Full wwPDB X-ray Structure Validation Report (i)

Sep 23, 2023 – 05:13 PM EDT

PDB ID	:	5T3Z
Title	:	3.5 Angstrom Crystal Structure of a Fully and Natively Glycosylated BG505 SOSIP.664 HIV-1 Env Trimer in Complex with the Broadly Neutralizing Antibodies IOMA and 10-1074
Authors	:	Gristick, H.B.; Bjorkman, P.J.
Deposited on	:	2016-08-26
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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

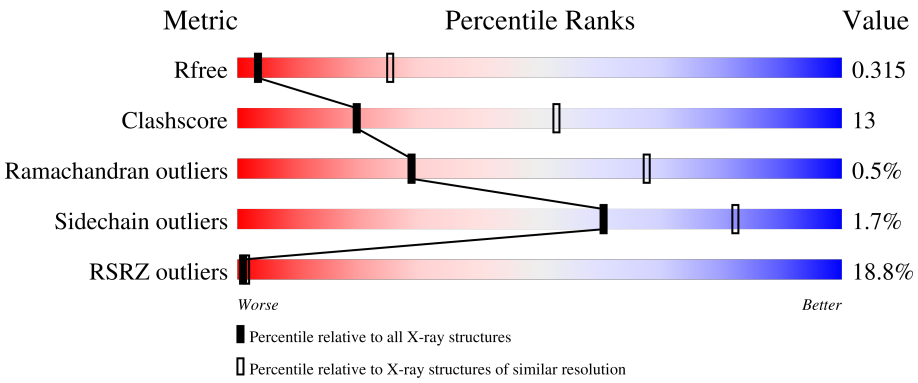
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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	B	153	6% 58% 24% • 18%
2	G	481	4% 67% 26% • 6%
3	H	238	19% 66% 30% •
4	L	214	24% 74% 23% ••
5	D	232	34% 62% 35% ••

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Mol	Chain	Length	Quality of chain
6	E	214	34% 71% 26%
7	A	2	100%
8	C	3	33% 67%
8	W	3	33% 67%
9	F	2	50% 50%
9	I	2	50% 50%
9	N	2	100%
9	Q	2	100%
10	J	11	9% 45% 45%
11	K	5	20% 40% 40%
11	U	5	20% 20% 60%
12	M	8	12% 25% 62%
13	O	7	29% 71%
14	P	8	38% 38% 25%
15	R	6	33% 67%
16	S	10	30% 40% 30%
17	T	7	29% 71%
18	V	4	50% 50%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	NAG	J	7	-	-	-	X
12	NAG	M	1	-	-	-	X
12	GAL	M	6	-	-	-	X
13	MAN	O	7	-	-	-	X
14	FUC	P	8	-	-	-	X
15	MAN	R	6	-	-	-	X
19	NAG	G	3390	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
9	NAG	F	2	-	-	-	X

2 Entry composition (i)

There are 19 unique types of molecules in this entry. The entry contains 12300 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 gp160.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	B	126	1001	633	172	190	6	0	0	0

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 2 is a protein called Envelope glycoprotein gp160.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	G	450	3538	2221	624	666	27	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	332	ASN	THR	engineered mutation	UNP Q2N0S6
G	501	CYS	ALA	engineered mutation	UNP Q2N0S6
G	509	ARG	-	expression tag	UNP Q2N0S6
G	510	ARG	-	expression tag	UNP Q2N0S6
G	512	ARG	-	expression tag	UNP Q2N0S6
G	513	ARG	-	expression tag	UNP Q2N0S6

- Molecule 3 is a protein called 10-1074 Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	H	230	1753	1108	293	345	7	0	0	0

- Molecule 4 is a protein called 10-1074 Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	L	211	1607	1006	281	314	6	0	0	0

- Molecule 5 is a protein called IOMA Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	D	229	1742	1100	298	332	12	0	0	0

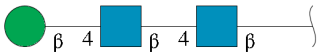
- Molecule 6 is a protein called IOMA Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	E	210	1558	976	261	317	4	0	0	0

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
7	A	2	24	14	1	9	0	0	0

- 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.

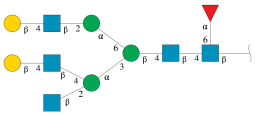


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
8	C	3	39	22	2	15	0	0	0
8	W	3	39	22	2	15	0	0	0

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

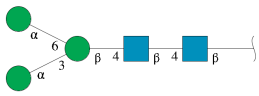
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
9	F	2	28	16	2	10	0	0	0
9	I	2	28	16	2	10	0	0	0
9	N	2	28	16	2	10	0	0	0
9	Q	2	28	16	2	10	0	0	0

- Molecule 10 is an oligosaccharide called beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)]alpha-D-mannopyranose-(1-3)-[beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



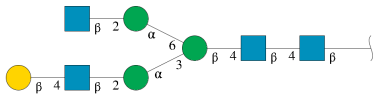
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
10	J	11	135	76	5	54	0	0	0

- 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.



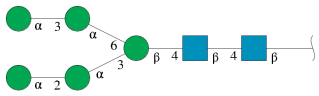
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
11	K	5	61	34	2	25	0	0	0
11	U	5	61	34	2	25	0	0	0

- Molecule 12 is an oligosaccharide called beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



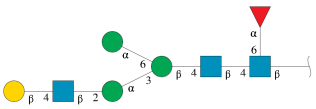
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
12	M	8	100	56	4	40	0	0	0

- Molecule 13 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



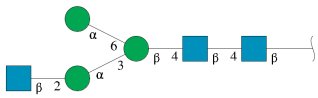
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
13	O	7	83	46	2	35	0	0	0

- Molecule 14 is an oligosaccharide called beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(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)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



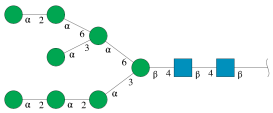
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
14	P	8	96	54	3	39	0	0	0

- Molecule 15 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(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.



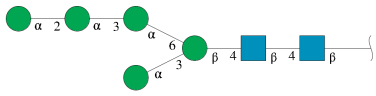
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
15	R	6	75	42	3	30	0	0	0

- Molecule 16 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.



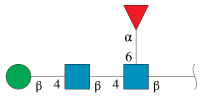
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
16	S	10	116	64	2	50	0	0	0

- Molecule 17 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



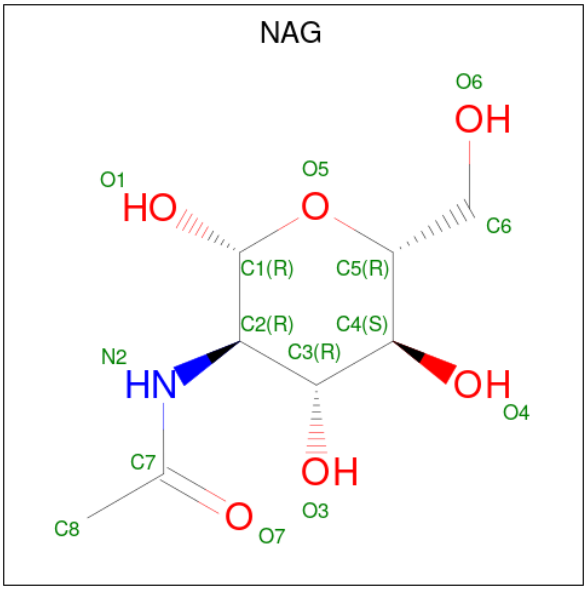
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
17	T	7	83	46	2	35	0	0	0

- Molecule 18 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
18	V	4	49	28	2	19	0	0	0

- Molecule 19 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



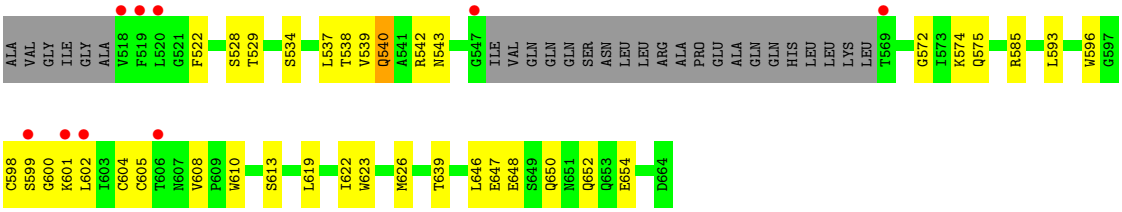
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
19	G	1	14	8	1	5	0	0
			Total	C	N	O		
19	G	1	14	8	1	5	0	0

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.

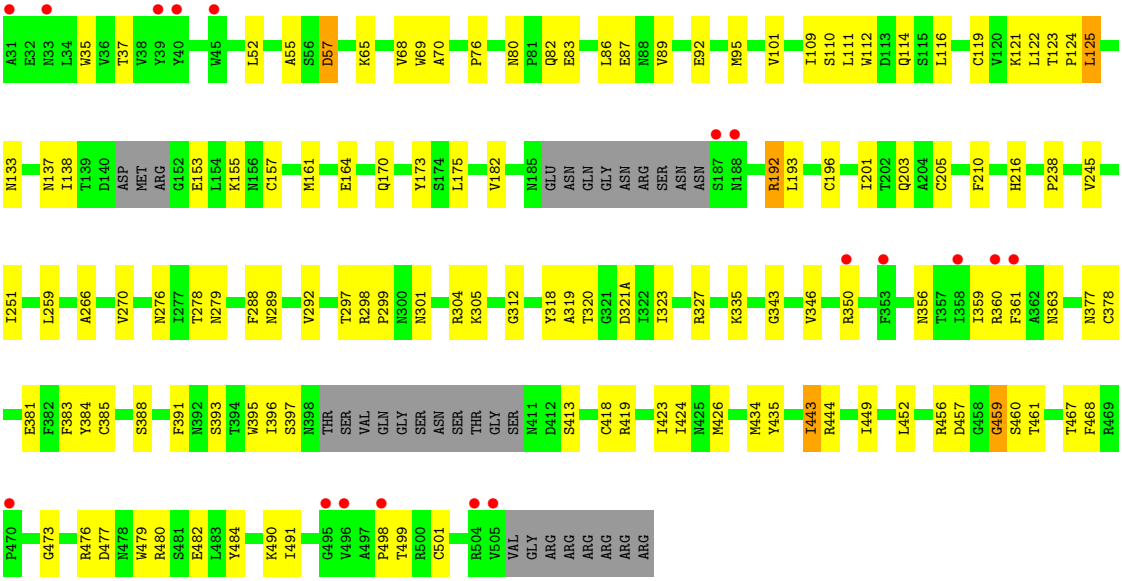
• Molecule 1: Envelope glycoprotein gp160

Chain B:



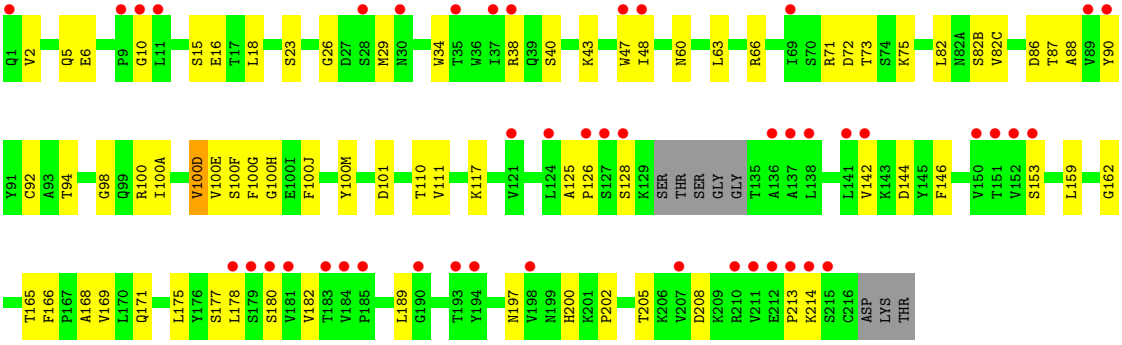
• Molecule 2: Envelope glycoprotein gp160

Chain G:



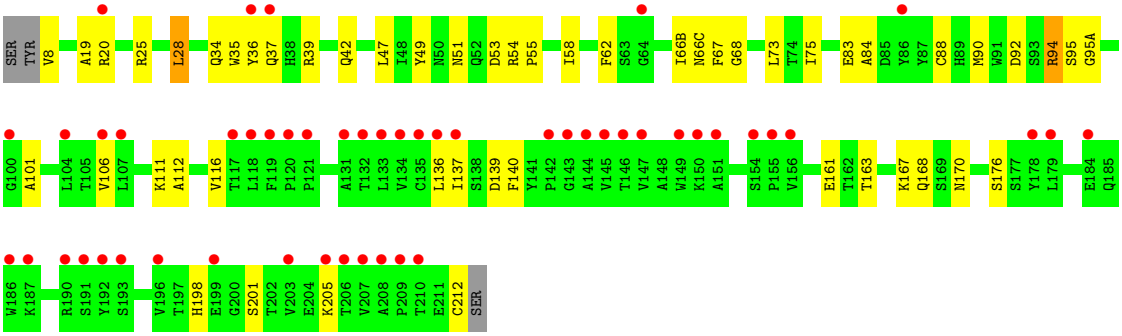
• Molecule 3: 10-1074 Heavy Chain

Chain H:



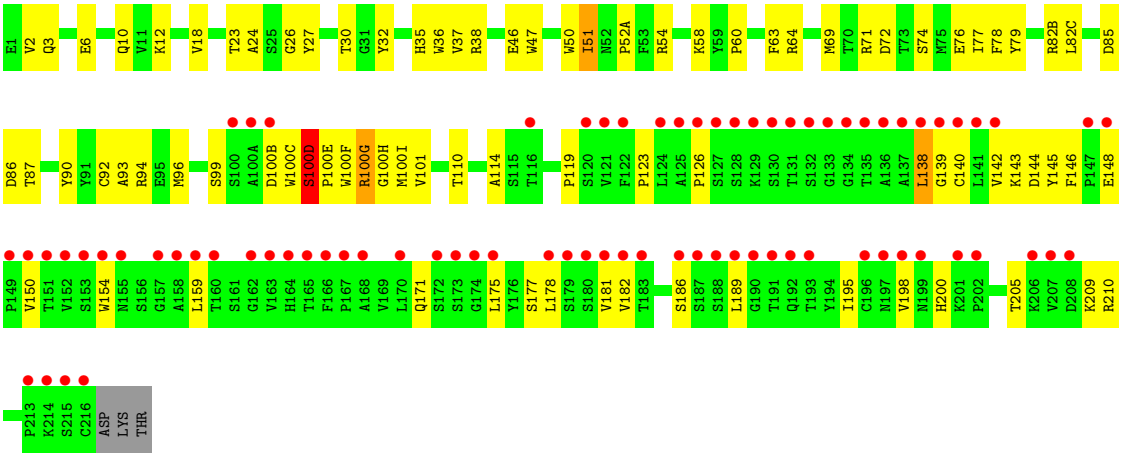
- Molecule 4: 10-1074 Light Chain

Chain L:



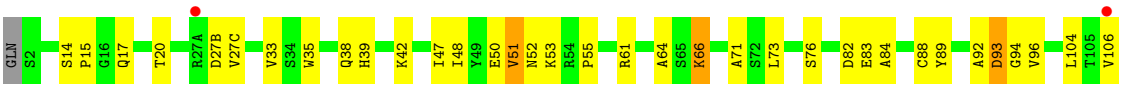
- Molecule 5: IOMA Heavy Chain

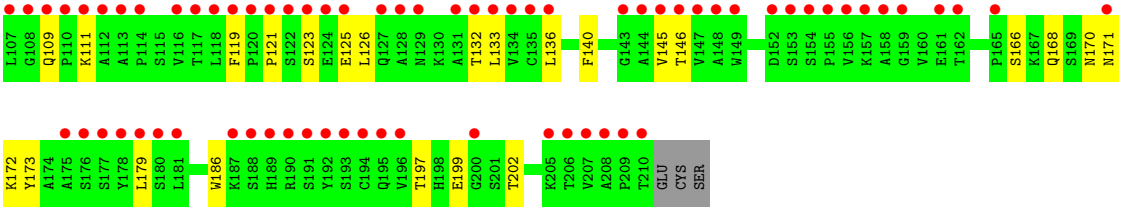
Chain D:



- Molecule 6: IOMA Light Chain

Chain E:





• Molecule 7: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain A: 100%

• 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: 33% 67%

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

Chain W: 33% 67%

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

Chain F: 50% 50%

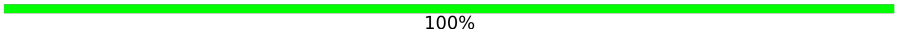
• Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I: 50% 50%

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

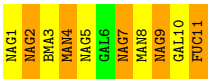
Chain N: 100%

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

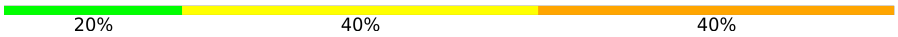
Chain Q: 

• Molecule 10: beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)]alpha-D-mannopyranose-(1-3)-[beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:



• 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 K: 

• 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 U:

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

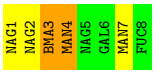
Chain M:

• Molecule 13: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O: 29% 71%

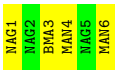
• Molecule 14: beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain P: 38% 38% 25%



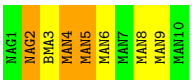
• Molecule 15: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain R: 33% 67%



• Molecule 16: 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 S: 30% 40% 30%



• Molecule 17: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain T: 29% 71%

• Molecule 18: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain V: 50% 50%

4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α, β, γ	217.26Å 217.26Å 154.94Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	64.63 – 3.50 80.41 – 3.50	Depositor EDS
% Data completeness (in resolution range)	100.0 (64.63-3.50) 94.8 (80.41-3.50)	Depositor EDS
R_{merge}	0.68	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.36 (at 3.49Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.275 , 0.298 0.290 , 0.315	Depositor DCC
R_{free} test set	1755 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å^2)	112.0	Xtriage
Anisotropy	0.022	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 155.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	0.055 for h,-h-k,-l	Xtriage
Reported twinning fraction	0.130 for k,h,-l	Depositor
Outliers	0 of 34373 reflections	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	12300	wwPDB-VP
Average B, all atoms (Å^2)	211.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.57% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, FUC, GAL, NAG, 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	B	0.25	0/1019	0.45	0/1382
2	G	0.28	0/3611	0.50	0/4903
3	H	0.25	0/1796	0.47	0/2450
4	L	0.27	0/1649	0.47	0/2250
5	D	0.29	0/1790	0.57	2/2437 (0.1%)
6	E	0.25	0/1596	0.47	0/2175
All	All	0.27	0/11461	0.50	2/15597 (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})
5	D	100(D)	SER	C-N-CD	-7.65	103.77	120.60
5	D	100(D)	SER	C-N-CA	6.00	147.21	122.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1001	0	976	24	1
2	G	3538	0	3469	86	0
3	H	1753	0	1719	49	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	L	1607	0	1550	37	0
5	D	1742	0	1698	73	0
6	E	1558	0	1511	37	0
7	A	24	0	22	1	0
8	C	39	0	34	0	0
8	W	39	0	34	0	0
9	F	28	0	25	2	0
9	I	28	0	25	0	0
9	N	28	0	25	1	0
9	Q	28	0	25	0	0
10	J	135	0	115	6	0
11	K	61	0	52	1	0
11	U	61	0	52	2	0
12	M	100	0	85	4	0
13	O	83	0	70	0	0
14	P	96	0	82	1	0
15	R	75	0	64	0	0
16	S	116	0	97	3	0
17	T	83	0	70	7	0
18	V	49	0	43	0	0
19	G	28	0	26	0	0
All	All	12300	0	11869	306	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 13.

