Full wwPDB EM Validation Report (i)

Nov 21, 2022 – 01:39 AM JST

PDB ID	:	7CWS
EMDB ID	:	EMD-30486
Title	:	SARS-CoV-2 Spike Proteins Trimer in Complex with FC05 and H014 Fabs Cocktail
Authors	:	Wang, L.; Wang, X.
Deposited on	:	2020-08-31
Resolution	:	3.40 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 (i) symbol.

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

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

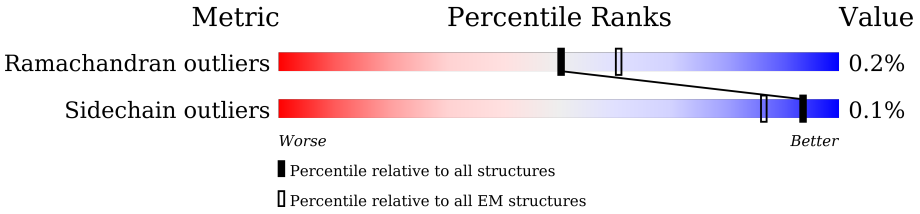
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

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 3.40 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)
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	L	120	98%
1	N	120	98%
1	P	120	98%
2	C	109	9%, 100%
2	K	109	11%, 100%
2	M	109	11%, 100%
3	D	107	22%, 98%
3	F	107	26%, 99%
3	H	107	28%, 99%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	E	122	100%
4	G	122	99%
4	I	122	100%
5	O	1134	94% 5%
5	Q	1134	94% 5%
5	R	1134	94% 5%
6	A	2	50% 50% 50%
6	B	2	100%
6	J	2	100%
6	S	2	100%
6	T	2	50% 100%
6	U	2	50% 50% 50%
6	V	2	100%
6	W	2	100%
6	X	2	100%
6	Y	2	100%
6	Z	2	50% 50% 50%
6	a	2	100%
6	b	2	100%
6	c	2	100%
6	d	2	100%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 36389 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 Heavy Chain of FC05 Fab.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	L	120	931	587	149	188	7	0	0
1	N	120	931	587	149	188	7	0	0
1	P	120	931	587	149	188	7	0	0

- Molecule 2 is a protein called Light Chain of FC05 Fab.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	C	109	789	492	132	163	2	0	0
2	K	109	789	492	132	163	2	0	0
2	M	109	789	492	132	163	2	0	0

- Molecule 3 is a protein called Light Chain of H014 Fab.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	D	107	844	540	140	162	2	0	0
3	F	107	844	540	140	162	2	0	0
3	H	107	844	540	140	162	2	0	0

- Molecule 4 is a protein called Heavy Chain of H014 Fab.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	E	122	939	598	148	189	4	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	G	122	939	598	148	189	4	0	0
4	I	122	939	598	148	189	4	0	0

- Molecule 5 is a protein called Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	O	1076	8414	5364	1406	1605	39	0	0
5	Q	1076	8411	5364	1403	1605	39	0	0
5	R	1076	8411	5364	1403	1605	39	0	0

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

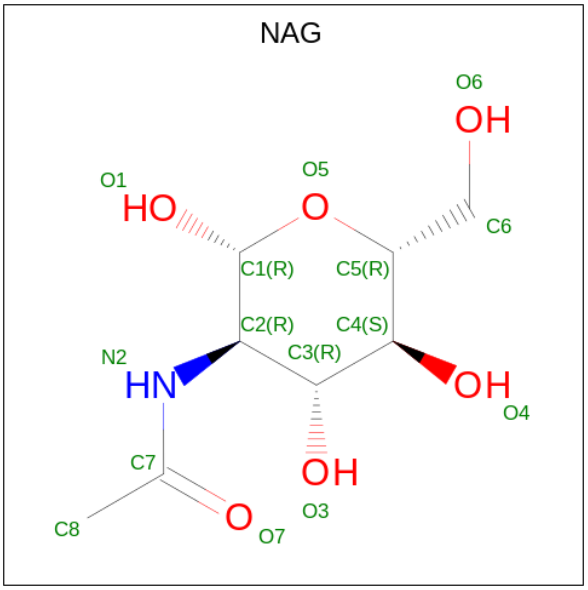
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
6	A	2	28	16	2	10	0	0
6	B	2	28	16	2	10	0	0
6	J	2	28	16	2	10	0	0
6	S	2	28	16	2	10	0	0
6	T	2	28	16	2	10	0	0
6	U	2	28	16	2	10	0	0
6	V	2	28	16	2	10	0	0
6	W	2	28	16	2	10	0	0
6	X	2	28	16	2	10	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
6	Y	2	28	16	2	10	0	0
			Total	C	N	O		
6	Z	2	28	16	2	10	0	0
			Total	C	N	O		
6	a	2	28	16	2	10	0	0
			Total	C	N	O		
6	b	2	28	16	2	10	0	0
			Total	C	N	O		
6	c	2	28	16	2	10	0	0
			Total	C	N	O		
6	d	2	28	16	2	10	0	0

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
7	O	1	70	40	5	25	0
			Total	C	N	O	
7	O	1	70	40	5	25	0
			Total	C	N	O	
7	O	1	70	40	5	25	0
			Total	C	N	O	
7	O	1	70	40	5	25	0
			Total	C	N	O	
7	O	1	70	40	5	25	0

Continued on next page...

Continued from previous page...

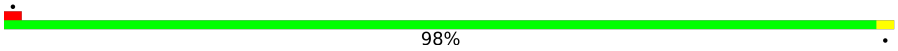
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
7	Q	1	84	48	6	30	0
7	Q	1	84	48	6	30	0
7	Q	1	84	48	6	30	0
7	Q	1	84	48	6	30	0
7	Q	1	84	48	6	30	0
7	Q	1	84	48	6	30	0
7	R	1	70	40	5	25	0
7	R	1	70	40	5	25	0
7	R	1	70	40	5	25	0
7	R	1	70	40	5	25	0
7	R	1	70	40	5	25	0

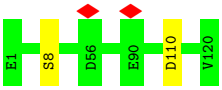
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and 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: Heavy Chain of FC05 Fab

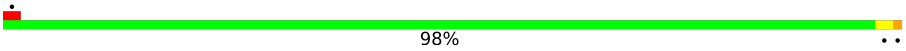
Chain L:

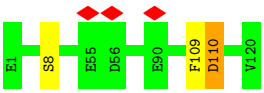




- Molecule 1: Heavy Chain of FC05 Fab

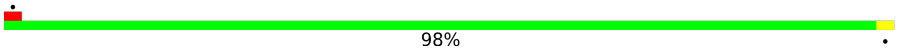
Chain N:

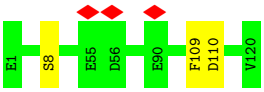




- Molecule 1: Heavy Chain of FC05 Fab

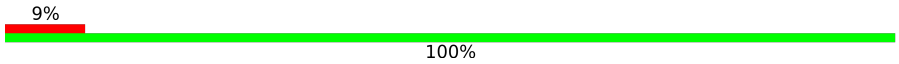
Chain P:

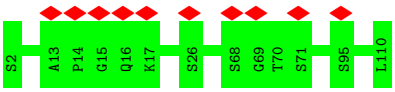




- Molecule 2: Light Chain of FC05 Fab

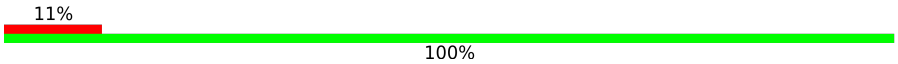
Chain C:

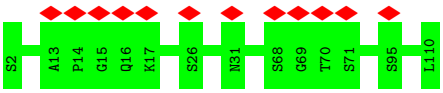




- Molecule 2: Light Chain of FC05 Fab

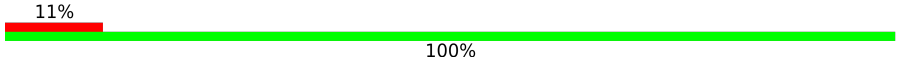
Chain K:

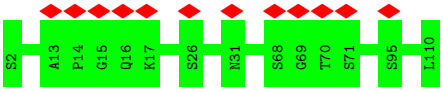




- Molecule 2: Light Chain of FC05 Fab

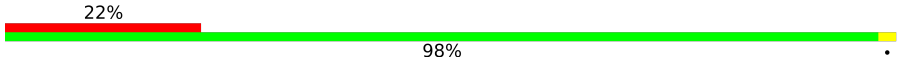
Chain M:

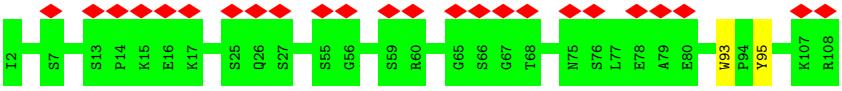




- Molecule 3: Light Chain of H014 Fab

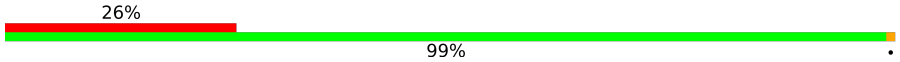
Chain D:

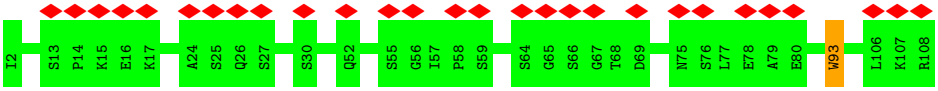




- Molecule 3: Light Chain of H014 Fab

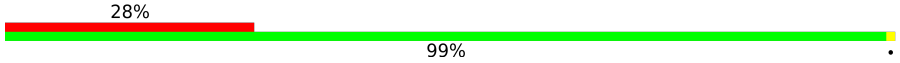
Chain F:

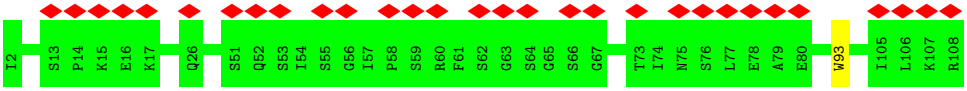




- Molecule 3: Light Chain of H014 Fab

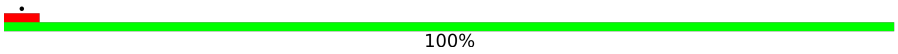
Chain H:

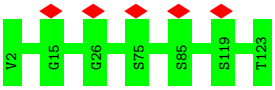




- Molecule 4: Heavy Chain of H014 Fab

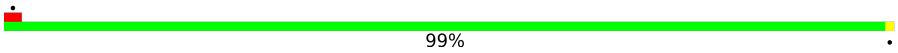
Chain E:

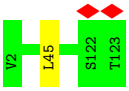




- Molecule 4: Heavy Chain of H014 Fab

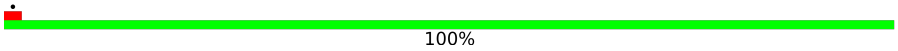
Chain G:

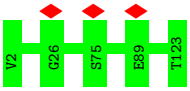




- Molecule 4: Heavy Chain of H014 Fab

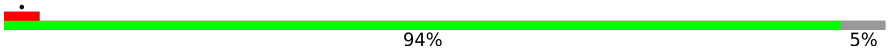
Chain I:

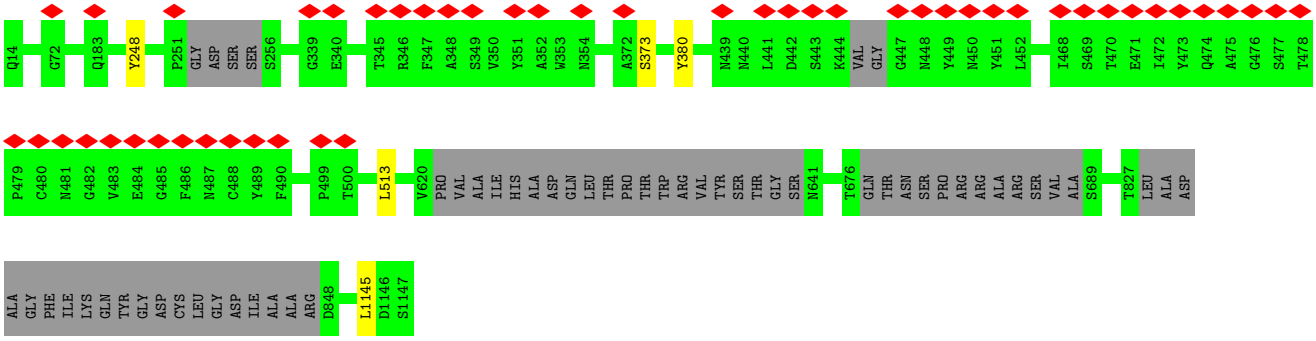




• Molecule 5: Spike glycoprotein

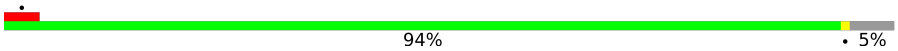
Chain O:

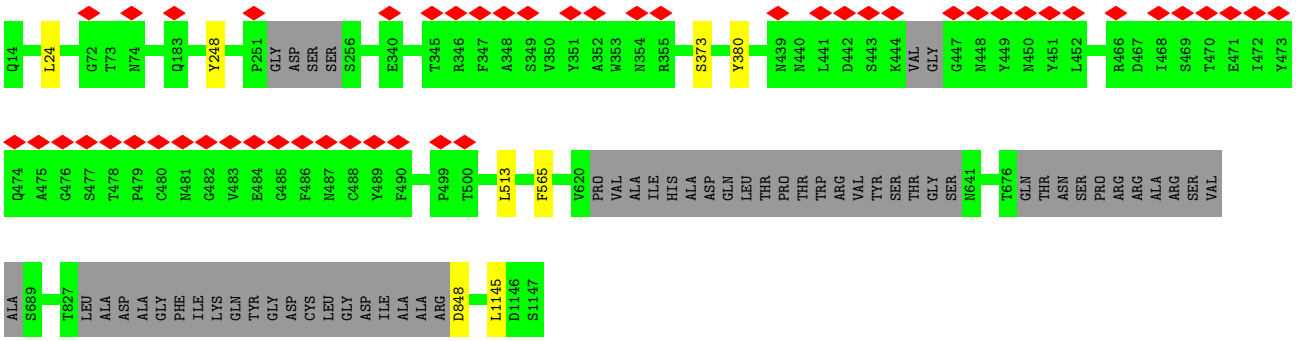




• Molecule 5: Spike glycoprotein

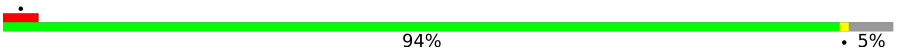
Chain Q:

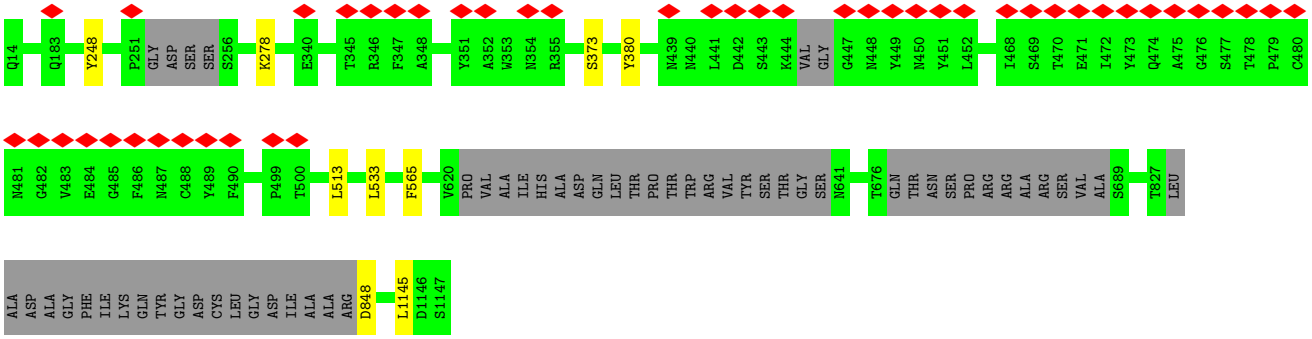




• Molecule 5: Spike glycoprotein

Chain R:

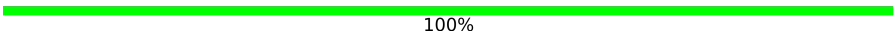




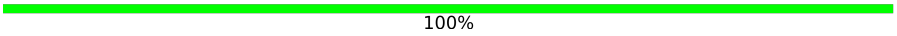
• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain A:

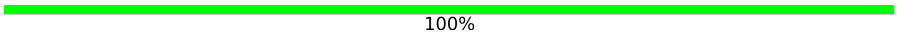
• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain B: 

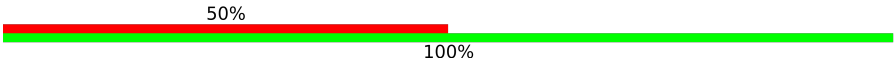
• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J: 

• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain S: 

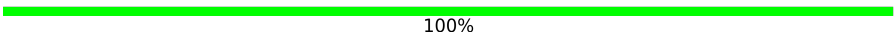
• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain T: 

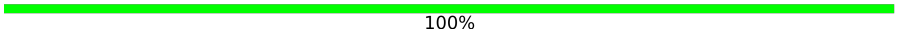
• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain U:

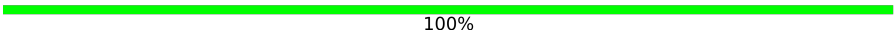
• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain V: 

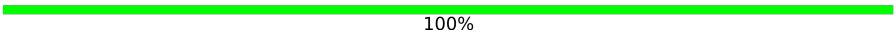
• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain W: 

• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain X: 

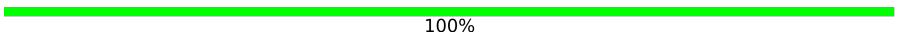
• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Y: 

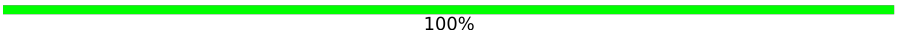
• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Z:

• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain a: 

• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain b: 

• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain c: 100%

NAG1
NAG2

• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain d: 100%

NAG1
NAG2

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	99382	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 ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.047	Depositor
Minimum map value	-0.012	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.003	Depositor
Map size (Å)	312.0, 312.0, 312.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.04, 1.04, 1.04	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	L	0.36	0/955	0.57	0/1299
1	N	0.37	0/955	0.59	1/1299 (0.1%)
1	P	0.37	0/955	0.58	0/1299
2	C	0.31	0/805	0.52	0/1097
2	K	0.32	0/805	0.52	0/1097
2	M	0.33	0/805	0.52	0/1097
3	D	0.40	0/865	0.67	1/1171 (0.1%)
3	F	0.45	0/865	0.72	2/1171 (0.2%)
3	H	0.41	0/865	0.63	0/1171
4	E	0.43	0/963	0.63	0/1311
4	G	0.45	0/963	0.69	1/1311 (0.1%)
4	I	0.43	0/963	0.61	0/1311
5	O	0.48	0/8606	0.61	1/11709 (0.0%)
5	Q	0.46	0/8603	0.59	2/11706 (0.0%)
5	R	0.47	0/8603	0.60	2/11706 (0.0%)
All	All	0.45	0/36576	0.60	10/49755 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	L	0	2
1	N	0	1
1	P	0	1
5	O	0	3
5	Q	0	4
5	R	0	5
All	All	0	16

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	95	TYR	CB-CA-C	6.93	124.25	110.40
3	F	93	TRP	CB-CA-C	6.77	123.94	110.40
3	F	93	TRP	CA-CB-CG	6.14	125.36	113.70
5	R	513	LEU	CA-CB-CG	5.61	128.20	115.30
5	O	513	LEU	CA-CB-CG	5.60	128.19	115.30
5	Q	513	LEU	CA-CB-CG	5.59	128.15	115.30
1	N	110	ASP	CB-CA-C	5.51	121.42	110.40
4	G	45	LEU	CA-CB-CG	5.47	127.89	115.30
5	Q	848	ASP	CB-CG-OD2	5.26	123.03	118.30
5	R	848	ASP	CB-CG-OD2	5.17	122.95	118.30

There are no chirality outliers.

All (16) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	L	110	ASP	Sidechain
1	L	8	SER	Peptide
1	N	8	SER	Peptide
5	O	1145	LEU	Peptide
5	O	248	TYR	Peptide
5	O	380	TYR	Peptide
1	P	8	SER	Peptide
5	Q	1145	LEU	Peptide
5	Q	248	TYR	Peptide
5	Q	380	TYR	Peptide
5	Q	565	PHE	Peptide
5	R	1145	LEU	Peptide
5	R	248	TYR	Peptide
5	R	278	LYS	Mainchain
5	R	380	TYR	Peptide
5	R	565	PHE	Peptide

5.2 Too-close contacts (i)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	L	118/120 (98%)	112 (95%)	6 (5%)	0	100	100
1	N	118/120 (98%)	109 (92%)	8 (7%)	1 (1%)	19	51
1	P	118/120 (98%)	108 (92%)	9 (8%)	1 (1%)	19	51
2	C	107/109 (98%)	101 (94%)	6 (6%)	0	100	100
2	K	107/109 (98%)	101 (94%)	6 (6%)	0	100	100
2	M	107/109 (98%)	100 (94%)	7 (6%)	0	100	100
3	D	105/107 (98%)	98 (93%)	6 (6%)	1 (1%)	15	46
3	F	105/107 (98%)	99 (94%)	5 (5%)	1 (1%)	15	46
3	H	105/107 (98%)	99 (94%)	5 (5%)	1 (1%)	15	46
4	E	120/122 (98%)	118 (98%)	2 (2%)	0	100	100
4	G	120/122 (98%)	114 (95%)	6 (5%)	0	100	100
4	I	120/122 (98%)	118 (98%)	2 (2%)	0	100	100
5	O	1064/1134 (94%)	979 (92%)	84 (8%)	1 (0%)	51	82
5	Q	1064/1134 (94%)	988 (93%)	74 (7%)	2 (0%)	47	78
5	R	1064/1134 (94%)	979 (92%)	84 (8%)	1 (0%)	51	82
All	All	4542/4776 (95%)	4223 (93%)	310 (7%)	9 (0%)	50	78

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	D	93	TRP
3	F	93	TRP
3	H	93	TRP
1	N	110	ASP
5	O	373	SER
5	R	373	SER
1	P	110	ASP
5	Q	373	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	Q	24	LEU

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	L	101/101 (100%)	101 (100%)	0	100	100
1	N	101/101 (100%)	100 (99%)	1 (1%)	76	88
1	P	101/101 (100%)	100 (99%)	1 (1%)	76	88
2	C	88/88 (100%)	88 (100%)	0	100	100
2	K	88/88 (100%)	88 (100%)	0	100	100
2	M	88/88 (100%)	88 (100%)	0	100	100
3	D	96/97 (99%)	96 (100%)	0	100	100
3	F	96/97 (99%)	96 (100%)	0	100	100
3	H	96/97 (99%)	96 (100%)	0	100	100
4	E	101/102 (99%)	101 (100%)	0	100	100
4	G	101/102 (99%)	101 (100%)	0	100	100
4	I	101/102 (99%)	101 (100%)	0	100	100
5	O	940/985 (95%)	940 (100%)	0	100	100
5	Q	940/985 (95%)	940 (100%)	0	100	100
5	R	940/985 (95%)	939 (100%)	1 (0%)	93	98
All	All	3978/4119 (97%)	3975 (100%)	3 (0%)	93	98

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	N	109	PHE
1	P	109	PHE
5	R	533	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (56)

such sidechains are listed below:

Mol	Chain	Res	Type
1	L	7	GLN
2	C	6	GLN
3	D	99	GLN
3	F	6	GLN
3	F	10	GLN
3	F	99	GLN
4	G	31	ASN
4	G	55	ASN
3	H	91	ASN
3	H	99	GLN
1	N	7	GLN
2	K	6	GLN
1	P	7	GLN
2	M	6	GLN
2	M	52	ASN
5	O	61	ASN
5	O	66	HIS
5	O	146	HIS
5	O	148	ASN
5	O	234	ASN
5	O	239	GLN
5	O	282	ASN
5	O	317	ASN
5	O	354	ASN
5	O	437	ASN
5	O	655	HIS
5	O	853	GLN
5	O	901	GLN
5	O	913	GLN
5	O	1119	ASN
5	O	1135	ASN
5	Q	122	ASN
5	Q	234	ASN
5	Q	239	GLN
5	Q	317	ASN
5	Q	354	ASN
5	Q	437	ASN
5	Q	779	GLN
5	Q	804	GLN
5	Q	853	GLN
5	Q	901	GLN
5	Q	935	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	Q	1011	GLN
5	R	121	ASN
5	R	234	ASN
5	R	239	GLN
5	R	317	ASN
5	R	414	GLN
5	R	437	ASN
5	R	779	GLN
5	R	804	GLN
5	R	853	GLN
5	R	901	GLN
5	R	913	GLN
5	R	935	GLN
5	R	1011	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

30 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	$\#\|Z\| > 2$
6	NAG	A	1	5,6	14,14,15	1.20	1 (7%)	17,19,21	1.10	2 (11%)
6	NAG	A	2	6	14,14,15	0.35	0	17,19,21	0.44	0
6	NAG	B	1	5,6	14,14,15	0.52	0	17,19,21	0.46	0
6	NAG	B	2	6	14,14,15	0.34	0	17,19,21	0.39	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	NAG	J	1	5,6	14,14,15	0.47	0	17,19,21	0.45	0
6	NAG	J	2	6	14,14,15	0.27	0	17,19,21	0.36	0
6	NAG	S	1	5,6	14,14,15	0.43	0	17,19,21	0.45	0
6	NAG	S	2	6	14,14,15	0.29	0	17,19,21	0.37	0
6	NAG	T	1	5,6	14,14,15	0.27	0	17,19,21	0.69	0
6	NAG	T	2	6	14,14,15	0.26	0	17,19,21	0.70	0
6	NAG	U	1	5,6	14,14,15	1.65	1 (7%)	17,19,21	1.39	2 (11%)
6	NAG	U	2	6	14,14,15	0.21	0	17,19,21	0.52	0
6	NAG	V	1	5,6	14,14,15	0.33	0	17,19,21	0.49	0
6	NAG	V	2	6	14,14,15	0.32	0	17,19,21	0.40	0
6	NAG	W	1	5,6	14,14,15	0.49	0	17,19,21	0.44	0
6	NAG	W	2	6	14,14,15	0.17	0	17,19,21	0.45	0
6	NAG	X	1	5,6	14,14,15	0.50	0	17,19,21	0.51	0
6	NAG	X	2	6	14,14,15	0.26	0	17,19,21	0.38	0
6	NAG	Y	1	5,6	14,14,15	0.50	0	17,19,21	0.39	0
6	NAG	Y	2	6	14,14,15	0.24	0	17,19,21	0.43	0
6	NAG	Z	1	6	14,14,15	1.66	1 (7%)	17,19,21	1.39	2 (11%)
6	NAG	Z	2	6	14,14,15	0.22	0	17,19,21	0.50	0
6	NAG	a	1	5,6	14,14,15	0.35	0	17,19,21	0.46	0
6	NAG	a	2	6	14,14,15	0.33	0	17,19,21	0.39	0
6	NAG	b	1	5,6	14,14,15	0.49	0	17,19,21	0.45	0
6	NAG	b	2	6	14,14,15	0.21	0	17,19,21	0.46	0
6	NAG	c	1	5,6	14,14,15	0.46	0	17,19,21	0.39	0
6	NAG	c	2	6	14,14,15	0.29	0	17,19,21	0.43	0
6	NAG	d	1	5,6	14,14,15	0.30	0	17,19,21	1.00	1 (5%)
6	NAG	d	2	6	14,14,15	0.47	0	17,19,21	1.21	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
6	NAG	A	1	5,6	-	2/6/23/26	0/1/1/1
6	NAG	A	2	6	-	2/6/23/26	0/1/1/1
6	NAG	B	1	5,6	-	0/6/23/26	0/1/1/1
6	NAG	B	2	6	-	2/6/23/26	0/1/1/1
6	NAG	J	1	5,6	-	2/6/23/26	0/1/1/1
6	NAG	J	2	6	-	2/6/23/26	0/1/1/1
6	NAG	S	1	5,6	-	2/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	S	2	6	-	2/6/23/26	0/1/1/1
6	NAG	T	1	5,6	-	3/6/23/26	0/1/1/1
6	NAG	T	2	6	-	2/6/23/26	0/1/1/1
6	NAG	U	1	5,6	-	4/6/23/26	0/1/1/1
6	NAG	U	2	6	-	0/6/23/26	0/1/1/1
6	NAG	V	1	5,6	-	2/6/23/26	0/1/1/1
6	NAG	V	2	6	-	2/6/23/26	0/1/1/1
6	NAG	W	1	5,6	-	2/6/23/26	0/1/1/1
6	NAG	W	2	6	-	2/6/23/26	0/1/1/1
6	NAG	X	1	5,6	-	0/6/23/26	0/1/1/1
6	NAG	X	2	6	-	1/6/23/26	0/1/1/1
6	NAG	Y	1	5,6	-	0/6/23/26	0/1/1/1
6	NAG	Y	2	6	-	2/6/23/26	0/1/1/1
6	NAG	Z	1	6	-	4/6/23/26	0/1/1/1
6	NAG	Z	2	6	-	0/6/23/26	0/1/1/1
6	NAG	a	1	5,6	-	2/6/23/26	0/1/1/1
6	NAG	a	2	6	-	2/6/23/26	0/1/1/1
6	NAG	b	1	5,6	-	2/6/23/26	0/1/1/1
6	NAG	b	2	6	-	2/6/23/26	0/1/1/1
6	NAG	c	1	5,6	-	0/6/23/26	0/1/1/1
6	NAG	c	2	6	-	2/6/23/26	0/1/1/1
6	NAG	d	1	5,6	-	3/6/23/26	0/1/1/1
6	NAG	d	2	6	-	0/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	Z	1	NAG	O5-C1	-5.99	1.34	1.43
6	U	1	NAG	O5-C1	-5.96	1.34	1.43
6	A	1	NAG	O5-C1	-3.88	1.37	1.43

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	d	2	NAG	C1-O5-C5	3.71	117.21	112.19
6	Z	1	NAG	C3-C4-C5	3.67	116.79	110.24
6	U	1	NAG	C3-C4-C5	3.65	116.76	110.24
6	A	1	NAG	C3-C4-C5	3.22	115.98	110.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	d	1	NAG	C4-C3-C2	-2.63	107.16	111.02
6	d	2	NAG	C1-C2-N2	2.44	114.66	110.49
6	U	1	NAG	C1-O5-C5	-2.27	109.11	112.19
6	Z	1	NAG	C1-O5-C5	-2.26	109.13	112.19
6	A	1	NAG	O4-C4-C5	-2.04	104.23	109.30

There are no chirality outliers.

