Full wwPDB EM Validation Report (i)

Sep 28, 2024 – 10:16 AM EDT

PDB ID	:	6NC3
EMDB ID	:	EMD-0434
Title	:	AMC011 v4.2 SOSIP Env trimer in complex with fusion peptide targeting antibody VRC34 fragment antigen binding
Authors	:	Cottrell, C.A.; Ozorowski, G.; Torres, J.L.; Ward, A.B.
Deposited on	:	2018-12-10
Resolution	:	4.50 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:

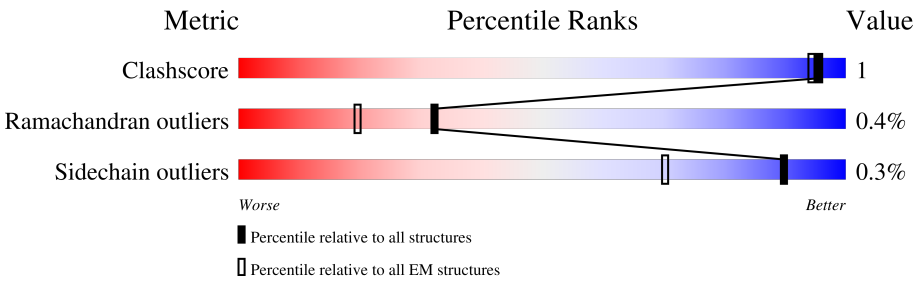
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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 4.50 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	512	7% 79% • 16%
1	C	512	7% 79% • 16%
1	D	512	7% 79% • 16%
1	E	512	7% 79% • 16%
1	F	512	7% 79% • 16%
1	G	512	7% 79% • 16%
2	B	153	• 81% • 16%
2	I	153	• 81% • 16%

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Mol	Chain	Length	Quality of chain
2	J	153	80% 16%
2	K	153	81% 16%
2	M	153	80% 16%
2	N	153	80% 16%
3	H	222	9% 51% 46%
3	O	222	9% 51% 46%
3	P	222	9% 51% 46%
3	Q	222	9% 51% 46%
3	R	222	9% 51% 46%
3	S	222	9% 51% 46%
4	L	210	17% 49% 50%
4	T	210	17% 49% 50%
4	U	210	17% 49% 50%
4	V	210	17% 49% 50%
4	W	210	17% 49% 50%
4	X	210	17% 49% 50%
5	0	5	40% 60% 40%
5	3	5	40% 80% 20%
5	7	5	40% 60% 40%
5	AA	5	40% 80% 20%
5	Y	5	40% 60% 40%
5	b	5	40% 100%
5	f	5	40% 100%
5	i	5	40% 100%
5	m	5	40% 100%

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Mol	Chain	Length	Quality of chain
5	p	5	40% 100%
5	t	5	40% 100%
5	w	5	40% 100%
6	1	2	50% 100%
6	4	2	50% 100%
6	8	2	50% 100%
6	BA	2	50% 100%
6	Z	2	50% 100%
6	c	2	50% 100%
6	g	2	50% 100%
6	j	2	50% 100%
6	n	2	50% 100%
6	q	2	50% 100%
6	u	2	50% 100%
6	x	2	50% 100%
7	2	4	25% 100%
7	9	4	25% 100%
7	a	4	25% 100%
7	h	4	25% 100%
7	o	4	25% 100%
7	v	4	25% 100%
8	5	3	67% 67% 33%
8	6	3	67% 33% 67%
8	CA	3	67% 67% 33%
8	DA	3	67% 33% 67%

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Mol	Chain	Length	Quality of chain
8	d	3	67% 67% 33%
8	e	3	67% 33% 67%
8	k	3	67% 67% 33%
8	l	3	67% 33% 67%
8	r	3	67% 67% 33%
8	s	3	67% 33% 67%
8	y	3	67% 67% 33%
8	z	3	67% 33% 67%

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 38904 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 HIV-1 Env AMC011 v4.2 SOSIP gp120.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	428	3387	2146	589	625	27	0	0
1	C	428	3387	2146	589	625	27	0	0
1	D	428	3387	2146	589	625	27	0	0
1	E	428	3387	2146	589	625	27	0	0
1	F	428	3387	2146	589	625	27	0	0
1	G	428	3387	2146	589	625	27	0	0

- Molecule 2 is a protein called HIV-1 Env AMC011 v4.2 SOSIP gp41.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	128	1017	644	171	195	7	0	0
2	I	128	1017	644	171	195	7	0	0
2	J	128	1017	644	171	195	7	0	0
2	K	128	1017	644	171	195	7	0	0
2	M	128	1017	644	171	195	7	0	0
2	N	128	1017	644	171	195	7	0	0

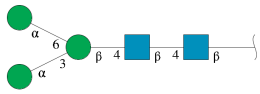
- Molecule 3 is a protein called Monoclonal antibody VRC34.01 fragment antigen binding heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	H	119	923	581	161	177	4	0	0
3	O	119	923	581	161	177	4	0	0
3	P	119	923	581	161	177	4	0	0
3	Q	119	923	581	161	177	4	0	0
3	R	119	923	581	161	177	4	0	0
3	S	119	923	581	161	177	4	0	0

- Molecule 4 is a protein called Monoclonal antibody VRC34.01 fragment antigen binding light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	L	106	809	515	135	156	3	0	0
4	T	106	809	515	135	156	3	0	0
4	U	106	809	515	135	156	3	0	0
4	V	106	809	515	135	156	3	0	0
4	W	106	809	515	135	156	3	0	0
4	X	106	809	515	135	156	3	0	0

- Molecule 5 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		
5	Y	5	61	34	2	25	0	0
5	b	5	61	34	2	25	0	0

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Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
5	f	5	61	34	2	25	0	0
5	i	5	61	34	2	25	0	0
5	m	5	61	34	2	25	0	0
5	p	5	61	34	2	25	0	0
5	t	5	61	34	2	25	0	0
5	w	5	61	34	2	25	0	0
5	0	5	61	34	2	25	0	0
5	3	5	61	34	2	25	0	0
5	7	5	61	34	2	25	0	0
5	AA	5	61	34	2	25	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
6	Z	2	28	16	2	10	0	0
6	c	2	28	16	2	10	0	0
6	g	2	28	16	2	10	0	0
6	j	2	28	16	2	10	0	0
6	n	2	28	16	2	10	0	0
6	q	2	28	16	2	10	0	0
6	u	2	28	16	2	10	0	0

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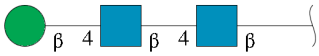
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
6	x	2	28	16	2	10	0	0
6	1	2	28	16	2	10	0	0
6	4	2	28	16	2	10	0	0
6	8	2	28	16	2	10	0	0
6	BA	2	28	16	2	10	0	0

- Molecule 7 is an oligosaccharide called 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.

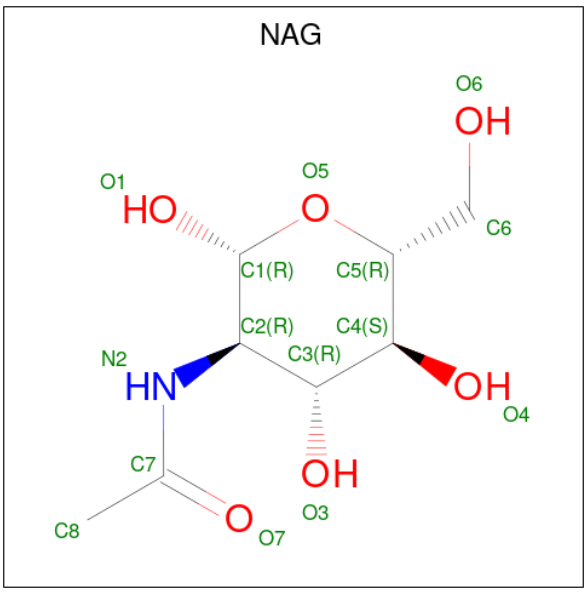
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
7	a	4	50	28	2	20	0	0
7	h	4	50	28	2	20	0	0
7	o	4	50	28	2	20	0	0
7	v	4	50	28	2	20	0	0
7	2	4	50	28	2	20	0	0
7	9	4	50	28	2	20	0	0

- 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	d	3	39	22	2	15	0	0
8	e	3	39	22	2	15	0	0
8	k	3	39	22	2	15	0	0
8	l	3	39	22	2	15	0	0
8	r	3	39	22	2	15	0	0
8	s	3	39	22	2	15	0	0
8	y	3	39	22	2	15	0	0
8	z	3	39	22	2	15	0	0
8	5	3	39	22	2	15	0	0
8	6	3	39	22	2	15	0	0
8	CA	3	39	22	2	15	0	0
8	DA	3	39	22	2	15	0	0

- Molecule 9 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



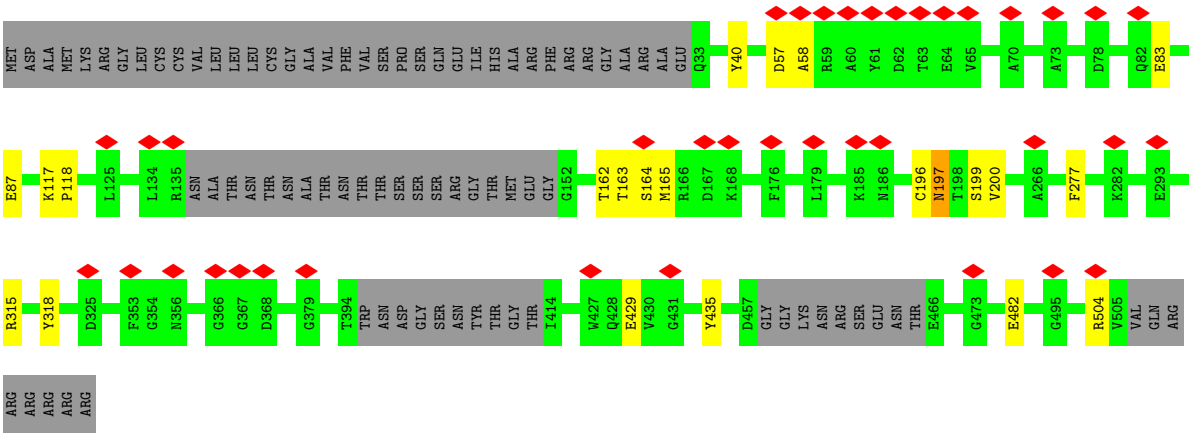
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
9	A	1	14	8	1	5	0
9	A	1	14	8	1	5	0
9	A	1	14	8	1	5	0
9	C	1	14	8	1	5	0
9	C	1	14	8	1	5	0
9	C	1	14	8	1	5	0
9	D	1	14	8	1	5	0
9	D	1	14	8	1	5	0
9	D	1	14	8	1	5	0
9	E	1	14	8	1	5	0
9	E	1	14	8	1	5	0
9	E	1	14	8	1	5	0
9	F	1	14	8	1	5	0
9	F	1	14	8	1	5	0
9	F	1	14	8	1	5	0
9	G	1	14	8	1	5	0
9	G	1	14	8	1	5	0
9	G	1	14	8	1	5	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.

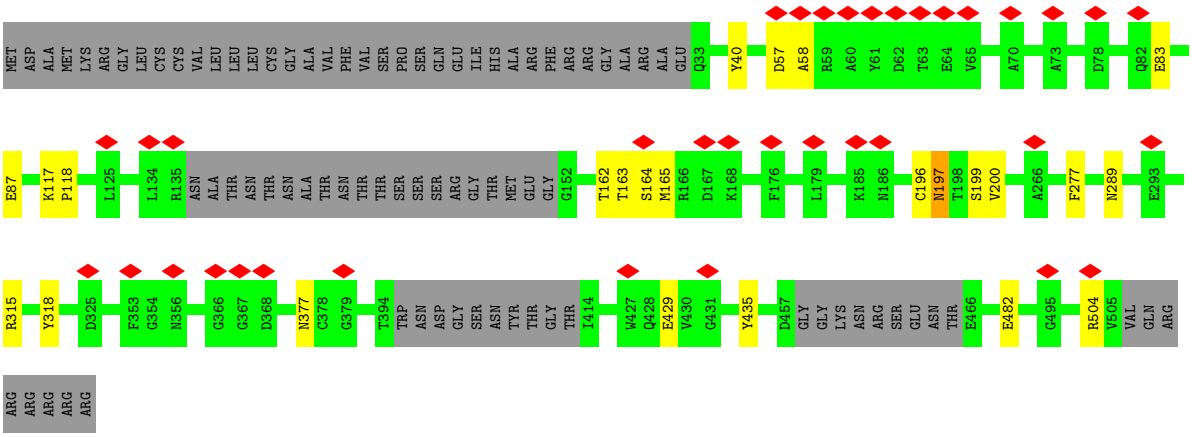
• Molecule 1: HIV-1 Env AMC011 v4.2 SOSIP gp120

Chain A:



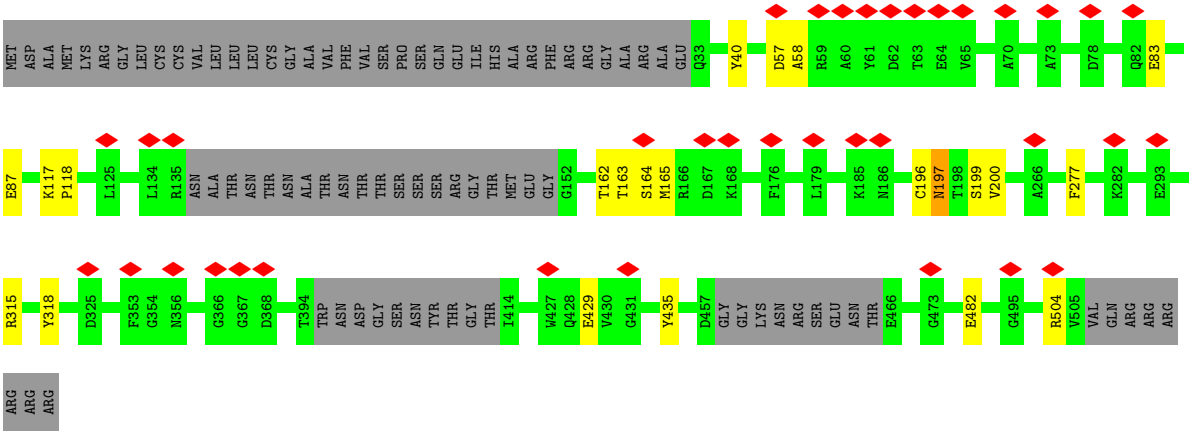
• Molecule 1: HIV-1 Env AMC011 v4.2 SOSIP gp120

Chain C:



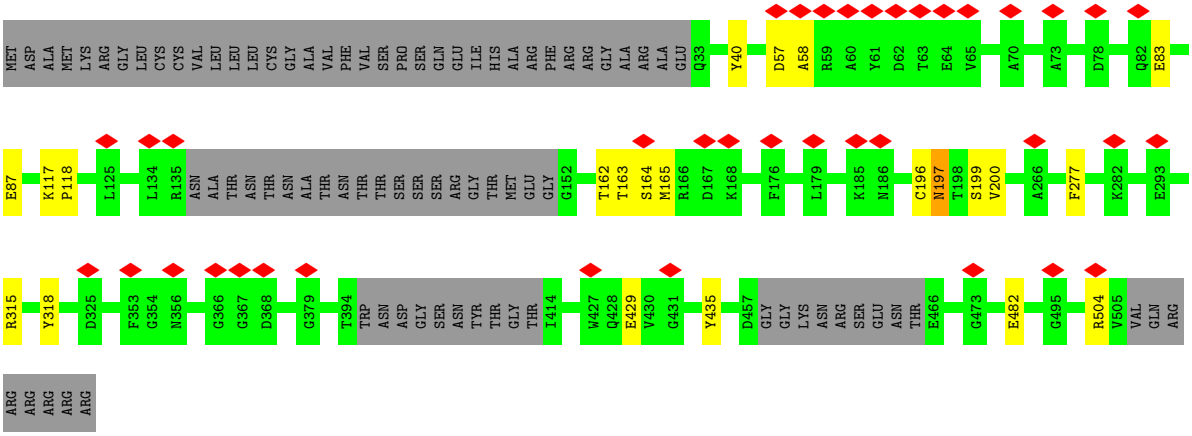
• Molecule 1: HIV-1 Env AMC011 v4.2 SOSIP gp120

Chain D:



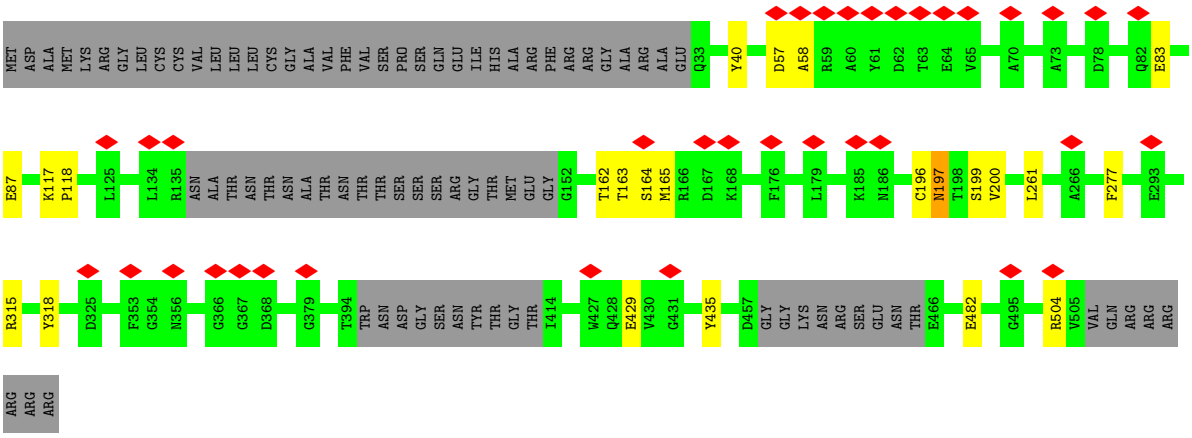
• Molecule 1: HIV-1 Env AMC011 v4.2 SOSIP gp120

Chain E:



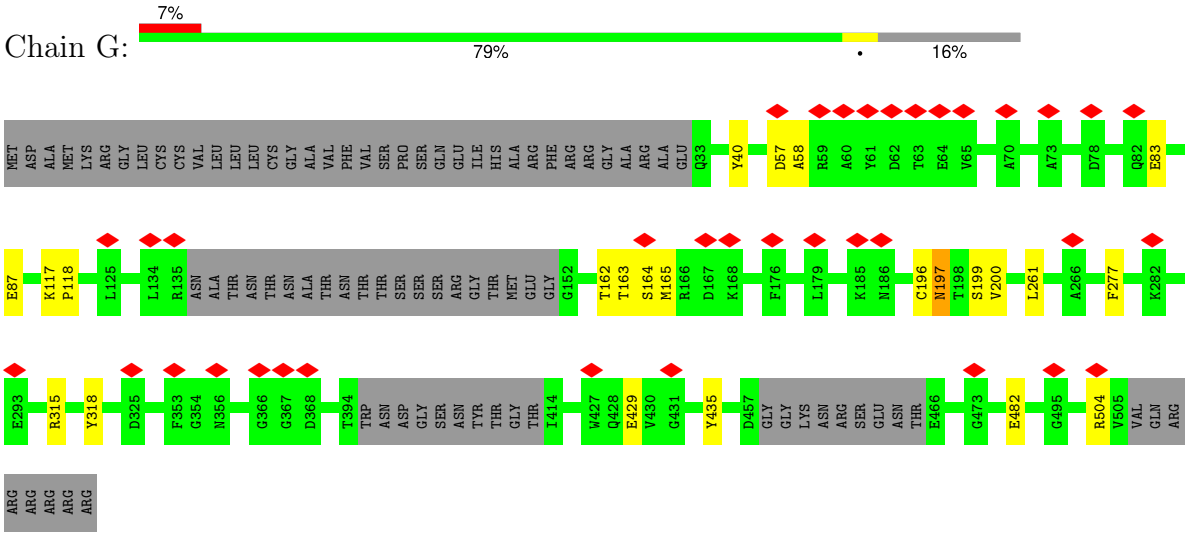
• Molecule 1: HIV-1 Env AMC011 v4.2 SOSIP gp120

Chain F:



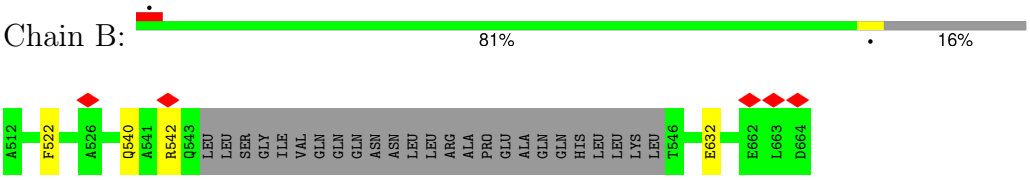
• Molecule 1: HIV-1 Env AMC011 v4.2 SOSIP gp120

Chain G:



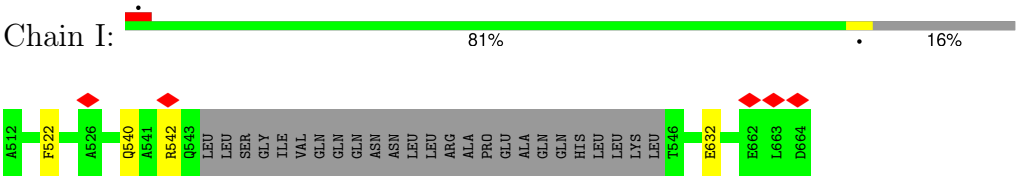
• Molecule 2: HIV-1 Env AMC011 v4.2 SOSIP gp41

Chain B:



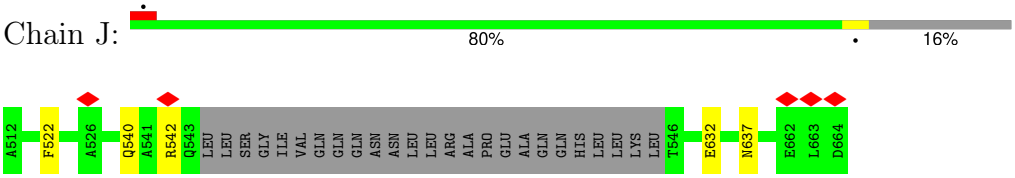
• Molecule 2: HIV-1 Env AMC011 v4.2 SOSIP gp41

Chain I:



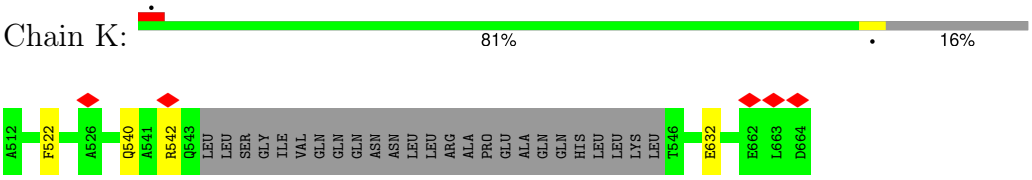
• Molecule 2: HIV-1 Env AMC011 v4.2 SOSIP gp41

Chain J:



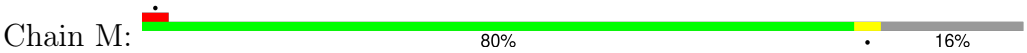
• Molecule 2: HIV-1 Env AMC011 v4.2 SOSIP gp41

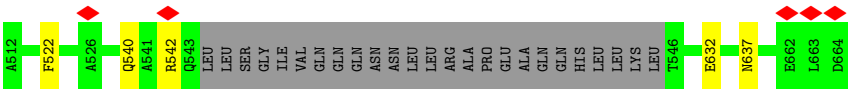
Chain K:



• Molecule 2: HIV-1 Env AMC011 v4.2 SOSIP gp41

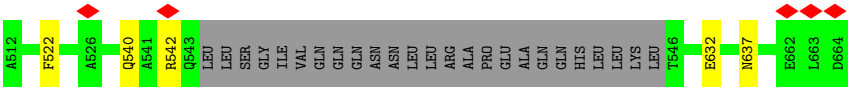
Chain M:





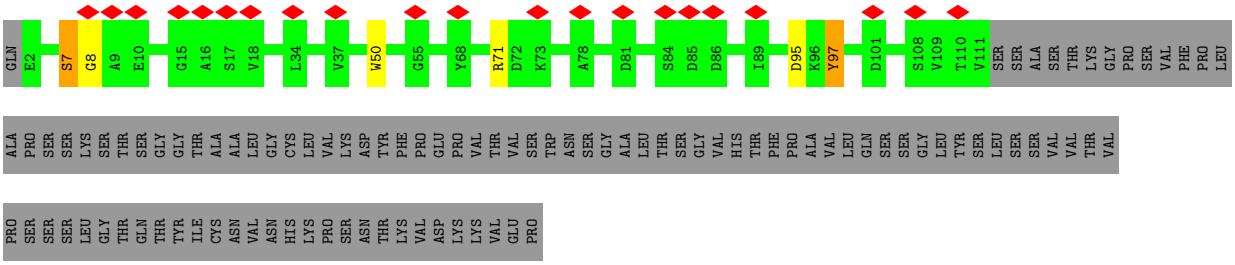
• Molecule 2: HIV-1 Env AMC011 v4.2 SOSIP gp41

Chain N:



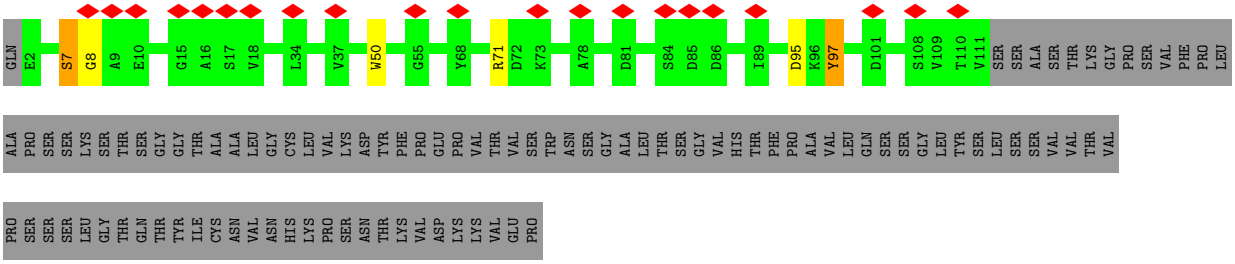
• Molecule 3: Monoclonal antibody VRC34.01 fragment antigen binding heavy chain

Chain H:



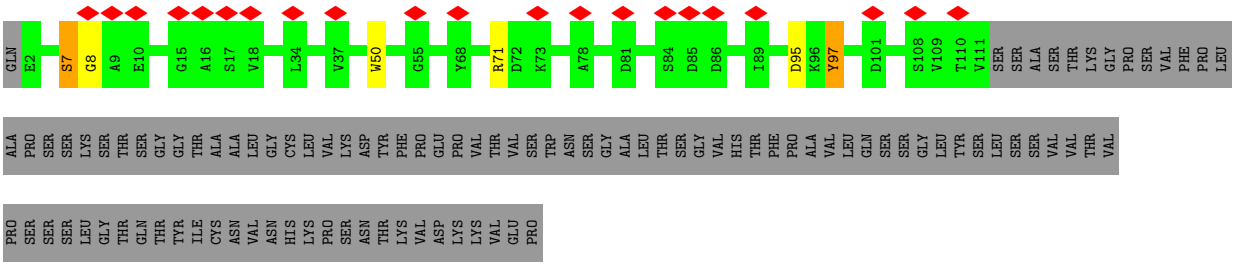
• Molecule 3: Monoclonal antibody VRC34.01 fragment antigen binding heavy chain

Chain O:



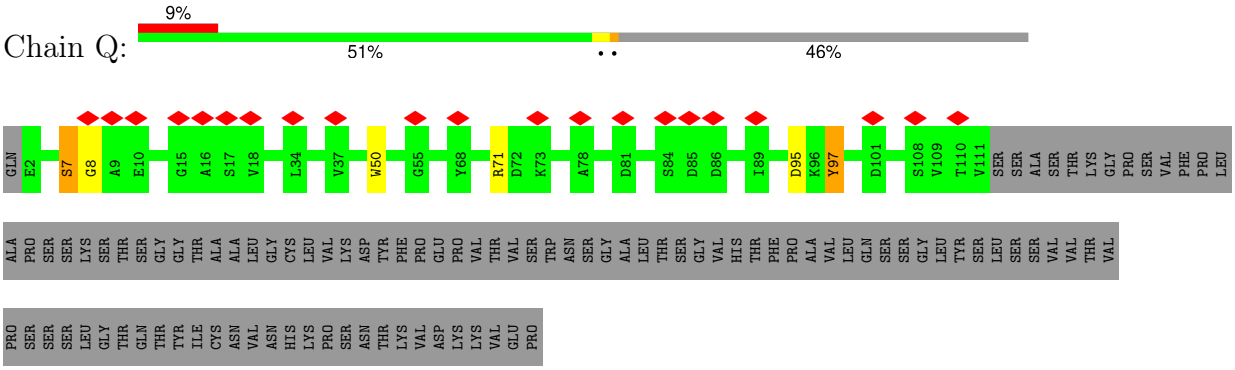
• Molecule 3: Monoclonal antibody VRC34.01 fragment antigen binding heavy chain

Chain P:



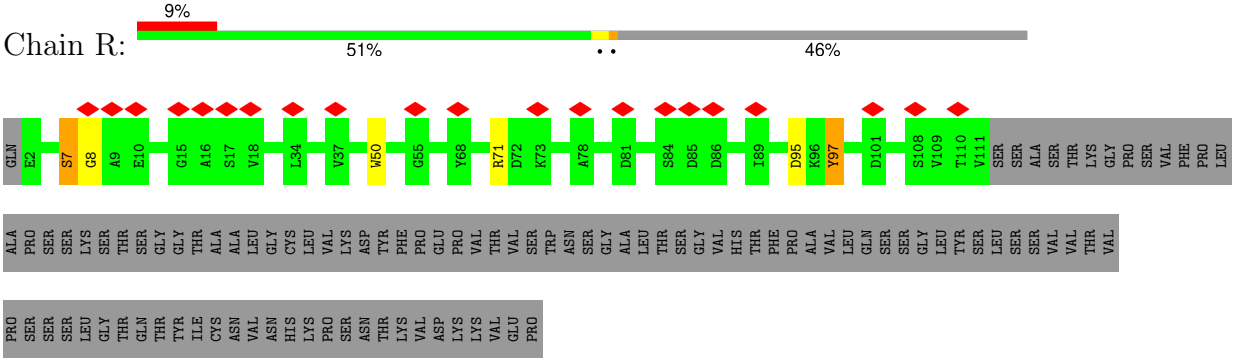
• Molecule 3: Monoclonal antibody VRC34.01 fragment antigen binding heavy chain

Chain Q:



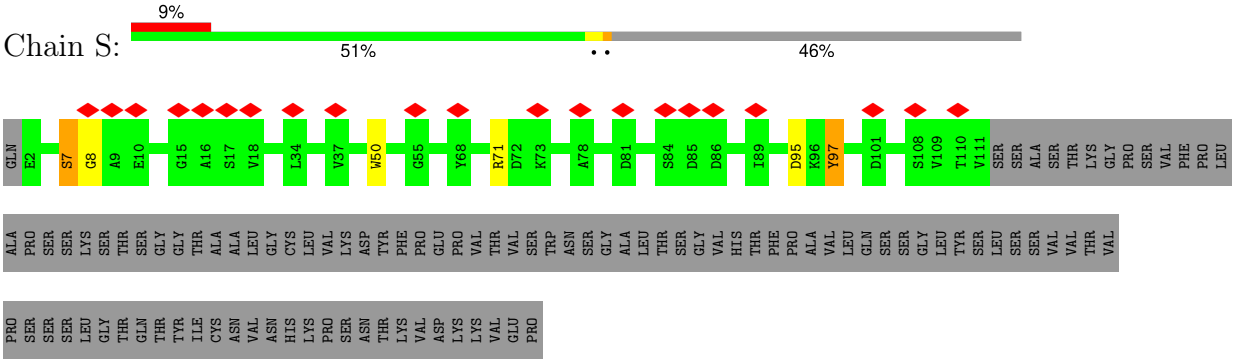
• Molecule 3: Monoclonal antibody VRC34.01 fragment antigen binding heavy chain

Chain R:



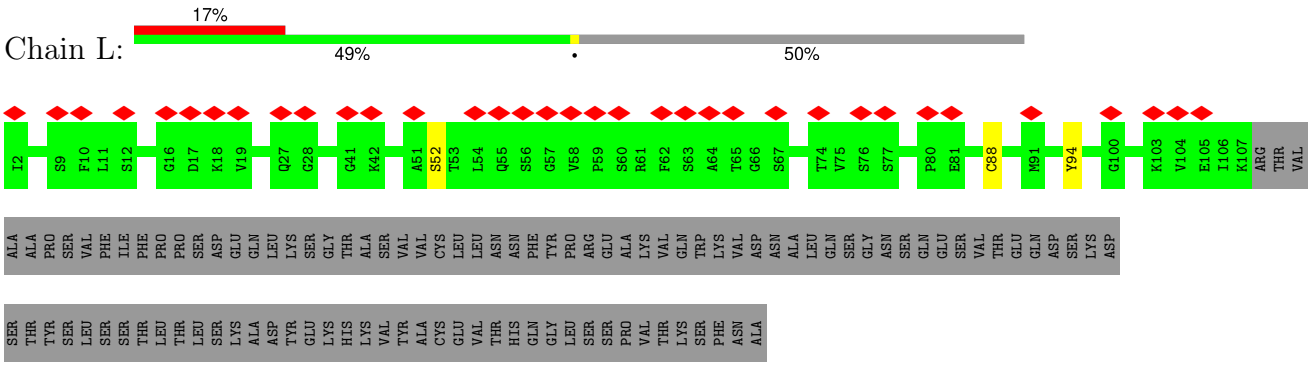
• Molecule 3: Monoclonal antibody VRC34.01 fragment antigen binding heavy chain

Chain S:



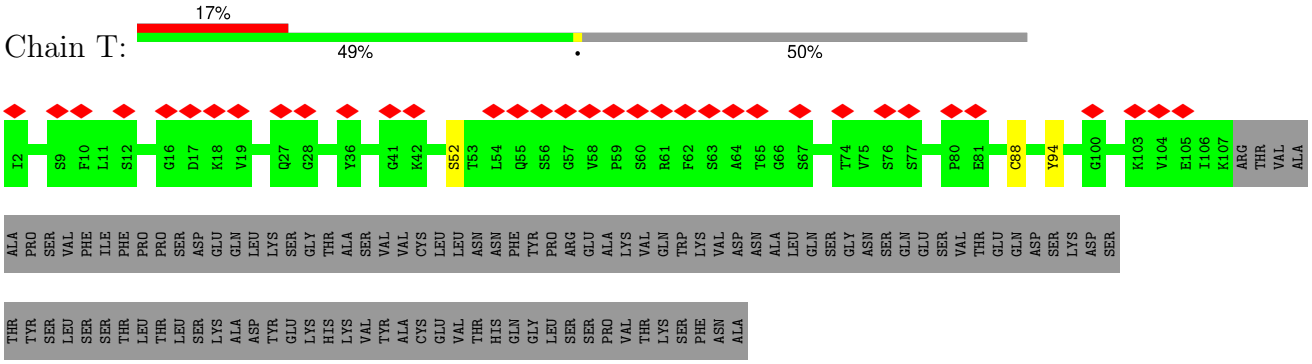
• Molecule 4: Monoclonal antibody VRC34.01 fragment antigen binding light chain

Chain L:



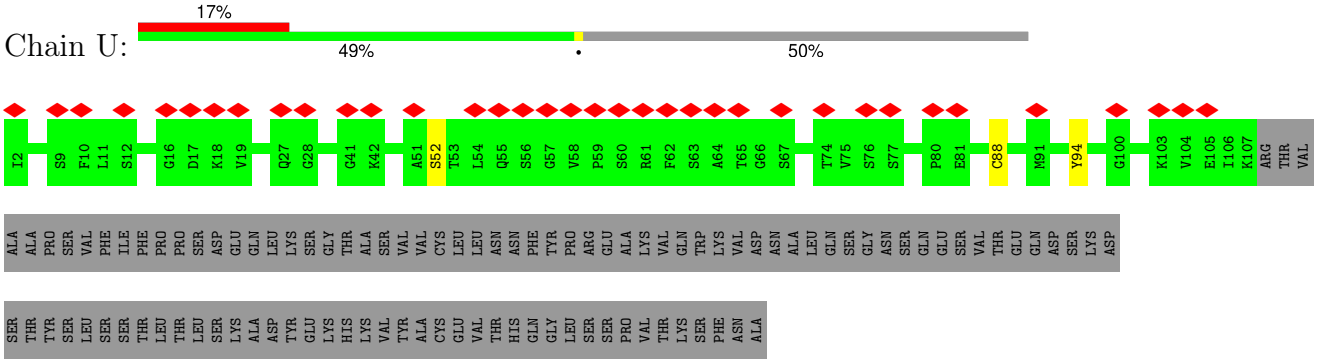
• Molecule 4: Monoclonal antibody VRC34.01 fragment antigen binding light chain

Chain T:



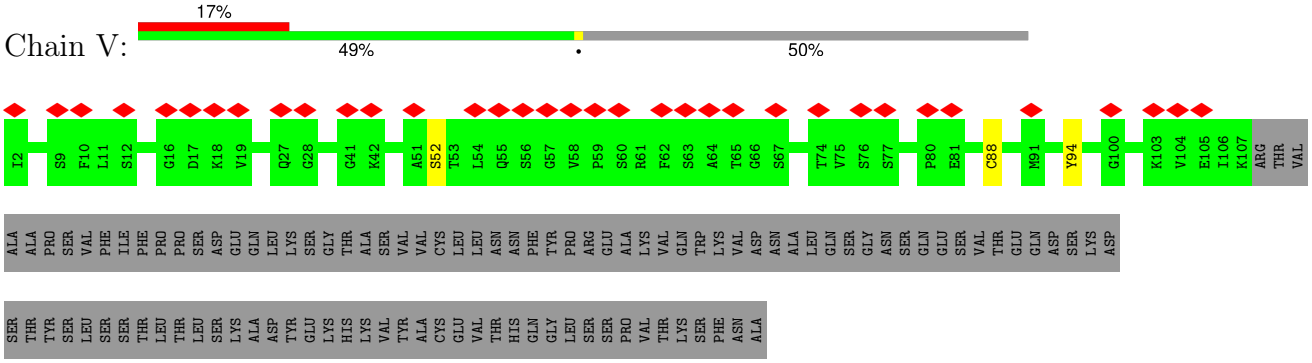
- Molecule 4: Monoclonal antibody VRC34.01 fragment antigen binding light chain

Chain U:



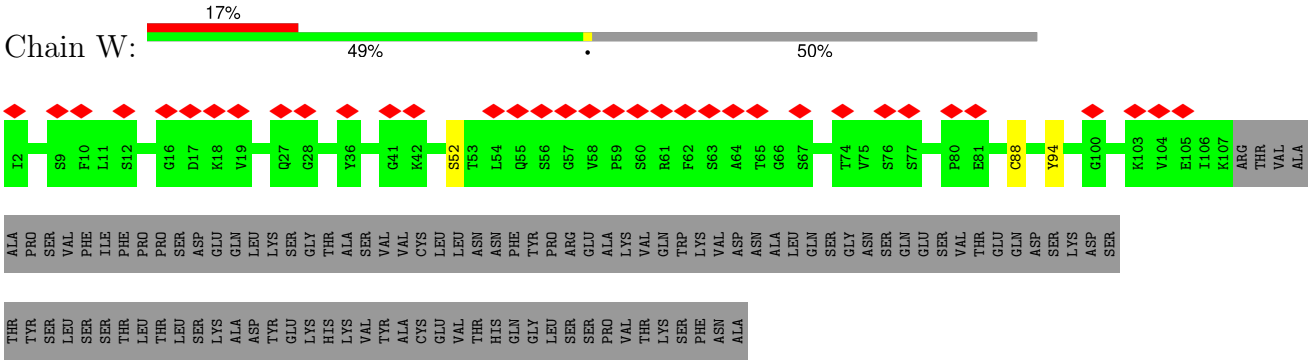
- Molecule 4: Monoclonal antibody VRC34.01 fragment antigen binding light chain

Chain V:



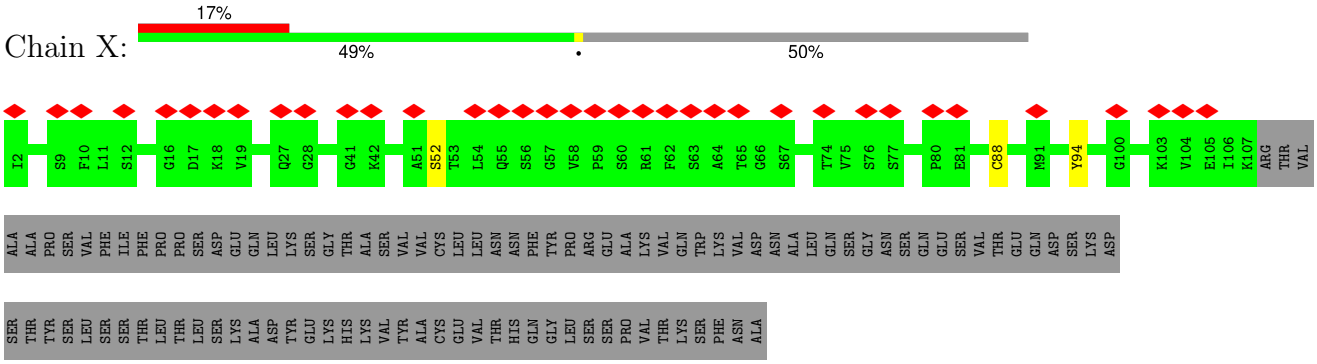
- Molecule 4: Monoclonal antibody VRC34.01 fragment antigen binding light chain

