wwPDB X-ray Structure Validation Summary Report (i)

Sep 24, 2023 – 04:54 PM EDT

PDB ID	:	5V7J
Title	:	Crystal Structure at 3.7 A Resolution of Glycosylated HIV-1 Clade A BG505 SOSIP.664 Prefusion Env Trimer with Four Glycans (N197, N276, N362, and N462) removed in Complex with Neutralizing Antibodies 3H+109L and 35O22.
Authors	:	Stewart-Jones, G.B.E.; Zhou, T.; Kwong, P.D.
Deposited on	:	2017-03-20
Resolution	:	2.91 Å(reported)

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

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

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

The following versions of software and data (see references (1)) were used in the production of this report:

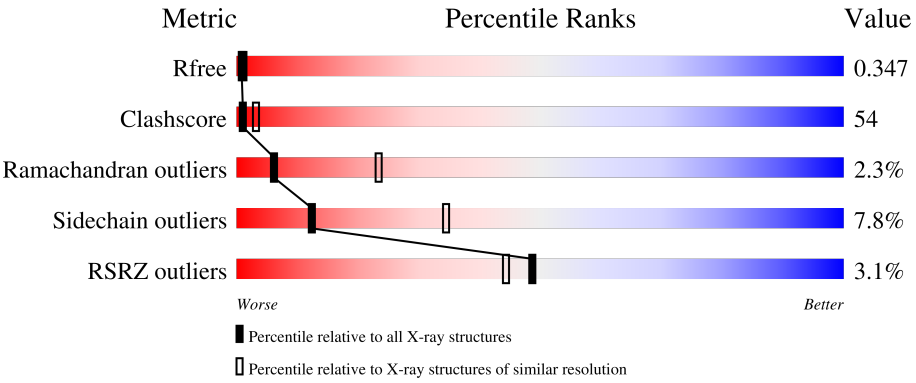
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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 2.91 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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

Mol	Chain	Length	Quality of chain
1	G	480	35% 53% 6% 6%
2	B	153	% 47% 44% 5% •
3	L	218	35% 51% 9% • •
4	H	236	% 30% 58% 9% • •
5	D	240	11% 39% 50% 8% •

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Mol	Chain	Length	Quality of chain
6	E	216	8% 35% 52% 10%
7	A	6	67% 33%
8	C	7	43% 57%
9	F	7	43% 57%
9	K	7	43% 57%
10	I	3	33% 67%
10	S	3	67% 33%
11	J	8	38% 50% 12%
11	M	8	25% 62% 12%
12	N	6	17% 67% 17%
13	O	10	50% 50%
14	P	7	86% 14%
15	Q	2	50% 50%
15	R	2	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
11	MAN	M	5	-	-	-	X
7	NAG	A	1	-	-	X	-

2 Entry composition (i)

There are 16 unique types of molecules in this entry. The entry contains 12436 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
1	G	452	Total	C	N	O	S	0	0	0
			3538	2222	625	664	27			

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	199	ALA	SER	engineered mutation	UNP Q2N0S6
G	278	ALA	THR	engineered mutation	UNP Q2N0S6
G	332	ASN	THR	engineered mutation	UNP Q2N0S6
G	365	ALA	SER	engineered mutation	UNP Q2N0S6
G	464	ALA	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	511	ARG	-	expression tag	UNP Q2N0S6
G	512	ARG	-	expression tag	UNP Q2N0S6
G	513	ARG	-	expression tag	UNP Q2N0S6

- Molecule 2 is a protein called Envelope glycoprotein gp160.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	148	Total	C	N	O	S	0	0	0
			1167	739	203	219	6			

There are 2 discrepancies between the modelled and reference sequences:

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

- Molecule 3 is a protein called Antibody 3H+109L Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	L	211	1603	1007	276	315	5	0	0	0

- Molecule 4 is a protein called Antibody 3H+109L Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	H	231	1744	1108	283	347	6	0	0	0

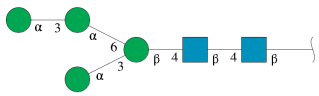
- Molecule 5 is a protein called Antibody 35O22 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	D	240	1813	1150	303	352	8	0	0	0

- Molecule 6 is a protein called Antibody 35O22 Fab heavy chain.

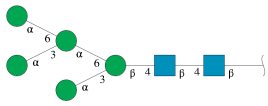
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	E	213	1615	1012	267	328	8	0	0	0

- Molecule 7 is an oligosaccharide called 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.



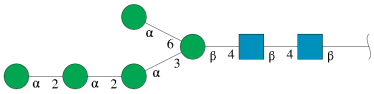
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
7	A	6	72	40	2	30	0	0	0

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



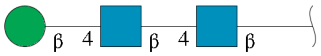
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
8	C	7	Total	C	N	O	0	0	0
			83	46	2	35			

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



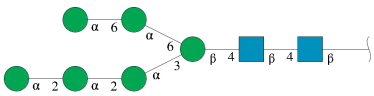
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	F	7	Total	C	N	O	0	0	0
			83	46	2	35			
9	K	7	Total	C	N	O	0	0	0
			83	46	2	35			

- Molecule 10 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.



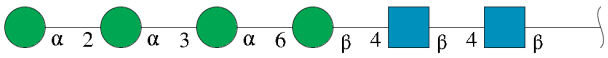
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	I	3	Total	C	N	O	0	0	0
			39	22	2	15			
10	S	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 11 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



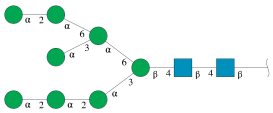
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
11	J	8	Total	C	N	O	0	0	0
			94	52	2	40			
11	M	8	Total	C	N	O	0	0	0
			94	52	2	40			

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



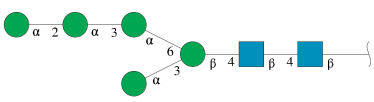
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
12	N	6	Total	C	N	O	0	0	0
			72	40	2	30			

- Molecule 13 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
13	O	10	Total	C	N	O	0	0	0
			116	64	2	50			

- Molecule 14 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.

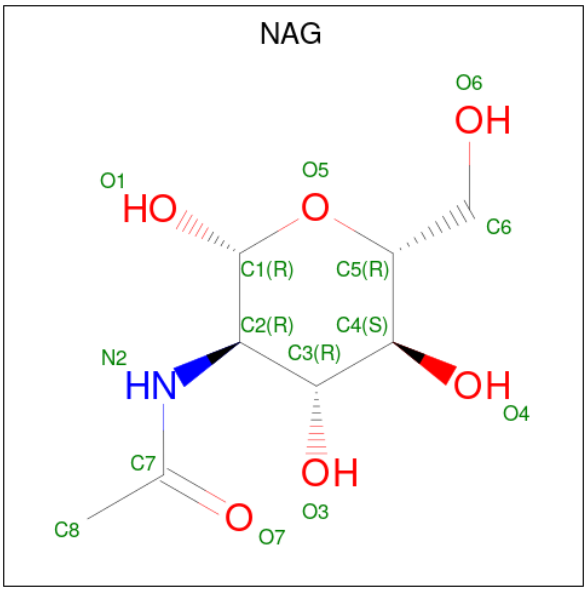


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
14	P	7	Total C N O 83 46 2 35	0	0	0

- Molecule 15 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
15	Q	2	Total C N O 28 16 2 10	0	0	0
15	R	2	Total C N O 28 16 2 10	0	0	0

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



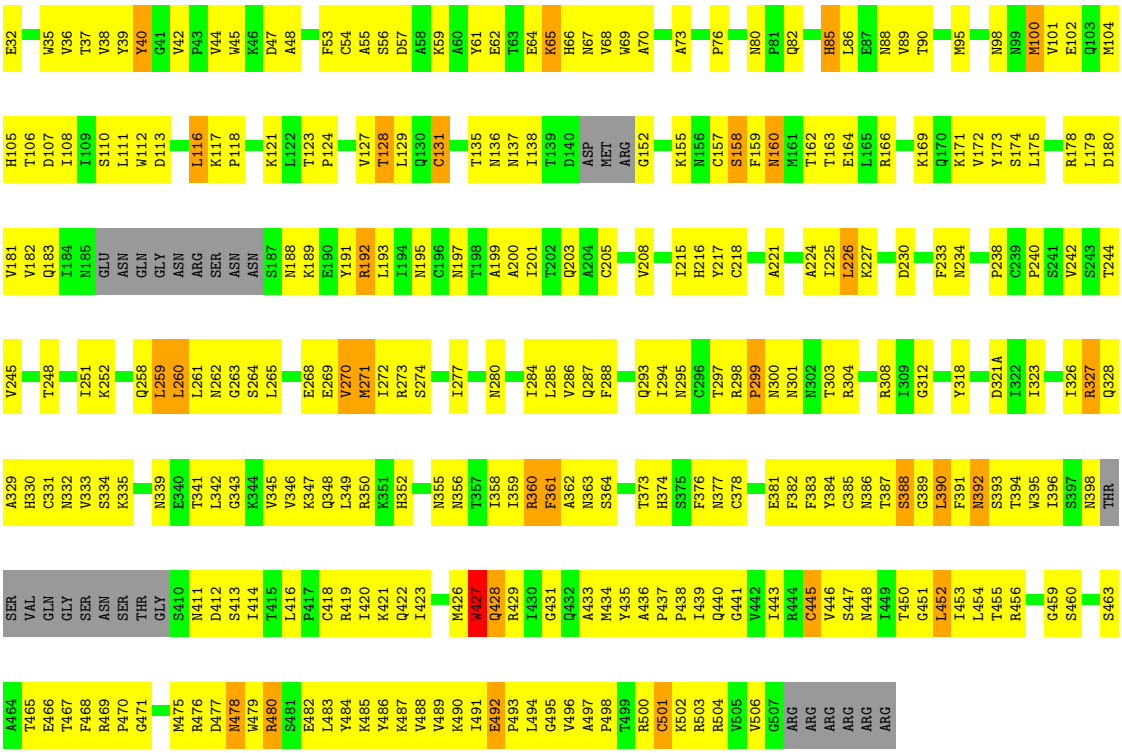
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	G	1	Total C N O 14 8 1 5	0	0
16	B	1	Total C N O 14 8 1 5	0	0
16	B	1	Total C N O 14 8 1 5	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

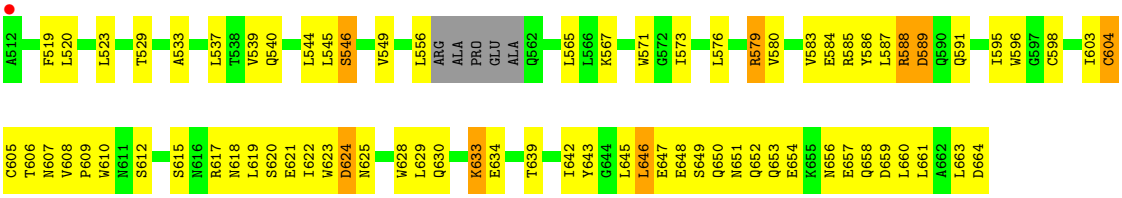
• Molecule 1: Envelope glycoprotein gp160

Chain G:



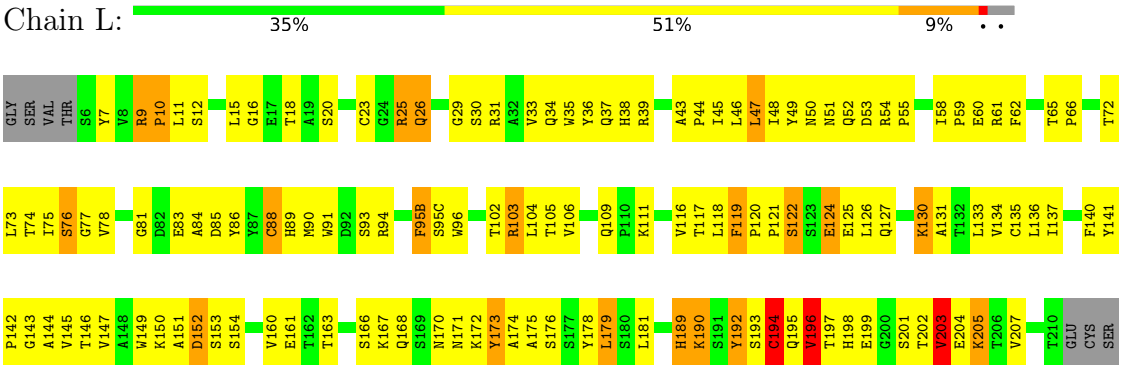
• Molecule 2: Envelope glycoprotein gp160

Chain B:



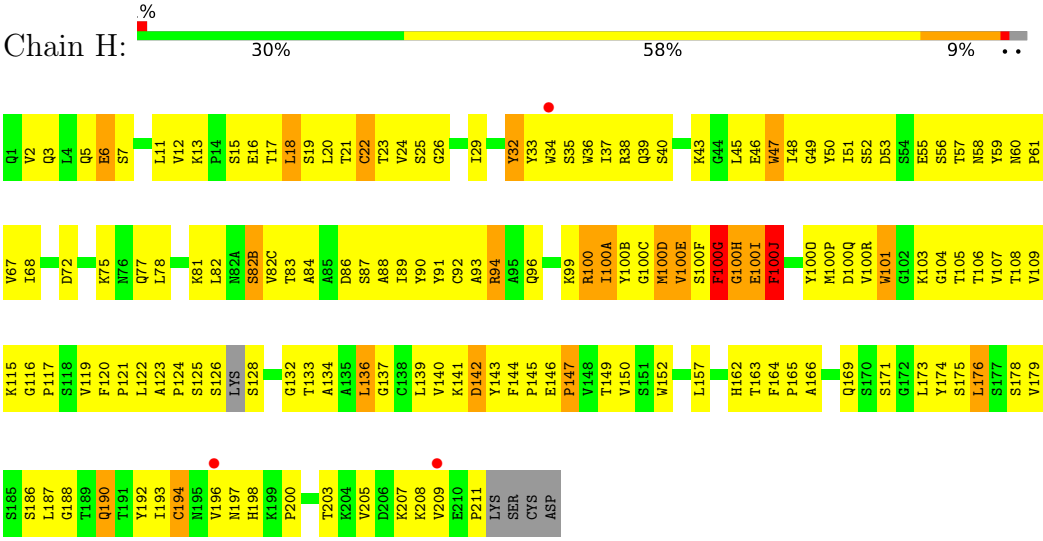
• Molecule 3: Antibody 3H+109L Fab light chain

Chain L:



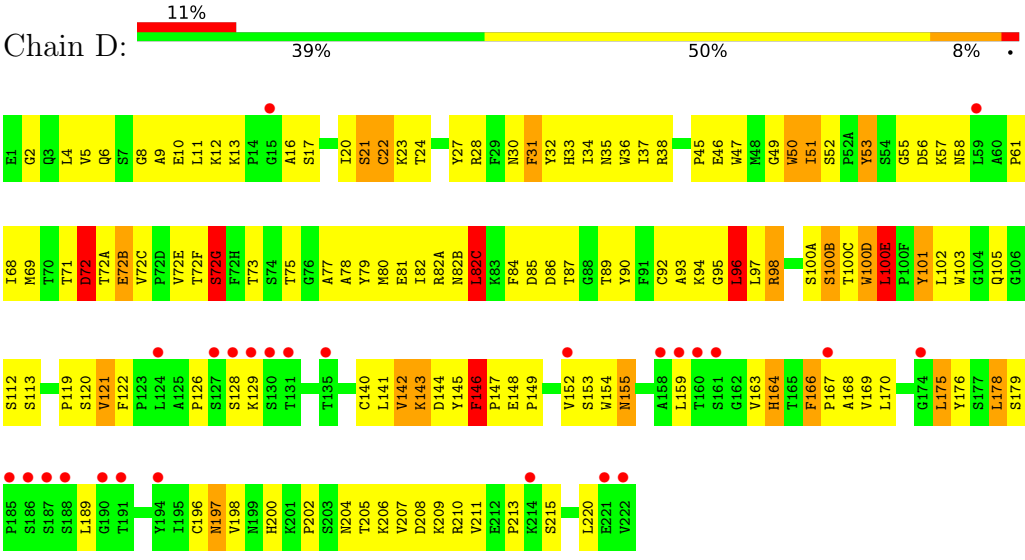
• Molecule 4: Antibody 3H+109L Fab heavy chain

