Full wwPDB X-ray Structure Validation Report ⓘ

Sep 20, 2023 – 07:57 AM EDT

PDB ID	:	5JSA
Title	:	Uncleaved prefusion optimized gp140 trimer with an engineered 10-residue HR1 turn bound to broadly neutralizing antibodies 8ANC195 and PGT128
Authors	:	Kong, L.; Wilson, I.A.
Deposited on	:	2016-05-07
Resolution	:	6.31 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:

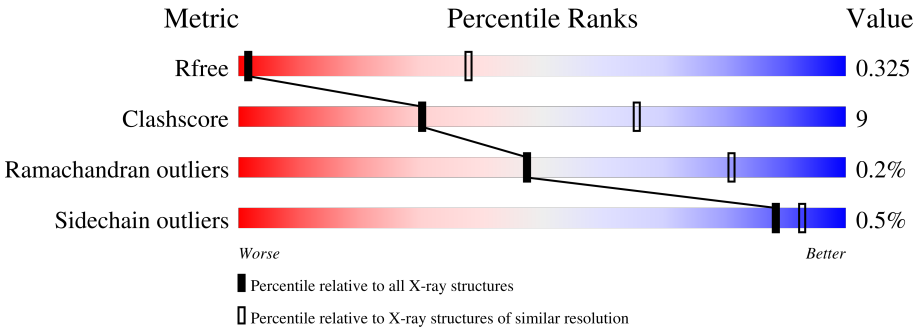
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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 6.31 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	1009 (8.70-3.88)
Clashscore	141614	1058 (8.70-3.90)
Ramachandran outliers	138981	1006 (8.70-3.88)
Sidechain outliers	138945	1005 (8.70-3.84)

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%

Mol	Chain	Length	Quality of chain
1	A	239	74% 23% .
2	B	211	74% 22% .
3	C	480	71% 22% 7%
4	D	142	65% 25% . 7%
5	E	238	75% 19% 6%
6	F	215	82% 17% .
7	G	2	50% 50%

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Mol	Chain	Length	Quality of chain
7	H	2	100%
7	I	2	50% 50%
8	J	8	25% 75%
9	K	10	30% 40% 30%
10	L	9	33% 67%
11	M	7	71% 29%
12	N	5	60% 40%
13	O	3	100%
13	P	3	100%
13	Q	3	33% 67%
13	R	3	100%
13	S	3	100%
14	T	4	25% 50% 25%
15	U	11	27% 73%

2 Entry composition (i)

There are 16 unique types of molecules in this entry. The entry contains 12075 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 broadly neutralizing antibody PGT128 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	230	Total	C	N	O	S	0	0	0
			1735	1105	292	332	6			

- Molecule 2 is a protein called broadly neutralizing antibody PGT128 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	204	Total	C	N	O	S	0	0	0
			1514	950	254	306	4			

- Molecule 3 is a protein called gp120.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	447	Total	C	N	O	S	0	0	0
			3519	2210	622	659	28			

- Molecule 4 is a protein called gp41.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	132	Total	C	N	O	S	0	0	0
			1052	663	178	205	6			

- Molecule 5 is a protein called broadly neutralizing antibody 8ANC195 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	224	Total	C	N	O	S	0	0	0
			1686	1072	284	325	5			

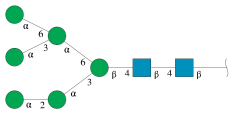
- Molecule 6 is a protein called broadly neutralizing antibody 8ANC195 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	212	Total	C	N	O	S	0	0	0
			1626	1018	279	324	5			

- Molecule 7 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

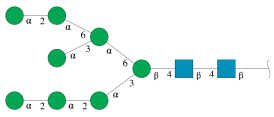
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	G	2	Total	C	N	O	0	0	0
			28	16	2	10			
7	H	2	Total	C	N	O	0	0	0
			28	16	2	10			
7	I	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 8 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[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
8	J	8	Total	C	N	O	0	0	0
			94	52	2	40			

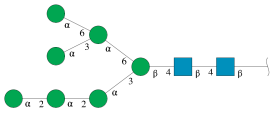
- Molecule 9 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	K	10	Total	C	N	O	0	0	0
			116	64	2	50			

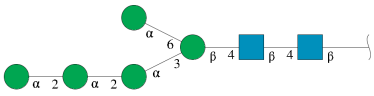
- Molecule 10 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-[alpha-D-mannopy

ranose-(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.



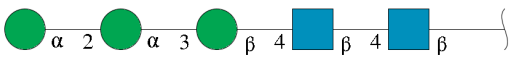
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	L	9	Total	C	N	O	0	0	0
			105	58	2	45			

- Molecule 11 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-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.



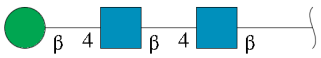
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
11	M	7	Total	C	N	O	0	0	0
			83	46	2	35			

- Molecule 12 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



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

- Molecule 13 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.

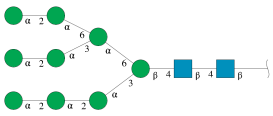


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
13	O	3	Total C N O 39 22 2 15	0	0	0
13	P	3	Total C N O 39 22 2 15	0	0	0
13	Q	3	Total C N O 39 22 2 15	0	0	0
13	R	3	Total C N O 39 22 2 15	0	0	0
13	S	3	Total C N O 39 22 2 15	0	0	0

- Molecule 14 is an oligosaccharide called 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.

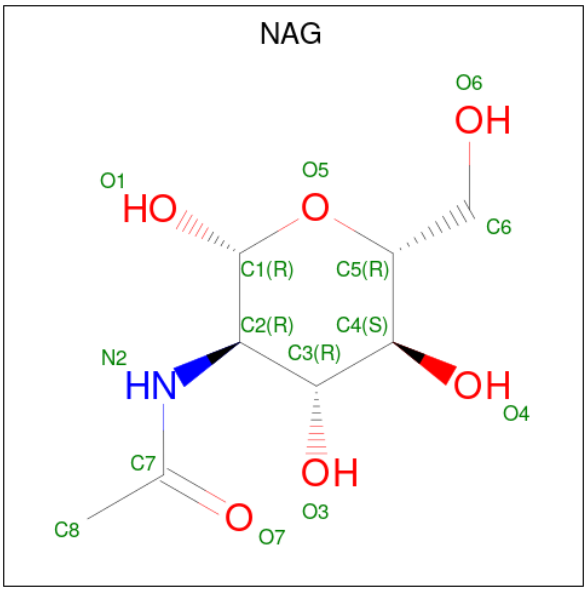
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
14	T	4	Total C N O 50 28 2 20	0	0	0

- Molecule 15 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-(1-2)-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
15	U	11	Total C N O 127 70 2 55	0	0	0

- Molecule 16 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



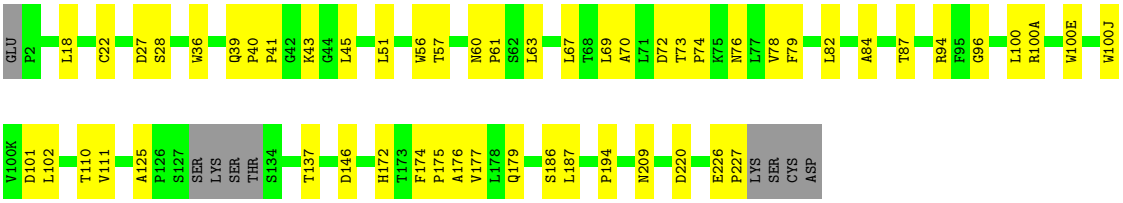
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	C	1	Total C N O 14 8 1 5	0	0
16	D	1	Total C N O 14 8 1 5	0	0

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. 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. 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.

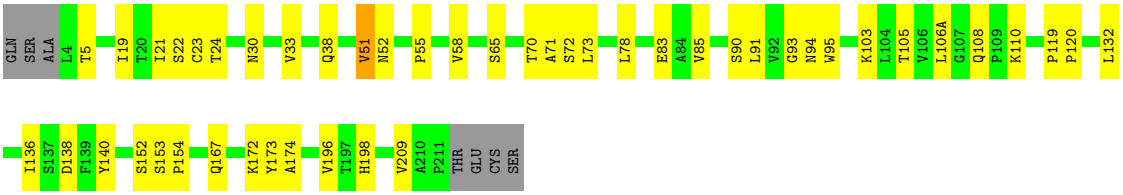
- Molecule 1: broadly neutralizing antibody PGT128 heavy chain

Chain A:



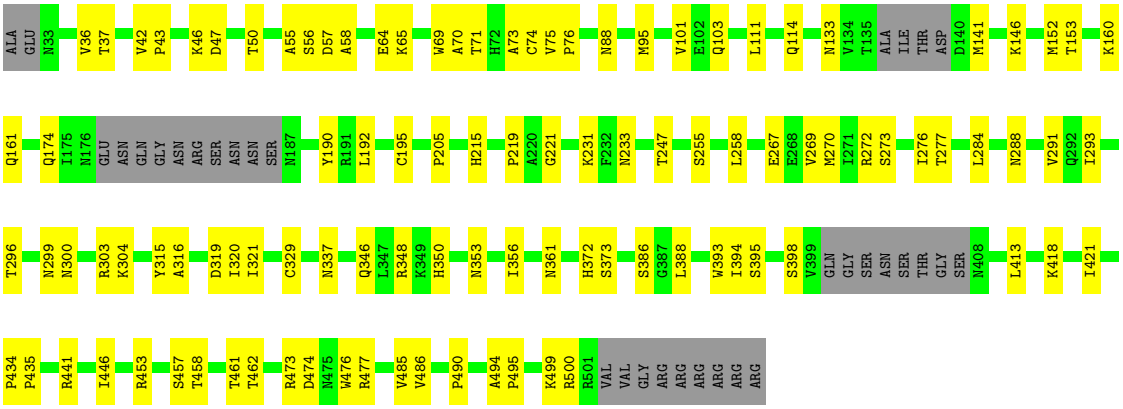
- Molecule 2: broadly neutralizing antibody PGT128 light chain

Chain B:



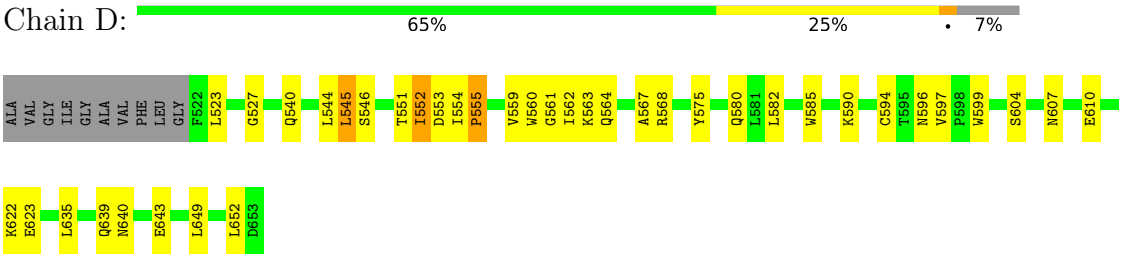
- Molecule 3: gp120

Chain C:



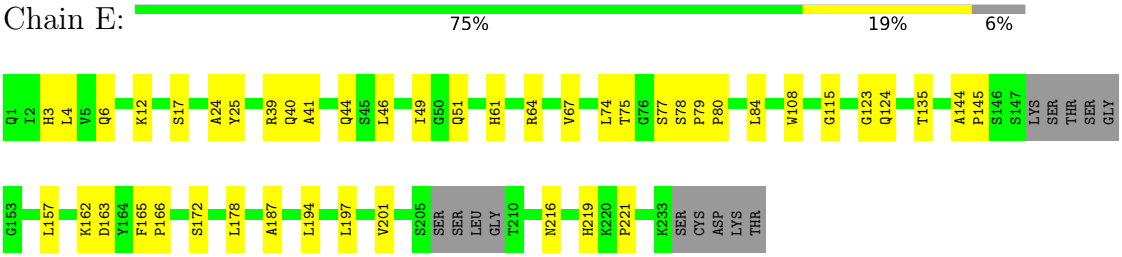
- Molecule 4: gp41

Chain D:



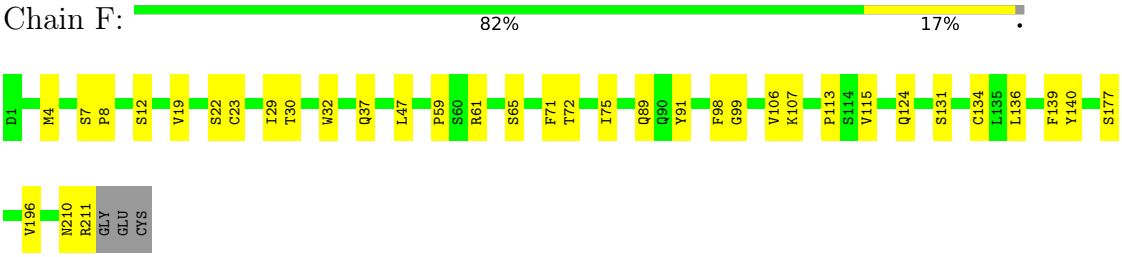
• Molecule 5: broadly neutralizing antibody 8ANC195 heavy chain

Chain E:



• Molecule 6: broadly neutralizing antibody 8ANC195 light chain

Chain F:

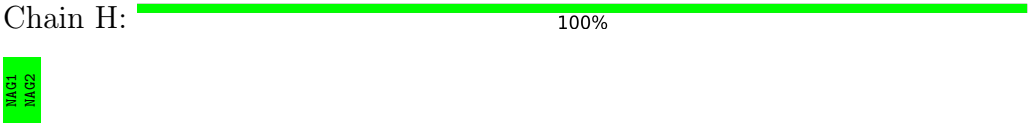


• Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:

• Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:



• Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

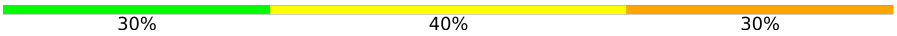
Chain I:

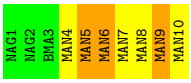
• Molecule 8: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:

• Molecule 9: 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

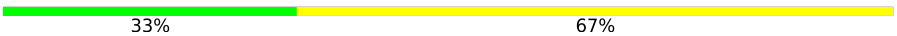
Chain K:





• Molecule 10: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[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 L:

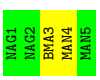


• Molecule 11: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:

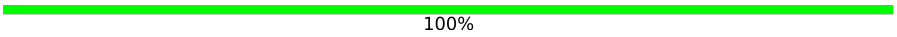
• Molecule 12: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N:



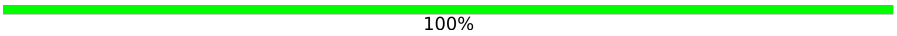
• Molecule 13: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O:



• Molecule 13: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain P:

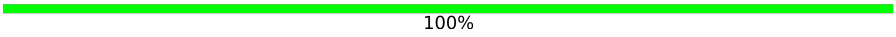


• Molecule 13: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Q:

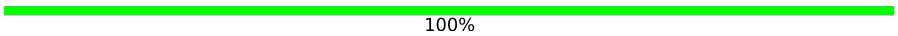
• Molecule 13: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain R:



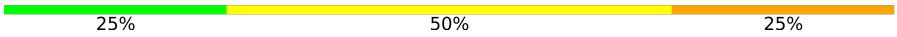
• Molecule 13: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain S:



• Molecule 14: 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:



• Molecule 15: 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-(1-2)-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-glucopyranos
e

Chain U:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 2 3	Depositor
Cell constants a, b, c, α, β, γ	266.28Å 266.28Å 266.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.14 – 6.31 47.07 – 6.31	Depositor EDS
% Data completeness (in resolution range)	99.9 (40.14-6.31) 99.9 (47.07-6.31)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	2.35 (at 6.15Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.281 , 0.322 0.285 , 0.325	Depositor DCC
R_{free} test set	685 reflections (9.92%)	wwPDB-VP
Wilson B-factor (Å^2)	357.6	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 304.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.049 for -l,-k,-h	Xtriage
F_o,F_c correlation	0.80	EDS
Total number of atoms	12075	wwPDB-VP
Average B, all atoms (Å^2)	350.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.31% 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, MAN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.20	0/1786	0.40	0/2449
2	B	0.21	0/1552	0.44	1/2121 (0.0%)
3	C	0.22	0/3592	0.42	0/4875
4	D	0.27	0/1072	0.58	1/1458 (0.1%)
5	E	0.21	0/1730	0.39	0/2361
6	F	0.22	0/1661	0.40	0/2256
All	All	0.22	0/11393	0.43	2/15520 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	545	LEU	CA-CB-CG	8.87	135.71	115.30
2	B	108	GLN	C-N-CD	-6.56	106.17	120.60

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	1735	0	1690	37	0
2	B	1514	0	1473	35	0
3	C	3519	0	3461	73	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	1052	0	1017	37	1
5	E	1686	0	1658	30	0
6	F	1626	0	1581	27	0
7	G	28	0	25	4	0
7	H	28	0	25	0	0
7	I	28	0	25	0	0
8	J	94	0	79	1	0
9	K	116	0	97	5	0
10	L	105	0	88	0	0
11	M	83	0	70	4	0
12	N	61	0	52	0	0
13	O	39	0	34	0	0
13	P	39	0	34	0	0
13	Q	39	0	34	1	0
13	R	39	0	34	0	0
13	S	39	0	34	0	0
14	T	50	0	43	2	0
15	U	127	0	104	0	0
16	C	14	0	13	0	0
16	D	14	0	13	0	0
All	All	12075	0	11684	220	1

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 9.

