



Full wwPDB EM Validation Report ⓘ

Jul 4, 2026 – 12:45 PM JST

PDB ID : 9UFE / pdb_00009ufe
EMDB ID : EMD-64106
Title : Cryo-EM structure of the tubular mastigoneme (the central tube) from golden algae 2.17 angstrom resolution
Authors : Huang, J.; Tao, H.; Chen, S.; Cui, Y.; Xu, Y.; Yan, C.; Yan, N.
Deposited on : 2025-04-10
Resolution : 2.17 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

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A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

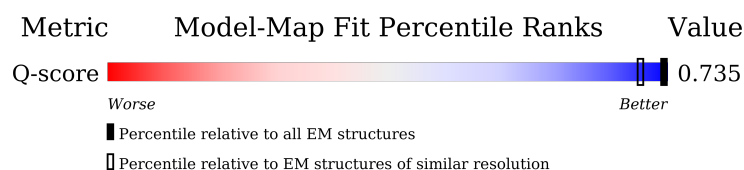
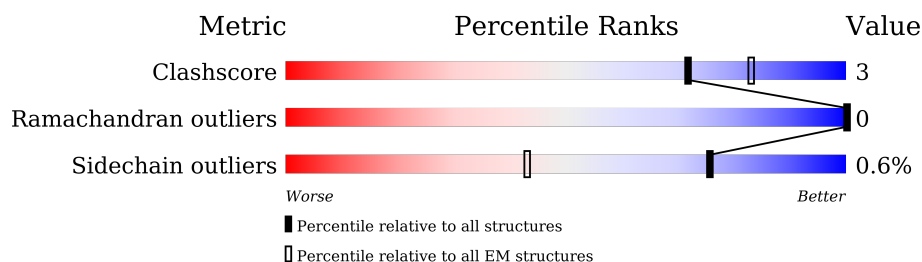
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.17 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	2651 (1.67 - 2.67)

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 $\leq 5\%$. 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	EA	368	
1	EB	368	
1	EC	368	
2	FA	723	

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Mol	Chain	Length	Quality of chain
2	FB	723	
2	FC	723	
3	DA	209	
3	DB	209	
3	DC	209	
4	CA	349	
4	CB	349	
4	CC	349	
5	AA	748	
5	AB	748	
5	AC	748	
6	BA	366	
6	BB	366	
6	BC	366	
7	aA	14	
7	aF	14	
7	aK	14	
8	aB	16	
8	aG	16	
8	aL	16	
9	aC	16	
9	aH	16	
9	aM	16	
10	aD	9	
10	aI	9	

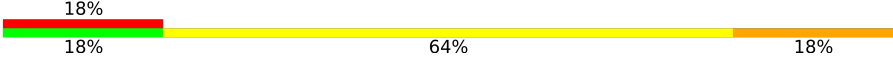
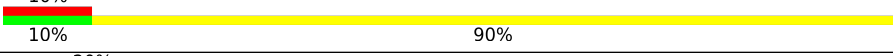
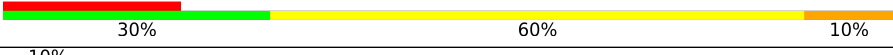
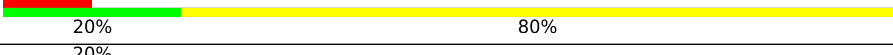
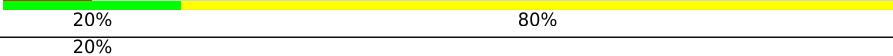
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Mol	Chain	Length	Quality of chain
10	aN	9	
11	aE	15	
11	aJ	15	
11	aO	15	
12	bA	9	
12	bD	9	
12	bG	9	
13	bB	5	
13	bE	5	
13	bH	5	
14	bC	10	
14	bF	10	
14	bI	10	
15	cA	4	
15	cB	4	
15	cC	4	
16	dA	7	
16	dB	7	
16	dC	7	
17	eA	11	
17	eC	11	
17	eE	11	
17	fC	11	
17	fD	11	
17	fH	11	

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Mol	Chain	Length	Quality of chain
17	fI	11	
17	fM	11	
17	fN	11	
18	eB	14	
18	eD	14	
18	eF	14	
19	fB	10	
19	fE	10	
19	fG	10	
19	fJ	10	
19	fL	10	
19	fO	10	
20	fF	14	
20	fK	14	
20	fP	14	