All (306) 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)
5:D:82(B):ARG:HH22	17:T:5:MAN:H5	1.24	0.98
5:D:119:PRO:HD2	5:D:205:THR:HB	1.62	0.80
2:G:87:GLU:HB3	9:F:1:NAG:H82	1.67	0.76
2:G:457:ASP:OD2	2:G:467:THR:HB	1.85	0.76
2:G:92:GLU:HA	2:G:238:PRO:HA	1.67	0.74
10:J:5:NAG:H81	10:J:9:NAG:H82	1.71	0.73
1:B:647:GLU:HG3	1:B:648:GLU:HG3	1.71	0.72
5:D:96:MET:HG3	5:D:100(H):GLY:HA3	1.69	0.72
2:G:297:THR:HG22	2:G:444:ARG:HG3	1.72	0.71
2:G:95:MET:HB3	2:G:484:TYR:HA	1.73	0.71
1:B:605:CYS:HA	2:G:37:THR:HG22	1.74	0.70
3:H:197:ASN:ND2	3:H:208:ASP:OD2	2.26	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:87:THR:HG23	5:D:110:THR:HA	1.76	0.68
6:E:27(B):ASP:HB3	6:E:92:ALA:HB2	1.76	0.66
2:G:350:ARG:NH2	2:G:396:ILE:O	2.28	0.66
4:L:83:GLU:HG2	4:L:106:VAL:H	1.61	0.66
5:D:60:PRO:HG2	5:D:63:PHE:HD2	1.61	0.66
3:H:88:ALA:HB3	3:H:90:TYR:HE1	1.61	0.65
5:D:52(A):PRO:HG3	5:D:78:PHE:HZ	1.61	0.65
2:G:473:GLY:O	5:D:54:ARG:NH1	2.30	0.65
11:K:1:NAG:H61	11:K:2:NAG:H82	1.79	0.65
3:H:15:SER:HA	3:H:82(B):SER:HA	1.78	0.64
2:G:298:ARG:HB3	2:G:443:ILE:HB	1.80	0.64
5:D:12:LYS:HG3	5:D:18:VAL:HG21	1.80	0.64
5:D:82(B):ARG:NH2	17:T:5:MAN:H5	2.06	0.63
4:L:39:ARG:NH1	4:L:83:GLU:O	2.30	0.63
6:E:50:GLU:OE1	6:E:53:LYS:NZ	2.28	0.62
17:T:3:BMA:H3	17:T:7:MAN:H5	1.81	0.62
2:G:460:SER:OG	2:G:461:THR:N	2.33	0.62
2:G:35:TRP:O	2:G:498:PRO:HA	1.99	0.62
2:G:456:ARG:NH2	6:E:93:ASP:OD1	2.23	0.62
6:E:133:LEU:HD12	6:E:179:LEU:HD23	1.83	0.61
5:D:72:ASP:OD1	5:D:74:SER:OG	2.16	0.61
2:G:321(A):ASP:HB2	10:J:11:FUC:C6	2.30	0.61
4:L:83:GLU:OE2	4:L:167:LYS:NZ	2.26	0.61
6:E:48:ILE:HG21	6:E:64:ALA:HB3	1.81	0.61
5:D:32:TYR:HB3	5:D:94:ARG:HD2	1.82	0.60
2:G:321(A):ASP:HB2	10:J:11:FUC:H61	1.82	0.60
4:L:51:ASN:ND2	16:S:5:MAN:O3	2.33	0.60
5:D:30:THR:HA	5:D:52(A):PRO:HB2	1.84	0.60
5:D:195:ILE:HG12	5:D:210:ARG:HG2	1.82	0.60
5:D:60:PRO:HD2	5:D:63:PHE:HB2	1.83	0.60
1:B:613:SER:HB2	7:A:2:FUC:H5	1.83	0.59
2:G:477:ASP:OD1	2:G:480:ARG:NH1	2.34	0.59
3:H:169:VAL:HG21	4:L:161:GLU:HB3	1.82	0.59
2:G:279:ASN:OD1	5:D:100(F):TRP:NE1	2.34	0.59
6:E:66:LYS:HA	6:E:71:ALA:HA	1.84	0.59
2:G:192:ARG:NH1	2:G:193:LEU:O	2.35	0.59
6:E:15:PRO:HD3	6:E:106:VAL:HG13	1.84	0.59
2:G:499:THR:HG23	2:G:501:CYS:H	1.68	0.59
2:G:456:ARG:HG2	2:G:457:ASP:H	1.68	0.59
4:L:8:VAL:HG12	4:L:101:ALA:HB3	1.85	0.58
5:D:2:VAL:HG11	5:D:94:ARG:HH12	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:92:ALA:O	6:E:94:GLY:N	2.29	0.58
2:G:83:GLU:HG3	2:G:245:VAL:HG22	1.86	0.58
2:G:259:LEU:HD23	2:G:452:LEU:HD21	1.84	0.58
2:G:182:VAL:HG23	2:G:192:ARG:HD3	1.84	0.58
3:H:6:GLU:N	3:H:6:GLU:OE1	2.36	0.58
3:H:200:HIS:HB3	3:H:205:THR:HB	1.85	0.58
2:G:292:VAL:HB	2:G:449:ILE:HB	1.85	0.58
3:H:10:GLY:HA3	3:H:202:PRO:HG3	1.85	0.58
14:P:3:BMA:H2	14:P:4:MAN:H5	1.85	0.58
5:D:159:LEU:HD21	5:D:182:VAL:HG21	1.86	0.58
5:D:144:ASP:HA	5:D:175:LEU:HB3	1.85	0.57
2:G:70:ALA:HA	2:G:111:LEU:HD21	1.86	0.57
2:G:363:ASN:HB3	2:G:388:SER:HA	1.87	0.57
5:D:36:TRP:HB2	5:D:69:MET:HE1	1.85	0.57
1:B:598:CYS:C	1:B:600:GLY:H	2.08	0.57
1:B:648:GLU:O	1:B:652:GLN:HB3	2.05	0.57
2:G:304:ARG:HD3	2:G:318:TYR:HB3	1.85	0.57
2:G:424:ILE:HG22	2:G:426:MET:H	1.69	0.57
10:J:4:MAN:O3	10:J:7:NAG:O5	2.20	0.57
5:D:27:TYR:HE2	5:D:32:TYR:HB2	1.69	0.57
4:L:55:PRO:HD2	4:L:58:ILE:HG13	1.87	0.56
3:H:100(D):VAL:HG22	3:H:100(G):PHE:H	1.71	0.56
4:L:19:ALA:HB3	4:L:75:ILE:HB	1.88	0.56
2:G:266:ALA:N	2:G:288:PHE:O	2.27	0.56
6:E:61:ARG:NH1	6:E:82:ASP:OD2	2.39	0.56
5:D:46:GLU:HB3	5:D:63:PHE:HZ	1.72	0.55
5:D:100(E):PRO:HB3	5:D:100(G):ARG:NH1	2.21	0.55
5:D:146:PHE:H	5:D:200:HIS:CE1	2.25	0.55
4:L:163:THR:HG1	4:L:176:SER:H	1.55	0.55
3:H:117:LYS:HD3	3:H:175:LEU:HD22	1.88	0.54
4:L:19:ALA:N	4:L:75:ILE:O	2.28	0.54
5:D:139:GLY:HA2	5:D:154:TRP:HH2	1.72	0.54
5:D:23:THR:HG22	5:D:77:ILE:HG23	1.89	0.54
2:G:335:LYS:H	2:G:413:SER:HA	1.72	0.54
5:D:37:VAL:HG22	5:D:47:TRP:HA	1.90	0.54
5:D:38:ARG:HD3	5:D:63:PHE:HE1	1.72	0.54
6:E:121:PRO:HD2	6:E:186:TRP:CZ2	2.43	0.54
2:G:384:TYR:O	2:G:419:ARG:N	2.40	0.54
2:G:69:TRP:CG	2:G:70:ALA:N	2.75	0.53
5:D:186:SER:HA	5:D:189:LEU:HG	1.91	0.53
5:D:60:PRO:O	5:D:64:ARG:HB2	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:86:LEU:HB3	2:G:89:VAL:HG21	1.90	0.53
4:L:94:ARG:HB3	4:L:94:ARG:HH21	1.73	0.53
3:H:94:THR:OG1	3:H:101:ASP:OD1	2.27	0.53
2:G:161:MET:N	2:G:170:GLN:O	2.30	0.52
4:L:28:LEU:HA	4:L:67:PHE:HZ	1.75	0.52
3:H:72:ASP:HB3	3:H:75:LYS:HB2	1.91	0.52
2:G:476:ARG:HA	2:G:479:TRP:CD1	2.45	0.52
6:E:145:VAL:HG12	6:E:146:THR:N	2.25	0.52
5:D:150:VAL:HB	5:D:178:LEU:HD21	1.91	0.52
6:E:166:SER:O	6:E:168:GLN:NE2	2.43	0.52
2:G:161:MET:O	2:G:170:GLN:N	2.36	0.52
5:D:38:ARG:HD3	5:D:63:PHE:CE1	2.45	0.52
5:D:119:PRO:HB3	5:D:145:TYR:HB3	1.92	0.52
2:G:193:LEU:HB2	2:G:196:CYS:SG	2.50	0.52
5:D:123:PRO:HD3	5:D:209:LYS:HE2	1.90	0.52
6:E:47:ILE:O	6:E:55:PRO:HD2	2.10	0.52
4:L:39:ARG:HB2	4:L:42:GLN:HB2	1.92	0.51
2:G:101:VAL:HG13	2:G:479:TRP:HB2	1.92	0.51
2:G:133:ASN:OD1	2:G:155:LYS:NZ	2.41	0.51
3:H:126:PRO:HD2	3:H:213:PRO:HA	1.93	0.51
4:L:116:VAL:HG22	4:L:137:ILE:HG23	1.92	0.51
2:G:385:CYS:HA	2:G:418:CYS:HA	1.91	0.51
3:H:142:VAL:HB	3:H:178:LEU:HG	1.92	0.51
3:H:159:LEU:HG	3:H:182:VAL:HG21	1.93	0.51
5:D:24:ALA:HB1	5:D:27:TYR:HE1	1.76	0.50
5:D:99:SER:OG	5:D:100(B):ASP:O	2.29	0.50
2:G:276:ASN:OD1	2:G:278:THR:OG1	2.29	0.50
6:E:92:ALA:C	6:E:94:GLY:H	2.11	0.50
1:B:538:THR:O	1:B:542:ARG:NH1	2.45	0.50
3:H:38:ARG:HH12	3:H:86:ASP:HA	1.75	0.50
6:E:83:GLU:HG3	6:E:104:LEU:O	2.12	0.50
2:G:210:PHE:HB2	2:G:377:ASN:ND2	2.26	0.50
6:E:61:ARG:HB3	6:E:76:SER:O	2.11	0.50
3:H:100(D):VAL:HA	16:S:2:NAG:H2	1.93	0.50
6:E:145:VAL:HG12	6:E:146:THR:H	1.76	0.50
5:D:38:ARG:HB3	5:D:90:TYR:CD2	2.47	0.50
2:G:55:ALA:HB3	2:G:216:HIS:HB2	1.93	0.49
2:G:116:LEU:HD21	2:G:434:MET:HG3	1.94	0.49
2:G:305:LYS:O	2:G:319:ALA:N	2.35	0.49
3:H:40:SER:HB3	3:H:43:LYS:HD2	1.94	0.49
4:L:20:ARG:HA	4:L:73:LEU:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:93:ALA:HB1	5:D:100(I):MET:HB3	1.94	0.49
1:B:608:VAL:HG21	1:B:646:LEU:HD23	1.94	0.49
5:D:94:ARG:O	5:D:100(I):MET:HA	2.12	0.49
2:G:201:ILE:HD13	2:G:423:ILE:HG23	1.94	0.49
3:H:5:GLN:O	3:H:23:SER:N	2.41	0.49
4:L:39:ARG:HD2	4:L:84:ALA:HB2	1.94	0.49
5:D:10:GLN:HB3	5:D:12:LYS:NZ	2.28	0.49
6:E:170:ASN:O	6:E:171:ASN:HB2	2.13	0.49
12:M:3:BMA:O5	12:M:7:MAN:H5	2.12	0.49
3:H:125:ALA:HB3	3:H:214:LYS:HE3	1.95	0.49
2:G:378:CYS:HB3	2:G:383:PHE:CE1	2.48	0.49
5:D:38:ARG:NH1	5:D:85:ASP:O	2.41	0.49
3:H:29:MET:HA	3:H:34:TRP:HZ2	1.77	0.48
6:E:109:GLN:HE22	6:E:172:LYS:HG2	1.78	0.48
3:H:100(H):GLY:HA2	3:H:100(J):PHE:CE2	2.48	0.48
3:H:171:GLN:NE2	3:H:177:SER:OG	2.45	0.48
2:G:153:GLU:HG3	2:G:419:ARG:HH21	1.78	0.48
3:H:166:PHE:CG	4:L:136:LEU:HD22	2.48	0.48
5:D:72:ASP:O	5:D:76:GLU:N	2.45	0.48
4:L:66(B):ILE:O	4:L:66(C):ASN:HB2	2.13	0.48
5:D:58:LYS:HE3	5:D:58:LYS:HB2	1.75	0.48
2:G:298:ARG:NH1	2:G:381:GLU:HG3	2.28	0.48
2:G:57:ASP:O	2:G:76:PRO:HA	2.13	0.48
3:H:100:ARG:NH2	16:S:4:MAN:O6	2.46	0.48
4:L:34:GLN:HB3	4:L:36:TYR:CE2	2.49	0.48
1:B:622:ILE:O	1:B:626:MET:HB2	2.13	0.47
3:H:168:ALA:HB2	3:H:178:LEU:HB3	1.96	0.47
5:D:86:ASP:O	5:D:90:TYR:OH	2.30	0.47
12:M:1:NAG:O3	12:M:2:NAG:N2	2.46	0.47
1:B:539:VAL:HG22	1:B:542:ARG:HH22	1.79	0.47
6:E:39:HIS:HD2	6:E:84:ALA:HB2	1.79	0.47
6:E:47:ILE:HG22	6:E:48:ILE:HG12	1.96	0.47
4:L:111:LYS:HG3	4:L:198:HIS:HE1	1.78	0.47
5:D:145:TYR:HE1	5:D:148:GLU:HA	1.78	0.47
6:E:123:SER:HA	6:E:126:LEU:HB2	1.96	0.47
3:H:47:TRP:HD1	3:H:48:ILE:H	1.63	0.47
2:G:137:ASN:HB2	4:L:95(A):GLY:HA2	1.97	0.47
5:D:46:GLU:HB3	5:D:63:PHE:CZ	2.50	0.47
5:D:47:TRP:CE3	5:D:60:PRO:HG3	2.49	0.47
5:D:146:PHE:H	5:D:200:HIS:HE1	1.61	0.47
3:H:166:PHE:CZ	4:L:136:LEU:HB3	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:396:ILE:HG22	2:G:397:SER:H	1.80	0.47
1:B:522:PHE:CE1	1:B:540:GLN:HA	2.50	0.46
1:B:522:PHE:CE1	1:B:543:ASN:HB2	2.50	0.46
5:D:100(C):TRP:O	5:D:100(D):SER:HB2	2.15	0.46
2:G:259:LEU:HD22	2:G:449:ILE:HG21	1.97	0.46
4:L:37:GLN:HB2	4:L:47:LEU:HD11	1.97	0.46
2:G:203:GLN:HG3	2:G:435:TYR:HD2	1.79	0.46
6:E:38:GLN:O	6:E:84:ALA:HB1	2.15	0.46
2:G:298:ARG:CB	2:G:443:ILE:HB	2.43	0.46
1:B:650:GLN:NE2	1:B:654:GLU:OE1	2.49	0.46
1:B:574:LYS:HG3	2:G:52:LEU:O	2.16	0.46
4:L:112:ALA:HB3	4:L:140:PHE:HA	1.97	0.46
5:D:82(B):ARG:NH2	17:T:4:MAN:O2	2.49	0.46
4:L:54:ARG:HG2	4:L:58:ILE:HB	1.98	0.46
10:J:2:NAG:H4	10:J:11:FUC:O2	2.16	0.46
17:T:3:BMA:H3	17:T:7:MAN:H3	1.96	0.46
3:H:66:ARG:HD2	3:H:82(B):SER:HB2	1.98	0.46
9:N:1:NAG:H62	9:N:2:NAG:C7	2.46	0.45
4:L:49:TYR:O	4:L:53:ASP:HB2	2.15	0.45
6:E:33:VAL:HB	6:E:51:VAL:HG22	1.98	0.45
2:G:251:ILE:HG23	2:G:482:GLU:HG3	1.97	0.45
2:G:301:ASN:HB3	2:G:323:ILE:HB	1.98	0.45
3:H:16:GLU:H	3:H:82(C):VAL:HG22	1.82	0.45
4:L:116:VAL:O	4:L:205:LYS:HE3	2.16	0.45
1:B:596:TRP:CD1	1:B:646:LEU:HB2	2.51	0.45
2:G:119:CYS:SG	2:G:205:CYS:N	2.87	0.45
6:E:27(B):ASP:OD1	6:E:27(C):VAL:N	2.44	0.45
12:M:1:NAG:O3	12:M:2:NAG:C7	2.65	0.45
2:G:361:PHE:HB3	2:G:391:PHE:HB3	1.99	0.45
5:D:96:MET:HG2	5:D:101:VAL:CG2	2.47	0.45
5:D:181:VAL:HG12	6:E:136:LEU:HD13	1.99	0.45
3:H:71:ARG:HH21	3:H:73:THR:HG22	1.80	0.45
3:H:87:THR:OG1	3:H:111:VAL:N	2.48	0.45
3:H:2:VAL:HA	3:H:26:GLY:HA3	1.98	0.45
2:G:65:LYS:HB2	2:G:68:VAL:HG13	1.99	0.45
2:G:452:LEU:HD23	2:G:452:LEU:HA	1.85	0.45
5:D:143:LYS:HG2	5:D:144:ASP:H	1.82	0.45
2:G:155:LYS:O	2:G:175:LEU:HA	2.17	0.44
2:G:270:VAL:HG12	2:G:289:ASN:H	1.82	0.44
2:G:122:LEU:O	2:G:125:LEU:HB2	2.18	0.44
3:H:165:THR:HA	3:H:180:SER:HA	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:92:ASP:OD1	4:L:95:SER:N	2.42	0.44
5:D:6:GLU:OE2	5:D:92:CYS:N	2.51	0.44
5:D:18:VAL:HB	5:D:82(C):LEU:HD11	1.99	0.44
5:D:126:PRO:HD3	5:D:138:LEU:HB3	1.99	0.44
6:E:52:ASN:HB3	6:E:64:ALA:O	2.17	0.44
4:L:67:PHE:HB3	4:L:68:GLY:H	1.47	0.44
3:H:87:THR:HG23	3:H:110:THR:HA	2.00	0.44
6:E:111:LYS:NZ	6:E:199:GLU:OE2	2.37	0.44
2:G:384:TYR:N	2:G:419:ARG:O	2.47	0.44
5:D:36:TRP:HB2	5:D:69:MET:CE	2.47	0.44
5:D:100(C):TRP:HB3	5:D:100(D):SER:O	2.18	0.44
5:D:119:PRO:HG3	5:D:200:HIS:HB2	1.99	0.44
2:G:164:GLU:HA	2:G:312:GLY:O	2.18	0.43
12:M:3:BMA:H3	12:M:4:MAN:H5	1.99	0.43
1:B:572:GLY:O	1:B:575:GLN:NE2	2.52	0.43
11:U:3:BMA:H61	11:U:5:MAN:H3	1.99	0.43
2:G:359:ILE:O	2:G:395:TRP:N	2.49	0.43
5:D:38:ARG:HH12	5:D:86:ASP:HA	1.84	0.43
6:E:125:GLU:OE2	6:E:132:THR:OG1	2.31	0.43
4:L:35:TRP:CZ3	4:L:88:CYS:HB2	2.53	0.43
6:E:20:THR:HA	6:E:73:LEU:O	2.18	0.43
2:G:360:ARG:NH2	2:G:467:THR:OG1	2.51	0.43
3:H:60:ASN:HB3	3:H:63:LEU:HD13	1.99	0.43
3:H:6:GLU:HG3	3:H:92:CYS:SG	2.58	0.43
6:E:197:THR:HA	6:E:202:THR:HA	2.00	0.43
1:B:593:LEU:HD21	1:B:601:LYS:HA	2.01	0.43
2:G:343:GLY:HA2	2:G:346:VAL:HG12	2.00	0.43
3:H:88:ALA:HB3	3:H:90:TYR:CE1	2.49	0.43
3:H:98:GLY:N	3:H:100(M):TYR:O	2.42	0.43
2:G:109:ILE:O	2:G:112:TRP:HB3	2.19	0.42
2:G:175:LEU:O	2:G:320:THR:OG1	2.36	0.42
17:T:3:BMA:H2	17:T:7:MAN:H3	2.00	0.42
1:B:528:SER:HA	9:F:1:NAG:O7	2.19	0.42
1:B:585:ARG:HH22	2:G:490:LYS:HD2	1.85	0.42
1:B:585:ARG:NH2	2:G:491:ILE:O	2.43	0.42
1:B:646:LEU:O	1:B:650:GLN:HB2	2.19	0.42
2:G:361:PHE:CD2	2:G:393:SER:HB2	2.54	0.42
3:H:100:ARG:NH1	3:H:100(A):ILE:O	2.52	0.42
4:L:19:ALA:O	4:L:75:ILE:N	2.37	0.42
5:D:35:HIS:ND1	5:D:50:TRP:HB3	2.34	0.42
2:G:157:CYS:O	2:G:173:TYR:HA	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:189:LEU:HD23	3:H:189:LEU:HA	1.80	0.42
5:D:38:ARG:NH1	5:D:86:ASP:HA	2.34	0.42
4:L:198:HIS:N	4:L:201:SER:O	2.46	0.42
1:B:598:CYS:C	1:B:600:GLY:N	2.71	0.42
5:D:114:ALA:HB3	5:D:146:PHE:CD2	2.55	0.42
2:G:321(A):ASP:HB2	10:J:11:FUC:H63	2.01	0.42
5:D:38:ARG:HB3	5:D:90:TYR:CE2	2.54	0.42
2:G:55:ALA:N	2:G:216:HIS:O	2.53	0.42
4:L:139:ASP:OD1	4:L:170:ASN:ND2	2.53	0.42
3:H:144:ASP:OD1	3:H:171:GLN:NE2	2.42	0.41
5:D:119:PRO:HD3	5:D:200:HIS:ND1	2.35	0.41
2:G:80:ASN:O	2:G:82:GLN:N	2.53	0.41
2:G:456:ARG:HG3	2:G:468:PHE:CE2	2.55	0.41
3:H:117:LYS:HB3	3:H:146:PHE:N	2.36	0.41
5:D:69:MET:HA	5:D:79:TYR:O	2.20	0.41
17:T:2:NAG:O7	11:U:1:NAG:O3	2.30	0.41
5:D:51:ILE:HG12	5:D:69:MET:HB3	2.03	0.41
6:E:121:PRO:HD2	6:E:186:TRP:CH2	2.55	0.41
1:B:610:TRP:CD2	2:G:498:PRO:HB3	2.56	0.41
3:H:153:SER:OG	3:H:197:ASN:HB2	2.20	0.41
5:D:126:PRO:HA	6:E:119:PHE:HE1	1.86	0.41
3:H:18:LEU:HB3	3:H:82:LEU:HB3	2.03	0.41
1:B:537:LEU:HB3	1:B:602:LEU:HD22	2.02	0.41
4:L:25:ARG:HH22	4:L:90:MET:H	1.68	0.41
5:D:142:VAL:O	5:D:177:SER:HA	2.21	0.41
1:B:529:THR:HB	1:B:623:TRP:O	2.20	0.41
5:D:139:GLY:HA2	5:D:154:TRP:CH2	2.55	0.41
6:E:35:TRP:CZ3	6:E:88:CYS:HB3	2.55	0.41
2:G:121:LYS:HE3	2:G:121:LYS:HB2	1.81	0.41
2:G:299:PRO:HG2	2:G:327:ARG:HB2	2.02	0.41
3:H:29:MET:HA	3:H:34:TRP:CZ2	2.55	0.41
3:H:101:ASP:OD1	3:H:101:ASP:N	2.42	0.41
5:D:2:VAL:HA	5:D:26:GLY:HA3	2.03	0.41
5:D:150:VAL:HG11	5:D:198:VAL:HG13	2.02	0.41
3:H:162:GLY:O	3:H:182:VAL:HA	2.21	0.41
3:H:169:VAL:HG12	3:H:177:SER:HB2	2.03	0.41
4:L:168:GLN:HB2	4:L:170:ASN:OD1	2.21	0.41
3:H:128:SER:OG	4:L:212:CYS:O	2.38	0.40
4:L:62:PHE:CD2	4:L:75:ILE:HG12	2.56	0.40
6:E:14:SER:HB3	6:E:17:GLN:HG3	2.03	0.40
2:G:65:LYS:HA	2:G:65:LYS:HD3	1.90	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:89:TYR:CE1	6:E:96:VAL:HG13	2.56	0.40
2:G:110:SER:O	2:G:114:GLN:HG2	2.20	0.40
2:G:123:THR:N	2:G:124:PRO:HD2	2.36	0.40
5:D:24:ALA:HB1	5:D:27:TYR:CE1	2.56	0.40
5:D:143:LYS:HE3	5:D:171:GLN:NE2	2.37	0.40
6:E:140:PHE:CE2	6:E:173:TYR:HB2	2.55	0.40
2:G:459:GLY:O	2:G:460:SER:C	2.59	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)
1:B:534:SER:O	1:B:652:GLN:NE2[3_555]	2.15	0.05

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	B	122/153 (80%)	109 (89%)	12 (10%)	1 (1%)	19	58
2	G	442/481 (92%)	417 (94%)	22 (5%)	3 (1%)	22	61
3	H	226/238 (95%)	216 (96%)	10 (4%)	0	100	100
4	L	209/214 (98%)	201 (96%)	8 (4%)	0	100	100
5	D	227/232 (98%)	218 (96%)	8 (4%)	1 (0%)	34	72
6	E	208/214 (97%)	198 (95%)	8 (4%)	2 (1%)	15	54
All	All	1434/1532 (94%)	1359 (95%)	68 (5%)	7 (0%)	29	68

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	G	57	ASP

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Mol	Chain	Res	Type
2	G	459	GLY
6	E	93	ASP
2	G	138	ILE
5	D	100(D)	SER
1	B	599	SER
6	E	51	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	108/129 (84%)	104 (96%)	4 (4%)	34	65
2	G	401/428 (94%)	397 (99%)	4 (1%)	76	88
3	H	202/208 (97%)	199 (98%)	3 (2%)	65	84
4	L	175/178 (98%)	173 (99%)	2 (1%)	73	88
5	D	194/197 (98%)	188 (97%)	6 (3%)	40	70
6	E	173/177 (98%)	171 (99%)	2 (1%)	71	87
All	All	1253/1317 (95%)	1232 (98%)	21 (2%)	60	82

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	540	GLN
1	B	604	CYS
1	B	619	LEU
1	B	639	THR
2	G	125	LEU
2	G	192	ARG
2	G	356	ASN
2	G	443	ILE
3	H	100(D)	VAL
3	H	100(E)	VAL
3	H	100(F)	SER
4	L	28	LEU

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Mol	Chain	Res	Type
4	L	94	ARG
5	D	3	GLN
5	D	51	ILE
5	D	71	ARG
5	D	100(G)	ARG
5	D	138	LEU
5	D	140	CYS
6	E	42	LYS
6	E	66	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	650	GLN
4	L	198	HIS
5	D	33	HIS
5	D	39	GLN
5	D	155	ASN
6	E	38	GLN
6	E	109	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)