Chain H:



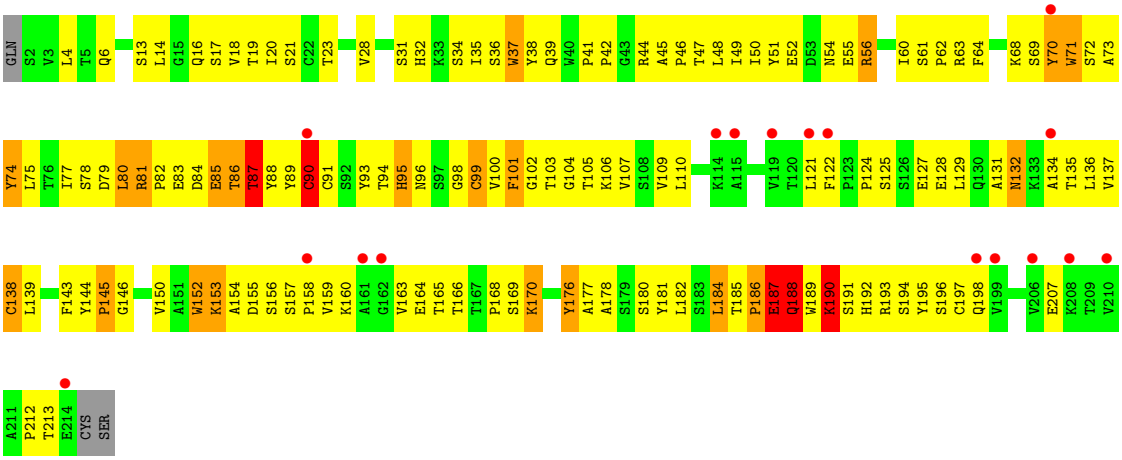
• Molecule 5: Antibody 35O22 Fab light chain

Chain D:



• Molecule 6: Antibody 35O22 Fab heavy chain

Chain E:



• Molecule 7: 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 A:

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

Chain C:

• Molecule 9: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:

• Molecule 9: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:

• Molecule 10: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:

• Molecule 10: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

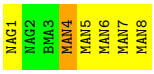
Chain S:

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

Chain J:

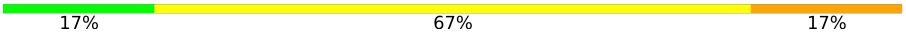
• Molecule 11: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

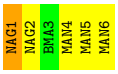
Chain M:



• Molecule 12: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N:





• Molecule 13: 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 O:

• Molecule 14: 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 P:

• Molecule 15: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Q:

• Molecule 15: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain R:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α, β, γ	131.16Å 131.16Å 315.24Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	41.42 – 2.91 41.42 – 2.91	Depositor EDS
% Data completeness (in resolution range)	49.9 (41.42-2.91) 49.9 (41.42-2.91)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.45 (at 2.90Å)	Xtriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R, R_{free}	0.316 , 0.339 0.320 , 0.347	Depositor DCC
R_{free} test set	1972 reflections (5.88%)	wwPDB-VP
Wilson B-factor (Å^2)	65.3	Xtriage
Anisotropy	0.129	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.19 , -9.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.39$, $< L^2 > = 0.22$	Xtriage
Estimated twinning fraction	0.340 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.77	EDS
Total number of atoms	12436	wwPDB-VP
Average B, all atoms (Å^2)	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.34% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	G	0.43	2/3611 (0.1%)	0.69	4/4903 (0.1%)
2	B	0.51	2/1186 (0.2%)	0.71	1/1608 (0.1%)
3	L	0.57	1/1646 (0.1%)	0.79	4/2247 (0.2%)
4	H	0.46	0/1787	0.79	5/2436 (0.2%)
5	D	0.51	1/1860 (0.1%)	0.87	8/2533 (0.3%)
6	E	0.68	4/1659 (0.2%)	0.94	8/2269 (0.4%)
All	All	0.52	10/11749 (0.1%)	0.79	30/15996 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	G	0	3
3	L	0	3
4	H	0	2
5	D	0	4
6	E	0	7
All	All	0	19

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	22	CYS	CB-SG	-11.40	1.62	1.82
2	B	604	CYS	CB-SG	-8.39	1.68	1.82
2	B	598	CYS	CB-SG	-7.02	1.70	1.82
6	E	187	GLU	CA-C	-6.82	1.35	1.52
6	E	85	GLU	CA-C	-6.26	1.36	1.52

The worst 5 of 30 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	D	82(C)	LEU	CB-CG-CD1	-11.09	92.14	111.00
5	D	100(E)	LEU	CA-CB-CG	9.36	136.84	115.30
6	E	85	GLU	N-CA-C	8.28	133.36	111.00
6	E	86	THR	OG1-CB-CG2	-8.02	91.54	110.00
4	H	194	CYS	CA-CB-SG	7.51	127.51	114.00

There are no chirality outliers.

5 of 19 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	G	128	THR	Peptide
1	G	158	SER	Peptide
1	G	492	GLU	Peptide
3	L	119	PHE	Peptide
3	L	202	THR	Peptide

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	G	3538	0	3469	368	0
2	B	1167	0	1158	117	0
3	L	1603	0	1546	195	0
4	H	1744	0	1710	232	0
5	D	1813	0	1784	243	0
6	E	1615	0	1544	220	0
7	A	72	0	61	9	0
8	C	83	0	70	8	0
9	F	83	0	70	6	0
9	K	83	0	70	8	0
10	I	39	0	34	2	0
10	S	39	0	34	0	0
11	J	94	0	79	1	0
11	M	94	0	79	2	0
12	N	72	0	61	1	0
13	O	116	0	97	11	0
14	P	83	0	70	3	0
15	Q	28	0	25	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	R	28	0	25	0	0
16	B	28	0	26	5	0
16	G	14	0	13	1	0
All	All	12436	0	12025	1323	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 54.

The worst 5 of 1323 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:234:ASN:HD21	9:K:1:NAG:C1	1.12	1.60
5:D:22:CYS:O	5:D:23:LYS:HE2	1.42	1.15
4:H:113:SER:O	4:H:144:PHE:CE2	2.01	1.13
5:D:22:CYS:C	5:D:23:LYS:HE2	1.72	1.09
1:G:226:LEU:HD11	1:G:244:THR:HA	1.28	1.08

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	G	444/480 (92%)	378 (85%)	62 (14%)	4 (1%)	17 48
2	B	144/153 (94%)	127 (88%)	16 (11%)	1 (1%)	22 54
3	L	209/218 (96%)	171 (82%)	34 (16%)	4 (2%)	8 28
4	H	227/236 (96%)	184 (81%)	35 (15%)	8 (4%)	3 14
5	D	238/240 (99%)	190 (80%)	36 (15%)	12 (5%)	2 7
6	E	211/216 (98%)	177 (84%)	29 (14%)	5 (2%)	6 22
All	All	1473/1543 (96%)	1227 (83%)	212 (14%)	34 (2%)	6 23

5 of 34 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	88	ASN
4	H	100	ARG
4	H	100(E)	VAL
4	H	100(G)	PHE
5	D	72(B)	GLU

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	G	397/424 (94%)	369 (93%)	28 (7%)	14 40
2	B	126/129 (98%)	117 (93%)	9 (7%)	14 40
3	L	175/181 (97%)	157 (90%)	18 (10%)	7 22
4	H	200/205 (98%)	183 (92%)	17 (8%)	10 31
5	D	203/203 (100%)	187 (92%)	16 (8%)	12 34
6	E	186/189 (98%)	173 (93%)	13 (7%)	15 41
All	All	1287/1331 (97%)	1186 (92%)	101 (8%)	12 34

5 of 101 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	H	32	TYR
4	H	194	CYS
6	E	176	TYR
4	H	61	PRO
4	H	101	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
5	D	33	HIS
5	D	105	GLN

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Mol	Chain	Res	Type
6	E	192	HIS
5	D	155	ASN
2	B	653	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

76 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
7	NAG	A	1	7,1	14,14,15	2.57	2 (14%)	17,19,21	1.71	3 (17%)
7	NAG	A	2	7	14,14,15	1.47	2 (14%)	17,19,21	0.93	1 (5%)
7	BMA	A	3	7	11,11,12	1.68	4 (36%)	15,15,17	1.84	4 (26%)
7	MAN	A	4	7	11,11,12	1.08	1 (9%)	15,15,17	0.92	0
7	MAN	A	5	7	11,11,12	0.80	0	15,15,17	0.98	1 (6%)
7	MAN	A	6	7	11,11,12	0.75	0	15,15,17	0.89	1 (6%)
8	NAG	C	1	8,1	14,14,15	1.14	1 (7%)	17,19,21	1.65	2 (11%)
8	NAG	C	2	8	14,14,15	1.04	2 (14%)	17,19,21	1.29	2 (11%)
8	BMA	C	3	8	11,11,12	0.93	1 (9%)	15,15,17	0.99	1 (6%)
8	MAN	C	4	8	11,11,12	1.00	1 (9%)	15,15,17	1.30	3 (20%)
8	MAN	C	5	8	11,11,12	0.59	0	15,15,17	1.01	2 (13%)
8	MAN	C	6	8	11,11,12	0.94	1 (9%)	15,15,17	1.51	3 (20%)
8	MAN	C	7	8	11,11,12	0.89	1 (9%)	15,15,17	1.19	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
9	NAG	F	1	9,1	14,14,15	0.22	0	17,19,21	0.53	0
9	NAG	F	2	9	14,14,15	0.60	0	17,19,21	1.04	1 (5%)
9	BMA	F	3	9	11,11,12	1.91	2 (18%)	15,15,17	1.23	2 (13%)
9	MAN	F	4	9	11,11,12	2.09	3 (27%)	15,15,17	1.58	3 (20%)
9	MAN	F	5	9	11,11,12	1.19	2 (18%)	15,15,17	1.68	3 (20%)
9	MAN	F	6	9	11,11,12	0.75	0	15,15,17	1.01	2 (13%)
9	MAN	F	7	9	11,11,12	0.67	0	15,15,17	1.00	2 (13%)
10	NAG	I	1	10,1	14,14,15	0.32	0	17,19,21	0.67	0
10	NAG	I	2	10	14,14,15	0.26	0	17,19,21	0.54	0
10	BMA	I	3	10	11,11,12	0.50	0	15,15,17	0.81	0
11	NAG	J	1	11,1	14,14,15	0.20	0	17,19,21	0.51	0
11	NAG	J	2	11	14,14,15	0.22	0	17,19,21	0.44	0
11	BMA	J	3	11	11,11,12	0.52	0	15,15,17	0.86	0
11	MAN	J	4	11	11,11,12	0.69	0	15,15,17	1.31	2 (13%)
11	MAN	J	5	11	11,11,12	0.78	0	15,15,17	1.20	2 (13%)
11	MAN	J	6	11	11,11,12	0.81	0	15,15,17	1.05	2 (13%)
11	MAN	J	7	11	11,11,12	0.67	0	15,15,17	1.19	2 (13%)
11	MAN	J	8	11	11,11,12	0.73	0	15,15,17	0.88	1 (6%)
9	NAG	K	1	9,1	14,14,15	0.71	1 (7%)	17,19,21	0.43	0
9	NAG	K	2	9	14,14,15	0.71	1 (7%)	17,19,21	0.94	1 (5%)
9	BMA	K	3	9	11,11,12	0.34	0	15,15,17	1.74	2 (13%)
9	MAN	K	4	9	11,11,12	1.35	2 (18%)	15,15,17	1.53	4 (26%)
9	MAN	K	5	9	11,11,12	1.07	0	15,15,17	1.64	3 (20%)
9	MAN	K	6	9	11,11,12	0.98	1 (9%)	15,15,17	1.11	2 (13%)
9	MAN	K	7	9	11,11,12	0.34	0	15,15,17	1.11	2 (13%)
11	NAG	M	1	11,1	14,14,15	0.22	0	17,19,21	0.55	0
11	NAG	M	2	11	14,14,15	0.20	0	17,19,21	0.41	0
11	BMA	M	3	11	11,11,12	0.59	0	15,15,17	0.76	0
11	MAN	M	4	11	11,11,12	0.81	0	15,15,17	1.27	2 (13%)
11	MAN	M	5	11	11,11,12	0.69	0	15,15,17	1.19	2 (13%)
11	MAN	M	6	11	11,11,12	0.82	1 (9%)	15,15,17	0.92	1 (6%)
11	MAN	M	7	11	11,11,12	0.79	1 (9%)	15,15,17	1.13	2 (13%)
11	MAN	M	8	11	11,11,12	0.61	0	15,15,17	0.99	2 (13%)
12	NAG	N	1	12,1	14,14,15	1.87	1 (7%)	17,19,21	1.08	1 (5%)
12	NAG	N	2	12	14,14,15	0.40	0	17,19,21	0.67	1 (5%)
12	BMA	N	3	12	11,11,12	0.76	0	15,15,17	0.87	0
12	MAN	N	4	12	11,11,12	0.82	1 (9%)	15,15,17	1.12	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
12	MAN	N	5	12	11,11,12	1.41	1 (9%)	15,15,17	1.41	2 (13%)
12	MAN	N	6	12	11,11,12	0.92	1 (9%)	15,15,17	1.54	2 (13%)
13	NAG	O	1	13,1	14,14,15	0.92	1 (7%)	17,19,21	1.41	2 (11%)
13	MAN	O	10	13	11,11,12	0.58	0	15,15,17	1.10	2 (13%)
13	NAG	O	2	13	14,14,15	0.34	0	17,19,21	0.51	0
13	BMA	O	3	13	11,11,12	1.02	1 (9%)	15,15,17	1.07	1 (6%)
13	MAN	O	4	13	11,11,12	0.86	1 (9%)	15,15,17	1.20	2 (13%)
13	MAN	O	5	13	11,11,12	0.97	2 (18%)	15,15,17	1.21	1 (6%)
13	MAN	O	6	13	11,11,12	1.00	1 (9%)	15,15,17	0.83	1 (6%)
13	MAN	O	7	13	11,11,12	0.57	0	15,15,17	1.16	2 (13%)
13	MAN	O	8	13	11,11,12	0.76	1 (9%)	15,15,17	1.06	1 (6%)
13	MAN	O	9	13	11,11,12	0.68	0	15,15,17	1.18	2 (13%)
14	NAG	P	1	14,1	14,14,15	2.16	4 (28%)	17,19,21	1.01	0
14	NAG	P	2	14	14,14,15	0.36	0	17,19,21	0.59	0
14	BMA	P	3	14	11,11,12	0.61	0	15,15,17	1.71	3 (20%)
14	MAN	P	4	14	11,11,12	0.94	1 (9%)	15,15,17	1.42	1 (6%)
14	MAN	P	5	14	11,11,12	1.12	1 (9%)	15,15,17	1.41	3 (20%)
14	MAN	P	6	14	11,11,12	1.09	1 (9%)	15,15,17	1.02	2 (13%)
14	MAN	P	7	14	11,11,12	1.08	1 (9%)	15,15,17	0.89	1 (6%)
15	NAG	Q	1	15,1	14,14,15	0.56	0	17,19,21	1.07	1 (5%)
15	NAG	Q	2	15	14,14,15	0.63	1 (7%)	17,19,21	0.98	1 (5%)
15	NAG	R	1	15,1	14,14,15	0.15	0	17,19,21	0.79	1 (5%)
15	NAG	R	2	15	14,14,15	0.33	0	17,19,21	0.51	0
10	NAG	S	1	2,10	14,14,15	0.44	0	17,19,21	0.60	0
10	NAG	S	2	10	14,14,15	0.24	0	17,19,21	0.55	0
10	BMA	S	3	10	11,11,12	0.53	0	15,15,17	1.16	1 (6%)

