Full wwPDB EM Validation Report (i)

Nov 8, 2022 – 06:50 AM EST

PDB ID	:	6OLP
EMDB ID	:	EMD-20118
Title	:	Full length HIV-1 Env AMC011 in complex with PGT151 Fab
Authors	:	Rantalainen, K.; Cottrell, C.A.
Deposited on	:	2019-04-16
Resolution	:	4.20 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:

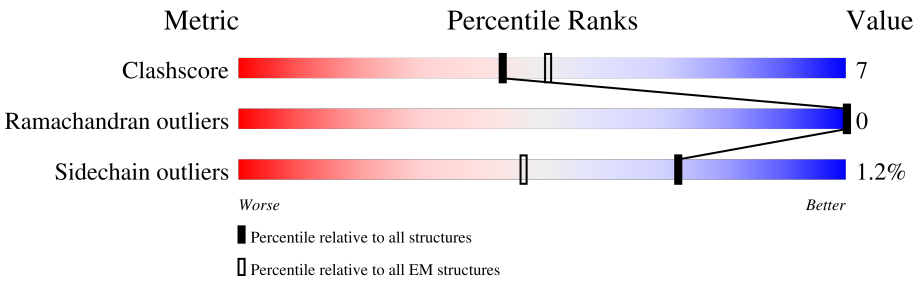
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al.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

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 4.20 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	506	5% 67% 17% 15%
1	C	506	10% 66% 20% 13%
1	E	506	9% 63% 19% • 17%
2	B	345	• 35% 7% 59%
2	D	345	• 33% • 63%
2	F	345	6% 33% 6% 61%
3	G	240	• 45% 10% 44%
3	H	240	5% 43% 13% 44%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	I	219	8% 40% 10% 50%
4	L	219	13% 42% 9% 49%
5	J	2	50% 50% 50%
5	M	2	50% 100%
5	N	2	100%
5	O	2	50% 50% 50%
5	Q	2	50% 100%
5	S	2	50% 100%
5	T	2	100%
5	U	2	50% 50% 50%
5	Y	2	50% 100%
5	Z	2	50% 50% 50%
5	a	2	100% 100%
5	d	2	50% 100%
5	g	2	100%
5	h	2	50% 100%
6	K	2	50% 100%
7	P	4	25% 75% 25%
8	R	3	67% 33% 67%
8	i	3	67% 33%
9	V	9	22% 11% 89%
10	W	8	12% 50% 38% 12%
11	X	2	50% 100%
11	c	2	50% 50%
12	b	5	20% 40% 60%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
13	e	9	22% 33% 67%
14	f	10	40% 20% 80%

2 Entry composition (i)

There are 15 unique types of molecules in this entry. The entry contains 18868 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Envelope glycoprotein gp120.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	430	3392	2148	586	632	26	1	0
1	C	438	3454	2185	600	643	26	0	0
1	E	419	3298	2092	573	607	26	0	0

- Molecule 2 is a protein called Envelope glycoprotein gp41.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	143	1152	728	198	220	6	0	0
2	D	129	1014	643	170	195	6	0	0
2	F	134	1063	674	183	200	6	0	0

- Molecule 3 is a protein called Immunoglobulin G PGT151 Fab, Heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	G	134	1062	676	184	196	6	0	0
3	H	135	1073	682	188	197	6	0	0

- Molecule 4 is a protein called Immunoglobulin G PGT151 Fab, Light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	I	109	838	527	142	165	4	0	0
4	L	111	854	537	144	169	4	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
5	J	2	28	16	2	10	0	0
5	M	2	28	16	2	10	0	0
5	N	2	28	16	2	10	0	0
5	O	2	28	16	2	10	0	0
5	Q	2	28	16	2	10	0	0
5	S	2	28	16	2	10	0	0
5	T	2	28	16	2	10	0	0
5	U	2	28	16	2	10	0	0
5	Y	2	28	16	2	10	0	0
5	Z	2	28	16	2	10	0	0
5	a	2	28	16	2	10	0	0
5	d	2	28	16	2	10	0	0
5	g	2	28	16	2	10	0	0
5	h	2	28	16	2	10	0	0

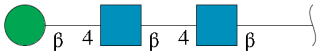
- Molecule 6 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
6	K	2	28	16	2	10	0	0

- Molecule 7 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

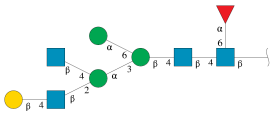
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
7	P	4	50	28	2	20	0	0

- Molecule 8 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



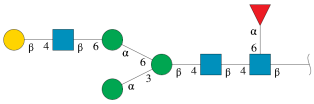
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
8	R	3	39	22	2	15	0	0
8	i	3	39	22	2	15	0	0

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



Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
9	V	9	110	62	4	44	0	0

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

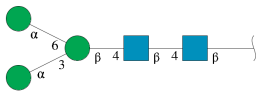


Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
10	W	8	96	54	3	39	0	0

- Molecule 11 is an oligosaccharide called alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose.

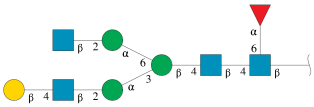
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
11	X	2	24	14	1	9	0	0
11	c	2	24	14	1	9	0	0

- Molecule 12 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.



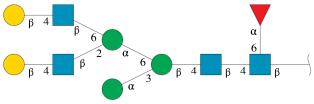
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
12	b	5	61	34	2	25	0	0

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



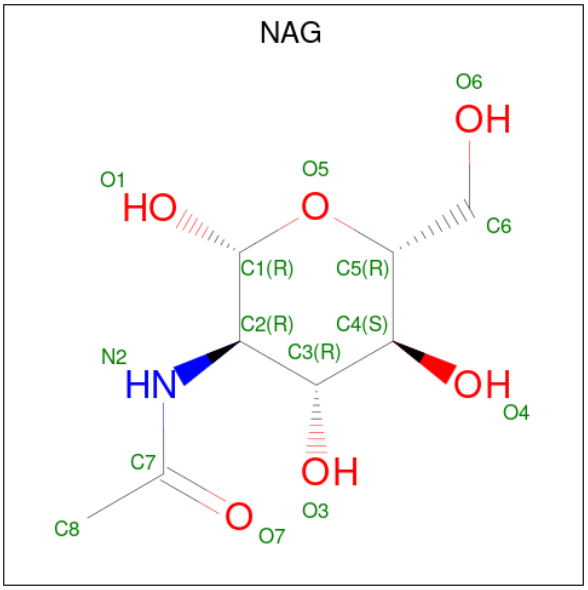
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
13	e	9	110	62	4	44	0	0

- Molecule 14 is an oligosaccharide called beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-[beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
14	f	10	121	68	4	49	0	0

- Molecule 15 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	
15	A	1	112	64	8	40	0
15	A	1	112	64	8	40	0
15	A	1	112	64	8	40	0
15	A	1	112	64	8	40	0
15	A	1	112	64	8	40	0
15	A	1	112	64	8	40	0
15	A	1	112	64	8	40	0
15	A	1	112	64	8	40	0
15	C	1	182	104	13	65	0
15	C	1	182	104	13	65	0
15	C	1	182	104	13	65	0
15	C	1	182	104	13	65	0
15	C	1	182	104	13	65	0
15	C	1	182	104	13	65	0
15	C	1	182	104	13	65	0
15	C	1	182	104	13	65	0
15	C	1	182	104	13	65	0
15	C	1	182	104	13	65	0
15	C	1	182	104	13	65	0
15	C	1	182	104	13	65	0
15	C	1	182	104	13	65	0
15	D	1	14	8	1	5	0

Continued on next page...

Continued from previous page...

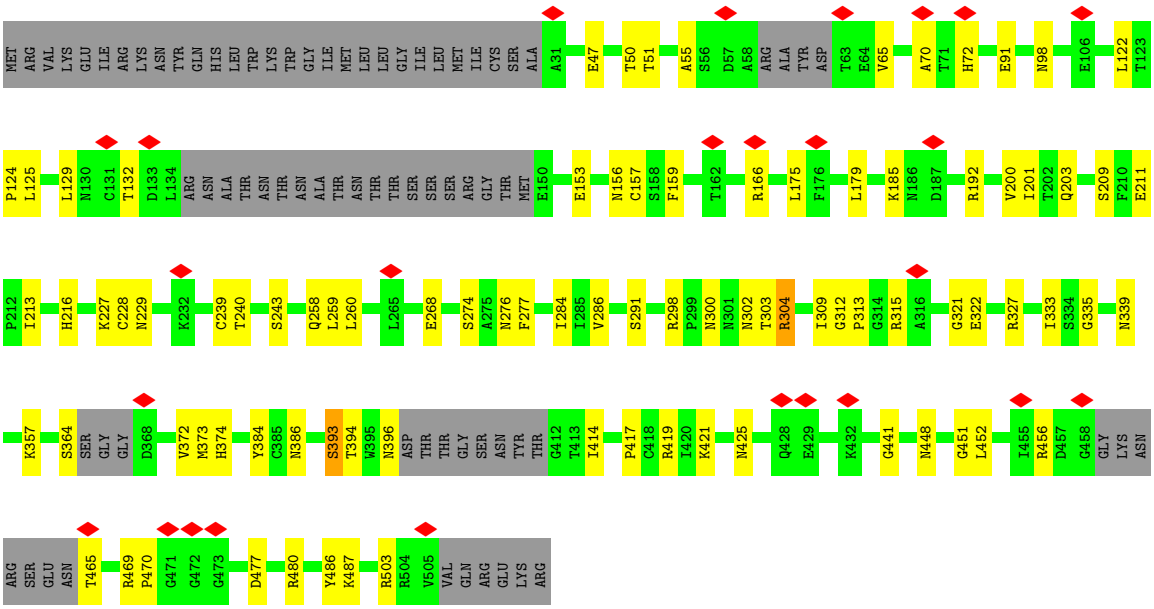
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
15	E	1	210	120	15	75	0
			Total	C	N	O	
15	E	1	210	120	15	75	0
			Total	C	N	O	
15	E	1	210	120	15	75	0
			Total	C	N	O	
15	E	1	210	120	15	75	0
			Total	C	N	O	
15	E	1	210	120	15	75	0
			Total	C	N	O	
15	E	1	210	120	15	75	0
			Total	C	N	O	
15	E	1	210	120	15	75	0
			Total	C	N	O	
15	E	1	210	120	15	75	0
			Total	C	N	O	
15	E	1	210	120	15	75	0
			Total	C	N	O	
15	E	1	210	120	15	75	0
			Total	C	N	O	
15	E	1	210	120	15	75	0
			Total	C	N	O	
15	E	1	210	120	15	75	0
			Total	C	N	O	
15	E	1	210	120	15	75	0
			Total	C	N	O	
15	E	1	210	120	15	75	0
			Total	C	N	O	
15	E	1	210	120	15	75	0
			Total	C	N	O	
15	F	1	56	32	4	20	0
			Total	C	N	O	
15	F	1	56	32	4	20	0
			Total	C	N	O	
15	F	1	56	32	4	20	0
			Total	C	N	O	
15	F	1	56	32	4	20	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.

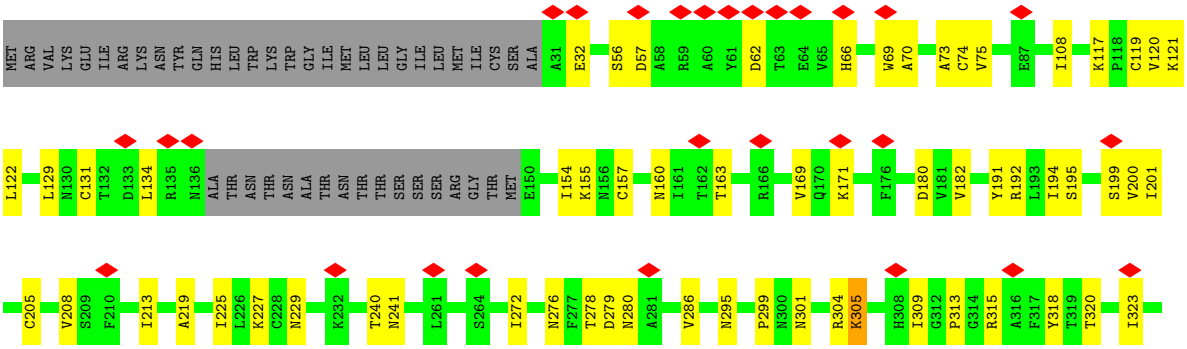
• Molecule 1: Envelope glycoprotein gp120

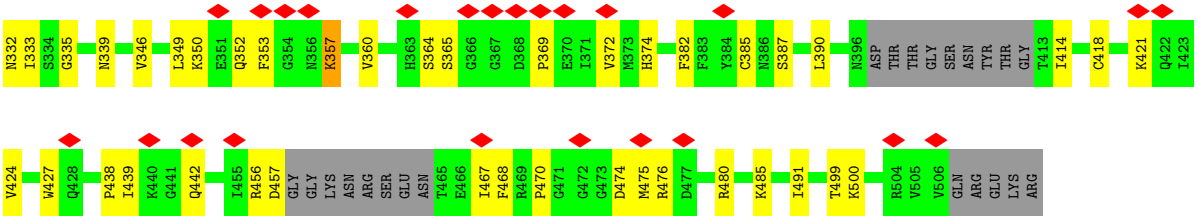
Chain A:



• Molecule 1: Envelope glycoprotein gp120

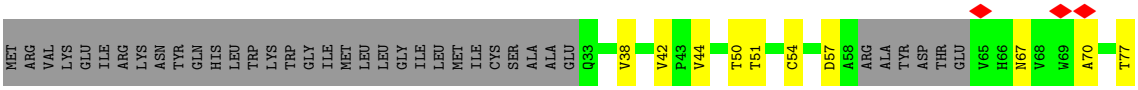
Chain C:

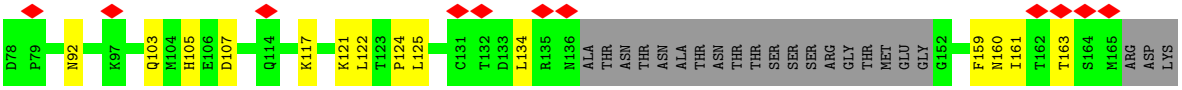


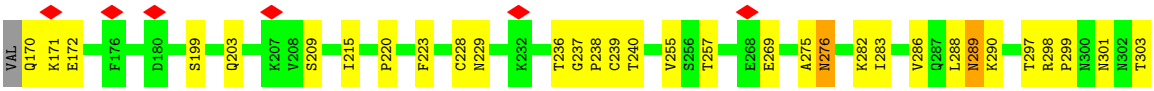


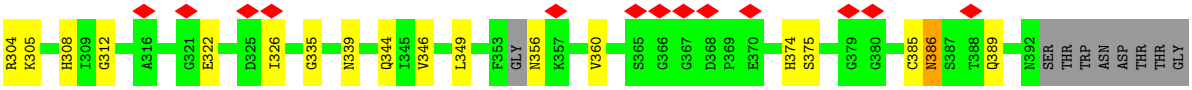
• Molecule 1: Envelope glycoprotein gp120

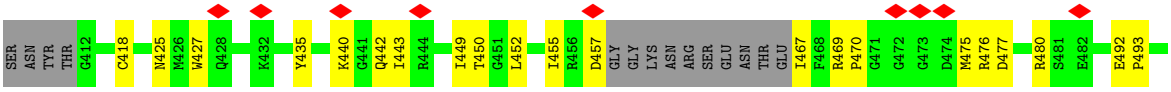
Chain E:

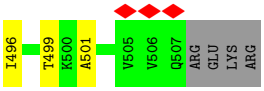






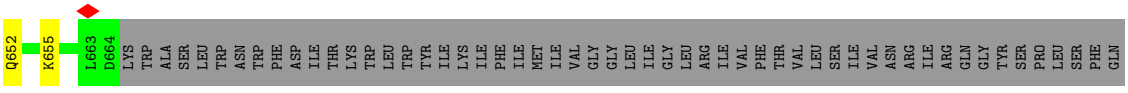






• Molecule 2: Envelope glycoprotein gp41

Chain B:

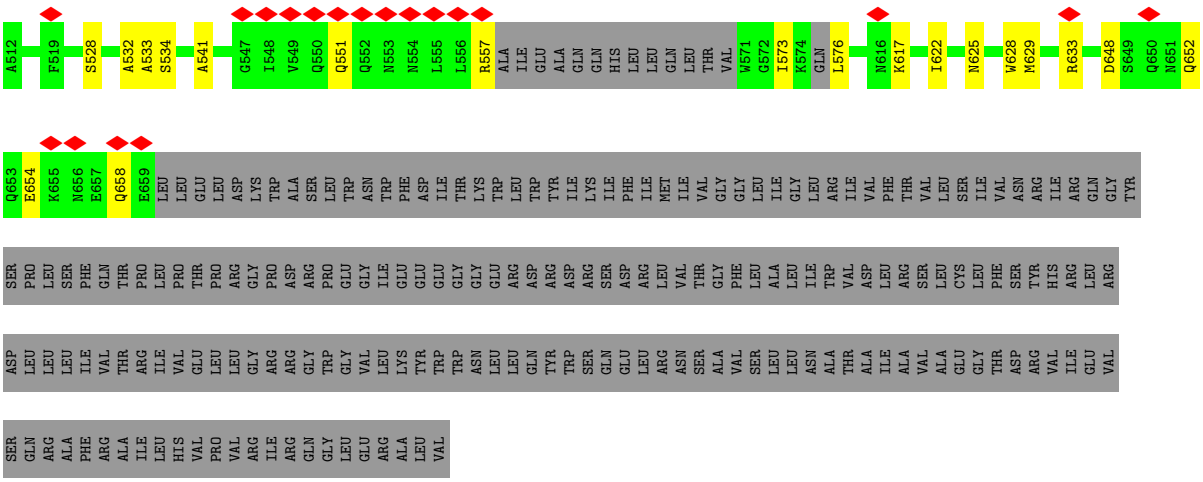


• Molecule 2: Envelope glycoprotein gp41

Chain D:

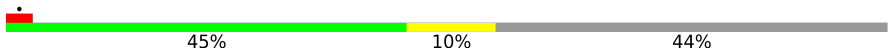
• Molecule 2: Envelope glycoprotein gp41

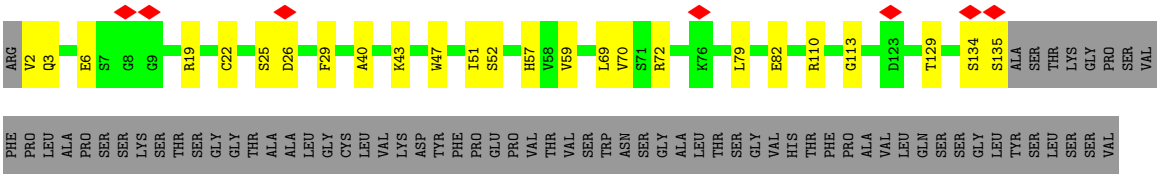
Chain F:



• Molecule 3: Immunoglobulin G PGT151 Fab, Heavy chain

Chain G:

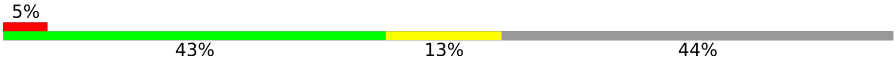


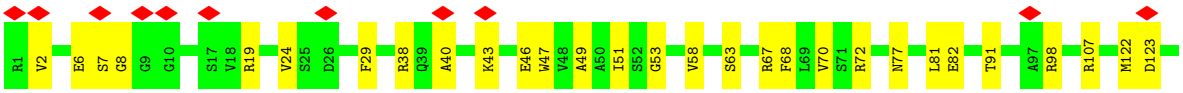


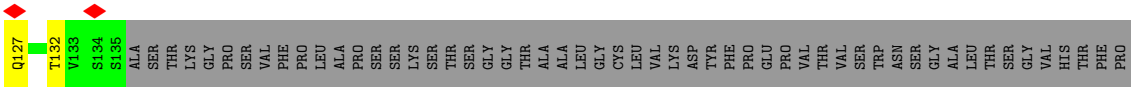
VAL THR VAL PRO SER SER SER LEU GLY THR GLN THR TYR ILE CYS ASN VAL ASN HIS LYS PRO SER ASN THR LYS VAL ASP LYS ARG VAL GLU PRO LYS SER CYS ASP LYS

• Molecule 3: Immunoglobulin G PGT151 Fab, Heavy chain

Chain H:

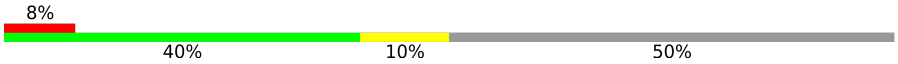


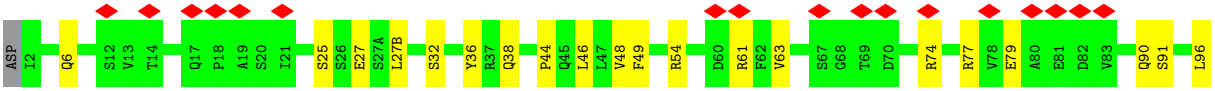




• Molecule 4: Immunoglobulin G PGT151 Fab, Light chain

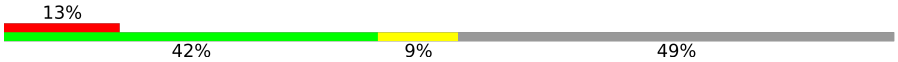
Chain I:

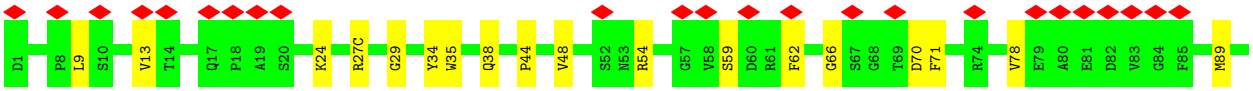


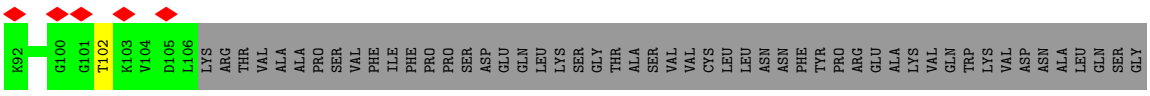


• Molecule 4: Immunoglobulin G PGT151 Fab, Light chain

Chain L:



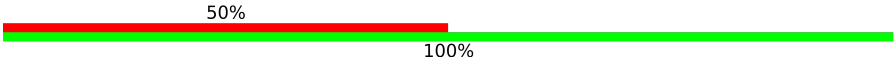




• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:

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

Chain M: 

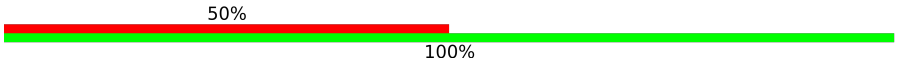
• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N:

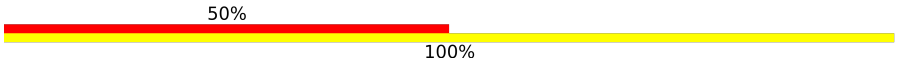
• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O:

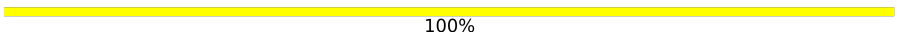
• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Q: 

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

Chain S: 

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

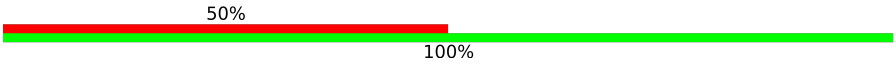
Chain T: 

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

Chain U:

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

Chain Y:



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

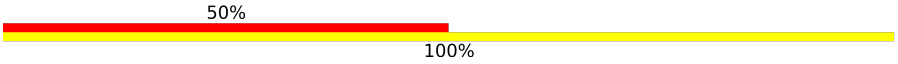
Chain Z:

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

Chain a:

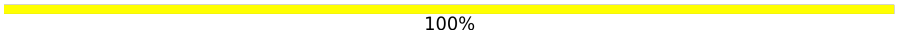
• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain d:



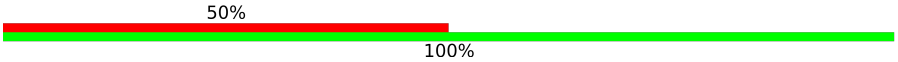
• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain g:



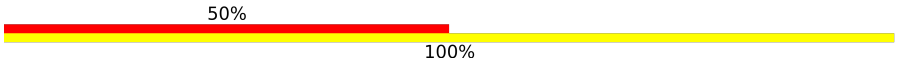
• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain h:



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

Chain K:



• Molecule 7: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain P:

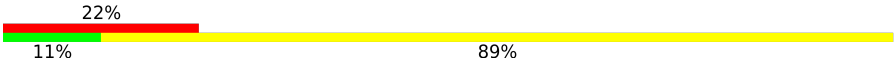
• Molecule 8: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

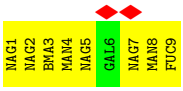
Chain R:

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

Chain i:

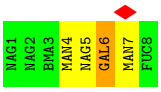
• Molecule 9: beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain V: 



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

Chain W:



• Molecule 11: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

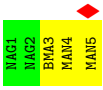
Chain X:

• Molecule 11: alpha-L-fucopyranose-(1-6)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain c:

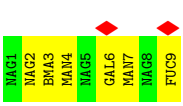
• Molecule 12: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain b:



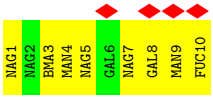
• Molecule 13: beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain e:



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

Chain f:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	74889	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 ($e^-/Å^2$)	51	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.067	Depositor
Minimum map value	-0.034	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.0218	Depositor
Map size (Å)	360.5, 360.5, 360.5	wwPDB
Map dimensions	350, 350, 350	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.03, 1.03, 1.03	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, MAN, BMA, FUC, GAL

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| >5$	RMSZ	$\#\|Z\| >5$
1	A	0.43	0/3462	0.61	0/4699
1	C	0.41	0/3527	0.60	0/4790
1	E	0.41	0/3365	0.58	0/4565
2	B	0.47	0/1172	0.62	0/1592
2	D	0.50	0/1031	0.58	0/1397
2	F	0.45	0/1081	0.58	0/1464
3	G	0.48	0/1091	0.56	0/1482
3	H	0.47	0/1102	0.55	0/1496
4	I	0.44	0/856	0.64	1/1156 (0.1%)
4	L	0.37	0/872	0.55	0/1178
All	All	0.43	0/17559	0.59	1/23819 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	I	96	LEU	CA-CB-CG	5.79	128.61	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3392	0	3345	50	0
1	C	3454	0	3406	63	0
1	E	3298	0	3269	63	0
2	B	1152	0	1136	14	0
2	D	1014	0	995	11	0
2	F	1063	0	1043	11	0
3	G	1062	0	1024	14	0
3	H	1073	0	1040	19	0
4	I	838	0	817	12	0
4	L	854	0	835	11	0
5	J	28	0	25	0	0
5	M	28	0	25	0	0
5	N	28	0	25	0	0
5	O	28	0	25	0	0
5	Q	28	0	25	0	0
5	S	28	0	25	0	0
5	T	28	0	25	0	0
5	U	28	0	25	1	0
5	Y	28	0	25	0	0
5	Z	28	0	25	1	0
5	a	28	0	25	0	0
5	d	28	0	25	0	0
5	g	28	0	25	0	0
5	h	28	0	25	0	0
6	K	28	0	25	0	0
7	P	50	0	43	2	0
8	R	39	0	34	0	0
8	i	39	0	34	0	0
9	V	110	0	94	0	0
10	W	96	0	82	1	0
11	X	24	0	22	0	0
11	c	24	0	22	0	0
12	b	61	0	52	0	0
13	e	110	0	94	0	0
14	f	121	0	103	0	0
15	A	112	0	104	0	0
15	C	182	0	169	0	0
15	D	14	0	13	0	0
15	E	210	0	195	4	0
15	F	56	0	52	1	0
All	All	18868	0	18398	259	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 7.

