Full wwPDB EM Validation Report ⓘ

Nov 12, 2022 – 07:49 PM EST

PDB ID	:	6VKN
EMDB ID	:	EMD-21227
Title	:	BG505 SOSIP.v5.2.N241.N289 in complex with rhesus macaque Fab RM19R
Authors	:	Cottrell, C.A.; Ward, A.B.
Deposited on	:	2020-01-21
Resolution	:	3.70 Å(reported)

This is a Full wwPDB EM 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/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

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

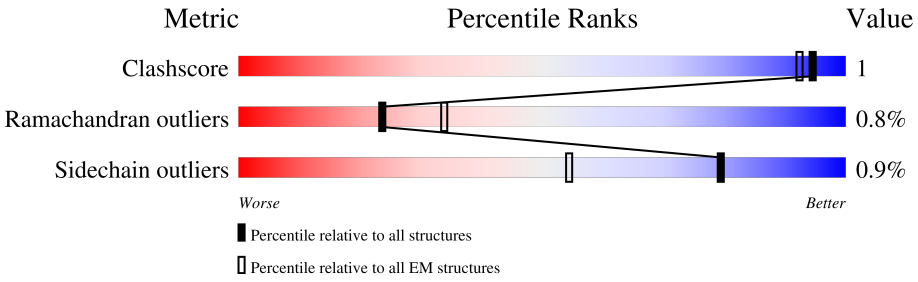
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.70 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)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	475	88% 5% 7%
1	C	475	88% 5% 7%
1	D	475	88% • 7%
2	B	153	80% 5% • 14%
2	E	153	80% 5% • 14%
2	F	153	80% 5% • 14%
3	J	107	10% 92% 6% ••
3	K	107	10% 92% 6% ••

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Mol	Chain	Length	Quality of chain
3	L	107	11% 92% 6%
4	G	121	18% 94% 5%
4	H	121	18% 94% 5%
4	I	121	19% 94% 5%
5	M	2	50% 100%
5	N	2	50% 50% 50%
5	O	2	50% 100%
5	P	2	100%
5	R	2	50% 100%
5	T	2	100% 100%
5	U	2	50% 100%
5	V	2	50% 50% 50%
5	W	2	50% 100%
5	X	2	100%
5	Z	2	100%
5	b	2	100% 100%
5	c	2	50% 100%
5	d	2	50% 50% 50%
5	e	2	50% 100%
5	f	2	100%
5	h	2	100%
5	j	2	100% 100%
6	Q	6	33% 100%
6	Y	6	33% 100%
6	g	6	33% 100%

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Mol	Chain	Length	Quality of chain
7	S	3	67% 100%
7	a	3	67% 100%
7	i	3	67% 100%

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 20220 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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					AltConf	Trace
1	A	441	Total	C	N	O	S	0	0
			3475	2183	614	650	28		
1	C	441	Total	C	N	O	S	0	0
			3475	2183	614	650	28		
1	D	441	Total	C	N	O	S	0	0
			3475	2183	614	650	28		

There are 33 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	64	LYS	GLU	engineered mutation	UNP Q2N0S6
A	73	CYS	ALA	engineered mutation	UNP Q2N0S6
A	240	THR	PRO	engineered mutation	UNP Q2N0S6
A	241	ASN	SER	engineered mutation	UNP Q2N0S6
A	271	ILE	MET	engineered mutation	UNP Q2N0S6
A	288	LEU	PHE	engineered mutation	UNP Q2N0S6
A	290	GLU	THR	engineered mutation	UNP Q2N0S6
A	291	SER	PRO	engineered mutation	UNP Q2N0S6
A	316	TRP	ALA	engineered mutation	UNP Q2N0S6
A	332	ASN	THR	engineered mutation	UNP Q2N0S6
A	501	CYS	ALA	engineered mutation	UNP Q2N0S6
C	64	LYS	GLU	engineered mutation	UNP Q2N0S6
C	73	CYS	ALA	engineered mutation	UNP Q2N0S6
C	240	THR	PRO	engineered mutation	UNP Q2N0S6
C	241	ASN	SER	engineered mutation	UNP Q2N0S6
C	271	ILE	MET	engineered mutation	UNP Q2N0S6
C	288	LEU	PHE	engineered mutation	UNP Q2N0S6
C	290	GLU	THR	engineered mutation	UNP Q2N0S6
C	291	SER	PRO	engineered mutation	UNP Q2N0S6
C	316	TRP	ALA	engineered mutation	UNP Q2N0S6
C	332	ASN	THR	engineered mutation	UNP Q2N0S6
C	501	CYS	ALA	engineered mutation	UNP Q2N0S6
D	64	LYS	GLU	engineered mutation	UNP Q2N0S6
D	73	CYS	ALA	engineered mutation	UNP Q2N0S6

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Chain	Residue	Modelled	Actual	Comment	Reference
D	240	THR	PRO	engineered mutation	UNP Q2N0S6
D	241	ASN	SER	engineered mutation	UNP Q2N0S6
D	271	ILE	MET	engineered mutation	UNP Q2N0S6
D	288	LEU	PHE	engineered mutation	UNP Q2N0S6
D	290	GLU	THR	engineered mutation	UNP Q2N0S6
D	291	SER	PRO	engineered mutation	UNP Q2N0S6
D	316	TRP	ALA	engineered mutation	UNP Q2N0S6
D	332	ASN	THR	engineered mutation	UNP Q2N0S6
D	501	CYS	ALA	engineered mutation	UNP Q2N0S6

- Molecule 2 is a protein called BG505 SOSIPv5.2 gp41.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	132	Total	C	N	O	S	0	0
			1057	669	183	198	7		
2	E	132	Total	C	N	O	S	0	0
			1057	669	183	198	7		
2	F	132	Total	C	N	O	S	0	0
			1057	669	183	198	7		

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	559	PRO	ILE	engineered mutation	UNP Q2N0S6
B	561	CYS	ALA	engineered mutation	UNP Q2N0S6
B	605	CYS	THR	engineered mutation	UNP Q2N0S6
E	559	PRO	ILE	engineered mutation	UNP Q2N0S6
E	561	CYS	ALA	engineered mutation	UNP Q2N0S6
E	605	CYS	THR	engineered mutation	UNP Q2N0S6
F	559	PRO	ILE	engineered mutation	UNP Q2N0S6
F	561	CYS	ALA	engineered mutation	UNP Q2N0S6
F	605	CYS	THR	engineered mutation	UNP Q2N0S6

- Molecule 3 is a protein called RM19R Kappa Light Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	L	105	Total	C	N	O	S	0	0
			818	511	142	162	3		
3	J	105	Total	C	N	O	S	0	0
			818	511	142	162	3		
3	K	105	Total	C	N	O	S	0	0
			818	511	142	162	3		

- Molecule 4 is a protein called RM19R Heavy Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	H	120	Total	C	N	O	S	0	0
			930	587	160	181	2		
4	G	120	Total	C	N	O	S	0	0
			930	587	160	181	2		
4	I	120	Total	C	N	O	S	0	0
			930	587	160	181	2		

- Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	M	2	Total	C	N	O	0	0
			28	16	2	10		
5	N	2	Total	C	N	O	0	0
			28	16	2	10		
5	O	2	Total	C	N	O	0	0
			28	16	2	10		
5	P	2	Total	C	N	O	0	0
			28	16	2	10		
5	R	2	Total	C	N	O	0	0
			28	16	2	10		
5	T	2	Total	C	N	O	0	0
			28	16	2	10		
5	U	2	Total	C	N	O	0	0
			28	16	2	10		
5	V	2	Total	C	N	O	0	0
			28	16	2	10		
5	W	2	Total	C	N	O	0	0
			28	16	2	10		
5	X	2	Total	C	N	O	0	0
			28	16	2	10		
5	Z	2	Total	C	N	O	0	0
			28	16	2	10		
5	b	2	Total	C	N	O	0	0
			28	16	2	10		
5	c	2	Total	C	N	O	0	0
			28	16	2	10		

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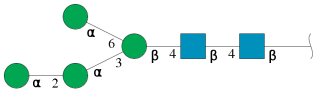
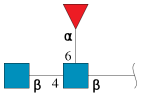
Mol	Chain	Residues	Atoms				AltConf	Trace
5	d	2	Total	C	N	O	0	0
			28	16	2	10		
5	e	2	Total	C	N	O	0	0
			28	16	2	10		
5	f	2	Total	C	N	O	0	0
			28	16	2	10		
5	h	2	Total	C	N	O	0	0
			28	16	2	10		
5	j	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 6 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.



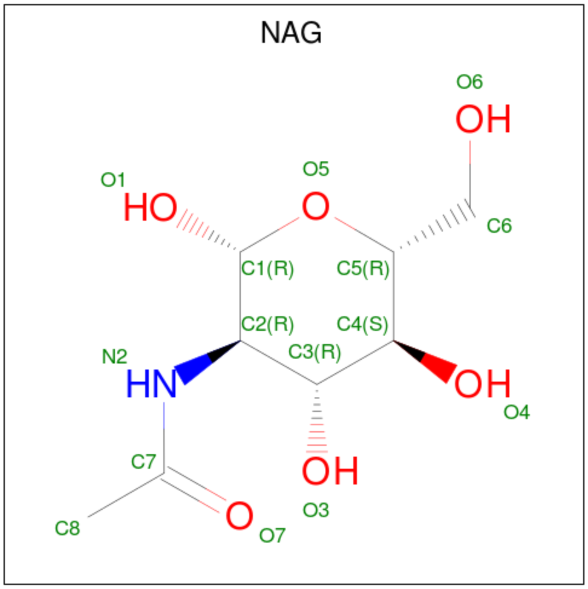
Mol	Chain	Residues	Atoms				AltConf	Trace
6	Q	6	Total	C	N	O	0	0
			72	40	2	30		
6	Y	6	Total	C	N	O	0	0
			72	40	2	30		
6	g	6	Total	C	N	O	0	0
			72	40	2	30		

- Molecule 7 is an oligosaccharide called 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				AltConf	Trace
7	S	3	Total	C	N	O	0	0
			38	22	2	14		
7	a	3	Total	C	N	O	0	0
			38	22	2	14		
7	i	3	Total	C	N	O	0	0
			38	22	2	14		

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



Mol	Chain	Residues	Atoms	AltConf
8	A	1	Total C N O 168 96 12 60	0
8	A	1	Total C N O 168 96 12 60	0
8	A	1	Total C N O 168 96 12 60	0
8	A	1	Total C N O 168 96 12 60	0
8	A	1	Total C N O 168 96 12 60	0
8	A	1	Total C N O 168 96 12 60	0
8	A	1	Total C N O 168 96 12 60	0
8	A	1	Total C N O 168 96 12 60	0
8	A	1	Total C N O 168 96 12 60	0
8	A	1	Total C N O 168 96 12 60	0
8	A	1	Total C N O 168 96 12 60	0
8	A	1	Total C N O 168 96 12 60	0

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Mol	Chain	Residues	Atoms	AltConf
8	B	1	Total C N O 14 8 1 5	0
8	C	1	Total C N O 168 96 12 60	0
8	C	1	Total C N O 168 96 12 60	0
8	C	1	Total C N O 168 96 12 60	0
8	C	1	Total C N O 168 96 12 60	0
8	C	1	Total C N O 168 96 12 60	0
8	C	1	Total C N O 168 96 12 60	0
8	C	1	Total C N O 168 96 12 60	0
8	C	1	Total C N O 168 96 12 60	0
8	C	1	Total C N O 168 96 12 60	0
8	C	1	Total C N O 168 96 12 60	0
8	C	1	Total C N O 168 96 12 60	0
8	C	1	Total C N O 168 96 12 60	0
8	E	1	Total C N O 14 8 1 5	0
8	D	1	Total C N O 168 96 12 60	0
8	D	1	Total C N O 168 96 12 60	0
8	D	1	Total C N O 168 96 12 60	0
8	D	1	Total C N O 168 96 12 60	0
8	D	1	Total C N O 168 96 12 60	0
8	D	1	Total C N O 168 96 12 60	0
8	D	1	Total C N O 168 96 12 60	0

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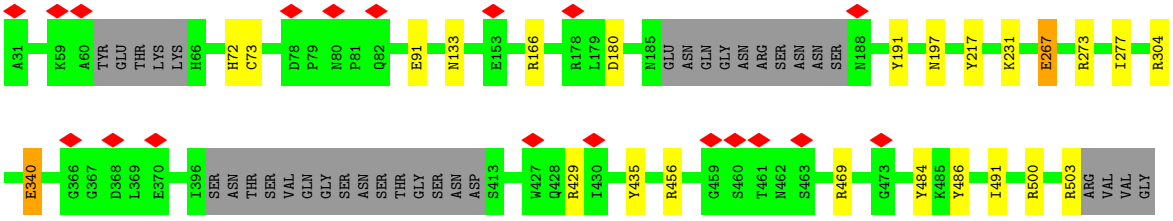
Mol	Chain	Residues	Atoms				AltConf
8	D	1	Total	C	N	O	0
			168	96	12	60	
8	D	1	Total	C	N	O	0
			168	96	12	60	
8	D	1	Total	C	N	O	0
			168	96	12	60	
8	D	1	Total	C	N	O	0
			168	96	12	60	
8	D	1	Total	C	N	O	0
			168	96	12	60	
8	F	1	Total	C	N	O	0
			14	8	1	5	

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 atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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.

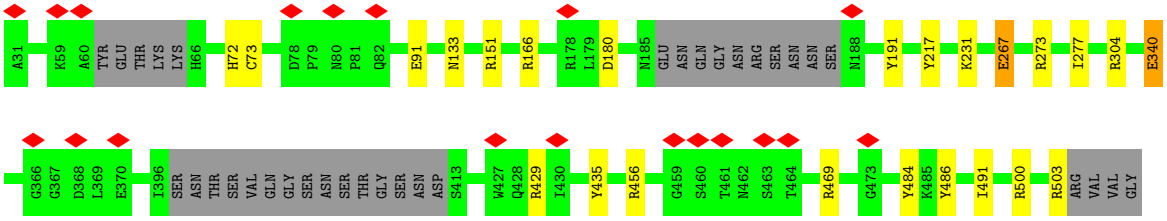
• Molecule 1: Envelope glycoprotein gp160

Chain A:



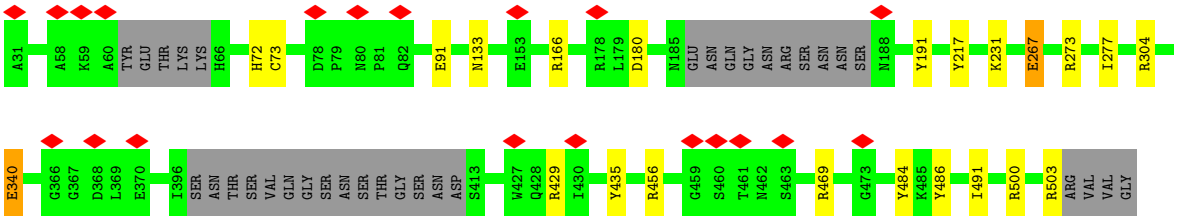
• Molecule 1: Envelope glycoprotein gp160

Chain C:



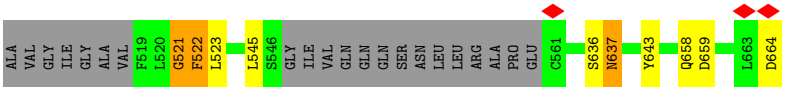
• Molecule 1: Envelope glycoprotein gp160

Chain D:

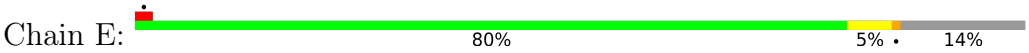


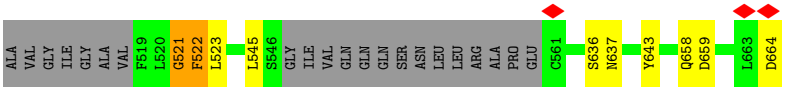
• Molecule 2: BG505 SOSIPv5.2 gp41

Chain B:

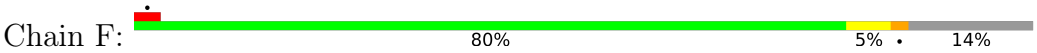


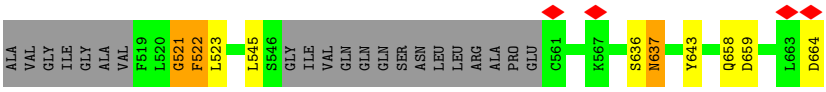
• Molecule 2: BG505 SOSIPv5.2 gp41



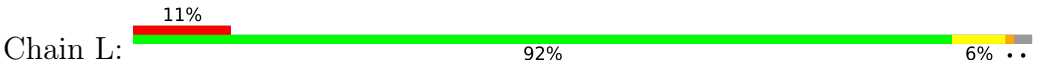


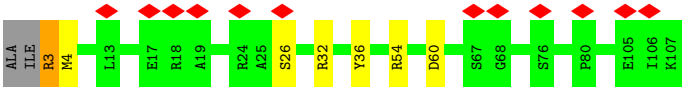
• Molecule 2: BG505 SOSIPv5.2 gp41



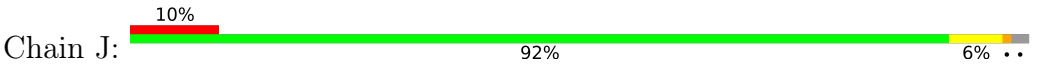


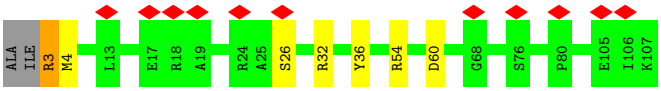
• Molecule 3: RM19R Kappa Light Chain



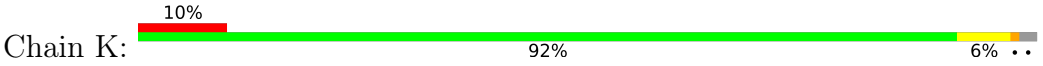


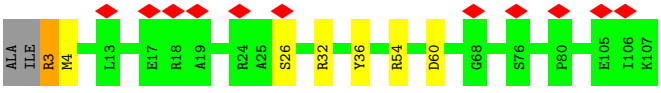
• Molecule 3: RM19R Kappa Light Chain



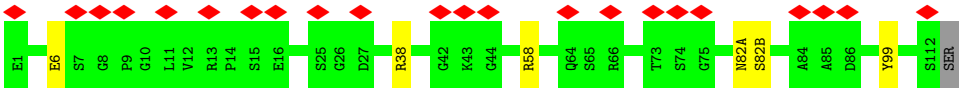


• Molecule 3: RM19R Kappa Light Chain



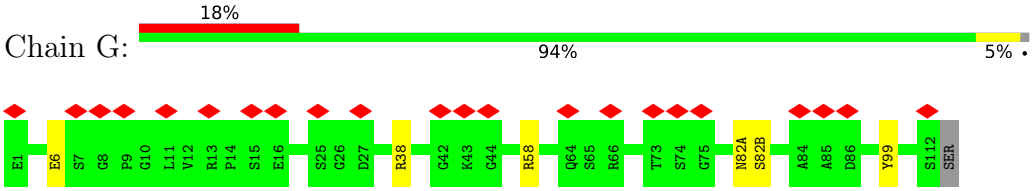


• Molecule 4: RM19R Heavy Chain



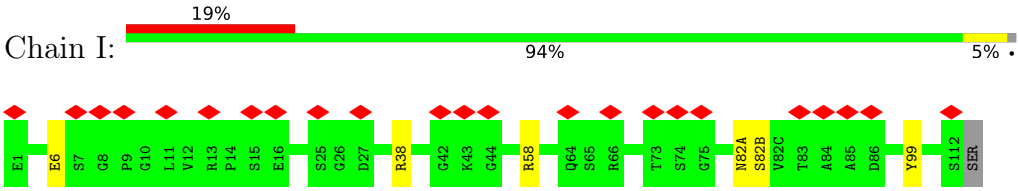
• Molecule 4: RM19R Heavy Chain

Chain G:



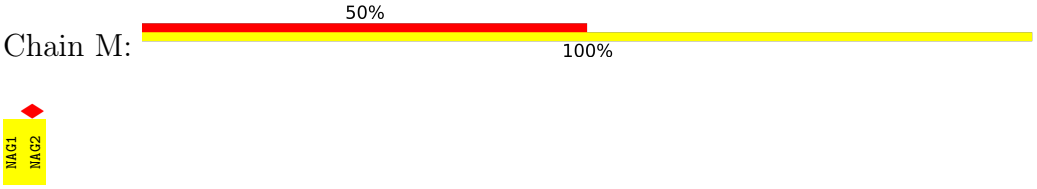
• Molecule 4: RM19R Heavy Chain

Chain I:



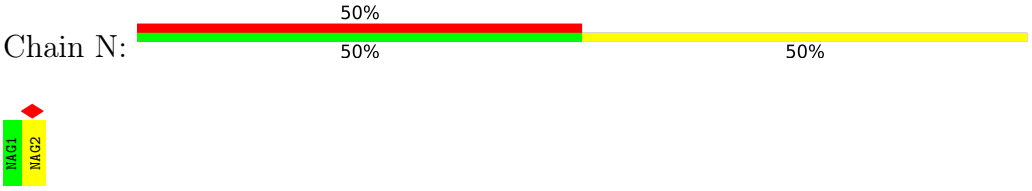
• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:



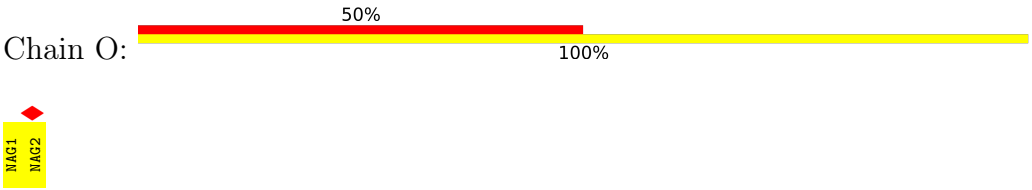
• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N:



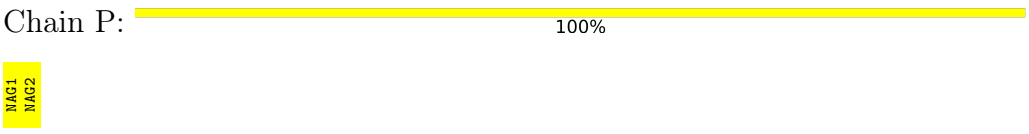
• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O:



• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain P:



• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain R:

• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain T:

• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

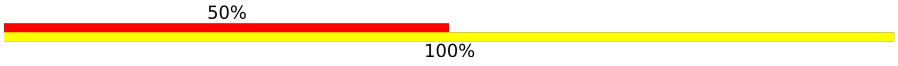
Chain U:

• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain V:

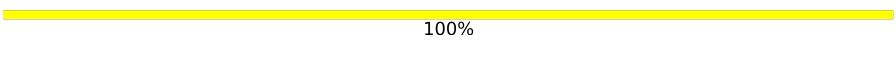
• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain W:



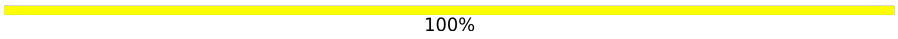
• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain X:



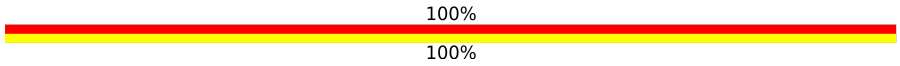
• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Z:



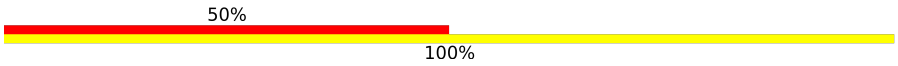
• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain b:



• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain c:



• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

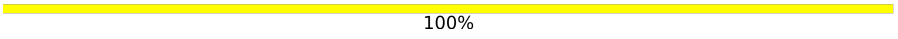
Chain d:

• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain e:

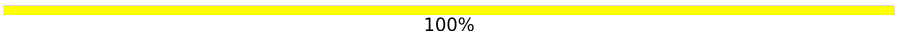
• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain f:



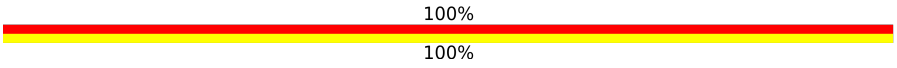
• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain h:



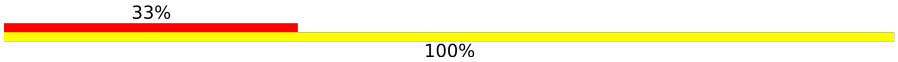
• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain j:



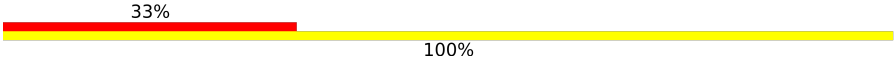
• Molecule 6: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Q:



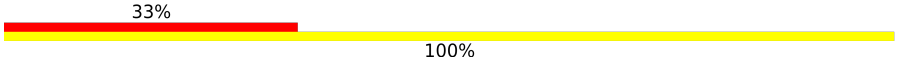
• Molecule 6: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Y:



• Molecule 6: 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 g:



• Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain S:

• Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain a:

• Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain i:

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	191556	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	67	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.305	Depositor
Minimum map value	-0.174	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.010	Depositor
Recommended contour level	0.05	Depositor
Map size (Å)	296.63998, 296.63998, 296.63998	wwPDB
Map dimensions	288, 288, 288	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.03, 1.03, 1.03	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.99	7/3546 (0.2%)	0.96	15/4814 (0.3%)
1	C	0.99	7/3546 (0.2%)	0.96	16/4814 (0.3%)
1	D	0.99	7/3546 (0.2%)	0.96	15/4814 (0.3%)
2	B	1.02	0/1076	0.83	1/1458 (0.1%)
2	E	1.02	0/1076	0.83	1/1458 (0.1%)
2	F	1.02	0/1076	0.83	1/1458 (0.1%)
3	J	0.96	0/838	0.94	3/1137 (0.3%)
3	K	0.96	0/838	0.94	3/1137 (0.3%)
3	L	0.96	0/838	0.94	3/1137 (0.3%)
4	G	1.01	2/954 (0.2%)	0.94	2/1301 (0.2%)
4	H	1.01	2/954 (0.2%)	0.94	2/1301 (0.2%)
4	I	1.01	2/954 (0.2%)	0.94	2/1301 (0.2%)
All	All	0.99	27/19242 (0.1%)	0.93	64/26130 (0.2%)

