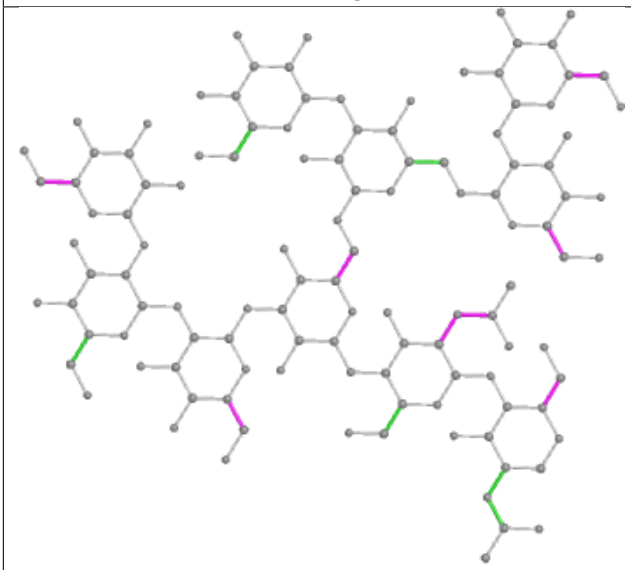
Oligosaccharide Chain A



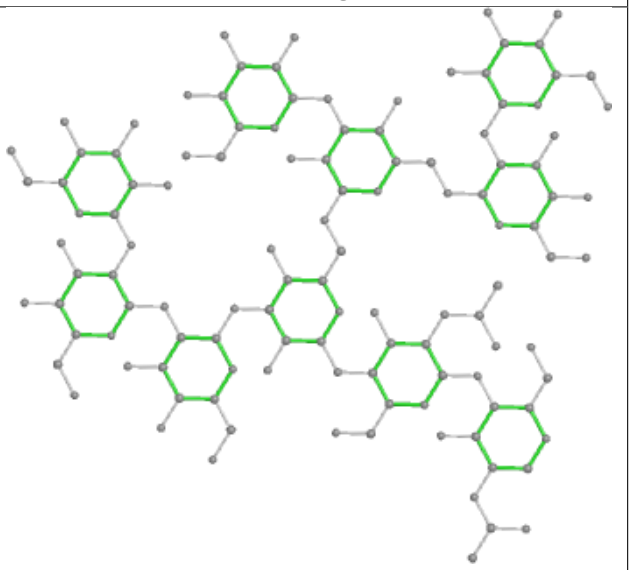
Bond lengths



Bond angles

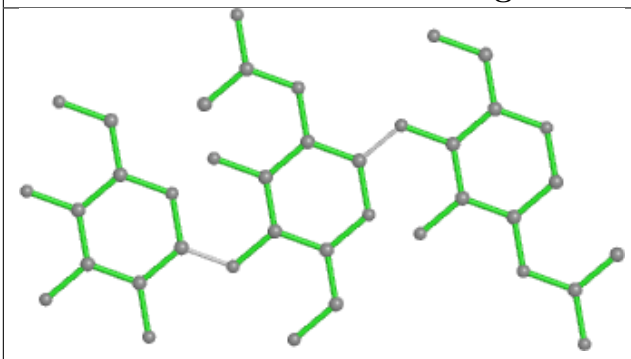


Torsions

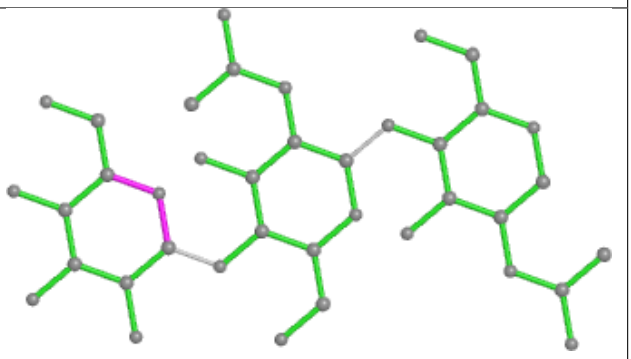


Rings

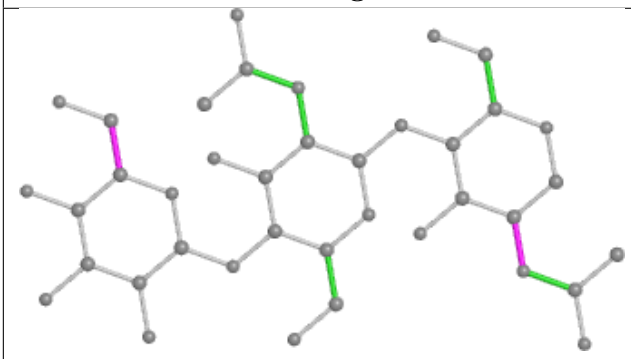
Oligosaccharide Chain C



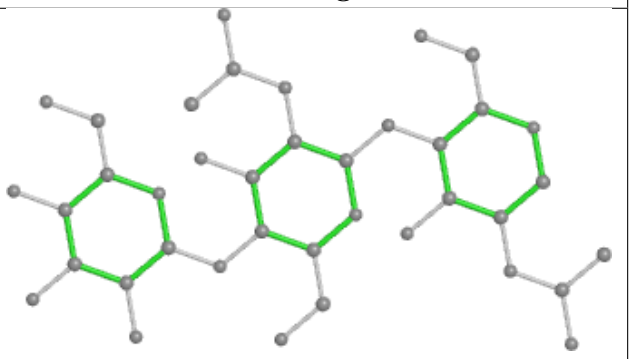
Bond lengths



Bond angles

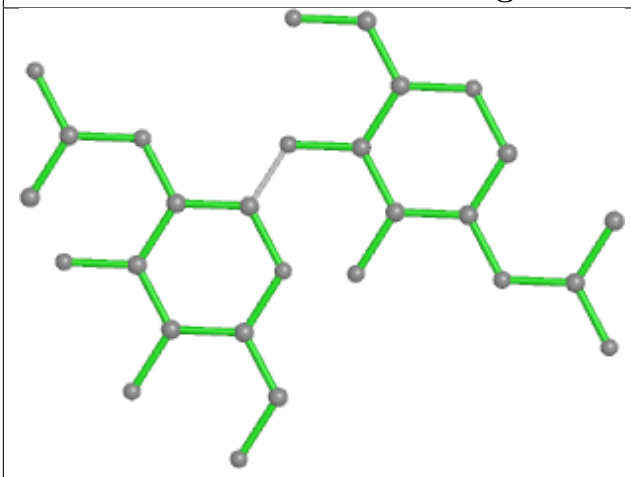


Torsions

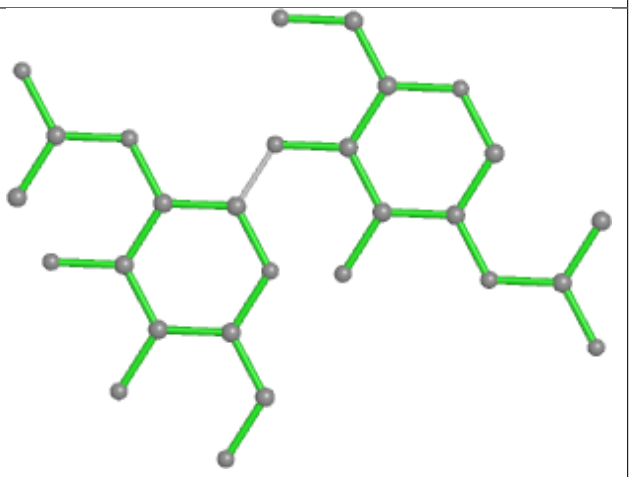


Rings

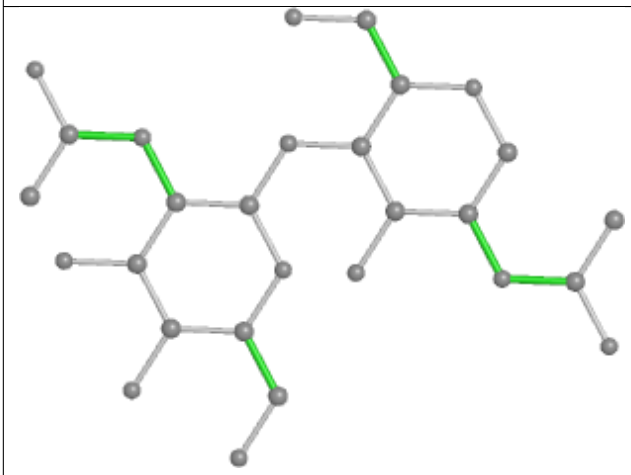
Oligosaccharide Chain F



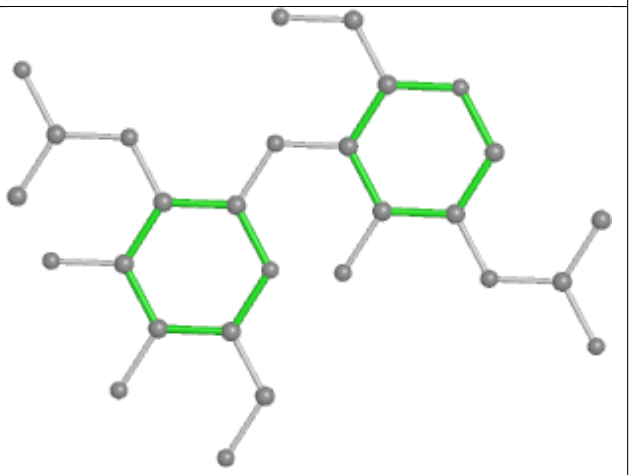
Bond lengths



Bond angles

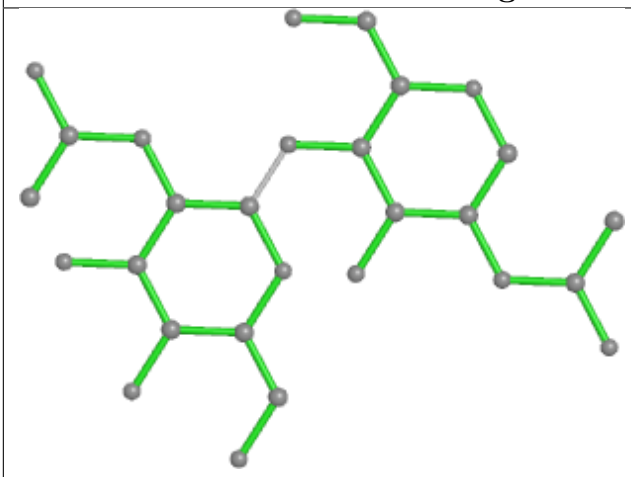


Torsions

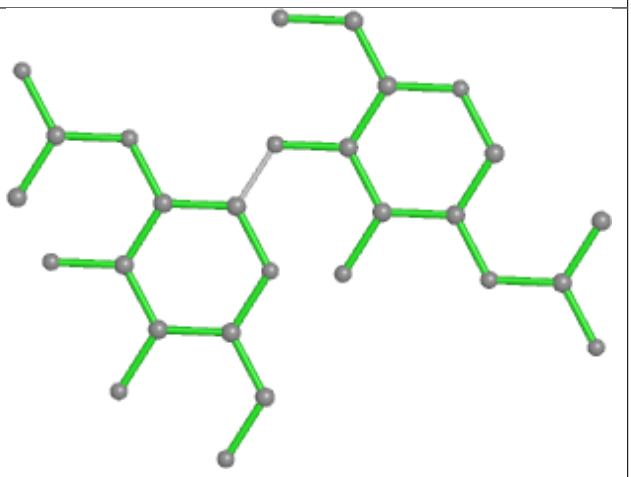


Rings

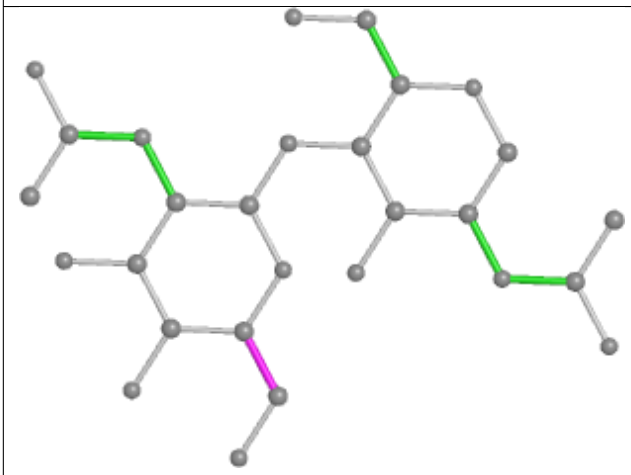
Oligosaccharide Chain J



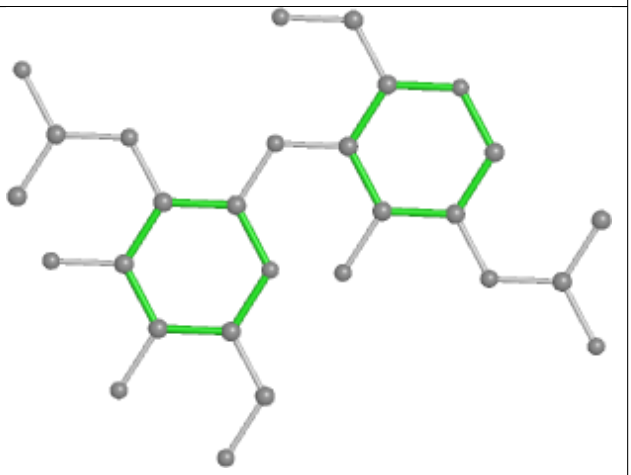
Bond lengths



Bond angles

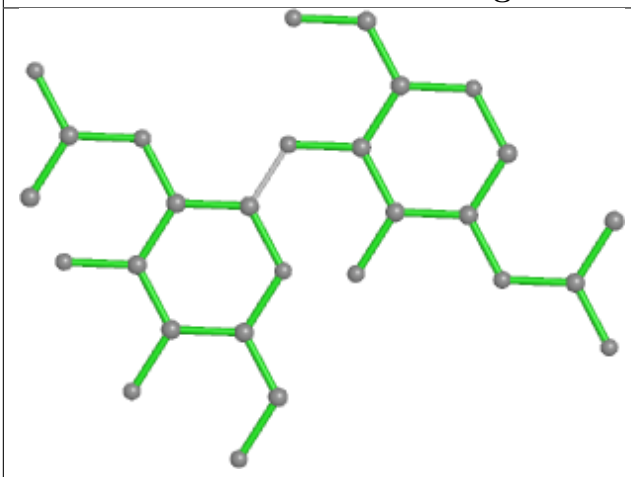


Torsions

