Full wwPDB EM Validation Report

Nov 13, 2022 – 11:22 AM EST

PDB ID	:	6VO3
EMDB ID	:	EMD-21258
Title	:	AMC009 SOSIP.v4.2 in complex with PGV04 Fab
Authors	:	Cottrell, C.A.; de Val, N.; Ward, A.B.
Deposited on	:	2020-01-29
Resolution	:	4.25 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:

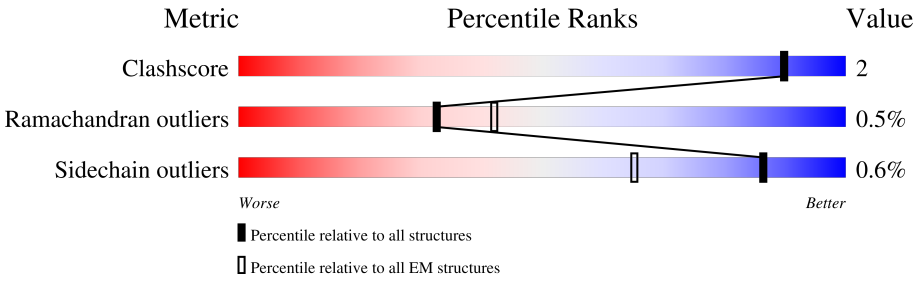
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (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 4.25 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	G	228	51% · 45%
1	H	228	51% · 45%
1	I	228	51% · 45%
2	J	208	46% · 52%
2	K	208	46% · 52%
2	L	208	46% · 52%
3	A	482	81% 7% 11%
3	C	482	81% 7% 11%

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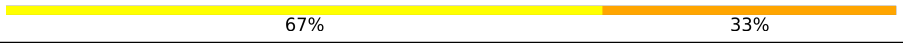
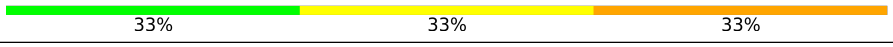
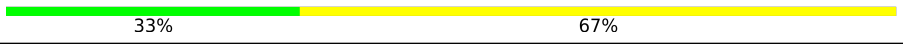
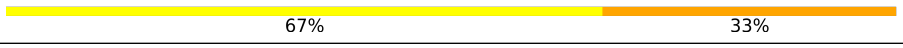
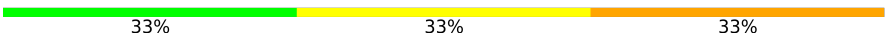
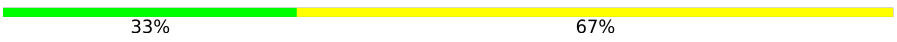
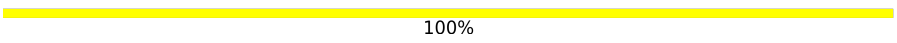
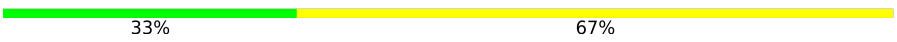
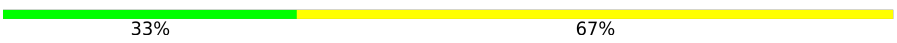
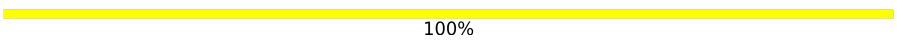
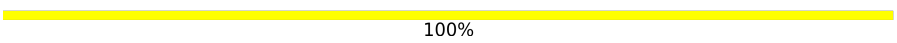
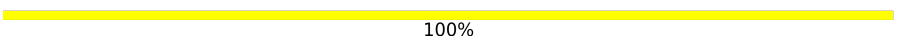
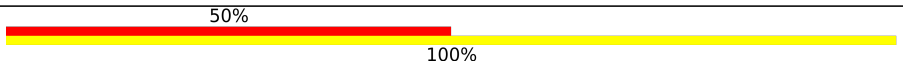
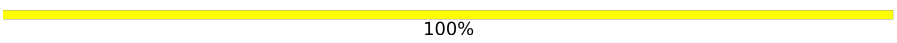
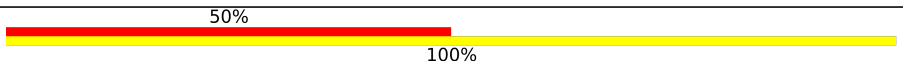
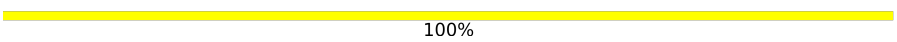
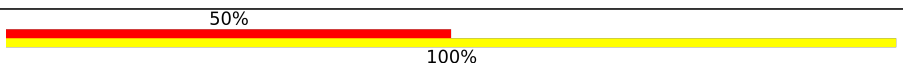
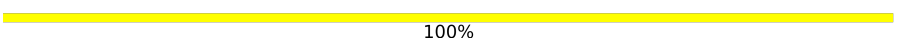
Mol	Chain	Length	Quality of chain
3	D	482	
4	B	154	
4	E	154	
4	F	154	
5	M	3	
5	O	3	
5	Q	3	
5	T	3	
5	V	3	
5	X	3	
5	a	3	
5	c	3	
5	e	3	
6	N	5	
6	U	5	
6	b	5	
7	P	2	
7	R	2	
7	S	2	
7	W	2	
7	Y	2	
7	Z	2	
7	d	2	
7	f	2	
7	g	2	

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 19554 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 PGV04 heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	H	125	Total	C	N	O	S	0	0
			994	632	179	180	3		
1	G	125	Total	C	N	O	S	0	0
			994	632	179	180	3		
1	I	125	Total	C	N	O	S	0	0
			994	632	179	180	3		

- Molecule 2 is a protein called PGV04 light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	L	100	Total	C	N	O	S	0	0
			784	500	131	149	4		
2	J	100	Total	C	N	O	S	0	0
			784	500	131	149	4		
2	K	100	Total	C	N	O	S	0	0
			784	500	131	149	4		

- Molecule 3 is a protein called AMC009 SOSIP.v4.2 envelope glycoprotein gp120.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	429	Total	C	N	O	S	0	0
			3402	2149	598	629	26		
3	C	429	Total	C	N	O	S	0	0
			3402	2149	598	629	26		
3	D	429	Total	C	N	O	S	0	0
			3402	2149	598	629	26		

- Molecule 4 is a protein called AMC009 SOSIP.v4.2 envelope glycoprotein gp41.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	B	124	Total	C	N	O	S	0	0
			992	623	172	190	7		

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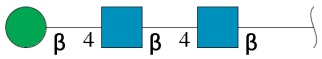
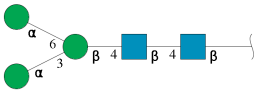
Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	124	Total	C	N	O	S	0	0
			992	623	172	190	7		
4	F	124	Total	C	N	O	S	0	0
			992	623	172	190	7		

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



Mol	Chain	Residues	Atoms				AltConf	Trace
5	M	3	Total	C	N	O	0	0
			39	22	2	15		
5	O	3	Total	C	N	O	0	0
			39	22	2	15		
5	Q	3	Total	C	N	O	0	0
			39	22	2	15		
5	T	3	Total	C	N	O	0	0
			39	22	2	15		
5	V	3	Total	C	N	O	0	0
			39	22	2	15		
5	X	3	Total	C	N	O	0	0
			39	22	2	15		
5	a	3	Total	C	N	O	0	0
			39	22	2	15		
5	c	3	Total	C	N	O	0	0
			39	22	2	15		
5	e	3	Total	C	N	O	0	0
			39	22	2	15		

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

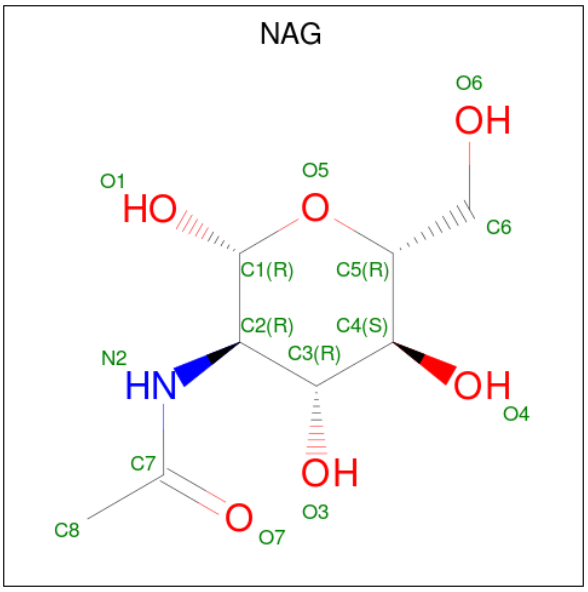


Mol	Chain	Residues	Atoms	AltConf	Trace
6	N	5	Total C N O 61 34 2 25	0	0
6	U	5	Total C N O 61 34 2 25	0	0
6	b	5	Total C N O 61 34 2 25	0	0

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

Mol	Chain	Residues	Atoms	AltConf	Trace
7	P	2	Total C N O 28 16 2 10	0	0
7	R	2	Total C N O 28 16 2 10	0	0
7	S	2	Total C N O 28 16 2 10	0	0
7	W	2	Total C N O 28 16 2 10	0	0
7	Y	2	Total C N O 28 16 2 10	0	0
7	Z	2	Total C N O 28 16 2 10	0	0
7	d	2	Total C N O 28 16 2 10	0	0
7	f	2	Total C N O 28 16 2 10	0	0
7	g	2	Total C N O 28 16 2 10	0	0

- 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	0
			70	40	5	25	
8	A	1	Total	C	N	O	0
			70	40	5	25	
8	A	1	Total	C	N	O	0
			70	40	5	25	
8	A	1	Total	C	N	O	0
			70	40	5	25	
8	A	1	Total	C	N	O	0
			70	40	5	25	
8	B	1	Total	C	N	O	0
			14	8	1	5	
8	C	1	Total	C	N	O	0
			70	40	5	25	
8	C	1	Total	C	N	O	0
			70	40	5	25	
8	C	1	Total	C	N	O	0
			70	40	5	25	
8	C	1	Total	C	N	O	0
			70	40	5	25	
8	C	1	Total	C	N	O	0
			70	40	5	25	
8	E	1	Total	C	N	O	0
			14	8	1	5	
8	D	1	Total	C	N	O	0
			70	40	5	25	
8	D	1	Total	C	N	O	0
			70	40	5	25	

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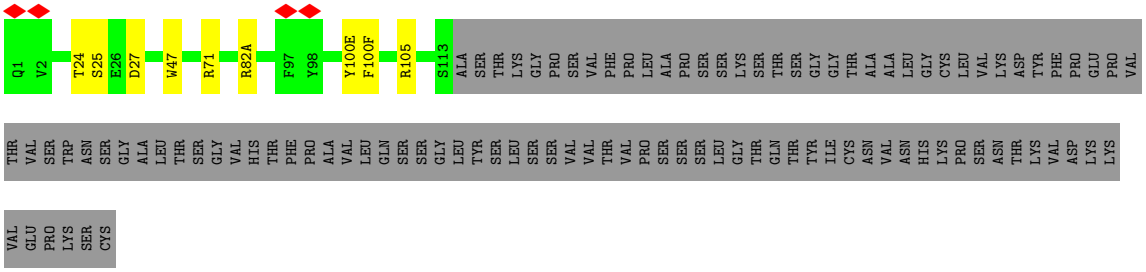
Mol	Chain	Residues	Atoms				AltConf
8	D	1	Total	C	N	O	0
			70	40	5	25	
8	D	1	Total	C	N	O	0
			70	40	5	25	
8	D	1	Total	C	N	O	0
			70	40	5	25	
8	F	1	Total	C	N	O	0
			14	8	1	5	

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.

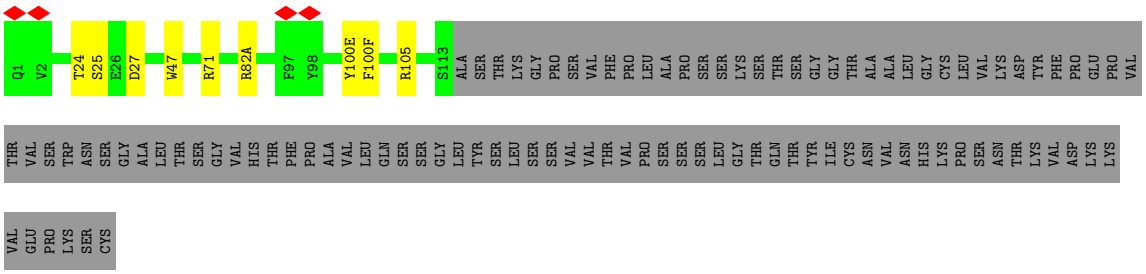
• Molecule 1: PGV04 heavy chain

Chain H:



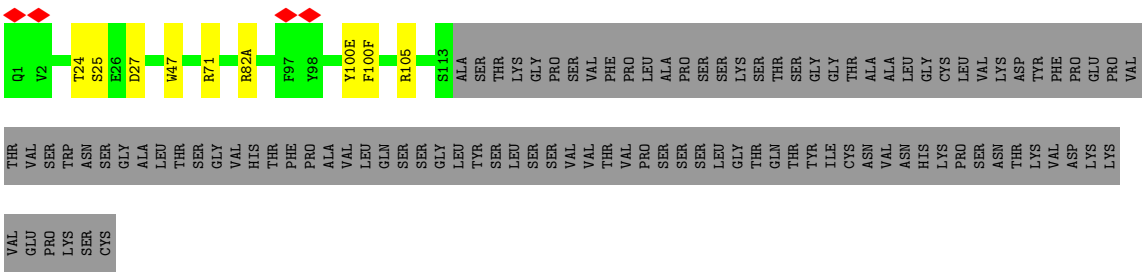
• Molecule 1: PGV04 heavy chain

Chain G:



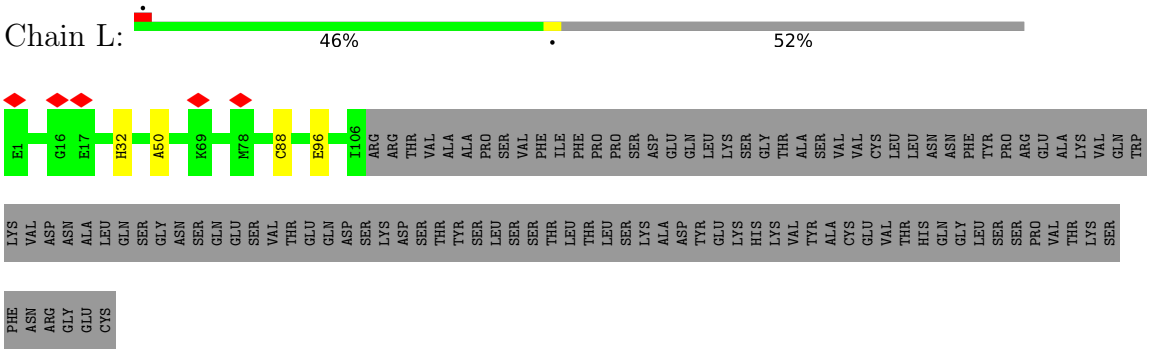
• Molecule 1: PGV04 heavy chain

Chain I:



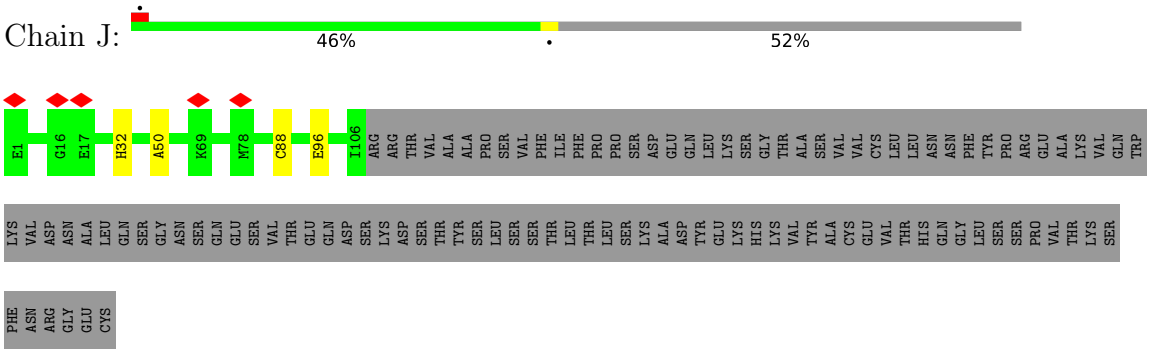
• Molecule 2: PGV04 light chain

Chain L:



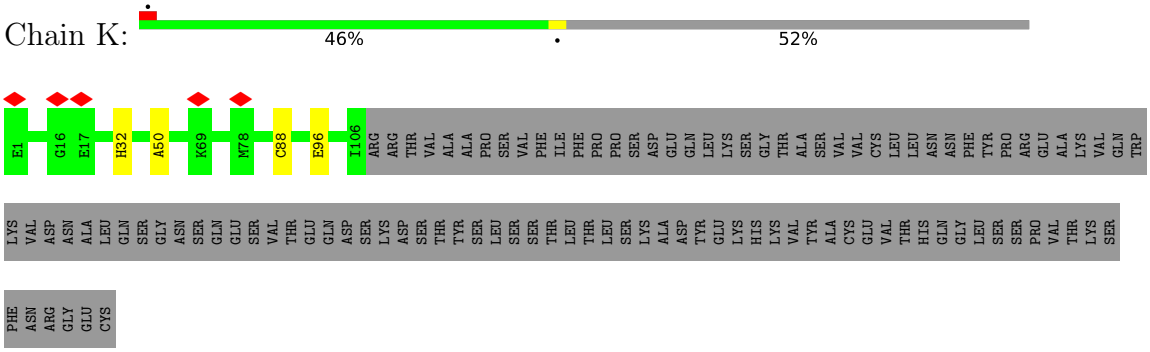
• Molecule 2: PGV04 light chain

Chain J:



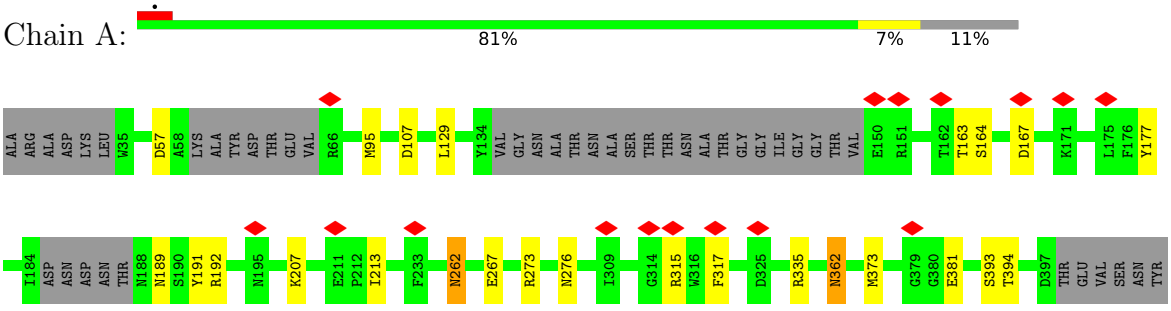
• Molecule 2: PGV04 light chain

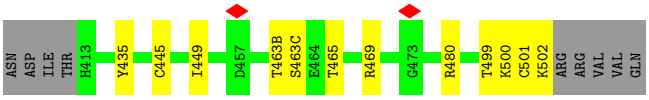
Chain K:



• Molecule 3: AMC009 SOSIP.v4.2 envelope glycoprotein gp120

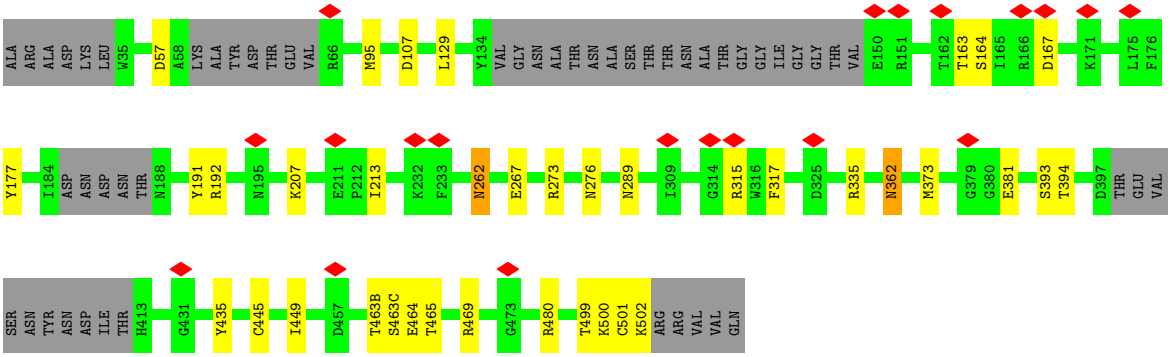
Chain A:





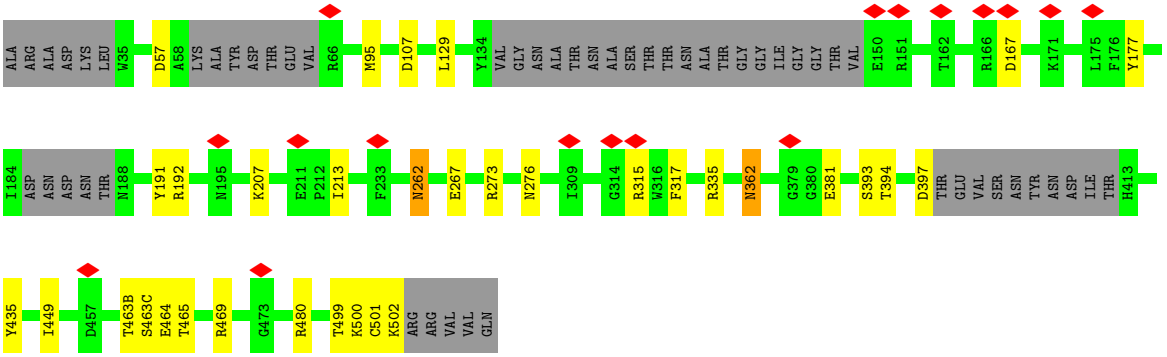
• Molecule 3: AMC009 SOSIP.v4.2 envelope glycoprotein gp120

Chain C:



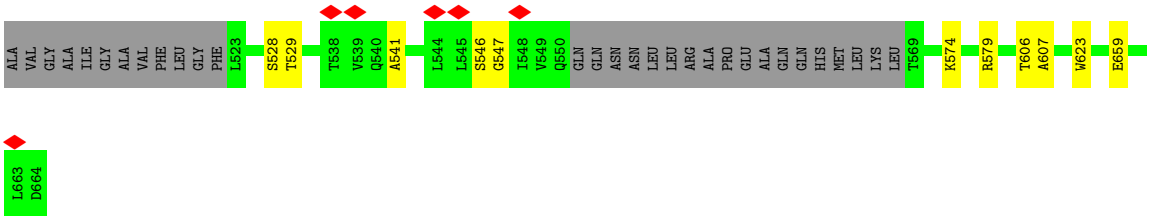
• Molecule 3: AMC009 SOSIP.v4.2 envelope glycoprotein gp120

Chain D:



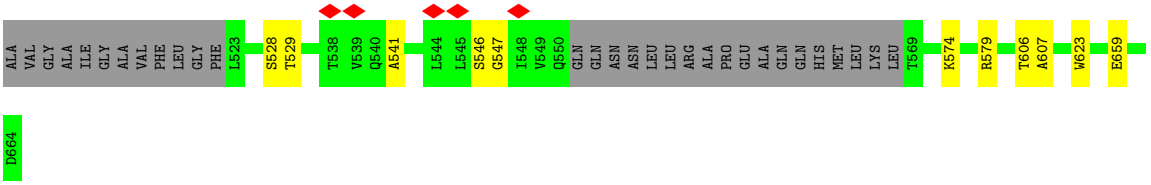
• Molecule 4: AMC009 SOSIP.v4.2 envelope glycoprotein gp41

Chain B:



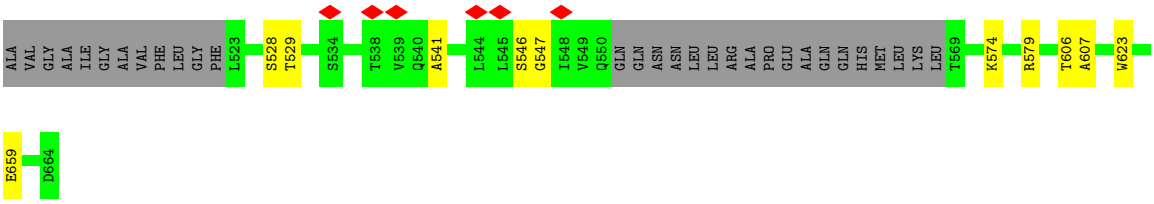
• Molecule 4: AMC009 SOSIP.v4.2 envelope glycoprotein gp41

Chain E:



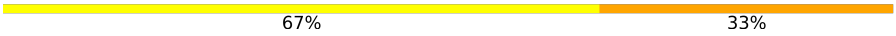
• Molecule 4: AMC009 SOSIP.v4.2 envelope glycoprotein gp41

Chain F:



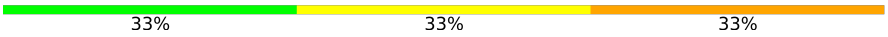
• Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:



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

Chain O:

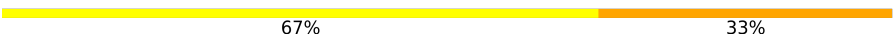


• Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

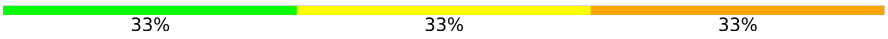
Chain Q:

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

Chain T:



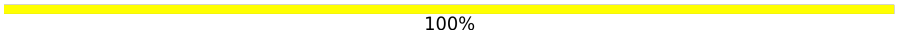
• Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain V: 

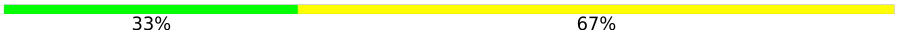
• Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain X: 

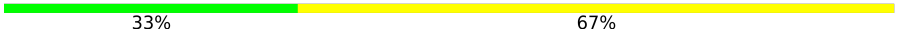
• Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain a: 

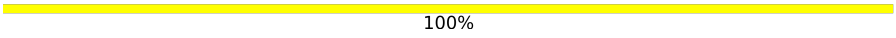
• Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain c: 

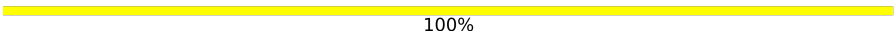
• Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain e: 

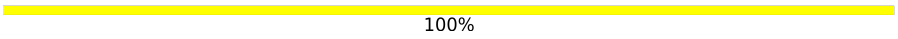
• Molecule 6: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N: 

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

Chain U: 

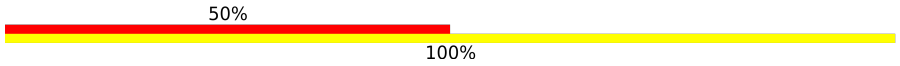
• Molecule 6: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain b: 

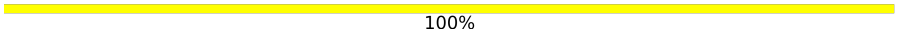
• Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain P: 

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

Chain R: 

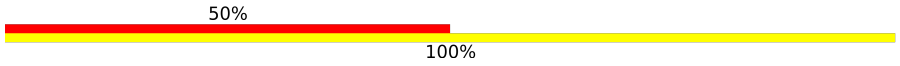
• Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain S: 

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

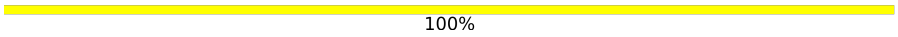
Chain W: 

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

Chain Y: 

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

Chain Z:

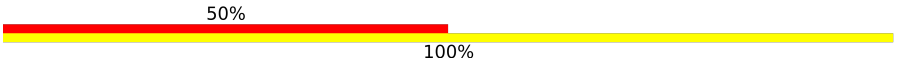


• Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain d:

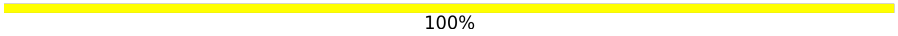
• Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain f:



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

Chain g:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	128752	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 ($e^-/Å^2$)	32	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	1.361	Depositor
Minimum map value	-0.778	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.049	Depositor
Recommended contour level	0.33	Depositor
Map size (Å)	335.36, 335.36, 335.36	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.31, 1.31, 1.31	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: MAN, BMA, 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	G	1.03	2/1020 (0.2%)	1.01	3/1383 (0.2%)
1	H	1.03	2/1020 (0.2%)	1.01	3/1383 (0.2%)
1	I	1.03	2/1020 (0.2%)	1.01	3/1383 (0.2%)
2	J	1.07	2/804 (0.2%)	0.98	0/1087
2	K	1.07	2/804 (0.2%)	0.98	0/1087
2	L	1.07	2/804 (0.2%)	0.98	0/1087
3	A	0.94	4/3475 (0.1%)	0.92	7/4717 (0.1%)
3	C	0.94	4/3475 (0.1%)	0.92	7/4717 (0.1%)
3	D	0.94	4/3475 (0.1%)	0.92	7/4717 (0.1%)
4	B	1.08	2/1008 (0.2%)	0.87	1/1367 (0.1%)
4	E	1.08	2/1008 (0.2%)	0.87	1/1367 (0.1%)
4	F	1.08	2/1008 (0.2%)	0.87	1/1367 (0.1%)
All	All	1.00	30/18921 (0.2%)	0.93	33/25662 (0.1%)

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	88	CYS	CB-SG	-10.77	1.64	1.82
2	J	88	CYS	CB-SG	-10.76	1.64	1.82
2	K	88	CYS	CB-SG	-10.75	1.64	1.82
1	H	100(E)	TYR	CB-CG	-7.31	1.40	1.51
1	I	100(E)	TYR	CB-CG	-7.31	1.40	1.51
1	G	100(E)	TYR	CB-CG	-7.31	1.40	1.51
3	D	381	GLU	CD-OE1	-5.74	1.19	1.25
3	C	381	GLU	CD-OE1	-5.72	1.19	1.25
1	I	47	TRP	CE2-CZ2	-5.72	1.30	1.39
3	A	381	GLU	CD-OE1	-5.72	1.19	1.25
1	H	47	TRP	CE2-CZ2	-5.71	1.30	1.39
1	G	47	TRP	CE2-CZ2	-5.68	1.30	1.39
4	E	659	GLU	CD-OE1	-5.44	1.19	1.25
4	B	659	GLU	CD-OE1	-5.44	1.19	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	659	GLU	CD-OE1	-5.42	1.19	1.25
3	C	435	TYR	CG-CD2	-5.27	1.32	1.39
3	D	435	TYR	CG-CD2	-5.26	1.32	1.39
3	A	435	TYR	CG-CD2	-5.25	1.32	1.39
4	B	623	TRP	CB-CG	5.17	1.59	1.50
4	F	623	TRP	CB-CG	5.16	1.59	1.50
3	A	317	PHE	CB-CG	-5.14	1.42	1.51
3	D	317	PHE	CB-CG	-5.14	1.42	1.51
4	E	623	TRP	CB-CG	5.13	1.59	1.50
3	C	317	PHE	CB-CG	-5.12	1.42	1.51
3	A	267	GLU	CD-OE2	-5.09	1.20	1.25
3	C	267	GLU	CD-OE2	-5.06	1.20	1.25
3	D	267	GLU	CD-OE2	-5.05	1.20	1.25
2	J	96	GLU	CD-OE1	-5.03	1.20	1.25
2	K	96	GLU	CD-OE1	-5.02	1.20	1.25
2	L	96	GLU	CD-OE1	-5.01	1.20	1.25

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	I	105	ARG	NE-CZ-NH2	-7.89	116.36	120.30
1	G	105	ARG	NE-CZ-NH2	-7.86	116.37	120.30
1	H	105	ARG	NE-CZ-NH2	-7.86	116.37	120.30
3	D	335	ARG	NE-CZ-NH2	-6.98	116.81	120.30
3	C	335	ARG	NE-CZ-NH2	-6.97	116.82	120.30
3	A	335	ARG	NE-CZ-NH2	-6.89	116.86	120.30
3	D	315	ARG	NE-CZ-NH2	-6.79	116.91	120.30
3	A	315	ARG	NE-CZ-NH2	-6.76	116.92	120.30
3	C	315	ARG	NE-CZ-NH2	-6.71	116.94	120.30
4	B	579	ARG	NE-CZ-NH2	-6.56	117.02	120.30
4	F	579	ARG	NE-CZ-NH2	-6.55	117.03	120.30
4	E	579	ARG	NE-CZ-NH2	-6.53	117.03	120.30
3	A	480	ARG	NE-CZ-NH1	6.16	123.38	120.30
3	D	480	ARG	NE-CZ-NH1	6.15	123.37	120.30
3	A	95	MET	CG-SD-CE	6.11	109.98	100.20
3	C	95	MET	CG-SD-CE	6.11	109.97	100.20
3	C	480	ARG	NE-CZ-NH1	6.10	123.35	120.30
3	D	95	MET	CG-SD-CE	6.10	109.95	100.20
3	C	177	TYR	CB-CG-CD2	-5.94	117.44	121.00
3	D	177	TYR	CB-CG-CD2	-5.92	117.45	121.00
3	A	177	TYR	CB-CG-CD2	-5.91	117.45	121.00
1	I	82(A)	ARG	NE-CZ-NH2	-5.76	117.42	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	H	82(A)	ARG	NE-CZ-NH2	-5.74	117.43	120.30
1	G	82(A)	ARG	NE-CZ-NH2	-5.72	117.44	120.30
1	H	100(F)	PHE	CB-CG-CD1	5.63	124.74	120.80
1	I	100(F)	PHE	CB-CG-CD1	5.62	124.73	120.80
1	G	100(F)	PHE	CB-CG-CD1	5.61	124.73	120.80
3	C	192	ARG	NE-CZ-NH2	-5.36	117.62	120.30
3	A	192	ARG	NE-CZ-NH2	-5.36	117.62	120.30
3	D	192	ARG	NE-CZ-NH2	-5.35	117.63	120.30
3	A	273	ARG	NE-CZ-NH1	5.24	122.92	120.30
3	C	273	ARG	NE-CZ-NH1	5.21	122.90	120.30
3	D	273	ARG	NE-CZ-NH1	5.18	122.89	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	G	994	0	964	2	0
1	H	994	0	964	2	0
1	I	994	0	964	2	0
2	J	784	0	771	1	0
2	K	784	0	771	1	0
2	L	784	0	771	1	0
3	A	3402	0	3358	15	0
3	C	3402	0	3358	16	0
3	D	3402	0	3358	13	0
4	B	992	0	970	4	0
4	E	992	0	970	4	0
4	F	992	0	970	4	0
5	M	39	0	33	1	0
5	O	39	0	33	1	0
5	Q	39	0	33	0	0
5	T	39	0	33	1	0
5	V	39	0	33	1	0
5	X	39	0	33	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	a	39	0	33	0	0
5	c	39	0	33	0	0
5	e	39	0	33	0	0
6	N	61	0	49	0	0
6	U	61	0	49	0	0
6	b	61	0	49	0	0
7	P	28	0	25	0	0
7	R	28	0	25	0	0
7	S	28	0	25	0	0
7	W	28	0	25	0	0
7	Y	28	0	25	0	0
7	Z	28	0	25	0	0
7	d	28	0	25	0	0
7	f	28	0	25	0	0
7	g	28	0	25	0	0
8	A	70	0	65	1	0
8	B	14	0	13	0	0
8	C	70	0	65	1	0
8	D	70	0	65	1	0
8	E	14	0	13	0	0
8	F	14	0	13	0	0
All	All	19554	0	19092	62	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 2.

All (62) 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)
3:A:207:LYS:NZ	1:I:27:ASP:OD1	2.39	0.56
1:G:27:ASP:OD1	3:D:207:LYS:NZ	2.39	0.56
3:C:57:ASP:N	3:C:57:ASP:OD1	2.38	0.56
3:D:57:ASP:N	3:D:57:ASP:OD1	2.39	0.56
1:H:27:ASP:OD1	3:C:207:LYS:NZ	2.39	0.56
3:A:57:ASP:N	3:A:57:ASP:OD1	2.38	0.55
3:A:167:ASP:OD1	3:A:167:ASP:N	2.40	0.54
3:A:107:ASP:OD1	4:B:574:LYS:NZ	2.40	0.54
3:C:107:ASP:OD1	4:E:574:LYS:NZ	2.40	0.54
4:E:606:THR:OG1	4:E:607:ALA:N	2.41	0.54
3:D:107:ASP:OD1	4:F:574:LYS:NZ	2.40	0.54
4:B:606:THR:OG1	4:B:607:ALA:N	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:167:ASP:N	3:C:167:ASP:OD1	2.40	0.53
3:C:362:ASN:O	3:C:469:ARG:NH1	2.42	0.53
4:F:606:THR:OG1	4:F:607:ALA:N	2.41	0.52
3:A:362:ASN:O	3:A:469:ARG:NH1	2.42	0.52
3:D:362:ASN:O	3:D:469:ARG:NH1	2.42	0.51
3:A:262:ASN:OD1	3:A:262:ASN:N	2.44	0.50
3:D:167:ASP:N	3:D:167:ASP:OD1	2.40	0.49
2:L:32:HIS:HB3	2:L:50:ALA:HB1	1.96	0.48
3:A:501:CYS:O	3:A:502:LYS:C	2.52	0.48
2:J:32:HIS:HB3	2:J:50:ALA:HB1	1.96	0.48
3:C:501:CYS:O	3:C:502:LYS:C	2.52	0.48
2:K:32:HIS:HB3	2:K:50:ALA:HB1	1.96	0.47
3:C:262:ASN:OD1	3:C:262:ASN:N	2.44	0.47
3:D:499:THR:OG1	3:D:500:LYS:N	2.48	0.47
3:D:129:LEU:HB2	3:D:191:TYR:CE2	2.51	0.46
3:C:129:LEU:HB2	3:C:191:TYR:CE2	2.51	0.46
3:D:501:CYS:O	3:D:502:LYS:C	2.52	0.46
3:A:499:THR:OG1	3:A:500:LYS:N	2.48	0.46
3:A:129:LEU:HB2	3:A:191:TYR:CE2	2.51	0.46
3:C:499:THR:OG1	3:C:500:LYS:N	2.48	0.46
3:D:262:ASN:OD1	3:D:262:ASN:N	2.44	0.45
4:E:546:SER:OG	4:E:547:GLY:N	2.50	0.45
4:E:528:SER:OG	4:E:529:THR:N	2.49	0.45
3:A:393:SER:OG	3:A:394:THR:N	2.50	0.45
3:C:393:SER:OG	3:C:394:THR:N	2.50	0.45
4:F:546:SER:OG	4:F:547:GLY:N	2.50	0.44
4:F:528:SER:OG	4:F:529:THR:N	2.49	0.44
4:B:546:SER:OG	4:B:547:GLY:N	2.50	0.43
3:A:189:ASN:OD1	3:A:189:ASN:N	2.51	0.43
3:D:393:SER:OG	3:D:394:THR:N	2.50	0.43
3:D:463(B):THR:OG1	3:D:463(C):SER:N	2.52	0.43
3:C:445:CYS:HB3	5:T:2:NAG:H83	2.01	0.42
3:C:463(B):THR:OG1	3:C:463(C):SER:N	2.52	0.42
3:A:373:MET:HG2	5:O:1:NAG:H81	2.01	0.42
3:C:289:ASN:OD1	3:C:289:ASN:N	2.52	0.42
3:C:373:MET:HG2	5:V:1:NAG:H81	2.01	0.42
3:D:463(C):SER:OG	3:D:464:GLU:N	2.53	0.42
1:H:24:THR:OG1	1:H:25:SER:N	2.53	0.42
3:A:463(B):THR:OG1	3:A:463(C):SER:N	2.52	0.42
3:A:163:THR:OG1	3:A:164:SER:N	2.50	0.42
3:C:163:THR:OG1	3:C:164:SER:N	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:24:THR:OG1	1:I:25:SER:N	2.53	0.41
3:A:445:CYS:HB3	5:M:2:NAG:H83	2.01	0.41
1:G:24:THR:OG1	1:G:25:SER:N	2.53	0.41
4:B:528:SER:OG	4:B:529:THR:N	2.49	0.41
8:C:619:NAG:O7	8:C:619:NAG:C3	2.69	0.41
3:C:463(C):SER:OG	3:C:464:GLU:N	2.53	0.40
3:D:397:ASP:C	3:D:397:ASP:OD1	2.59	0.40
8:A:619:NAG:O7	8:A:619:NAG:C3	2.69	0.40
8:D:619:NAG:O7	8:D:619:NAG:C3	2.69	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	G	123/228 (54%)	122 (99%)	1 (1%)	0	100	100
1	H	123/228 (54%)	122 (99%)	1 (1%)	0	100	100
1	I	123/228 (54%)	122 (99%)	1 (1%)	0	100	100
2	J	98/208 (47%)	94 (96%)	4 (4%)	0	100	100
2	K	98/208 (47%)	94 (96%)	4 (4%)	0	100	100
2	L	98/208 (47%)	94 (96%)	4 (4%)	0	100	100
3	A	419/482 (87%)	397 (95%)	19 (4%)	3 (1%)	22	62
3	C	419/482 (87%)	397 (95%)	19 (4%)	3 (1%)	22	62
3	D	419/482 (87%)	397 (95%)	19 (4%)	3 (1%)	22	62
4	B	120/154 (78%)	114 (95%)	5 (4%)	1 (1%)	19	60
4	E	120/154 (78%)	114 (95%)	5 (4%)	1 (1%)	19	60
4	F	120/154 (78%)	114 (95%)	5 (4%)	1 (1%)	19	60
All	All	2280/3216 (71%)	2181 (96%)	87 (4%)	12 (0%)	32	68

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	465	THR
3	C	465	THR
3	D	465	THR
3	A	213	ILE
3	C	213	ILE
3	D	213	ILE
3	A	449	ILE
4	B	541	ALA
3	C	449	ILE
4	E	541	ALA
3	D	449	ILE
4	F	541	ALA

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	G	104/193 (54%)	103 (99%)	1 (1%)	76 86
1	H	104/193 (54%)	103 (99%)	1 (1%)	76 86
1	I	104/193 (54%)	103 (99%)	1 (1%)	76 86
2	J	85/182 (47%)	85 (100%)	0	100 100
2	K	85/182 (47%)	85 (100%)	0	100 100
2	L	85/182 (47%)	85 (100%)	0	100 100
3	A	386/428 (90%)	383 (99%)	3 (1%)	81 89
3	C	386/428 (90%)	383 (99%)	3 (1%)	81 89
3	D	386/428 (90%)	383 (99%)	3 (1%)	81 89
4	B	107/129 (83%)	107 (100%)	0	100 100
4	E	107/129 (83%)	107 (100%)	0	100 100
4	F	107/129 (83%)	107 (100%)	0	100 100
All	All	2046/2796 (73%)	2034 (99%)	12 (1%)	86 92

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	71	ARG
3	A	262	ASN
3	A	276	ASN
3	A	362	ASN
1	G	71	ARG
3	C	262	ASN
3	C	276	ASN
3	C	362	ASN
1	I	71	ARG
3	D	262	ASN
3	D	276	ASN
3	D	362	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	114	GLN
3	A	229	ASN
3	C	114	GLN
3	C	229	ASN
3	D	114	GLN
3	D	229	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