Chain W:



- Molecule 4: Monoclonal antibody VRC34.01 fragment antigen binding light chain

Chain X:

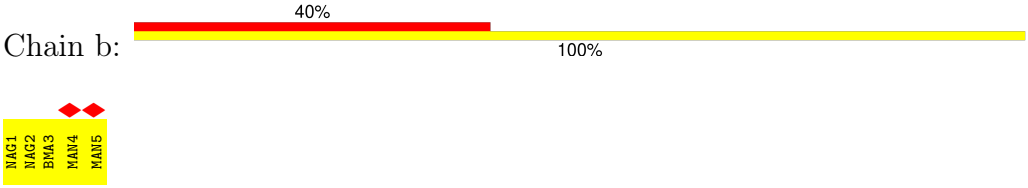


• Molecule 5: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Y:

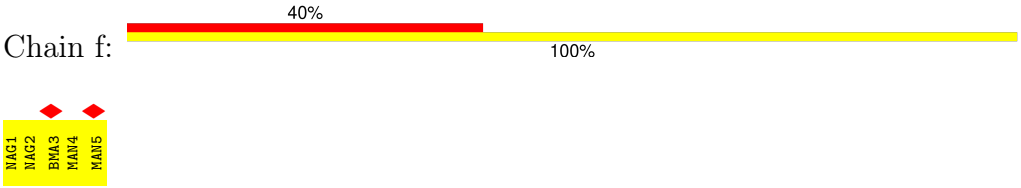
• Molecule 5: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain b:



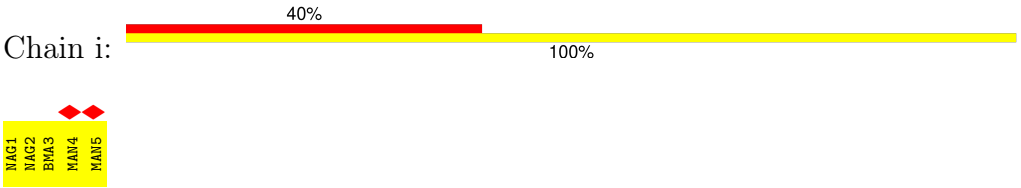
• Molecule 5: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain f:



• Molecule 5: 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 i:

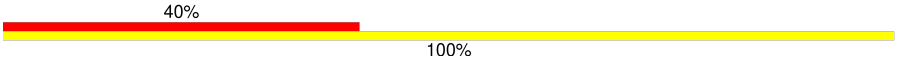


• Molecule 5: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain m:

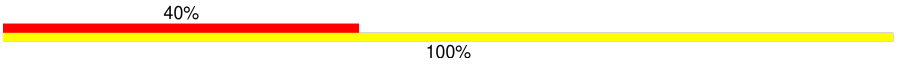
• Molecule 5: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain p:



• Molecule 5: 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 t:

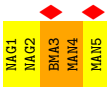


• Molecule 5: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain w:

• Molecule 5: 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

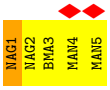
Chain 0:



• Molecule 5: 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-glucopyra

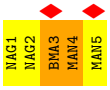
nose

Chain 3:



• Molecule 5: 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

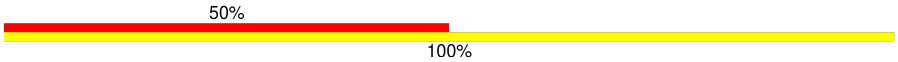
Chain 7:



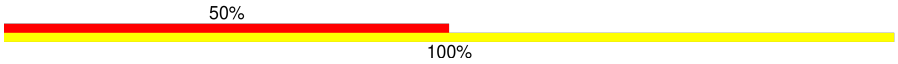
• Molecule 5: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain AA:

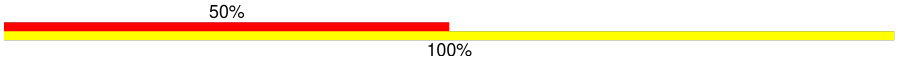
• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Z: 

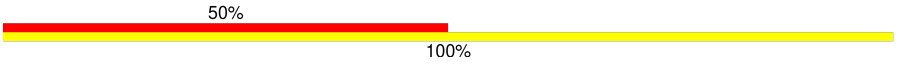
• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain c: 

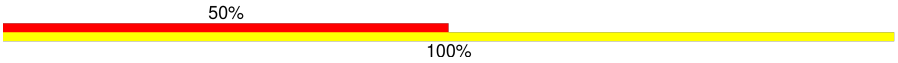
• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain g: 

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

Chain j: 

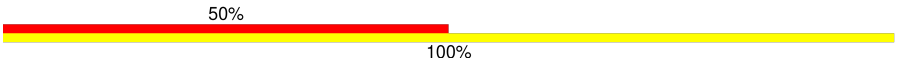
• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain n: 

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

Chain q:

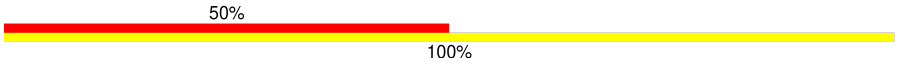
• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain u: 

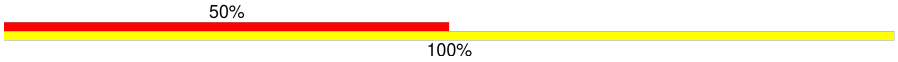
• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain x:

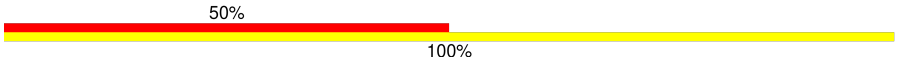
• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 1: 

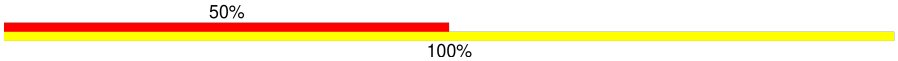
• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 4: 

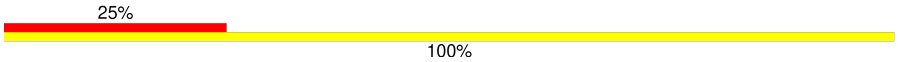
• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 8: 

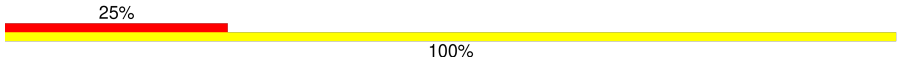
• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain BA: 

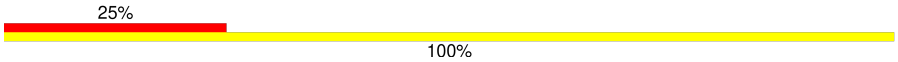
• Molecule 7: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain a: 

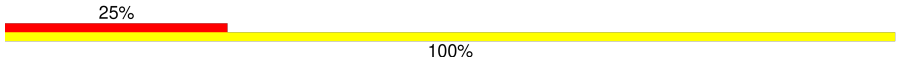
• Molecule 7: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain h: 

• Molecule 7: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain o: 

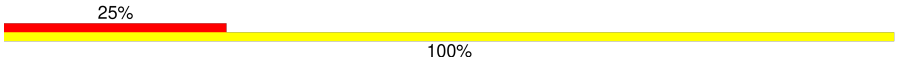
• Molecule 7: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain v: 

• Molecule 7: 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 2:

• Molecule 7: 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 9: 

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

Chain d:

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

Chain e:

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

Chain k:

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

Chain l:

• 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 s:

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

Chain y:

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

Chain z:

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

Chain 5:

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

Chain 6:

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

Chain CA:

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

Chain DA:

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, D3	Depositor
Number of particles used	35611	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 ($e^-/Å^2$)	56	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	29000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	2.395	Depositor
Minimum map value	-0.857	Depositor
Average map value	0.012	Depositor
Map value standard deviation	0.164	Depositor
Recommended contour level	0.9	Depositor
Map size (Å)	362.56, 362.56, 362.56	wwPDB
Map dimensions	352, 352, 352	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, BMA, MAN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
1	A	1.00	11/3459 (0.3%)	0.91	3/4695 (0.1%)
1	C	1.00	11/3459 (0.3%)	0.91	3/4695 (0.1%)
1	D	1.00	11/3459 (0.3%)	0.91	3/4695 (0.1%)
1	E	1.00	11/3459 (0.3%)	0.91	3/4695 (0.1%)
1	F	1.00	11/3459 (0.3%)	0.91	3/4695 (0.1%)
1	G	1.00	11/3459 (0.3%)	0.91	3/4695 (0.1%)
2	B	1.13	1/1036 (0.1%)	0.85	1/1404 (0.1%)
2	I	1.13	1/1036 (0.1%)	0.85	1/1404 (0.1%)
2	J	1.13	1/1036 (0.1%)	0.85	1/1404 (0.1%)
2	K	1.13	1/1036 (0.1%)	0.85	1/1404 (0.1%)
2	M	1.13	1/1036 (0.1%)	0.85	1/1404 (0.1%)
2	N	1.13	1/1036 (0.1%)	0.85	1/1404 (0.1%)
3	H	1.03	2/945 (0.2%)	0.87	0/1283
3	O	1.03	2/945 (0.2%)	0.88	0/1283
3	P	1.03	2/945 (0.2%)	0.87	0/1283
3	Q	1.03	2/945 (0.2%)	0.87	0/1283
3	R	1.03	2/945 (0.2%)	0.88	0/1283
3	S	1.03	2/945 (0.2%)	0.87	0/1283
4	L	0.95	2/829 (0.2%)	0.92	0/1126
4	T	0.95	2/829 (0.2%)	0.92	0/1126
4	U	0.95	2/829 (0.2%)	0.92	0/1126
4	V	0.95	2/829 (0.2%)	0.92	0/1126
4	W	0.95	2/829 (0.2%)	0.92	0/1126
4	X	0.95	2/829 (0.2%)	0.92	0/1126
All	All	1.02	96/37614 (0.3%)	0.90	24/51048 (0.0%)

All (96) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	U	88	CYS	CB-SG	-8.32	1.68	1.82
4	X	88	CYS	CB-SG	-8.32	1.68	1.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	T	88	CYS	CB-SG	-8.30	1.68	1.82
4	W	88	CYS	CB-SG	-8.30	1.68	1.82
4	L	88	CYS	CB-SG	-8.29	1.68	1.82
4	V	88	CYS	CB-SG	-8.29	1.68	1.82
1	C	429	GLU	CG-CD	-6.54	1.42	1.51
1	F	429	GLU	CG-CD	-6.54	1.42	1.51
1	A	429	GLU	CG-CD	-6.52	1.42	1.51
1	E	429	GLU	CG-CD	-6.52	1.42	1.51
1	D	429	GLU	CG-CD	-6.52	1.42	1.51
1	G	429	GLU	CG-CD	-6.52	1.42	1.51
1	C	429	GLU	CD-OE2	-5.93	1.19	1.25
1	F	429	GLU	CD-OE2	-5.93	1.19	1.25
1	A	429	GLU	CD-OE2	-5.93	1.19	1.25
1	E	429	GLU	CD-OE2	-5.93	1.19	1.25
1	D	429	GLU	CD-OE2	-5.87	1.19	1.25
1	G	429	GLU	CD-OE2	-5.87	1.19	1.25
1	D	482	GLU	CG-CD	-5.86	1.43	1.51
1	G	482	GLU	CG-CD	-5.86	1.43	1.51
1	C	482	GLU	CG-CD	-5.83	1.43	1.51
1	F	482	GLU	CG-CD	-5.83	1.43	1.51
1	A	482	GLU	CG-CD	-5.80	1.43	1.51
1	E	482	GLU	CG-CD	-5.80	1.43	1.51
1	D	196	CYS	CB-SG	-5.77	1.72	1.81
1	G	196	CYS	CB-SG	-5.77	1.72	1.81
1	C	196	CYS	CB-SG	-5.75	1.72	1.81
1	F	196	CYS	CB-SG	-5.75	1.72	1.81
1	A	196	CYS	CB-SG	-5.75	1.72	1.81
1	E	196	CYS	CB-SG	-5.75	1.72	1.81
1	C	318	TYR	CB-CG	-5.38	1.43	1.51
1	F	318	TYR	CB-CG	-5.38	1.43	1.51
1	A	318	TYR	CB-CG	-5.34	1.43	1.51
1	E	318	TYR	CB-CG	-5.34	1.43	1.51
1	D	318	TYR	CB-CG	-5.34	1.43	1.51
1	G	318	TYR	CB-CG	-5.34	1.43	1.51
1	D	87	GLU	CD-OE2	-5.26	1.19	1.25
1	G	87	GLU	CD-OE2	-5.26	1.19	1.25
1	A	87	GLU	CD-OE2	-5.25	1.19	1.25
1	E	87	GLU	CD-OE2	-5.25	1.19	1.25
4	L	94	TYR	CB-CG	-5.24	1.43	1.51
4	V	94	TYR	CB-CG	-5.24	1.43	1.51
1	C	87	GLU	CD-OE2	-5.24	1.19	1.25
1	F	87	GLU	CD-OE2	-5.24	1.19	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	U	94	TYR	CB-CG	-5.22	1.43	1.51
4	X	94	TYR	CB-CG	-5.22	1.43	1.51
4	T	94	TYR	CB-CG	-5.21	1.43	1.51
4	W	94	TYR	CB-CG	-5.21	1.43	1.51
1	D	435	TYR	CB-CG	-5.21	1.43	1.51
1	G	435	TYR	CB-CG	-5.21	1.43	1.51
1	A	435	TYR	CB-CG	-5.20	1.43	1.51
1	E	435	TYR	CB-CG	-5.20	1.43	1.51
1	C	435	TYR	CB-CG	-5.18	1.43	1.51
1	F	435	TYR	CB-CG	-5.18	1.43	1.51
3	H	50	TRP	NE1-CE2	-5.17	1.30	1.37
3	Q	50	TRP	NE1-CE2	-5.17	1.30	1.37
3	P	50	TRP	NE1-CE2	-5.16	1.30	1.37
3	S	50	TRP	NE1-CE2	-5.16	1.30	1.37
3	H	97	TYR	CB-CG	-5.16	1.44	1.51
3	Q	97	TYR	CB-CG	-5.16	1.44	1.51
2	J	632	GLU	CD-OE1	-5.16	1.20	1.25
2	N	632	GLU	CD-OE1	-5.16	1.20	1.25
3	O	50	TRP	NE1-CE2	-5.15	1.30	1.37
3	R	50	TRP	NE1-CE2	-5.15	1.30	1.37
3	P	97	TYR	CB-CG	-5.15	1.44	1.51
3	S	97	TYR	CB-CG	-5.15	1.44	1.51
2	I	632	GLU	CD-OE1	-5.14	1.20	1.25
2	M	632	GLU	CD-OE1	-5.14	1.20	1.25
2	B	632	GLU	CD-OE1	-5.14	1.20	1.25
3	O	97	TYR	CB-CG	-5.14	1.44	1.51
2	K	632	GLU	CD-OE1	-5.14	1.20	1.25
3	R	97	TYR	CB-CG	-5.14	1.44	1.51
1	C	277	PHE	CB-CG	-5.08	1.42	1.51
1	F	277	PHE	CB-CG	-5.08	1.42	1.51
1	A	277	PHE	CB-CG	-5.08	1.42	1.51
1	E	277	PHE	CB-CG	-5.08	1.42	1.51
1	C	83	GLU	CD-OE2	-5.08	1.20	1.25
1	F	83	GLU	CD-OE2	-5.08	1.20	1.25
1	C	482	GLU	CD-OE1	-5.06	1.20	1.25
1	F	482	GLU	CD-OE1	-5.06	1.20	1.25
1	D	277	PHE	CB-CG	-5.05	1.42	1.51
1	G	277	PHE	CB-CG	-5.05	1.42	1.51
1	D	57	ASP	CB-CG	5.05	1.62	1.51
1	G	57	ASP	CB-CG	5.05	1.62	1.51
1	D	482	GLU	CD-OE1	-5.05	1.20	1.25
1	G	482	GLU	CD-OE1	-5.05	1.20	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	83	GLU	CD-OE2	-5.04	1.20	1.25
1	G	83	GLU	CD-OE2	-5.04	1.20	1.25
1	A	57	ASP	CB-CG	5.04	1.62	1.51
1	E	57	ASP	CB-CG	5.04	1.62	1.51
1	C	57	ASP	CB-CG	5.04	1.62	1.51
1	F	57	ASP	CB-CG	5.04	1.62	1.51
1	A	482	GLU	CD-OE1	-5.03	1.20	1.25
1	E	482	GLU	CD-OE1	-5.03	1.20	1.25
1	A	83	GLU	CD-OE2	-5.02	1.20	1.25
1	E	83	GLU	CD-OE2	-5.02	1.20	1.25

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	315	ARG	NE-CZ-NH2	-6.77	116.92	120.30
1	G	315	ARG	NE-CZ-NH2	-6.77	116.92	120.30
1	A	315	ARG	NE-CZ-NH2	-6.70	116.95	120.30
1	E	315	ARG	NE-CZ-NH2	-6.70	116.95	120.30
1	C	315	ARG	NE-CZ-NH2	-6.69	116.95	120.30
1	F	315	ARG	NE-CZ-NH2	-6.69	116.95	120.30
1	C	40	TYR	CB-CG-CD1	-6.56	117.06	121.00
1	F	40	TYR	CB-CG-CD1	-6.56	117.06	121.00
1	A	40	TYR	CB-CG-CD1	-6.56	117.07	121.00
1	E	40	TYR	CB-CG-CD1	-6.56	117.07	121.00
1	D	40	TYR	CB-CG-CD1	-6.54	117.07	121.00
1	G	40	TYR	CB-CG-CD1	-6.54	117.07	121.00
1	C	504	ARG	NE-CZ-NH2	-6.01	117.30	120.30
1	F	504	ARG	NE-CZ-NH2	-6.01	117.30	120.30
1	A	504	ARG	NE-CZ-NH2	-6.01	117.30	120.30
1	E	504	ARG	NE-CZ-NH2	-6.01	117.30	120.30
1	D	504	ARG	NE-CZ-NH2	-5.99	117.30	120.30
1	G	504	ARG	NE-CZ-NH2	-5.99	117.30	120.30
2	B	542	ARG	NE-CZ-NH2	-5.65	117.48	120.30
2	K	542	ARG	NE-CZ-NH2	-5.65	117.48	120.30
2	I	542	ARG	NE-CZ-NH2	-5.62	117.49	120.30
2	J	542	ARG	NE-CZ-NH2	-5.62	117.49	120.30
2	M	542	ARG	NE-CZ-NH2	-5.62	117.49	120.30
2	N	542	ARG	NE-CZ-NH2	-5.62	117.49	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3387	0	3362	5	0
1	C	3387	0	3362	7	0
1	D	3387	0	3362	5	0
1	E	3387	0	3362	5	0
1	F	3387	0	3362	6	0
1	G	3387	0	3362	6	0
2	B	1017	0	989	1	0
2	I	1017	0	989	1	0
2	J	1017	0	989	2	0
2	K	1017	0	989	1	0
2	M	1017	0	989	2	0
2	N	1017	0	989	2	0
3	H	923	0	883	3	0
3	O	923	0	883	3	0
3	P	923	0	883	3	0
3	Q	923	0	883	3	0
3	R	923	0	883	3	0
3	S	923	0	883	3	0
4	L	809	0	793	0	0
4	T	809	0	793	0	0
4	U	809	0	793	0	0
4	V	809	0	793	0	0
4	W	809	0	793	0	0
4	X	809	0	793	0	0
5	0	61	0	50	1	0
5	3	61	0	49	1	0
5	7	61	0	50	1	0
5	AA	61	0	49	1	0
5	Y	61	0	50	1	0
5	b	61	0	49	0	0
5	f	61	0	50	0	0
5	i	61	0	49	0	0
5	m	61	0	50	0	0
5	p	61	0	49	0	0
5	t	61	0	50	0	0
5	w	61	0	49	0	0
6	1	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	4	28	0	25	0	0
6	8	28	0	25	0	0
6	BA	28	0	25	0	0
6	Z	28	0	25	0	0
6	c	28	0	25	0	0
6	g	28	0	25	0	0
6	j	28	0	25	0	0
6	n	28	0	25	0	0
6	q	28	0	25	0	0
6	u	28	0	25	0	0
6	x	28	0	25	0	0
7	2	50	0	41	0	0
7	9	50	0	41	0	0
7	a	50	0	41	0	0
7	h	50	0	41	0	0
7	o	50	0	41	0	0
7	v	50	0	41	0	0
8	5	39	0	33	0	0
8	6	39	0	33	0	0
8	CA	39	0	33	0	0
8	DA	39	0	33	0	0
8	d	39	0	33	0	0
8	e	39	0	33	0	0
8	k	39	0	33	0	0
8	l	39	0	33	0	0
8	r	39	0	33	0	0
8	s	39	0	33	0	0
8	y	39	0	33	0	0
8	z	39	0	33	0	0
9	A	42	0	39	0	0
9	C	42	0	39	0	0
9	D	42	0	39	0	0
9	E	42	0	39	0	0
9	F	42	0	39	0	0
9	G	42	0	39	0	0
All	All	38904	0	37932	64	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 1.

All (64) 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:A:197:ASN:OD1	1:A:197:ASN:N	2.38	0.57
1:F:197:ASN:OD1	1:F:197:ASN:N	2.38	0.57
5:0:3:BMA:O2	5:0:4:MAN:C1	2.53	0.56
5:7:3:BMA:O2	5:7:4:MAN:C1	2.53	0.55
5:Y:3:BMA:O2	5:Y:4:MAN:C1	2.53	0.55
1:F:261:LEU:HD11	5:3:1:NAG:H82	1.90	0.54
3:O:7:SER:OG	3:O:8:GLY:N	2.42	0.53
1:D:197:ASN:OD1	1:D:197:ASN:N	2.38	0.53
3:R:7:SER:OG	3:R:8:GLY:N	2.42	0.52
1:G:261:LEU:HD11	5:AA:1:NAG:H82	1.90	0.52
3:Q:7:SER:OG	3:Q:8:GLY:N	2.42	0.52
1:E:197:ASN:OD1	1:E:197:ASN:N	2.38	0.52
3:H:7:SER:OG	3:H:8:GLY:N	2.42	0.52
1:G:197:ASN:OD1	1:G:197:ASN:N	2.38	0.52
3:P:7:SER:OG	3:P:8:GLY:N	2.42	0.50
1:E:199:SER:OG	1:E:200:VAL:N	2.46	0.48
1:C:199:SER:OG	1:C:200:VAL:N	2.46	0.48
1:D:199:SER:OG	1:D:200:VAL:N	2.46	0.48
1:C:197:ASN:OD1	1:C:197:ASN:N	2.38	0.48
1:E:162:THR:O	1:E:163:THR:C	2.52	0.48
1:G:164:SER:OG	1:G:165:MET:N	2.47	0.48
1:C:162:THR:O	1:C:163:THR:C	2.52	0.48
1:F:199:SER:OG	1:F:200:VAL:N	2.46	0.48
1:G:199:SER:OG	1:G:200:VAL:N	2.46	0.48
1:F:162:THR:O	1:F:163:THR:C	2.52	0.48
3:S:7:SER:OG	3:S:8:GLY:N	2.42	0.47
1:A:162:THR:O	1:A:163:THR:C	2.52	0.47
1:C:164:SER:OG	1:C:165:MET:N	2.47	0.47
1:D:162:THR:O	1:D:163:THR:C	2.52	0.47
1:A:164:SER:OG	1:A:165:MET:N	2.47	0.47
2:M:637:ASN:OD1	2:M:637:ASN:N	2.46	0.47
1:A:199:SER:OG	1:A:200:VAL:N	2.46	0.47
1:F:164:SER:OG	1:F:165:MET:N	2.47	0.47
2:J:637:ASN:OD1	2:J:637:ASN:N	2.46	0.47
1:E:164:SER:OG	1:E:165:MET:N	2.47	0.46
1:D:164:SER:OG	1:D:165:MET:N	2.47	0.46
2:N:522:PHE:O	2:N:540:GLN:NE2	2.49	0.45
2:K:522:PHE:O	2:K:540:GLN:NE2	2.49	0.45
2:M:522:PHE:O	2:M:540:GLN:NE2	2.49	0.45
2:J:522:PHE:O	2:J:540:GLN:NE2	2.49	0.45
1:G:162:THR:O	1:G:163:THR:C	2.52	0.45
2:B:522:PHE:O	2:B:540:GLN:NE2	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:522:PHE:O	2:I:540:GLN:NE2	2.49	0.43
3:H:95:ASP:HB3	3:H:97:TYR:CZ	2.54	0.43
3:O:95:ASP:HB3	3:O:97:TYR:CZ	2.54	0.43
1:F:117:LYS:N	1:F:118:PRO:CD	2.82	0.43
3:R:95:ASP:HB3	3:R:97:TYR:CZ	2.54	0.43
3:S:95:ASP:HB3	3:S:97:TYR:CZ	2.54	0.43
1:D:117:LYS:N	1:D:118:PRO:CD	2.82	0.43
1:G:117:LYS:N	1:G:118:PRO:CD	2.82	0.43
1:A:117:LYS:N	1:A:118:PRO:CD	2.82	0.42
3:P:95:ASP:HB3	3:P:97:TYR:CZ	2.54	0.42
1:E:117:LYS:N	1:E:118:PRO:CD	2.82	0.42
3:Q:95:ASP:HB3	3:Q:97:TYR:CZ	2.54	0.42
1:C:117:LYS:N	1:C:118:PRO:CD	2.82	0.42
3:Q:95:ASP:HB3	3:Q:97:TYR:CE1	2.55	0.42
3:R:95:ASP:HB3	3:R:97:TYR:CE1	2.55	0.42
2:N:637:ASN:OD1	2:N:637:ASN:N	2.46	0.41
3:S:95:ASP:HB3	3:S:97:TYR:CE1	2.55	0.41
1:C:377:ASN:OD1	1:C:377:ASN:N	2.48	0.41
3:P:95:ASP:HB3	3:P:97:TYR:CE1	2.55	0.41
1:C:289:ASN:OD1	1:C:289:ASN:N	2.50	0.41
3:O:95:ASP:HB3	3:O:97:TYR:CE1	2.55	0.41
3:H:95:ASP:HB3	3:H:97:TYR:CE1	2.55	0.41

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	420/512 (82%)	408 (97%)	11 (3%)	1 (0%)	44	78
1	C	420/512 (82%)	408 (97%)	11 (3%)	1 (0%)	44	78
1	D	420/512 (82%)	408 (97%)	11 (3%)	1 (0%)	44	78

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	420/512 (82%)	408 (97%)	11 (3%)	1 (0%)	44	78
1	F	420/512 (82%)	408 (97%)	11 (3%)	1 (0%)	44	78
1	G	420/512 (82%)	408 (97%)	11 (3%)	1 (0%)	44	78
2	B	124/153 (81%)	118 (95%)	6 (5%)	0	100	100
2	I	124/153 (81%)	118 (95%)	6 (5%)	0	100	100
2	J	124/153 (81%)	118 (95%)	6 (5%)	0	100	100
2	K	124/153 (81%)	118 (95%)	6 (5%)	0	100	100
2	M	124/153 (81%)	118 (95%)	6 (5%)	0	100	100
2	N	124/153 (81%)	118 (95%)	6 (5%)	0	100	100
3	H	117/222 (53%)	116 (99%)	0	1 (1%)	14	51
3	O	117/222 (53%)	116 (99%)	0	1 (1%)	14	51
3	P	117/222 (53%)	116 (99%)	0	1 (1%)	14	51
3	Q	117/222 (53%)	116 (99%)	0	1 (1%)	14	51
3	R	117/222 (53%)	116 (99%)	0	1 (1%)	14	51
3	S	117/222 (53%)	116 (99%)	0	1 (1%)	14	51
4	L	104/210 (50%)	96 (92%)	7 (7%)	1 (1%)	13	49
4	T	104/210 (50%)	96 (92%)	7 (7%)	1 (1%)	13	49
4	U	104/210 (50%)	96 (92%)	7 (7%)	1 (1%)	13	49
4	V	104/210 (50%)	96 (92%)	7 (7%)	1 (1%)	13	49
4	W	104/210 (50%)	96 (92%)	7 (7%)	1 (1%)	13	49
4	X	104/210 (50%)	96 (92%)	7 (7%)	1 (1%)	13	49
All	All	4590/6582 (70%)	4428 (96%)	144 (3%)	18 (0%)	32	68

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	58	ALA
1	C	58	ALA
1	D	58	ALA
1	E	58	ALA
1	F	58	ALA
1	G	58	ALA
3	H	7	SER
4	L	52	SER
3	O	7	SER

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Mol	Chain	Res	Type
4	T	52	SER
3	P	7	SER
4	U	52	SER
3	Q	7	SER
4	V	52	SER
3	R	7	SER
4	W	52	SER
3	S	7	SER
4	X	52	SER

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	386/454 (85%)	385 (100%)	1 (0%)	91	91
1	C	386/454 (85%)	385 (100%)	1 (0%)	91	91
1	D	386/454 (85%)	385 (100%)	1 (0%)	91	91
1	E	386/454 (85%)	385 (100%)	1 (0%)	91	91
1	F	386/454 (85%)	385 (100%)	1 (0%)	91	91
1	G	386/454 (85%)	385 (100%)	1 (0%)	91	91
2	B	108/130 (83%)	108 (100%)	0	100	100
2	I	108/130 (83%)	108 (100%)	0	100	100
2	J	108/130 (83%)	108 (100%)	0	100	100
2	K	108/130 (83%)	108 (100%)	0	100	100
2	M	108/130 (83%)	108 (100%)	0	100	100
2	N	108/130 (83%)	108 (100%)	0	100	100
3	H	97/186 (52%)	96 (99%)	1 (1%)	73	81
3	O	97/186 (52%)	96 (99%)	1 (1%)	73	81
3	P	97/186 (52%)	96 (99%)	1 (1%)	73	81
3	Q	97/186 (52%)	96 (99%)	1 (1%)	73	81
3	R	97/186 (52%)	96 (99%)	1 (1%)	73	81

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	S	97/186 (52%)	96 (99%)	1 (1%)	73	81
4	L	90/183 (49%)	90 (100%)	0	100	100
4	T	90/183 (49%)	90 (100%)	0	100	100
4	U	90/183 (49%)	90 (100%)	0	100	100
4	V	90/183 (49%)	90 (100%)	0	100	100
4	W	90/183 (49%)	90 (100%)	0	100	100
4	X	90/183 (49%)	90 (100%)	0	100	100
All	All	4086/5718 (72%)	4074 (100%)	12 (0%)	90	91

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

Mol	Chain	Res	Type
1	A	197	ASN
3	H	71	ARG
1	C	197	ASN
3	O	71	ARG
1	D	197	ASN
3	P	71	ARG
1	E	197	ASN
3	Q	71	ARG
1	F	197	ASN
3	R	71	ARG
1	G	197	ASN
3	S	71	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	422	GLN
3	H	64	GLN
1	C	422	GLN
3	O	64	GLN
1	D	422	GLN
3	P	64	GLN
1	E	422	GLN
3	Q	64	GLN
1	F	422	GLN
3	R	64	GLN

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Mol	Chain	Res	Type
1	G	422	GLN
3	S	64	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)