All (51) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	T	1	NAG	C8-C7-N2-C2
6	T	1	NAG	O7-C7-N2-C2
6	d	1	NAG	C8-C7-N2-C2
6	d	1	NAG	O7-C7-N2-C2
6	V	2	NAG	O5-C5-C6-O6
6	a	2	NAG	O5-C5-C6-O6
6	J	1	NAG	O5-C5-C6-O6
6	A	1	NAG	C4-C5-C6-O6
6	V	2	NAG	C4-C5-C6-O6
6	a	2	NAG	C4-C5-C6-O6
6	S	2	NAG	O5-C5-C6-O6
6	W	2	NAG	O5-C5-C6-O6
6	b	2	NAG	O5-C5-C6-O6
6	V	1	NAG	O5-C5-C6-O6
6	a	1	NAG	O5-C5-C6-O6
6	J	1	NAG	C4-C5-C6-O6
6	U	1	NAG	C1-C2-N2-C7
6	Z	1	NAG	C1-C2-N2-C7
6	V	1	NAG	C4-C5-C6-O6
6	a	1	NAG	C4-C5-C6-O6
6	A	2	NAG	C4-C5-C6-O6
6	W	2	NAG	C4-C5-C6-O6
6	b	2	NAG	C4-C5-C6-O6
6	A	1	NAG	O5-C5-C6-O6
6	W	1	NAG	O5-C5-C6-O6
6	b	1	NAG	O5-C5-C6-O6
6	c	2	NAG	C4-C5-C6-O6
6	U	1	NAG	C4-C5-C6-O6
6	Y	2	NAG	C4-C5-C6-O6
6	Z	1	NAG	C4-C5-C6-O6
6	A	2	NAG	O5-C5-C6-O6
6	S	2	NAG	C4-C5-C6-O6

Continued on next page...

Continued from previous page...

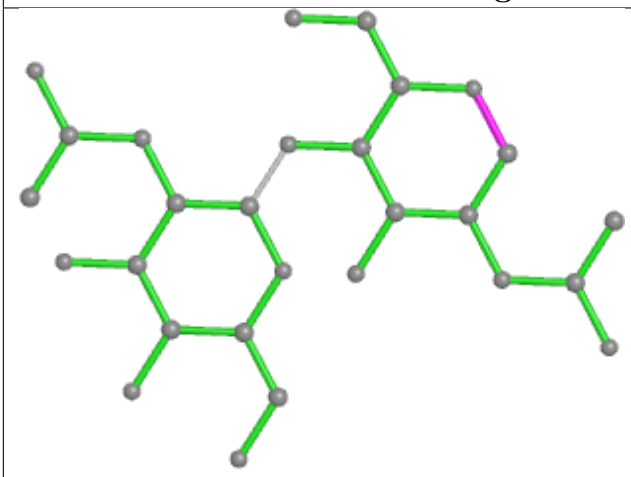
Mol	Chain	Res	Type	Atoms
6	b	1	NAG	C4-C5-C6-O6
6	T	1	NAG	C1-C2-N2-C7
6	W	1	NAG	C4-C5-C6-O6
6	T	2	NAG	C1-C2-N2-C7
6	B	2	NAG	C4-C5-C6-O6
6	J	2	NAG	C4-C5-C6-O6
6	c	2	NAG	O5-C5-C6-O6
6	Y	2	NAG	O5-C5-C6-O6
6	X	2	NAG	O5-C5-C6-O6
6	d	1	NAG	O5-C5-C6-O6
6	S	1	NAG	C4-C5-C6-O6
6	T	2	NAG	C3-C2-N2-C7
6	B	2	NAG	O5-C5-C6-O6
6	J	2	NAG	O5-C5-C6-O6
6	Z	1	NAG	O5-C5-C6-O6
6	U	1	NAG	O5-C5-C6-O6
6	S	1	NAG	O5-C5-C6-O6
6	U	1	NAG	C3-C2-N2-C7
6	Z	1	NAG	C3-C2-N2-C7

There are no ring outliers.

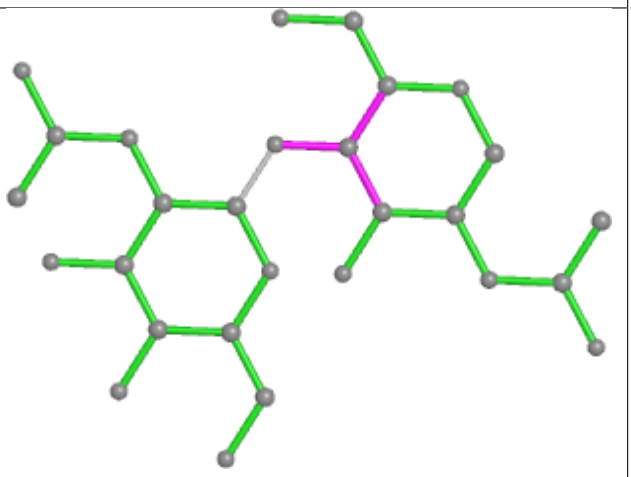
No monomer is involved in short contacts.