All (259) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:288:LEU:HD11	1:E:452:LEU:CD1	2.20	0.70
1:E:288:LEU:HD11	1:E:452:LEU:HD11	1.77	0.66
4:I:61:ARG:HH22	4:I:79:GLU:HB2	1.62	0.63
3:H:29:PHE:O	3:H:72:ARG:NH2	2.33	0.62
3:H:40:ALA:HB3	3:H:43:LYS:HB2	1.82	0.62
1:E:161:ILE:HG22	1:E:170:GLN:HG3	1.81	0.61
1:A:357:LYS:HB3	1:A:465:THR:HA	1.83	0.60
1:A:335:GLY:O	1:A:339:ASN:ND2	2.35	0.60
1:E:344:GLN:NE2	15:E:611:NAG:O7	2.35	0.59
2:F:617:LYS:HD3	2:F:622:ILE:HD11	1.84	0.59
2:F:654:GLU:O	2:F:658:GLN:NE2	2.34	0.59
1:A:373:MET:HG2	1:A:384:TYR:HB3	1.84	0.59
1:C:346:VAL:HA	1:C:349:LEU:HB2	1.84	0.59
3:G:29:PHE:O	3:G:72:ARG:NH2	2.34	0.59
1:E:290:LYS:O	1:E:290:LYS:HG3	2.02	0.58
2:B:546:SER:O	2:B:550:GLN:NE2	2.37	0.57
1:A:209:SER:OG	1:A:211:GLU:OE1	2.22	0.57
1:C:122:LEU:HB2	1:C:201:ILE:HG23	1.86	0.57
1:A:277:PHE:O	1:A:456:ARG:NH1	2.34	0.57
1:C:305:LYS:HD3	1:C:318:TYR:HB3	1.87	0.57
1:C:350:LYS:NZ	1:C:357:LYS:O	2.29	0.56
4:L:34:TYR:HB2	4:L:89:MET:HB3	1.87	0.56
1:E:477:ASP:OD1	1:E:480:ARG:NH1	2.38	0.56
1:A:239:CYS:SG	1:A:240:THR:N	2.79	0.56
2:D:594:GLY:HA2	2:D:599:SER:HB3	1.87	0.56
4:L:35:TRP:HB2	4:L:48:VAL:HB	1.87	0.56
2:B:655:LYS:HB3	2:D:603:ILE:HG12	1.88	0.56
1:E:304:ARG:HG2	1:E:440:LYS:HD3	1.88	0.56
1:A:300:ASN:HD21	1:A:327:ARG:H	1.52	0.56
1:A:393[B]:SER:OG	1:A:394:THR:N	2.39	0.56
4:I:25:SER:OG	4:I:27:GLU:O	2.24	0.56
3:H:6:GLU:O	3:H:127:GLN:NE2	2.39	0.56
2:B:551:GLN:O	2:B:555:LEU:N	2.37	0.55
1:C:476:ARG:O	1:C:480:ARG:N	2.38	0.55
1:A:393[A]:SER:OG	1:A:394:THR:N	2.39	0.55
1:E:288:LEU:N	1:E:450:THR:O	2.40	0.55
1:E:276:ASN:H	1:E:282:LYS:HG3	1.72	0.55
1:C:74:CYS:SG	1:C:75:VAL:N	2.80	0.55
1:C:457:ASP:HB3	1:C:467:ILE:HB	1.89	0.55
1:A:298:ARG:NH2	1:A:441:GLY:O	2.39	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:54:ARG:NH1	4:L:59:SER:O	2.40	0.54
1:E:122:LEU:HD13	1:E:125:LEU:HD12	1.87	0.54
1:E:290:LYS:O	1:E:290:LYS:CG	2.56	0.54
1:E:386:ASN:HB3	1:E:389:GLN:HE22	1.71	0.54
2:D:591:GLN:NE2	2:F:541:ALA:O	2.40	0.54
1:E:160:ASN:HA	1:E:171:LYS:H	1.71	0.54
2:B:652:GLN:NE2	2:D:534:SER:O	2.41	0.54
1:C:117:LYS:O	1:C:121:LYS:NZ	2.40	0.54
1:A:98:ASN:ND2	1:A:486:TYR:O	2.36	0.54
1:C:272:ILE:HG12	1:C:286:VAL:HA	1.88	0.54
1:E:269:GLU:O	1:E:289:ASN:HB3	2.07	0.54
2:D:639:THR:HA	2:D:642:ILE:HD12	1.88	0.54
2:B:546:SER:OG	2:B:550:GLN:NE2	2.38	0.54
1:C:456:ARG:HG2	1:C:468:PHE:HE1	1.73	0.54
3:H:38:ARG:NH2	3:H:46:GLU:OE1	2.41	0.54
1:A:129:LEU:HD12	1:A:157:CYS:HB3	1.89	0.53
3:H:63:SER:O	3:H:67:ARG:NH1	2.41	0.53
3:H:51:ILE:HD13	3:H:72:ARG:HG3	1.89	0.53
4:L:24:LYS:HA	4:L:70:ASP:HA	1.90	0.53
1:A:313:PRO:HB2	1:E:199:SER:HA	1.89	0.53
1:A:503:ARG:HD2	2:B:650:GLN:HE22	1.74	0.53
1:C:299:PRO:O	1:C:442:GLN:NE2	2.42	0.53
4:I:32:SER:HB3	4:I:91:SER:HB2	1.90	0.53
1:A:122:LEU:HB3	1:A:125:LEU:HD12	1.91	0.52
1:C:32:GLU:HG3	1:C:500:LYS:HG2	1.90	0.52
2:B:563:GLN:HB3	2:B:566:LEU:HG	1.91	0.52
1:C:427:TRP:HZ2	1:C:475:MET:H	1.56	0.52
1:C:491:ILE:O	2:D:585:ARG:NH2	2.42	0.52
4:L:66:GLY:HA3	4:L:71:PHE:HA	1.91	0.52
1:C:56:SER:OG	1:C:57:ASP:N	2.41	0.52
1:E:308:HIS:NE2	1:E:312:GLY:O	2.42	0.52
3:H:19:ARG:HE	3:H:82:GLU:HB2	1.74	0.52
1:A:304:ARG:HA	1:A:321:GLY:H	1.74	0.52
1:E:344:GLN:NE2	15:E:611:NAG:O3	2.43	0.52
3:G:69:LEU:HB3	3:G:82:GLU:HB3	1.90	0.52
1:A:274:SER:HB2	1:A:284:ILE:HA	1.92	0.52
1:E:159:PHE:O	1:E:172:GLU:N	2.39	0.52
3:G:40:ALA:HB3	3:G:43:LYS:HB2	1.92	0.51
1:E:288:LEU:HD11	1:E:452:LEU:HD12	1.90	0.51
1:A:91:GLU:OE2	1:A:487:LYS:NZ	2.43	0.51
1:C:364:SER:HB2	1:C:470:PRO:HG2	1.91	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:134:LEU:HD23	1:E:326:ILE:HD11	1.93	0.51
3:H:19:ARG:NH2	3:H:82:GLU:OE1	2.41	0.51
1:A:122:LEU:HD12	1:A:201:ILE:HG22	1.93	0.51
1:C:369:PRO:HA	1:C:372:VAL:HB	1.91	0.51
1:C:387:SER:HB2	1:C:390:LEU:HD12	1.93	0.50
4:L:54:ARG:HH12	4:L:62:PHE:H	1.58	0.50
1:A:179:LEU:O	1:A:421:LYS:NZ	2.35	0.50
1:E:38:VAL:HA	1:E:496:ILE:HG22	1.93	0.50
1:A:55:ALA:HB3	1:A:216:HIS:HB2	1.94	0.50
1:E:161:ILE:HB	1:E:170:GLN:HA	1.93	0.50
1:E:289:ASN:O	1:E:290:LYS:HG2	2.12	0.50
4:L:27(C):ARG:HE	4:L:29:GLY:HA2	1.76	0.50
1:C:276:ASN:HD22	1:C:279:ASP:HB2	1.76	0.50
1:A:65:VAL:HG22	1:A:72:HIS:HB3	1.93	0.50
1:C:382:PHE:HD2	1:C:424:VAL:HG21	1.75	0.50
1:E:105:HIS:CD2	1:E:476:ARG:HE	2.30	0.50
4:I:63:VAL:HG23	4:I:74:ARG:HB3	1.94	0.50
2:D:652:GLN:NE2	2:F:534:SER:O	2.45	0.49
2:F:629:MET:HB3	2:F:633:ARG:HH12	1.77	0.49
1:E:457:ASP:O	1:E:469:ARG:NH2	2.44	0.49
1:A:129:LEU:HD23	1:A:192:ARG:HA	1.94	0.49
4:I:6:GLN:HE21	4:I:101:GLY:H	1.60	0.49
4:I:90:GLN:HE21	4:I:97:THR:H	1.59	0.49
2:B:569:THR:HG23	2:B:572:GLY:H	1.78	0.49
1:E:385:CYS:HA	1:E:418:CYS:HA	1.94	0.49
1:E:228:CYS:SG	1:E:229:ASN:N	2.85	0.49
1:A:200:VAL:HG22	1:C:313:PRO:HB2	1.95	0.49
2:B:539:VAL:O	2:B:541:ALA:N	2.46	0.49
1:E:117:LYS:O	1:E:121:LYS:NZ	2.46	0.49
1:A:386:ASN:HB3	1:A:417:PRO:HG2	1.95	0.49
1:C:333:ILE:HG23	1:C:414:ILE:HB	1.94	0.49
1:E:288:LEU:HD12	1:E:449:ILE:HG22	1.95	0.49
1:C:69:TRP:HZ3	1:C:108:ILE:HD12	1.77	0.48
4:I:61:ARG:NH1	4:I:77:ARG:O	2.45	0.48
1:C:134:LEU:N	1:C:154:ILE:O	2.46	0.48
1:E:236:THR:OG1	1:E:237:GLY:N	2.45	0.48
3:H:70:VAL:HG22	3:H:81:LEU:HD13	1.93	0.48
1:A:129:LEU:HD13	1:A:159:PHE:HB3	1.94	0.48
1:E:44:VAL:HG23	1:E:492:GLU:HB2	1.94	0.48
3:H:51:ILE:HG13	3:H:58:VAL:HG22	1.94	0.48
2:D:650:GLN:O	2:D:654:GLU:N	2.42	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:67:ASN:HB3	1:E:70:ALA:HB2	1.95	0.48
3:G:51:ILE:HD11	3:G:70:VAL:HB	1.96	0.48
1:A:228:CYS:SG	1:A:229:ASN:N	2.87	0.48
1:E:92:ASN:HA	1:E:238:PRO:HA	1.96	0.48
1:A:258:GLN:NE2	1:A:372:VAL:O	2.41	0.48
2:B:540:GLN:HB2	2:B:543:LEU:HD23	1.96	0.48
1:E:298:ARG:N	1:E:443:ILE:O	2.46	0.48
1:E:286:VAL:CG1	1:E:452:LEU:HB2	2.44	0.47
1:E:303:THR:OG1	1:E:322:GLU:N	2.47	0.47
1:C:119:CYS:SG	1:C:205:CYS:N	2.87	0.47
1:A:312:GLY:HA3	1:A:315:ARG:HB2	1.97	0.47
1:C:421:LYS:HE3	1:C:424:VAL:HA	1.95	0.47
1:E:42:VAL:N	1:E:493:PRO:O	2.47	0.47
1:C:301:ASN:HD22	1:C:323:ILE:HD12	1.79	0.47
1:C:304:ARG:HG3	1:C:305:LYS:H	1.79	0.47
1:C:499:THR:OG1	1:C:500:LYS:N	2.48	0.47
1:E:50:THR:OG1	1:E:51:THR:N	2.44	0.47
1:A:70:ALA:HB2	1:A:213:ILE:HD13	1.96	0.47
1:C:70:ALA:HB1	1:C:73:ALA:H	1.79	0.47
1:E:57:ASP:HA	1:E:77:THR:HA	1.96	0.47
3:G:19:ARG:NH1	10:W:6:GAL:O3	2.47	0.47
4:I:46:LEU:HD21	4:I:49:PHE:HB3	1.96	0.47
1:A:477:ASP:OD1	1:A:480:ARG:NH1	2.48	0.47
1:E:220:PRO:HG2	1:E:223:PHE:HD2	1.80	0.47
1:E:257:THR:HG1	1:E:375:SER:H	1.62	0.47
3:G:52:SER:HB3	3:G:57:HIS:HB3	1.96	0.47
1:E:427:TRP:CD1	1:E:475:MET:HG2	2.50	0.47
1:C:360:VAL:HG21	1:C:467:ILE:HD13	1.98	0.46
1:A:298:ARG:NH1	1:A:302:ASN:HD22	2.14	0.46
3:H:68:PHE:HB3	3:H:81:LEU:HD11	1.97	0.46
4:L:38:GLN:HB3	4:L:44:PRO:HA	1.97	0.46
1:A:364:SER:HA	1:A:469:ARG:HD2	1.98	0.46
1:A:364:SER:HB2	1:A:470:PRO:HD2	1.96	0.46
1:A:286:VAL:HB	1:A:452:LEU:HB3	1.96	0.46
2:F:528:SER:HB2	2:F:533:ALA:HB2	1.97	0.46
3:H:98:ARG:NH2	3:H:123:ASP:OD2	2.49	0.46
1:C:229:ASN:ND2	1:C:241:ASN:O	2.39	0.46
1:A:166:ARG:HD2	1:E:124:PRO:HA	1.98	0.46
1:A:268:GLU:HA	5:U:1:NAG:HN2	1.81	0.46
1:E:54:CYS:HB2	1:E:215:ILE:HD11	1.97	0.46
1:C:70:ALA:HB2	1:C:213:ILE:HD11	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:283:ILE:HG12	1:E:455:ILE:HD11	1.98	0.46
1:E:269:GLU:HA	15:E:611:NAG:H82	1.96	0.45
1:E:335:GLY:O	1:E:339:ASN:ND2	2.48	0.45
1:E:103:GLN:NE2	1:E:107:ASP:OD2	2.41	0.45
1:E:269:GLU:HG2	15:E:611:NAG:H82	1.98	0.45
1:E:360:VAL:HG22	1:E:467:ILE:HB	1.99	0.45
4:I:27(B):LEU:HD21	4:I:90:GLN:HB2	1.99	0.45
3:G:22:CYS:HB3	3:G:79:LEU:HB3	1.98	0.45
3:H:53:GLY:O	3:H:72:ARG:NH1	2.50	0.45
1:C:180:ASP:HA	1:C:194:ILE:HG12	1.99	0.45
1:C:163:THR:OG1	1:C:309:ILE:O	2.29	0.44
3:H:2:VAL:HG11	3:H:98:ARG:HD3	1.99	0.44
1:C:350:LYS:HD2	1:C:350:LYS:HA	1.63	0.44
3:H:91:THR:HG23	3:H:132:THR:HA	1.99	0.44
1:C:295:ASN:O	1:C:332:ASN:N	2.49	0.44
1:C:364:SER:OG	1:C:365:SER:N	2.49	0.44
2:F:533:ALA:HB3	2:F:628:TRP:HE1	1.82	0.44
3:G:3:GLN:HB3	3:G:25:SER:HB2	1.98	0.44
1:C:66:HIS:HB2	1:C:208:VAL:HA	2.00	0.44
1:E:203:GLN:HA	1:E:435:TYR:HB3	2.00	0.44
2:B:559:ILE:HA	2:B:562:GLN:HB2	1.99	0.44
1:A:303:THR:OG1	1:A:322:GLU:O	2.26	0.44
1:C:352:GLN:HG2	1:C:353:PHE:HD1	1.83	0.44
2:D:518:VAL:N	3:G:113:GLY:O	2.45	0.43
3:G:47:TRP:HH2	3:G:59:VAL:HG12	1.82	0.43
4:I:36:TYR:HB3	4:I:46:LEU:HD12	2.00	0.43
1:E:374:HIS:HB3	1:E:385:CYS:HB2	2.00	0.43
1:A:50:THR:OG1	1:A:51:THR:N	2.51	0.43
2:F:573:ILE:O	2:F:576:LEU:N	2.52	0.43
2:F:617:LYS:HA	15:F:901:NAG:H82	2.00	0.43
4:L:13:VAL:HB	4:L:78:VAL:HG11	2.00	0.43
1:E:67:ASN:HA	1:E:209:SER:HB3	2.01	0.43
1:E:297:THR:HG23	1:E:299:PRO:HD3	2.01	0.43
7:P:4:MAN:O6	7:P:4:MAN:O4	2.33	0.43
2:B:552:GLN:HA	2:B:555:LEU:HB3	2.01	0.43
1:E:275:ALA:HB3	1:E:282:LYS:HG3	1.99	0.43
1:E:499:THR:HG23	1:E:501:ALA:H	1.83	0.43
1:A:47:GLU:OE2	1:A:487:LYS:NZ	2.45	0.43
1:C:474:ASP:OD2	1:C:476:ARG:NE	2.45	0.43
1:E:346:VAL:HA	1:E:349:LEU:HB2	2.00	0.43
3:G:134:SER:OG	3:G:135:SER:N	2.49	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:182:VAL:HG23	1:C:194:ILE:HG22	2.01	0.43
1:A:153:GLU:OE1	1:A:419:ARG:NH2	2.52	0.43
1:C:219:ALA:HB2	1:C:225:ILE:HG13	2.01	0.43
1:C:227:LYS:HG3	1:C:485:LYS:HB3	2.00	0.43
3:G:2:VAL:HG21	3:G:26:ASP:H	1.84	0.43
1:A:259:LEU:HB2	1:A:374:HIS:HE1	1.84	0.42
2:F:648:ASP:HA	2:F:652:GLN:HB3	2.01	0.42
1:A:333:ILE:O	1:A:414:ILE:N	2.48	0.42
1:C:304:ARG:HE	1:C:305:LYS:HD2	1.84	0.42
2:D:523:LEU:HA	2:D:540:GLN:HE21	1.84	0.42
1:C:160:ASN:HB3	1:C:169:VAL:HB	2.00	0.42
1:C:374:HIS:N	1:C:385:CYS:O	2.46	0.42
1:A:227:LYS:O	1:A:243:SER:N	2.51	0.42
4:L:54:ARG:HH22	4:L:62:PHE:H	1.67	0.42
1:A:156:ASN:HA	1:A:175:LEU:HD23	2.01	0.42
1:C:439:ILE:H	1:C:439:ILE:HG13	1.58	0.42
1:E:163:THR:HA	1:E:308:HIS:HD2	1.84	0.42
1:E:255:VAL:HG22	1:E:475:MET:HE2	2.02	0.42
3:H:47:TRP:NE1	3:H:49:ALA:O	2.52	0.42
2:D:649:SER:OG	2:D:650:GLN:N	2.52	0.42
2:B:590:GLN:O	2:B:594:GLY:N	2.53	0.42
1:C:320:THR:HG22	1:C:438:PRO:HD2	2.02	0.42
1:C:385:CYS:HA	1:C:418:CYS:HA	2.01	0.42
4:I:38:GLN:HB3	4:I:44:PRO:HB3	2.02	0.42
1:A:122:LEU:HD11	1:A:203:GLN:HB2	2.02	0.42
1:C:280:ASN:OD1	1:C:456:ARG:NH1	2.53	0.42
1:A:291:SER:HB2	1:A:448:ASN:HB3	2.02	0.41
2:B:644:THR:OG1	3:G:110:ARG:NH1	2.46	0.41
1:C:70:ALA:O	1:C:74:CYS:N	2.53	0.41
1:E:239:CYS:SG	1:E:240:THR:N	2.93	0.41
1:C:131:CYS:HB3	1:C:155:LYS:HB3	2.03	0.41
1:A:260:LEU:HB2	1:A:451:GLY:HA3	2.01	0.41
2:F:528:SER:HB3	2:F:532:ALA:HB3	2.02	0.41
3:G:6:GLU:HB2	3:G:129:THR:HG23	2.03	0.41
1:E:469:ARG:HA	1:E:470:PRO:HD3	1.89	0.41
1:C:199:SER:OG	1:C:200:VAL:N	2.51	0.41
7:P:4:MAN:HO4	7:P:4:MAN:HO6	1.68	0.41
1:C:194:ILE:HD12	1:C:195:SER:HB3	2.01	0.41
3:H:7:SER:OG	3:H:8:GLY:N	2.54	0.41
1:C:62:ASP:OD1	1:C:62:ASP:N	2.51	0.41
4:I:48:VAL:HG12	4:I:54:ARG:HA	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:124:PRO:HB2	1:A:309:ILE:HD11	2.01	0.41
1:C:129:LEU:HD22	1:C:157:CYS:HB3	2.02	0.41
1:A:132:THR:O	1:A:156:ASN:N	2.54	0.41
1:C:335:GLY:O	1:C:339:ASN:ND2	2.54	0.41
4:L:9:LEU:HB3	4:L:102:THR:HA	2.03	0.41
1:C:120:VAL:HG22	1:C:315:ARG:HD2	2.02	0.41
1:C:278:THR:O	1:C:456:ARG:NH1	2.53	0.41
1:E:286:VAL:O	1:E:286:VAL:HG13	2.20	0.41
1:E:301:ASN:HB2	1:E:442:GLN:HE21	1.85	0.41
3:H:24:VAL:HG22	3:H:77:ASN:HB3	2.03	0.41
1:C:160:ASN:HD22	5:Z:1:NAG:H83	1.86	0.40
3:H:6:GLU:H	3:H:127:GLN:HE22	1.70	0.40
1:C:155:LYS:HG3	1:C:191:TYR:HE2	1.86	0.40
1:C:240:THR:OG1	1:C:241:ASN:N	2.54	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	419/506 (83%)	370 (88%)	49 (12%)	0	100	100
1	C	430/506 (85%)	371 (86%)	59 (14%)	0	100	100
1	E	405/506 (80%)	358 (88%)	47 (12%)	0	100	100
2	B	141/345 (41%)	129 (92%)	12 (8%)	0	100	100
2	D	125/345 (36%)	113 (90%)	12 (10%)	0	100	100
2	F	128/345 (37%)	108 (84%)	20 (16%)	0	100	100
3	G	132/240 (55%)	118 (89%)	14 (11%)	0	100	100
3	H	133/240 (55%)	119 (90%)	14 (10%)	0	100	100
4	I	107/219 (49%)	95 (89%)	12 (11%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	L	109/219 (50%)	98 (90%)	11 (10%)	0	100	100
All	All	2129/3471 (61%)	1879 (88%)	250 (12%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	386/450 (86%)	379 (98%)	7 (2%)	59	76
1	C	392/450 (87%)	388 (99%)	4 (1%)	76	86
1	E	376/450 (84%)	370 (98%)	6 (2%)	62	79
2	B	125/298 (42%)	123 (98%)	2 (2%)	62	79
2	D	108/298 (36%)	108 (100%)	0	100	100
2	F	113/298 (38%)	110 (97%)	3 (3%)	44	66
3	G	115/207 (56%)	115 (100%)	0	100	100
3	H	116/207 (56%)	114 (98%)	2 (2%)	60	78
4	I	96/195 (49%)	96 (100%)	0	100	100
4	L	98/195 (50%)	98 (100%)	0	100	100
All	All	1925/3048 (63%)	1901 (99%)	24 (1%)	72	83

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	185	LYS
1	A	276	ASN
1	A	304	ARG
1	A	393[A]	SER
1	A	393[B]	SER
1	A	396	ASN
1	A	425	ASN
2	B	616	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	625	ASN
1	C	171	LYS
1	C	192	ARG
1	C	305	LYS
1	C	357	LYS
1	E	276	ASN
1	E	289	ASN
1	E	305	LYS
1	E	356	ASN
1	E	386	ASN
1	E	425	ASN
2	F	551	GLN
2	F	557	ARG
2	F	625	ASN
3	H	107	ARG
3	H	122	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	105	HIS
1	A	216	HIS
1	A	300	ASN
1	A	339	ASN
1	A	396	ASN
1	A	425	ASN
2	B	550	GLN
2	B	616	ASN
1	C	82	GLN
1	C	287	GLN
1	C	300	ASN
1	C	339	ASN
2	D	590	GLN
2	D	651	ASN
1	E	105	HIS
1	E	339	ASN
1	E	344	GLN
1	E	386	ASN
1	E	422	GLN
1	E	425	ASN
1	E	442	GLN
4	I	6	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	H	39	GLN
4	L	38	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)