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	73	CYS	CB-SG	-8.21	1.68	1.82
1	A	73	CYS	CB-SG	-8.21	1.68	1.82
1	D	73	CYS	CB-SG	-8.18	1.68	1.82
1	A	484	TYR	CB-CG	-6.55	1.41	1.51
1	C	484	TYR	CB-CG	-6.55	1.41	1.51
1	D	484	TYR	CB-CG	-6.54	1.41	1.51
4	G	6	GLU	CG-CD	-6.19	1.42	1.51
4	H	6	GLU	CG-CD	-6.18	1.42	1.51
4	I	6	GLU	CG-CD	-6.17	1.42	1.51
1	D	91	GLU	CG-CD	-5.67	1.43	1.51
1	A	91	GLU	CG-CD	-5.66	1.43	1.51
1	C	91	GLU	CG-CD	-5.61	1.43	1.51
1	C	91	GLU	CD-OE2	-5.49	1.19	1.25
1	A	91	GLU	CD-OE2	-5.45	1.19	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	91	GLU	CD-OE2	-5.43	1.19	1.25
1	C	486	TYR	CB-CG	-5.18	1.43	1.51
4	I	6	GLU	CD-OE1	-5.17	1.20	1.25
1	C	340	GLU	CD-OE1	-5.16	1.20	1.25
1	A	340	GLU	CD-OE1	-5.15	1.20	1.25
1	D	486	TYR	CB-CG	-5.15	1.44	1.51
1	D	191	TYR	CG-CD1	-5.15	1.32	1.39
1	A	486	TYR	CB-CG	-5.14	1.44	1.51
1	D	340	GLU	CD-OE1	-5.12	1.20	1.25
4	H	6	GLU	CD-OE1	-5.12	1.20	1.25
1	C	191	TYR	CG-CD1	-5.12	1.32	1.39
1	A	191	TYR	CG-CD1	-5.11	1.32	1.39
4	G	6	GLU	CD-OE1	-5.07	1.20	1.25

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	484	TYR	CB-CG-CD2	-11.95	113.83	121.00
1	C	484	TYR	CB-CG-CD2	-11.93	113.84	121.00
1	A	484	TYR	CB-CG-CD2	-11.93	113.84	121.00
1	C	469	ARG	NE-CZ-NH2	-9.84	115.38	120.30
1	A	469	ARG	NE-CZ-NH2	-9.83	115.38	120.30
1	D	469	ARG	NE-CZ-NH2	-9.79	115.40	120.30
1	D	456	ARG	NE-CZ-NH2	-9.52	115.54	120.30
1	A	456	ARG	NE-CZ-NH2	-9.52	115.54	120.30
1	C	456	ARG	NE-CZ-NH2	-9.48	115.56	120.30
1	D	166	ARG	NE-CZ-NH2	-7.98	116.31	120.30
1	A	166	ARG	NE-CZ-NH2	-7.94	116.33	120.30
1	C	166	ARG	NE-CZ-NH2	-7.91	116.35	120.30
1	A	304	ARG	NE-CZ-NH2	-7.48	116.56	120.30
1	C	304	ARG	NE-CZ-NH2	-7.46	116.57	120.30
1	D	304	ARG	NE-CZ-NH2	-7.43	116.58	120.30
1	C	429	ARG	NE-CZ-NH1	7.42	124.01	120.30
1	D	429	ARG	NE-CZ-NH1	7.38	123.99	120.30
1	A	429	ARG	NE-CZ-NH1	7.36	123.98	120.30
3	L	54	ARG	NE-CZ-NH2	-7.21	116.69	120.30
3	J	54	ARG	NE-CZ-NH2	-7.21	116.70	120.30
3	K	54	ARG	NE-CZ-NH2	-7.21	116.70	120.30
1	A	484	TYR	CB-CG-CD1	6.93	125.16	121.00
1	C	484	TYR	CB-CG-CD1	6.92	125.15	121.00
1	D	484	TYR	CB-CG-CD1	6.91	125.15	121.00
1	C	456	ARG	NE-CZ-NH1	6.72	123.66	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	456	ARG	NE-CZ-NH1	6.72	123.66	120.30
1	D	456	ARG	NE-CZ-NH1	6.68	123.64	120.30
1	D	273	ARG	NE-CZ-NH2	-6.65	116.97	120.30
1	A	273	ARG	NE-CZ-NH2	-6.65	116.97	120.30
1	C	273	ARG	NE-CZ-NH2	-6.64	116.98	120.30
1	C	429	ARG	NE-CZ-NH2	-6.50	117.05	120.30
1	A	429	ARG	NE-CZ-NH2	-6.45	117.08	120.30
1	D	429	ARG	NE-CZ-NH2	-6.40	117.10	120.30
1	D	217	TYR	CB-CG-CD2	-6.20	117.28	121.00
1	A	217	TYR	CB-CG-CD2	-6.18	117.29	121.00
1	C	217	TYR	CB-CG-CD2	-6.18	117.29	121.00
4	G	99	TYR	CB-CG-CD2	-6.05	117.37	121.00
4	H	99	TYR	CB-CG-CD2	-6.02	117.39	121.00
4	H	38	ARG	NE-CZ-NH2	-5.98	117.31	120.30
4	G	38	ARG	NE-CZ-NH2	-5.98	117.31	120.30
4	I	99	TYR	CB-CG-CD2	-5.97	117.42	121.00
4	I	38	ARG	NE-CZ-NH2	-5.92	117.34	120.30
3	K	32	ARG	NE-CZ-NH1	5.68	123.14	120.30
3	L	32	ARG	NE-CZ-NH1	5.68	123.14	120.30
3	J	32	ARG	NE-CZ-NH1	5.67	123.14	120.30
1	A	435	TYR	CB-CG-CD2	-5.48	117.71	121.00
1	C	435	TYR	CB-CG-CD2	-5.45	117.73	121.00
1	D	435	TYR	CB-CG-CD2	-5.44	117.74	121.00
1	A	503	ARG	NE-CZ-NH2	-5.31	117.65	120.30
1	C	503	ARG	NE-CZ-NH2	-5.29	117.66	120.30
1	C	500	ARG	NE-CZ-NH2	-5.28	117.66	120.30
1	D	503	ARG	NE-CZ-NH2	-5.26	117.67	120.30
1	A	500	ARG	NE-CZ-NH2	-5.23	117.69	120.30
1	D	500	ARG	NE-CZ-NH2	-5.19	117.70	120.30
3	L	36	TYR	CB-CG-CD2	-5.19	117.89	121.00
1	C	180	ASP	CB-CG-OD1	5.19	122.97	118.30
3	J	36	TYR	CB-CG-CD2	-5.17	117.90	121.00
1	A	180	ASP	CB-CG-OD1	5.17	122.95	118.30
3	K	36	TYR	CB-CG-CD2	-5.17	117.90	121.00
2	B	643	TYR	CB-CG-CD2	-5.15	117.91	121.00
2	E	643	TYR	CB-CG-CD2	-5.13	117.92	121.00
1	D	180	ASP	CB-CG-OD1	5.13	122.92	118.30
2	F	643	TYR	CB-CG-CD2	-5.13	117.92	121.00
1	C	151	ARG	NE-CZ-NH2	-5.07	117.76	120.30

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	A	3475	0	3414	4	0
1	C	3475	0	3414	3	0
1	D	3475	0	3414	3	0
2	B	1057	0	1037	8	0
2	E	1057	0	1037	7	0
2	F	1057	0	1037	8	0
3	J	818	0	786	3	0
3	K	818	0	786	3	0
3	L	818	0	786	3	0
4	G	930	0	897	2	0
4	H	930	0	897	2	0
4	I	930	0	897	2	0
5	M	28	0	25	0	0
5	N	28	0	25	0	0
5	O	28	0	25	0	0
5	P	28	0	25	0	0
5	R	28	0	25	0	0
5	T	28	0	25	0	0
5	U	28	0	25	0	0
5	V	28	0	25	0	0
5	W	28	0	25	0	0
5	X	28	0	25	0	0
5	Z	28	0	25	0	0
5	b	28	0	25	0	0
5	c	28	0	25	0	0
5	d	28	0	25	0	0
5	e	28	0	25	0	0
5	f	28	0	25	0	0
5	h	28	0	25	0	0
5	j	28	0	25	0	0
6	Q	72	0	58	0	0
6	Y	72	0	58	0	0
6	g	72	0	58	0	0
7	S	38	0	34	0	0
7	a	38	0	34	0	0
7	i	38	0	34	0	0
8	A	168	0	156	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	B	14	0	13	0	0
8	C	168	0	156	0	0
8	D	168	0	156	0	0
8	E	14	0	13	0	0
8	F	14	0	13	0	0
All	All	20220	0	19635	42	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 1.

All (42) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:522:PHE:O	2:F:523:LEU:HD12	1.78	0.83
2:E:522:PHE:O	2:E:523:LEU:HD12	1.78	0.83
2:B:522:PHE:O	2:B:523:LEU:HD12	1.78	0.83
2:E:521:GLY:O	2:E:523:LEU:N	2.27	0.67
2:B:521:GLY:O	2:B:523:LEU:N	2.27	0.67
2:F:521:GLY:O	2:F:523:LEU:N	2.27	0.66
3:J:3:ARG:N	3:J:26:SER:HG	1.99	0.61
3:L:3:ARG:N	3:L:26:SER:HG	1.98	0.61
3:K:3:ARG:N	3:K:26:SER:HG	1.99	0.60
2:B:521:GLY:O	2:B:522:PHE:C	2.42	0.58
2:F:521:GLY:O	2:F:522:PHE:C	2.42	0.56
2:E:521:GLY:O	2:E:522:PHE:C	2.42	0.56
3:J:60:ASP:OD1	3:J:60:ASP:N	2.41	0.53
1:A:72:HIS:CG	1:A:72:HIS:O	2.62	0.52
3:L:60:ASP:OD1	3:L:60:ASP:N	2.41	0.52
1:C:72:HIS:O	1:C:72:HIS:CG	2.62	0.52
1:D:72:HIS:CG	1:D:72:HIS:O	2.62	0.51
3:K:60:ASP:OD1	3:K:60:ASP:N	2.41	0.50
3:L:3:ARG:HD2	3:L:4:MET:H	1.78	0.48
3:J:3:ARG:HD2	3:J:4:MET:H	1.78	0.48
2:E:522:PHE:C	2:E:523:LEU:HD12	2.34	0.47
3:K:3:ARG:HD2	3:K:4:MET:H	1.78	0.47
1:D:231:LYS:NZ	1:D:267:GLU:OE2	2.47	0.47
2:B:522:PHE:C	2:B:523:LEU:HD12	2.34	0.47
2:F:521:GLY:C	2:F:523:LEU:N	2.68	0.47
2:B:521:GLY:C	2:B:523:LEU:N	2.69	0.46
2:F:522:PHE:C	2:F:523:LEU:HD12	2.34	0.46
2:B:637:ASN:OD1	2:B:637:ASN:N	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:521:GLY:C	2:E:523:LEU:N	2.69	0.45
1:A:231:LYS:NZ	1:A:267:GLU:OE2	2.47	0.45
1:C:231:LYS:NZ	1:C:267:GLU:OE2	2.47	0.45
2:F:637:ASN:OD1	2:F:637:ASN:N	2.49	0.44
1:C:491:ILE:HG13	2:E:522:PHE:CZ	2.54	0.43
1:D:491:ILE:HG13	2:F:522:PHE:CZ	2.54	0.43
1:A:491:ILE:HG13	2:B:522:PHE:CZ	2.54	0.43
2:B:664:ASP:OD2	4:I:58:ARG:NH2	2.54	0.40
4:H:82(A):ASN:O	4:H:82(B):SER:C	2.59	0.40
1:A:197:ASN:OD1	1:A:197:ASN:N	2.52	0.40
4:G:58:ARG:NH2	2:F:664:ASP:OD2	2.54	0.40
4:I:82(A):ASN:O	4:I:82(B):SER:C	2.59	0.40
4:H:58:ARG:NH2	2:E:664:ASP:OD2	2.54	0.40
4:G:82(A):ASN:O	4:G:82(B):SER:C	2.59	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	433/475 (91%)	413 (95%)	17 (4%)	3 (1%)	22	59
1	C	433/475 (91%)	413 (95%)	17 (4%)	3 (1%)	22	59
1	D	433/475 (91%)	413 (95%)	17 (4%)	3 (1%)	22	59
2	B	128/153 (84%)	119 (93%)	6 (5%)	3 (2%)	6	36
2	E	128/153 (84%)	119 (93%)	6 (5%)	3 (2%)	6	36
2	F	128/153 (84%)	119 (93%)	6 (5%)	3 (2%)	6	36
3	J	103/107 (96%)	100 (97%)	3 (3%)	0	100	100
3	K	103/107 (96%)	100 (97%)	3 (3%)	0	100	100
3	L	103/107 (96%)	100 (97%)	3 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
4	G	118/121 (98%)	116 (98%)	2 (2%)	0	100 100
4	H	118/121 (98%)	116 (98%)	2 (2%)	0	100 100
4	I	118/121 (98%)	116 (98%)	2 (2%)	0	100 100
All	All	2346/2568 (91%)	2244 (96%)	84 (4%)	18 (1%)	24 56

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	636	SER
2	E	636	SER
2	F	636	SER
1	A	267	GLU
1	A	340	GLU
2	B	522	PHE
1	C	267	GLU
1	C	340	GLU
2	E	522	PHE
1	D	267	GLU
1	D	340	GLU
2	F	522	PHE
2	B	521	GLY
2	E	521	GLY
2	F	521	GLY
1	A	277	ILE
1	C	277	ILE
1	D	277	ILE

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 PDB entries followed by that with respect to all EM entries.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	394/424 (93%)	393 (100%)	1 (0%)	92 96
1	C	394/424 (93%)	393 (100%)	1 (0%)	92 96
1	D	394/424 (93%)	393 (100%)	1 (0%)	92 96

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	B	115/130 (88%)	111 (96%)	4 (4%)	36 63
2	E	115/130 (88%)	111 (96%)	4 (4%)	36 63
2	F	115/130 (88%)	111 (96%)	4 (4%)	36 63
3	J	91/92 (99%)	90 (99%)	1 (1%)	73 85
3	K	91/92 (99%)	90 (99%)	1 (1%)	73 85
3	L	91/92 (99%)	90 (99%)	1 (1%)	73 85
4	G	103/104 (99%)	103 (100%)	0	100 100
4	H	103/104 (99%)	103 (100%)	0	100 100
4	I	103/104 (99%)	103 (100%)	0	100 100
All	All	2109/2250 (94%)	2091 (99%)	18 (1%)	79 88

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	133	ASN
2	B	545	LEU
2	B	637	ASN
2	B	658	GLN
2	B	659	ASP
3	L	3	ARG
1	C	133	ASN
2	E	545	LEU
2	E	637	ASN
2	E	658	GLN
2	E	659	ASP
3	J	3	ARG
1	D	133	ASN
2	F	545	LEU
2	F	637	ASN
2	F	658	GLN
2	F	659	ASP
3	K	3	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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

63 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	$\#\|Z\| > 2$
5	NAG	M	1	5,1	14,14,15	0.82	0	17,19,21	1.23	1 (5%)
5	NAG	M	2	5	14,14,15	0.80	0	17,19,21	0.93	1 (5%)
5	NAG	N	1	5,1	14,14,15	0.77	0	17,19,21	0.92	0
5	NAG	N	2	5	14,14,15	0.76	0	17,19,21	0.98	1 (5%)
5	NAG	O	1	5,1	14,14,15	0.84	0	17,19,21	1.38	3 (17%)
5	NAG	O	2	5	14,14,15	0.83	0	17,19,21	0.90	1 (5%)
5	NAG	P	1	5,1	14,14,15	0.76	0	17,19,21	0.94	1 (5%)
5	NAG	P	2	5	14,14,15	0.81	0	17,19,21	1.26	2 (11%)
6	NAG	Q	1	6,1	14,14,15	0.81	0	17,19,21	1.29	3 (17%)
6	NAG	Q	2	6	14,14,15	0.79	0	17,19,21	1.22	2 (11%)
6	BMA	Q	3	6	11,11,12	1.84	2 (18%)	15,15,17	1.20	2 (13%)
6	MAN	Q	4	6	11,11,12	1.51	1 (9%)	15,15,17	1.02	1 (6%)
6	MAN	Q	5	6	11,11,12	1.86	3 (27%)	15,15,17	1.13	3 (20%)
6	MAN	Q	6	6	11,11,12	1.84	2 (18%)	15,15,17	1.08	2 (13%)
5	NAG	R	1	5,1	14,14,15	0.76	0	17,19,21	0.85	1 (5%)
5	NAG	R	2	5	14,14,15	0.83	0	17,19,21	0.89	1 (5%)
7	NAG	S	1	2,7	14,14,15	0.79	0	17,19,21	0.97	1 (5%)
7	NAG	S	2	7	14,14,15	0.86	0	17,19,21	0.94	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
7	FUC	S	3	7	10,10,11	0.86	0	14,14,16	1.50	4 (28%)
5	NAG	T	1	2,5	14,14,15	0.88	1 (7%)	17,19,21	1.04	1 (5%)
5	NAG	T	2	5	14,14,15	0.82	0	17,19,21	0.97	1 (5%)
5	NAG	U	1	5,1	14,14,15	0.82	0	17,19,21	1.23	1 (5%)
5	NAG	U	2	5	14,14,15	0.81	0	17,19,21	0.93	1 (5%)
5	NAG	V	1	5,1	14,14,15	0.77	0	17,19,21	0.92	0
5	NAG	V	2	5	14,14,15	0.77	0	17,19,21	0.97	1 (5%)
5	NAG	W	1	5,1	14,14,15	0.84	0	17,19,21	1.38	3 (17%)
5	NAG	W	2	5	14,14,15	0.83	0	17,19,21	0.90	1 (5%)
5	NAG	X	1	5,1	14,14,15	0.77	0	17,19,21	0.95	1 (5%)
5	NAG	X	2	5	14,14,15	0.81	0	17,19,21	1.26	2 (11%)
6	NAG	Y	1	6,1	14,14,15	0.81	0	17,19,21	1.29	3 (17%)
6	NAG	Y	2	6	14,14,15	0.79	0	17,19,21	1.22	2 (11%)
6	BMA	Y	3	6	11,11,12	1.84	2 (18%)	15,15,17	1.20	2 (13%)
6	MAN	Y	4	6	11,11,12	1.51	1 (9%)	15,15,17	1.01	1 (6%)
6	MAN	Y	5	6	11,11,12	1.85	3 (27%)	15,15,17	1.14	3 (20%)
6	MAN	Y	6	6	11,11,12	1.84	2 (18%)	15,15,17	1.08	2 (13%)
5	NAG	Z	1	5,1	14,14,15	0.76	0	17,19,21	0.85	1 (5%)
5	NAG	Z	2	5	14,14,15	0.83	0	17,19,21	0.89	1 (5%)
7	NAG	a	1	2,7	14,14,15	0.79	0	17,19,21	0.98	1 (5%)
7	NAG	a	2	7	14,14,15	0.87	0	17,19,21	0.94	1 (5%)
7	FUC	a	3	7	10,10,11	0.86	0	14,14,16	1.50	4 (28%)
5	NAG	b	1	2,5	14,14,15	0.88	1 (7%)	17,19,21	1.04	1 (5%)
5	NAG	b	2	5	14,14,15	0.81	0	17,19,21	0.97	1 (5%)
5	NAG	c	1	5,1	14,14,15	0.82	0	17,19,21	1.23	1 (5%)
5	NAG	c	2	5	14,14,15	0.80	0	17,19,21	0.93	1 (5%)
5	NAG	d	1	5,1	14,14,15	0.76	0	17,19,21	0.92	0
5	NAG	d	2	5	14,14,15	0.76	0	17,19,21	0.98	1 (5%)
5	NAG	e	1	5,1	14,14,15	0.84	0	17,19,21	1.38	3 (17%)
5	NAG	e	2	5	14,14,15	0.83	0	17,19,21	0.89	1 (5%)
5	NAG	f	1	5,1	14,14,15	0.76	0	17,19,21	0.94	1 (5%)
5	NAG	f	2	5	14,14,15	0.80	0	17,19,21	1.26	2 (11%)
6	NAG	g	1	6,1	14,14,15	0.81	0	17,19,21	1.29	3 (17%)
6	NAG	g	2	6	14,14,15	0.78	0	17,19,21	1.22	2 (11%)
6	BMA	g	3	6	11,11,12	1.84	2 (18%)	15,15,17	1.20	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	MAN	g	4	6	11,11,12	1.50	1 (9%)	15,15,17	1.02	1 (6%)
6	MAN	g	5	6	11,11,12	1.86	3 (27%)	15,15,17	1.13	3 (20%)
6	MAN	g	6	6	11,11,12	1.85	2 (18%)	15,15,17	1.09	2 (13%)
5	NAG	h	1	5,1	14,14,15	0.76	0	17,19,21	0.85	1 (5%)
5	NAG	h	2	5	14,14,15	0.84	0	17,19,21	0.89	1 (5%)
7	NAG	i	1	2,7	14,14,15	0.79	0	17,19,21	0.97	1 (5%)
7	NAG	i	2	7	14,14,15	0.86	0	17,19,21	0.94	1 (5%)
7	FUC	i	3	7	10,10,11	0.86	0	14,14,16	1.50	4 (28%)
5	NAG	j	1	2,5	14,14,15	0.89	1 (7%)	17,19,21	1.04	1 (5%)
5	NAG	j	2	5	14,14,15	0.81	0	17,19,21	0.97	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
5	NAG	M	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	M	2	5	-	2/6/23/26	0/1/1/1
5	NAG	N	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	N	2	5	-	1/6/23/26	0/1/1/1
5	NAG	O	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	O	2	5	-	1/6/23/26	0/1/1/1
5	NAG	P	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	P	2	5	-	2/6/23/26	0/1/1/1
6	NAG	Q	1	6,1	-	2/6/23/26	0/1/1/1
6	NAG	Q	2	6	-	0/6/23/26	0/1/1/1
6	BMA	Q	3	6	-	2/2/19/22	0/1/1/1
6	MAN	Q	4	6	-	1/2/19/22	0/1/1/1
6	MAN	Q	5	6	-	1/2/19/22	0/1/1/1
6	MAN	Q	6	6	-	1/2/19/22	0/1/1/1
5	NAG	R	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	R	2	5	-	2/6/23/26	0/1/1/1
7	NAG	S	1	2,7	-	0/6/23/26	0/1/1/1
7	NAG	S	2	7	-	2/6/23/26	0/1/1/1
7	FUC	S	3	7	-	-	0/1/1/1
5	NAG	T	1	2,5	-	0/6/23/26	0/1/1/1
5	NAG	T	2	5	-	1/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	U	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	U	2	5	-	2/6/23/26	0/1/1/1
5	NAG	V	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	V	2	5	-	1/6/23/26	0/1/1/1
5	NAG	W	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	W	2	5	-	1/6/23/26	0/1/1/1
5	NAG	X	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	X	2	5	-	2/6/23/26	0/1/1/1
6	NAG	Y	1	6,1	-	2/6/23/26	0/1/1/1
6	NAG	Y	2	6	-	0/6/23/26	0/1/1/1
6	BMA	Y	3	6	-	2/2/19/22	0/1/1/1
6	MAN	Y	4	6	-	1/2/19/22	0/1/1/1
6	MAN	Y	5	6	-	1/2/19/22	0/1/1/1
6	MAN	Y	6	6	-	1/2/19/22	0/1/1/1
5	NAG	Z	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	Z	2	5	-	2/6/23/26	0/1/1/1
7	NAG	a	1	2,7	-	0/6/23/26	0/1/1/1
7	NAG	a	2	7	-	2/6/23/26	0/1/1/1
7	FUC	a	3	7	-	-	0/1/1/1
5	NAG	b	1	2,5	-	0/6/23/26	0/1/1/1
5	NAG	b	2	5	-	1/6/23/26	0/1/1/1
5	NAG	c	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	c	2	5	-	2/6/23/26	0/1/1/1
5	NAG	d	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	d	2	5	-	1/6/23/26	0/1/1/1
5	NAG	e	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	e	2	5	-	1/6/23/26	0/1/1/1
5	NAG	f	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	f	2	5	-	2/6/23/26	0/1/1/1
6	NAG	g	1	6,1	-	2/6/23/26	0/1/1/1
6	NAG	g	2	6	-	0/6/23/26	0/1/1/1
6	BMA	g	3	6	-	2/2/19/22	0/1/1/1
6	MAN	g	4	6	-	1/2/19/22	0/1/1/1
6	MAN	g	5	6	-	1/2/19/22	0/1/1/1
6	MAN	g	6	6	-	1/2/19/22	0/1/1/1
5	NAG	h	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	h	2	5	-	2/6/23/26	0/1/1/1
7	NAG	i	1	2,7	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	i	2	7	-	2/6/23/26	0/1/1/1
7	FUC	i	3	7	-	-	0/1/1/1
5	NAG	j	1	2,5	-	0/6/23/26	0/1/1/1
5	NAG	j	2	5	-	1/6/23/26	0/1/1/1

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	g	6	MAN	O2-C2	-4.19	1.34	1.43
6	Q	6	MAN	O2-C2	-4.18	1.34	1.43
6	Y	6	MAN	O2-C2	-4.14	1.34	1.43
6	g	3	BMA	O2-C2	-4.13	1.34	1.43
6	Y	3	BMA	O2-C2	-4.12	1.34	1.43
6	Q	3	BMA	O2-C2	-4.12	1.34	1.43
6	g	5	MAN	O2-C2	-4.11	1.34	1.43
6	Q	5	MAN	O2-C2	-4.09	1.34	1.43
6	Y	5	MAN	O2-C2	-4.07	1.34	1.43
6	Q	4	MAN	O2-C2	-2.93	1.37	1.43
6	Y	4	MAN	O2-C2	-2.92	1.37	1.43
6	g	4	MAN	O2-C2	-2.91	1.37	1.43
6	Y	3	BMA	C2-C3	-2.35	1.49	1.52
6	Q	3	BMA	C2-C3	-2.35	1.49	1.52
6	g	3	BMA	C2-C3	-2.33	1.49	1.52
6	g	6	MAN	C2-C3	-2.27	1.49	1.52
6	Q	6	MAN	C2-C3	-2.24	1.49	1.52
6	Y	6	MAN	C2-C3	-2.24	1.49	1.52
6	Y	5	MAN	C2-C3	-2.15	1.49	1.52
6	g	5	MAN	C2-C3	-2.14	1.49	1.52
6	Q	5	MAN	C2-C3	-2.14	1.49	1.52
6	g	5	MAN	O5-C1	2.13	1.47	1.43
6	Q	5	MAN	O5-C1	2.12	1.47	1.43
5	j	1	NAG	C3-C2	-2.11	1.48	1.52
6	Y	5	MAN	O5-C1	2.10	1.47	1.43
5	b	1	NAG	C3-C2	-2.10	1.48	1.52
5	T	1	NAG	C3-C2	-2.10	1.48	1.52