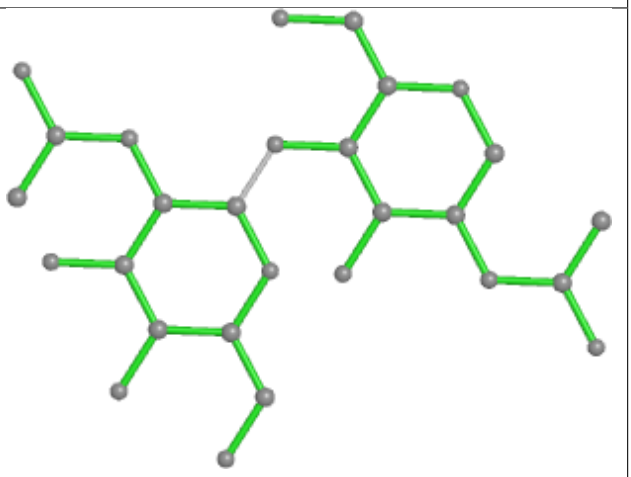


Rings

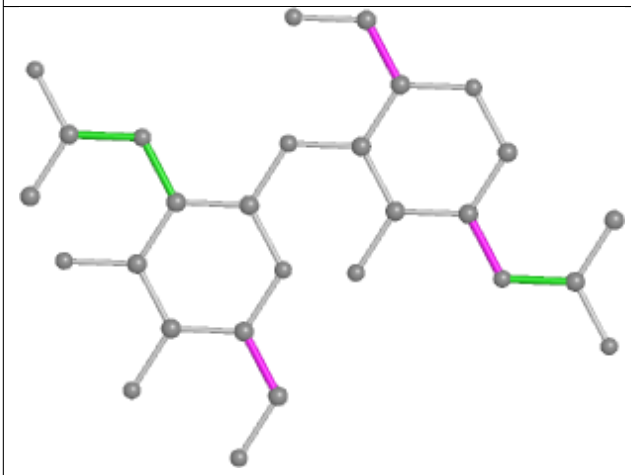
Oligosaccharide Chain K



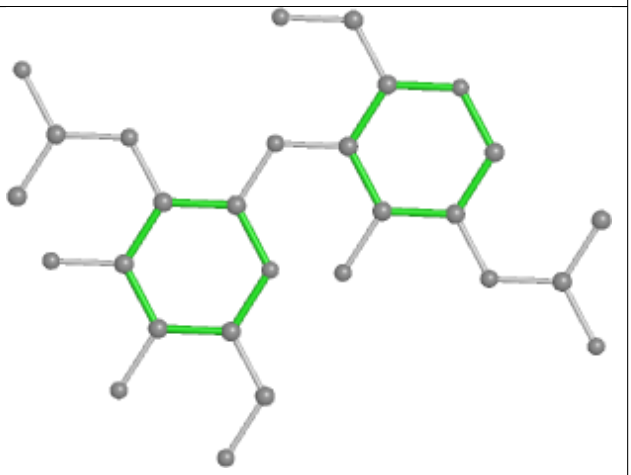
Bond lengths



Bond angles

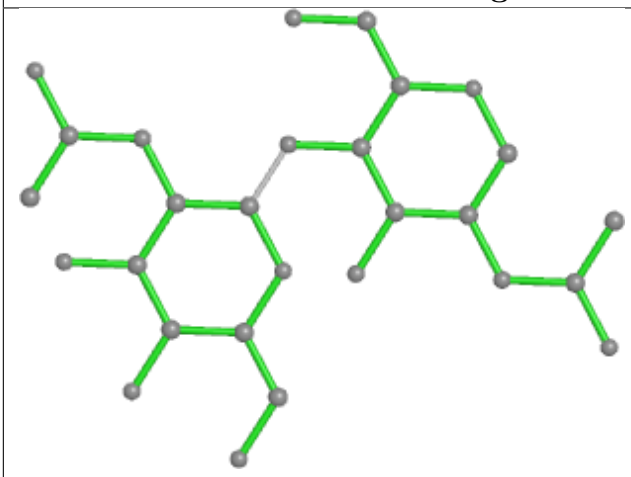


Torsions

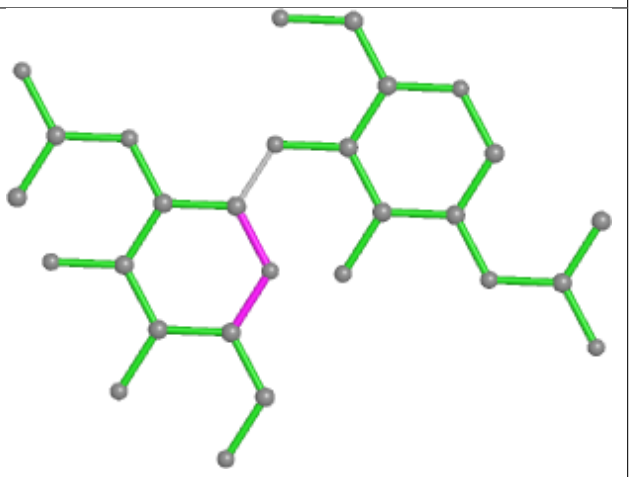


Rings

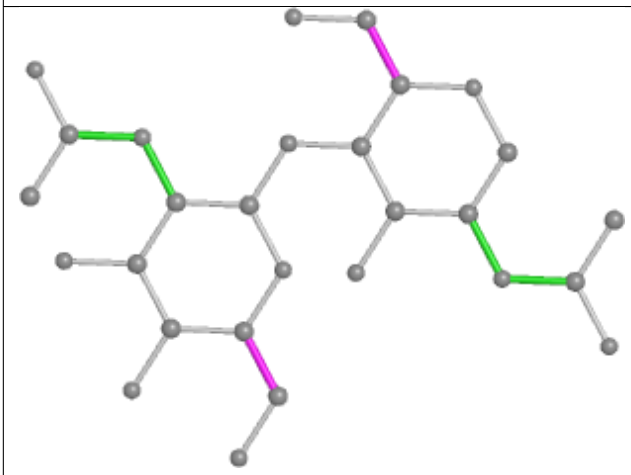
Oligosaccharide Chain M



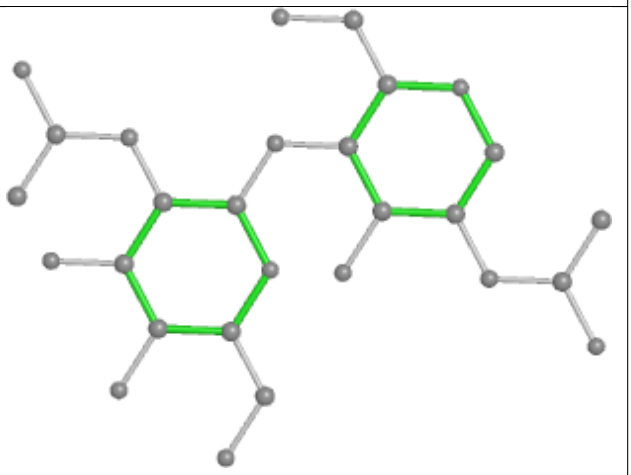
Bond lengths



Bond angles

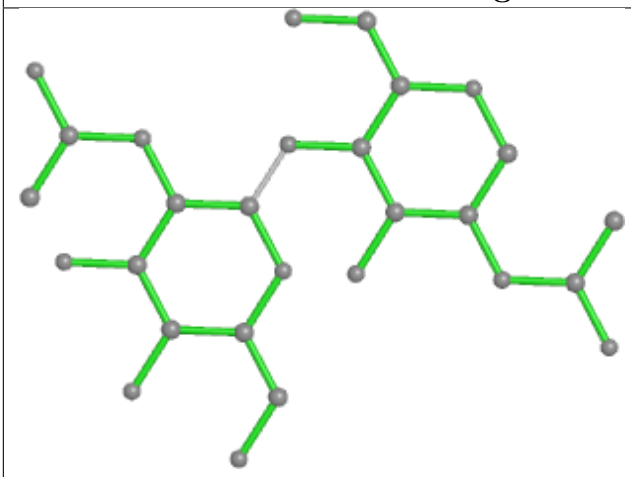


Torsions

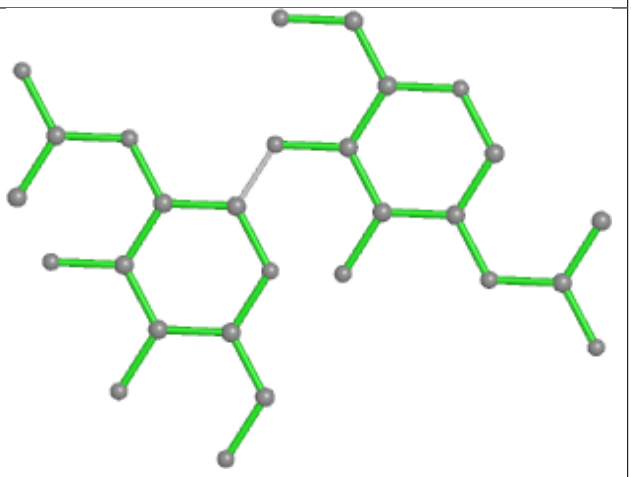


Rings

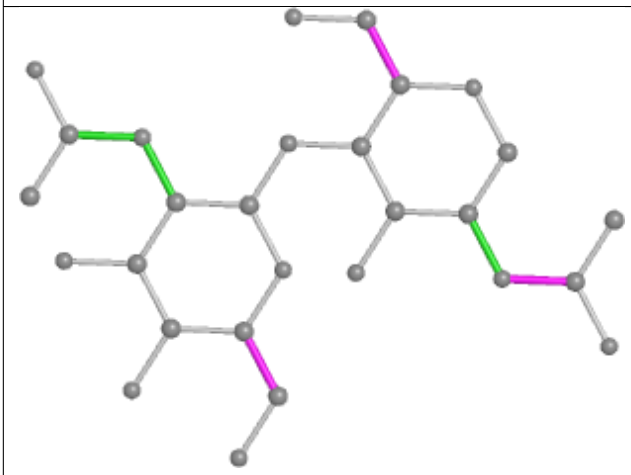
Oligosaccharide Chain N



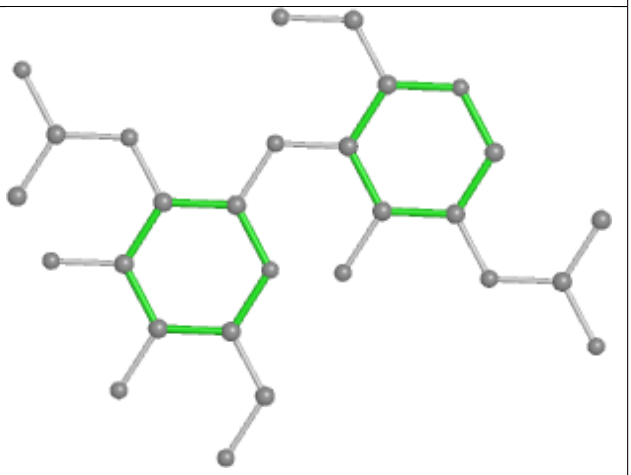
Bond lengths



Bond angles

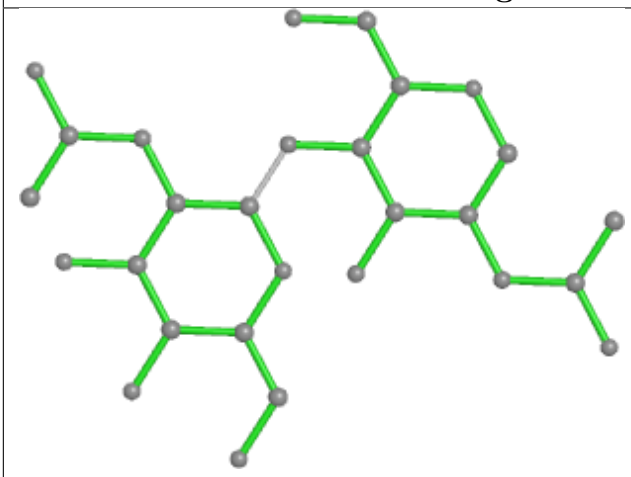


Torsions

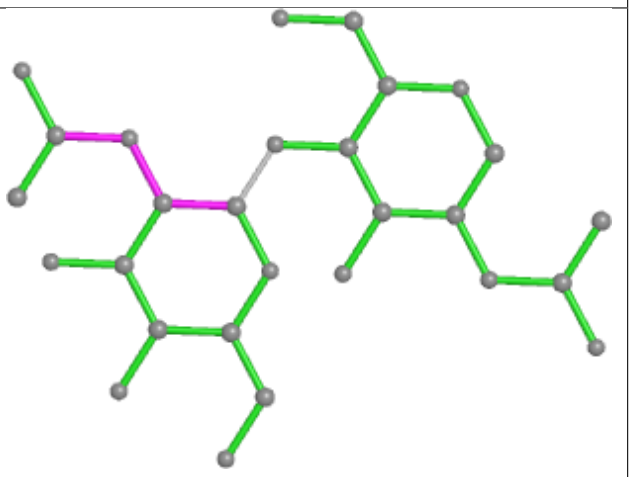


Rings

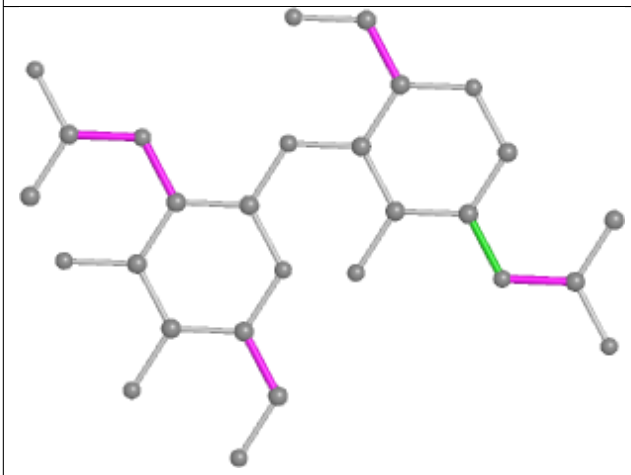
Oligosaccharide Chain P



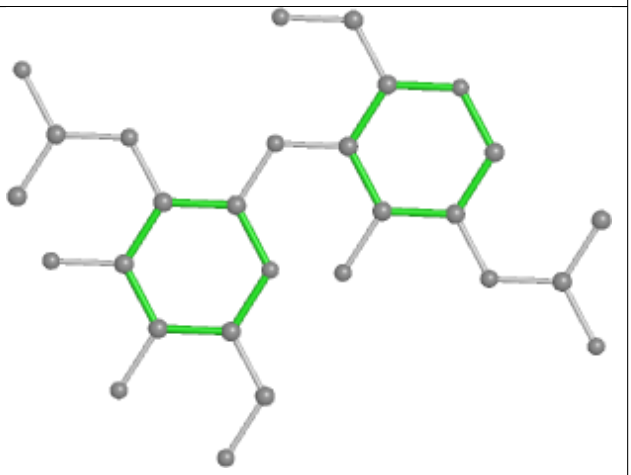
Bond lengths



Bond angles

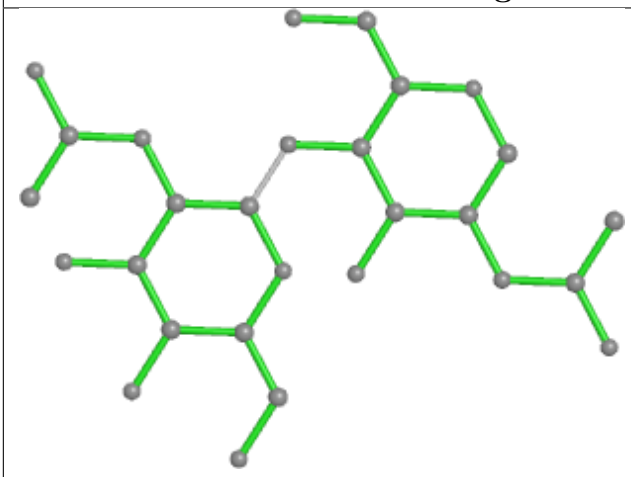