85 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	J	1	1,5	14,14,15	0.53	0	17,19,21	1.00	1 (5%)
5	NAG	J	2	5	14,14,15	0.32	0	17,19,21	0.42	0
6	NAG	K	1	1,6	14,14,15	0.46	0	17,19,21	0.67	1 (5%)
6	NAG	K	2	6	14,14,15	0.51	0	17,19,21	1.01	1 (5%)
5	NAG	M	1	1,5	14,14,15	0.27	0	17,19,21	0.65	0
5	NAG	M	2	5	14,14,15	0.33	0	17,19,21	0.43	0
5	NAG	N	1	1,5	14,14,15	0.41	0	17,19,21	0.62	0
5	NAG	N	2	5	14,14,15	0.47	0	17,19,21	0.44	0
5	NAG	O	1	1,5	14,14,15	0.27	0	17,19,21	1.00	1 (5%)
5	NAG	O	2	5	14,14,15	0.39	0	17,19,21	0.58	0
7	NAG	P	1	1,7	14,14,15	0.38	0	17,19,21	0.46	0
7	NAG	P	2	7	14,14,15	0.24	0	17,19,21	0.56	0
7	BMA	P	3	7	11,11,12	0.79	0	15,15,17	1.02	0
7	MAN	P	4	7	11,11,12	0.88	1 (9%)	15,15,17	1.53	2 (13%)
5	NAG	Q	1	1,5	14,14,15	0.45	0	17,19,21	0.61	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	NAG	Q	2	5	14,14,15	0.24	0	17,19,21	0.56	0
8	NAG	R	1	1,8	14,14,15	0.31	0	17,19,21	0.54	0
8	NAG	R	2	8	14,14,15	0.24	0	17,19,21	0.86	1 (5%)
8	BMA	R	3	8	11,11,12	0.70	0	15,15,17	0.80	1 (6%)
5	NAG	S	1	1,5	14,14,15	0.70	1 (7%)	17,19,21	0.91	0
5	NAG	S	2	5	14,14,15	0.37	0	17,19,21	0.91	1 (5%)
5	NAG	T	1	1,5	14,14,15	0.51	0	17,19,21	1.02	1 (5%)
5	NAG	T	2	5	14,14,15	0.21	0	17,19,21	0.74	1 (5%)
5	NAG	U	1	1,5	14,14,15	0.63	0	17,19,21	0.94	1 (5%)
5	NAG	U	2	5	14,14,15	0.44	0	17,19,21	0.96	1 (5%)
9	NAG	V	1	9,2	14,14,15	0.67	1 (7%)	17,19,21	0.82	0
9	NAG	V	2	9	14,14,15	0.48	0	17,19,21	1.04	1 (5%)
9	BMA	V	3	9	11,11,12	1.08	1 (9%)	15,15,17	1.75	4 (26%)
9	MAN	V	4	9	11,11,12	0.99	1 (9%)	15,15,17	1.76	2 (13%)
9	NAG	V	5	9	14,14,15	0.21	0	17,19,21	0.75	1 (5%)
9	GAL	V	6	9	11,11,12	0.65	0	15,15,17	1.14	0
9	NAG	V	7	9	14,14,15	0.37	0	17,19,21	0.93	1 (5%)
9	MAN	V	8	9	11,11,12	0.97	1 (9%)	15,15,17	1.00	1 (6%)
9	FUC	V	9	9	10,10,11	1.00	1 (10%)	14,14,16	0.96	0
10	NAG	W	1	2,10	14,14,15	0.57	0	17,19,21	0.50	0
10	NAG	W	2	10	14,14,15	0.34	0	17,19,21	0.67	0
10	BMA	W	3	10	11,11,12	0.89	0	15,15,17	0.90	0
10	MAN	W	4	10	11,11,12	0.90	0	15,15,17	1.39	2 (13%)
10	NAG	W	5	10	14,14,15	0.24	0	17,19,21	0.71	1 (5%)
10	GAL	W	6	10	11,11,12	0.86	0	15,15,17	1.19	2 (13%)
10	MAN	W	7	10	11,11,12	1.04	1 (9%)	15,15,17	1.43	3 (20%)
10	FUC	W	8	10	10,10,11	0.67	0	14,14,16	0.74	0
11	NAG	X	1	11,2	14,14,15	0.77	1 (7%)	17,19,21	2.29	4 (23%)
11	FUC	X	2	11	10,10,11	1.40	2 (20%)	14,14,16	1.64	3 (21%)
5	NAG	Y	1	1,5	14,14,15	0.19	0	17,19,21	0.58	0
5	NAG	Y	2	5	14,14,15	0.22	0	17,19,21	0.58	0
5	NAG	Z	1	1,5	14,14,15	0.33	0	17,19,21	0.63	0
5	NAG	Z	2	5	14,14,15	0.24	0	17,19,21	0.57	0
5	NAG	a	1	1,5	14,14,15	0.54	0	17,19,21	1.09	2 (11%)
5	NAG	a	2	5	14,14,15	0.41	0	17,19,21	0.62	1 (5%)
12	NAG	b	1	1,12	14,14,15	0.46	0	17,19,21	0.63	0
12	NAG	b	2	12	14,14,15	0.21	0	17,19,21	0.62	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
12	BMA	b	3	12	11,11,12	0.70	0	15,15,17	1.16	2 (13%)
12	MAN	b	4	12	11,11,12	1.14	1 (9%)	15,15,17	1.60	3 (20%)
12	MAN	b	5	12	11,11,12	0.86	1 (9%)	15,15,17	1.32	2 (13%)
11	NAG	c	1	1,11	14,14,15	0.42	0	17,19,21	0.57	0
11	FUC	c	2	11	10,10,11	0.86	0	14,14,16	1.25	1 (7%)
5	NAG	d	1	1,5	14,14,15	0.35	0	17,19,21	0.98	1 (5%)
5	NAG	d	2	5	14,14,15	0.48	0	17,19,21	0.94	1 (5%)
13	NAG	e	1	13,2	14,14,15	0.42	0	17,19,21	0.63	0
13	NAG	e	2	13	14,14,15	0.66	1 (7%)	17,19,21	0.71	0
13	BMA	e	3	13	11,11,12	0.87	0	15,15,17	1.01	2 (13%)
13	MAN	e	4	13	11,11,12	0.84	1 (9%)	15,15,17	1.46	1 (6%)
13	NAG	e	5	13	14,14,15	0.21	0	17,19,21	0.52	0
13	GAL	e	6	13	11,11,12	1.08	1 (9%)	15,15,17	1.36	1 (6%)
13	MAN	e	7	13	11,11,12	0.73	0	15,15,17	1.38	1 (6%)
13	NAG	e	8	13	14,14,15	0.48	0	17,19,21	0.41	0
13	FUC	e	9	13	10,10,11	0.75	0	14,14,16	1.11	1 (7%)
14	NAG	f	1	14,2	14,14,15	0.77	1 (7%)	17,19,21	1.23	1 (5%)
14	FUC	f	10	14	10,10,11	1.06	1 (10%)	14,14,16	0.98	1 (7%)
14	NAG	f	2	14	14,14,15	0.21	0	17,19,21	0.43	0
14	BMA	f	3	14	11,11,12	0.88	0	15,15,17	1.09	1 (6%)
14	MAN	f	4	14	11,11,12	1.01	1 (9%)	15,15,17	1.66	3 (20%)
14	NAG	f	5	14	14,14,15	0.58	1 (7%)	17,19,21	0.57	0
14	GAL	f	6	14	11,11,12	0.72	0	15,15,17	0.92	0
14	NAG	f	7	14	14,14,15	0.19	0	17,19,21	0.62	1 (5%)
14	GAL	f	8	14	11,11,12	0.71	0	15,15,17	1.36	2 (13%)
14	MAN	f	9	14	11,11,12	0.87	0	15,15,17	1.07	2 (13%)
5	NAG	g	1	1,5	14,14,15	0.86	1 (7%)	17,19,21	1.04	1 (5%)
5	NAG	g	2	5	14,14,15	0.57	0	17,19,21	0.73	1 (5%)
5	NAG	h	1	1,5	14,14,15	0.50	0	17,19,21	0.63	0
5	NAG	h	2	5	14,14,15	0.37	0	17,19,21	0.45	0
8	NAG	i	1	1,8	14,14,15	0.35	0	17,19,21	0.58	0
8	NAG	i	2	8	14,14,15	0.37	0	17,19,21	0.76	0
8	BMA	i	3	8	11,11,12	0.69	0	15,15,17	1.01	1 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	J	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	J	2	5	-	2/6/23/26	0/1/1/1
6	NAG	K	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	K	2	6	-	2/6/23/26	0/1/1/1
5	NAG	M	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	M	2	5	-	2/6/23/26	0/1/1/1
5	NAG	N	1	1,5	-	1/6/23/26	0/1/1/1
5	NAG	N	2	5	-	2/6/23/26	0/1/1/1
5	NAG	O	1	1,5	-	3/6/23/26	0/1/1/1
5	NAG	O	2	5	-	2/6/23/26	0/1/1/1
7	NAG	P	1	1,7	-	0/6/23/26	0/1/1/1
7	NAG	P	2	7	-	2/6/23/26	0/1/1/1
7	BMA	P	3	7	-	1/2/19/22	0/1/1/1
7	MAN	P	4	7	-	2/2/19/22	0/1/1/1
5	NAG	Q	1	1,5	-	1/6/23/26	0/1/1/1
5	NAG	Q	2	5	-	2/6/23/26	0/1/1/1
8	NAG	R	1	1,8	-	2/6/23/26	0/1/1/1
8	NAG	R	2	8	-	2/6/23/26	0/1/1/1
8	BMA	R	3	8	-	1/2/19/22	0/1/1/1
5	NAG	S	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	S	2	5	-	3/6/23/26	0/1/1/1
5	NAG	T	1	1,5	-	3/6/23/26	0/1/1/1
5	NAG	T	2	5	-	2/6/23/26	0/1/1/1
5	NAG	U	1	1,5	-	1/6/23/26	0/1/1/1
5	NAG	U	2	5	-	1/6/23/26	0/1/1/1
9	NAG	V	1	9,2	-	0/6/23/26	0/1/1/1
9	NAG	V	2	9	-	1/6/23/26	0/1/1/1
9	BMA	V	3	9	-	2/2/19/22	0/1/1/1
9	MAN	V	4	9	-	0/2/19/22	0/1/1/1
9	NAG	V	5	9	-	0/6/23/26	0/1/1/1
9	GAL	V	6	9	-	2/2/19/22	0/1/1/1
9	NAG	V	7	9	-	3/6/23/26	0/1/1/1
9	MAN	V	8	9	-	2/2/19/22	0/1/1/1
9	FUC	V	9	9	-	-	0/1/1/1
10	NAG	W	1	2,10	-	0/6/23/26	0/1/1/1
10	NAG	W	2	10	-	2/6/23/26	0/1/1/1
10	BMA	W	3	10	-	0/2/19/22	0/1/1/1
10	MAN	W	4	10	-	0/2/19/22	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	NAG	W	5	10	-	1/6/23/26	0/1/1/1
10	GAL	W	6	10	-	0/2/19/22	0/1/1/1
10	MAN	W	7	10	-	2/2/19/22	0/1/1/1
10	FUC	W	8	10	-	-	0/1/1/1
11	NAG	X	1	11,2	-	5/6/23/26	0/1/1/1
11	FUC	X	2	11	-	-	0/1/1/1
5	NAG	Y	1	1,5	-	1/6/23/26	0/1/1/1
5	NAG	Y	2	5	-	2/6/23/26	0/1/1/1
5	NAG	Z	1	1,5	-	4/6/23/26	0/1/1/1
5	NAG	Z	2	5	-	4/6/23/26	0/1/1/1
5	NAG	a	1	1,5	-	3/6/23/26	0/1/1/1
5	NAG	a	2	5	-	2/6/23/26	0/1/1/1
12	NAG	b	1	1,12	-	2/6/23/26	0/1/1/1
12	NAG	b	2	12	-	3/6/23/26	0/1/1/1
12	BMA	b	3	12	-	2/2/19/22	0/1/1/1
12	MAN	b	4	12	-	2/2/19/22	0/1/1/1
12	MAN	b	5	12	-	1/2/19/22	0/1/1/1
11	NAG	c	1	1,11	-	4/6/23/26	0/1/1/1
11	FUC	c	2	11	-	-	0/1/1/1
5	NAG	d	1	1,5	-	3/6/23/26	0/1/1/1
5	NAG	d	2	5	-	3/6/23/26	0/1/1/1
13	NAG	e	1	13,2	-	1/6/23/26	0/1/1/1
13	NAG	e	2	13	-	2/6/23/26	0/1/1/1
13	BMA	e	3	13	-	1/2/19/22	0/1/1/1
13	MAN	e	4	13	-	1/2/19/22	0/1/1/1
13	NAG	e	5	13	-	2/6/23/26	0/1/1/1
13	GAL	e	6	13	-	0/2/19/22	0/1/1/1
13	MAN	e	7	13	-	2/2/19/22	0/1/1/1
13	NAG	e	8	13	-	1/6/23/26	0/1/1/1
13	FUC	e	9	13	-	-	0/1/1/1
14	NAG	f	1	14,2	-	0/6/23/26	0/1/1/1
14	FUC	f	10	14	-	-	0/1/1/1
14	NAG	f	2	14	-	4/6/23/26	0/1/1/1
14	BMA	f	3	14	-	2/2/19/22	0/1/1/1
14	MAN	f	4	14	-	0/2/19/22	0/1/1/1
14	NAG	f	5	14	-	1/6/23/26	0/1/1/1
14	GAL	f	6	14	-	0/2/19/22	0/1/1/1
14	NAG	f	7	14	-	1/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	GAL	f	8	14	-	2/2/19/22	0/1/1/1
14	MAN	f	9	14	-	1/2/19/22	0/1/1/1
5	NAG	g	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	g	2	5	-	1/6/23/26	0/1/1/1
5	NAG	h	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	h	2	5	-	2/6/23/26	0/1/1/1
8	NAG	i	1	1,8	-	0/6/23/26	0/1/1/1
8	NAG	i	2	8	-	2/6/23/26	0/1/1/1
8	BMA	i	3	8	-	1/2/19/22	0/1/1/1

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	b	4	MAN	C1-C2	3.49	1.60	1.52
10	W	7	MAN	C1-C2	2.85	1.58	1.52
13	e	6	GAL	C1-C2	2.82	1.58	1.52
5	g	1	NAG	O5-C1	2.77	1.48	1.43
14	f	10	FUC	C1-C2	2.74	1.58	1.52
11	X	2	FUC	C2-C3	2.70	1.56	1.52
14	f	1	NAG	O5-C1	-2.62	1.39	1.43
12	b	5	MAN	C1-C2	2.47	1.57	1.52
14	f	4	MAN	O5-C5	2.45	1.48	1.43
5	S	1	NAG	O5-C1	-2.41	1.39	1.43
9	V	9	FUC	O5-C1	-2.36	1.39	1.43
9	V	1	NAG	O5-C1	-2.35	1.40	1.43
13	e	2	NAG	O5-C1	-2.28	1.40	1.43
7	P	4	MAN	C1-C2	2.19	1.57	1.52
13	e	4	MAN	C1-C2	2.17	1.57	1.52
9	V	4	MAN	C2-C3	-2.17	1.49	1.52
11	X	2	FUC	C4-C3	2.14	1.57	1.52
11	X	1	NAG	C1-C2	2.14	1.55	1.52
9	V	3	BMA	C1-C2	2.10	1.57	1.52
14	f	5	NAG	O5-C1	-2.07	1.40	1.43
9	V	8	MAN	O5-C1	-2.03	1.40	1.43

All (71) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	X	1	NAG	C2-N2-C7	7.96	134.24	122.90
9	V	4	MAN	C1-O5-C5	4.78	118.67	112.19
7	P	4	MAN	C1-O5-C5	4.43	118.19	112.19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	e	7	MAN	C1-O5-C5	4.02	117.63	112.19
14	f	4	MAN	O2-C2-C3	-3.93	102.26	110.14
12	b	4	MAN	C1-O5-C5	3.81	117.36	112.19
14	f	1	NAG	C1-O5-C5	3.77	117.30	112.19
13	e	4	MAN	C1-O5-C5	3.75	117.28	112.19
9	V	3	BMA	C1-C2-C3	3.73	114.25	109.67
9	V	4	MAN	O2-C2-C3	-3.72	102.69	110.14
12	b	5	MAN	C1-O5-C5	3.71	117.22	112.19
14	f	8	GAL	C1-O5-C5	3.70	117.20	112.19
14	f	4	MAN	C1-O5-C5	3.53	116.98	112.19
10	W	7	MAN	C1-O5-C5	3.52	116.97	112.19
11	c	2	FUC	C1-O5-C5	3.42	120.52	112.78
5	T	1	NAG	C2-N2-C7	3.26	127.55	122.90
10	W	4	MAN	C1-O5-C5	3.23	116.58	112.19
5	g	1	NAG	C1-O5-C5	3.23	116.57	112.19
5	J	1	NAG	C2-N2-C7	3.23	127.50	122.90
11	X	2	FUC	C1-O5-C5	3.22	120.07	112.78
11	X	1	NAG	C1-C2-N2	3.17	115.90	110.49
5	d	2	NAG	C2-N2-C7	3.12	127.34	122.90
13	e	6	GAL	O2-C2-C3	-3.11	103.90	110.14
5	O	1	NAG	C2-N2-C7	3.09	127.31	122.90
10	W	4	MAN	O2-C2-C3	-3.09	103.94	110.14
5	S	2	NAG	C2-N2-C7	3.08	127.29	122.90
9	V	2	NAG	C2-N2-C7	3.08	127.29	122.90
9	V	7	NAG	C2-N2-C7	3.07	127.27	122.90
9	V	3	BMA	C1-O5-C5	3.04	116.31	112.19
6	K	2	NAG	C2-N2-C7	3.03	127.22	122.90
5	U	1	NAG	C2-N2-C7	3.02	127.21	122.90
9	V	3	BMA	O5-C1-C2	3.01	115.42	110.77
11	X	2	FUC	O5-C5-C4	3.01	114.92	109.52
5	U	2	NAG	C2-N2-C7	2.97	127.13	122.90
5	d	1	NAG	C2-N2-C7	2.92	127.07	122.90
5	a	1	NAG	C2-N2-C7	2.88	127.00	122.90
14	f	4	MAN	C1-C2-C3	-2.80	106.22	109.67
12	b	4	MAN	C1-C2-C3	2.79	113.10	109.67
12	b	3	BMA	C1-O5-C5	2.70	115.85	112.19
14	f	3	BMA	C1-O5-C5	2.68	115.82	112.19
8	R	2	NAG	C1-O5-C5	2.67	115.80	112.19
12	b	5	MAN	O2-C2-C3	-2.62	104.88	110.14
14	f	9	MAN	C1-O5-C5	2.61	115.73	112.19
5	a	1	NAG	C1-O5-C5	2.59	115.70	112.19
12	b	4	MAN	O2-C2-C3	-2.51	105.11	110.14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	T	2	NAG	C1-O5-C5	2.45	115.52	112.19
10	W	5	NAG	C1-O5-C5	2.44	115.50	112.19
14	f	10	FUC	O2-C2-C1	2.44	114.15	109.15
9	V	5	NAG	C1-O5-C5	2.42	115.47	112.19
11	X	2	FUC	C2-C3-C4	2.41	115.07	110.89
11	X	1	NAG	C1-O5-C5	-2.40	108.94	112.19
10	W	7	MAN	O2-C2-C3	-2.39	105.36	110.14
5	g	2	NAG	C1-O5-C5	2.34	115.37	112.19
10	W	6	GAL	C1-C2-C3	2.33	112.53	109.67
13	e	3	BMA	C1-C2-C3	2.32	112.52	109.67
7	P	4	MAN	O2-C2-C3	-2.31	105.50	110.14
6	K	1	NAG	C1-O5-C5	2.28	115.28	112.19
9	V	3	BMA	O2-C2-C3	-2.22	105.69	110.14
13	e	3	BMA	O2-C2-C3	-2.22	105.70	110.14
11	X	1	NAG	C8-C7-N2	2.22	119.85	116.10
14	f	8	GAL	O5-C5-C6	-2.16	103.81	107.20
9	V	8	MAN	C1-O5-C5	2.15	115.11	112.19
14	f	9	MAN	O2-C2-C3	-2.12	105.89	110.14
5	a	2	NAG	C1-O5-C5	2.11	115.06	112.19
10	W	7	MAN	C1-C2-C3	2.11	112.26	109.67
13	e	9	FUC	C1-O5-C5	2.09	117.50	112.78
10	W	6	GAL	O2-C2-C3	-2.07	106.00	110.14
8	i	3	BMA	O2-C2-C3	-2.04	106.05	110.14
8	R	3	BMA	O2-C2-C3	-2.03	106.06	110.14
14	f	7	NAG	C1-O5-C5	2.03	114.94	112.19
12	b	3	BMA	O2-C2-C3	-2.02	106.10	110.14

There are no chirality outliers.

All (130) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	a	2	NAG	C4-C5-C6-O6
5	Z	2	NAG	O5-C5-C6-O6
8	R	2	NAG	O5-C5-C6-O6
12	b	1	NAG	O5-C5-C6-O6
9	V	8	MAN	O5-C5-C6-O6
13	e	7	MAN	O5-C5-C6-O6
5	a	2	NAG	O5-C5-C6-O6
5	M	2	NAG	C4-C5-C6-O6
5	d	2	NAG	C4-C5-C6-O6
13	e	5	NAG	C4-C5-C6-O6
5	Y	2	NAG	C4-C5-C6-O6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	Q	2	NAG	O5-C5-C6-O6
7	P	4	MAN	O5-C5-C6-O6
12	b	4	MAN	O5-C5-C6-O6
5	d	1	NAG	O5-C5-C6-O6
10	W	7	MAN	O5-C5-C6-O6
13	e	2	NAG	O5-C5-C6-O6
12	b	1	NAG	C4-C5-C6-O6
13	e	5	NAG	O5-C5-C6-O6
5	T	1	NAG	C4-C5-C6-O6
5	Z	2	NAG	C4-C5-C6-O6
5	T	1	NAG	O5-C5-C6-O6
5	g	1	NAG	O5-C5-C6-O6
6	K	1	NAG	O5-C5-C6-O6
5	N	2	NAG	C4-C5-C6-O6
8	R	2	NAG	C4-C5-C6-O6
10	W	2	NAG	C4-C5-C6-O6
5	M	2	NAG	O5-C5-C6-O6
5	d	2	NAG	O5-C5-C6-O6
5	h	2	NAG	O5-C5-C6-O6
5	N	2	NAG	O5-C5-C6-O6
10	W	2	NAG	O5-C5-C6-O6
5	S	2	NAG	O5-C5-C6-O6
9	V	8	MAN	C4-C5-C6-O6
13	e	7	MAN	C4-C5-C6-O6
5	O	1	NAG	C4-C5-C6-O6
14	f	2	NAG	O5-C5-C6-O6
5	h	2	NAG	C4-C5-C6-O6
13	e	2	NAG	C4-C5-C6-O6
8	R	1	NAG	O5-C5-C6-O6
10	W	7	MAN	C4-C5-C6-O6
12	b	4	MAN	C4-C5-C6-O6
5	T	2	NAG	C8-C7-N2-C2
5	T	2	NAG	O7-C7-N2-C2
5	Z	1	NAG	C8-C7-N2-C2
5	Z	1	NAG	O7-C7-N2-C2
5	Z	2	NAG	C8-C7-N2-C2
5	Z	2	NAG	O7-C7-N2-C2
11	X	1	NAG	C8-C7-N2-C2
11	X	1	NAG	O7-C7-N2-C2
11	c	1	NAG	C8-C7-N2-C2
11	c	1	NAG	O7-C7-N2-C2
12	b	2	NAG	C8-C7-N2-C2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
12	b	2	NAG	O7-C7-N2-C2
14	f	2	NAG	C8-C7-N2-C2
14	f	2	NAG	O7-C7-N2-C2
5	d	1	NAG	C4-C5-C6-O6
5	g	1	NAG	C4-C5-C6-O6
5	Y	2	NAG	O5-C5-C6-O6
5	Q	2	NAG	C4-C5-C6-O6
11	X	1	NAG	C4-C5-C6-O6
5	Z	1	NAG	O5-C5-C6-O6
12	b	5	MAN	O5-C5-C6-O6
13	e	4	MAN	O5-C5-C6-O6
14	f	8	GAL	O5-C5-C6-O6
8	R	1	NAG	C4-C5-C6-O6
5	O	1	NAG	O5-C5-C6-O6
7	P	4	MAN	C4-C5-C6-O6
14	f	3	BMA	C4-C5-C6-O6
5	S	2	NAG	C4-C5-C6-O6
7	P	2	NAG	C4-C5-C6-O6
8	i	2	NAG	O5-C5-C6-O6
9	V	3	BMA	O5-C5-C6-O6
5	M	1	NAG	C4-C5-C6-O6
5	O	2	NAG	C4-C5-C6-O6
7	P	2	NAG	O5-C5-C6-O6
12	b	3	BMA	C4-C5-C6-O6
5	N	1	NAG	O5-C5-C6-O6
5	a	1	NAG	O5-C5-C6-O6
11	X	1	NAG	O5-C5-C6-O6
5	J	2	NAG	C4-C5-C6-O6
13	e	8	NAG	O5-C5-C6-O6
5	O	2	NAG	O5-C5-C6-O6
7	P	3	BMA	O5-C5-C6-O6
14	f	9	MAN	O5-C5-C6-O6
9	V	7	NAG	C4-C5-C6-O6
5	Z	1	NAG	C4-C5-C6-O6
5	S	1	NAG	C4-C5-C6-O6
11	c	1	NAG	C4-C5-C6-O6
6	K	2	NAG	O5-C5-C6-O6
14	f	8	GAL	C4-C5-C6-O6
8	R	3	BMA	O5-C5-C6-O6
10	W	5	NAG	O5-C5-C6-O6
9	V	3	BMA	C4-C5-C6-O6
8	i	3	BMA	O5-C5-C6-O6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	M	1	NAG	O5-C5-C6-O6
14	f	3	BMA	O5-C5-C6-O6
13	e	1	NAG	O5-C5-C6-O6
5	J	2	NAG	O5-C5-C6-O6
14	f	2	NAG	C4-C5-C6-O6
6	K	1	NAG	C4-C5-C6-O6
5	Y	1	NAG	O5-C5-C6-O6
5	S	1	NAG	O5-C5-C6-O6
9	V	7	NAG	O5-C5-C6-O6
13	e	3	BMA	O5-C5-C6-O6
9	V	6	GAL	C4-C5-C6-O6
11	c	1	NAG	O5-C5-C6-O6
12	b	3	BMA	O5-C5-C6-O6
5	J	1	NAG	C3-C2-N2-C7
6	K	2	NAG	C3-C2-N2-C7
14	f	7	NAG	C4-C5-C6-O6
14	f	5	NAG	O5-C5-C6-O6
5	a	1	NAG	C4-C5-C6-O6
8	i	2	NAG	C4-C5-C6-O6
9	V	6	GAL	O5-C5-C6-O6
5	Q	1	NAG	C4-C5-C6-O6
5	g	2	NAG	C4-C5-C6-O6
12	b	2	NAG	C4-C5-C6-O6
5	J	1	NAG	C1-C2-N2-C7
5	O	1	NAG	C3-C2-N2-C7
5	S	2	NAG	C3-C2-N2-C7
5	T	1	NAG	C3-C2-N2-C7
5	U	1	NAG	C3-C2-N2-C7
5	U	2	NAG	C3-C2-N2-C7
5	a	1	NAG	C3-C2-N2-C7
5	d	1	NAG	C3-C2-N2-C7
5	d	2	NAG	C3-C2-N2-C7
9	V	2	NAG	C3-C2-N2-C7
9	V	7	NAG	C3-C2-N2-C7
11	X	1	NAG	C3-C2-N2-C7

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	W	6	GAL	1	0
7	P	4	MAN	2	0

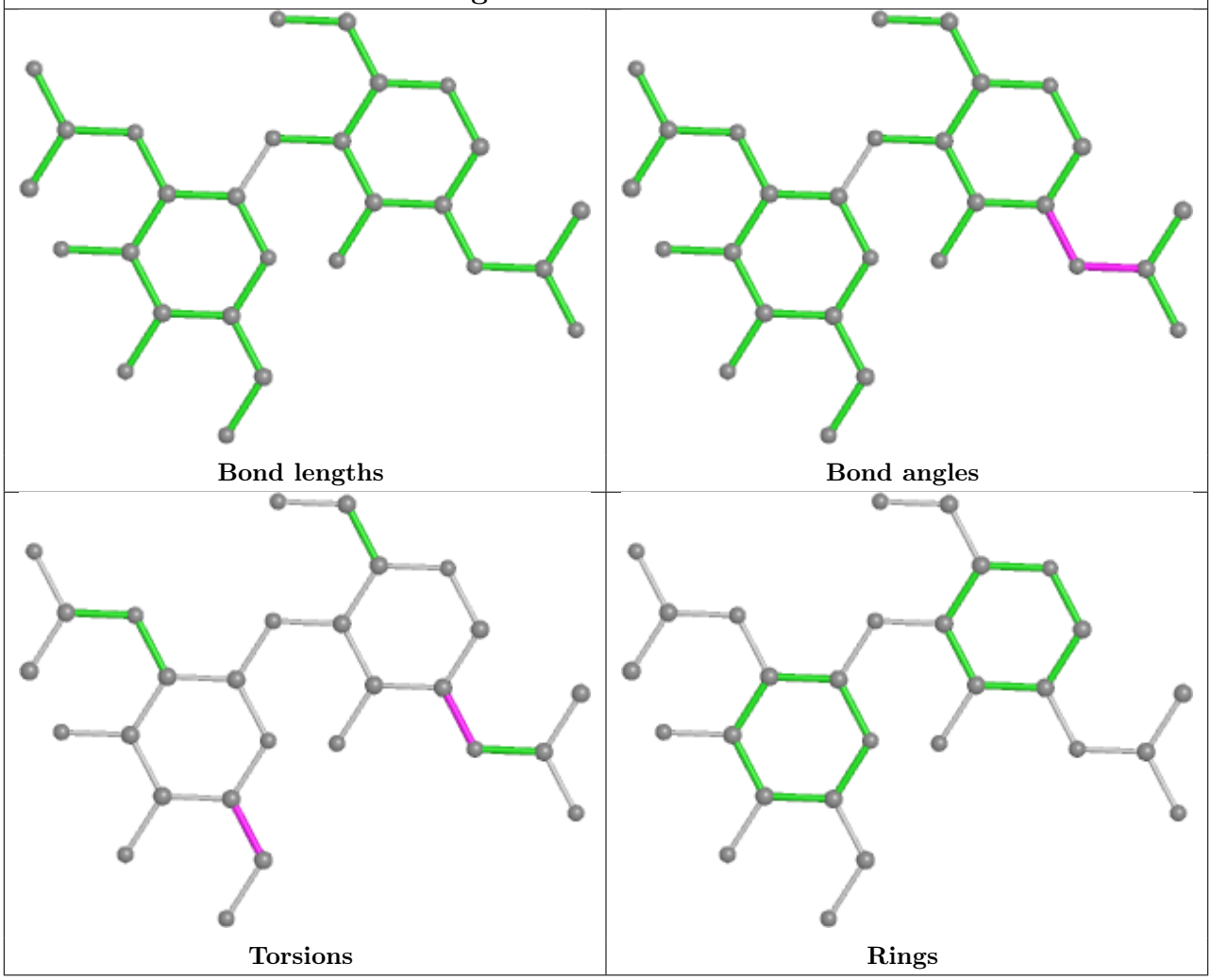
Continued on next page...