60 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	3,5	14,14,15	0.89	1 (7%)	17,19,21	2.15	4 (23%)
5	NAG	M	2	5	14,14,15	0.82	0	17,19,21	1.29	2 (11%)
5	BMA	M	3	5	11,11,12	1.84	2 (18%)	15,15,17	0.97	0
6	NAG	N	1	3,6	14,14,15	0.87	0	17,19,21	1.12	2 (11%)
6	NAG	N	2	6	14,14,15	1.08	1 (7%)	17,19,21	1.29	2 (11%)
6	BMA	N	3	6	11,11,12	1.99	3 (27%)	15,15,17	1.13	1 (6%)
6	MAN	N	4	6	11,11,12	1.86	3 (27%)	15,15,17	1.16	3 (20%)
6	MAN	N	5	6	11,11,12	1.84	2 (18%)	15,15,17	1.24	3 (20%)
5	NAG	O	1	3,5	14,14,15	0.86	0	17,19,21	2.41	5 (29%)
5	NAG	O	2	5	14,14,15	0.78	0	17,19,21	0.92	0
5	BMA	O	3	5	11,11,12	1.82	2 (18%)	15,15,17	0.90	1 (6%)
7	NAG	P	1	3,7	14,14,15	0.79	0	17,19,21	0.92	0
7	NAG	P	2	7	14,14,15	0.80	0	17,19,21	0.89	1 (5%)
5	NAG	Q	1	3,5	14,14,15	0.79	0	17,19,21	0.91	0
5	NAG	Q	2	5	14,14,15	0.83	0	17,19,21	0.95	1 (5%)
5	BMA	Q	3	5	11,11,12	1.81	2 (18%)	15,15,17	0.89	1 (6%)
7	NAG	R	1	3,7	14,14,15	0.81	0	17,19,21	1.50	3 (17%)
7	NAG	R	2	7	14,14,15	0.83	0	17,19,21	1.11	1 (5%)
7	NAG	S	1	3,7	14,14,15	0.83	0	17,19,21	1.29	2 (11%)
7	NAG	S	2	7	14,14,15	0.81	0	17,19,21	0.95	1 (5%)
5	NAG	T	1	3,5	14,14,15	0.89	1 (7%)	17,19,21	2.16	4 (23%)
5	NAG	T	2	5	14,14,15	0.82	0	17,19,21	1.29	2 (11%)
5	BMA	T	3	5	11,11,12	1.83	2 (18%)	15,15,17	0.97	0
6	NAG	U	1	3,6	14,14,15	0.87	0	17,19,21	1.13	2 (11%)
6	NAG	U	2	6	14,14,15	1.07	1 (7%)	17,19,21	1.29	2 (11%)
6	BMA	U	3	6	11,11,12	1.99	3 (27%)	15,15,17	1.13	1 (6%)
6	MAN	U	4	6	11,11,12	1.86	3 (27%)	15,15,17	1.17	3 (20%)
6	MAN	U	5	6	11,11,12	1.84	2 (18%)	15,15,17	1.24	3 (20%)
5	NAG	V	1	3,5	14,14,15	0.86	0	17,19,21	2.41	5 (29%)
5	NAG	V	2	5	14,14,15	0.78	0	17,19,21	0.93	0
5	BMA	V	3	5	11,11,12	1.83	2 (18%)	15,15,17	0.90	1 (6%)
7	NAG	W	1	3,7	14,14,15	0.78	0	17,19,21	0.92	0
7	NAG	W	2	7	14,14,15	0.81	0	17,19,21	0.89	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	NAG	X	1	3,5	14,14,15	0.79	0	17,19,21	0.90	0
5	NAG	X	2	5	14,14,15	0.83	0	17,19,21	0.95	1 (5%)
5	BMA	X	3	5	11,11,12	1.82	2 (18%)	15,15,17	0.89	1 (6%)
7	NAG	Y	1	3,7	14,14,15	0.81	0	17,19,21	1.50	3 (17%)
7	NAG	Y	2	7	14,14,15	0.84	0	17,19,21	1.11	1 (5%)
7	NAG	Z	1	3,7	14,14,15	0.83	0	17,19,21	1.29	2 (11%)
7	NAG	Z	2	7	14,14,15	0.80	0	17,19,21	0.95	1 (5%)
5	NAG	a	1	3,5	14,14,15	0.89	1 (7%)	17,19,21	2.15	4 (23%)
5	NAG	a	2	5	14,14,15	0.82	0	17,19,21	1.29	2 (11%)
5	BMA	a	3	5	11,11,12	1.84	2 (18%)	15,15,17	0.97	0
6	NAG	b	1	3,6	14,14,15	0.87	0	17,19,21	1.12	2 (11%)
6	NAG	b	2	6	14,14,15	1.08	1 (7%)	17,19,21	1.29	2 (11%)
6	BMA	b	3	6	11,11,12	1.99	3 (27%)	15,15,17	1.13	1 (6%)
6	MAN	b	4	6	11,11,12	1.86	3 (27%)	15,15,17	1.17	3 (20%)
6	MAN	b	5	6	11,11,12	1.85	2 (18%)	15,15,17	1.24	3 (20%)
5	NAG	c	1	3,5	14,14,15	0.85	0	17,19,21	2.41	5 (29%)
5	NAG	c	2	5	14,14,15	0.78	0	17,19,21	0.92	0
5	BMA	c	3	5	11,11,12	1.82	2 (18%)	15,15,17	0.90	1 (6%)
7	NAG	d	1	3,7	14,14,15	0.79	0	17,19,21	0.92	0
7	NAG	d	2	7	14,14,15	0.81	0	17,19,21	0.90	1 (5%)
5	NAG	e	1	3,5	14,14,15	0.79	0	17,19,21	0.91	0
5	NAG	e	2	5	14,14,15	0.83	0	17,19,21	0.95	1 (5%)
5	BMA	e	3	5	11,11,12	1.82	2 (18%)	15,15,17	0.89	1 (6%)
7	NAG	f	1	3,7	14,14,15	0.81	0	17,19,21	1.50	3 (17%)
7	NAG	f	2	7	14,14,15	0.84	0	17,19,21	1.11	1 (5%)
7	NAG	g	1	3,7	14,14,15	0.84	0	17,19,21	1.29	2 (11%)
7	NAG	g	2	7	14,14,15	0.81	0	17,19,21	0.95	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	3,5	-	2/6/23/26	0/1/1/1
5	NAG	M	2	5	-	2/6/23/26	0/1/1/1
5	BMA	M	3	5	-	2/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	N	1	3,6	-	0/6/23/26	0/1/1/1
6	NAG	N	2	6	-	0/6/23/26	0/1/1/1
6	BMA	N	3	6	-	2/2/19/22	0/1/1/1
6	MAN	N	4	6	-	1/2/19/22	0/1/1/1
6	MAN	N	5	6	-	1/2/19/22	0/1/1/1
5	NAG	O	1	3,5	-	2/6/23/26	0/1/1/1
5	NAG	O	2	5	-	0/6/23/26	0/1/1/1
5	BMA	O	3	5	-	1/2/19/22	0/1/1/1
7	NAG	P	1	3,7	-	0/6/23/26	0/1/1/1
7	NAG	P	2	7	-	1/6/23/26	0/1/1/1
5	NAG	Q	1	3,5	-	0/6/23/26	0/1/1/1
5	NAG	Q	2	5	-	0/6/23/26	0/1/1/1
5	BMA	Q	3	5	-	1/2/19/22	0/1/1/1
7	NAG	R	1	3,7	-	2/6/23/26	0/1/1/1
7	NAG	R	2	7	-	1/6/23/26	0/1/1/1
7	NAG	S	1	3,7	-	2/6/23/26	0/1/1/1
7	NAG	S	2	7	-	2/6/23/26	0/1/1/1
5	NAG	T	1	3,5	-	2/6/23/26	0/1/1/1
5	NAG	T	2	5	-	2/6/23/26	0/1/1/1
5	BMA	T	3	5	-	2/2/19/22	0/1/1/1
6	NAG	U	1	3,6	-	0/6/23/26	0/1/1/1
6	NAG	U	2	6	-	0/6/23/26	0/1/1/1
6	BMA	U	3	6	-	2/2/19/22	0/1/1/1
6	MAN	U	4	6	-	1/2/19/22	0/1/1/1
6	MAN	U	5	6	-	1/2/19/22	0/1/1/1
5	NAG	V	1	3,5	-	2/6/23/26	0/1/1/1
5	NAG	V	2	5	-	0/6/23/26	0/1/1/1
5	BMA	V	3	5	-	1/2/19/22	0/1/1/1
7	NAG	W	1	3,7	-	0/6/23/26	0/1/1/1
7	NAG	W	2	7	-	1/6/23/26	0/1/1/1
5	NAG	X	1	3,5	-	0/6/23/26	0/1/1/1
5	NAG	X	2	5	-	0/6/23/26	0/1/1/1
5	BMA	X	3	5	-	1/2/19/22	0/1/1/1
7	NAG	Y	1	3,7	-	2/6/23/26	0/1/1/1
7	NAG	Y	2	7	-	1/6/23/26	0/1/1/1
7	NAG	Z	1	3,7	-	2/6/23/26	0/1/1/1
7	NAG	Z	2	7	-	2/6/23/26	0/1/1/1
5	NAG	a	1	3,5	-	2/6/23/26	0/1/1/1
5	NAG	a	2	5	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	BMA	a	3	5	-	2/2/19/22	0/1/1/1
6	NAG	b	1	3,6	-	0/6/23/26	0/1/1/1
6	NAG	b	2	6	-	0/6/23/26	0/1/1/1
6	BMA	b	3	6	-	2/2/19/22	0/1/1/1
6	MAN	b	4	6	-	1/2/19/22	0/1/1/1
6	MAN	b	5	6	-	1/2/19/22	0/1/1/1
5	NAG	c	1	3,5	-	2/6/23/26	0/1/1/1
5	NAG	c	2	5	-	0/6/23/26	0/1/1/1
5	BMA	c	3	5	-	1/2/19/22	0/1/1/1
7	NAG	d	1	3,7	-	0/6/23/26	0/1/1/1
7	NAG	d	2	7	-	1/6/23/26	0/1/1/1
5	NAG	e	1	3,5	-	0/6/23/26	0/1/1/1
5	NAG	e	2	5	-	0/6/23/26	0/1/1/1
5	BMA	e	3	5	-	1/2/19/22	0/1/1/1
7	NAG	f	1	3,7	-	2/6/23/26	0/1/1/1
7	NAG	f	2	7	-	1/6/23/26	0/1/1/1
7	NAG	g	1	3,7	-	2/6/23/26	0/1/1/1
7	NAG	g	2	7	-	2/6/23/26	0/1/1/1

All (48) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	e	3	BMA	O2-C2	-4.19	1.34	1.43
5	X	3	BMA	O2-C2	-4.17	1.34	1.43
5	Q	3	BMA	O2-C2	-4.16	1.34	1.43
6	b	5	MAN	O2-C2	-4.15	1.34	1.43
6	U	5	MAN	O2-C2	-4.14	1.34	1.43
6	N	5	MAN	O2-C2	-4.13	1.34	1.43
6	N	3	BMA	O2-C2	-4.10	1.34	1.43
6	U	3	BMA	O2-C2	-4.10	1.34	1.43
6	b	3	BMA	O2-C2	-4.09	1.34	1.43
6	N	4	MAN	O2-C2	-4.07	1.34	1.43
6	b	4	MAN	O2-C2	-4.07	1.34	1.43
6	U	4	MAN	O2-C2	-4.07	1.34	1.43
5	M	3	BMA	O2-C2	-4.07	1.34	1.43
5	V	3	BMA	O2-C2	-4.06	1.34	1.43
5	O	3	BMA	O2-C2	-4.06	1.34	1.43
5	c	3	BMA	O2-C2	-4.06	1.34	1.43
5	T	3	BMA	O2-C2	-4.05	1.34	1.43
5	a	3	BMA	O2-C2	-4.04	1.34	1.43
5	V	3	BMA	C2-C3	-2.42	1.48	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	b	3	BMA	C2-C3	-2.40	1.49	1.52
5	O	3	BMA	C2-C3	-2.40	1.49	1.52
6	N	5	MAN	C2-C3	-2.40	1.49	1.52
5	c	3	BMA	C2-C3	-2.39	1.49	1.52
6	U	3	BMA	C2-C3	-2.39	1.49	1.52
6	b	5	MAN	C2-C3	-2.37	1.49	1.52
6	N	3	BMA	C2-C3	-2.37	1.49	1.52
6	U	5	MAN	C2-C3	-2.36	1.49	1.52
6	N	4	MAN	O5-C1	2.28	1.47	1.43
5	a	3	BMA	C2-C3	-2.28	1.49	1.52
6	b	4	MAN	O5-C1	2.27	1.47	1.43
6	U	4	MAN	O5-C1	2.27	1.47	1.43
5	X	3	BMA	C2-C3	-2.26	1.49	1.52
5	M	1	NAG	C3-C2	-2.25	1.47	1.52
5	T	1	NAG	C3-C2	-2.25	1.47	1.52
5	a	1	NAG	C3-C2	-2.25	1.47	1.52
5	e	3	BMA	C2-C3	-2.25	1.49	1.52
5	M	3	BMA	C2-C3	-2.24	1.49	1.52
5	Q	3	BMA	C2-C3	-2.24	1.49	1.52
5	T	3	BMA	C2-C3	-2.23	1.49	1.52
6	b	2	NAG	C3-C2	-2.20	1.47	1.52
6	N	2	NAG	C3-C2	-2.20	1.47	1.52
6	U	2	NAG	C3-C2	-2.20	1.47	1.52
6	U	4	MAN	C2-C3	-2.19	1.49	1.52
6	N	4	MAN	C2-C3	-2.18	1.49	1.52
6	b	4	MAN	C2-C3	-2.17	1.49	1.52
6	N	3	BMA	C6-C5	2.10	1.58	1.51
6	U	3	BMA	C6-C5	2.10	1.58	1.51
6	b	3	BMA	C6-C5	2.08	1.58	1.51

All (99) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	c	1	NAG	O5-C5-C6	-5.87	98.01	107.20
5	V	1	NAG	O5-C5-C6	-5.86	98.01	107.20
5	O	1	NAG	O5-C5-C6	-5.85	98.04	107.20
5	c	1	NAG	O4-C4-C3	-5.32	98.04	110.35
5	V	1	NAG	O4-C4-C3	-5.31	98.06	110.35
5	O	1	NAG	O4-C4-C3	-5.31	98.08	110.35
5	T	1	NAG	O4-C4-C3	-5.19	98.36	110.35
5	M	1	NAG	O4-C4-C3	-5.18	98.37	110.35
5	a	1	NAG	O4-C4-C3	-5.18	98.37	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	T	1	NAG	O5-C5-C6	-4.54	100.08	107.20
5	a	1	NAG	O5-C5-C6	-4.53	100.10	107.20
5	M	1	NAG	O5-C5-C6	-4.52	100.12	107.20
6	b	1	NAG	C3-C4-C5	-3.60	103.83	110.24
6	U	1	NAG	C3-C4-C5	-3.59	103.83	110.24
6	N	1	NAG	C3-C4-C5	-3.59	103.83	110.24
5	V	1	NAG	C3-C4-C5	-3.45	104.08	110.24
5	O	1	NAG	C3-C4-C5	-3.45	104.08	110.24
5	c	1	NAG	C3-C4-C5	-3.44	104.10	110.24
7	g	1	NAG	C4-C3-C2	-3.42	106.00	111.02
5	M	2	NAG	C4-C3-C2	-3.40	106.03	111.02
7	Z	1	NAG	C4-C3-C2	-3.40	106.04	111.02
7	S	1	NAG	C4-C3-C2	-3.40	106.04	111.02
5	a	2	NAG	C4-C3-C2	-3.40	106.04	111.02
5	T	2	NAG	C4-C3-C2	-3.39	106.05	111.02
7	f	2	NAG	C4-C3-C2	-3.33	106.14	111.02
7	Y	2	NAG	C4-C3-C2	-3.32	106.15	111.02
5	T	1	NAG	O4-C4-C5	3.32	117.53	109.30
7	R	2	NAG	C4-C3-C2	-3.32	106.16	111.02
5	a	1	NAG	O4-C4-C5	3.31	117.53	109.30
5	M	1	NAG	O4-C4-C5	3.31	117.52	109.30
5	c	1	NAG	O4-C4-C5	3.21	117.26	109.30
5	O	1	NAG	O4-C4-C5	3.21	117.26	109.30
5	V	1	NAG	O4-C4-C5	3.20	117.23	109.30
7	f	1	NAG	O5-C5-C6	-3.18	102.22	107.20
7	R	1	NAG	O5-C5-C6	-3.18	102.22	107.20
7	Y	1	NAG	O5-C5-C6	-3.18	102.22	107.20
7	f	1	NAG	O4-C4-C3	-3.05	103.31	110.35
7	Y	1	NAG	O4-C4-C3	-3.04	103.31	110.35
7	R	1	NAG	O4-C4-C3	-3.04	103.32	110.35
6	N	2	NAG	O5-C1-C2	-2.99	106.57	111.29
6	U	2	NAG	O5-C1-C2	-2.99	106.57	111.29
6	b	2	NAG	O5-C1-C2	-2.98	106.58	111.29
5	M	2	NAG	C1-C2-N2	-2.95	105.45	110.49
5	a	2	NAG	C1-C2-N2	-2.95	105.45	110.49
5	T	2	NAG	C1-C2-N2	-2.94	105.47	110.49
7	Y	1	NAG	C3-C4-C5	-2.84	105.17	110.24
7	R	1	NAG	C3-C4-C5	-2.83	105.19	110.24
7	f	1	NAG	C3-C4-C5	-2.83	105.20	110.24
5	T	1	NAG	C3-C4-C5	-2.73	105.37	110.24
5	a	1	NAG	C3-C4-C5	-2.73	105.37	110.24
5	M	1	NAG	C3-C4-C5	-2.73	105.38	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	S	2	NAG	C4-C3-C2	-2.65	107.13	111.02
7	g	2	NAG	C4-C3-C2	-2.65	107.13	111.02
7	Z	2	NAG	C4-C3-C2	-2.64	107.14	111.02
6	N	5	MAN	C1-C2-C3	2.55	112.80	109.67
5	O	1	NAG	C4-C3-C2	2.54	114.75	111.02
6	U	5	MAN	C1-C2-C3	2.54	112.79	109.67
5	V	1	NAG	C4-C3-C2	2.53	114.73	111.02
6	b	5	MAN	C1-C2-C3	2.52	112.77	109.67
5	c	1	NAG	C4-C3-C2	2.52	114.70	111.02
7	S	1	NAG	O5-C1-C2	-2.48	107.37	111.29
7	Z	1	NAG	O5-C1-C2	-2.47	107.38	111.29
7	g	1	NAG	O5-C1-C2	-2.47	107.38	111.29
7	d	2	NAG	C4-C3-C2	-2.46	107.41	111.02
6	b	4	MAN	C1-C2-C3	2.46	112.69	109.67
6	U	4	MAN	C1-C2-C3	2.46	112.69	109.67
7	W	2	NAG	C4-C3-C2	-2.45	107.42	111.02
7	P	2	NAG	C4-C3-C2	-2.45	107.43	111.02
6	N	4	MAN	C1-C2-C3	2.44	112.67	109.67
6	b	3	BMA	O3-C3-C4	2.40	115.90	110.35
6	N	3	BMA	O3-C3-C4	2.40	115.90	110.35
6	U	3	BMA	O3-C3-C4	2.40	115.90	110.35
5	X	2	NAG	C4-C3-C2	-2.29	107.66	111.02
5	Q	2	NAG	C4-C3-C2	-2.29	107.66	111.02
5	e	2	NAG	C4-C3-C2	-2.29	107.66	111.02
6	N	5	MAN	C2-C3-C4	-2.29	106.94	110.89
6	U	5	MAN	C2-C3-C4	-2.28	106.94	110.89
6	b	5	MAN	C2-C3-C4	-2.28	106.95	110.89
6	U	4	MAN	C2-C3-C4	-2.24	107.02	110.89
6	b	4	MAN	C2-C3-C4	-2.23	107.03	110.89
6	N	1	NAG	O5-C1-C2	-2.23	107.77	111.29
6	U	1	NAG	O5-C1-C2	-2.23	107.77	111.29
6	b	1	NAG	O5-C1-C2	-2.22	107.78	111.29
6	N	4	MAN	C2-C3-C4	-2.22	107.06	110.89
6	N	5	MAN	O5-C1-C2	-2.19	107.38	110.77
6	b	5	MAN	O5-C1-C2	-2.19	107.39	110.77
6	U	5	MAN	O5-C1-C2	-2.18	107.41	110.77
6	U	2	NAG	C4-C3-C2	-2.17	107.84	111.02
6	b	2	NAG	C4-C3-C2	-2.16	107.86	111.02
6	N	2	NAG	C4-C3-C2	-2.15	107.86	111.02
6	b	4	MAN	O5-C1-C2	-2.13	107.48	110.77
6	U	4	MAN	O5-C1-C2	-2.13	107.49	110.77
6	N	4	MAN	O5-C1-C2	-2.12	107.49	110.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	Q	3	BMA	C2-C3-C4	-2.10	107.25	110.89
5	X	3	BMA	C2-C3-C4	-2.10	107.26	110.89
5	e	3	BMA	C2-C3-C4	-2.09	107.28	110.89
5	O	3	BMA	C2-C3-C4	-2.08	107.30	110.89
5	V	3	BMA	C2-C3-C4	-2.08	107.30	110.89
5	c	3	BMA	C2-C3-C4	-2.07	107.31	110.89

There are no chirality outliers.