All (99) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	f	2	NAG	C4-C3-C2	-3.67	105.64	111.02
5	P	2	NAG	C4-C3-C2	-3.65	105.67	111.02
5	X	2	NAG	C4-C3-C2	-3.64	105.68	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	c	1	NAG	C4-C3-C2	-3.07	106.52	111.02
5	M	1	NAG	C4-C3-C2	-3.06	106.54	111.02
5	U	1	NAG	C4-C3-C2	-3.05	106.55	111.02
6	g	3	BMA	C2-C3-C4	-3.05	105.62	110.89
5	W	1	NAG	C3-C4-C5	-3.05	104.80	110.24
6	Y	3	BMA	C2-C3-C4	-3.04	105.63	110.89
5	O	1	NAG	C3-C4-C5	-3.03	104.83	110.24
6	Q	3	BMA	C2-C3-C4	-3.03	105.65	110.89
5	e	1	NAG	C3-C4-C5	-3.01	104.86	110.24
5	T	2	NAG	C4-C3-C2	-2.91	106.75	111.02
5	b	2	NAG	C4-C3-C2	-2.91	106.75	111.02
5	d	2	NAG	C4-C3-C2	-2.91	106.76	111.02
5	j	2	NAG	C4-C3-C2	-2.91	106.76	111.02
5	N	2	NAG	C4-C3-C2	-2.90	106.77	111.02
5	V	2	NAG	C4-C3-C2	-2.90	106.77	111.02
6	Y	1	NAG	C3-C4-C5	-2.81	105.23	110.24
6	Q	1	NAG	C3-C4-C5	-2.79	105.26	110.24
6	g	1	NAG	C3-C4-C5	-2.79	105.26	110.24
5	e	1	NAG	O4-C4-C3	-2.78	103.91	110.35
5	W	1	NAG	O4-C4-C3	-2.77	103.94	110.35
5	O	1	NAG	O4-C4-C3	-2.76	103.96	110.35
7	i	3	FUC	O2-C2-C1	2.73	114.74	109.15
7	a	3	FUC	O2-C2-C1	2.73	114.74	109.15
7	S	3	FUC	O2-C2-C1	2.73	114.74	109.15
6	Y	2	NAG	O5-C1-C2	-2.68	107.05	111.29
6	Q	2	NAG	O5-C1-C2	-2.68	107.05	111.29
6	g	2	NAG	O5-C1-C2	-2.68	107.06	111.29
7	S	3	FUC	C6-C5-C4	-2.62	108.23	113.07
7	a	3	FUC	C6-C5-C4	-2.62	108.23	113.07
7	i	3	FUC	C6-C5-C4	-2.61	108.25	113.07
5	M	2	NAG	C4-C3-C2	-2.59	107.22	111.02
5	c	2	NAG	C4-C3-C2	-2.59	107.22	111.02
7	i	2	NAG	C4-C3-C2	-2.58	107.23	111.02
5	U	2	NAG	C4-C3-C2	-2.58	107.23	111.02
7	S	2	NAG	C4-C3-C2	-2.58	107.24	111.02
7	a	2	NAG	C4-C3-C2	-2.57	107.25	111.02
5	W	2	NAG	C4-C3-C2	-2.54	107.29	111.02
5	O	2	NAG	C4-C3-C2	-2.54	107.30	111.02
5	W	1	NAG	O5-C5-C6	-2.54	103.22	107.20
5	O	1	NAG	O5-C5-C6	-2.53	103.24	107.20
5	e	1	NAG	O5-C5-C6	-2.53	103.24	107.20
5	e	2	NAG	C4-C3-C2	-2.53	107.31	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	Z	2	NAG	C4-C3-C2	-2.49	107.37	111.02
5	h	2	NAG	C4-C3-C2	-2.48	107.38	111.02
5	R	2	NAG	C4-C3-C2	-2.48	107.38	111.02
7	S	3	FUC	C2-C3-C4	-2.47	106.61	110.89
7	i	3	FUC	C2-C3-C4	-2.47	106.62	110.89
7	a	3	FUC	C2-C3-C4	-2.47	106.63	110.89
7	i	3	FUC	O5-C1-C2	-2.43	107.02	110.77
7	a	3	FUC	O5-C1-C2	-2.43	107.03	110.77
7	S	3	FUC	O5-C1-C2	-2.42	107.03	110.77
6	Y	1	NAG	O5-C1-C2	-2.40	107.49	111.29
6	Q	1	NAG	O5-C1-C2	-2.40	107.49	111.29
5	h	1	NAG	C3-C4-C5	-2.40	105.96	110.24
5	R	1	NAG	C3-C4-C5	-2.39	105.97	110.24
6	g	1	NAG	O5-C1-C2	-2.39	107.51	111.29
5	Z	1	NAG	C3-C4-C5	-2.39	105.97	110.24
6	Y	5	MAN	C1-C2-C3	2.35	112.56	109.67
5	f	2	NAG	O5-C1-C2	-2.34	107.59	111.29
5	P	2	NAG	O5-C1-C2	-2.34	107.60	111.29
6	Q	5	MAN	C1-C2-C3	2.33	112.53	109.67
5	X	2	NAG	O5-C1-C2	-2.32	107.63	111.29
6	Y	5	MAN	C2-C3-C4	-2.28	106.95	110.89
6	g	5	MAN	C1-C2-C3	2.28	112.47	109.67
6	Q	5	MAN	C2-C3-C4	-2.28	106.95	110.89
6	g	1	NAG	C8-C7-N2	2.27	119.95	116.10
6	Q	4	MAN	C2-C3-C4	-2.27	106.97	110.89
6	g	5	MAN	C2-C3-C4	-2.27	106.97	110.89
6	Y	4	MAN	C2-C3-C4	-2.26	106.98	110.89
6	g	4	MAN	C2-C3-C4	-2.26	106.99	110.89
6	Q	1	NAG	C8-C7-N2	2.25	119.92	116.10
6	Y	1	NAG	C8-C7-N2	2.24	119.89	116.10
7	i	1	NAG	C4-C3-C2	-2.16	107.85	111.02
7	a	1	NAG	C4-C3-C2	-2.16	107.86	111.02
7	S	1	NAG	C4-C3-C2	-2.16	107.86	111.02
6	Y	2	NAG	O5-C5-C6	-2.11	103.89	107.20
6	g	3	BMA	C1-C2-C3	2.11	112.25	109.67
6	Q	2	NAG	O5-C5-C6	-2.09	103.92	107.20
6	g	2	NAG	O5-C5-C6	-2.09	103.93	107.20
6	Y	3	BMA	C1-C2-C3	2.08	112.22	109.67
6	Q	3	BMA	C1-C2-C3	2.08	112.22	109.67
5	X	1	NAG	C3-C4-C5	-2.07	106.54	110.24
5	P	1	NAG	C3-C4-C5	-2.06	106.56	110.24
6	Q	6	MAN	C2-C3-C4	-2.06	107.33	110.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	g	6	MAN	C2-C3-C4	-2.06	107.33	110.89
5	f	1	NAG	C3-C4-C5	-2.06	106.57	110.24
6	Y	6	MAN	C2-C3-C4	-2.05	107.35	110.89
6	Q	6	MAN	O5-C1-C2	-2.04	107.62	110.77
6	g	6	MAN	O5-C1-C2	-2.03	107.63	110.77
5	b	1	NAG	O5-C1-C2	-2.03	108.09	111.29
5	j	1	NAG	O5-C1-C2	-2.02	108.09	111.29
6	Y	5	MAN	O5-C1-C2	-2.02	107.65	110.77
5	T	1	NAG	O5-C1-C2	-2.02	108.10	111.29
6	Y	6	MAN	O5-C1-C2	-2.02	107.66	110.77
6	Q	5	MAN	O5-C1-C2	-2.01	107.67	110.77
6	g	5	MAN	O5-C1-C2	-2.01	107.67	110.77

There are no chirality outliers.

All (72) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	P	1	NAG	O5-C5-C6-O6
5	X	1	NAG	O5-C5-C6-O6
5	f	1	NAG	O5-C5-C6-O6
5	P	2	NAG	C4-C5-C6-O6
5	X	2	NAG	C4-C5-C6-O6
5	f	2	NAG	C4-C5-C6-O6
6	Q	3	BMA	C4-C5-C6-O6
6	Y	3	BMA	C4-C5-C6-O6
6	g	3	BMA	C4-C5-C6-O6
5	d	1	NAG	O5-C5-C6-O6
7	S	2	NAG	O5-C5-C6-O6
7	a	2	NAG	O5-C5-C6-O6
7	i	2	NAG	O5-C5-C6-O6
5	M	1	NAG	O5-C5-C6-O6
5	N	1	NAG	O5-C5-C6-O6
5	U	1	NAG	O5-C5-C6-O6
5	V	1	NAG	O5-C5-C6-O6
5	c	1	NAG	O5-C5-C6-O6
5	P	1	NAG	C4-C5-C6-O6
5	X	1	NAG	C4-C5-C6-O6
5	f	1	NAG	C4-C5-C6-O6
5	M	2	NAG	O5-C5-C6-O6
5	U	2	NAG	O5-C5-C6-O6
5	c	2	NAG	O5-C5-C6-O6
5	P	2	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
5	R	2	NAG	O5-C5-C6-O6
5	X	2	NAG	O5-C5-C6-O6
5	Z	2	NAG	O5-C5-C6-O6
5	f	2	NAG	O5-C5-C6-O6
5	h	2	NAG	O5-C5-C6-O6
6	Q	3	BMA	O5-C5-C6-O6
6	Y	3	BMA	O5-C5-C6-O6
6	g	3	BMA	O5-C5-C6-O6
5	N	1	NAG	C4-C5-C6-O6
5	d	1	NAG	C4-C5-C6-O6
5	M	1	NAG	C4-C5-C6-O6
5	U	1	NAG	C4-C5-C6-O6
5	V	1	NAG	C4-C5-C6-O6
5	c	1	NAG	C4-C5-C6-O6
6	Q	1	NAG	C8-C7-N2-C2
6	Q	1	NAG	O7-C7-N2-C2
6	Y	1	NAG	C8-C7-N2-C2
6	Y	1	NAG	O7-C7-N2-C2
6	g	1	NAG	C8-C7-N2-C2
6	g	1	NAG	O7-C7-N2-C2
5	N	2	NAG	O5-C5-C6-O6
5	V	2	NAG	O5-C5-C6-O6
5	d	2	NAG	O5-C5-C6-O6
6	Q	4	MAN	O5-C5-C6-O6
6	Y	4	MAN	O5-C5-C6-O6
6	g	4	MAN	O5-C5-C6-O6
6	Q	5	MAN	O5-C5-C6-O6
6	Y	5	MAN	O5-C5-C6-O6
6	g	5	MAN	O5-C5-C6-O6
5	T	2	NAG	O5-C5-C6-O6
5	b	2	NAG	O5-C5-C6-O6
5	j	2	NAG	O5-C5-C6-O6
7	S	2	NAG	C4-C5-C6-O6
7	a	2	NAG	C4-C5-C6-O6
7	i	2	NAG	C4-C5-C6-O6
6	Q	6	MAN	O5-C5-C6-O6
6	Y	6	MAN	O5-C5-C6-O6
6	g	6	MAN	O5-C5-C6-O6
5	e	2	NAG	O5-C5-C6-O6
5	O	2	NAG	O5-C5-C6-O6
5	W	2	NAG	O5-C5-C6-O6
5	R	2	NAG	C4-C5-C6-O6

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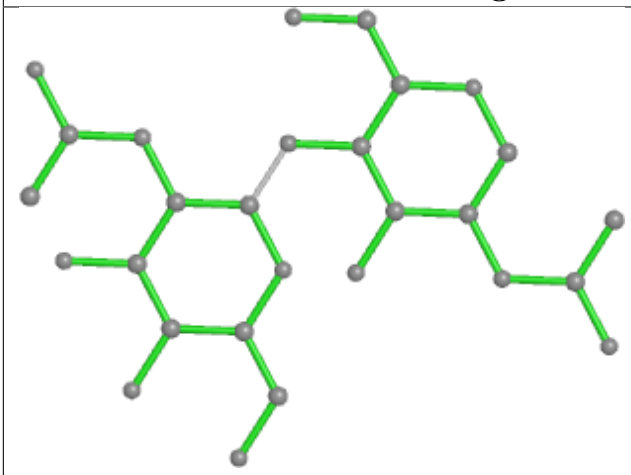
Mol	Chain	Res	Type	Atoms
5	Z	2	NAG	C4-C5-C6-O6
5	h	2	NAG	C4-C5-C6-O6
5	U	2	NAG	C4-C5-C6-O6
5	M	2	NAG	C4-C5-C6-O6
5	c	2	NAG	C4-C5-C6-O6

There are no ring outliers.

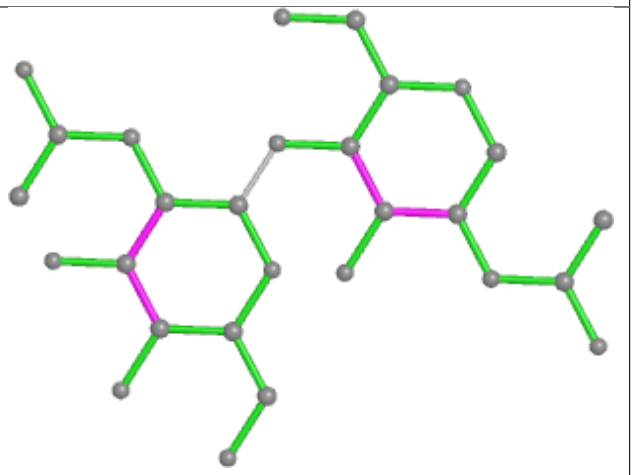
No monomer is involved in short contacts.