All (220) 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:95:TRP:HE1	9:K:6:MAN:HO4	1.12	0.93
4:D:553:ASP:OD1	4:D:564:GLN:NE2	2.07	0.85
3:C:499:LYS:HG2	3:C:500:ARG:H	1.50	0.77
2:B:95:TRP:NE1	9:K:6:MAN:O4	2.16	0.75
3:C:394:ILE:HG22	3:C:395:SER:H	1.53	0.72
3:C:55:ALA:HB3	3:C:215:HIS:HB2	1.71	0.71
5:E:178:LEU:HD21	5:E:201:VAL:HG11	1.75	0.69
2:B:106(A):LEU:HB3	2:B:140:TYR:HE1	1.57	0.69
3:C:329:CYS:HB3	3:C:413:LEU:HB2	1.75	0.69
5:E:61:HIS:HA	5:E:64:ARG:HG3	1.77	0.66
3:C:291:VAL:HB	3:C:446:ILE:HB	1.79	0.65
3:C:50:THR:O	3:C:103:GLN:NE2	2.24	0.64
3:C:73:ALA:O	4:D:552:ILE:HG13	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:114:GLN:CD	4:D:559:VAL:HG21	2.18	0.64
3:C:277:THR:O	3:C:453:ARG:NH2	2.30	0.64
4:D:639:GLN:O	4:D:643:GLU:N	2.21	0.64
13:Q:1:NAG:O7	13:Q:1:NAG:O3	2.13	0.62
3:C:350:HIS:O	5:E:75:THR:OG1	2.18	0.62
6:F:12:SER:HB3	6:F:107:LYS:HD3	1.81	0.62
3:C:58:ALA:HB2	3:C:76:PRO:HB3	1.81	0.62
3:C:152:MET:O	3:C:161:GLN:N	2.33	0.61
3:C:174:GLN:HA	3:C:190:TYR:HA	1.83	0.61
11:M:4:MAN:O3	11:M:6:MAN:O6	2.19	0.61
5:E:25:TYR:HD1	8:J:2:NAG:H2	1.66	0.60
1:A:176:ALA:HA	1:A:187:LEU:HB3	1.83	0.60
4:D:552:ILE:HG12	4:D:553:ASP:H	1.67	0.59
3:C:37:THR:HG22	4:D:594:CYS:HA	1.85	0.59
3:C:219:PRO:HG3	4:D:567:ALA:HB1	1.84	0.59
2:B:138:ASP:HA	2:B:172:LYS:HB3	1.84	0.59
3:C:101:VAL:HG21	3:C:477:ARG:HG2	1.85	0.58
4:D:604:SER:H	6:F:30:THR:HG21	1.68	0.58
5:E:39:ARG:HB3	5:E:49:ILE:HD11	1.84	0.58
4:D:561:GLY:O	4:D:564:GLN:HG3	2.04	0.58
3:C:418:LYS:HE3	3:C:421:ILE:HG22	1.84	0.58
5:E:40:GLN:HB2	5:E:46:LEU:HD23	1.85	0.58
4:D:545:LEU:HD12	4:D:575:TYR:HE1	1.69	0.58
4:D:545:LEU:HD12	4:D:575:TYR:CE1	2.38	0.57
4:D:551:THR:O	4:D:552:ILE:HG22	2.04	0.57
4:D:622:LYS:HG3	6:F:32:TRP:HH2	1.70	0.57
5:E:12:LYS:NZ	5:E:17:SER:O	2.27	0.57
3:C:277:THR:OG1	5:E:75:THR:O	2.23	0.57
6:F:113:PRO:HB3	6:F:139:PHE:HB3	1.87	0.56
11:M:1:NAG:H61	11:M:2:NAG:N2	2.20	0.56
7:G:1:NAG:O3	7:G:1:NAG:H83	2.05	0.56
2:B:5:THR:OG1	2:B:24:THR:OG1	2.23	0.56
5:E:4:LEU:HB2	5:E:123:GLY:HA2	1.88	0.56
4:D:585:TRP:O	4:D:640:ASN:ND2	2.39	0.55
1:A:72:ASP:HB2	1:A:79:PHE:HE1	1.70	0.55
3:C:141:MET:SD	3:C:141:MET:N	2.79	0.55
5:E:135:THR:HG22	5:E:166:PRO:HD3	1.88	0.55
6:F:59:PRO:HB2	6:F:61:ARG:HG2	1.88	0.55
2:B:93:GLY:HA3	9:K:9:MAN:O2	2.06	0.55
3:C:47:ASP:HA	3:C:486:VAL:HG12	1.88	0.55
4:D:553:ASP:OD2	4:D:568:ARG:NH1	2.38	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:296:THR:HG22	3:C:441:ARG:HA	1.89	0.54
6:F:22:SER:HA	6:F:72:THR:HA	1.89	0.54
6:F:115:VAL:HG21	6:F:196:VAL:HG21	1.90	0.54
3:C:215:HIS:ND1	3:C:247:THR:O	2.36	0.54
3:C:304:LYS:HB2	3:C:316:ALA:HB3	1.89	0.54
14:T:2:NAG:H83	14:T:2:NAG:H3	1.88	0.54
3:C:152:MET:SD	3:C:153:THR:N	2.81	0.53
3:C:71:THR:HA	3:C:74:CYS:HB2	1.90	0.53
3:C:300:ASN:HB3	3:C:321:ILE:O	2.09	0.53
4:D:582:LEU:HD21	4:D:590:LYS:HA	1.89	0.53
1:A:40:PRO:HB2	1:A:43:LYS:HD2	1.90	0.53
2:B:24:THR:HG22	2:B:70:THR:HG22	1.91	0.53
7:G:1:NAG:H83	7:G:1:NAG:C3	2.37	0.53
5:E:219:HIS:CD2	5:E:221:PRO:HD2	2.43	0.53
3:C:36:VAL:HG22	4:D:597:VAL:HB	1.91	0.52
1:A:28:SER:HA	1:A:76:ASN:HD21	1.74	0.52
5:E:162:LYS:NZ	6:F:131:SER:OG	2.40	0.52
3:C:36:VAL:HG12	4:D:599:TRP:HE3	1.73	0.52
11:M:4:MAN:HO3	11:M:6:MAN:HO6	1.57	0.52
3:C:37:THR:OG1	3:C:494:ALA:O	2.21	0.51
1:A:96:GLY:N	1:A:100(J):TRP:O	2.35	0.51
2:B:106(A):LEU:HD22	2:B:173:TYR:HE1	1.76	0.51
3:C:73:ALA:HB2	4:D:555:PRO:HG2	1.93	0.51
1:A:84:ALA:HA	1:A:111:VAL:HB	1.91	0.51
2:B:120:PRO:HD3	2:B:132:LEU:HG	1.92	0.51
6:F:37:GLN:HB2	6:F:47:LEU:HD11	1.93	0.51
3:C:133:ASN:OD1	3:C:146:LYS:NZ	2.42	0.51
3:C:76:PRO:HD2	4:D:551:THR:HB	1.92	0.50
1:A:18:LEU:HD23	1:A:82:LEU:HD12	1.93	0.50
1:A:22:CYS:HB3	1:A:78:VAL:HB	1.93	0.50
3:C:269:VAL:HG23	3:C:346:GLN:HG3	1.94	0.50
1:A:177:VAL:N	1:A:186:SER:O	2.45	0.50
3:C:500:ARG:HB2	4:D:596:ASN:OD1	2.12	0.50
4:D:560:TRP:CZ3	4:D:564:GLN:HG2	2.47	0.50
5:E:41:ALA:HB3	5:E:44:GLN:HB2	1.93	0.50
3:C:284:LEU:HD21	3:C:474:ASP:HB3	1.93	0.50
4:D:622:LYS:HG3	6:F:32:TRP:CH2	2.46	0.50
3:C:361:ASN:HB3	3:C:386:SER:HA	1.94	0.50
5:E:172:SER:HB3	5:E:216:ASN:HB2	1.94	0.49
2:B:23:CYS:N	2:B:71:ALA:O	2.44	0.49
4:D:607:ASN:HB3	4:D:610:GLU:HB2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:70:ALA:HB2	3:C:111:LEU:HD11	1.94	0.49
2:B:19:ILE:HG13	2:B:78:LEU:HD11	1.95	0.49
2:B:91:LEU:HD11	2:B:95:TRP:HA	1.95	0.49
3:C:299:ASN:HB3	3:C:320:ILE:HD13	1.95	0.48
3:C:273:SER:HB3	3:C:276:ILE:HG12	1.94	0.48
3:C:221:GLY:HA2	4:D:544:LEU:CD1	2.43	0.48
3:C:114:GLN:NE2	4:D:559:VAL:HG21	2.28	0.48
6:F:65:SER:HB3	6:F:72:THR:HG23	1.95	0.48
4:D:523:LEU:H	4:D:540:GLN:CD	2.14	0.48
4:D:554:ILE:HB	4:D:555:PRO:HD3	1.94	0.48
4:D:604:SER:N	6:F:30:THR:HG21	2.28	0.48
1:A:87:THR:HG23	1:A:110:THR:HA	1.95	0.48
6:F:124:GLN:OE1	6:F:131:SER:N	2.47	0.48
3:C:499:LYS:HG2	3:C:500:ARG:N	2.25	0.47
1:A:125:ALA:HB1	1:A:227:PRO:HA	1.96	0.47
3:C:356:ILE:O	3:C:462:THR:OG1	2.24	0.47
5:E:187:ALA:HB2	5:E:197:LEU:HD23	1.96	0.47
2:B:110:LYS:HG2	2:B:140:TYR:CD2	2.49	0.47
3:C:258:LEU:HD12	3:C:372:HIS:CD2	2.50	0.47
1:A:27:ASP:OD1	1:A:28:SER:N	2.45	0.47
1:A:63:LEU:HB3	1:A:67:LEU:HD23	1.97	0.47
2:B:110:LYS:HG2	2:B:140:TYR:HD2	1.80	0.47
5:E:135:THR:HA	5:E:165:PHE:HD2	1.79	0.47
1:A:51:LEU:HB3	1:A:57:THR:HG23	1.97	0.46
2:B:65:SER:O	2:B:72:SER:N	2.35	0.46
5:E:145:PRO:HG3	5:E:157:LEU:HB3	1.97	0.46
5:E:163:ASP:HA	5:E:194:LEU:HB3	1.97	0.46
2:B:33:VAL:HA	2:B:90:SER:HB2	1.97	0.46
3:C:56:SER:O	3:C:57:ASP:HB2	2.16	0.46
3:C:192:LEU:HB2	3:C:195:CYS:SG	2.56	0.46
3:C:319:ASP:HB3	7:G:1:NAG:H82	1.97	0.46
4:D:552:ILE:O	4:D:553:ASP:HB2	2.15	0.46
1:A:73:THR:HB	1:A:74:PRO:HD3	1.98	0.46
2:B:105:THR:HG22	2:B:106(A):LEU:H	1.81	0.46
6:F:32:TRP:HE3	6:F:91:TYR:HE2	1.64	0.46
1:A:100(E):TRP:CD1	2:B:95:TRP:HE3	2.34	0.45
2:B:51:VAL:HG12	2:B:52:ASN:N	2.31	0.45
5:E:6:GLN:O	5:E:124:GLN:NE2	2.50	0.45
3:C:293:ILE:HD12	3:C:446:ILE:HD11	1.97	0.45
6:F:23:CYS:N	6:F:71:PHE:O	2.44	0.45
1:A:100(E):TRP:NE1	2:B:94:ASN:O	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:106:VAL:O	6:F:140:TYR:OH	2.32	0.45
14:T:2:NAG:O3	14:T:3:BMA:O5	2.23	0.45
2:B:119:PRO:HD3	2:B:209:VAL:HG11	1.99	0.45
6:F:29:ILE:HB	6:F:71:PHE:HZ	1.82	0.45
3:C:46:LYS:HG2	5:E:108:TRP:NE1	2.32	0.45
4:D:635:LEU:O	4:D:639:GLN:HB2	2.17	0.44
1:A:56:TRP:CE3	9:K:5:MAN:H62	2.53	0.44
2:B:85:VAL:HG22	2:B:103:LYS:HG2	1.98	0.44
2:B:153:SER:HA	2:B:154:PRO:HD3	1.80	0.44
2:B:21:ILE:HD11	2:B:73:LEU:HD23	1.99	0.44
1:A:146:ASP:OD1	1:A:179:GLN:NE2	2.42	0.44
1:A:209:ASN:ND2	1:A:220:ASP:OD2	2.51	0.44
1:A:39:GLN:HB2	1:A:45:LEU:HD23	2.00	0.44
3:C:348:ARG:HD3	3:C:353:ASN:O	2.17	0.43
3:C:388:LEU:HD11	3:C:413:LEU:HD11	1.99	0.43
1:A:137:THR:HG22	1:A:194:PRO:HA	1.99	0.43
1:A:27:ASP:OD2	1:A:94:ARG:NH2	2.51	0.43
1:A:51:LEU:HD23	1:A:69:LEU:HB3	2.00	0.43
5:E:25:TYR:CE1	5:E:79:PRO:HG3	2.53	0.43
2:B:136:ILE:HG12	2:B:196:VAL:HG11	1.99	0.43
5:E:51:GLN:NE2	5:E:115:GLY:O	2.43	0.43
6:F:136:LEU:HD11	6:F:196:VAL:HG11	2.01	0.43
1:A:70:ALA:HB3	1:A:79:PHE:HB2	2.01	0.43
1:A:101:ASP:OD1	1:A:102:LEU:N	2.52	0.43
3:C:461:THR:OG1	3:C:462:THR:N	2.52	0.43
2:B:22:SER:OG	2:B:23:CYS:N	2.52	0.42
3:C:50:THR:HG22	3:C:485:VAL:HG11	2.01	0.42
3:C:329:CYS:O	3:C:413:LEU:N	2.52	0.42
5:E:24:ALA:O	5:E:79:PRO:HB2	2.18	0.42
5:E:25:TYR:CD1	5:E:79:PRO:HG3	2.54	0.42
2:B:83:GLU:HG3	2:B:105:THR:HA	2.01	0.42
3:C:255:SER:HA	3:C:373:SER:O	2.19	0.42
3:C:457:SER:HA	3:C:458:THR:OG1	2.19	0.42
6:F:134:CYS:HB3	6:F:177:SER:HB3	2.00	0.42
3:C:88:ASN:ND2	4:D:527:GLY:O	2.53	0.42
3:C:490:PRO:HB3	4:D:544:LEU:HD23	2.01	0.42
1:A:100:LEU:HD12	3:C:321:ILE:HG23	2.02	0.42
3:C:64:GLU:HG3	3:C:65:LYS:H	1.84	0.42
4:D:552:ILE:HG23	4:D:553:ASP:N	2.34	0.42
1:A:22:CYS:HB2	1:A:36:TRP:CH2	2.54	0.42
2:B:167:GLN:NE2	2:B:174:ALA:HB2	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:649:LEU:HA	4:D:652:LEU:HD23	2.02	0.42
1:A:60:ASN:HA	1:A:61:PRO:HD3	1.94	0.42
3:C:42:VAL:HA	3:C:43:PRO:HD3	1.90	0.42
3:C:95:MET:SD	3:C:272:ARG:HD3	2.60	0.42
5:E:75:THR:HG23	5:E:77:SER:H	1.84	0.42
3:C:393:TRP:CD2	3:C:398:SER:HB3	2.54	0.42
3:C:434:PRO:HA	3:C:435:PRO:HD3	1.87	0.42
1:A:100(A):ARG:NH2	7:G:1:NAG:O7	2.53	0.42
2:B:55:PRO:HG2	2:B:58:VAL:HG21	2.02	0.42
6:F:7:SER:HA	6:F:8:PRO:HA	1.90	0.42
1:A:174:PHE:HA	1:A:175:PRO:HD3	1.89	0.41
3:C:231:LYS:HA	3:C:270:MET:HE1	2.02	0.41
2:B:51:VAL:HG12	2:B:52:ASN:H	1.85	0.41
3:C:69:TRP:CG	3:C:70:ALA:N	2.88	0.41
3:C:75:VAL:HG22	4:D:552:ILE:HB	2.02	0.41
6:F:210:ASN:O	6:F:211:ARG:HG2	2.20	0.41
1:A:226:GLU:HA	1:A:227:PRO:HD3	1.85	0.41
3:C:473:ARG:HA	3:C:476:TRP:CD1	2.55	0.41
5:E:67:VAL:HG13	5:E:84:LEU:HD11	2.03	0.41
1:A:18:LEU:HB3	1:A:82:LEU:HB2	2.01	0.41
6:F:4:MET:HB2	6:F:99:GLY:HA2	2.03	0.41
2:B:30:ASN:ND2	2:B:91:LEU:O	2.51	0.41
2:B:94:ASN:HB3	2:B:95:TRP:CE3	2.56	0.41
3:C:494:ALA:HA	3:C:495:PRO:HD3	1.81	0.41
5:E:144:ALA:HA	5:E:145:PRO:HD3	1.95	0.41
11:M:1:NAG:H61	11:M:2:NAG:HN2	1.83	0.41
2:B:140:TYR:O	2:B:198:HIS:NE2	2.52	0.41
6:F:29:ILE:HB	6:F:71:PHE:CZ	2.56	0.41
4:D:623:GLU:HG2	6:F:32:TRP:HE1	1.86	0.40
6:F:107:LYS:HA	6:F:140:TYR:OH	2.21	0.40
1:A:172:HIS:NE2	2:B:167:GLN:OE1	2.55	0.40
5:E:75:THR:HG23	5:E:78:SER:H	1.86	0.40
6:F:19:VAL:N	6:F:75:ILE:O	2.43	0.40
6:F:89:GLN:HB2	6:F:98:PHE:CD2	2.56	0.40
1:A:56:TRP:HE3	9:K:5:MAN:H62	1.87	0.40
3:C:160:LYS:HE2	3:C:160:LYS:HB2	1.89	0.40
3:C:267:GLU:O	3:C:288:ASN:ND2	2.54	0.40
3:C:394:ILE:HG22	3:C:395:SER:N	2.30	0.40
5:E:74:LEU:HD13	5:E:80:PRO:HD3	2.04	0.40
1:A:39:GLN:NE2	2:B:38:GLN:OE1	2.51	0.40
1:A:40:PRO:HA	1:A:41:PRO:HD3	1.93	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:205:PRO:HG3	3:C:315:TYR:CE2	2.57	0.40
5:E:3:HIS:HB2	5:E:25:TYR:HB2	2.04	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:546:SER:OG	4:D:580:GLN:OE1[5_555]	2.09	0.11

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	226/239 (95%)	212 (94%)	14 (6%)	0	100 100
2	B	202/211 (96%)	194 (96%)	7 (4%)	1 (0%)	29 69
3	C	439/480 (92%)	417 (95%)	22 (5%)	0	100 100
4	D	130/142 (92%)	119 (92%)	9 (7%)	2 (2%)	10 45
5	E	218/238 (92%)	209 (96%)	9 (4%)	0	100 100
6	F	210/215 (98%)	205 (98%)	5 (2%)	0	100 100
All	All	1425/1525 (93%)	1356 (95%)	66 (5%)	3 (0%)	47 81

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	552	ILE
2	B	51	VAL
4	D	555	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	194/203 (96%)	194 (100%)	0	100 100
2	B	171/177 (97%)	170 (99%)	1 (1%)	86 92
3	C	399/426 (94%)	396 (99%)	3 (1%)	81 89
4	D	115/120 (96%)	113 (98%)	2 (2%)	60 78
5	E	192/204 (94%)	192 (100%)	0	100 100
6	F	180/182 (99%)	180 (100%)	0	100 100
All	All	1251/1312 (95%)	1245 (100%)	6 (0%)	88 93