2 Entry composition [i](#)

There are 25 unique types of molecules in this entry. The entry contains 71986 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 OCM5.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	EA	351	Total	C	N	O	S	0	0
			2672	1651	460	532	29		
1	EB	351	Total	C	N	O	S	0	0
			2672	1651	460	532	29		
1	EC	351	Total	C	N	O	S	0	0
			2672	1651	460	532	29		

- Molecule 2 is a protein called OCM6.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	FA	699	Total	C	N	O	S	0	0
			5350	3333	898	1078	41		
2	FB	699	Total	C	N	O	S	0	0
			5350	3333	898	1078	41		
2	FC	699	Total	C	N	O	S	0	0
			5350	3333	898	1078	41		

- Molecule 3 is a protein called Tubular mastigoneme protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	DA	192	Total	C	N	O	S	0	0
			1409	850	251	284	24		
3	DB	192	Total	C	N	O	S	0	0
			1409	850	251	284	24		
3	DC	192	Total	C	N	O	S	0	0
			1409	850	251	284	24		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
DA	106	SER	PRO	conflict	UNP C4B7Q8
DB	106	SER	PRO	conflict	UNP C4B7Q8
DC	106	SER	PRO	conflict	UNP C4B7Q8

- Molecule 4 is a protein called OCM3.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	CA	227	Total	C	N	O	S	0	0
			1728	1047	313	343	25		
4	CB	227	Total	C	N	O	S	0	0
			1728	1047	313	343	25		
4	CC	227	Total	C	N	O	S	0	0
			1728	1047	313	343	25		

- Molecule 5 is a protein called Tubular mastigoneme protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	AA	727	Total	C	N	O	S	0	0
			5689	3561	936	1150	42		
5	AB	727	Total	C	N	O	S	0	0
			5689	3561	936	1150	42		
5	AC	727	Total	C	N	O	S	0	0
			5689	3561	936	1150	42		

- Molecule 6 is a protein called Tubular mastigoneme protein.

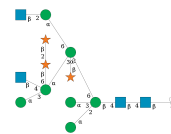
Mol	Chain	Residues	Atoms					AltConf	Trace
6	BA	348	Total	C	N	O	S	0	0
			2725	1678	462	558	27		
6	BB	348	Total	C	N	O	S	0	0
			2725	1678	462	558	27		
6	BC	348	Total	C	N	O	S	0	0
			2725	1678	462	558	27		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BA	72	GLY	VAL	conflict	UNP C4B7Q7
BA	112	ASP	ALA	conflict	UNP C4B7Q7
BB	72	GLY	VAL	conflict	UNP C4B7Q7
BB	112	ASP	ALA	conflict	UNP C4B7Q7
BC	72	GLY	VAL	conflict	UNP C4B7Q7
BC	112	ASP	ALA	conflict	UNP C4B7Q7

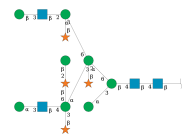
- Molecule 7 is an oligosaccharide called beta-D-xylopyranose-(1-2)-beta-D-xylopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)][2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]alpha-D-mannopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)][beta-D-xylopyranose-(1-2)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyra

nose-(1-2)][alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



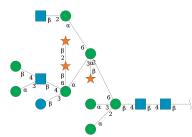
Mol	Chain	Residues	Atoms				AltConf	Trace
7	aA	14	Total	C	N	O	0	0
			160	89	4	67		
7	aF	14	Total	C	N	O	0	0
			160	89	4	67		
7	aK	14	Total	C	N	O	0	0
			160	89	4	67		

- Molecule 8 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[beta-D-mannopyranose-(1-2)-beta-D-xylopyranose-(1-6)][beta-D-xylopyranose-(1-3)]alpha-D-mannopyranose-(1-3)-[beta-D-mannopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-[beta-D-xylopyranose-(1-3)]alpha-D-mannopyranose-(1-6)][beta-D-xylopyranose-(1-2)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



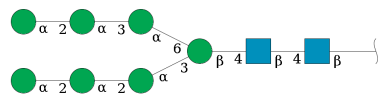
Mol	Chain	Residues	Atoms				AltConf	Trace
8	aB	16	Total	C	N	O	0	0
			180	100	4	76		
8	aG	16	Total	C	N	O	0	0
			180	100	4	76		
8	aL	16	Total	C	N	O	0	0
			180	100	4	76		