All (66) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	S	1	NAG	O5-C5-C6-O6
7	Z	1	NAG	O5-C5-C6-O6
7	g	1	NAG	O5-C5-C6-O6
7	R	1	NAG	O5-C5-C6-O6
7	Y	1	NAG	O5-C5-C6-O6
7	f	1	NAG	O5-C5-C6-O6
7	S	2	NAG	O5-C5-C6-O6
7	Z	2	NAG	O5-C5-C6-O6
7	g	2	NAG	O5-C5-C6-O6
7	S	1	NAG	C4-C5-C6-O6
7	Z	1	NAG	C4-C5-C6-O6
7	g	1	NAG	C4-C5-C6-O6
5	M	3	BMA	O5-C5-C6-O6
5	O	1	NAG	O5-C5-C6-O6
5	T	3	BMA	O5-C5-C6-O6
5	V	1	NAG	O5-C5-C6-O6
5	a	3	BMA	O5-C5-C6-O6
5	c	1	NAG	O5-C5-C6-O6
6	N	3	BMA	O5-C5-C6-O6
6	U	3	BMA	O5-C5-C6-O6
6	b	3	BMA	O5-C5-C6-O6
5	O	1	NAG	C4-C5-C6-O6
5	V	1	NAG	C4-C5-C6-O6
5	c	1	NAG	C4-C5-C6-O6
5	Q	3	BMA	O5-C5-C6-O6
5	X	3	BMA	O5-C5-C6-O6
5	e	3	BMA	O5-C5-C6-O6
7	R	2	NAG	O5-C5-C6-O6
7	Y	2	NAG	O5-C5-C6-O6
7	f	2	NAG	O5-C5-C6-O6
6	N	3	BMA	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
6	U	3	BMA	C4-C5-C6-O6
6	b	3	BMA	C4-C5-C6-O6
5	O	3	BMA	O5-C5-C6-O6
5	V	3	BMA	O5-C5-C6-O6
5	c	3	BMA	O5-C5-C6-O6
7	P	2	NAG	O5-C5-C6-O6
7	W	2	NAG	O5-C5-C6-O6
7	d	2	NAG	O5-C5-C6-O6
6	N	4	MAN	O5-C5-C6-O6
6	U	4	MAN	O5-C5-C6-O6
6	b	4	MAN	O5-C5-C6-O6
7	R	1	NAG	C4-C5-C6-O6
7	Y	1	NAG	C4-C5-C6-O6
7	f	1	NAG	C4-C5-C6-O6
5	M	1	NAG	C4-C5-C6-O6
5	T	1	NAG	C4-C5-C6-O6
5	a	1	NAG	C4-C5-C6-O6
5	M	2	NAG	O5-C5-C6-O6
5	T	2	NAG	O5-C5-C6-O6
5	a	2	NAG	O5-C5-C6-O6
7	S	2	NAG	C4-C5-C6-O6
7	Z	2	NAG	C4-C5-C6-O6
7	g	2	NAG	C4-C5-C6-O6
6	N	5	MAN	O5-C5-C6-O6
6	U	5	MAN	O5-C5-C6-O6
6	b	5	MAN	O5-C5-C6-O6
5	M	1	NAG	O5-C5-C6-O6
5	T	1	NAG	O5-C5-C6-O6
5	a	1	NAG	O5-C5-C6-O6
5	M	2	NAG	C4-C5-C6-O6
5	a	2	NAG	C4-C5-C6-O6
5	T	2	NAG	C4-C5-C6-O6
5	M	3	BMA	C4-C5-C6-O6
5	T	3	BMA	C4-C5-C6-O6
5	a	3	BMA	C4-C5-C6-O6

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	O	1	NAG	1	0
5	M	2	NAG	1	0

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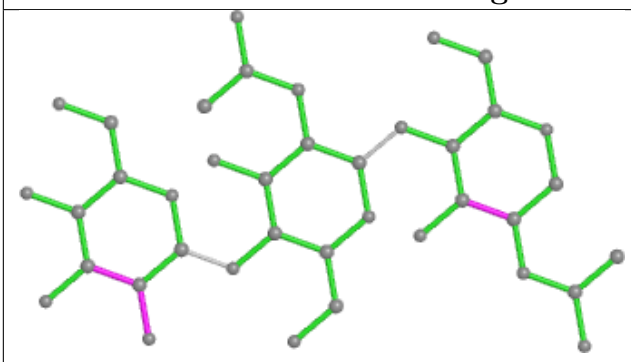
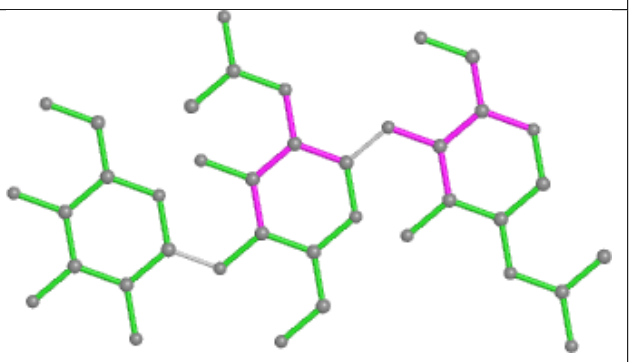
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	V	1	NAG	1	0
5	T	2	NAG	1	0

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

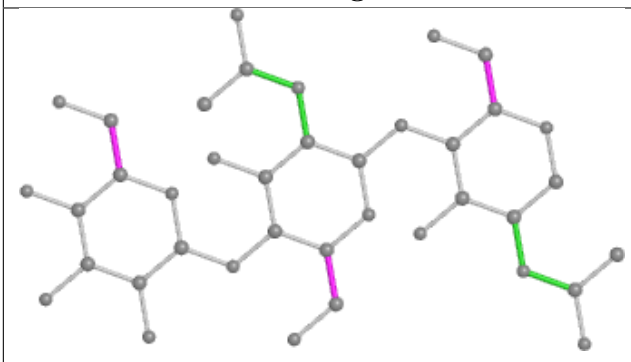
Oligosaccharide Chain M



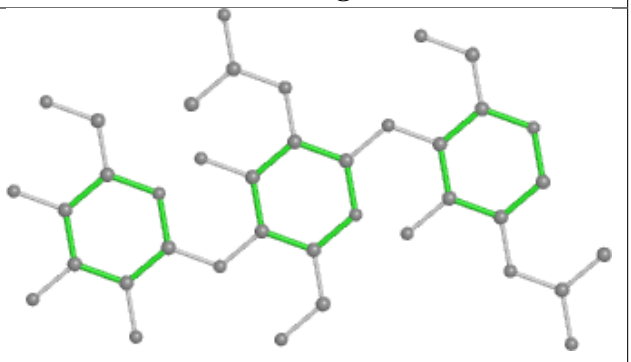
Bond lengths



Bond angles

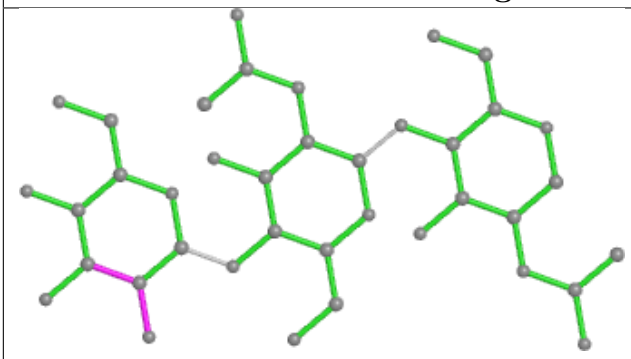


Torsions

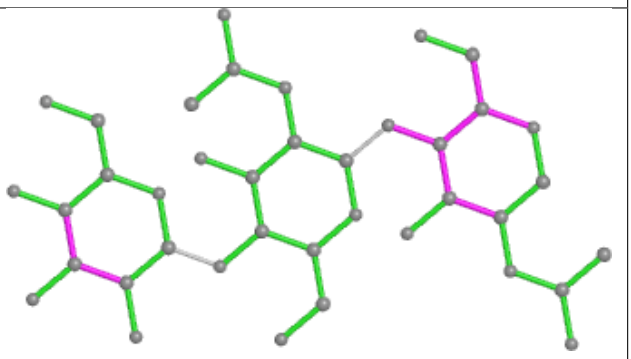


Rings

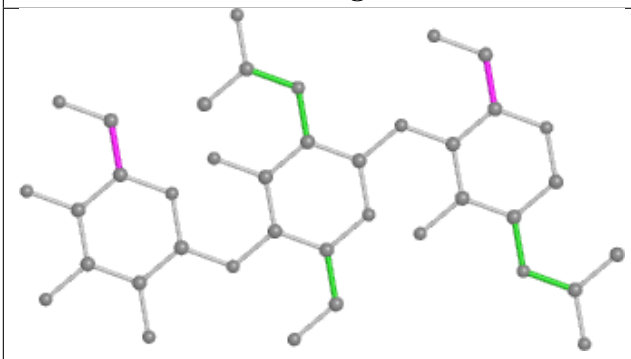
Oligosaccharide Chain O



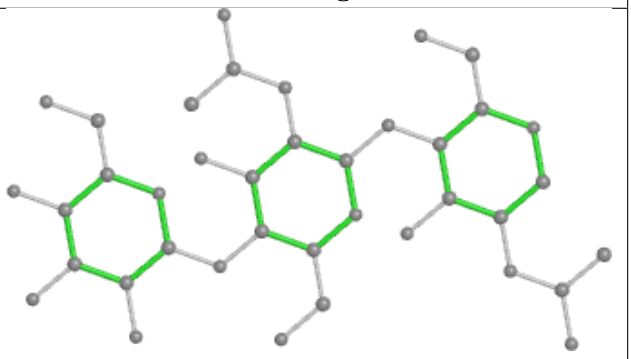
Bond lengths



Bond angles

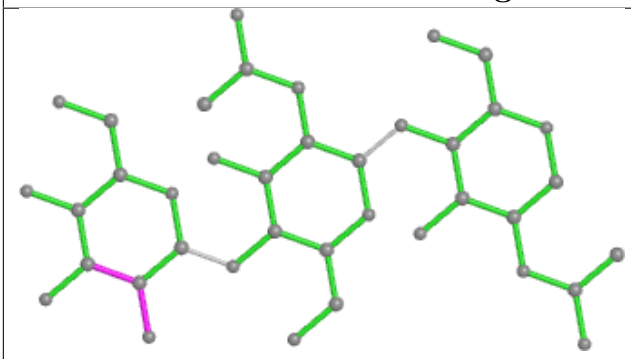


Torsions

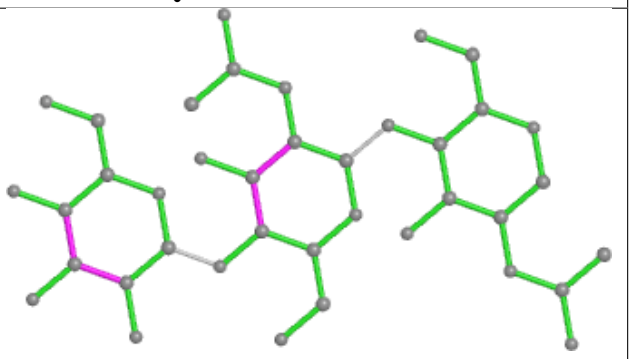


Rings

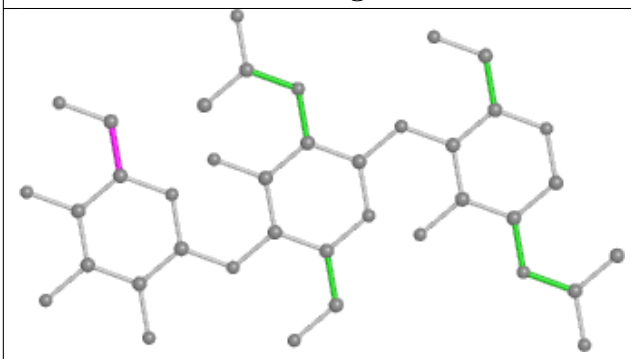
Oligosaccharide Chain Q



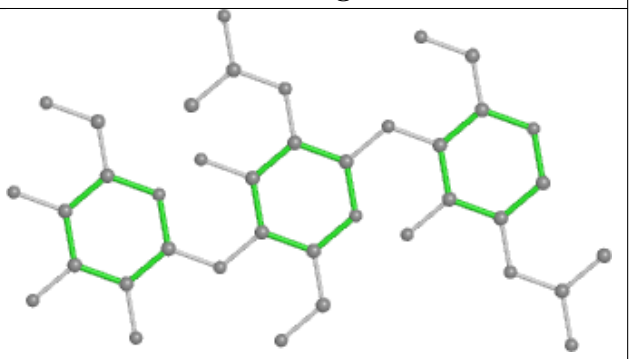
Bond lengths



Bond angles

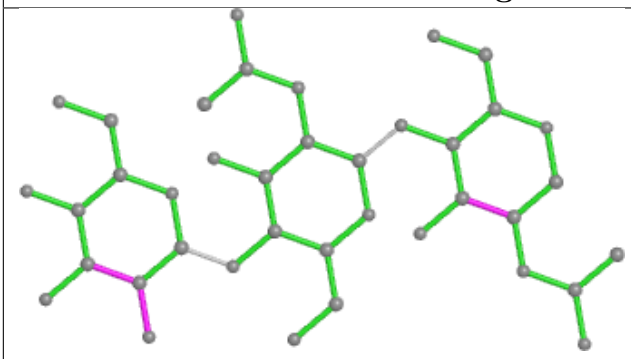


Torsions

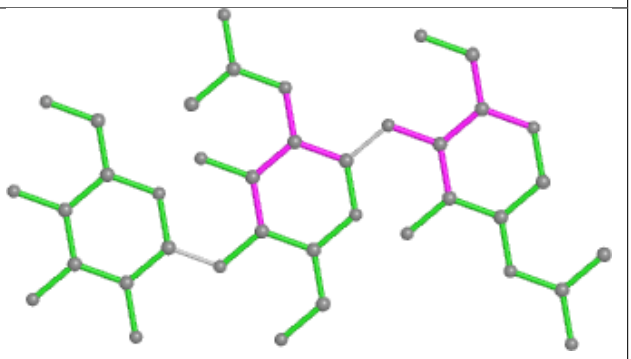


Rings

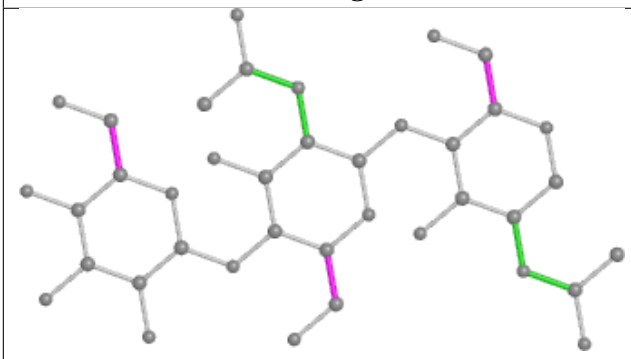
Oligosaccharide Chain T



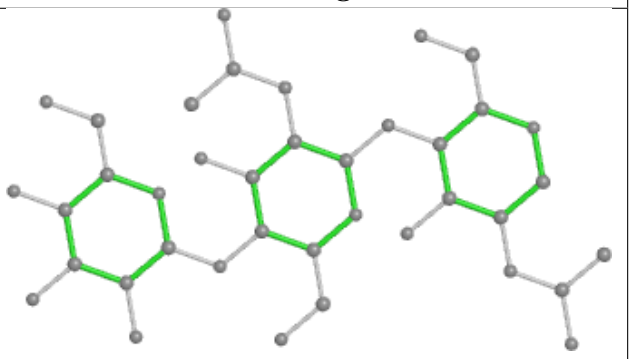
Bond lengths



Bond angles

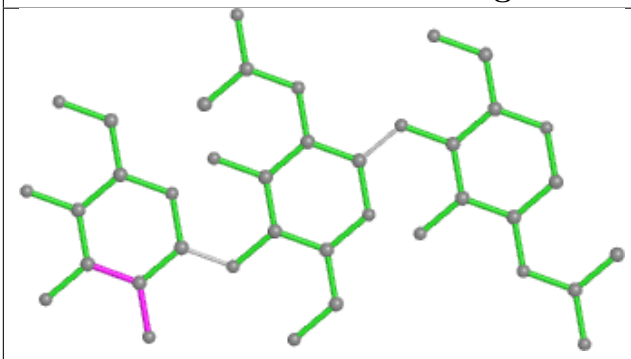


Torsions

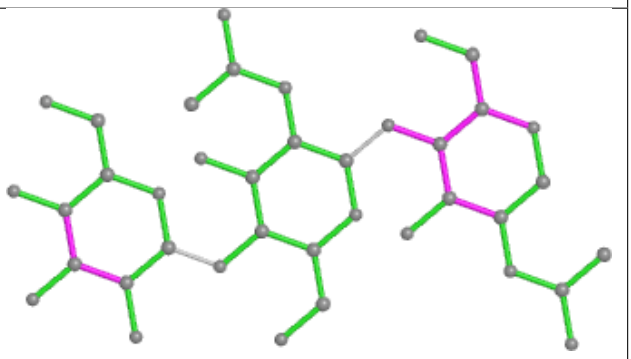


Rings

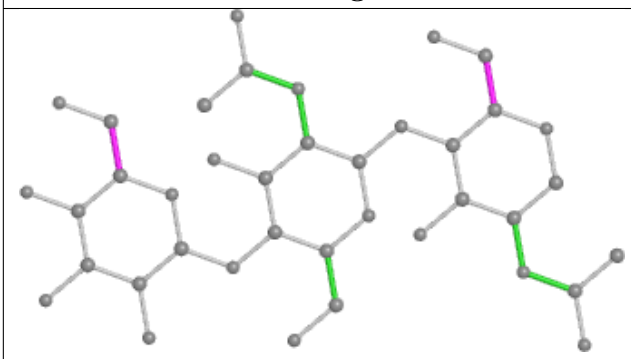
Oligosaccharide Chain V



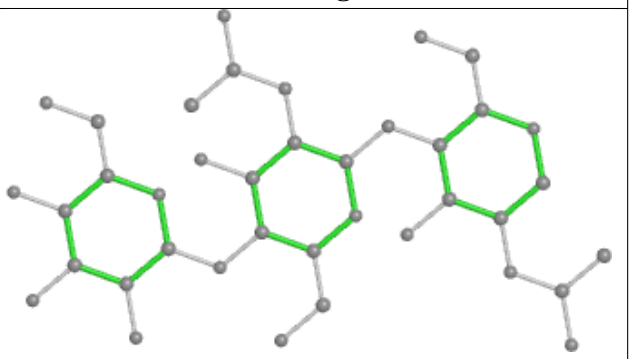
Bond lengths



Bond angles

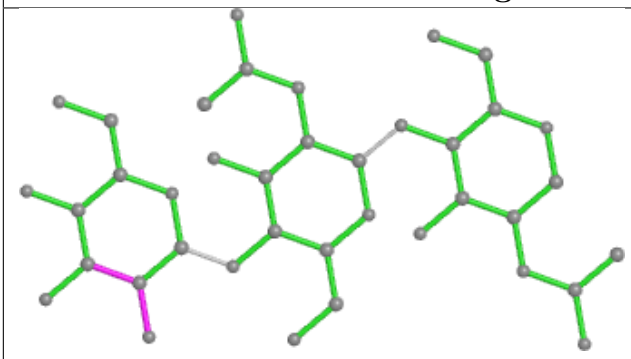


Torsions



Rings

Oligosaccharide Chain X



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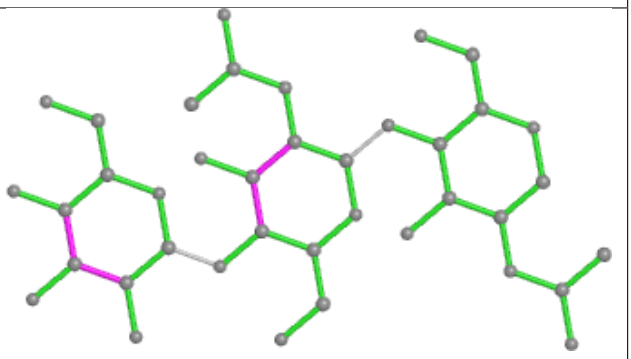
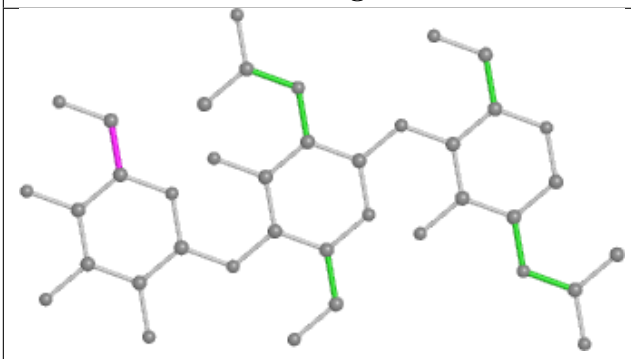


Bond angles



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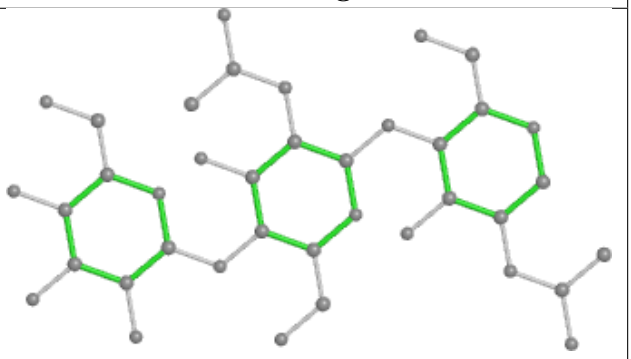
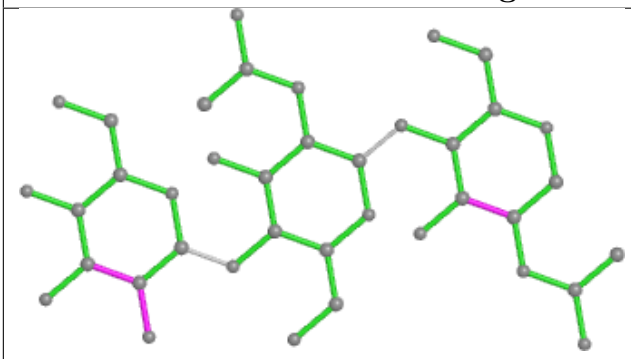


Rings

Oligosaccharide Chain a



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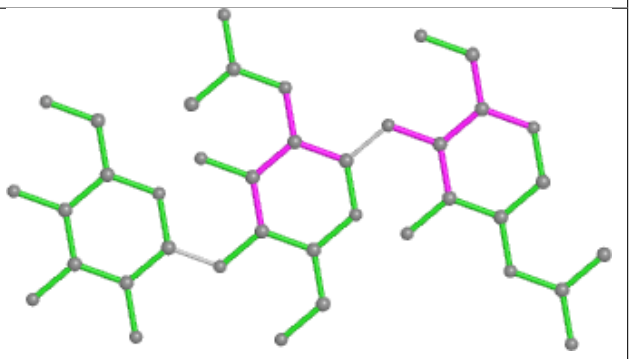
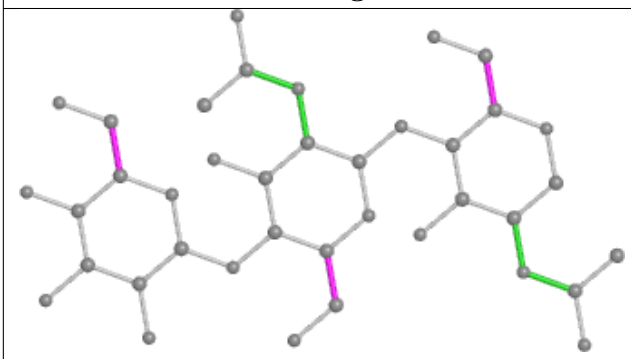


Bond angles



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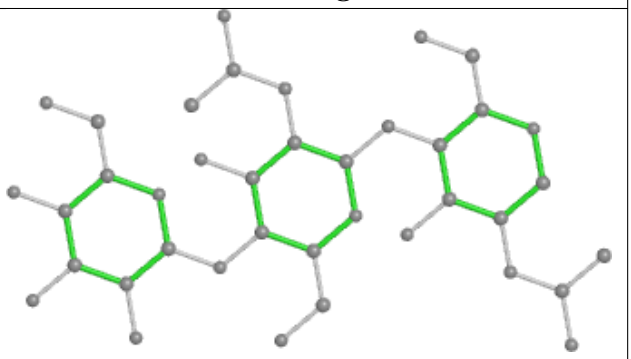
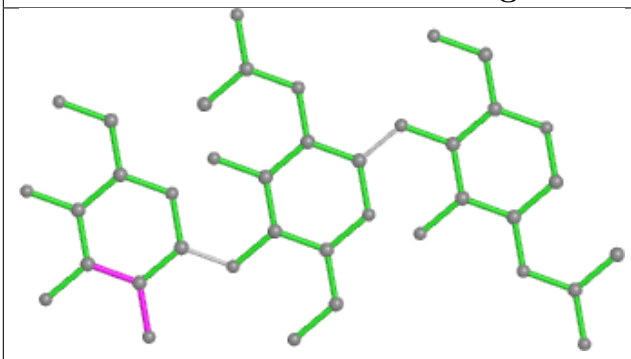