87 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	1,7	14,14,15	0.33	0	17,19,21	0.97	1 (5%)
7	FUC	A	2	7	10,10,11	0.73	0	14,14,16	0.90	0
8	NAG	C	1	8,1	14,14,15	0.37	0	17,19,21	1.30	2 (11%)
8	NAG	C	2	8	14,14,15	0.27	0	17,19,21	1.02	1 (5%)
8	BMA	C	3	8	11,11,12	0.25	0	15,15,17	0.74	0
9	NAG	F	1	9,2	14,14,15	0.29	0	17,19,21	0.88	1 (5%)
9	NAG	F	2	9	14,14,15	0.27	0	17,19,21	0.68	0
9	NAG	I	1	9,2	14,14,15	0.45	0	17,19,21	2.28	6 (35%)
9	NAG	I	2	9	14,14,15	0.29	0	17,19,21	0.90	0
10	NAG	J	1	10,2	14,14,15	0.41	0	17,19,21	1.79	6 (35%)
10	GAL	J	10	10	11,11,12	0.56	0	15,15,17	1.02	1 (6%)
10	FUC	J	11	10	10,10,11	1.41	2 (20%)	14,14,16	1.25	1 (7%)
10	NAG	J	2	10	14,14,15	0.55	0	17,19,21	1.41	2 (11%)
10	BMA	J	3	10	11,11,12	0.48	0	15,15,17	2.00	4 (26%)
10	MAN	J	4	10	11,11,12	0.41	0	15,15,17	2.01	4 (26%)
10	NAG	J	5	10	14,14,15	0.35	0	17,19,21	0.82	0
10	GAL	J	6	10	11,11,12	0.50	0	15,15,17	0.92	0
10	NAG	J	7	10	14,14,15	0.27	0	17,19,21	1.07	1 (5%)
10	MAN	J	8	10	11,11,12	0.65	0	15,15,17	1.96	2 (13%)
10	NAG	J	9	10	14,14,15	0.34	0	17,19,21	0.85	1 (5%)
11	NAG	K	1	11,2	14,14,15	0.39	0	17,19,21	1.38	4 (23%)
11	NAG	K	2	11	14,14,15	0.38	0	17,19,21	2.12	4 (23%)
11	BMA	K	3	11	11,11,12	0.24	0	15,15,17	1.23	2 (13%)
11	MAN	K	4	11	11,11,12	0.29	0	15,15,17	0.87	1 (6%)
11	MAN	K	5	11	11,11,12	0.26	0	15,15,17	0.80	0
12	NAG	M	1	12,2	14,14,15	0.52	0	17,19,21	2.35	4 (23%)
12	NAG	M	2	12	14,14,15	0.51	0	17,19,21	1.93	5 (29%)
12	BMA	M	3	12	11,11,12	0.60	0	15,15,17	1.75	2 (13%)
12	MAN	M	4	12	11,11,12	0.51	0	15,15,17	1.52	3 (20%)
12	NAG	M	5	12	14,14,15	0.30	0	17,19,21	0.80	0
12	GAL	M	6	12	11,11,12	0.58	0	15,15,17	1.02	1 (6%)
12	MAN	M	7	12	11,11,12	0.27	0	15,15,17	1.18	1 (6%)
12	NAG	M	8	12	14,14,15	0.29	0	17,19,21	0.79	1 (5%)
9	NAG	N	1	9,2	14,14,15	0.38	0	17,19,21	0.86	1 (5%)
9	NAG	N	2	9	14,14,15	0.29	0	17,19,21	0.80	1 (5%)
13	NAG	O	1	13,2	14,14,15	0.36	0	17,19,21	0.90	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
13	NAG	O	2	13	14,14,15	0.35	0	17,19,21	1.39	3 (17%)
13	BMA	O	3	13	11,11,12	0.30	0	15,15,17	1.05	1 (6%)
13	MAN	O	4	13	11,11,12	0.47	0	15,15,17	1.03	1 (6%)
13	MAN	O	5	13	11,11,12	0.49	0	15,15,17	1.13	2 (13%)
13	MAN	O	6	13	11,11,12	0.24	0	15,15,17	0.85	0
13	MAN	O	7	13	11,11,12	0.26	0	15,15,17	0.78	0
14	NAG	P	1	14,2	14,14,15	0.54	0	17,19,21	1.42	2 (11%)
14	NAG	P	2	14	14,14,15	0.32	0	17,19,21	1.12	2 (11%)
14	BMA	P	3	14	11,11,12	0.28	0	15,15,17	1.42	2 (13%)
14	MAN	P	4	14	11,11,12	0.49	0	15,15,17	1.82	3 (20%)
14	NAG	P	5	14	14,14,15	0.28	0	17,19,21	0.63	0
14	GAL	P	6	14	11,11,12	0.48	0	15,15,17	0.94	0
14	MAN	P	7	14	11,11,12	0.50	0	15,15,17	1.25	2 (13%)
14	FUC	P	8	14	10,10,11	0.61	0	14,14,16	0.92	0
9	NAG	Q	1	9,2	14,14,15	0.29	0	17,19,21	0.53	0
9	NAG	Q	2	9	14,14,15	0.30	0	17,19,21	0.67	0
15	NAG	R	1	15,2	14,14,15	0.35	0	17,19,21	0.97	2 (11%)
15	NAG	R	2	15	14,14,15	0.34	0	17,19,21	0.77	0
15	BMA	R	3	15	11,11,12	0.24	0	15,15,17	1.48	2 (13%)
15	MAN	R	4	15	11,11,12	0.21	0	15,15,17	1.19	1 (6%)
15	NAG	R	5	15	14,14,15	0.28	0	17,19,21	0.76	0
15	MAN	R	6	15	11,11,12	0.88	0	15,15,17	1.47	1 (6%)
16	NAG	S	1	16,2	14,14,15	0.34	0	17,19,21	0.78	0
16	MAN	S	10	16	11,11,12	0.28	0	15,15,17	0.75	0
16	NAG	S	2	16	14,14,15	0.28	0	17,19,21	1.36	2 (11%)
16	BMA	S	3	16	11,11,12	0.31	0	15,15,17	1.04	1 (6%)
16	MAN	S	4	16	11,11,12	0.23	0	15,15,17	1.11	2 (13%)
16	MAN	S	5	16	11,11,12	0.33	0	15,15,17	1.51	3 (20%)
16	MAN	S	6	16	11,11,12	0.28	0	15,15,17	0.88	1 (6%)
16	MAN	S	7	16	11,11,12	0.27	0	15,15,17	0.78	0
16	MAN	S	8	16	11,11,12	0.29	0	15,15,17	1.38	3 (20%)
16	MAN	S	9	16	11,11,12	0.28	0	15,15,17	0.97	1 (6%)
17	NAG	T	1	17,2	14,14,15	0.43	0	17,19,21	1.06	2 (11%)
17	NAG	T	2	17	14,14,15	0.40	0	17,19,21	1.65	4 (23%)
17	BMA	T	3	17	11,11,12	0.61	0	15,15,17	1.92	3 (20%)
17	MAN	T	4	17	11,11,12	0.85	0	15,15,17	1.92	5 (33%)
17	MAN	T	5	17	11,11,12	0.51	0	15,15,17	1.25	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
17	MAN	T	6	17	11,11,12	0.81	0	15,15,17	1.98	5 (33%)
17	MAN	T	7	17	11,11,12	1.39	2 (18%)	15,15,17	1.81	3 (20%)
11	NAG	U	1	11,2	14,14,15	0.37	0	17,19,21	1.05	2 (11%)
11	NAG	U	2	11	14,14,15	0.39	0	17,19,21	1.27	1 (5%)
11	BMA	U	3	11	11,11,12	0.46	0	15,15,17	1.51	3 (20%)
11	MAN	U	4	11	11,11,12	0.33	0	15,15,17	0.98	0
11	MAN	U	5	11	11,11,12	1.20	2 (18%)	15,15,17	2.42	3 (20%)
18	NAG	V	1	18,2	14,14,15	0.32	0	17,19,21	1.14	3 (17%)
18	NAG	V	2	18	14,14,15	0.29	0	17,19,21	0.89	0
18	BMA	V	3	18	11,11,12	0.27	0	15,15,17	0.75	0
18	FUC	V	4	18	10,10,11	1.02	0	14,14,16	1.28	2 (14%)
8	NAG	W	1	8,2	14,14,15	0.29	0	17,19,21	0.77	1 (5%)
8	NAG	W	2	8	14,14,15	0.31	0	17,19,21	1.20	2 (11%)
8	BMA	W	3	8	11,11,12	0.33	0	15,15,17	0.60	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
7	NAG	A	1	1,7	-	0/6/23/26	0/1/1/1
7	FUC	A	2	7	-	-	0/1/1/1
8	NAG	C	1	8,1	-	1/6/23/26	0/1/1/1
8	NAG	C	2	8	-	3/6/23/26	0/1/1/1
8	BMA	C	3	8	-	0/2/19/22	0/1/1/1
9	NAG	F	1	9,2	-	0/6/23/26	0/1/1/1
9	NAG	F	2	9	-	0/6/23/26	0/1/1/1
9	NAG	I	1	9,2	-	0/6/23/26	0/1/1/1
9	NAG	I	2	9	-	2/6/23/26	0/1/1/1
10	NAG	J	1	10,2	-	2/6/23/26	0/1/1/1
10	GAL	J	10	10	-	0/2/19/22	0/1/1/1
10	FUC	J	11	10	-	-	0/1/1/1
10	NAG	J	2	10	-	1/6/23/26	0/1/1/1
10	BMA	J	3	10	-	0/2/19/22	0/1/1/1
10	MAN	J	4	10	-	0/2/19/22	0/1/1/1
10	NAG	J	5	10	-	0/6/23/26	0/1/1/1
10	GAL	J	6	10	-	0/2/19/22	0/1/1/1
10	NAG	J	7	10	-	0/6/23/26	0/1/1/1
10	MAN	J	8	10	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	NAG	J	9	10	-	2/6/23/26	0/1/1/1
11	NAG	K	1	11,2	-	2/6/23/26	0/1/1/1
11	NAG	K	2	11	-	3/6/23/26	0/1/1/1
11	BMA	K	3	11	-	2/2/19/22	0/1/1/1
11	MAN	K	4	11	-	0/2/19/22	0/1/1/1
11	MAN	K	5	11	-	0/2/19/22	0/1/1/1
12	NAG	M	1	12,2	-	2/6/23/26	0/1/1/1
12	NAG	M	2	12	-	3/6/23/26	0/1/1/1
12	BMA	M	3	12	-	2/2/19/22	0/1/1/1
12	MAN	M	4	12	-	2/2/19/22	0/1/1/1
12	NAG	M	5	12	-	2/6/23/26	0/1/1/1
12	GAL	M	6	12	-	2/2/19/22	0/1/1/1
12	MAN	M	7	12	-	0/2/19/22	0/1/1/1
12	NAG	M	8	12	-	2/6/23/26	0/1/1/1
9	NAG	N	1	9,2	-	0/6/23/26	0/1/1/1
9	NAG	N	2	9	-	0/6/23/26	0/1/1/1
13	NAG	O	1	13,2	-	2/6/23/26	0/1/1/1
13	NAG	O	2	13	-	2/6/23/26	0/1/1/1
13	BMA	O	3	13	-	1/2/19/22	0/1/1/1
13	MAN	O	4	13	-	1/2/19/22	0/1/1/1
13	MAN	O	5	13	-	0/2/19/22	0/1/1/1
13	MAN	O	6	13	-	2/2/19/22	0/1/1/1
13	MAN	O	7	13	-	0/2/19/22	0/1/1/1
14	NAG	P	1	14,2	-	2/6/23/26	0/1/1/1
14	NAG	P	2	14	-	0/6/23/26	0/1/1/1
14	BMA	P	3	14	-	2/2/19/22	0/1/1/1
14	MAN	P	4	14	-	2/2/19/22	0/1/1/1
14	NAG	P	5	14	-	2/6/23/26	0/1/1/1
14	GAL	P	6	14	-	2/2/19/22	0/1/1/1
14	MAN	P	7	14	-	2/2/19/22	0/1/1/1
14	FUC	P	8	14	-	-	0/1/1/1
9	NAG	Q	1	9,2	-	2/6/23/26	0/1/1/1
9	NAG	Q	2	9	-	0/6/23/26	0/1/1/1
15	NAG	R	1	15,2	-	0/6/23/26	0/1/1/1
15	NAG	R	2	15	-	0/6/23/26	0/1/1/1
15	BMA	R	3	15	-	2/2/19/22	0/1/1/1
15	MAN	R	4	15	-	1/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	NAG	R	5	15	-	2/6/23/26	0/1/1/1
15	MAN	R	6	15	-	0/2/19/22	0/1/1/1
16	NAG	S	1	16,2	-	0/6/23/26	0/1/1/1
16	MAN	S	10	16	-	0/2/19/22	0/1/1/1
16	NAG	S	2	16	-	1/6/23/26	0/1/1/1
16	BMA	S	3	16	-	0/2/19/22	0/1/1/1
16	MAN	S	4	16	-	0/2/19/22	0/1/1/1
16	MAN	S	5	16	-	0/2/19/22	0/1/1/1
16	MAN	S	6	16	-	0/2/19/22	0/1/1/1
16	MAN	S	7	16	-	2/2/19/22	0/1/1/1
16	MAN	S	8	16	-	0/2/19/22	0/1/1/1
16	MAN	S	9	16	-	2/2/19/22	0/1/1/1
17	NAG	T	1	17,2	-	1/6/23/26	0/1/1/1
17	NAG	T	2	17	-	1/6/23/26	0/1/1/1
17	BMA	T	3	17	-	0/2/19/22	0/1/1/1
17	MAN	T	4	17	-	0/2/19/22	0/1/1/1
17	MAN	T	5	17	-	0/2/19/22	0/1/1/1
17	MAN	T	6	17	-	1/2/19/22	0/1/1/1
17	MAN	T	7	17	-	2/2/19/22	0/1/1/1
11	NAG	U	1	11,2	-	0/6/23/26	0/1/1/1
11	NAG	U	2	11	-	0/6/23/26	0/1/1/1
11	BMA	U	3	11	-	2/2/19/22	0/1/1/1
11	MAN	U	4	11	-	0/2/19/22	0/1/1/1
11	MAN	U	5	11	-	2/2/19/22	0/1/1/1
18	NAG	V	1	18,2	-	0/6/23/26	0/1/1/1
18	NAG	V	2	18	-	1/6/23/26	0/1/1/1
18	BMA	V	3	18	-	0/2/19/22	0/1/1/1
18	FUC	V	4	18	-	-	0/1/1/1
8	NAG	W	1	8,2	-	2/6/23/26	0/1/1/1
8	NAG	W	2	8	-	0/6/23/26	0/1/1/1
8	BMA	W	3	8	-	2/2/19/22	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	T	7	MAN	O5-C1	3.25	1.48	1.43
11	U	5	MAN	O5-C1	3.16	1.48	1.43
17	T	7	MAN	C1-C2	3.01	1.59	1.52
10	J	11	FUC	O2-C2	-2.38	1.38	1.43
11	U	5	MAN	C1-C2	2.30	1.57	1.52
10	J	11	FUC	C1-C2	2.18	1.57	1.52

All (142) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	K	2	NAG	C2-N2-C7	6.57	132.26	122.90
9	I	1	NAG	O4-C4-C5	6.05	124.32	109.30
10	J	8	MAN	O2-C2-C3	5.91	121.98	110.14
11	U	5	MAN	C1-C2-C3	5.88	116.89	109.67
10	J	4	MAN	C1-C2-C3	-5.41	103.02	109.67
11	U	5	MAN	C1-O5-C5	5.40	119.52	112.19
17	T	3	BMA	O3-C3-C2	5.06	119.69	109.99
17	T	4	MAN	C1-C2-C3	5.06	115.89	109.67
12	M	1	NAG	O4-C4-C3	-5.05	98.66	110.35
14	P	1	NAG	O4-C4-C5	-4.49	98.15	109.30
10	J	3	BMA	C1-C2-C3	4.48	115.17	109.67
10	J	3	BMA	O3-C3-C2	-4.42	101.52	109.99
9	I	1	NAG	C1-O5-C5	4.28	117.99	112.19
12	M	1	NAG	O3-C3-C2	-4.23	100.71	109.47
14	P	4	MAN	O5-C1-C2	-4.22	104.25	110.77
12	M	1	NAG	O4-C4-C5	-4.22	98.81	109.30
11	U	5	MAN	O5-C1-C2	-4.18	104.32	110.77
12	M	1	NAG	O5-C1-C2	-4.17	104.70	111.29
17	T	2	NAG	O4-C4-C5	-4.07	99.18	109.30
10	J	2	NAG	O5-C1-C2	-4.05	104.89	111.29
17	T	6	MAN	O3-C3-C2	4.00	117.66	109.99
12	M	3	BMA	O5-C1-C2	-3.96	104.66	110.77
17	T	7	MAN	C1-C2-C3	3.85	114.40	109.67
10	J	4	MAN	O4-C4-C5	3.85	118.85	109.30
15	R	3	BMA	O3-C3-C2	-3.84	102.64	109.99
10	J	1	NAG	O4-C4-C3	-3.79	101.59	110.35
8	C	1	NAG	O4-C4-C3	-3.78	101.62	110.35
12	M	2	NAG	C4-C3-C2	3.76	116.53	111.02
14	P	4	MAN	C1-O5-C5	3.69	117.19	112.19
12	M	2	NAG	O4-C4-C5	-3.58	100.41	109.30
15	R	6	MAN	O5-C5-C6	3.58	112.81	107.20
17	T	7	MAN	O5-C1-C2	-3.56	105.27	110.77
12	M	4	MAN	O5-C1-C2	-3.55	105.29	110.77
12	M	2	NAG	O4-C4-C3	-3.55	102.14	110.35
9	I	1	NAG	O4-C4-C3	3.54	118.54	110.35
14	P	7	MAN	O5-C5-C6	3.50	112.69	107.20
17	T	7	MAN	C1-O5-C5	3.42	116.82	112.19
12	M	2	NAG	O5-C1-C2	-3.39	105.94	111.29
11	U	2	NAG	O5-C1-C2	-3.34	106.01	111.29
11	K	2	NAG	C8-C7-N2	3.32	121.71	116.10
11	U	3	BMA	C1-C2-C3	3.27	113.69	109.67
10	J	8	MAN	O3-C3-C2	3.27	116.25	109.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	T	6	MAN	O5-C5-C6	3.21	112.24	107.20
12	M	3	BMA	O3-C3-C4	3.18	117.70	110.35
17	T	2	NAG	O5-C5-C6	3.12	112.10	107.20
16	S	5	MAN	O5-C1-C2	-3.10	105.98	110.77
13	O	2	NAG	O4-C4-C5	-3.10	101.61	109.30
17	T	6	MAN	O3-C3-C4	3.00	117.28	110.35
18	V	4	FUC	O2-C2-C1	2.99	115.28	109.15
17	T	6	MAN	C3-C4-C5	-2.98	104.92	110.24
16	S	8	MAN	C1-C2-C3	-2.97	106.01	109.67
10	J	7	NAG	C1-O5-C5	2.95	116.19	112.19
12	M	4	MAN	C1-O5-C5	2.93	116.17	112.19
17	T	5	MAN	C1-C2-C3	2.93	113.27	109.67
16	S	5	MAN	O2-C2-C1	-2.92	103.18	109.15
10	J	1	NAG	O5-C5-C6	2.91	111.77	107.20
10	J	1	NAG	C1-O5-C5	-2.90	108.26	112.19
11	K	1	NAG	O4-C4-C3	-2.84	103.78	110.35
16	S	2	NAG	O4-C4-C5	-2.81	102.33	109.30
17	T	3	BMA	O5-C1-C2	-2.75	106.52	110.77
17	T	4	MAN	O4-C4-C3	2.71	116.62	110.35
17	T	2	NAG	O4-C4-C3	-2.71	104.09	110.35
8	W	2	NAG	O4-C4-C5	-2.68	102.64	109.30
9	N	1	NAG	O4-C4-C5	-2.64	102.75	109.30
14	P	4	MAN	O2-C2-C1	-2.63	103.77	109.15
14	P	2	NAG	O4-C4-C3	-2.62	104.30	110.35
15	R	4	MAN	O5-C1-C2	-2.61	106.73	110.77
11	K	1	NAG	O5-C1-C2	-2.61	107.16	111.29
16	S	4	MAN	C1-C2-C3	2.59	112.84	109.67
14	P	2	NAG	O4-C4-C5	-2.58	102.89	109.30
11	K	1	NAG	C1-O5-C5	2.58	115.68	112.19
12	M	7	MAN	O5-C1-C2	-2.57	106.80	110.77
11	U	3	BMA	O5-C5-C6	2.57	111.23	107.20
13	O	5	MAN	O5-C1-C2	-2.56	106.81	110.77
8	C	1	NAG	O5-C5-C6	-2.56	103.20	107.20
12	M	4	MAN	O2-C2-C3	-2.52	105.08	110.14
10	J	1	NAG	C4-C3-C2	2.52	114.71	111.02
11	U	1	NAG	C1-O5-C5	2.50	115.57	112.19
10	J	9	NAG	C1-O5-C5	2.49	115.57	112.19
14	P	3	BMA	C3-C4-C5	-2.49	105.80	110.24
12	M	8	NAG	O5-C5-C6	2.47	111.07	107.20
16	S	8	MAN	O5-C1-C2	-2.47	106.97	110.77
17	T	1	NAG	O4-C4-C3	-2.46	104.66	110.35
7	A	1	NAG	O5-C5-C6	2.46	111.05	107.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	J	11	FUC	C1-C2-C3	2.45	112.68	109.67
16	S	5	MAN	O2-C2-C3	-2.44	105.25	110.14
17	T	5	MAN	O5-C5-C6	2.43	111.01	107.20
11	U	3	BMA	O3-C3-C2	-2.41	105.38	109.99
10	J	3	BMA	C6-C5-C4	-2.39	107.40	113.00
11	K	1	NAG	O5-C5-C6	-2.38	103.47	107.20
17	T	4	MAN	O3-C3-C2	-2.37	105.46	109.99
9	F	1	NAG	O4-C4-C3	-2.34	104.94	110.35
8	W	2	NAG	O5-C1-C2	-2.33	107.61	111.29
14	P	3	BMA	O5-C5-C6	2.32	110.84	107.20
13	O	2	NAG	O5-C1-C2	-2.32	107.62	111.29
17	T	2	NAG	O5-C1-C2	-2.31	107.64	111.29
15	R	3	BMA	C1-C2-C3	2.31	112.51	109.67
14	P	1	NAG	O5-C1-C2	-2.30	107.66	111.29
16	S	3	BMA	O3-C3-C2	-2.30	105.59	109.99
9	I	1	NAG	C4-C3-C2	-2.30	107.65	111.02
11	K	2	NAG	C1-C2-N2	2.28	114.39	110.49
16	S	9	MAN	O5-C5-C6	2.27	110.77	107.20
13	O	2	NAG	O4-C4-C3	-2.26	105.11	110.35
15	R	1	NAG	C1-O5-C5	2.25	115.24	112.19
16	S	2	NAG	O4-C4-C3	-2.24	105.16	110.35
12	M	2	NAG	O3-C3-C2	-2.23	104.84	109.47
17	T	6	MAN	O5-C1-C2	-2.22	107.35	110.77
10	J	4	MAN	O2-C2-C1	-2.18	104.70	109.15
10	J	4	MAN	O5-C1-C2	-2.17	107.42	110.77
10	J	1	NAG	O4-C4-C5	-2.17	103.91	109.30
11	K	2	NAG	O5-C5-C6	2.17	110.60	107.20
10	J	10	GAL	C1-O5-C5	2.16	115.11	112.19
15	R	1	NAG	O5-C1-C2	-2.16	107.88	111.29
18	V	1	NAG	C6-C5-C4	-2.15	107.97	113.00
18	V	4	FUC	O5-C5-C4	2.15	113.37	109.52
8	C	2	NAG	O5-C5-C6	2.14	110.55	107.20
13	O	5	MAN	C1-O5-C5	-2.14	109.30	112.19
17	T	1	NAG	C1-O5-C5	-2.13	109.31	112.19
18	V	1	NAG	O4-C4-C3	-2.12	105.44	110.35
10	J	1	NAG	C3-C4-C5	-2.12	106.46	110.24
17	T	4	MAN	O4-C4-C5	2.12	114.56	109.30
11	K	3	BMA	O3-C3-C2	-2.11	105.94	109.99
10	J	3	BMA	C2-C3-C4	-2.11	107.24	110.89
17	T	3	BMA	O5-C5-C6	2.11	110.51	107.20
8	W	1	NAG	C1-O5-C5	2.10	115.04	112.19
16	S	8	MAN	O2-C2-C3	-2.10	105.93	110.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	P	7	MAN	C1-O5-C5	-2.09	109.36	112.19
10	J	2	NAG	C1-C2-N2	2.09	114.06	110.49
11	K	3	BMA	O5-C5-C6	2.09	110.48	107.20
16	S	6	MAN	O5-C1-C2	-2.07	107.58	110.77
9	I	1	NAG	C3-C4-C5	2.06	113.92	110.24
13	O	1	NAG	C1-O5-C5	2.05	114.97	112.19
13	O	4	MAN	C1-C2-C3	2.04	112.18	109.67
9	N	2	NAG	O5-C5-C6	2.04	110.40	107.20
16	S	4	MAN	O5-C1-C2	-2.04	107.62	110.77
13	O	3	BMA	C1-C2-C3	2.04	112.17	109.67
12	M	6	GAL	C1-O5-C5	2.03	114.94	112.19
11	K	4	MAN	O5-C5-C6	2.03	110.38	107.20
17	T	4	MAN	C2-C3-C4	-2.03	107.39	110.89
18	V	1	NAG	O5-C1-C2	-2.02	108.09	111.29
9	I	1	NAG	O5-C5-C4	-2.02	105.92	110.83
11	U	1	NAG	O5-C1-C2	-2.01	108.12	111.29

There are no chirality outliers.