Torsions

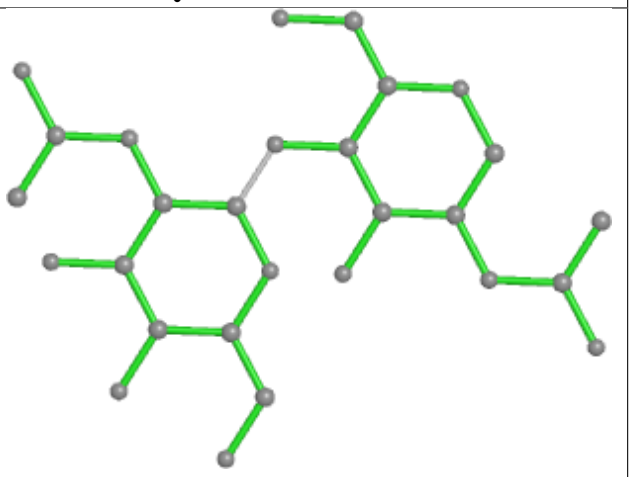


Rings

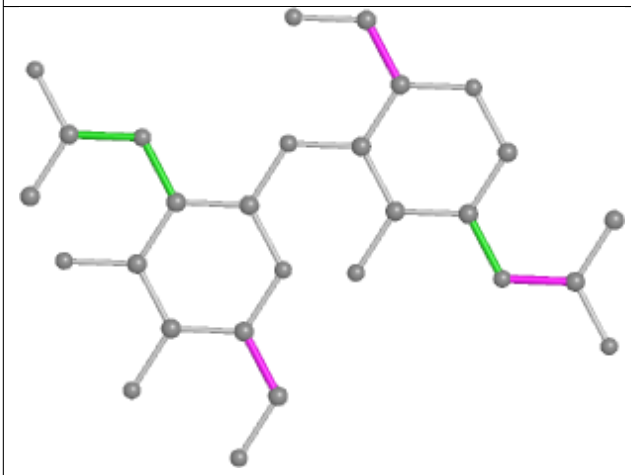
Oligosaccharide Chain Q



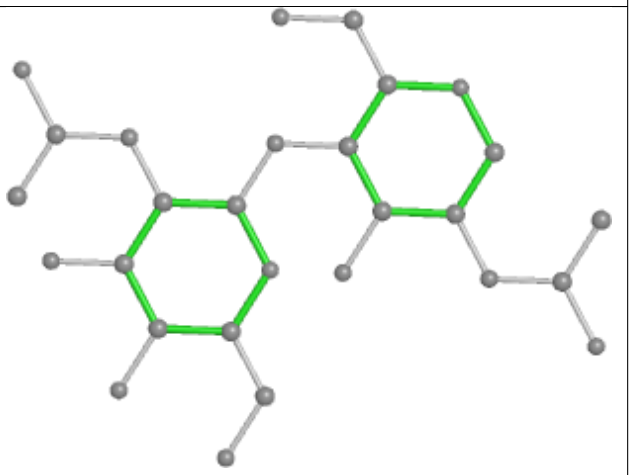
Bond lengths



Bond angles

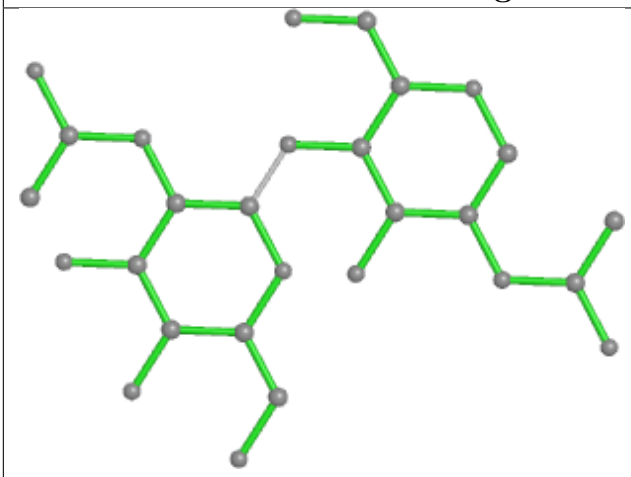


Torsions

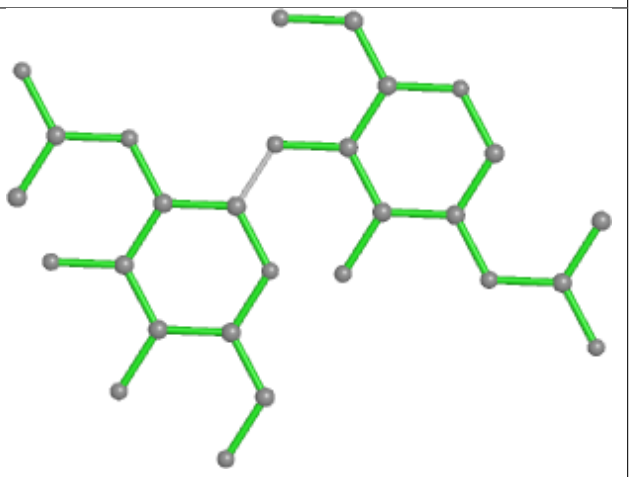


Rings

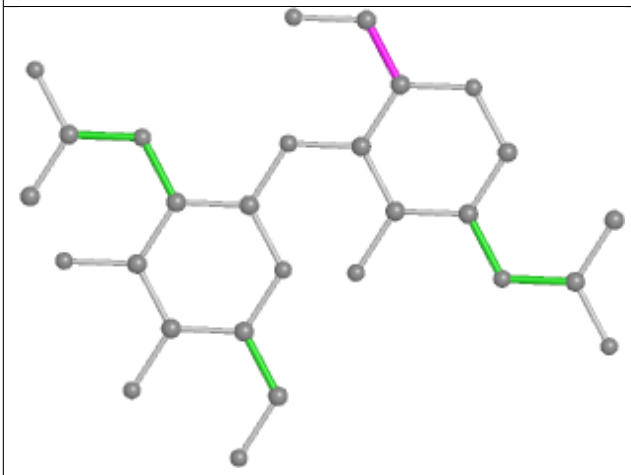
Oligosaccharide Chain R



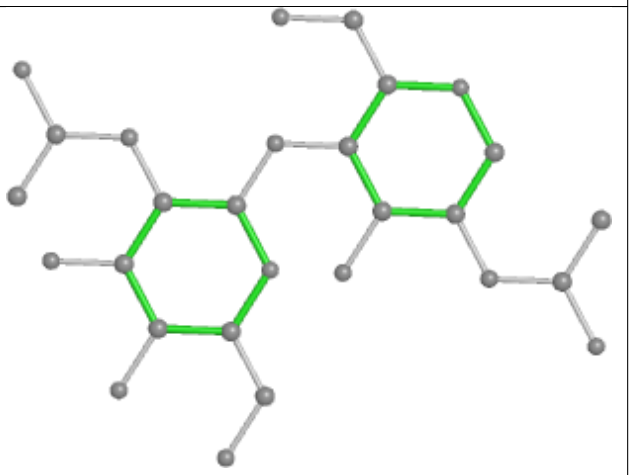
Bond lengths



Bond angles

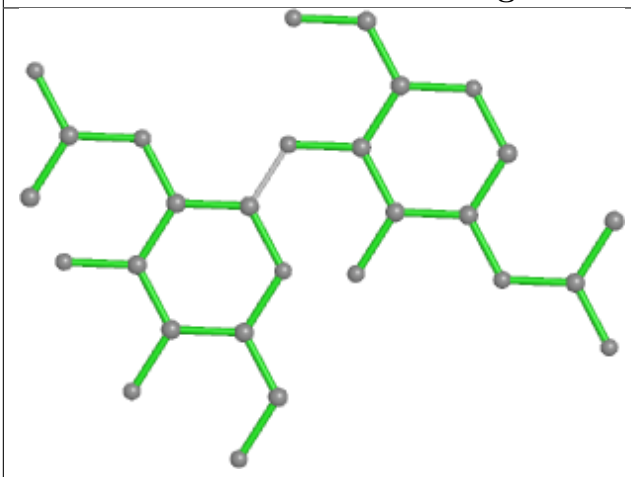


Torsions

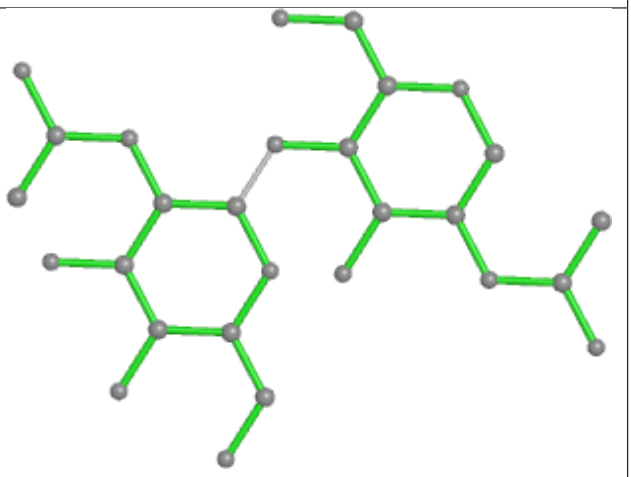


Rings

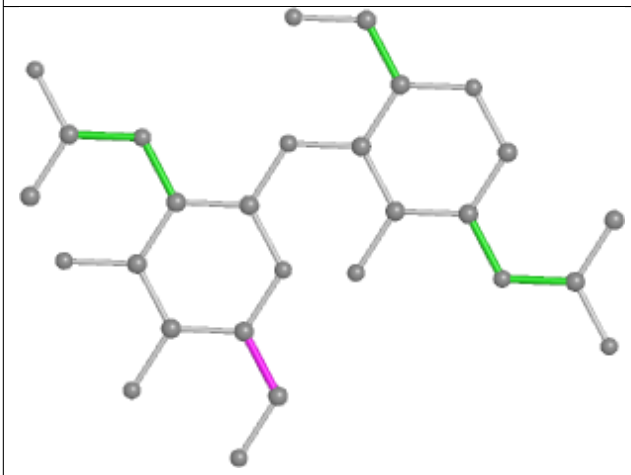
Oligosaccharide Chain S



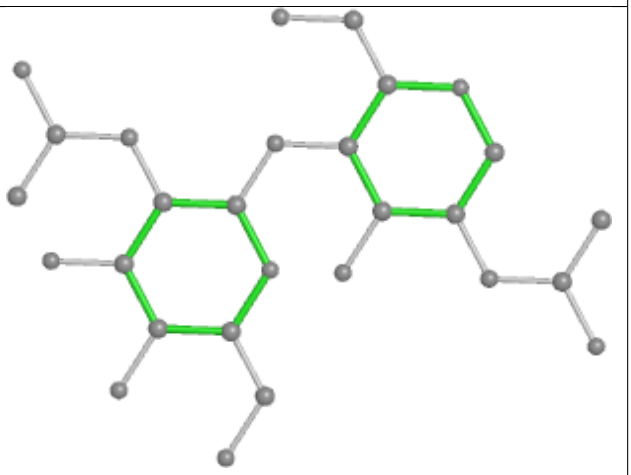
Bond lengths



Bond angles

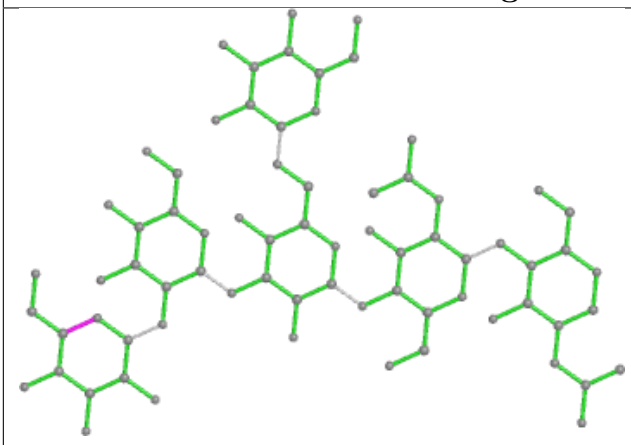


Torsions

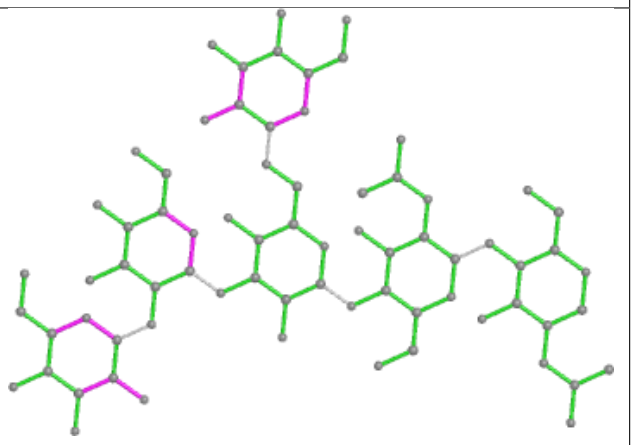


Rings

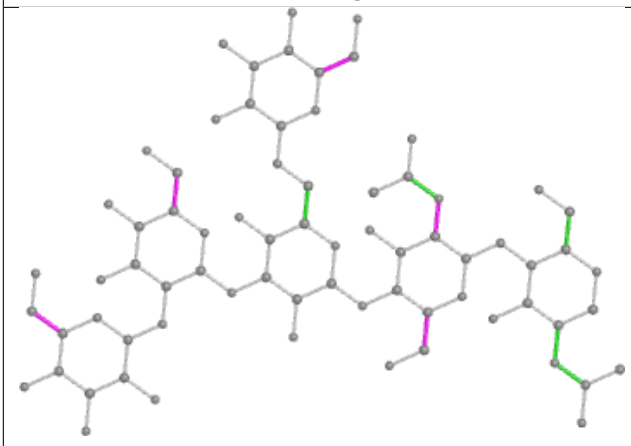
Oligosaccharide Chain I



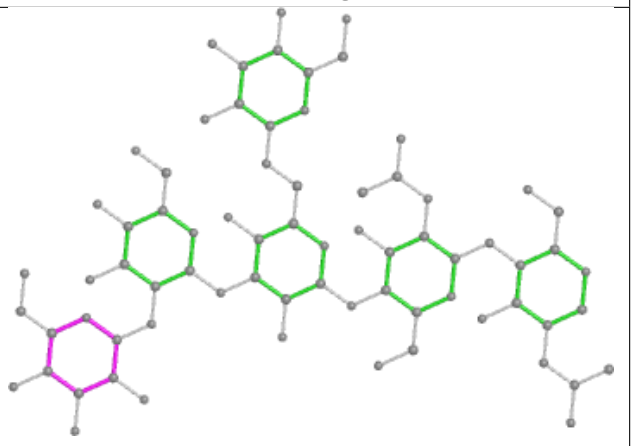
Bond lengths



Bond angles