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

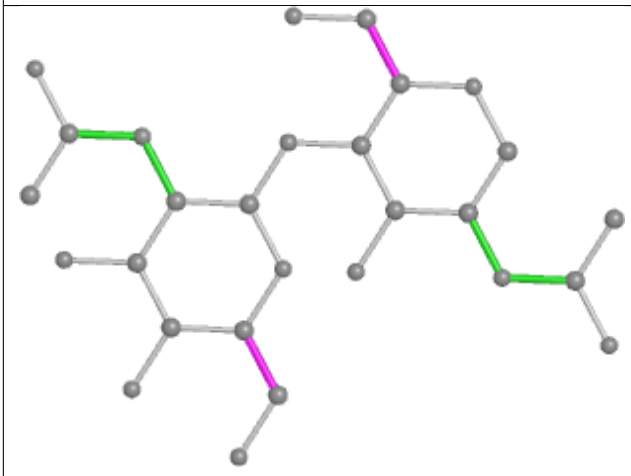
Oligosaccharide Chain M



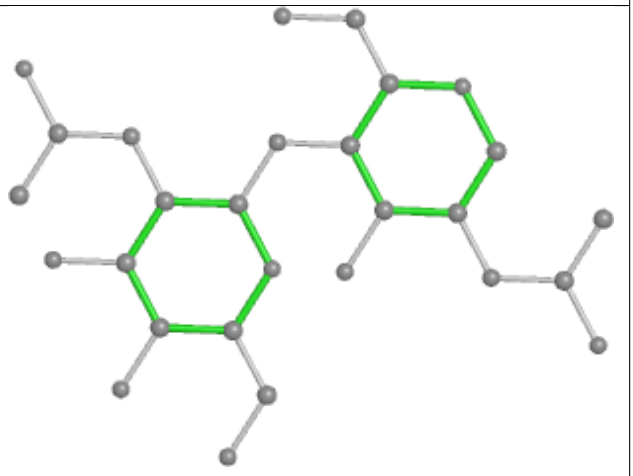
Bond lengths



Bond angles

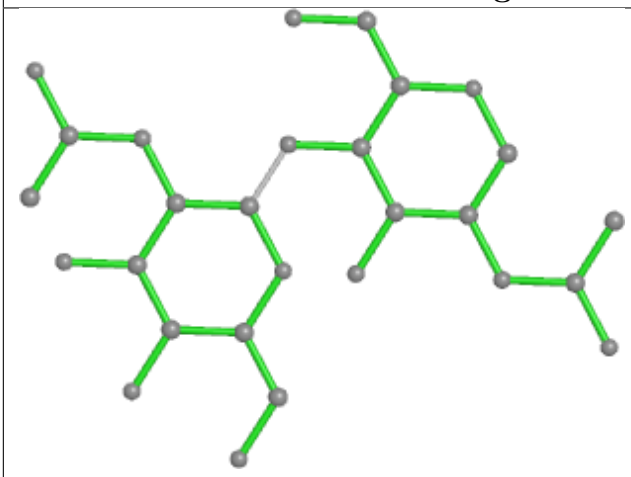


Torsions

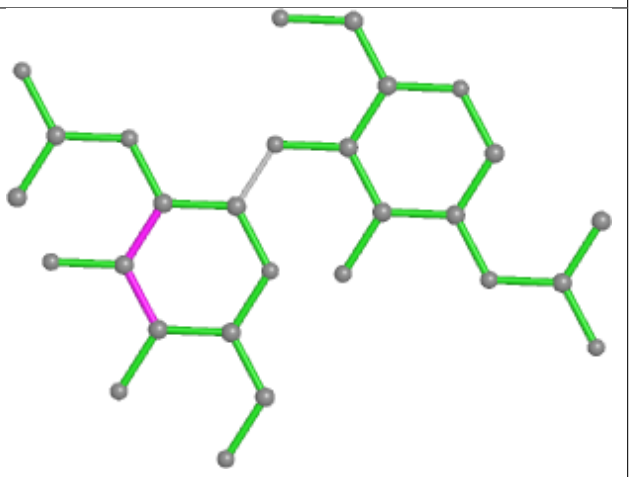


Rings

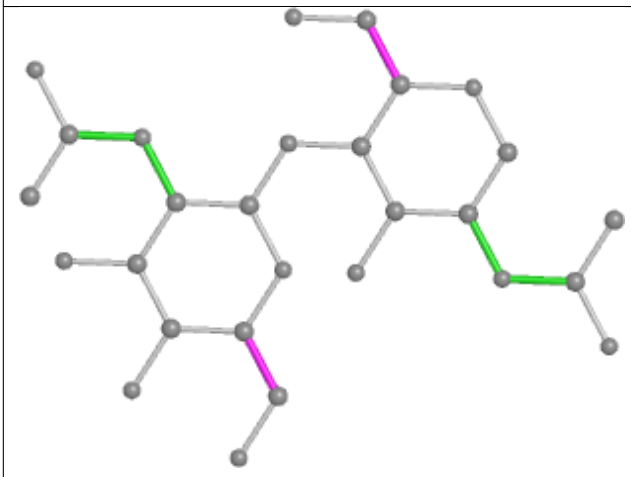
Oligosaccharide Chain N



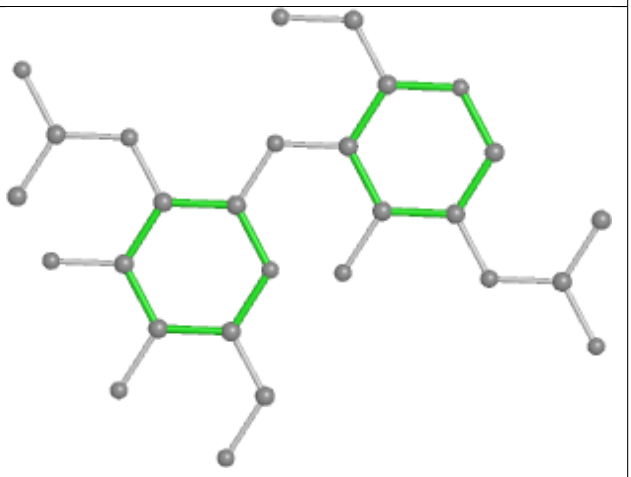
Bond lengths



Bond angles

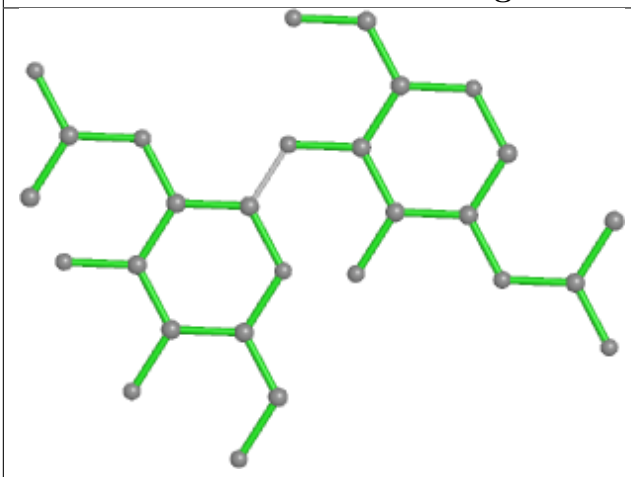


Torsions

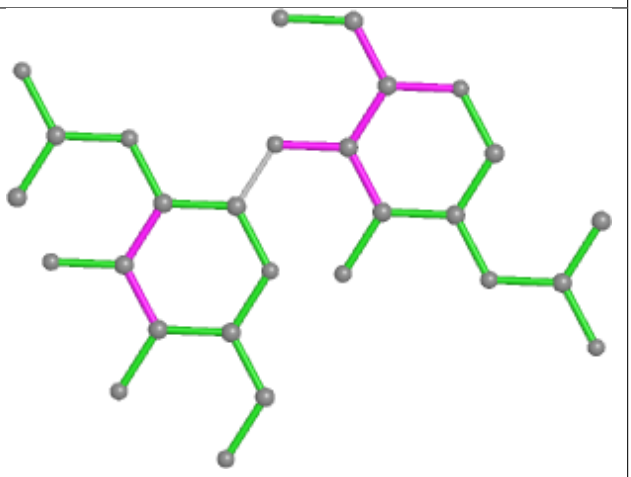


Rings

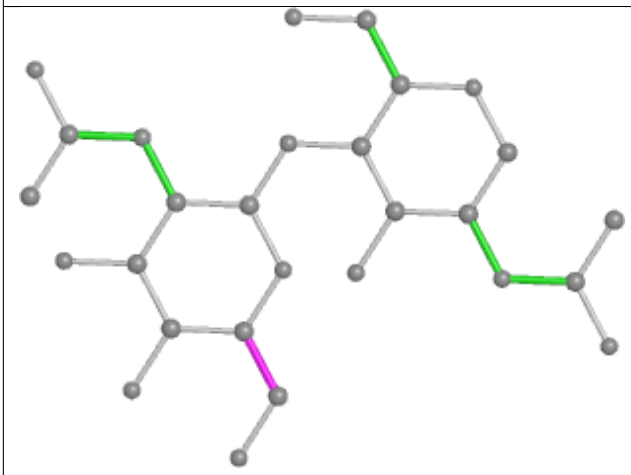
Oligosaccharide Chain O



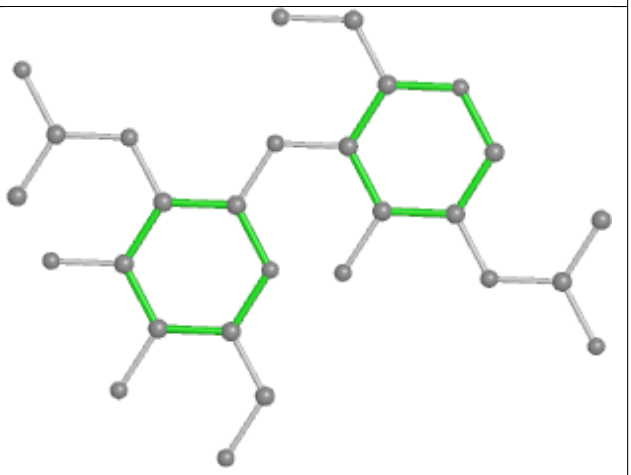
Bond lengths



Bond angles

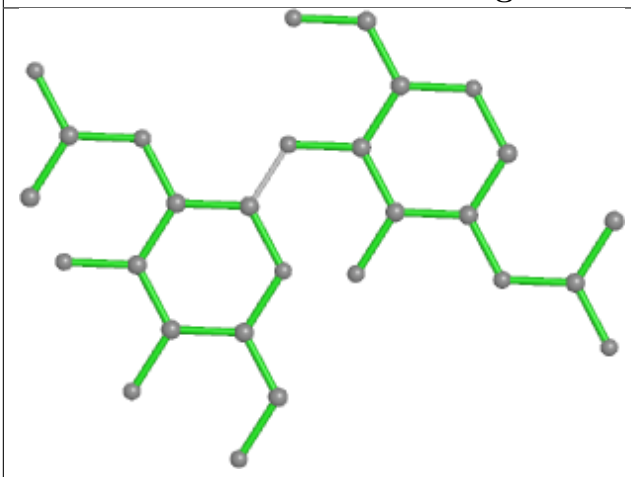


Torsions

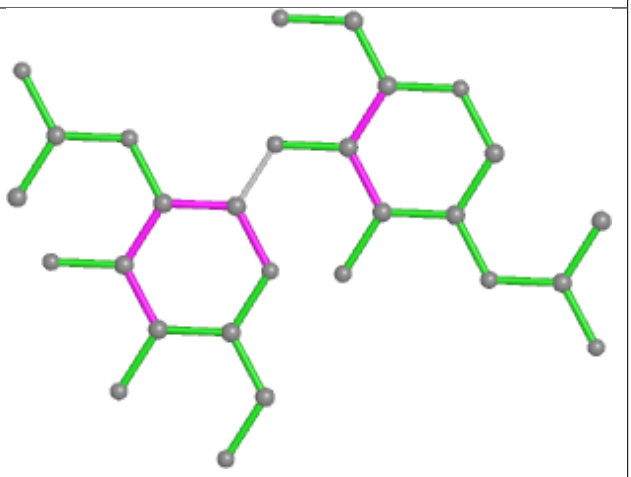


Rings

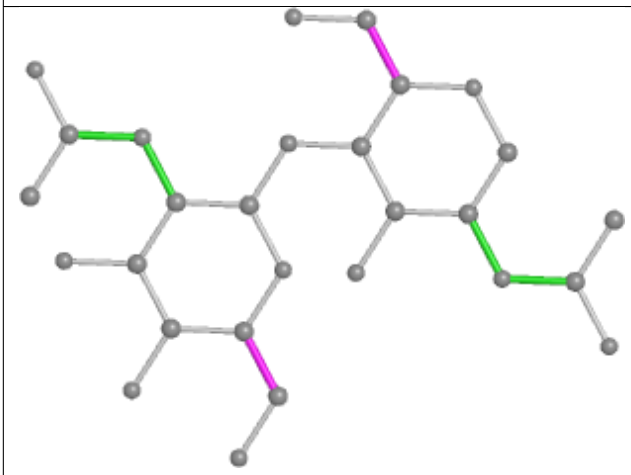
Oligosaccharide Chain P



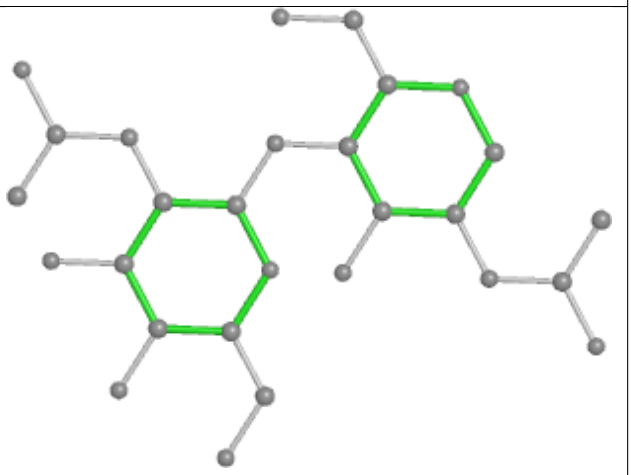
Bond lengths



Bond angles

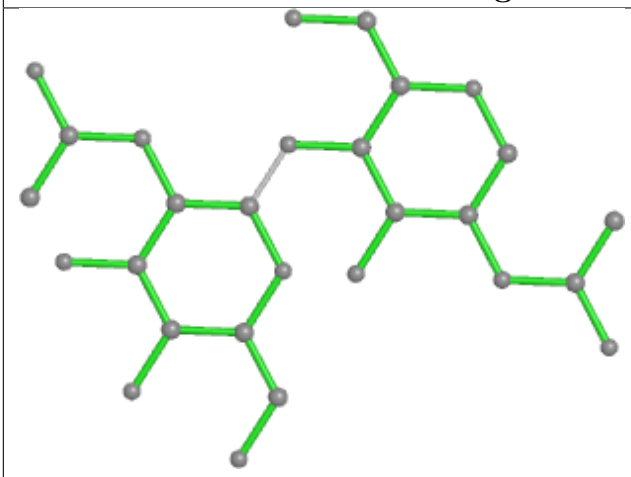


Torsions

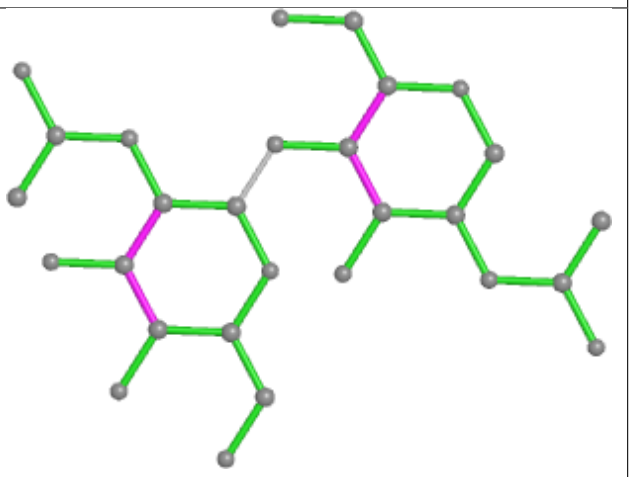


Rings

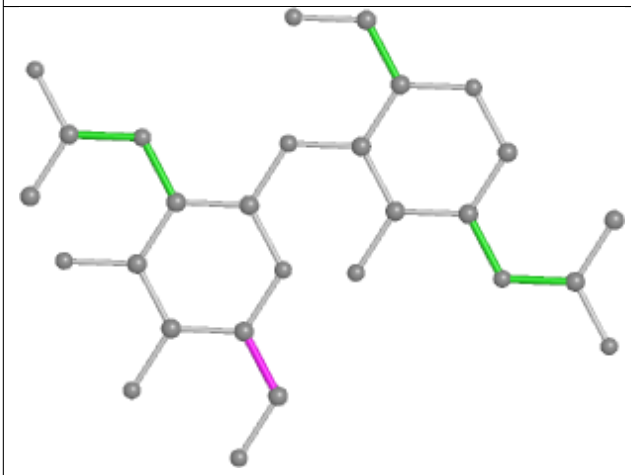
Oligosaccharide Chain R



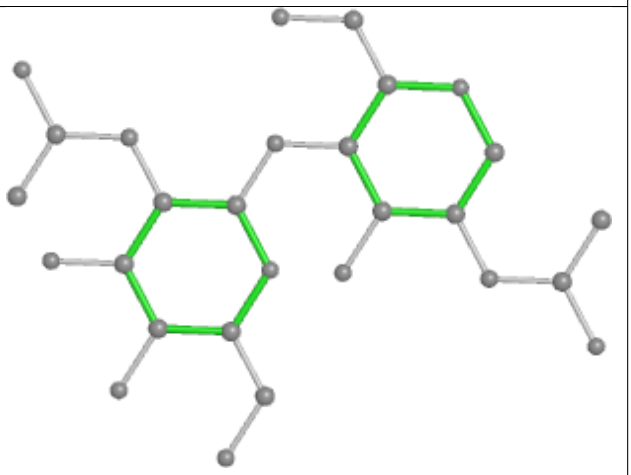
Bond lengths



Bond angles

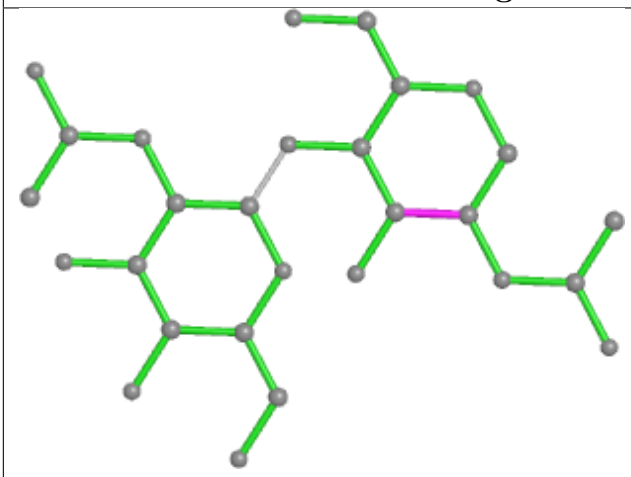


Torsions



Rings

Oligosaccharide Chain T



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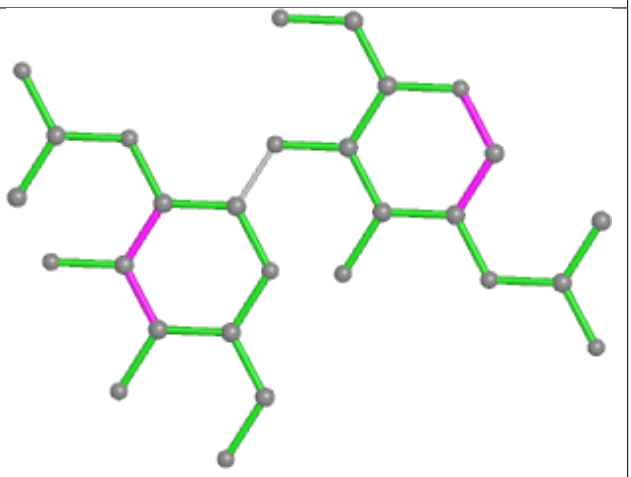
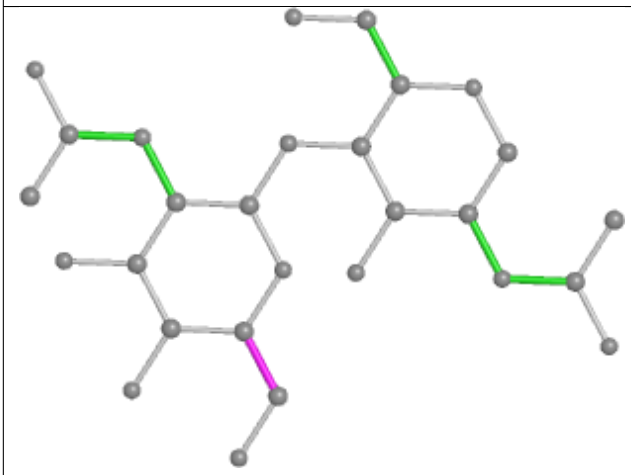


Bond angles



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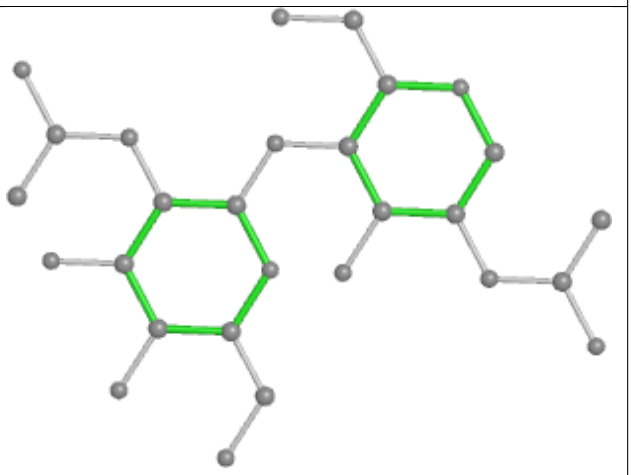
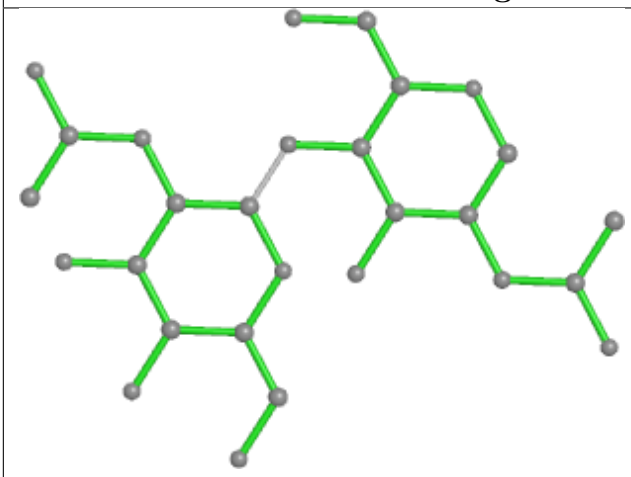


Rings

Oligosaccharide Chain U



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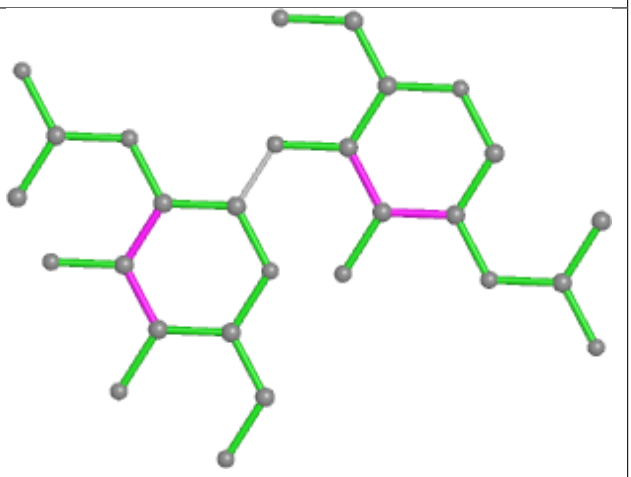
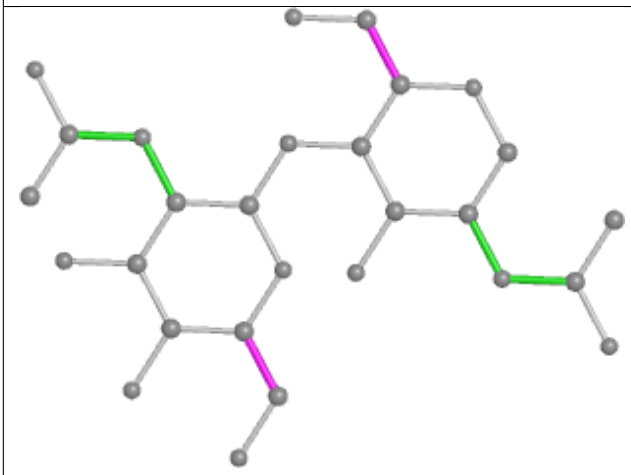


Bond angles



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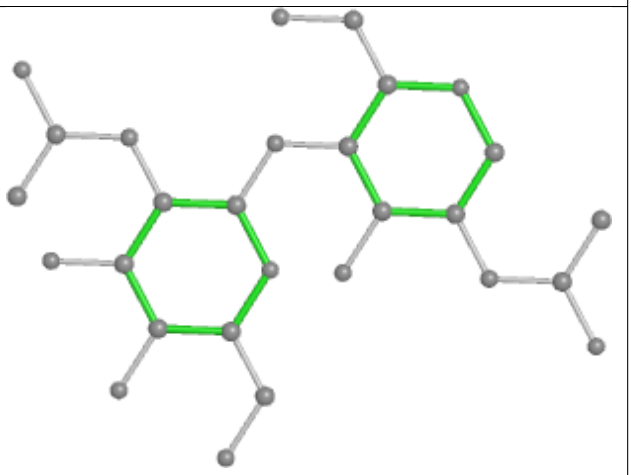
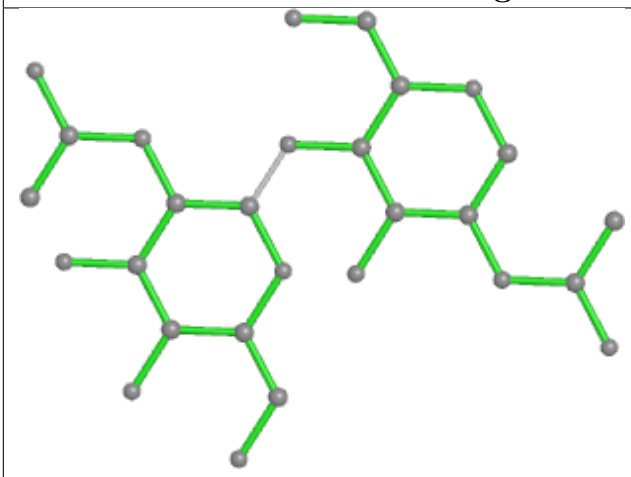


Rings

Oligosaccharide Chain V



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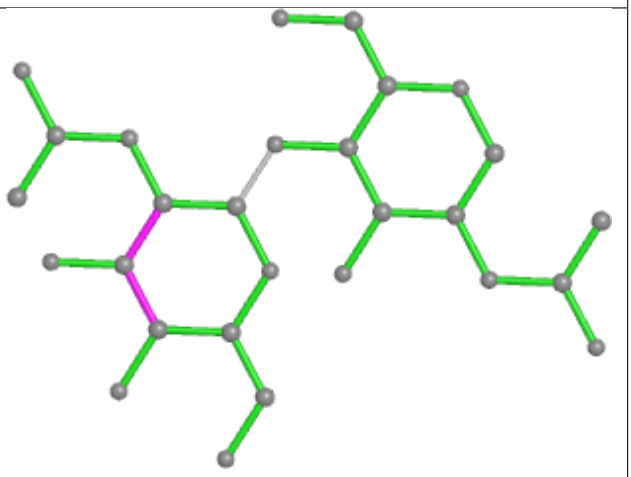
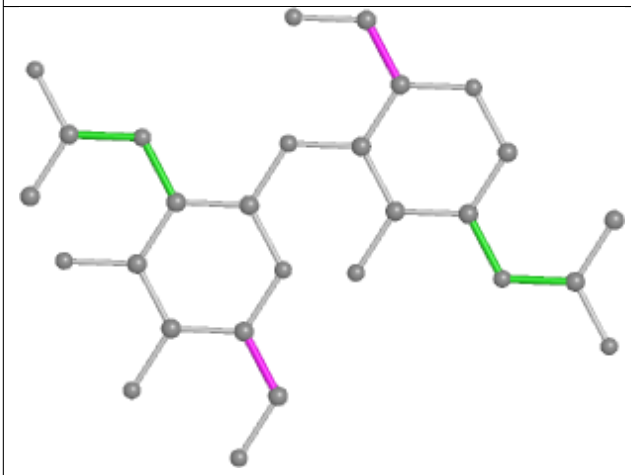


Bond angles



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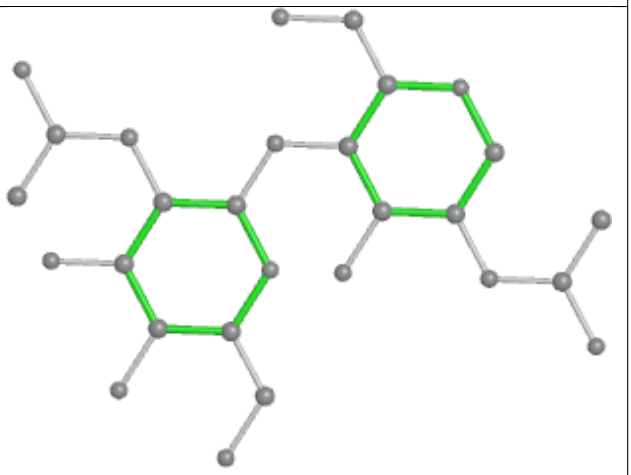
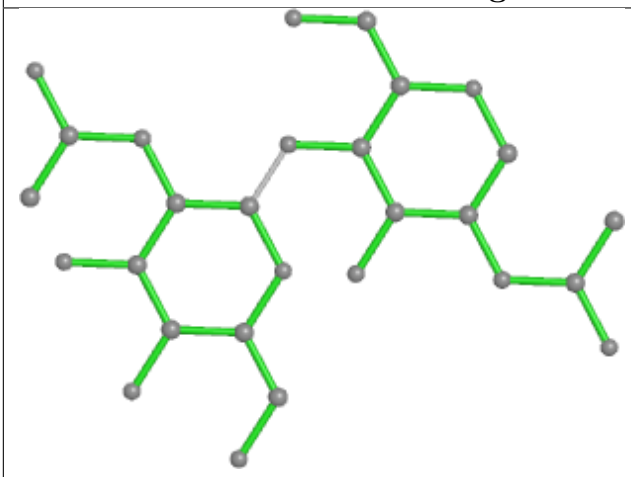


Rings

Oligosaccharide Chain W



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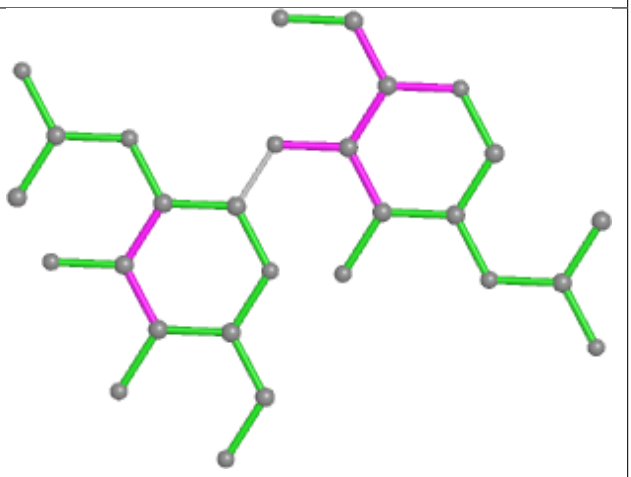
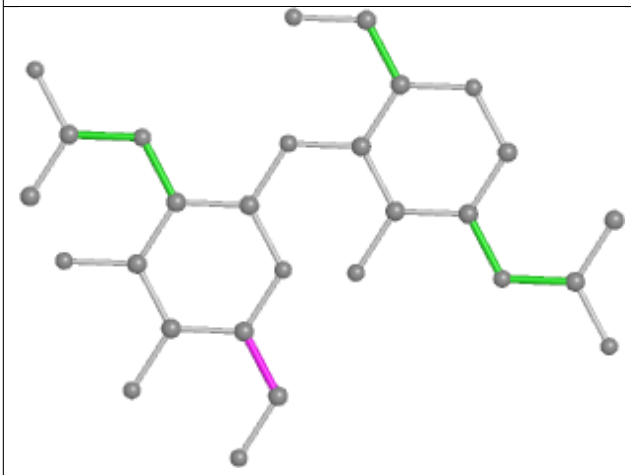


Bond angles



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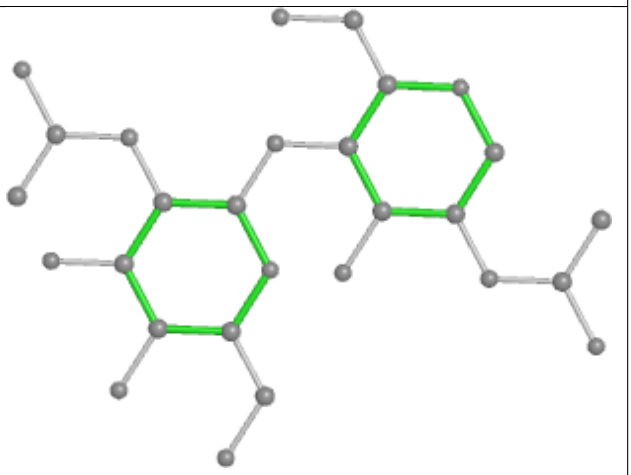
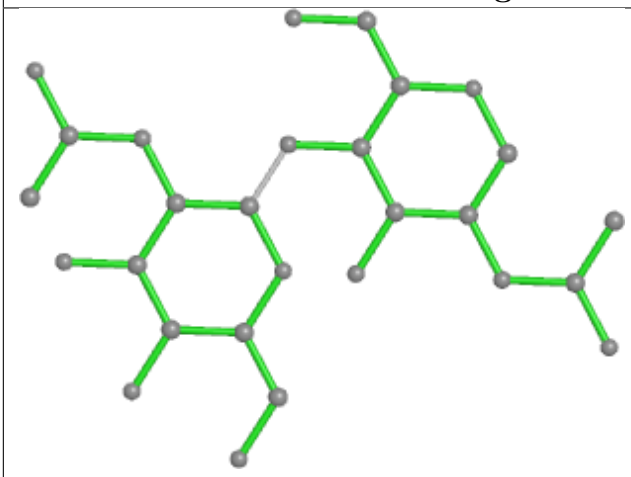


Rings

Oligosaccharide Chain X



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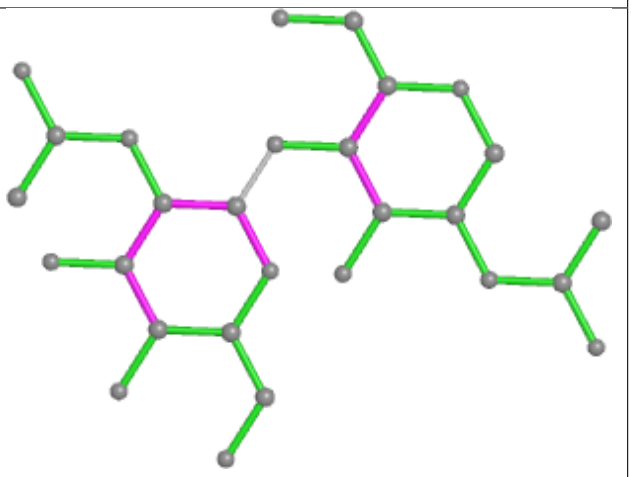
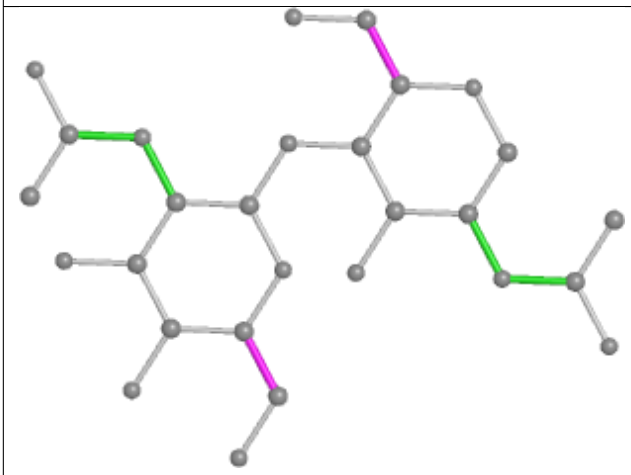


Bond angles



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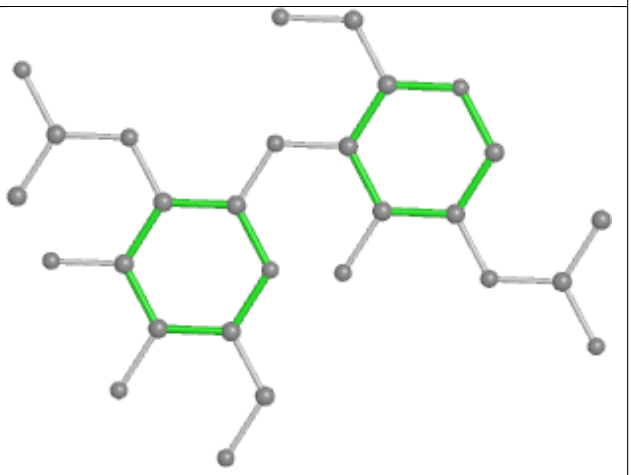
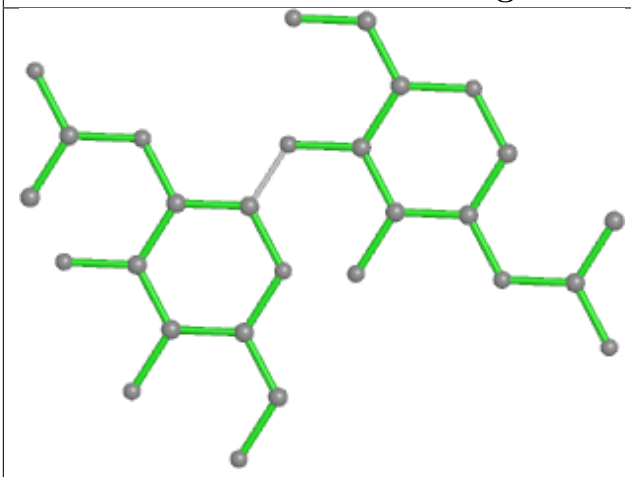