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	152	SER
3	C	233	ASN
3	C	303	ARG
3	C	337	ASN
4	D	562	ILE
4	D	563	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	114	GLN
3	C	194	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

75 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	G	1	3,7	14,14,15	0.30	0	17,19,21	0.63	0
7	NAG	G	2	7	14,14,15	0.20	0	17,19,21	0.38	0
7	NAG	H	1	3,7	14,14,15	0.22	0	17,19,21	0.42	0
7	NAG	H	2	7	14,14,15	0.28	0	17,19,21	0.41	0
7	NAG	I	1	3,7	14,14,15	0.23	0	17,19,21	1.02	1 (5%)
7	NAG	I	2	7	14,14,15	0.24	0	17,19,21	0.37	0
8	NAG	J	1	3,8	14,14,15	0.60	0	17,19,21	0.53	0
8	NAG	J	2	8	14,14,15	0.58	0	17,19,21	0.48	0
8	BMA	J	3	8	11,11,12	0.55	0	15,15,17	0.69	0
8	MAN	J	4	8	11,11,12	0.69	0	15,15,17	1.07	1 (6%)
8	MAN	J	5	8	11,11,12	0.59	0	15,15,17	1.04	1 (6%)
8	MAN	J	6	8	11,11,12	0.90	0	15,15,17	0.92	2 (13%)
8	MAN	J	7	8	11,11,12	0.64	0	15,15,17	1.03	2 (13%)
8	MAN	J	8	8	11,11,12	0.82	1 (9%)	15,15,17	1.47	2 (13%)
9	NAG	K	1	3,9	14,14,15	0.25	0	17,19,21	0.44	0
9	MAN	K	10	9	11,11,12	0.69	0	15,15,17	1.00	2 (13%)
9	NAG	K	2	9	14,14,15	0.23	0	17,19,21	0.39	0
9	BMA	K	3	9	11,11,12	0.81	0	15,15,17	0.87	0
9	MAN	K	4	9	11,11,12	0.76	1 (9%)	15,15,17	1.14	2 (13%)
9	MAN	K	5	9	11,11,12	0.68	0	15,15,17	1.14	2 (13%)
9	MAN	K	6	9	11,11,12	0.80	0	15,15,17	0.96	1 (6%)
9	MAN	K	7	9	11,11,12	0.69	0	15,15,17	1.05	2 (13%)
9	MAN	K	8	9	11,11,12	0.68	0	15,15,17	1.24	2 (13%)
9	MAN	K	9	9	11,11,12	0.70	0	15,15,17	0.92	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
10	NAG	L	1	3,10	14,14,15	0.51	0	17,19,21	0.63	0
10	NAG	L	2	10	14,14,15	0.20	0	17,19,21	0.71	0
10	BMA	L	3	10	11,11,12	0.82	0	15,15,17	1.03	0
10	MAN	L	4	10	11,11,12	0.79	0	15,15,17	1.35	2 (13%)
10	MAN	L	5	10	11,11,12	0.61	0	15,15,17	1.15	2 (13%)
10	MAN	L	6	10	11,11,12	0.61	0	15,15,17	1.16	2 (13%)
10	MAN	L	7	10	11,11,12	0.72	0	15,15,17	0.98	2 (13%)
10	MAN	L	8	10	11,11,12	0.68	0	15,15,17	0.97	2 (13%)
10	MAN	L	9	10	11,11,12	0.64	0	15,15,17	1.01	2 (13%)
11	NAG	M	1	11,3	14,14,15	0.30	0	17,19,21	0.45	0
11	NAG	M	2	11	14,14,15	0.41	0	17,19,21	0.52	0
11	BMA	M	3	11	11,11,12	0.66	0	15,15,17	1.03	1 (6%)
11	MAN	M	4	11	11,11,12	0.71	0	15,15,17	1.35	1 (6%)
11	MAN	M	5	11	11,11,12	0.55	0	15,15,17	1.15	1 (6%)
11	MAN	M	6	11	11,11,12	0.68	0	15,15,17	1.28	2 (13%)
11	MAN	M	7	11	11,11,12	0.77	1 (9%)	15,15,17	1.17	2 (13%)
12	NAG	N	1	3,12	14,14,15	0.47	0	17,19,21	0.45	0
12	NAG	N	2	12	14,14,15	0.23	0	17,19,21	0.60	0
12	BMA	N	3	12	11,11,12	0.66	0	15,15,17	1.23	1 (6%)
12	MAN	N	4	12	11,11,12	0.63	0	15,15,17	1.33	2 (13%)
12	MAN	N	5	12	11,11,12	0.22	0	15,15,17	0.59	0
13	NAG	O	1	3,13	14,14,15	0.41	0	17,19,21	0.40	0
13	NAG	O	2	13	14,14,15	0.28	0	17,19,21	0.62	0
13	BMA	O	3	13	11,11,12	0.65	0	15,15,17	0.78	0
13	NAG	P	1	3,13	14,14,15	0.31	0	17,19,21	0.49	0
13	NAG	P	2	13	14,14,15	0.39	0	17,19,21	0.62	0
13	BMA	P	3	13	11,11,12	0.69	0	15,15,17	0.81	0
13	NAG	Q	1	3,13	14,14,15	0.31	0	17,19,21	0.74	0
13	NAG	Q	2	13	14,14,15	0.24	0	17,19,21	0.67	1 (5%)
13	BMA	Q	3	13	11,11,12	0.64	0	15,15,17	0.76	0
13	NAG	R	1	3,13	14,14,15	0.32	0	17,19,21	0.50	0
13	NAG	R	2	13	14,14,15	0.39	0	17,19,21	0.62	0
13	BMA	R	3	13	11,11,12	0.69	0	15,15,17	0.80	0
13	NAG	S	1	3,13	14,14,15	0.32	0	17,19,21	0.50	0
13	NAG	S	2	13	14,14,15	0.39	0	17,19,21	0.61	0
13	BMA	S	3	13	11,11,12	0.69	0	15,15,17	0.80	0
14	NAG	T	1	4,14	14,14,15	0.26	0	17,19,21	0.41	0
14	NAG	T	2	14	14,14,15	0.42	0	17,19,21	1.52	3 (17%)
14	BMA	T	3	14	11,11,12	0.74	0	15,15,17	0.98	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
14	MAN	T	4	14	11,11,12	1.55	3 (27%)	15,15,17	1.38	2 (13%)
15	NAG	U	1	3,15	14,14,15	0.18	0	17,19,21	0.38	0
15	MAN	U	10	15	11,11,12	0.64	0	15,15,17	1.19	2 (13%)
15	MAN	U	11	15	11,11,12	0.67	0	15,15,17	0.96	2 (13%)
15	NAG	U	2	15	14,14,15	0.38	0	17,19,21	0.45	0
15	BMA	U	3	15	11,11,12	0.53	0	15,15,17	0.70	0
15	MAN	U	4	15	11,11,12	0.54	0	15,15,17	1.12	2 (13%)
15	MAN	U	5	15	11,11,12	0.73	0	15,15,17	1.07	1 (6%)
15	MAN	U	6	15	11,11,12	0.55	0	15,15,17	1.00	2 (13%)
15	MAN	U	7	15	11,11,12	0.59	0	15,15,17	1.17	2 (13%)
15	MAN	U	8	15	11,11,12	0.85	0	15,15,17	1.43	3 (20%)
15	MAN	U	9	15	11,11,12	0.59	0	15,15,17	1.04	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	G	1	3,7	-	4/6/23/26	0/1/1/1
7	NAG	G	2	7	-	2/6/23/26	0/1/1/1
7	NAG	H	1	3,7	-	2/6/23/26	0/1/1/1
7	NAG	H	2	7	-	2/6/23/26	0/1/1/1
7	NAG	I	1	3,7	-	1/6/23/26	0/1/1/1
7	NAG	I	2	7	-	0/6/23/26	0/1/1/1
8	NAG	J	1	3,8	-	2/6/23/26	0/1/1/1
8	NAG	J	2	8	-	2/6/23/26	0/1/1/1
8	BMA	J	3	8	-	0/2/19/22	0/1/1/1
8	MAN	J	4	8	-	0/2/19/22	0/1/1/1
8	MAN	J	5	8	-	0/2/19/22	0/1/1/1
8	MAN	J	6	8	-	2/2/19/22	0/1/1/1
8	MAN	J	7	8	-	0/2/19/22	0/1/1/1
8	MAN	J	8	8	-	0/2/19/22	0/1/1/1
9	NAG	K	1	3,9	-	0/6/23/26	0/1/1/1
9	MAN	K	10	9	-	1/2/19/22	0/1/1/1
9	NAG	K	2	9	-	2/6/23/26	0/1/1/1
9	BMA	K	3	9	-	0/2/19/22	0/1/1/1
9	MAN	K	4	9	-	1/2/19/22	0/1/1/1
9	MAN	K	5	9	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	MAN	K	6	9	-	0/2/19/22	0/1/1/1
9	MAN	K	7	9	-	0/2/19/22	0/1/1/1
9	MAN	K	8	9	-	0/2/19/22	0/1/1/1
9	MAN	K	9	9	-	0/2/19/22	0/1/1/1
10	NAG	L	1	3,10	-	1/6/23/26	0/1/1/1
10	NAG	L	2	10	-	1/6/23/26	0/1/1/1
10	BMA	L	3	10	-	0/2/19/22	0/1/1/1
10	MAN	L	4	10	-	0/2/19/22	0/1/1/1
10	MAN	L	5	10	-	0/2/19/22	0/1/1/1
10	MAN	L	6	10	-	0/2/19/22	0/1/1/1
10	MAN	L	7	10	-	0/2/19/22	0/1/1/1
10	MAN	L	8	10	-	0/2/19/22	0/1/1/1
10	MAN	L	9	10	-	0/2/19/22	0/1/1/1
11	NAG	M	1	11,3	-	0/6/23/26	0/1/1/1
11	NAG	M	2	11	-	0/6/23/26	0/1/1/1
11	BMA	M	3	11	-	0/2/19/22	0/1/1/1
11	MAN	M	4	11	-	1/2/19/22	0/1/1/1
11	MAN	M	5	11	-	0/2/19/22	0/1/1/1
11	MAN	M	6	11	-	1/2/19/22	0/1/1/1
11	MAN	M	7	11	-	0/2/19/22	0/1/1/1
12	NAG	N	1	3,12	-	0/6/23/26	0/1/1/1
12	NAG	N	2	12	-	2/6/23/26	0/1/1/1
12	BMA	N	3	12	-	0/2/19/22	0/1/1/1
12	MAN	N	4	12	-	2/2/19/22	0/1/1/1
12	MAN	N	5	12	-	0/2/19/22	0/1/1/1
13	NAG	O	1	3,13	-	0/6/23/26	0/1/1/1
13	NAG	O	2	13	-	1/6/23/26	0/1/1/1
13	BMA	O	3	13	-	0/2/19/22	0/1/1/1
13	NAG	P	1	3,13	-	0/6/23/26	0/1/1/1
13	NAG	P	2	13	-	2/6/23/26	0/1/1/1
13	BMA	P	3	13	-	0/2/19/22	0/1/1/1
13	NAG	Q	1	3,13	-	4/6/23/26	0/1/1/1
13	NAG	Q	2	13	-	0/6/23/26	0/1/1/1
13	BMA	Q	3	13	-	0/2/19/22	0/1/1/1
13	NAG	R	1	3,13	-	0/6/23/26	0/1/1/1
13	NAG	R	2	13	-	2/6/23/26	0/1/1/1
13	BMA	R	3	13	-	0/2/19/22	0/1/1/1
13	NAG	S	1	3,13	-	0/6/23/26	0/1/1/1
13	NAG	S	2	13	-	2/6/23/26	0/1/1/1
13	BMA	S	3	13	-	0/2/19/22	0/1/1/1
14	NAG	T	1	4,14	-	1/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	NAG	T	2	14	-	5/6/23/26	0/1/1/1
14	BMA	T	3	14	-	2/2/19/22	0/1/1/1
14	MAN	T	4	14	-	2/2/19/22	0/1/1/1
15	NAG	U	1	3,15	-	2/6/23/26	0/1/1/1
15	MAN	U	10	15	-	2/2/19/22	0/1/1/1
15	MAN	U	11	15	-	2/2/19/22	0/1/1/1
15	NAG	U	2	15	-	2/6/23/26	0/1/1/1
15	BMA	U	3	15	-	0/2/19/22	0/1/1/1
15	MAN	U	4	15	-	0/2/19/22	0/1/1/1
15	MAN	U	5	15	-	2/2/19/22	0/1/1/1
15	MAN	U	6	15	-	0/2/19/22	0/1/1/1
15	MAN	U	7	15	-	0/2/19/22	0/1/1/1
15	MAN	U	8	15	-	0/2/19/22	0/1/1/1
15	MAN	U	9	15	-	1/2/19/22	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	T	4	MAN	C2-C3	2.98	1.56	1.52
14	T	4	MAN	O2-C2	2.74	1.49	1.43
14	T	4	MAN	C1-C2	2.66	1.58	1.52
11	M	7	MAN	C1-C2	2.30	1.57	1.52
8	J	8	MAN	C1-C2	2.23	1.57	1.52
9	K	4	MAN	C1-C2	2.16	1.57	1.52

All (65) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	J	8	MAN	C1-O5-C5	4.62	118.46	112.19
11	M	4	MAN	C1-O5-C5	4.51	118.30	112.19
14	T	2	NAG	C2-N2-C7	4.50	129.31	122.90
10	L	4	MAN	C1-O5-C5	4.34	118.08	112.19
11	M	6	MAN	C1-O5-C5	4.02	117.64	112.19
11	M	5	MAN	C1-O5-C5	3.55	117.00	112.19
10	L	5	MAN	C1-O5-C5	3.49	116.92	112.19
10	L	6	MAN	C1-O5-C5	3.34	116.72	112.19
12	N	4	MAN	O2-C2-C1	3.32	115.95	109.15
15	U	8	MAN	O2-C2-C3	-3.29	103.55	110.14
7	I	1	NAG	C2-N2-C7	3.27	127.56	122.90
15	U	4	MAN	C1-O5-C5	3.20	116.53	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	U	7	MAN	C1-O5-C5	3.20	116.53	112.19
9	K	5	MAN	O2-C2-C3	-3.13	103.86	110.14
9	K	8	MAN	C1-O5-C5	3.08	116.37	112.19
9	K	4	MAN	C1-O5-C5	3.06	116.33	112.19
15	U	8	MAN	C1-O5-C5	3.03	116.30	112.19
12	N	3	BMA	C1-C2-C3	3.01	113.37	109.67
9	K	8	MAN	O2-C2-C3	-2.97	104.18	110.14
14	T	2	NAG	C1-C2-N2	2.96	115.54	110.49
8	J	5	MAN	C1-O5-C5	2.93	116.16	112.19
14	T	4	MAN	O2-C2-C1	2.90	115.09	109.15
12	N	4	MAN	C1-O5-C5	2.90	116.12	112.19
15	U	10	MAN	C1-O5-C5	2.85	116.06	112.19
11	M	3	BMA	C1-C2-C3	-2.85	106.16	109.67
11	M	7	MAN	C1-O5-C5	2.81	116.00	112.19
9	K	7	MAN	C1-O5-C5	2.66	115.80	112.19
15	U	6	MAN	C1-O5-C5	2.63	115.76	112.19
8	J	7	MAN	C1-O5-C5	2.62	115.74	112.19
15	U	9	MAN	C1-O5-C5	2.60	115.71	112.19
14	T	2	NAG	C1-O5-C5	2.57	115.68	112.19
15	U	8	MAN	C1-C2-C3	-2.52	106.56	109.67
14	T	4	MAN	C1-O5-C5	2.48	115.56	112.19
15	U	9	MAN	O2-C2-C3	-2.48	105.17	110.14
10	L	9	MAN	C1-O5-C5	2.44	115.50	112.19
9	K	4	MAN	O2-C2-C3	-2.42	105.29	110.14
9	K	5	MAN	C1-O5-C5	2.42	115.47	112.19
9	K	7	MAN	O2-C2-C3	-2.32	105.49	110.14
10	L	7	MAN	C1-O5-C5	2.29	115.30	112.19
8	J	4	MAN	C1-O5-C5	2.27	115.27	112.19
15	U	11	MAN	C1-O5-C5	2.27	115.26	112.19
9	K	10	MAN	C1-O5-C5	2.25	115.24	112.19
10	L	8	MAN	O2-C2-C3	-2.25	105.64	110.14
10	L	6	MAN	O2-C2-C3	-2.25	105.64	110.14
15	U	6	MAN	O2-C2-C3	-2.24	105.65	110.14
10	L	5	MAN	O2-C2-C3	-2.23	105.67	110.14
15	U	7	MAN	O2-C2-C3	-2.23	105.67	110.14
10	L	7	MAN	O2-C2-C3	-2.22	105.69	110.14
9	K	9	MAN	O2-C2-C3	-2.21	105.72	110.14
11	M	6	MAN	O2-C2-C3	-2.20	105.73	110.14
8	J	7	MAN	O2-C2-C3	-2.19	105.75	110.14
9	K	10	MAN	O2-C2-C3	-2.18	105.76	110.14
15	U	11	MAN	O2-C2-C3	-2.18	105.77	110.14
8	J	6	MAN	O2-C2-C3	-2.18	105.78	110.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	L	9	MAN	O2-C2-C3	-2.17	105.80	110.14
15	U	4	MAN	O2-C2-C3	-2.16	105.80	110.14
9	K	6	MAN	O2-C2-C3	-2.16	105.81	110.14
13	Q	2	NAG	C1-O5-C5	2.12	115.07	112.19
8	J	8	MAN	O2-C2-C3	-2.11	105.91	110.14
11	M	7	MAN	O2-C2-C3	-2.10	105.94	110.14
10	L	4	MAN	O2-C2-C3	-2.09	105.96	110.14
10	L	8	MAN	C1-O5-C5	2.09	115.02	112.19
15	U	10	MAN	O2-C2-C3	-2.07	105.98	110.14
8	J	6	MAN	C1-O5-C5	2.05	114.98	112.19
15	U	5	MAN	C1-O5-C5	2.02	114.93	112.19

There are no chirality outliers.