All (79) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	W	3	BMA	C4-C5-C6-O6
12	M	4	MAN	O5-C5-C6-O6
14	P	6	GAL	O5-C5-C6-O6
8	W	3	BMA	O5-C5-C6-O6
14	P	1	NAG	O5-C5-C6-O6
15	R	5	NAG	O5-C5-C6-O6
9	Q	1	NAG	O5-C5-C6-O6
11	U	5	MAN	O5-C5-C6-O6
14	P	3	BMA	O5-C5-C6-O6
12	M	3	BMA	O5-C5-C6-O6
12	M	6	GAL	C4-C5-C6-O6
14	P	1	NAG	C4-C5-C6-O6
14	P	6	GAL	C4-C5-C6-O6
12	M	2	NAG	O5-C5-C6-O6
12	M	4	MAN	C4-C5-C6-O6
15	R	5	NAG	C4-C5-C6-O6
12	M	6	GAL	O5-C5-C6-O6
9	Q	1	NAG	C4-C5-C6-O6
11	U	5	MAN	C4-C5-C6-O6
14	P	3	BMA	C4-C5-C6-O6
8	C	2	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
17	T	7	MAN	O5-C5-C6-O6
12	M	3	BMA	C4-C5-C6-O6
8	W	1	NAG	C8-C7-N2-C2
8	W	1	NAG	O7-C7-N2-C2
11	K	1	NAG	C8-C7-N2-C2
11	K	1	NAG	O7-C7-N2-C2
11	K	2	NAG	C8-C7-N2-C2
11	K	2	NAG	O7-C7-N2-C2
12	M	5	NAG	C8-C7-N2-C2
12	M	5	NAG	O7-C7-N2-C2
12	M	8	NAG	C8-C7-N2-C2
12	M	8	NAG	O7-C7-N2-C2
14	P	5	NAG	C8-C7-N2-C2
14	P	5	NAG	O7-C7-N2-C2
12	M	2	NAG	C4-C5-C6-O6
17	T	7	MAN	C4-C5-C6-O6
14	P	4	MAN	O5-C5-C6-O6
15	R	3	BMA	O5-C5-C6-O6
8	C	2	NAG	O5-C5-C6-O6
17	T	2	NAG	O5-C5-C6-O6
10	J	1	NAG	O5-C5-C6-O6
16	S	7	MAN	O5-C5-C6-O6
16	S	7	MAN	C4-C5-C6-O6
11	K	3	BMA	O5-C5-C6-O6
13	O	6	MAN	C4-C5-C6-O6
14	P	7	MAN	C4-C5-C6-O6
15	R	3	BMA	C4-C5-C6-O6
14	P	4	MAN	C4-C5-C6-O6
16	S	9	MAN	C4-C5-C6-O6
10	J	1	NAG	C4-C5-C6-O6
9	I	2	NAG	O5-C5-C6-O6
10	J	2	NAG	O5-C5-C6-O6
13	O	6	MAN	O5-C5-C6-O6
12	M	1	NAG	C4-C5-C6-O6
12	M	2	NAG	C1-C2-N2-C7
10	J	9	NAG	O5-C5-C6-O6
13	O	1	NAG	O5-C5-C6-O6
13	O	1	NAG	C4-C5-C6-O6
10	J	9	NAG	C4-C5-C6-O6
11	K	3	BMA	C4-C5-C6-O6
11	U	3	BMA	C4-C5-C6-O6
17	T	1	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
8	C	2	NAG	C3-C2-N2-C7
11	K	2	NAG	C3-C2-N2-C7
16	S	2	NAG	C3-C2-N2-C7
16	S	9	MAN	O5-C5-C6-O6
13	O	3	BMA	C4-C5-C6-O6
15	R	4	MAN	O5-C5-C6-O6
12	M	1	NAG	O5-C5-C6-O6
13	O	4	MAN	O5-C5-C6-O6
8	C	1	NAG	C1-C2-N2-C7
11	U	3	BMA	O5-C5-C6-O6
9	I	2	NAG	C1-C2-N2-C7
18	V	2	NAG	O5-C5-C6-O6
17	T	6	MAN	C4-C5-C6-O6
13	O	2	NAG	C3-C2-N2-C7
13	O	2	NAG	C1-C2-N2-C7
14	P	7	MAN	O5-C5-C6-O6

There are no ring outliers.

30 monomers are involved in 27 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	J	7	NAG	1	0
10	J	9	NAG	1	0
17	T	4	MAN	1	0
11	K	2	NAG	1	0
11	U	5	MAN	1	0
12	M	1	NAG	2	0
11	U	3	BMA	1	0
14	P	3	BMA	1	0
12	M	3	BMA	2	0
10	J	5	NAG	1	0
9	N	1	NAG	1	0
16	S	2	NAG	1	0
10	J	11	FUC	4	0
12	M	4	MAN	1	0
12	M	7	MAN	1	0
9	N	2	NAG	1	0
17	T	5	MAN	2	0
16	S	5	MAN	1	0
10	J	2	NAG	1	0
7	A	2	FUC	1	0
17	T	7	MAN	3	0

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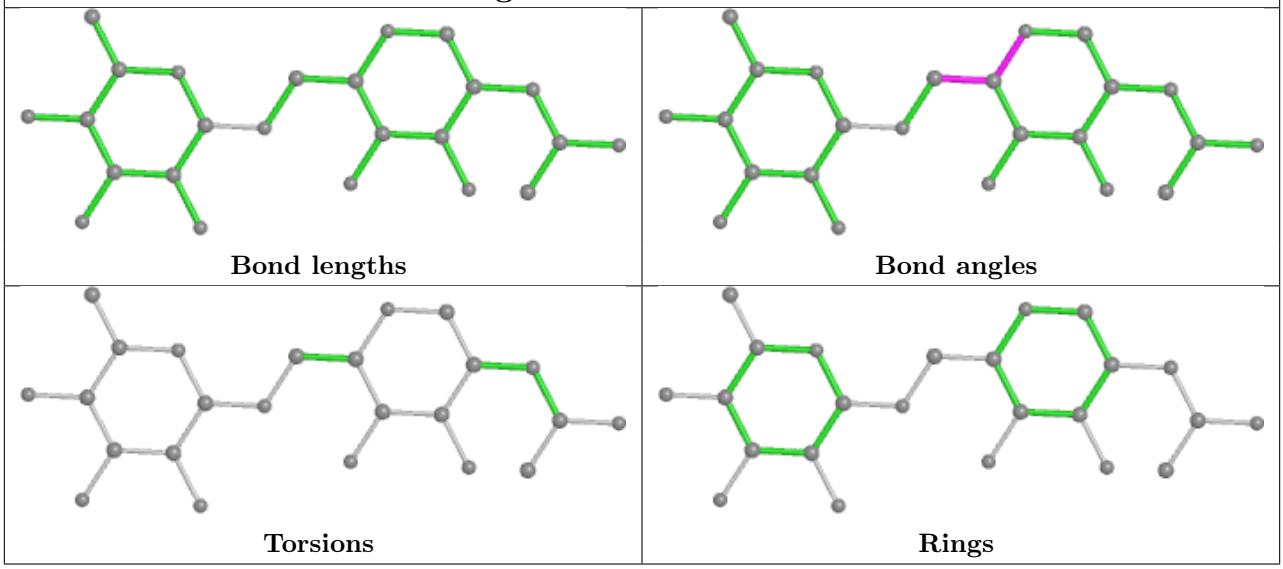
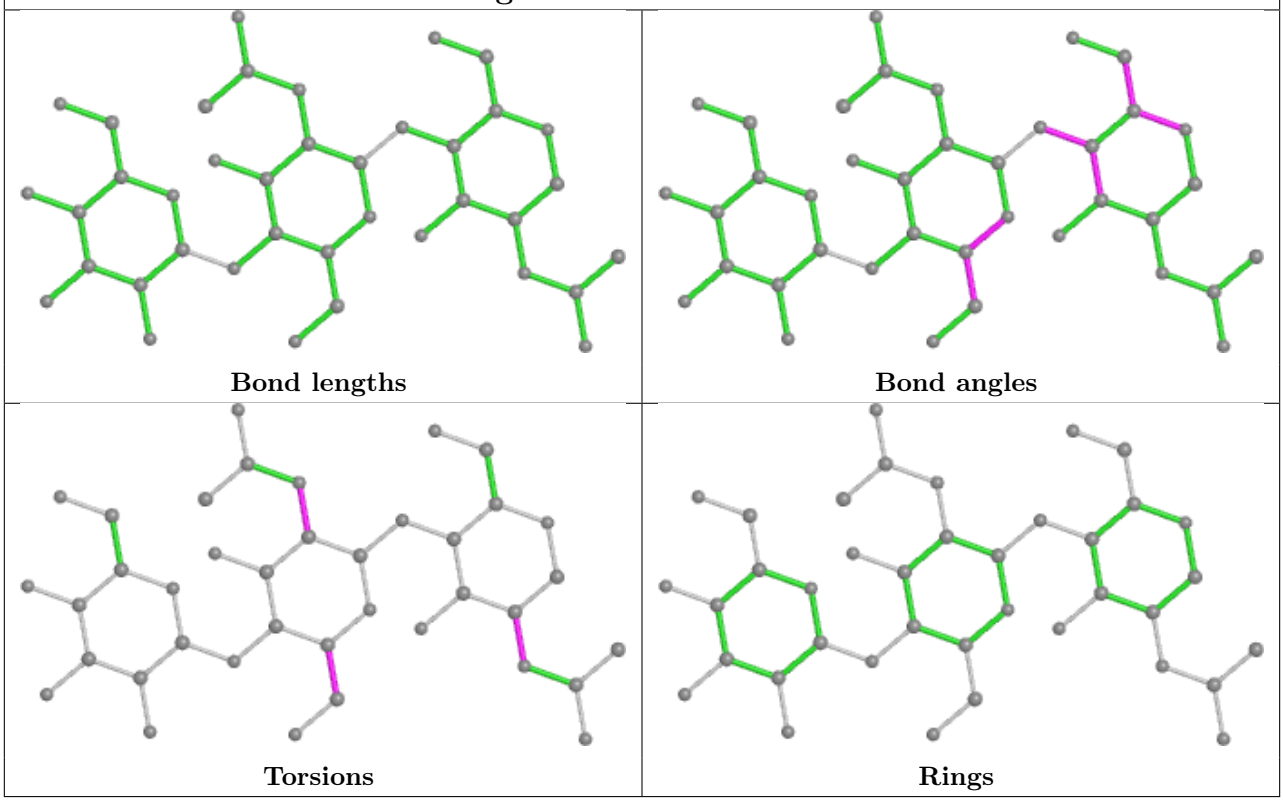
Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	T	3	BMA	3	0
10	J	4	MAN	1	0
11	U	1	NAG	1	0
12	M	2	NAG	2	0
16	S	4	MAN	1	0
9	F	1	NAG	2	0
17	T	2	NAG	1	0
14	P	4	MAN	1	0
11	K	1	NAG	1	0