144 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	0	1	1,5	14,14,15	0.94	0	17,19,21	1.87	5 (29%)
5	NAG	0	2	5	14,14,15	0.81	0	17,19,21	1.25	3 (17%)
5	BMA	0	3	5	11,11,12	1.83	1 (9%)	15,15,17	1.05	1 (6%)
5	MAN	0	4	5	11,11,12	0.56	0	15,15,17	2.58	4 (26%)
5	MAN	0	5	5	11,11,12	1.84	2 (18%)	15,15,17	0.95	1 (6%)
6	NAG	1	1	1,6	14,14,15	0.88	0	17,19,21	0.94	1 (5%)
6	NAG	1	2	6	14,14,15	0.80	0	17,19,21	1.00	1 (5%)
7	NAG	2	1	1,7	14,14,15	0.78	0	17,19,21	1.09	1 (5%)
7	NAG	2	2	7	14,14,15	0.81	0	17,19,21	0.95	1 (5%)
7	BMA	2	3	7	11,11,12	1.91	3 (27%)	15,15,17	1.08	1 (6%)
7	MAN	2	4	7	11,11,12	1.82	2 (18%)	15,15,17	0.99	2 (13%)
5	NAG	3	1	1,5	14,14,15	1.05	1 (7%)	17,19,21	1.37	3 (17%)
5	NAG	3	2	5	14,14,15	0.80	0	17,19,21	1.41	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	BMA	3	3	5	11,11,12	1.82	2 (18%)	15,15,17	0.86	1 (6%)
5	MAN	3	4	5	11,11,12	1.80	2 (18%)	15,15,17	1.08	2 (13%)
5	MAN	3	5	5	11,11,12	1.80	2 (18%)	15,15,17	0.91	0
6	NAG	4	1	1,6	14,14,15	0.66	0	17,19,21	1.69	3 (17%)
6	NAG	4	2	6	14,14,15	1.18	1 (7%)	17,19,21	1.20	2 (11%)
8	NAG	5	1	1,8	14,14,15	0.84	0	17,19,21	0.86	0
8	NAG	5	2	8	14,14,15	0.83	0	17,19,21	0.94	0
8	BMA	5	3	8	11,11,12	1.79	2 (18%)	15,15,17	0.84	1 (6%)
8	NAG	6	1	1,8	14,14,15	0.87	0	17,19,21	0.84	0
8	NAG	6	2	8	14,14,15	0.76	0	17,19,21	0.91	1 (5%)
8	BMA	6	3	8	11,11,12	1.82	2 (18%)	15,15,17	0.79	0
5	NAG	7	1	1,5	14,14,15	0.93	0	17,19,21	1.87	5 (29%)
5	NAG	7	2	5	14,14,15	0.81	0	17,19,21	1.26	3 (17%)
5	BMA	7	3	5	11,11,12	1.83	1 (9%)	15,15,17	1.05	1 (6%)
5	MAN	7	4	5	11,11,12	0.56	0	15,15,17	2.58	4 (26%)
5	MAN	7	5	5	11,11,12	1.84	2 (18%)	15,15,17	0.95	1 (6%)
6	NAG	8	1	1,6	14,14,15	0.88	0	17,19,21	0.94	1 (5%)
6	NAG	8	2	6	14,14,15	0.80	0	17,19,21	1.01	1 (5%)
7	NAG	9	1	1,7	14,14,15	0.78	0	17,19,21	1.09	1 (5%)
7	NAG	9	2	7	14,14,15	0.81	0	17,19,21	0.95	1 (5%)
7	BMA	9	3	7	11,11,12	1.91	3 (27%)	15,15,17	1.08	1 (6%)
7	MAN	9	4	7	11,11,12	1.82	2 (18%)	15,15,17	0.98	2 (13%)
5	NAG	AA	1	1,5	14,14,15	1.05	1 (7%)	17,19,21	1.36	3 (17%)
5	NAG	AA	2	5	14,14,15	0.80	0	17,19,21	1.41	2 (11%)
5	BMA	AA	3	5	11,11,12	1.83	2 (18%)	15,15,17	0.87	1 (6%)
5	MAN	AA	4	5	11,11,12	1.80	2 (18%)	15,15,17	1.08	2 (13%)
5	MAN	AA	5	5	11,11,12	1.81	2 (18%)	15,15,17	0.91	0
6	NAG	BA	1	1,6	14,14,15	0.66	0	17,19,21	1.68	3 (17%)
6	NAG	BA	2	6	14,14,15	1.18	1 (7%)	17,19,21	1.20	2 (11%)
8	NAG	CA	1	1,8	14,14,15	0.83	0	17,19,21	0.86	0
8	NAG	CA	2	8	14,14,15	0.83	0	17,19,21	0.94	0
8	BMA	CA	3	8	11,11,12	1.79	2 (18%)	15,15,17	0.84	1 (6%)
8	NAG	DA	1	1,8	14,14,15	0.86	0	17,19,21	0.84	0
8	NAG	DA	2	8	14,14,15	0.76	0	17,19,21	0.91	1 (5%)
8	BMA	DA	3	8	11,11,12	1.82	2 (18%)	15,15,17	0.79	0
5	NAG	Y	1	1,5	14,14,15	0.93	0	17,19,21	1.87	5 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	NAG	Y	2	5	14,14,15	0.81	0	17,19,21	1.25	3 (17%)
5	BMA	Y	3	5	11,11,12	1.84	1 (9%)	15,15,17	1.05	1 (6%)
5	MAN	Y	4	5	11,11,12	0.56	0	15,15,17	2.58	4 (26%)
5	MAN	Y	5	5	11,11,12	1.84	2 (18%)	15,15,17	0.95	1 (6%)
6	NAG	Z	1	1,6	14,14,15	0.88	0	17,19,21	0.94	1 (5%)
6	NAG	Z	2	6	14,14,15	0.81	0	17,19,21	1.01	1 (5%)
7	NAG	a	1	1,7	14,14,15	0.78	0	17,19,21	1.10	1 (5%)
7	NAG	a	2	7	14,14,15	0.80	0	17,19,21	0.95	1 (5%)
7	BMA	a	3	7	11,11,12	1.91	3 (27%)	15,15,17	1.08	1 (6%)
7	MAN	a	4	7	11,11,12	1.81	2 (18%)	15,15,17	0.99	2 (13%)
5	NAG	b	1	1,5	14,14,15	1.05	1 (7%)	17,19,21	1.37	3 (17%)
5	NAG	b	2	5	14,14,15	0.79	0	17,19,21	1.41	2 (11%)
5	BMA	b	3	5	11,11,12	1.83	2 (18%)	15,15,17	0.87	1 (6%)
5	MAN	b	4	5	11,11,12	1.80	2 (18%)	15,15,17	1.08	2 (13%)
5	MAN	b	5	5	11,11,12	1.81	2 (18%)	15,15,17	0.92	0
6	NAG	c	1	1,6	14,14,15	0.66	0	17,19,21	1.69	3 (17%)
6	NAG	c	2	6	14,14,15	1.18	1 (7%)	17,19,21	1.20	2 (11%)
8	NAG	d	1	1,8	14,14,15	0.84	0	17,19,21	0.86	0
8	NAG	d	2	8	14,14,15	0.83	0	17,19,21	0.93	0
8	BMA	d	3	8	11,11,12	1.78	2 (18%)	15,15,17	0.84	1 (6%)
8	NAG	e	1	1,8	14,14,15	0.87	0	17,19,21	0.83	0
8	NAG	e	2	8	14,14,15	0.76	0	17,19,21	0.91	1 (5%)
8	BMA	e	3	8	11,11,12	1.82	2 (18%)	15,15,17	0.79	0
5	NAG	f	1	1,5	14,14,15	0.94	0	17,19,21	1.87	5 (29%)
5	NAG	f	2	5	14,14,15	0.81	0	17,19,21	1.25	3 (17%)
5	BMA	f	3	5	11,11,12	1.83	1 (9%)	15,15,17	1.05	1 (6%)
5	MAN	f	4	5	11,11,12	0.56	0	15,15,17	2.58	4 (26%)
5	MAN	f	5	5	11,11,12	1.84	2 (18%)	15,15,17	0.95	1 (6%)
6	NAG	g	1	1,6	14,14,15	0.88	0	17,19,21	0.94	1 (5%)
6	NAG	g	2	6	14,14,15	0.80	0	17,19,21	1.00	1 (5%)
7	NAG	h	1	1,7	14,14,15	0.78	0	17,19,21	1.09	1 (5%)
7	NAG	h	2	7	14,14,15	0.81	0	17,19,21	0.95	1 (5%)
7	BMA	h	3	7	11,11,12	1.91	3 (27%)	15,15,17	1.08	1 (6%)
7	MAN	h	4	7	11,11,12	1.82	2 (18%)	15,15,17	0.99	2 (13%)
5	NAG	i	1	1,5	14,14,15	1.05	1 (7%)	17,19,21	1.37	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	NAG	i	2	5	14,14,15	0.80	0	17,19,21	1.41	2 (11%)
5	BMA	i	3	5	11,11,12	1.82	2 (18%)	15,15,17	0.86	1 (6%)
5	MAN	i	4	5	11,11,12	1.80	2 (18%)	15,15,17	1.08	2 (13%)
5	MAN	i	5	5	11,11,12	1.80	2 (18%)	15,15,17	0.91	0
6	NAG	j	1	1,6	14,14,15	0.66	0	17,19,21	1.69	3 (17%)
6	NAG	j	2	6	14,14,15	1.18	1 (7%)	17,19,21	1.20	2 (11%)
8	NAG	k	1	1,8	14,14,15	0.84	0	17,19,21	0.86	0
8	NAG	k	2	8	14,14,15	0.83	0	17,19,21	0.94	0
8	BMA	k	3	8	11,11,12	1.79	2 (18%)	15,15,17	0.84	1 (6%)
8	NAG	l	1	1,8	14,14,15	0.87	0	17,19,21	0.84	0
8	NAG	l	2	8	14,14,15	0.76	0	17,19,21	0.91	1 (5%)
8	BMA	l	3	8	11,11,12	1.82	2 (18%)	15,15,17	0.79	0
5	NAG	m	1	1,5	14,14,15	0.93	0	17,19,21	1.87	5 (29%)
5	NAG	m	2	5	14,14,15	0.81	0	17,19,21	1.26	3 (17%)
5	BMA	m	3	5	11,11,12	1.83	1 (9%)	15,15,17	1.05	1 (6%)
5	MAN	m	4	5	11,11,12	0.56	0	15,15,17	2.58	4 (26%)
5	MAN	m	5	5	11,11,12	1.84	2 (18%)	15,15,17	0.95	1 (6%)
6	NAG	n	1	1,6	14,14,15	0.88	0	17,19,21	0.94	1 (5%)
6	NAG	n	2	6	14,14,15	0.80	0	17,19,21	1.01	1 (5%)
7	NAG	o	1	1,7	14,14,15	0.78	0	17,19,21	1.09	1 (5%)
7	NAG	o	2	7	14,14,15	0.81	0	17,19,21	0.95	1 (5%)
7	BMA	o	3	7	11,11,12	1.91	3 (27%)	15,15,17	1.08	1 (6%)
7	MAN	o	4	7	11,11,12	1.82	2 (18%)	15,15,17	0.98	2 (13%)
5	NAG	p	1	1,5	14,14,15	1.05	1 (7%)	17,19,21	1.36	3 (17%)
5	NAG	p	2	5	14,14,15	0.80	0	17,19,21	1.41	2 (11%)
5	BMA	p	3	5	11,11,12	1.83	2 (18%)	15,15,17	0.87	1 (6%)
5	MAN	p	4	5	11,11,12	1.80	2 (18%)	15,15,17	1.08	2 (13%)
5	MAN	p	5	5	11,11,12	1.81	2 (18%)	15,15,17	0.91	0
6	NAG	q	1	1,6	14,14,15	0.66	0	17,19,21	1.68	3 (17%)
6	NAG	q	2	6	14,14,15	1.18	1 (7%)	17,19,21	1.20	2 (11%)
8	NAG	r	1	1,8	14,14,15	0.83	0	17,19,21	0.86	0
8	NAG	r	2	8	14,14,15	0.83	0	17,19,21	0.94	0
8	BMA	r	3	8	11,11,12	1.79	2 (18%)	15,15,17	0.84	1 (6%)
8	NAG	s	1	1,8	14,14,15	0.86	0	17,19,21	0.84	0
8	NAG	s	2	8	14,14,15	0.76	0	17,19,21	0.91	1 (5%)
8	BMA	s	3	8	11,11,12	1.82	2 (18%)	15,15,17	0.79	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	NAG	t	1	1,5	14,14,15	0.93	0	17,19,21	1.87	5 (29%)
5	NAG	t	2	5	14,14,15	0.81	0	17,19,21	1.25	3 (17%)
5	BMA	t	3	5	11,11,12	1.84	1 (9%)	15,15,17	1.05	1 (6%)
5	MAN	t	4	5	11,11,12	0.56	0	15,15,17	2.58	4 (26%)
5	MAN	t	5	5	11,11,12	1.84	2 (18%)	15,15,17	0.95	1 (6%)
6	NAG	u	1	1,6	14,14,15	0.88	0	17,19,21	0.94	1 (5%)
6	NAG	u	2	6	14,14,15	0.81	0	17,19,21	1.01	1 (5%)
7	NAG	v	1	1,7	14,14,15	0.78	0	17,19,21	1.10	1 (5%)
7	NAG	v	2	7	14,14,15	0.80	0	17,19,21	0.95	1 (5%)
7	BMA	v	3	7	11,11,12	1.91	3 (27%)	15,15,17	1.08	1 (6%)
7	MAN	v	4	7	11,11,12	1.81	2 (18%)	15,15,17	0.99	2 (13%)
5	NAG	w	1	1,5	14,14,15	1.05	1 (7%)	17,19,21	1.37	3 (17%)
5	NAG	w	2	5	14,14,15	0.79	0	17,19,21	1.41	2 (11%)
5	BMA	w	3	5	11,11,12	1.83	2 (18%)	15,15,17	0.87	1 (6%)
5	MAN	w	4	5	11,11,12	1.80	2 (18%)	15,15,17	1.08	2 (13%)
5	MAN	w	5	5	11,11,12	1.81	2 (18%)	15,15,17	0.92	0
6	NAG	x	1	1,6	14,14,15	0.66	0	17,19,21	1.69	3 (17%)
6	NAG	x	2	6	14,14,15	1.18	1 (7%)	17,19,21	1.20	2 (11%)
8	NAG	y	1	1,8	14,14,15	0.84	0	17,19,21	0.86	0
8	NAG	y	2	8	14,14,15	0.83	0	17,19,21	0.93	0
8	BMA	y	3	8	11,11,12	1.78	2 (18%)	15,15,17	0.84	1 (6%)
8	NAG	z	1	1,8	14,14,15	0.87	0	17,19,21	0.83	0
8	NAG	z	2	8	14,14,15	0.76	0	17,19,21	0.91	1 (5%)
8	BMA	z	3	8	11,11,12	1.82	2 (18%)	15,15,17	0.79	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
5	NAG	0	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	0	2	5	-	2/6/23/26	0/1/1/1
5	BMA	0	3	5	-	2/2/19/22	0/1/1/1
5	MAN	0	4	5	-	2/2/19/22	0/1/1/1
5	MAN	0	5	5	-	2/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	1	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	1	2	6	-	1/6/23/26	0/1/1/1
7	NAG	2	1	1,7	-	0/6/23/26	0/1/1/1
7	NAG	2	2	7	-	1/6/23/26	0/1/1/1
7	BMA	2	3	7	-	1/2/19/22	0/1/1/1
7	MAN	2	4	7	-	2/2/19/22	0/1/1/1
5	NAG	3	1	1,5	-	3/6/23/26	0/1/1/1
5	NAG	3	2	5	-	2/6/23/26	0/1/1/1
5	BMA	3	3	5	-	2/2/19/22	0/1/1/1
5	MAN	3	4	5	-	2/2/19/22	0/1/1/1
5	MAN	3	5	5	-	1/2/19/22	0/1/1/1
6	NAG	4	1	1,6	-	1/6/23/26	0/1/1/1
6	NAG	4	2	6	-	2/6/23/26	0/1/1/1
8	NAG	5	1	1,8	-	2/6/23/26	0/1/1/1
8	NAG	5	2	8	-	0/6/23/26	0/1/1/1
8	BMA	5	3	8	-	1/2/19/22	0/1/1/1
8	NAG	6	1	1,8	-	0/6/23/26	0/1/1/1
8	NAG	6	2	8	-	1/6/23/26	0/1/1/1
8	BMA	6	3	8	-	1/2/19/22	0/1/1/1
5	NAG	7	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	7	2	5	-	2/6/23/26	0/1/1/1
5	BMA	7	3	5	-	2/2/19/22	0/1/1/1
5	MAN	7	4	5	-	2/2/19/22	0/1/1/1
5	MAN	7	5	5	-	2/2/19/22	0/1/1/1
6	NAG	8	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	8	2	6	-	1/6/23/26	0/1/1/1
7	NAG	9	1	1,7	-	0/6/23/26	0/1/1/1
7	NAG	9	2	7	-	1/6/23/26	0/1/1/1
7	BMA	9	3	7	-	1/2/19/22	0/1/1/1
7	MAN	9	4	7	-	2/2/19/22	0/1/1/1
5	NAG	AA	1	1,5	-	3/6/23/26	0/1/1/1
5	NAG	AA	2	5	-	2/6/23/26	0/1/1/1
5	BMA	AA	3	5	-	2/2/19/22	0/1/1/1
5	MAN	AA	4	5	-	2/2/19/22	0/1/1/1
5	MAN	AA	5	5	-	1/2/19/22	0/1/1/1
6	NAG	BA	1	1,6	-	1/6/23/26	0/1/1/1
6	NAG	BA	2	6	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	NAG	CA	1	1,8	-	2/6/23/26	0/1/1/1
8	NAG	CA	2	8	-	0/6/23/26	0/1/1/1
8	BMA	CA	3	8	-	1/2/19/22	0/1/1/1
8	NAG	DA	1	1,8	-	0/6/23/26	0/1/1/1
8	NAG	DA	2	8	-	1/6/23/26	0/1/1/1
8	BMA	DA	3	8	-	1/2/19/22	0/1/1/1
5	NAG	Y	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	Y	2	5	-	2/6/23/26	0/1/1/1
5	BMA	Y	3	5	-	2/2/19/22	0/1/1/1
5	MAN	Y	4	5	-	2/2/19/22	0/1/1/1
5	MAN	Y	5	5	-	2/2/19/22	0/1/1/1
6	NAG	Z	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	Z	2	6	-	1/6/23/26	0/1/1/1
7	NAG	a	1	1,7	-	0/6/23/26	0/1/1/1
7	NAG	a	2	7	-	1/6/23/26	0/1/1/1
7	BMA	a	3	7	-	1/2/19/22	0/1/1/1
7	MAN	a	4	7	-	2/2/19/22	0/1/1/1
5	NAG	b	1	1,5	-	3/6/23/26	0/1/1/1
5	NAG	b	2	5	-	2/6/23/26	0/1/1/1
5	BMA	b	3	5	-	2/2/19/22	0/1/1/1
5	MAN	b	4	5	-	2/2/19/22	0/1/1/1
5	MAN	b	5	5	-	1/2/19/22	0/1/1/1
6	NAG	c	1	1,6	-	1/6/23/26	0/1/1/1
6	NAG	c	2	6	-	2/6/23/26	0/1/1/1
8	NAG	d	1	1,8	-	2/6/23/26	0/1/1/1
8	NAG	d	2	8	-	0/6/23/26	0/1/1/1
8	BMA	d	3	8	-	1/2/19/22	0/1/1/1
8	NAG	e	1	1,8	-	0/6/23/26	0/1/1/1
8	NAG	e	2	8	-	1/6/23/26	0/1/1/1
8	BMA	e	3	8	-	1/2/19/22	0/1/1/1
5	NAG	f	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	f	2	5	-	2/6/23/26	0/1/1/1
5	BMA	f	3	5	-	2/2/19/22	0/1/1/1
5	MAN	f	4	5	-	2/2/19/22	0/1/1/1
5	MAN	f	5	5	-	2/2/19/22	0/1/1/1
6	NAG	g	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	g	2	6	-	1/6/23/26	0/1/1/1
7	NAG	h	1	1,7	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	h	2	7	-	1/6/23/26	0/1/1/1
7	BMA	h	3	7	-	1/2/19/22	0/1/1/1
7	MAN	h	4	7	-	2/2/19/22	0/1/1/1
5	NAG	i	1	1,5	-	3/6/23/26	0/1/1/1
5	NAG	i	2	5	-	2/6/23/26	0/1/1/1
5	BMA	i	3	5	-	2/2/19/22	0/1/1/1
5	MAN	i	4	5	-	2/2/19/22	0/1/1/1
5	MAN	i	5	5	-	1/2/19/22	0/1/1/1
6	NAG	j	1	1,6	-	1/6/23/26	0/1/1/1
6	NAG	j	2	6	-	2/6/23/26	0/1/1/1
8	NAG	k	1	1,8	-	2/6/23/26	0/1/1/1
8	NAG	k	2	8	-	0/6/23/26	0/1/1/1
8	BMA	k	3	8	-	1/2/19/22	0/1/1/1
8	NAG	l	1	1,8	-	0/6/23/26	0/1/1/1
8	NAG	l	2	8	-	1/6/23/26	0/1/1/1
8	BMA	l	3	8	-	1/2/19/22	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	BMA	m	3	5	-	2/2/19/22	0/1/1/1
5	MAN	m	4	5	-	2/2/19/22	0/1/1/1
5	MAN	m	5	5	-	2/2/19/22	0/1/1/1
6	NAG	n	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	n	2	6	-	1/6/23/26	0/1/1/1
7	NAG	o	1	1,7	-	0/6/23/26	0/1/1/1
7	NAG	o	2	7	-	1/6/23/26	0/1/1/1
7	BMA	o	3	7	-	1/2/19/22	0/1/1/1
7	MAN	o	4	7	-	2/2/19/22	0/1/1/1
5	NAG	p	1	1,5	-	3/6/23/26	0/1/1/1
5	NAG	p	2	5	-	2/6/23/26	0/1/1/1
5	BMA	p	3	5	-	2/2/19/22	0/1/1/1
5	MAN	p	4	5	-	2/2/19/22	0/1/1/1
5	MAN	p	5	5	-	1/2/19/22	0/1/1/1
6	NAG	q	1	1,6	-	1/6/23/26	0/1/1/1
6	NAG	q	2	6	-	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	-	0/6/23/26	0/1/1/1
8	BMA	r	3	8	-	1/2/19/22	0/1/1/1
8	NAG	s	1	1,8	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	NAG	s	2	8	-	1/6/23/26	0/1/1/1
8	BMA	s	3	8	-	1/2/19/22	0/1/1/1
5	NAG	t	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	t	2	5	-	2/6/23/26	0/1/1/1
5	BMA	t	3	5	-	2/2/19/22	0/1/1/1
5	MAN	t	4	5	-	2/2/19/22	0/1/1/1
5	MAN	t	5	5	-	2/2/19/22	0/1/1/1
6	NAG	u	1	1,6	-	2/6/23/26	0/1/1/1
6	NAG	u	2	6	-	1/6/23/26	0/1/1/1
7	NAG	v	1	1,7	-	0/6/23/26	0/1/1/1
7	NAG	v	2	7	-	1/6/23/26	0/1/1/1
7	BMA	v	3	7	-	1/2/19/22	0/1/1/1
7	MAN	v	4	7	-	2/2/19/22	0/1/1/1
5	NAG	w	1	1,5	-	3/6/23/26	0/1/1/1
5	NAG	w	2	5	-	2/6/23/26	0/1/1/1
5	BMA	w	3	5	-	2/2/19/22	0/1/1/1
5	MAN	w	4	5	-	2/2/19/22	0/1/1/1
5	MAN	w	5	5	-	1/2/19/22	0/1/1/1
6	NAG	x	1	1,6	-	1/6/23/26	0/1/1/1
6	NAG	x	2	6	-	2/6/23/26	0/1/1/1
8	NAG	y	1	1,8	-	2/6/23/26	0/1/1/1
8	NAG	y	2	8	-	0/6/23/26	0/1/1/1
8	BMA	y	3	8	-	1/2/19/22	0/1/1/1
8	NAG	z	1	1,8	-	0/6/23/26	0/1/1/1
8	NAG	z	2	8	-	1/6/23/26	0/1/1/1
8	BMA	z	3	8	-	1/2/19/22	0/1/1/1

All (120) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	f	5	MAN	O2-C2	-4.28	1.34	1.43
5	0	5	MAN	O2-C2	-4.28	1.34	1.43
7	o	4	MAN	O2-C2	-4.28	1.34	1.43
7	9	4	MAN	O2-C2	-4.28	1.34	1.43
7	h	4	MAN	O2-C2	-4.28	1.34	1.43
7	2	4	MAN	O2-C2	-4.28	1.34	1.43
7	a	4	MAN	O2-C2	-4.28	1.34	1.43
7	v	4	MAN	O2-C2	-4.28	1.34	1.43
5	m	5	MAN	O2-C2	-4.27	1.34	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	7	5	MAN	O2-C2	-4.27	1.34	1.43
5	Y	5	MAN	O2-C2	-4.25	1.34	1.43
5	t	5	MAN	O2-C2	-4.25	1.34	1.43
7	o	3	BMA	O2-C2	-4.22	1.34	1.43
7	9	3	BMA	O2-C2	-4.22	1.34	1.43
7	h	3	BMA	O2-C2	-4.22	1.34	1.43
7	2	3	BMA	O2-C2	-4.22	1.34	1.43
7	a	3	BMA	O2-C2	-4.22	1.34	1.43
7	v	3	BMA	O2-C2	-4.22	1.34	1.43
8	s	3	BMA	O2-C2	-4.18	1.34	1.43
8	DA	3	BMA	O2-C2	-4.18	1.34	1.43
8	l	3	BMA	O2-C2	-4.18	1.34	1.43
8	6	3	BMA	O2-C2	-4.18	1.34	1.43
5	p	5	MAN	O2-C2	-4.17	1.34	1.43
5	AA	5	MAN	O2-C2	-4.17	1.34	1.43
8	e	3	BMA	O2-C2	-4.17	1.34	1.43
8	z	3	BMA	O2-C2	-4.17	1.34	1.43
5	b	5	MAN	O2-C2	-4.16	1.34	1.43
5	w	5	MAN	O2-C2	-4.16	1.34	1.43
5	p	3	BMA	O2-C2	-4.16	1.34	1.43
5	AA	3	BMA	O2-C2	-4.16	1.34	1.43
5	b	3	BMA	O2-C2	-4.15	1.34	1.43
5	w	3	BMA	O2-C2	-4.15	1.34	1.43
5	i	5	MAN	O2-C2	-4.15	1.34	1.43
5	3	5	MAN	O2-C2	-4.15	1.34	1.43
5	f	3	BMA	O2-C2	-4.15	1.34	1.43
5	0	3	BMA	O2-C2	-4.15	1.34	1.43
5	Y	3	BMA	O2-C2	-4.14	1.34	1.43
5	t	3	BMA	O2-C2	-4.14	1.34	1.43
5	i	3	BMA	O2-C2	-4.14	1.34	1.43
5	m	3	BMA	O2-C2	-4.14	1.34	1.43
5	3	3	BMA	O2-C2	-4.14	1.34	1.43
5	7	3	BMA	O2-C2	-4.14	1.34	1.43
8	k	3	BMA	O2-C2	-4.13	1.34	1.43
8	5	3	BMA	O2-C2	-4.13	1.34	1.43
5	i	4	MAN	O2-C2	-4.13	1.34	1.43
5	3	4	MAN	O2-C2	-4.13	1.34	1.43
8	d	3	BMA	O2-C2	-4.12	1.34	1.43
8	y	3	BMA	O2-C2	-4.12	1.34	1.43
8	r	3	BMA	O2-C2	-4.12	1.34	1.43
8	CA	3	BMA	O2-C2	-4.12	1.34	1.43
5	p	4	MAN	O2-C2	-4.12	1.34	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	AA	4	MAN	O2-C2	-4.12	1.34	1.43
5	b	4	MAN	O2-C2	-4.12	1.34	1.43
5	w	4	MAN	O2-C2	-4.12	1.34	1.43
6	j	2	NAG	C1-C2	3.37	1.56	1.52
6	4	2	NAG	C1-C2	3.37	1.56	1.52
6	c	2	NAG	C1-C2	3.36	1.56	1.52
6	q	2	NAG	C1-C2	3.36	1.56	1.52
6	x	2	NAG	C1-C2	3.36	1.56	1.52
6	BA	2	NAG	C1-C2	3.36	1.56	1.52
7	o	3	BMA	C2-C3	-2.52	1.48	1.52
7	9	3	BMA	C2-C3	-2.52	1.48	1.52
7	a	3	BMA	C2-C3	-2.50	1.48	1.52
7	v	3	BMA	C2-C3	-2.50	1.48	1.52
7	h	3	BMA	C2-C3	-2.50	1.48	1.52
7	2	3	BMA	C2-C3	-2.50	1.48	1.52
5	m	5	MAN	C2-C3	-2.34	1.48	1.52
5	7	5	MAN	C2-C3	-2.34	1.48	1.52
5	Y	5	MAN	C2-C3	-2.33	1.48	1.52
5	t	5	MAN	C2-C3	-2.33	1.48	1.52
5	f	5	MAN	C2-C3	-2.32	1.48	1.52
5	0	5	MAN	C2-C3	-2.32	1.48	1.52
7	h	4	MAN	C2-C3	-2.22	1.49	1.52
7	2	4	MAN	C2-C3	-2.22	1.49	1.52
7	o	4	MAN	C2-C3	-2.20	1.49	1.52
7	9	4	MAN	C2-C3	-2.20	1.49	1.52
5	i	4	MAN	C2-C3	-2.19	1.49	1.52
5	3	4	MAN	C2-C3	-2.19	1.49	1.52
8	s	3	BMA	C2-C3	-2.18	1.49	1.52
8	DA	3	BMA	C2-C3	-2.18	1.49	1.52
7	a	4	MAN	C2-C3	-2.18	1.49	1.52
7	v	4	MAN	C2-C3	-2.18	1.49	1.52
5	b	5	MAN	C2-C3	-2.16	1.49	1.52
5	w	5	MAN	C2-C3	-2.16	1.49	1.52
8	e	3	BMA	C2-C3	-2.16	1.49	1.52
8	z	3	BMA	C2-C3	-2.16	1.49	1.52
5	p	5	MAN	C2-C3	-2.16	1.49	1.52
5	AA	5	MAN	C2-C3	-2.16	1.49	1.52
8	l	3	BMA	C2-C3	-2.15	1.49	1.52
8	6	3	BMA	C2-C3	-2.15	1.49	1.52
5	p	4	MAN	C2-C3	-2.15	1.49	1.52
5	AA	4	MAN	C2-C3	-2.15	1.49	1.52
5	b	4	MAN	C2-C3	-2.15	1.49	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	w	4	MAN	C2-C3	-2.15	1.49	1.52
5	i	5	MAN	C2-C3	-2.14	1.49	1.52
5	3	5	MAN	C2-C3	-2.14	1.49	1.52
8	k	3	BMA	C2-C3	-2.14	1.49	1.52
8	5	3	BMA	C2-C3	-2.14	1.49	1.52
8	r	3	BMA	C2-C3	-2.12	1.49	1.52
8	CA	3	BMA	C2-C3	-2.12	1.49	1.52
8	d	3	BMA	C2-C3	-2.11	1.49	1.52
8	y	3	BMA	C2-C3	-2.11	1.49	1.52
7	h	3	BMA	C6-C5	2.06	1.58	1.51
7	2	3	BMA	C6-C5	2.06	1.58	1.51
5	i	1	NAG	C3-C2	-2.06	1.48	1.52
5	3	1	NAG	C3-C2	-2.06	1.48	1.52
5	b	1	NAG	C3-C2	-2.06	1.48	1.52
5	w	1	NAG	C3-C2	-2.06	1.48	1.52
7	o	3	BMA	C6-C5	2.06	1.58	1.51
7	9	3	BMA	C6-C5	2.06	1.58	1.51
7	a	3	BMA	C6-C5	2.05	1.58	1.51
7	v	3	BMA	C6-C5	2.05	1.58	1.51
5	p	3	BMA	C2-C3	-2.05	1.49	1.52
5	AA	3	BMA	C2-C3	-2.05	1.49	1.52
5	p	1	NAG	C3-C2	-2.04	1.48	1.52
5	AA	1	NAG	C3-C2	-2.04	1.48	1.52
5	b	3	BMA	C2-C3	-2.03	1.49	1.52
5	w	3	BMA	C2-C3	-2.03	1.49	1.52
5	i	3	BMA	C2-C3	-2.02	1.49	1.52
5	3	3	BMA	C2-C3	-2.02	1.49	1.52

All (216) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	Y	4	MAN	O3-C3-C4	-5.85	96.58	110.38
5	t	4	MAN	O3-C3-C4	-5.85	96.58	110.38
5	m	4	MAN	O3-C3-C4	-5.84	96.61	110.38
5	7	4	MAN	O3-C3-C4	-5.84	96.61	110.38
5	f	4	MAN	O3-C3-C4	-5.83	96.63	110.38
5	0	4	MAN	O3-C3-C4	-5.83	96.63	110.38
5	Y	4	MAN	O4-C4-C5	-5.79	95.05	109.32
5	t	4	MAN	O4-C4-C5	-5.79	95.05	109.32
5	m	4	MAN	O4-C4-C5	-5.78	95.08	109.32
5	7	4	MAN	O4-C4-C5	-5.78	95.08	109.32
5	f	4	MAN	O4-C4-C5	-5.78	95.10	109.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	0	4	MAN	O4-C4-C5	-5.78	95.10	109.32
6	j	1	NAG	C4-C3-C2	-4.83	103.94	111.02
6	4	1	NAG	C4-C3-C2	-4.83	103.94	111.02
6	c	1	NAG	C4-C3-C2	-4.83	103.94	111.02
6	x	1	NAG	C4-C3-C2	-4.83	103.94	111.02
6	q	1	NAG	C4-C3-C2	-4.82	103.95	111.02
6	BA	1	NAG	C4-C3-C2	-4.82	103.95	111.02
5	m	4	MAN	O5-C5-C6	-4.33	99.23	107.66
5	7	4	MAN	O5-C5-C6	-4.33	99.23	107.66
5	f	4	MAN	O5-C5-C6	-4.32	99.25	107.66
5	0	4	MAN	O5-C5-C6	-4.32	99.25	107.66
5	Y	4	MAN	O5-C5-C6	-4.32	99.26	107.66
5	t	4	MAN	O5-C5-C6	-4.32	99.26	107.66
5	m	1	NAG	O5-C1-C2	-3.81	105.40	111.29
5	7	1	NAG	O5-C1-C2	-3.81	105.40	111.29
5	Y	1	NAG	O5-C1-C2	-3.80	105.41	111.29
5	t	1	NAG	O5-C1-C2	-3.80	105.41	111.29
5	f	1	NAG	O5-C1-C2	-3.80	105.42	111.29
5	0	1	NAG	O5-C1-C2	-3.80	105.42	111.29
5	b	2	NAG	C4-C3-C2	-3.37	106.07	111.02
5	w	2	NAG	C4-C3-C2	-3.37	106.07	111.02
5	i	2	NAG	C4-C3-C2	-3.37	106.08	111.02
5	3	2	NAG	C4-C3-C2	-3.37	106.08	111.02
5	p	2	NAG	C4-C3-C2	-3.36	106.09	111.02
5	AA	2	NAG	C4-C3-C2	-3.36	106.09	111.02
5	b	1	NAG	O5-C1-C2	-3.10	106.49	111.29
5	w	1	NAG	O5-C1-C2	-3.10	106.49	111.29
5	i	1	NAG	O5-C1-C2	-3.10	106.49	111.29
5	3	1	NAG	O5-C1-C2	-3.10	106.49	111.29
5	p	1	NAG	O5-C1-C2	-3.10	106.50	111.29
5	AA	1	NAG	O5-C1-C2	-3.10	106.50	111.29
5	i	2	NAG	O5-C1-C2	-3.03	106.60	111.29
5	3	2	NAG	O5-C1-C2	-3.03	106.60	111.29
5	b	2	NAG	O5-C1-C2	-3.02	106.62	111.29
5	w	2	NAG	O5-C1-C2	-3.02	106.62	111.29
5	p	2	NAG	O5-C1-C2	-3.01	106.63	111.29
5	AA	2	NAG	O5-C1-C2	-3.01	106.63	111.29
6	j	2	NAG	O5-C1-C2	-3.01	106.63	111.29
6	q	2	NAG	O5-C1-C2	-3.01	106.63	111.29
6	4	2	NAG	O5-C1-C2	-3.01	106.63	111.29
6	BA	2	NAG	O5-C1-C2	-3.01	106.63	111.29
6	c	2	NAG	O5-C1-C2	-3.01	106.64	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	x	2	NAG	O5-C1-C2	-3.01	106.64	111.29
6	n	2	NAG	C4-C3-C2	-3.01	106.61	111.02
6	8	2	NAG	C4-C3-C2	-3.01	106.61	111.02
6	Z	2	NAG	C4-C3-C2	-2.99	106.63	111.02
6	u	2	NAG	C4-C3-C2	-2.99	106.63	111.02
6	q	1	NAG	C1-C2-N2	-2.98	105.73	110.43
6	BA	1	NAG	C1-C2-N2	-2.98	105.73	110.43
6	g	2	NAG	C4-C3-C2	-2.98	106.65	111.02
6	1	2	NAG	C4-C3-C2	-2.98	106.65	111.02
6	c	1	NAG	C1-C2-N2	-2.97	105.75	110.43
6	x	1	NAG	C1-C2-N2	-2.97	105.75	110.43
6	j	1	NAG	C1-C2-N2	-2.97	105.75	110.43
6	4	1	NAG	C1-C2-N2	-2.97	105.75	110.43
5	Y	1	NAG	C3-C4-C5	-2.89	105.00	110.23
5	m	1	NAG	C3-C4-C5	-2.89	105.00	110.23
5	t	1	NAG	C3-C4-C5	-2.89	105.00	110.23
5	7	1	NAG	C3-C4-C5	-2.89	105.00	110.23
5	f	1	NAG	C3-C4-C5	-2.88	105.01	110.23
5	0	1	NAG	C3-C4-C5	-2.88	105.01	110.23
5	f	1	NAG	O3-C3-C4	2.87	117.14	110.38
5	0	1	NAG	O3-C3-C4	2.87	117.14	110.38
5	Y	1	NAG	O3-C3-C4	2.86	117.13	110.38
5	t	1	NAG	O3-C3-C4	2.86	117.13	110.38
5	m	1	NAG	O3-C3-C4	2.86	117.12	110.38
5	7	1	NAG	O3-C3-C4	2.86	117.12	110.38
7	a	1	NAG	C4-C3-C2	-2.83	106.87	111.02
7	v	1	NAG	C4-C3-C2	-2.83	106.87	111.02
7	h	1	NAG	C4-C3-C2	-2.82	106.88	111.02
7	o	1	NAG	C4-C3-C2	-2.82	106.88	111.02
7	2	1	NAG	C4-C3-C2	-2.82	106.88	111.02
7	9	1	NAG	C4-C3-C2	-2.82	106.88	111.02
5	Y	2	NAG	O4-C4-C3	-2.79	103.80	110.38
5	t	2	NAG	O4-C4-C3	-2.79	103.80	110.38
5	m	2	NAG	O4-C4-C3	-2.78	103.82	110.38
5	7	2	NAG	O4-C4-C3	-2.78	103.82	110.38
5	f	2	NAG	O4-C4-C3	-2.78	103.82	110.38
5	0	2	NAG	O4-C4-C3	-2.78	103.82	110.38
5	m	1	NAG	C4-C3-C2	-2.66	107.11	111.02
5	7	1	NAG	C4-C3-C2	-2.66	107.11	111.02
5	Y	1	NAG	C4-C3-C2	-2.66	107.12	111.02
5	t	1	NAG	C4-C3-C2	-2.66	107.12	111.02
5	m	4	MAN	O2-C2-C3	-2.64	104.69	110.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	7	4	MAN	O2-C2-C3	-2.64	104.69	110.15
5	f	4	MAN	O2-C2-C3	-2.63	104.70	110.15
5	0	4	MAN	O2-C2-C3	-2.63	104.70	110.15
5	Y	4	MAN	O2-C2-C3	-2.63	104.71	110.15
5	t	4	MAN	O2-C2-C3	-2.63	104.71	110.15
5	f	1	NAG	C4-C3-C2	-2.63	107.17	111.02
5	0	1	NAG	C4-C3-C2	-2.63	107.17	111.02
6	j	1	NAG	O4-C4-C3	2.62	116.56	110.38
6	4	1	NAG	O4-C4-C3	2.62	116.56	110.38
6	c	1	NAG	O4-C4-C3	2.62	116.56	110.38
6	x	1	NAG	O4-C4-C3	2.62	116.56	110.38
6	q	1	NAG	O4-C4-C3	2.62	116.55	110.38
6	BA	1	NAG	O4-C4-C3	2.62	116.55	110.38
6	c	2	NAG	C1-O5-C5	2.51	115.55	112.19
6	x	2	NAG	C1-O5-C5	2.51	115.55	112.19
6	j	2	NAG	C1-O5-C5	2.50	115.54	112.19
6	q	2	NAG	C1-O5-C5	2.50	115.54	112.19
6	4	2	NAG	C1-O5-C5	2.50	115.54	112.19
6	BA	2	NAG	C1-O5-C5	2.50	115.54	112.19
5	m	3	BMA	O3-C3-C4	2.49	116.24	110.38
5	7	3	BMA	O3-C3-C4	2.49	116.24	110.38
5	f	3	BMA	O3-C3-C4	2.49	116.24	110.38
5	0	3	BMA	O3-C3-C4	2.49	116.24	110.38
5	Y	3	BMA	O3-C3-C4	2.49	116.24	110.38
5	t	3	BMA	O3-C3-C4	2.49	116.24	110.38
5	f	2	NAG	O5-C5-C6	-2.46	102.88	107.66
5	0	2	NAG	O5-C5-C6	-2.46	102.88	107.66
5	m	2	NAG	O5-C5-C6	-2.45	102.89	107.66
5	7	2	NAG	O5-C5-C6	-2.45	102.89	107.66
5	Y	2	NAG	O5-C5-C6	-2.45	102.90	107.66
5	t	2	NAG	O5-C5-C6	-2.45	102.90	107.66
5	i	1	NAG	O4-C4-C3	-2.43	104.65	110.38
5	3	1	NAG	O4-C4-C3	-2.43	104.65	110.38
5	b	1	NAG	O4-C4-C3	-2.42	104.66	110.38
5	p	1	NAG	O4-C4-C3	-2.42	104.66	110.38
5	w	1	NAG	O4-C4-C3	-2.42	104.66	110.38
5	AA	1	NAG	O4-C4-C3	-2.42	104.66	110.38
5	b	1	NAG	C3-C4-C5	-2.40	105.89	110.23
5	w	1	NAG	C3-C4-C5	-2.40	105.89	110.23
5	i	1	NAG	C3-C4-C5	-2.37	105.93	110.23
5	3	1	NAG	C3-C4-C5	-2.37	105.93	110.23
5	p	1	NAG	C3-C4-C5	-2.36	105.95	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	AA	1	NAG	C3-C4-C5	-2.36	105.95	110.23
5	f	5	MAN	C2-C3-C4	-2.31	106.80	110.86
5	0	5	MAN	C2-C3-C4	-2.31	106.80	110.86
6	g	1	NAG	C1-C2-N2	-2.30	106.81	110.43
6	1	1	NAG	C1-C2-N2	-2.30	106.81	110.43
5	f	1	NAG	C1-C2-N2	2.30	114.05	110.43
5	0	1	NAG	C1-C2-N2	2.30	114.05	110.43
5	m	1	NAG	C1-C2-N2	2.30	114.05	110.43
5	7	1	NAG	C1-C2-N2	2.30	114.05	110.43
5	Y	1	NAG	C1-C2-N2	2.30	114.05	110.43
5	t	1	NAG	C1-C2-N2	2.30	114.05	110.43
5	m	5	MAN	C2-C3-C4	-2.29	106.83	110.86
5	7	5	MAN	C2-C3-C4	-2.29	106.83	110.86
6	n	1	NAG	C1-C2-N2	-2.29	106.82	110.43
6	8	1	NAG	C1-C2-N2	-2.29	106.82	110.43
5	Y	5	MAN	C2-C3-C4	-2.29	106.84	110.86
5	t	5	MAN	C2-C3-C4	-2.29	106.84	110.86
6	Z	1	NAG	C1-C2-N2	-2.29	106.83	110.43
6	u	1	NAG	C1-C2-N2	-2.29	106.83	110.43
5	b	4	MAN	C2-C3-C4	-2.26	106.88	110.86
5	w	4	MAN	C2-C3-C4	-2.26	106.88	110.86
5	i	4	MAN	C2-C3-C4	-2.26	106.89	110.86
5	3	4	MAN	C2-C3-C4	-2.26	106.89	110.86
5	p	4	MAN	C2-C3-C4	-2.25	106.91	110.86
5	AA	4	MAN	C2-C3-C4	-2.25	106.91	110.86
7	h	3	BMA	C2-C3-C4	-2.21	106.97	110.86
7	2	3	BMA	C2-C3-C4	-2.21	106.97	110.86
7	a	3	BMA	C2-C3-C4	-2.21	106.98	110.86
7	o	3	BMA	C2-C3-C4	-2.21	106.98	110.86
7	v	3	BMA	C2-C3-C4	-2.21	106.98	110.86
7	9	3	BMA	C2-C3-C4	-2.21	106.98	110.86
7	a	4	MAN	C2-C3-C4	-2.20	107.00	110.86
7	v	4	MAN	C2-C3-C4	-2.20	107.00	110.86
7	o	4	MAN	C2-C3-C4	-2.19	107.00	110.86
7	9	4	MAN	C2-C3-C4	-2.19	107.00	110.86
7	h	4	MAN	C2-C3-C4	-2.19	107.00	110.86
7	2	4	MAN	C2-C3-C4	-2.19	107.00	110.86
5	i	4	MAN	C1-C2-C3	2.17	112.80	109.64
5	3	4	MAN	C1-C2-C3	2.17	112.80	109.64
5	p	4	MAN	C1-C2-C3	2.16	112.79	109.64
5	AA	4	MAN	C1-C2-C3	2.16	112.79	109.64
5	b	4	MAN	C1-C2-C3	2.15	112.77	109.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	w	4	MAN	C1-C2-C3	2.15	112.77	109.64
7	h	2	NAG	C3-C4-C5	-2.12	106.39	110.23
7	2	2	NAG	C3-C4-C5	-2.12	106.39	110.23
7	a	2	NAG	C3-C4-C5	-2.11	106.40	110.23
7	v	2	NAG	C3-C4-C5	-2.11	106.40	110.23
7	o	2	NAG	C3-C4-C5	-2.11	106.41	110.23
7	9	2	NAG	C3-C4-C5	-2.11	106.41	110.23
8	s	2	NAG	C4-C3-C2	-2.10	107.94	111.02
8	DA	2	NAG	C4-C3-C2	-2.10	107.94	111.02
8	l	2	NAG	C4-C3-C2	-2.10	107.95	111.02
8	6	2	NAG	C4-C3-C2	-2.10	107.95	111.02
8	e	2	NAG	C4-C3-C2	-2.09	107.95	111.02
8	z	2	NAG	C4-C3-C2	-2.09	107.95	111.02
5	b	3	BMA	C2-C3-C4	-2.09	107.18	110.86
5	w	3	BMA	C2-C3-C4	-2.09	107.18	110.86
5	p	3	BMA	C2-C3-C4	-2.08	107.21	110.86
5	AA	3	BMA	C2-C3-C4	-2.08	107.21	110.86
5	i	3	BMA	C2-C3-C4	-2.07	107.23	110.86
5	3	3	BMA	C2-C3-C4	-2.07	107.23	110.86
5	m	2	NAG	C3-C4-C5	-2.06	106.50	110.23
5	7	2	NAG	C3-C4-C5	-2.06	106.50	110.23
5	f	2	NAG	C3-C4-C5	-2.05	106.51	110.23
5	0	2	NAG	C3-C4-C5	-2.05	106.51	110.23
5	Y	2	NAG	C3-C4-C5	-2.05	106.51	110.23
5	t	2	NAG	C3-C4-C5	-2.05	106.51	110.23
7	h	4	MAN	C1-C2-C3	2.04	112.61	109.64
7	2	4	MAN	C1-C2-C3	2.04	112.61	109.64
7	a	4	MAN	C1-C2-C3	2.03	112.60	109.64
7	v	4	MAN	C1-C2-C3	2.03	112.60	109.64
8	k	3	BMA	C2-C3-C4	-2.03	107.29	110.86
8	5	3	BMA	C2-C3-C4	-2.03	107.29	110.86
8	r	3	BMA	C2-C3-C4	-2.03	107.30	110.86
8	CA	3	BMA	C2-C3-C4	-2.03	107.30	110.86
7	o	4	MAN	C1-C2-C3	2.02	112.59	109.64
7	9	4	MAN	C1-C2-C3	2.02	112.59	109.64
8	d	3	BMA	C2-C3-C4	-2.02	107.31	110.86
8	y	3	BMA	C2-C3-C4	-2.02	107.31	110.86

There are no chirality outliers.