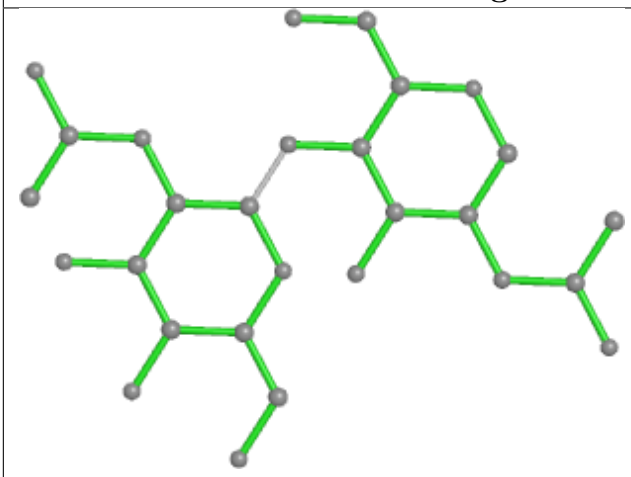
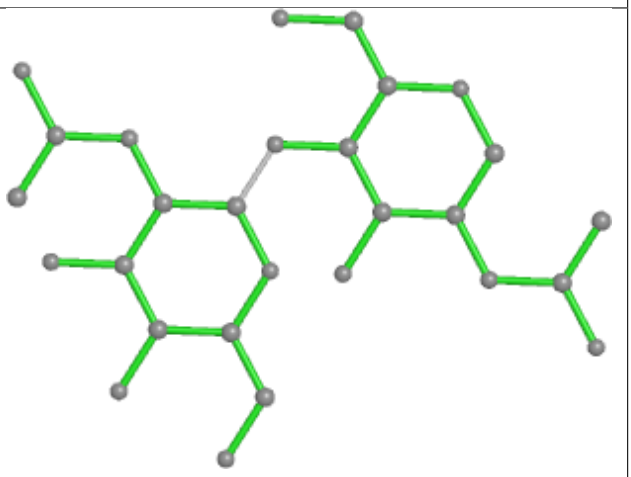
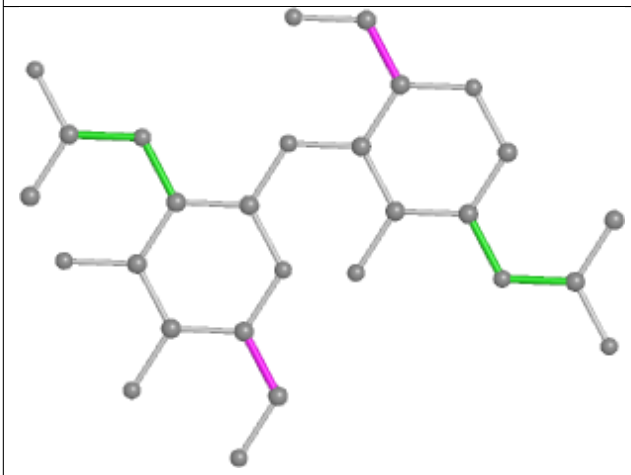
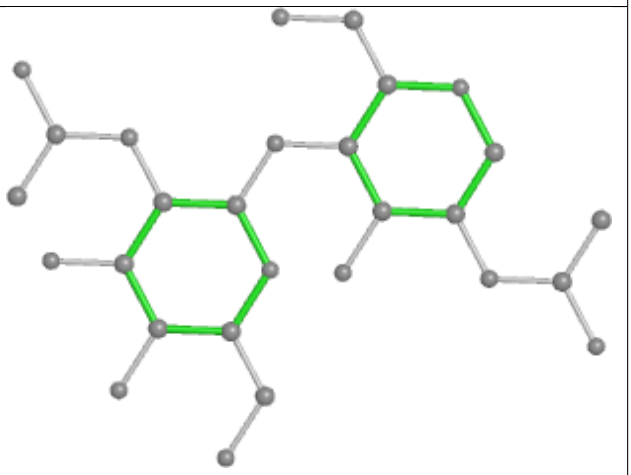
Continued from previous page...

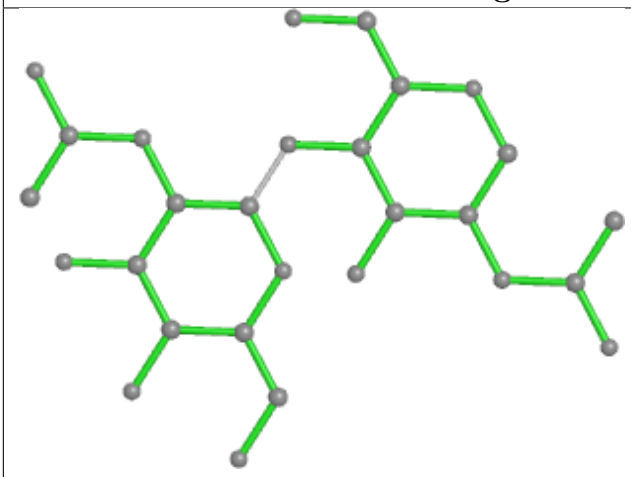
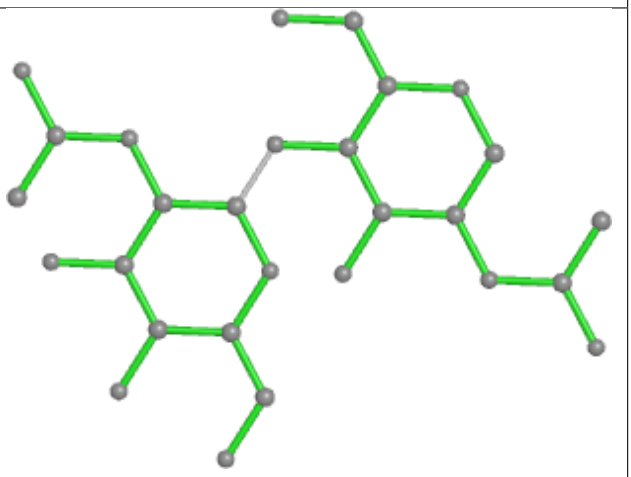
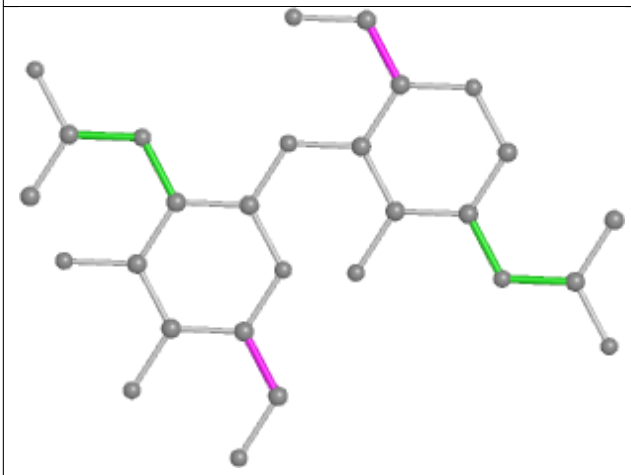
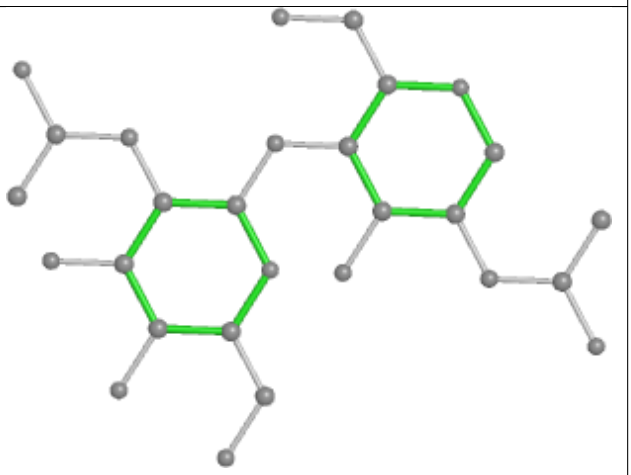
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	U	1	NAG	1	0
5	Z	1	NAG	1	0

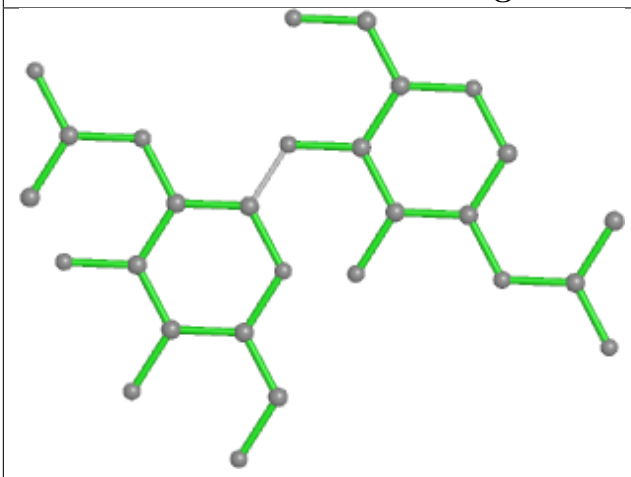
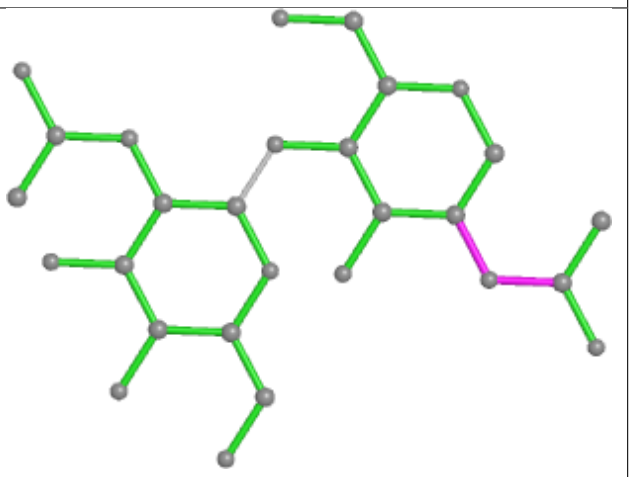
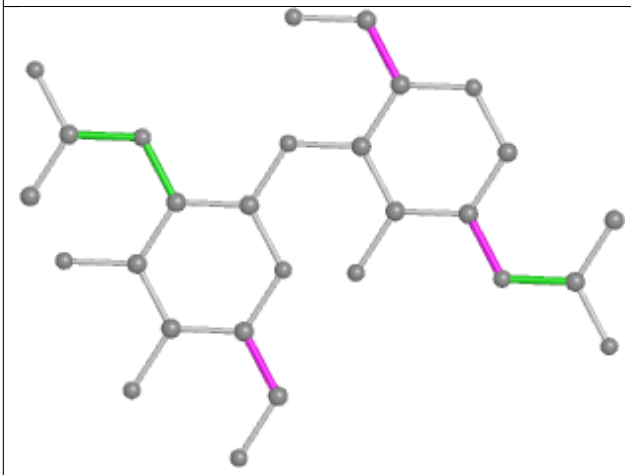
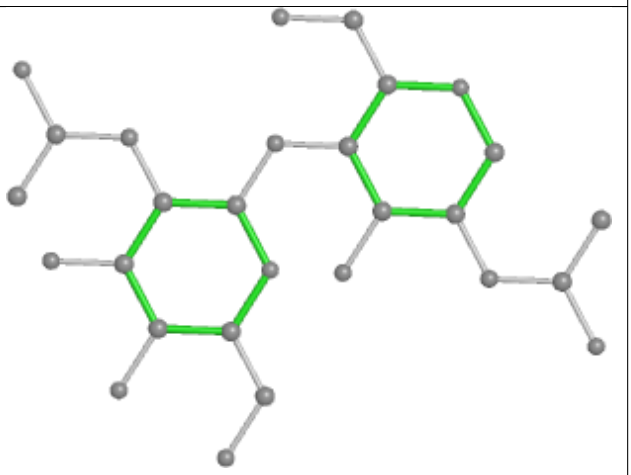
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

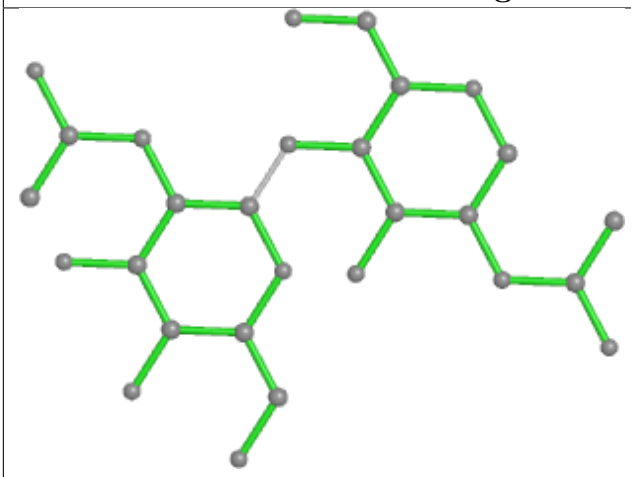
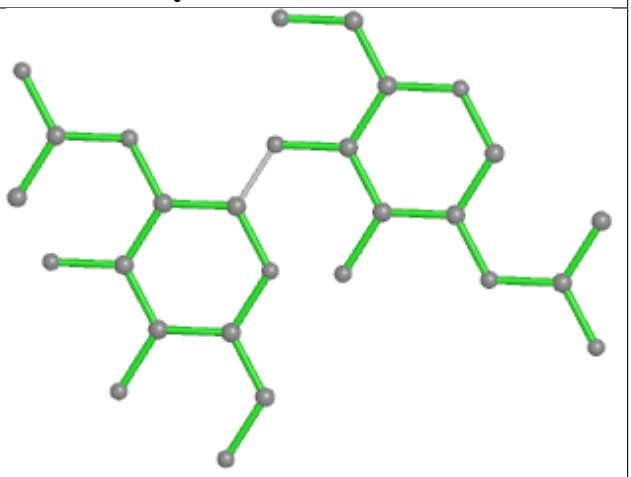
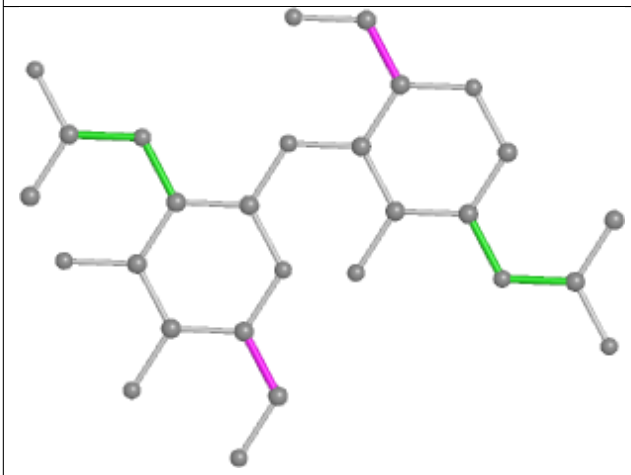
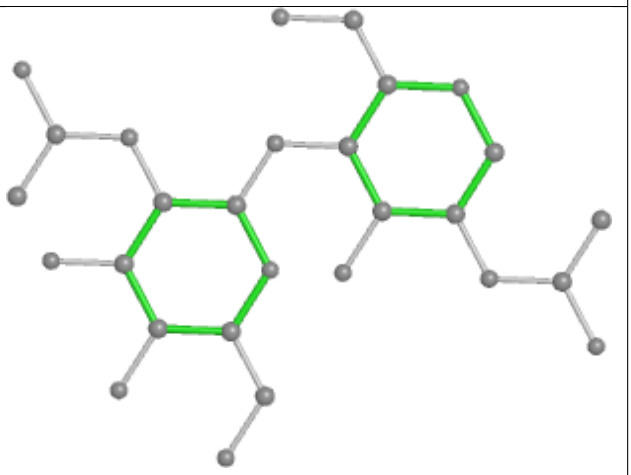
Oligosaccharide Chain J



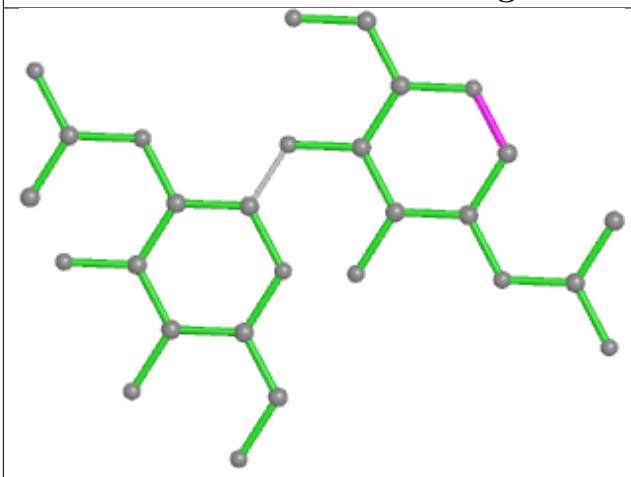
Oligosaccharide Chain M	
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain N	
 Bond lengths	 Bond angles
 Torsions	 Rings

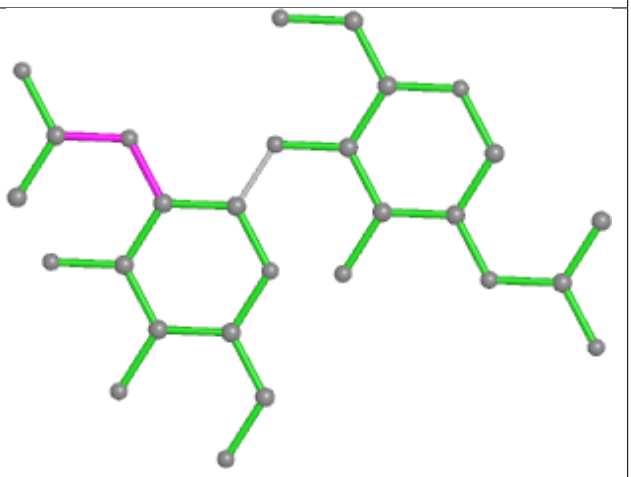
Oligosaccharide Chain O	
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain Q	
 Bond lengths	 Bond angles
 Torsions	 Rings

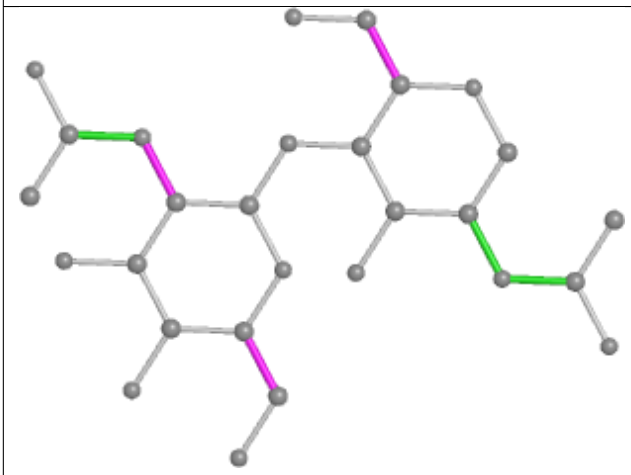
Oligosaccharide Chain S



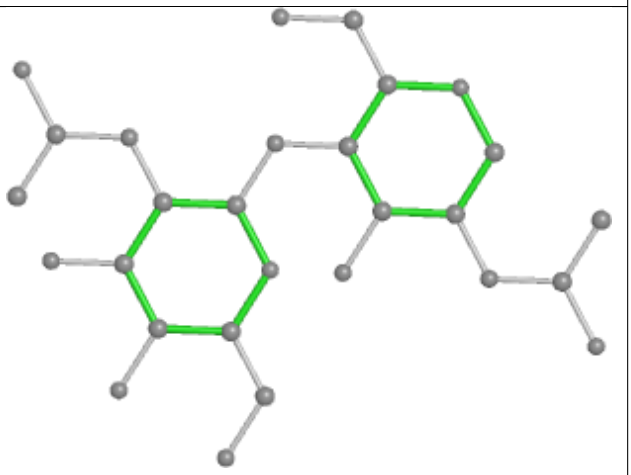
Bond lengths



Bond angles

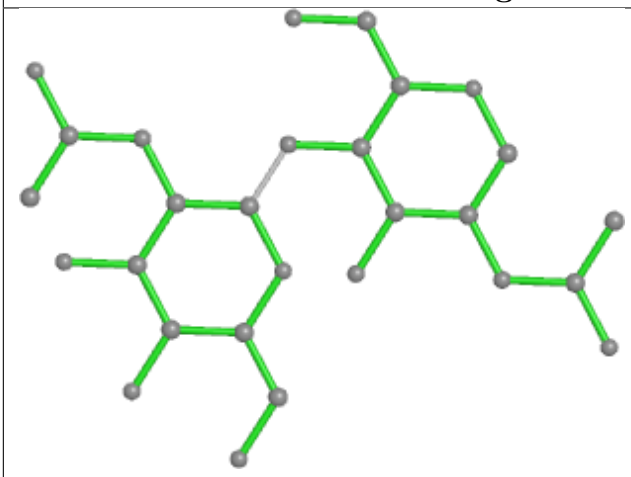


Torsions

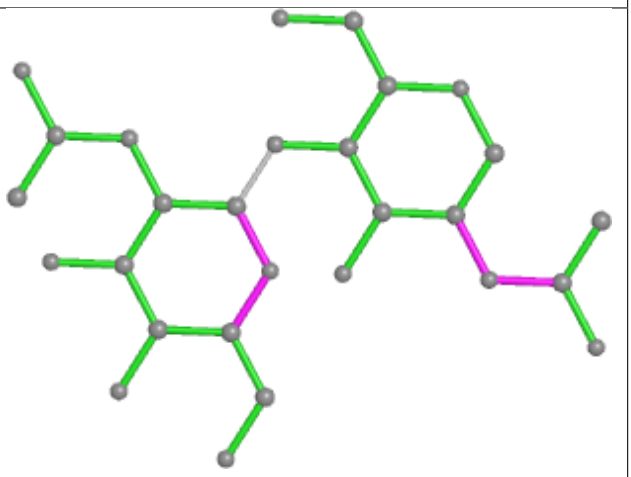


Rings

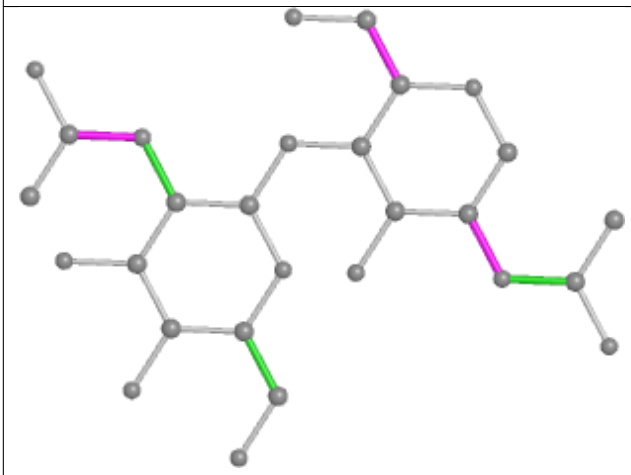
Oligosaccharide Chain T



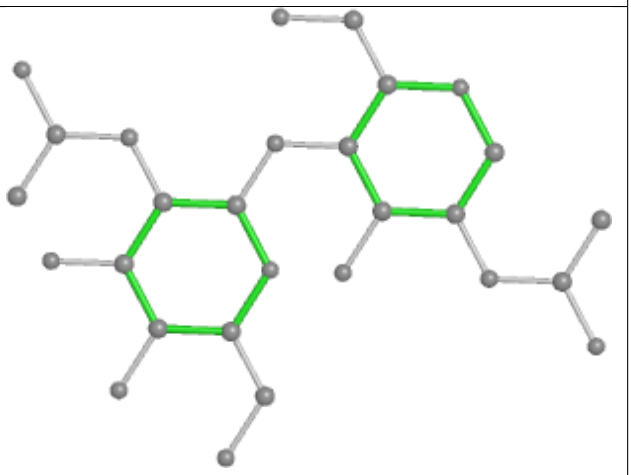
Bond lengths



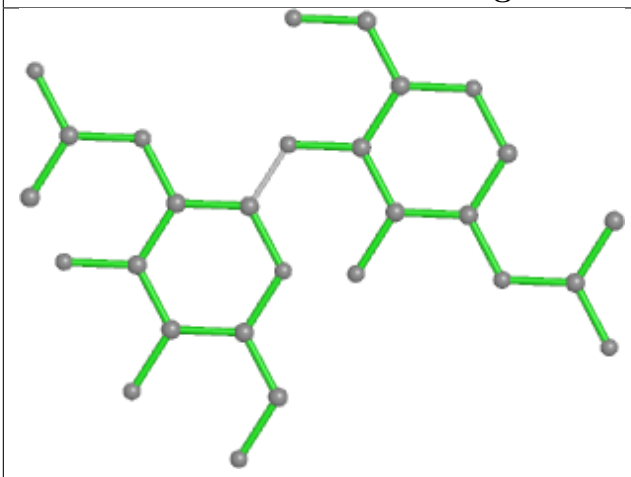
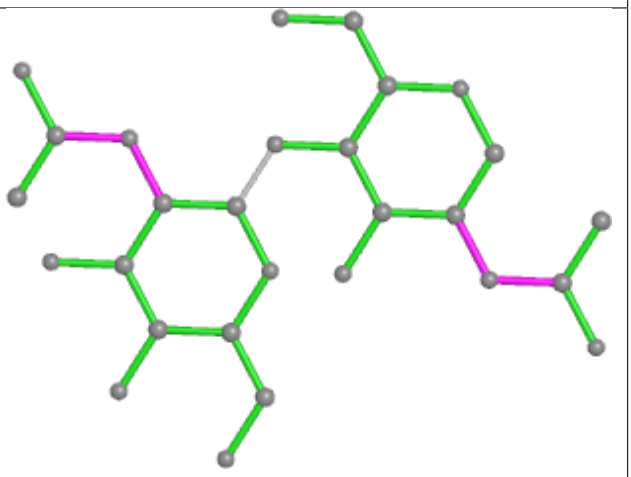
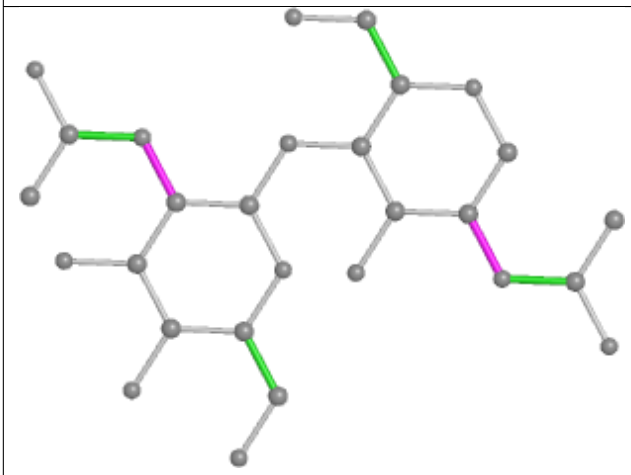
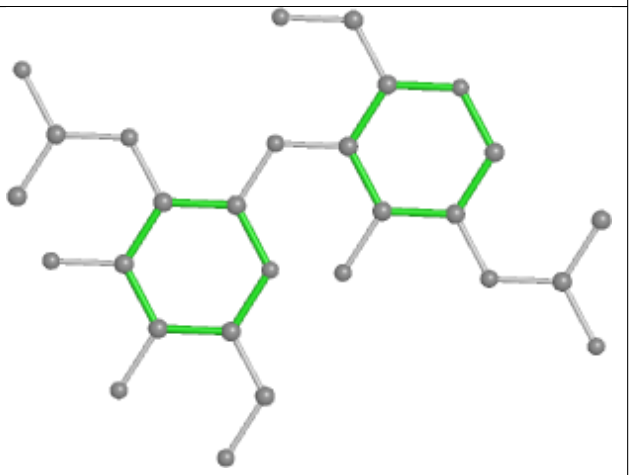
Bond angles