All (61) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	G	1	NAG	C3-C2-N2-C7
7	G	1	NAG	C8-C7-N2-C2
7	G	1	NAG	O7-C7-N2-C2
7	I	1	NAG	C3-C2-N2-C7
13	Q	1	NAG	C8-C7-N2-C2
13	Q	1	NAG	O7-C7-N2-C2
8	J	1	NAG	O5-C5-C6-O6
14	T	2	NAG	C4-C5-C6-O6
15	U	1	NAG	O5-C5-C6-O6
8	J	1	NAG	C4-C5-C6-O6
7	G	2	NAG	O5-C5-C6-O6
7	G	2	NAG	C4-C5-C6-O6
12	N	2	NAG	O5-C5-C6-O6
14	T	2	NAG	O5-C5-C6-O6
8	J	2	NAG	C4-C5-C6-O6
15	U	10	MAN	O5-C5-C6-O6
13	Q	1	NAG	C1-C2-N2-C7
7	H	2	NAG	O5-C5-C6-O6
8	J	2	NAG	O5-C5-C6-O6
12	N	2	NAG	C4-C5-C6-O6
7	H	1	NAG	C8-C7-N2-C2
7	H	1	NAG	O7-C7-N2-C2
14	T	2	NAG	C8-C7-N2-C2
14	T	2	NAG	O7-C7-N2-C2
9	K	2	NAG	O5-C5-C6-O6
15	U	1	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
15	U	10	MAN	C4-C5-C6-O6
8	J	6	MAN	O5-C5-C6-O6
15	U	5	MAN	O5-C5-C6-O6
8	J	6	MAN	C4-C5-C6-O6
14	T	3	BMA	O5-C5-C6-O6
15	U	11	MAN	O5-C5-C6-O6
15	U	5	MAN	C4-C5-C6-O6
12	N	4	MAN	O5-C5-C6-O6
14	T	3	BMA	C4-C5-C6-O6
12	N	4	MAN	C4-C5-C6-O6
9	K	2	NAG	C4-C5-C6-O6
15	U	9	MAN	O5-C5-C6-O6
9	K	4	MAN	O5-C5-C6-O6
9	K	10	MAN	O5-C5-C6-O6
7	H	2	NAG	C4-C5-C6-O6
14	T	1	NAG	O5-C5-C6-O6
15	U	2	NAG	C4-C5-C6-O6
7	G	1	NAG	C1-C2-N2-C7
13	Q	1	NAG	C3-C2-N2-C7
15	U	11	MAN	C4-C5-C6-O6
13	P	2	NAG	C4-C5-C6-O6
13	R	2	NAG	C4-C5-C6-O6
13	S	2	NAG	C4-C5-C6-O6
14	T	4	MAN	C4-C5-C6-O6
11	M	4	MAN	O5-C5-C6-O6
15	U	2	NAG	O5-C5-C6-O6
13	O	2	NAG	C4-C5-C6-O6
10	L	1	NAG	C3-C2-N2-C7
14	T	2	NAG	C3-C2-N2-C7
14	T	4	MAN	O5-C5-C6-O6
13	S	2	NAG	O5-C5-C6-O6
13	P	2	NAG	O5-C5-C6-O6
13	R	2	NAG	O5-C5-C6-O6
11	M	6	MAN	O5-C5-C6-O6
10	L	2	NAG	C3-C2-N2-C7

There are no ring outliers.

12 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	G	1	NAG	4	0
11	M	2	NAG	2	0

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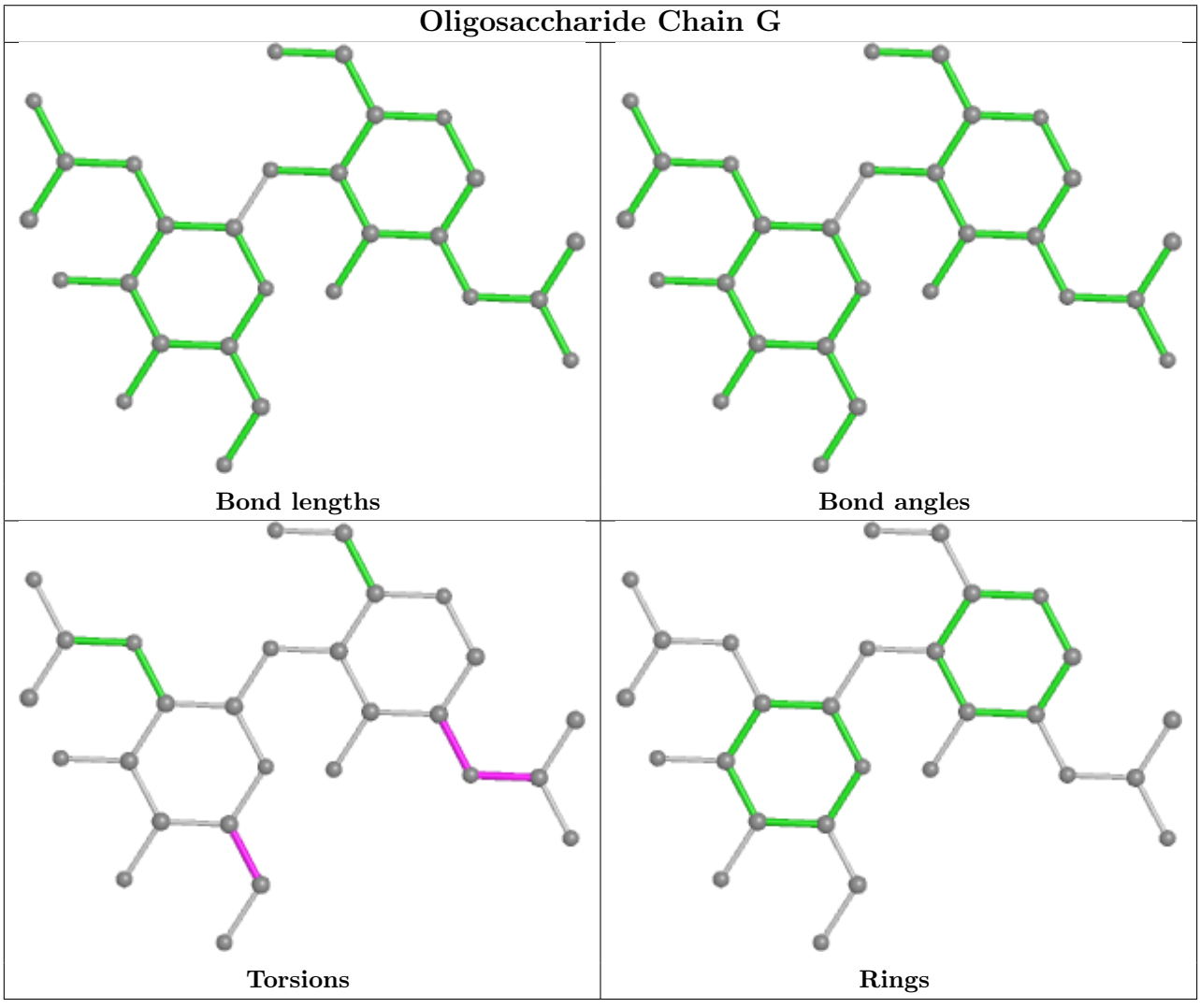
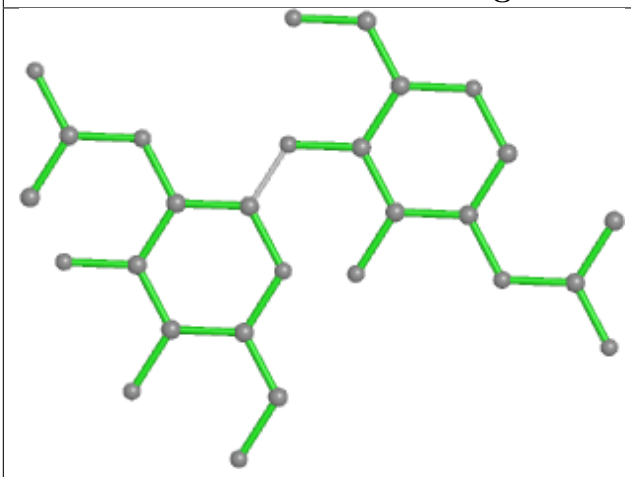
Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	T	2	NAG	2	0
13	Q	1	NAG	1	0
11	M	6	MAN	2	0
14	T	3	BMA	1	0
9	K	5	MAN	2	0
8	J	2	NAG	1	0
9	K	9	MAN	1	0
11	M	1	NAG	2	0
9	K	6	MAN	2	0
11	M	4	MAN	2	0

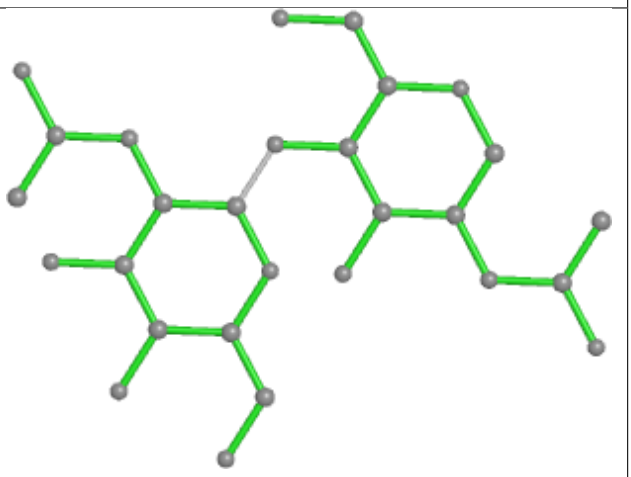
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