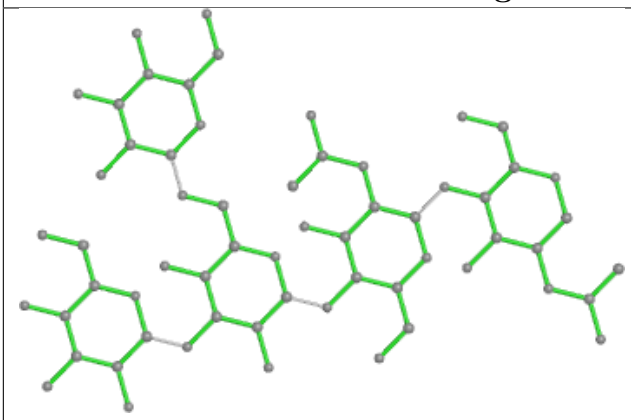


Torsions

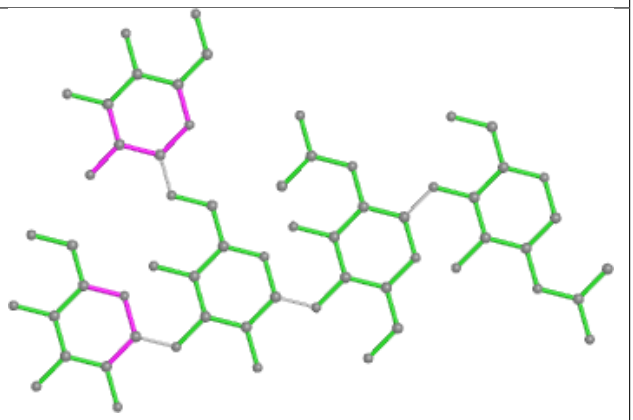


Rings

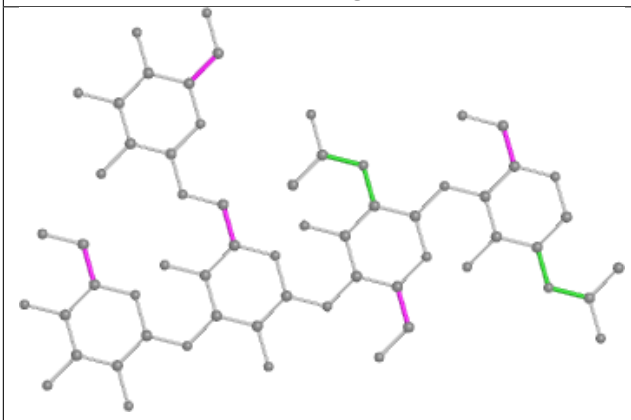
Oligosaccharide Chain O



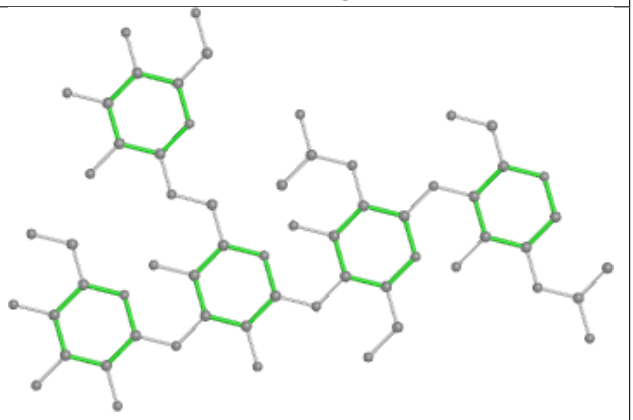
Bond lengths



Bond angles

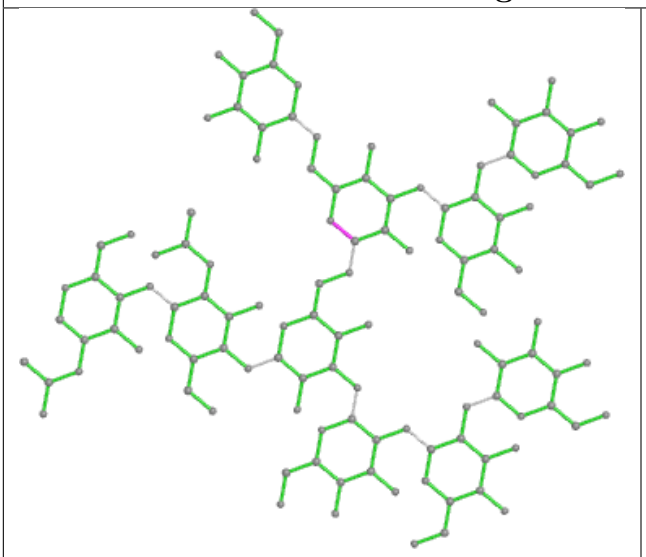


Torsions

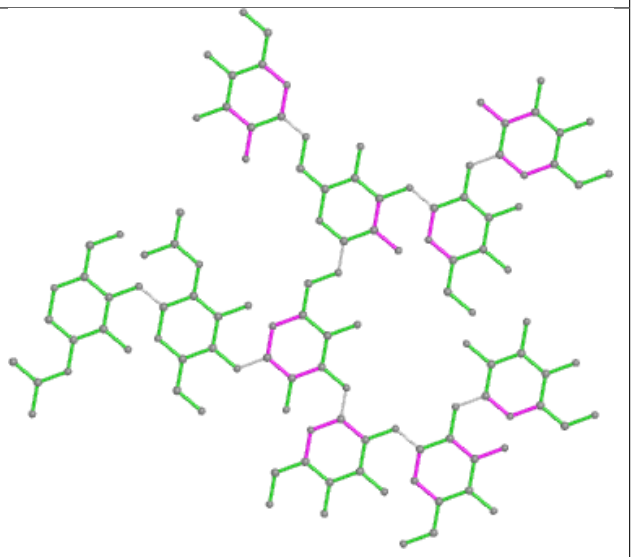


Rings

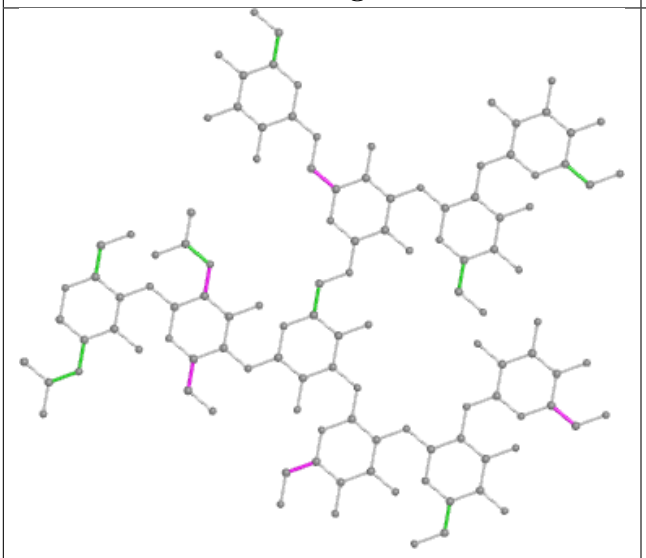
Oligosaccharide Chain T



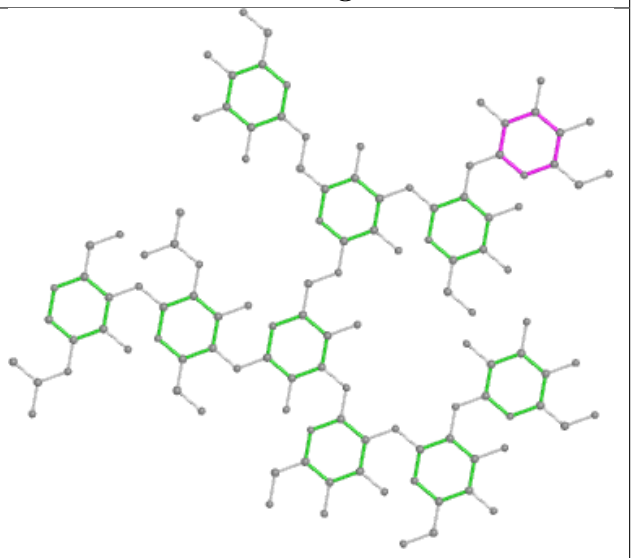
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry (i)

7 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
13	NAG	G	623	1	14,14,15	0.41	0	17,19,21	0.39	0
13	NAG	G	622	1	14,14,15	0.58	0	17,19,21	1.23	1 (5%)
13	NAG	G	633	1	14,14,15	0.44	0	17,19,21	0.65	1 (5%)
13	NAG	B	702	2	14,14,15	0.32	0	17,19,21	0.36	0
13	NAG	B	703	2	14,14,15	0.46	0	17,19,21	0.40	0
13	NAG	B	701	2	14,14,15	0.32	0	17,19,21	0.58	0
13	NAG	G	624	1	14,14,15	0.20	0	17,19,21	0.52	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