Rings

Oligosaccharide Chain c



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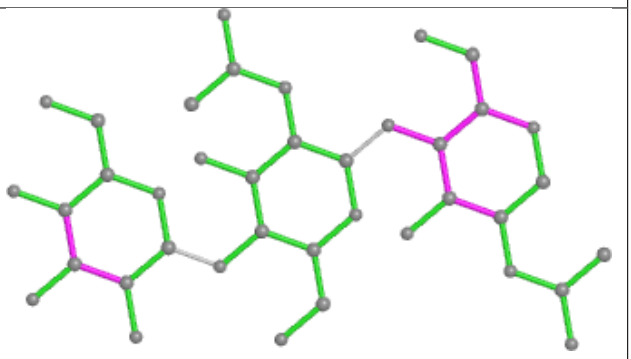
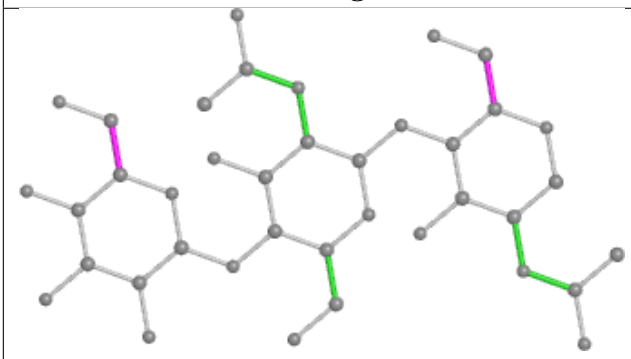
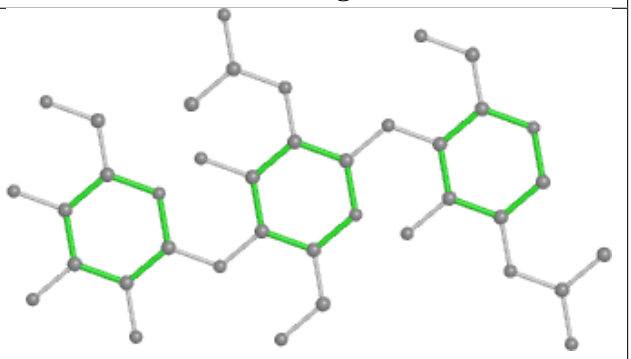


Bond angles

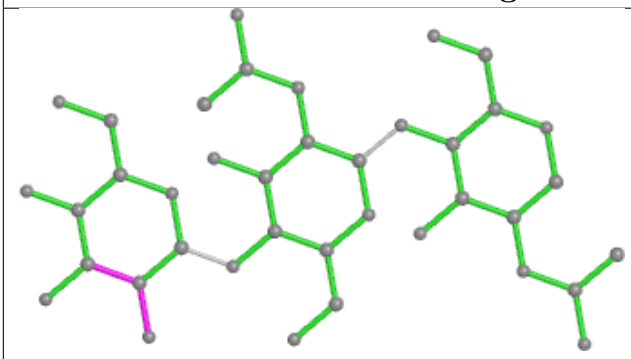


Torsions



Rings

Oligosaccharide Chain e



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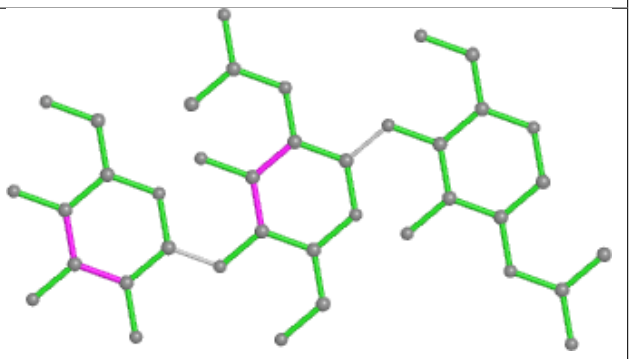
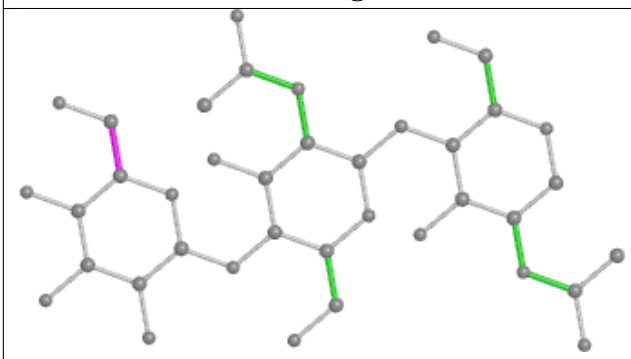


Bond angles



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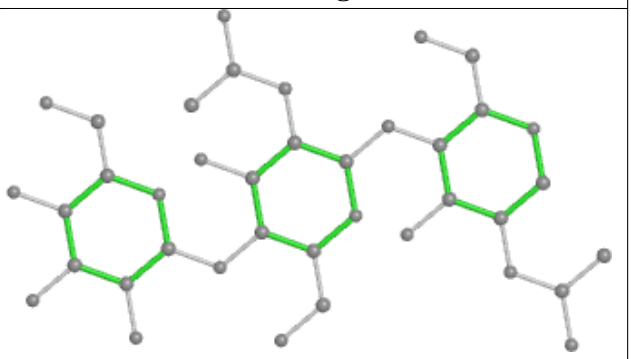
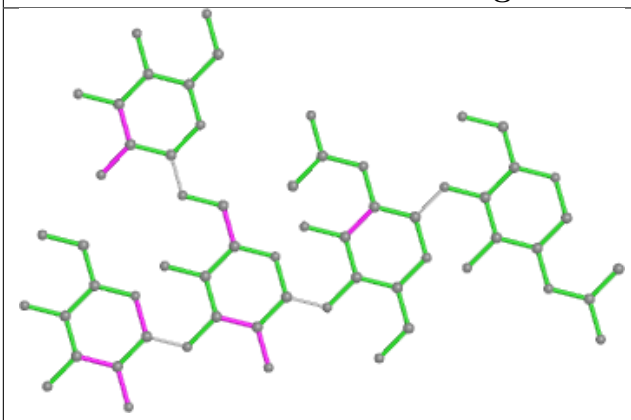


Rings

Oligosaccharide Chain N



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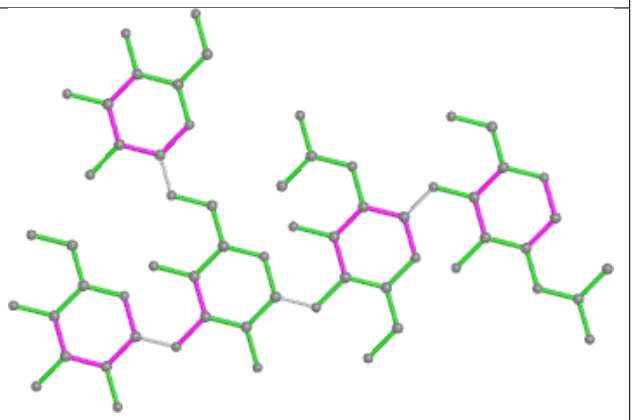
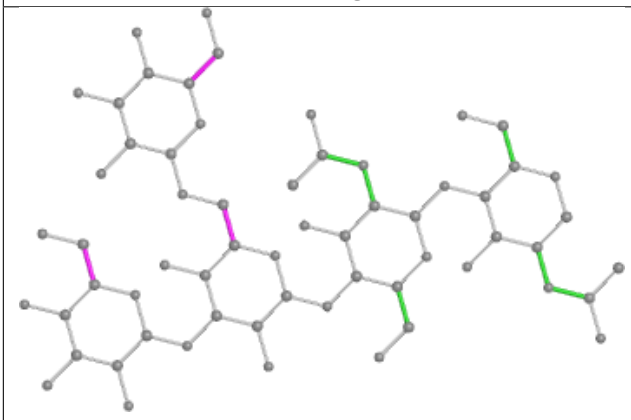


Bond angles



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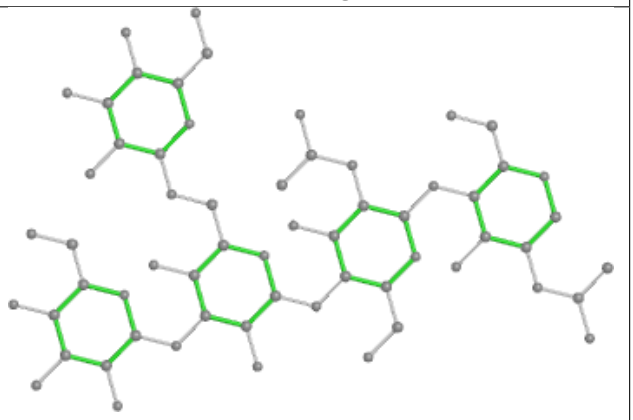
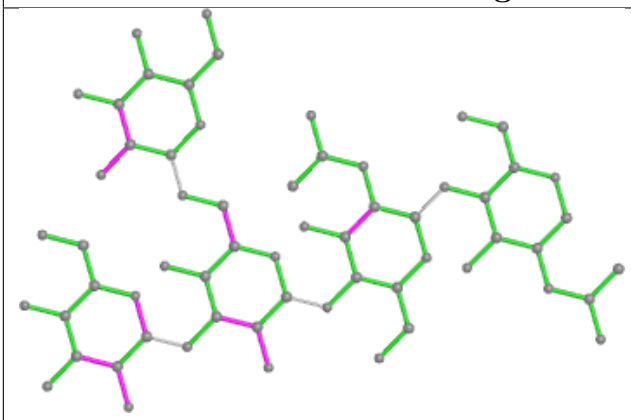


Rings

Oligosaccharide Chain U



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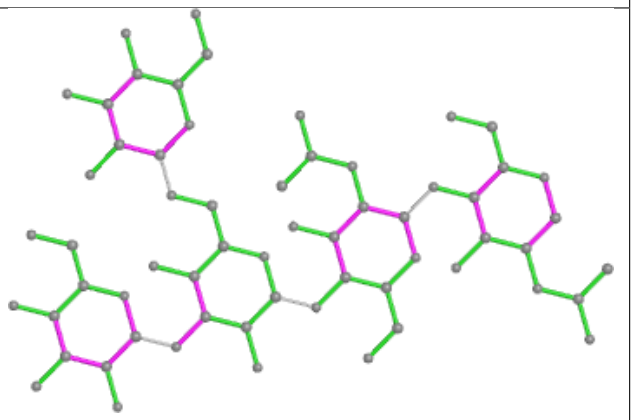
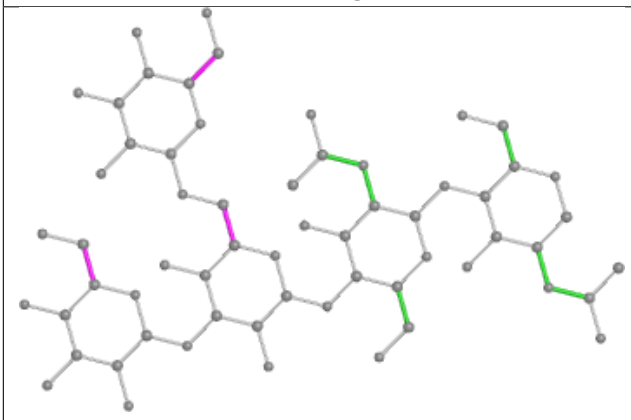
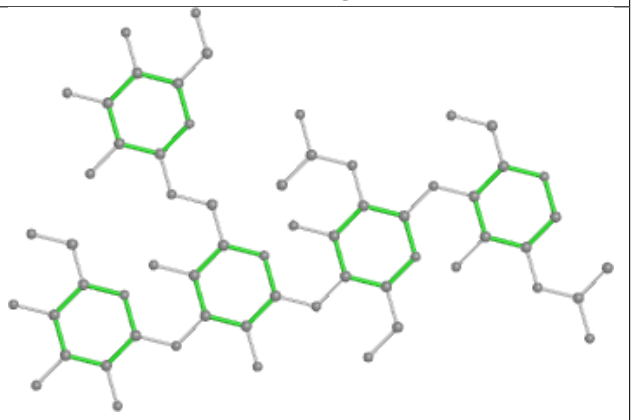


Bond angles

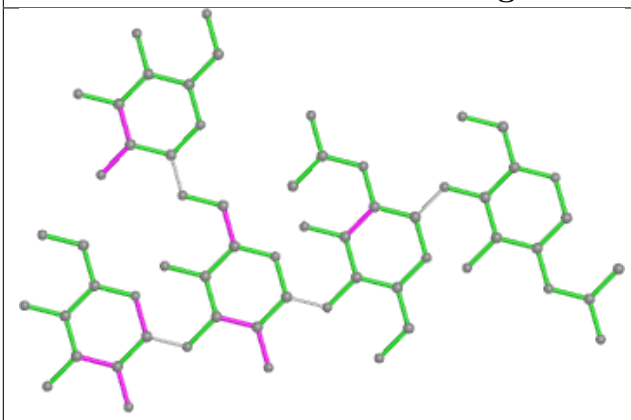


Torsions



Rings

Oligosaccharide Chain b



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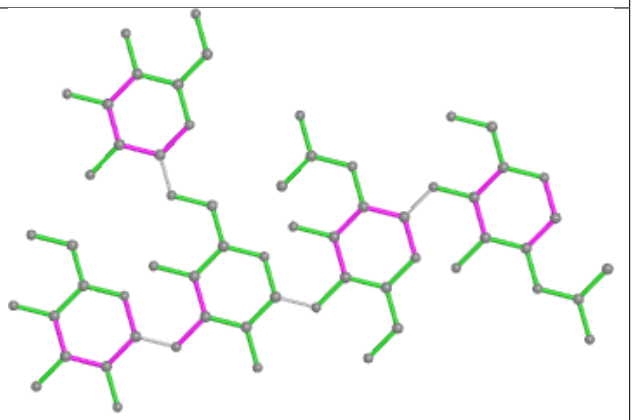
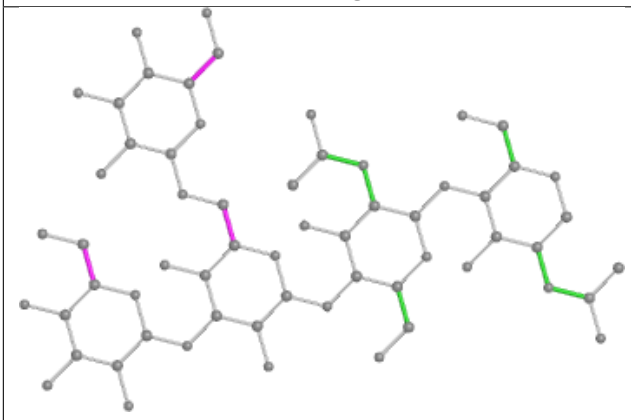


Bond angles



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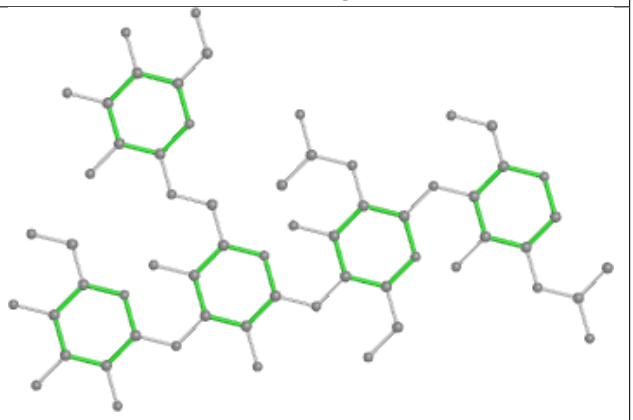
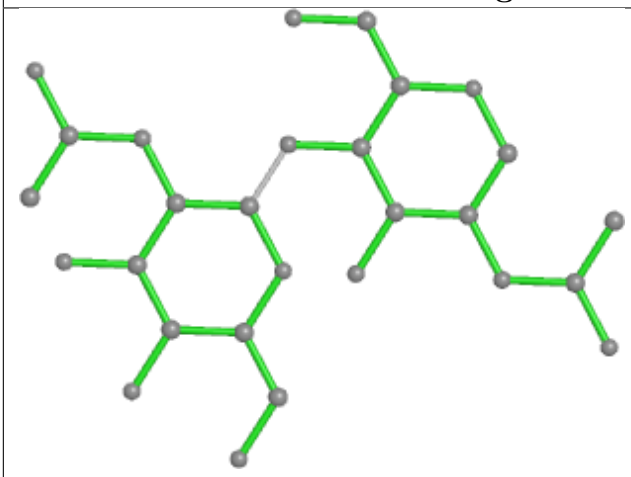


Rings

Oligosaccharide Chain P



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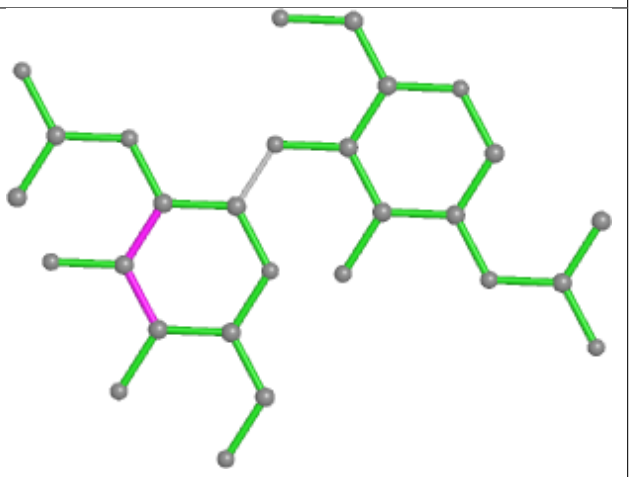
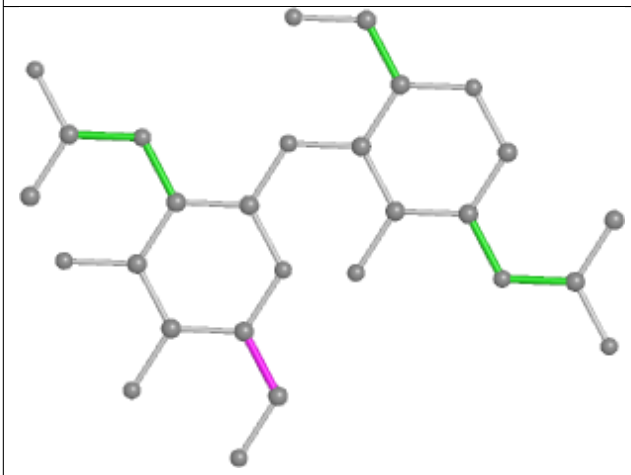
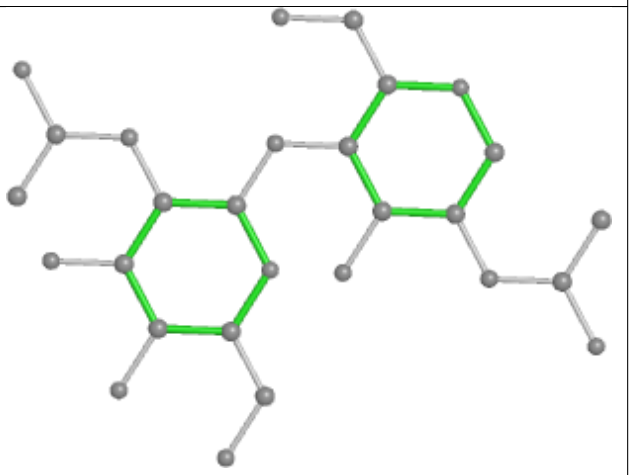


Bond angles

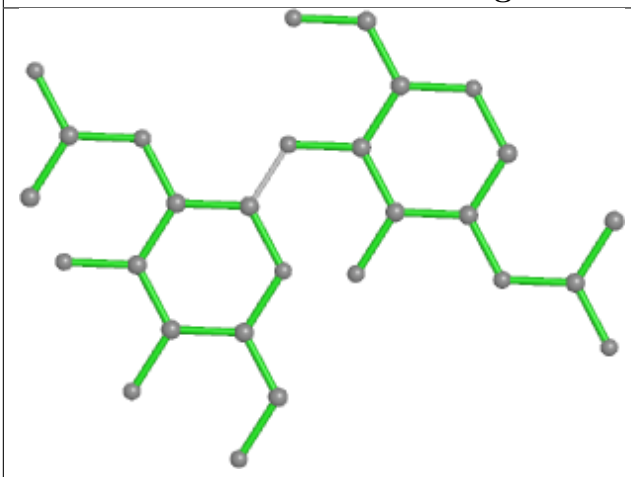


Torsions



Rings

Oligosaccharide Chain R



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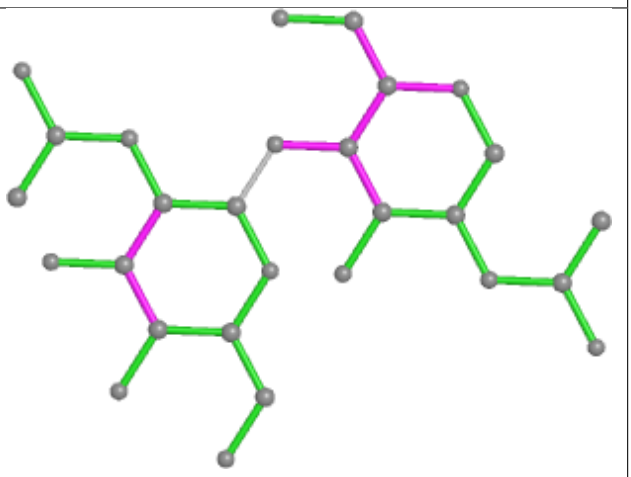
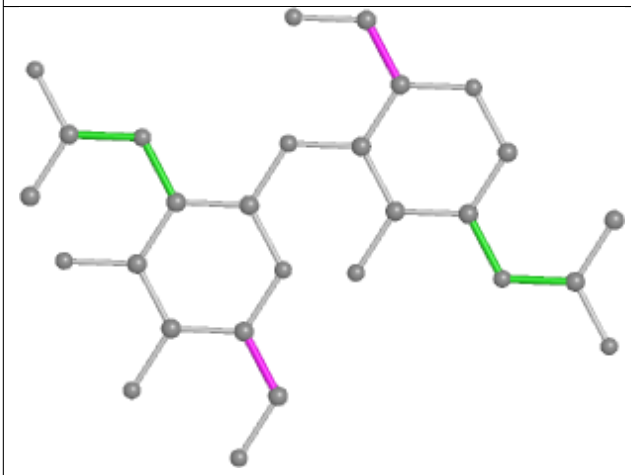
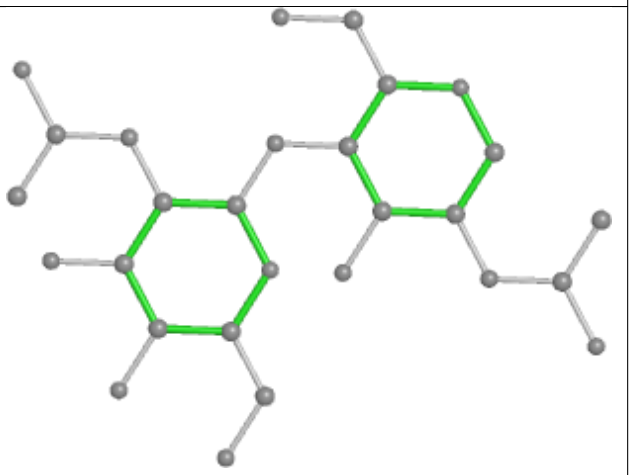