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

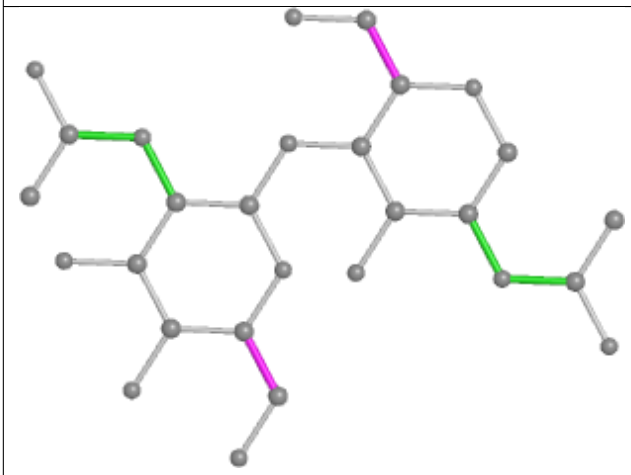
Oligosaccharide Chain A



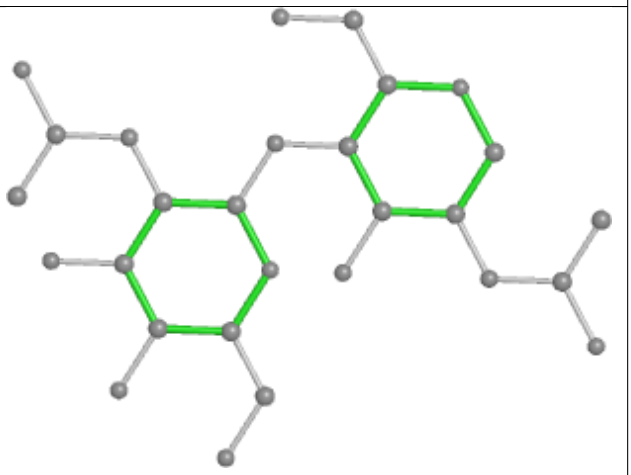
Bond lengths



Bond angles

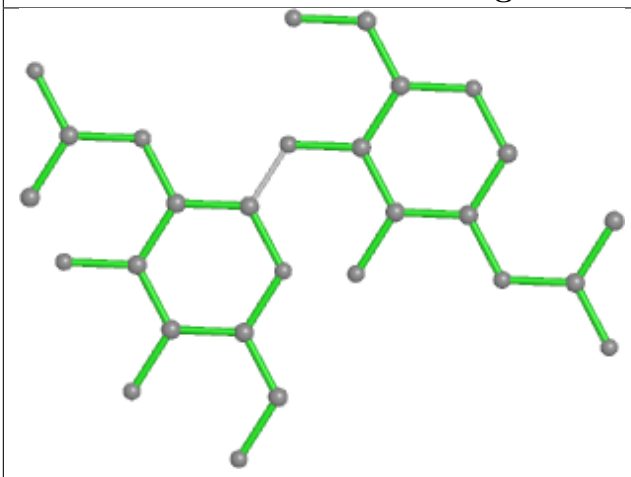


Torsions

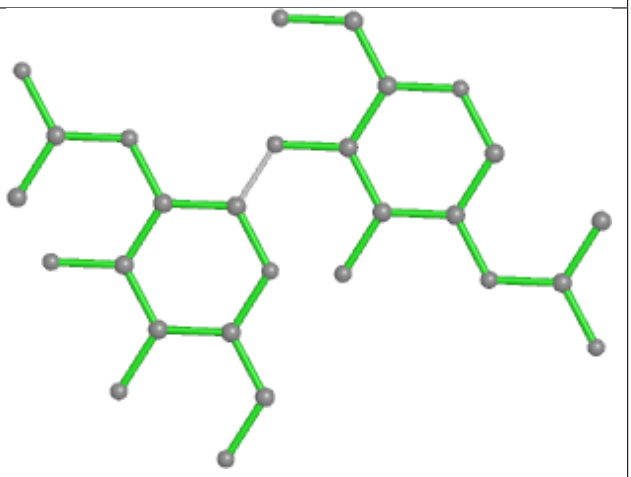


Rings

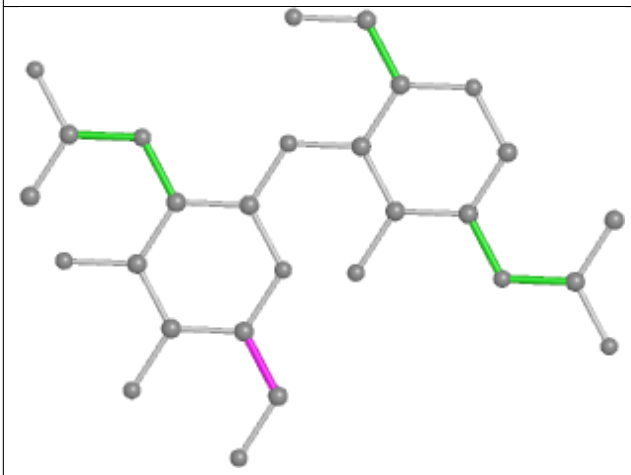
Oligosaccharide Chain B



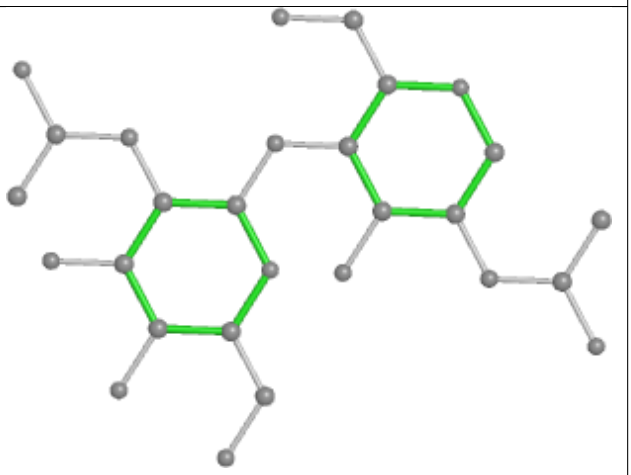
Bond lengths



Bond angles

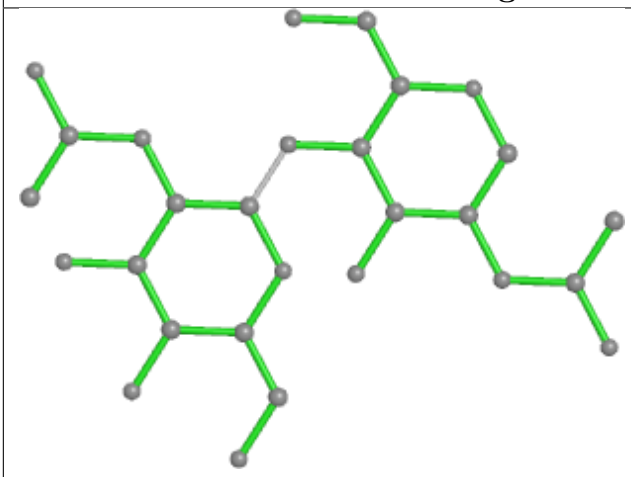


Torsions

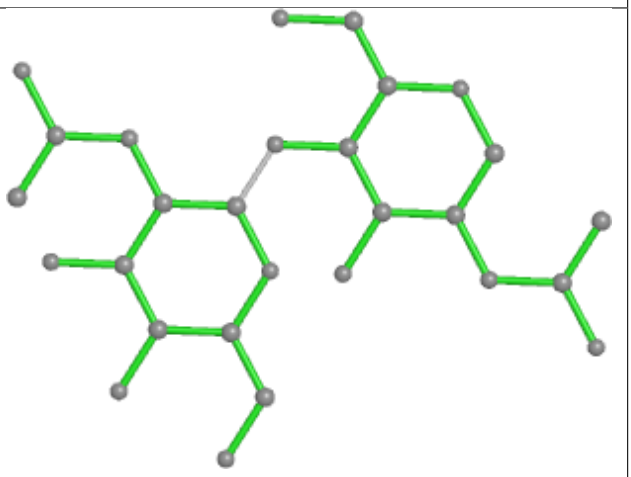


Rings

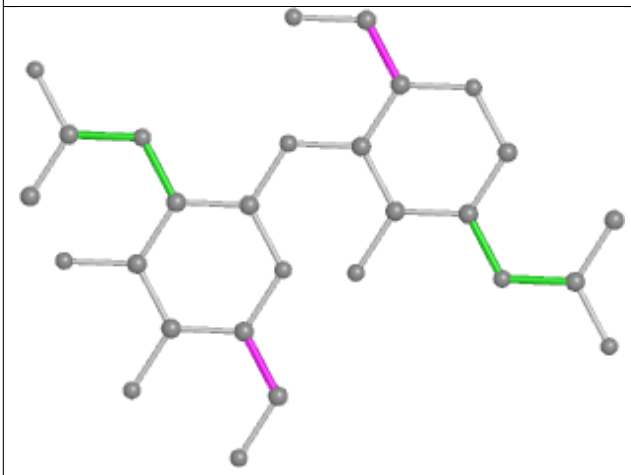
Oligosaccharide Chain J



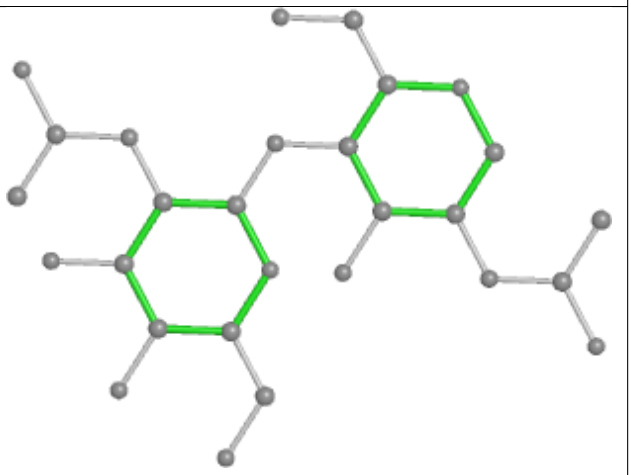
Bond lengths



Bond angles

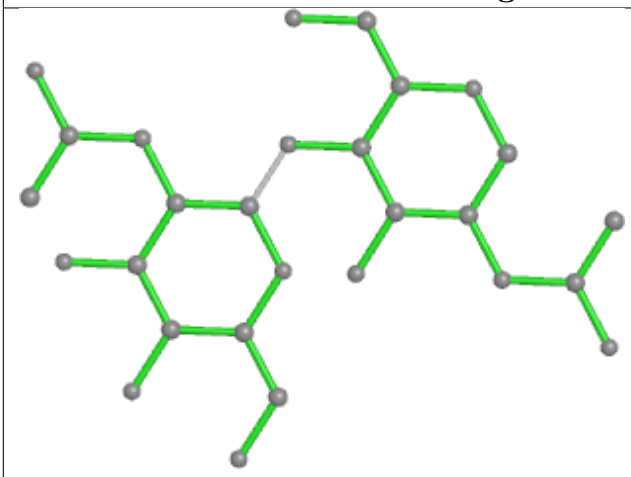


Torsions

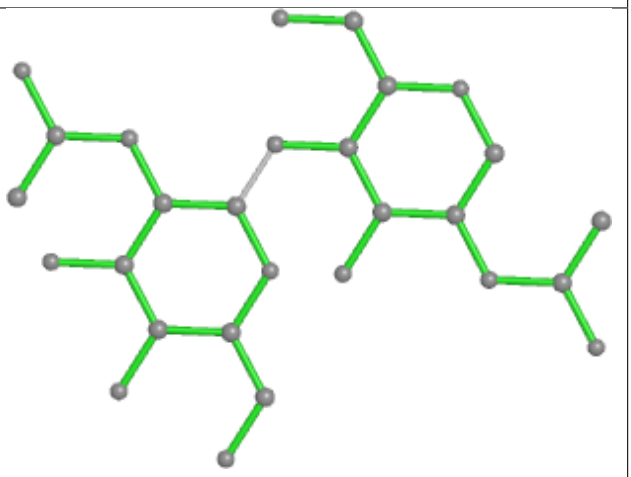


Rings

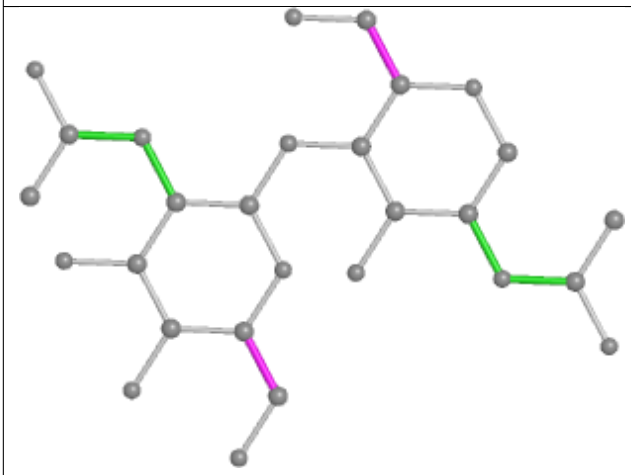
Oligosaccharide Chain S



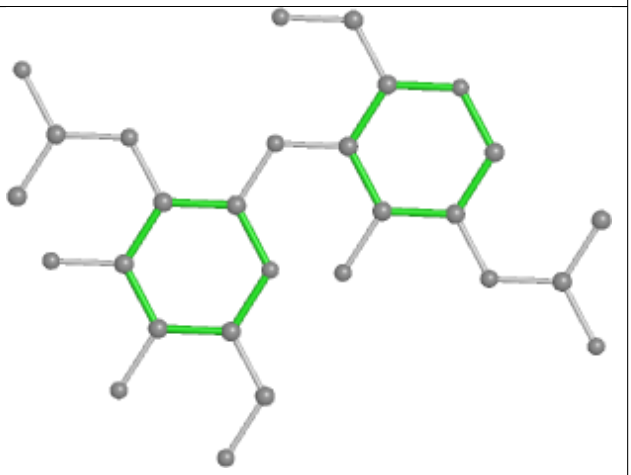
Bond lengths



Bond angles

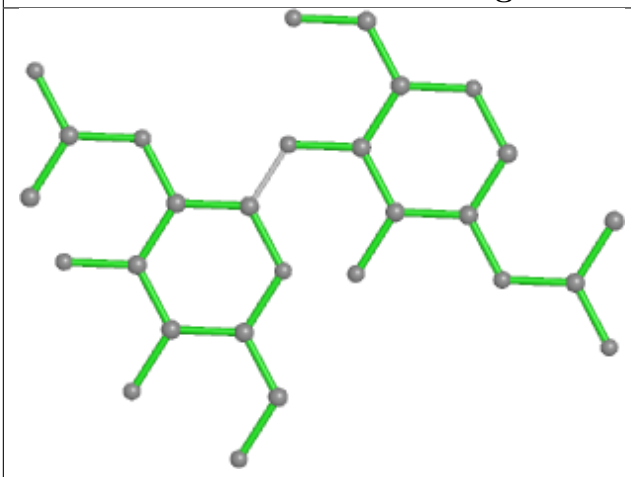


Torsions

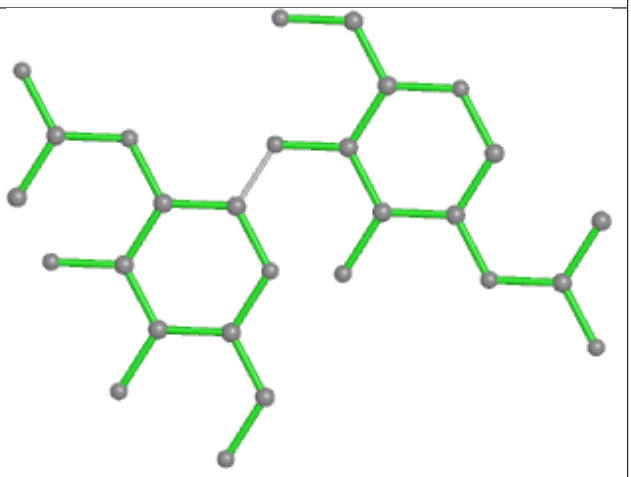


Rings

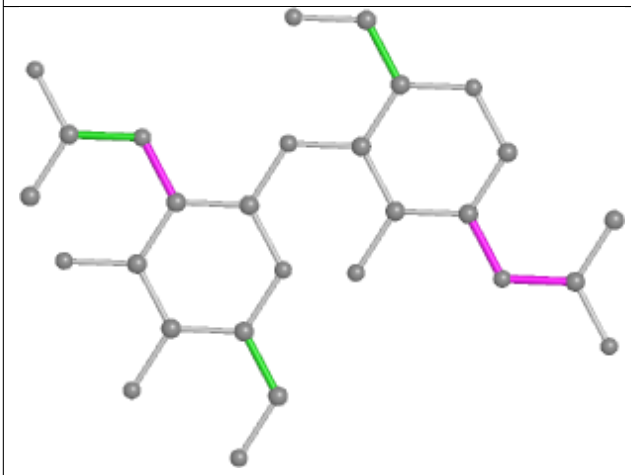
Oligosaccharide Chain T



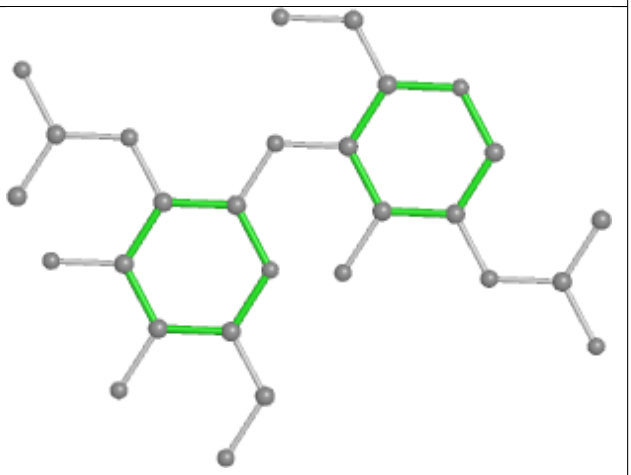
Bond lengths



Bond angles

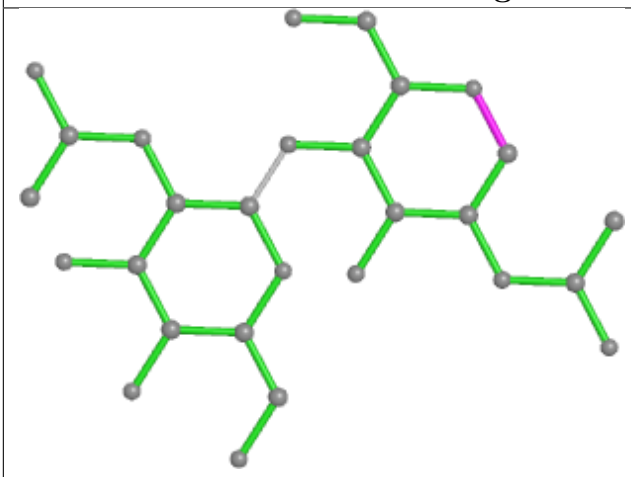


Torsions

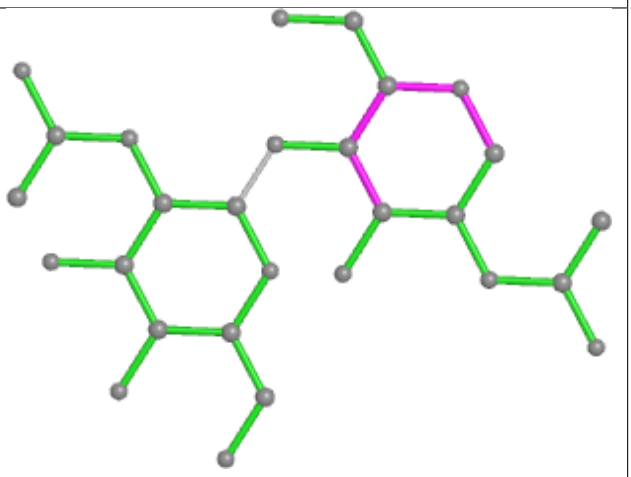


Rings

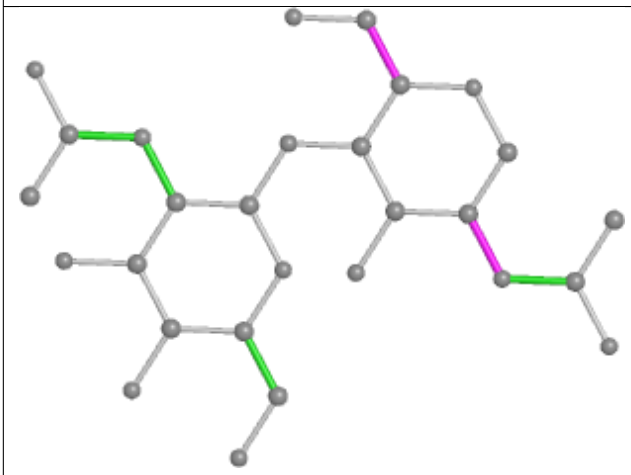
Oligosaccharide Chain U



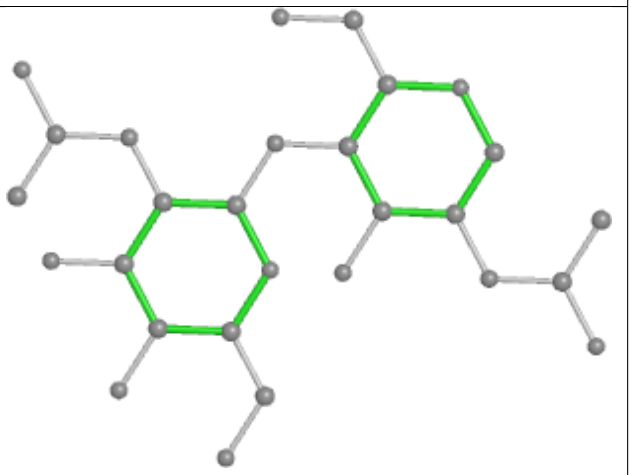
Bond lengths



Bond angles

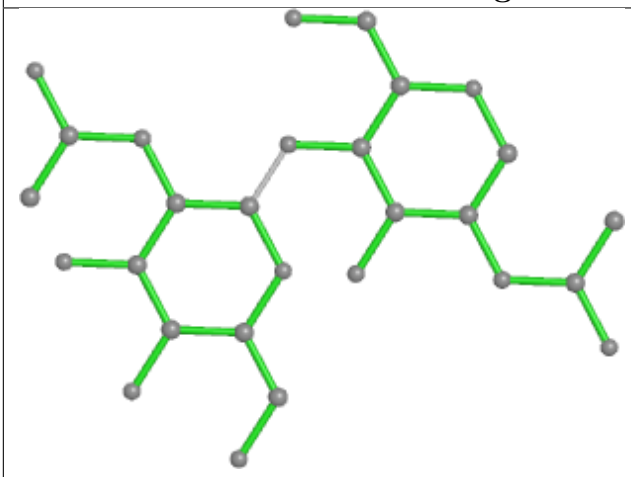


Torsions

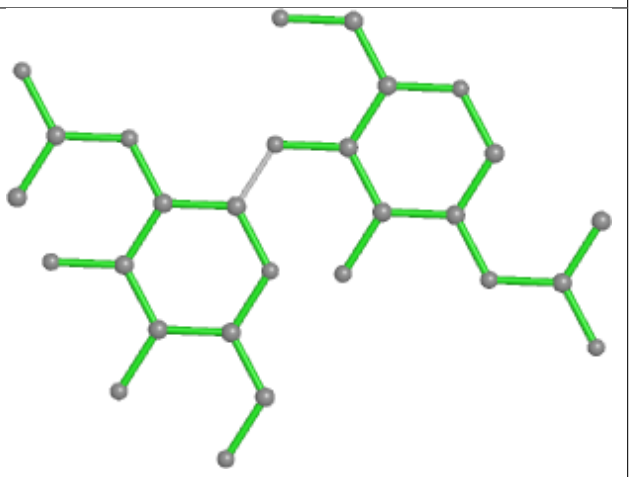


Rings

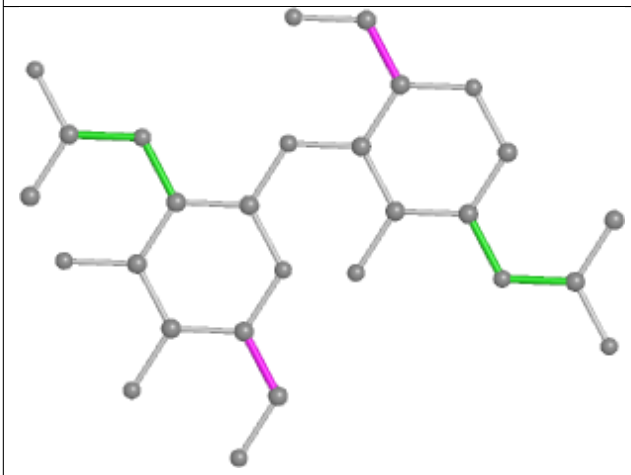
Oligosaccharide Chain V



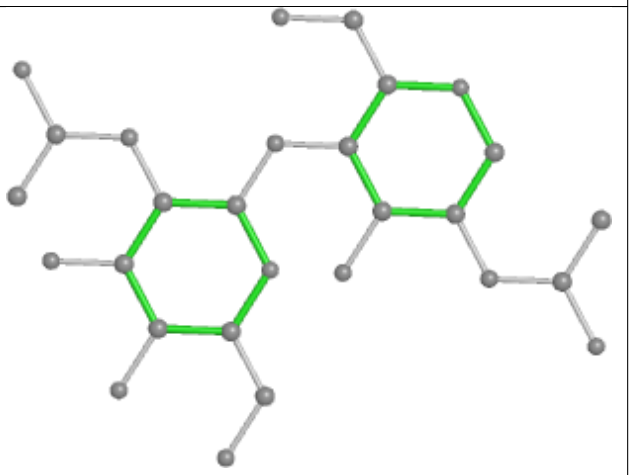