All (210) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	Y	2	NAG	O5-C5-C6-O6
5	f	2	NAG	O5-C5-C6-O6
5	m	2	NAG	O5-C5-C6-O6
5	t	2	NAG	O5-C5-C6-O6
5	0	2	NAG	O5-C5-C6-O6
5	7	2	NAG	O5-C5-C6-O6
6	c	2	NAG	O5-C5-C6-O6
6	j	2	NAG	O5-C5-C6-O6
6	q	2	NAG	O5-C5-C6-O6
6	x	2	NAG	O5-C5-C6-O6
6	4	2	NAG	O5-C5-C6-O6
6	BA	2	NAG	O5-C5-C6-O6
5	b	4	MAN	O5-C5-C6-O6
5	i	4	MAN	O5-C5-C6-O6
5	p	4	MAN	O5-C5-C6-O6
5	w	4	MAN	O5-C5-C6-O6
5	3	4	MAN	O5-C5-C6-O6
5	AA	4	MAN	O5-C5-C6-O6
5	Y	2	NAG	C4-C5-C6-O6
5	f	2	NAG	C4-C5-C6-O6
5	m	2	NAG	C4-C5-C6-O6
5	t	2	NAG	C4-C5-C6-O6
5	0	2	NAG	C4-C5-C6-O6
5	7	2	NAG	C4-C5-C6-O6
5	Y	5	MAN	O5-C5-C6-O6
5	f	5	MAN	O5-C5-C6-O6
5	m	5	MAN	O5-C5-C6-O6
5	t	5	MAN	O5-C5-C6-O6
5	0	5	MAN	O5-C5-C6-O6
5	7	5	MAN	O5-C5-C6-O6
7	a	4	MAN	O5-C5-C6-O6
7	h	4	MAN	O5-C5-C6-O6
7	o	4	MAN	O5-C5-C6-O6
7	v	4	MAN	O5-C5-C6-O6
7	2	4	MAN	O5-C5-C6-O6
7	9	4	MAN	O5-C5-C6-O6
5	Y	3	BMA	O5-C5-C6-O6
5	f	3	BMA	O5-C5-C6-O6
5	m	3	BMA	O5-C5-C6-O6
5	t	3	BMA	O5-C5-C6-O6
5	0	3	BMA	O5-C5-C6-O6
5	7	3	BMA	O5-C5-C6-O6
8	d	3	BMA	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
8	k	3	BMA	O5-C5-C6-O6
8	y	3	BMA	O5-C5-C6-O6
8	5	3	BMA	O5-C5-C6-O6
5	b	4	MAN	C4-C5-C6-O6
5	i	4	MAN	C4-C5-C6-O6
5	p	4	MAN	C4-C5-C6-O6
5	w	4	MAN	C4-C5-C6-O6
5	3	4	MAN	C4-C5-C6-O6
5	AA	4	MAN	C4-C5-C6-O6
8	r	3	BMA	O5-C5-C6-O6
8	CA	3	BMA	O5-C5-C6-O6
8	d	1	NAG	O5-C5-C6-O6
8	k	1	NAG	O5-C5-C6-O6
8	r	1	NAG	O5-C5-C6-O6
8	y	1	NAG	O5-C5-C6-O6
8	5	1	NAG	O5-C5-C6-O6
8	CA	1	NAG	O5-C5-C6-O6
5	Y	3	BMA	C4-C5-C6-O6
5	f	3	BMA	C4-C5-C6-O6
5	m	3	BMA	C4-C5-C6-O6
5	t	3	BMA	C4-C5-C6-O6
5	0	3	BMA	C4-C5-C6-O6
5	7	3	BMA	C4-C5-C6-O6
5	b	1	NAG	O5-C5-C6-O6
5	i	1	NAG	O5-C5-C6-O6
5	p	1	NAG	O5-C5-C6-O6
5	w	1	NAG	O5-C5-C6-O6
5	3	1	NAG	O5-C5-C6-O6
5	AA	1	NAG	O5-C5-C6-O6
6	Z	2	NAG	O5-C5-C6-O6
6	g	2	NAG	O5-C5-C6-O6
6	n	2	NAG	O5-C5-C6-O6
6	u	2	NAG	O5-C5-C6-O6
6	1	2	NAG	O5-C5-C6-O6
6	8	2	NAG	O5-C5-C6-O6
8	e	3	BMA	O5-C5-C6-O6
8	l	3	BMA	O5-C5-C6-O6
8	s	3	BMA	O5-C5-C6-O6
8	z	3	BMA	O5-C5-C6-O6
8	6	3	BMA	O5-C5-C6-O6
8	DA	3	BMA	O5-C5-C6-O6
5	b	5	MAN	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
5	i	5	MAN	O5-C5-C6-O6
5	p	5	MAN	O5-C5-C6-O6
5	w	5	MAN	O5-C5-C6-O6
5	3	5	MAN	O5-C5-C6-O6
5	AA	5	MAN	O5-C5-C6-O6
6	Z	1	NAG	O5-C5-C6-O6
6	n	1	NAG	O5-C5-C6-O6
6	u	1	NAG	O5-C5-C6-O6
6	8	1	NAG	O5-C5-C6-O6
6	g	1	NAG	O5-C5-C6-O6
6	1	1	NAG	O5-C5-C6-O6
8	d	1	NAG	C4-C5-C6-O6
8	r	1	NAG	C4-C5-C6-O6
8	y	1	NAG	C4-C5-C6-O6
8	CA	1	NAG	C4-C5-C6-O6
7	a	3	BMA	O5-C5-C6-O6
7	h	3	BMA	O5-C5-C6-O6
7	o	3	BMA	O5-C5-C6-O6
7	v	3	BMA	O5-C5-C6-O6
7	2	3	BMA	O5-C5-C6-O6
7	9	3	BMA	O5-C5-C6-O6
6	j	2	NAG	C4-C5-C6-O6
6	q	2	NAG	C4-C5-C6-O6
6	4	2	NAG	C4-C5-C6-O6
6	BA	2	NAG	C4-C5-C6-O6
8	k	1	NAG	C4-C5-C6-O6
8	5	1	NAG	C4-C5-C6-O6
6	c	2	NAG	C4-C5-C6-O6
6	x	2	NAG	C4-C5-C6-O6
5	Y	4	MAN	O5-C5-C6-O6
5	f	4	MAN	O5-C5-C6-O6
5	m	4	MAN	O5-C5-C6-O6
5	t	4	MAN	O5-C5-C6-O6
5	0	4	MAN	O5-C5-C6-O6
5	7	4	MAN	O5-C5-C6-O6
5	Y	1	NAG	O5-C5-C6-O6
5	f	1	NAG	O5-C5-C6-O6
5	m	1	NAG	O5-C5-C6-O6
5	t	1	NAG	O5-C5-C6-O6
5	0	1	NAG	O5-C5-C6-O6
5	7	1	NAG	O5-C5-C6-O6
5	b	1	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
5	i	1	NAG	C4-C5-C6-O6
5	p	1	NAG	C4-C5-C6-O6
5	w	1	NAG	C4-C5-C6-O6
5	3	1	NAG	C4-C5-C6-O6
5	AA	1	NAG	C4-C5-C6-O6
8	e	2	NAG	O5-C5-C6-O6
8	l	2	NAG	O5-C5-C6-O6
8	s	2	NAG	O5-C5-C6-O6
8	z	2	NAG	O5-C5-C6-O6
8	6	2	NAG	O5-C5-C6-O6
8	DA	2	NAG	O5-C5-C6-O6
7	a	2	NAG	O5-C5-C6-O6
7	h	2	NAG	O5-C5-C6-O6
7	o	2	NAG	O5-C5-C6-O6
7	v	2	NAG	O5-C5-C6-O6
7	2	2	NAG	O5-C5-C6-O6
7	9	2	NAG	O5-C5-C6-O6
6	c	1	NAG	O5-C5-C6-O6
6	j	1	NAG	O5-C5-C6-O6
6	q	1	NAG	O5-C5-C6-O6
6	x	1	NAG	O5-C5-C6-O6
6	4	1	NAG	O5-C5-C6-O6
6	BA	1	NAG	O5-C5-C6-O6
5	Y	5	MAN	C4-C5-C6-O6
5	f	5	MAN	C4-C5-C6-O6
5	m	5	MAN	C4-C5-C6-O6
5	t	5	MAN	C4-C5-C6-O6
5	0	5	MAN	C4-C5-C6-O6
5	7	5	MAN	C4-C5-C6-O6
6	g	1	NAG	C4-C5-C6-O6
6	1	1	NAG	C4-C5-C6-O6
6	Z	1	NAG	C4-C5-C6-O6
6	n	1	NAG	C4-C5-C6-O6
6	u	1	NAG	C4-C5-C6-O6
6	8	1	NAG	C4-C5-C6-O6
5	b	2	NAG	C1-C2-N2-C7
5	i	2	NAG	C1-C2-N2-C7
5	p	2	NAG	C1-C2-N2-C7
5	w	2	NAG	C1-C2-N2-C7
5	3	2	NAG	C1-C2-N2-C7
5	AA	2	NAG	C1-C2-N2-C7
7	a	4	MAN	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
7	v	4	MAN	C4-C5-C6-O6
5	Y	4	MAN	C4-C5-C6-O6
5	f	4	MAN	C4-C5-C6-O6
5	m	4	MAN	C4-C5-C6-O6
5	t	4	MAN	C4-C5-C6-O6
5	0	4	MAN	C4-C5-C6-O6
5	7	4	MAN	C4-C5-C6-O6
7	h	4	MAN	C4-C5-C6-O6
7	o	4	MAN	C4-C5-C6-O6
7	2	4	MAN	C4-C5-C6-O6
7	9	4	MAN	C4-C5-C6-O6
5	b	3	BMA	O5-C5-C6-O6
5	p	3	BMA	O5-C5-C6-O6
5	w	3	BMA	O5-C5-C6-O6
5	AA	3	BMA	O5-C5-C6-O6
5	Y	1	NAG	C3-C2-N2-C7
5	b	2	NAG	C3-C2-N2-C7
5	f	1	NAG	C3-C2-N2-C7
5	i	2	NAG	C3-C2-N2-C7
5	m	1	NAG	C3-C2-N2-C7
5	p	2	NAG	C3-C2-N2-C7
5	t	1	NAG	C3-C2-N2-C7
5	w	2	NAG	C3-C2-N2-C7
5	0	1	NAG	C3-C2-N2-C7
5	3	2	NAG	C3-C2-N2-C7
5	7	1	NAG	C3-C2-N2-C7
5	AA	2	NAG	C3-C2-N2-C7
5	i	3	BMA	O5-C5-C6-O6
5	3	3	BMA	O5-C5-C6-O6
5	b	1	NAG	C1-C2-N2-C7
5	i	1	NAG	C1-C2-N2-C7
5	p	1	NAG	C1-C2-N2-C7
5	w	1	NAG	C1-C2-N2-C7
5	3	1	NAG	C1-C2-N2-C7
5	AA	1	NAG	C1-C2-N2-C7
5	b	3	BMA	C4-C5-C6-O6
5	w	3	BMA	C4-C5-C6-O6
5	i	3	BMA	C4-C5-C6-O6
5	3	3	BMA	C4-C5-C6-O6
5	p	3	BMA	C4-C5-C6-O6
5	AA	3	BMA	C4-C5-C6-O6

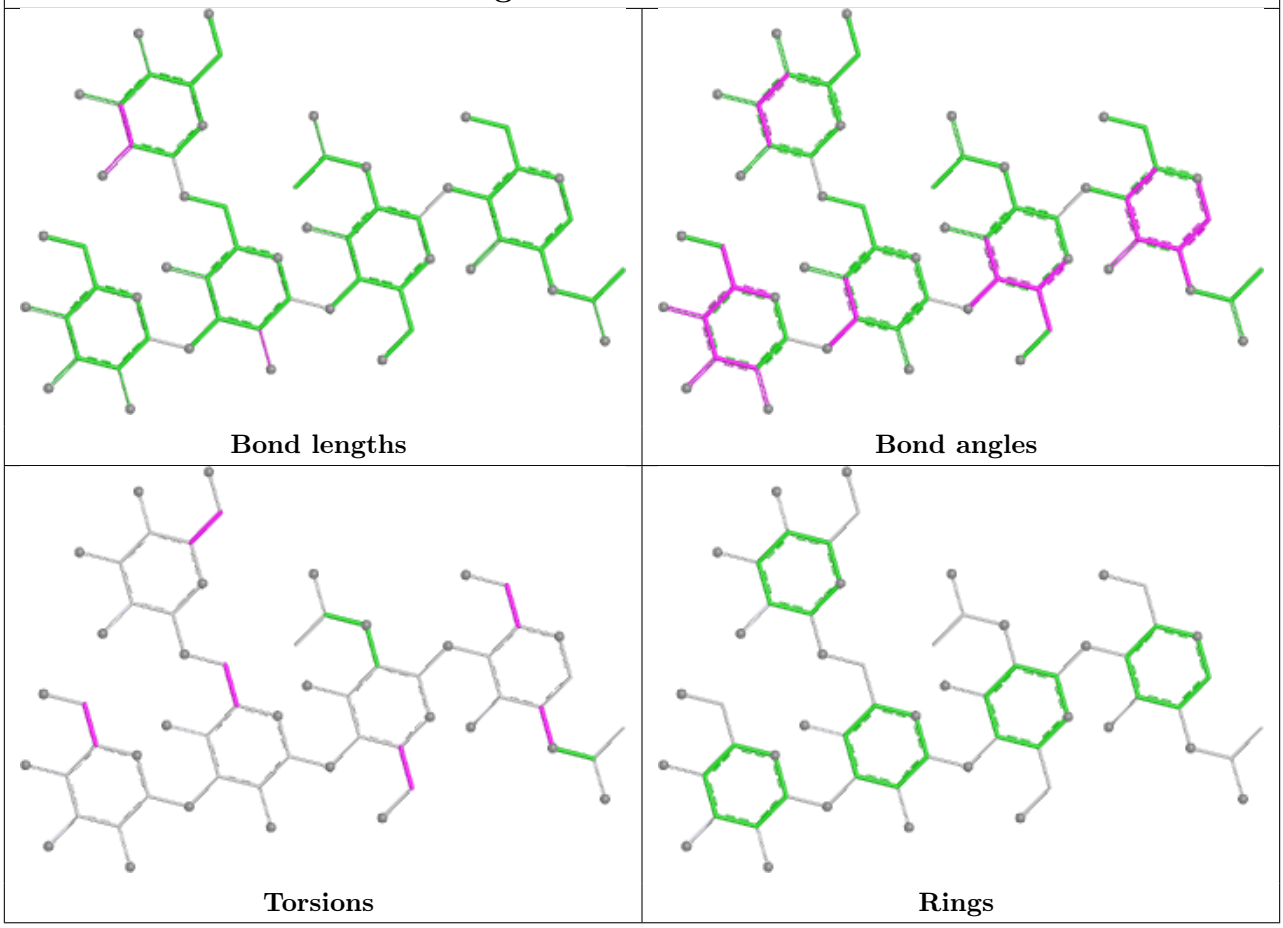
There are no ring outliers.

8 monomers are involved in 5 short contacts:

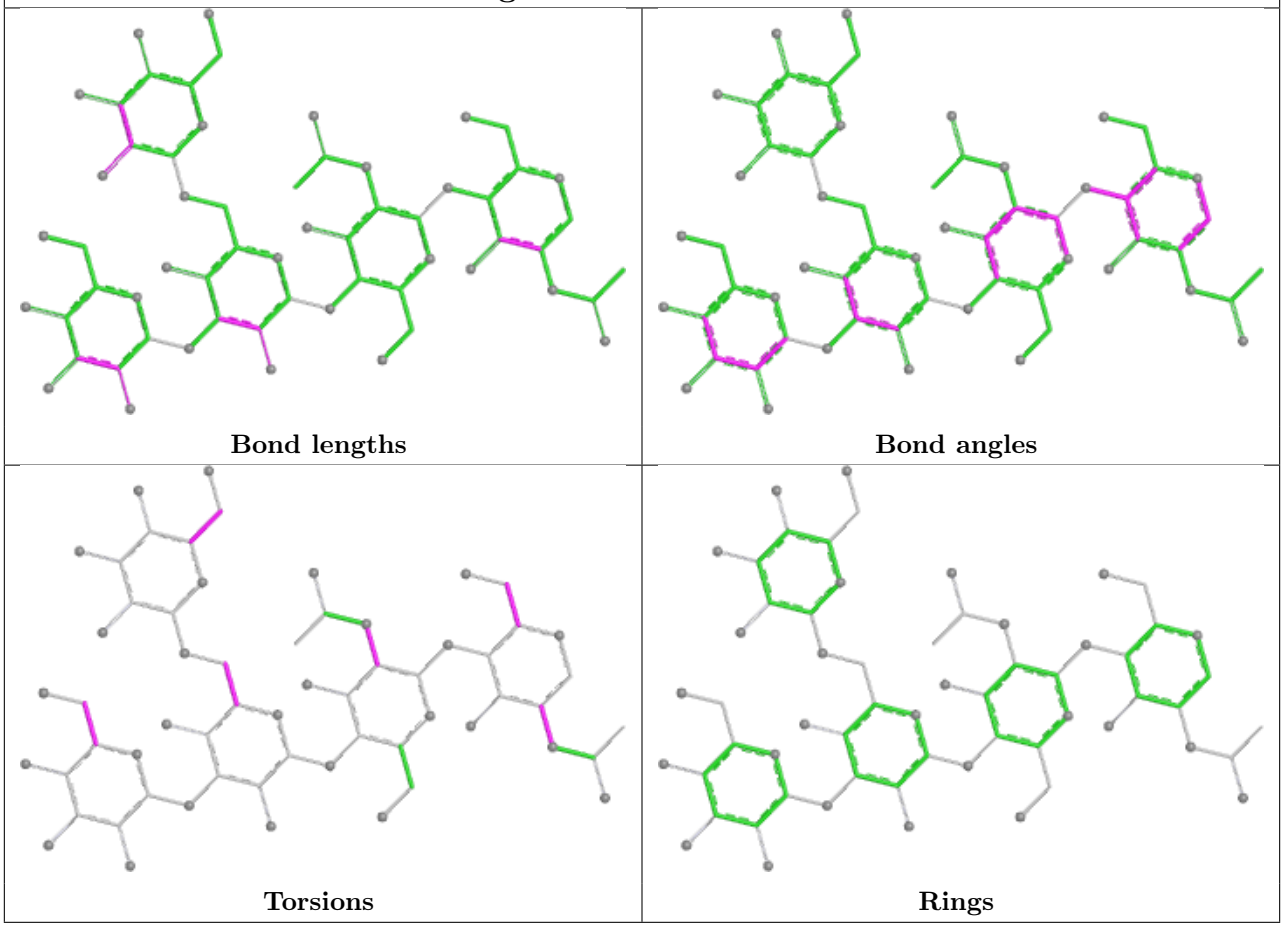
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	7	4	MAN	1	0
5	Y	3	BMA	1	0
5	0	3	BMA	1	0
5	3	1	NAG	1	0
5	AA	1	NAG	1	0
5	0	4	MAN	1	0
5	7	3	BMA	1	0
5	Y	4	MAN	1	0

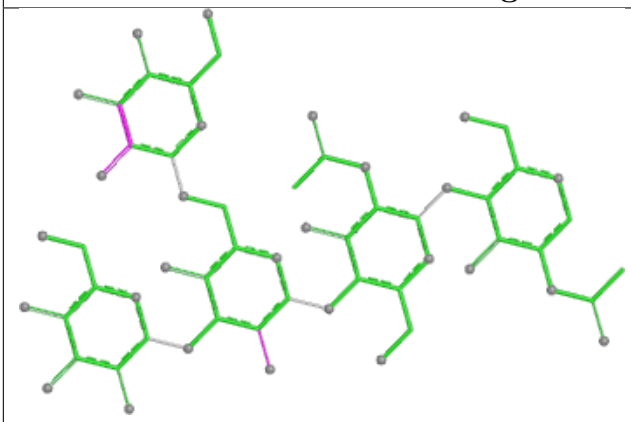
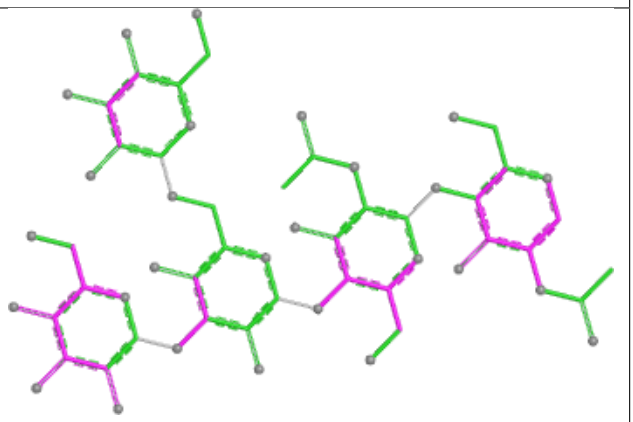
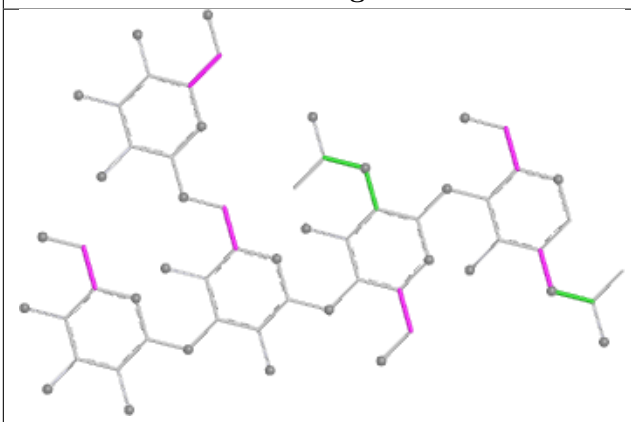
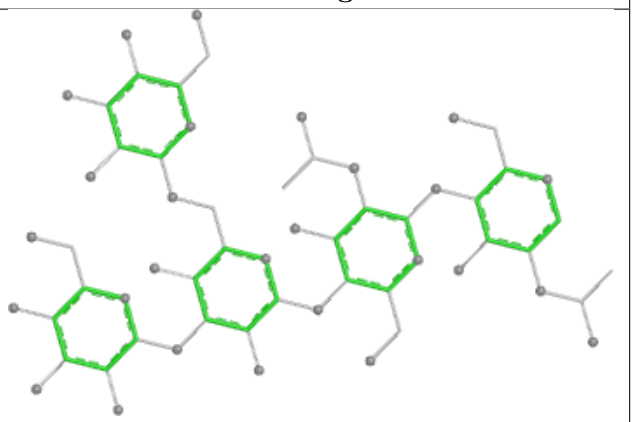
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

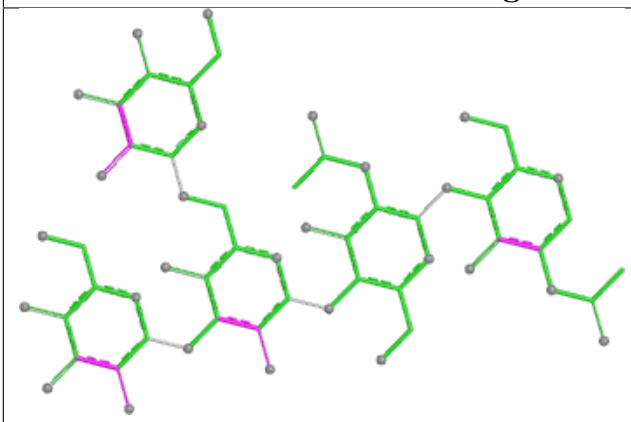
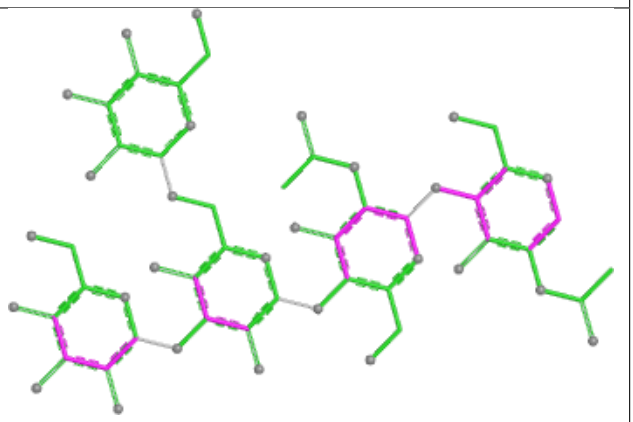
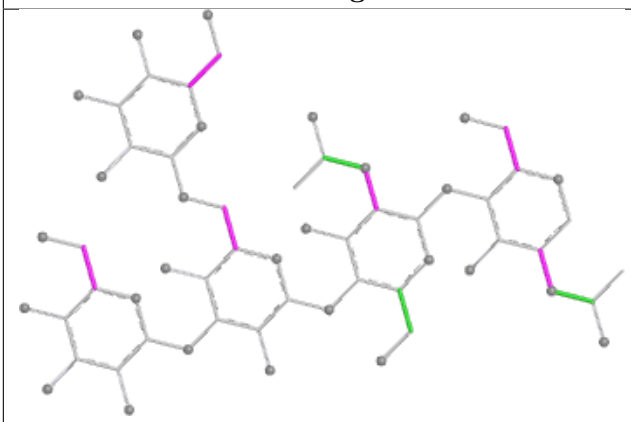
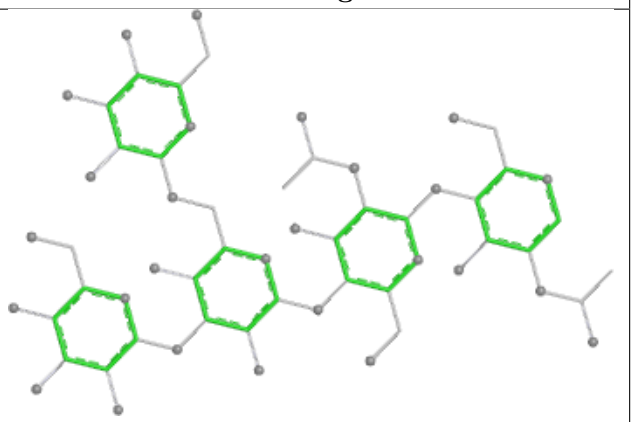
Oligosaccharide Chain Y

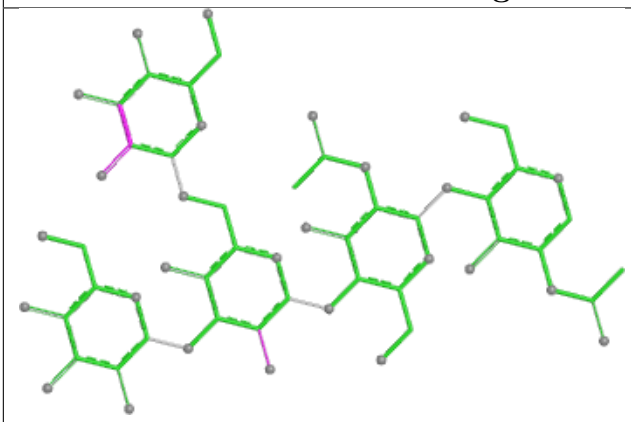
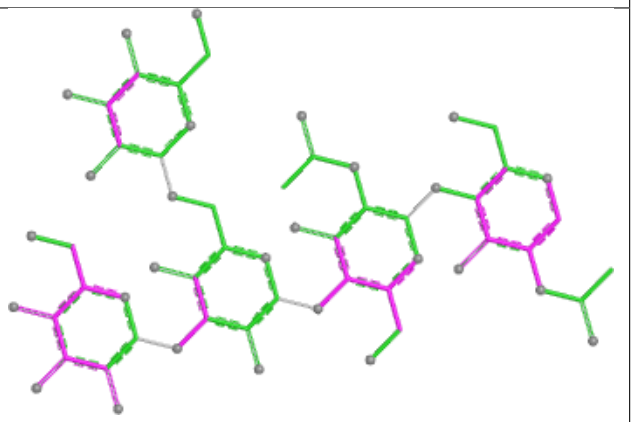
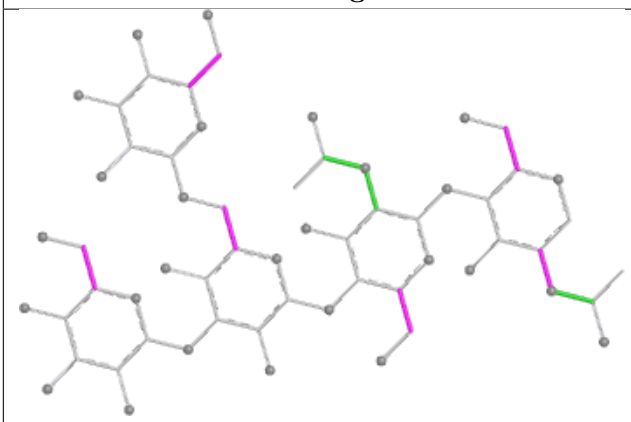
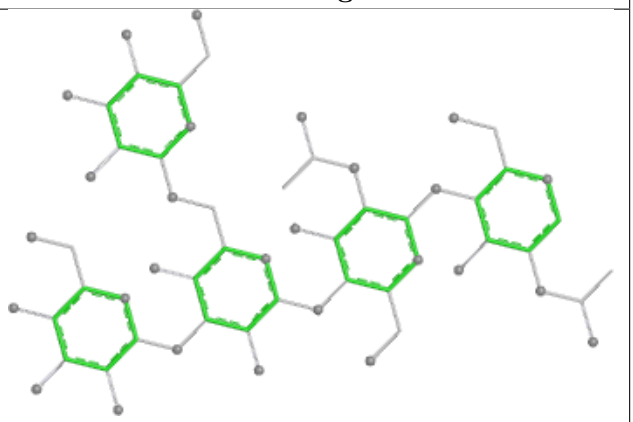


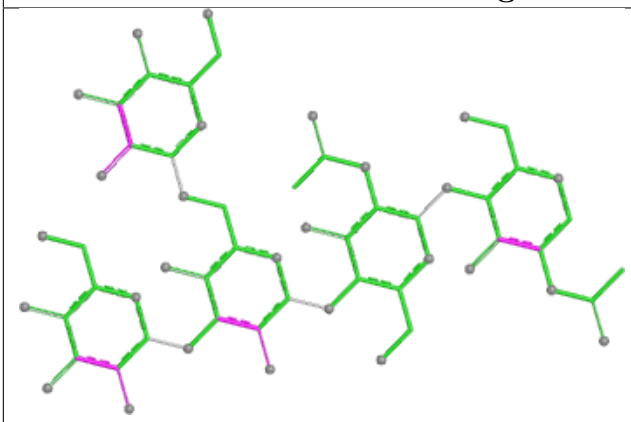
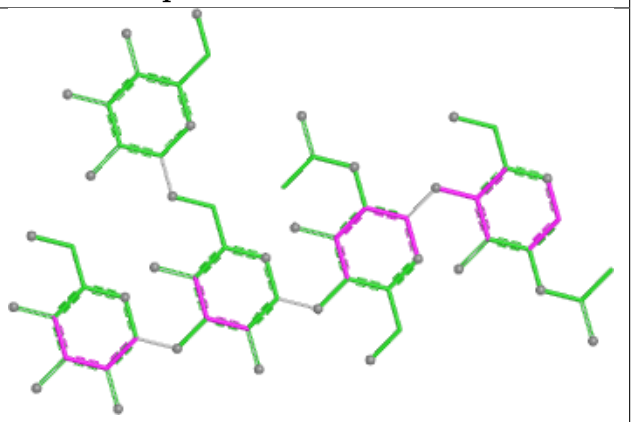
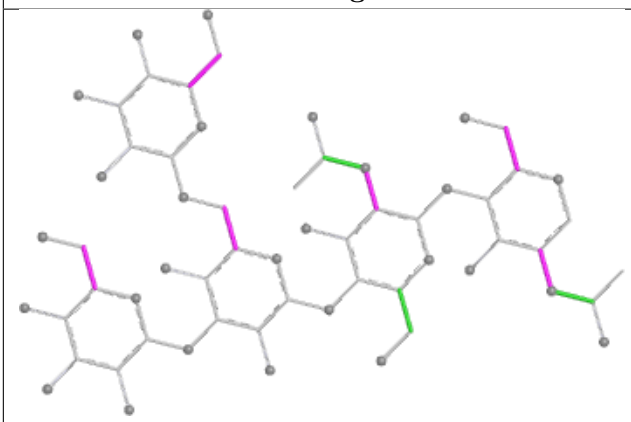
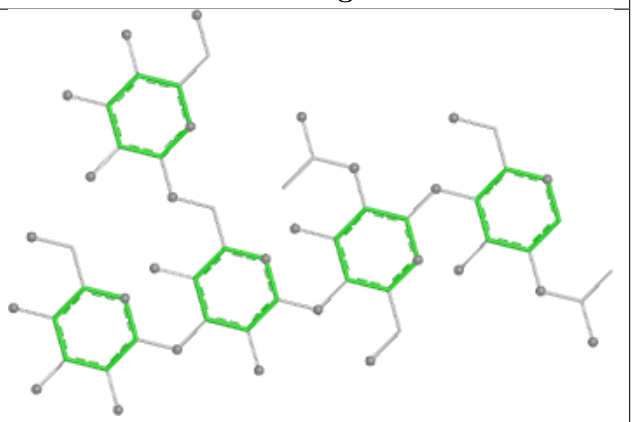
Oligosaccharide Chain b

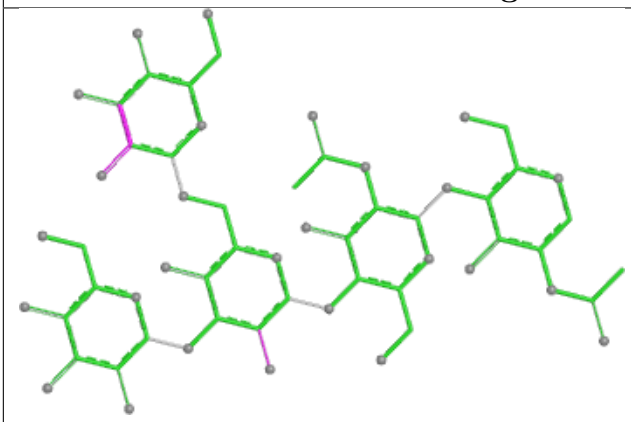
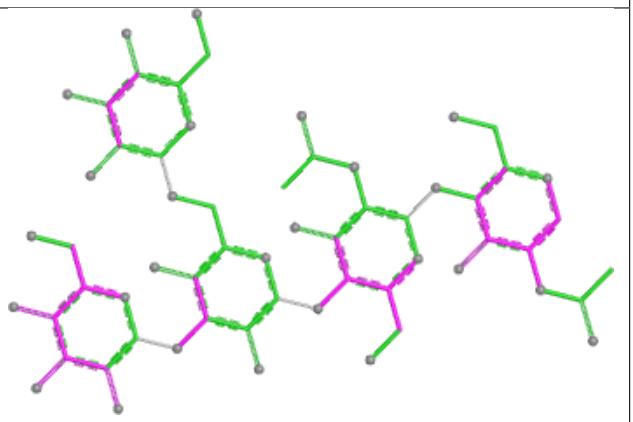
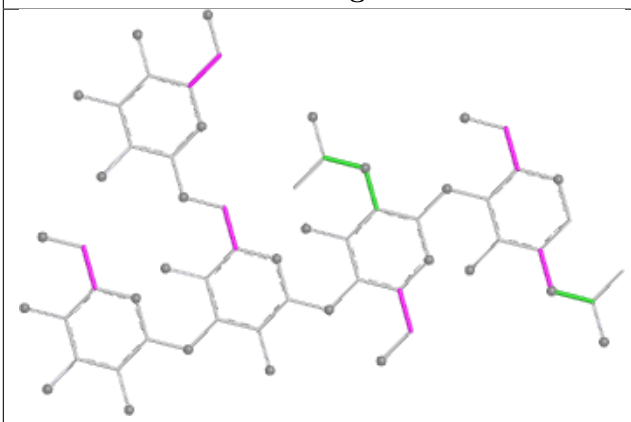
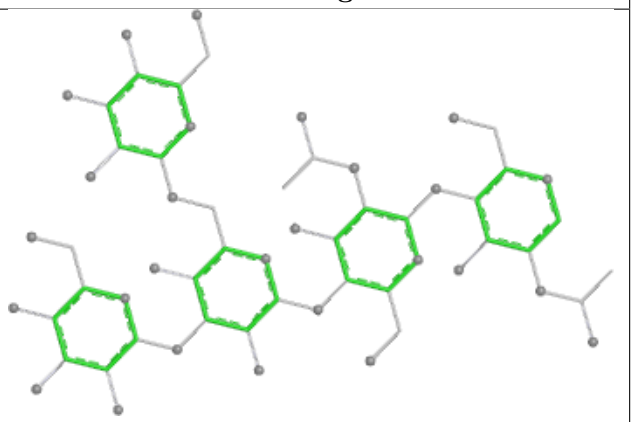


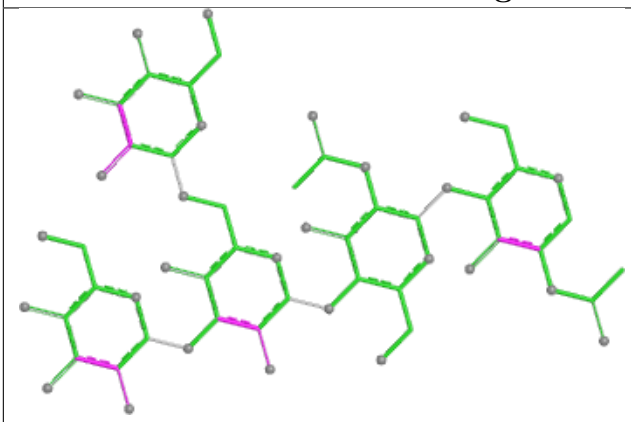
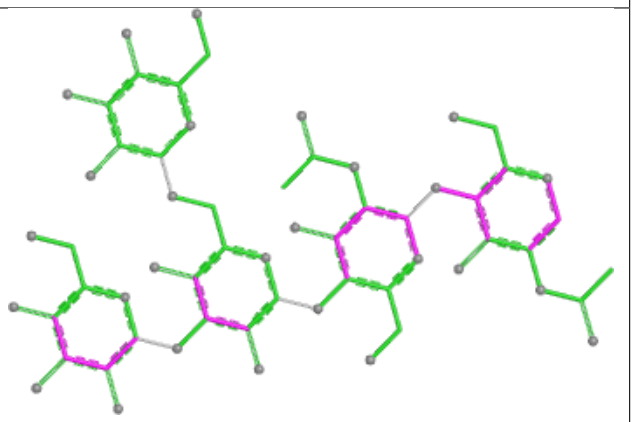
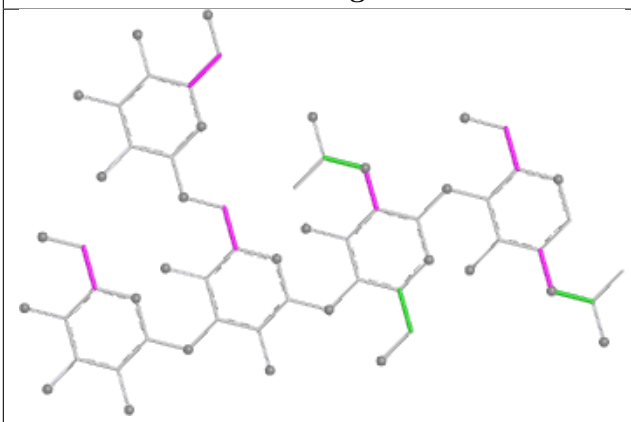
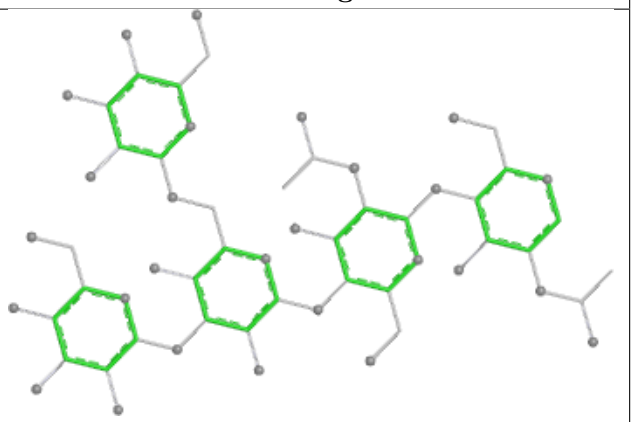
Oligosaccharide Chain f	
 Bond lengths	 Bond angles
 Torsions	 Rings

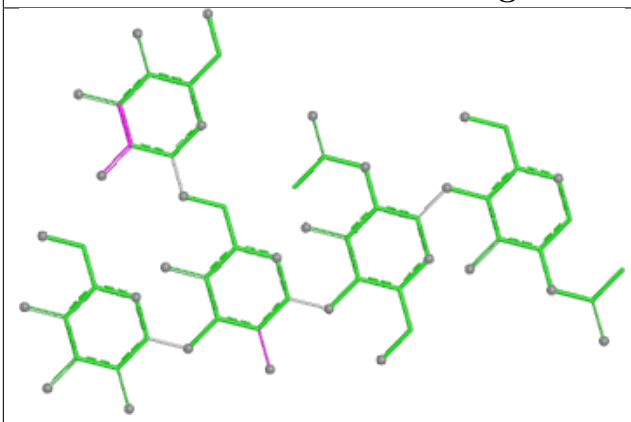
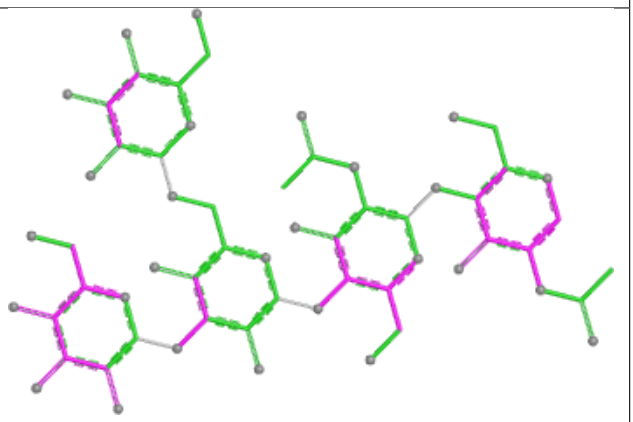
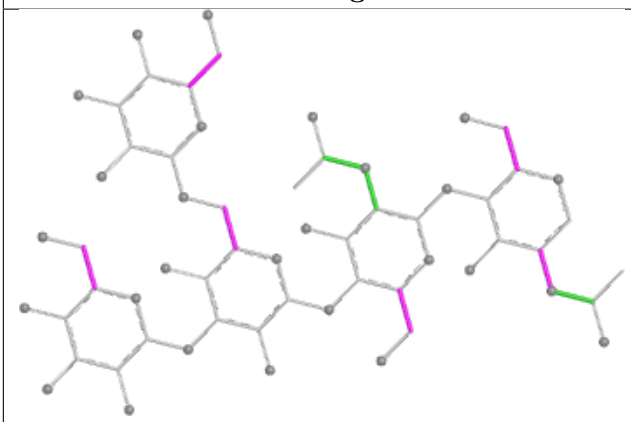
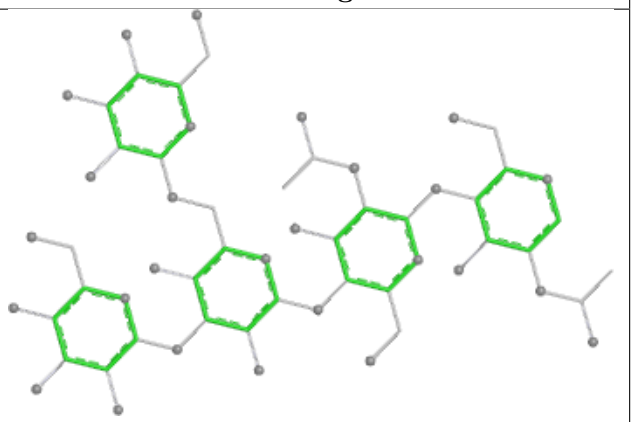
Oligosaccharide Chain i	
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain m	
 Bond lengths	 Bond angles
 Torsions	 Rings