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

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	MAN	A	5	7	-	0/2/19/22	0/1/1/1
7	MAN	A	6	7	-	0/2/19/22	0/1/1/1
8	NAG	C	1	8,1	-	2/6/23/26	0/1/1/1
8	NAG	C	2	8	-	3/6/23/26	0/1/1/1
8	BMA	C	3	8	-	2/2/19/22	0/1/1/1
8	MAN	C	4	8	-	0/2/19/22	0/1/1/1
8	MAN	C	5	8	-	0/2/19/22	0/1/1/1
8	MAN	C	6	8	-	0/2/19/22	0/1/1/1
8	MAN	C	7	8	-	0/2/19/22	0/1/1/1
9	NAG	F	1	9,1	-	0/6/23/26	0/1/1/1
9	NAG	F	2	9	-	2/6/23/26	0/1/1/1
9	BMA	F	3	9	-	2/2/19/22	0/1/1/1
9	MAN	F	4	9	-	2/2/19/22	0/1/1/1
9	MAN	F	5	9	-	0/2/19/22	0/1/1/1
9	MAN	F	6	9	-	0/2/19/22	0/1/1/1
9	MAN	F	7	9	-	0/2/19/22	0/1/1/1
10	NAG	I	1	10,1	-	1/6/23/26	0/1/1/1
10	NAG	I	2	10	-	2/6/23/26	0/1/1/1
10	BMA	I	3	10	-	0/2/19/22	0/1/1/1
11	NAG	J	1	11,1	-	2/6/23/26	0/1/1/1
11	NAG	J	2	11	-	2/6/23/26	0/1/1/1
11	BMA	J	3	11	-	2/2/19/22	0/1/1/1
11	MAN	J	4	11	-	1/2/19/22	0/1/1/1
11	MAN	J	5	11	-	0/2/19/22	0/1/1/1
11	MAN	J	6	11	-	0/2/19/22	0/1/1/1
11	MAN	J	7	11	-	2/2/19/22	0/1/1/1
11	MAN	J	8	11	-	0/2/19/22	0/1/1/1
9	NAG	K	1	9,1	-	1/6/23/26	0/1/1/1
9	NAG	K	2	9	-	2/6/23/26	0/1/1/1
9	BMA	K	3	9	-	2/2/19/22	0/1/1/1
9	MAN	K	4	9	-	0/2/19/22	0/1/1/1
9	MAN	K	5	9	-	2/2/19/22	0/1/1/1
9	MAN	K	6	9	-	0/2/19/22	0/1/1/1
9	MAN	K	7	9	-	0/2/19/22	0/1/1/1
11	NAG	M	1	11,1	-	2/6/23/26	0/1/1/1
11	NAG	M	2	11	-	0/6/23/26	0/1/1/1
11	BMA	M	3	11	-	0/2/19/22	0/1/1/1
11	MAN	M	4	11	-	1/2/19/22	0/1/1/1

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

The worst 5 of 50 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	1	NAG	O5-C1	9.12	1.58	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	N	1	NAG	O5-C1	6.33	1.53	1.43
14	P	1	NAG	O5-C1	5.17	1.52	1.43
14	P	1	NAG	C1-C2	-4.93	1.45	1.52
9	F	4	MAN	O2-C2	4.65	1.53	1.43

The worst 5 of 106 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	C	1	NAG	C1-O5-C5	5.34	119.43	112.19
12	N	6	MAN	C1-O5-C5	4.87	118.79	112.19
7	A	1	NAG	C2-N2-C7	4.80	129.74	122.90
9	K	3	BMA	C1-O5-C5	4.67	118.52	112.19
7	A	3	BMA	O3-C3-C2	4.54	118.68	109.99

There are no chirality outliers.

5 of 81 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	1	NAG	C3-C2-N2-C7
8	C	1	NAG	O5-C5-C6-O6
11	J	1	NAG	O5-C5-C6-O6
14	P	1	NAG	C4-C5-C6-O6
12	N	1	NAG	O5-C5-C6-O6

There are no ring outliers.

30 monomers are involved in 53 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	K	1	NAG	6	0
9	F	6	MAN	1	0
7	A	2	NAG	1	0
9	K	2	NAG	2	0
10	I	2	NAG	1	0
11	M	1	NAG	1	0
9	K	7	MAN	2	0
9	F	5	MAN	1	0
9	F	4	MAN	3	0
13	O	1	NAG	2	0
8	C	7	MAN	1	0
14	P	1	NAG	3	0
13	O	5	MAN	3	0

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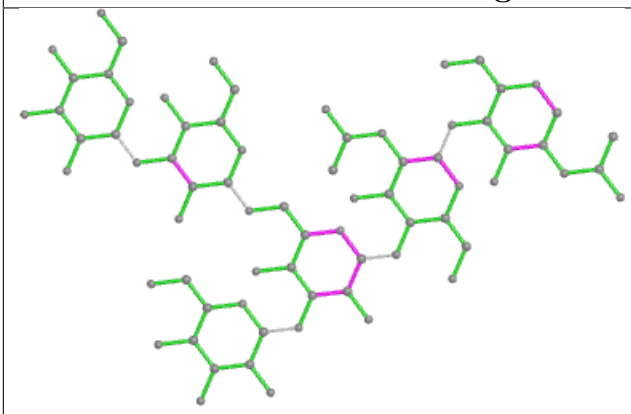
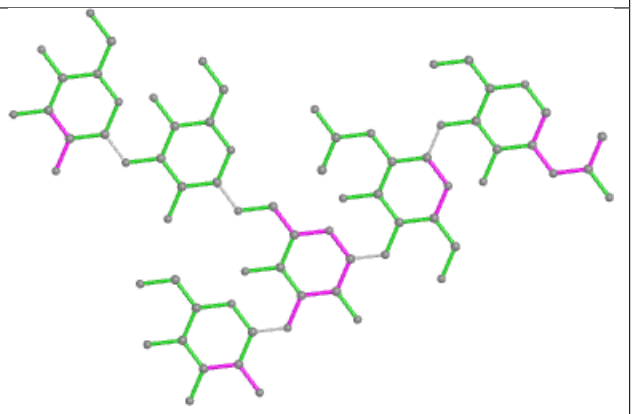
Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	N	1	NAG	1	0
9	F	3	BMA	3	0
14	P	2	NAG	1	0
13	O	3	BMA	1	0
11	J	5	MAN	1	0
13	O	4	MAN	1	0
8	C	1	NAG	3	0
9	F	1	NAG	2	0
10	I	1	NAG	2	0
7	A	1	NAG	8	0
8	C	2	NAG	2	0
13	O	2	NAG	3	0
15	Q	1	NAG	2	0
13	O	9	MAN	1	0
11	M	4	MAN	1	0
9	K	3	BMA	2	0
8	C	6	MAN	2	0