Bond lengths



Bond angles

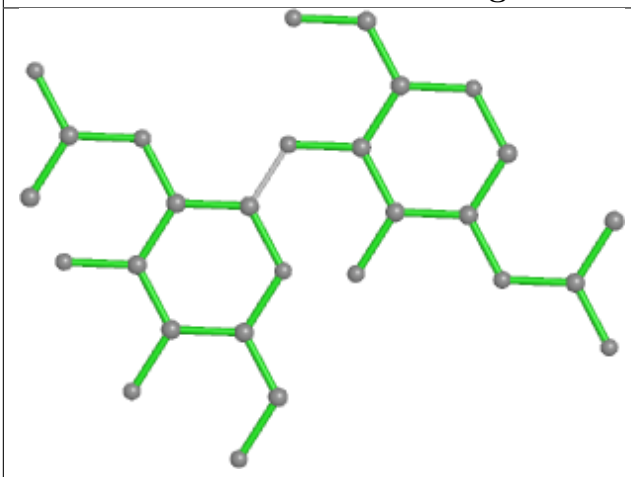


Torsions

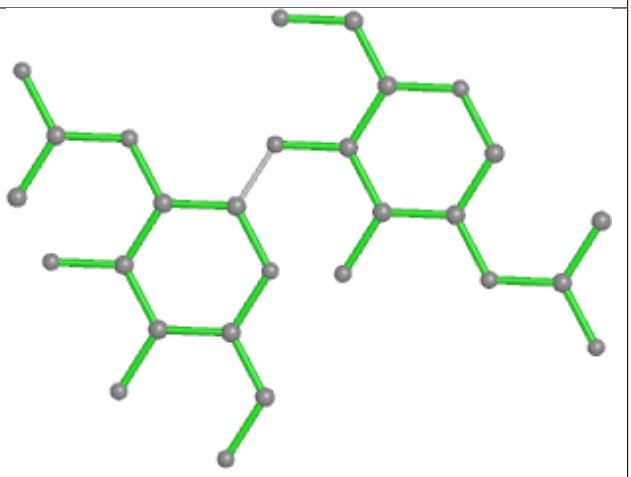


Rings

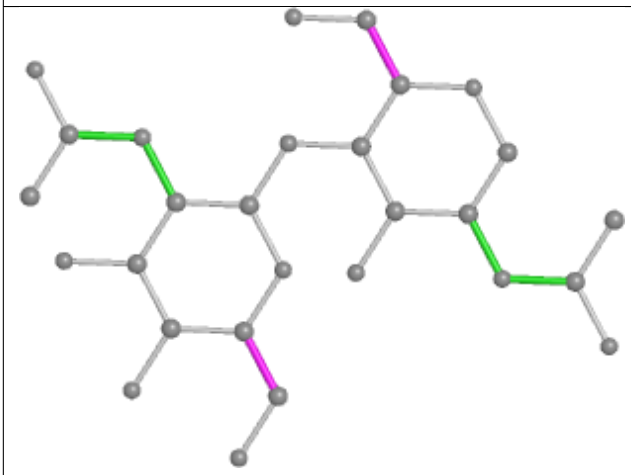
Oligosaccharide Chain W



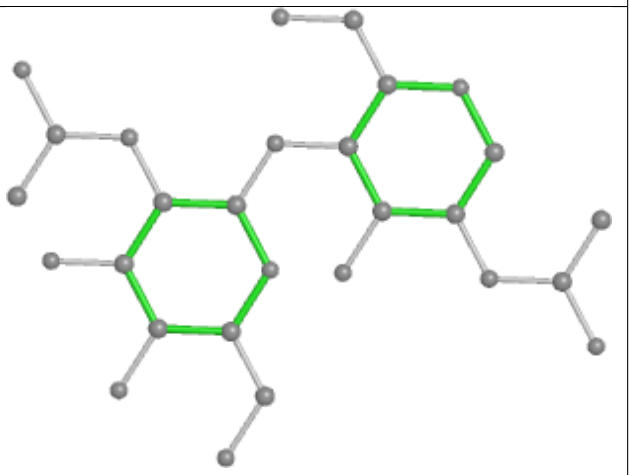
Bond lengths



Bond angles

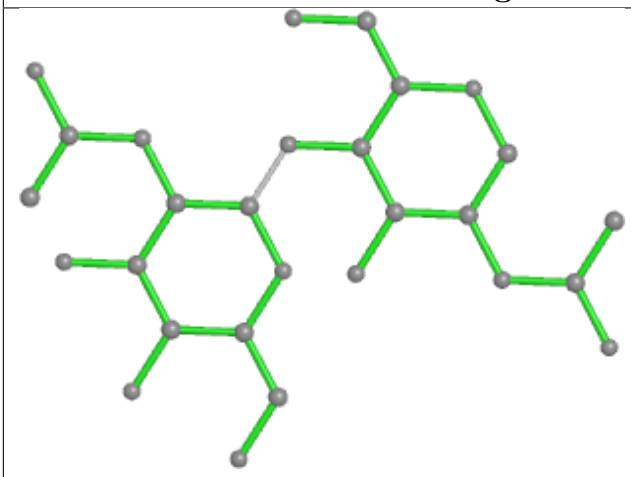


Torsions

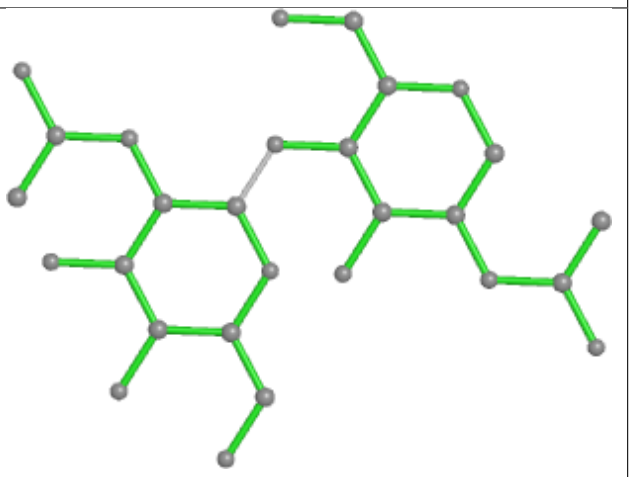


Rings

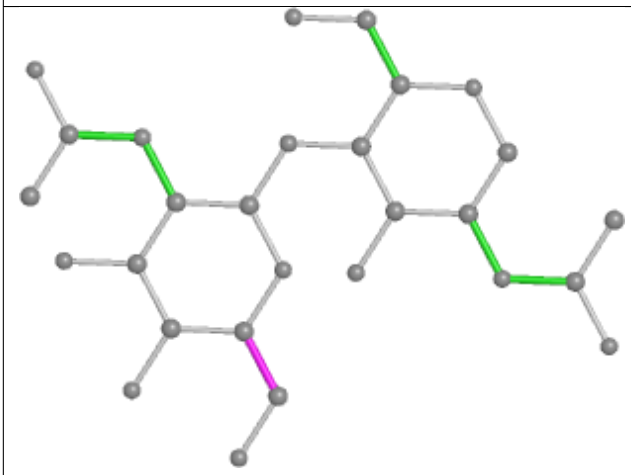
Oligosaccharide Chain X



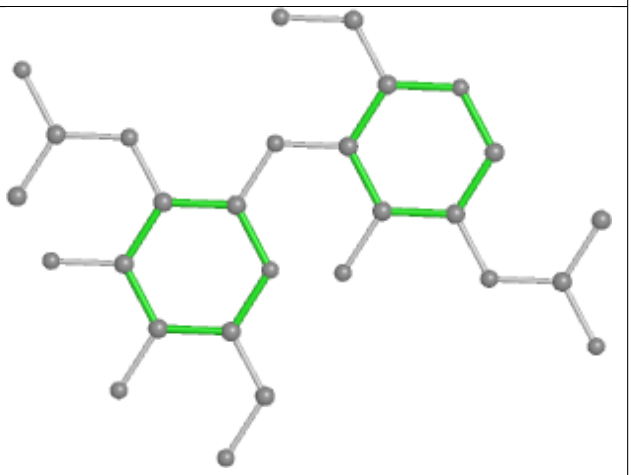
Bond lengths



Bond angles

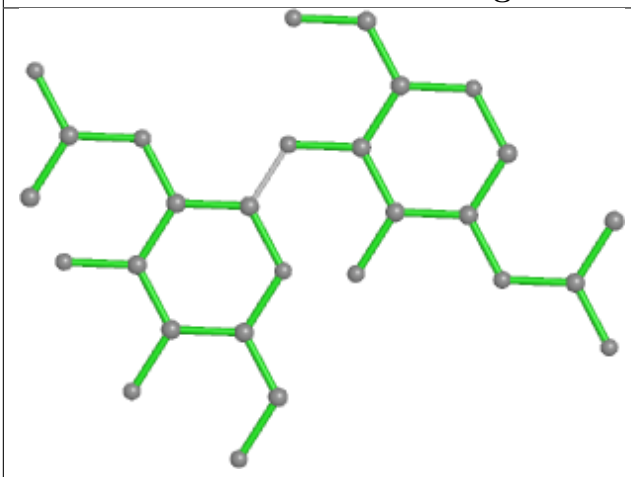


Torsions

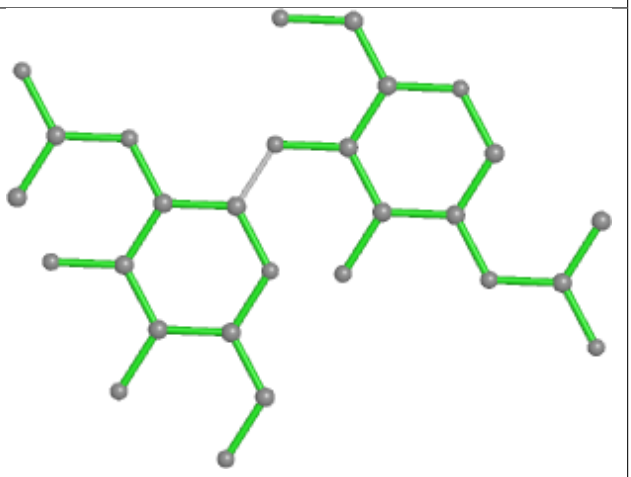


Rings

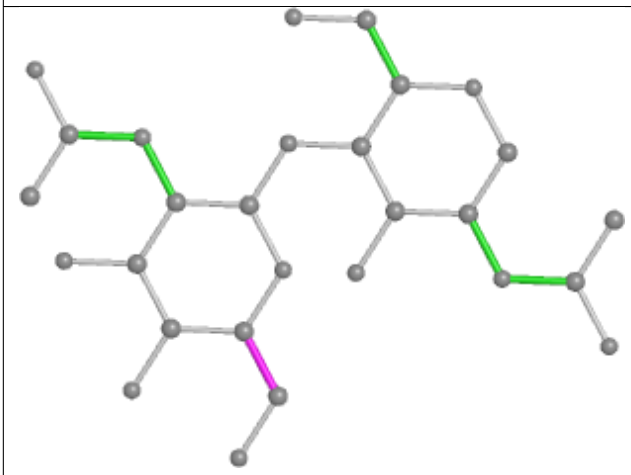
Oligosaccharide Chain Y



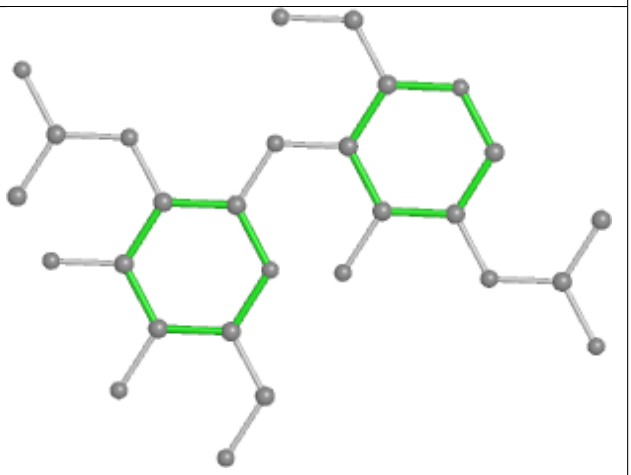
Bond lengths



Bond angles

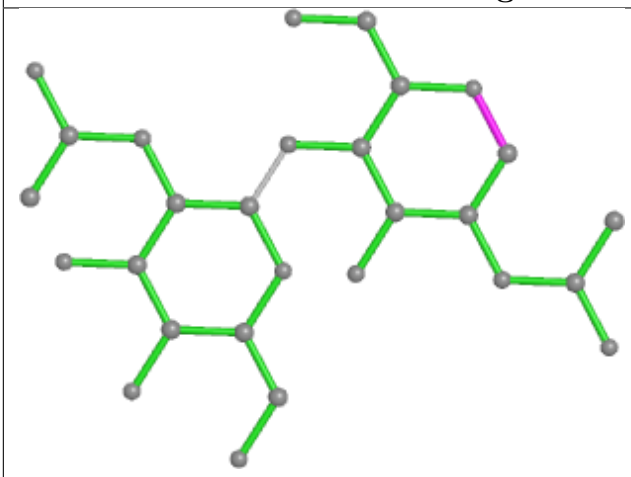


Torsions

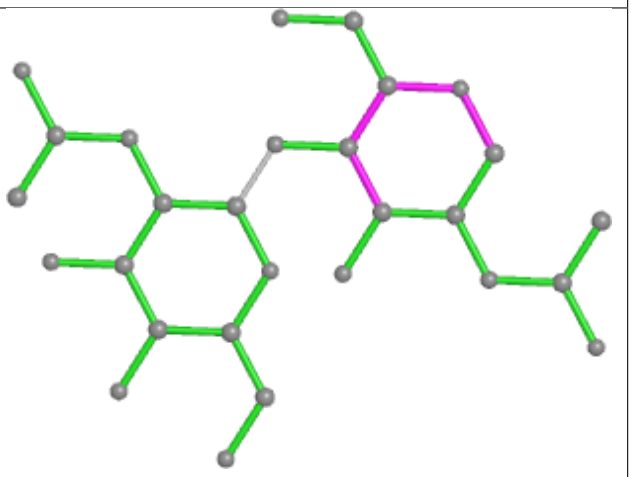


Rings

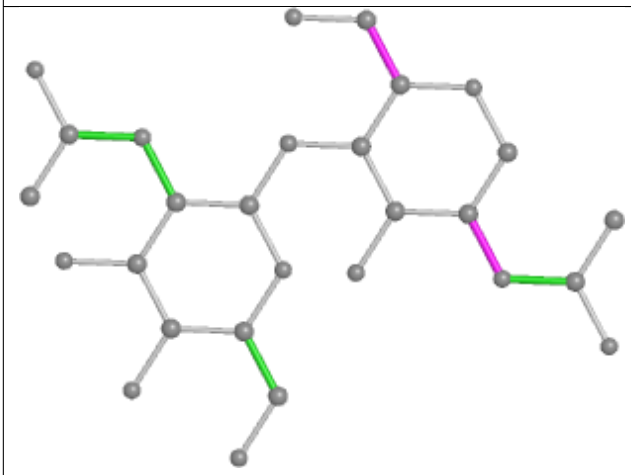
Oligosaccharide Chain Z



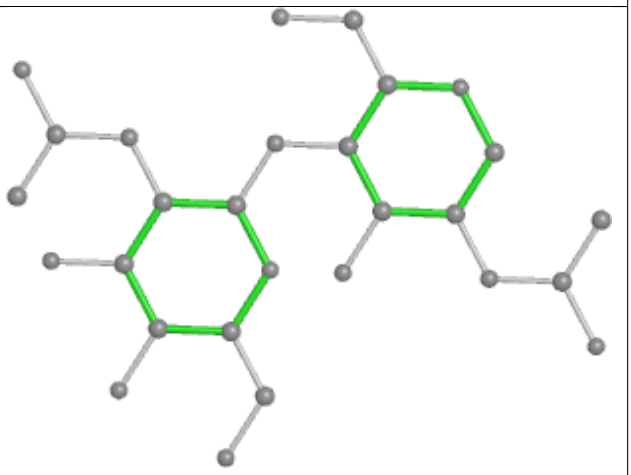
Bond lengths



Bond angles

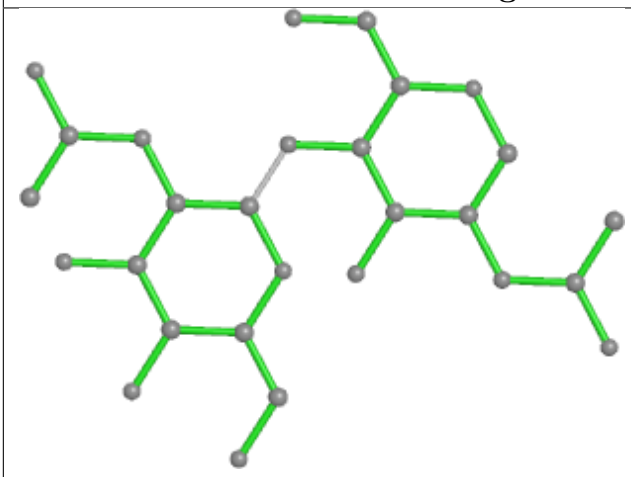


Torsions

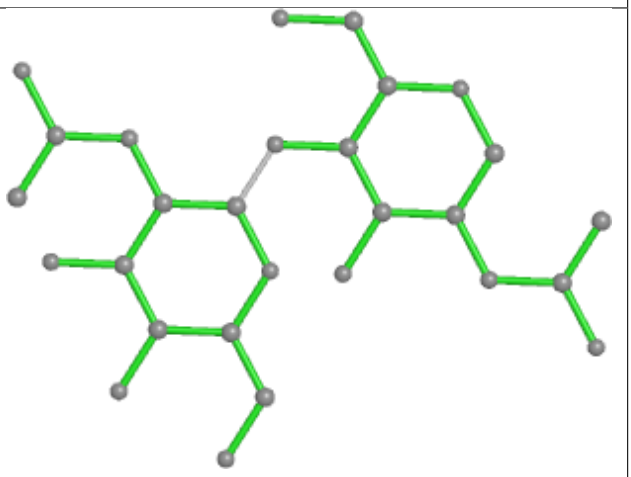


Rings

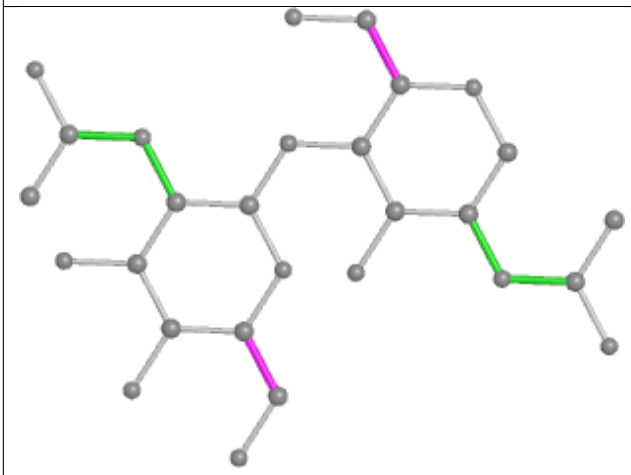
Oligosaccharide Chain a



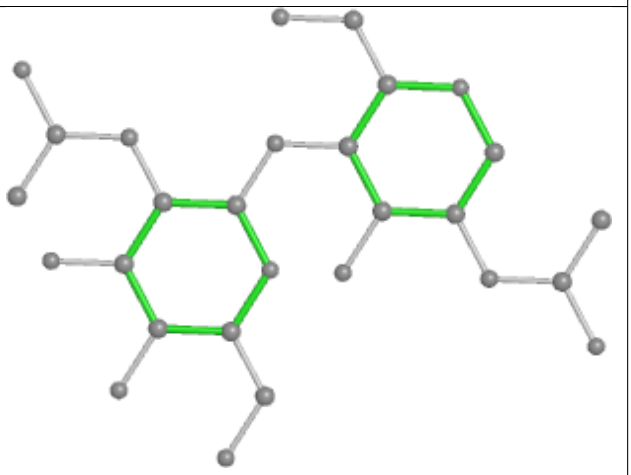
Bond lengths



Bond angles

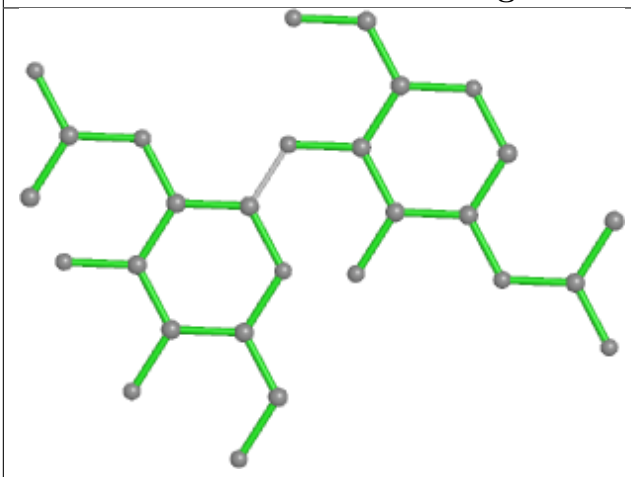


Torsions

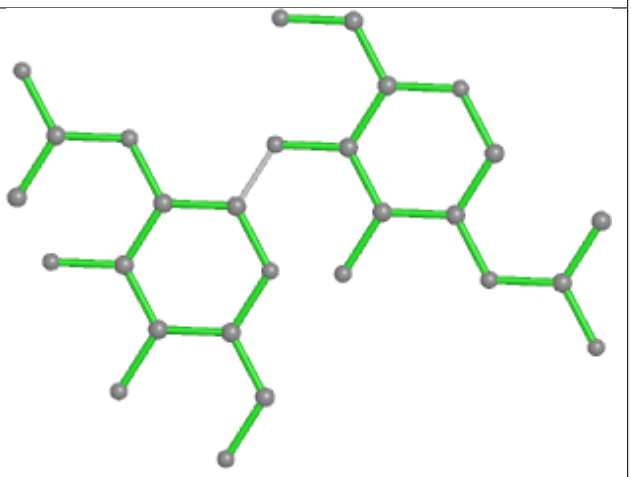


Rings

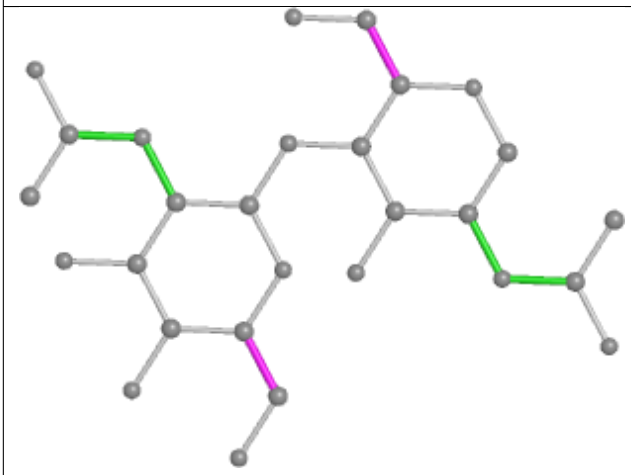
Oligosaccharide Chain b



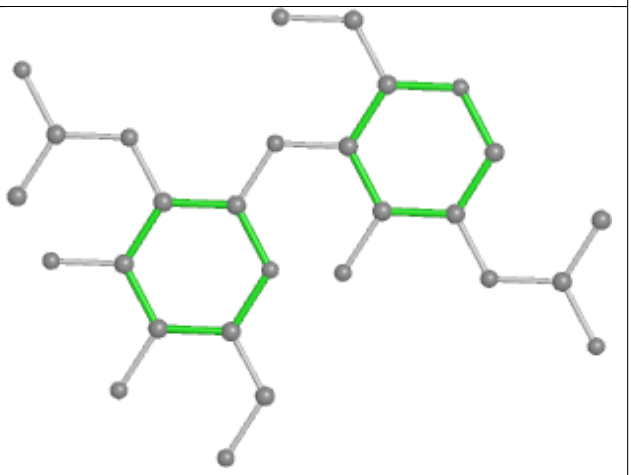
Bond lengths



Bond angles

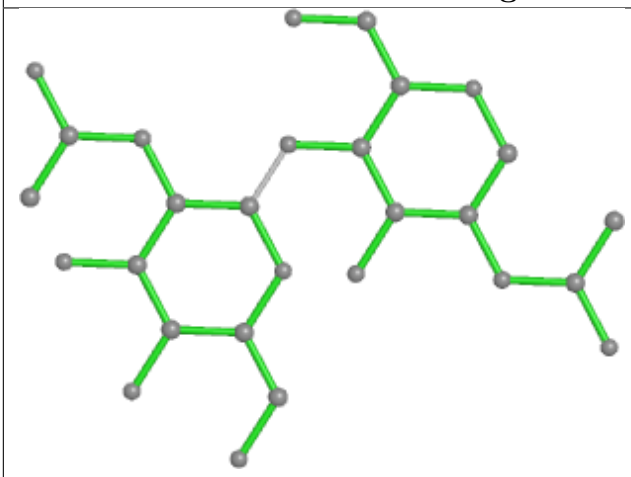


Torsions

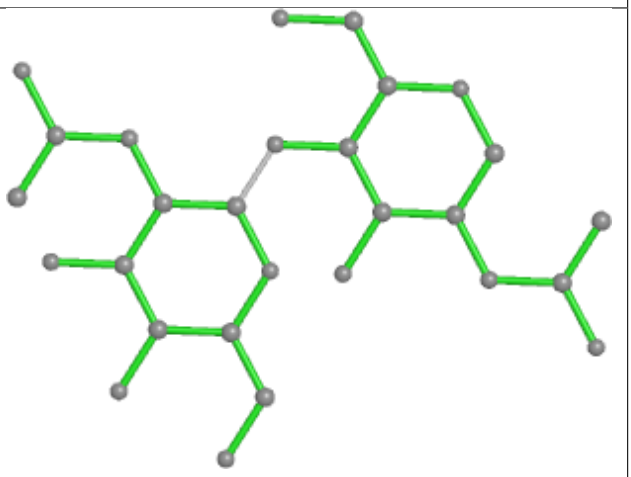


Rings

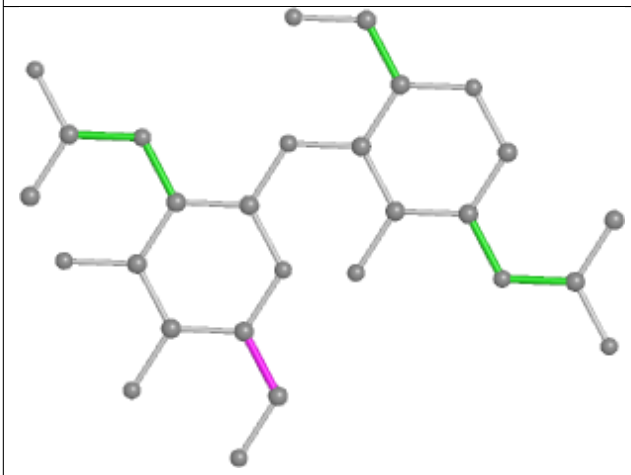