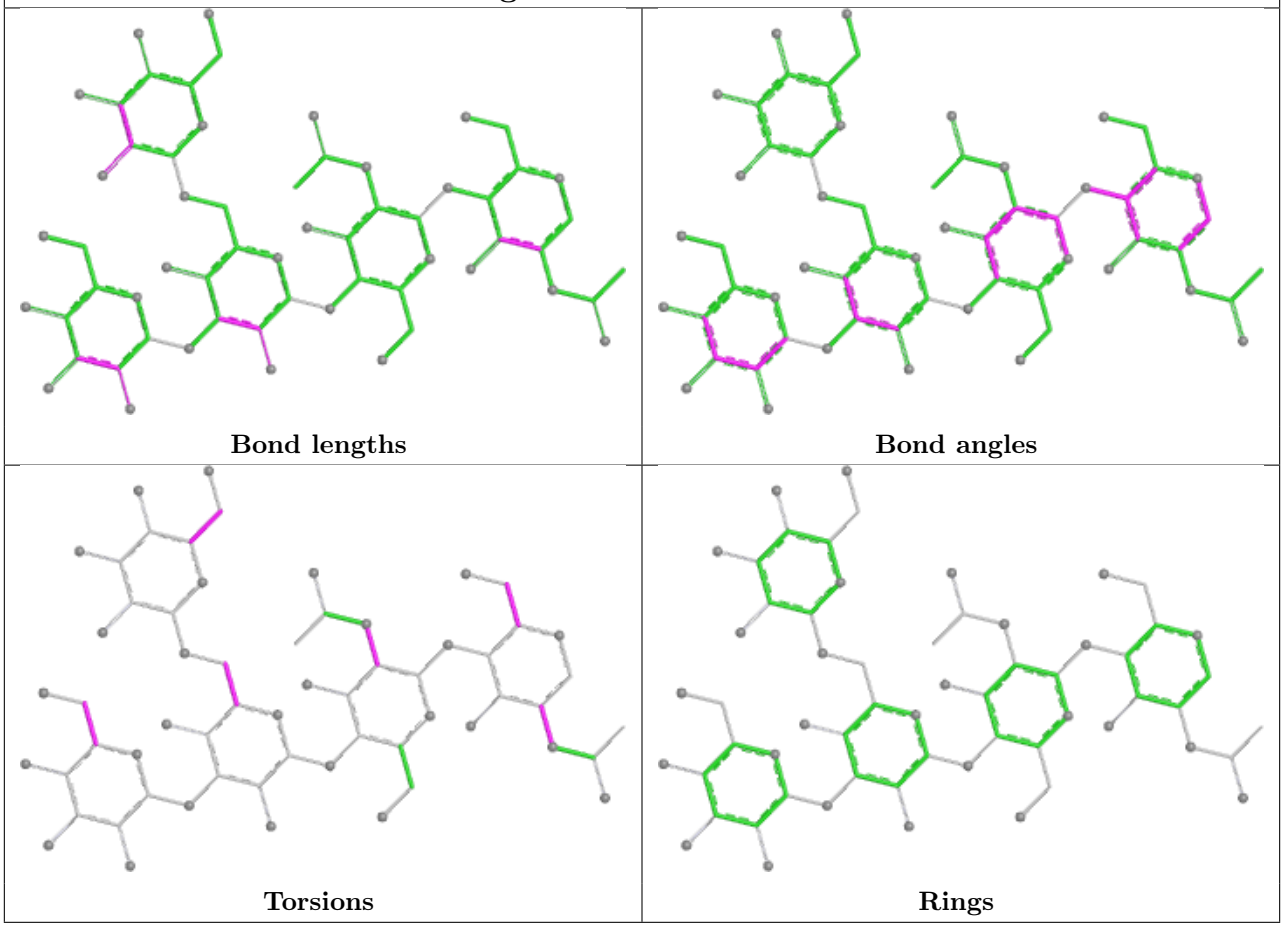
Oligosaccharide Chain p	
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain t	
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain w	
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain 0	
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain 3



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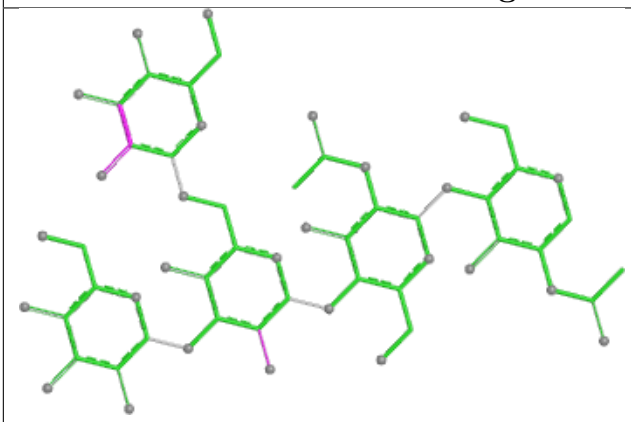
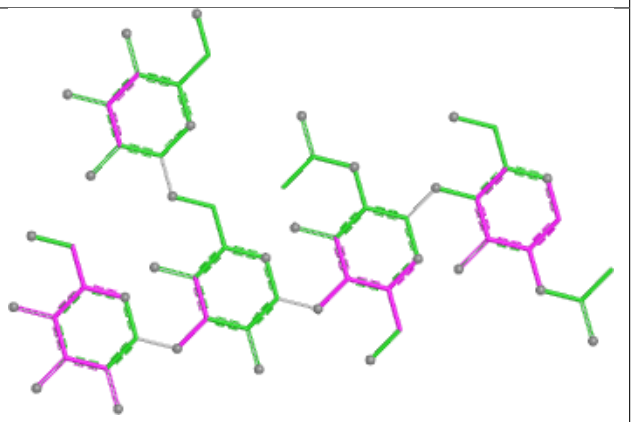
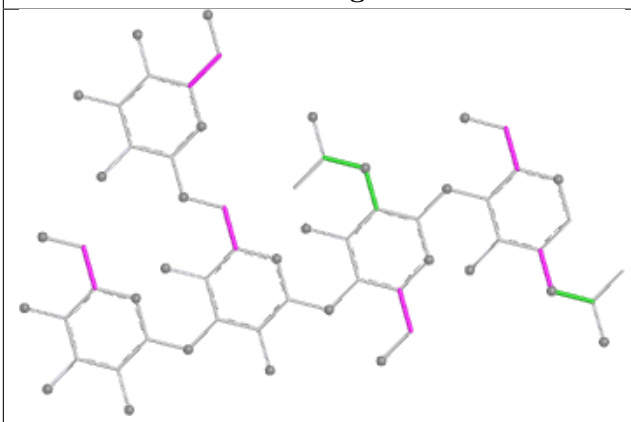
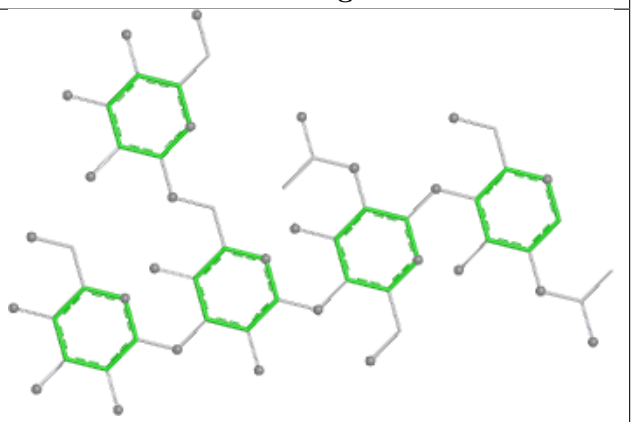
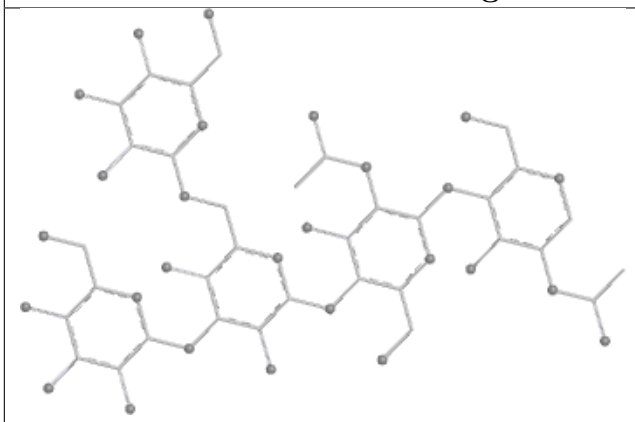
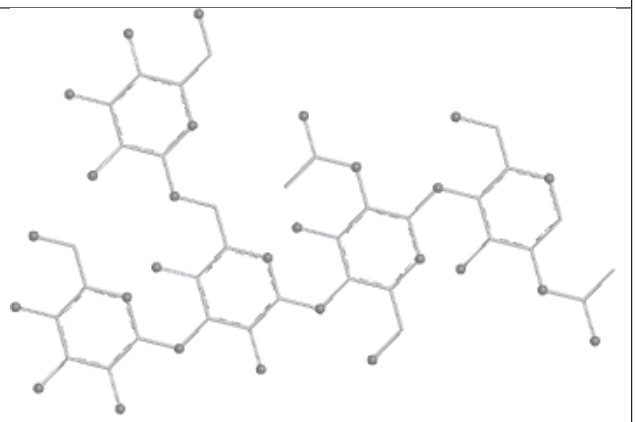
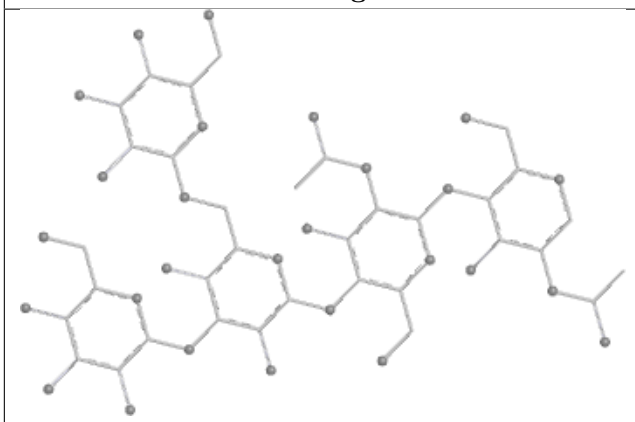
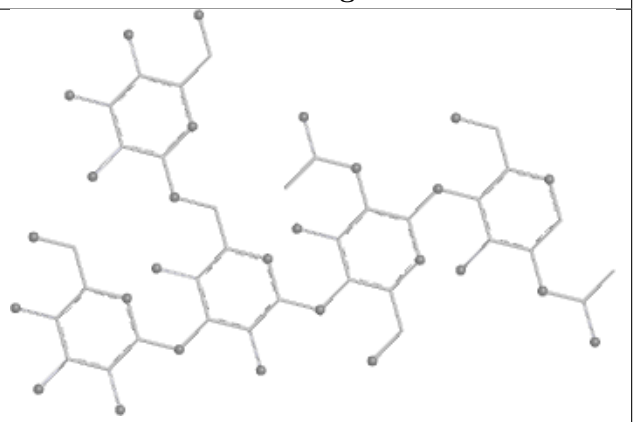
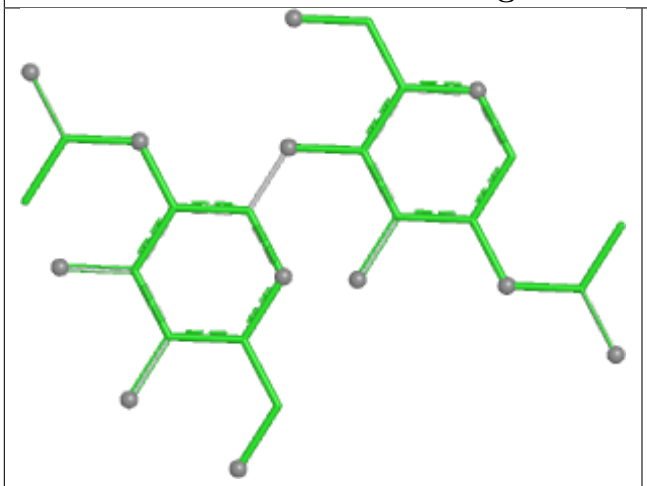
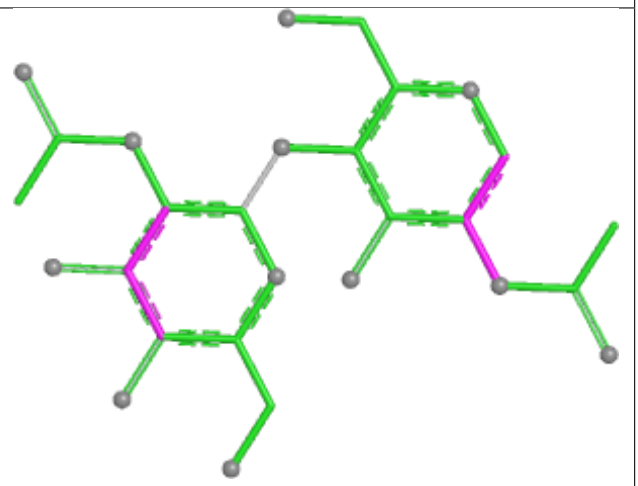
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain AA	
 Bond lengths	 Bond angles
 Torsions	 Rings

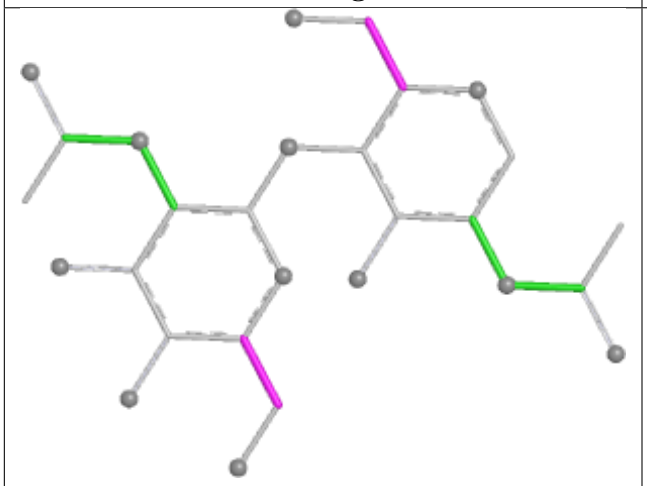
Oligosaccharide Chain Z



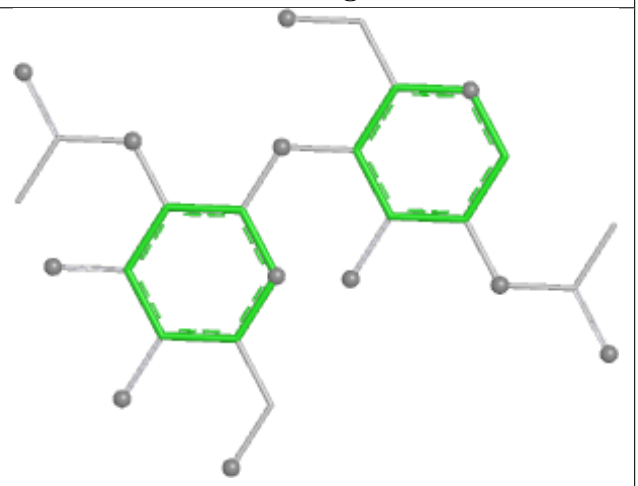
Bond lengths



Bond angles

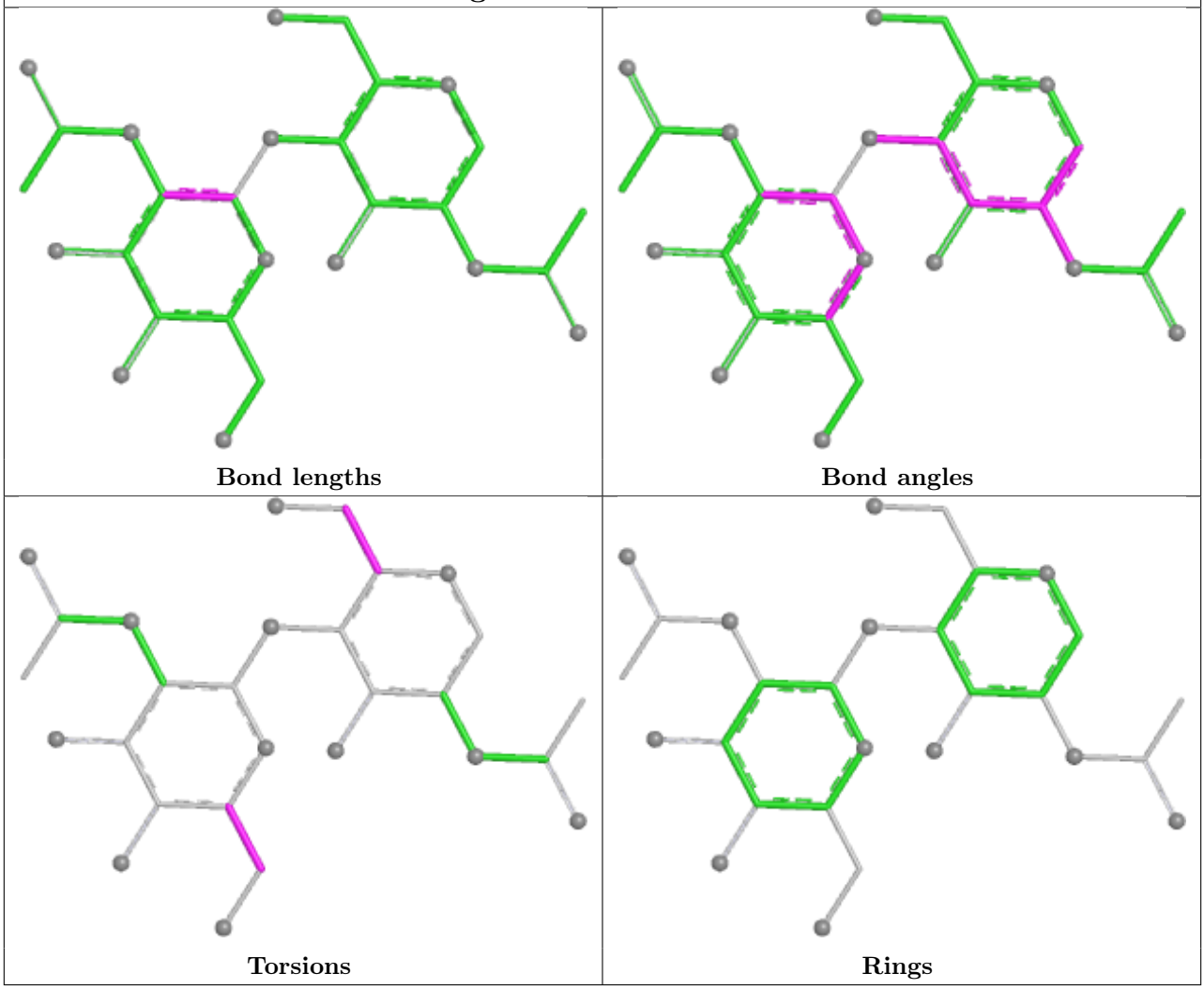


Torsions

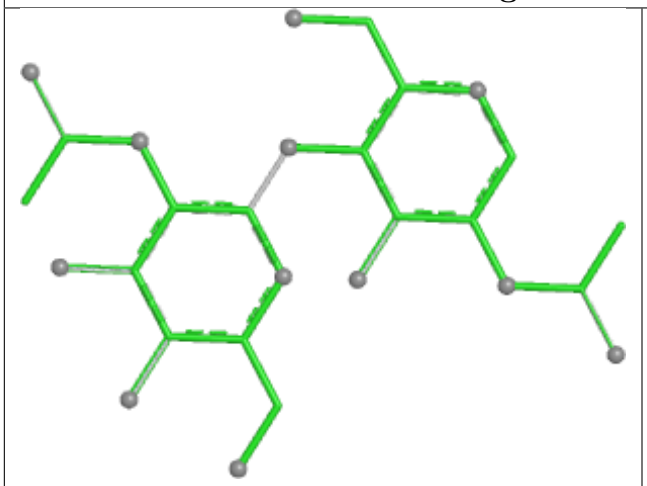


Rings

Oligosaccharide Chain c



Oligosaccharide Chain g



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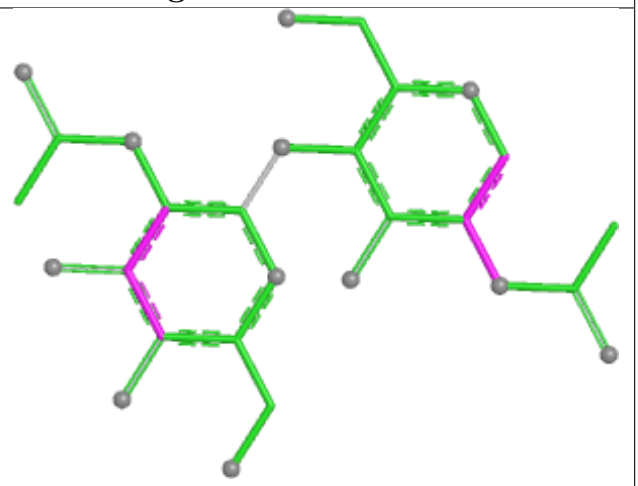

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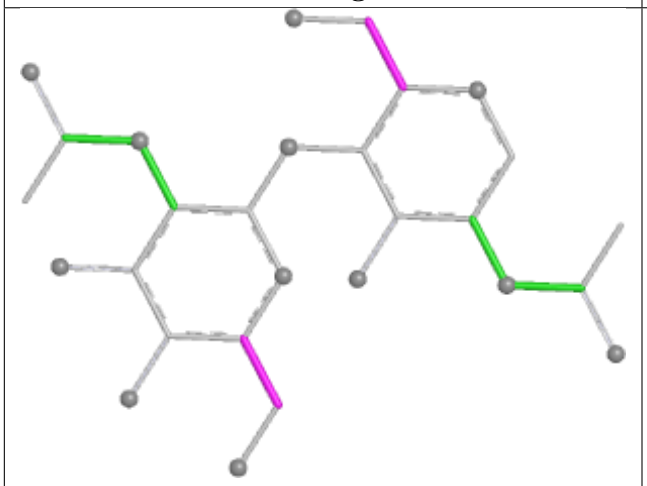

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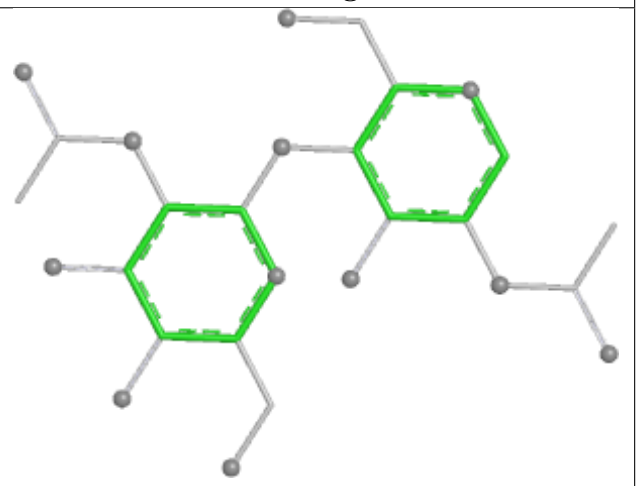
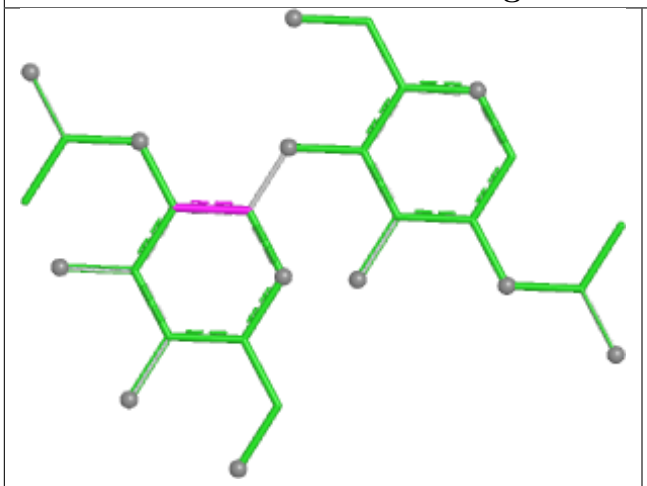


Rings

Oligosaccharide Chain j



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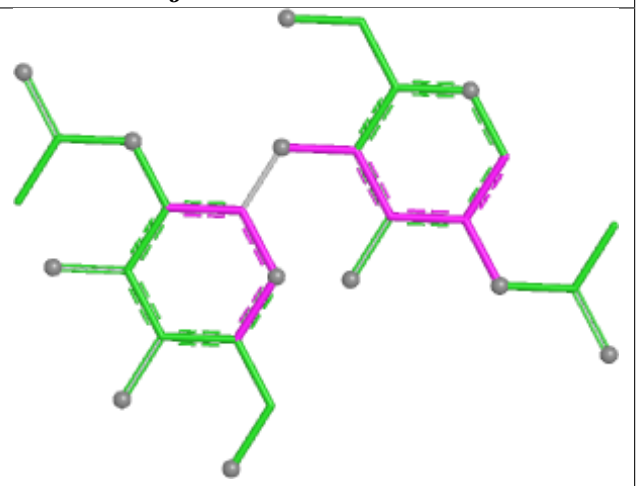
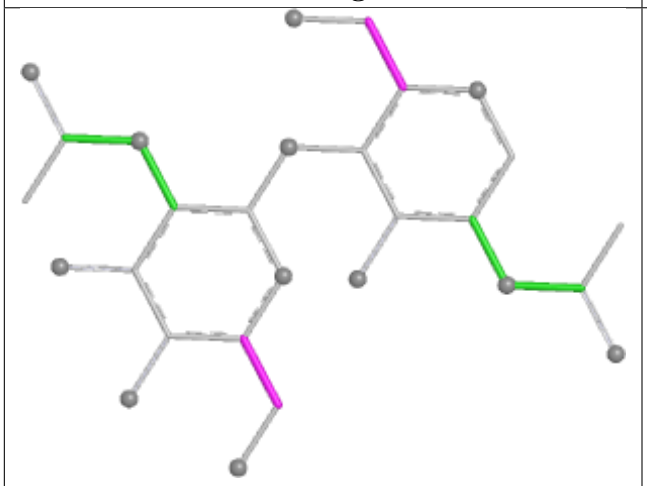


Bond angles



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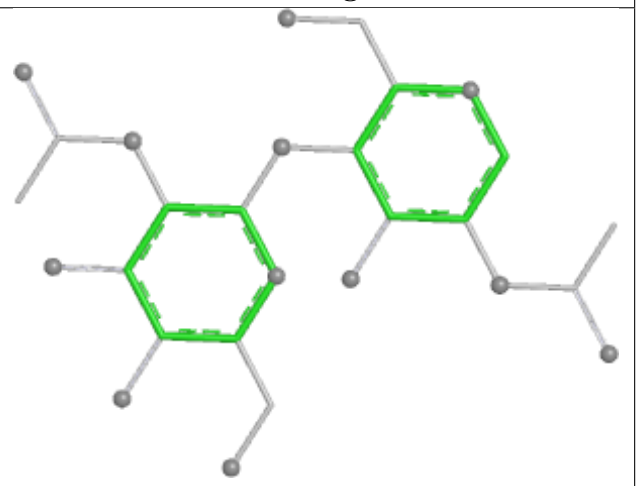
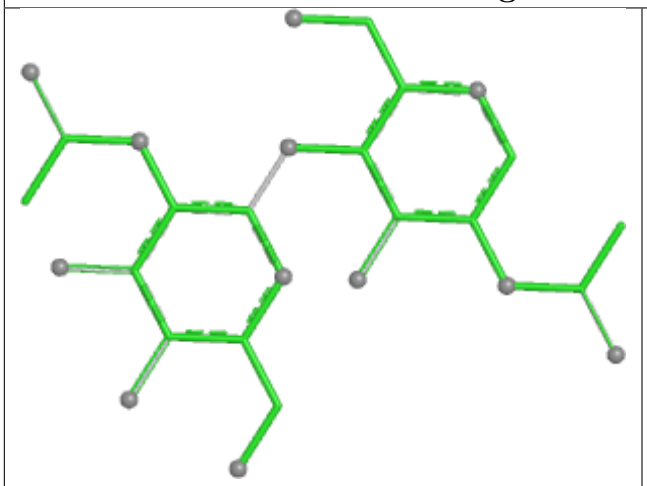


Rings

Oligosaccharide Chain n



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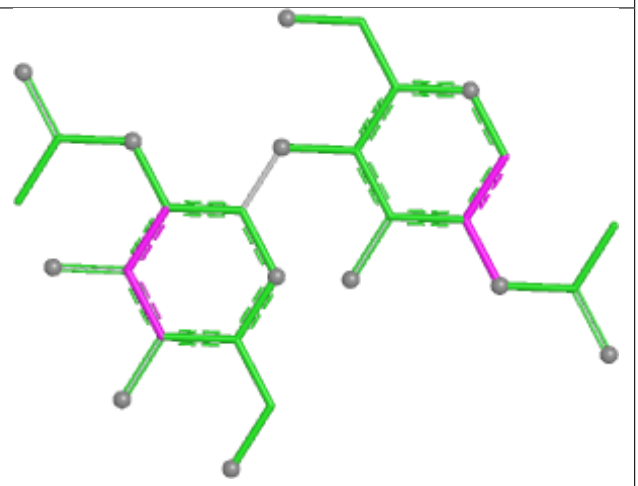
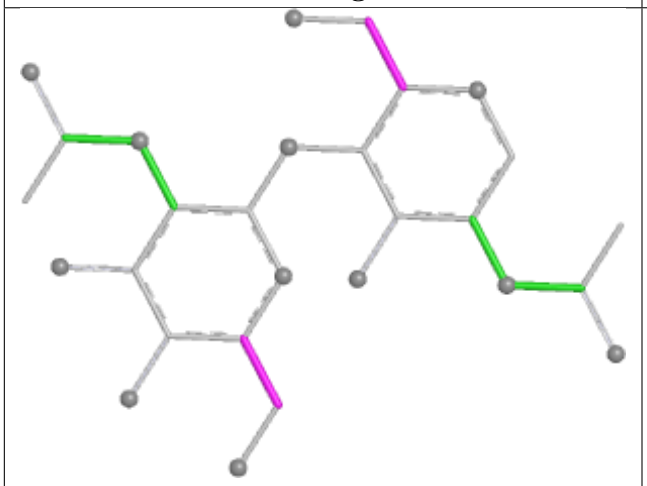


Bond angles



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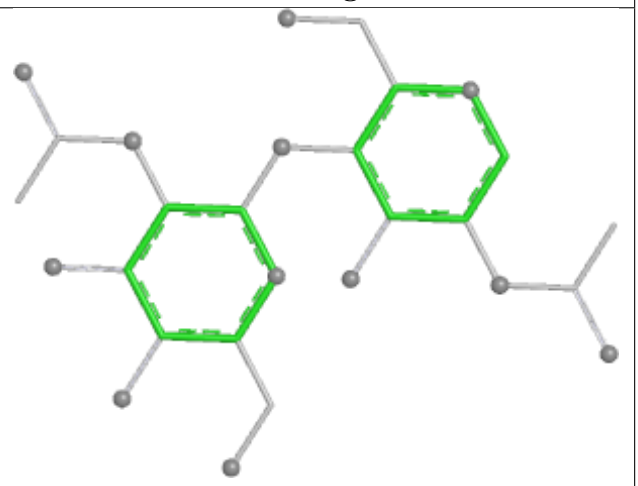
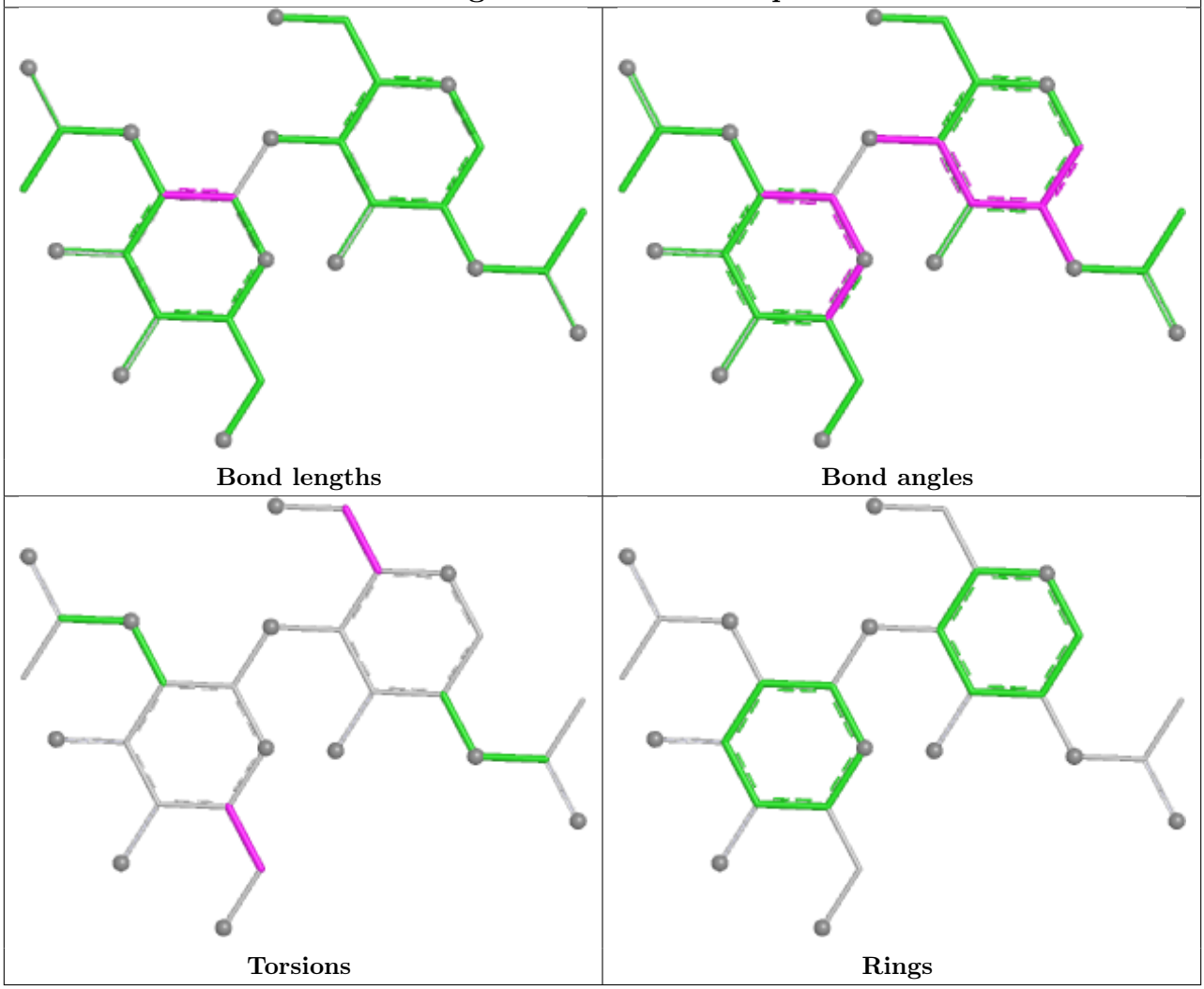


Rings

Oligosaccharide Chain q



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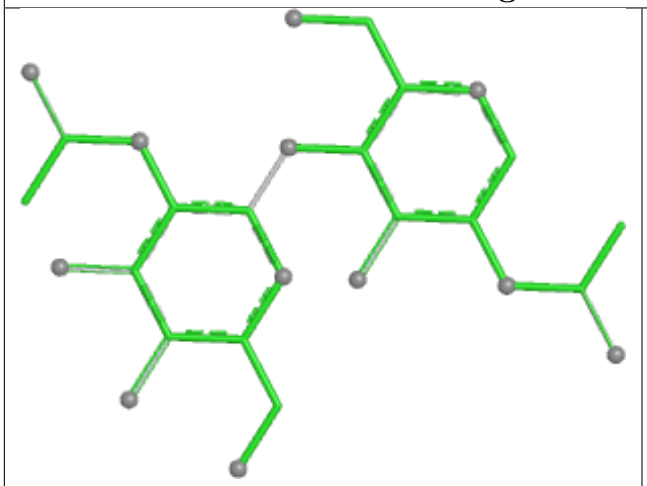

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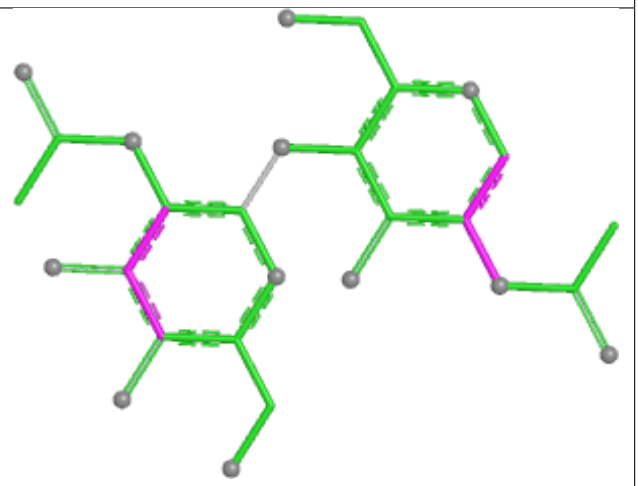
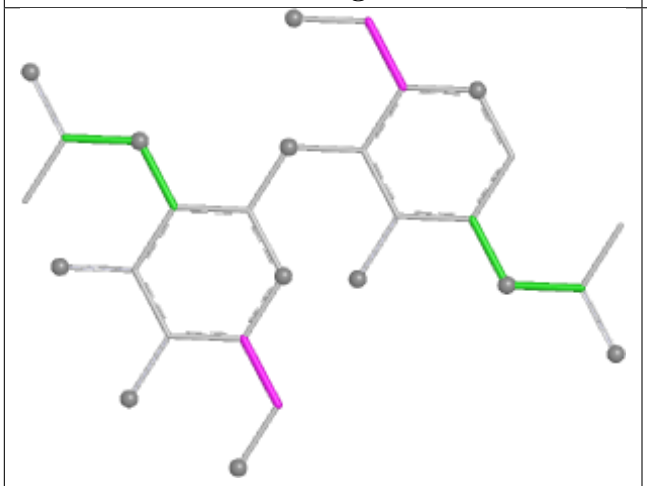