Bond angles

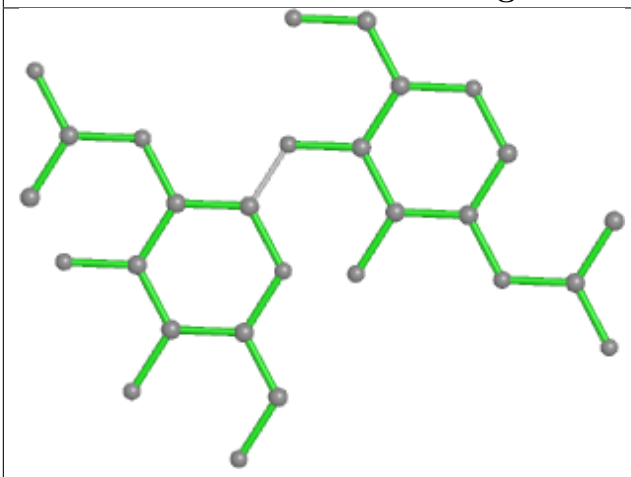


Torsions



Rings

Oligosaccharide Chain S



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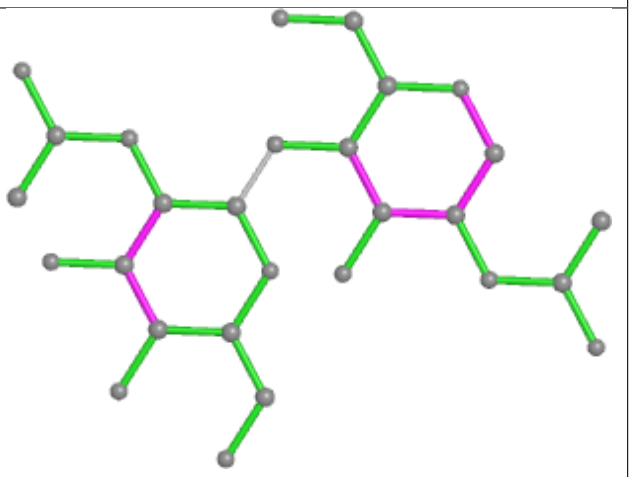
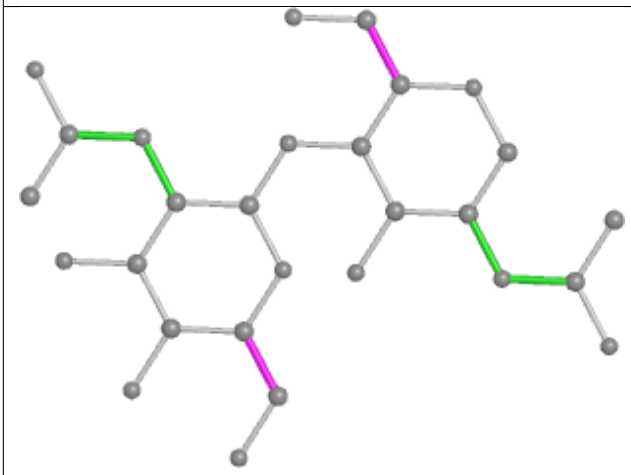
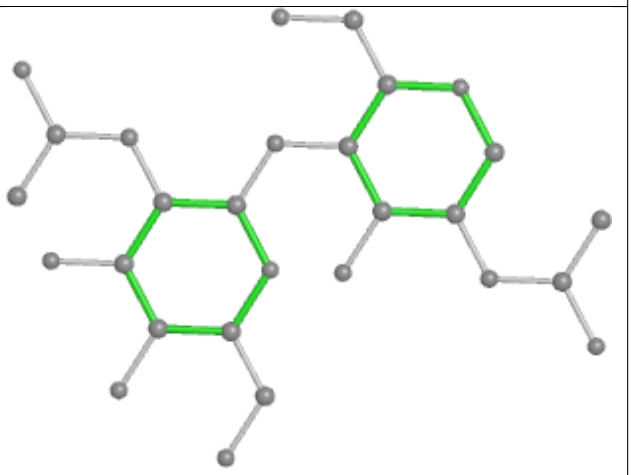


Bond angles

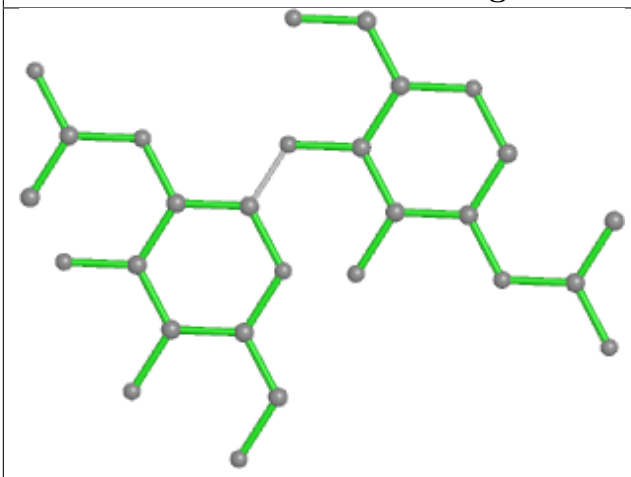


Torsions



Rings

Oligosaccharide Chain W



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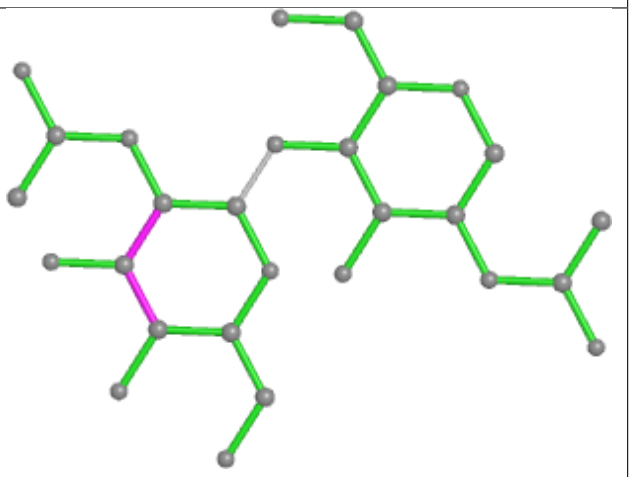
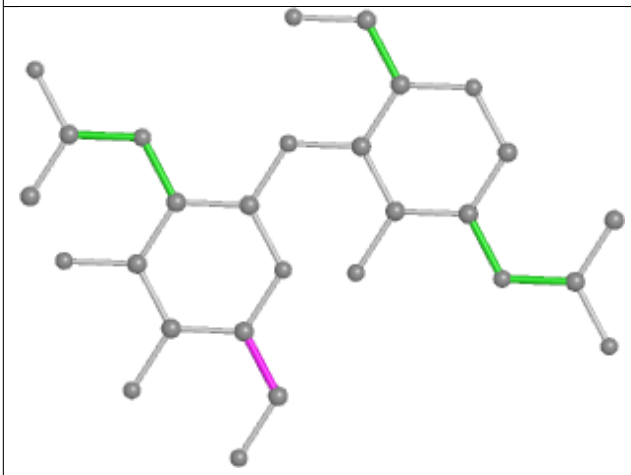
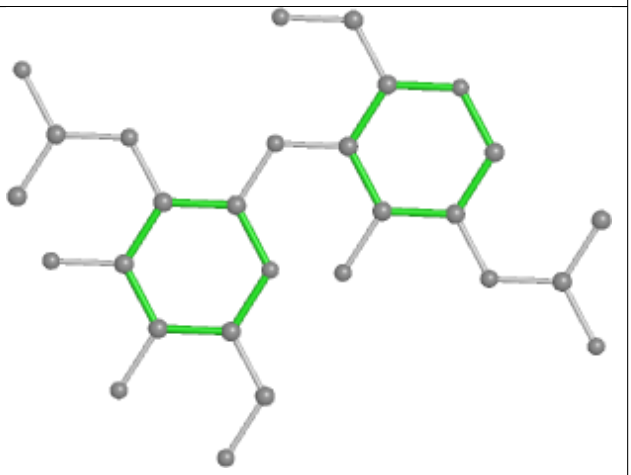


Bond angles

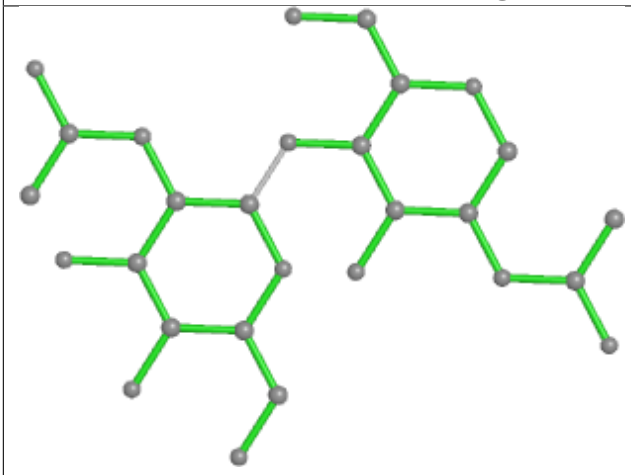


Torsions



Rings

Oligosaccharide Chain Y



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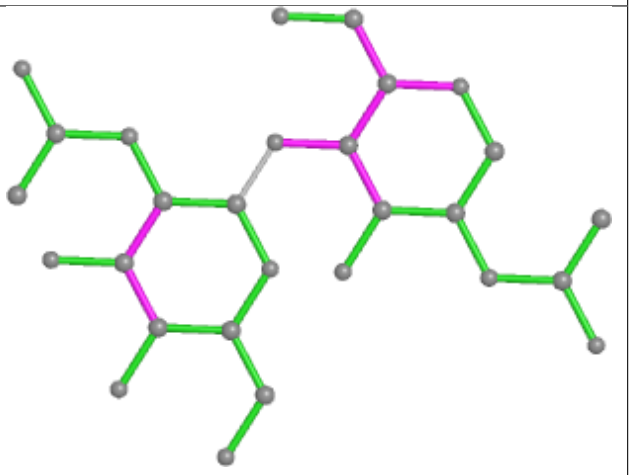
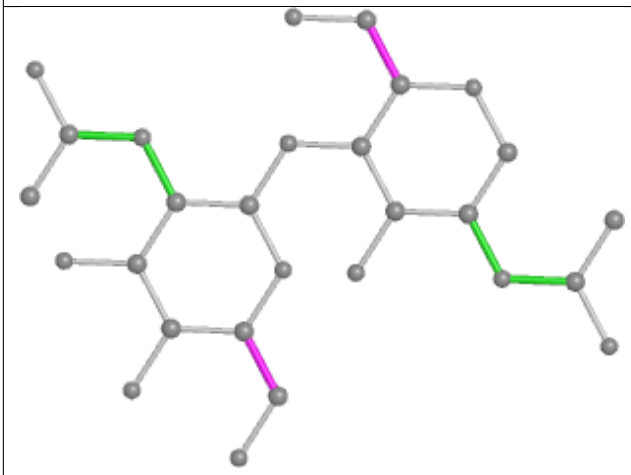
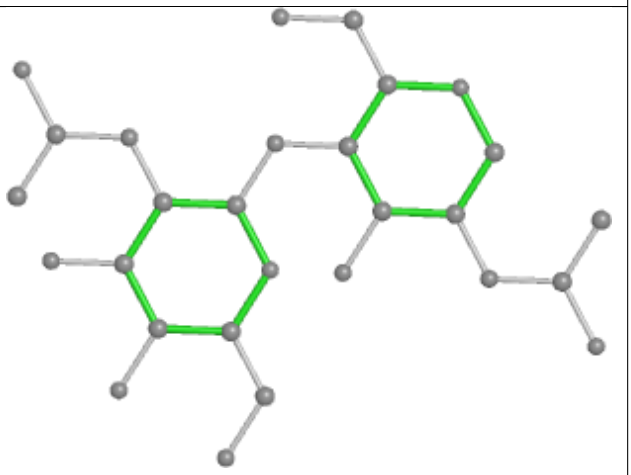


Bond angles

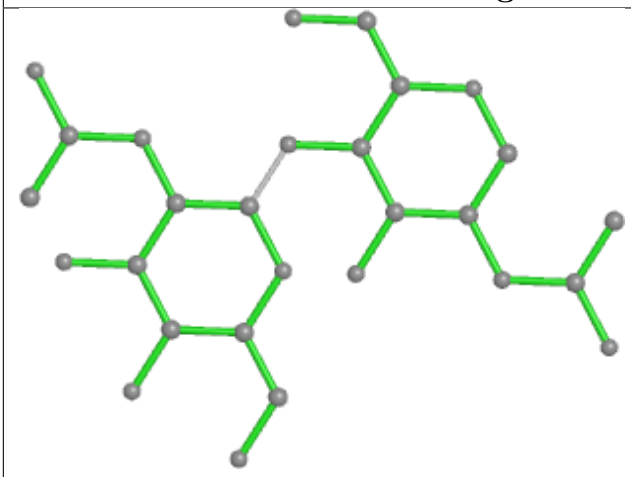


Torsions



Rings

Oligosaccharide Chain Z



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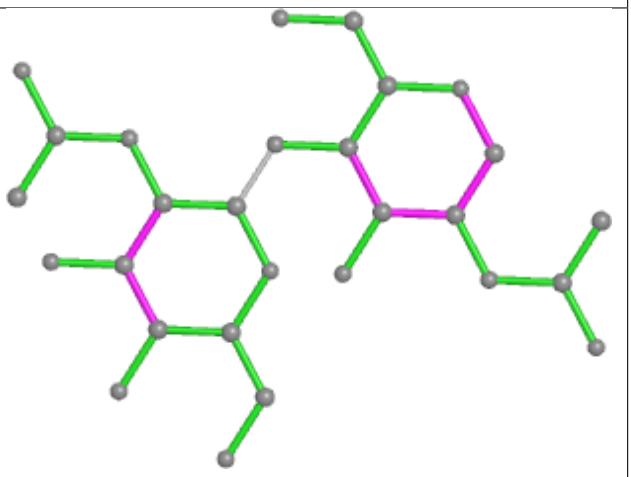
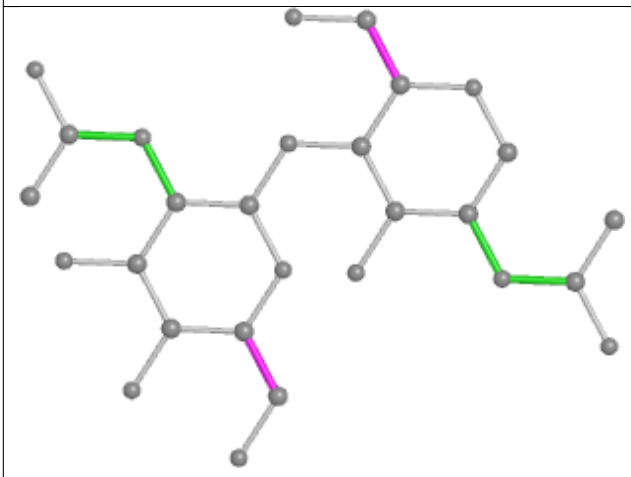
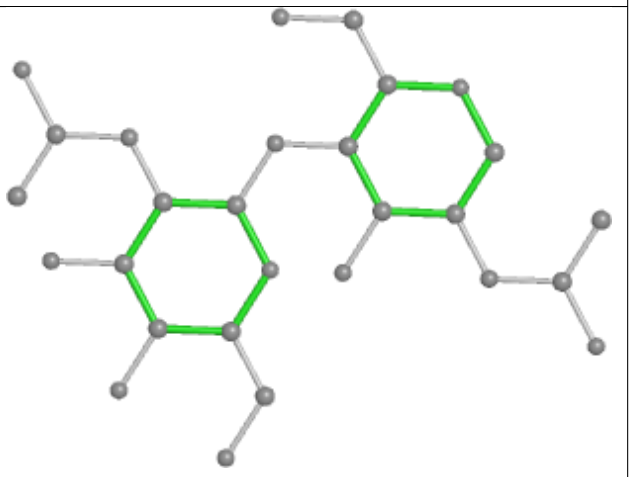