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



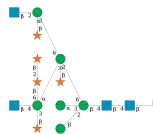
Mol	Chain	Residues	Atoms				AltConf	Trace
9	aC	16	Total	C	N	O	0	0
			182	101	4	77		
9	aH	16	Total	C	N	O	0	0
			182	101	4	77		
9	aM	16	Total	C	N	O	0	0
			182	101	4	77		

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



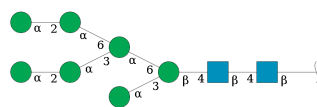
Mol	Chain	Residues	Atoms				AltConf	Trace
10	aD	9	Total	C	N	O	0	0
			105	58	2	45		
10	aI	9	Total	C	N	O	0	0
			105	58	2	45		
10	aN	9	Total	C	N	O	0	0
			105	58	2	45		

- Molecule 11 is an oligosaccharide called beta-D-xylopyranose-(1-2)-beta-D-xylopyranose-(1-6)-[beta-D-xylopyranose-(1-3)][2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]alpha-D-mannopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-[beta-D-xylopyranose-(1-3)]alpha-D-mannopyranose-(1-6)][beta-D-xylopyranose-(1-2)]alpha-D-mannopyranose-(1-6)-[beta-D-mannopyranose-(1-2)][alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



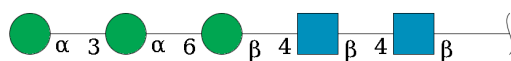
Mol	Chain	Residues	Atoms				AltConf	Trace
11	aE	15	Total	C	N	O	0	0
			167	93	4	70		
11	aJ	15	Total	C	N	O	0	0
			167	93	4	70		
11	aO	15	Total	C	N	O	0	0
			167	93	4	70		

- Molecule 12 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
12	bA	9	Total	C	N	O	0	0
			105	58	2	45		
12	bD	9	Total	C	N	O	0	0
			105	58	2	45		
12	bG	9	Total	C	N	O	0	0
			105	58	2	45		

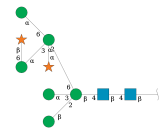
- Molecule 13 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
13	bB	5	Total	C	N	O	0	0
			61	34	2	25		
13	bE	5	Total	C	N	O	0	0
			61	34	2	25		
13	bH	5	Total	C	N	O	0	0
			61	34	2	25		

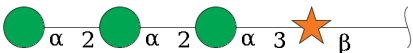
- Molecule 14 is an oligosaccharide called beta-D-xylopyranose-(1-6)-alpha-D-mannopyranose-(1-3)-[alpha-D-xylopyranose-(1-2)][alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[beta-D-mannopyranose-(1-2)][alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(

1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



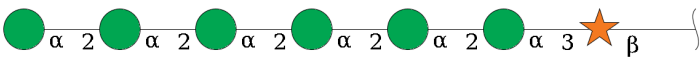
Mol	Chain	Residues	Atoms				AltConf	Trace
14	bC	10	Total	C	N	O	0	0
			112	62	2	48		
14	bF	10	Total	C	N	O	0	0
			112	62	2	48		
14	bI	10	Total	C	N	O	0	0
			112	62	2	48		

- Molecule 15 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-beta-D-xylopyranose.



Mol	Chain	Residues	Atoms			AltConf	Trace
15	cA	4	Total	C	O	0	0
			42	23	19		
15	cB	4	Total	C	O	0	0
			42	23	19		
15	cC	4	Total	C	O	0	0
			42	23	19		

- Molecule 16 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-beta-D-xylopyranose.



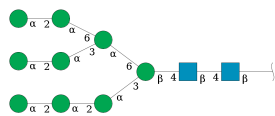
Mol	Chain	Residues	Atoms			AltConf	Trace
16	dA	7	Total	C	O	0	0
			75	41	34		
16	dB	7	Total	C	O	0	0
			75	41	34		

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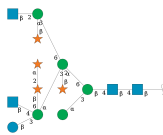
Mol	Chain	Residues	Atoms			AltConf	Trace
16	dC	7	Total	C	O	0	0
			75	41	34		

- Molecule 17 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]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.