Bond angles



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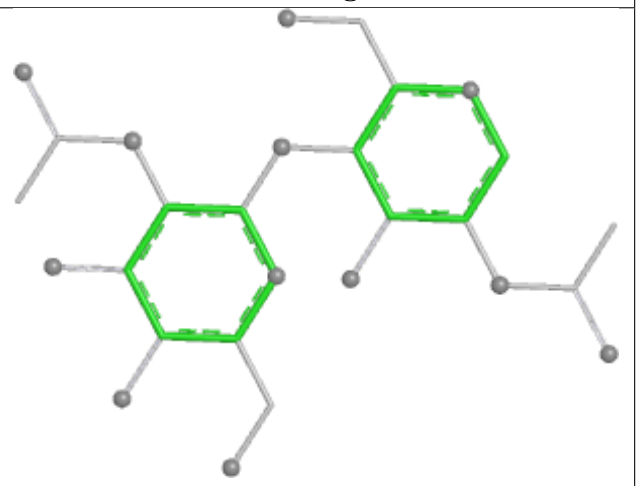
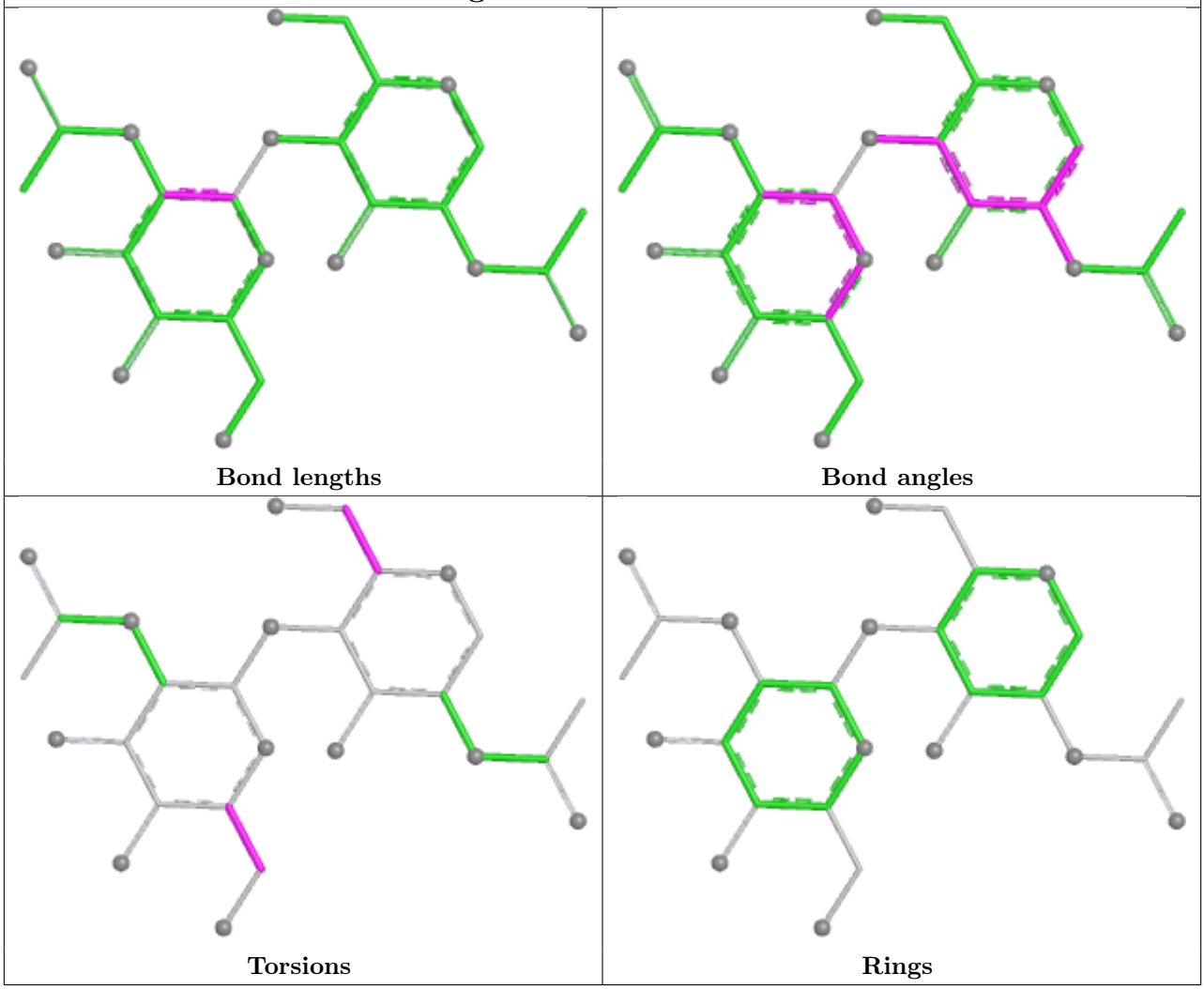
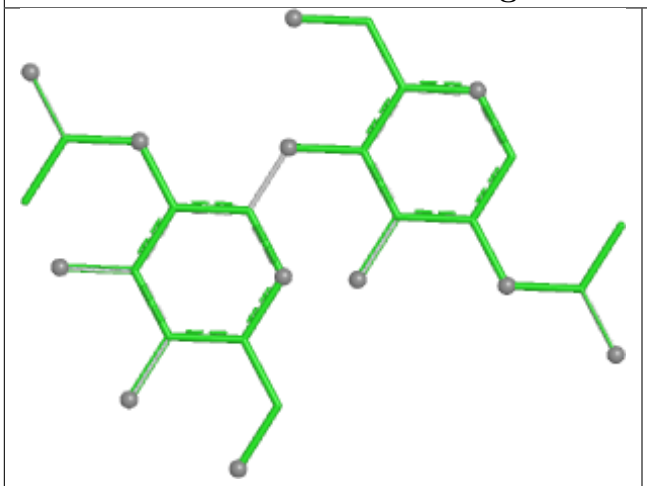


Rings

Oligosaccharide Chain x



Oligosaccharide Chain 1



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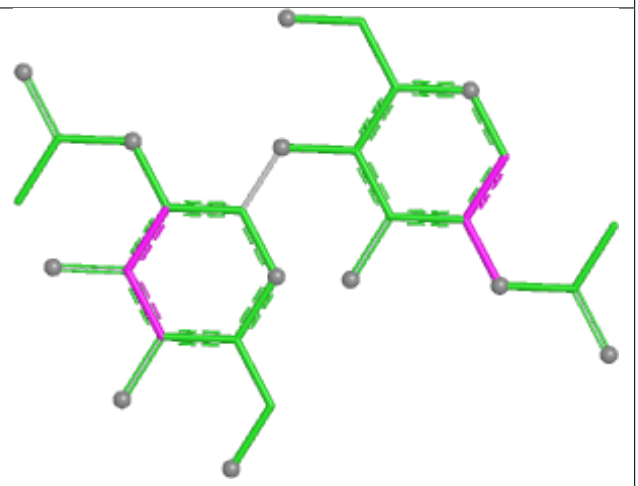
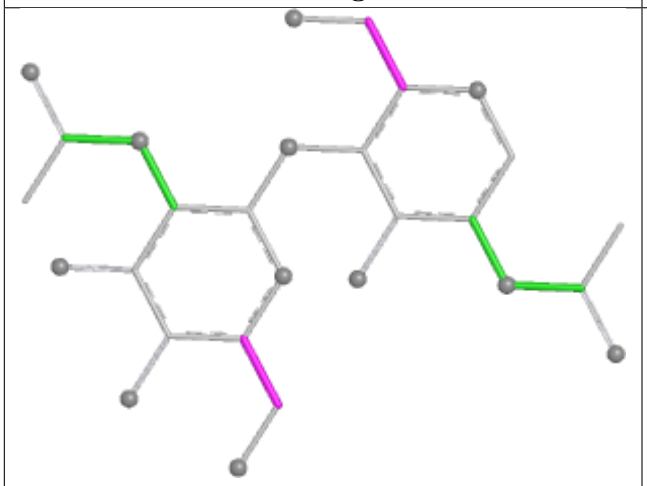


Bond angles



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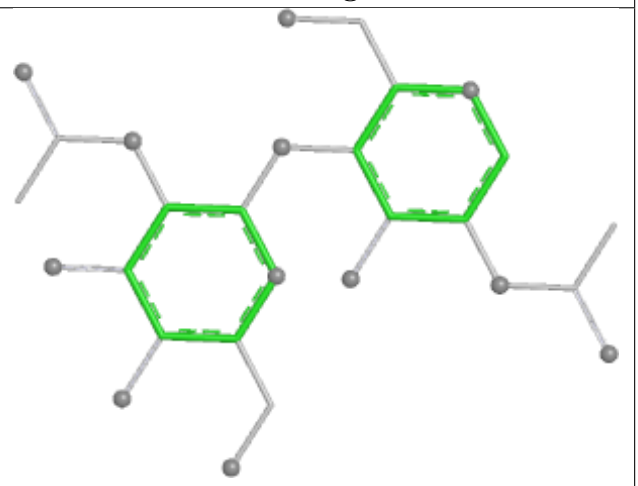
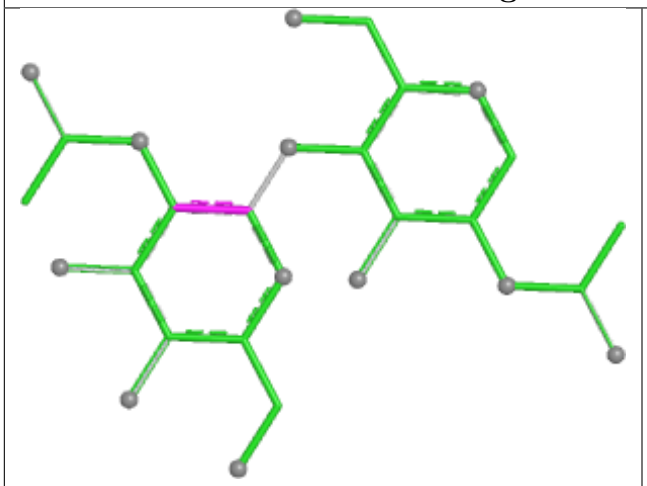


Rings

Oligosaccharide Chain 4



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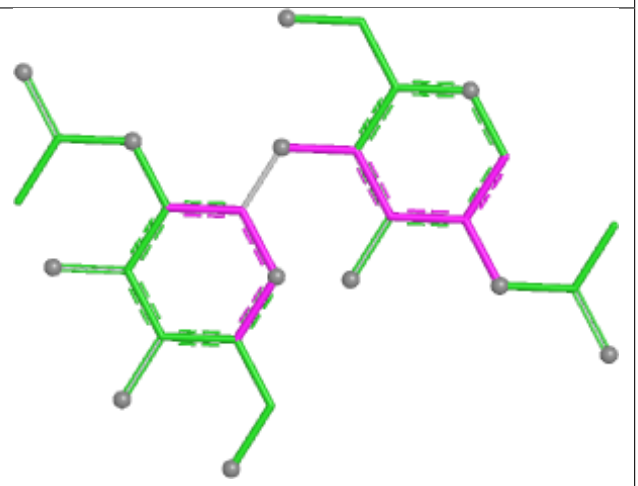

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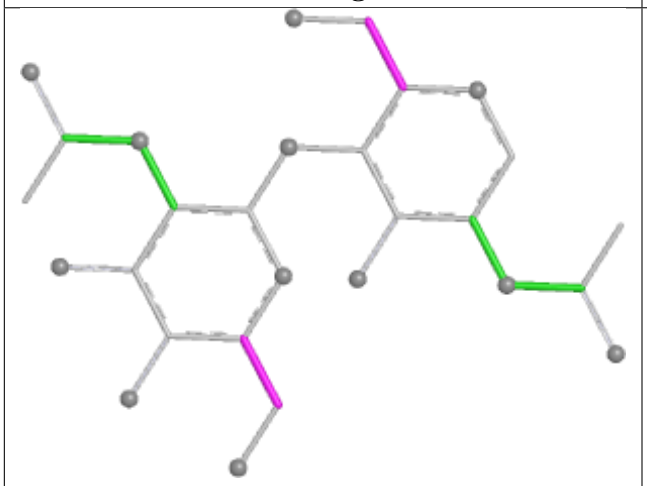

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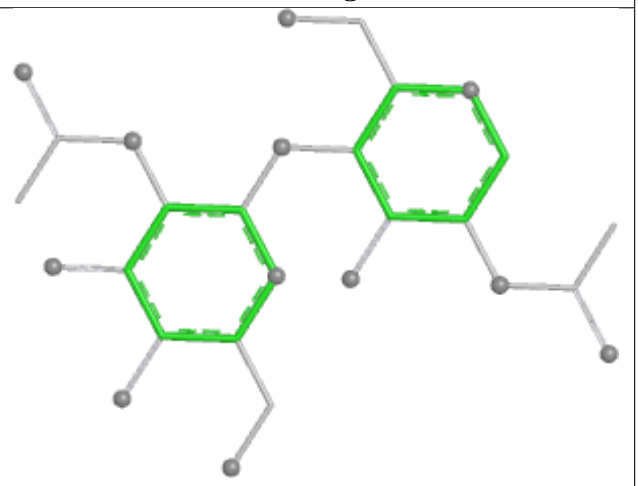
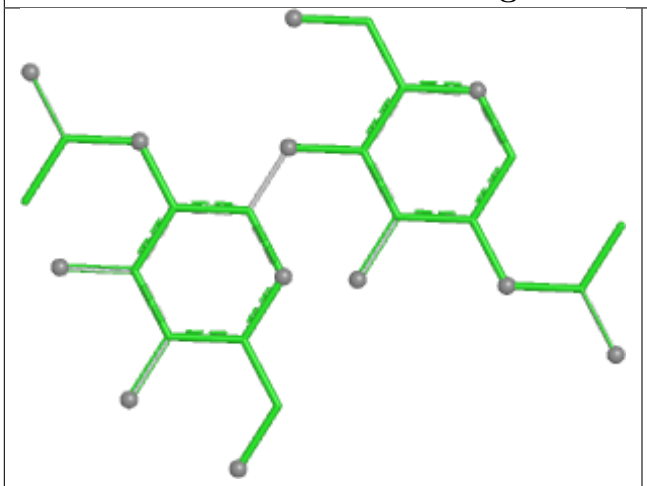


Rings

Oligosaccharide Chain 8



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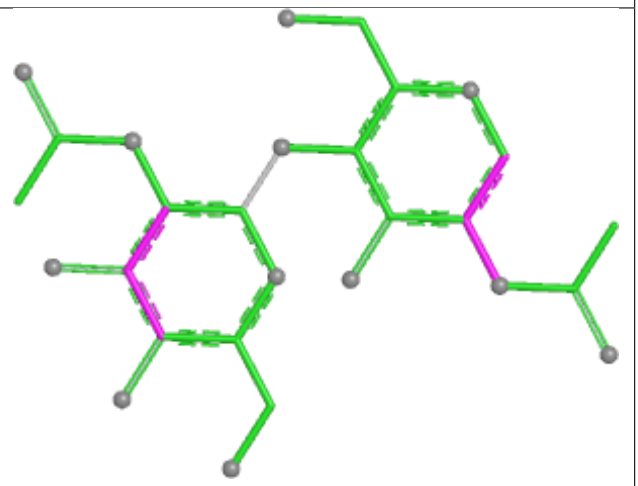
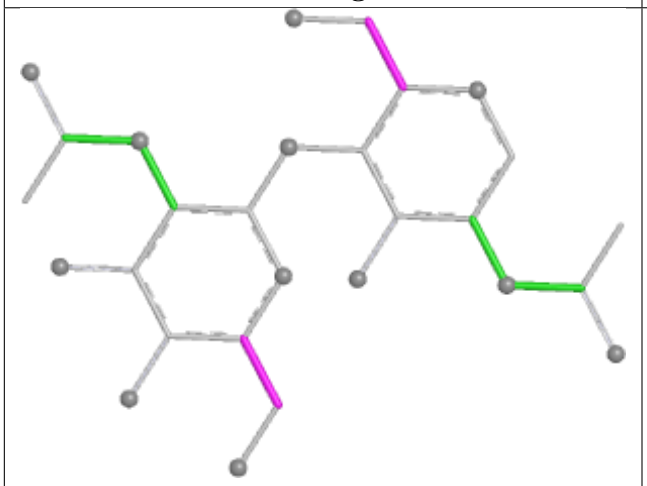


Bond angles



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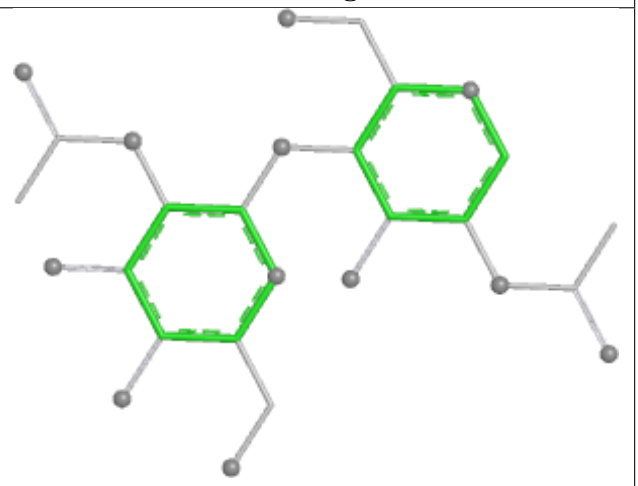
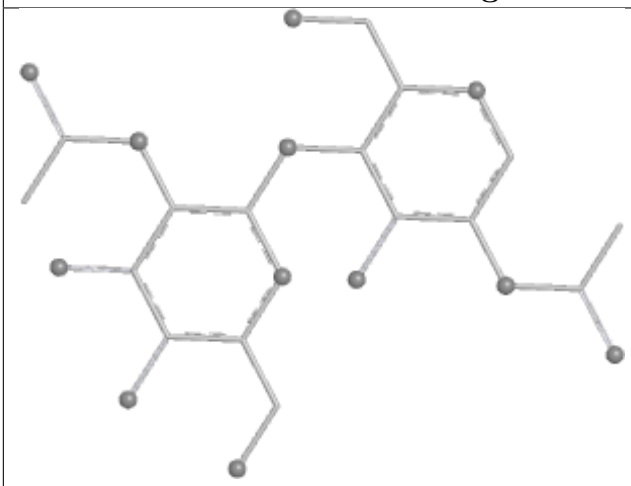
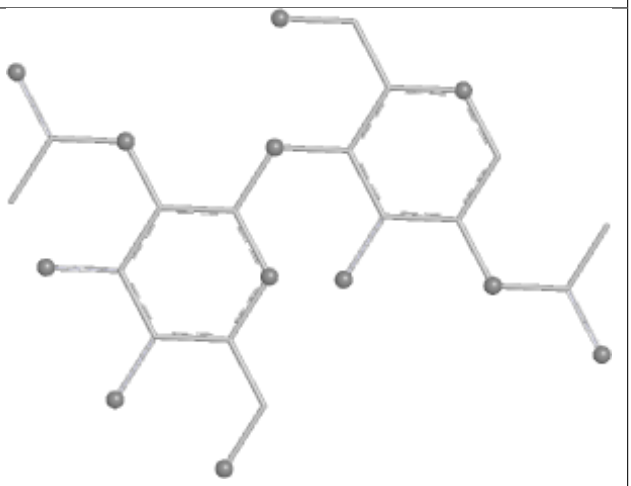
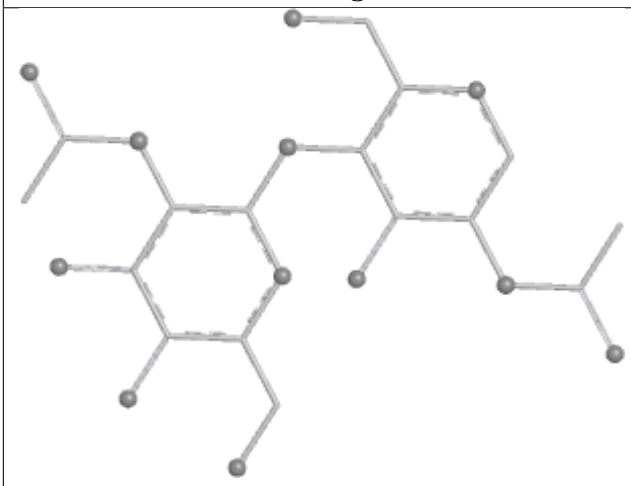
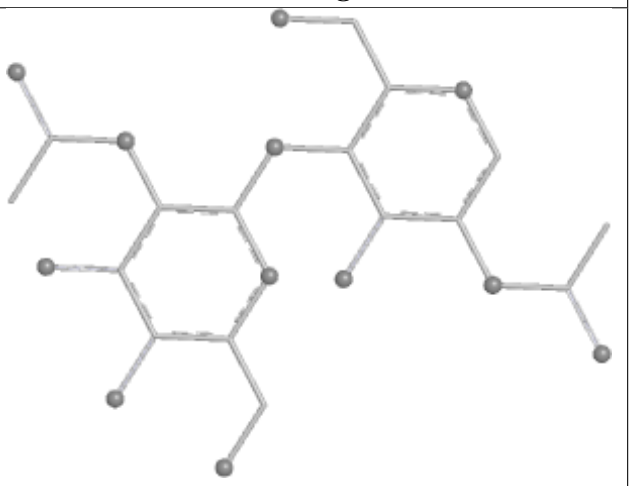
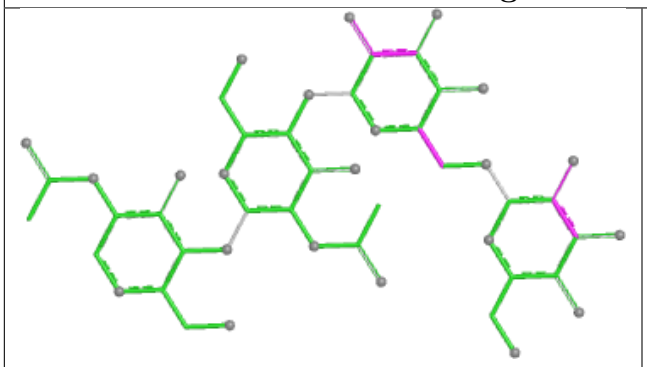


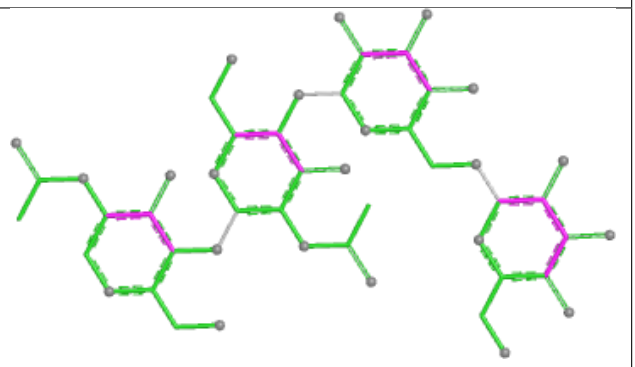
Rings

Oligosaccharide Chain BA	
 Bond lengths	 Bond angles
 Torsions	 Rings

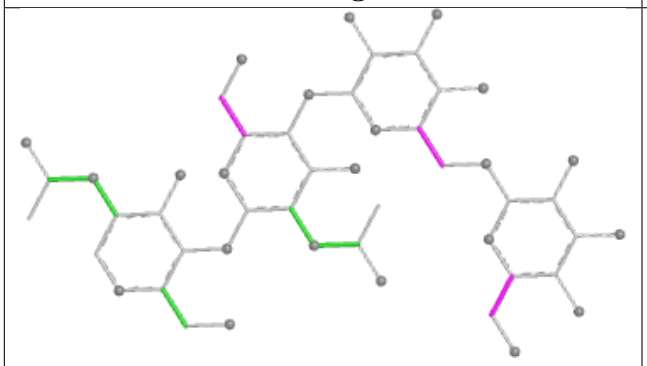
Oligosaccharide Chain a



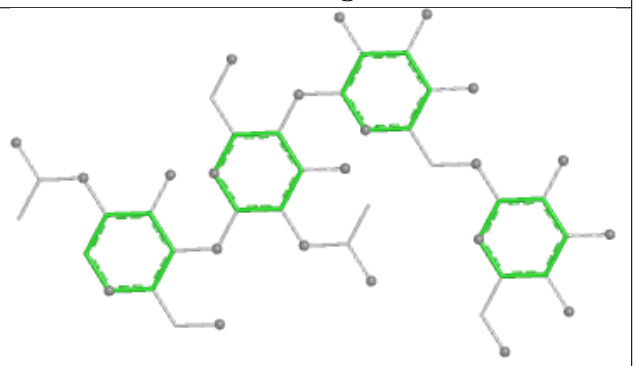
Bond lengths



Bond angles

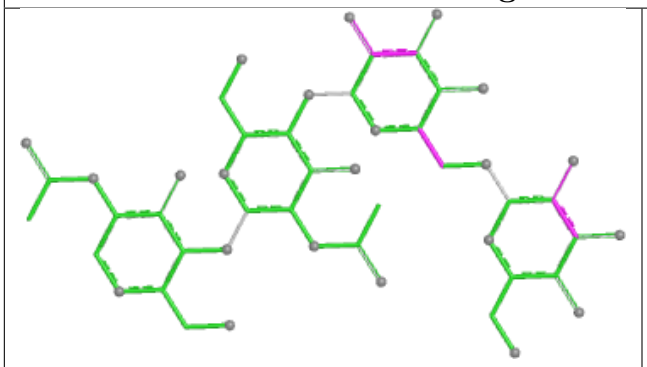


Torsions

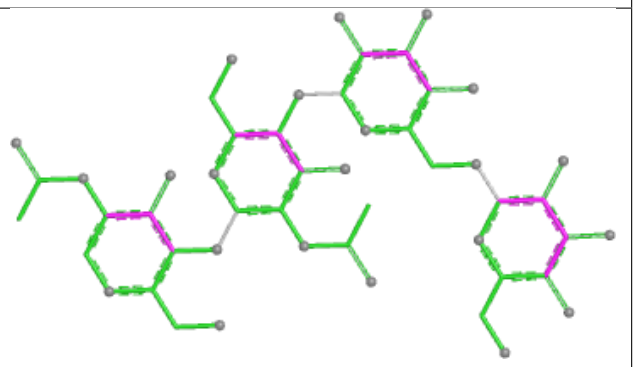


Rings

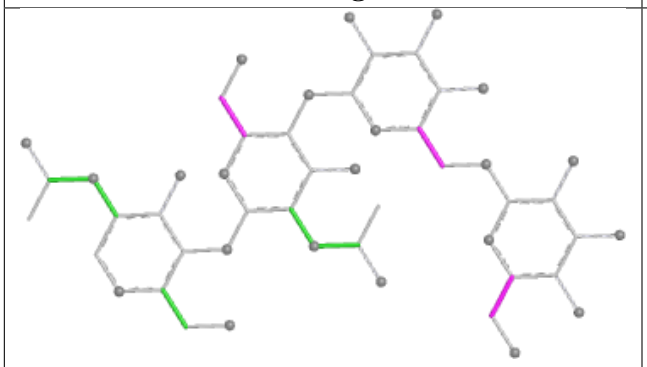
Oligosaccharide Chain h



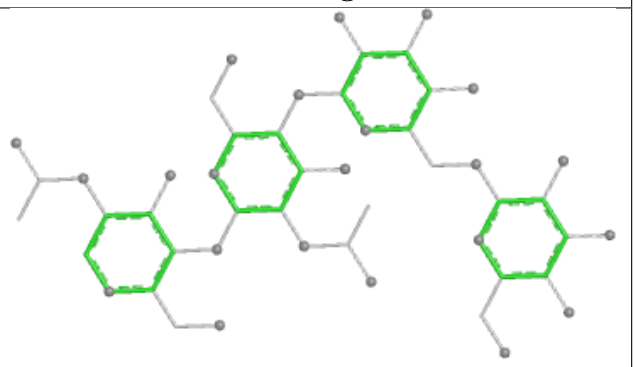
Bond lengths



Bond angles

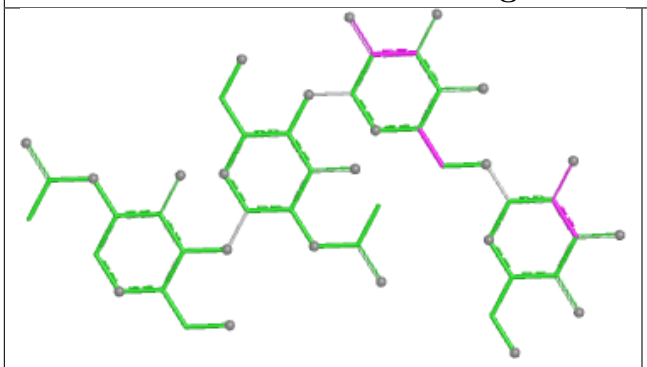


Torsions

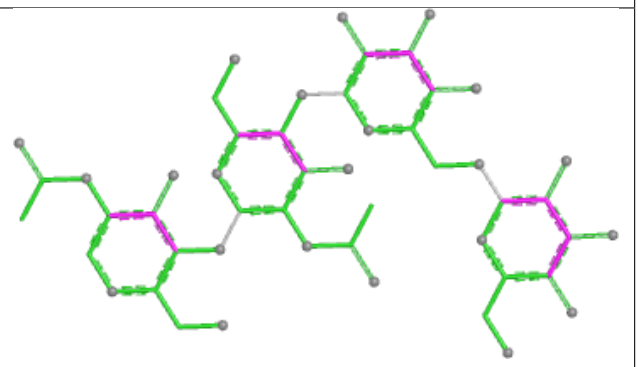


Rings

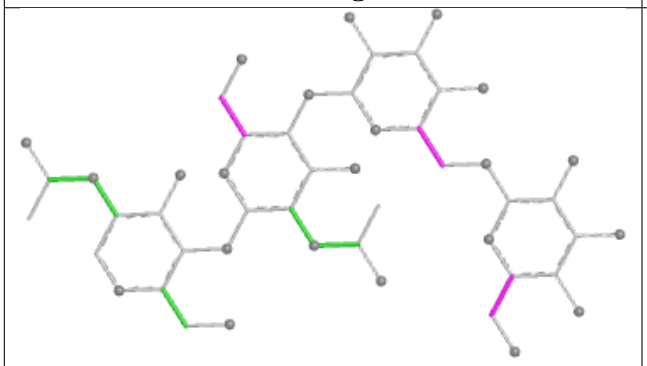
Oligosaccharide Chain o



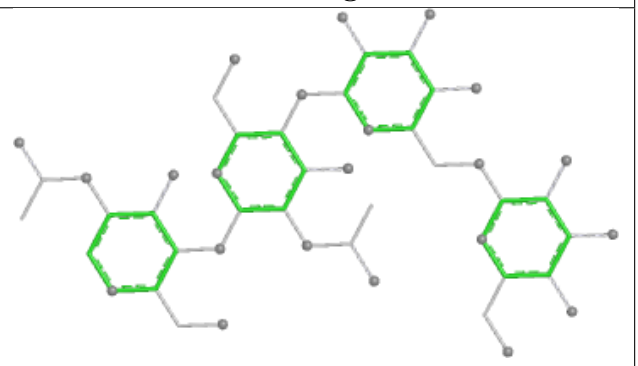
Bond lengths



Bond angles

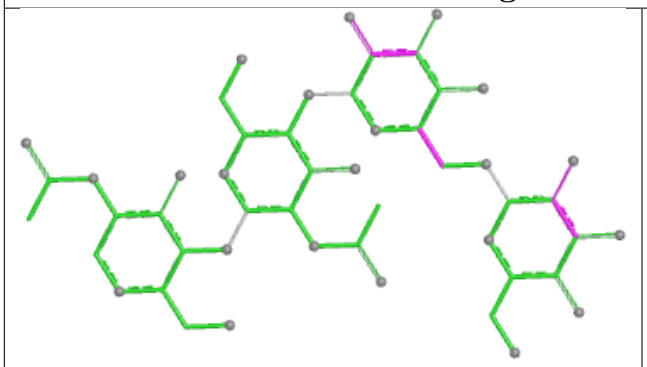


Torsions

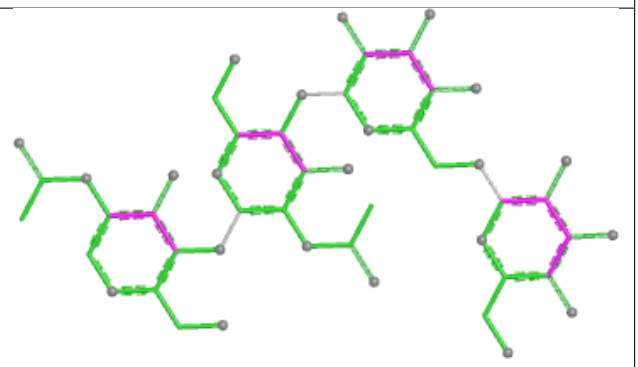


Rings

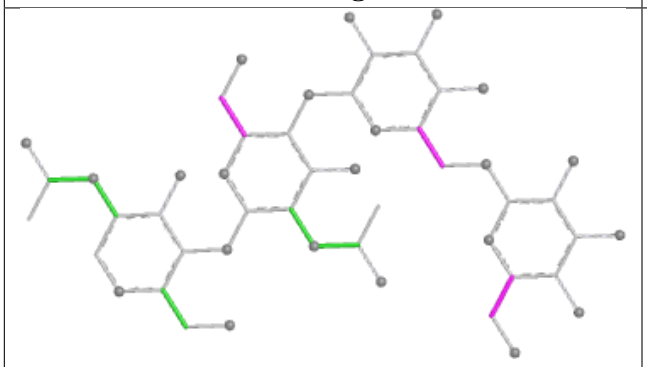
Oligosaccharide Chain v



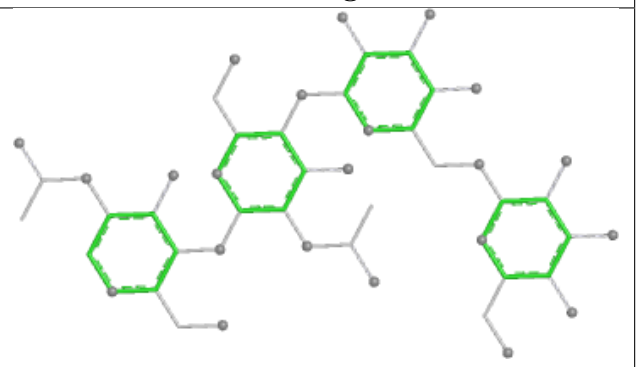
Bond lengths



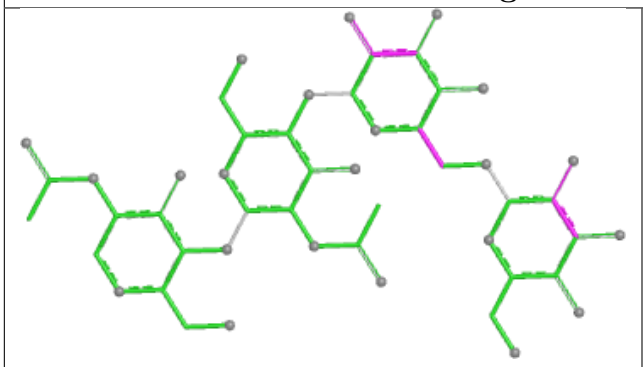
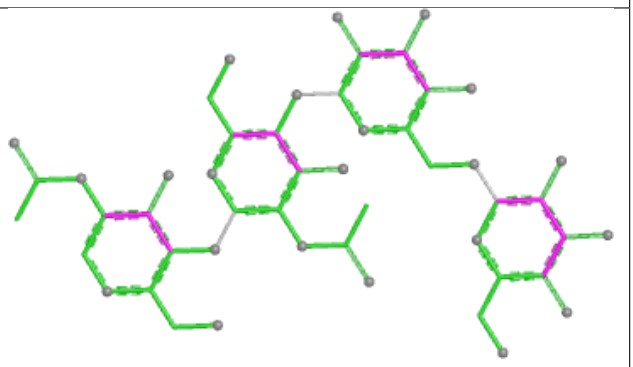
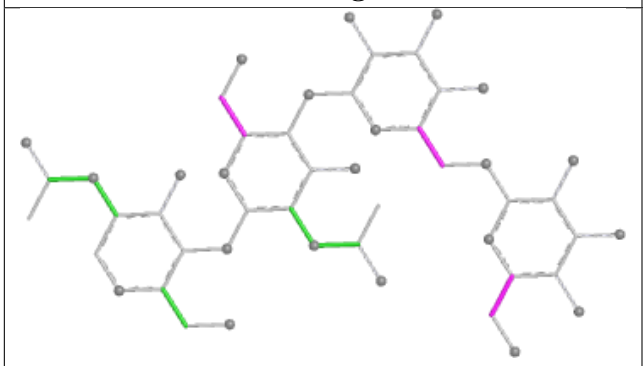
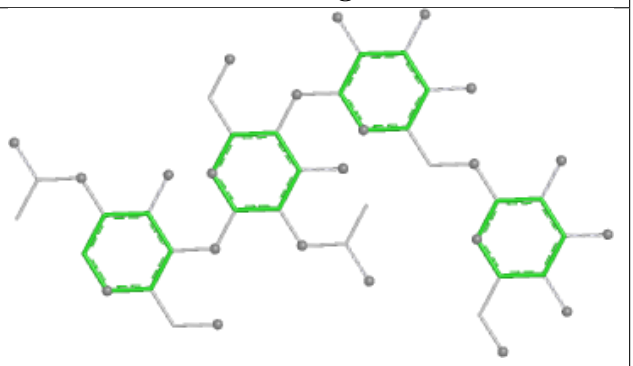
Bond angles

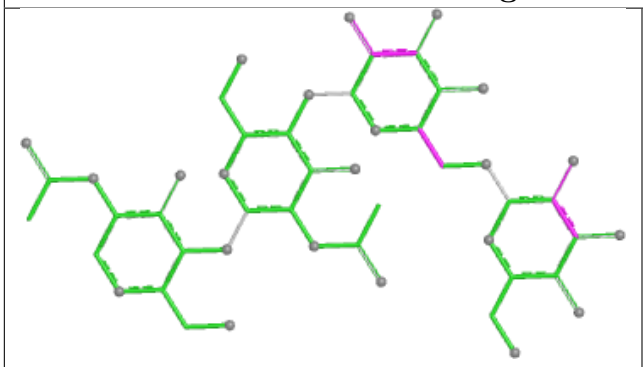
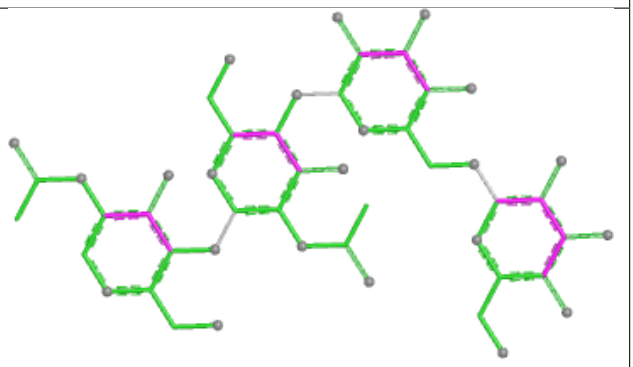
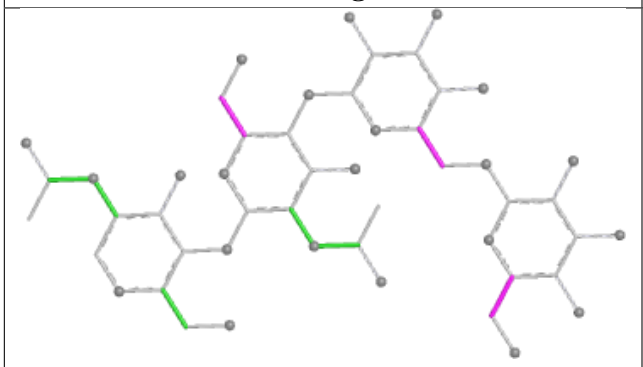
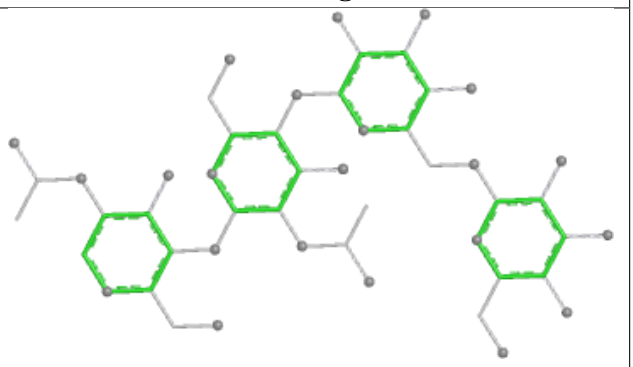


Torsions

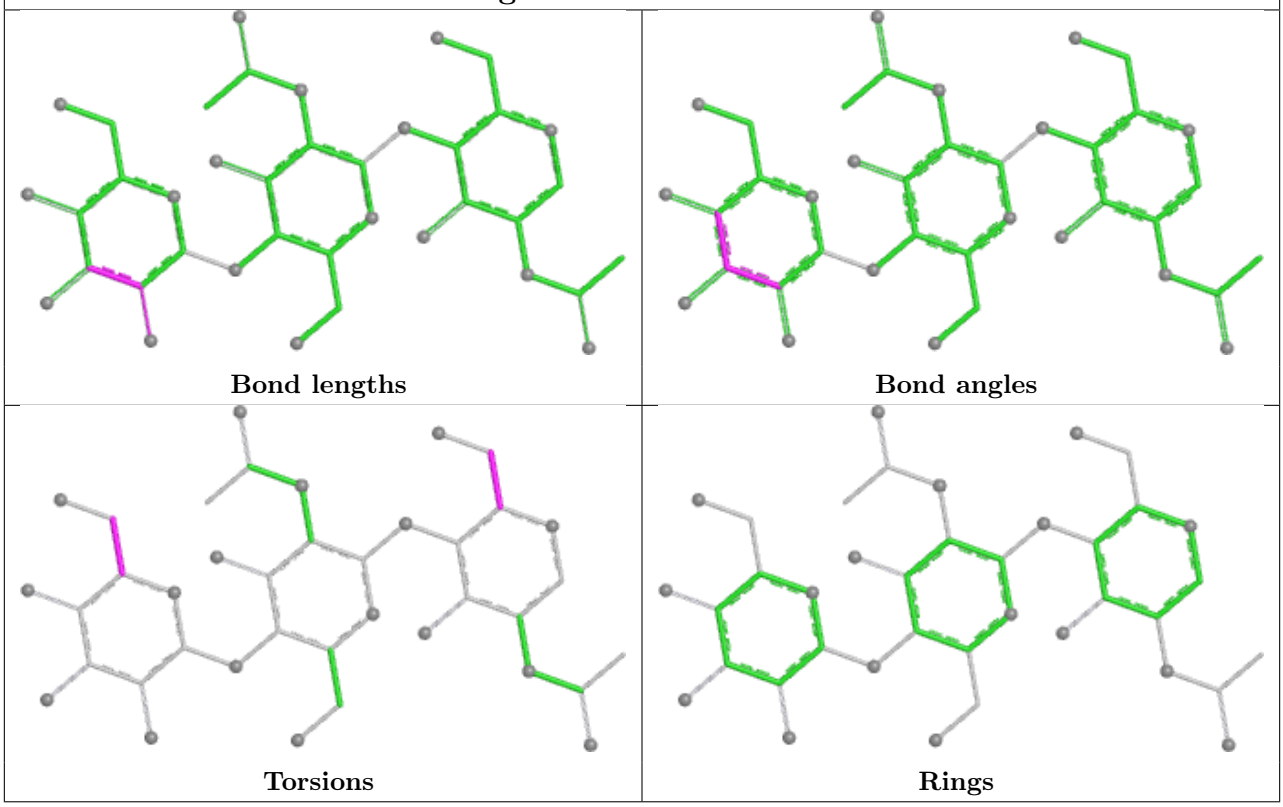


Rings

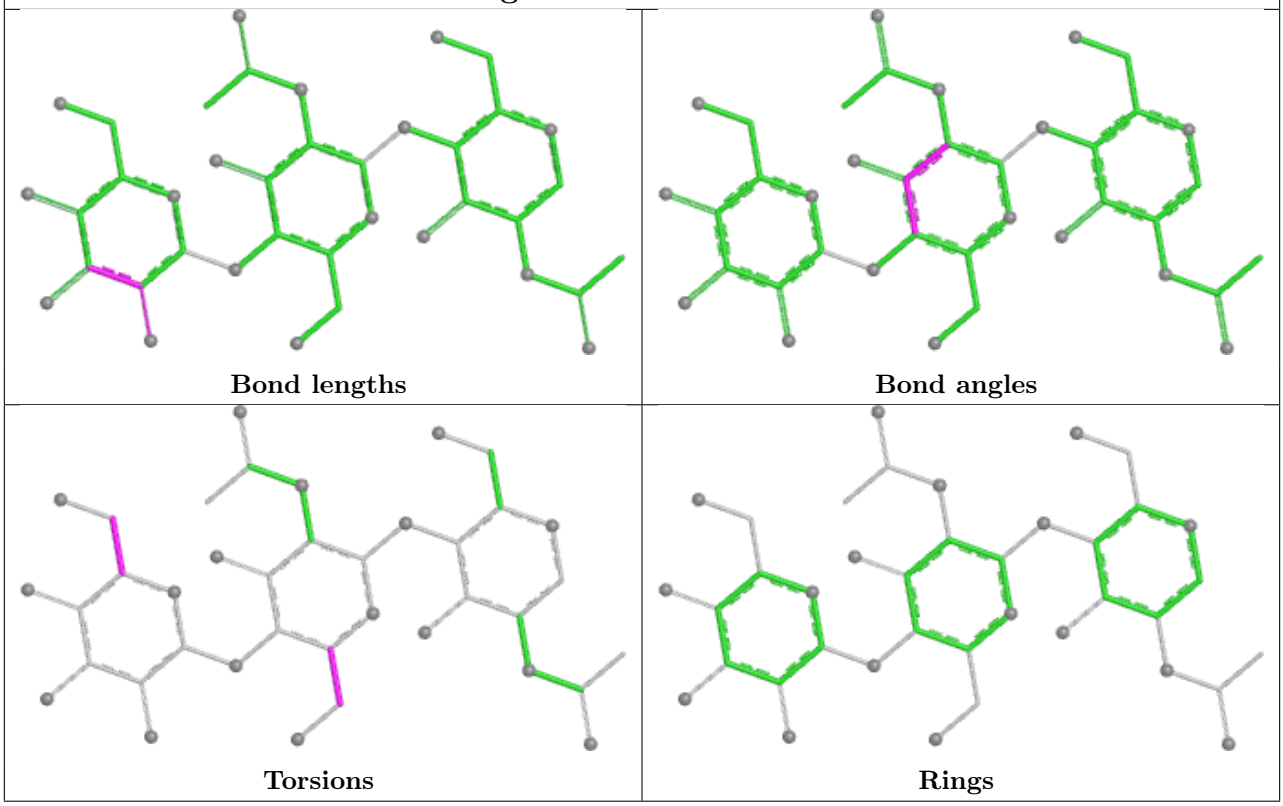
Oligosaccharide Chain 2	
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain 9	
 Bond lengths	 Bond angles
 Torsions	 Rings