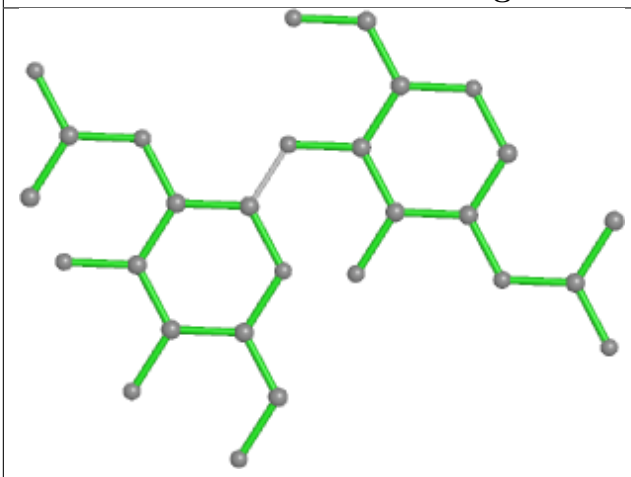
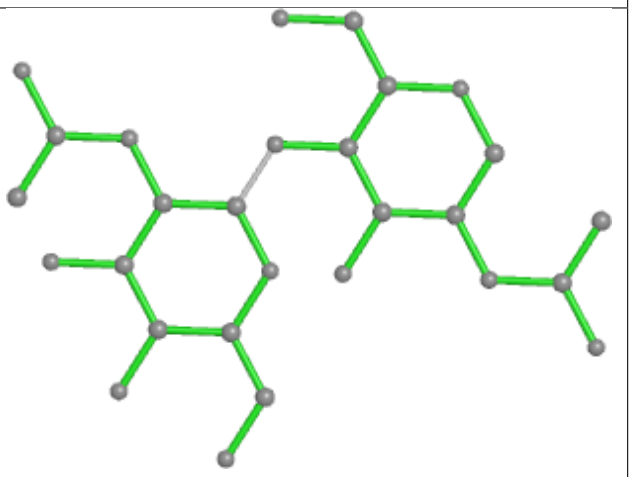
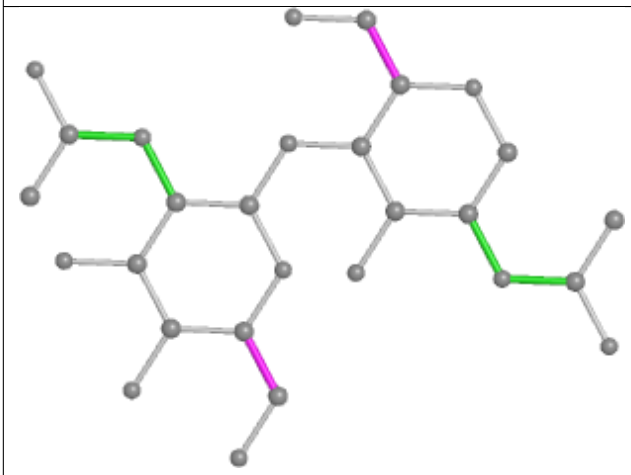
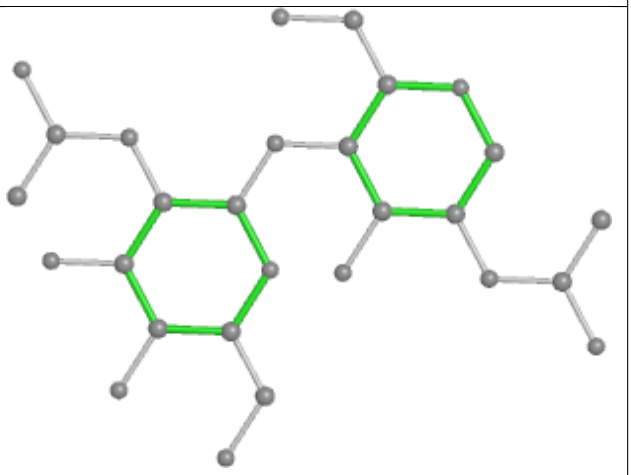


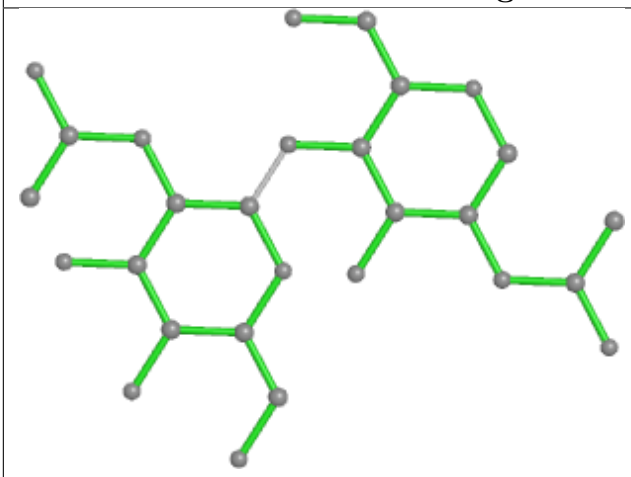
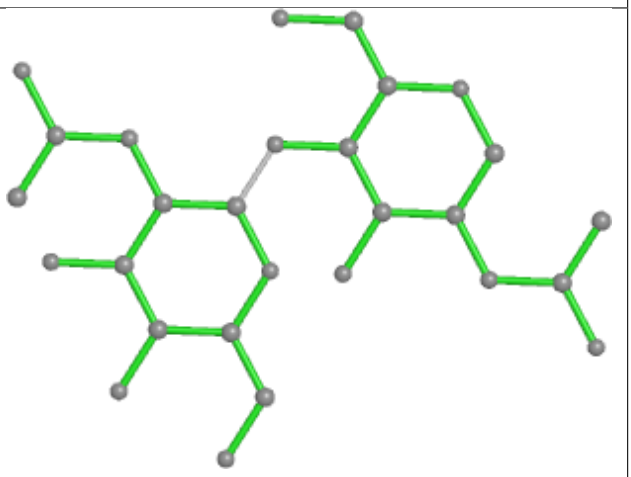
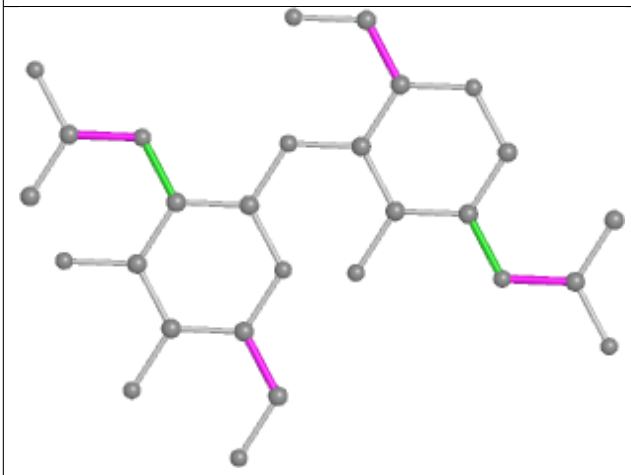
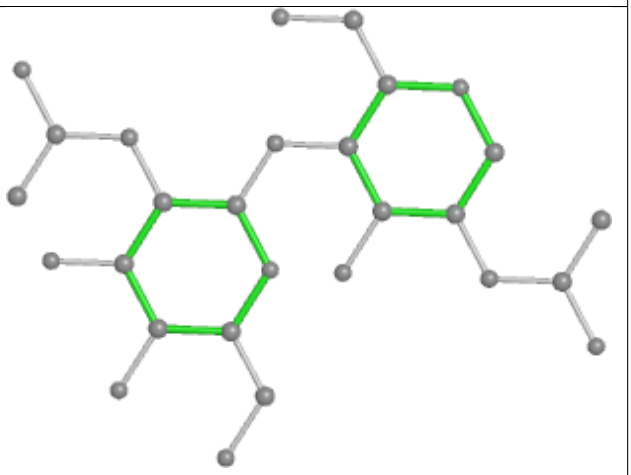
Torsions



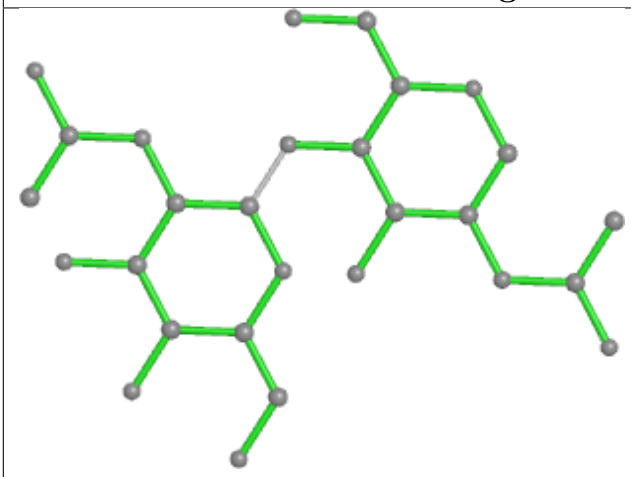
Rings

Oligosaccharide Chain U	
 Bond lengths	 Bond angles
 Torsions	 Rings

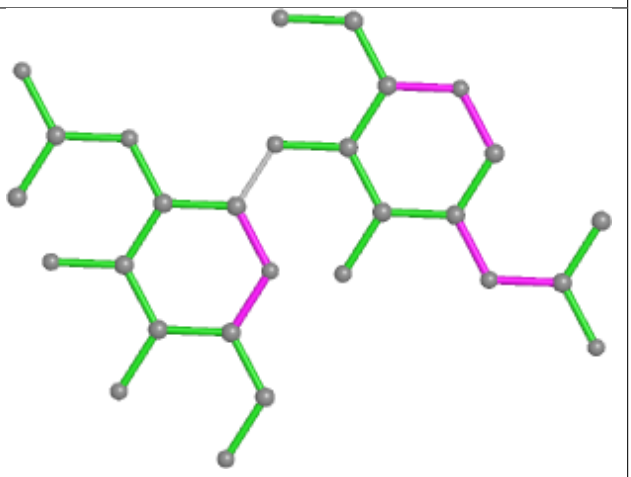
Oligosaccharide Chain Y	
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain Z	
 Bond lengths	 Bond angles
 Torsions	 Rings

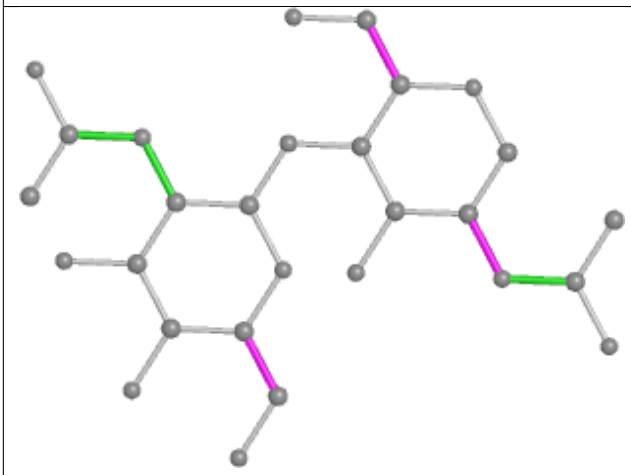
Oligosaccharide Chain a



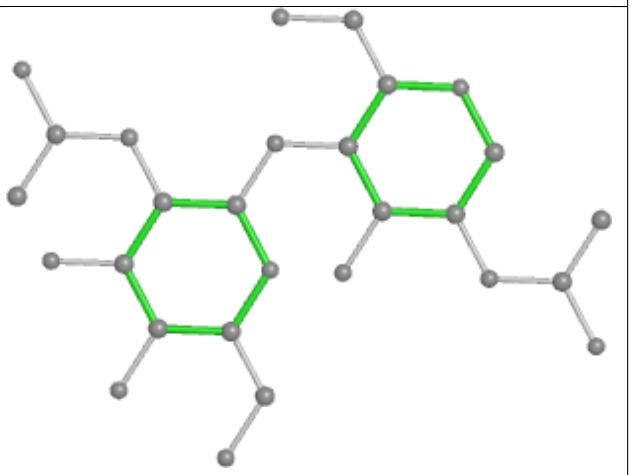
Bond lengths



Bond angles

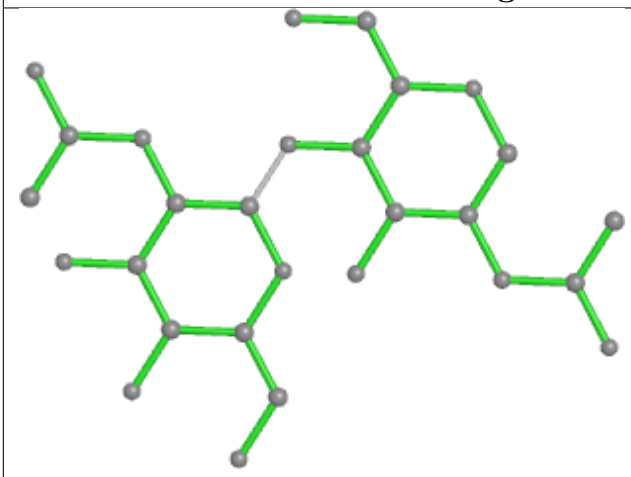


Torsions

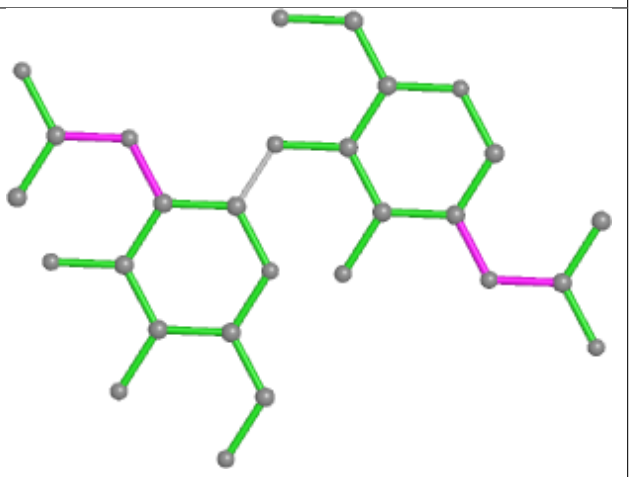


Rings

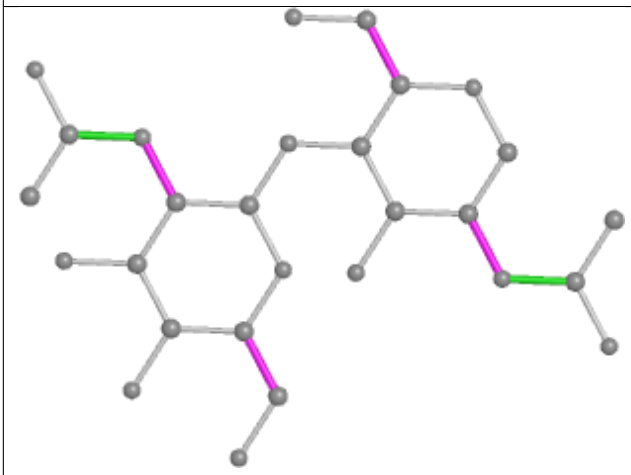
Oligosaccharide Chain d



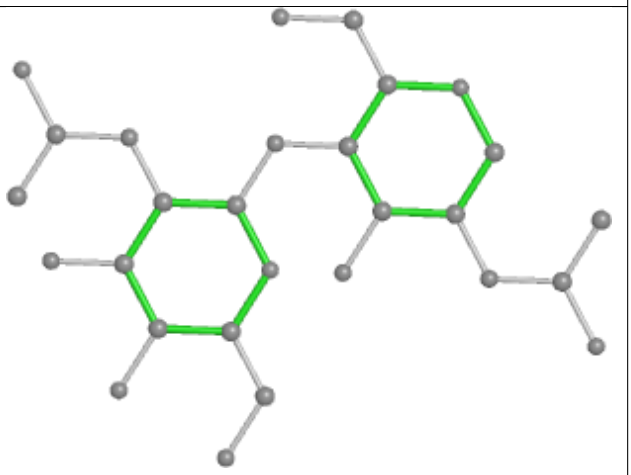
Bond lengths



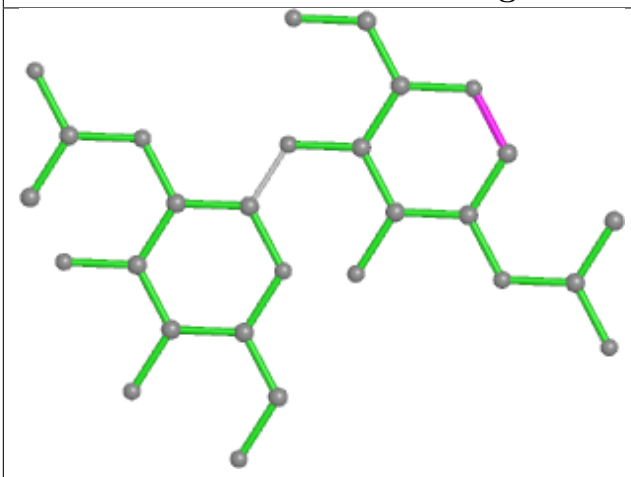
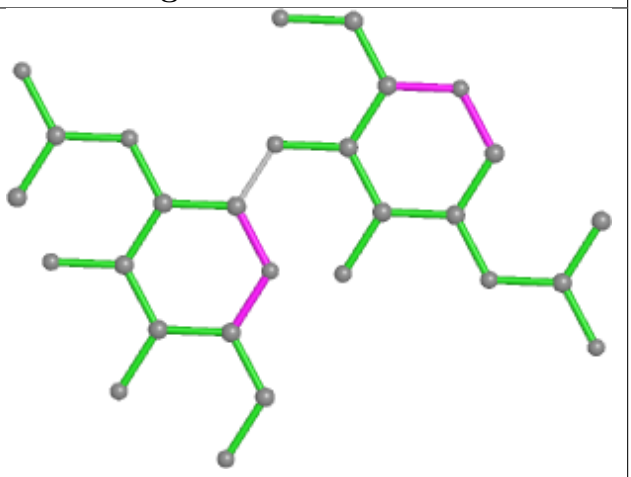
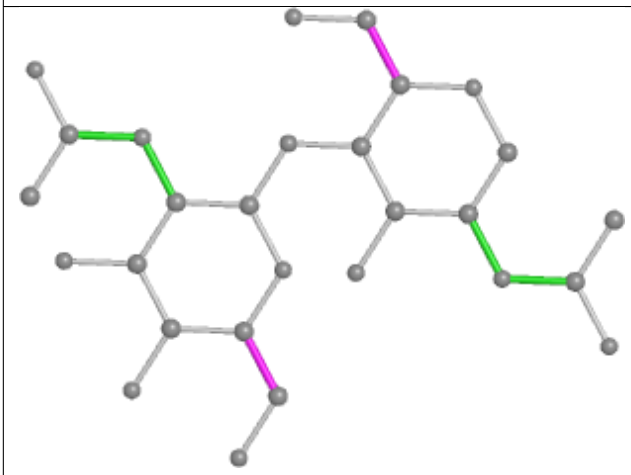
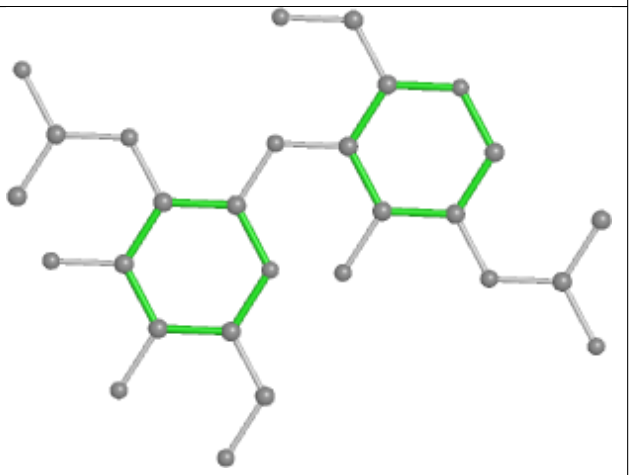
Bond angles

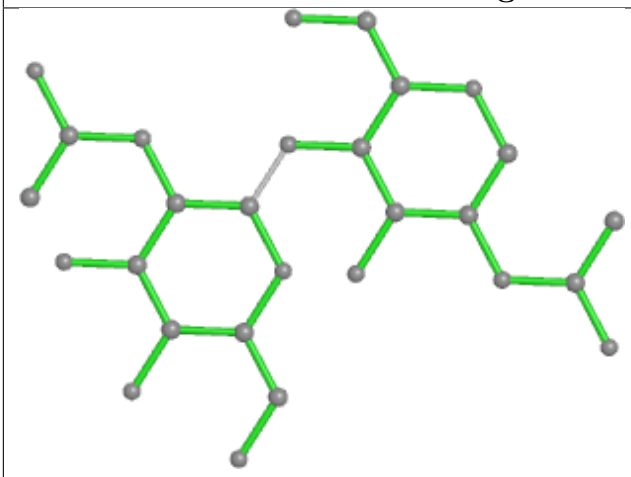
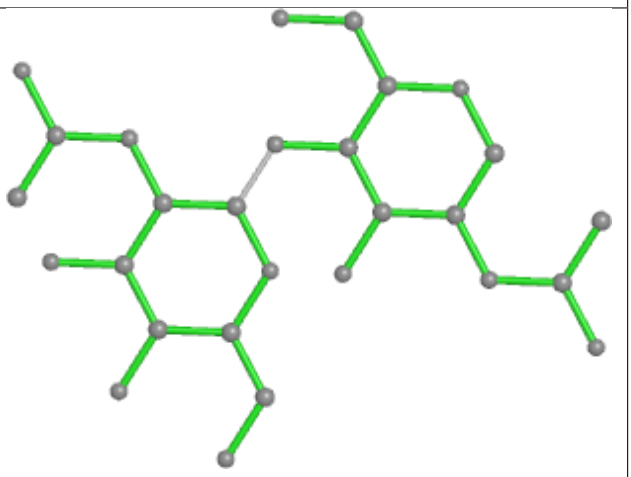
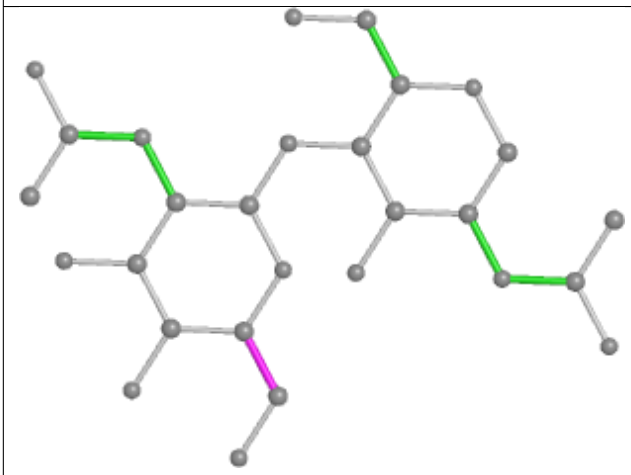
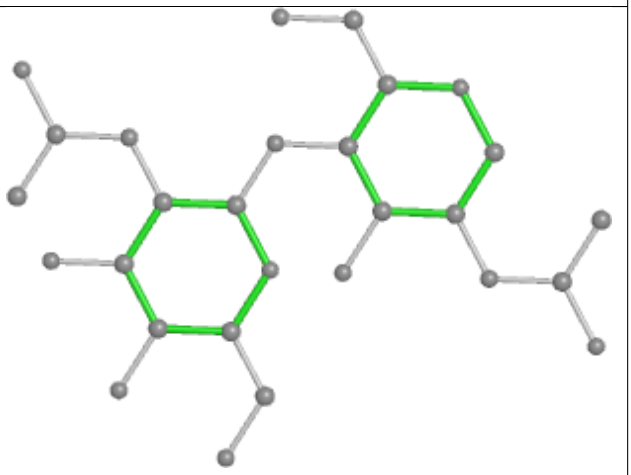


Torsions

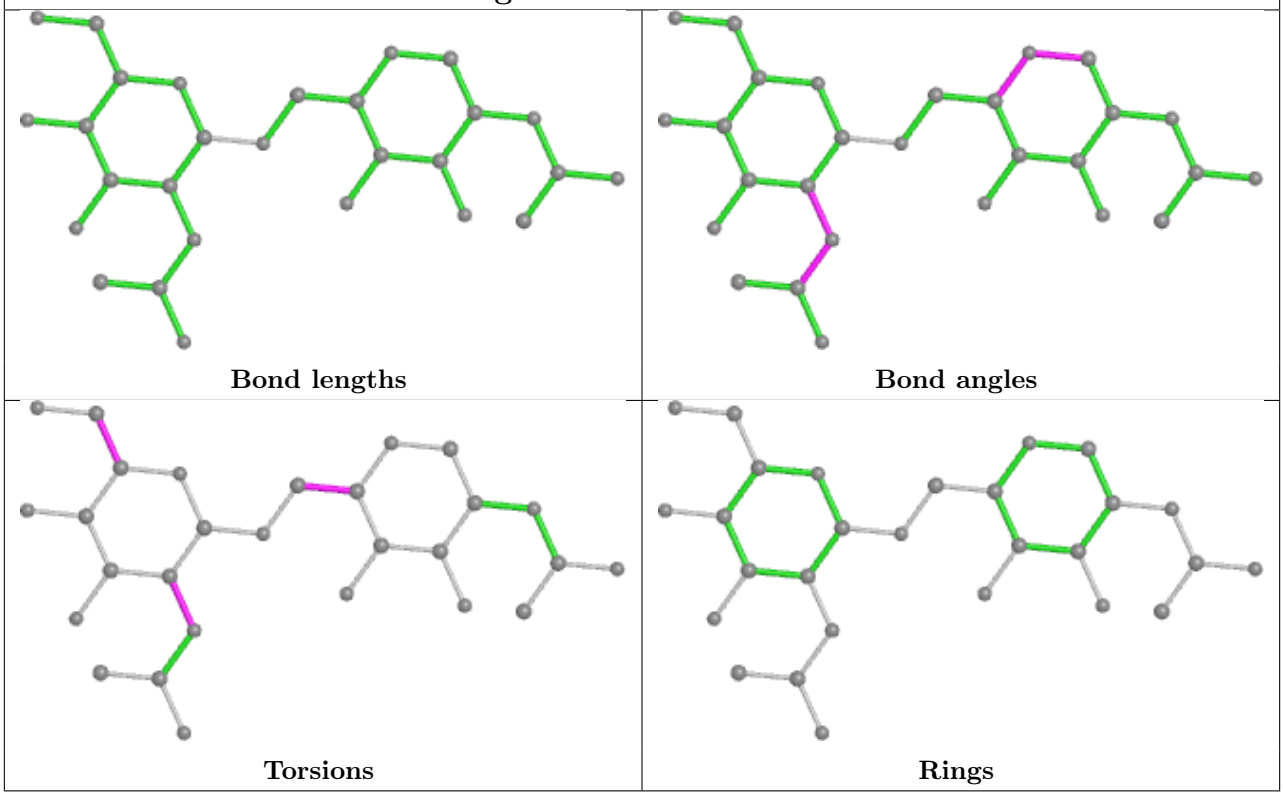


Rings

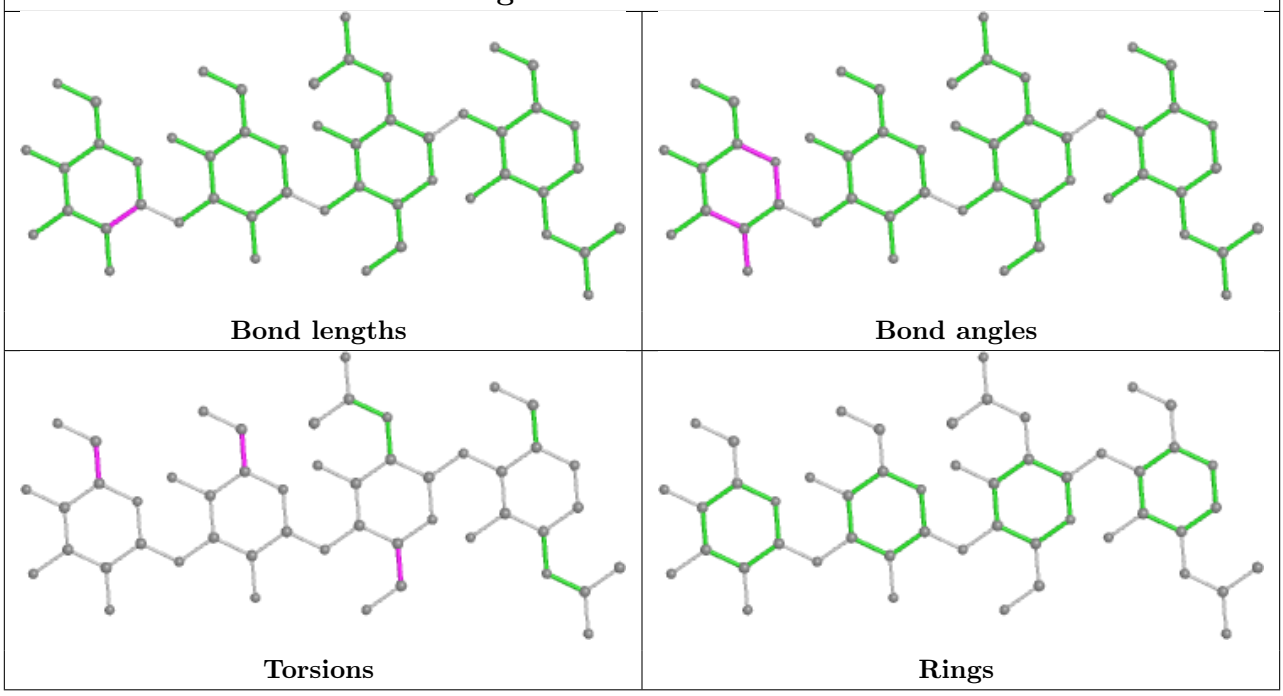
Oligosaccharide Chain g	
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain h	
 Bond lengths	 Bond angles
 Torsions	 Rings