Oligosaccharide Chain c



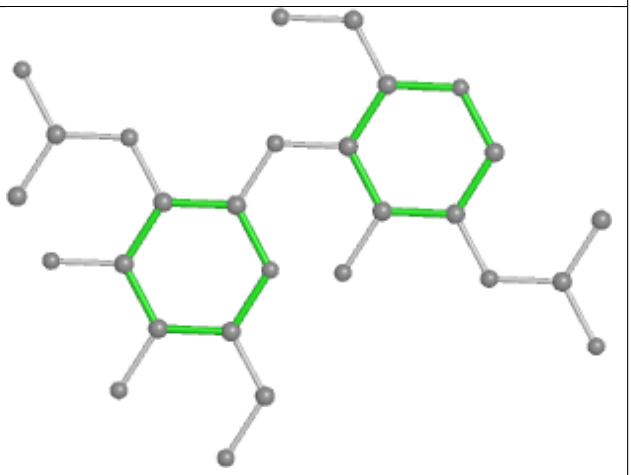
Bond lengths



Bond angles

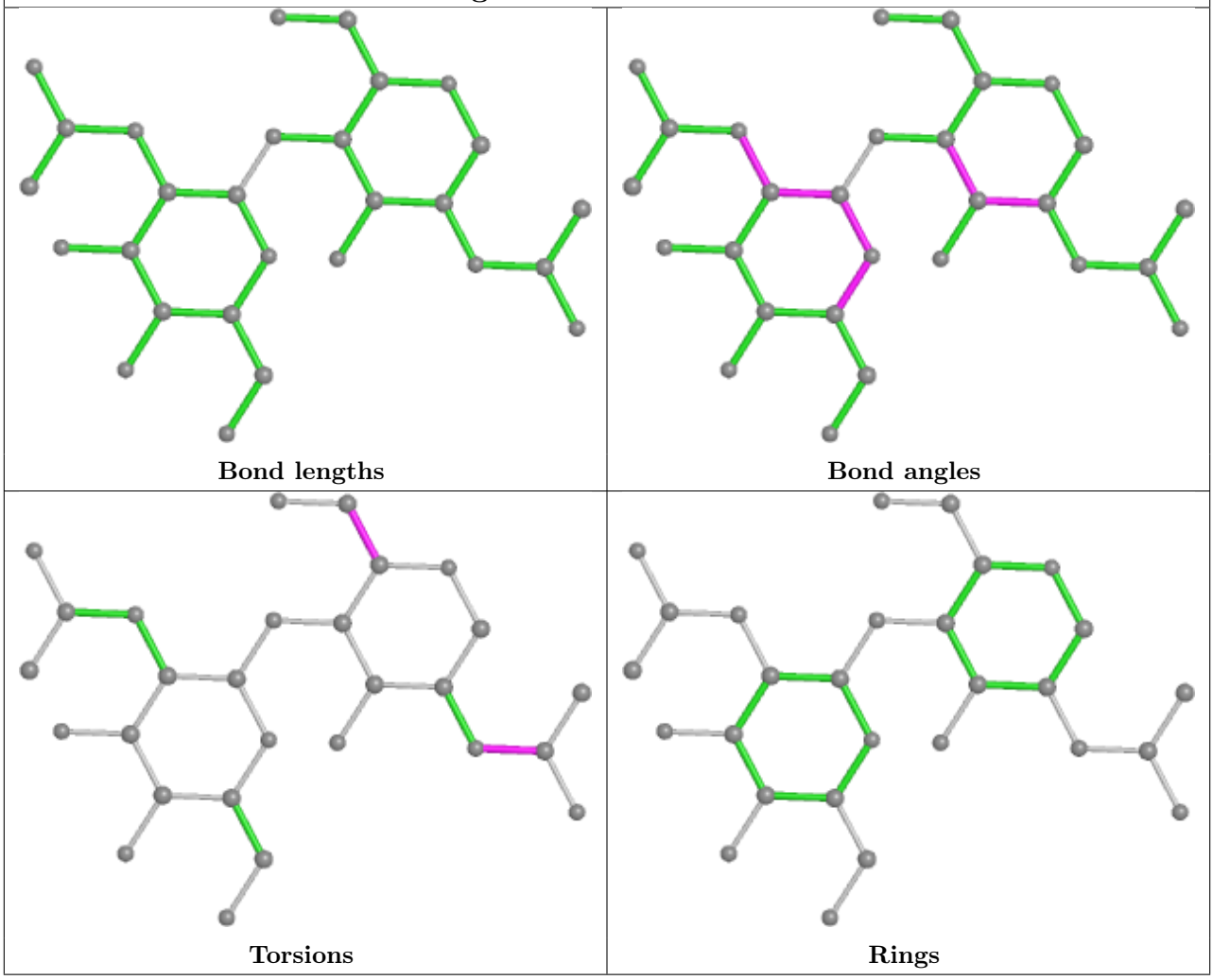


Torsions



Rings

Oligosaccharide Chain d



5.6 Ligand geometry (i)

16 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	$\#\|Z\| > 2$
7	NAG	Q	1305	5	14,14,15	0.57	0	17,19,21	0.36	0
7	NAG	Q	1301	5	14,14,15	0.35	0	17,19,21	0.38	0
7	NAG	R	1204	5	14,14,15	0.58	0	17,19,21	0.37	0
7	NAG	O	1201	5	14,14,15	0.39	0	17,19,21	0.41	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
7	NAG	Q	1304	5	14,14,15	0.21	0	17,19,21	0.43	0
7	NAG	O	1203	5	14,14,15	0.31	0	17,19,21	0.37	0
7	NAG	R	1203	5	14,14,15	0.18	0	17,19,21	0.44	0
7	NAG	Q	1302	5	14,14,15	0.22	0	17,19,21	0.34	0
7	NAG	R	1201	5	14,14,15	0.22	0	17,19,21	0.35	0
7	NAG	O	1205	5	14,14,15	0.25	0	17,19,21	0.51	0
7	NAG	O	1202	5	14,14,15	0.67	0	17,19,21	0.44	0
7	NAG	O	1204	5	14,14,15	0.48	0	17,19,21	0.51	0
7	NAG	R	1205	5	14,14,15	0.23	0	17,19,21	0.61	0
7	NAG	Q	1303	5	14,14,15	0.46	0	17,19,21	0.48	0
7	NAG	R	1202	5	14,14,15	0.49	0	17,19,21	0.49	0
7	NAG	Q	1306	5	14,14,15	0.22	0	17,19,21	0.59	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	Q	1305	5	-	2/6/23/26	0/1/1/1
7	NAG	Q	1301	5	-	0/6/23/26	0/1/1/1
7	NAG	R	1204	5	-	2/6/23/26	0/1/1/1
7	NAG	O	1201	5	-	0/6/23/26	0/1/1/1
7	NAG	Q	1304	5	-	0/6/23/26	0/1/1/1
7	NAG	O	1203	5	-	0/6/23/26	0/1/1/1
7	NAG	R	1203	5	-	0/6/23/26	0/1/1/1
7	NAG	Q	1302	5	-	0/6/23/26	0/1/1/1
7	NAG	R	1201	5	-	0/6/23/26	0/1/1/1
7	NAG	O	1205	5	-	1/6/23/26	0/1/1/1
7	NAG	O	1202	5	-	2/6/23/26	0/1/1/1
7	NAG	O	1204	5	-	2/6/23/26	0/1/1/1
7	NAG	R	1205	5	-	1/6/23/26	0/1/1/1
7	NAG	Q	1303	5	-	1/6/23/26	0/1/1/1