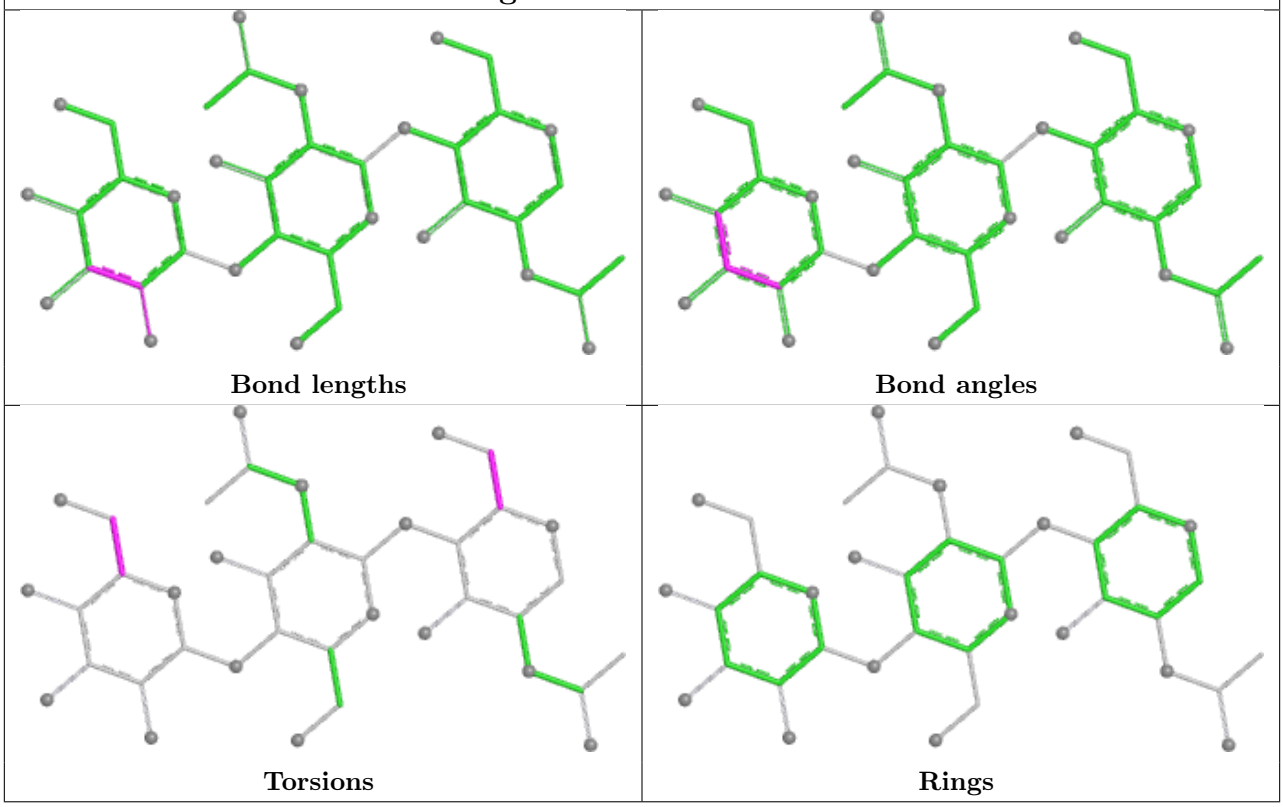
Oligosaccharide Chain d



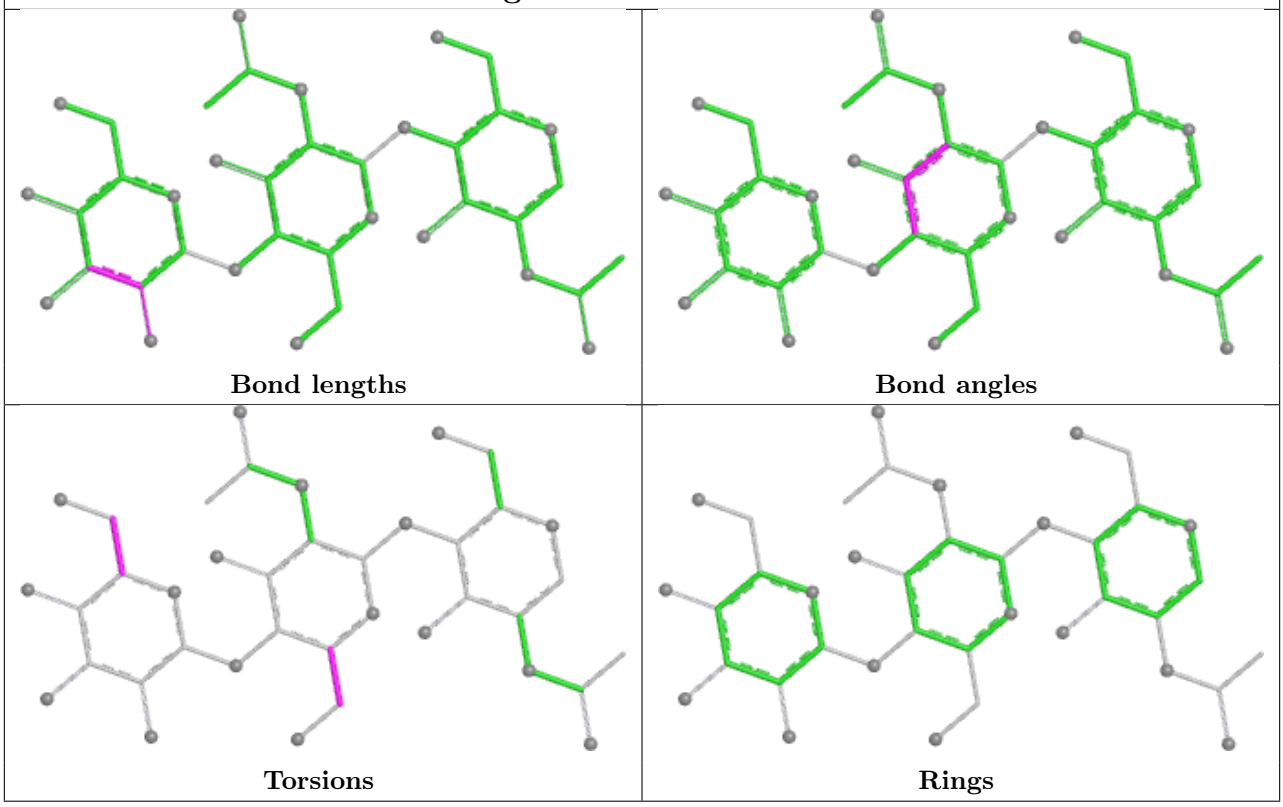
Oligosaccharide Chain e



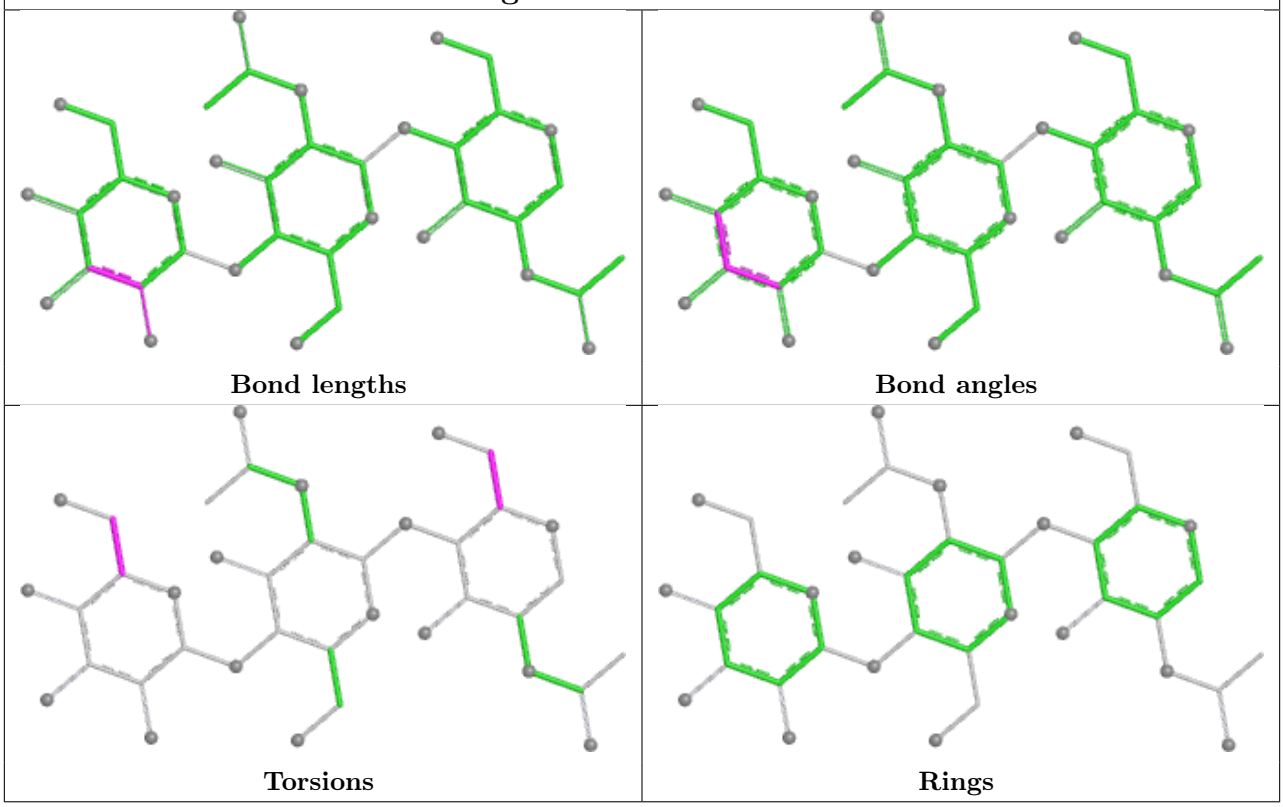
Oligosaccharide Chain k



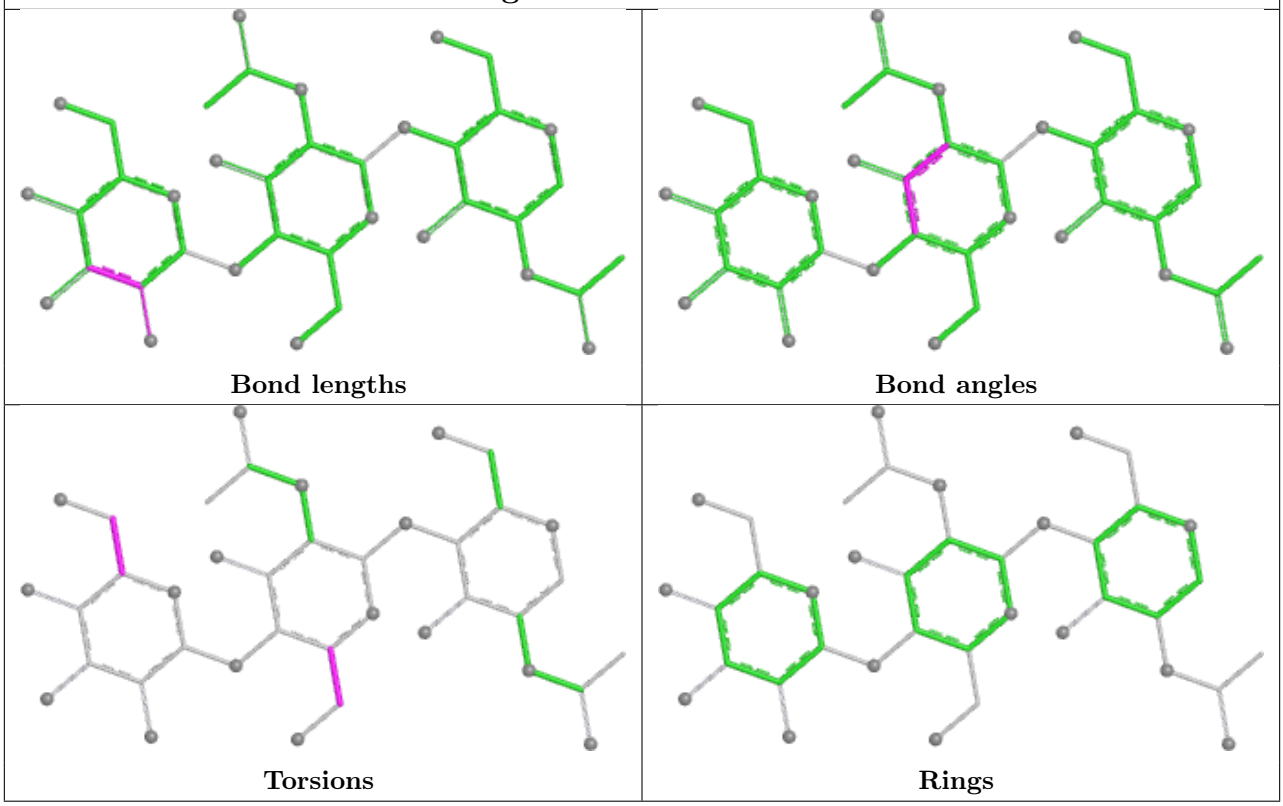
Oligosaccharide Chain l



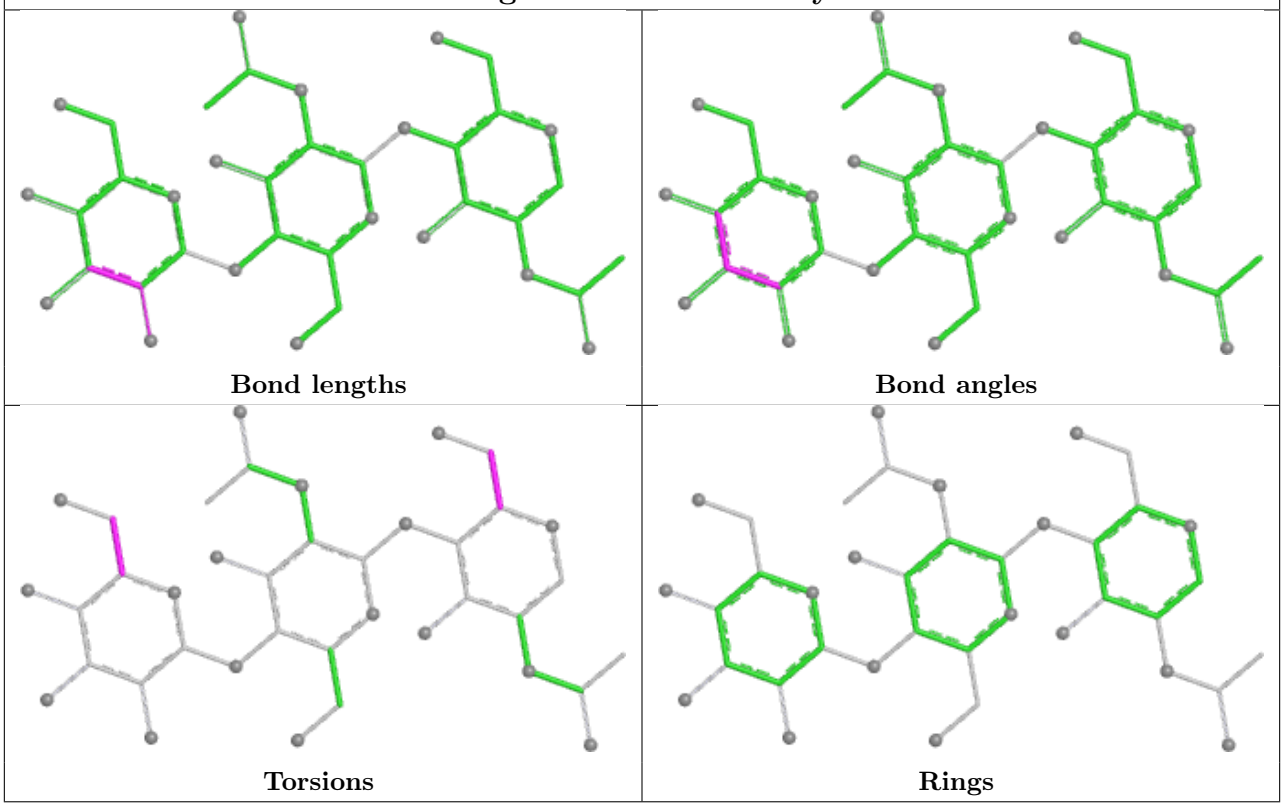
Oligosaccharide Chain r



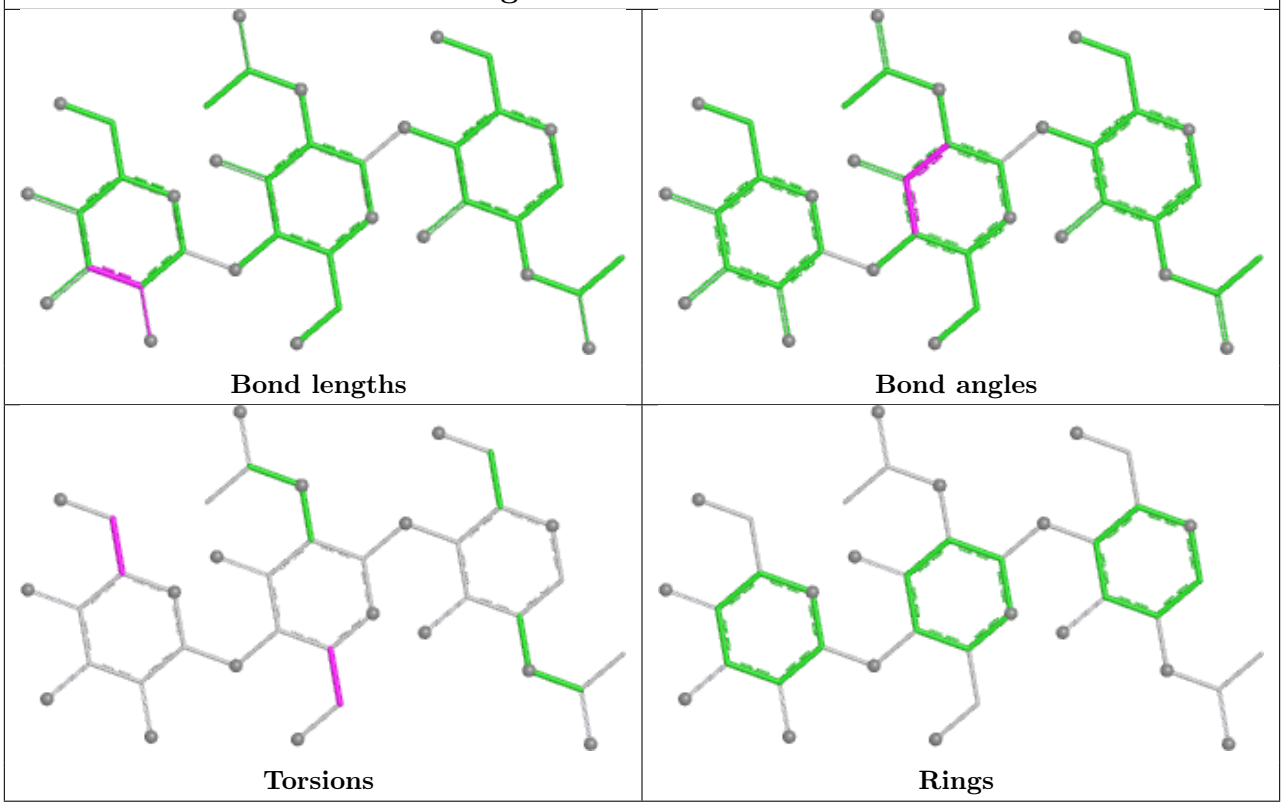
Oligosaccharide Chain s



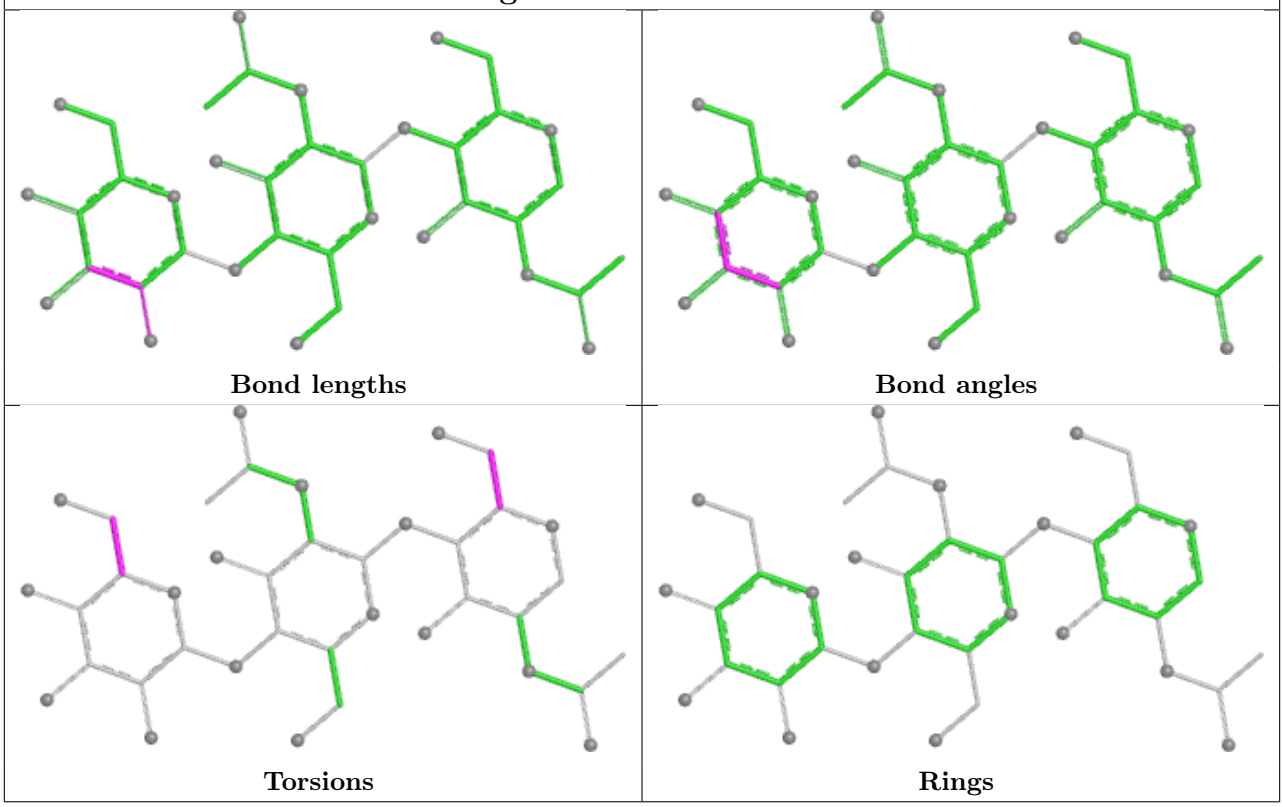
Oligosaccharide Chain y



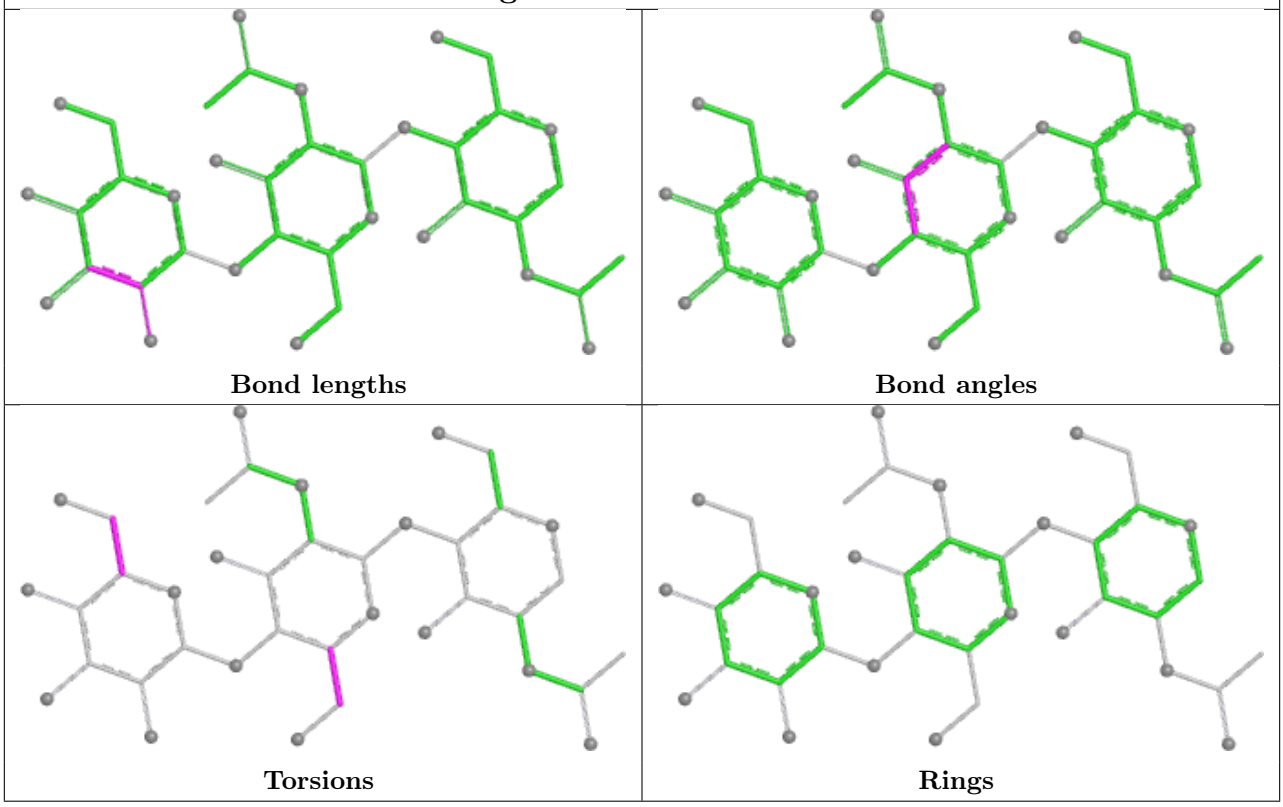
Oligosaccharide Chain z



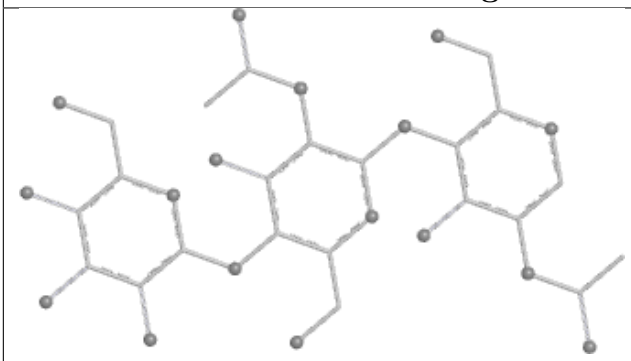
Oligosaccharide Chain 5



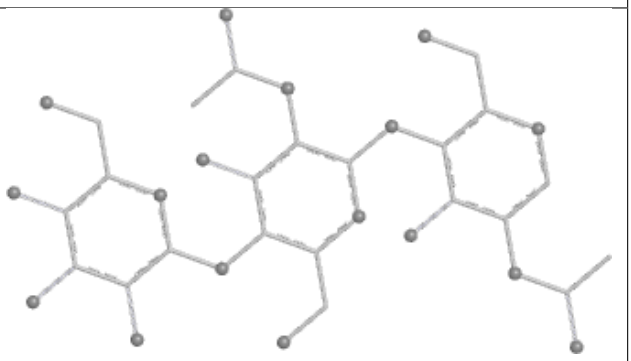
Oligosaccharide Chain 6



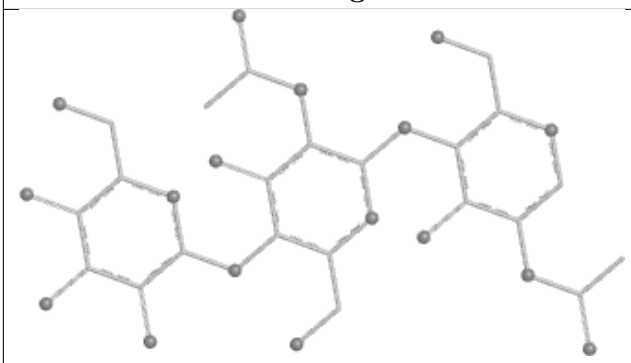
Oligosaccharide Chain CA



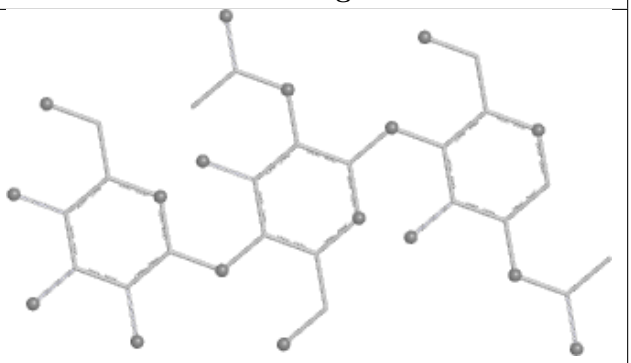
Bond lengths



Bond angles

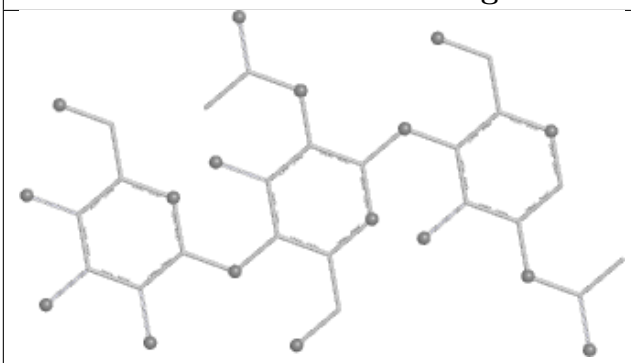


Torsions

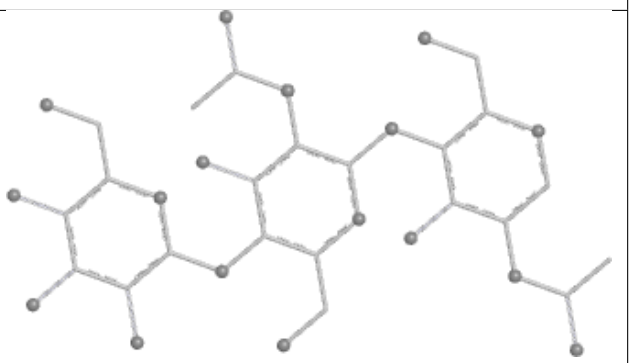


Rings

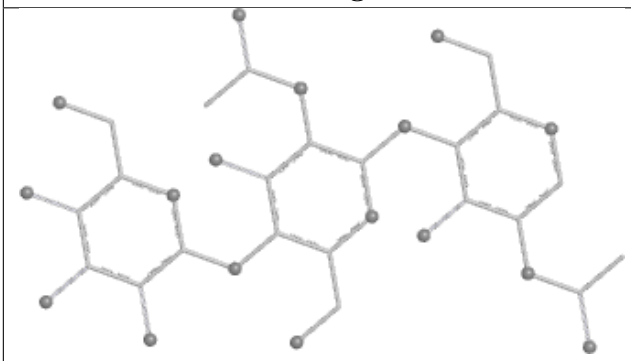
Oligosaccharide Chain DA



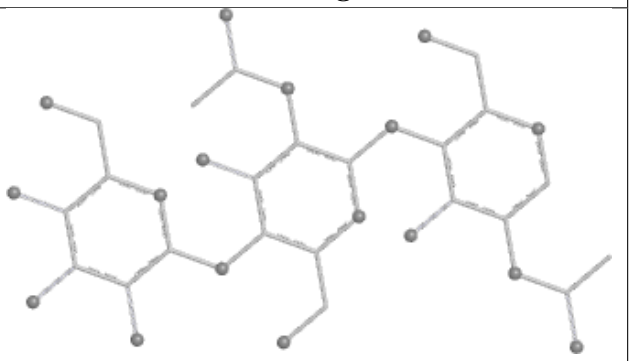
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry (i)

18 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
9	NAG	G	620	1	14,14,15	0.88	0	17,19,21	0.90	1 (5%)
9	NAG	C	608	1	14,14,15	0.84	0	17,19,21	0.94	1 (5%)
9	NAG	E	627	1	14,14,15	0.90	0	17,19,21	0.91	1 (5%)
9	NAG	G	608	1	14,14,15	0.83	0	17,19,21	0.94	1 (5%)
9	NAG	D	608	1	14,14,15	0.83	0	17,19,21	0.94	1 (5%)
9	NAG	A	608	1	14,14,15	0.83	0	17,19,21	0.94	1 (5%)
9	NAG	D	620	1	14,14,15	0.88	0	17,19,21	0.90	1 (5%)
9	NAG	A	627	1	14,14,15	0.90	0	17,19,21	0.91	1 (5%)
9	NAG	E	608	1	14,14,15	0.83	0	17,19,21	0.94	1 (5%)
9	NAG	F	620	1	14,14,15	0.88	0	17,19,21	0.90	1 (5%)
9	NAG	G	627	1	14,14,15	0.90	0	17,19,21	0.90	1 (5%)
9	NAG	A	620	1	14,14,15	0.88	0	17,19,21	0.90	1 (5%)
9	NAG	C	627	1	14,14,15	0.89	0	17,19,21	0.91	1 (5%)
9	NAG	E	620	1	14,14,15	0.88	0	17,19,21	0.90	1 (5%)
9	NAG	C	620	1	14,14,15	0.88	0	17,19,21	0.90	1 (5%)
9	NAG	F	608	1	14,14,15	0.84	0	17,19,21	0.94	1 (5%)
9	NAG	F	627	1	14,14,15	0.89	0	17,19,21	0.91	1 (5%)
9	NAG	D	627	1	14,14,15	0.90	0	17,19,21	0.90	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	NAG	G	620	1	-	1/6/23/26	0/1/1/1
9	NAG	C	608	1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	NAG	E	627	1	-	2/6/23/26	0/1/1/1
9	NAG	G	608	1	-	2/6/23/26	0/1/1/1
9	NAG	D	608	1	-	2/6/23/26	0/1/1/1
9	NAG	A	608	1	-	2/6/23/26	0/1/1/1
9	NAG	D	620	1	-	1/6/23/26	0/1/1/1
9	NAG	A	627	1	-	2/6/23/26	0/1/1/1
9	NAG	E	608	1	-	2/6/23/26	0/1/1/1
9	NAG	F	620	1	-	1/6/23/26	0/1/1/1
9	NAG	G	627	1	-	2/6/23/26	0/1/1/1
9	NAG	A	620	1	-	1/6/23/26	0/1/1/1
9	NAG	C	627	1	-	2/6/23/26	0/1/1/1
9	NAG	E	620	1	-	1/6/23/26	0/1/1/1
9	NAG	C	620	1	-	1/6/23/26	0/1/1/1
9	NAG	F	608	1	-	2/6/23/26	0/1/1/1
9	NAG	F	627	1	-	2/6/23/26	0/1/1/1
9	NAG	D	627	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	A	620	NAG	C4-C3-C2	-2.69	107.07	111.02
9	E	620	NAG	C4-C3-C2	-2.69	107.07	111.02
9	D	620	NAG	C4-C3-C2	-2.69	107.07	111.02
9	G	620	NAG	C4-C3-C2	-2.69	107.07	111.02
9	C	620	NAG	C4-C3-C2	-2.69	107.08	111.02
9	F	620	NAG	C4-C3-C2	-2.69	107.08	111.02
9	C	627	NAG	C4-C3-C2	-2.58	107.23	111.02
9	F	627	NAG	C4-C3-C2	-2.58	107.23	111.02
9	A	608	NAG	C4-C3-C2	-2.58	107.23	111.02
9	E	608	NAG	C4-C3-C2	-2.58	107.23	111.02
9	D	608	NAG	C4-C3-C2	-2.58	107.24	111.02
9	G	608	NAG	C4-C3-C2	-2.58	107.24	111.02
9	C	608	NAG	C4-C3-C2	-2.58	107.24	111.02
9	F	608	NAG	C4-C3-C2	-2.58	107.24	111.02
9	A	627	NAG	C4-C3-C2	-2.56	107.27	111.02
9	D	627	NAG	C4-C3-C2	-2.56	107.27	111.02
9	E	627	NAG	C4-C3-C2	-2.56	107.27	111.02
9	G	627	NAG	C4-C3-C2	-2.56	107.27	111.02

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	A	627	NAG	O5-C5-C6-O6
9	C	627	NAG	O5-C5-C6-O6
9	D	627	NAG	O5-C5-C6-O6
9	E	627	NAG	O5-C5-C6-O6
9	F	627	NAG	O5-C5-C6-O6
9	G	627	NAG	O5-C5-C6-O6
9	C	620	NAG	O5-C5-C6-O6
9	F	620	NAG	O5-C5-C6-O6
9	A	620	NAG	O5-C5-C6-O6
9	D	620	NAG	O5-C5-C6-O6
9	E	620	NAG	O5-C5-C6-O6
9	G	620	NAG	O5-C5-C6-O6
9	A	608	NAG	O5-C5-C6-O6
9	C	608	NAG	O5-C5-C6-O6
9	D	608	NAG	O5-C5-C6-O6
9	E	608	NAG	O5-C5-C6-O6
9	F	608	NAG	O5-C5-C6-O6
9	G	608	NAG	O5-C5-C6-O6
9	A	608	NAG	C1-C2-N2-C7
9	C	608	NAG	C1-C2-N2-C7
9	D	608	NAG	C1-C2-N2-C7
9	E	608	NAG	C1-C2-N2-C7
9	F	608	NAG	C1-C2-N2-C7
9	G	608	NAG	C1-C2-N2-C7
9	A	627	NAG	C4-C5-C6-O6
9	E	627	NAG	C4-C5-C6-O6
9	C	627	NAG	C4-C5-C6-O6
9	D	627	NAG	C4-C5-C6-O6
9	F	627	NAG	C4-C5-C6-O6
9	G	627	NAG	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

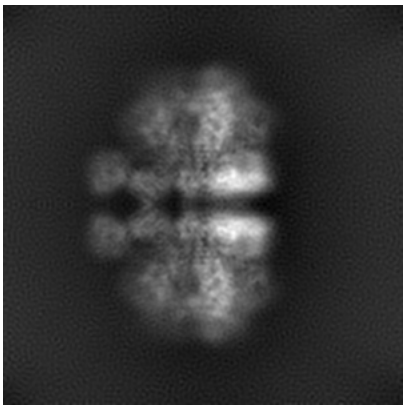
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-0434. These allow visual inspection of the internal detail of the map and identification of artifacts.