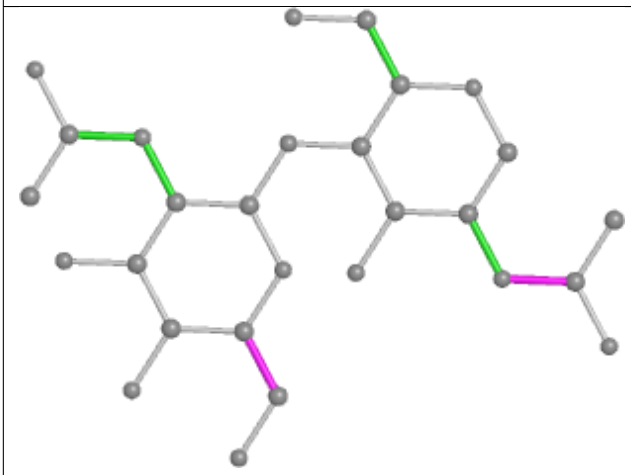
Oligosaccharide Chain H



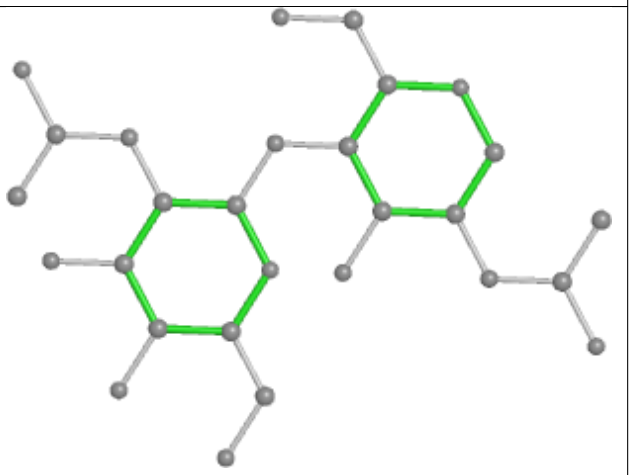
Bond lengths



Bond angles

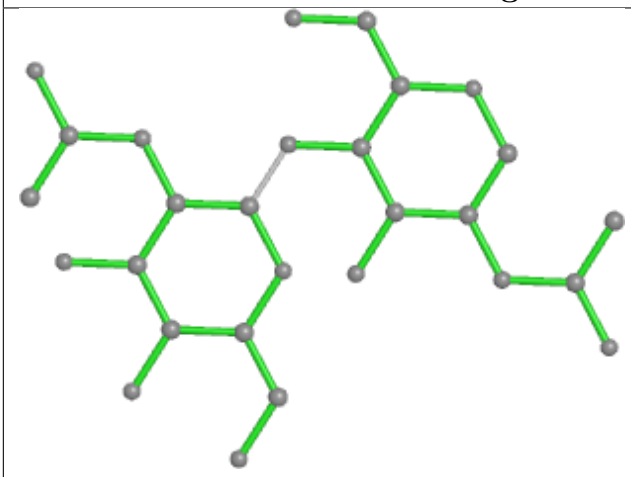


Torsions

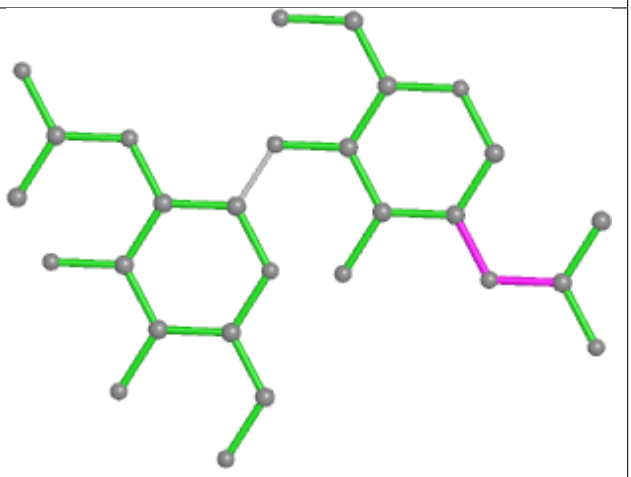


Rings

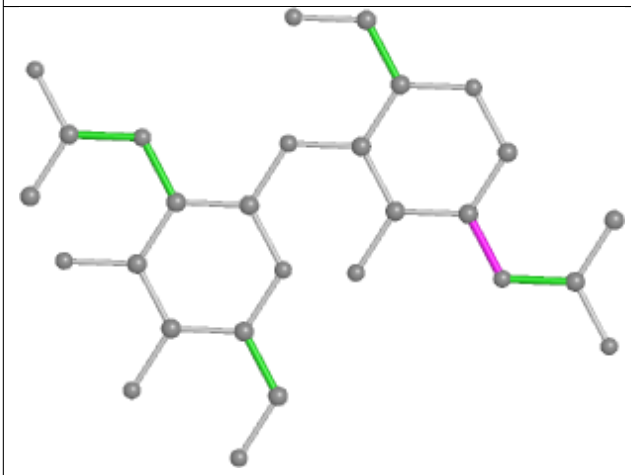
Oligosaccharide Chain I



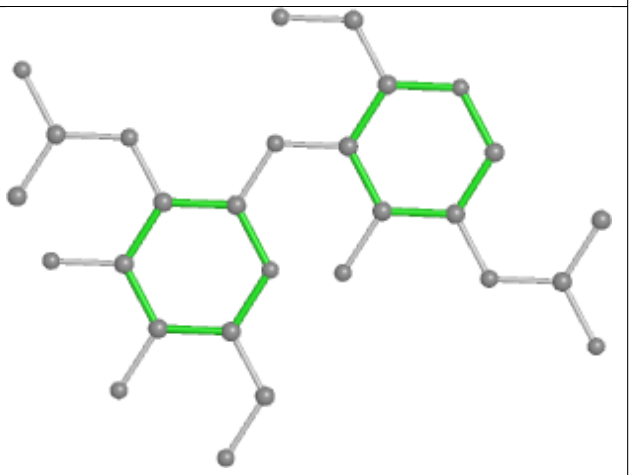
Bond lengths



Bond angles

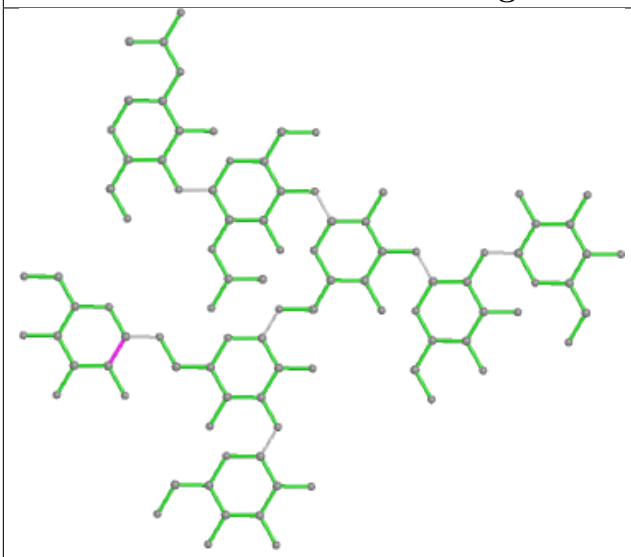


Torsions

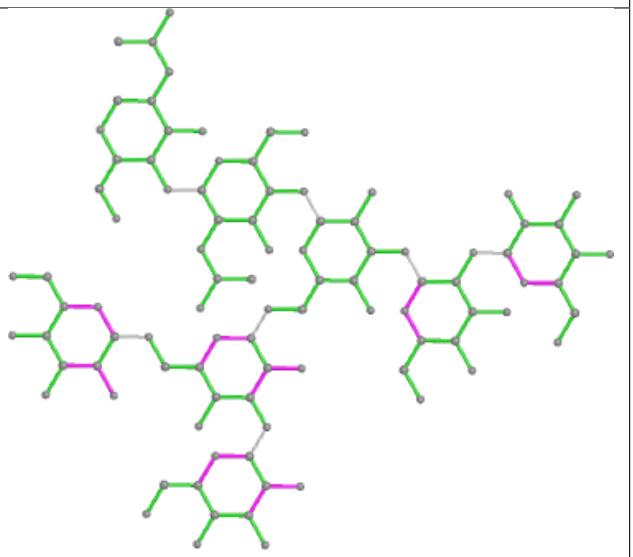


Rings

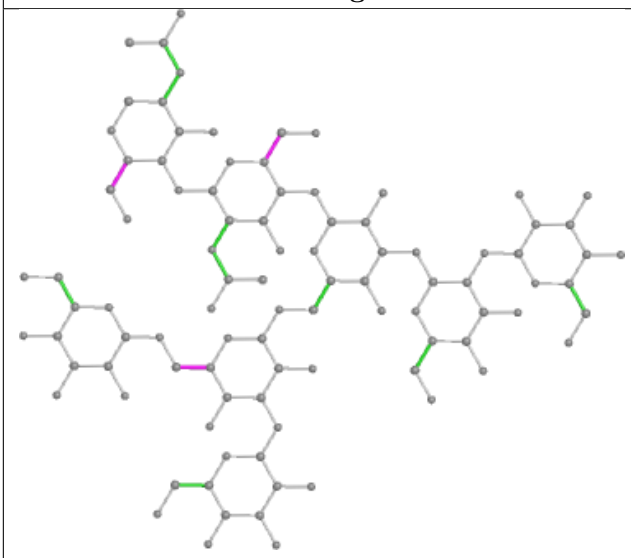
Oligosaccharide Chain J



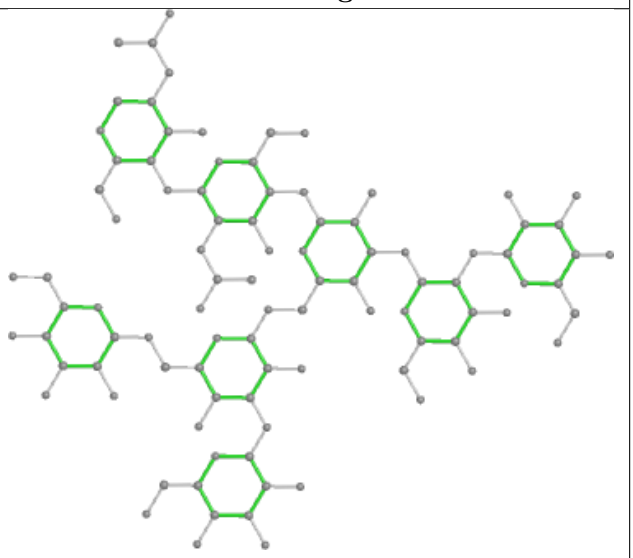
Bond lengths



Bond angles

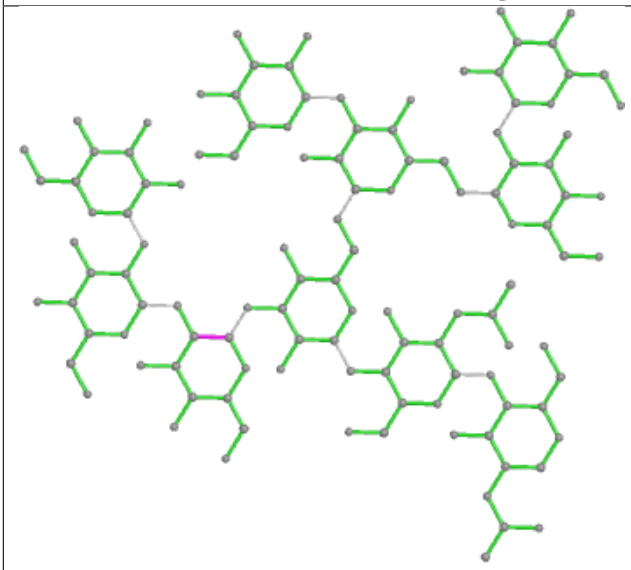


Torsions

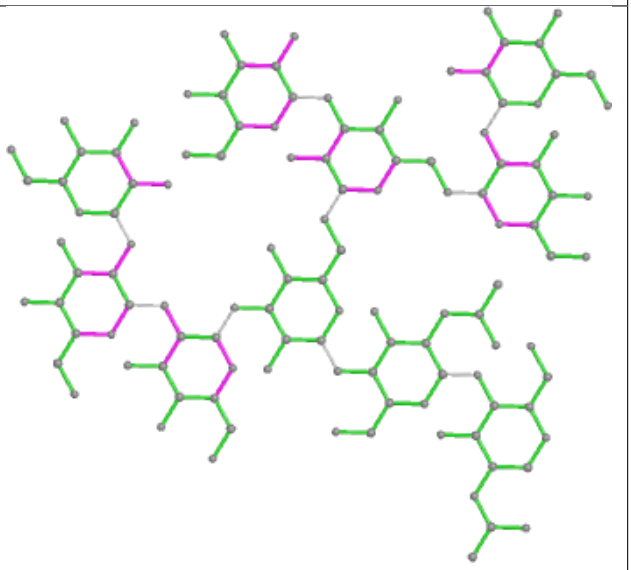


Rings

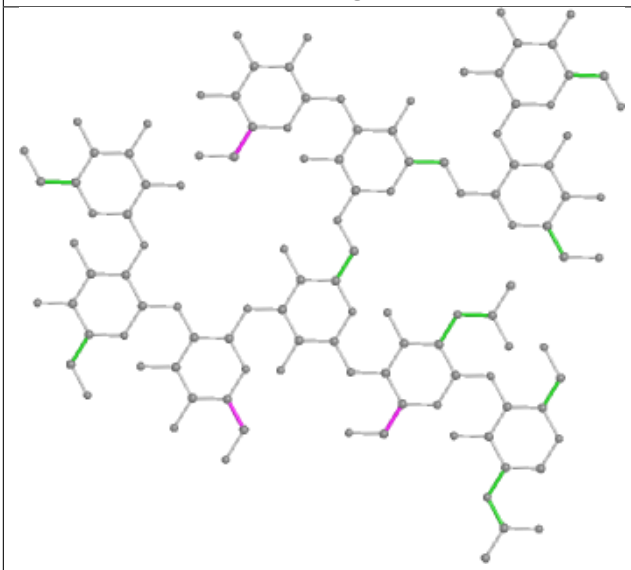
Oligosaccharide Chain K



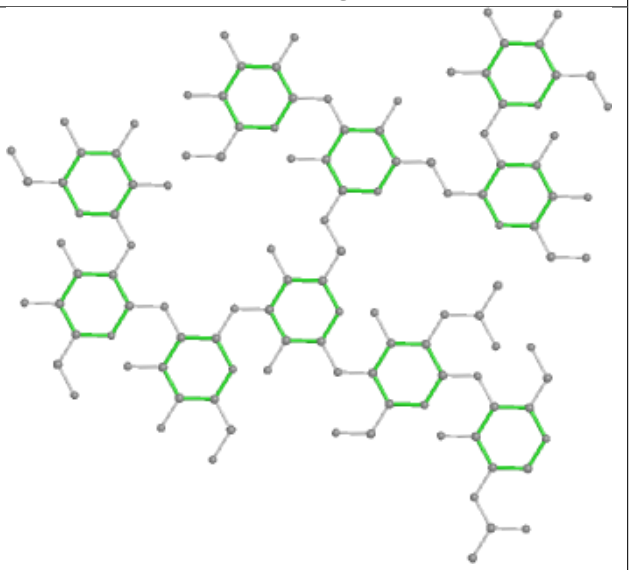
Bond lengths



Bond angles

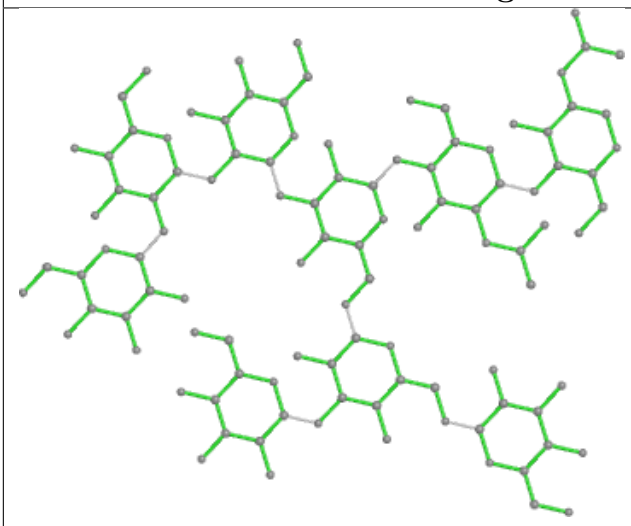


Torsions

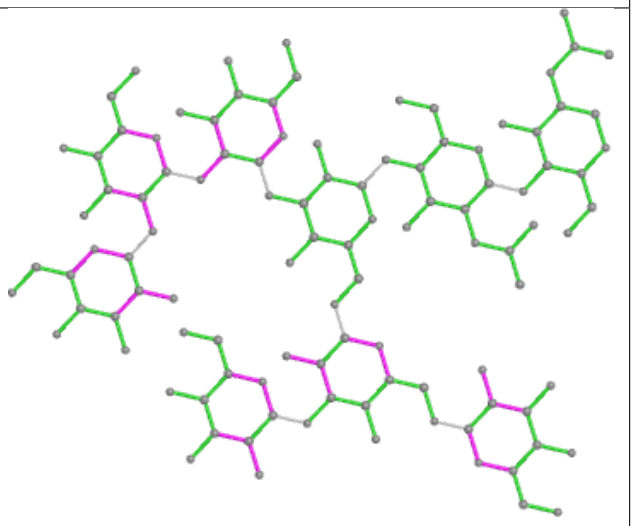


Rings

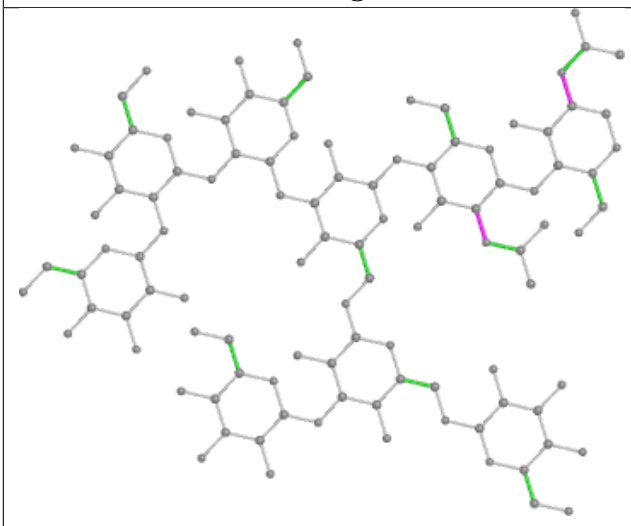
Oligosaccharide Chain L



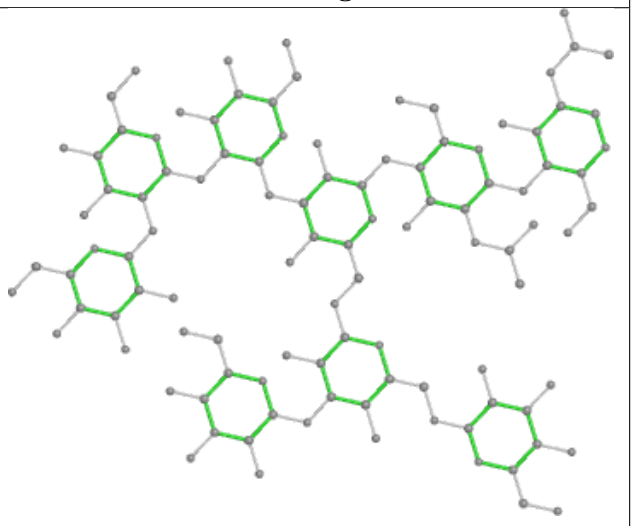
Bond lengths



Bond angles

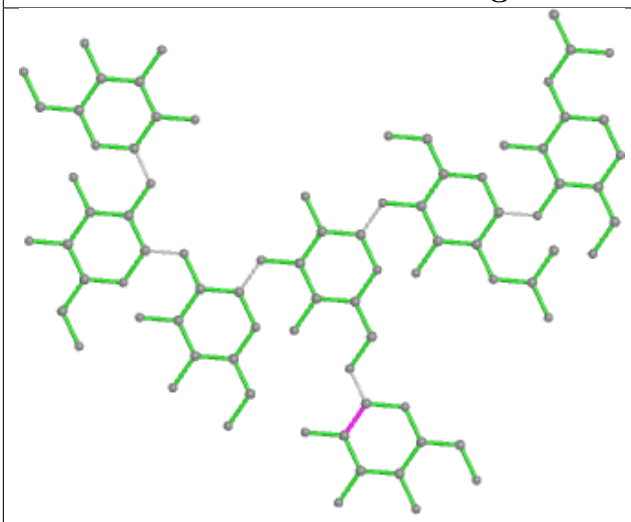


Torsions

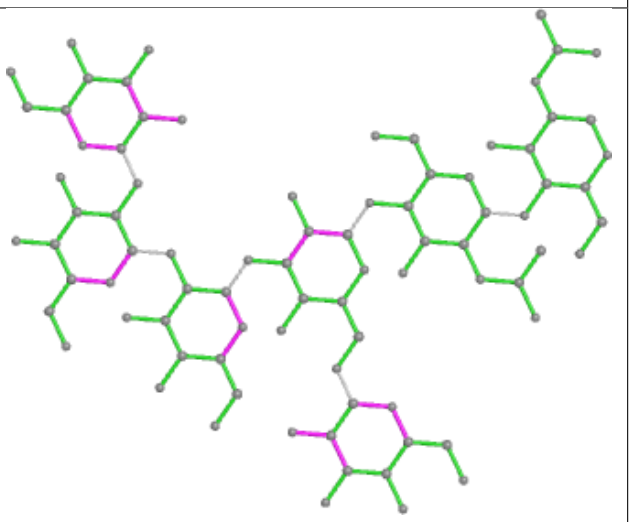


Rings

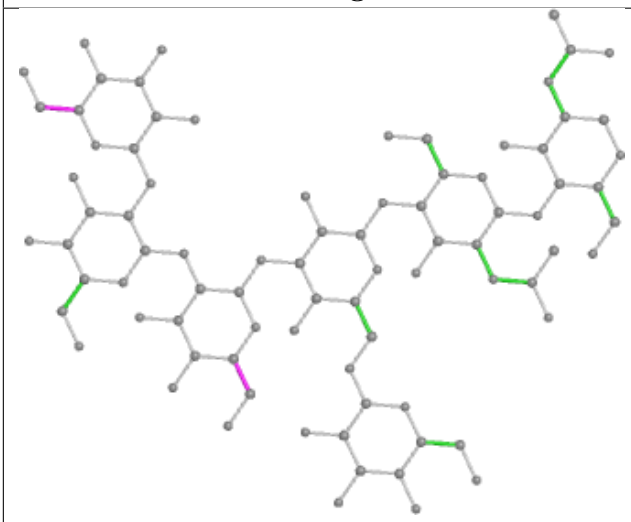
Oligosaccharide Chain M



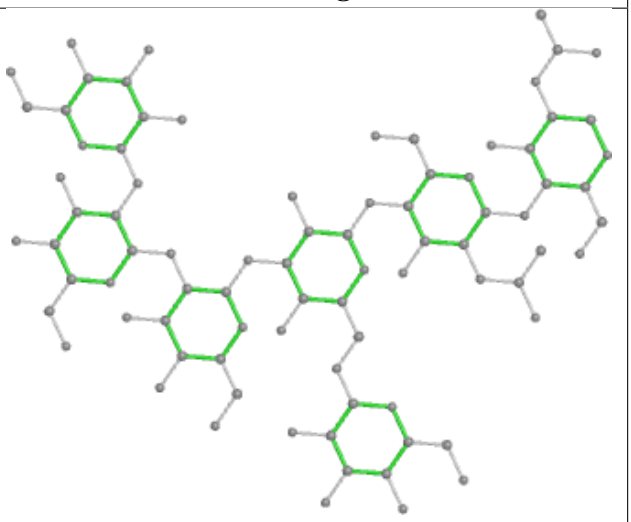
Bond lengths



Bond angles

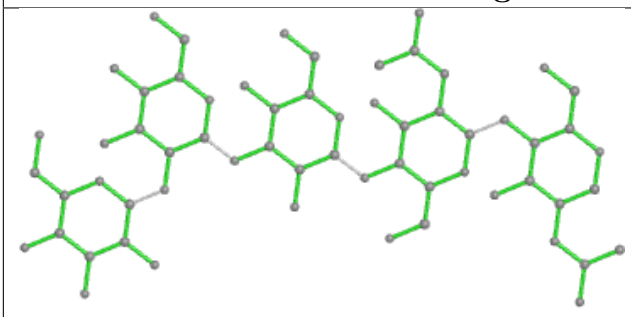


Torsions

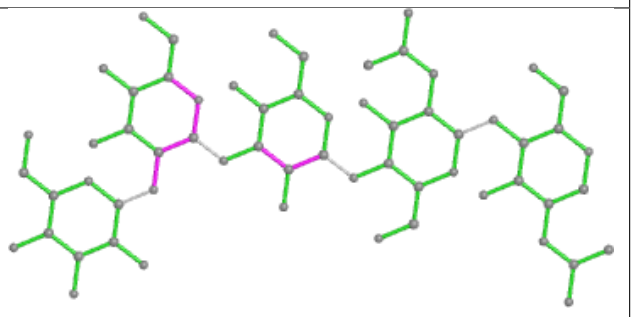


Rings

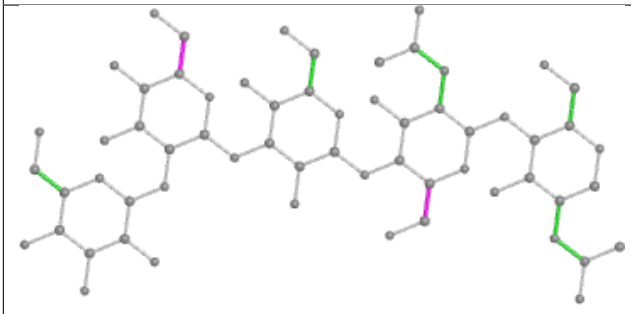