13	NAG	G	623	1	-	1/6/23/26	0/1/1/1
13	NAG	G	622	1	-	5/6/23/26	0/1/1/1
13	NAG	G	633	1	-	1/6/23/26	0/1/1/1
13	NAG	B	702	2	-	1/6/23/26	0/1/1/1
13	NAG	B	703	2	-	1/6/23/26	0/1/1/1
13	NAG	B	701	2	-	0/6/23/26	0/1/1/1
13	NAG	G	624	1	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	G	622	NAG	C2-N2-C7	4.27	128.98	122.90
13	G	633	NAG	C1-O5-C5	2.30	115.31	112.19

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	G	624	NAG	O5-C5-C6-O6
13	G	622	NAG	O5-C5-C6-O6
13	G	624	NAG	C4-C5-C6-O6
13	G	622	NAG	C4-C5-C6-O6
13	G	622	NAG	C8-C7-N2-C2
13	G	622	NAG	O7-C7-N2-C2
13	G	624	NAG	C8-C7-N2-C2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	G	624	NAG	O7-C7-N2-C2
13	G	633	NAG	O5-C5-C6-O6
13	B	702	NAG	O5-C5-C6-O6
13	B	703	NAG	O5-C5-C6-O6
13	G	622	NAG	C3-C2-N2-C7
13	G	623	NAG	C4-C5-C6-O6

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	G	622	NAG	1	0
13	G	633	NAG	1	0
13	B	702	NAG	2	0
13	B	703	NAG	1	0