Rings

Oligosaccharide Chain Z



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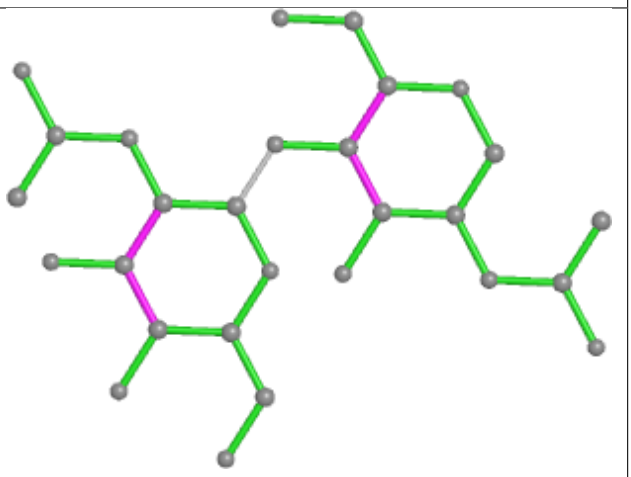

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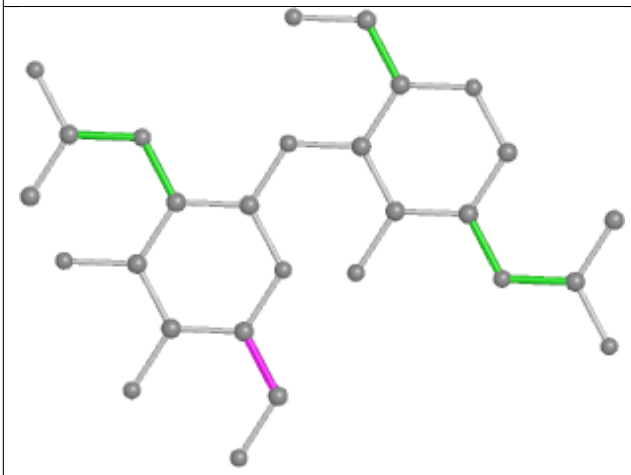

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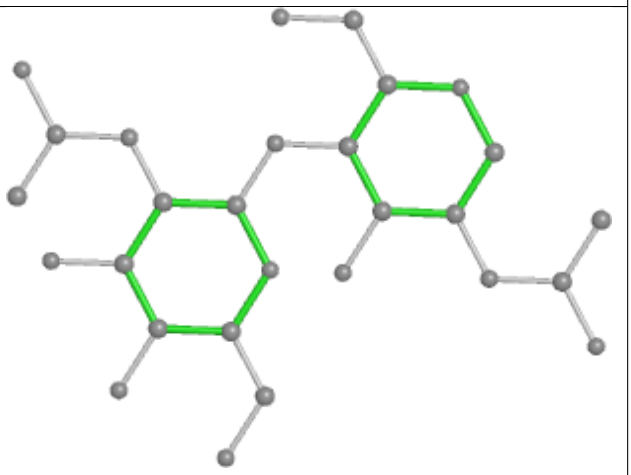
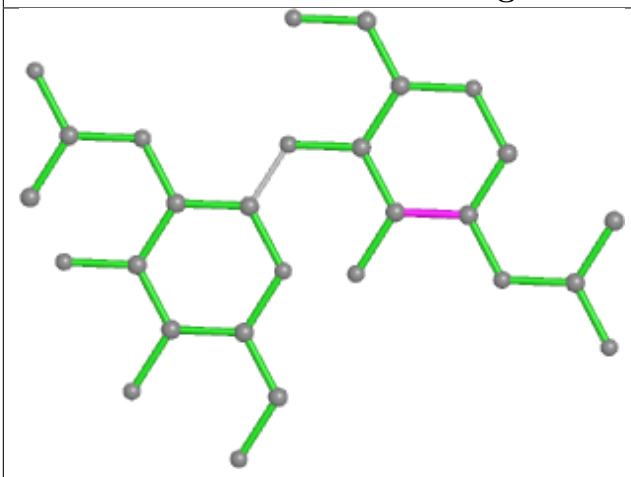


Rings

Oligosaccharide Chain b



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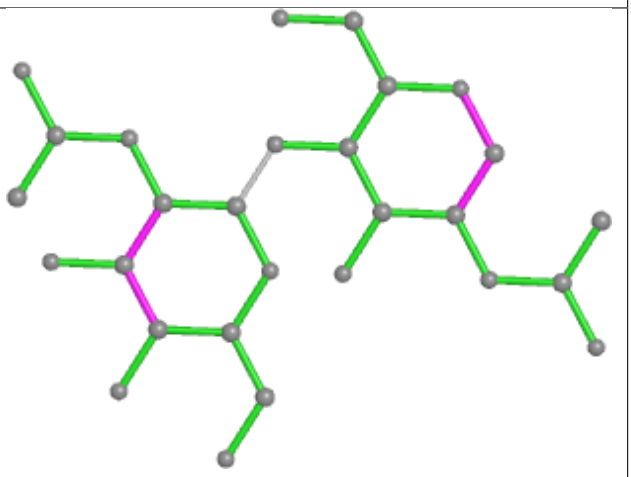

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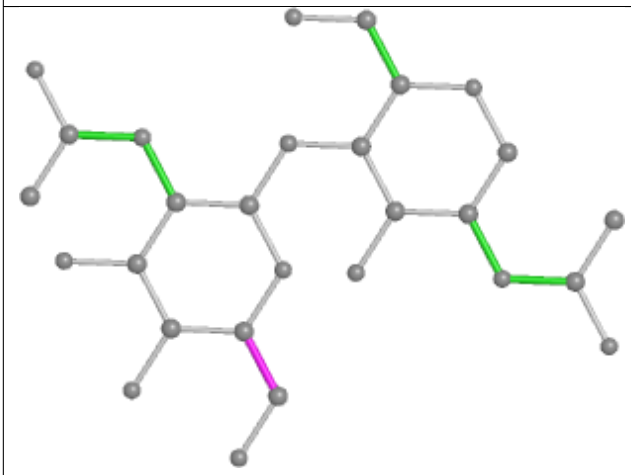

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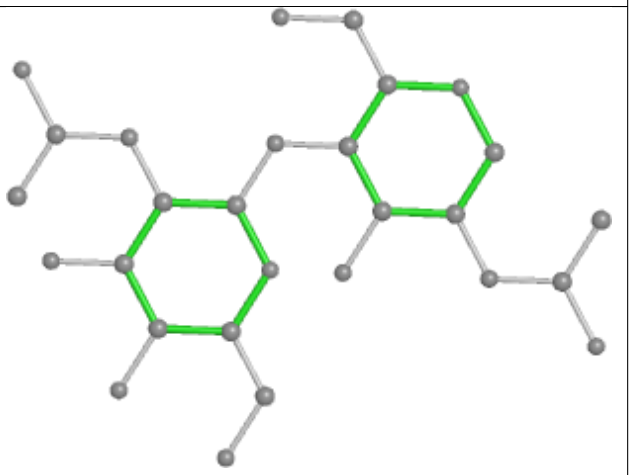
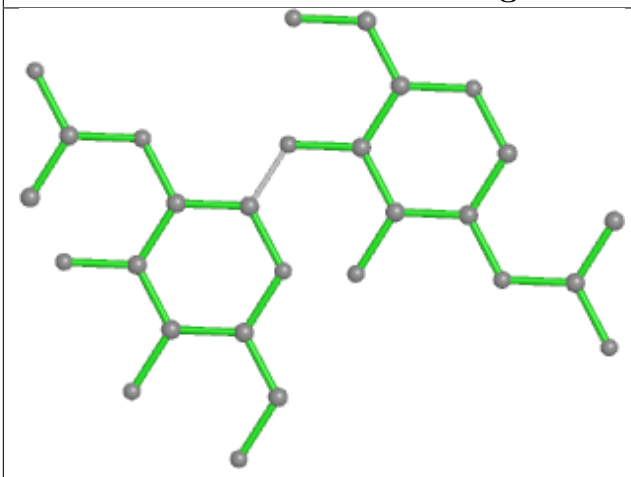


Rings

Oligosaccharide Chain c



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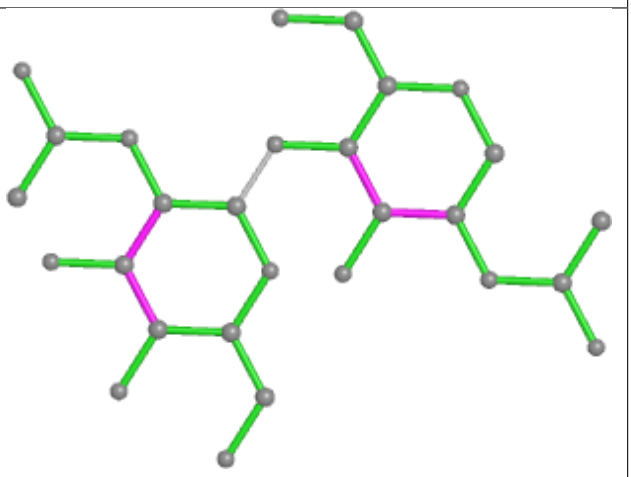

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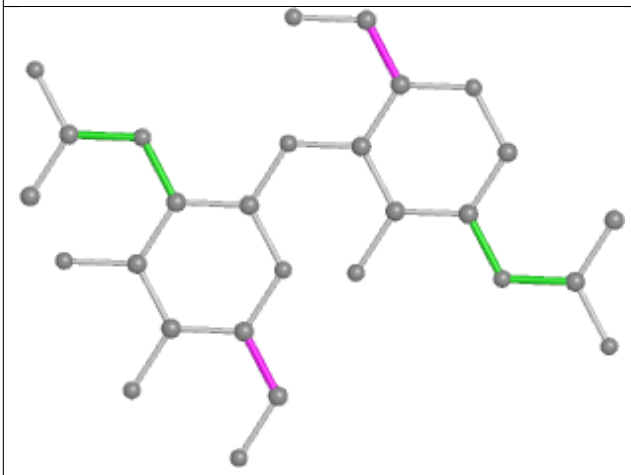

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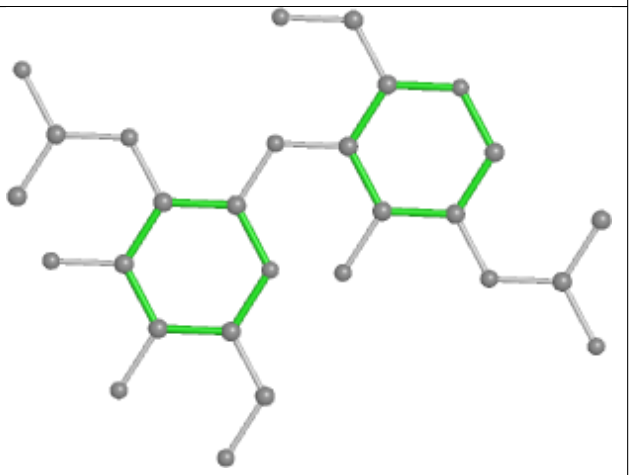
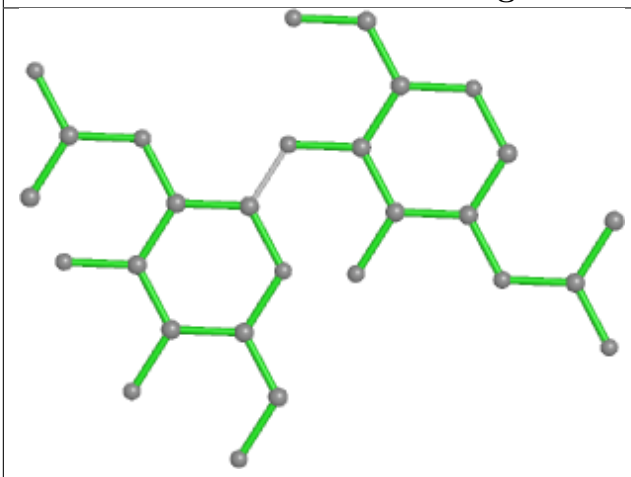


Rings

Oligosaccharide Chain d



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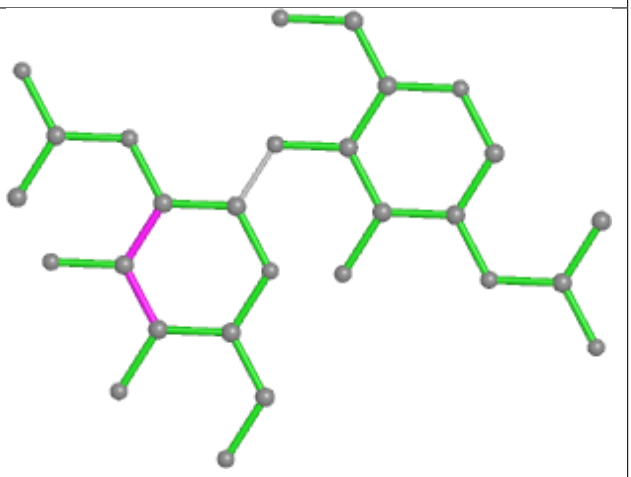

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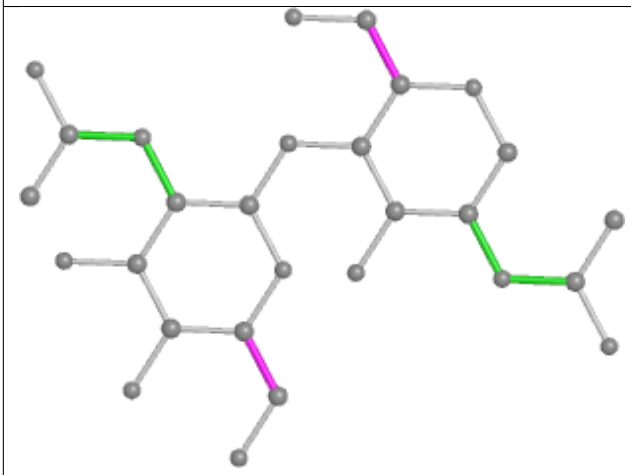

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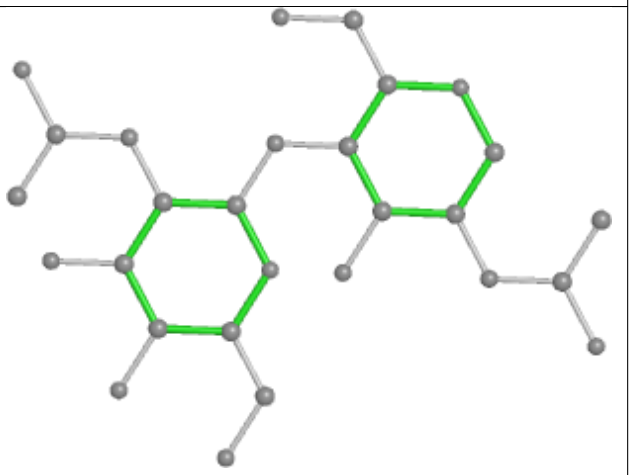
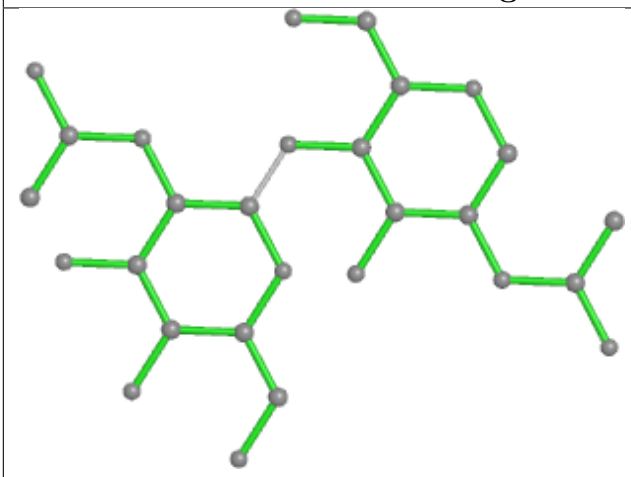


Rings

Oligosaccharide Chain e



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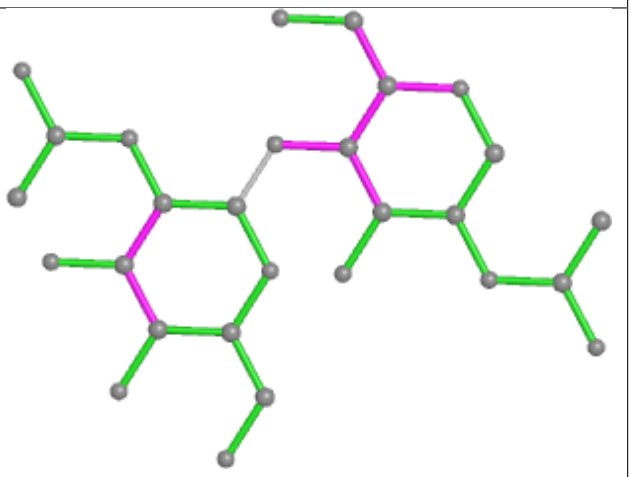

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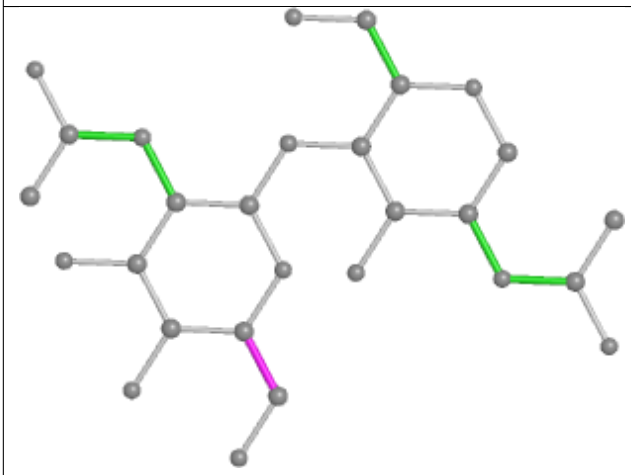

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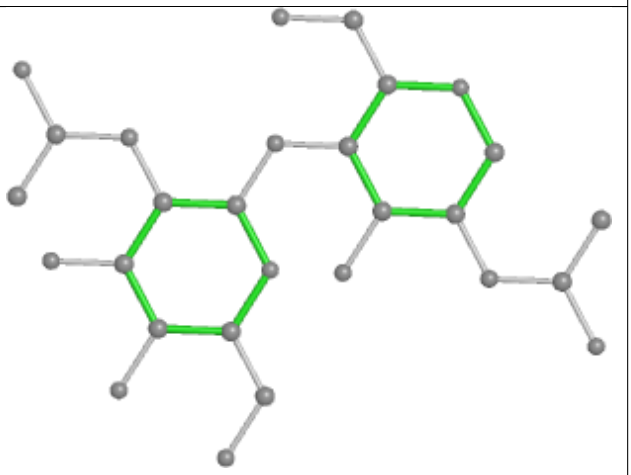
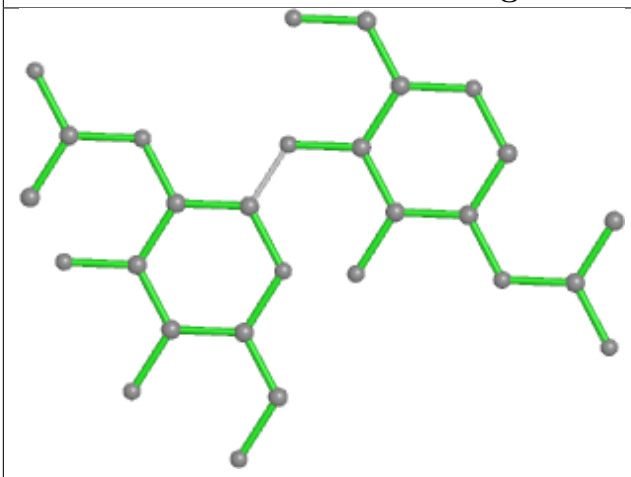


Rings

Oligosaccharide Chain f



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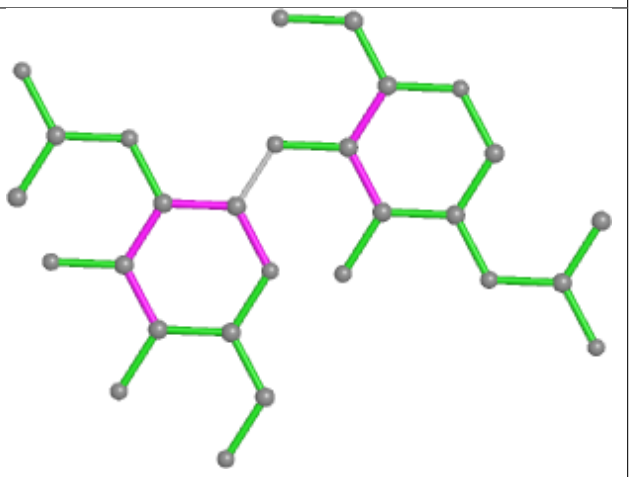

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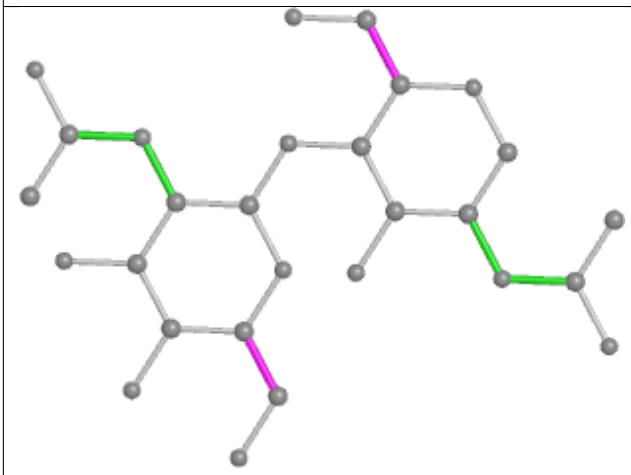

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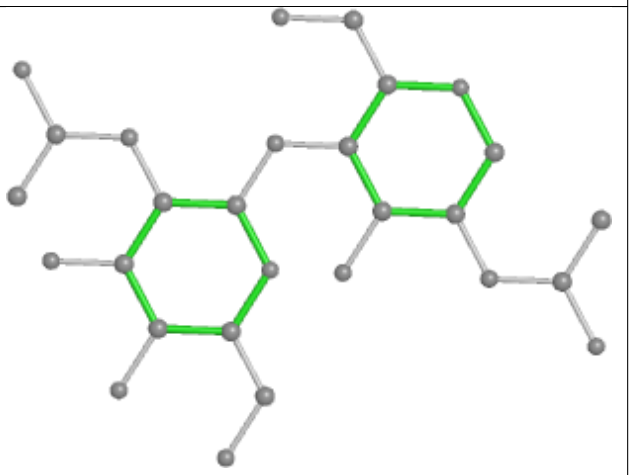
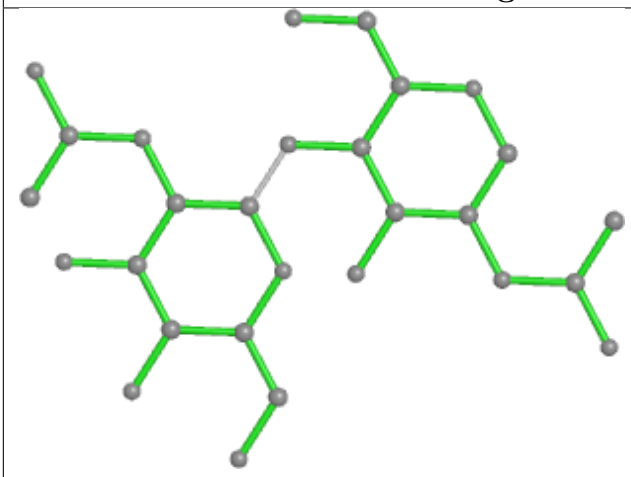


Rings

Oligosaccharide Chain h



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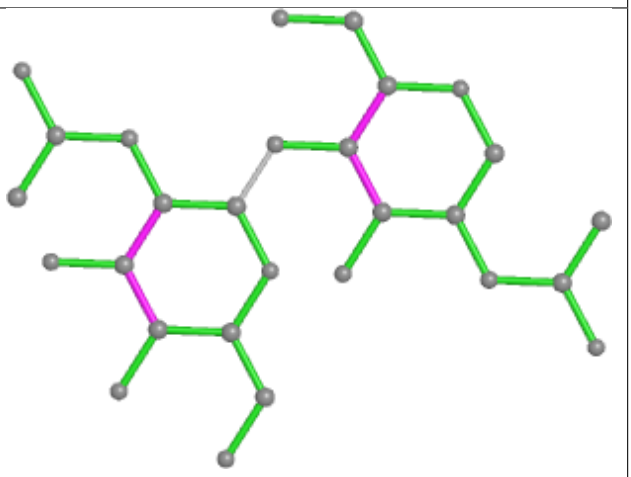
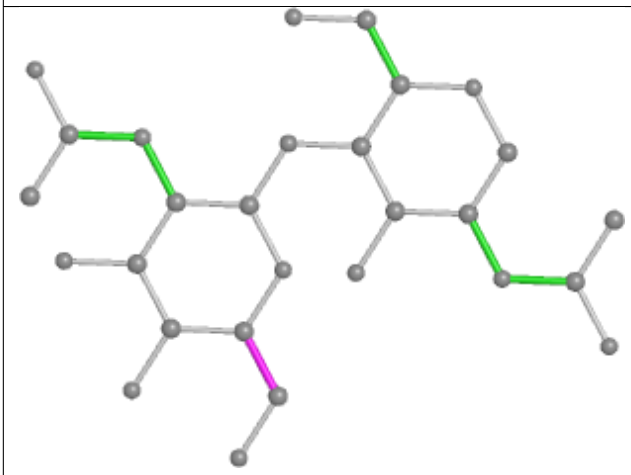