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

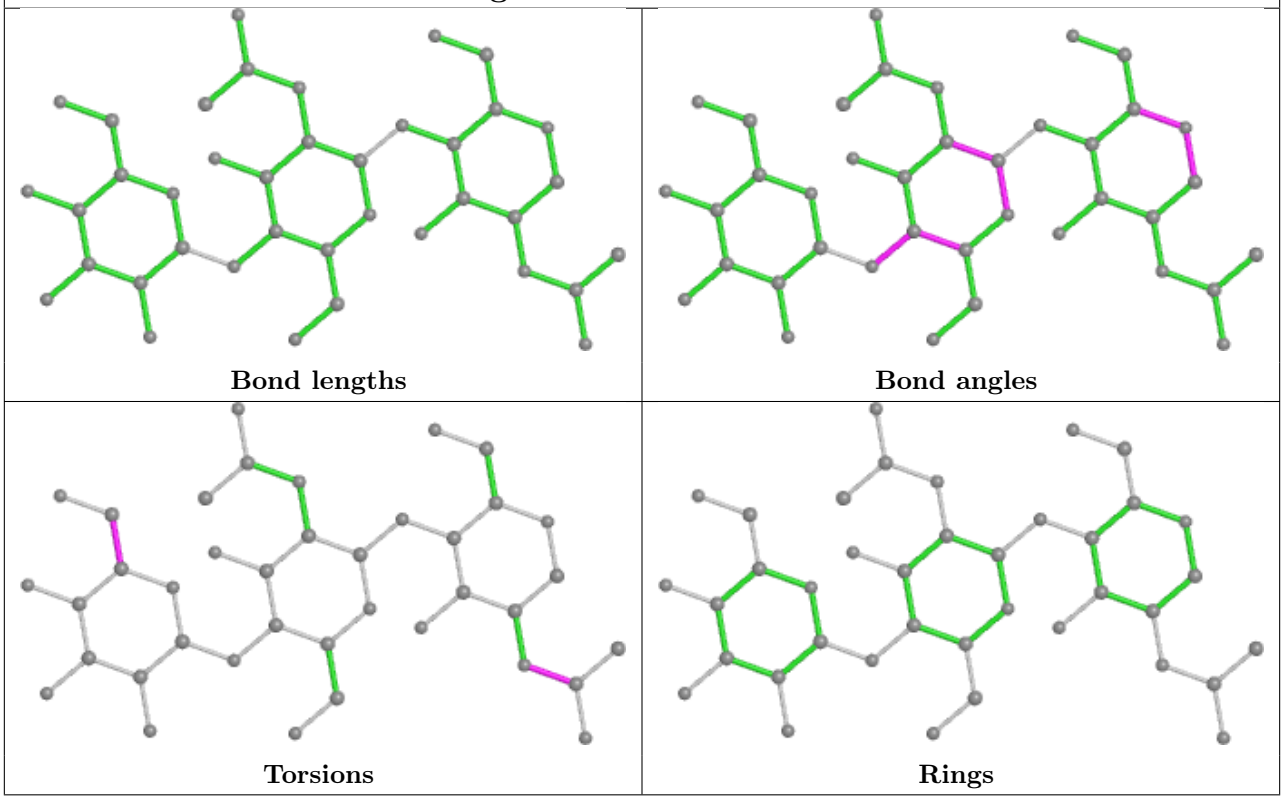
Oligosaccharide Chain A



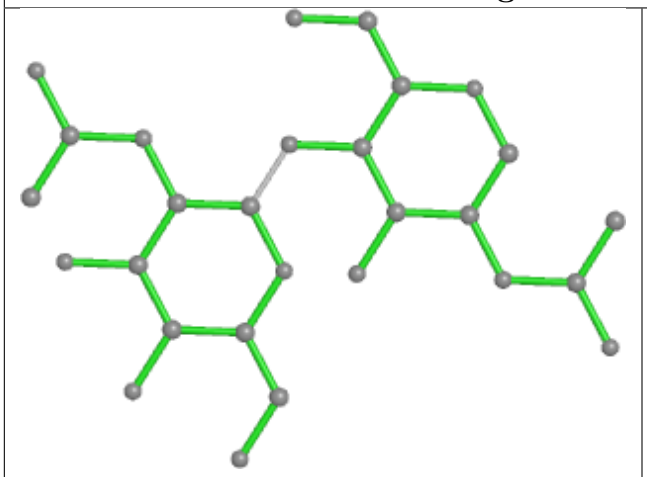
Oligosaccharide Chain C



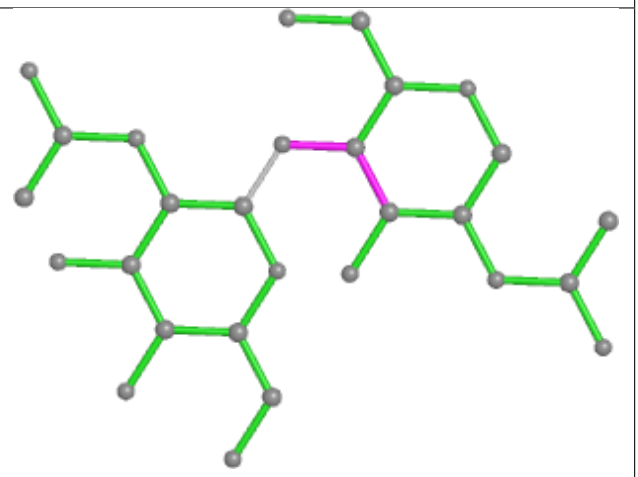
Oligosaccharide Chain W



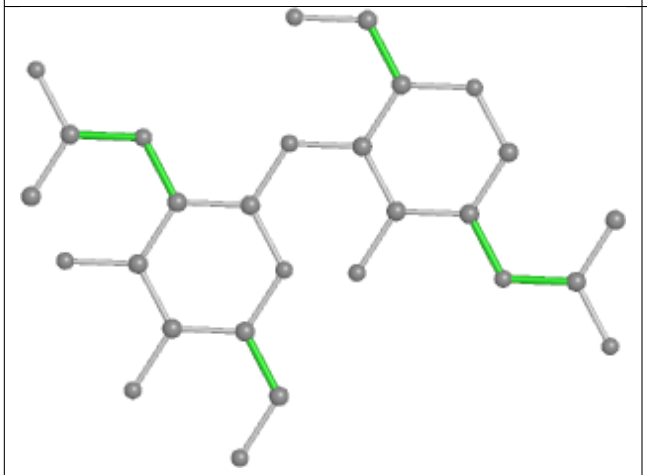
Oligosaccharide Chain F



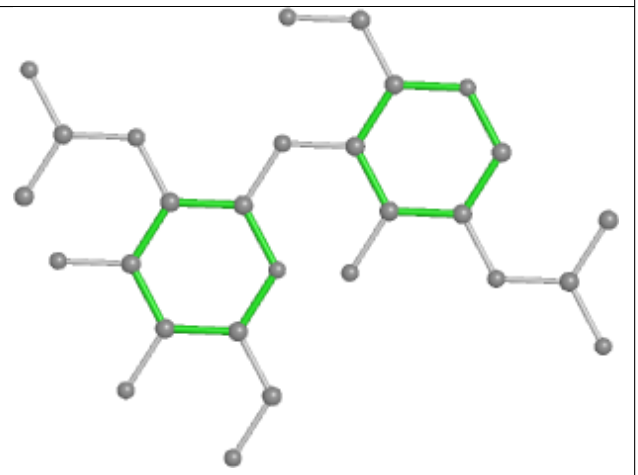
Bond lengths



Bond angles

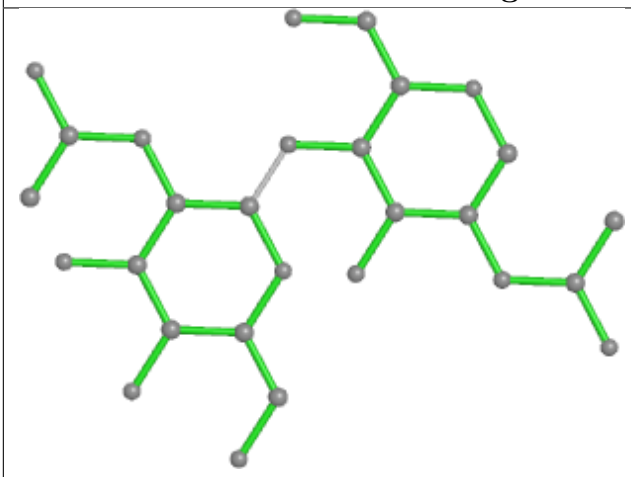


Torsions

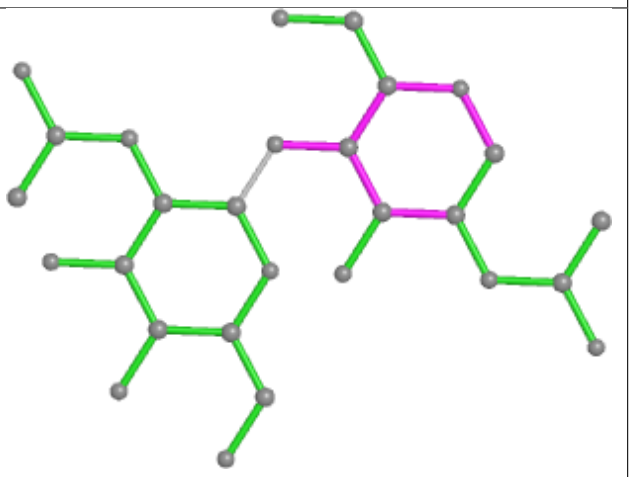


Rings

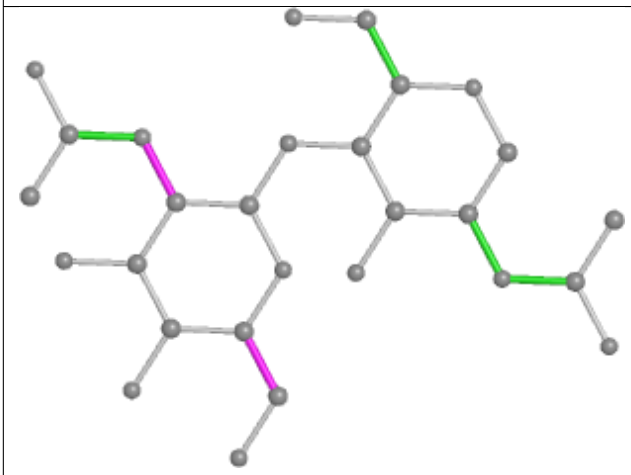
Oligosaccharide Chain I



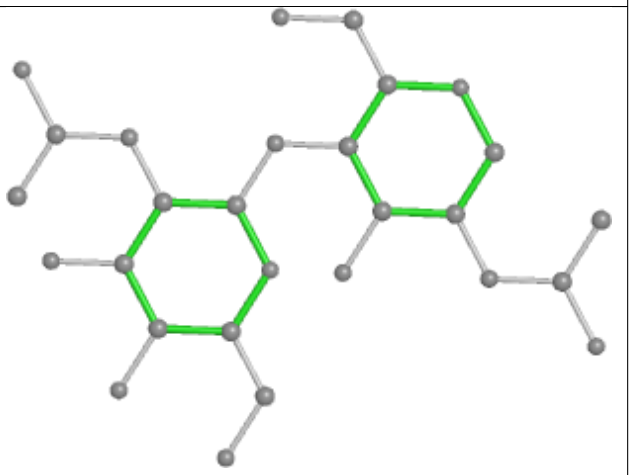
Bond lengths



Bond angles

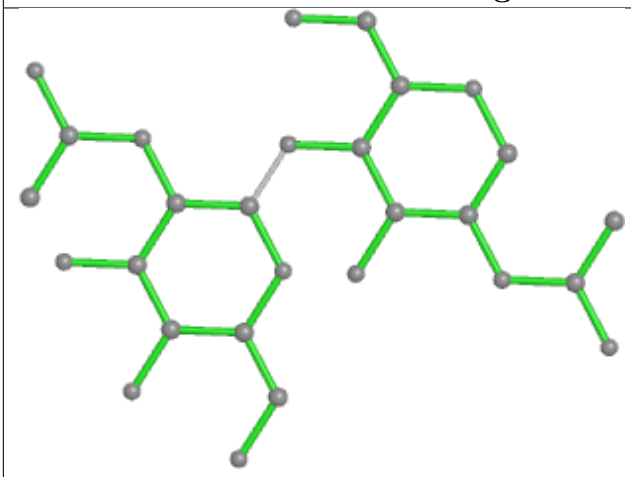


Torsions

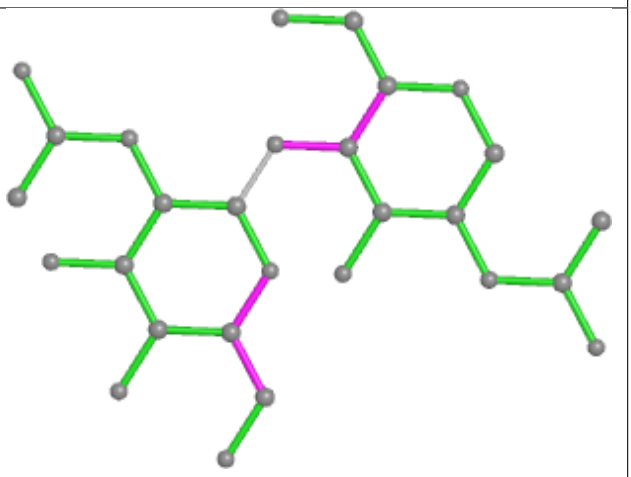


Rings

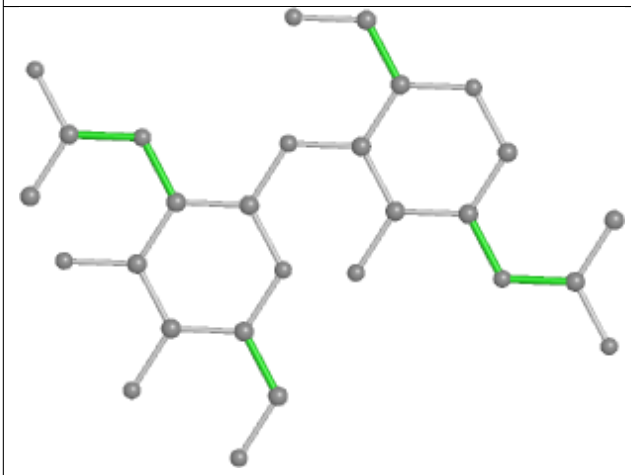
Oligosaccharide Chain N



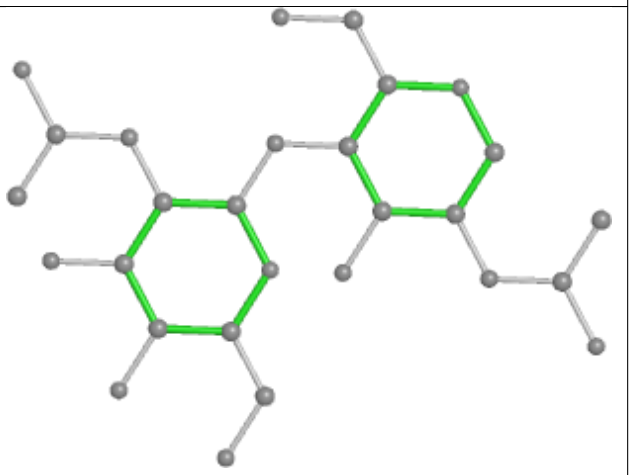
Bond lengths



Bond angles

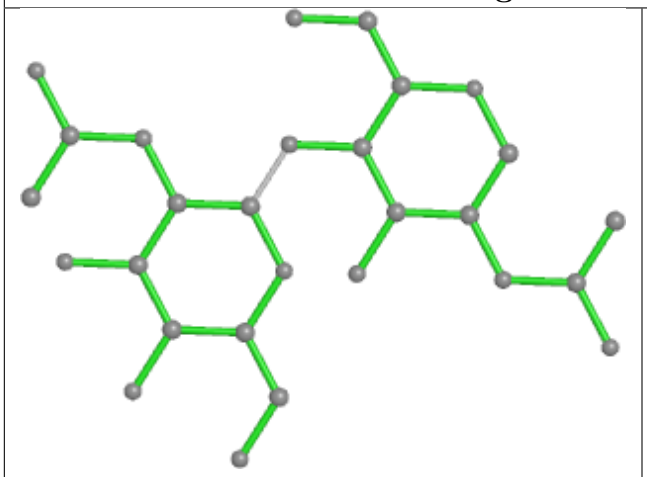


Torsions

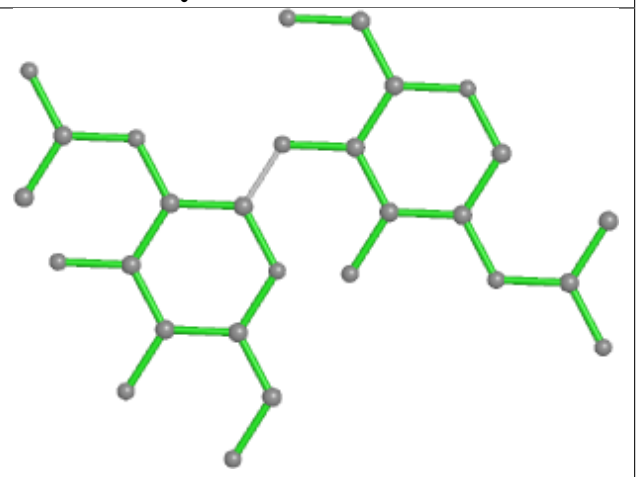


Rings

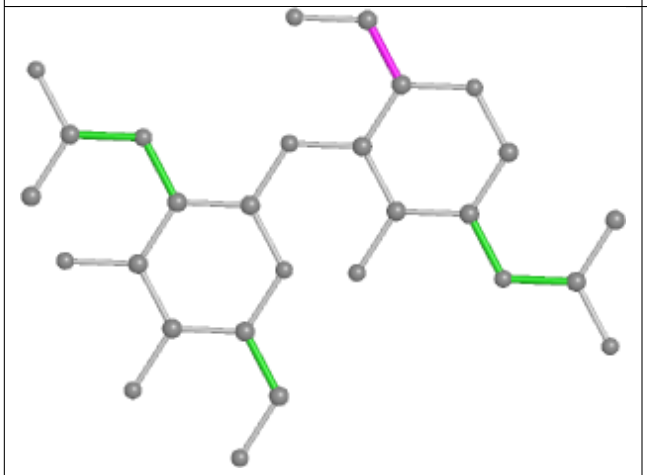
Oligosaccharide Chain Q



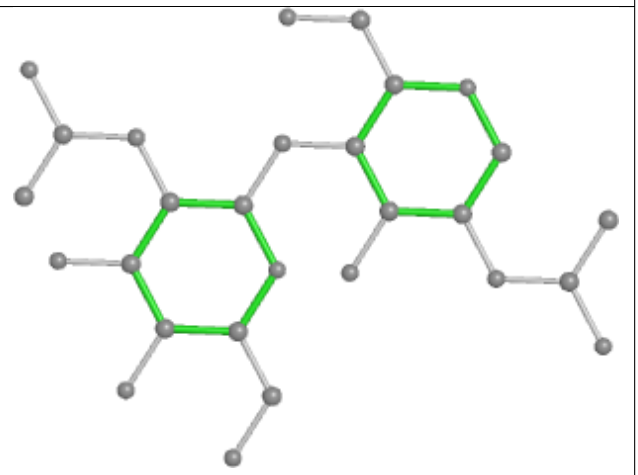
Bond lengths



Bond angles

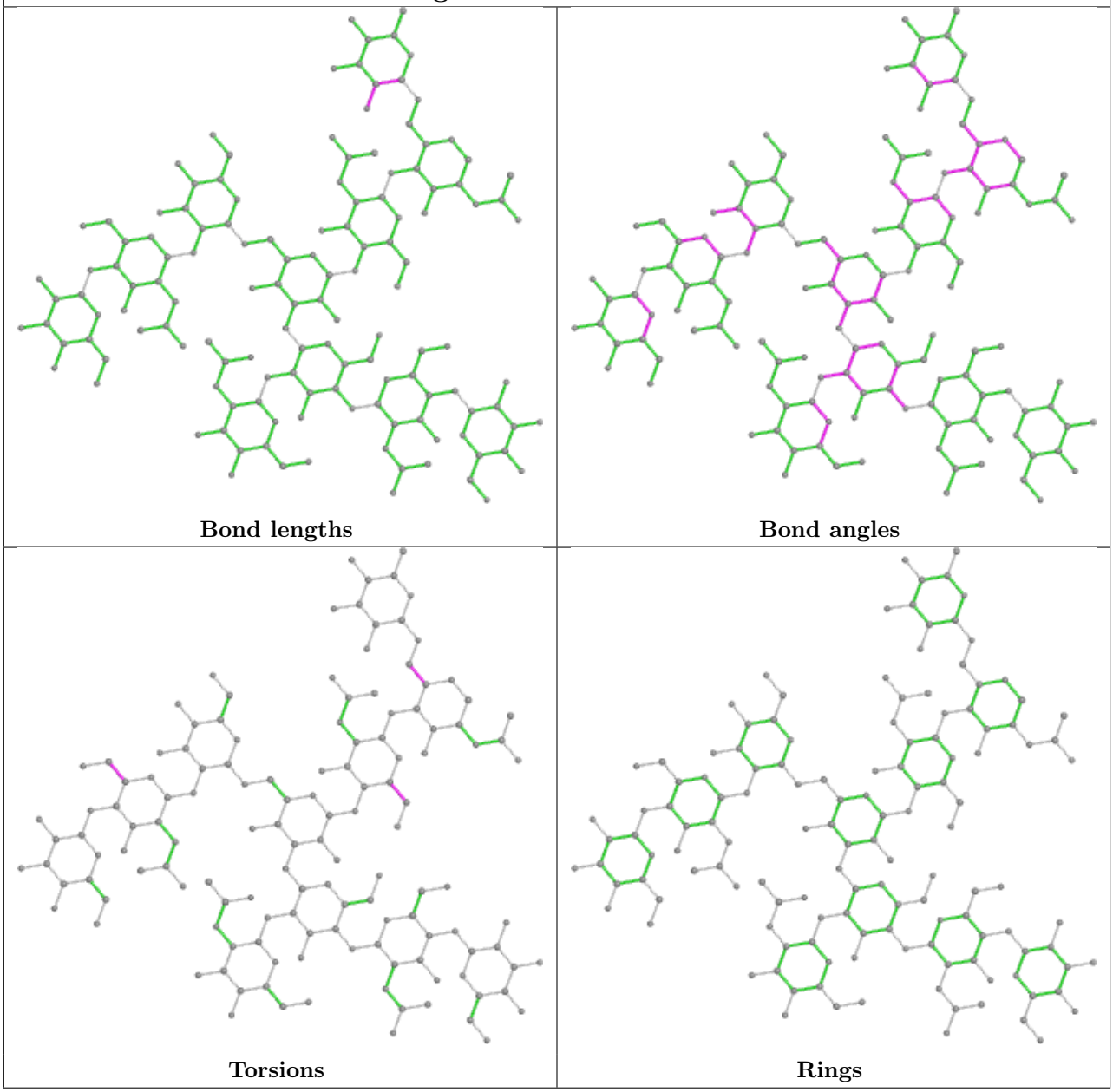


Torsions

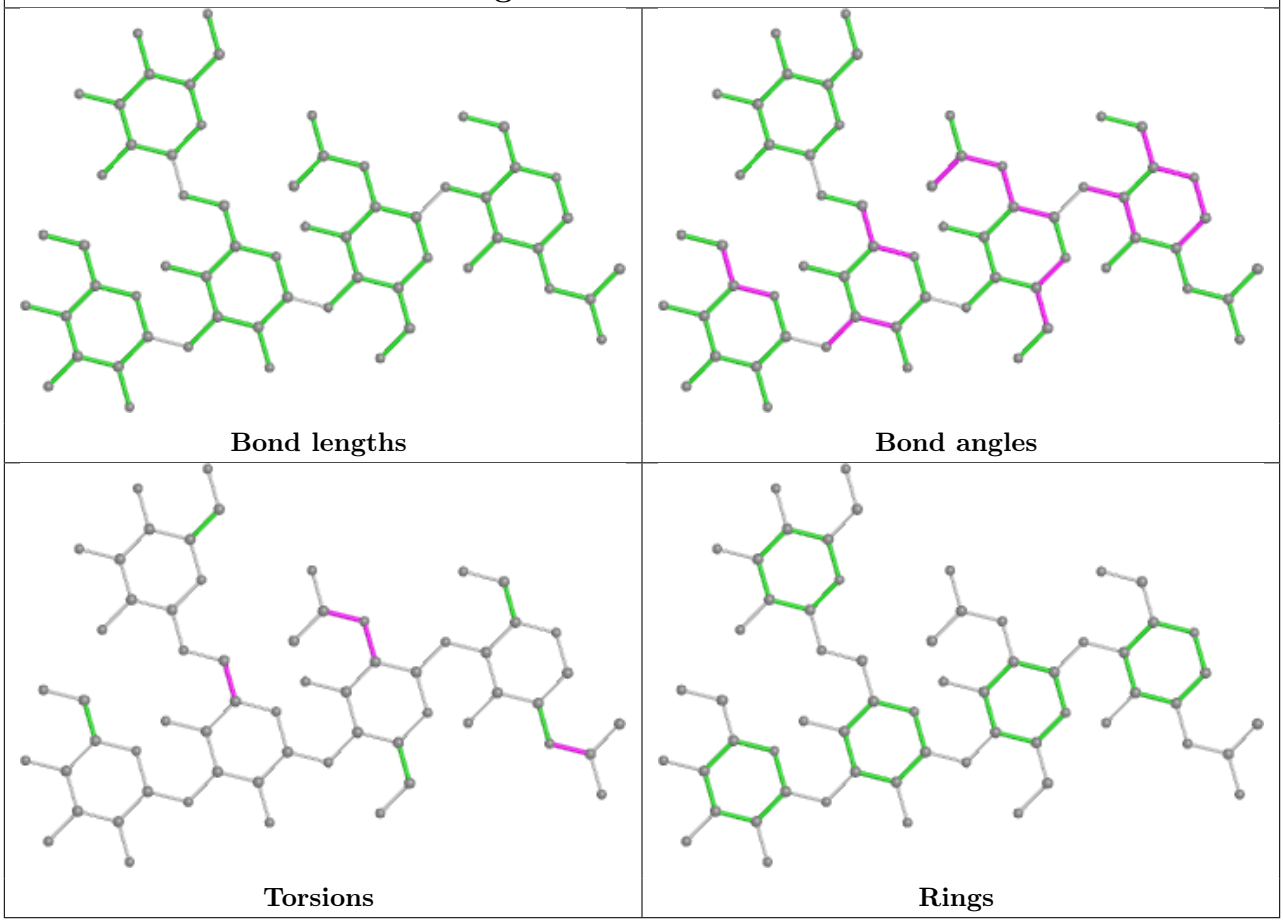


Rings

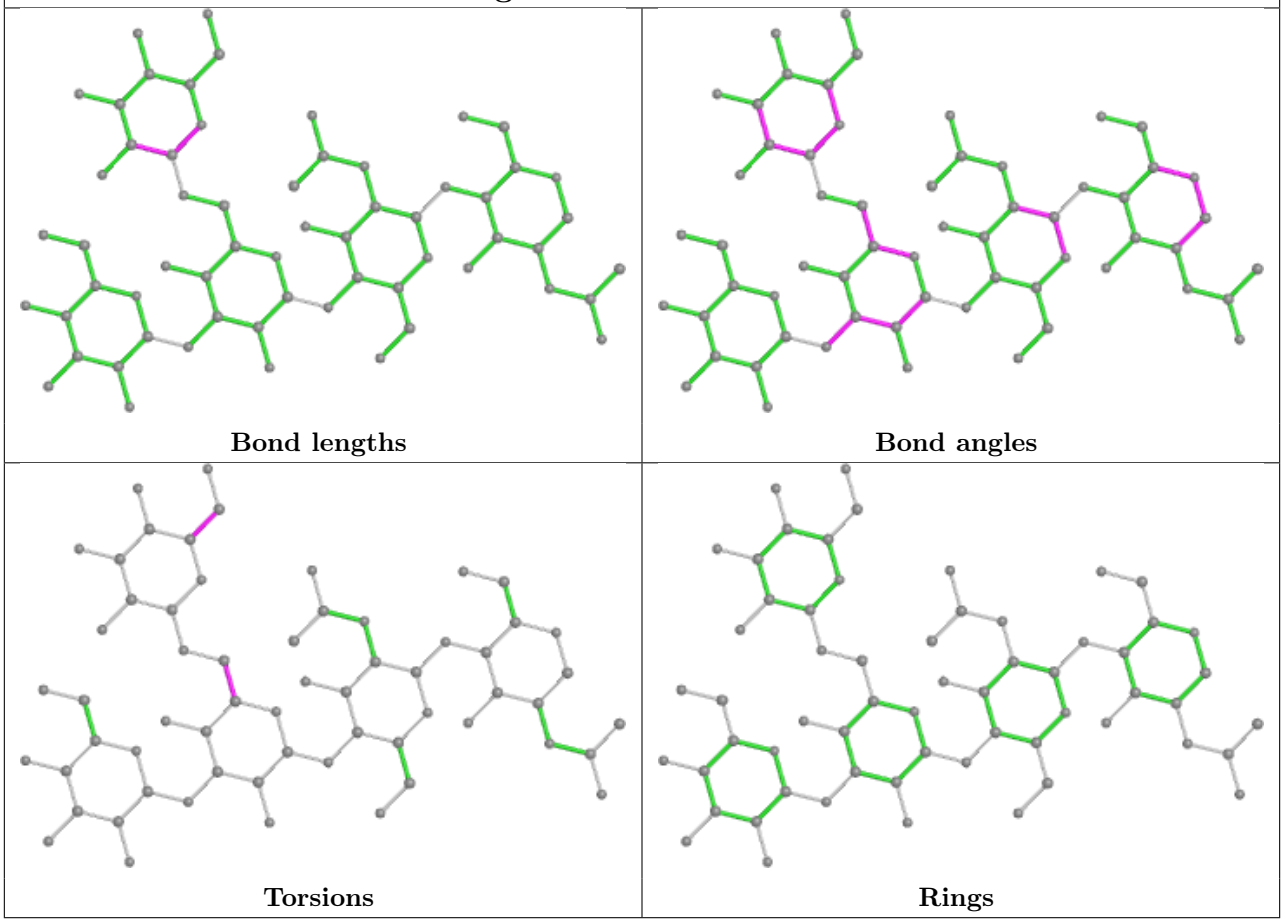
Oligosaccharide Chain J



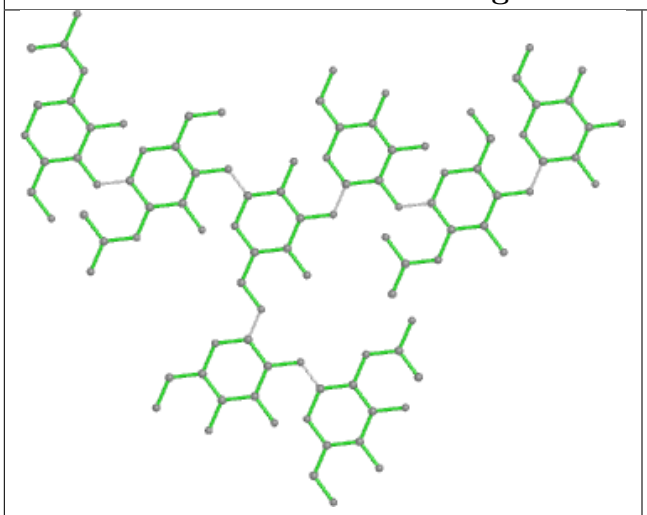
Oligosaccharide Chain K



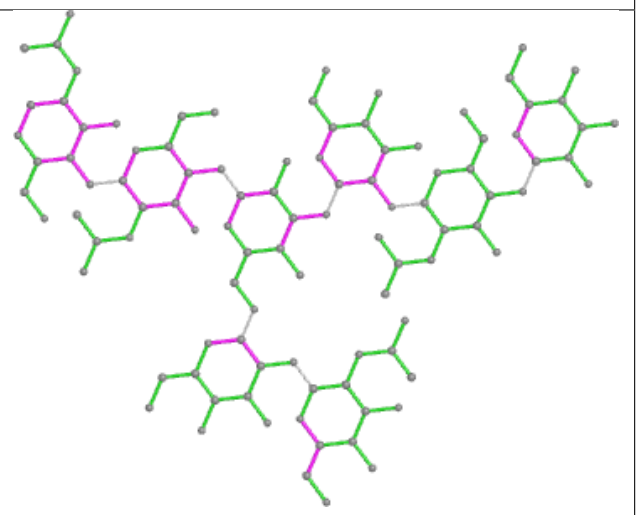
Oligosaccharide Chain U



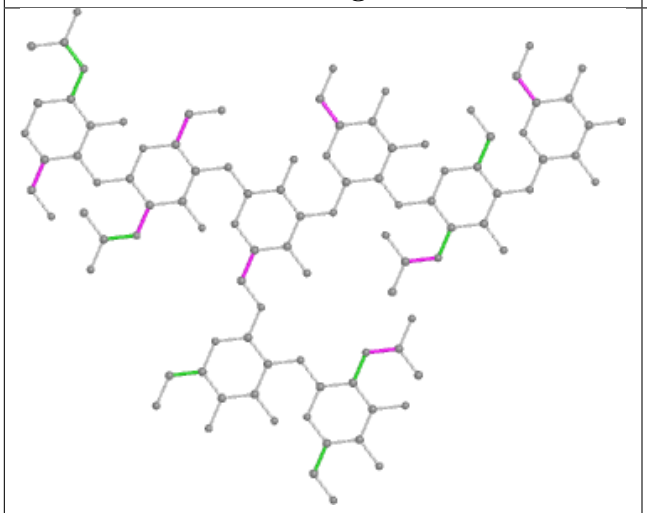
Oligosaccharide Chain M



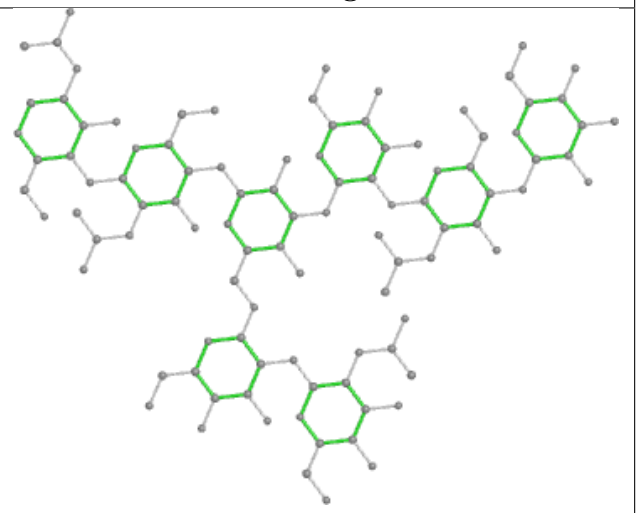
Bond lengths



Bond angles

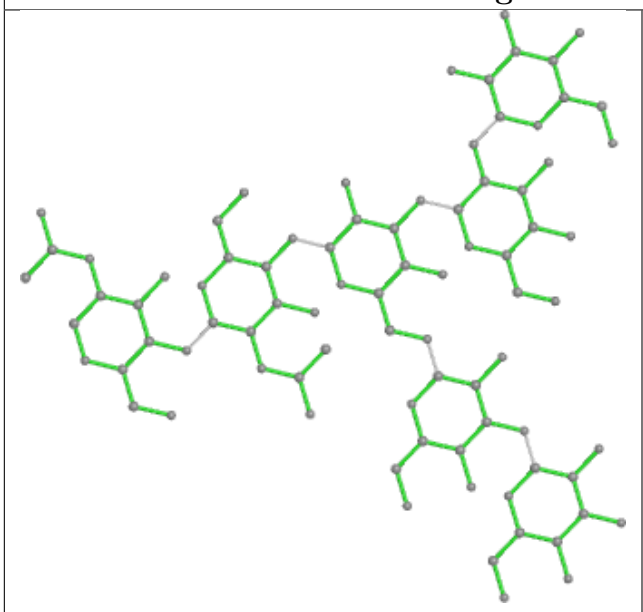


Torsions

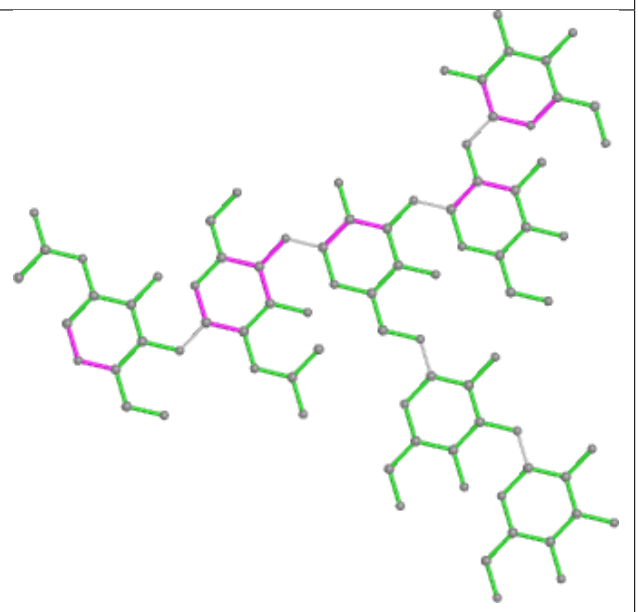


Rings

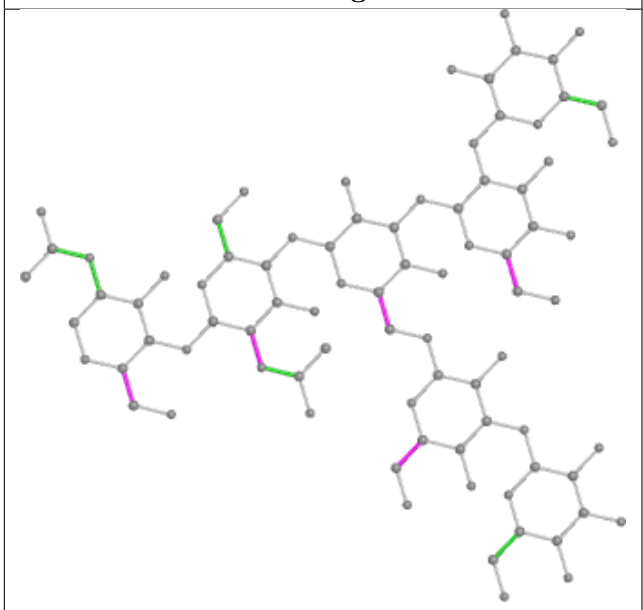
Oligosaccharide Chain O



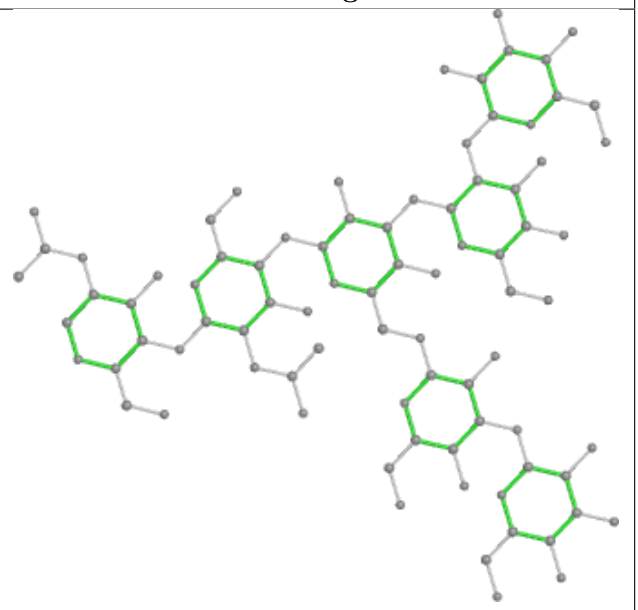
Bond lengths



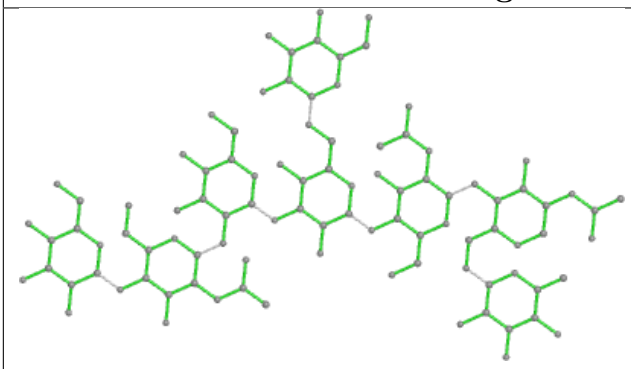
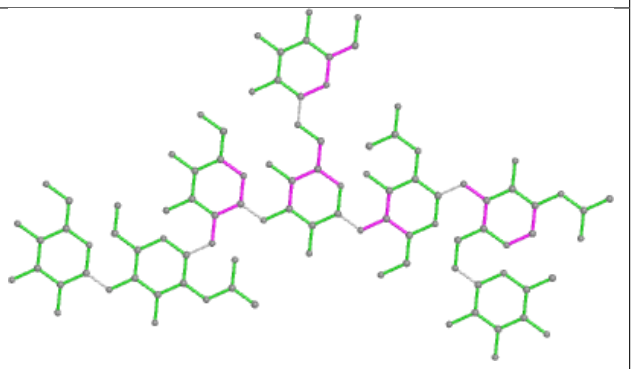
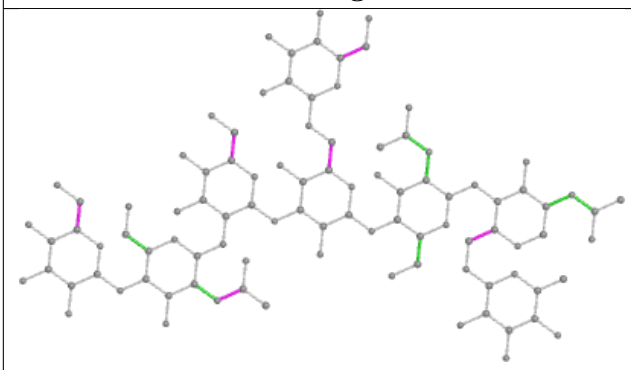
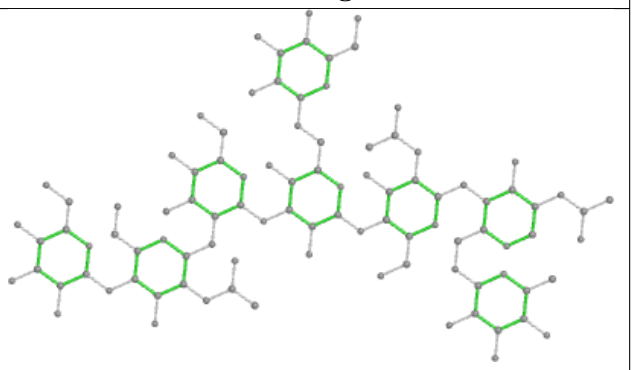
Bond angles