Oligosaccharide Chain N



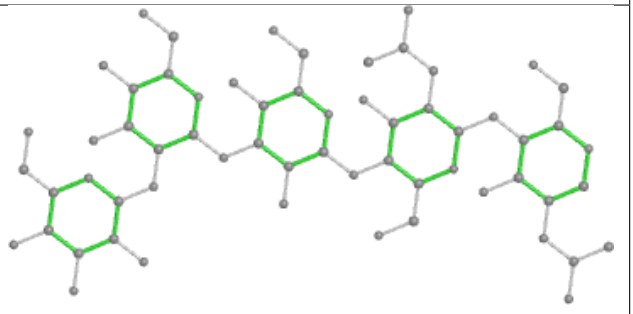
Bond lengths



Bond angles

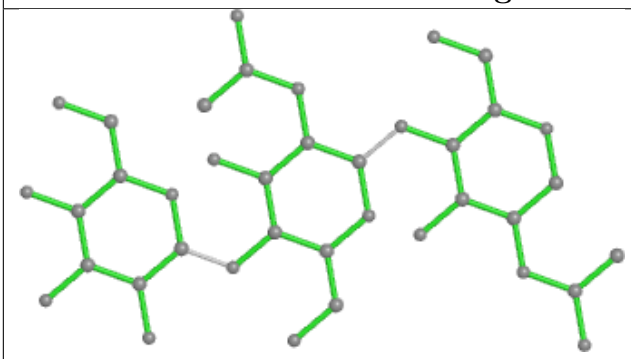


Torsions

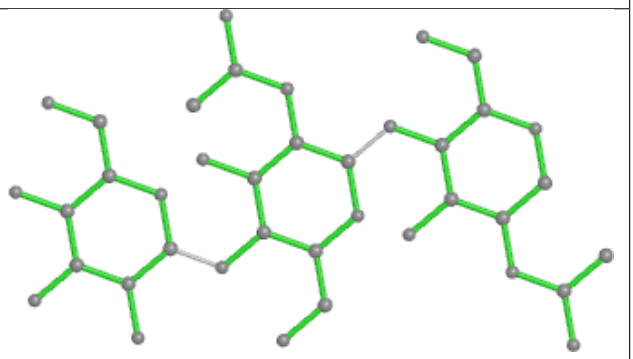


Rings

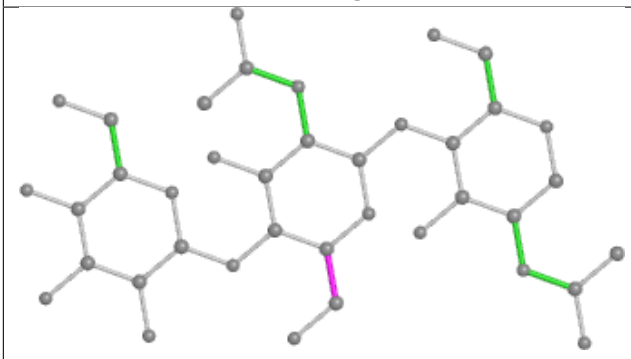
Oligosaccharide Chain O



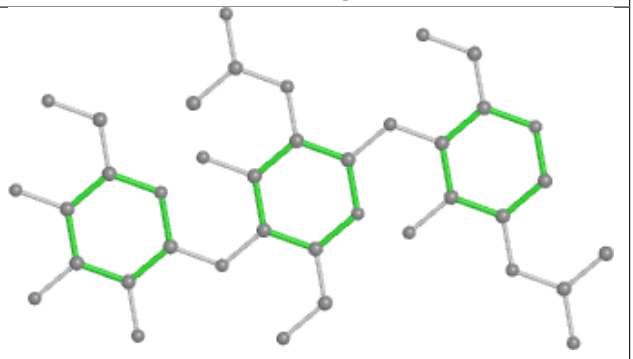
Bond lengths



Bond angles

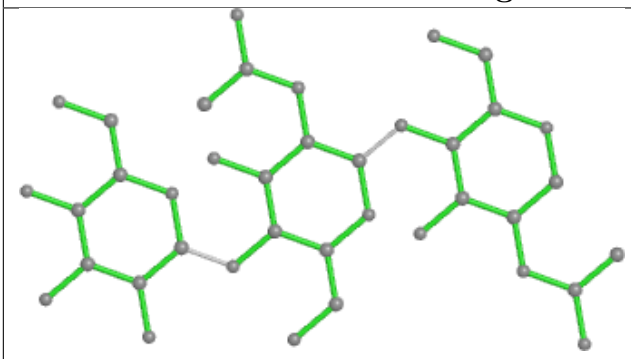


Torsions

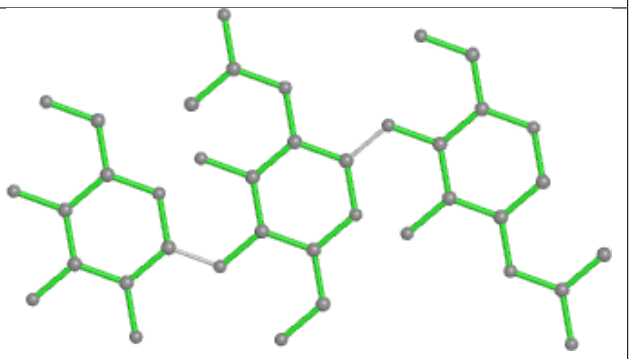


Rings

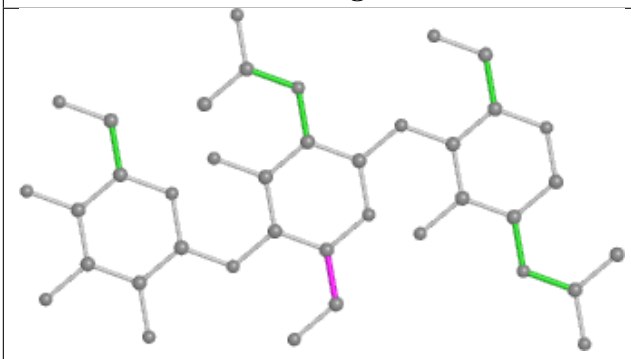
Oligosaccharide Chain P



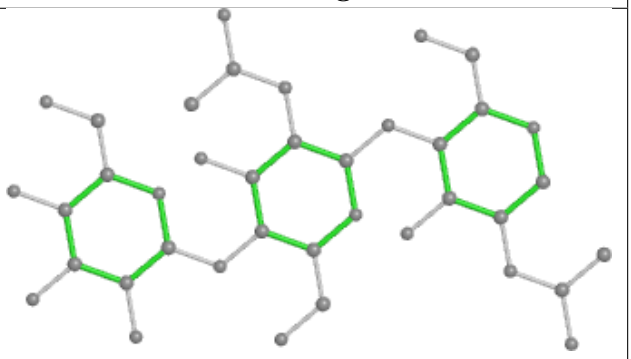
Bond lengths



Bond angles

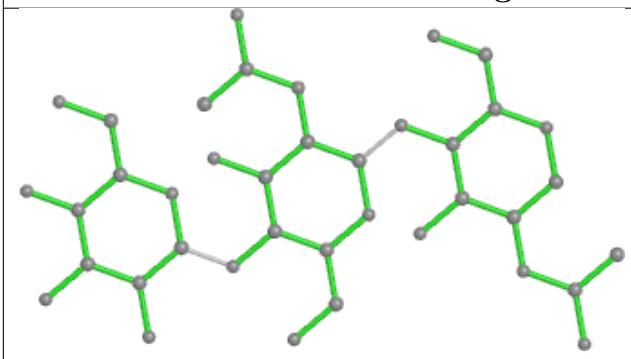


Torsions

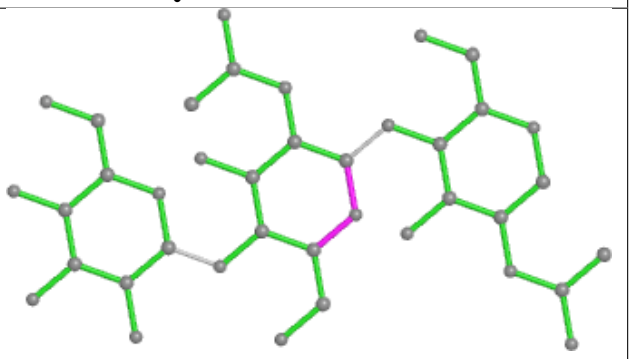


Rings

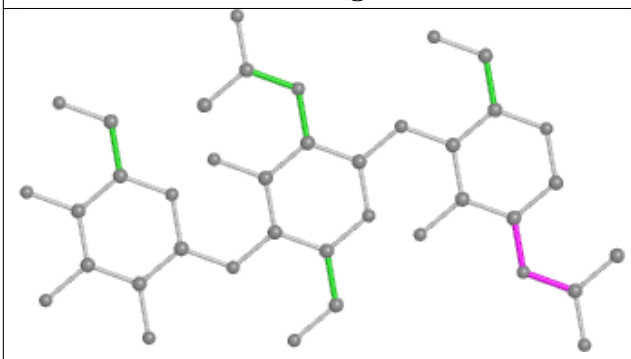
Oligosaccharide Chain Q



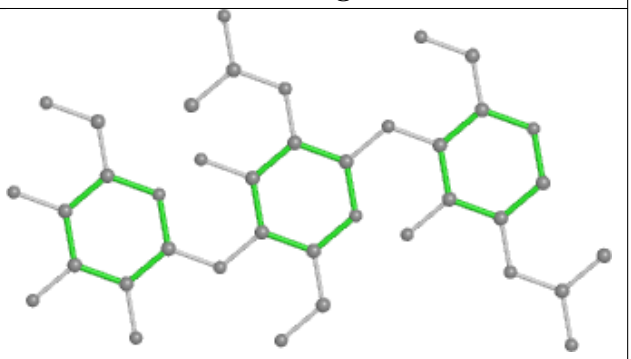
Bond lengths



Bond angles

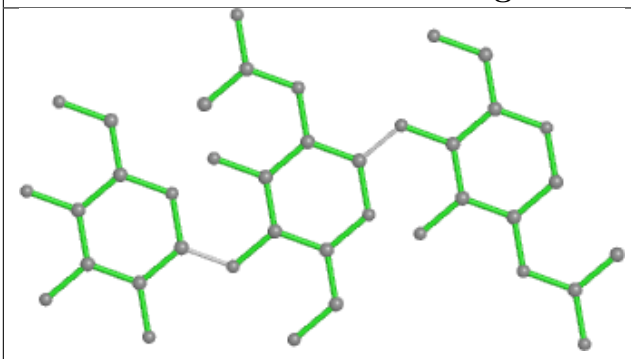


Torsions

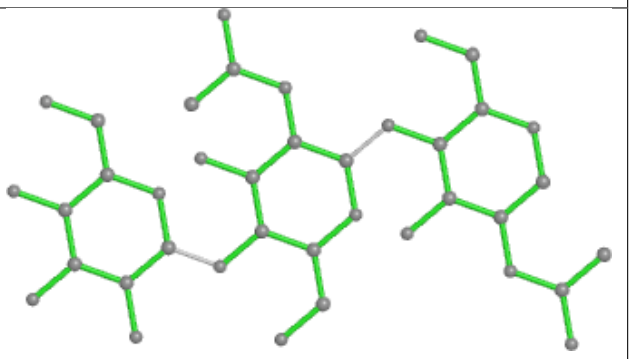


Rings

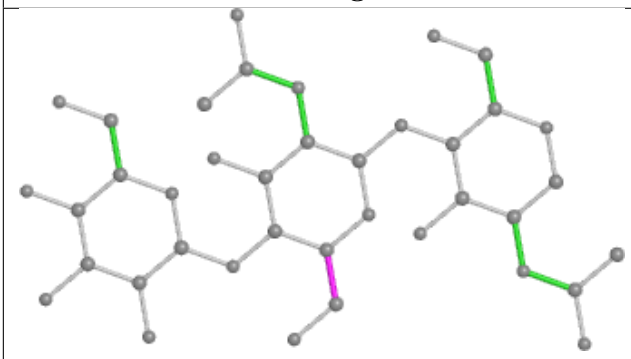
Oligosaccharide Chain R



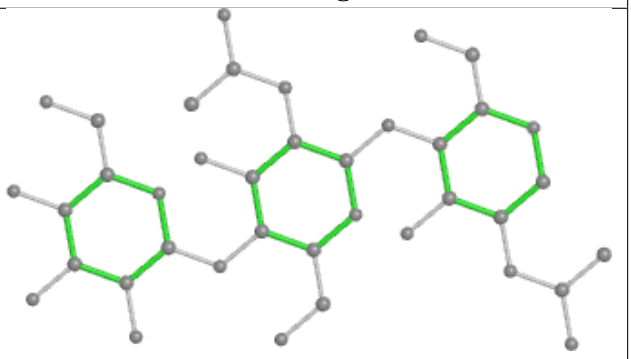
Bond lengths



Bond angles

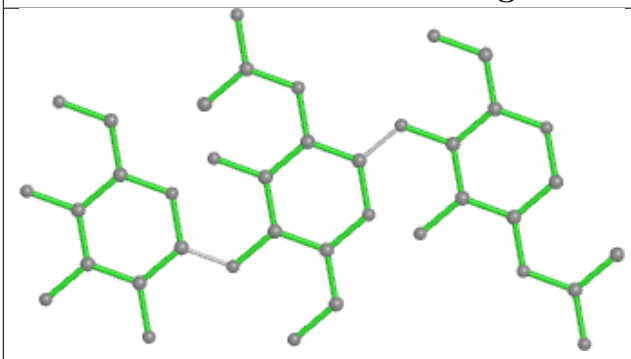


Torsions

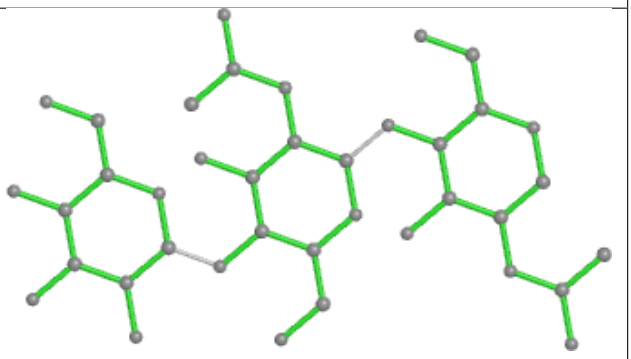


Rings

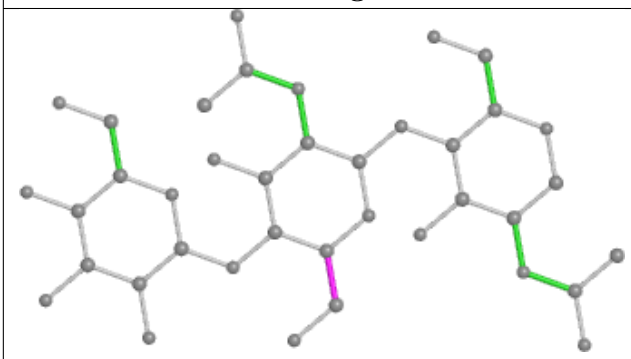
Oligosaccharide Chain S



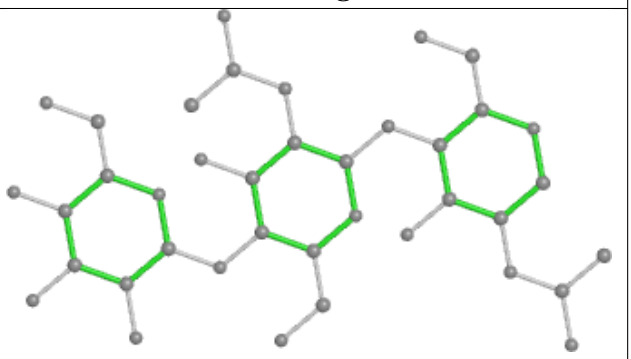
Bond lengths



Bond angles

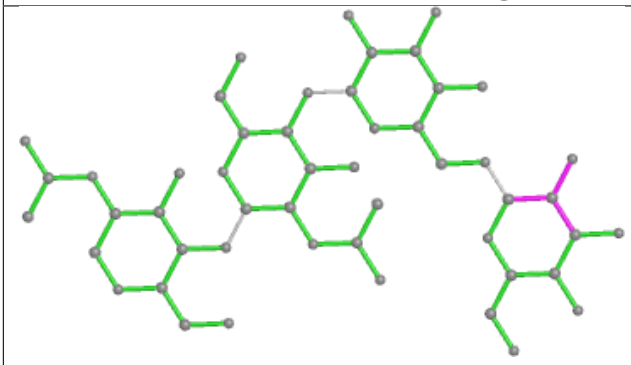


Torsions

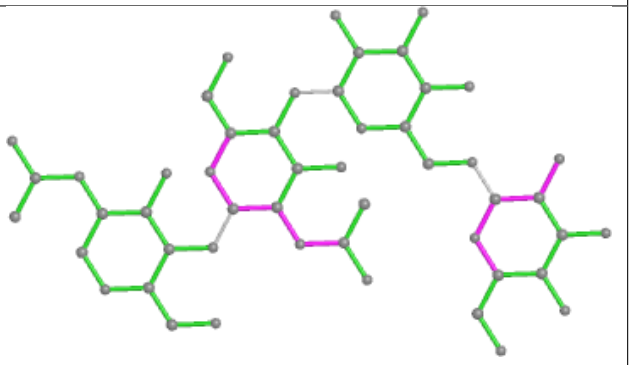


Rings

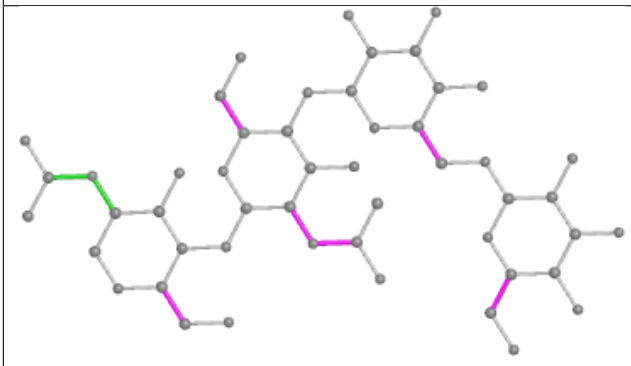