Bond angles



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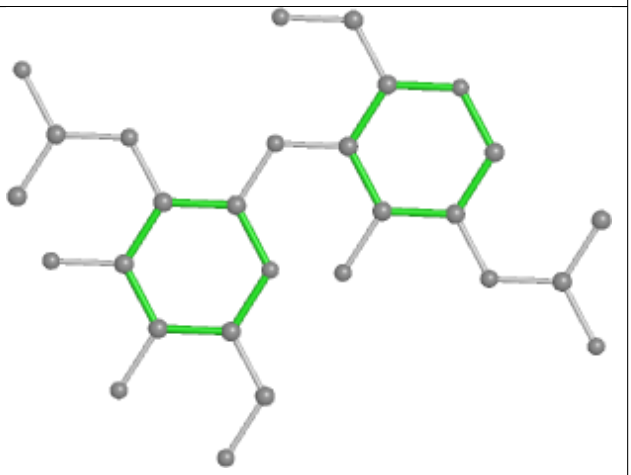
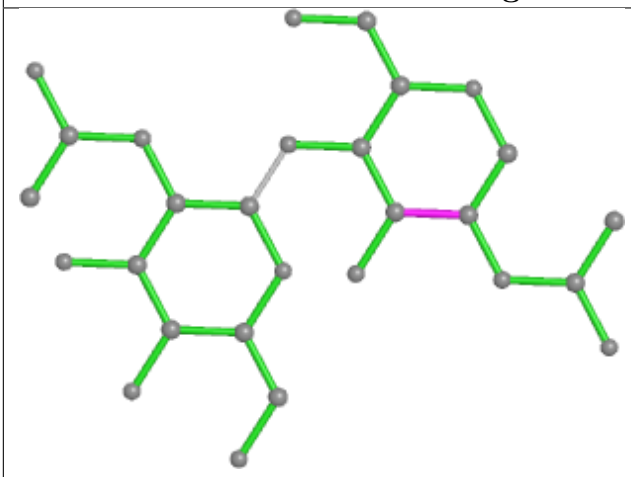


Rings

Oligosaccharide Chain j



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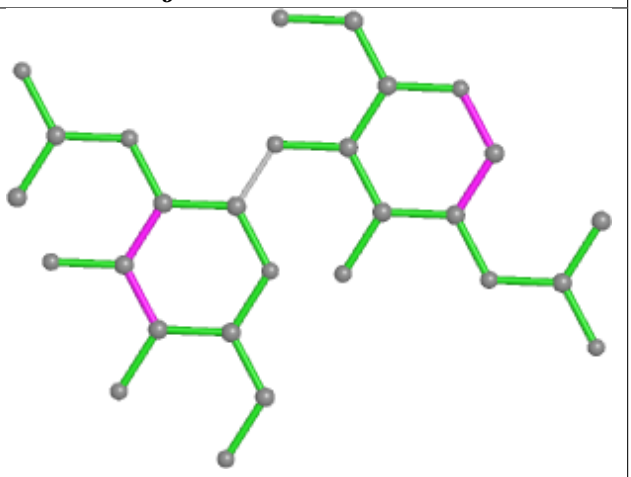

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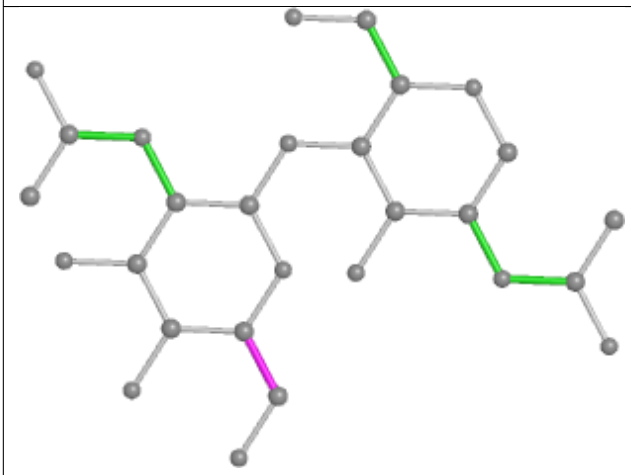
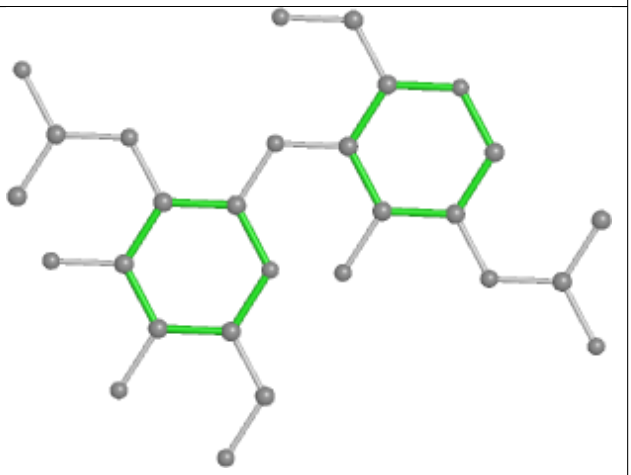
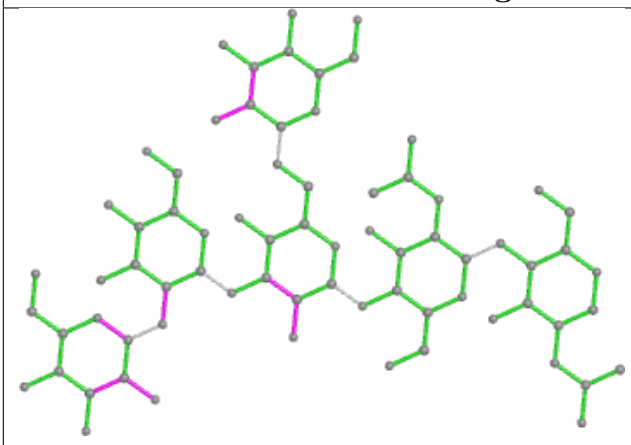


Torsions



Rings

Oligosaccharide Chain Q



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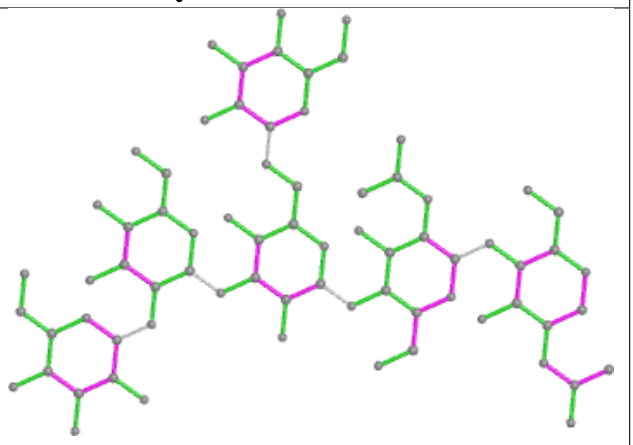
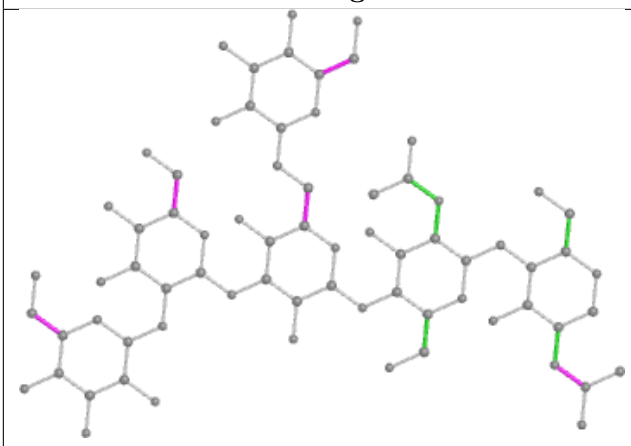


Bond angles



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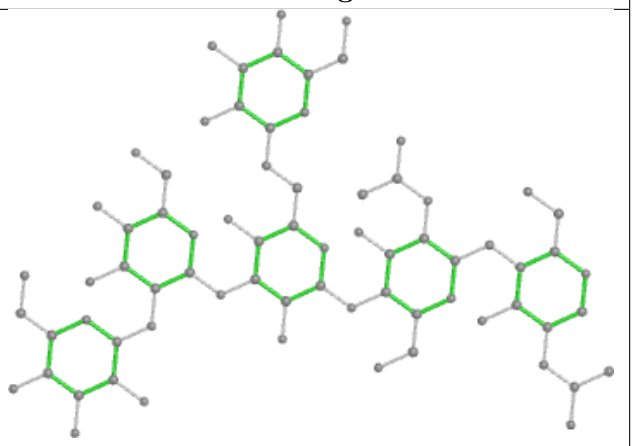
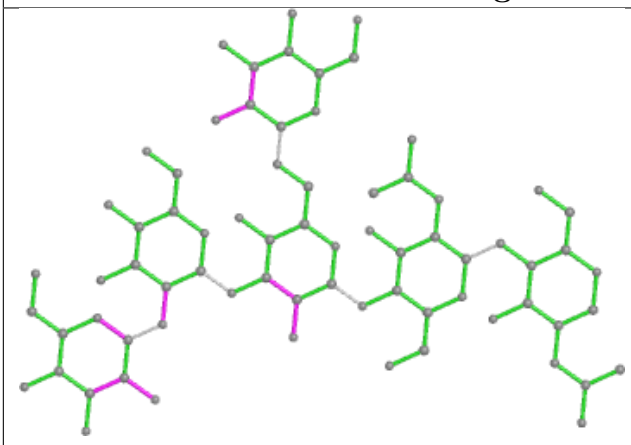
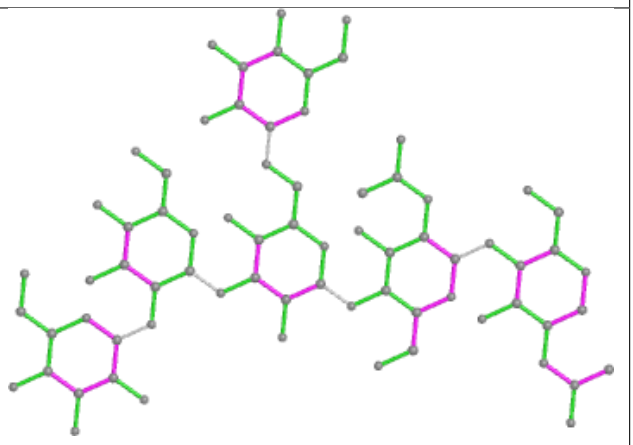