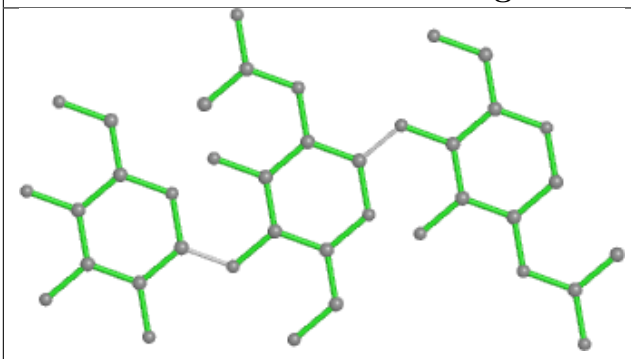
Oligosaccharide Chain K



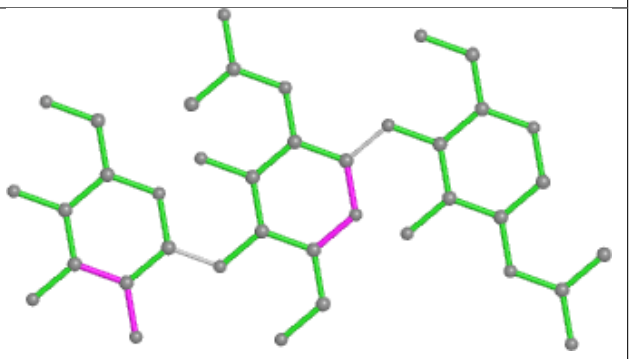
Oligosaccharide Chain P



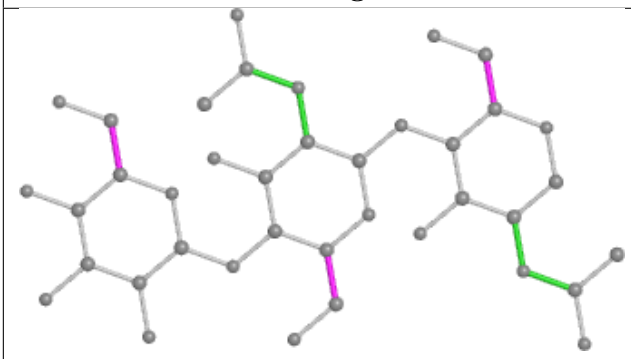
Oligosaccharide Chain R



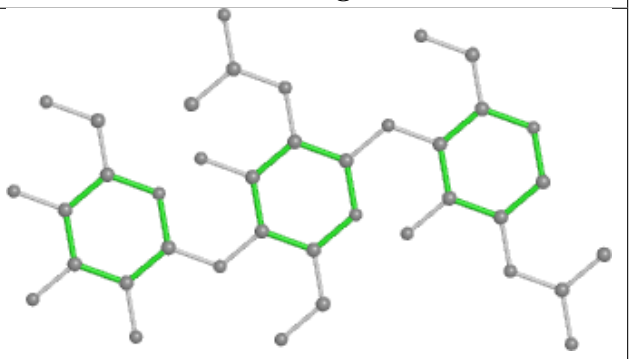
Bond lengths



Bond angles

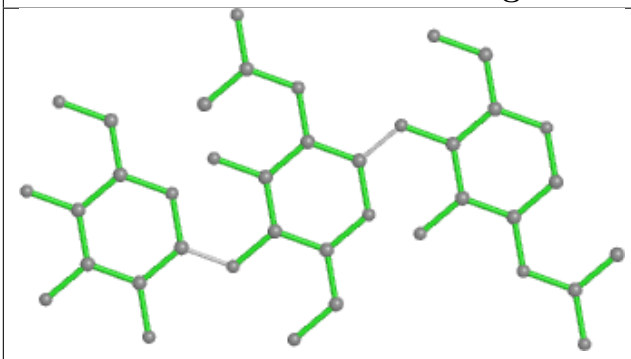


Torsions

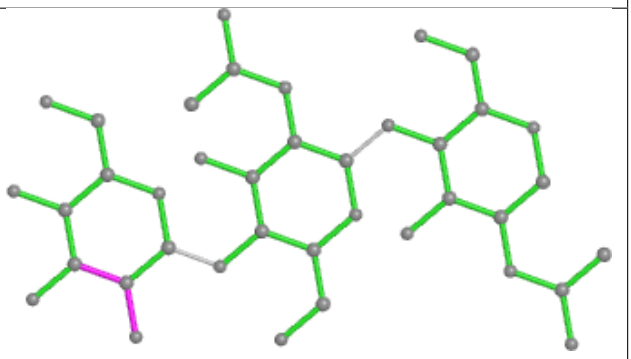


Rings

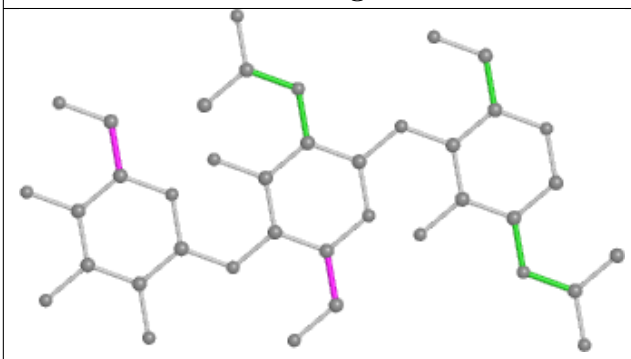
Oligosaccharide Chain i



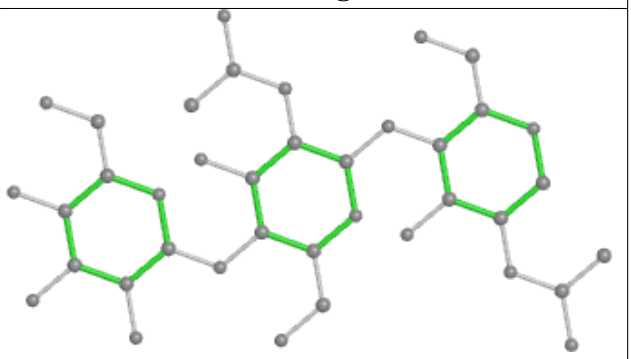
Bond lengths



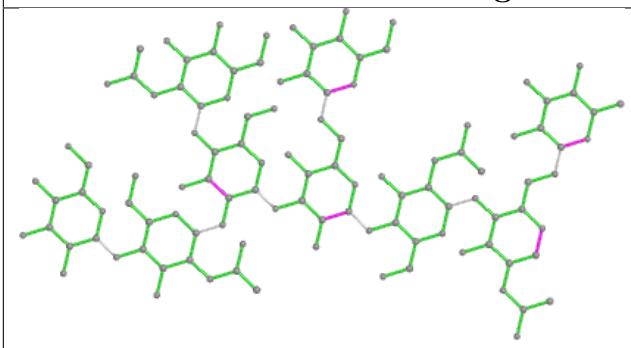
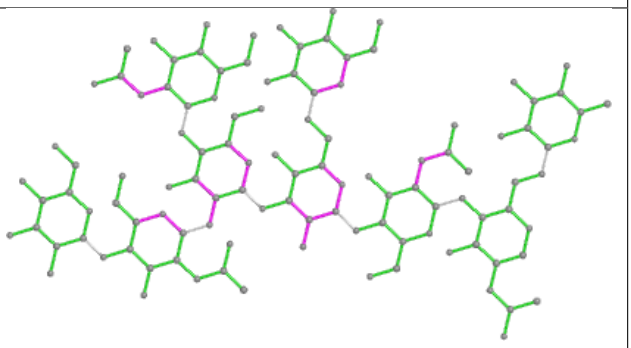
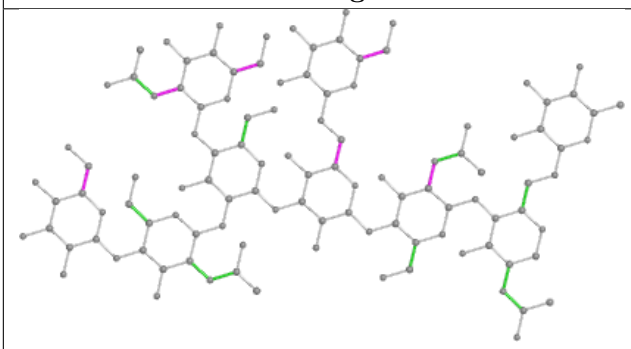
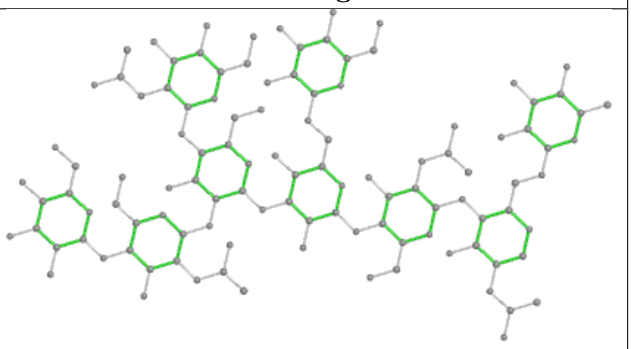
Bond angles



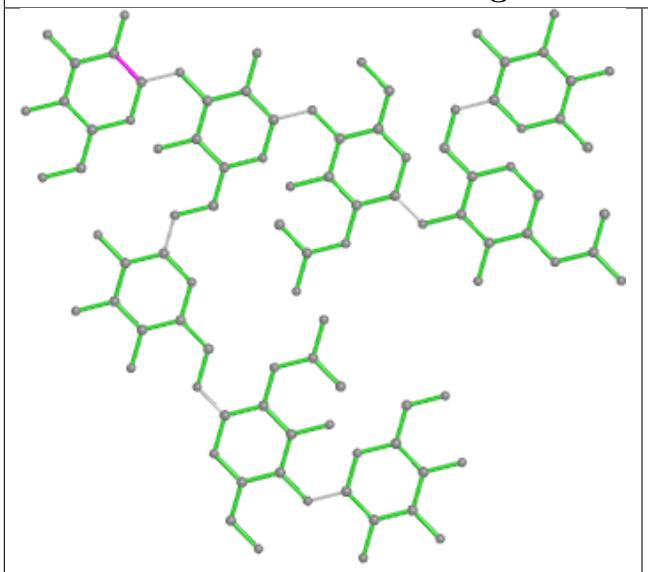
Torsions



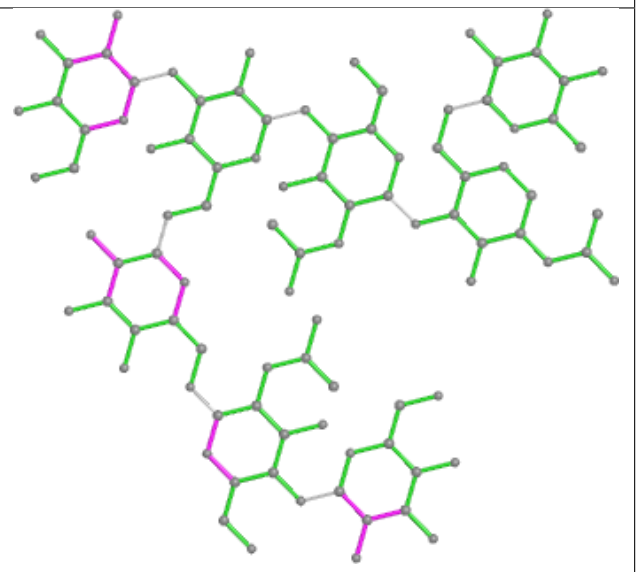
Rings

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

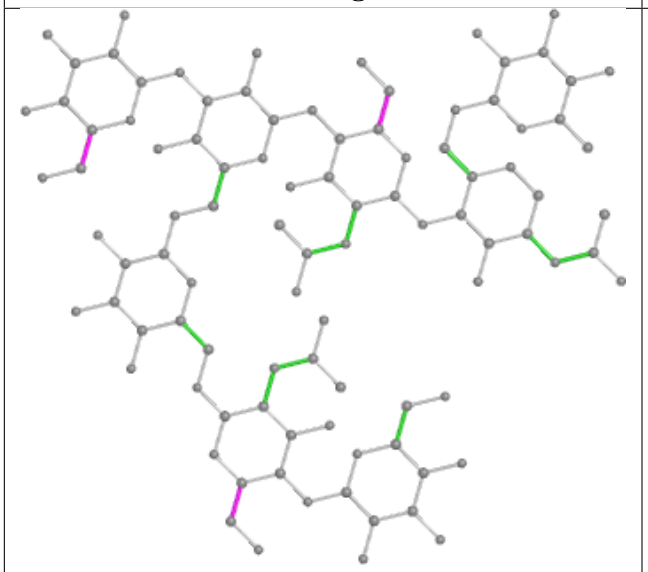
Oligosaccharide Chain W



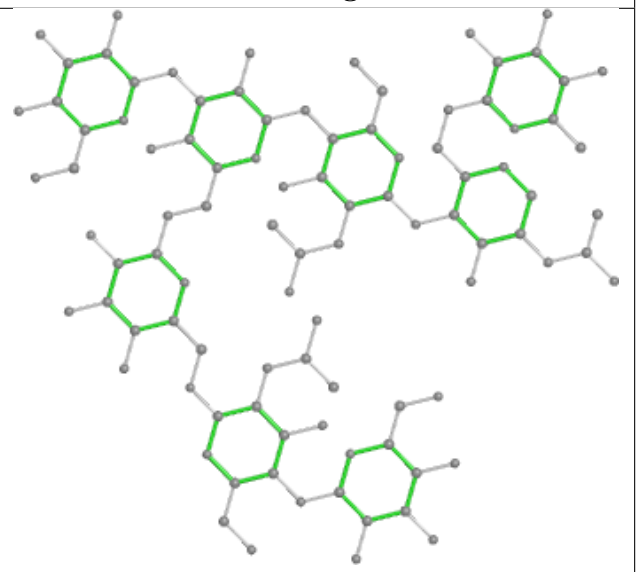
Bond lengths



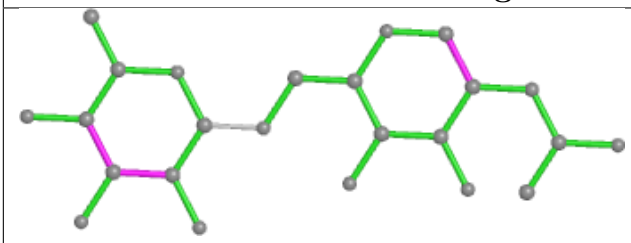
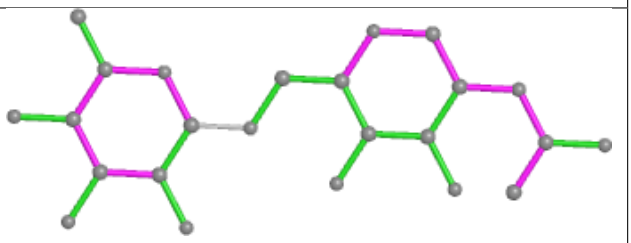
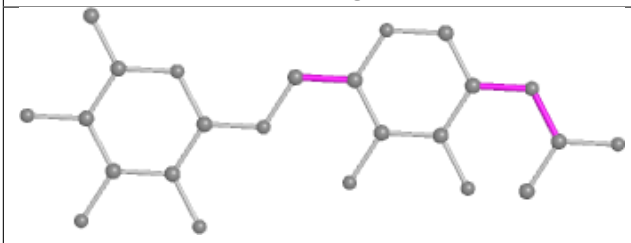
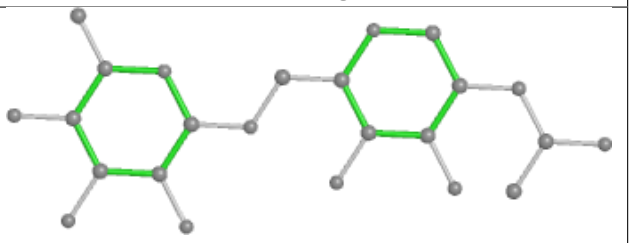
Bond angles

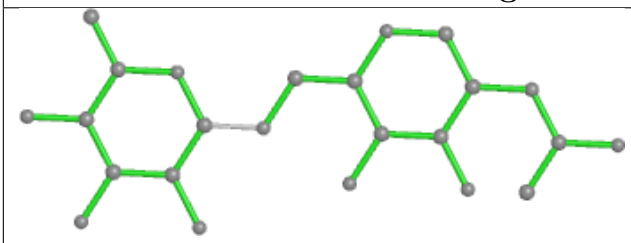
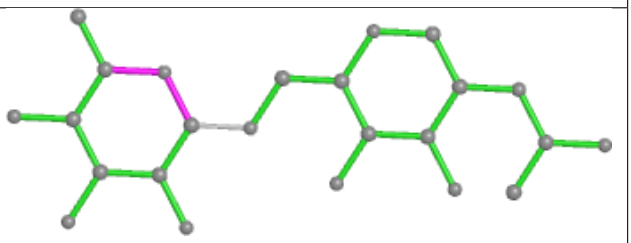
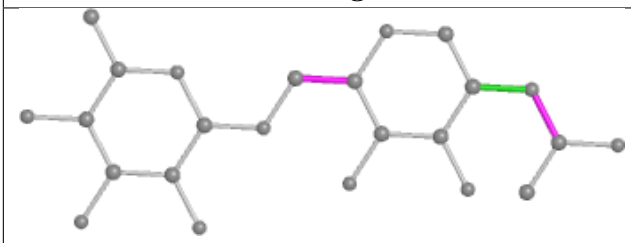
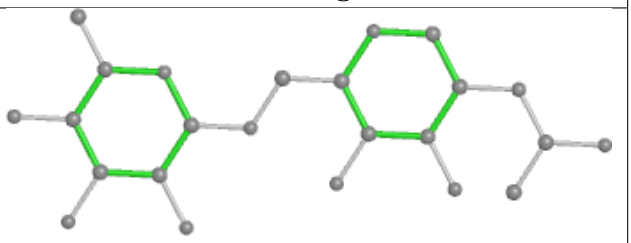


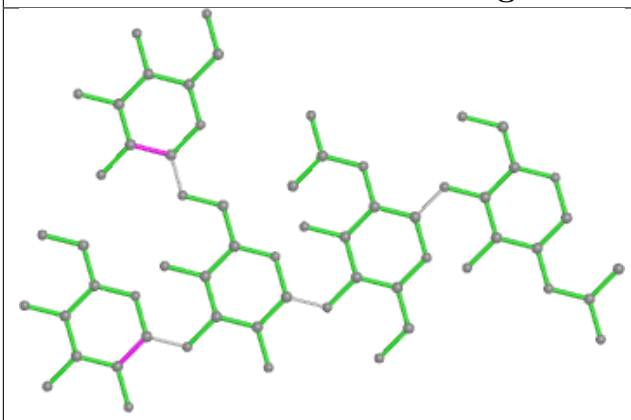
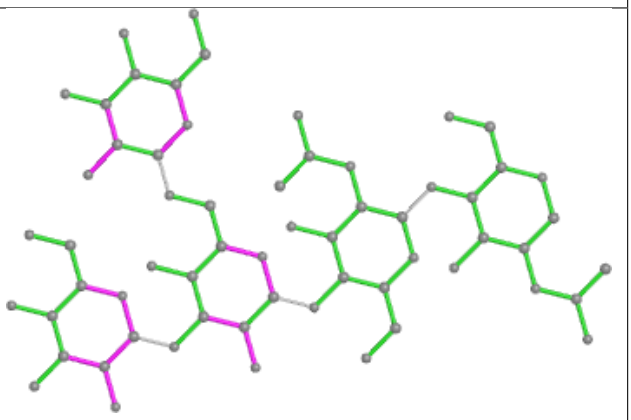
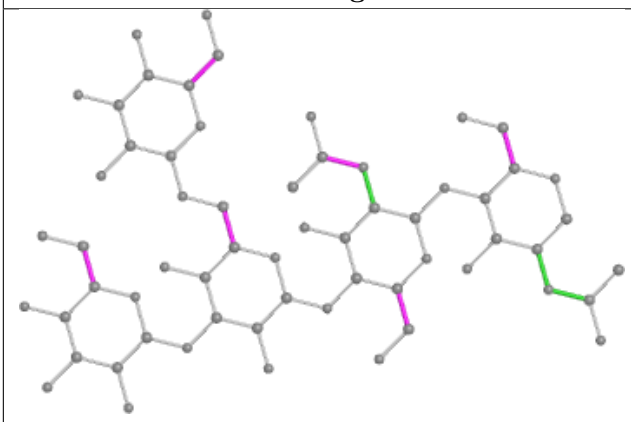
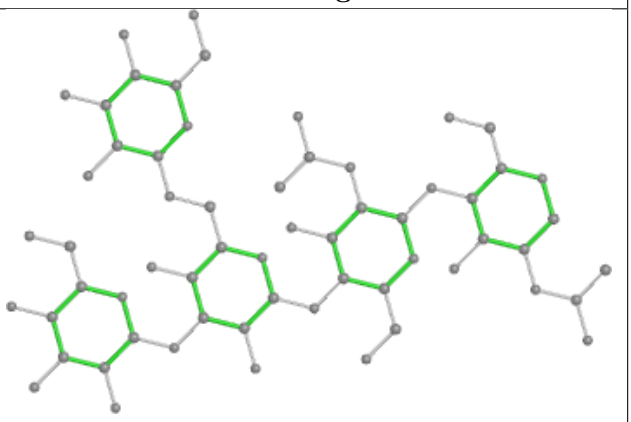
Torsions

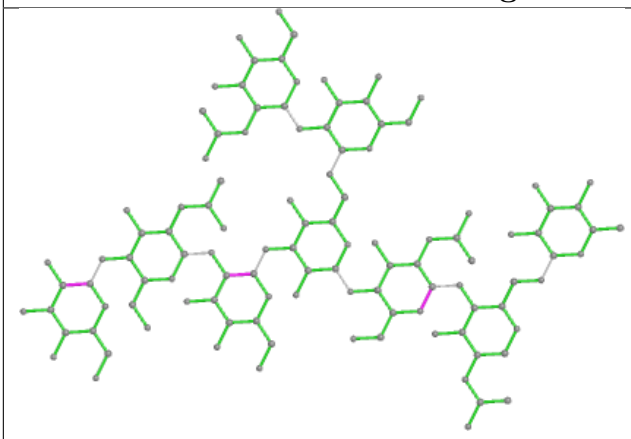
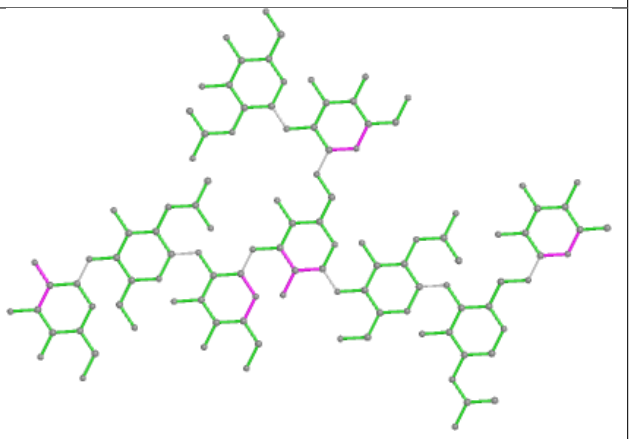
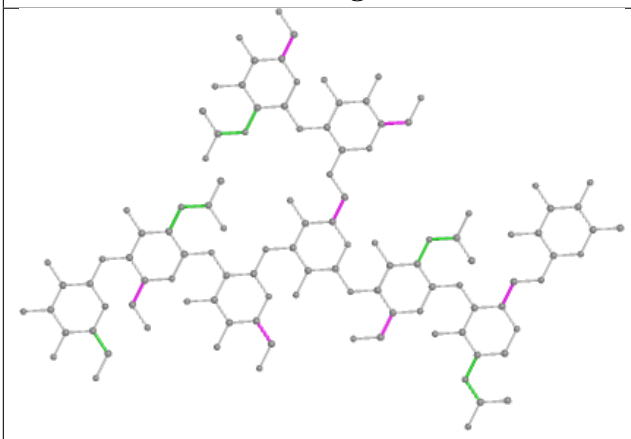
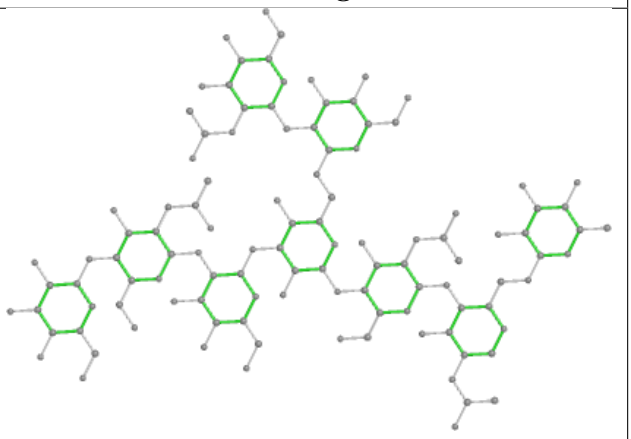