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

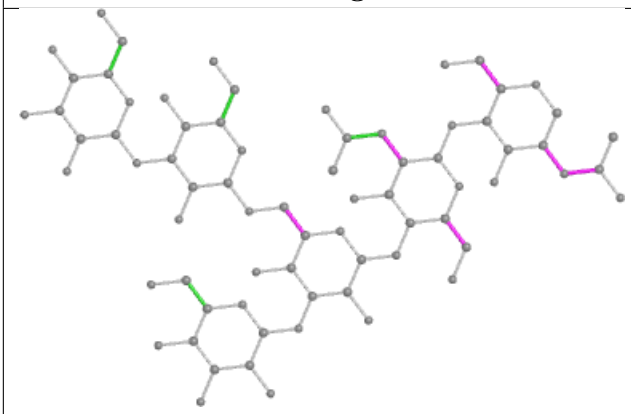
Oligosaccharide Chain A



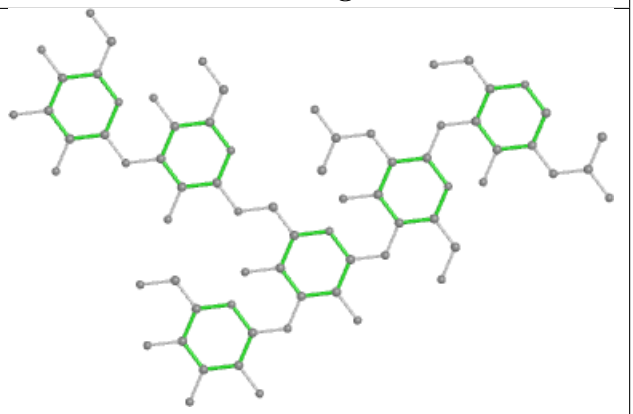
Bond lengths



Bond angles

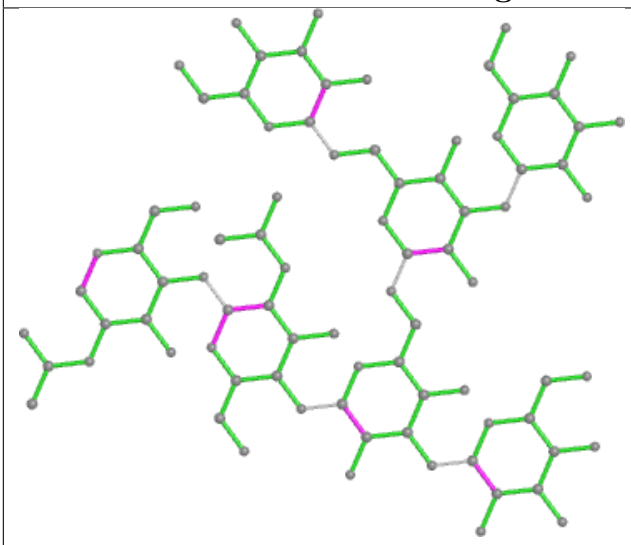


Torsions

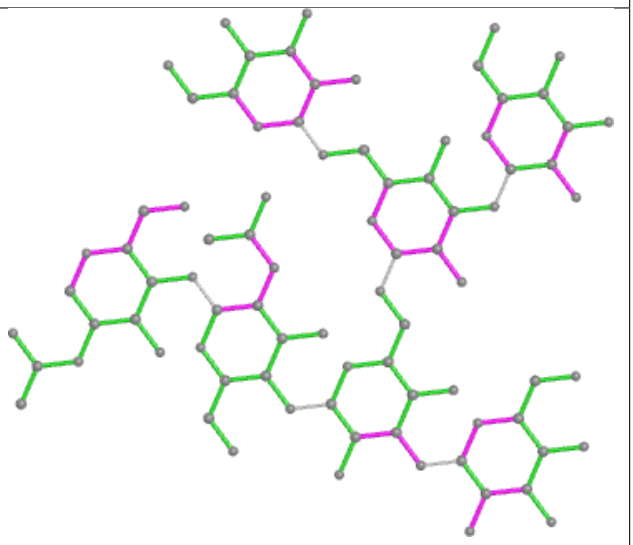


Rings

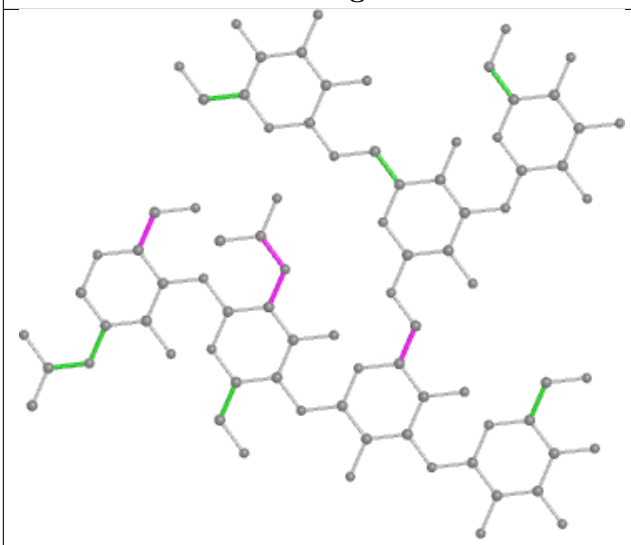
Oligosaccharide Chain C



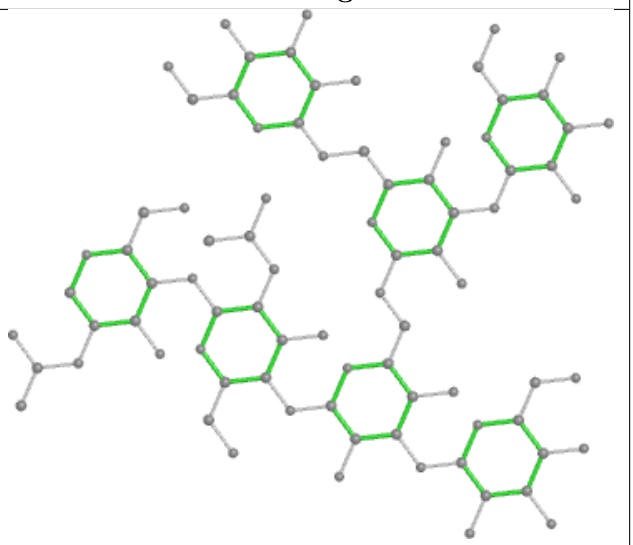
Bond lengths



Bond angles

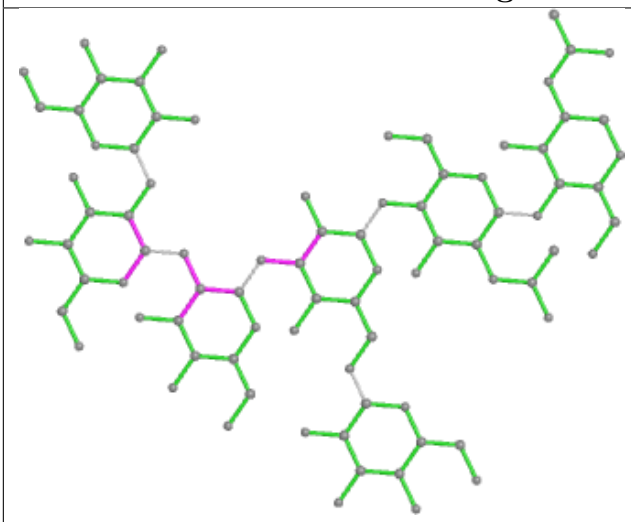


Torsions

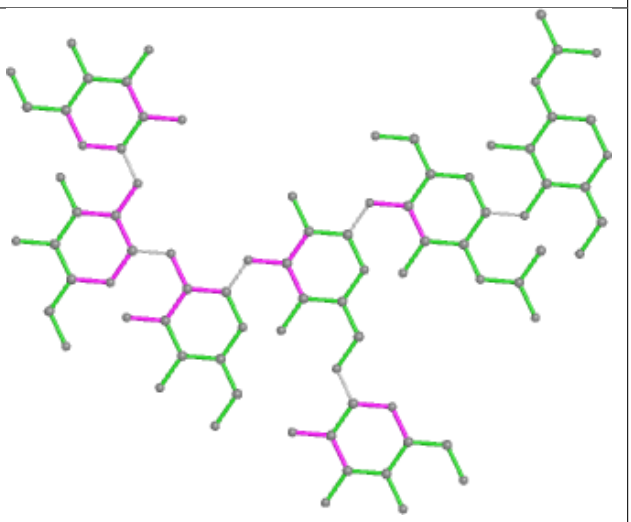


Rings

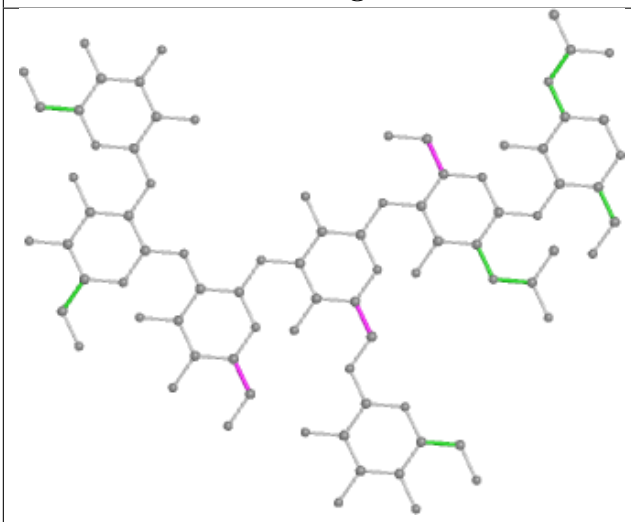
Oligosaccharide Chain F



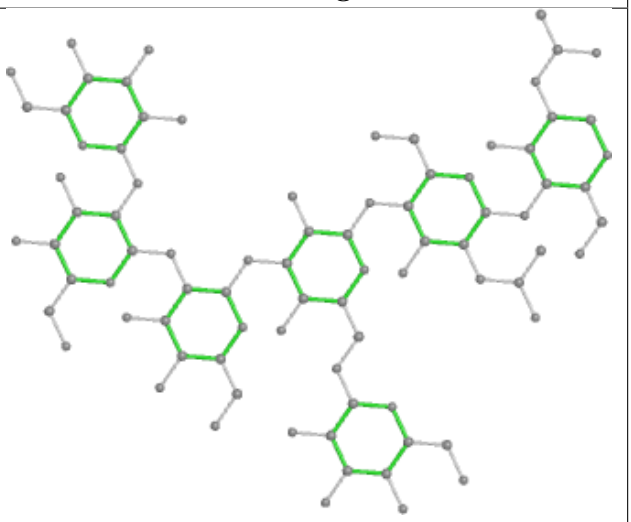
Bond lengths



Bond angles

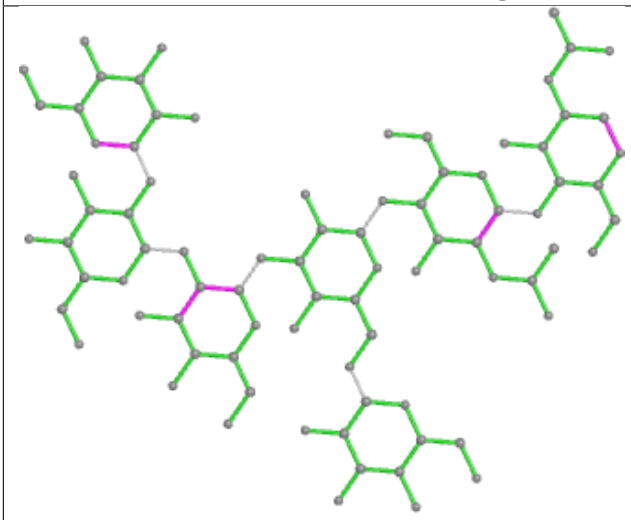


Torsions

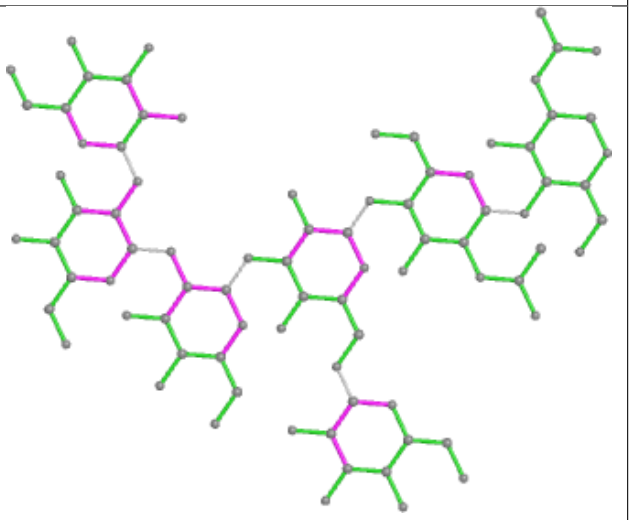


Rings

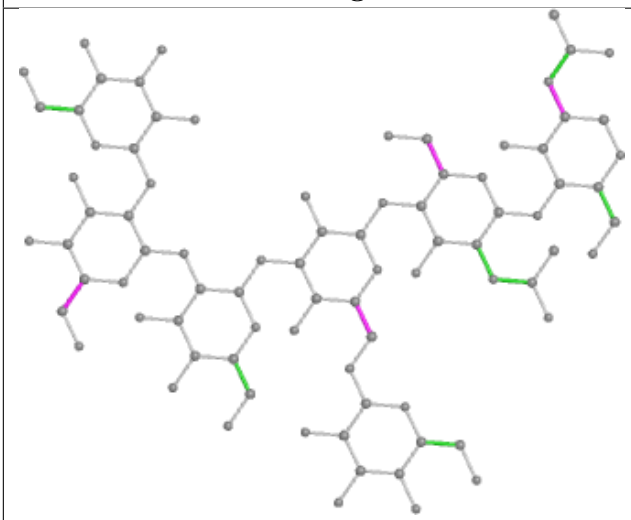
Oligosaccharide Chain K



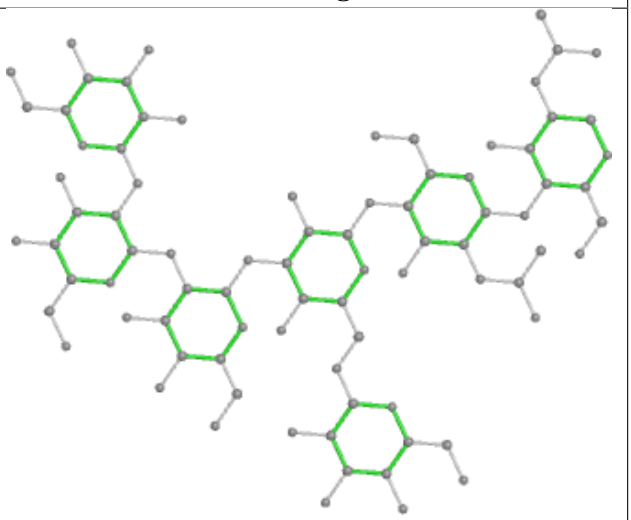
Bond lengths



Bond angles

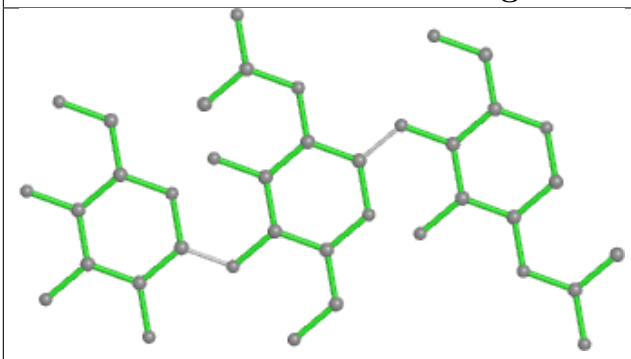


Torsions

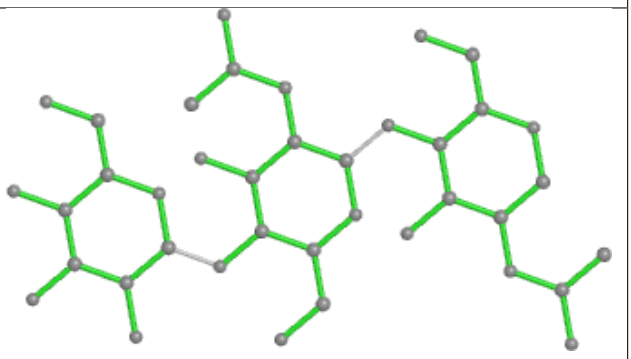


Rings

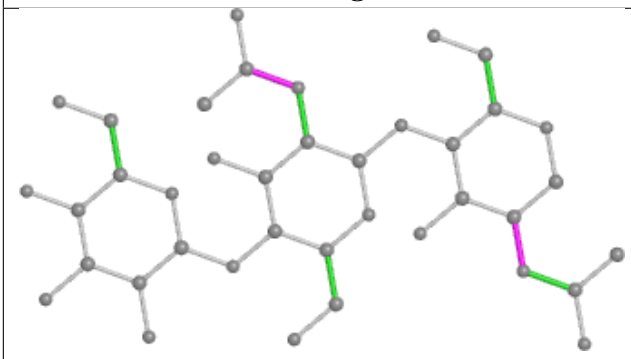
Oligosaccharide Chain I



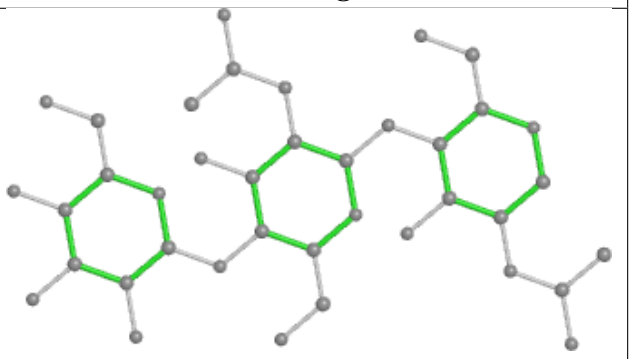
Bond lengths



Bond angles

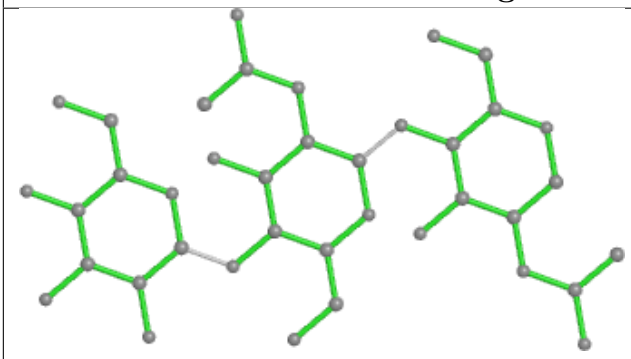


Torsions

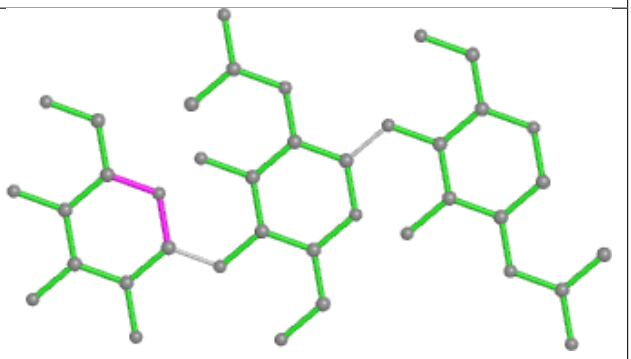


Rings

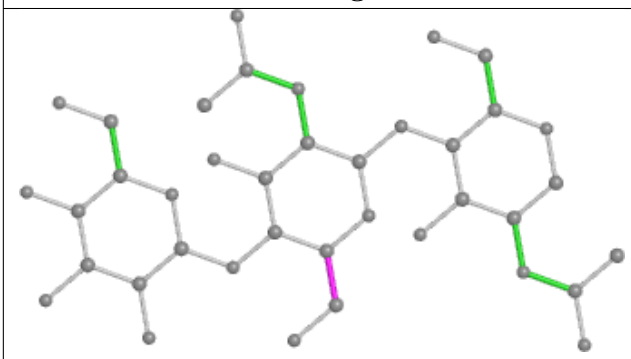
Oligosaccharide Chain S



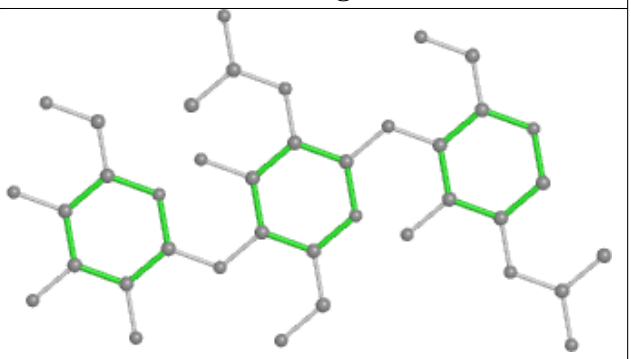
Bond lengths



Bond angles

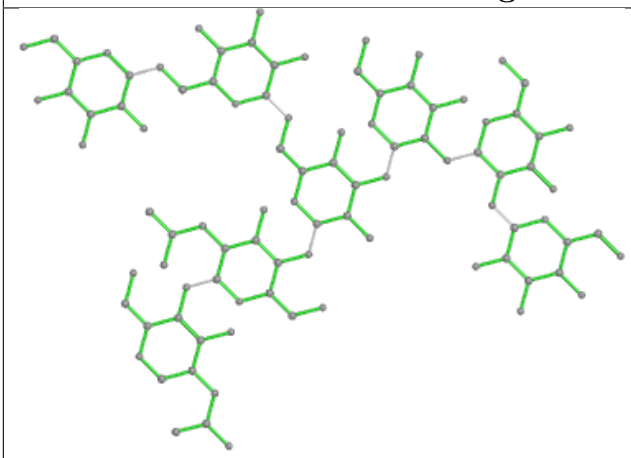


Torsions

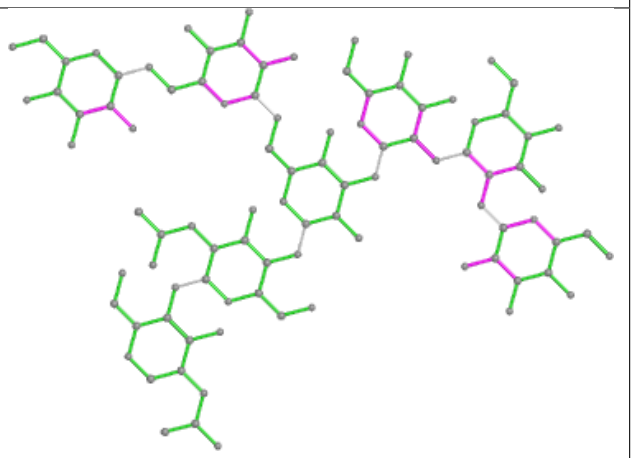


Rings

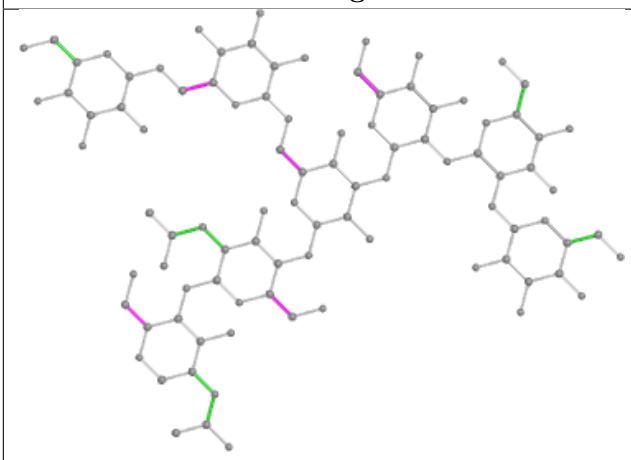
Oligosaccharide Chain J



Bond lengths



Bond angles



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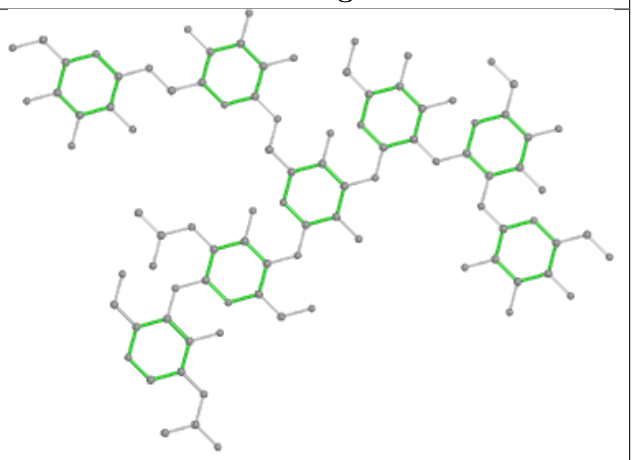
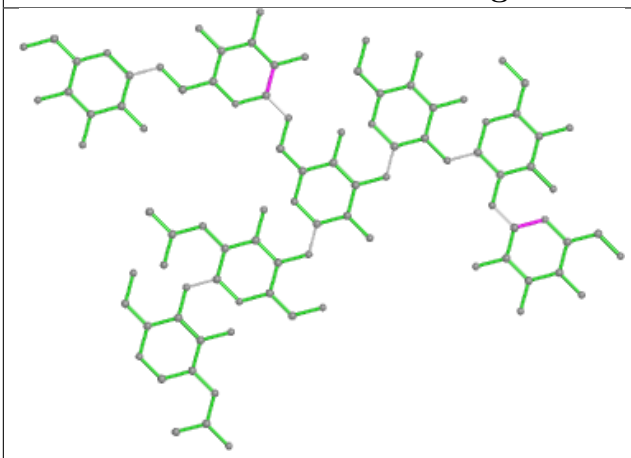
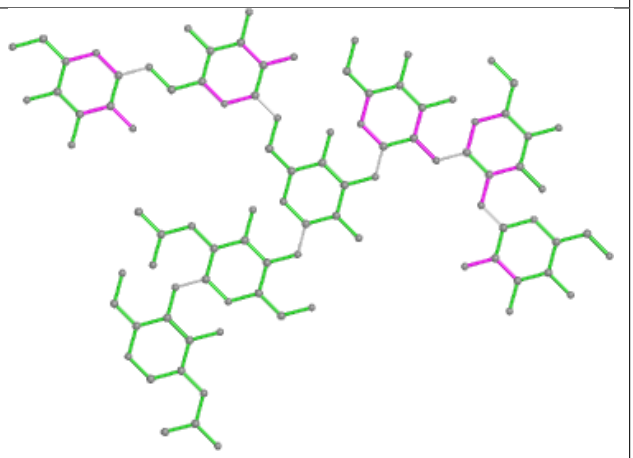