Rings

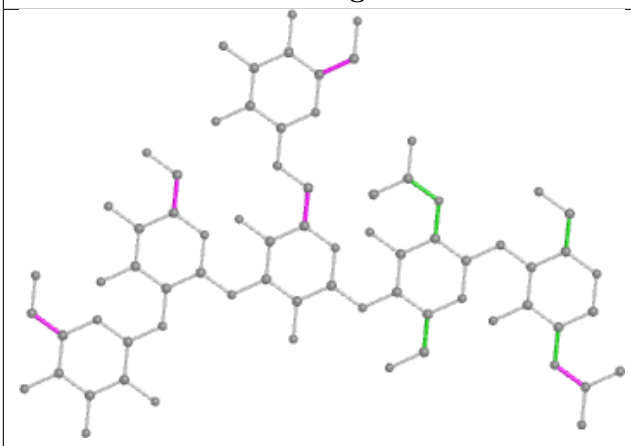
Oligosaccharide Chain Y



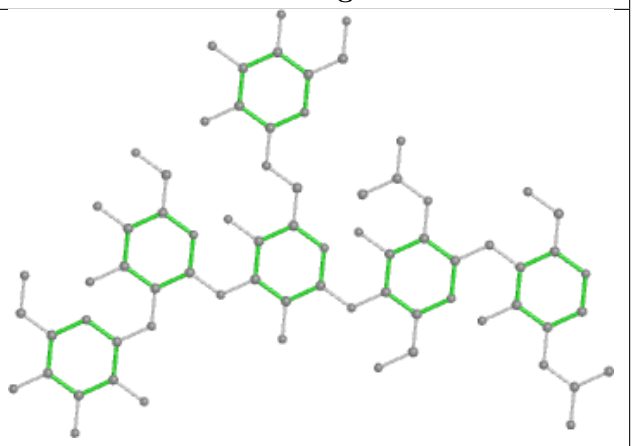
Bond lengths



Bond angles

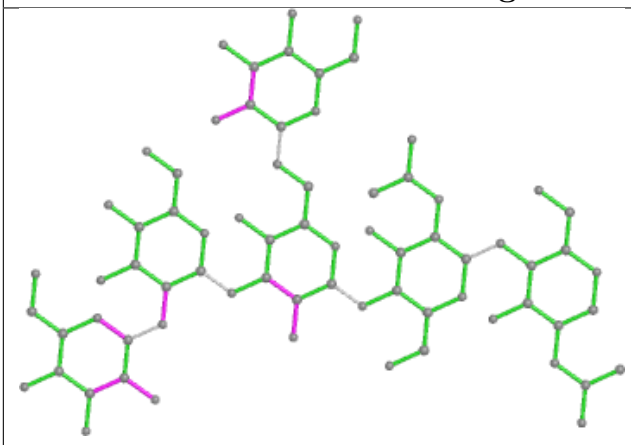


Torsions

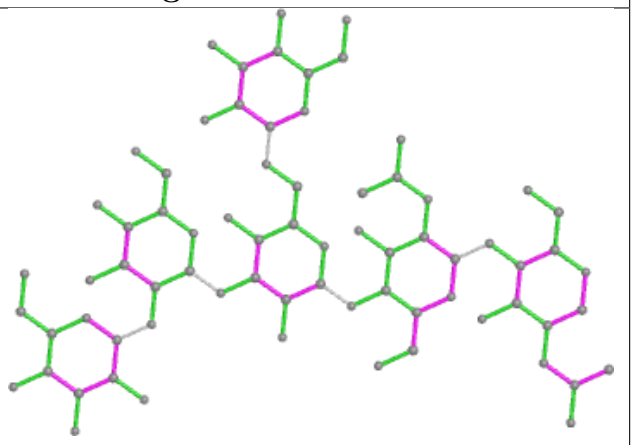


Rings

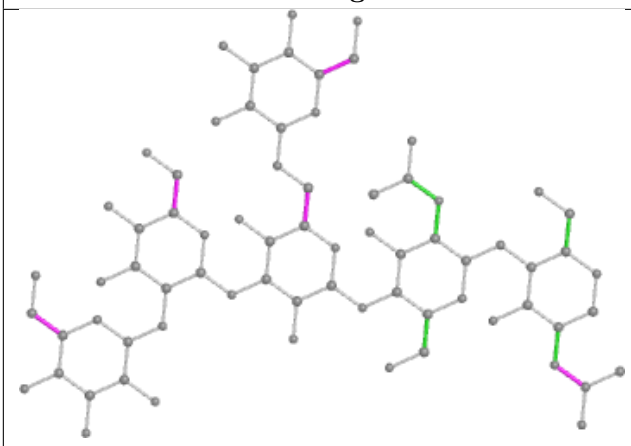
Oligosaccharide Chain g



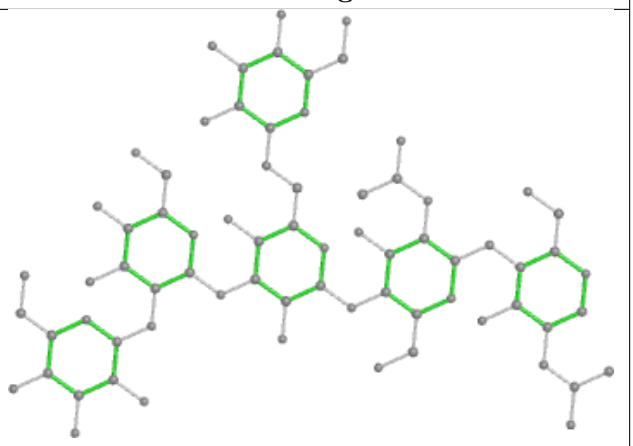
Bond lengths



Bond angles

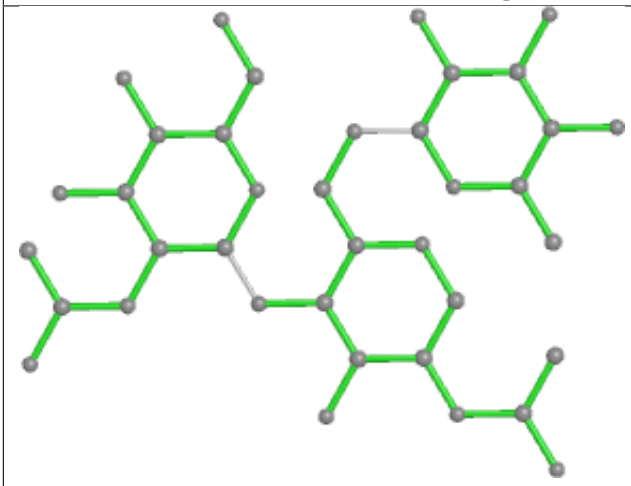


Torsions

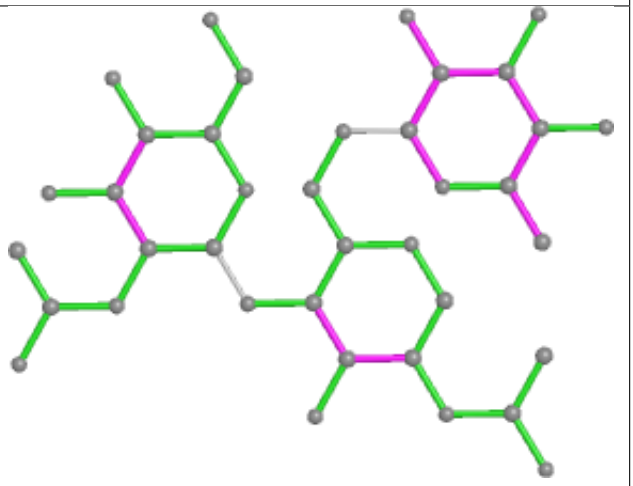


Rings

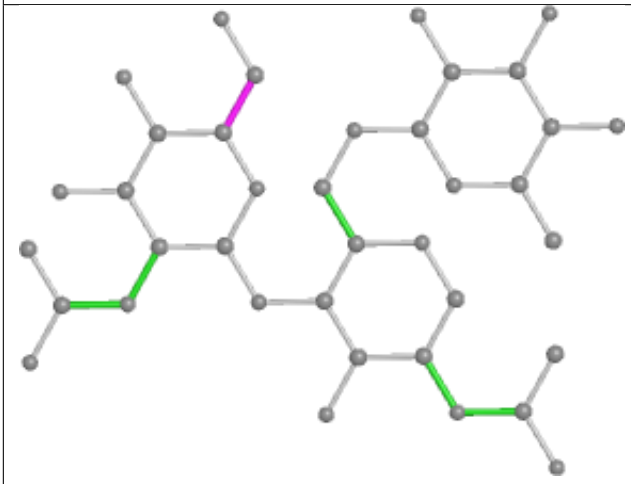
Oligosaccharide Chain S



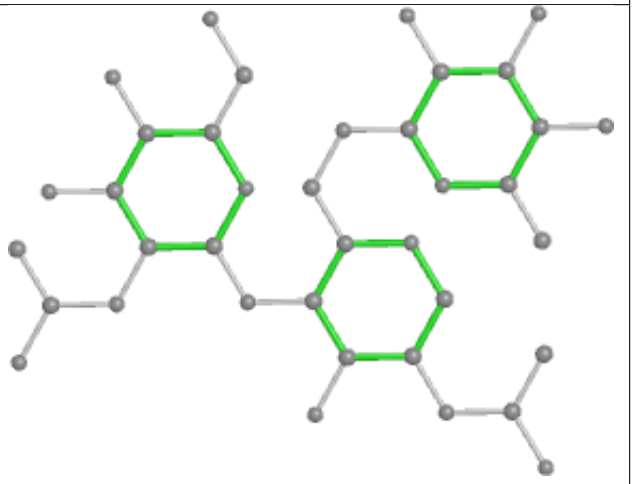
Bond lengths



Bond angles

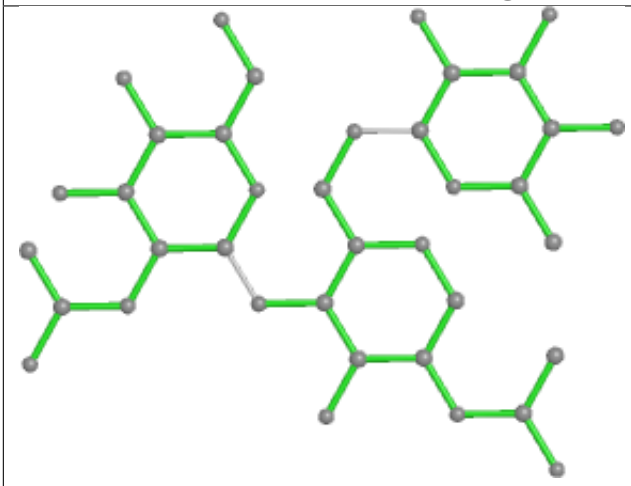


Torsions

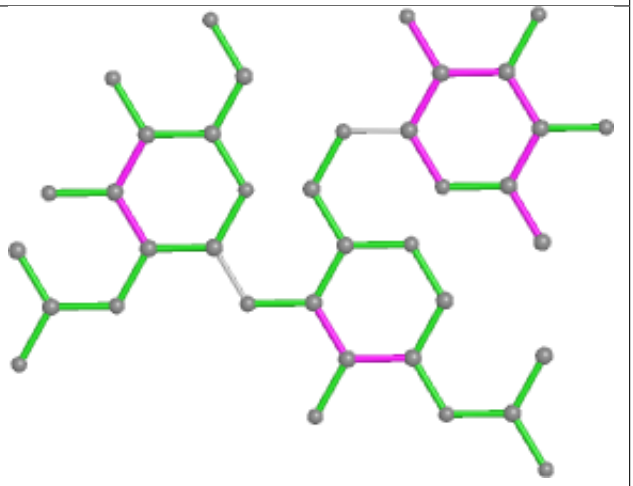


Rings

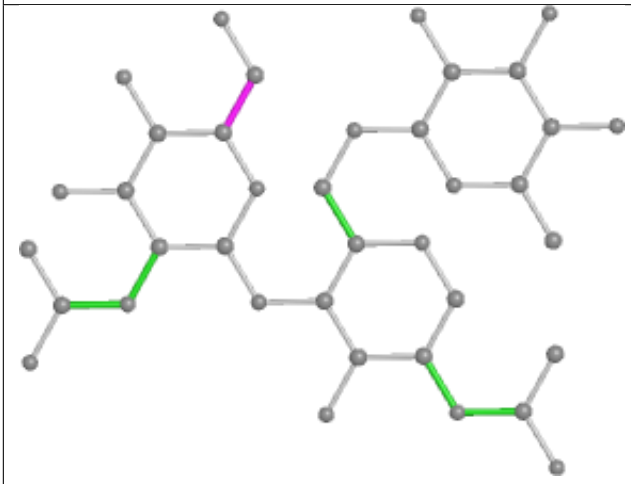
Oligosaccharide Chain a



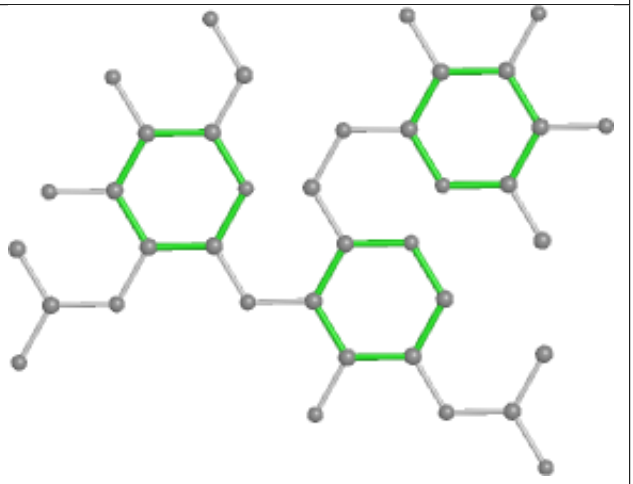
Bond lengths



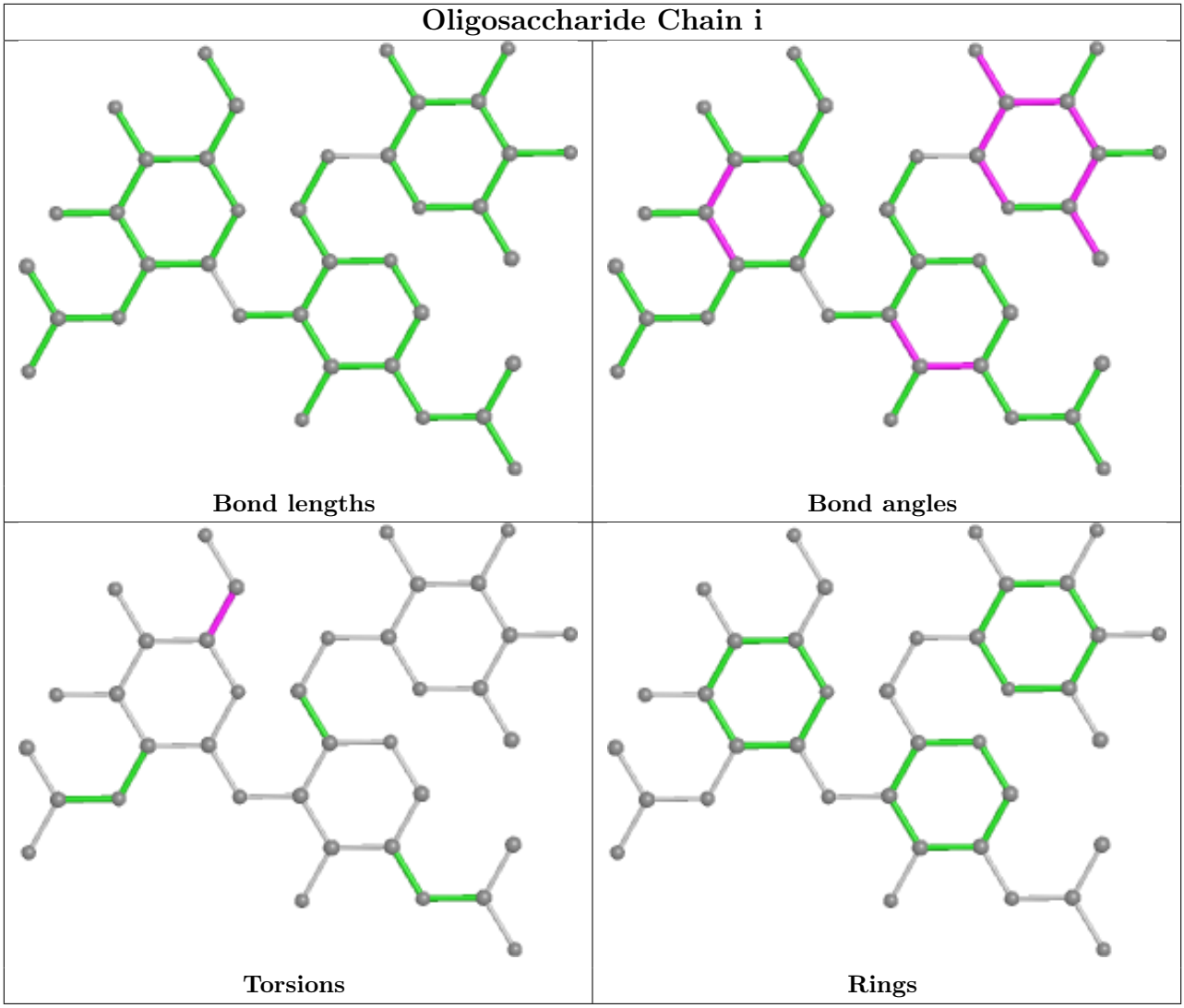
Bond angles



Torsions



Rings



5.6 Ligand geometry (i)

39 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	$\#\|Z\| > 2$
8	NAG	A	621	1	14,14,15	0.74	0	17,19,21	1.34	3 (17%)
8	NAG	D	627	1	14,14,15	0.85	0	17,19,21	0.88	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
8	NAG	C	613	1	14,14,15	0.78	0	17,19,21	0.86	1 (5%)
8	NAG	A	611	1	14,14,15	0.91	0	17,19,21	1.21	1 (5%)
8	NAG	C	624	1	14,14,15	0.85	0	17,19,21	0.81	0
8	NAG	D	611	1	14,14,15	0.91	0	17,19,21	1.20	1 (5%)
8	NAG	C	612	1	14,14,15	0.79	0	17,19,21	1.07	1 (5%)
8	NAG	D	626	1	14,14,15	0.89	0	17,19,21	1.35	1 (5%)
8	NAG	D	628	1	14,14,15	0.80	0	17,19,21	1.04	1 (5%)
8	NAG	C	614	1	14,14,15	0.80	0	17,19,21	1.06	1 (5%)
8	NAG	C	621	1	14,14,15	0.73	0	17,19,21	1.34	3 (17%)
8	NAG	A	608	1	14,14,15	0.74	0	17,19,21	1.18	2 (11%)
8	NAG	C	608	1	14,14,15	0.74	0	17,19,21	1.19	2 (11%)
8	NAG	A	626	1	14,14,15	0.89	0	17,19,21	1.35	1 (5%)
8	NAG	D	624	1	14,14,15	0.84	0	17,19,21	0.81	0
8	NAG	C	628	1	14,14,15	0.81	0	17,19,21	1.03	1 (5%)
8	NAG	D	613	1	14,14,15	0.77	0	17,19,21	0.85	1 (5%)
8	NAG	A	613	1	14,14,15	0.78	0	17,19,21	0.85	1 (5%)
8	NAG	A	612	1	14,14,15	0.80	0	17,19,21	1.07	1 (5%)
8	NAG	A	625	1	14,14,15	0.86	0	17,19,21	0.90	1 (5%)
8	NAG	A	627	1	14,14,15	0.84	0	17,19,21	0.88	1 (5%)
8	NAG	D	625	1	14,14,15	0.86	0	17,19,21	0.89	1 (5%)
8	NAG	D	612	1	14,14,15	0.80	0	17,19,21	1.06	1 (5%)
8	NAG	B	704	2	14,14,15	0.77	0	17,19,21	1.04	2 (11%)
8	NAG	C	603	1	14,14,15	0.84	0	17,19,21	1.31	2 (11%)
8	NAG	C	625	1	14,14,15	0.85	0	17,19,21	0.90	1 (5%)
8	NAG	C	626	1	14,14,15	0.89	0	17,19,21	1.36	1 (5%)
8	NAG	D	614	1	14,14,15	0.82	0	17,19,21	1.06	1 (5%)
8	NAG	E	704	2	14,14,15	0.78	0	17,19,21	1.04	2 (11%)
8	NAG	A	624	1	14,14,15	0.85	0	17,19,21	0.81	0
8	NAG	C	611	1	14,14,15	0.90	0	17,19,21	1.21	1 (5%)
8	NAG	A	603	1	14,14,15	0.85	0	17,19,21	1.30	2 (11%)
8	NAG	C	627	1	14,14,15	0.85	0	17,19,21	0.88	1 (5%)
8	NAG	F	704	2	14,14,15	0.77	0	17,19,21	1.04	2 (11%)
8	NAG	D	621	1	14,14,15	0.75	0	17,19,21	1.34	3 (17%)
8	NAG	A	614	1	14,14,15	0.81	0	17,19,21	1.06	1 (5%)
8	NAG	D	603	1	14,14,15	0.84	0	17,19,21	1.30	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
8	NAG	A	628	1	14,14,15	0.80	0	17,19,21	1.04	1 (5%)
8	NAG	D	608	1	14,14,15	0.74	0	17,19,21	1.19	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
8	NAG	A	621	1	-	4/6/23/26	0/1/1/1
8	NAG	D	627	1	-	2/6/23/26	0/1/1/1
8	NAG	C	613	1	-	1/6/23/26	0/1/1/1
8	NAG	A	611	1	-	1/6/23/26	0/1/1/1
8	NAG	C	624	1	-	1/6/23/26	0/1/1/1
8	NAG	D	611	1	-	1/6/23/26	0/1/1/1
8	NAG	C	612	1	-	1/6/23/26	0/1/1/1
8	NAG	D	626	1	-	1/6/23/26	0/1/1/1
8	NAG	D	628	1	-	1/6/23/26	0/1/1/1
8	NAG	C	614	1	-	2/6/23/26	0/1/1/1
8	NAG	C	621	1	-	4/6/23/26	0/1/1/1
8	NAG	A	608	1	-	2/6/23/26	0/1/1/1
8	NAG	C	608	1	-	2/6/23/26	0/1/1/1
8	NAG	A	626	1	-	1/6/23/26	0/1/1/1
8	NAG	D	624	1	-	1/6/23/26	0/1/1/1
8	NAG	C	628	1	-	1/6/23/26	0/1/1/1
8	NAG	D	613	1	-	1/6/23/26	0/1/1/1
8	NAG	A	613	1	-	1/6/23/26	0/1/1/1
8	NAG	A	612	1	-	1/6/23/26	0/1/1/1
8	NAG	A	625	1	-	1/6/23/26	0/1/1/1
8	NAG	A	627	1	-	2/6/23/26	0/1/1/1
8	NAG	D	625	1	-	1/6/23/26	0/1/1/1
8	NAG	D	612	1	-	1/6/23/26	0/1/1/1
8	NAG	B	704	2	-	1/6/23/26	0/1/1/1
8	NAG	C	603	1	-	2/6/23/26	0/1/1/1
8	NAG	C	625	1	-	1/6/23/26	0/1/1/1
8	NAG	C	626	1	-	1/6/23/26	0/1/1/1
8	NAG	D	614	1	-	2/6/23/26	0/1/1/1
8	NAG	E	704	2	-	1/6/23/26	0/1/1/1
8	NAG	A	624	1	-	1/6/23/26	0/1/1/1
8	NAG	C	611	1	-	1/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	NAG	A	603	1	-	2/6/23/26	0/1/1/1
8	NAG	C	627	1	-	2/6/23/26	0/1/1/1
8	NAG	F	704	2	-	1/6/23/26	0/1/1/1
8	NAG	D	621	1	-	4/6/23/26	0/1/1/1
8	NAG	A	614	1	-	2/6/23/26	0/1/1/1
8	NAG	D	603	1	-	2/6/23/26	0/1/1/1
8	NAG	A	628	1	-	1/6/23/26	0/1/1/1
8	NAG	D	608	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	C	626	NAG	C4-C3-C2	-4.35	104.65	111.02
8	A	626	NAG	C4-C3-C2	-4.34	104.66	111.02
8	D	626	NAG	C4-C3-C2	-4.33	104.67	111.02
8	C	603	NAG	C4-C3-C2	-4.05	105.08	111.02
8	A	603	NAG	C4-C3-C2	-4.03	105.11	111.02
8	D	603	NAG	C4-C3-C2	-4.03	105.11	111.02
8	C	611	NAG	C4-C3-C2	-3.89	105.32	111.02
8	A	611	NAG	C4-C3-C2	-3.86	105.36	111.02
8	D	611	NAG	C4-C3-C2	-3.84	105.39	111.02
8	C	614	NAG	C4-C3-C2	-3.27	106.22	111.02
8	A	614	NAG	C4-C3-C2	-3.27	106.22	111.02
8	D	614	NAG	C4-C3-C2	-3.25	106.26	111.02
8	C	621	NAG	C8-C7-N2	3.19	121.49	116.10
8	A	621	NAG	C8-C7-N2	3.17	121.47	116.10
8	D	621	NAG	C8-C7-N2	3.17	121.47	116.10
8	C	608	NAG	C4-C3-C2	-3.07	106.51	111.02
8	D	608	NAG	C4-C3-C2	-3.06	106.53	111.02
8	A	608	NAG	C4-C3-C2	-3.06	106.54	111.02
8	A	628	NAG	C4-C3-C2	-2.94	106.70	111.02
8	C	628	NAG	C4-C3-C2	-2.94	106.70	111.02
8	D	628	NAG	C4-C3-C2	-2.94	106.71	111.02
8	C	612	NAG	C4-C3-C2	-2.86	106.83	111.02
8	A	612	NAG	C4-C3-C2	-2.86	106.83	111.02
8	D	612	NAG	C4-C3-C2	-2.84	106.86	111.02
8	C	627	NAG	C4-C3-C2	-2.65	107.13	111.02
8	D	627	NAG	C4-C3-C2	-2.65	107.14	111.02
8	A	627	NAG	C4-C3-C2	-2.64	107.15	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	F	704	NAG	C4-C3-C2	-2.60	107.20	111.02
8	B	704	NAG	C4-C3-C2	-2.59	107.22	111.02
8	E	704	NAG	C4-C3-C2	-2.57	107.25	111.02
8	C	625	NAG	C4-C3-C2	-2.49	107.37	111.02
8	A	625	NAG	C4-C3-C2	-2.47	107.40	111.02
8	D	625	NAG	C4-C3-C2	-2.47	107.40	111.02
8	B	704	NAG	O5-C1-C2	-2.36	107.56	111.29
8	E	704	NAG	O5-C1-C2	-2.35	107.57	111.29
8	F	704	NAG	O5-C1-C2	-2.35	107.58	111.29
8	C	608	NAG	O5-C1-C2	-2.35	107.58	111.29
8	A	613	NAG	C4-C3-C2	-2.34	107.58	111.02
8	C	613	NAG	C4-C3-C2	-2.34	107.58	111.02
8	D	613	NAG	C4-C3-C2	-2.34	107.58	111.02
8	D	608	NAG	O5-C1-C2	-2.34	107.59	111.29
8	C	603	NAG	O5-C1-C2	-2.34	107.60	111.29
8	A	608	NAG	O5-C1-C2	-2.33	107.61	111.29
8	A	603	NAG	O5-C1-C2	-2.33	107.61	111.29
8	D	603	NAG	O5-C1-C2	-2.31	107.63	111.29
8	D	621	NAG	O5-C1-C2	-2.07	108.02	111.29
8	A	621	NAG	O5-C1-C2	-2.06	108.04	111.29
8	C	621	NAG	O5-C1-C2	-2.05	108.05	111.29
8	C	621	NAG	C4-C3-C2	-2.04	108.02	111.02
8	A	621	NAG	C4-C3-C2	-2.04	108.03	111.02
8	D	621	NAG	C4-C3-C2	-2.03	108.04	111.02

There are no chirality outliers.

All (60) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	614	NAG	O5-C5-C6-O6
8	A	621	NAG	O5-C5-C6-O6
8	C	614	NAG	O5-C5-C6-O6
8	C	621	NAG	O5-C5-C6-O6
8	D	614	NAG	O5-C5-C6-O6
8	D	621	NAG	O5-C5-C6-O6
8	C	608	NAG	O5-C5-C6-O6
8	A	608	NAG	O5-C5-C6-O6
8	D	608	NAG	O5-C5-C6-O6
8	A	627	NAG	O5-C5-C6-O6
8	D	627	NAG	O5-C5-C6-O6
8	C	627	NAG	O5-C5-C6-O6
8	B	704	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
8	E	704	NAG	O5-C5-C6-O6
8	F	704	NAG	O5-C5-C6-O6
8	A	603	NAG	C4-C5-C6-O6
8	C	603	NAG	C4-C5-C6-O6
8	D	603	NAG	C4-C5-C6-O6
8	A	621	NAG	C8-C7-N2-C2
8	A	621	NAG	O7-C7-N2-C2
8	C	621	NAG	C8-C7-N2-C2
8	C	621	NAG	O7-C7-N2-C2
8	D	621	NAG	C8-C7-N2-C2
8	D	621	NAG	O7-C7-N2-C2
8	A	624	NAG	O5-C5-C6-O6
8	C	624	NAG	O5-C5-C6-O6
8	D	624	NAG	O5-C5-C6-O6
8	A	612	NAG	O5-C5-C6-O6
8	C	612	NAG	O5-C5-C6-O6
8	D	612	NAG	O5-C5-C6-O6
8	A	628	NAG	O5-C5-C6-O6
8	C	628	NAG	O5-C5-C6-O6
8	D	628	NAG	O5-C5-C6-O6
8	A	621	NAG	C4-C5-C6-O6
8	C	621	NAG	C4-C5-C6-O6
8	D	621	NAG	C4-C5-C6-O6
8	A	614	NAG	C4-C5-C6-O6
8	C	614	NAG	C4-C5-C6-O6
8	D	614	NAG	C4-C5-C6-O6
8	A	613	NAG	O5-C5-C6-O6
8	C	613	NAG	O5-C5-C6-O6
8	D	613	NAG	O5-C5-C6-O6
8	A	625	NAG	O5-C5-C6-O6
8	C	625	NAG	O5-C5-C6-O6
8	D	625	NAG	O5-C5-C6-O6
8	A	611	NAG	O5-C5-C6-O6
8	C	611	NAG	O5-C5-C6-O6
8	D	611	NAG	O5-C5-C6-O6
8	A	626	NAG	O5-C5-C6-O6
8	C	626	NAG	O5-C5-C6-O6
8	D	626	NAG	O5-C5-C6-O6
8	A	603	NAG	O5-C5-C6-O6
8	C	603	NAG	O5-C5-C6-O6
8	D	603	NAG	O5-C5-C6-O6
8	A	627	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
8	C	627	NAG	C4-C5-C6-O6
8	D	627	NAG	C4-C5-C6-O6
8	C	608	NAG	C4-C5-C6-O6
8	A	608	NAG	C4-C5-C6-O6
8	D	608	NAG	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

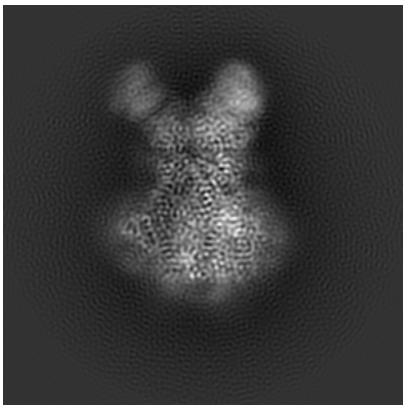
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-21227. These allow visual inspection of the internal detail of the map and identification of artifacts.

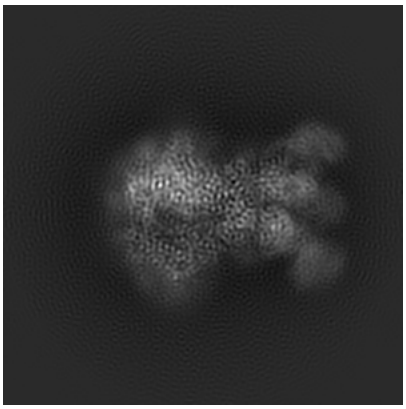
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

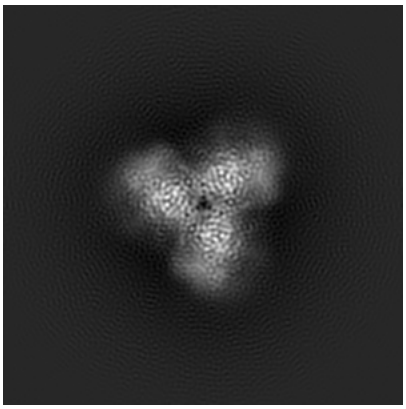
6.1.1 Primary map



X

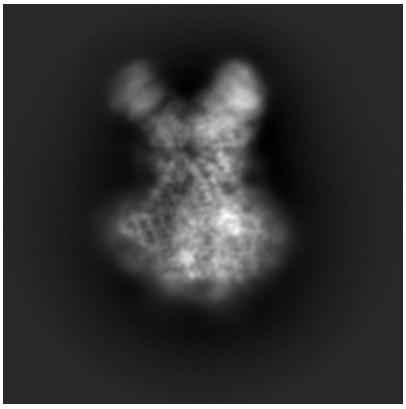


Y

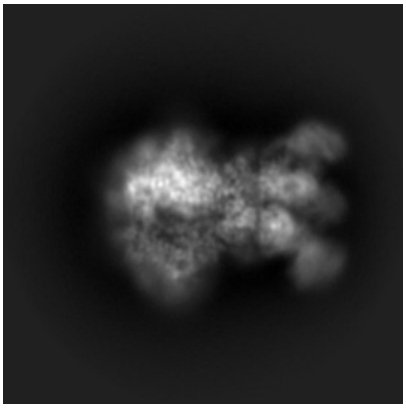


Z

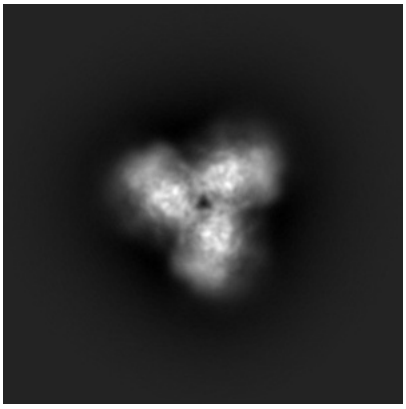
6.1.2 Raw map



X



Y

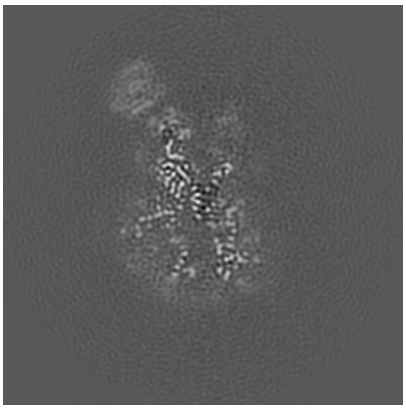


Z

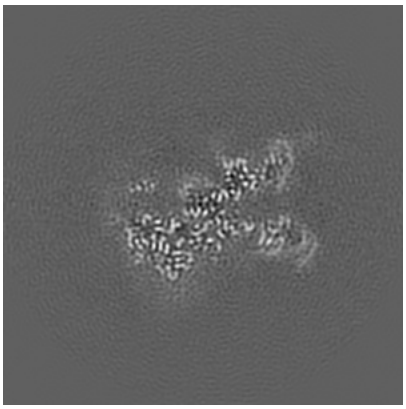
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

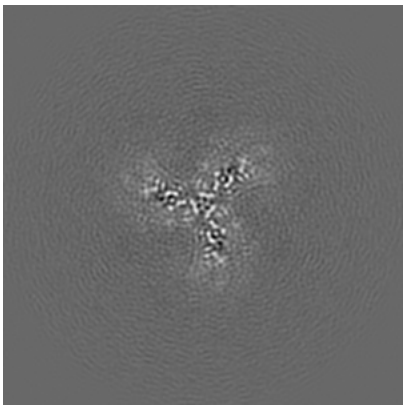
6.2.1 Primary map



X Index: 144

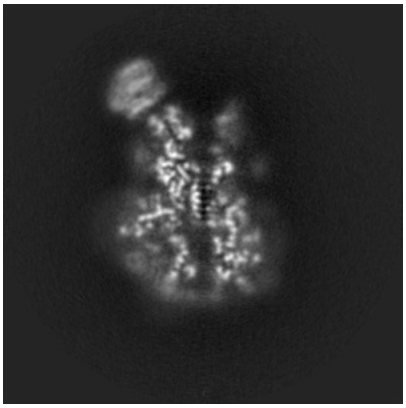


Y Index: 144

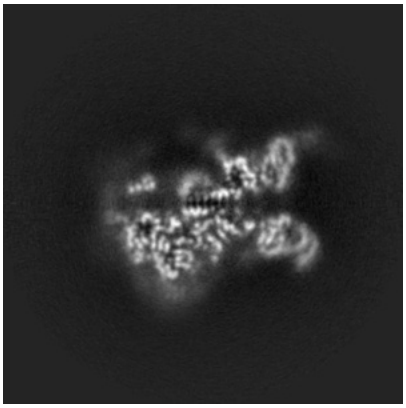


Z Index: 144

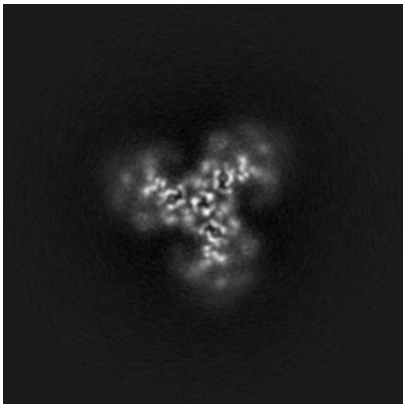
6.2.2 Raw map



X Index: 144



Y Index: 144

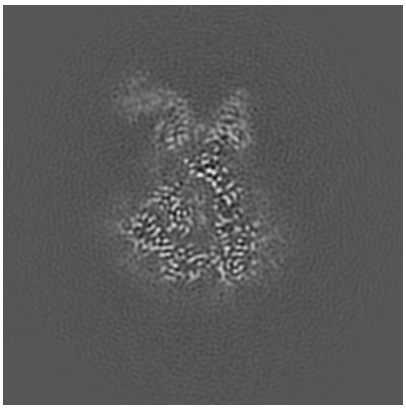


Z Index: 144

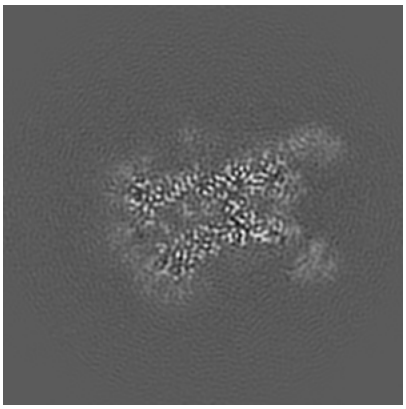
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

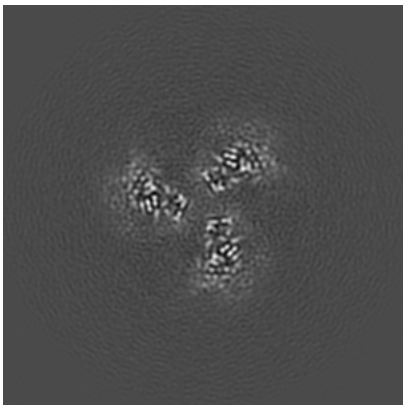
6.3.1 Primary map



X Index: 158

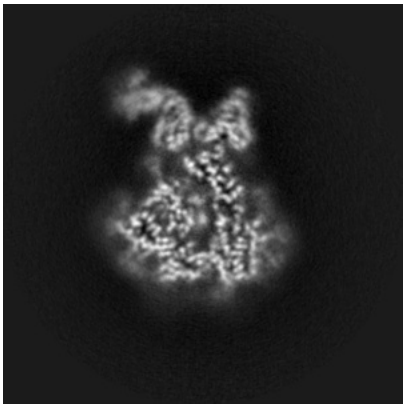


Y Index: 156

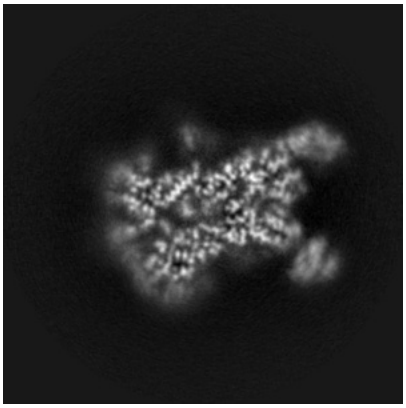


Z Index: 125

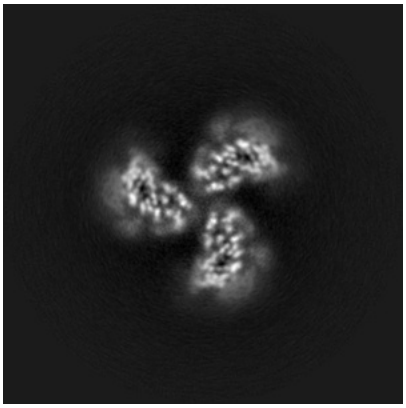
6.3.2 Raw map



X Index: 158



Y Index: 156

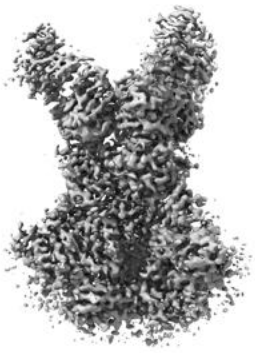


Z Index: 124

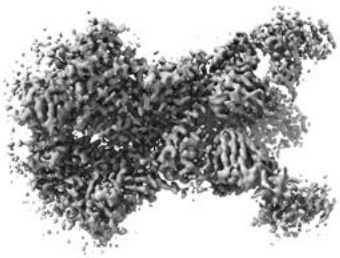
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

6.4.1 Primary map



X



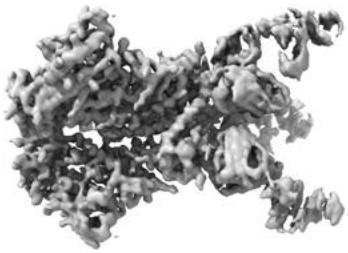
Y

Z

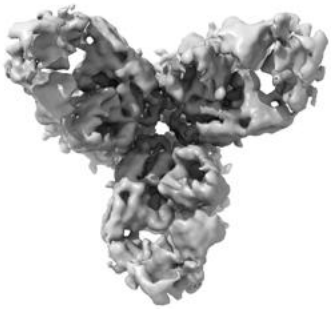
The images above show the 3D surface view of the map at the recommended contour level 0.05. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map

X



Y



Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

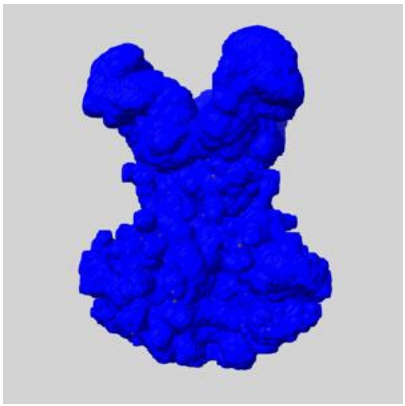
6.5 Mask visualisation (i)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