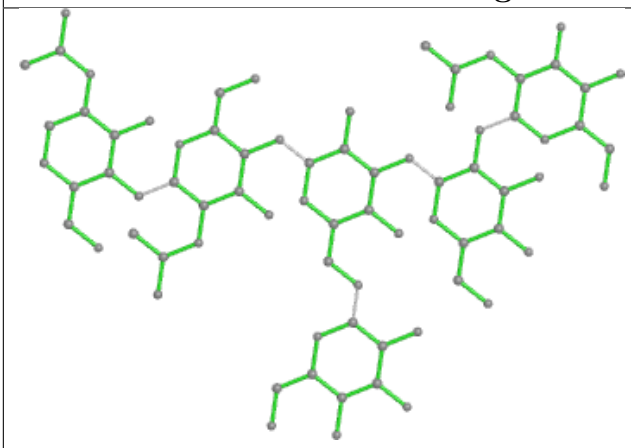
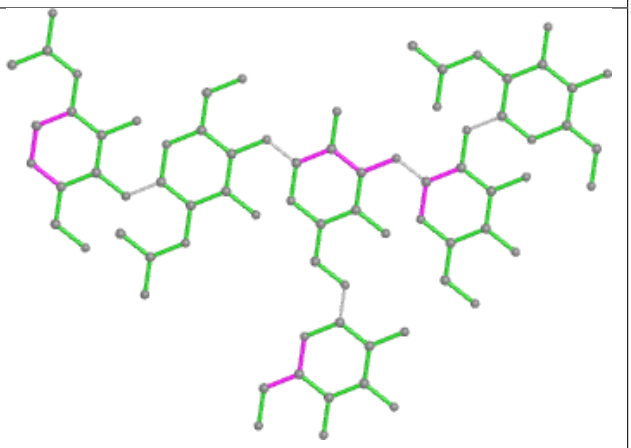
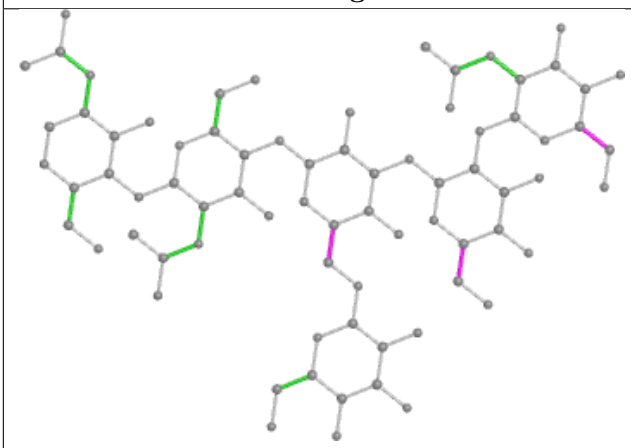
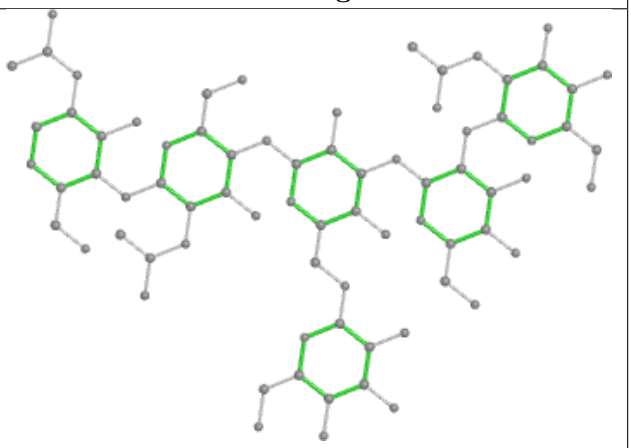


Torsions

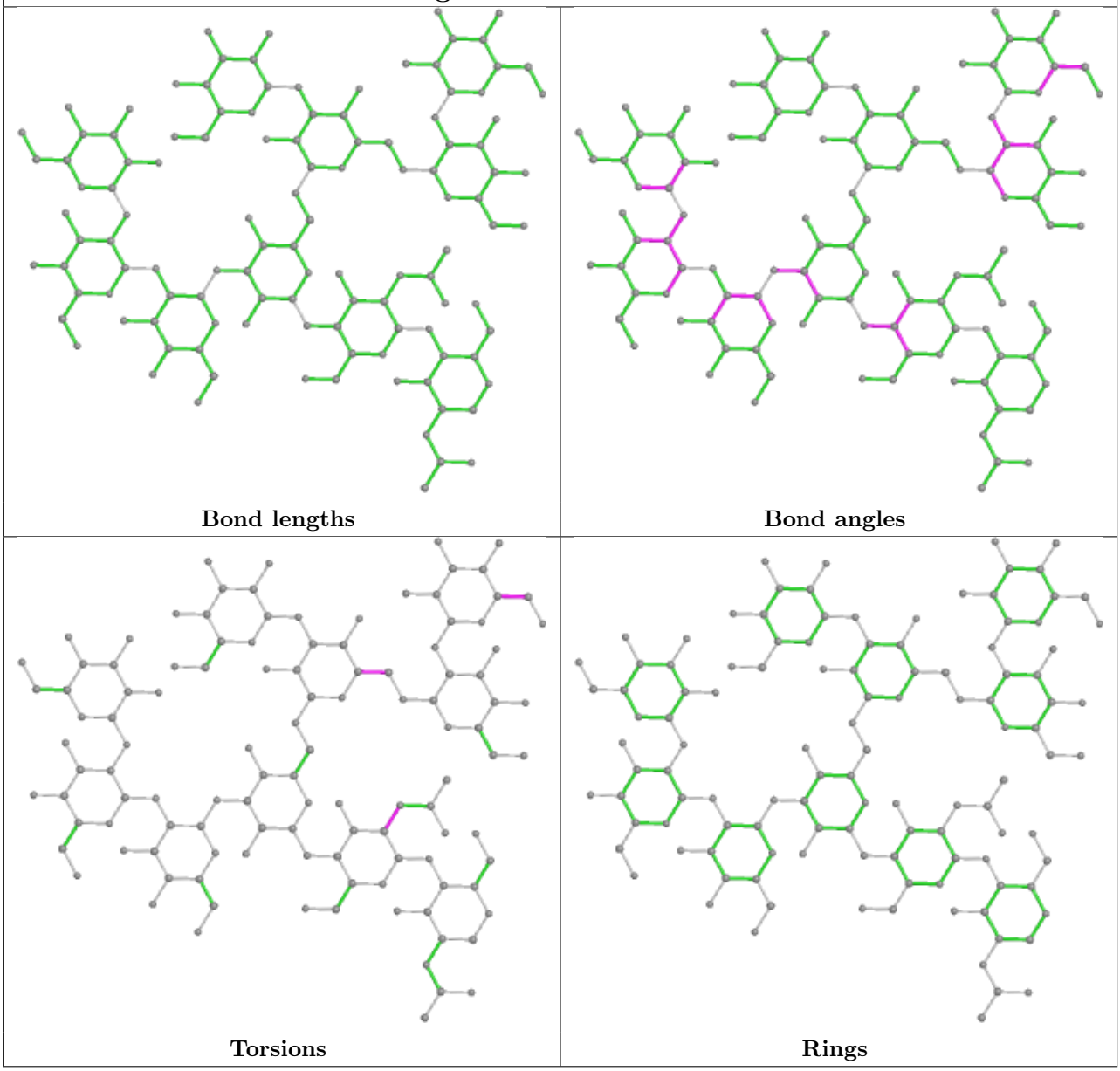


Rings

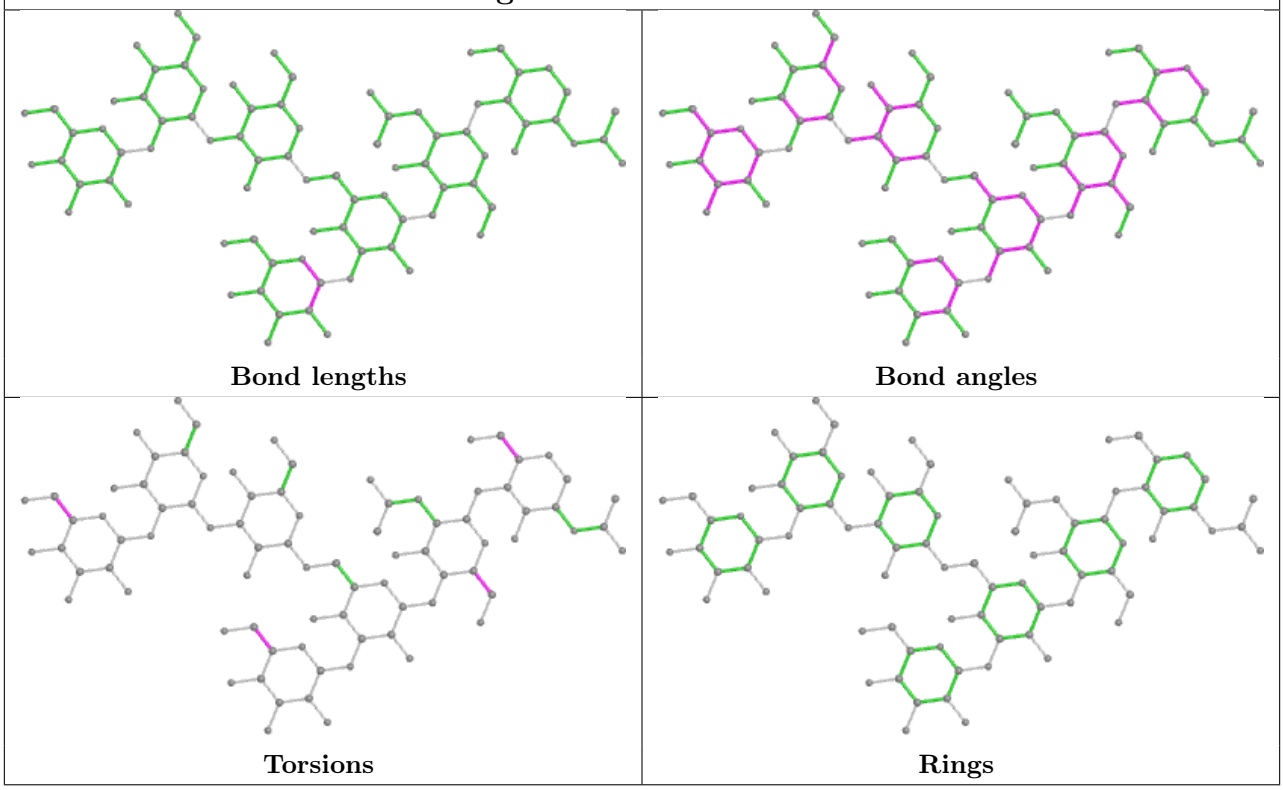
Oligosaccharide Chain P	
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain R	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

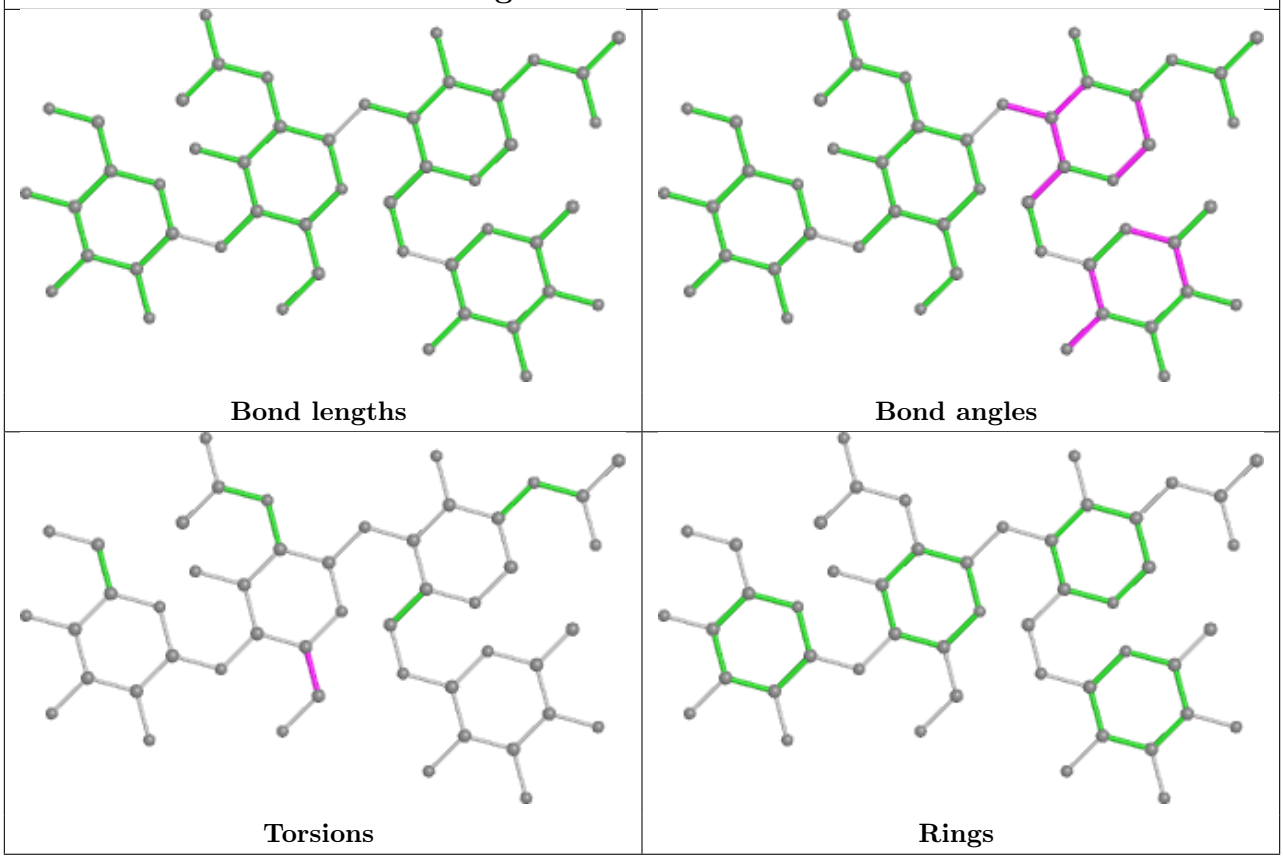
Oligosaccharide Chain S



Oligosaccharide Chain T



Oligosaccharide Chain V



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	$\#\|Z\| > 2$
19	NAG	G	3550	2	14,14,15	0.31	0	17,19,21	0.71	0
19	NAG	G	3390	2	14,14,15	0.29	0	17,19,21	0.77	1 (5%)

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
19	NAG	G	3550	2	-	4/6/23/26	0/1/1/1
19	NAG	G	3390	2	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	G	3390	NAG	O5-C5-C6	2.08	110.46	107.20

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
19	G	3550	NAG	C8-C7-N2-C2
19	G	3550	NAG	O7-C7-N2-C2
19	G	3550	NAG	C4-C5-C6-O6
19	G	3390	NAG	C4-C5-C6-O6
19	G	3550	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	B	126/153 (82%)	0.41	9 (7%)	16	15	134, 197, 240, 278	0
2	G	450/481 (93%)	0.56	18 (4%)	38	33	70, 138, 243, 334	0
3	H	230/238 (96%)	1.27	46 (20%)	1	1	106, 228, 348, 427	0
4	L	211/214 (98%)	1.37	51 (24%)	0	0	119, 258, 380, 414	0
5	D	229/232 (98%)	2.28	78 (34%)	0	0	89, 177, 439, 480	0
6	E	210/214 (98%)	2.02	72 (34%)	0	0	109, 243, 408, 444	0
All	All	1456/1532 (95%)	1.26	274 (18%)	1	1	70, 189, 390, 480	0

All (274) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	D	133	GLY	18.7
5	D	127	SER	18.1
6	E	210	THR	17.3
5	D	126	PRO	17.3
4	L	209	PRO	16.9
5	D	216	CYS	16.4
6	E	155	PRO	15.4
6	E	108	GLY	14.7
5	D	134	GLY	14.1
5	D	135	THR	13.5
3	H	127	SER	12.8
6	E	134	VAL	12.7
5	D	128	SER	12.6
4	L	145	VAL	11.9
3	H	212	GLU	11.8
5	D	125	ALA	11.7
6	E	117	THR	11.6
5	D	215	SER	11.4
5	D	165	THR	11.2

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Mol	Chain	Res	Type	RSRZ
6	E	133	LEU	11.2
5	D	199	ASN	10.8
6	E	147	VAL	10.8
5	D	140	CYS	10.7
6	E	190	ARG	10.5
4	L	192	TYR	10.5
3	H	136	ALA	10.1
6	E	208	ALA	9.8
4	L	118	LEU	9.1
3	H	138	LEU	9.1
5	D	192	GLN	8.9
3	H	152	VAL	8.7
6	E	136	LEU	8.7
6	E	206	THR	8.6
6	E	107	LEU	8.6
5	D	129	LYS	8.6
4	L	144	ALA	8.4
5	D	130	SER	8.0
5	D	141	LEU	8.0
4	L	132	THR	7.9
5	D	120	SER	7.5
6	E	143	GLY	7.3
5	D	151	THR	7.2
3	H	213	PRO	7.1
3	H	184	VAL	7.1
5	D	191	THR	7.1
3	H	183	THR	7.1
4	L	117	THR	7.0
6	E	135	CYS	7.0
3	H	194	TYR	6.8
6	E	118	LEU	6.8
5	D	147	PRO	6.8
5	D	189	LEU	6.7
5	D	152	VAL	6.7
4	L	206	THR	6.7
5	D	122	PHE	6.6
4	L	119	PHE	6.6
6	E	119	PHE	6.6
6	E	145	VAL	6.5
2	G	187	SER	6.5
5	D	121	VAL	6.4
3	H	179	SER	6.2

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Mol	Chain	Res	Type	RSRZ
5	D	148	GLU	6.2
6	E	127	GLN	6.2
5	D	160	THR	6.0
6	E	158	ALA	6.0
5	D	197	ASN	6.0
5	D	137	ALA	6.0
5	D	202	PRO	5.8
5	D	139	GLY	5.7
3	H	30	ASN	5.6
5	D	208	ASP	5.5
5	D	124	LEU	5.5
3	H	185	PRO	5.4
5	D	183	THR	5.4
3	H	126	PRO	5.4
5	D	149	PRO	5.4
3	H	137	ALA	5.4
4	L	191	SER	5.3
6	E	209	PRO	5.3
2	G	505	VAL	5.3
5	D	166	PHE	5.2
6	E	207	VAL	5.2
3	H	153	SER	5.2
5	D	201	LYS	5.2
4	L	207	VAL	5.2
3	H	181	VAL	5.2
5	D	167	PRO	5.1
5	D	162	GLY	5.1
6	E	148	ALA	5.1
6	E	120	PRO	5.1
6	E	113	ALA	5.0
6	E	196	VAL	5.0
5	D	153	SER	5.0
4	L	156	VAL	5.0
3	H	142	VAL	5.0
5	D	179	SER	5.0
6	E	156	VAL	4.9
6	E	111	LYS	4.9
1	B	518	VAL	4.8
6	E	176	SER	4.8
5	D	136	ALA	4.7
4	L	208	ALA	4.7
6	E	189	HIS	4.7

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Mol	Chain	Res	Type	RSRZ
5	D	132	SER	4.7
5	D	180	SER	4.7
6	E	159	GLY	4.7
5	D	193	THR	4.7
5	D	157	GLY	4.6
6	E	132	THR	4.6
6	E	122	SER	4.6
5	D	206	LYS	4.6
3	H	141	LEU	4.6
4	L	134	VAL	4.5
6	E	146	THR	4.5
6	E	179	LEU	4.5
4	L	107	LEU	4.5
6	E	109	GLN	4.5
6	E	149	TRP	4.5
5	D	178	LEU	4.5
5	D	154	TRP	4.4
1	B	602	LEU	4.3
3	H	214	LYS	4.3
3	H	150	VAL	4.2
5	D	138	LEU	4.2
4	L	133	LEU	4.2
3	H	124	LEU	4.1
6	E	114	PRO	4.1
3	H	198	VAL	4.1
4	L	186	TRP	4.1
2	G	504	ARG	4.1
3	H	151	THR	4.1
3	H	90	TYR	4.1
6	E	194	CYS	4.0
5	D	190	GLY	4.0
6	E	112	ALA	4.0
4	L	199	GLU	4.0
3	H	37	ILE	4.0
6	E	157	LYS	4.0
6	E	154	SER	4.0
6	E	191	SER	4.0
6	E	128	ALA	3.9
5	D	150	VAL	3.9
6	E	144	ALA	3.9
1	B	519	PHE	3.9
6	E	131	ALA	3.9