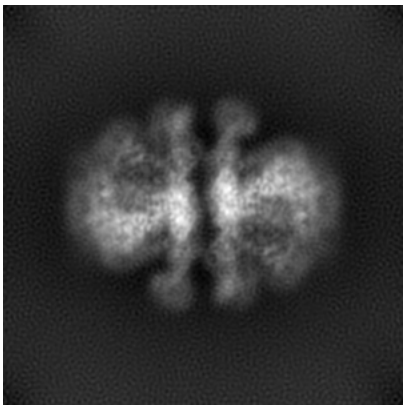
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

6.1.1 Primary map



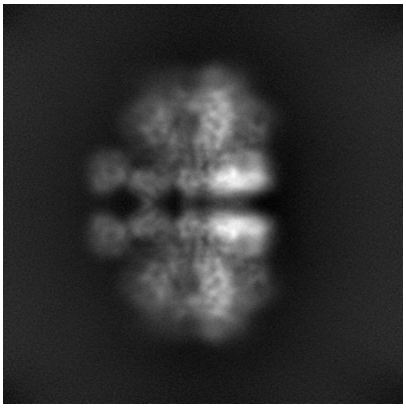
X



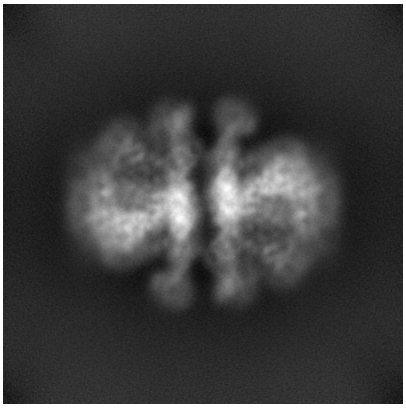
Y

Z

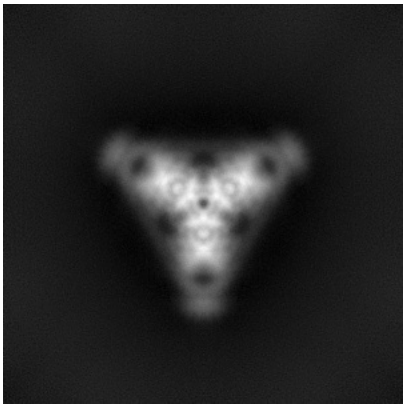
6.1.2 Raw map



X



Y

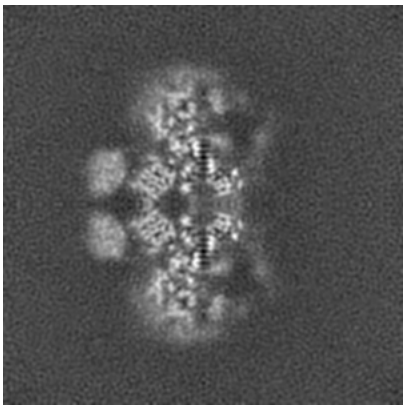


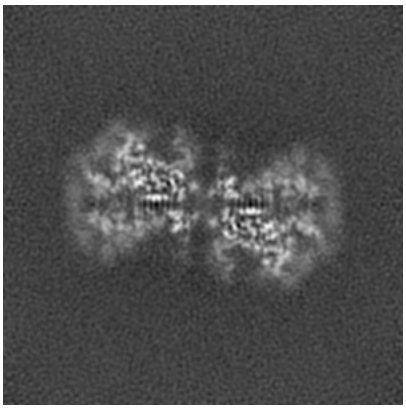
Z

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

6.2 Central slices (i)

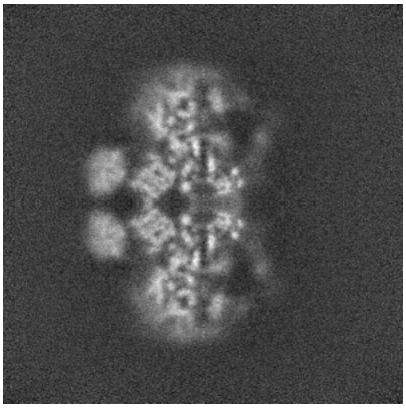
6.2.1 Primary map

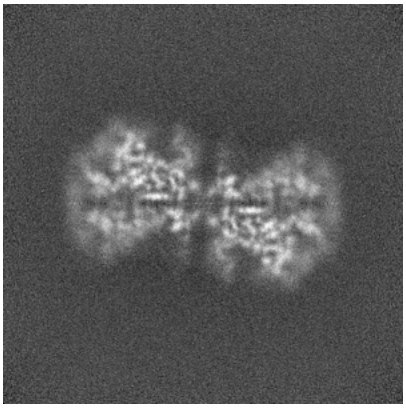

X Index: 176

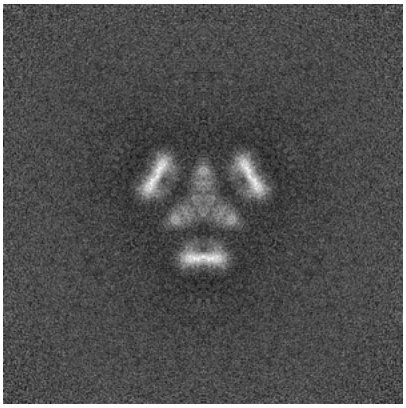

Y Index: 176

Z Index: 176

6.2.2 Raw map


X Index: 176

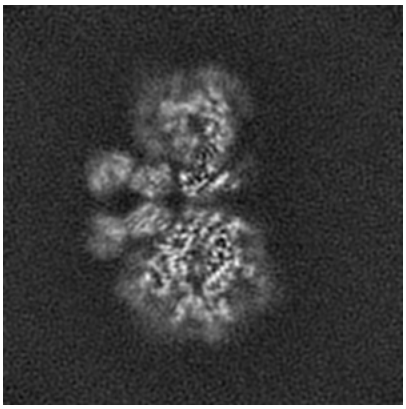

Y Index: 176

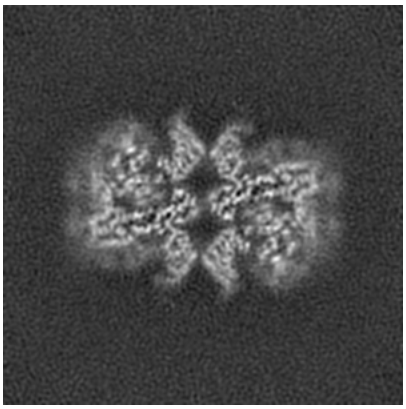

Z Index: 176

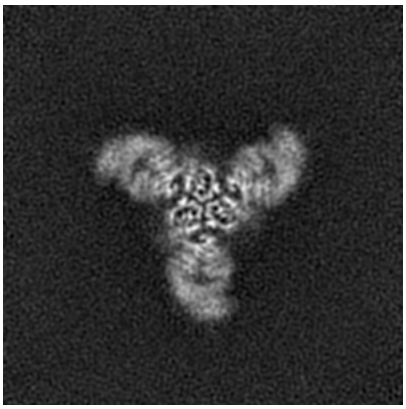
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

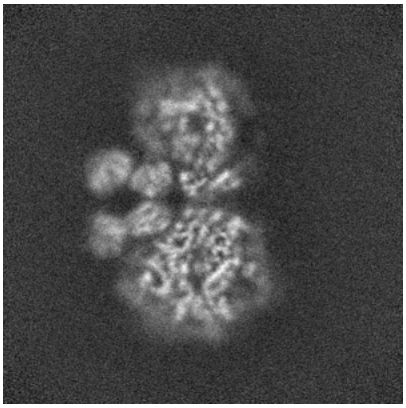
6.3.1 Primary map

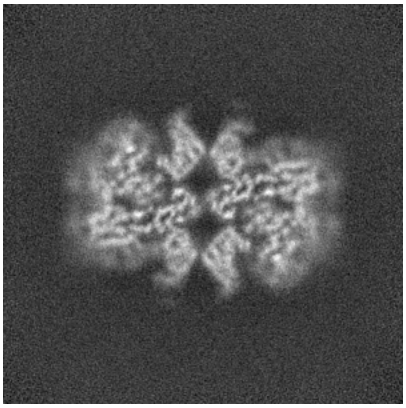

X Index: 165

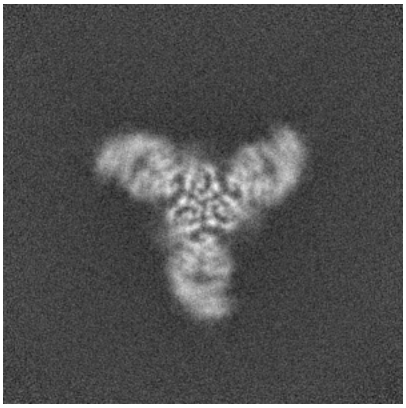

Y Index: 191


Z Index: 155

6.3.2 Raw map


X Index: 166

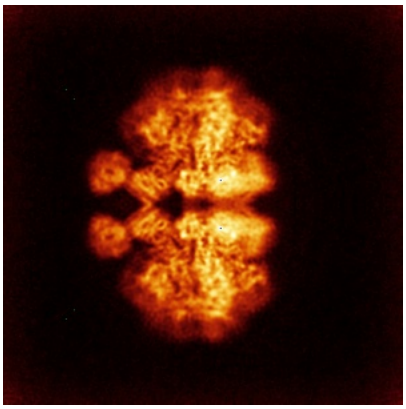

Y Index: 192

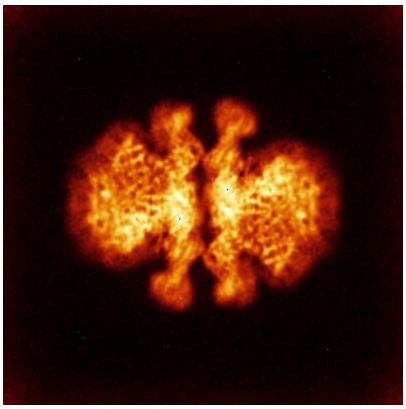

Z Index: 155

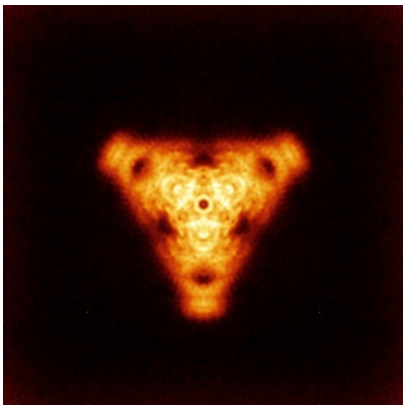
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

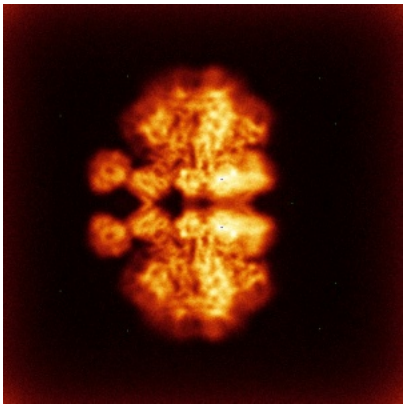
6.4.1 Primary map

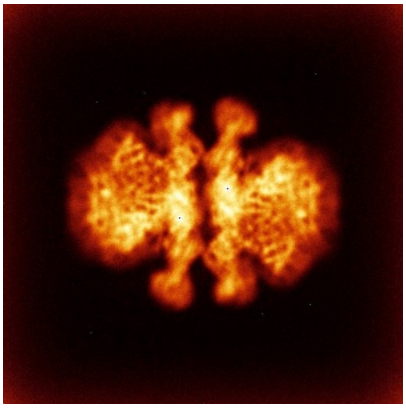

X

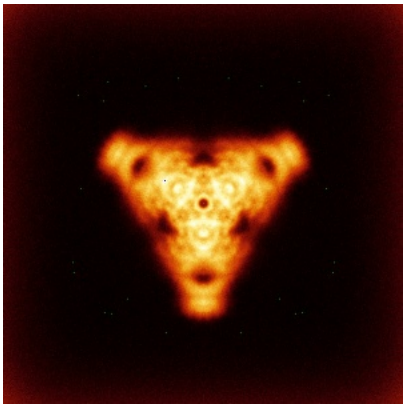

Y


Z

6.4.2 Raw map


X


Y


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

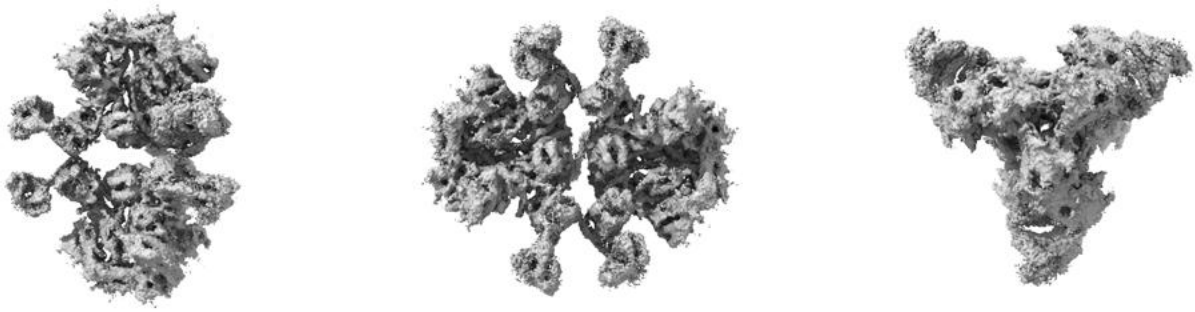
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.9. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 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.

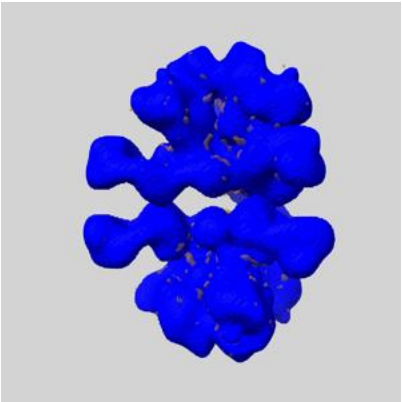
6.6 Mask visualisation (i)

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

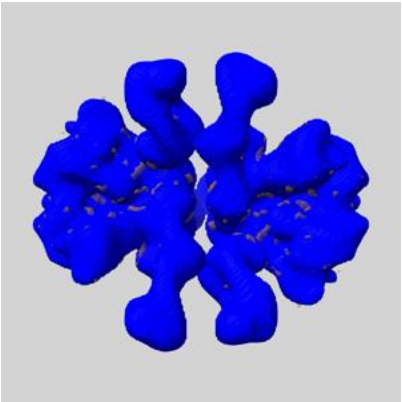
A mask typically either:

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

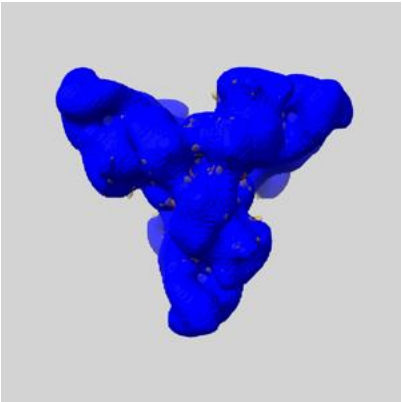
6.6.1 emd_0434_msk_1.map (i)



X



Y

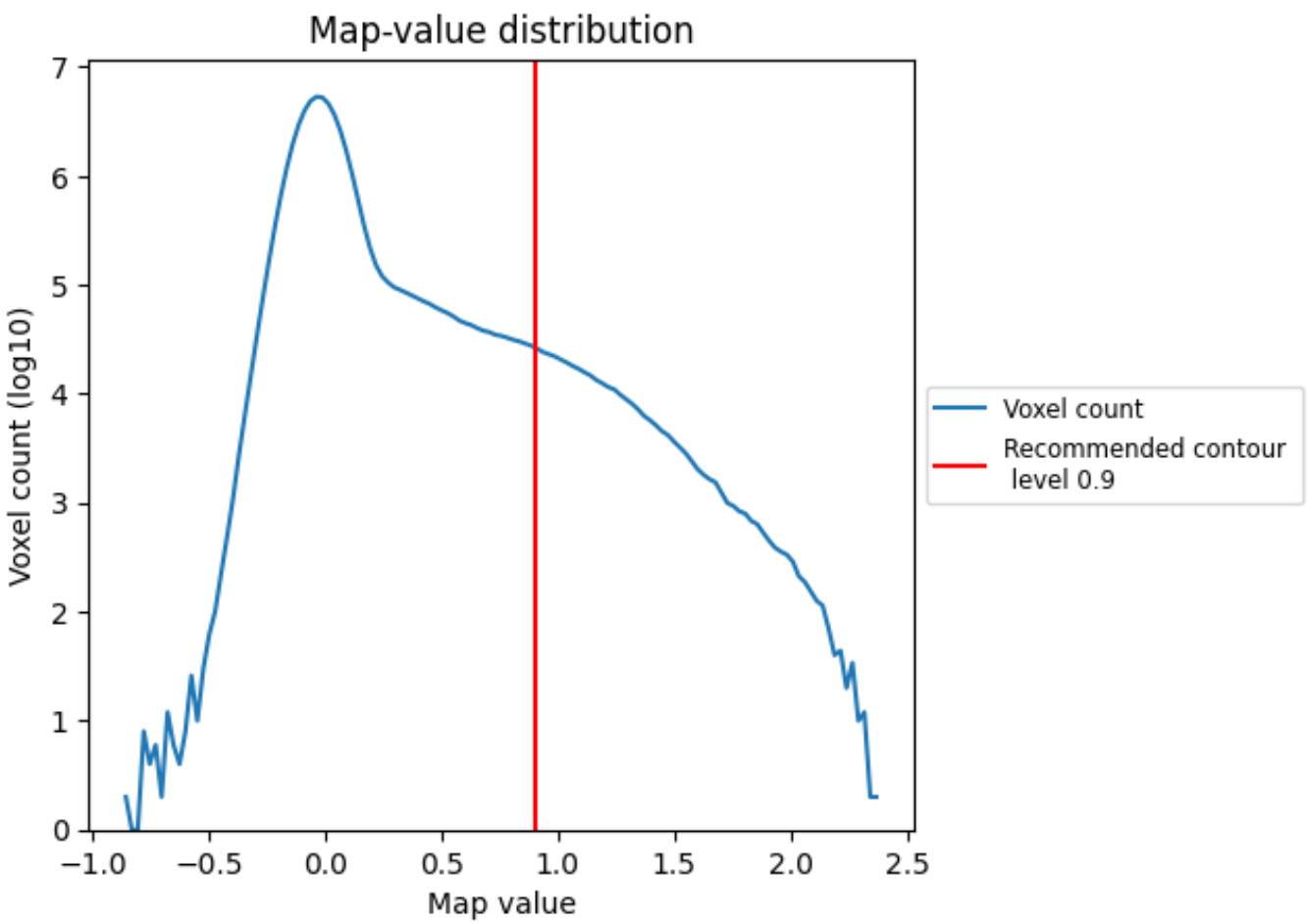


Z

7 Map analysis (i)

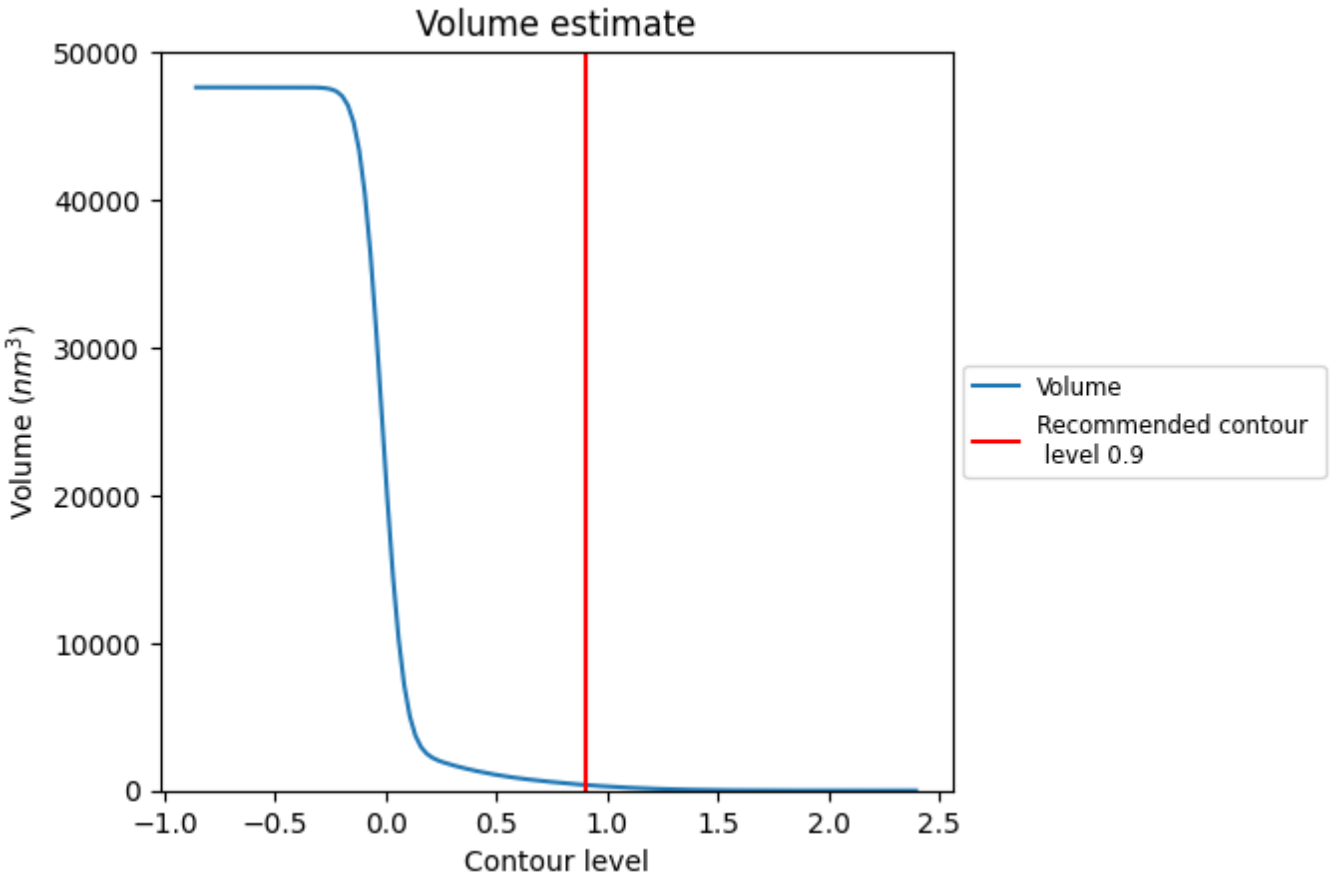
This section contains the results of statistical analysis of the map.

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.

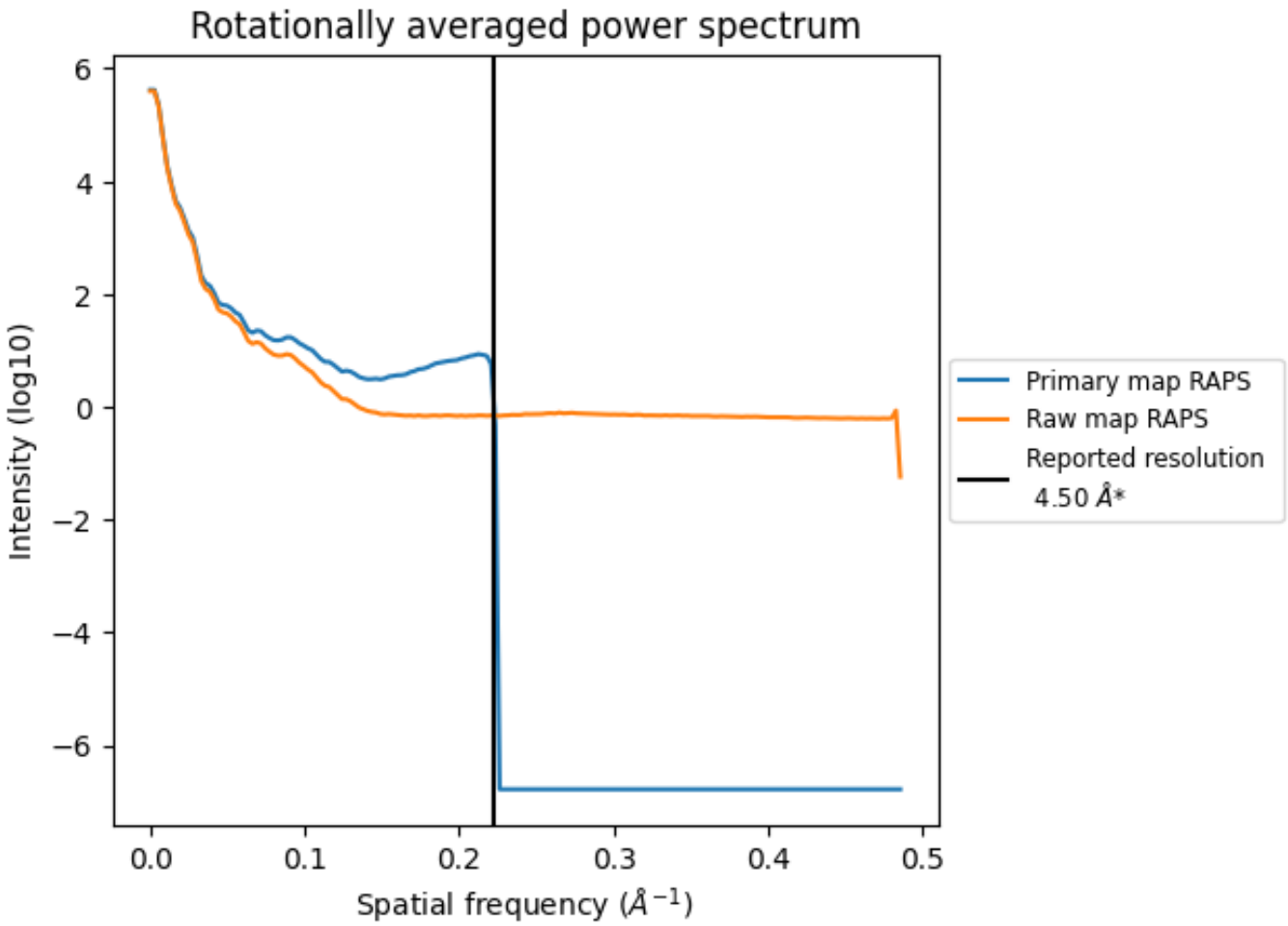
7.2 Volume estimate (i)



The volume at the recommended contour level is 382 nm^3; this corresponds to an approximate mass of 345 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)

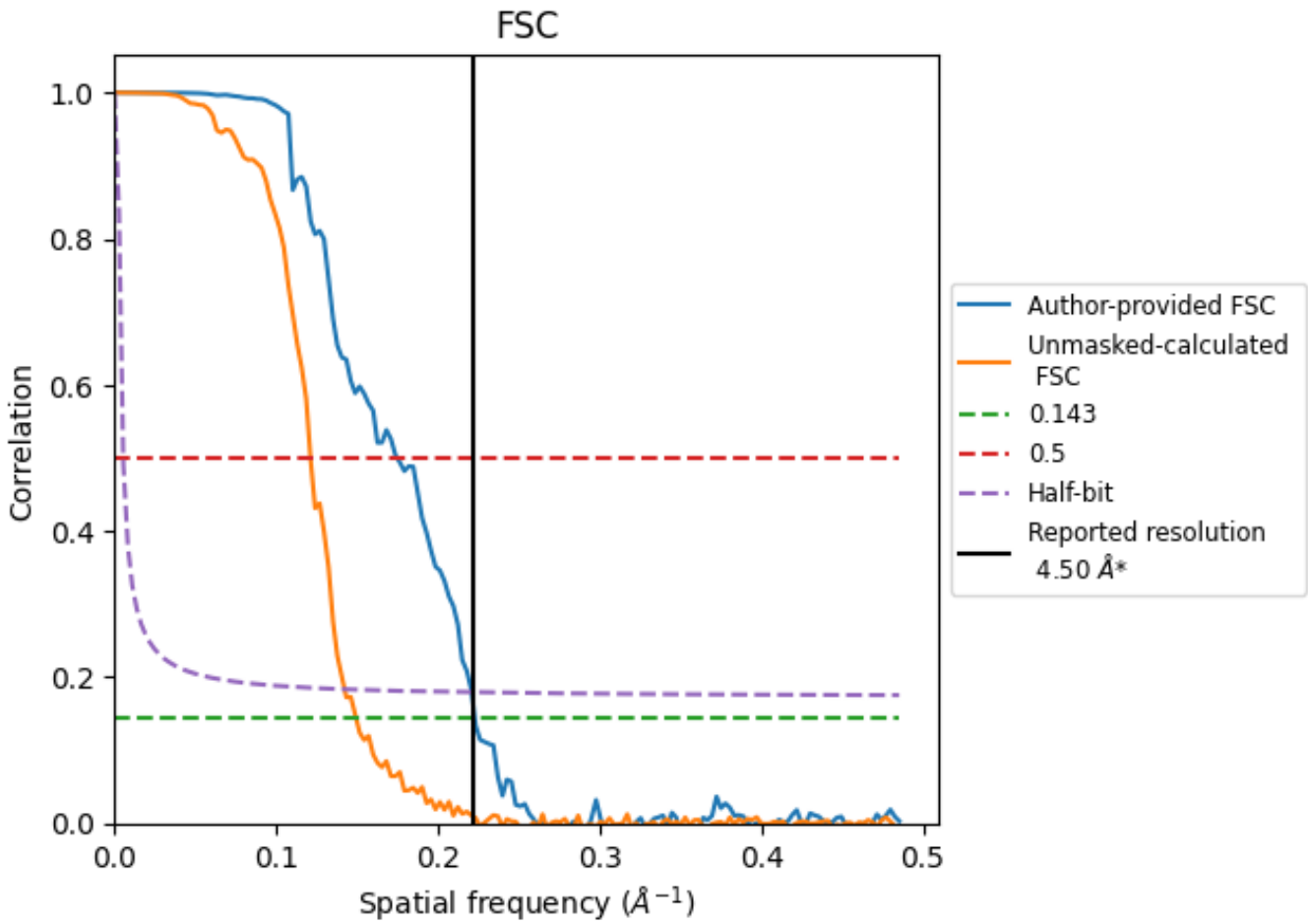


*Reported resolution corresponds to spatial frequency of 0.222 Å^{-1}

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 0.222 Å^{-1}

8.2 Resolution estimates (i)

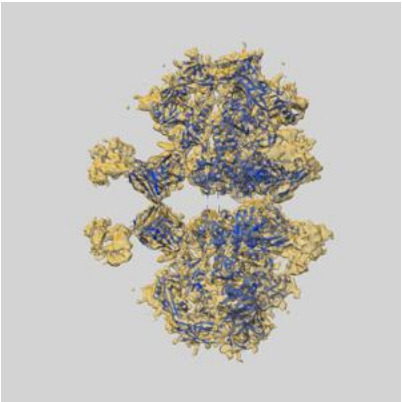
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.50	-	-
Author-provided FSC curve	4.49	5.72	4.53
Unmasked-calculated*	6.68	8.25	7.03

*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 6.68 differs from the reported value 4.5 by more than 10 %

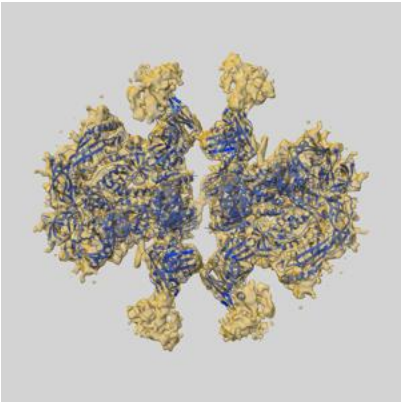
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-0434 and PDB model 6NC3. Per-residue inclusion information can be found in section 3 on page 12.

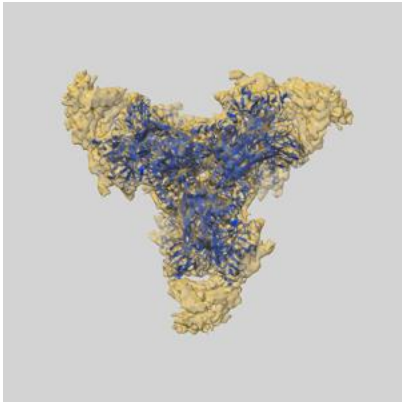
9.1 Map-model overlay (i)



X



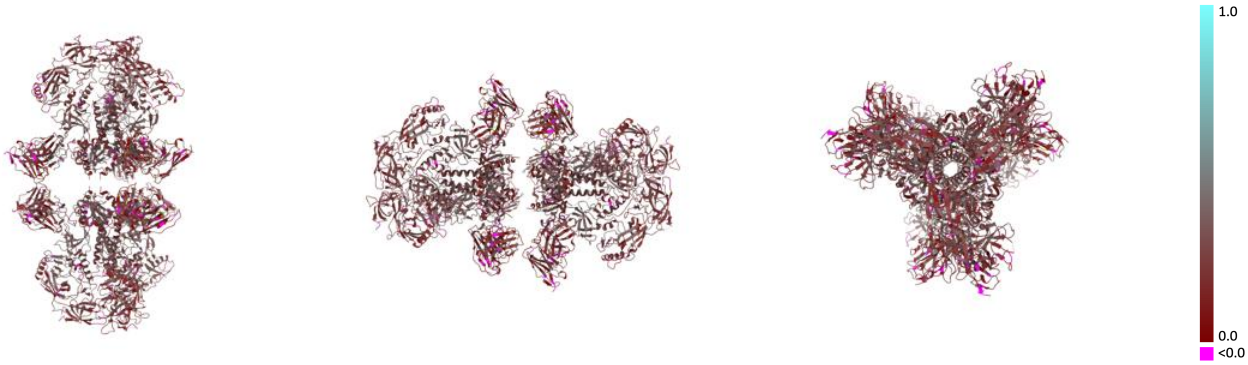
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.9 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.

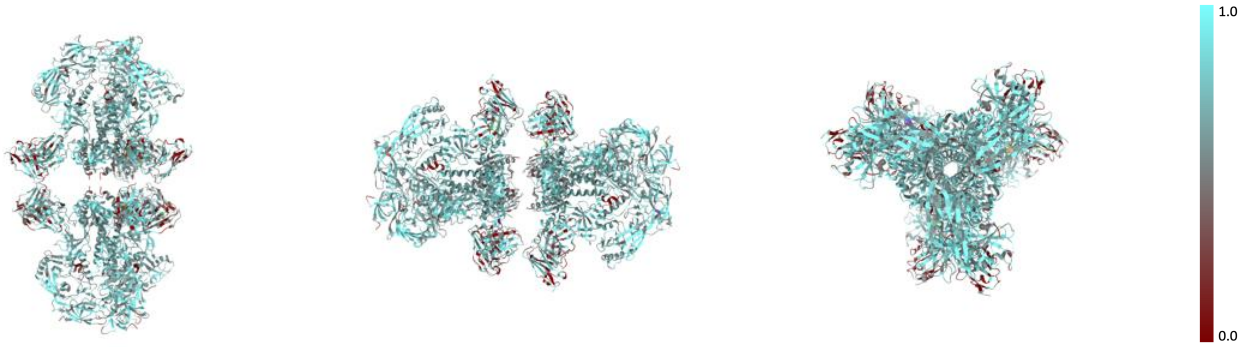
9.2 Q-score mapped to coordinate model (i)



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.

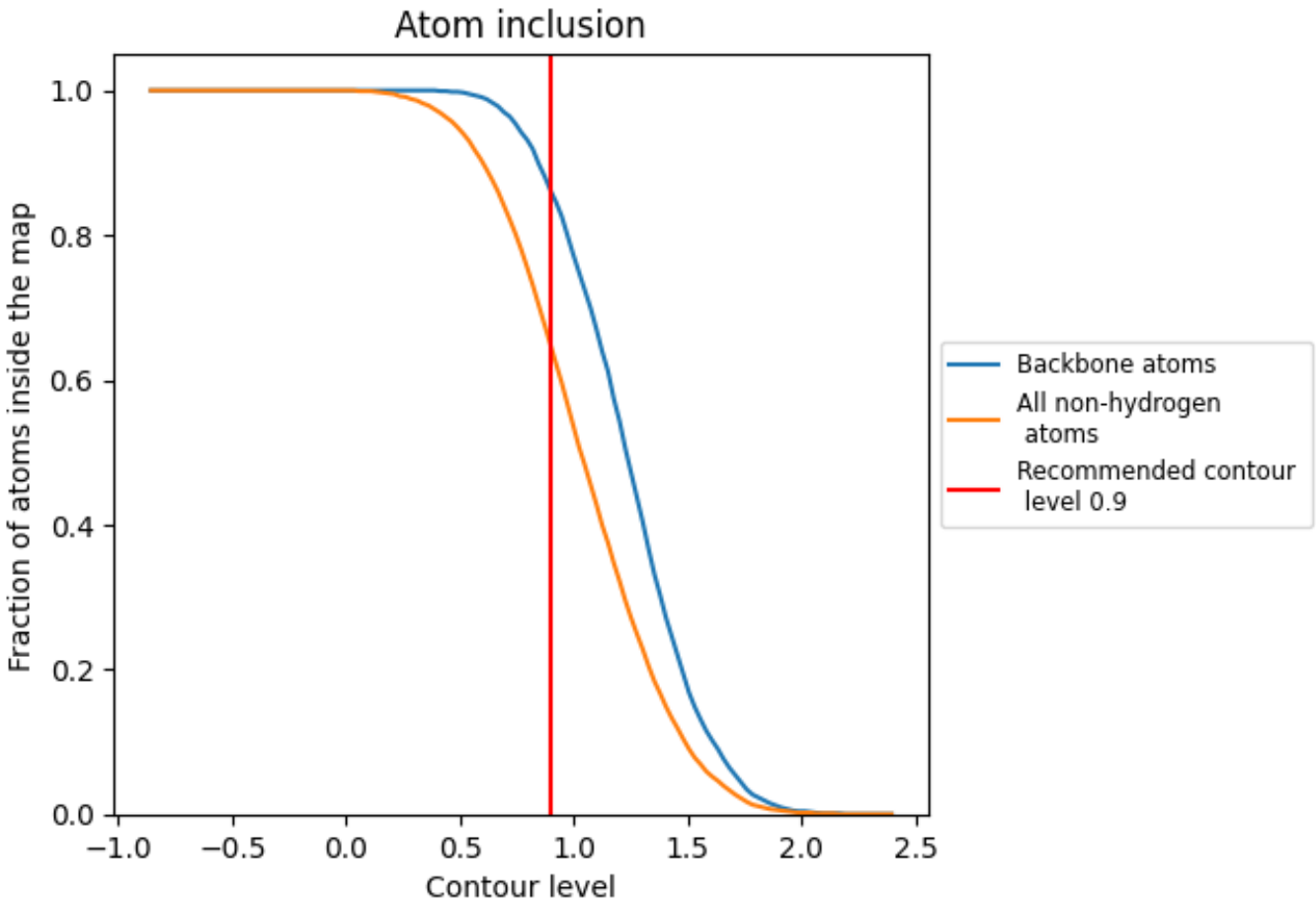
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.9).

9.4 Atom inclusion (i)



At the recommended contour level, 86% 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 (0.9) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6460	0.2550
0	0.5250	0.3280
1	0.2860	0.2100
2	0.7600	0.4320
3	0.5410	0.3750
4	0.2140	0.2870
5	0.3590	0.3230
6	0.2050	0.3200
7	0.5570	0.3240
8	0.2860	0.2090
9	0.7600	0.4320
A	0.6840	0.2700
AA	0.5570	0.3730
B	0.6900	0.2680
BA	0.2140	0.2790
C	0.6850	0.2710
CA	0.3590	0.3210
D	0.6860	0.2690
DA	0.2050	0.3360
E	0.6840	0.2690
F	0.6850	0.2690
G	0.6860	0.2680
H	0.6130	0.2110
I	0.6870	0.2680
J	0.6880	0.2670
K	0.6900	0.2650
L	0.5410	0.2000
M	0.6870	0.2680
N	0.6880	0.2710
O	0.6130	0.2100
P	0.6130	0.2100
Q	0.6130	0.2100
R	0.6130	0.2090
S	0.6130	0.2090
T	0.5360	0.1990

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
U	0.5380	0.1990
V	0.5410	0.1980
W	0.5360	0.1960
X	0.5380	0.1980
Y	0.5740	0.3210
Z	0.2860	0.2270
a	0.7600	0.4180
b	0.5250	0.3780
c	0.2140	0.2700
d	0.3590	0.3260
e	0.2310	0.3330
f	0.5250	0.3230
g	0.2860	0.2240
h	0.7600	0.4340
i	0.5410	0.3800
j	0.2140	0.2730
k	0.3590	0.3290
l	0.2050	0.3280
m	0.5570	0.3300
n	0.2860	0.2080
o	0.7600	0.4360
p	0.5570	0.3830
q	0.2140	0.2750
r	0.3590	0.3150
s	0.2050	0.3260
t	0.5740	0.3310
u	0.2860	0.2210
v	0.7600	0.4320
w	0.5250	0.3870
x	0.2140	0.2860
y	0.3590	0.3170
z	0.2310	0.3400