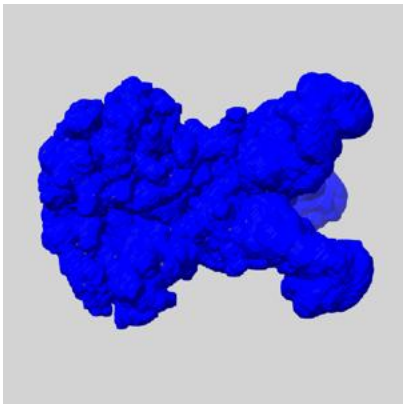
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

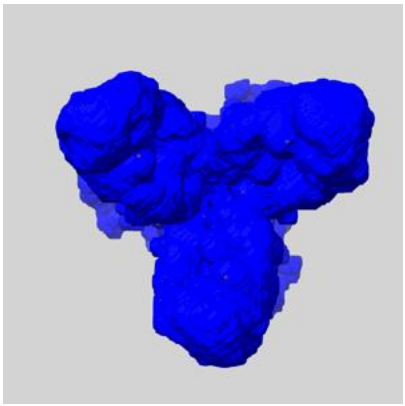
6.5.1 emd_21227_msk_1.map (i)



X



Y

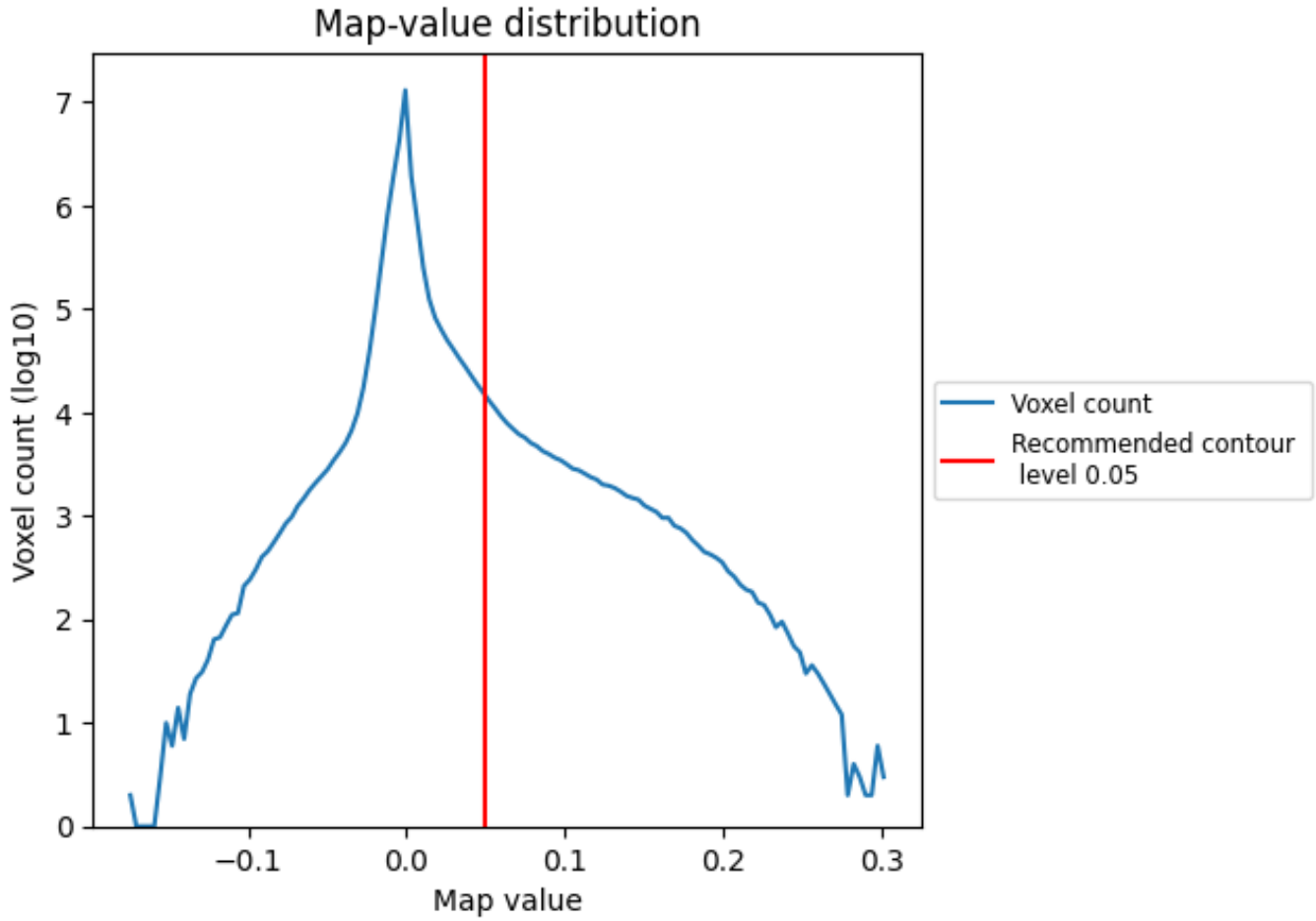


Z

7 Map analysis

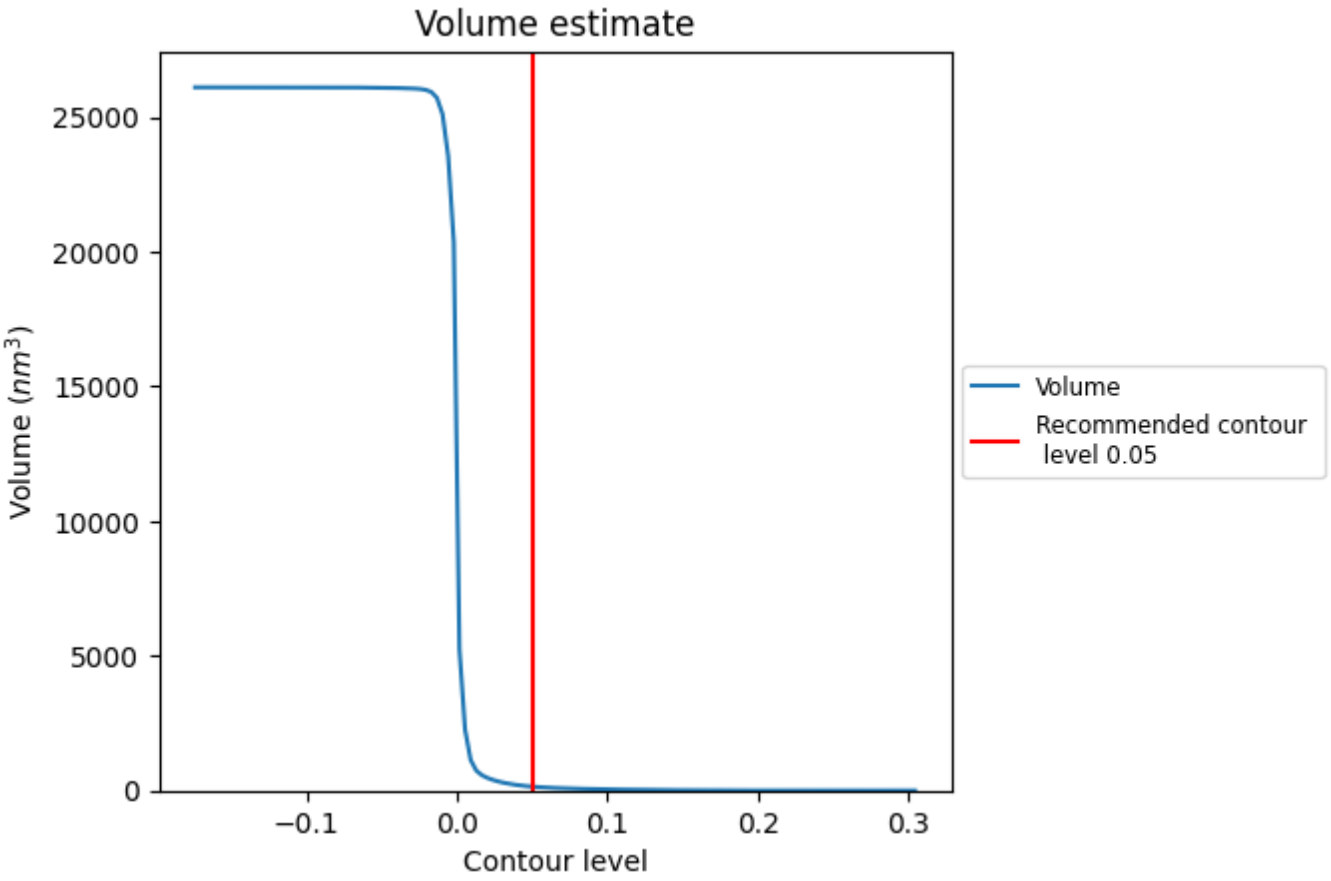
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

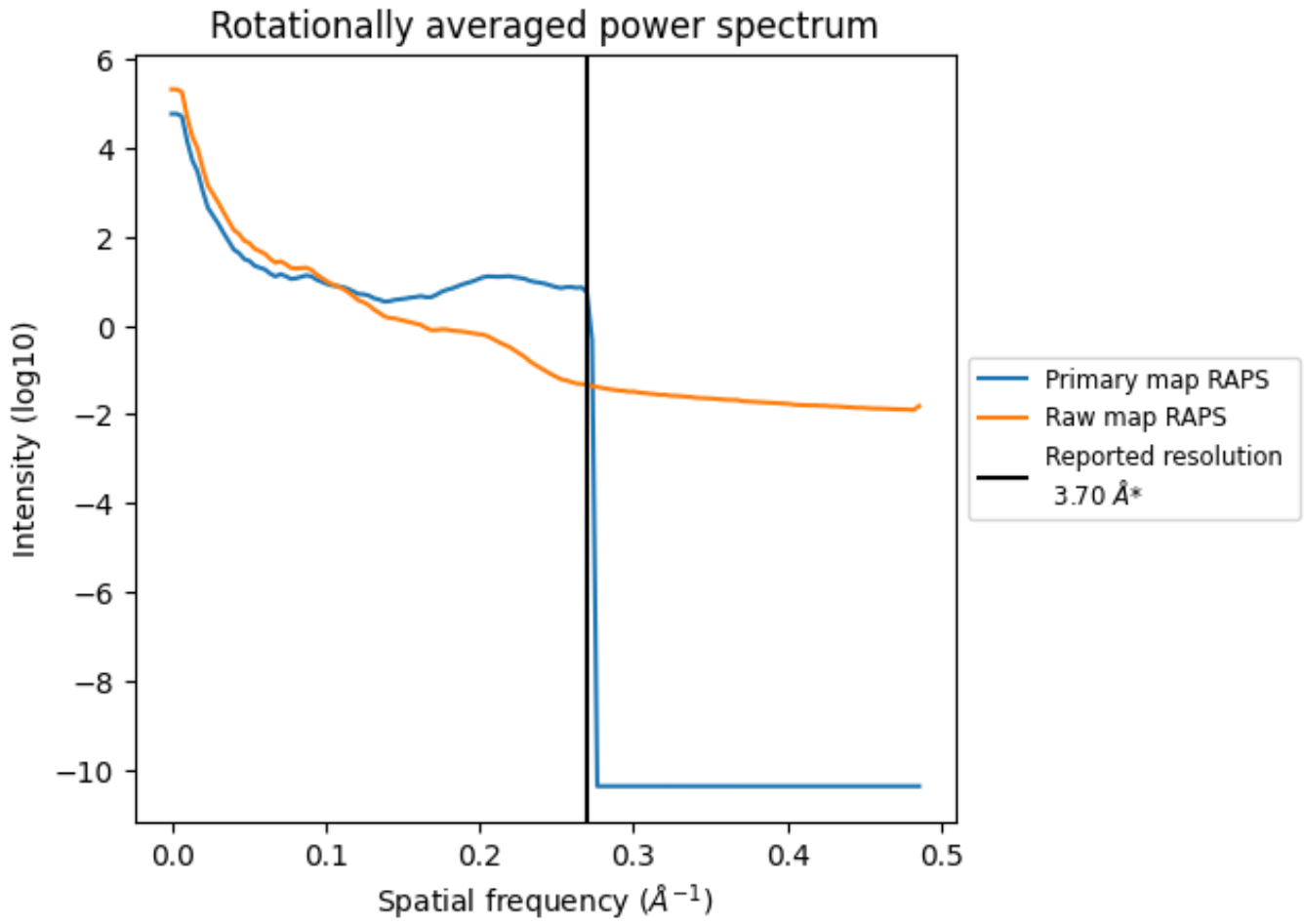
7.2 Volume estimate



The volume at the recommended contour level is 146 nm^3; this corresponds to an approximate mass of 132 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)

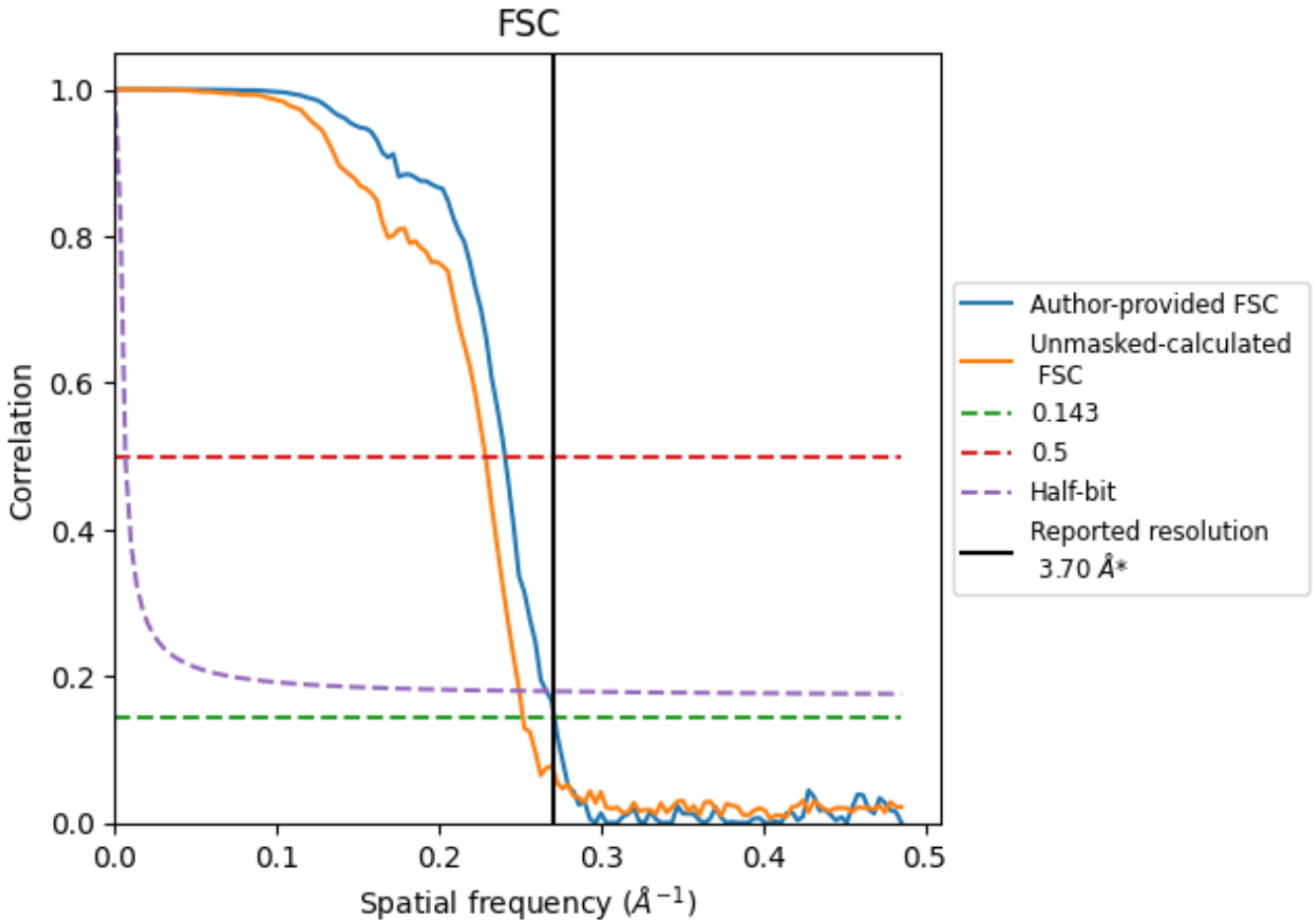


*Reported resolution corresponds to spatial frequency of 0.270 Å^{-1}

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.270 Å^{-1}

8.2 Resolution estimates (i)

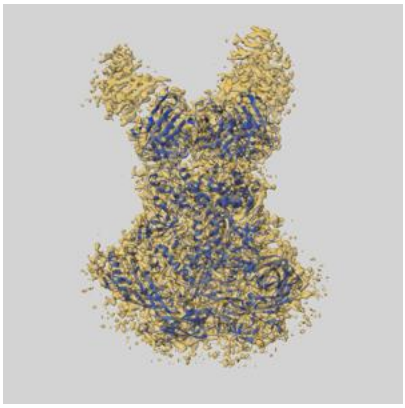
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.70	-	-
Author-provided FSC curve	3.69	4.15	3.75
Unmasked-calculated*	3.97	4.37	4.01

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

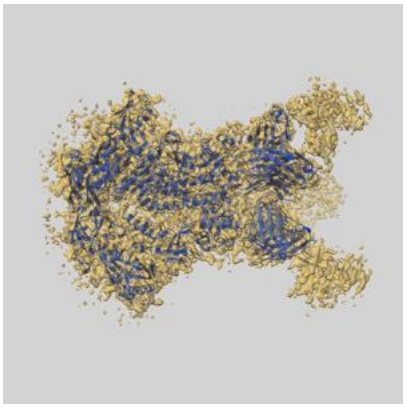
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-21227 and PDB model 6VKN. Per-residue inclusion information can be found in section 3 on page 12.

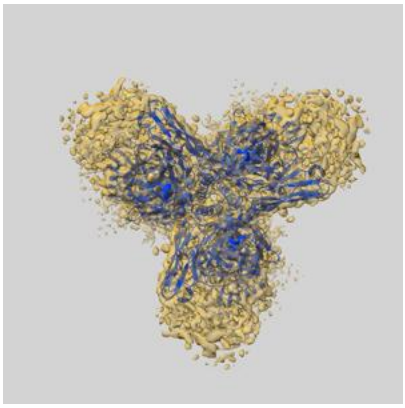
9.1 Map-model overlay



X



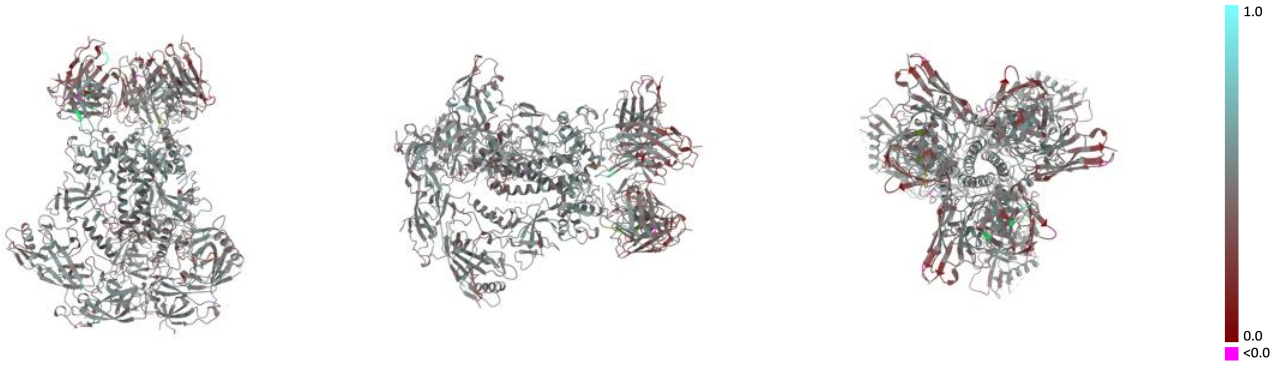
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

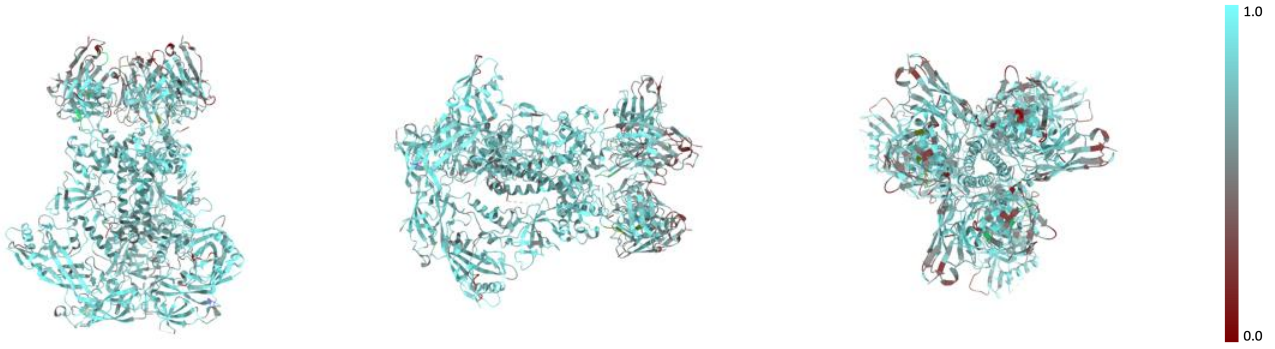
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

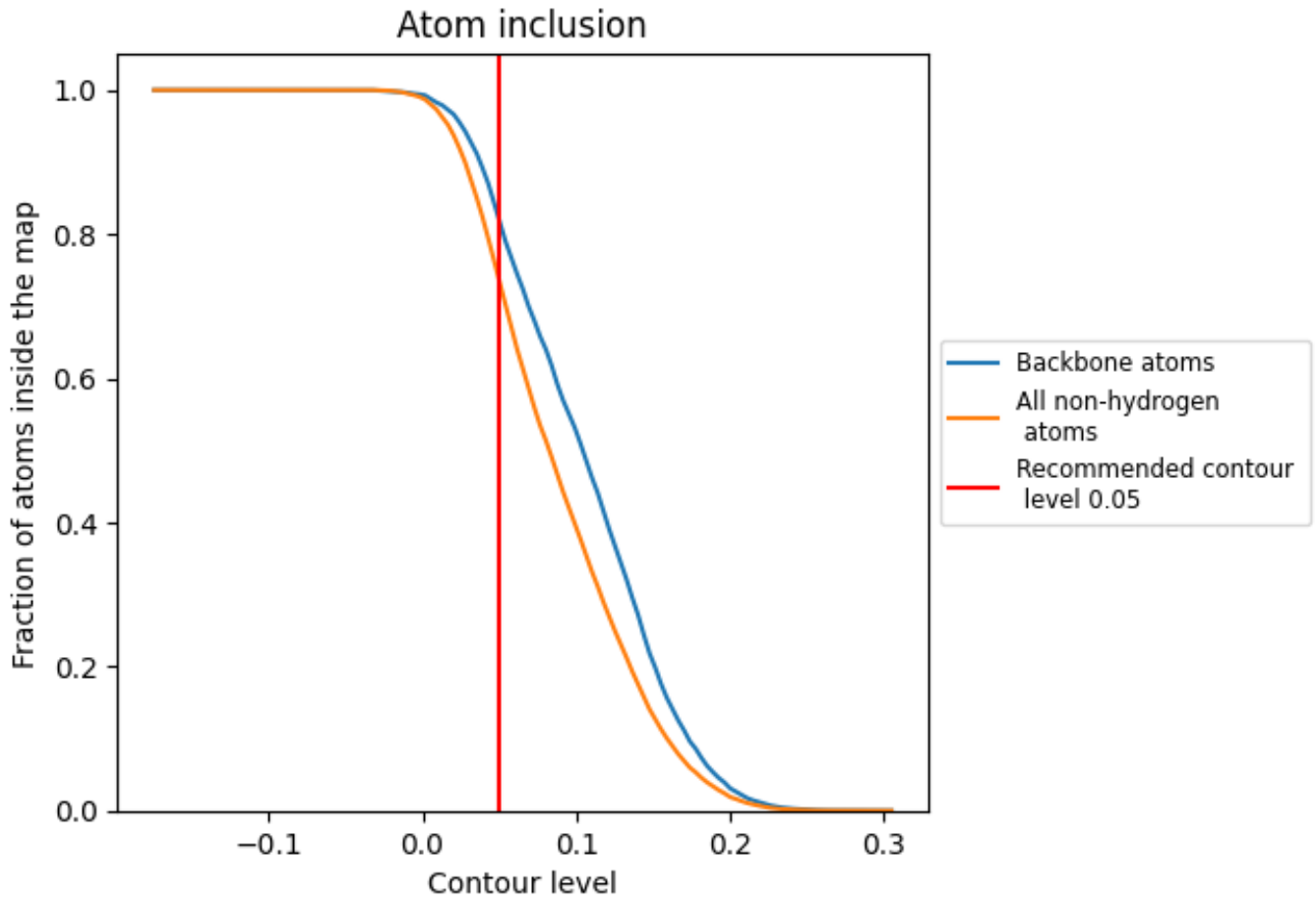
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.05).

9.4 Atom inclusion (i)



At the recommended contour level, 82% of all backbone atoms, 73% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7348	0.4520
A	0.7711	0.4680
B	0.7840	0.4940
C	0.7705	0.4680
D	0.7666	0.4680
E	0.7831	0.4940
F	0.7831	0.4930
G	0.6608	0.3990
H	0.6597	0.3990
I	0.6586	0.3980
J	0.6905	0.4160
K	0.6930	0.4160
L	0.6905	0.4170
M	0.4643	0.4090
N	0.4643	0.3090
O	0.3929	0.2730
P	0.6429	0.4330
Q	0.5833	0.4340
R	0.5357	0.4200
S	0.3421	0.3240
T	0.1786	0.1920
U	0.4643	0.4210
V	0.5000	0.3130
W	0.4286	0.2850
X	0.6429	0.4160
Y	0.5833	0.4420
Z	0.5714	0.4420
a	0.3421	0.3100
b	0.1429	0.2010
c	0.4643	0.4190
d	0.5000	0.2990
e	0.4286	0.2970
f	0.6786	0.4120
g	0.5833	0.4390
h	0.5357	0.4450

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Chain	Atom inclusion	Q-score
i	0.3421	0.3300
j	0.1786	0.1940