7	NAG	R	1202	5	-	1/6/23/26	0/1/1/1
7	NAG	Q	1306	5	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	O	1202	NAG	O5-C5-C6-O6
7	Q	1305	NAG	C4-C5-C6-O6
7	R	1204	NAG	C4-C5-C6-O6
7	Q	1305	NAG	O5-C5-C6-O6
7	R	1204	NAG	O5-C5-C6-O6
7	O	1204	NAG	C4-C5-C6-O6
7	O	1202	NAG	C4-C5-C6-O6
7	O	1204	NAG	O5-C5-C6-O6
7	O	1205	NAG	O5-C5-C6-O6
7	Q	1306	NAG	O5-C5-C6-O6
7	R	1205	NAG	O5-C5-C6-O6
7	R	1202	NAG	O5-C5-C6-O6
7	Q	1303	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Map visualisation (i)

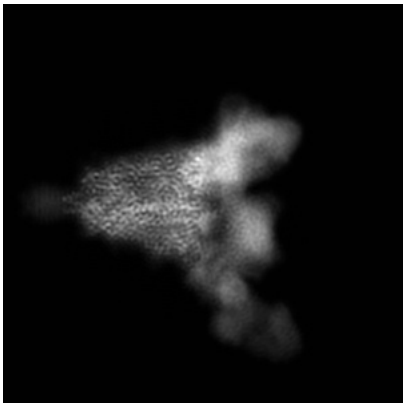
This section contains visualisations of the EMDB entry EMD-30486. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

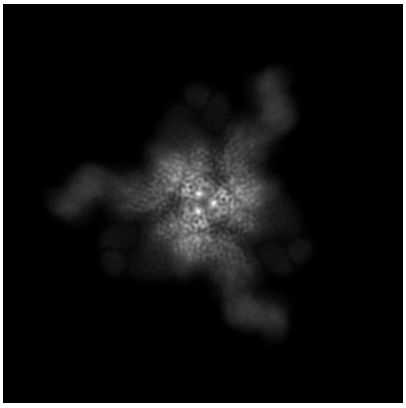
6.1 Orthogonal projections (i)

6.1.1 Primary map

X



Y

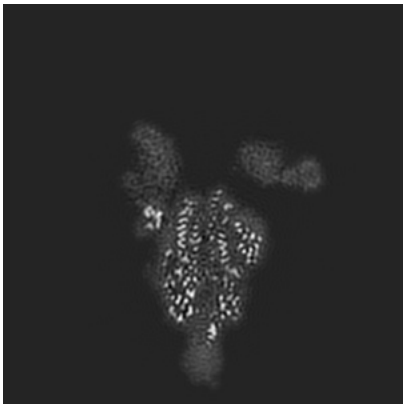


Z

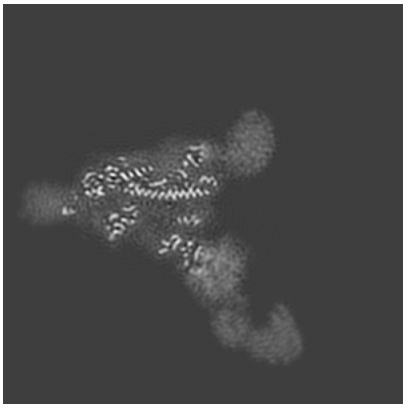
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

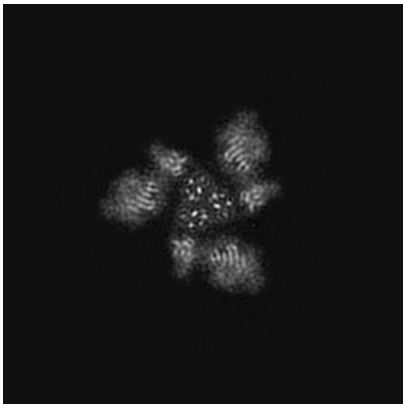
6.2.1 Primary map



X Index: 150



Y Index: 150

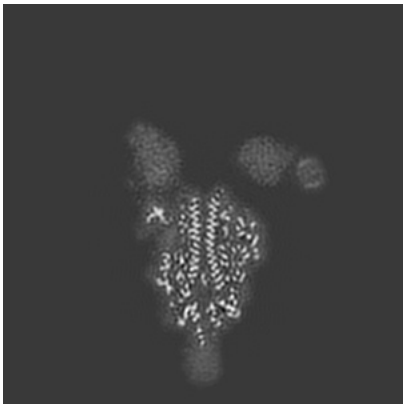


Z Index: 150

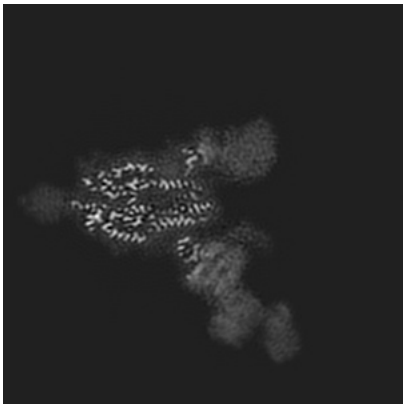
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

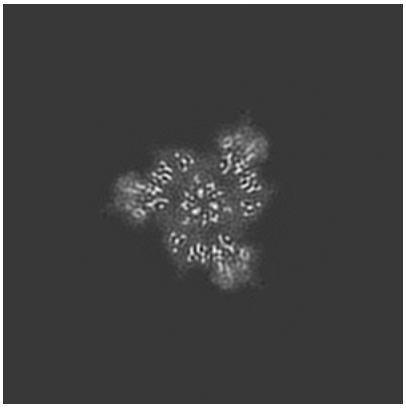
6.3.1 Primary map



X Index: 146



Y Index: 159



Z Index: 144

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 0.003. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

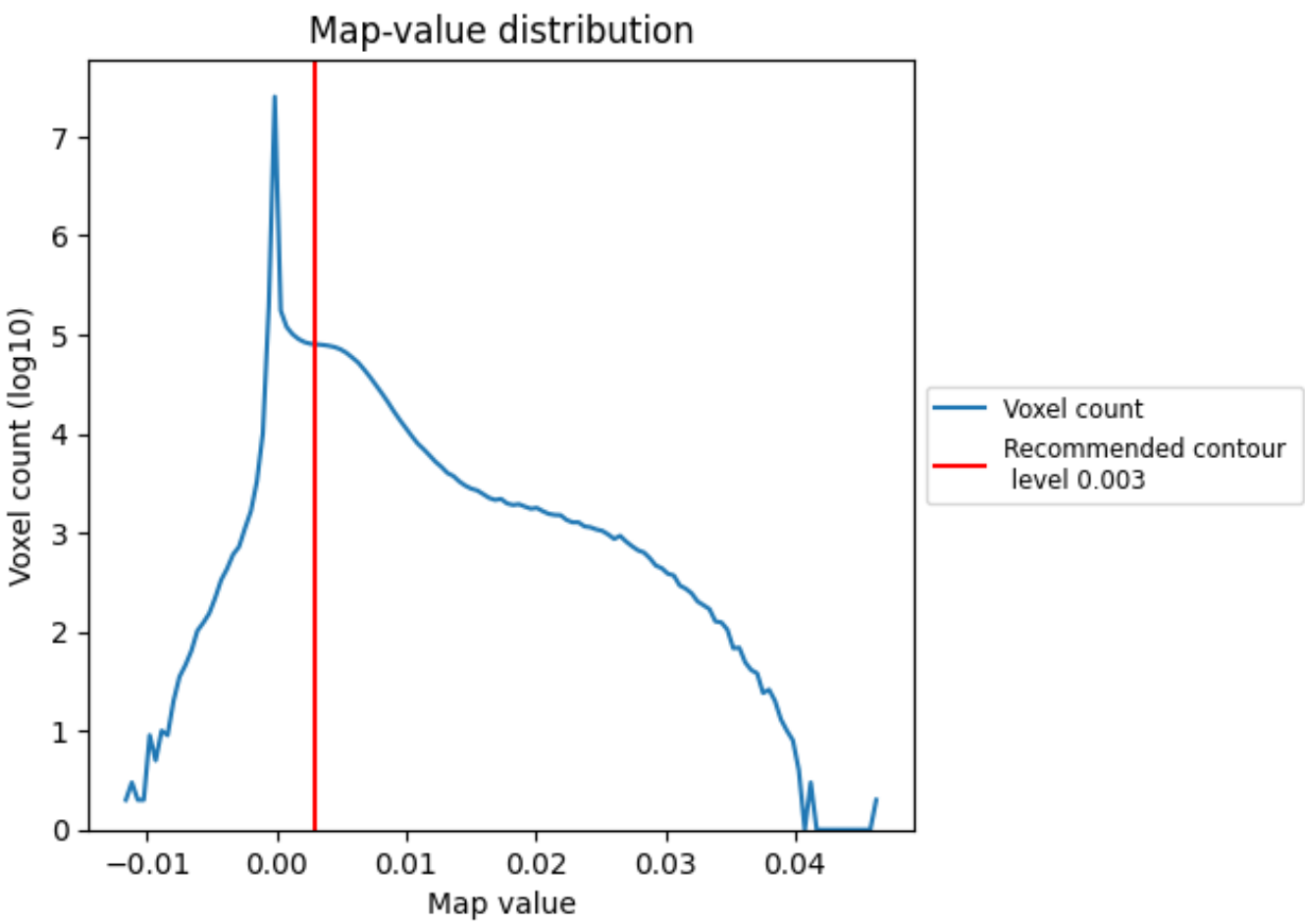
6.5 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis (i)

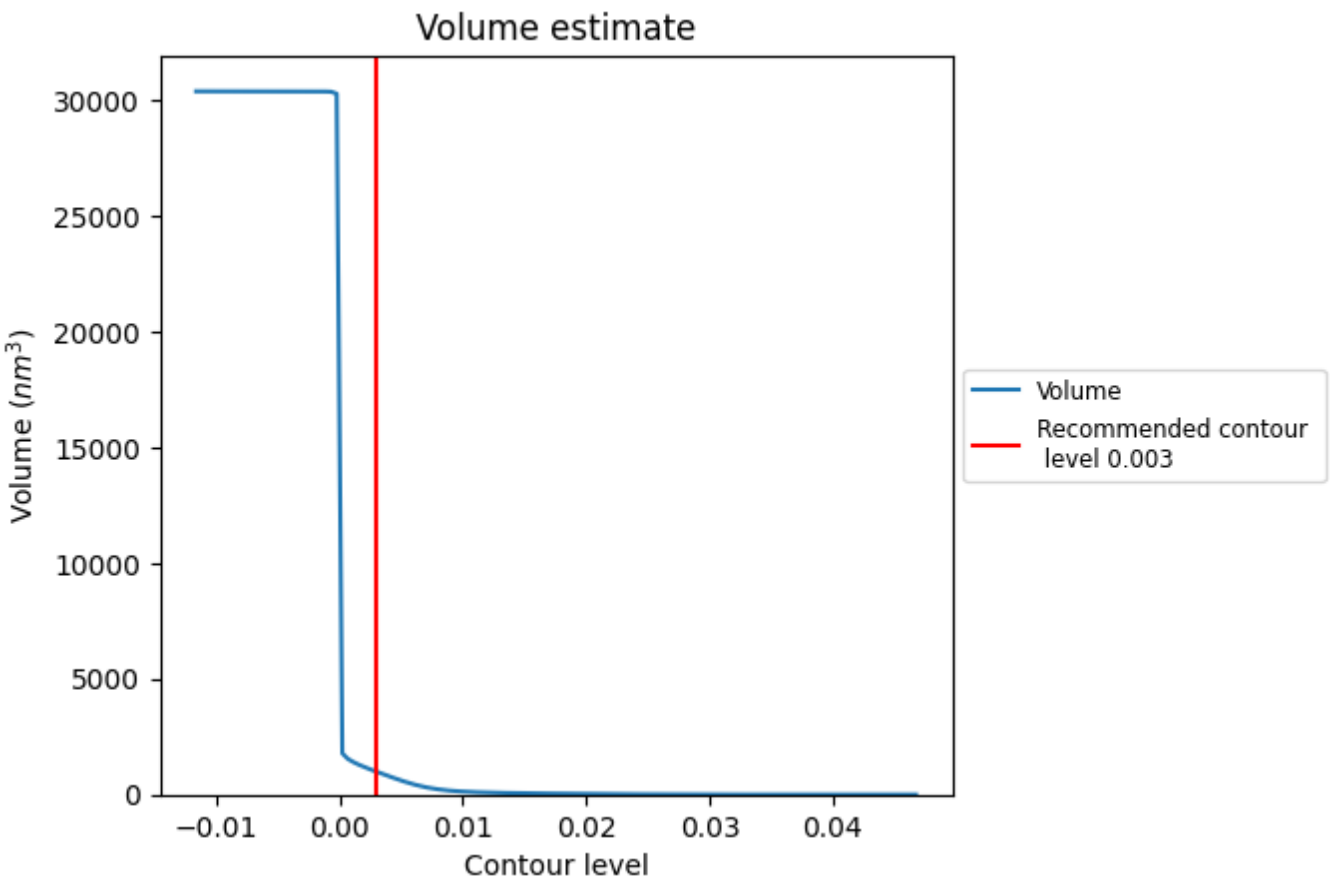
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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.