Rings

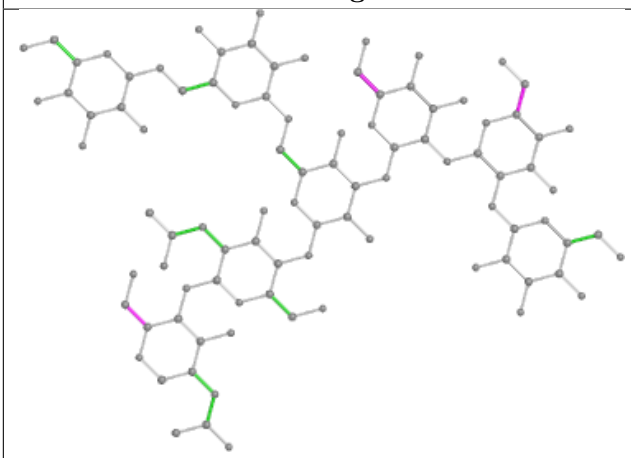
Oligosaccharide Chain M



Bond lengths



Bond angles



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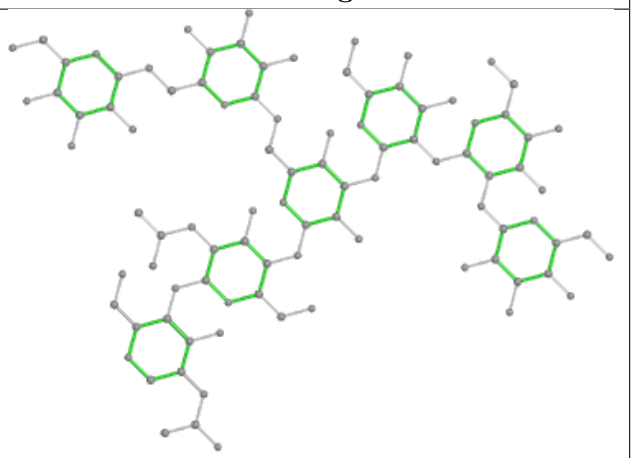
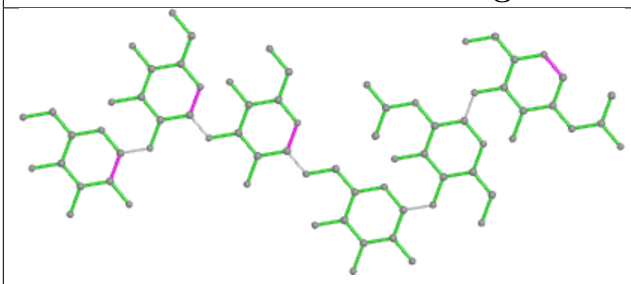
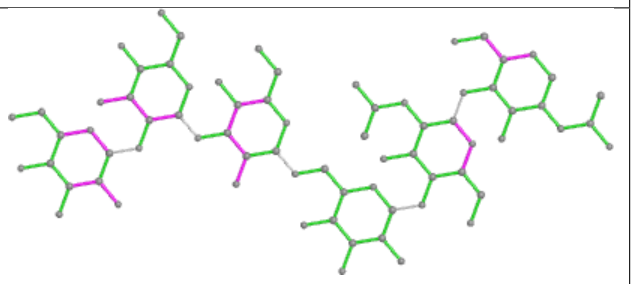


Rings

Oligosaccharide Chain N



Bond lengths



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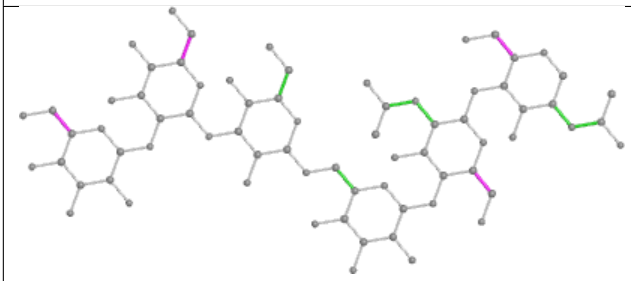
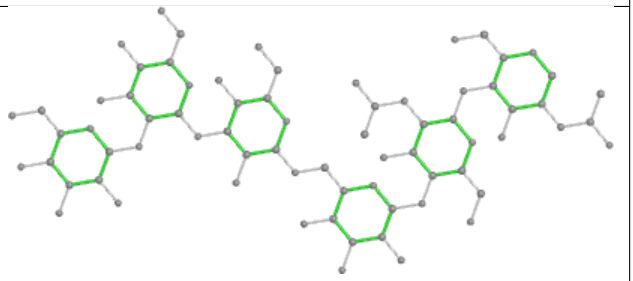
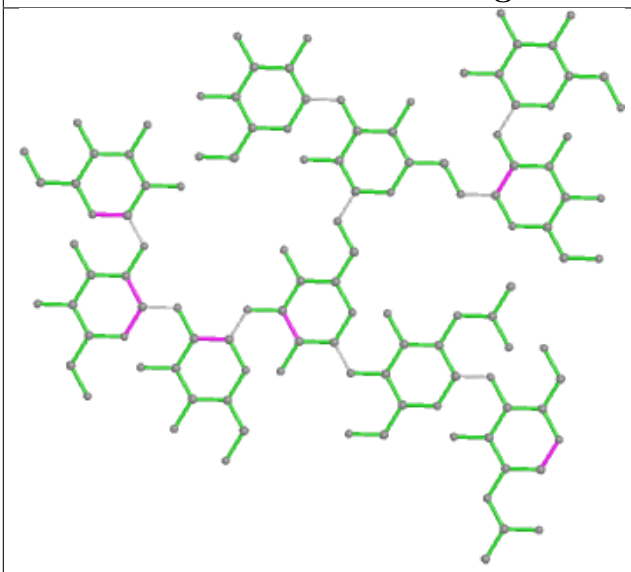