Rings

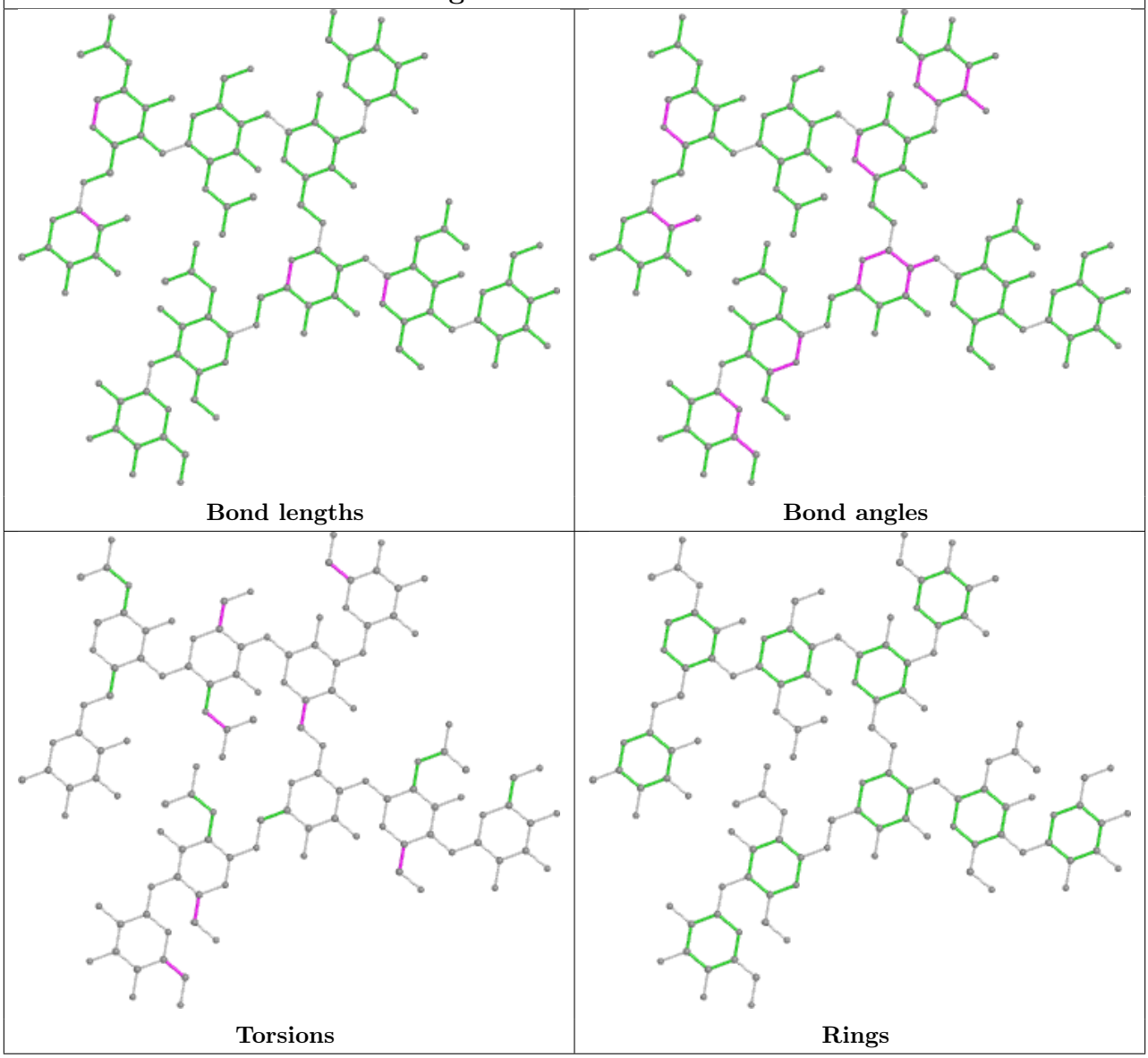
Oligosaccharide Chain X	
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain c	
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain b	
 Bond lengths	 Bond angles
 Torsions	 Rings

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

Oligosaccharide Chain f



5.6 Ligand geometry (i)

41 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	$\#\|Z\| > 2$
15	NAG	E	612	1	14,14,15	0.78	1 (7%)	17,19,21	2.24	3 (17%)
15	NAG	E	614	1	14,14,15	0.37	0	17,19,21	0.50	0
15	NAG	F	901	2	14,14,15	0.20	0	17,19,21	0.67	1 (5%)
15	NAG	F	903	2	14,14,15	0.43	0	17,19,21	0.83	1 (5%)
15	NAG	F	902	2	14,14,15	0.34	0	17,19,21	0.38	0
15	NAG	C	627	1	14,14,15	0.32	0	17,19,21	0.53	0
15	NAG	C	624	1	14,14,15	0.68	1 (7%)	17,19,21	0.89	1 (5%)
15	NAG	C	622	1	14,14,15	0.26	0	17,19,21	0.44	0
15	NAG	C	606	1	14,14,15	0.18	0	17,19,21	0.39	0
15	NAG	C	603	1	14,14,15	0.44	0	17,19,21	0.59	1 (5%)
15	NAG	C	623	1	14,14,15	0.32	0	17,19,21	0.42	0
15	NAG	D	901	2	14,14,15	0.47	0	17,19,21	0.46	0
15	NAG	C	617	1	14,14,15	0.29	0	17,19,21	0.58	0
15	NAG	E	608	1	14,14,15	0.28	0	17,19,21	0.45	0
15	NAG	C	628	1	14,14,15	0.44	0	17,19,21	0.65	1 (5%)
15	NAG	A	619	1	14,14,15	0.45	0	17,19,21	0.52	0
15	NAG	E	610	1	14,14,15	0.32	0	17,19,21	0.39	0
15	NAG	A	604	1	14,14,15	0.41	0	17,19,21	0.60	0
15	NAG	E	622	1	14,14,15	0.48	0	17,19,21	0.70	1 (5%)
15	NAG	C	615	1	14,14,15	1.28	1 (7%)	17,19,21	1.61	1 (5%)
15	NAG	E	618	1	14,14,15	0.62	1 (7%)	17,19,21	1.66	1 (5%)
15	NAG	E	621	1	14,14,15	0.30	0	17,19,21	0.40	0
15	NAG	E	611	1	14,14,15	0.92	1 (7%)	17,19,21	0.62	0
15	NAG	C	614	1	14,14,15	0.62	0	17,19,21	0.68	1 (5%)
15	NAG	C	621	1	14,14,15	0.35	0	17,19,21	0.55	0
15	NAG	A	603	1	14,14,15	0.29	0	17,19,21	0.52	0
15	NAG	E	616	1	14,14,15	0.51	0	17,19,21	1.02	2 (11%)
15	NAG	A	605	1	14,14,15	0.48	0	17,19,21	0.81	1 (5%)
15	NAG	A	629	1	14,14,15	0.21	0	17,19,21	0.57	0
15	NAG	E	615	1	14,14,15	0.26	0	17,19,21	0.43	0
15	NAG	E	617	1	14,14,15	0.27	0	17,19,21	0.41	0
15	NAG	E	619	1	14,14,15	0.78	1 (7%)	17,19,21	2.18	3 (17%)
15	NAG	A	632	1	14,14,15	0.53	0	17,19,21	0.60	1 (5%)
15	NAG	C	616	1	14,14,15	0.44	0	17,19,21	0.35	0
15	NAG	E	609	1	14,14,15	0.25	0	17,19,21	0.61	0
15	NAG	F	904	2	14,14,15	0.60	0	17,19,21	0.48	0
15	NAG	E	620	1	14,14,15	0.52	0	17,19,21	0.63	1 (5%)
15	NAG	A	633	1	14,14,15	0.64	1 (7%)	17,19,21	0.96	1 (5%)
15	NAG	A	618	1	14,14,15	0.19	0	17,19,21	0.49	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
15	NAG	E	613	1	14,14,15	0.26	0	17,19,21	0.51	0
15	NAG	C	620	1	14,14,15	0.25	0	17,19,21	0.64	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
15	NAG	E	612	1	-	5/6/23/26	0/1/1/1
15	NAG	E	614	1	-	1/6/23/26	0/1/1/1
15	NAG	F	901	2	-	2/6/23/26	0/1/1/1
15	NAG	F	903	2	-	0/6/23/26	0/1/1/1
15	NAG	F	902	2	-	2/6/23/26	0/1/1/1
15	NAG	C	627	1	-	2/6/23/26	0/1/1/1
15	NAG	C	624	1	-	2/6/23/26	0/1/1/1
15	NAG	C	622	1	-	2/6/23/26	0/1/1/1
15	NAG	C	606	1	-	2/6/23/26	0/1/1/1
15	NAG	C	603	1	-	1/6/23/26	0/1/1/1
15	NAG	C	623	1	-	1/6/23/26	0/1/1/1
15	NAG	D	901	2	-	2/6/23/26	0/1/1/1
15	NAG	C	617	1	-	4/6/23/26	0/1/1/1
15	NAG	E	608	1	-	2/6/23/26	0/1/1/1
15	NAG	C	628	1	-	0/6/23/26	0/1/1/1
15	NAG	A	619	1	-	4/6/23/26	0/1/1/1
15	NAG	E	610	1	-	2/6/23/26	0/1/1/1
15	NAG	A	604	1	-	2/6/23/26	0/1/1/1
15	NAG	E	622	1	-	2/6/23/26	0/1/1/1
15	NAG	C	615	1	-	4/6/23/26	0/1/1/1
15	NAG	E	618	1	-	4/6/23/26	0/1/1/1
15	NAG	E	621	1	-	2/6/23/26	0/1/1/1
15	NAG	E	611	1	-	3/6/23/26	0/1/1/1
15	NAG	C	614	1	-	2/6/23/26	0/1/1/1
15	NAG	C	621	1	-	2/6/23/26	0/1/1/1
15	NAG	A	603	1	-	2/6/23/26	0/1/1/1
15	NAG	E	616	1	-	2/6/23/26	0/1/1/1
15	NAG	A	605	1	-	0/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	NAG	A	629	1	-	2/6/23/26	0/1/1/1
15	NAG	E	615	1	-	2/6/23/26	0/1/1/1
15	NAG	E	617	1	-	1/6/23/26	0/1/1/1
15	NAG	E	619	1	-	5/6/23/26	0/1/1/1
15	NAG	A	632	1	-	2/6/23/26	0/1/1/1
15	NAG	C	616	1	-	2/6/23/26	0/1/1/1
15	NAG	E	609	1	-	4/6/23/26	0/1/1/1
15	NAG	F	904	2	-	0/6/23/26	0/1/1/1
15	NAG	E	620	1	-	1/6/23/26	0/1/1/1
15	NAG	A	633	1	-	3/6/23/26	0/1/1/1
15	NAG	A	618	1	-	2/6/23/26	0/1/1/1
15	NAG	E	613	1	-	2/6/23/26	0/1/1/1
15	NAG	C	620	1	-	4/6/23/26	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	C	615	NAG	O5-C1	4.65	1.51	1.43
15	E	611	NAG	C1-C2	3.09	1.57	1.52
15	C	624	NAG	C1-C2	2.27	1.55	1.52
15	E	619	NAG	C1-C2	2.22	1.55	1.52
15	A	633	NAG	C1-C2	2.14	1.55	1.52
15	E	618	NAG	O5-C1	2.14	1.47	1.43
15	E	612	NAG	C1-C2	2.07	1.55	1.52

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	E	619	NAG	C2-N2-C7	7.86	134.09	122.90
15	E	612	NAG	C2-N2-C7	7.70	133.86	122.90
15	C	615	NAG	C1-O5-C5	6.41	120.88	112.19
15	E	618	NAG	C1-O5-C5	6.21	120.61	112.19
15	E	612	NAG	C1-C2-N2	3.79	116.96	110.49
15	E	619	NAG	C1-C2-N2	3.21	115.98	110.49
15	F	903	NAG	C1-O5-C5	3.02	116.29	112.19
15	E	616	NAG	C2-N2-C7	3.00	127.17	122.90
15	A	605	NAG	C1-O5-C5	2.91	116.13	112.19
15	C	624	NAG	C2-N2-C7	2.85	126.96	122.90
15	A	633	NAG	C2-N2-C7	2.84	126.95	122.90
15	E	622	NAG	C1-O5-C5	2.49	115.57	112.19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	C	614	NAG	C1-O5-C5	2.35	115.38	112.19
15	E	619	NAG	C8-C7-N2	2.22	119.85	116.10
15	C	628	NAG	C1-O5-C5	2.20	115.17	112.19
15	E	620	NAG	C1-O5-C5	2.17	115.14	112.19
15	E	616	NAG	C1-O5-C5	2.11	115.05	112.19
15	E	612	NAG	C8-C7-N2	2.11	119.67	116.10
15	F	901	NAG	C1-O5-C5	2.09	115.03	112.19
15	C	603	NAG	C1-O5-C5	2.04	114.96	112.19
15	A	632	NAG	C1-O5-C5	2.03	114.94	112.19

There are no chirality outliers.

All (89) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	E	615	NAG	C4-C5-C6-O6
15	E	609	NAG	O5-C5-C6-O6
15	E	608	NAG	C4-C5-C6-O6
15	D	901	NAG	O5-C5-C6-O6
15	E	615	NAG	O5-C5-C6-O6
15	A	603	NAG	C4-C5-C6-O6
15	A	632	NAG	C4-C5-C6-O6
15	E	622	NAG	C4-C5-C6-O6
15	A	618	NAG	O5-C5-C6-O6
15	C	616	NAG	O5-C5-C6-O6
15	C	622	NAG	O5-C5-C6-O6
15	C	627	NAG	O5-C5-C6-O6
15	D	901	NAG	C4-C5-C6-O6
15	E	610	NAG	C4-C5-C6-O6
15	A	604	NAG	O5-C5-C6-O6
15	C	617	NAG	O5-C5-C6-O6
15	E	621	NAG	O5-C5-C6-O6
15	E	619	NAG	C4-C5-C6-O6
15	C	614	NAG	O5-C5-C6-O6
15	C	621	NAG	O5-C5-C6-O6
15	F	902	NAG	O5-C5-C6-O6
15	A	618	NAG	C4-C5-C6-O6
15	C	621	NAG	C4-C5-C6-O6
15	C	606	NAG	O5-C5-C6-O6
15	E	618	NAG	O5-C5-C6-O6
15	E	619	NAG	O5-C5-C6-O6
15	E	608	NAG	O5-C5-C6-O6
15	E	610	NAG	O5-C5-C6-O6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	E	622	NAG	O5-C5-C6-O6
15	A	629	NAG	C4-C5-C6-O6
15	C	620	NAG	C4-C5-C6-O6
15	E	609	NAG	C4-C5-C6-O6
15	A	632	NAG	O5-C5-C6-O6
15	E	611	NAG	O5-C5-C6-O6
15	A	633	NAG	O5-C5-C6-O6
15	C	622	NAG	C4-C5-C6-O6
15	C	627	NAG	C4-C5-C6-O6
15	A	619	NAG	C8-C7-N2-C2
15	A	619	NAG	O7-C7-N2-C2
15	C	615	NAG	C8-C7-N2-C2
15	C	615	NAG	O7-C7-N2-C2
15	C	617	NAG	C8-C7-N2-C2
15	C	617	NAG	O7-C7-N2-C2
15	C	620	NAG	C8-C7-N2-C2
15	C	620	NAG	O7-C7-N2-C2
15	E	609	NAG	C8-C7-N2-C2
15	E	609	NAG	O7-C7-N2-C2
15	E	612	NAG	C8-C7-N2-C2
15	E	612	NAG	O7-C7-N2-C2
15	E	613	NAG	C8-C7-N2-C2
15	E	613	NAG	O7-C7-N2-C2
15	E	618	NAG	C8-C7-N2-C2
15	E	618	NAG	O7-C7-N2-C2
15	E	619	NAG	C8-C7-N2-C2
15	E	619	NAG	O7-C7-N2-C2
15	A	604	NAG	C4-C5-C6-O6
15	E	611	NAG	C4-C5-C6-O6
15	A	603	NAG	O5-C5-C6-O6
15	C	617	NAG	C4-C5-C6-O6
15	A	619	NAG	O5-C5-C6-O6
15	E	612	NAG	C4-C5-C6-O6
15	E	614	NAG	O5-C5-C6-O6
15	C	616	NAG	C4-C5-C6-O6
15	E	621	NAG	C4-C5-C6-O6
15	F	902	NAG	C4-C5-C6-O6
15	A	629	NAG	O5-C5-C6-O6
15	E	618	NAG	C4-C5-C6-O6
15	C	620	NAG	O5-C5-C6-O6
15	C	614	NAG	C4-C5-C6-O6
15	E	612	NAG	O5-C5-C6-O6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	C	606	NAG	C4-C5-C6-O6
15	C	624	NAG	O5-C5-C6-O6
15	C	603	NAG	O5-C5-C6-O6
15	E	616	NAG	O5-C5-C6-O6
15	E	620	NAG	O5-C5-C6-O6
15	C	623	NAG	O5-C5-C6-O6
15	F	901	NAG	C4-C5-C6-O6
15	C	615	NAG	O5-C5-C6-O6
15	C	615	NAG	C4-C5-C6-O6
15	F	901	NAG	O5-C5-C6-O6
15	E	616	NAG	C3-C2-N2-C7
15	E	617	NAG	O5-C5-C6-O6
15	A	633	NAG	C4-C5-C6-O6
15	E	611	NAG	C1-C2-N2-C7
15	A	633	NAG	C3-C2-N2-C7
15	C	624	NAG	C3-C2-N2-C7
15	E	612	NAG	C3-C2-N2-C7
15	E	619	NAG	C3-C2-N2-C7
15	A	619	NAG	C4-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	F	901	NAG	1	0
15	E	611	NAG	4	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.

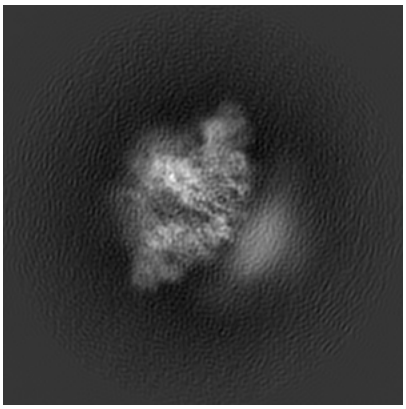
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-20118. These allow visual inspection of the internal detail of the map and identification of artifacts.

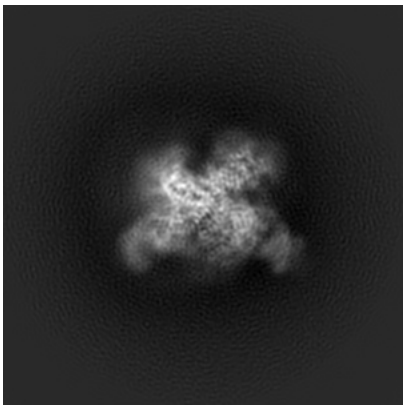
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

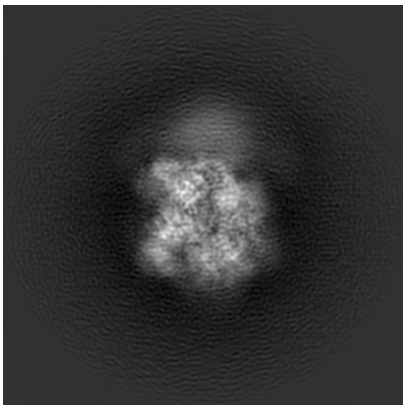
6.1.1 Primary map



X

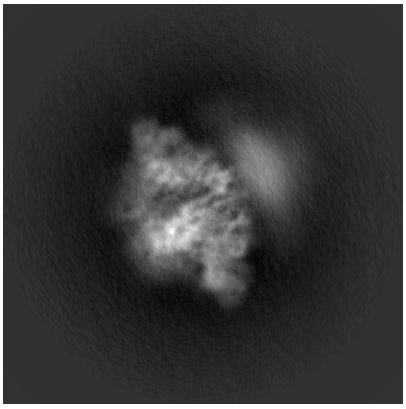


Y

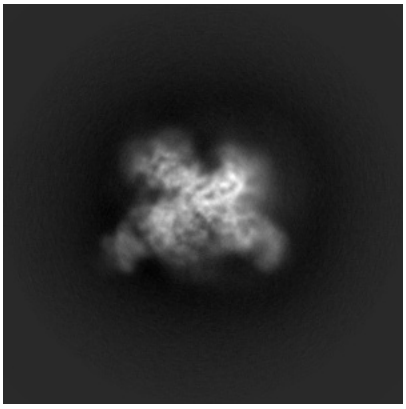


Z

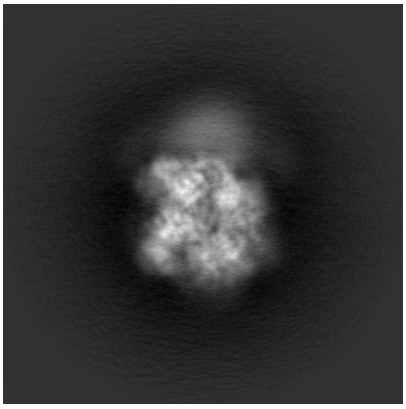
6.1.2 Raw map



X



Y

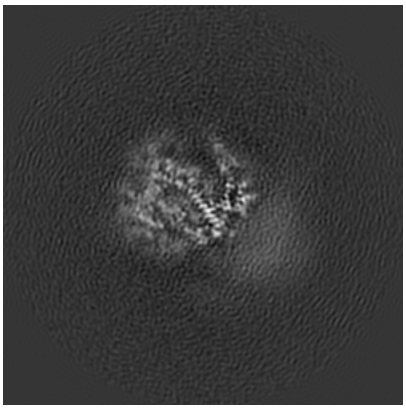


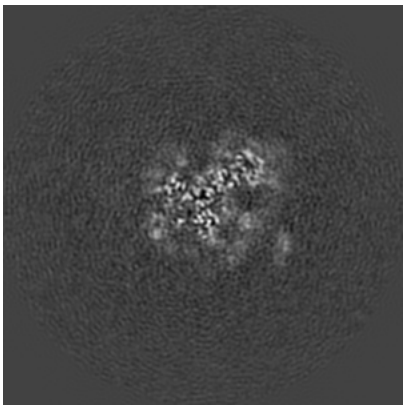
Z

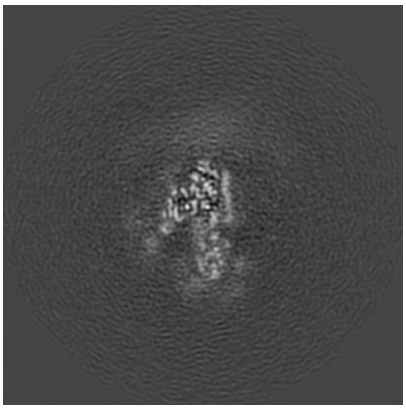
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

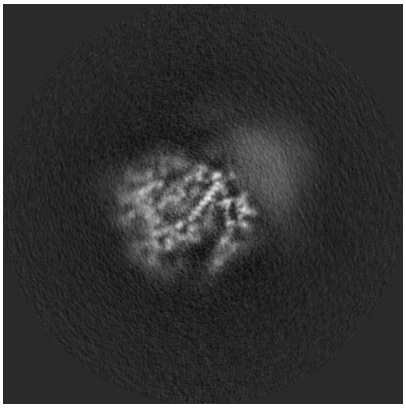
6.2.1 Primary map

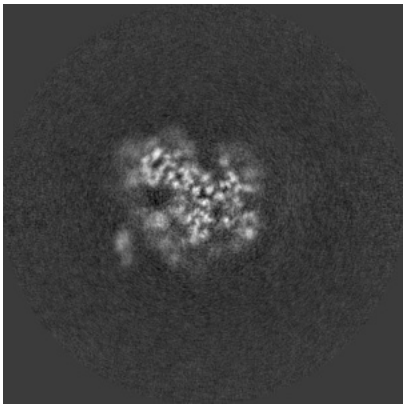

X Index: 175

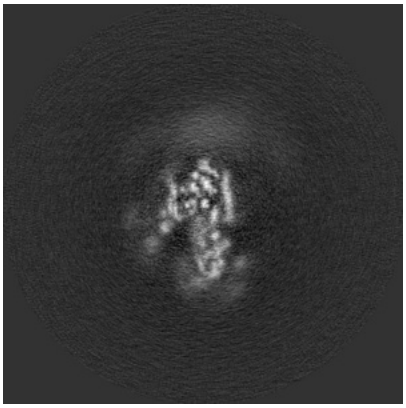

Y Index: 175


Z Index: 175

6.2.2 Raw map


X Index: 175

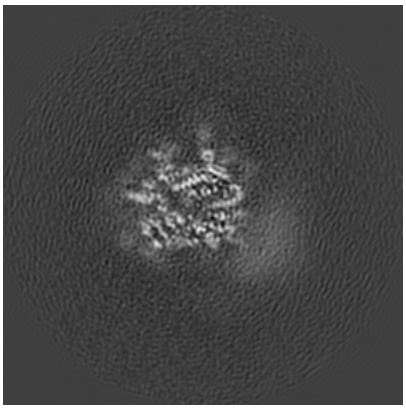

Y Index: 175

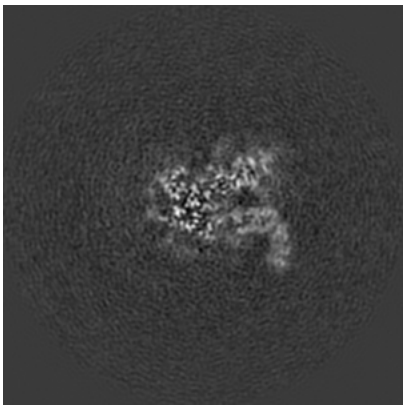

Z Index: 175

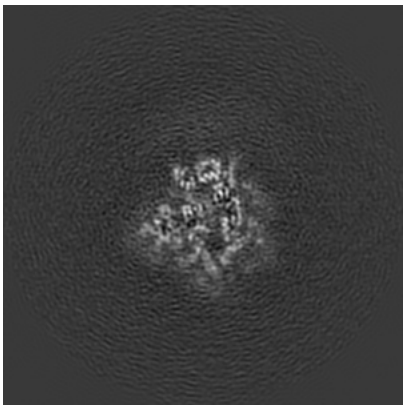
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

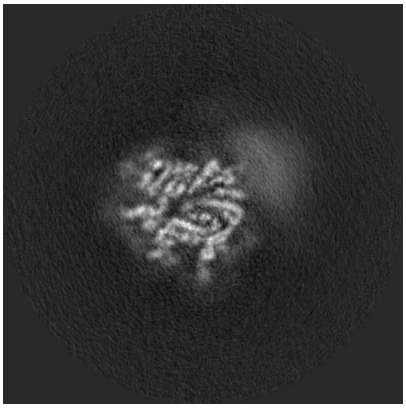
6.3.1 Primary map

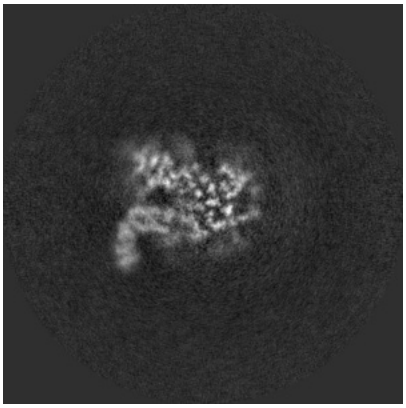

X Index: 193

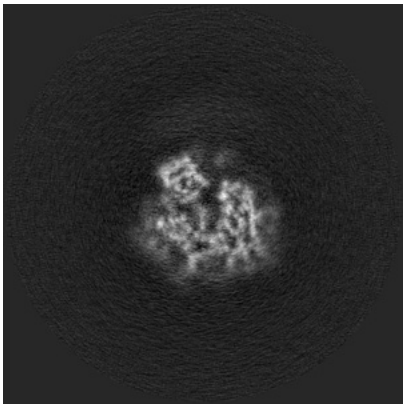

Y Index: 181


Z Index: 192

6.3.2 Raw map


X Index: 194

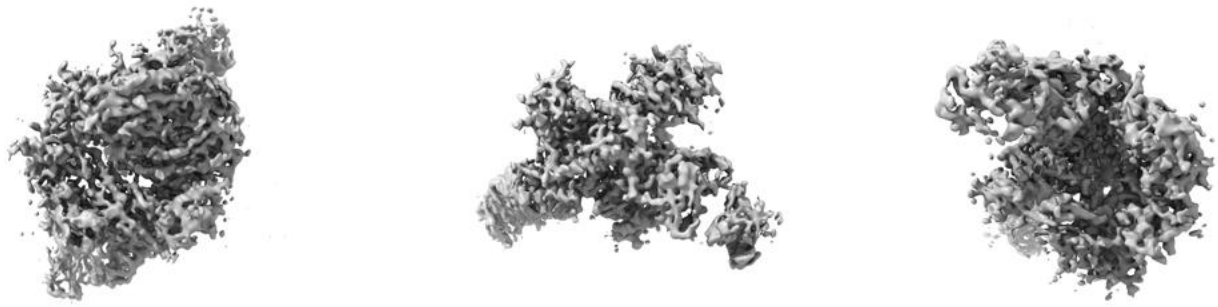

Y Index: 181


Z Index: 144

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

6.4 Orthogonal surface views (i)

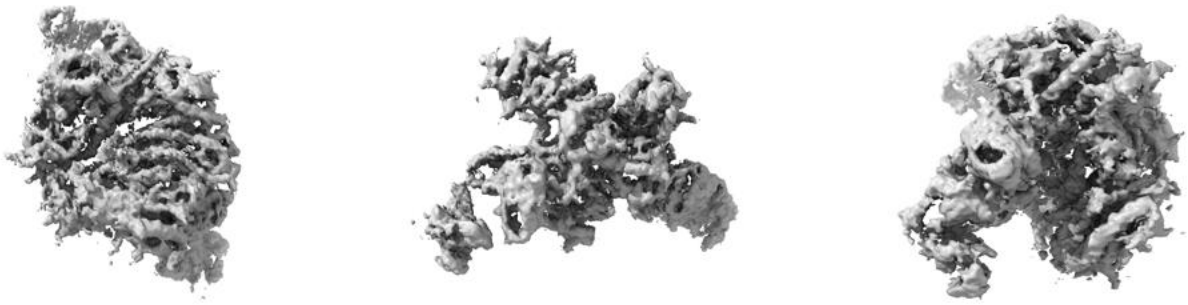
6.4.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.0218. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map