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Mol	Chain	Res	Type	RSRZ
3	H	38	ARG	3.8
1	B	547	GLY	3.7
6	E	195	GLN	3.7
5	D	155	ASN	3.6
5	D	158	ALA	3.6
4	L	120	PRO	3.6
3	H	190	GLY	3.6
4	L	150	LYS	3.6
4	L	187	LYS	3.6
6	E	175	ALA	3.6
3	H	28	SER	3.6
2	G	40	TYR	3.6
3	H	211	VAL	3.6
5	D	187	SER	3.5
6	E	205	LYS	3.5
4	L	104	LEU	3.5
2	G	353	PHE	3.5
4	L	210	THR	3.5
6	E	188	SER	3.5
2	G	39	TYR	3.4
3	H	178	LEU	3.4
3	H	215	SER	3.4
3	H	9	PRO	3.4
5	D	173	SER	3.3
5	D	182	VAL	3.2
6	E	171	ASN	3.2
4	L	136	LEU	3.2
4	L	155	PRO	3.2
1	B	520	LEU	3.2
4	L	203	VAL	3.1
5	D	168	ALA	3.1
4	L	154	SER	3.1
4	L	190	ARG	3.1
5	D	214	LYS	3.1
5	D	198	VAL	3.1
6	E	165	PRO	3.1
5	D	172	SER	3.0
3	H	69	ILE	3.0
4	L	100	GLY	3.0
4	L	151	ALA	3.0
2	G	496	VAL	3.0
4	L	137	ILE	3.0

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Mol	Chain	Res	Type	RSRZ
6	E	180	SER	3.0
6	E	193	SER	3.0
4	L	106	VAL	3.0
5	D	100	SER	2.9
2	G	358	ILE	2.9
3	H	210	ARG	2.9
2	G	360	ARG	2.9
5	D	131	THR	2.9
3	H	180	SER	2.9
4	L	149	TRP	2.9
3	H	1	GLN	2.9
4	L	142	PRO	2.9
4	L	121	PRO	2.9
3	H	128	SER	2.9
2	G	498	PRO	2.8
3	H	193	THR	2.8
4	L	146	THR	2.8
5	D	170	LEU	2.8
5	D	159	LEU	2.8
6	E	162	THR	2.8
5	D	164	HIS	2.8
3	H	207	VAL	2.8
4	L	205	LYS	2.8
4	L	20	ARG	2.8
5	D	116	THR	2.7
6	E	187	LYS	2.7
6	E	192	TYR	2.7
6	E	116	VAL	2.7
2	G	361	PHE	2.7
4	L	135	CYS	2.7
4	L	179	LEU	2.7
1	B	569	THR	2.7
4	L	86	TYR	2.7
4	L	64	GLY	2.7
5	D	181	VAL	2.6
1	B	599	SER	2.6
4	L	178	TYR	2.6
5	D	142	VAL	2.6
6	E	152	ASP	2.6
4	L	147	VAL	2.6
2	G	31	ALA	2.6
5	D	213	PRO	2.6

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Mol	Chain	Res	Type	RSRZ
6	E	27(A)	ARG	2.5
6	E	110	PRO	2.5
6	E	124	GLU	2.5
6	E	181	LEU	2.5
6	E	106	VAL	2.5
2	G	45	TRP	2.5
3	H	121	VAL	2.5
6	E	161	GLU	2.5
6	E	178	TYR	2.5
5	D	196	CYS	2.4
5	D	174	GLY	2.4
2	G	188	ASN	2.4
6	E	129	ASN	2.4
3	H	35	THR	2.3
5	D	163	VAL	2.3
2	G	33	ASN	2.3
4	L	36	TYR	2.3
5	D	186	SER	2.3
5	D	175	LEU	2.3
4	L	193	SER	2.3
6	E	123	SER	2.3
3	H	47	TRP	2.3
3	H	89	VAL	2.3
5	D	188	SER	2.2
3	H	10	GLY	2.2
2	G	495	GLY	2.2
3	H	48	ILE	2.2
2	G	350	ARG	2.2
2	G	470	PRO	2.2
5	D	100(B)	ASP	2.2
5	D	100(A)	ALA	2.2
4	L	196	VAL	2.1
4	L	37	GLN	2.1
4	L	143	GLY	2.1
6	E	200	GLY	2.1
4	L	184	GLU	2.1
6	E	153	SER	2.1
6	E	125	GLU	2.1
5	D	207	VAL	2.1
4	L	131	ALA	2.1
1	B	601	LYS	2.1
3	H	11	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	606	THR	2.0
6	E	121	PRO	2.0
6	E	177	SER	2.0

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

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

6.3 Carbohydrates (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
12	GAL	M	6	11/12	0.34	0.41	306,310,319,322	0
14	MAN	P	7	11/12	0.40	0.39	277,277,277,277	0
14	NAG	P	2	14/15	0.51	0.40	226,246,249,249	0
14	FUC	P	8	10/11	0.52	0.57	225,225,225,225	0
15	MAN	R	6	11/12	0.53	0.50	236,236,236,236	0
9	NAG	I	2	14/15	0.57	0.37	242,242,242,242	0
11	MAN	U	4	11/12	0.59	0.28	242,242,242,242	0
17	BMA	T	3	11/12	0.59	0.21	243,243,243,243	0
11	BMA	U	3	11/12	0.60	0.21	249,249,249,249	0
14	GAL	P	6	11/12	0.60	0.28	290,290,290,290	0
11	MAN	K	5	11/12	0.62	0.30	293,293,293,293	0
11	MAN	K	4	11/12	0.62	0.33	293,293,293,293	0
17	MAN	T	7	11/12	0.62	0.31	237,237,237,237	0
13	MAN	O	5	11/12	0.63	0.35	223,223,223,223	0
17	MAN	T	6	11/12	0.64	0.25	215,215,215,215	0
10	GAL	J	6	11/12	0.64	0.27	278,278,278,278	0
14	NAG	P	1	14/15	0.65	0.40	204,214,231,234	0
7	NAG	A	1	14/15	0.65	0.38	246,258,311,313	0
7	FUC	A	2	10/11	0.65	0.39	256,256,256,256	0
13	MAN	O	7	11/12	0.66	0.44	257,259,268,273	0
12	MAN	M	7	11/12	0.67	0.24	216,224,229,230	0
10	NAG	J	7	14/15	0.69	0.43	275,275,275,275	0
9	NAG	F	2	14/15	0.69	0.51	244,244,244,244	0
13	MAN	O	6	11/12	0.70	0.33	251,268,274,283	0
17	MAN	T	5	11/12	0.70	0.20	218,218,218,218	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
15	NAG	R	5	14/15	0.70	0.25	223,223,223,223	0
12	NAG	M	5	14/15	0.70	0.38	284,297,302,304	0
8	BMA	W	3	11/12	0.71	0.35	244,280,310,364	0
18	FUC	V	4	10/11	0.71	0.33	250,255,265,273	0
9	NAG	F	1	14/15	0.72	0.24	222,222,222,222	0
10	NAG	J	2	14/15	0.73	0.23	179,199,212,212	0
12	NAG	M	2	14/15	0.73	0.36	177,197,200,200	0
10	BMA	J	3	11/12	0.74	0.13	237,237,237,237	0
12	MAN	M	4	11/12	0.74	0.23	255,255,255,255	0
17	NAG	T	2	14/15	0.75	0.36	227,233,241,245	0
11	MAN	U	5	11/12	0.75	0.33	245,245,245,245	0
12	BMA	M	3	11/12	0.75	0.27	198,205,209,214	0
15	BMA	R	3	11/12	0.75	0.15	231,231,231,231	0
14	BMA	P	3	11/12	0.75	0.13	265,272,276,281	0
12	NAG	M	1	14/15	0.75	0.45	153,162,180,183	0
9	NAG	N	2	14/15	0.76	0.36	227,229,232,233	0
11	BMA	K	3	11/12	0.76	0.16	273,273,273,273	0
17	MAN	T	4	11/12	0.77	0.16	227,227,227,227	0
8	BMA	C	3	11/12	0.78	0.25	241,241,241,241	0
10	NAG	J	9	14/15	0.78	0.19	263,263,263,263	0
15	MAN	R	4	11/12	0.78	0.32	245,245,245,245	0
18	BMA	V	3	11/12	0.78	0.24	227,234,238,243	0
11	NAG	K	1	14/15	0.78	0.32	140,164,173,185	0
13	BMA	O	3	11/12	0.79	0.30	193,211,226,228	0
16	MAN	S	6	11/12	0.79	0.30	144,149,154,155	0
14	NAG	P	5	14/15	0.79	0.22	285,299,303,305	0
10	GAL	J	10	11/12	0.79	0.23	275,275,275,275	0
12	NAG	M	8	14/15	0.79	0.28	210,223,227,229	0
16	MAN	S	9	11/12	0.80	0.35	266,266,266,266	0
18	NAG	V	1	14/15	0.80	0.22	214,224,242,245	0
18	NAG	V	2	14/15	0.80	0.19	233,254,256,257	0
15	NAG	R	2	14/15	0.80	0.24	207,207,207,207	0
16	MAN	S	8	11/12	0.80	0.34	237,252,258,260	0
10	NAG	J	5	14/15	0.81	0.18	273,273,273,273	0
10	MAN	J	8	11/12	0.81	0.17	236,236,236,236	0
9	NAG	Q	1	14/15	0.82	0.27	164,179,205,214	0
14	MAN	P	4	11/12	0.83	0.18	302,302,302,302	0
16	MAN	S	10	11/12	0.83	0.29	186,188,197,203	0
9	NAG	Q	2	14/15	0.83	0.33	199,213,224,232	0
11	NAG	K	2	14/15	0.84	0.20	208,221,233,240	0
9	NAG	N	1	14/15	0.84	0.25	186,200,216,224	0
10	NAG	J	1	14/15	0.85	0.21	148,161,214,215	0

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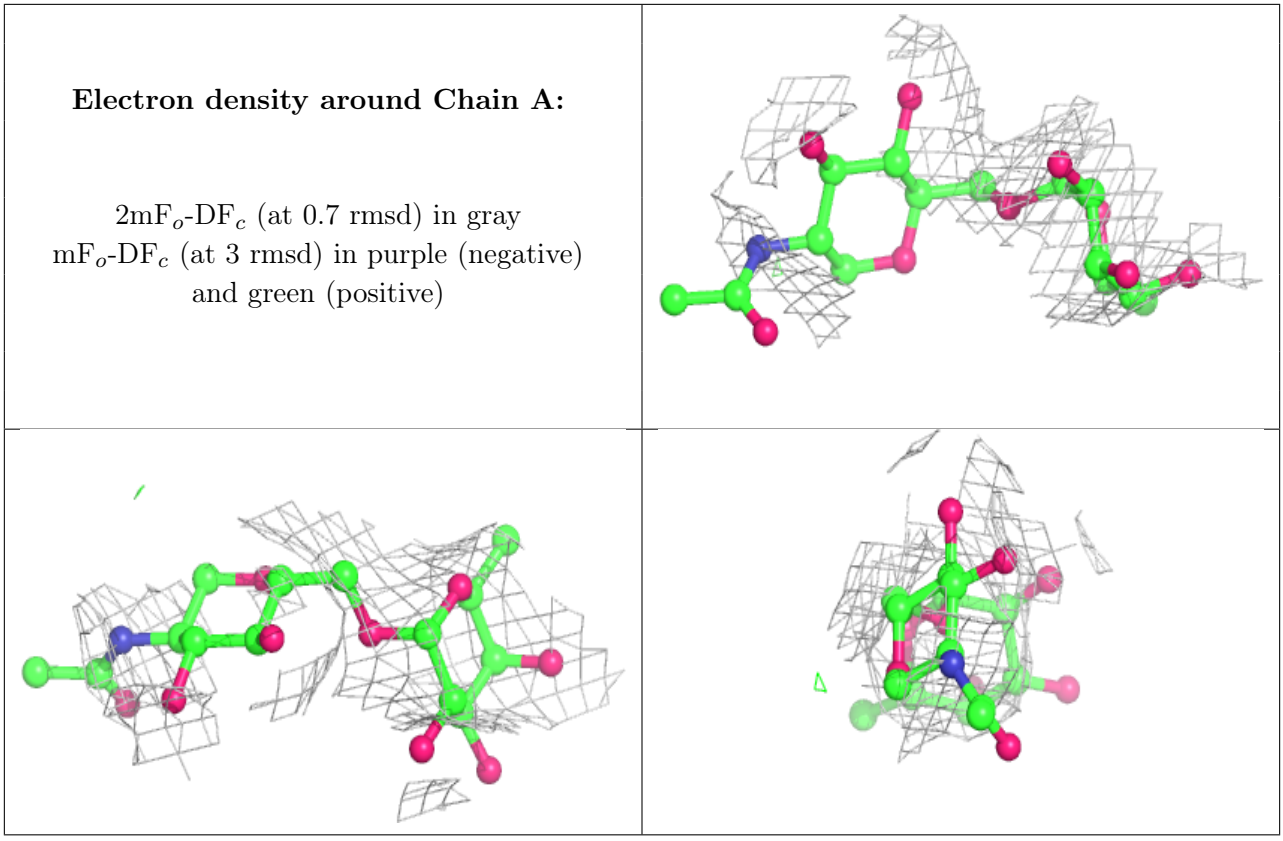
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
8	NAG	W	1	14/15	0.85	0.28	173,191,202,205	0
8	NAG	C	2	14/15	0.85	0.19	246,246,246,246	0
8	NAG	C	1	14/15	0.85	0.19	238,256,268,270	0
17	NAG	T	1	14/15	0.86	0.32	171,180,204,223	0
8	NAG	W	2	14/15	0.87	0.25	214,236,262,289	0
16	MAN	S	7	11/12	0.87	0.24	151,168,174,183	0
10	FUC	J	11	10/11	0.88	0.21	194,194,194,194	0
10	MAN	J	4	11/12	0.88	0.11	263,263,263,263	0
15	NAG	R	1	14/15	0.88	0.30	167,167,167,167	0
13	MAN	O	4	11/12	0.88	0.24	223,223,223,223	0
16	NAG	S	1	14/15	0.89	0.27	121,132,150,155	0
13	NAG	O	2	14/15	0.90	0.26	153,169,190,196	0
16	MAN	S	4	11/12	0.90	0.20	132,137,155,175	0
11	NAG	U	1	14/15	0.91	0.31	153,164,182,187	0
9	NAG	I	1	14/15	0.91	0.29	189,204,216,219	0
13	NAG	O	1	14/15	0.92	0.31	102,113,131,136	0
11	NAG	U	2	14/15	0.94	0.22	180,196,217,222	0
16	MAN	S	5	11/12	0.94	0.22	125,129,142,149	0
16	NAG	S	2	14/15	0.95	0.29	102,118,139,145	0
16	BMA	S	3	11/12	0.96	0.26	98,115,130,132	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.

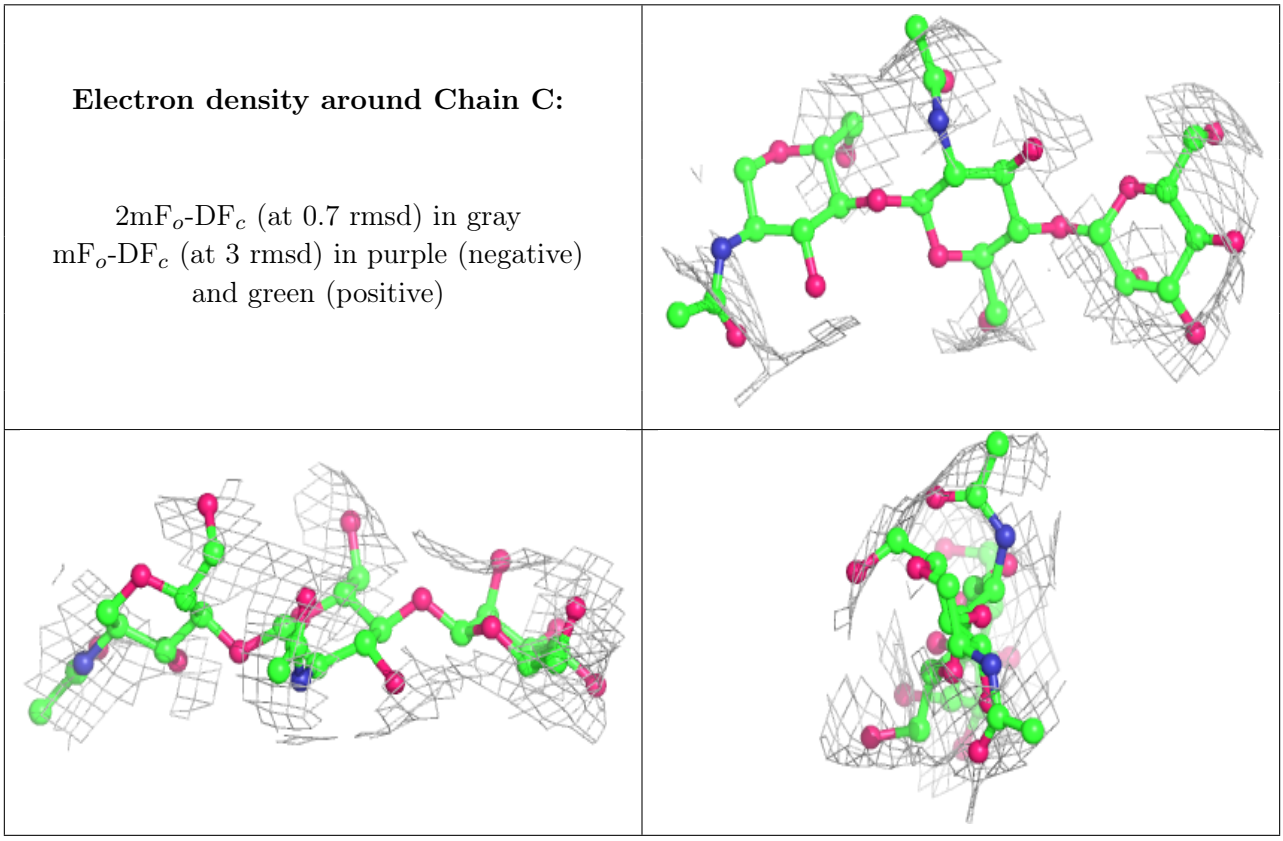
Electron density around Chain A:

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



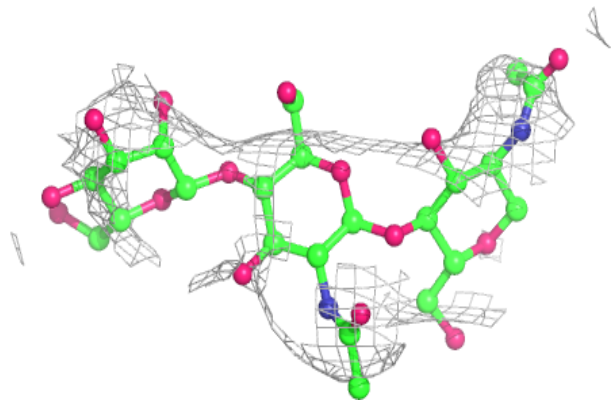
Electron density around Chain C:

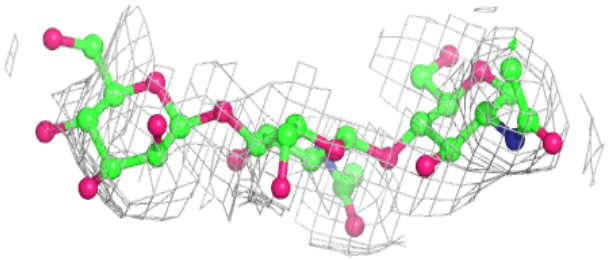
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

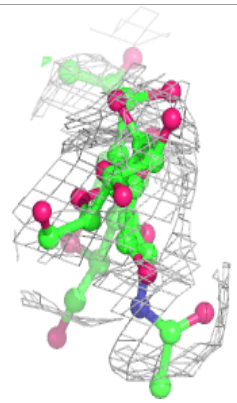


Electron density around Chain W:

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

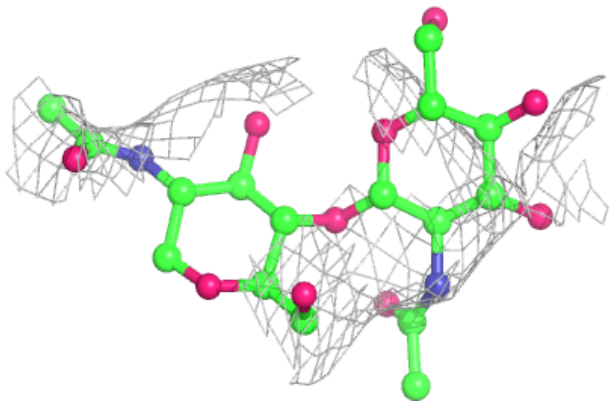


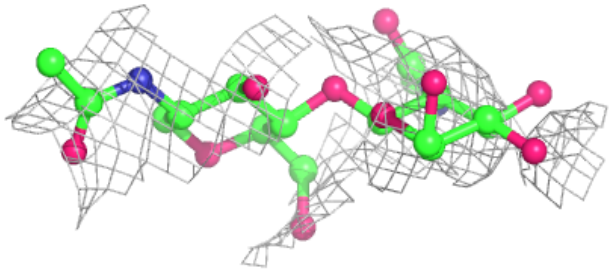


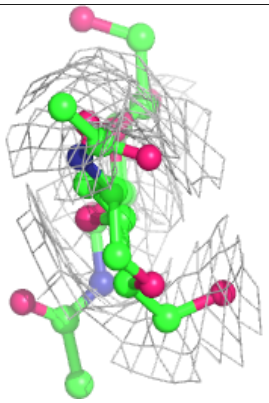


Electron density around Chain F:

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

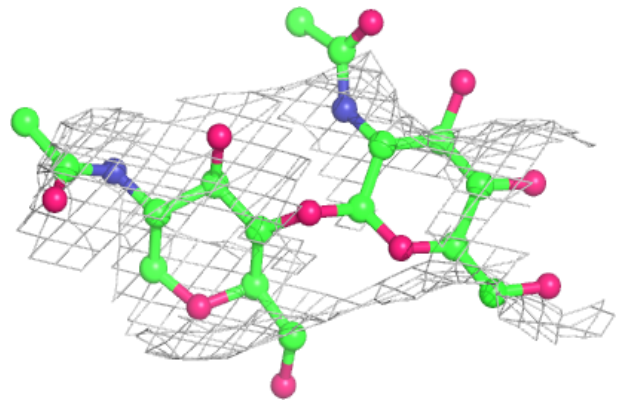


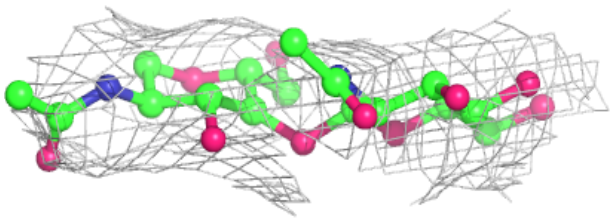


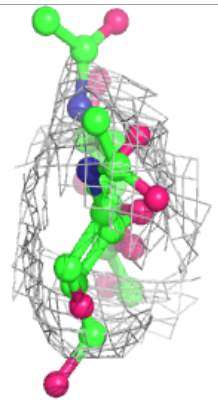


Electron density around Chain I:

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

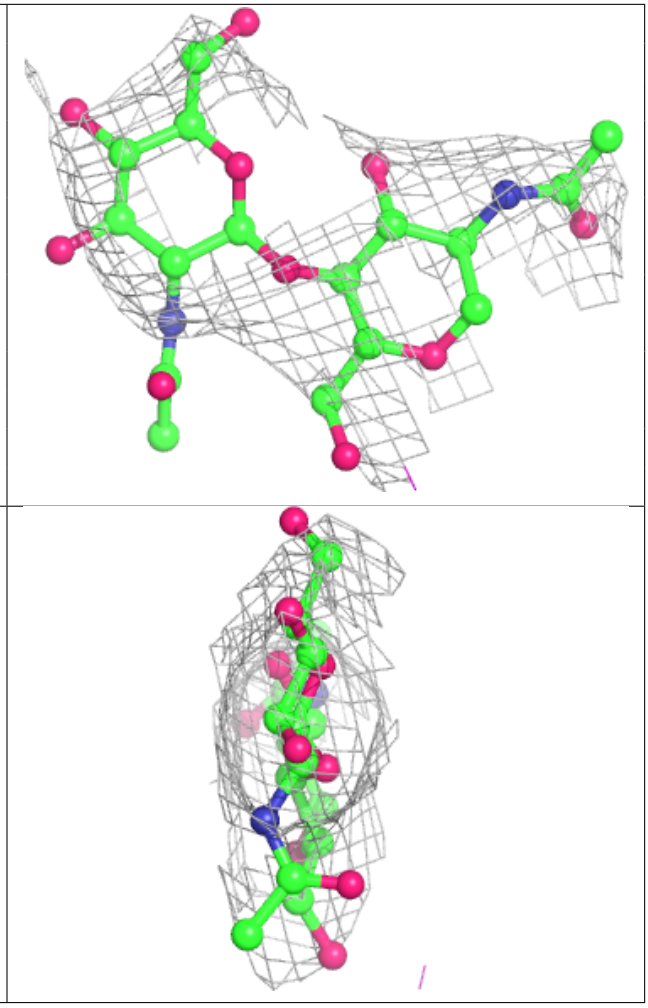






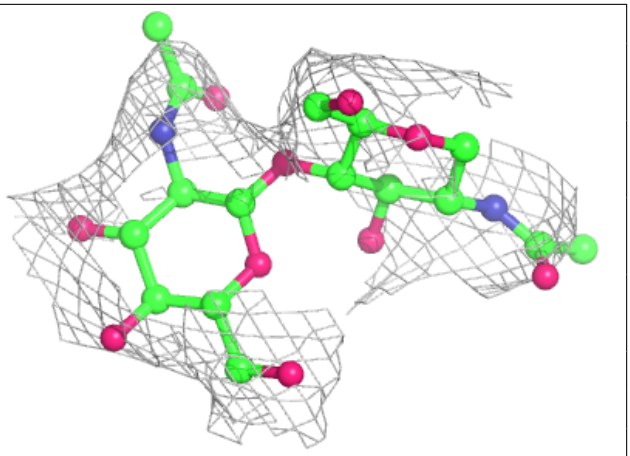
Electron density around Chain N:

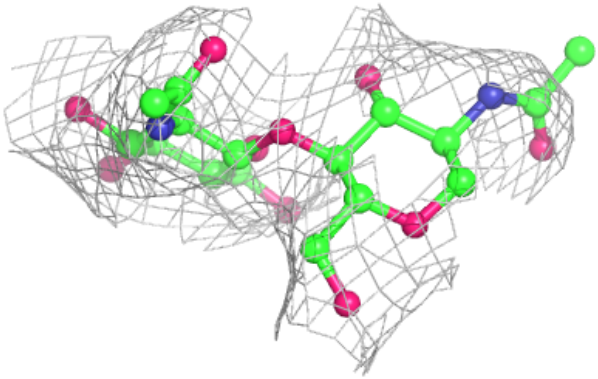
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

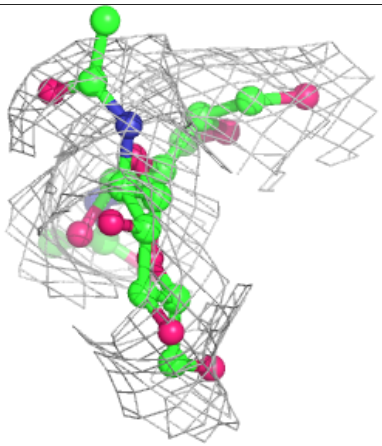


Electron density around Chain Q:

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

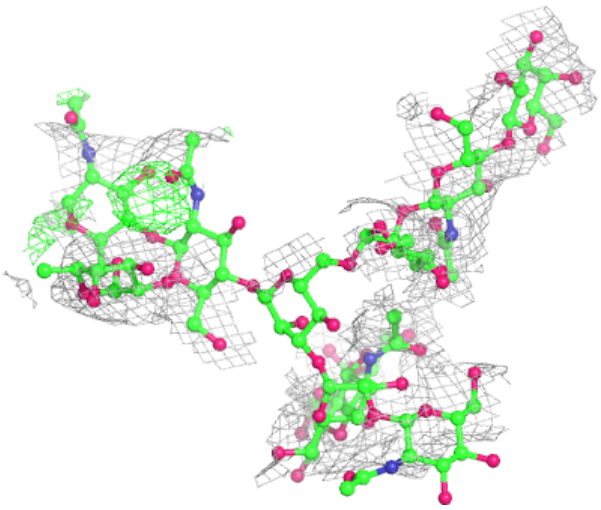


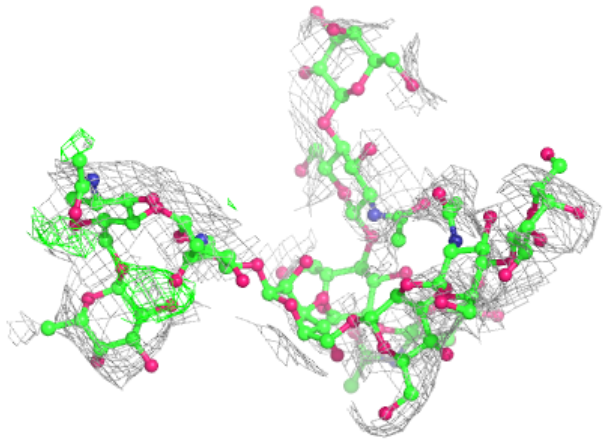


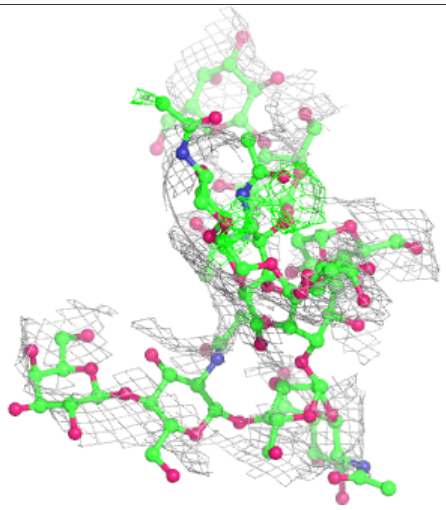


Electron density around Chain J:

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

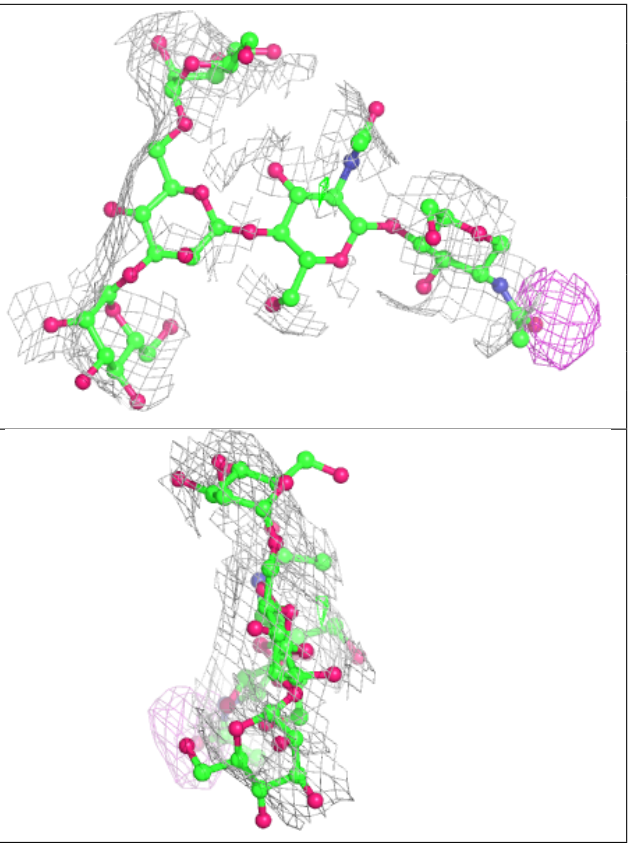






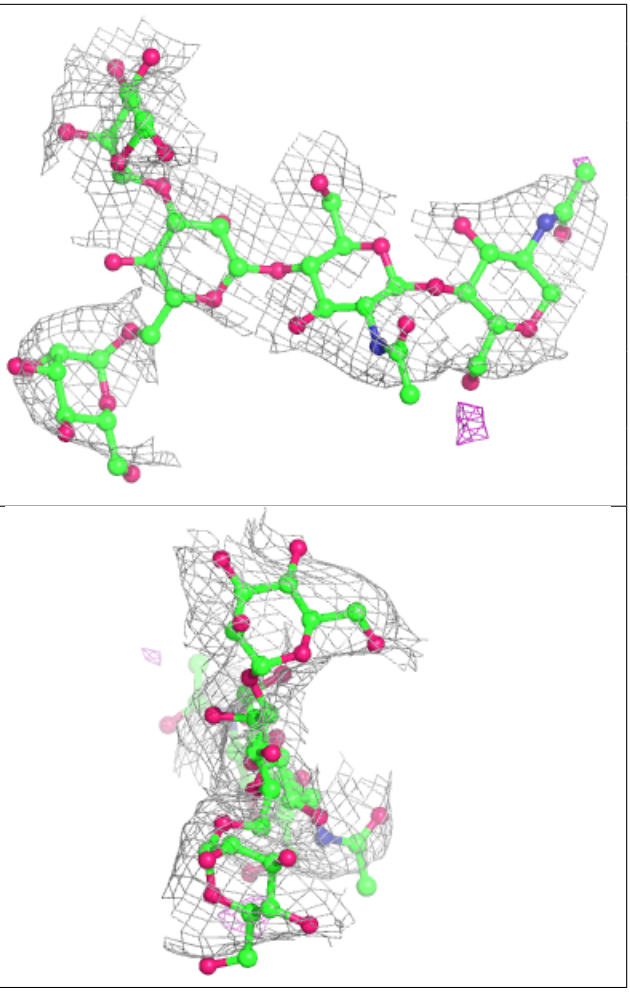
Electron density around Chain K:

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



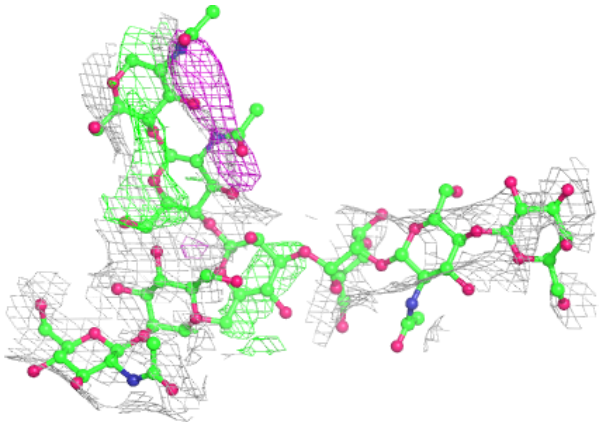
Electron density around Chain U:

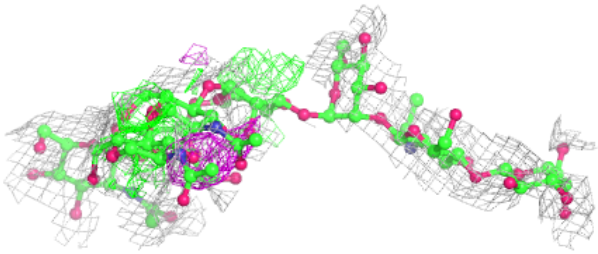
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

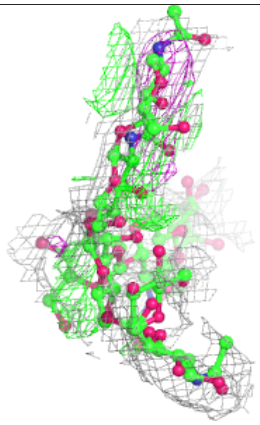


Electron density around Chain M:

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

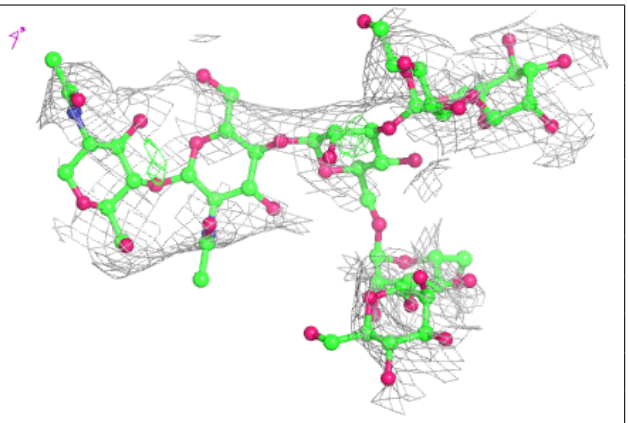


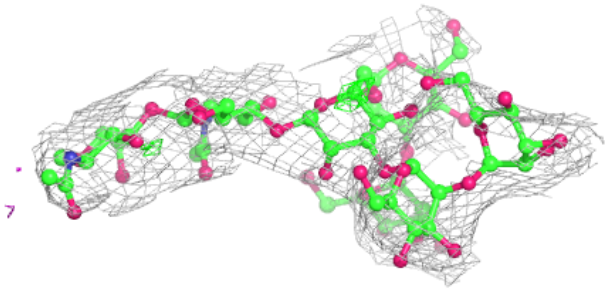


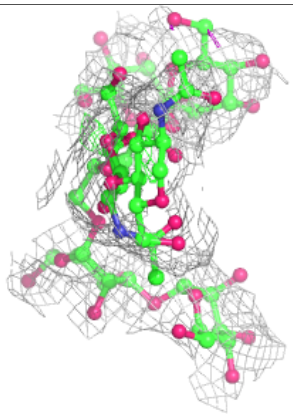


Electron density around Chain O:

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

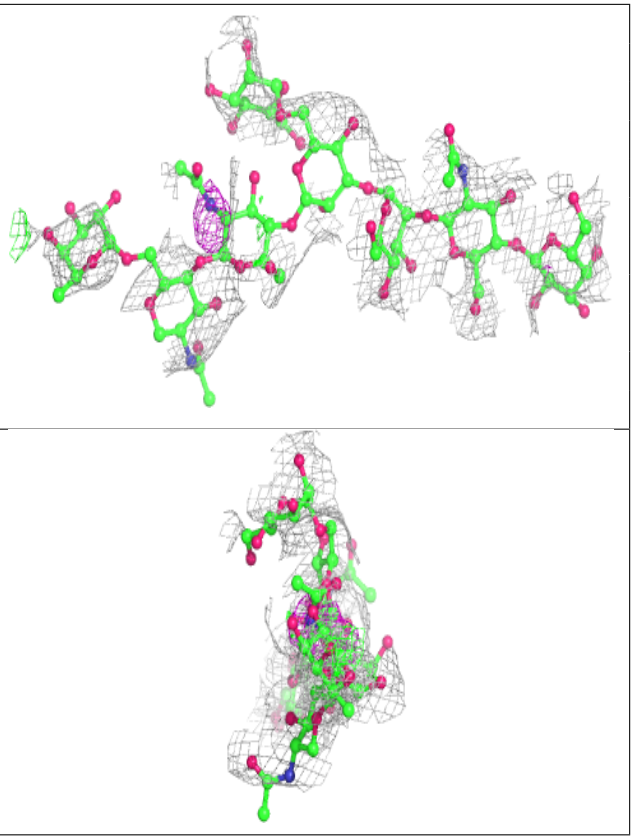






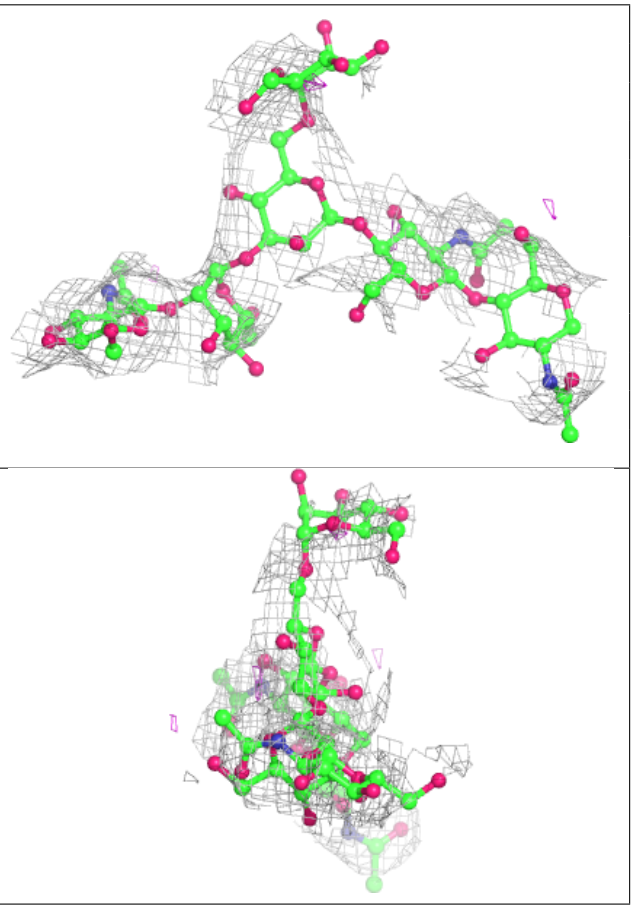
Electron density around Chain P:

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



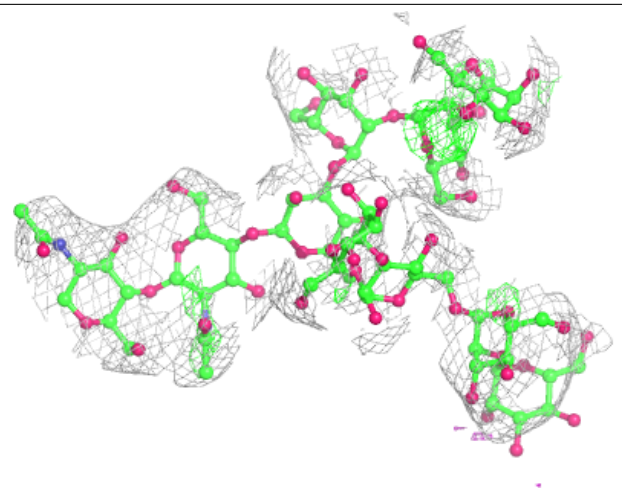
Electron density around Chain R:

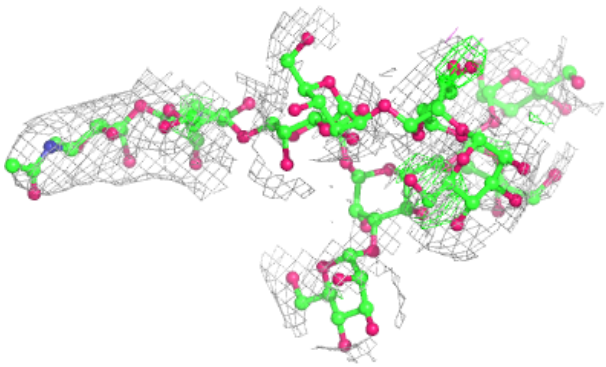
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

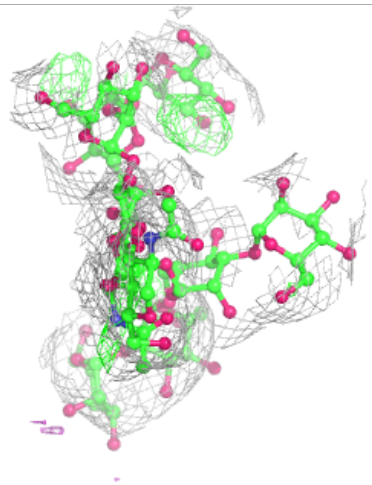


Electron density around Chain S:

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

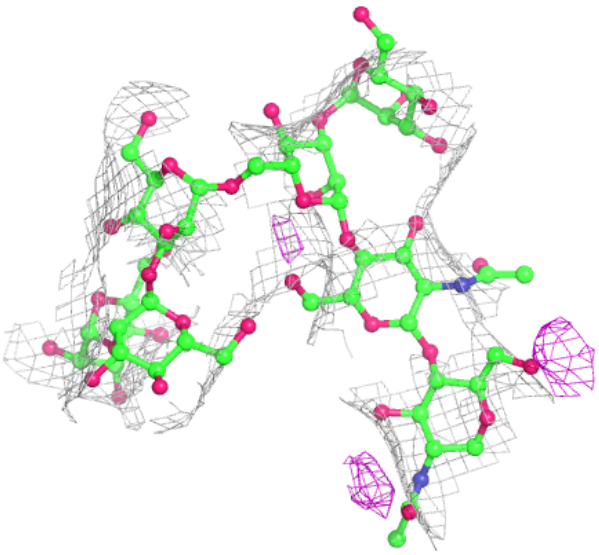


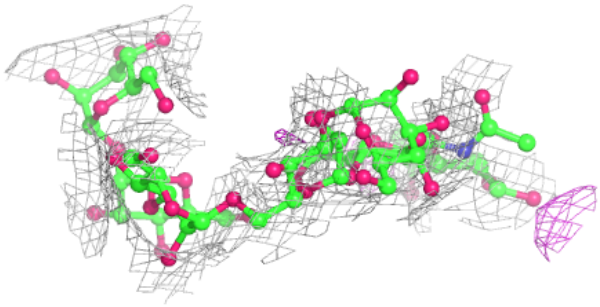


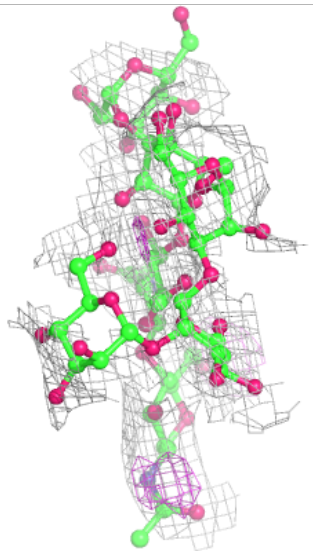


Electron density around Chain T:

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

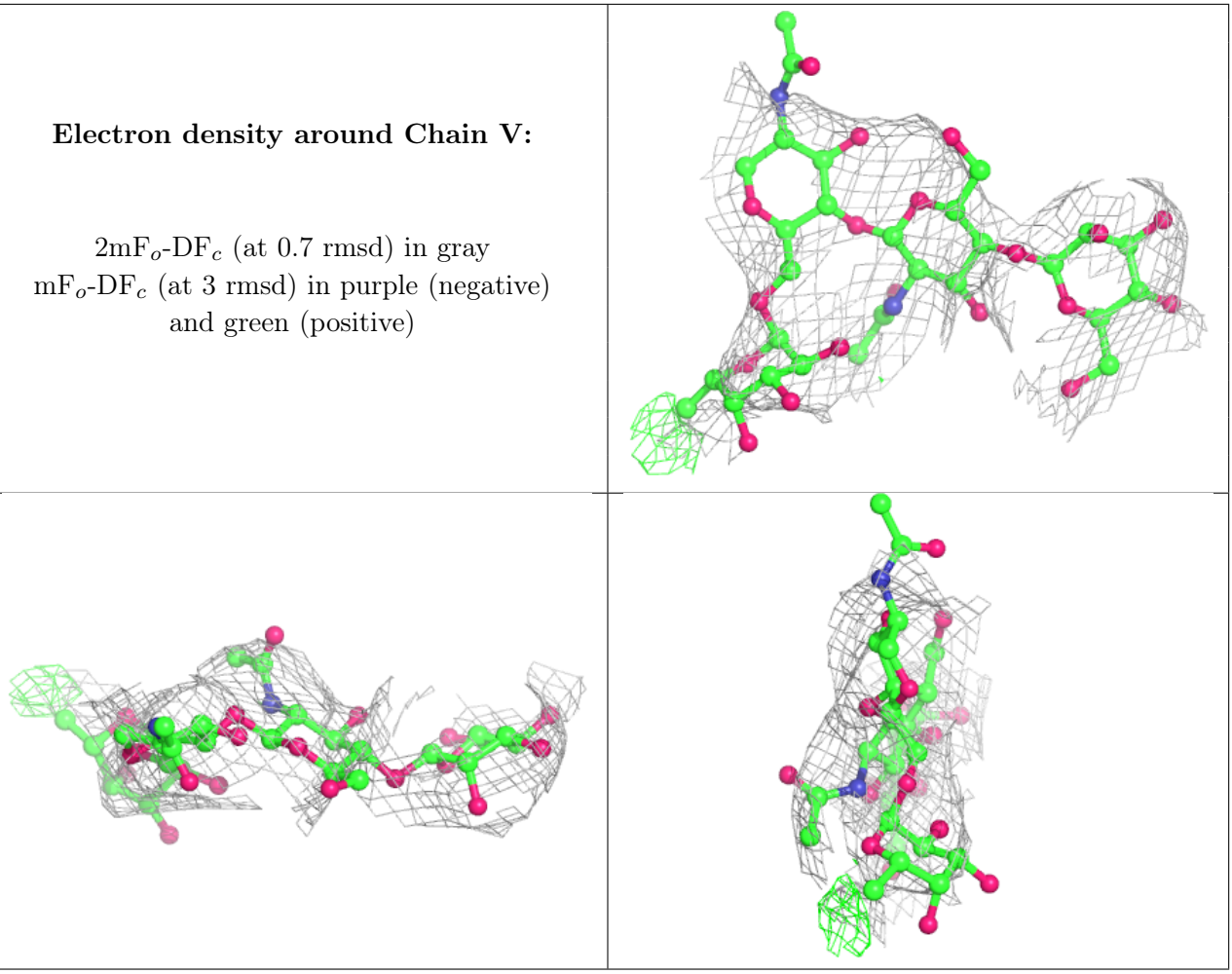






Electron density around Chain V:

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



6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
19	NAG	G	3550	14/15	0.60	0.25	279,296,303,305	0
19	NAG	G	3390	14/15	0.64	0.42	221,239,246,251	0

6.5 Other polymers (i)

There are no such residues in this entry.