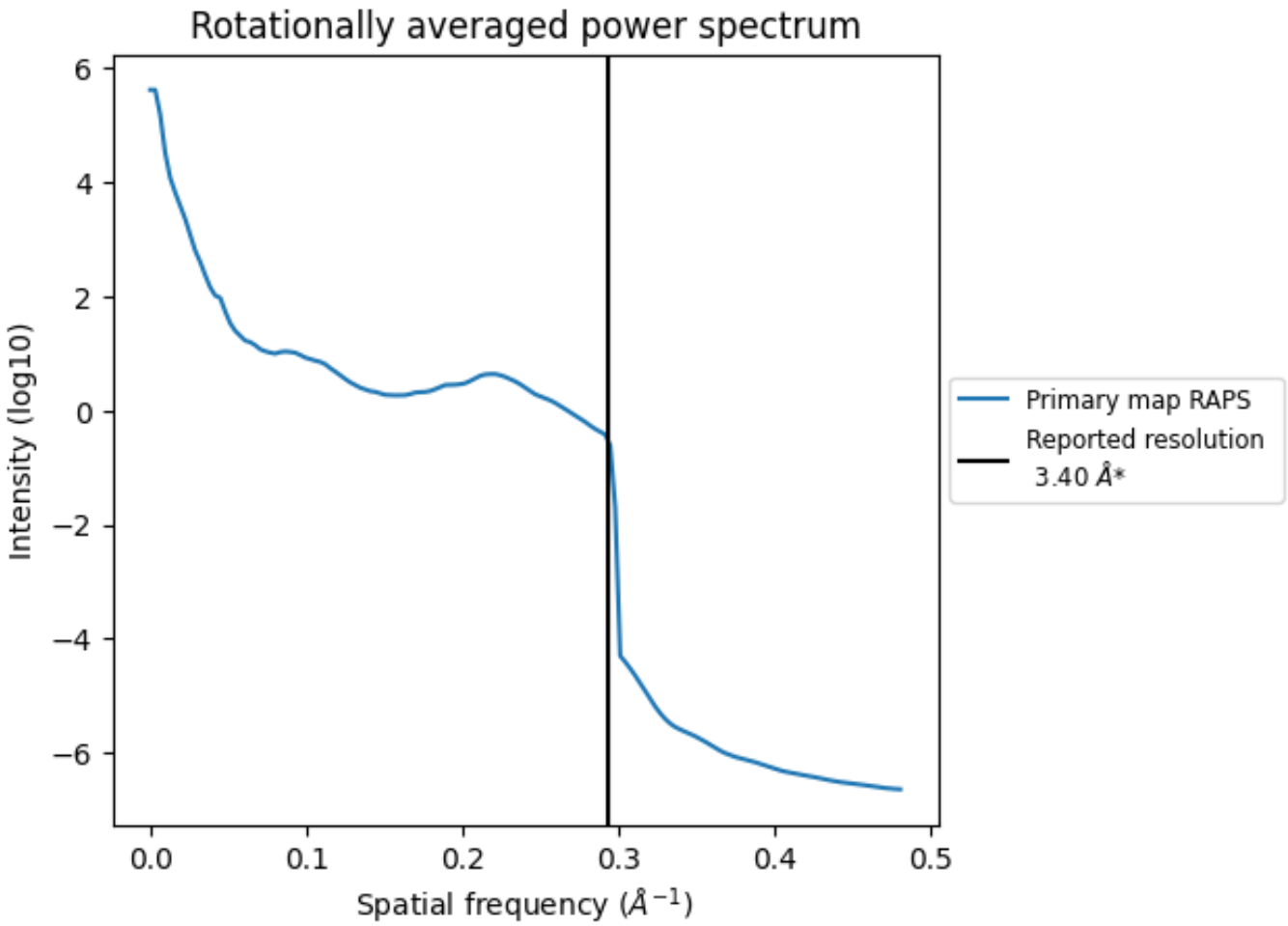
7.2 Volume estimate (i)



The volume at the recommended contour level is 988 nm^3; this corresponds to an approximate mass of 892 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 0.294 Å^{-1}

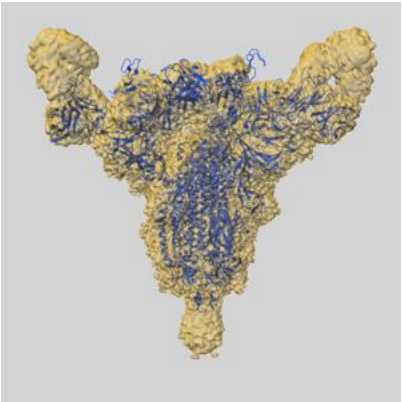
8 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.

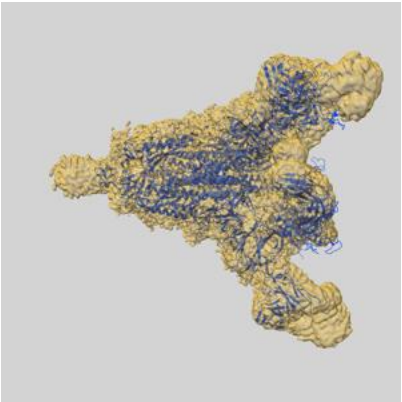
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-30486 and PDB model 7CWS. Per-residue inclusion information can be found in section 3 on page 8.

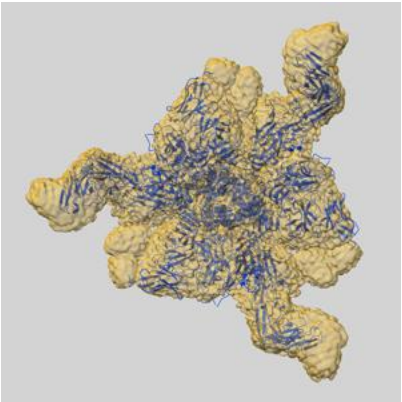
9.1 Map-model overlay (i)



X



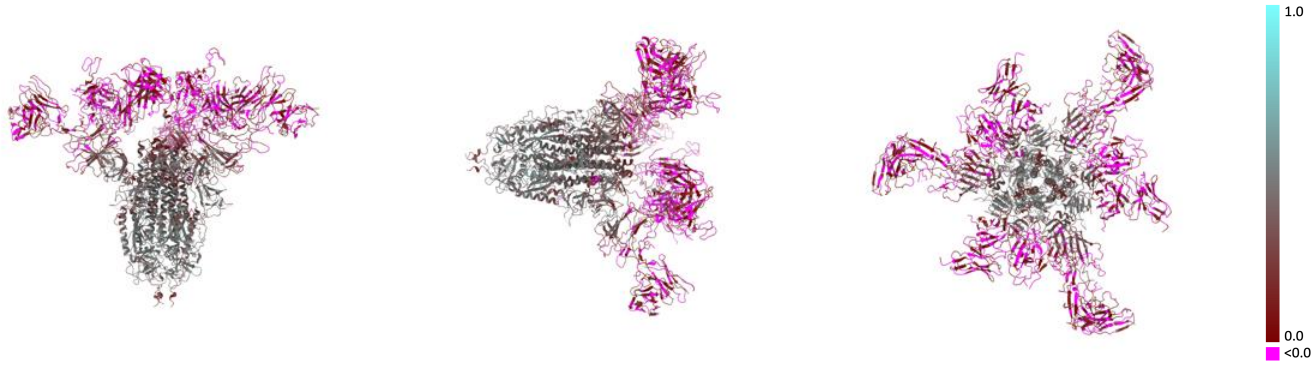
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.003 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.

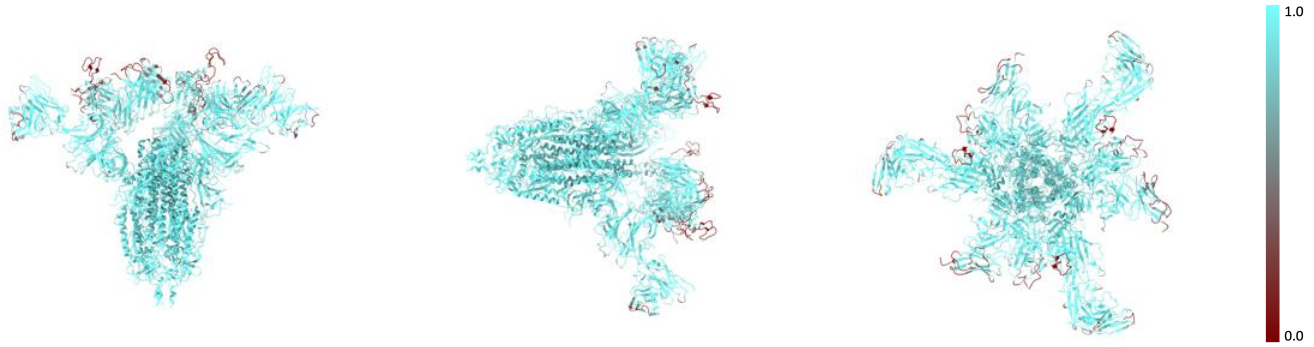
9.2 Q-score mapped to coordinate model (i)



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.

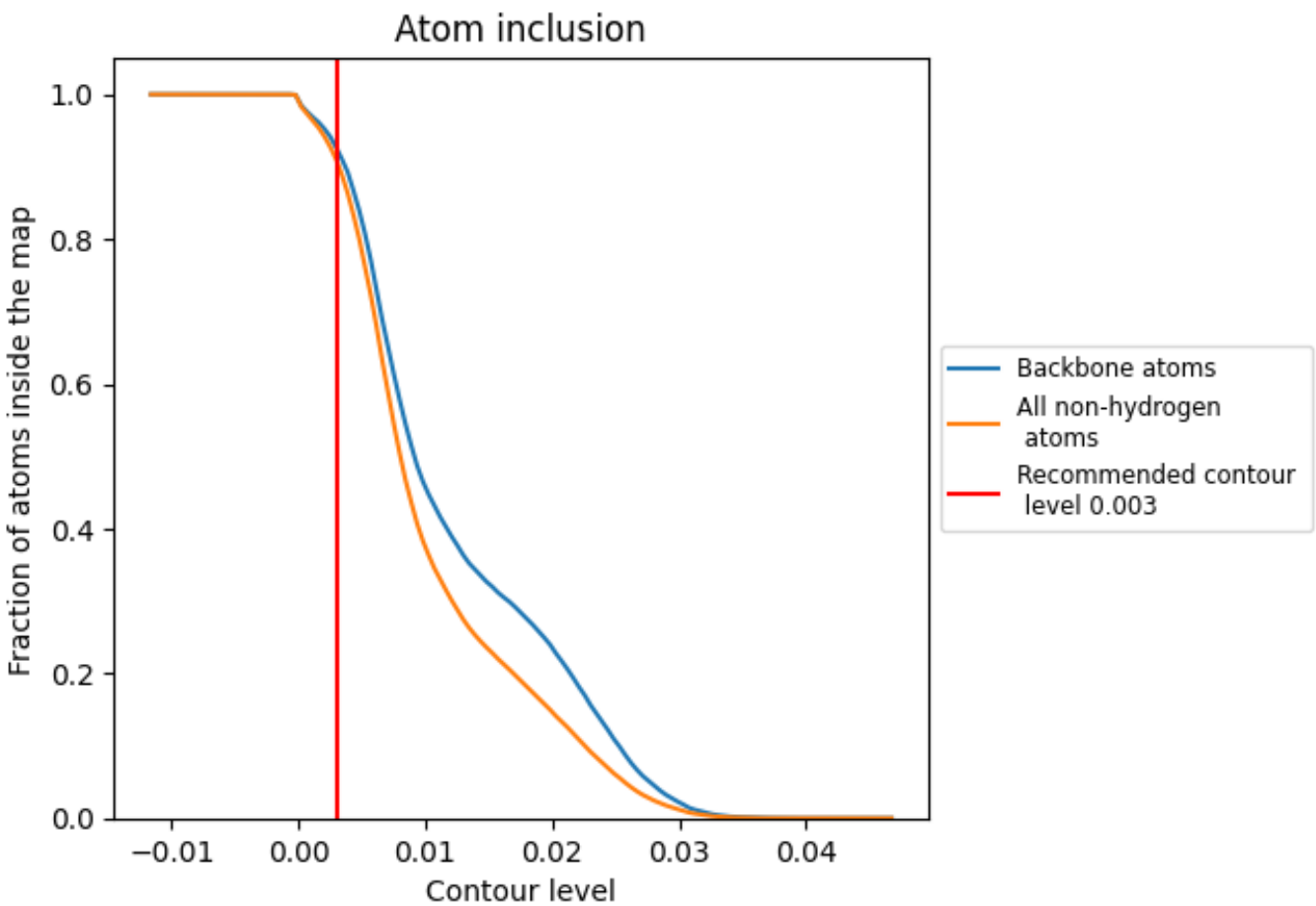
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.003).

9.4 Atom inclusion (i)



At the recommended contour level, 93% of all backbone atoms, 91% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.003) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9091	0.2150
A	0.5714	0.1620
B	0.9286	0.4610
C	0.8560	0.0700
D	0.7368	0.0510
E	0.9392	0.0350
F	0.7055	0.0270
G	0.9414	0.0590
H	0.7091	0.0260
I	0.9435	0.0420
J	0.8214	0.2520
K	0.8393	0.0730
L	0.9354	0.0590
M	0.8483	0.0710
N	0.9376	0.0720
O	0.9320	0.2800
P	0.9343	0.0810
Q	0.9281	0.2810
R	0.9303	0.2800
S	0.8214	0.3290
T	0.5000	0.1620
U	0.5000	0.0690
V	0.9286	0.4000
W	0.8214	0.2820
X	0.7857	0.3370
Y	0.7143	0.3690
Z	0.4643	0.0420
a	0.9286	0.4130
b	0.8214	0.2680
c	0.7143	0.3570
d	0.8214	0.2860