Bond angles

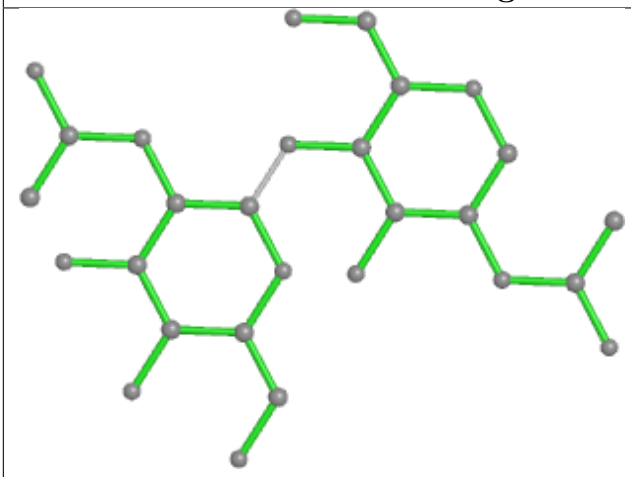


Torsions

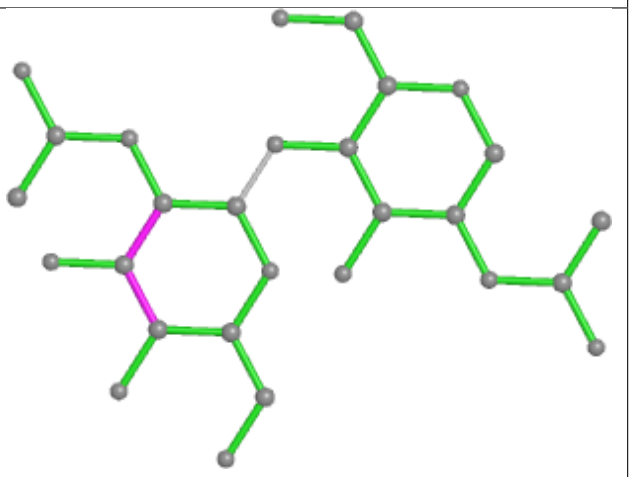


Rings

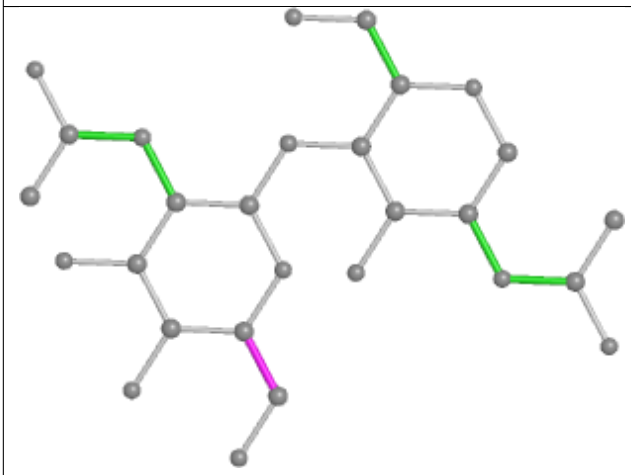
Oligosaccharide Chain d



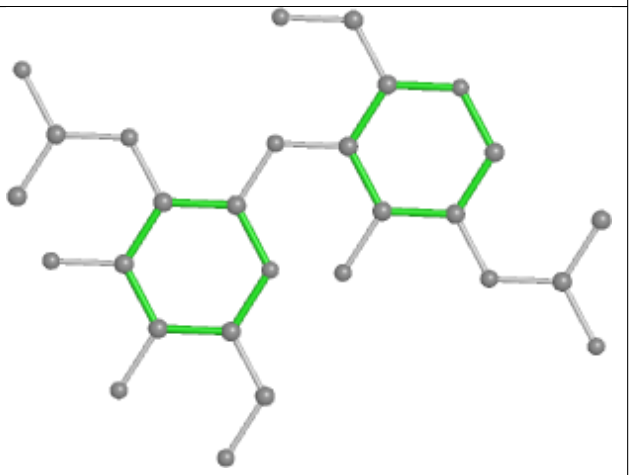
Bond lengths



Bond angles

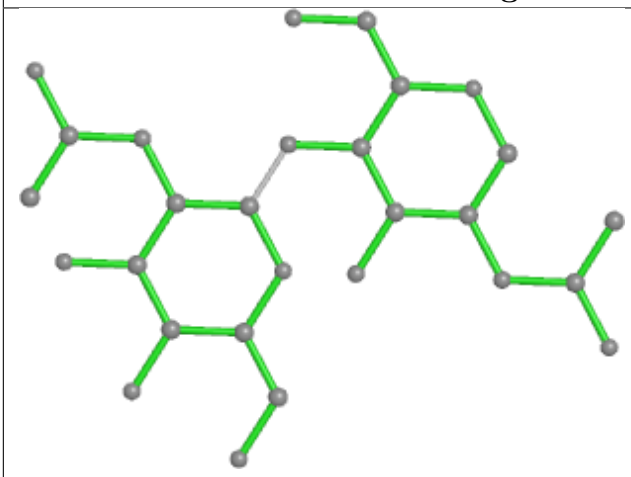


Torsions

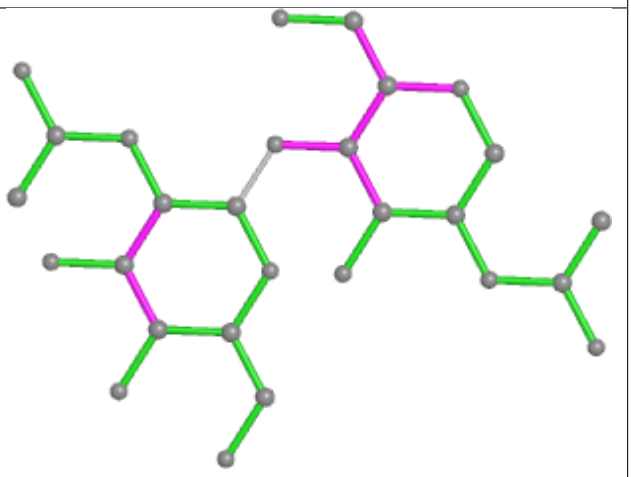


Rings

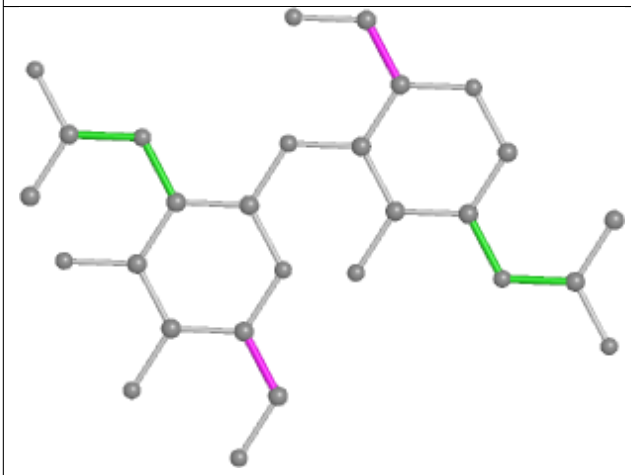
Oligosaccharide Chain f



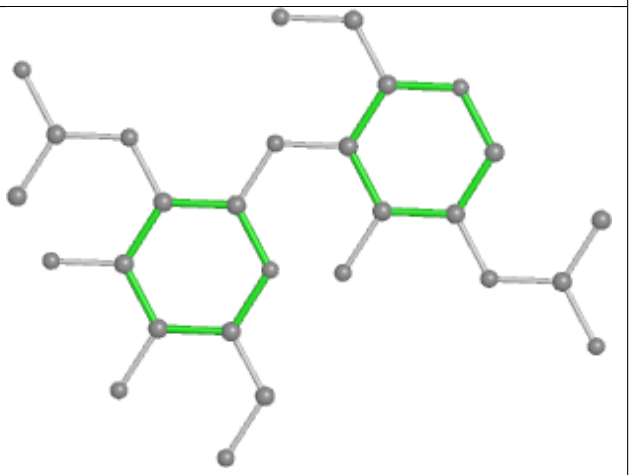
Bond lengths



Bond angles

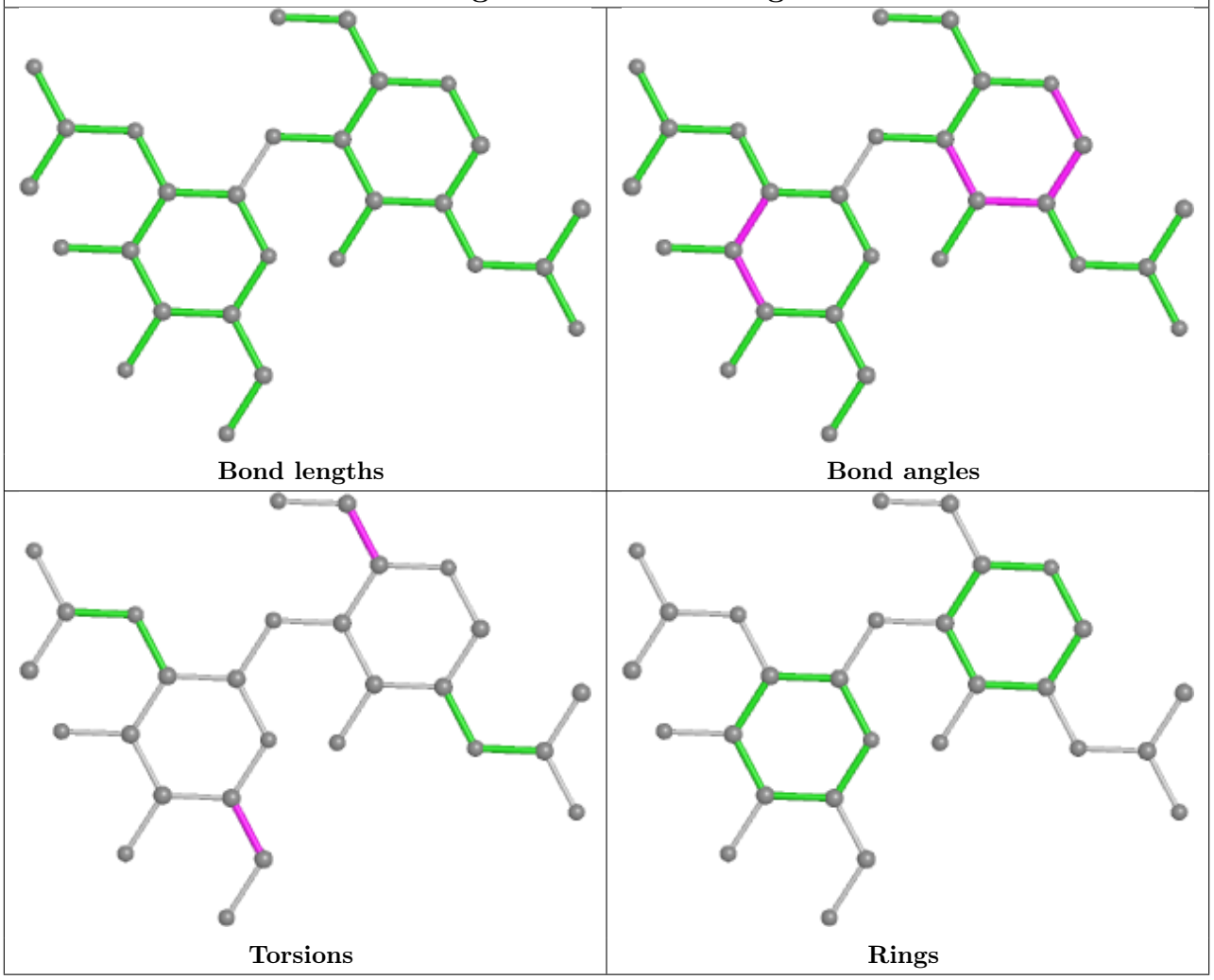


Torsions



Rings

Oligosaccharide Chain g



5.6 Ligand geometry (i)

18 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	C	619	3	14,14,15	0.82	0	17,19,21	1.52	2 (11%)
8	NAG	A	614	3	14,14,15	0.83	0	17,19,21	0.83	1 (5%)
8	NAG	D	619	3	14,14,15	0.81	0	17,19,21	1.52	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
8	NAG	A	615	3	14,14,15	0.73	0	17,19,21	1.13	1 (5%)
8	NAG	C	615	3	14,14,15	0.73	0	17,19,21	1.13	1 (5%)
8	NAG	F	701	4	14,14,15	0.83	0	17,19,21	0.77	1 (5%)
8	NAG	A	622	3	14,14,15	0.70	0	17,19,21	0.94	1 (5%)
8	NAG	D	614	3	14,14,15	0.83	0	17,19,21	0.83	1 (5%)
8	NAG	A	623	3	14,14,15	0.85	0	17,19,21	1.20	1 (5%)
8	NAG	D	615	3	14,14,15	0.74	0	17,19,21	1.13	1 (5%)
8	NAG	C	614	3	14,14,15	0.83	0	17,19,21	0.83	1 (5%)
8	NAG	D	622	3	14,14,15	0.70	0	17,19,21	0.95	1 (5%)
8	NAG	A	619	3	14,14,15	0.82	0	17,19,21	1.52	2 (11%)
8	NAG	E	701	4	14,14,15	0.84	0	17,19,21	0.77	1 (5%)
8	NAG	D	623	3	14,14,15	0.86	0	17,19,21	1.21	1 (5%)
8	NAG	B	701	4	14,14,15	0.84	0	17,19,21	0.77	1 (5%)
8	NAG	C	623	3	14,14,15	0.85	0	17,19,21	1.20	1 (5%)
8	NAG	C	622	3	14,14,15	0.70	0	17,19,21	0.94	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
8	NAG	C	619	3	-	2/6/23/26	0/1/1/1
8	NAG	A	614	3	-	1/6/23/26	0/1/1/1
8	NAG	D	619	3	-	2/6/23/26	0/1/1/1
8	NAG	A	615	3	-	3/6/23/26	0/1/1/1
8	NAG	C	615	3	-	3/6/23/26	0/1/1/1
8	NAG	F	701	4	-	1/6/23/26	0/1/1/1
8	NAG	A	622	3	-	1/6/23/26	0/1/1/1
8	NAG	D	614	3	-	1/6/23/26	0/1/1/1
8	NAG	A	623	3	-	2/6/23/26	0/1/1/1
8	NAG	D	615	3	-	3/6/23/26	0/1/1/1
8	NAG	C	614	3	-	1/6/23/26	0/1/1/1
8	NAG	D	622	3	-	1/6/23/26	0/1/1/1
8	NAG	A	619	3	-	2/6/23/26	0/1/1/1
8	NAG	E	701	4	-	1/6/23/26	0/1/1/1
8	NAG	D	623	3	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	NAG	B	701	4	-	1/6/23/26	0/1/1/1
8	NAG	C	623	3	-	2/6/23/26	0/1/1/1
8	NAG	C	622	3	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	C	619	NAG	C2-N2-C7	4.22	128.91	122.90
8	A	619	NAG	C2-N2-C7	4.20	128.88	122.90
8	D	619	NAG	C2-N2-C7	4.19	128.86	122.90
8	C	615	NAG	C4-C3-C2	-3.61	105.73	111.02
8	A	615	NAG	C4-C3-C2	-3.61	105.73	111.02
8	D	615	NAG	C4-C3-C2	-3.59	105.75	111.02
8	D	623	NAG	C4-C3-C2	-3.42	106.01	111.02
8	C	623	NAG	C4-C3-C2	-3.41	106.02	111.02
8	A	623	NAG	C4-C3-C2	-3.41	106.03	111.02
8	C	619	NAG	C4-C3-C2	-3.29	106.20	111.02
8	A	619	NAG	C4-C3-C2	-3.27	106.22	111.02
8	D	619	NAG	C4-C3-C2	-3.27	106.23	111.02
8	D	622	NAG	C4-C3-C2	-2.92	106.74	111.02
8	A	622	NAG	C4-C3-C2	-2.91	106.76	111.02
8	C	622	NAG	C4-C3-C2	-2.89	106.79	111.02
8	D	614	NAG	C4-C3-C2	-2.37	107.54	111.02
8	C	614	NAG	C4-C3-C2	-2.37	107.55	111.02
8	A	614	NAG	C4-C3-C2	-2.36	107.56	111.02
8	E	701	NAG	C4-C3-C2	-2.23	107.74	111.02
8	F	701	NAG	C4-C3-C2	-2.22	107.76	111.02
8	B	701	NAG	C4-C3-C2	-2.22	107.77	111.02

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	619	NAG	C3-C2-N2-C7
8	C	619	NAG	C3-C2-N2-C7
8	D	619	NAG	C3-C2-N2-C7
8	A	623	NAG	O5-C5-C6-O6
8	C	623	NAG	O5-C5-C6-O6
8	D	623	NAG	O5-C5-C6-O6
8	C	614	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
8	A	614	NAG	O5-C5-C6-O6
8	D	614	NAG	O5-C5-C6-O6
8	A	623	NAG	C4-C5-C6-O6
8	C	623	NAG	C4-C5-C6-O6
8	D	623	NAG	C4-C5-C6-O6
8	A	619	NAG	O5-C5-C6-O6
8	C	619	NAG	O5-C5-C6-O6
8	D	619	NAG	O5-C5-C6-O6
8	B	701	NAG	O5-C5-C6-O6
8	E	701	NAG	O5-C5-C6-O6
8	F	701	NAG	O5-C5-C6-O6
8	A	615	NAG	O5-C5-C6-O6
8	C	615	NAG	O5-C5-C6-O6
8	D	615	NAG	O5-C5-C6-O6
8	A	622	NAG	O5-C5-C6-O6
8	C	622	NAG	O5-C5-C6-O6
8	D	622	NAG	O5-C5-C6-O6
8	A	615	NAG	C3-C2-N2-C7
8	C	615	NAG	C3-C2-N2-C7
8	D	615	NAG	C3-C2-N2-C7
8	A	615	NAG	C1-C2-N2-C7
8	C	615	NAG	C1-C2-N2-C7
8	D	615	NAG	C1-C2-N2-C7

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	C	619	NAG	1	0
8	D	619	NAG	1	0
8	A	619	NAG	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

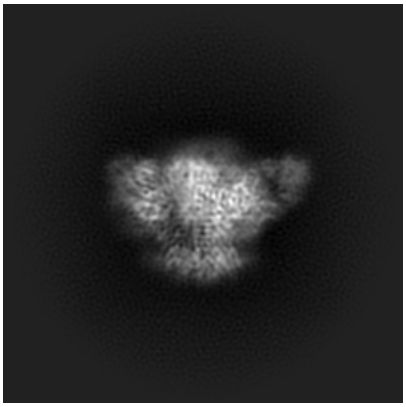
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-21258. These allow visual inspection of the internal detail of the map and identification of artifacts.

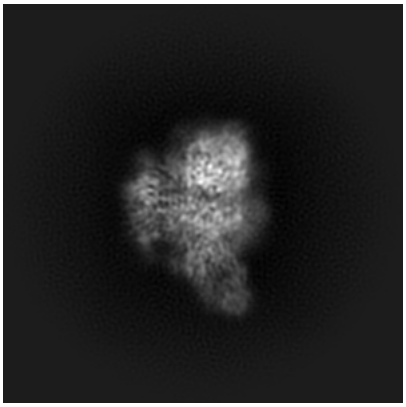
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

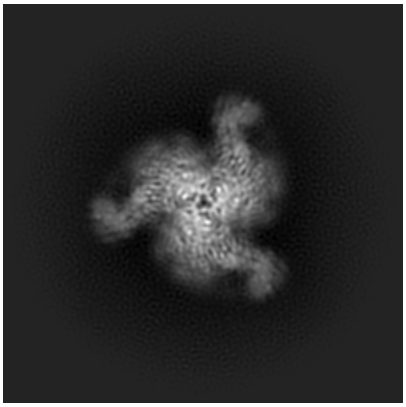
6.1.1 Primary map



X



Y

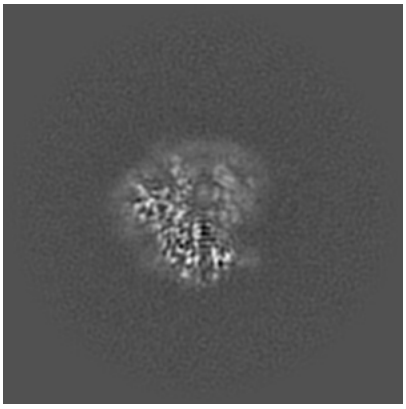


Z

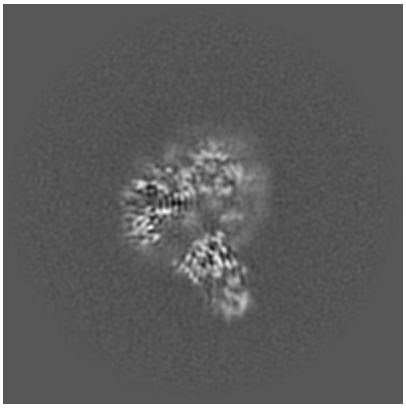
The images above show the map projected in three orthogonal directions.

6.2 Central slices

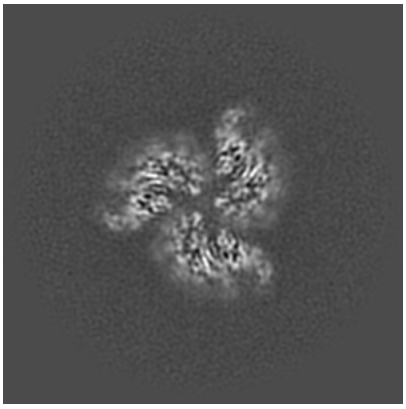
6.2.1 Primary map



X Index: 128



Y Index: 128

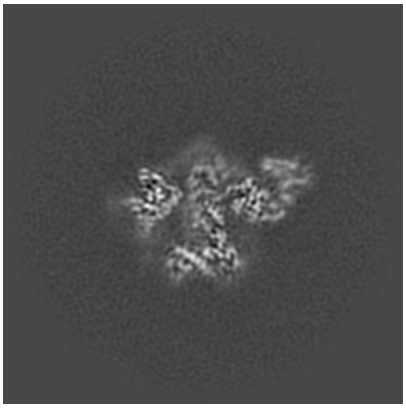


Z Index: 128

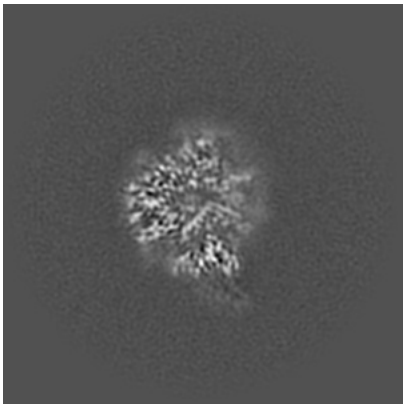
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

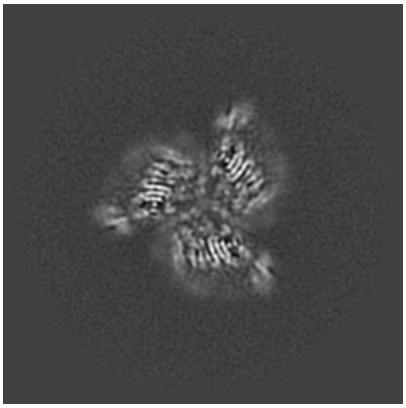
6.3.1 Primary map



X Index: 141



Y Index: 135

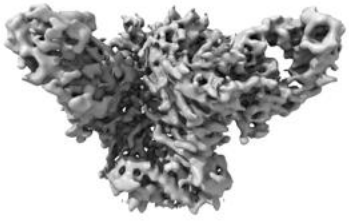


Z Index: 133

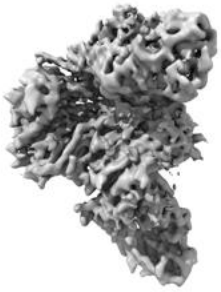
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

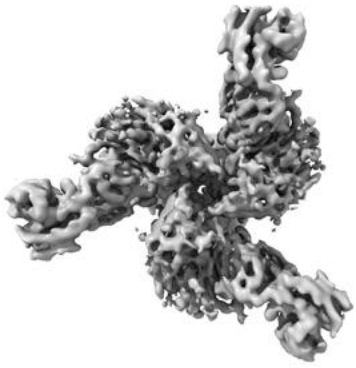
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.33. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

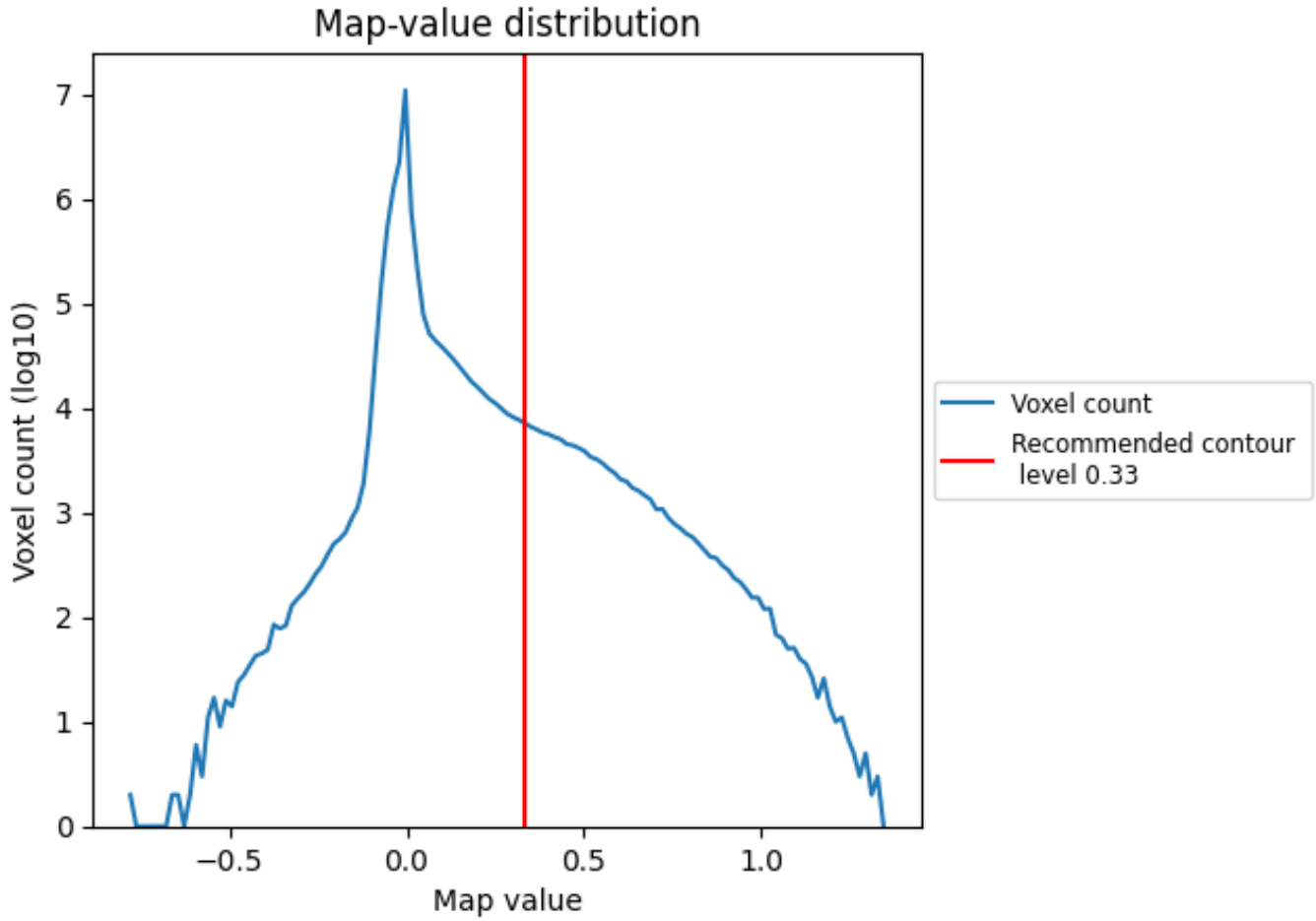
6.5 Mask visualisation (i)