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	G	439/481 (91%)	-0.43	2 (0%) 91 88	23, 80, 145, 229	0
2	B	123/153 (80%)	-0.32	1 (0%) 86 81	32, 69, 128, 181	0
3	L	208/213 (97%)	-0.53	0 100 100	52, 105, 158, 211	0
4	H	228/235 (97%)	-0.51	0 100 100	52, 124, 172, 217	0
5	D	242/243 (99%)	-0.22	5 (2%) 63 58	64, 135, 240, 310	0
6	E	213/216 (98%)	-0.32	5 (2%) 60 54	73, 152, 227, 271	0
All	All	1453/1541 (94%)	-0.40	13 (0%) 84 79	23, 106, 210, 310	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	547	GLY	6.8
5	D	213	PRO	5.5
5	D	222	VAL	4.8
6	E	209	THR	3.3
6	E	157	ALA	2.7
5	D	209	LYS	2.5
1	G	66	HIS	2.5
6	E	118	PHE	2.5
6	E	185	TRP	2.4
1	G	73	ALA	2.3
6	E	133	VAL	2.2
5	D	138	LEU	2.2
5	D	218	LYS	2.1

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

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

6.3 Carbohydrates (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
9	NAG	F	2	14/15	0.80	0.26	133,141,148,148	0
9	NAG	Q	1	14/15	0.80	0.19	130,153,164,168	0
8	NAG	C	1	14/15	0.81	0.24	77,115,139,154	0
9	NAG	M	2	14/15	0.82	0.36	182,188,193,194	0
9	NAG	R	2	14/15	0.83	0.28	111,132,138,138	0
9	NAG	Q	2	14/15	0.84	0.21	164,173,193,196	0
9	NAG	M	1	14/15	0.85	0.35	135,151,173,185	0
9	NAG	S	2	14/15	0.86	0.18	102,127,140,147	0
8	NAG	C	2	14/15	0.87	0.18	134,150,157,160	0
12	MAN	T	9	11/12	0.87	0.26	149,160,162,163	0
12	MAN	T	10	11/12	0.88	0.21	97,118,129,131	0
12	MAN	T	8	11/12	0.89	0.17	136,148,156,159	0
8	BMA	C	3	11/12	0.89	0.15	134,145,159,163	0
9	NAG	P	2	14/15	0.89	0.33	131,143,147,149	0
9	NAG	N	2	14/15	0.90	0.22	141,151,158,159	0
9	NAG	F	1	14/15	0.90	0.20	78,91,119,126	0
7	MAN	A	9	11/12	0.90	0.20	114,128,136,141	0
9	NAG	N	1	14/15	0.91	0.11	95,113,133,145	0
7	MAN	A	8	11/12	0.92	0.11	64,87,104,106	0
12	MAN	T	7	11/12	0.92	0.11	109,119,130,135	0
9	NAG	J	2	14/15	0.92	0.19	79,104,121,125	0
7	MAN	A	6	11/12	0.92	0.13	131,141,151,153	0
9	NAG	P	1	14/15	0.92	0.16	77,94,120,139	0
7	MAN	A	7	11/12	0.93	0.12	87,94,101,101	0
9	NAG	K	2	14/15	0.93	0.12	73,86,91,91	0
10	MAN	I	6	11/12	0.93	0.09	127,133,142,147	0
11	MAN	O	5	11/12	0.93	0.11	119,125,131,137	0
10	MAN	I	5	11/12	0.94	0.21	120,129,138,142	0
9	NAG	R	1	14/15	0.94	0.16	66,84,105,119	0
11	NAG	O	2	14/15	0.94	0.16	100,112,116,116	0
11	MAN	O	4	11/12	0.94	0.09	129,134,138,139	0
7	MAN	A	10	11/12	0.94	0.11	78,96,105,105	0
9	NAG	S	1	14/15	0.94	0.18	69,90,104,106	0
7	NAG	A	2	14/15	0.94	0.15	51,87,102,114	0
10	BMA	I	3	11/12	0.94	0.17	85,101,124,129	0
10	MAN	I	4	11/12	0.94	0.16	137,146,157,161	0
12	MAN	T	5	11/12	0.95	0.13	52,70,81,84	0

Continued on next page...

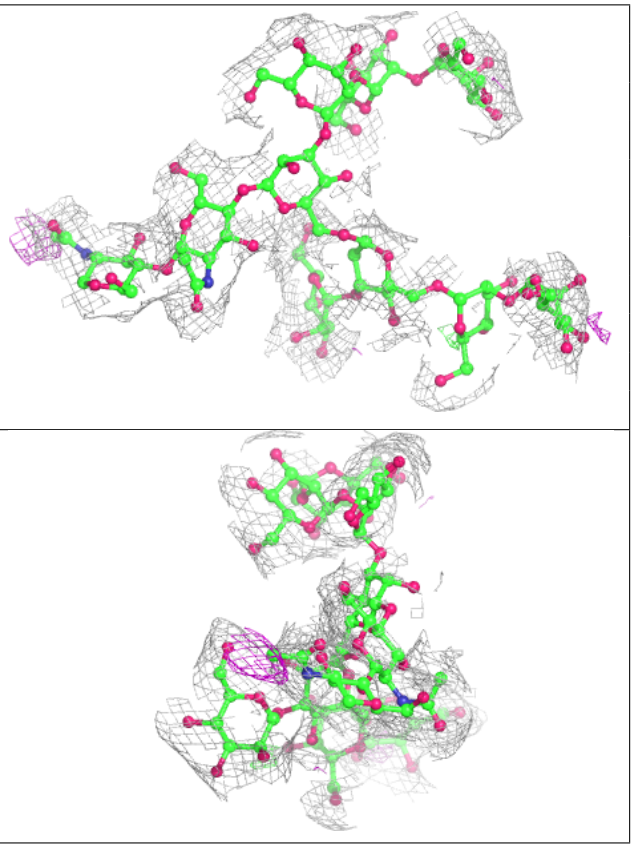
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
12	MAN	T	6	11/12	0.95	0.12	71,84,97,106	0
11	BMA	O	3	11/12	0.95	0.10	112,115,119,124	0
7	MAN	A	5	11/12	0.95	0.14	112,121,130,131	0
7	NAG	A	1	14/15	0.95	0.17	40,52,82,84	0
12	BMA	T	3	11/12	0.95	0.16	72,82,94,100	0
11	NAG	O	1	14/15	0.96	0.16	47,65,79,90	0
10	NAG	I	1	14/15	0.96	0.21	35,46,74,81	0
10	NAG	I	2	14/15	0.96	0.18	64,81,99,108	0
7	BMA	A	3	11/12	0.96	0.13	88,98,104,109	0
7	MAN	A	4	11/12	0.97	0.15	57,63,83,99	0
9	NAG	K	1	14/15	0.97	0.16	54,82,104,107	0
12	NAG	T	1	14/15	0.97	0.13	51,64,85,88	0
12	NAG	T	2	14/15	0.97	0.15	63,81,85,87	0
9	NAG	J	1	14/15	0.97	0.13	66,87,98,105	0
12	MAN	T	4	11/12	0.97	0.14	58,74,87,89	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.

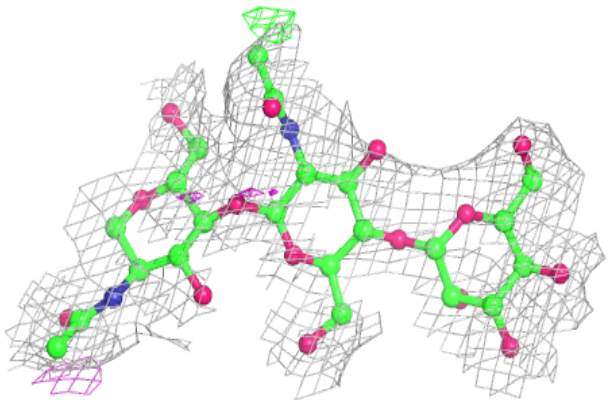
Electron density around Chain A:

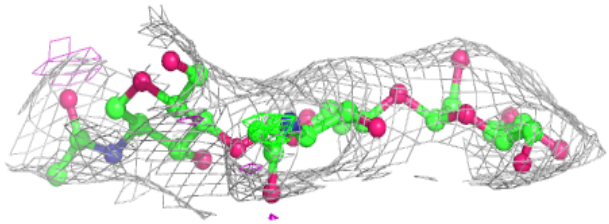
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

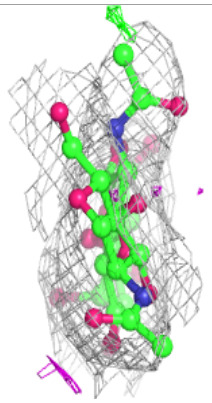


Electron density around Chain C:

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

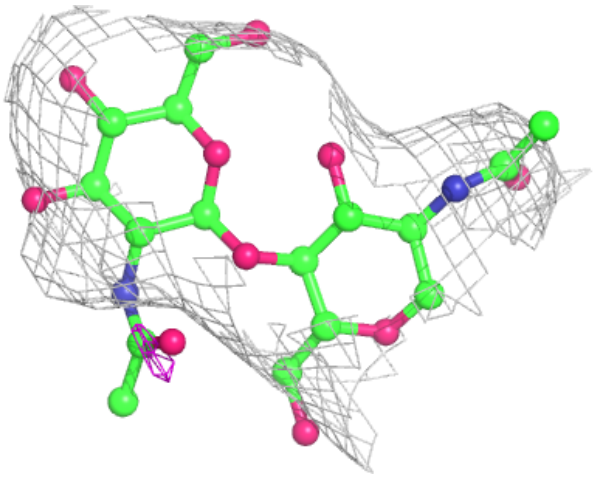


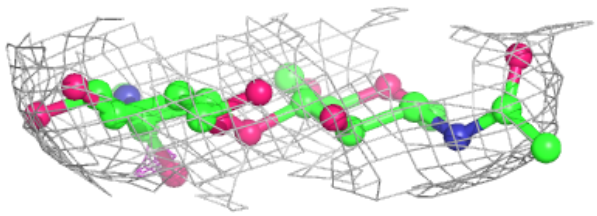


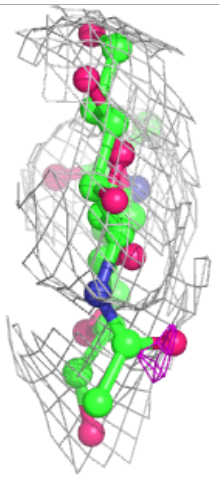


Electron density around Chain F:

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

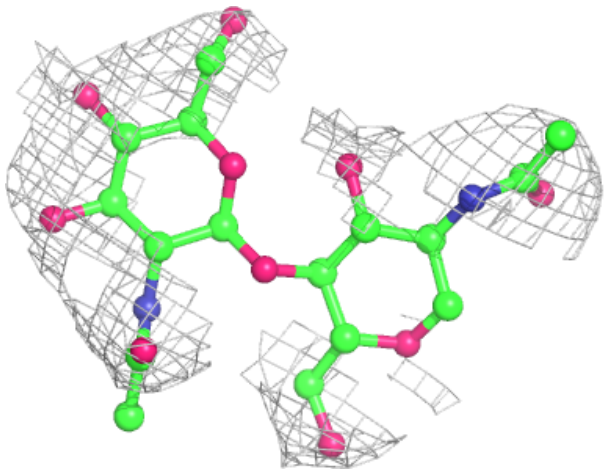


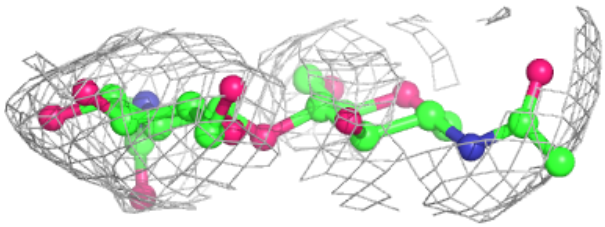


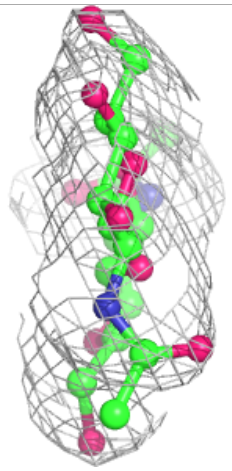


Electron density around Chain J:

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

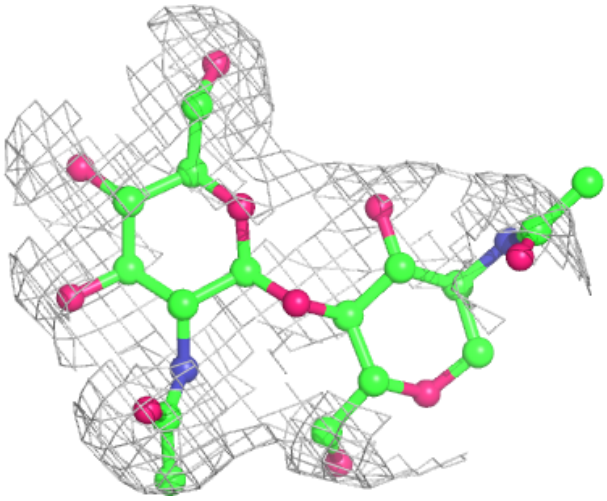


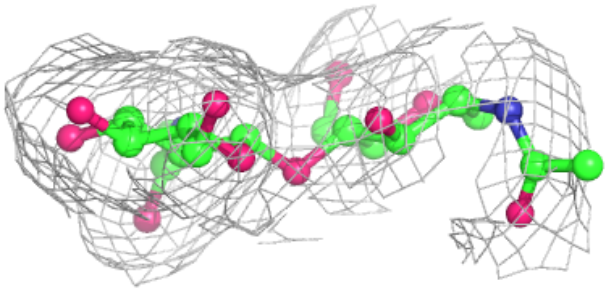


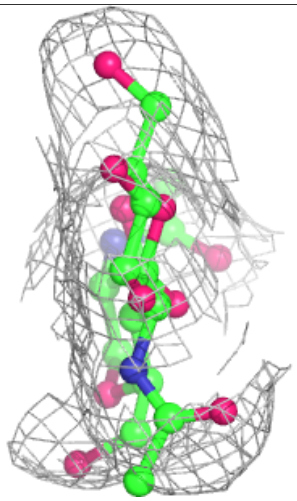


Electron density around Chain K:

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

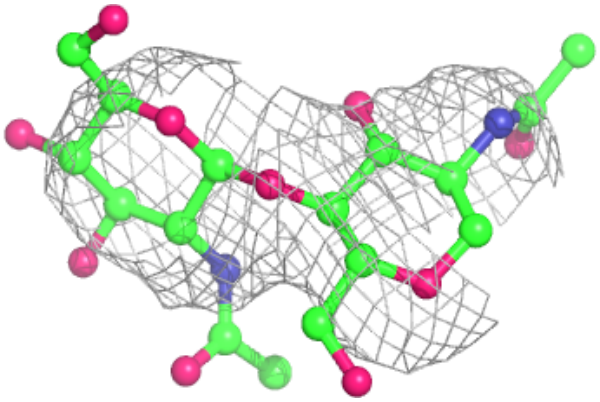


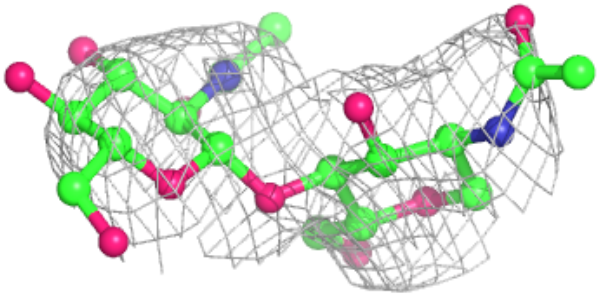


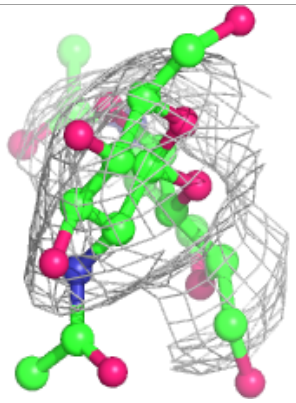


Electron density around Chain M:

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

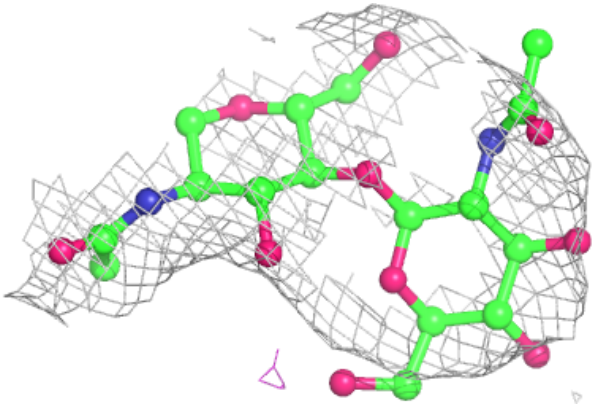


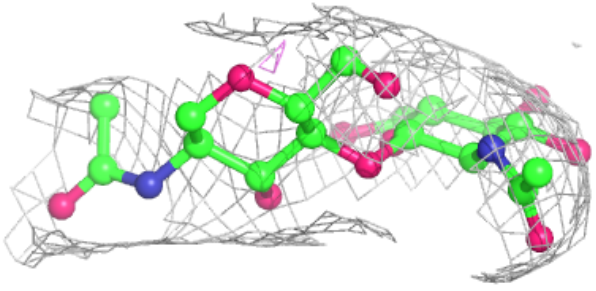


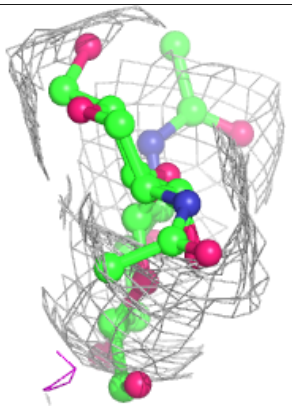


Electron density around Chain N:

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

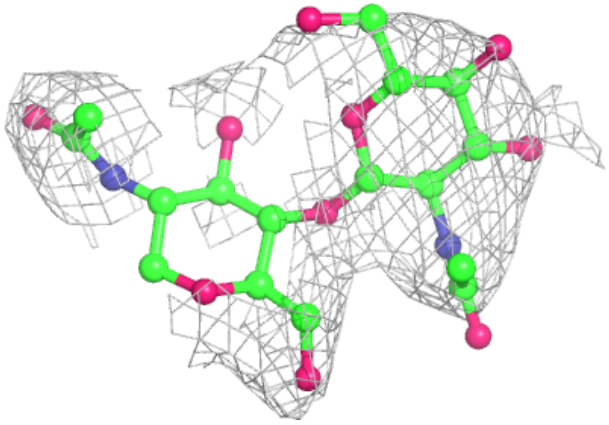


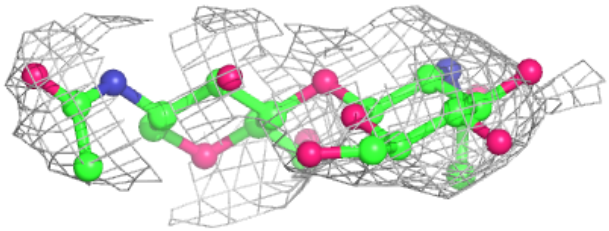


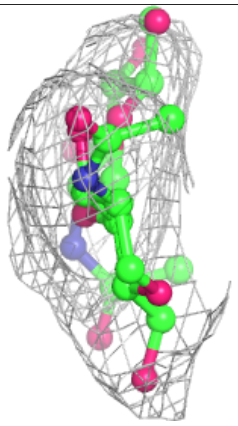


Electron density around Chain P:

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

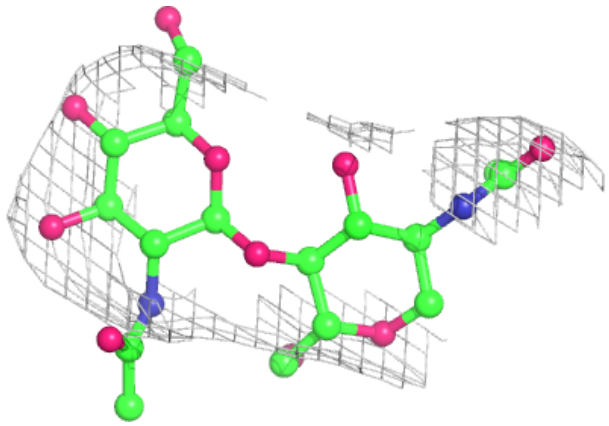


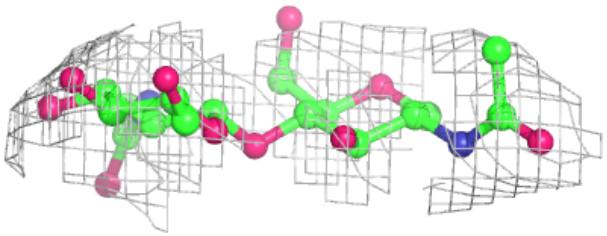


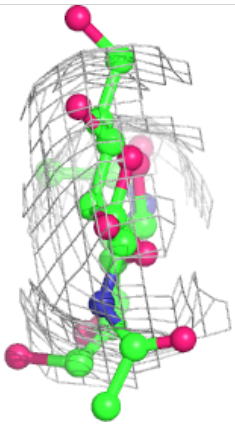


Electron density around Chain Q:

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

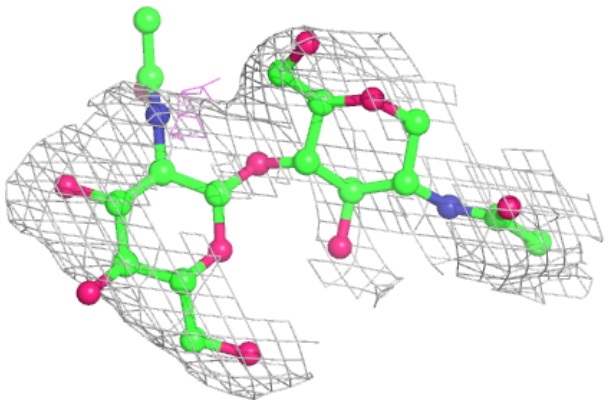


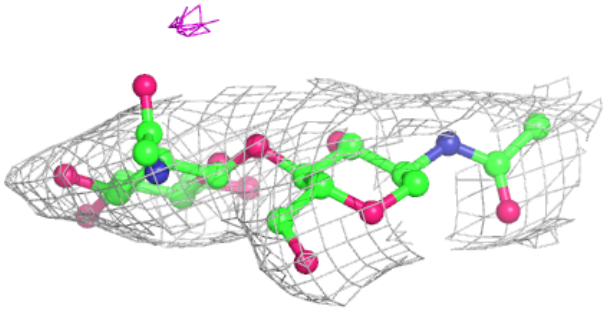


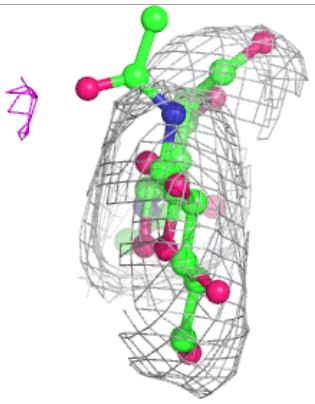


Electron density around Chain R:

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

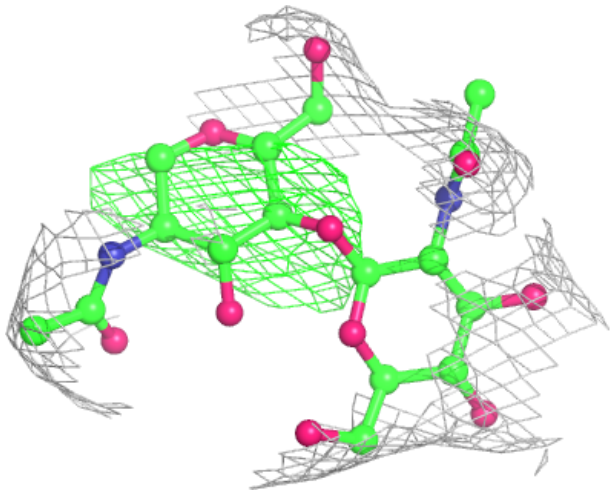


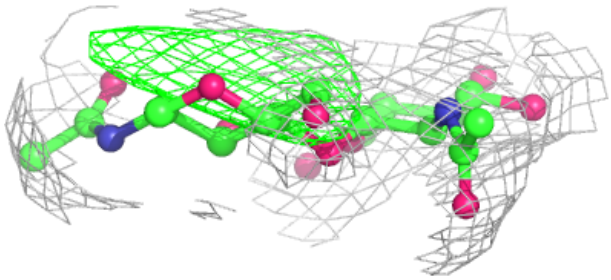


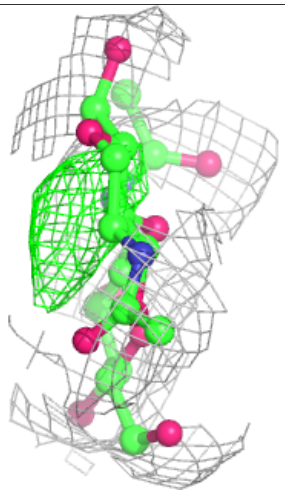


Electron density around Chain S:

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

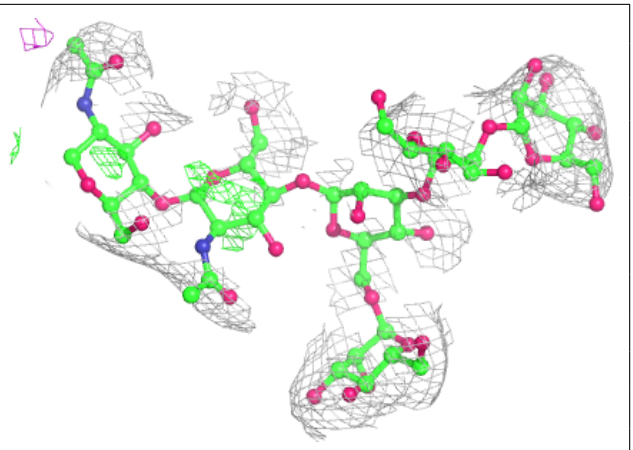


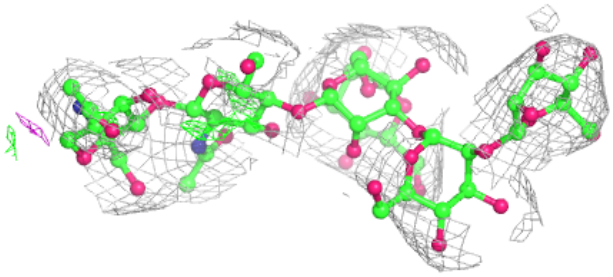


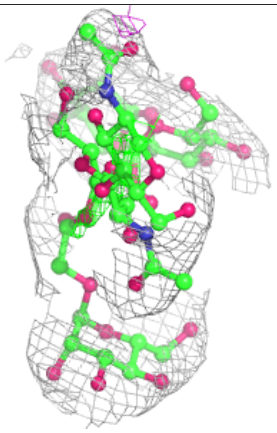


Electron density around Chain I:

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

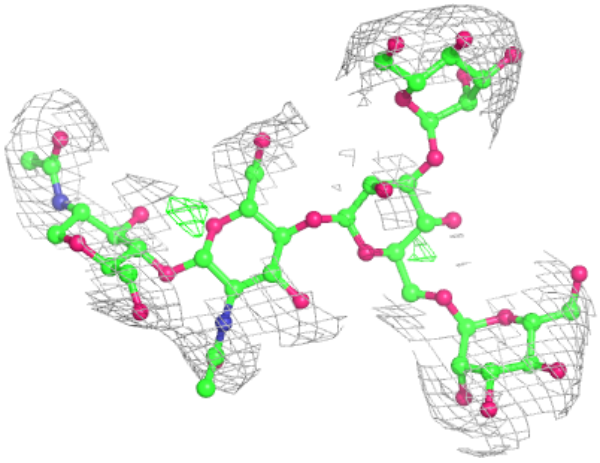


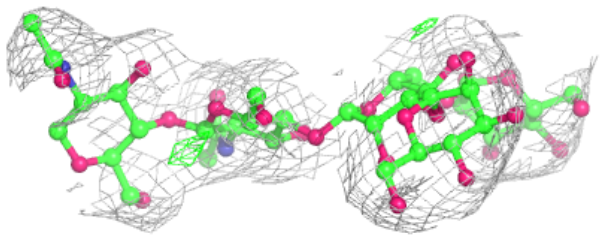


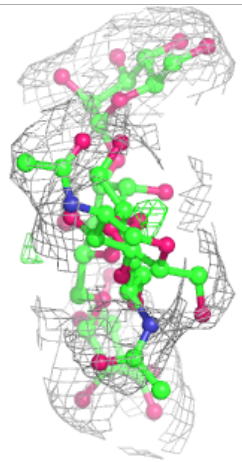


Electron density around Chain O:

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

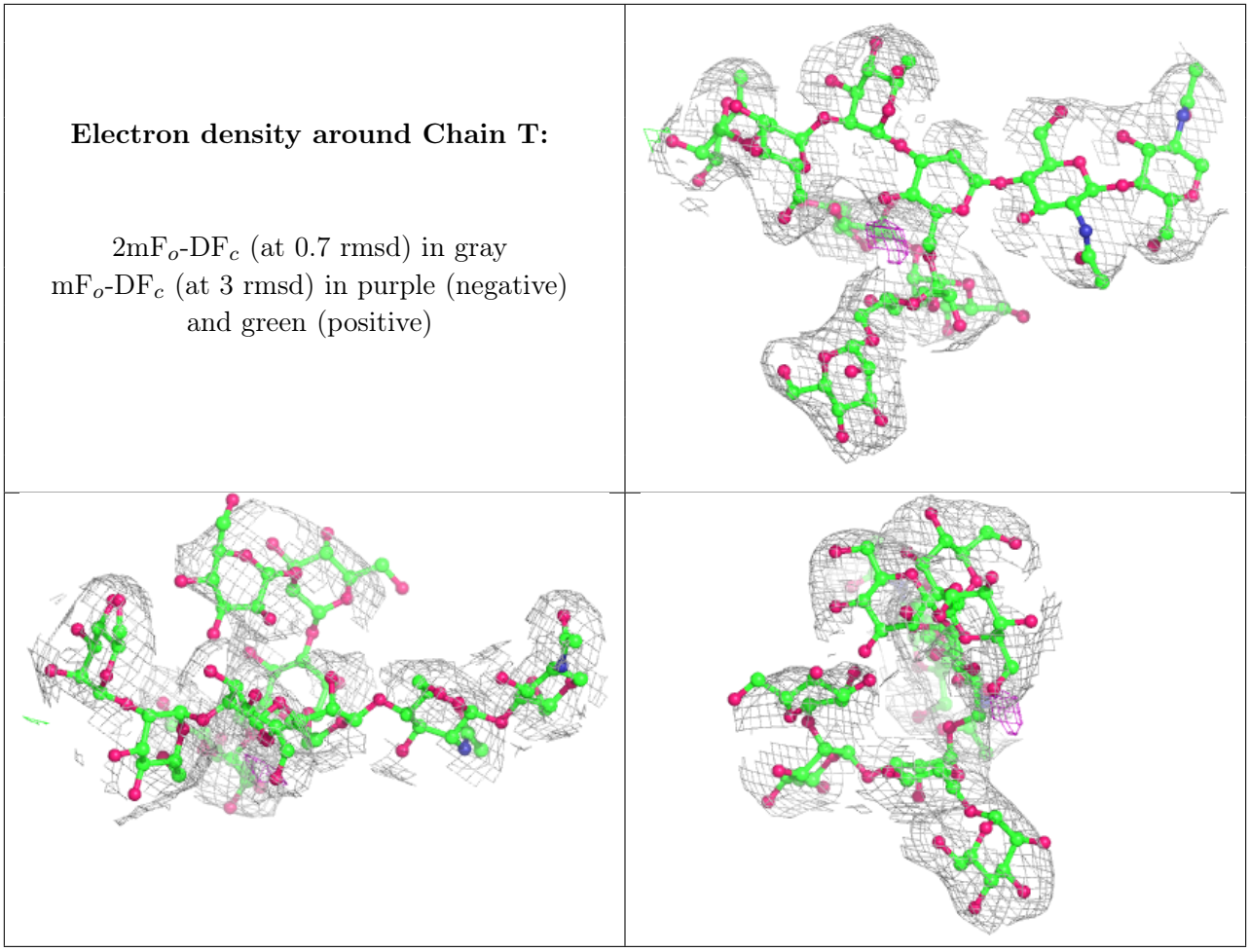






Electron density around Chain T:

$2mF_o$-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
13	NAG	G	624	14/15	0.71	0.40	147,163,168,171	0
13	NAG	G	633	14/15	0.82	0.25	120,140,153,155	0
13	NAG	B	701	14/15	0.83	0.22	127,140,159,161	0
13	NAG	B	702	14/15	0.86	0.28	120,125,132,132	0
13	NAG	G	623	14/15	0.88	0.24	79,108,130,137	0
13	NAG	G	622	14/15	0.91	0.17	94,99,101,102	0
13	NAG	B	703	14/15	0.93	0.15	94,102,111,114	0

6.5 Other polymers (i)

There are no such residues in this entry.