Oligosaccharide Chain T



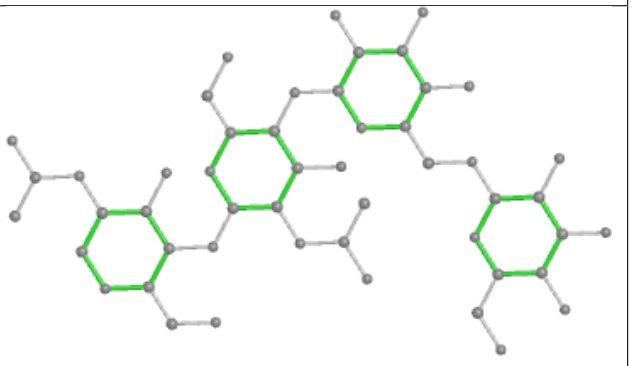
Bond lengths



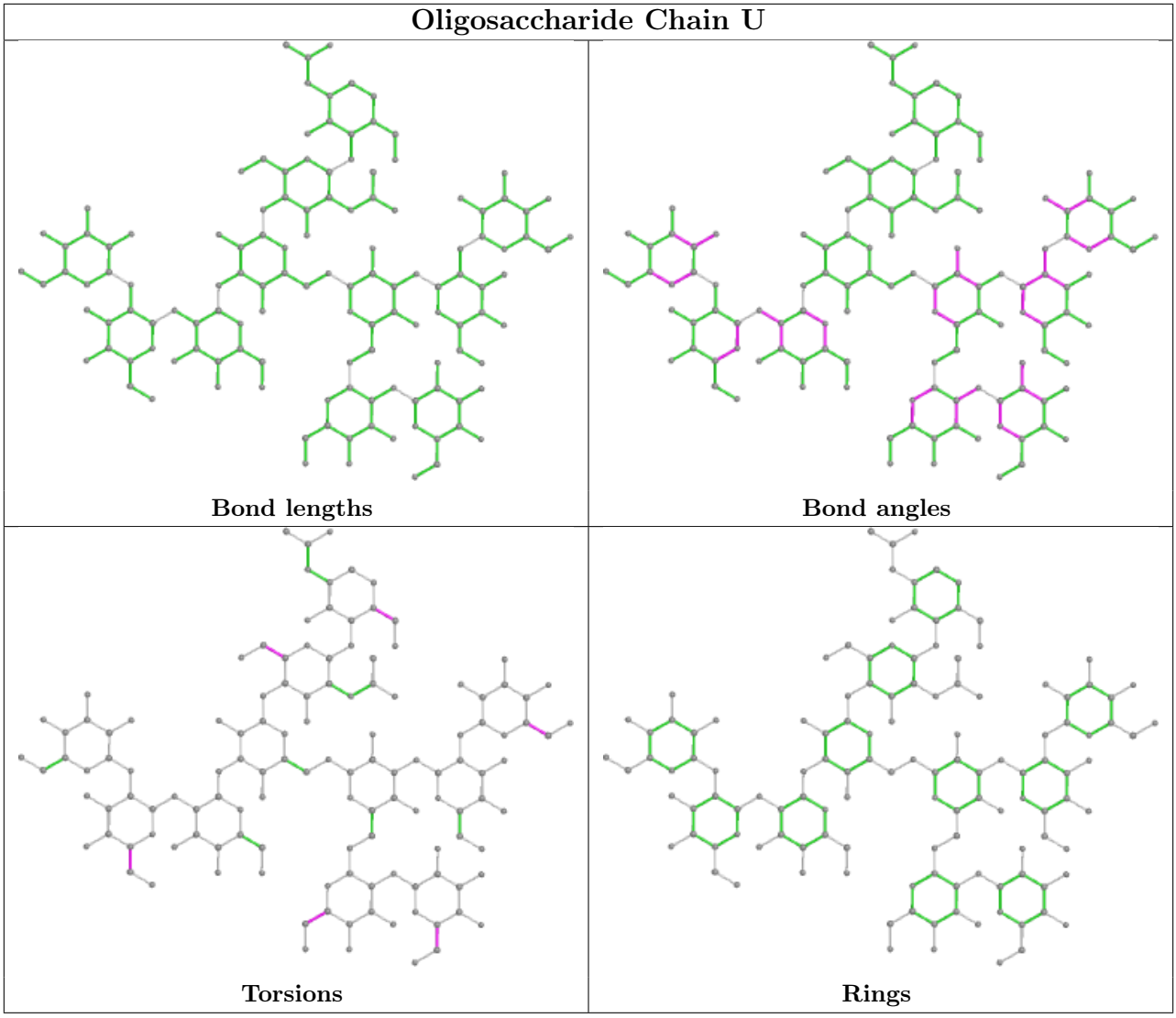
Bond angles



Torsions



Rings



5.6 Ligand geometry (i)

2 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	$\#\|Z\| > 2$
16	NAG	D	705	4	14,14,15	0.21	0	17,19,21	0.40	0
16	NAG	C	615	3	14,14,15	0.35	0	17,19,21	0.35	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
16	NAG	D	705	4	-	2/6/23/26	0/1/1/1
16	NAG	C	615	3	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
16	D	705	NAG	O5-C5-C6-O6
16	C	615	NAG	C4-C5-C6-O6
16	C	615	NAG	O5-C5-C6-O6
16	D	705	NAG	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

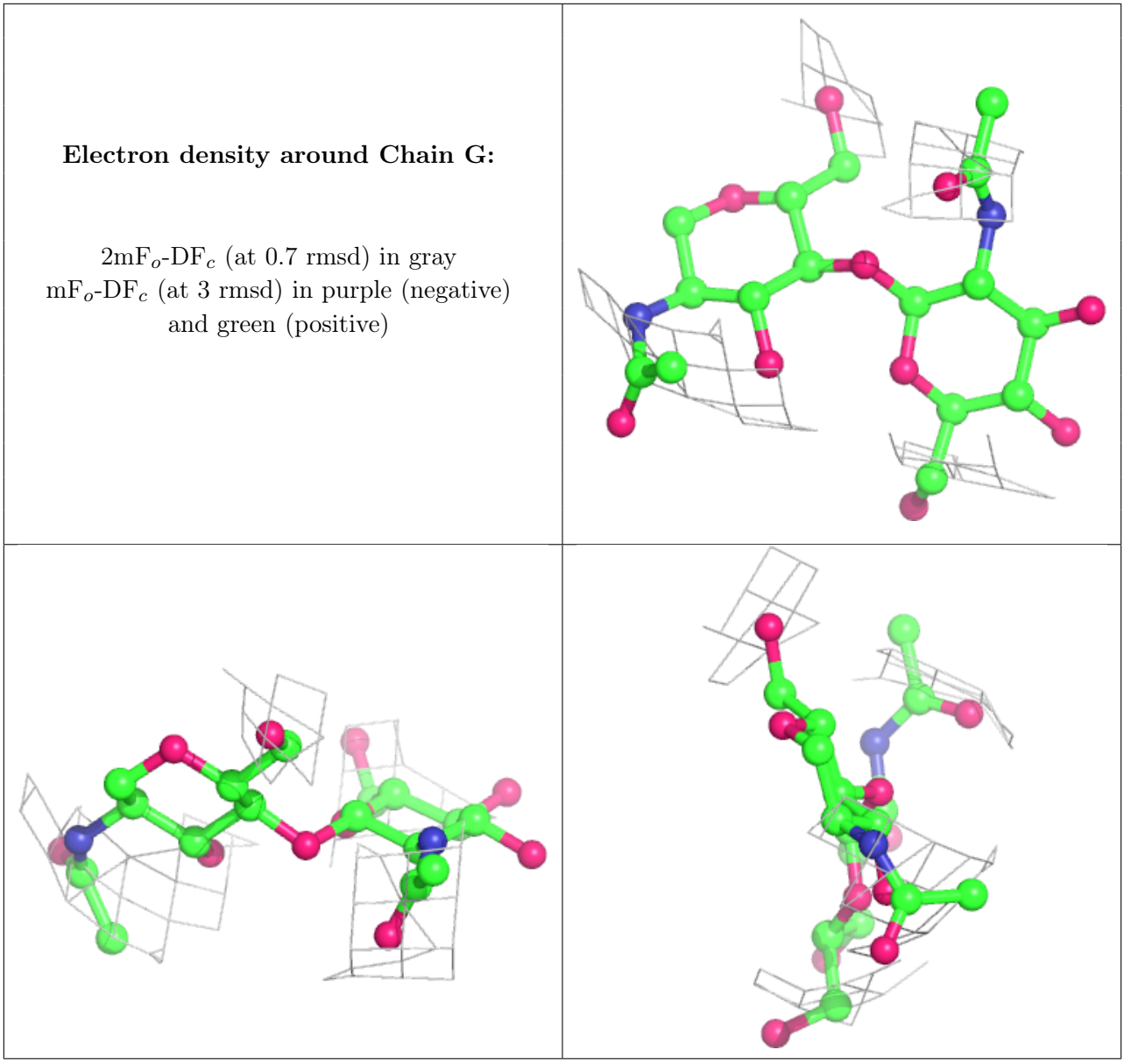
6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

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.

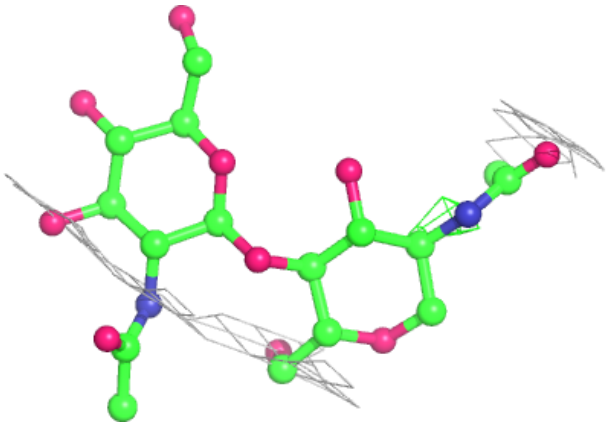
Electron density around Chain G:

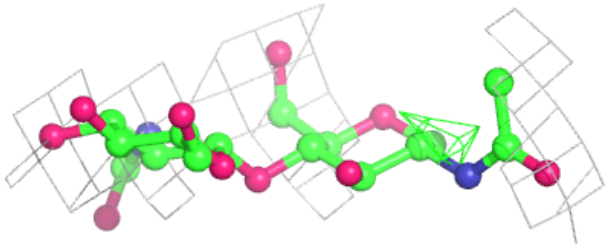
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

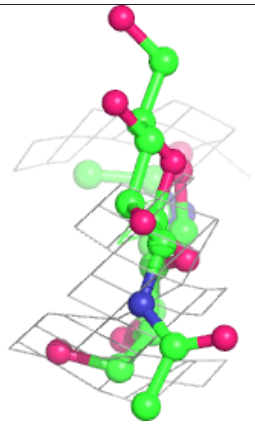


Electron density around Chain H:

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

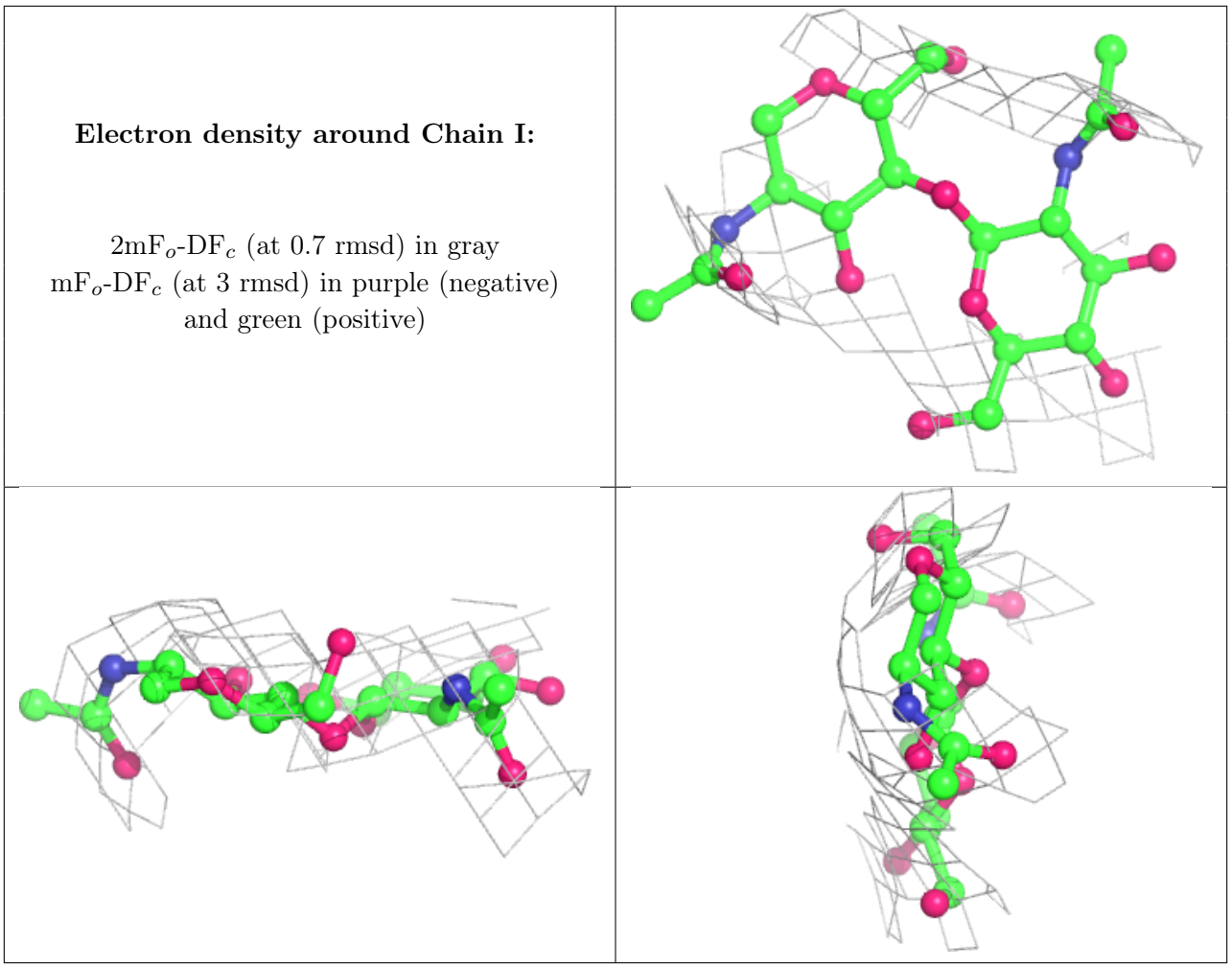






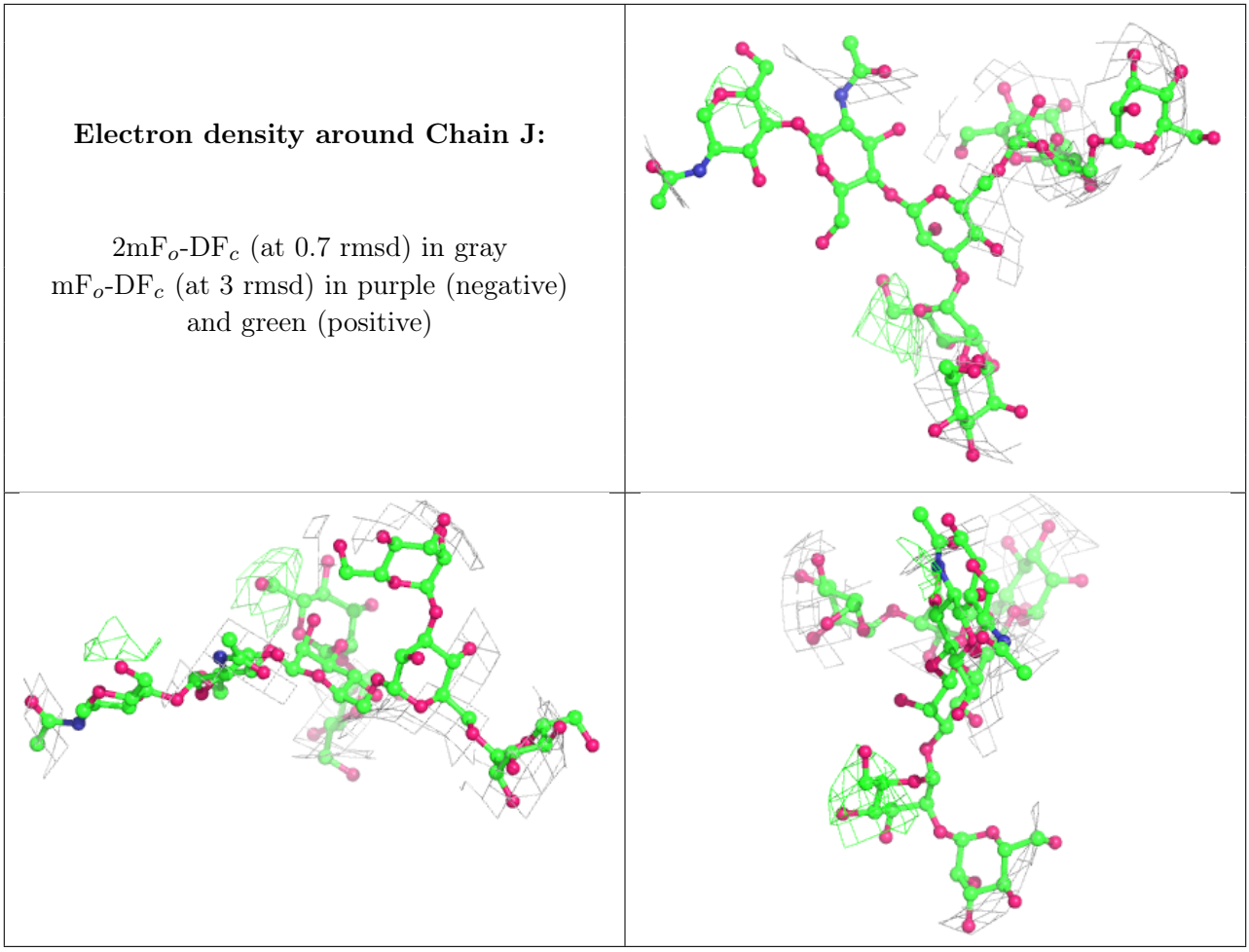
Electron density around Chain I:

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



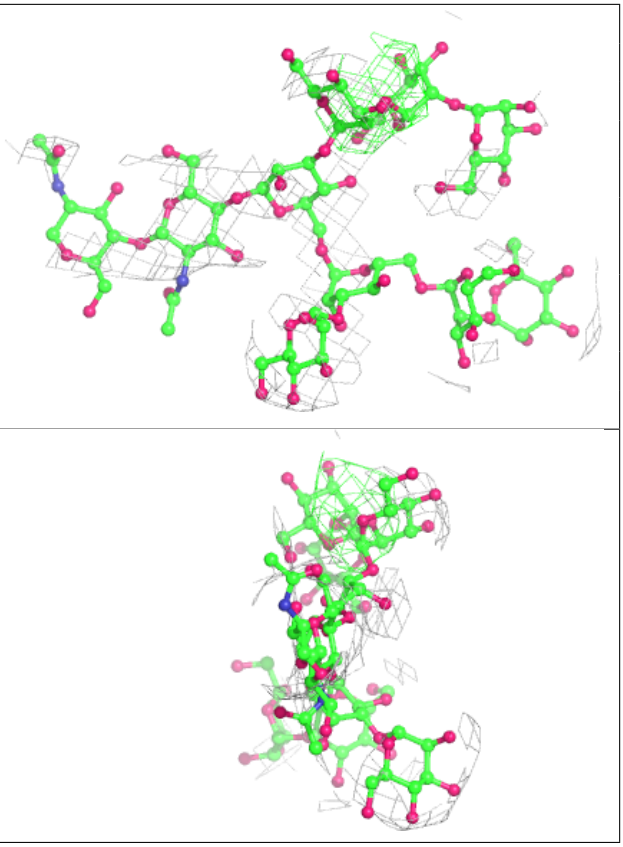
Electron density around Chain J:

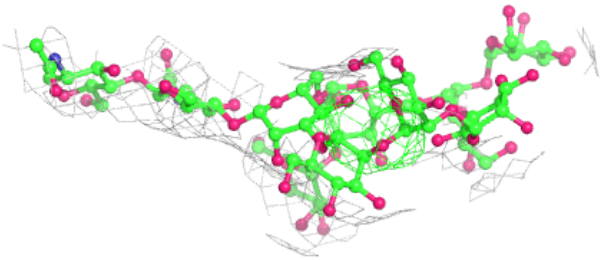
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around Chain K:

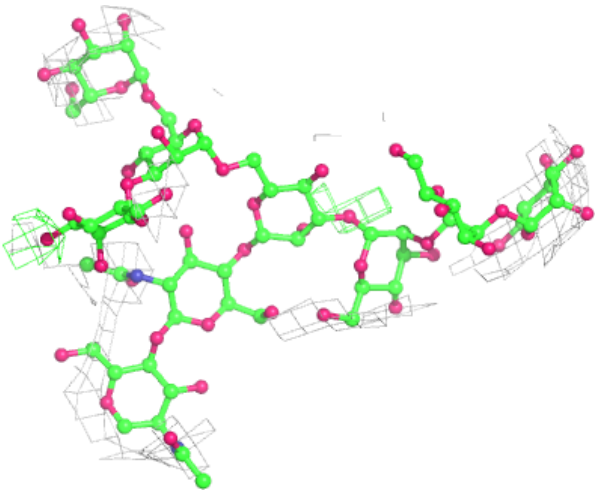
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

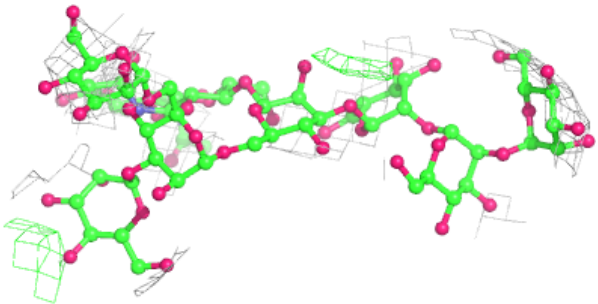


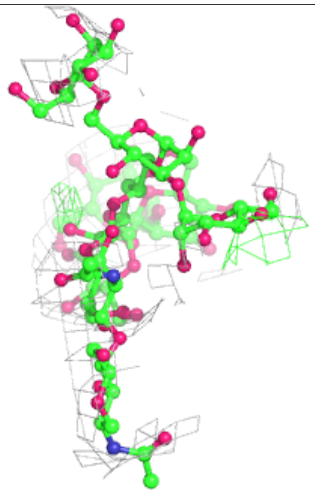


Electron density around Chain L:

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

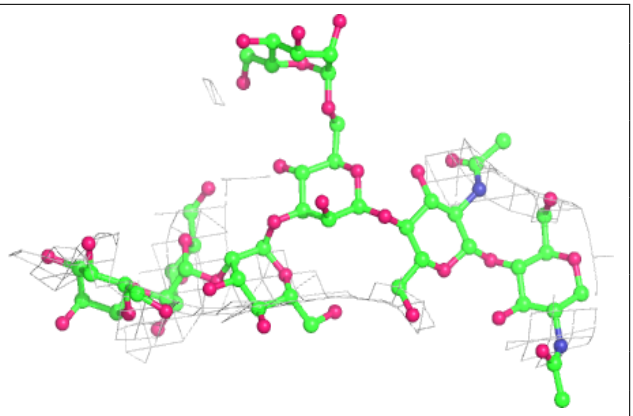


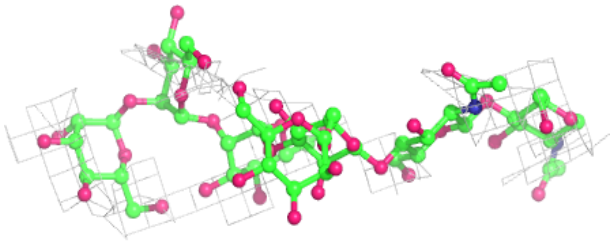


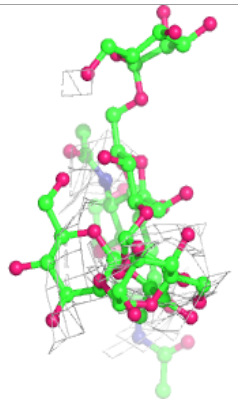


Electron density around Chain M:

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

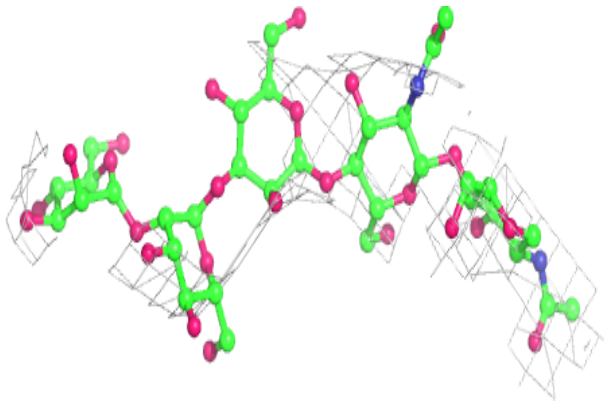


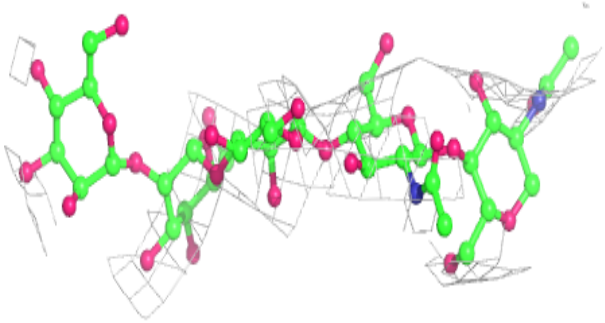


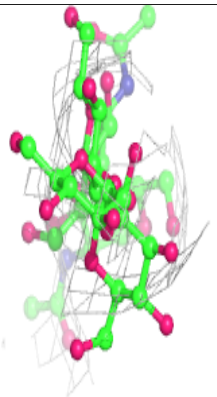


Electron density around Chain N:

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

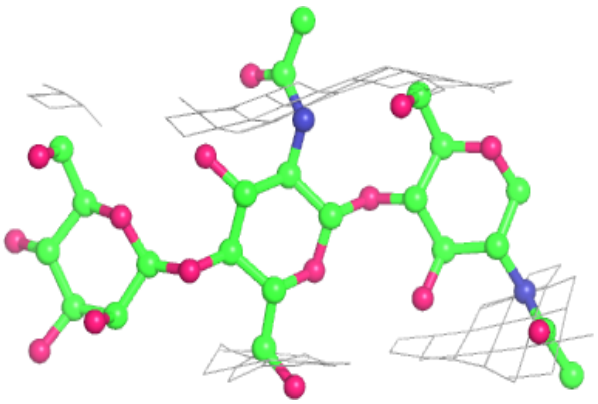


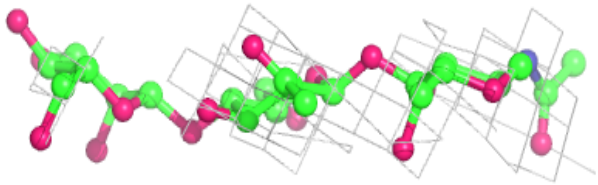


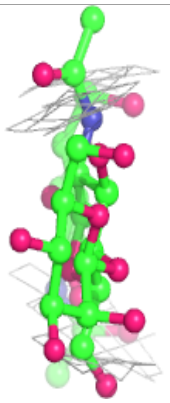


Electron density around Chain O:

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

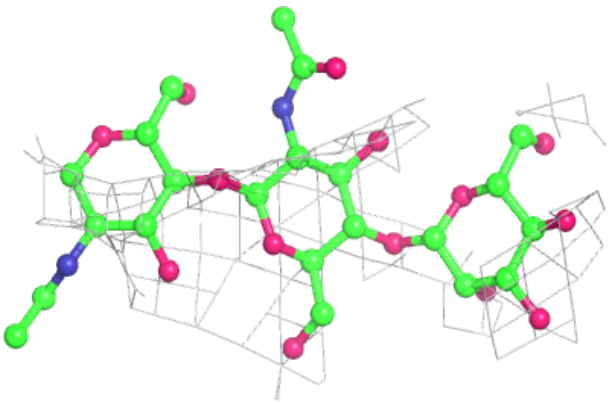


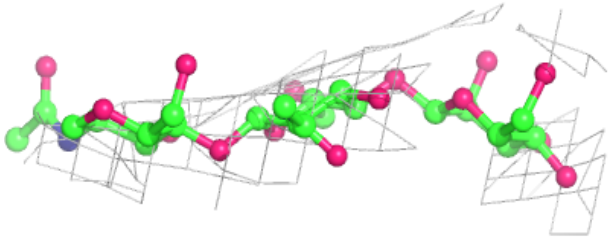


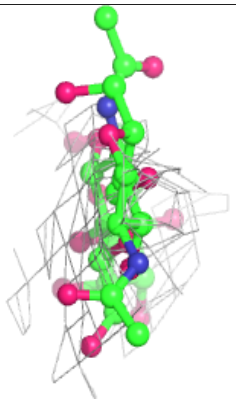


Electron density around Chain P:

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

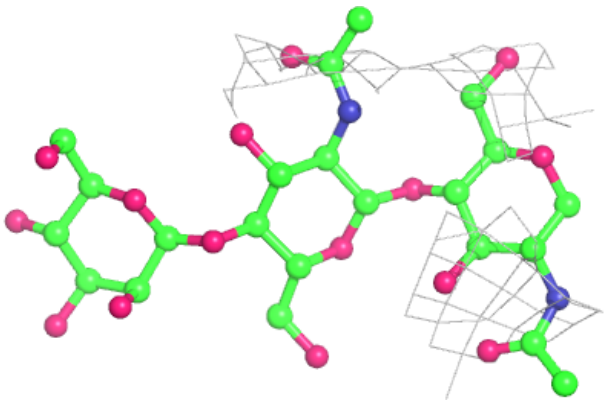


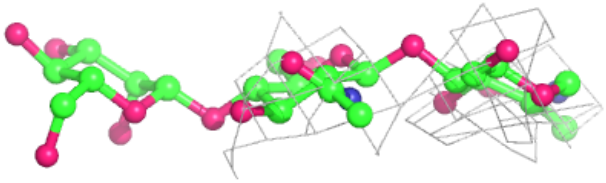


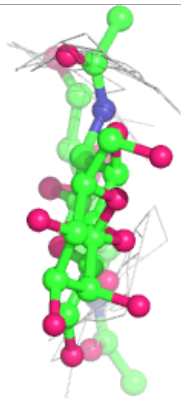


Electron density around Chain Q:

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

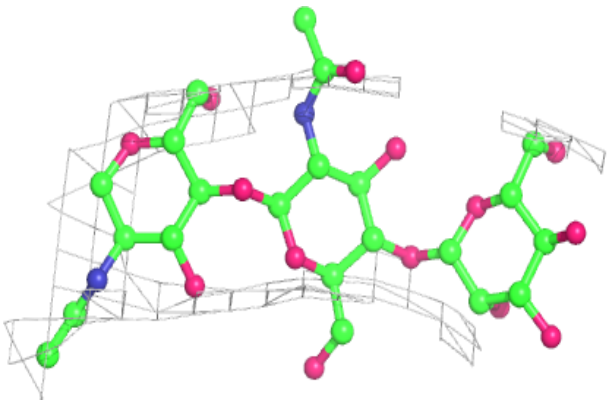


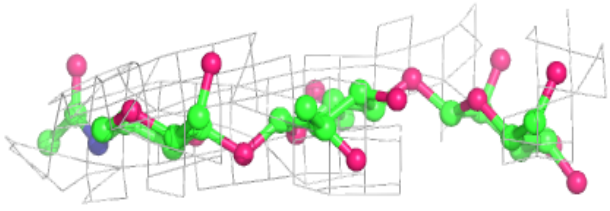


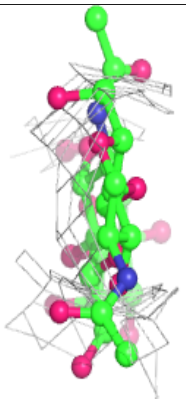


Electron density around Chain R:

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

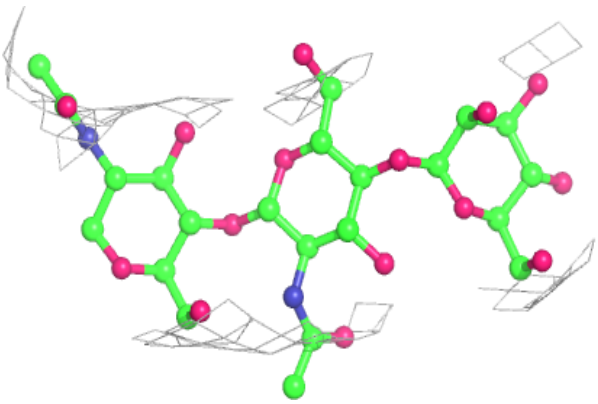


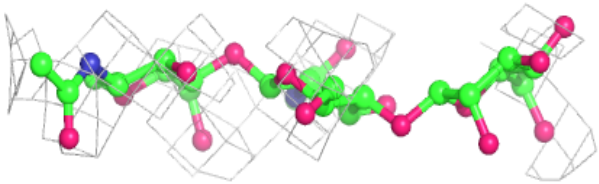


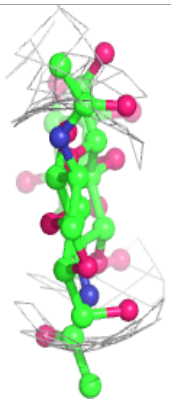


Electron density around Chain S:

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

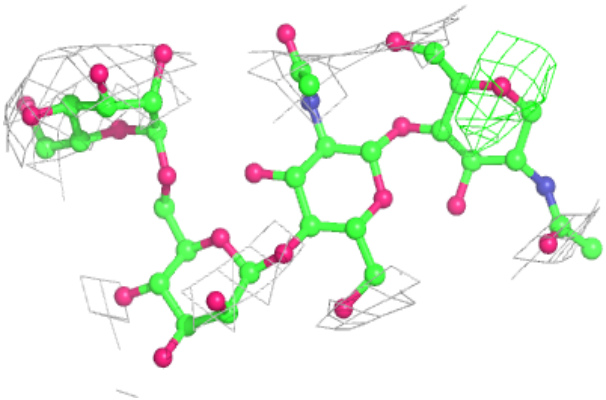


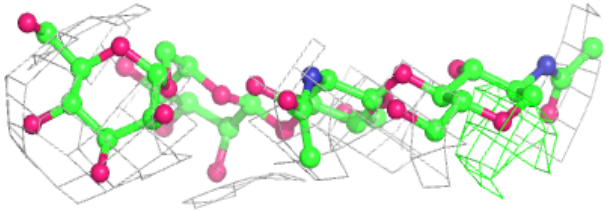


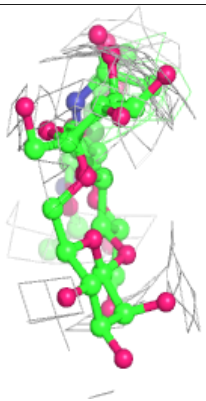


Electron density around Chain T:

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

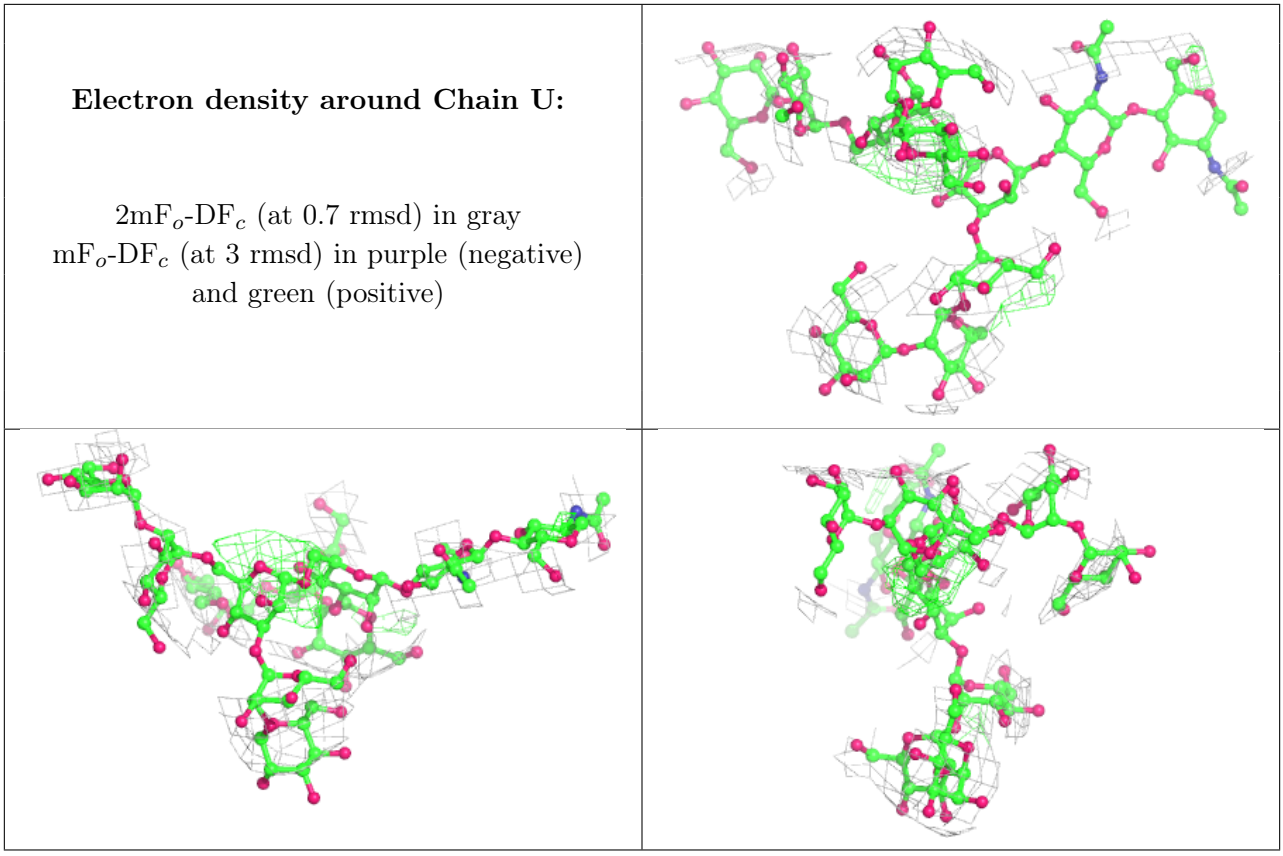






Electron density around Chain U:

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



6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers

Unable to reproduce the depositors R factor - this section is therefore empty.