Torsions

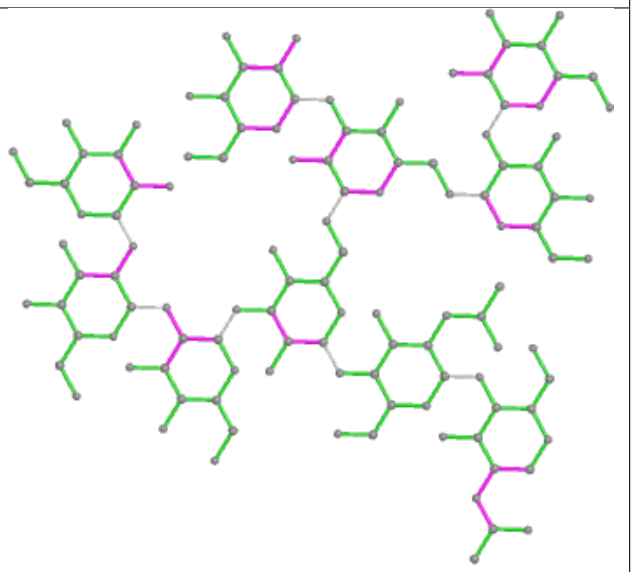


Rings

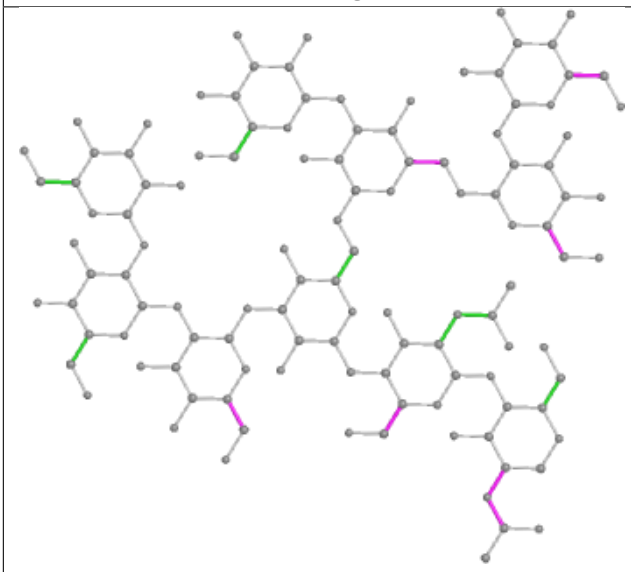
Oligosaccharide Chain O



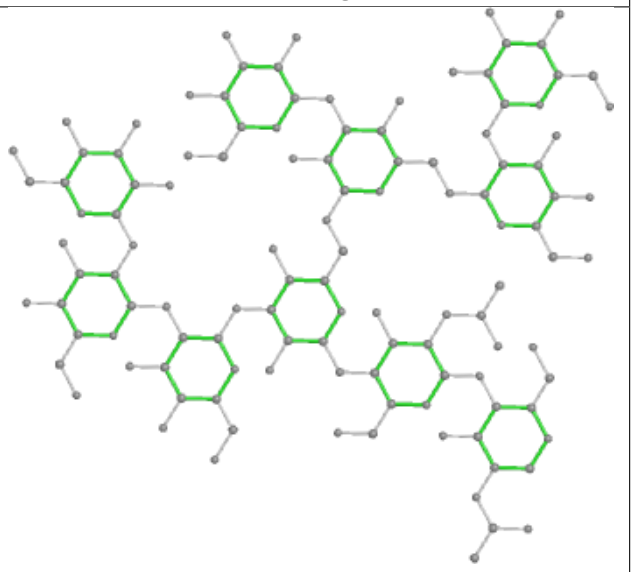
Bond lengths



Bond angles

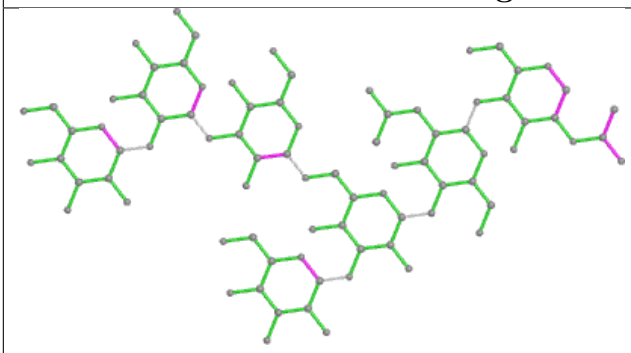


Torsions

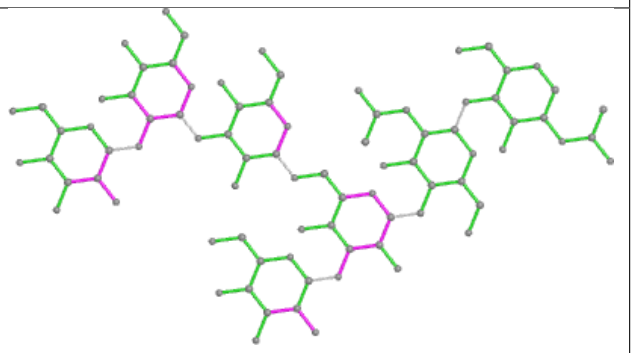


Rings

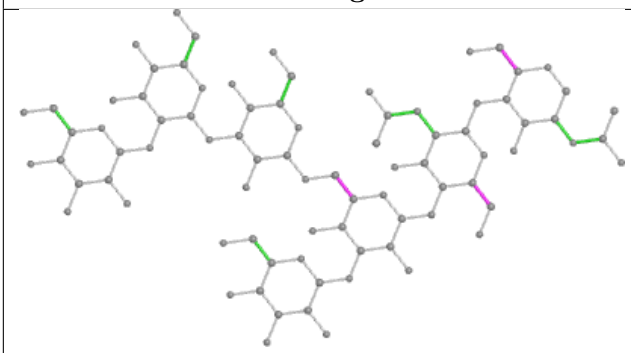
Oligosaccharide Chain P



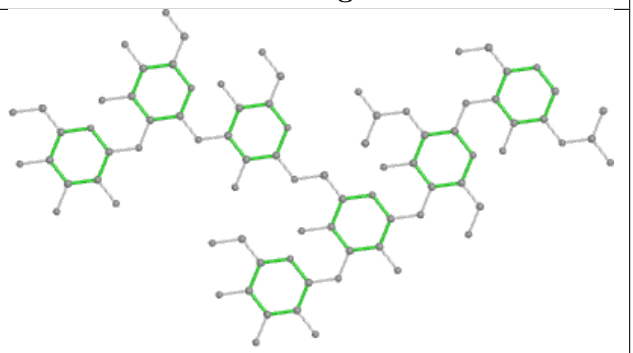
Bond lengths



Bond angles

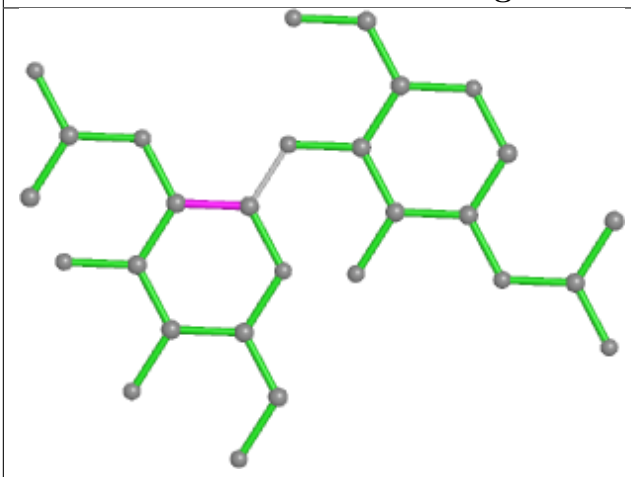


Torsions

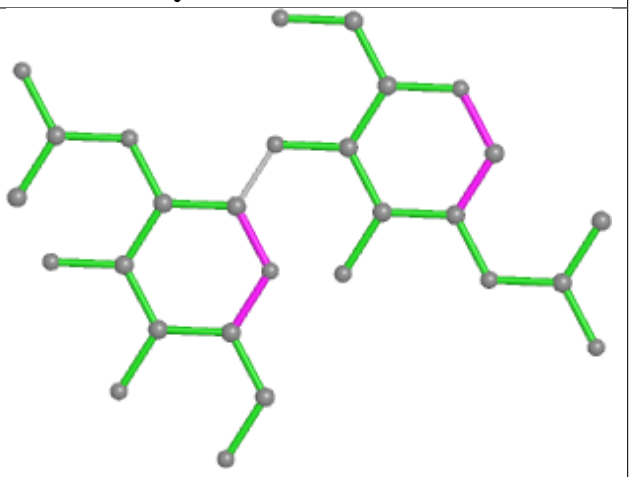


Rings

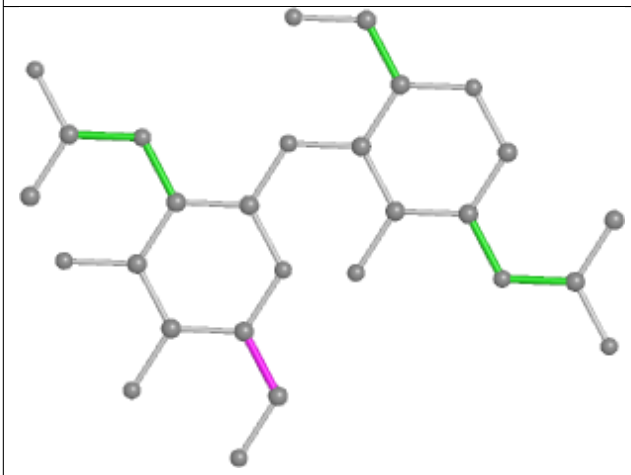
Oligosaccharide Chain Q



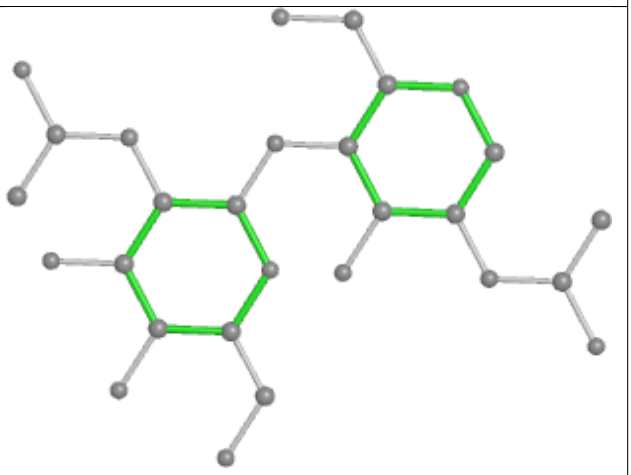
Bond lengths



Bond angles

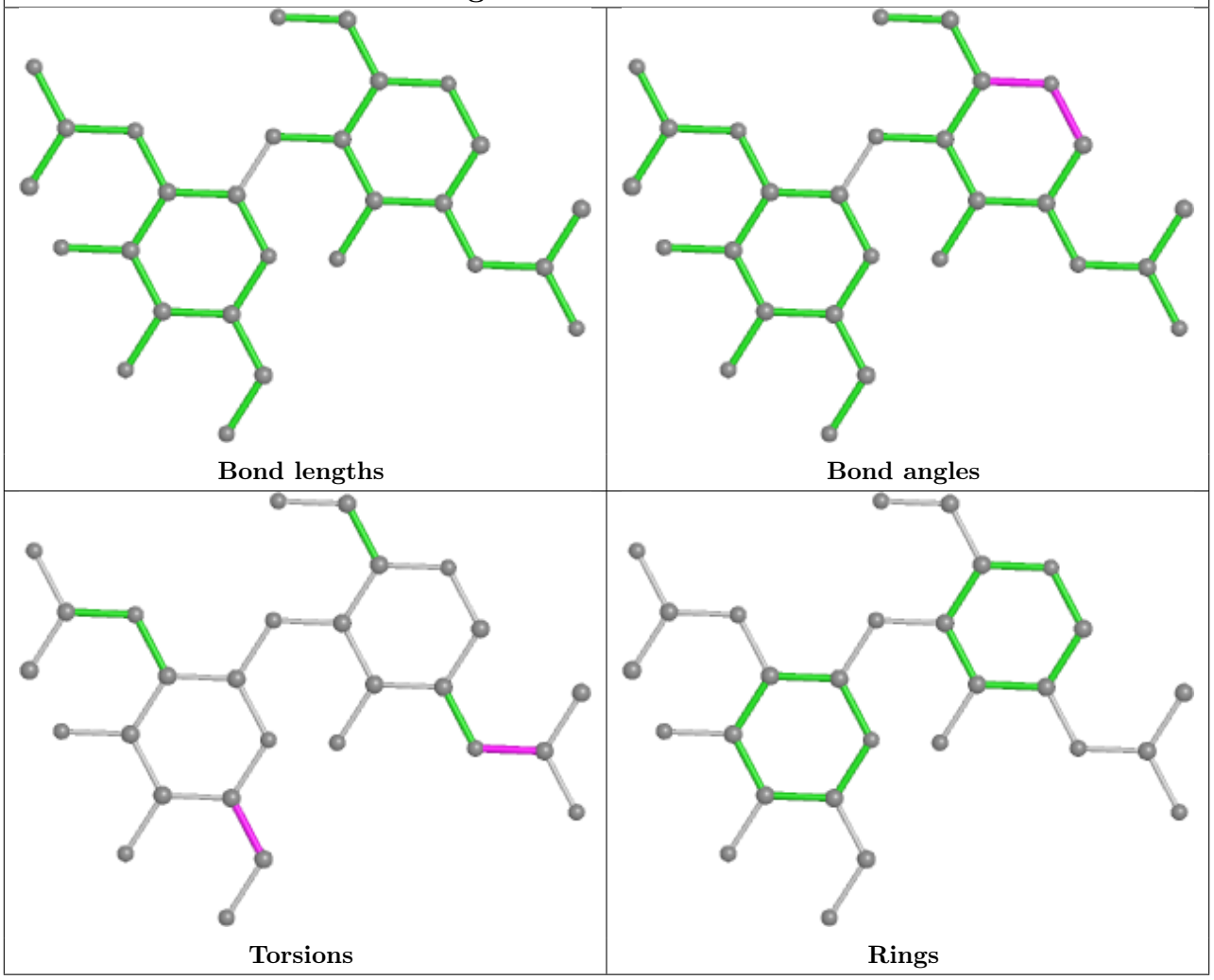


Torsions



Rings

Oligosaccharide Chain R



5.6 Ligand geometry (i)

3 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
16	NAG	G	1663	1	14,14,15	0.44	0	17,19,21	0.57	0
16	NAG	B	701	-	14,14,15	0.76	1 (7%)	17,19,21	0.37	0
16	NAG	B	702	2	14,14,15	2.37	2 (14%)	17,19,21	1.58	2 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	NAG	G	1663	1	-	2/6/23/26	0/1/1/1
16	NAG	B	701	-	-	0/6/23/26	0/1/1/1
16	NAG	B	702	2	-	2/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	B	702	NAG	C1-C2	-6.82	1.42	1.52
16	B	702	NAG	O5-C1	5.29	1.52	1.43
16	B	701	NAG	O5-C1	-2.80	1.39	1.43

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	B	702	NAG	C1-O5-C5	5.11	119.11	112.19
16	B	702	NAG	O5-C5-C4	-2.10	105.72	110.83

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
16	B	702	NAG	C4-C5-C6-O6
16	B	702	NAG	O5-C5-C6-O6
16	G	1663	NAG	O5-C5-C6-O6
16	G	1663	NAG	C4-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	G	1663	NAG	1	0
16	B	702	NAG	5	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	G	452/480 (94%)	-0.65	0 100 100	10, 33, 73, 120	0
2	B	148/153 (96%)	-0.46	1 (0%) 87 87	9, 37, 109, 192	0
3	L	211/218 (96%)	-0.69	0 100 100	19, 44, 79, 104	0
4	H	231/236 (97%)	-0.62	3 (1%) 77 77	32, 62, 91, 228	0
5	D	240/240 (100%)	-0.02	26 (10%) 5 4	36, 97, 226, 263	0
6	E	213/216 (98%)	-0.04	17 (7%) 12 9	55, 115, 172, 202	0
All	All	1495/1543 (96%)	-0.45	47 (3%) 49 44	9, 55, 165, 263	0

The worst 5 of 47 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	D	222	VAL	9.3
5	D	129	LYS	8.7
6	E	214	GLU	6.8
5	D	160	THR	6.7
6	E	198	GLN	6.1

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

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

6.3 Carbohydrates

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
10	NAG	I	2	14/15	0.52	0.21	213,239,249,255	0
7	NAG	A	1	14/15	0.56	0.30	142,152,164,166	0
14	BMA	P	3	11/12	0.62	0.14	235,247,263,263	0
14	MAN	P	7	11/12	0.67	0.35	262,267,270,273	0
12	BMA	N	3	11/12	0.69	0.40	212,225,229,231	0
11	MAN	M	5	11/12	0.71	0.42	267,278,283,284	0
9	NAG	F	2	14/15	0.71	0.28	146,153,166,167	0
11	MAN	M	6	11/12	0.73	0.18	246,261,264,268	0
8	NAG	C	1	14/15	0.73	0.19	134,135,138,145	0
11	MAN	J	7	11/12	0.74	0.15	241,243,257,260	0
10	NAG	S	2	14/15	0.74	0.40	191,196,215,219	0
11	MAN	M	7	11/12	0.77	0.22	150,181,209,210	0
14	MAN	P	6	11/12	0.77	0.38	201,208,212,213	0
11	MAN	J	8	11/12	0.77	0.17	263,269,274,275	0
11	MAN	M	4	11/12	0.78	0.23	243,244,255,265	0
7	MAN	A	6	11/12	0.79	0.30	160,167,172,173	0
10	BMA	S	3	11/12	0.79	0.19	181,186,191,191	0
8	NAG	C	2	14/15	0.79	0.25	135,141,146,148	0
10	NAG	S	1	14/15	0.79	0.40	143,170,181,191	0
15	NAG	R	2	14/15	0.79	0.21	176,181,183,186	0
8	MAN	C	4	11/12	0.80	0.16	170,172,183,187	0
9	NAG	F	1	14/15	0.81	0.19	122,130,140,142	0
9	MAN	F	7	11/12	0.81	0.37	160,171,179,190	0
9	BMA	K	3	11/12	0.81	0.09	231,234,240,242	0
8	BMA	C	3	11/12	0.82	0.11	127,140,157,159	0
10	BMA	I	3	11/12	0.82	0.20	263,271,276,280	0
14	MAN	P	5	11/12	0.83	0.23	209,221,224,226	0
12	NAG	N	2	14/15	0.83	0.22	181,190,208,215	0
9	MAN	K	7	11/12	0.83	0.45	233,243,248,257	0
8	MAN	C	5	11/12	0.83	0.17	165,172,184,185	0
12	MAN	N	4	11/12	0.84	0.13	191,199,207,208	0
14	NAG	P	1	14/15	0.84	0.20	178,191,199,199	0
9	NAG	K	2	14/15	0.84	0.33	231,240,257,259	0
15	NAG	R	1	14/15	0.84	0.13	154,165,171,171	0
14	MAN	P	4	11/12	0.84	0.14	228,240,254,255	0
9	MAN	F	6	11/12	0.85	0.16	98,102,105,106	0
13	NAG	O	2	14/15	0.85	0.24	127,131,150,172	0
11	MAN	J	6	11/12	0.86	0.16	209,227,238,239	0
11	BMA	M	3	11/12	0.86	0.21	214,223,228,232	0
14	NAG	P	2	14/15	0.86	0.17	204,213,217,225	0
15	NAG	Q	2	14/15	0.86	0.34	201,214,223,228	0
9	MAN	K	4	11/12	0.86	0.16	202,211,230,239	0
12	MAN	N	6	11/12	0.86	0.19	223,225,234,237	0

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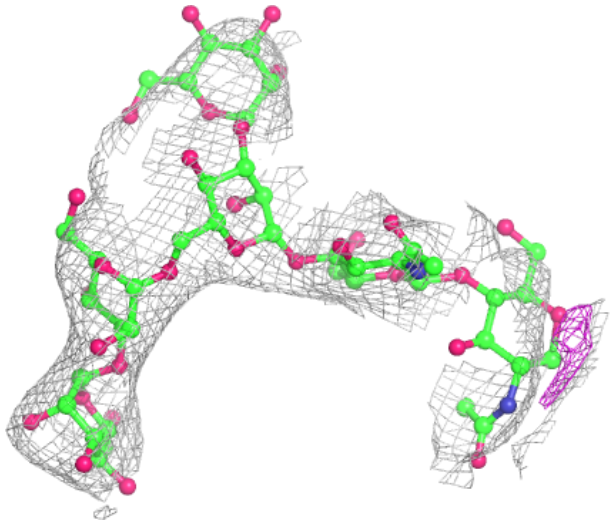
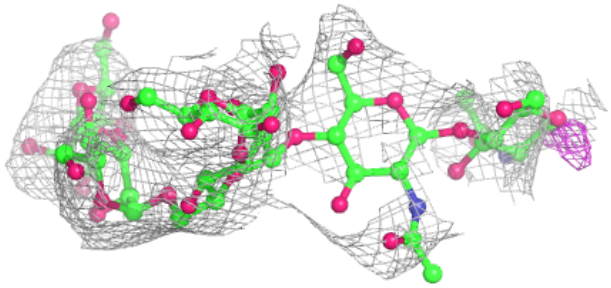
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
11	BMA	J	3	11/12	0.87	0.12	209,215,228,233	0
11	NAG	M	2	14/15	0.87	0.21	177,196,201,205	0
11	MAN	J	5	11/12	0.87	0.16	213,225,232,239	0
7	MAN	A	4	11/12	0.87	0.23	136,139,144,148	0
7	NAG	A	2	14/15	0.87	0.16	171,175,181,186	0
12	MAN	N	5	11/12	0.87	0.25	204,211,226,227	0
11	MAN	J	4	11/12	0.88	0.18	216,217,221,222	0
12	NAG	N	1	14/15	0.88	0.28	133,150,161,169	0
7	BMA	A	3	11/12	0.88	0.12	150,162,167,168	0
13	NAG	O	1	14/15	0.89	0.14	132,137,140,141	0
10	NAG	I	1	14/15	0.89	0.23	203,222,253,261	0
13	MAN	O	4	11/12	0.89	0.18	101,102,106,109	0
13	MAN	O	5	11/12	0.89	0.11	103,107,113,114	0
13	MAN	O	6	11/12	0.89	0.12	123,125,129,139	0
15	NAG	Q	1	14/15	0.89	0.19	152,164,180,193	0
13	MAN	O	9	11/12	0.89	0.16	152,157,169,174	0
8	MAN	C	7	11/12	0.89	0.14	117,120,133,134	0
9	BMA	F	3	11/12	0.89	0.10	160,165,168,172	0
9	MAN	F	5	11/12	0.90	0.10	108,116,127,131	0
11	NAG	J	1	14/15	0.90	0.14	165,173,182,184	0
13	MAN	O	7	11/12	0.90	0.13	149,154,159,163	0
11	NAG	J	2	14/15	0.90	0.23	182,193,199,201	0
7	MAN	A	5	11/12	0.90	0.20	133,137,149,150	0
9	MAN	K	5	11/12	0.91	0.12	187,195,205,208	0
11	NAG	M	1	14/15	0.91	0.22	181,187,211,221	0
11	MAN	M	8	11/12	0.91	0.13	99,118,144,152	0
9	MAN	F	4	11/12	0.92	0.12	136,155,161,171	0
8	MAN	C	6	11/12	0.92	0.10	184,191,198,199	0
9	NAG	K	1	14/15	0.92	0.28	168,198,226,229	0
13	MAN	O	8	11/12	0.92	0.08	146,151,154,154	0
13	MAN	O	10	11/12	0.93	0.12	165,174,180,184	0
9	MAN	K	6	11/12	0.93	0.23	219,223,235,238	0
13	BMA	O	3	11/12	0.94	0.10	119,126,138,145	0