X Y Z

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

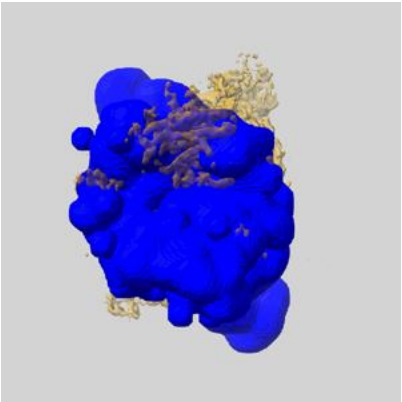
6.5 Mask visualisation (i)

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

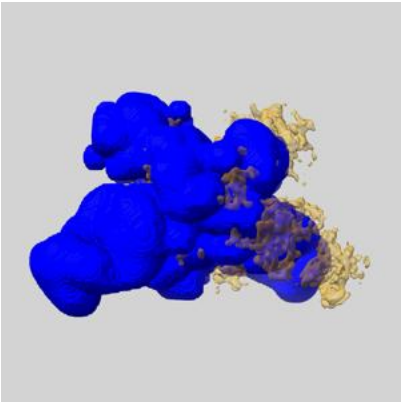
A mask typically either:

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

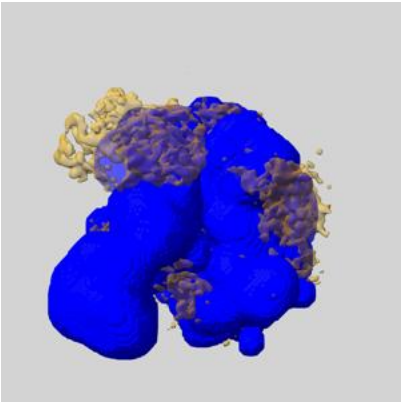
6.5.1 emd_20118_msk_1.map (i)



X



Y

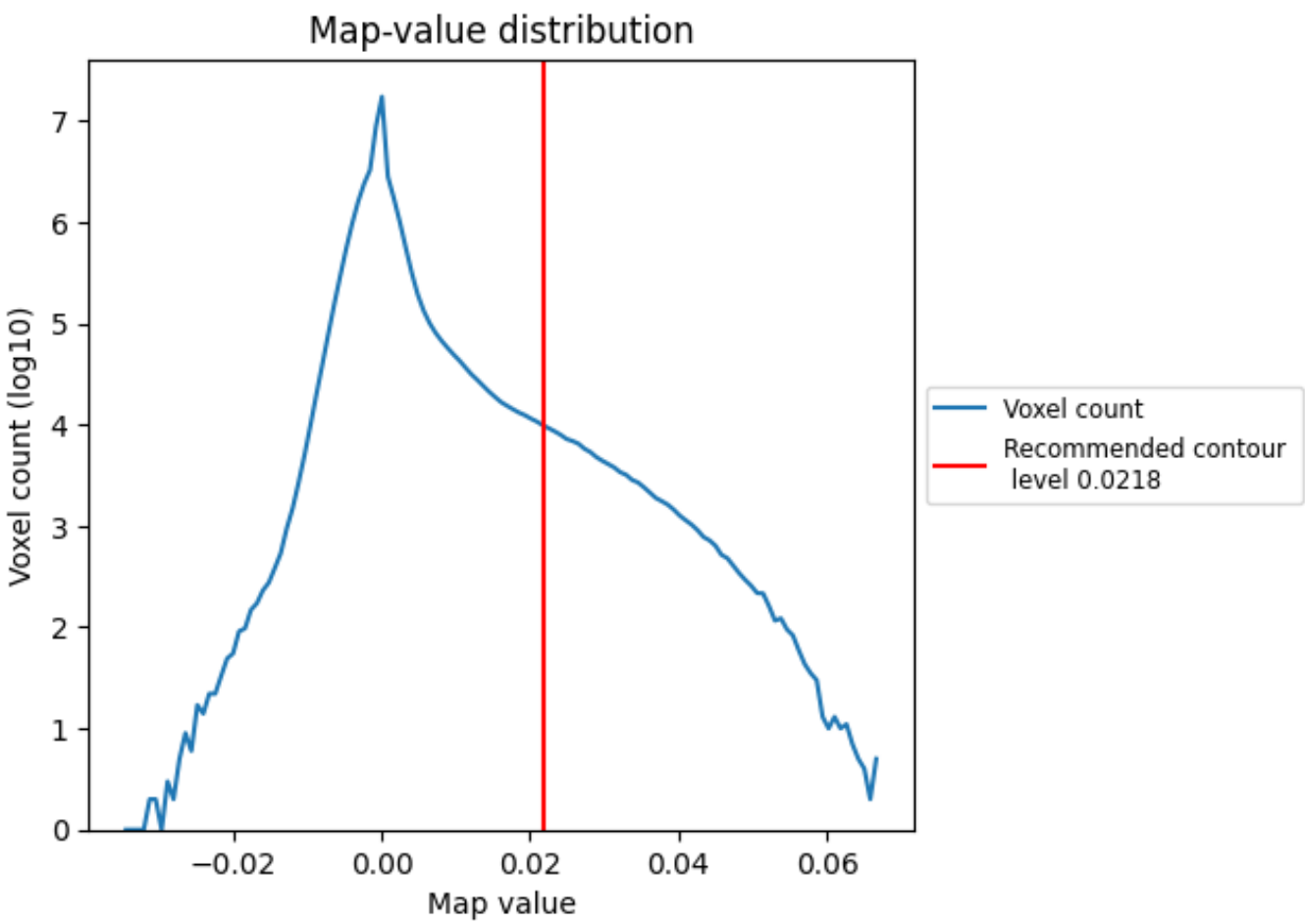


Z

7 Map analysis (i)

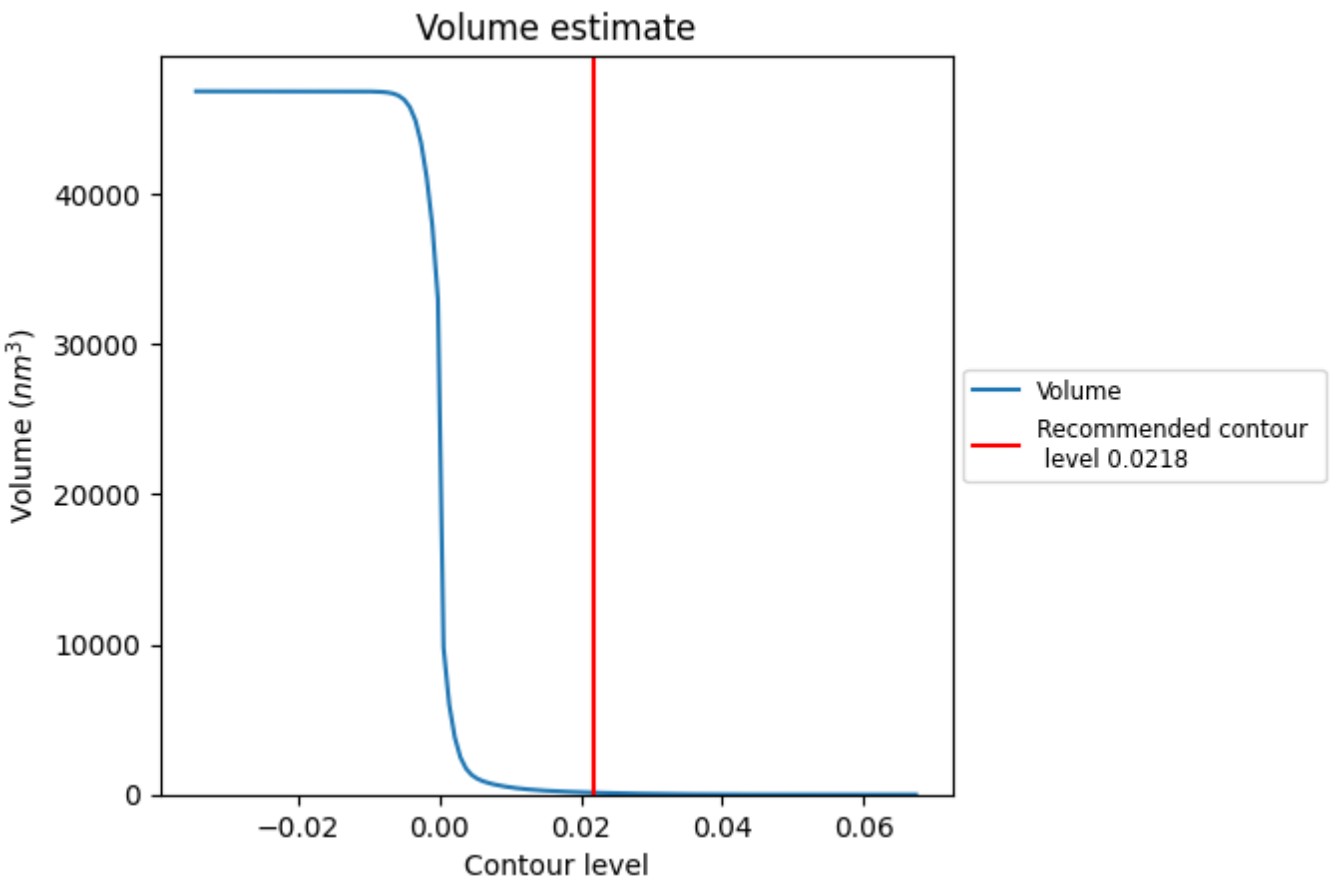
This section contains the results of statistical analysis of the map.

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.

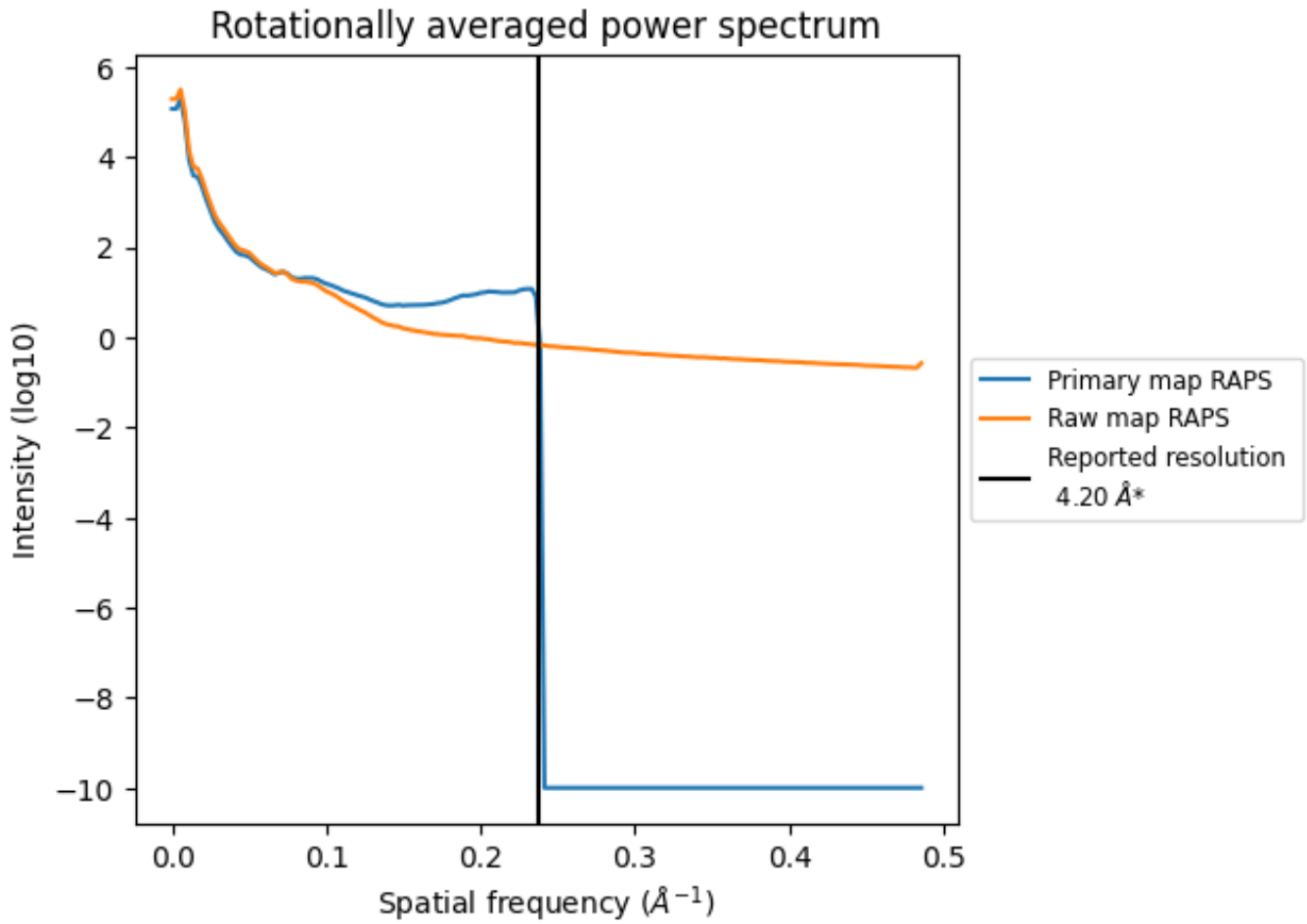
7.2 Volume estimate (i)



The volume at the recommended contour level is 127 nm^3; this corresponds to an approximate mass of 115 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)

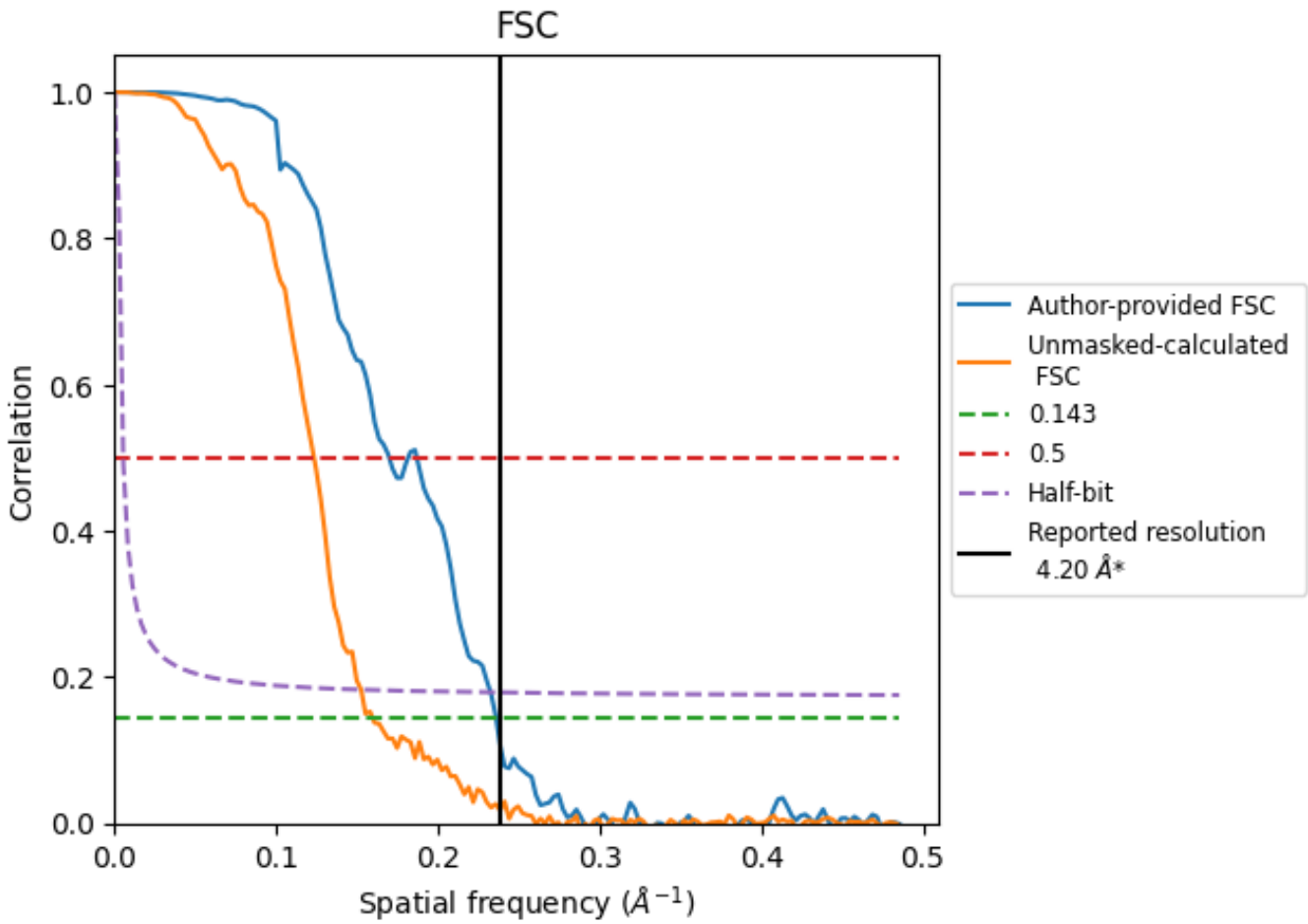


*Reported resolution corresponds to spatial frequency of 0.238 Å^{-1}

8 Fourier-Shell correlation (i)

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 (i)



*Reported resolution corresponds to spatial frequency of 0.238 Å^{-1}

8.2 Resolution estimates (i)

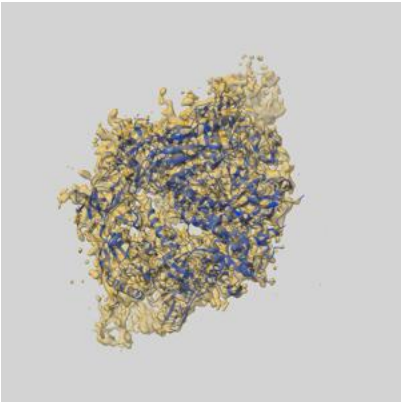
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.20	-	-
Author-provided FSC curve	4.24	5.89	4.30
Unmasked-calculated*	6.26	8.10	6.56

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.26 differs from the reported value 4.2 by more than 10 %

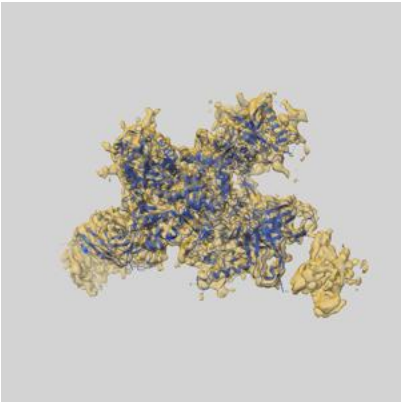
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-20118 and PDB model 6OLP. Per-residue inclusion information can be found in section 3 on page 12.

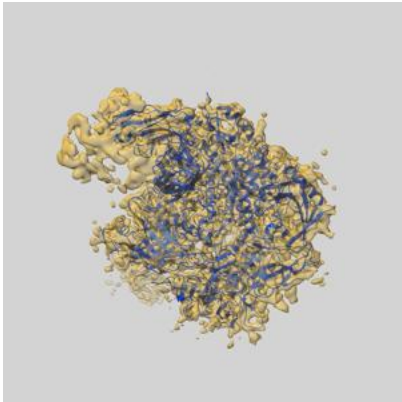
9.1 Map-model overlay (i)



X



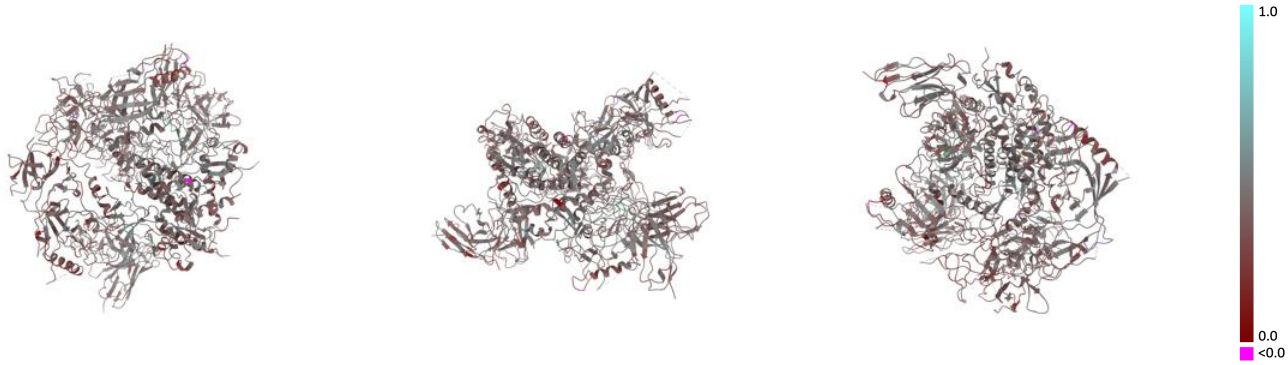
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0218 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.

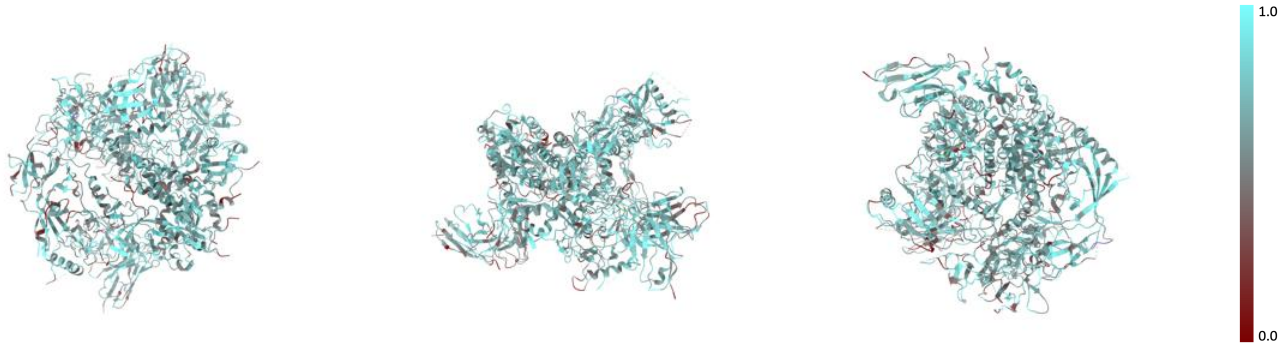
9.2 Q-score mapped to coordinate model (i)



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.

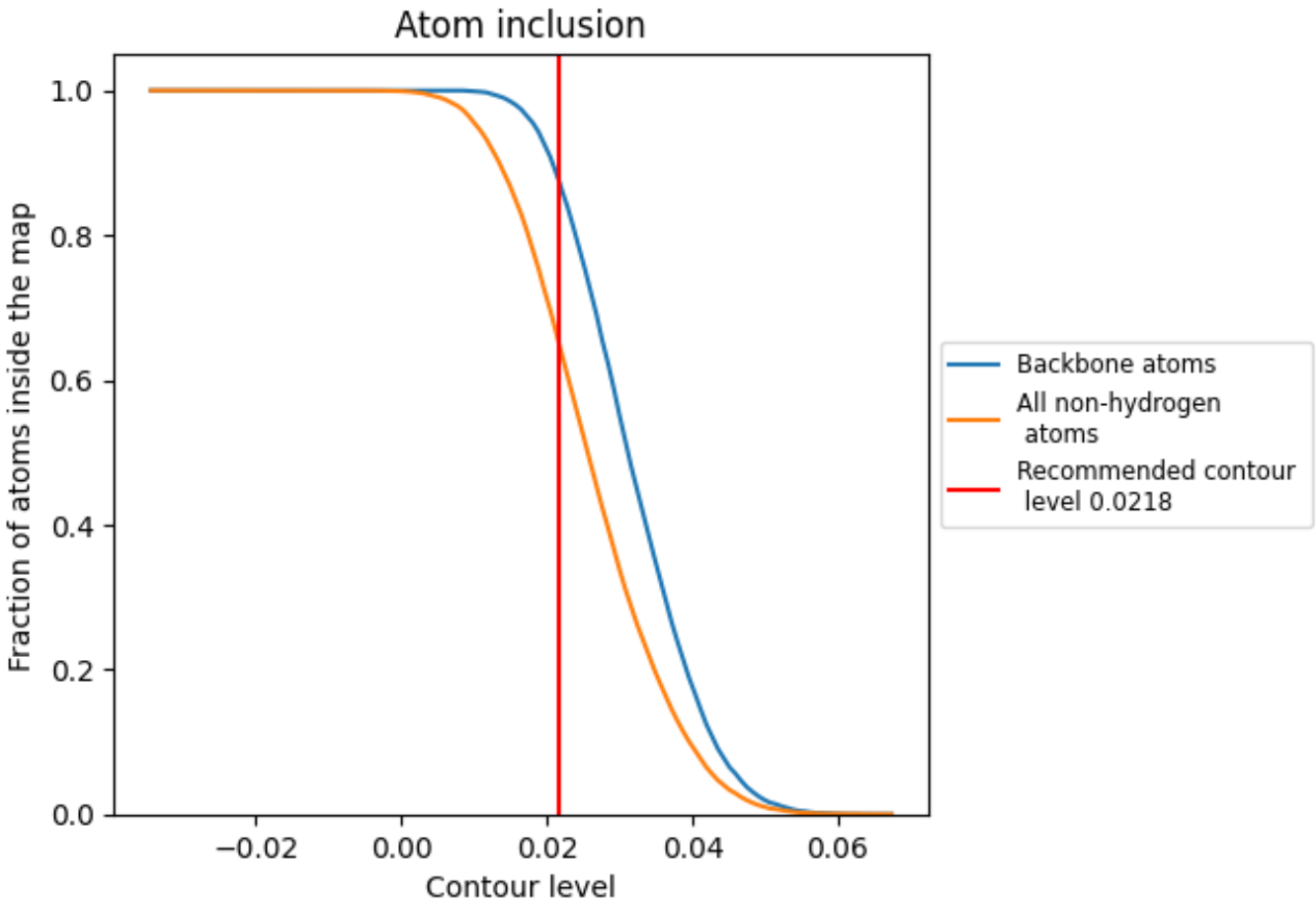
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.0218).

9.4 Atom inclusion (i)



At the recommended contour level, 87% of all backbone atoms, 65% 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 (0.0218) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6459	0.3990
A	0.6849	0.4110
B	0.6587	0.3910
C	0.6382	0.3880
D	0.6960	0.4240
E	0.6445	0.3860
F	0.6211	0.4020
G	0.7340	0.4170
H	0.6910	0.4060
I	0.5956	0.3790
J	0.4643	0.4100
K	0.3214	0.4210
L	0.5293	0.3670
M	0.3571	0.3750
N	0.6071	0.4390
O	0.4643	0.4010
P	0.6400	0.4760
Q	0.5357	0.4370
R	0.3846	0.4180
S	0.3571	0.2910
T	0.4643	0.3390
U	0.4286	0.3760
V	0.6182	0.4150
W	0.6458	0.4480
X	0.3750	0.4150
Y	0.4643	0.4760
Z	0.3571	0.3950
a	0.1786	0.3980
b	0.5902	0.4770
c	0.7500	0.4510
d	0.3929	0.4700
e	0.6182	0.4840
f	0.5041	0.4680
g	0.4643	0.4070
h	0.3214	0.4310
i	0.6667	0.4330