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

7 Map analysis

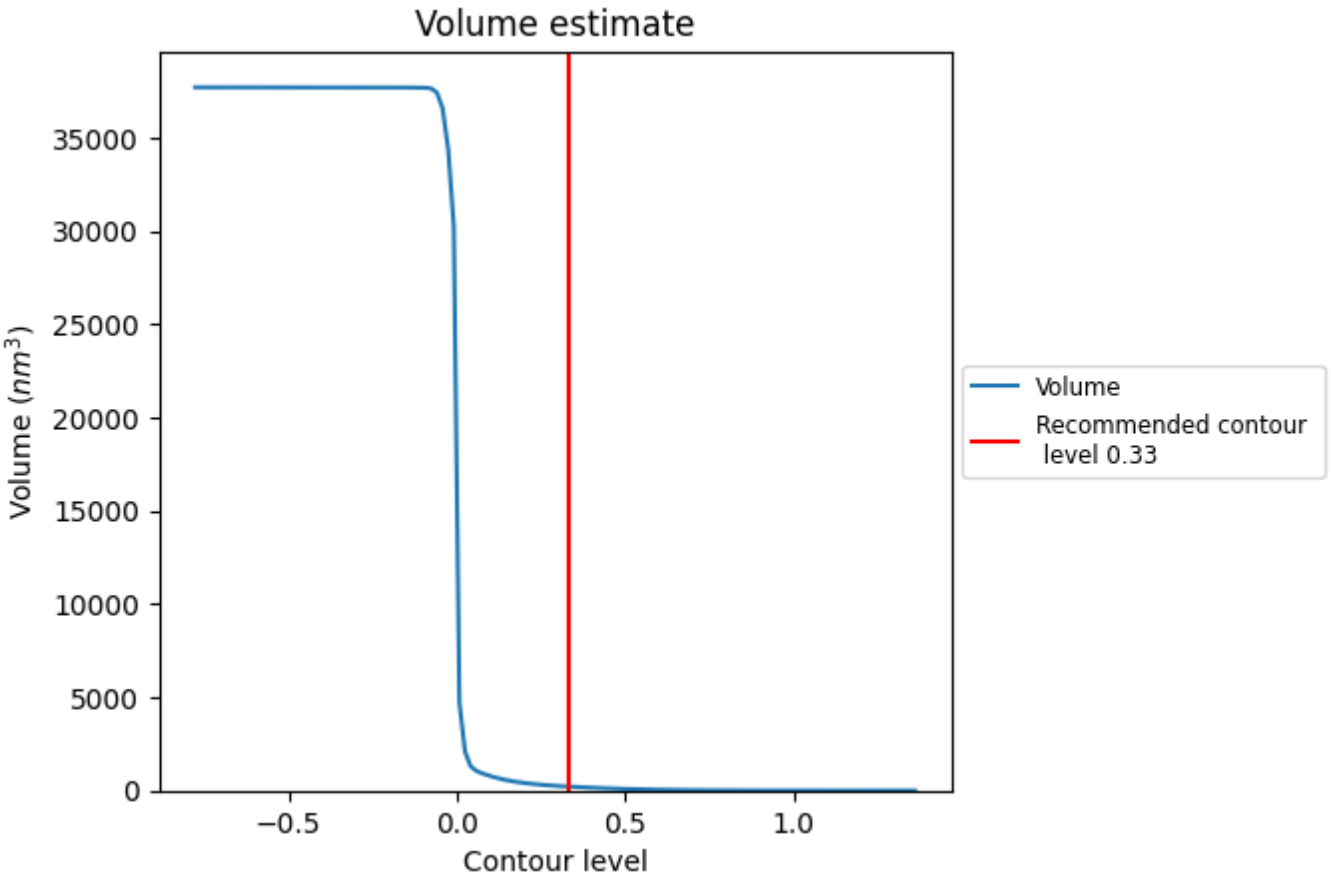
This section contains the results of statistical analysis of the map.

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.

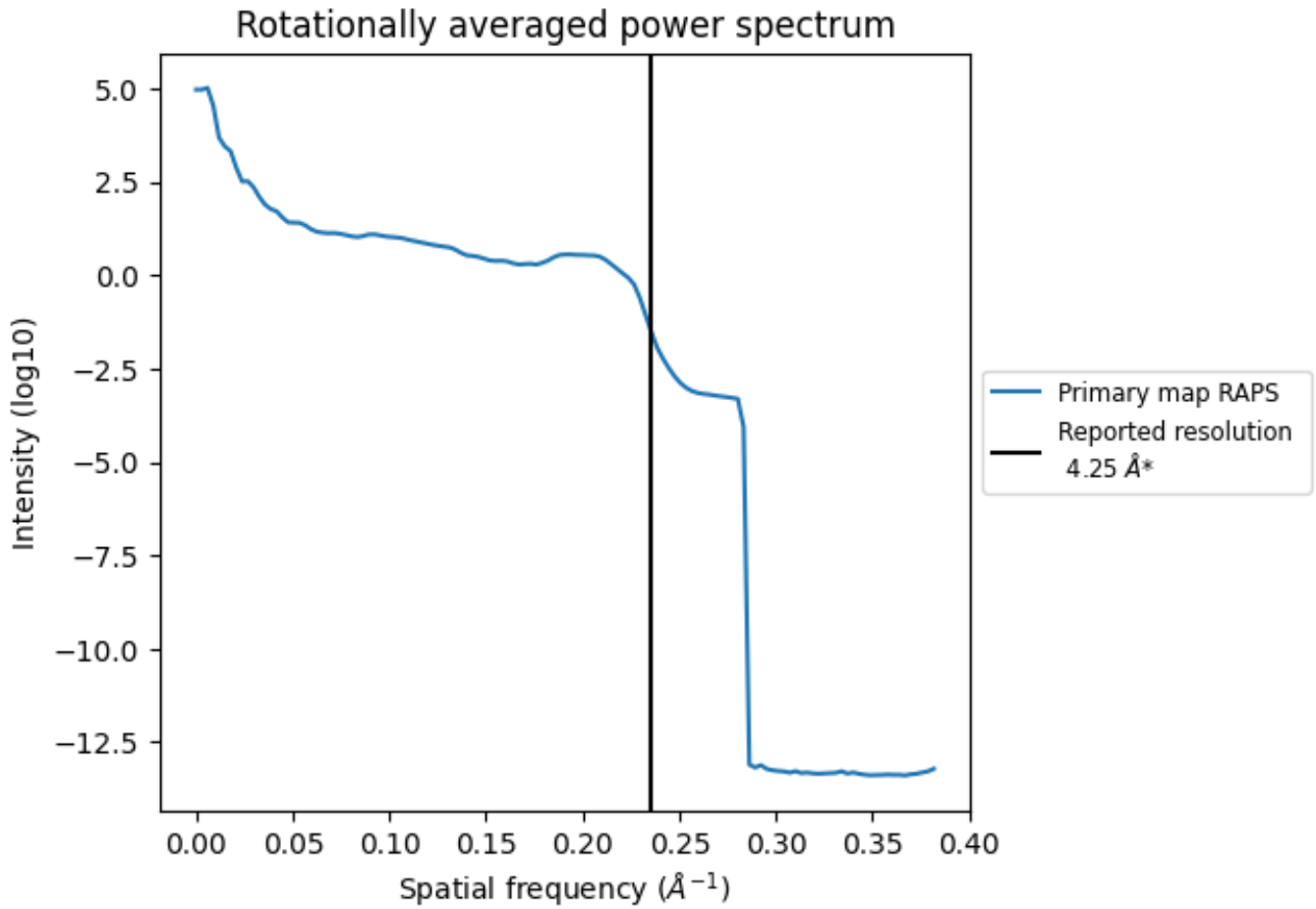
7.2 Volume estimate



The volume at the recommended contour level is 213 nm^3; this corresponds to an approximate mass of 192 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)

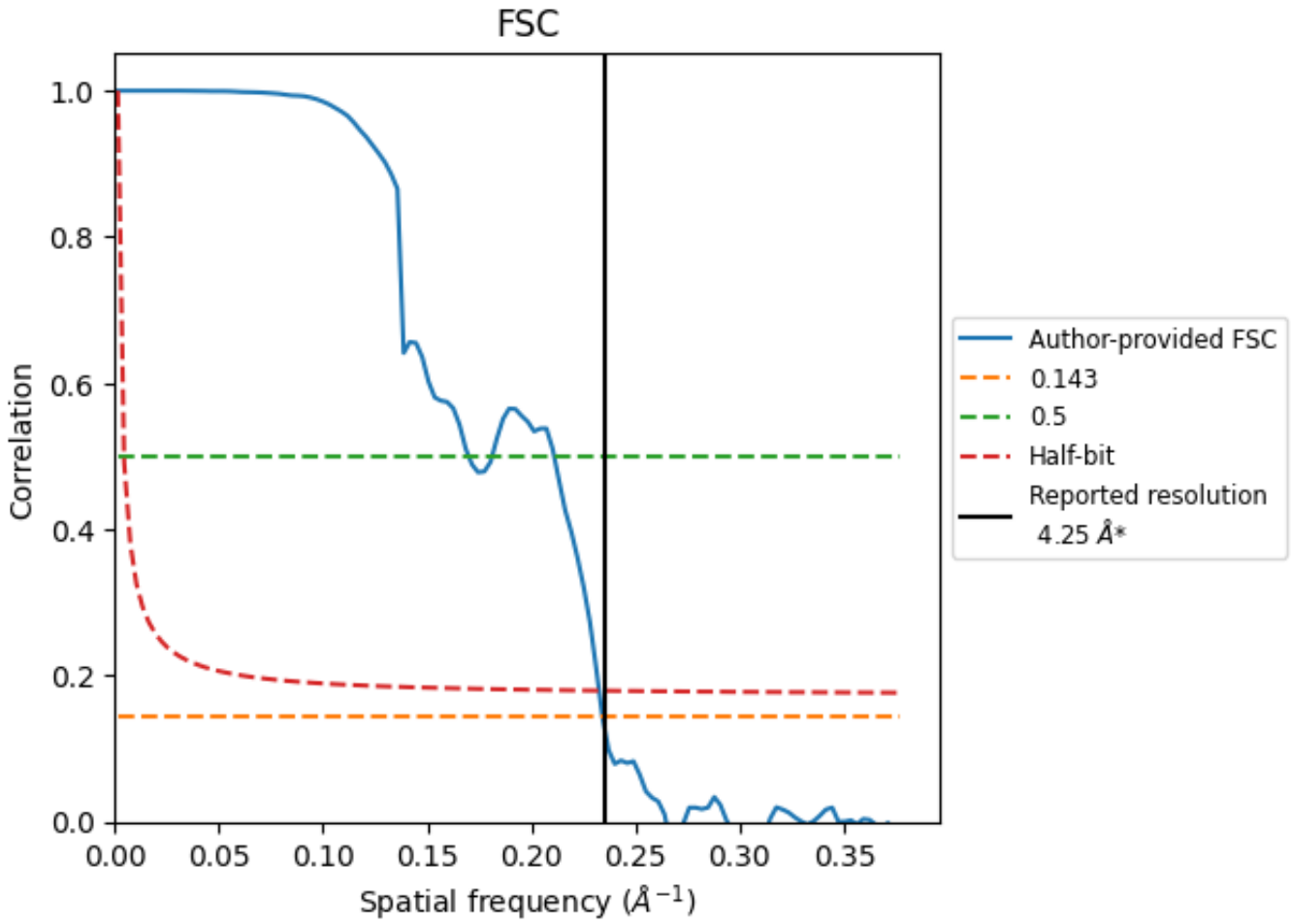


*Reported resolution corresponds to spatial frequency of 0.235 $Å^{-1}$

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 0.235 Å^{-1}

8.2 Resolution estimates (i)

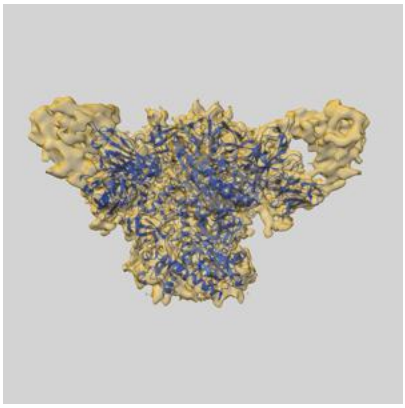
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.25	-	-
Author-provided FSC curve	4.27	5.89	4.30
Unmasked-calculated*	-	-	-

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

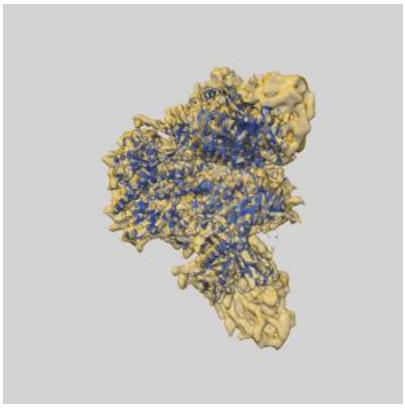
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-21258 and PDB model 6VO3. Per-residue inclusion information can be found in section 3 on page 9.

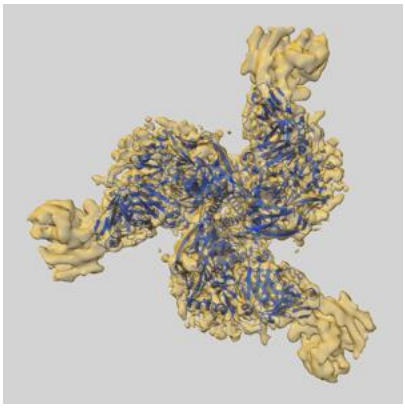
9.1 Map-model overlay



X



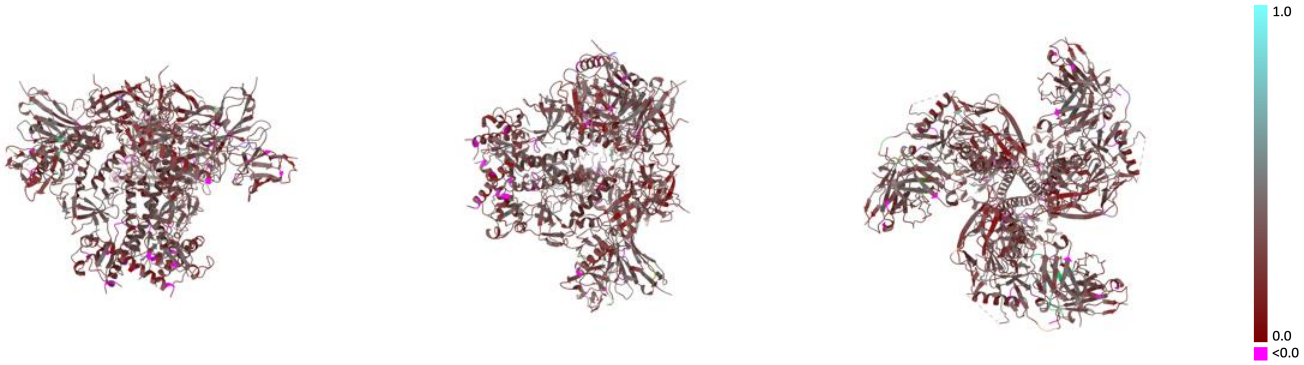
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.33 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.

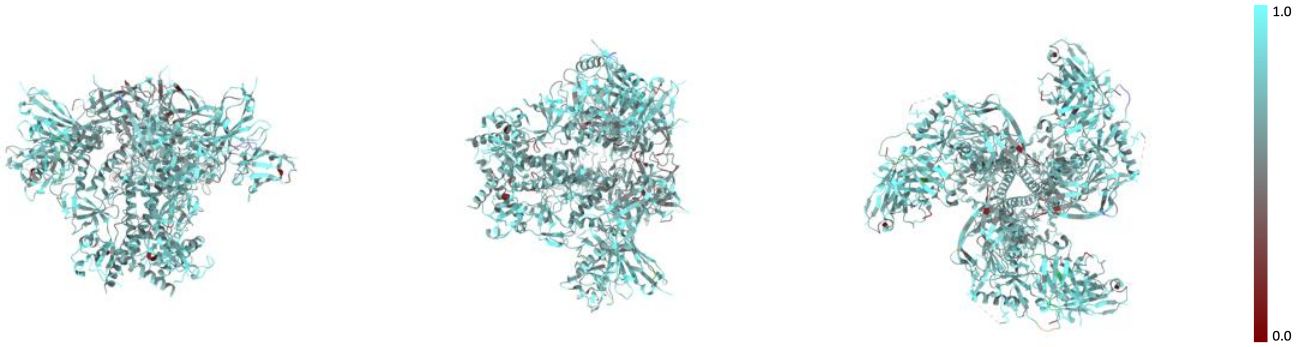
9.2 Q-score mapped to coordinate model (i)



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.

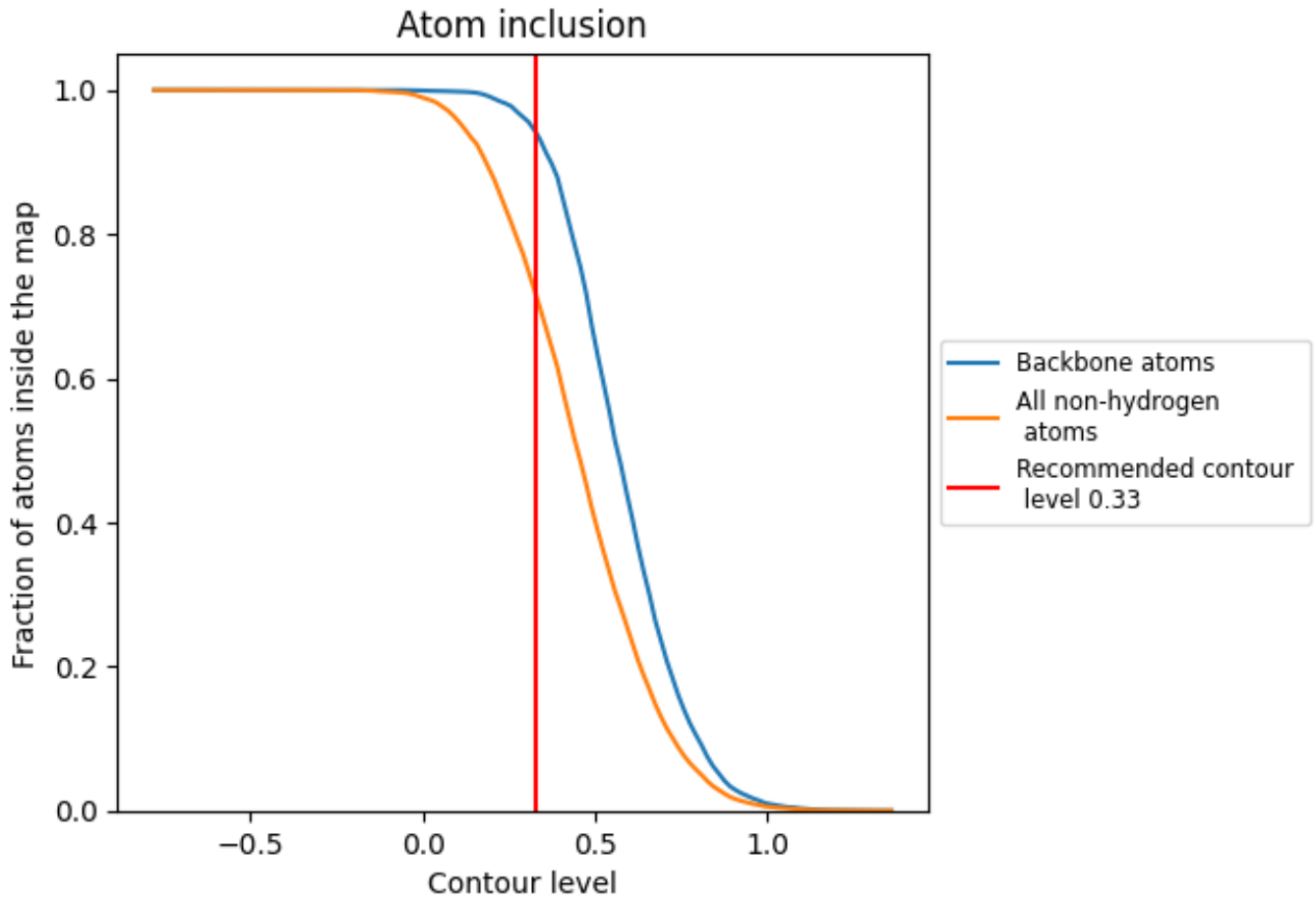
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.33).

9.4 Atom inclusion (i)



At the recommended contour level, 94% of all backbone atoms, 72% 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 (0.33) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7150	0.2900
A	0.7043	0.2950
B	0.7226	0.2510
C	0.7043	0.2940
D	0.7040	0.2930
E	0.7256	0.2540
F	0.7215	0.2520
G	0.7440	0.3250
H	0.7472	0.3220
I	0.7451	0.3200
J	0.7214	0.2630
K	0.7201	0.2660
L	0.7227	0.2620
M	0.5897	0.2400
N	0.7869	0.3400
O	0.6667	0.3130
P	0.7143	0.3850
Q	0.7949	0.3800
R	0.5357	0.3190
S	0.6071	0.4020
T	0.5897	0.2220
U	0.8033	0.3350
V	0.6667	0.3100
W	0.7143	0.4000
X	0.8205	0.3880
Y	0.5357	0.3330
Z	0.6071	0.4220
a	0.6154	0.2380
b	0.7869	0.3530
c	0.6667	0.3230
d	0.7500	0.3860
e	0.8205	0.3730
f	0.5714	0.3290
g	0.6071	0.4050