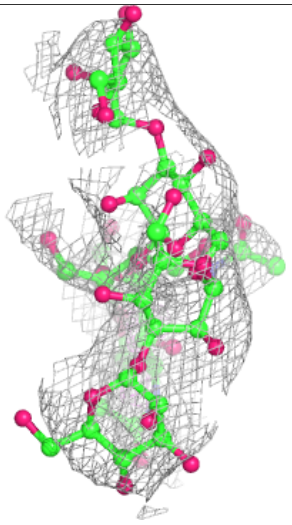
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain A:

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

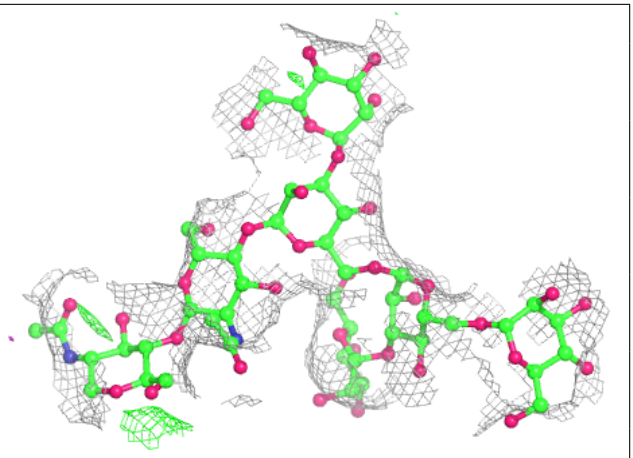


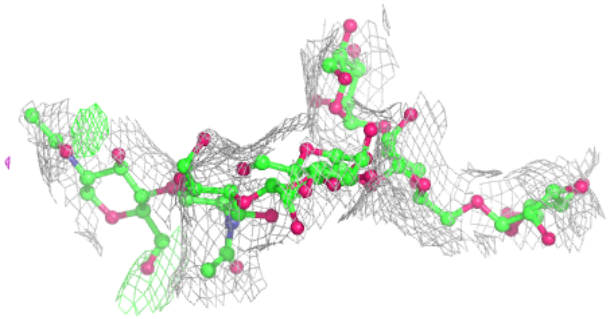


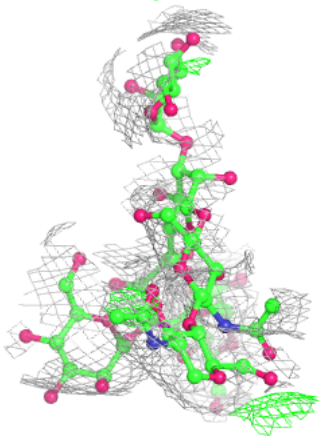


Electron density around Chain C:

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

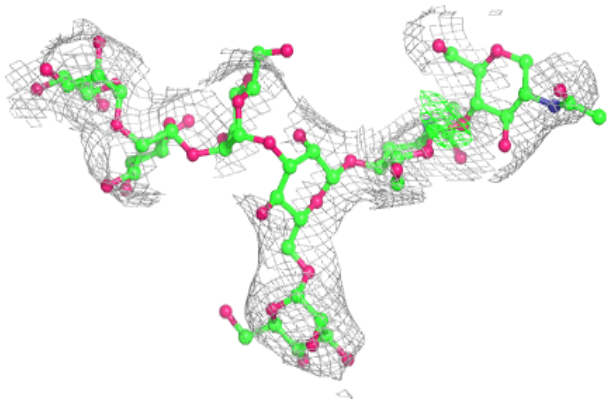


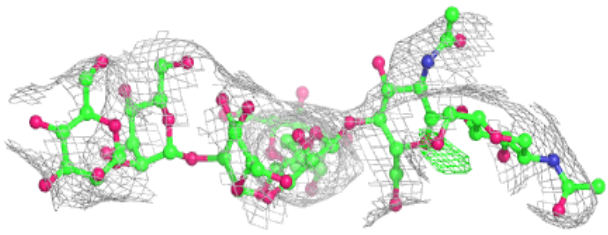


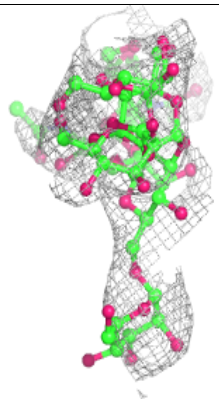


Electron density around Chain F:

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

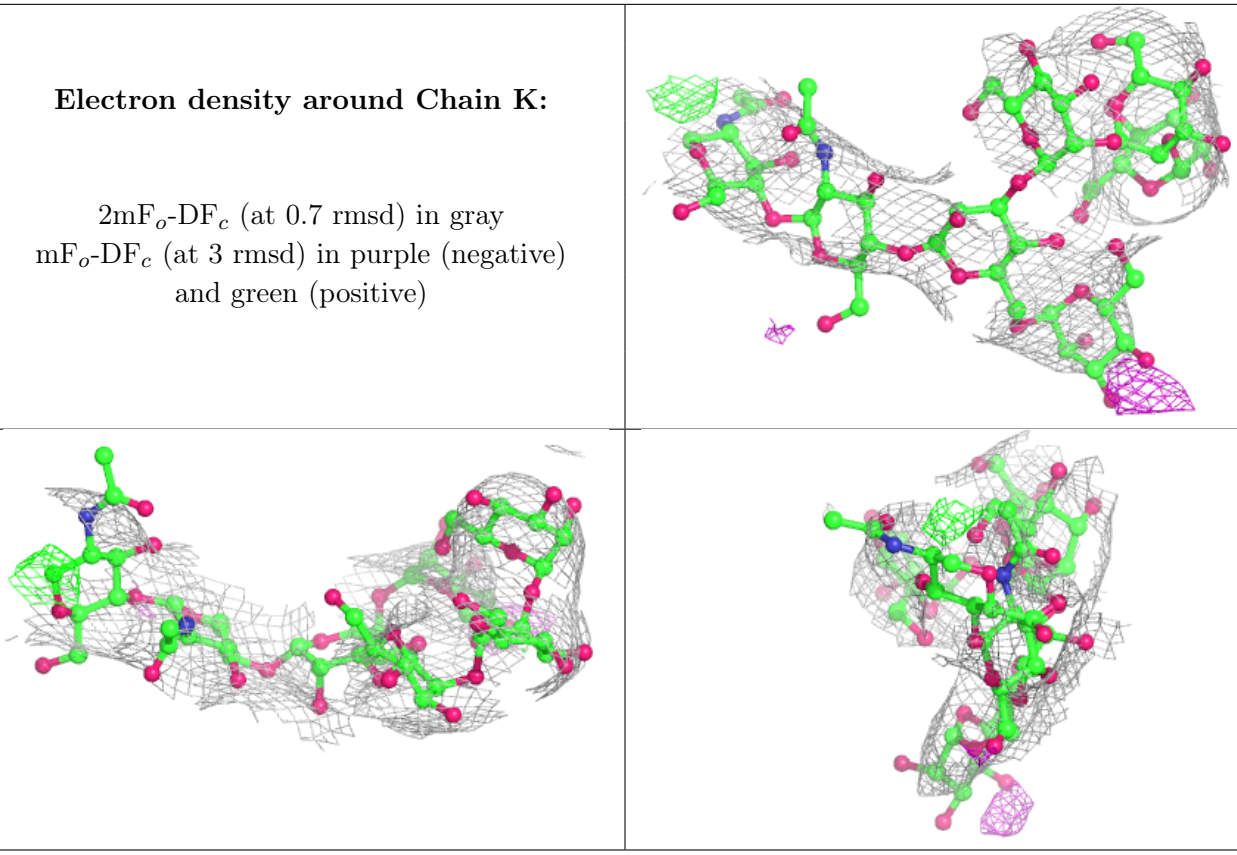






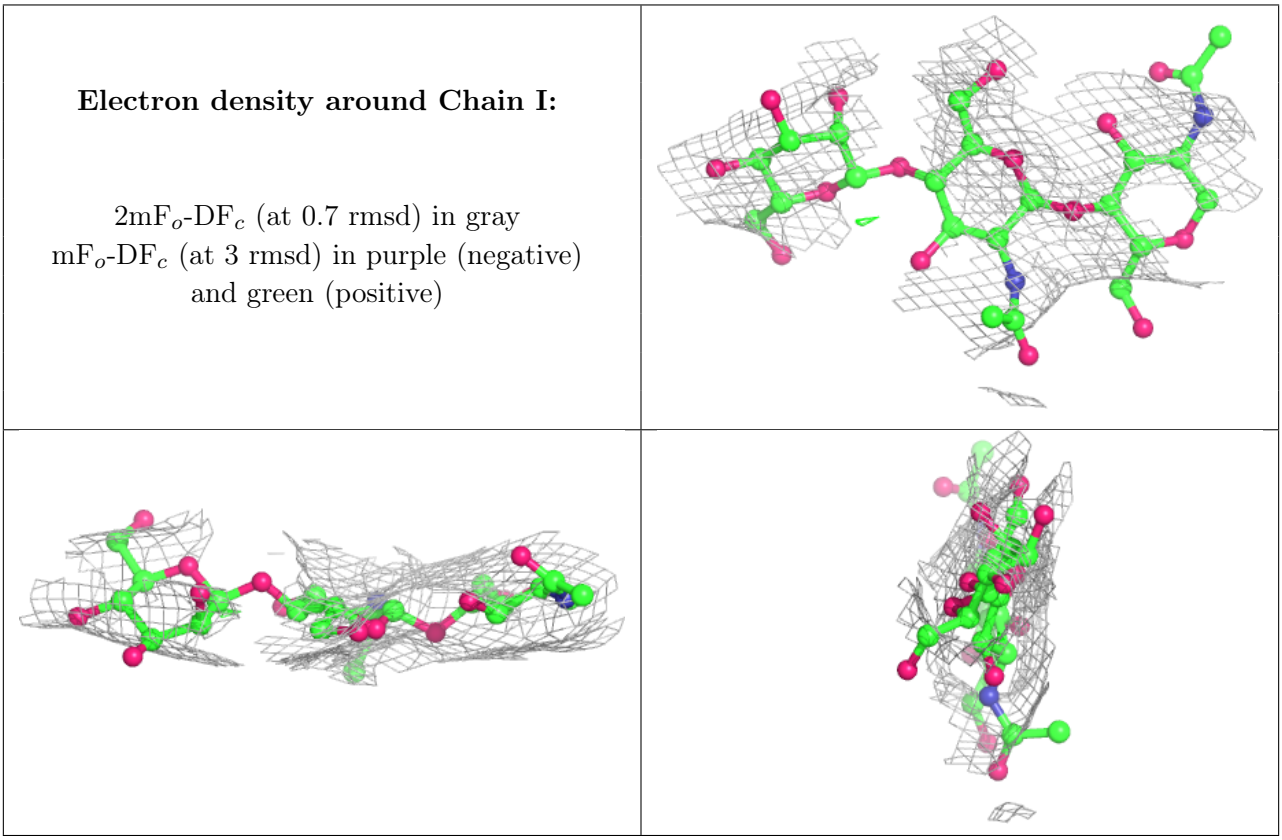
Electron density around Chain K:

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



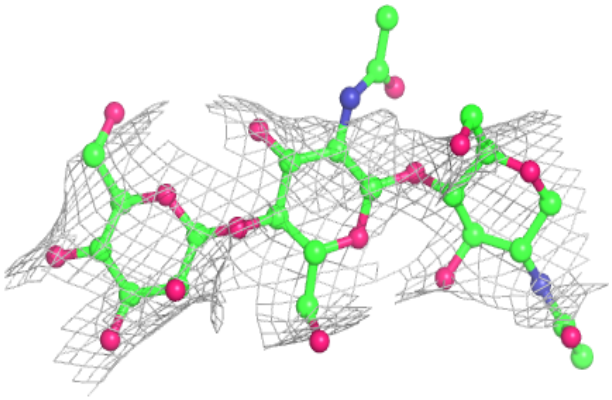
Electron density around Chain I:

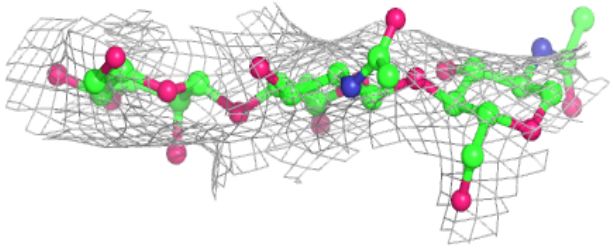
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

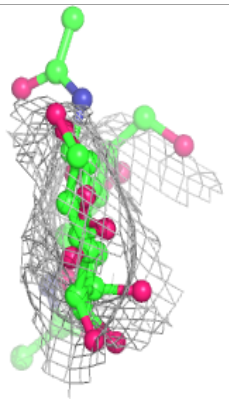


Electron density around Chain S:

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

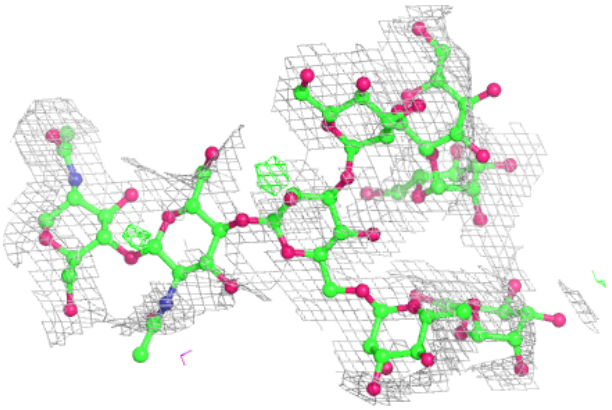


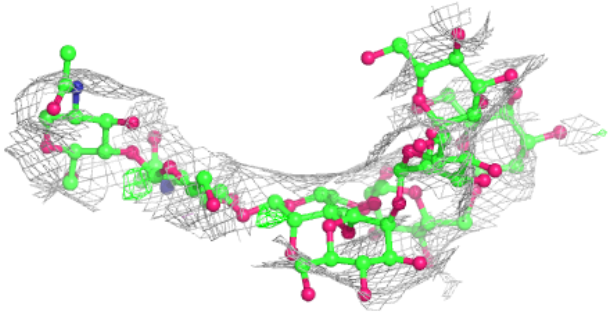


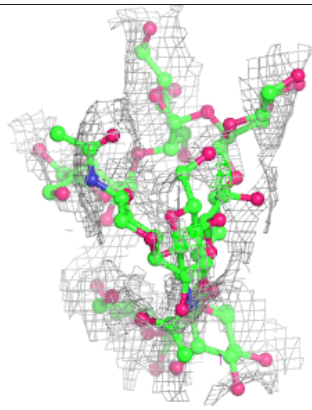


Electron density around Chain J:

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

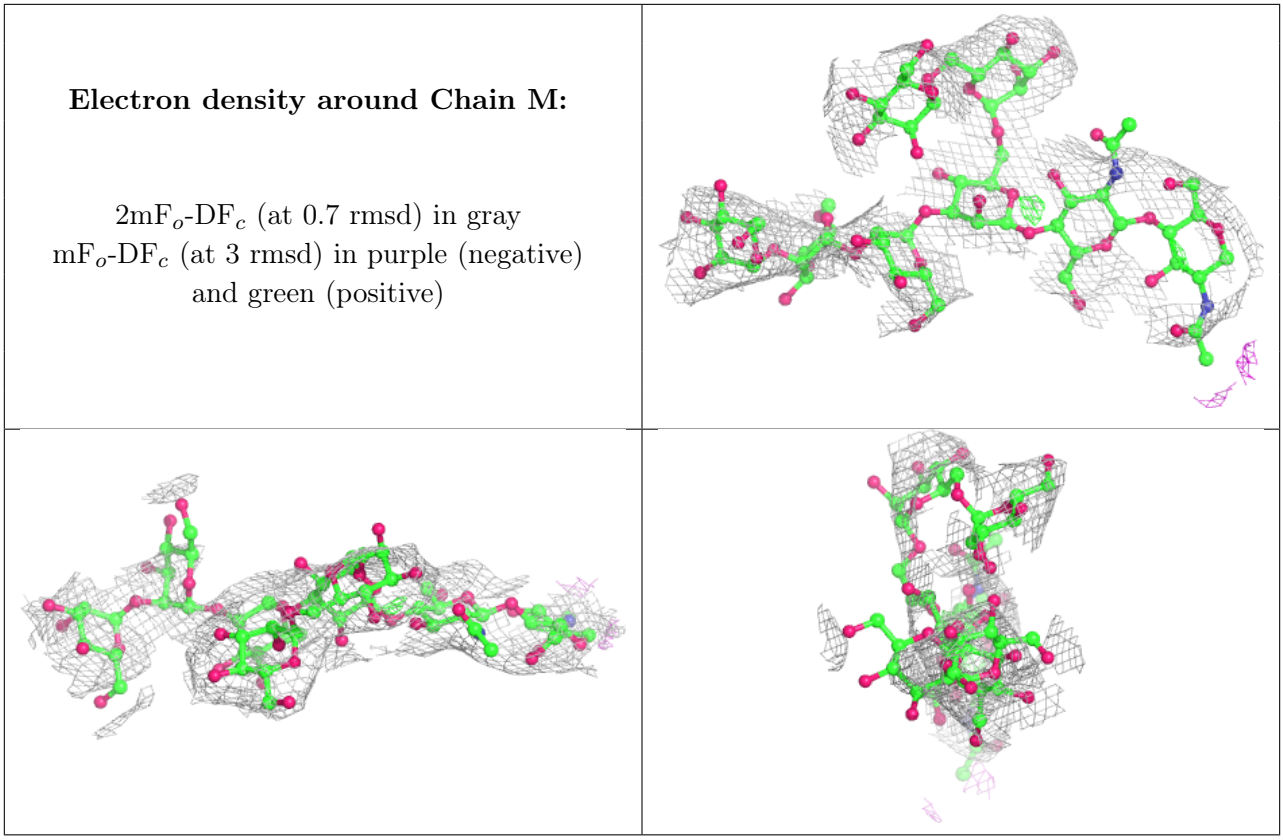






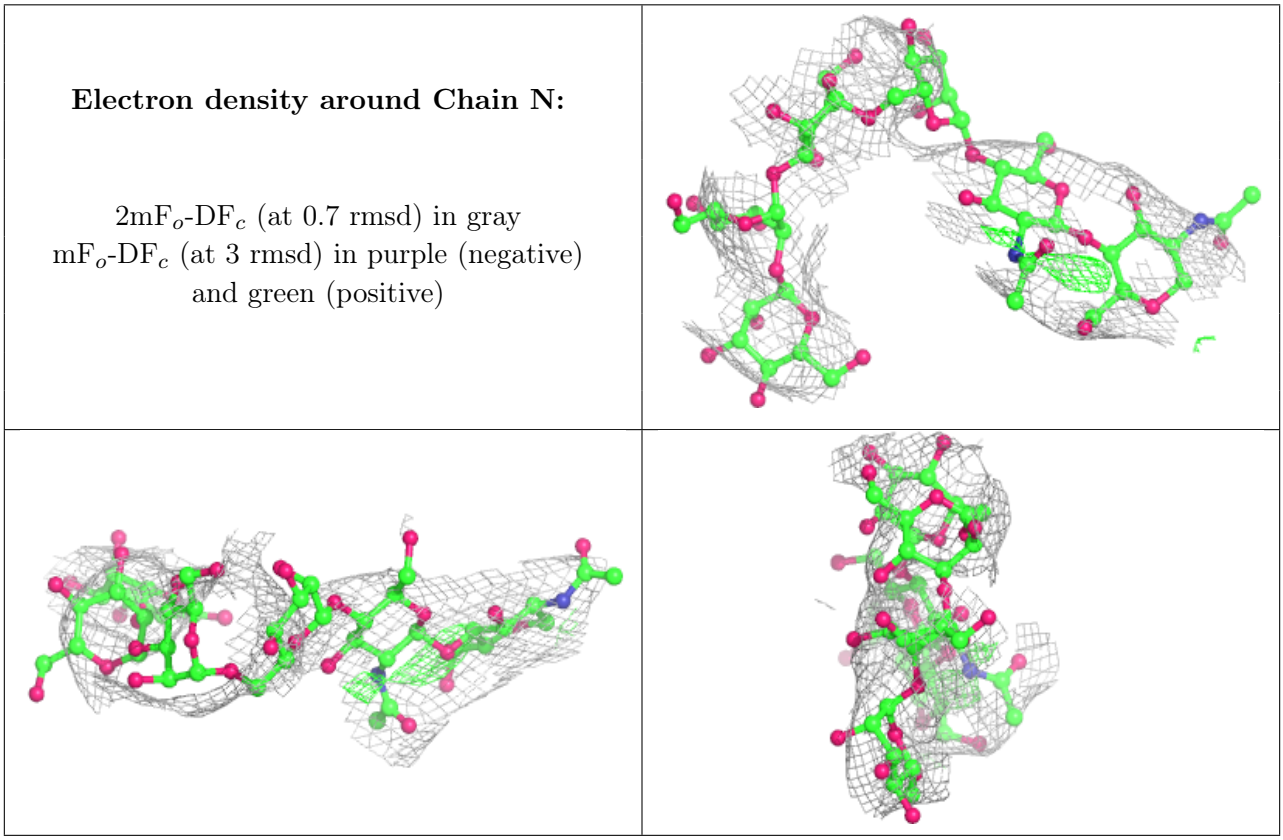
Electron density around Chain M:

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



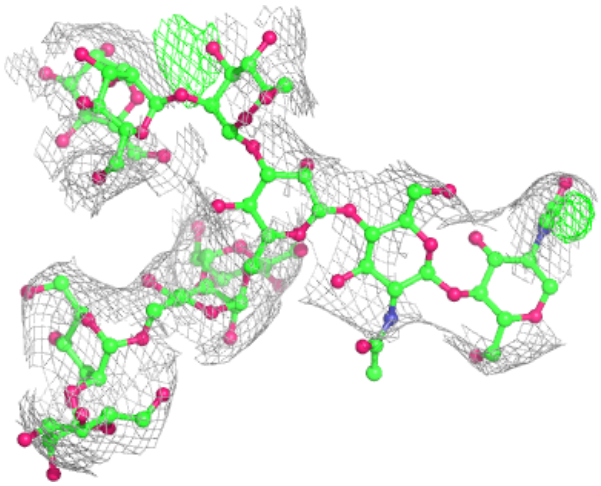
Electron density around Chain N:

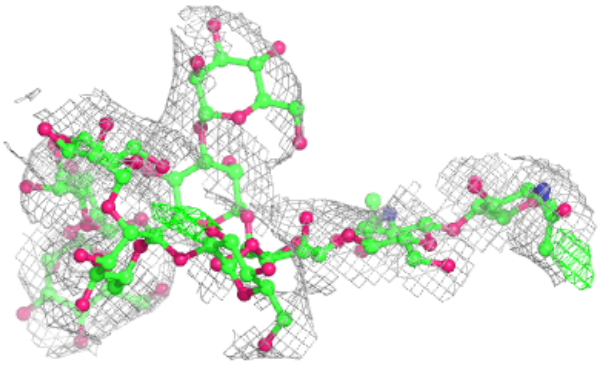
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

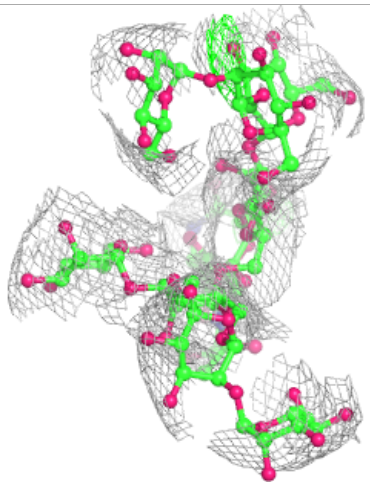


Electron density around Chain O:

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

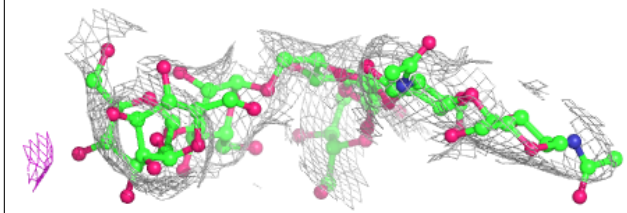


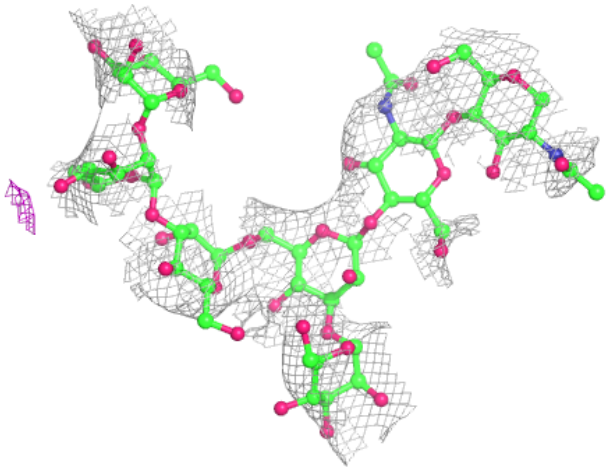


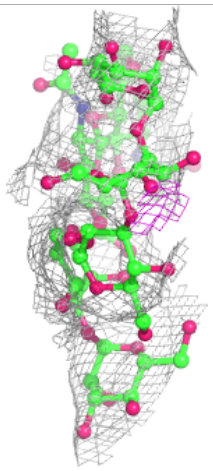


Electron density around Chain P:

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

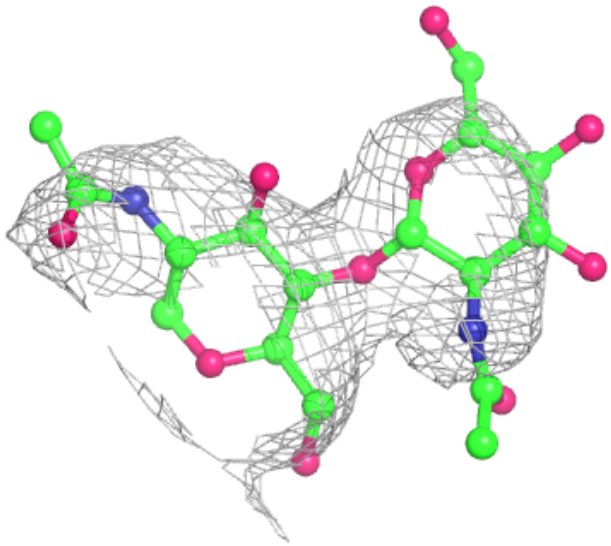


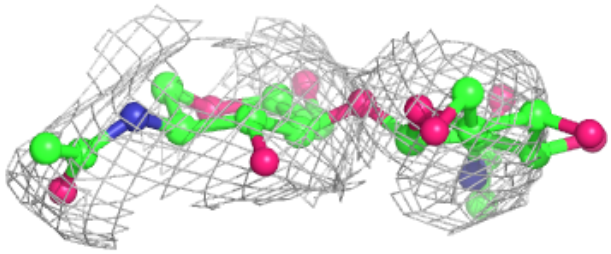


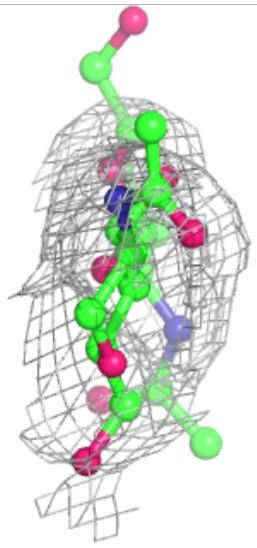


Electron density around Chain Q:

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

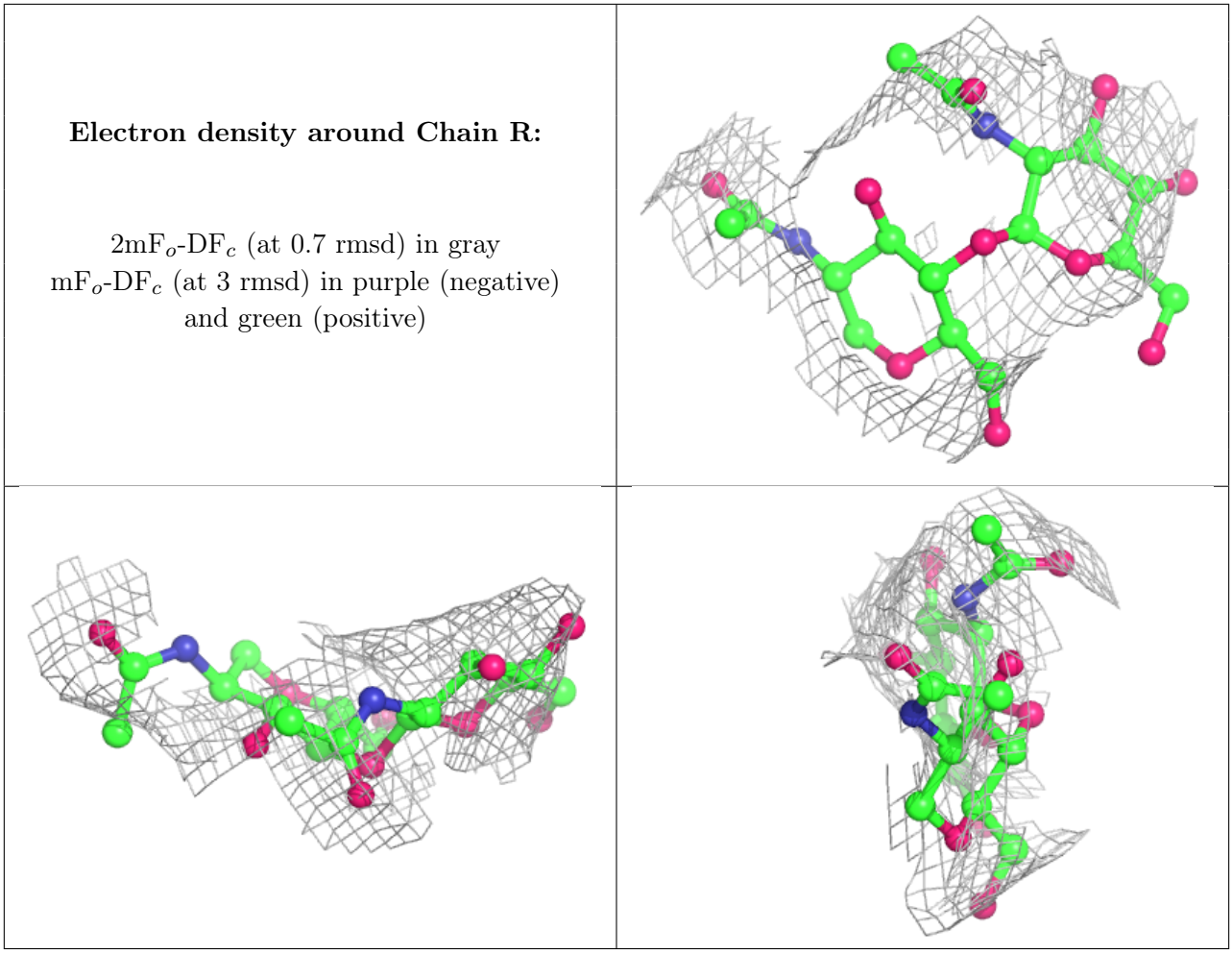






Electron density around Chain R:

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



6.4 Ligands

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
16	NAG	B	701	14/15	0.77	0.28	169,185,194,204	0
16	NAG	B	702	14/15	0.86	0.23	212,220,224,225	0
16	NAG	G	1663	14/15	0.88	0.22	134,144,154,161	0

6.5 Other polymers

There are no such residues in this entry.