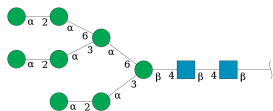
Mol	Chain	Residues	Atoms				AltConf	Trace
17	eA	11	Total	C	N	O	0	0
			127	70	2	55		
17	fC	11	Total	C	N	O	0	0
			127	70	2	55		
17	fD	11	Total	C	N	O	0	0
			127	70	2	55		
17	eC	11	Total	C	N	O	0	0
			127	70	2	55		
17	fH	11	Total	C	N	O	0	0
			127	70	2	55		
17	fI	11	Total	C	N	O	0	0
			127	70	2	55		
17	eE	11	Total	C	N	O	0	0
			127	70	2	55		
17	fM	11	Total	C	N	O	0	0
			127	70	2	55		
17	fN	11	Total	C	N	O	0	0
			127	70	2	55		

- Molecule 18 is an oligosaccharide called alpha-D-xylopyranose-(1-2)-beta-D-xylopyranose-(1-6)-[beta-D-glucopyranose-(1-3)][2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]alpha-D-mannopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-[beta-D-xylopyranose-(1-3)]alpha-D-mannopyranose-(1-6)][beta-D-xylopyranose-(1-2)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



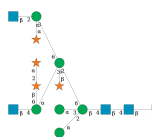
Mol	Chain	Residues	Atoms				AltConf	Trace
18	eB	14	Total	C	N	O	0	0
			158	88	4	66		
18	eD	14	Total	C	N	O	0	0
			158	88	4	66		
18	eF	14	Total	C	N	O	0	0
			158	88	4	66		

- Molecule 19 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
19	fB	10	Total	C	N	O	0	0
			116	64	2	50		
19	fE	10	Total	C	N	O	0	0
			116	64	2	50		
19	fG	10	Total	C	N	O	0	0
			116	64	2	50		
19	fJ	10	Total	C	N	O	0	0
			116	64	2	50		
19	fL	10	Total	C	N	O	0	0
			116	64	2	50		
19	fO	10	Total	C	N	O	0	0
			116	64	2	50		

- Molecule 20 is an oligosaccharide called alpha-D-xylopyranose-(1-2)-beta-D-xylopyranose-(1-6)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]alpha-D-mannopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-[alpha-D-xylopyranose-(1-3)]alpha-D-mannopyranose-(1-6)]beta-D-xylopyranose-(1-2)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-2)]alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
20	fF	14	Total	C	N	O	0	0
			158	88	4	66		
20	fK	14	Total	C	N	O	0	0
			158	88	4	66		
20	fP	14	Total	C	N	O	0	0
			158	88	4	66		

- Molecule 21 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

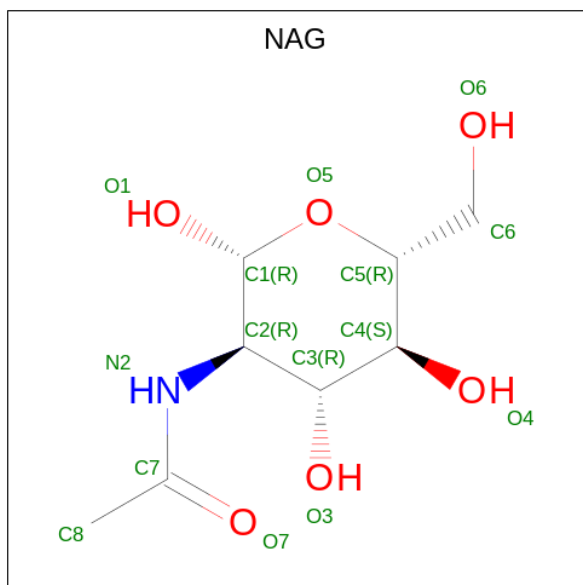
Mol	Chain	Residues	Atoms		AltConf
21	EA	2	Total	Ca	0
			2	2	
21	FA	6	Total	Ca	0
			6	6	
21	CA	1	Total	Ca	0
			1	1	
21	AA	7	Total	Ca	0
			7	7	
21	BA	3	Total	Ca	0
			3	3	
21	EB	1	Total	Ca	0
			1	1	
21	FB	6	Total	Ca	0
			6	6	
21	CB	1	Total	Ca	0
			1	1	
21	AB	7	Total	Ca	0
			7	7	
21	BB	3	Total	Ca	0
			3	3	
21	EC	1	Total	Ca	0
			1	1	
21	FC	6	Total	Ca	0
			6	6	
21	CC	1	Total	Ca	0
			1	1	
21	AC	7	Total	Ca	0
			7	7	

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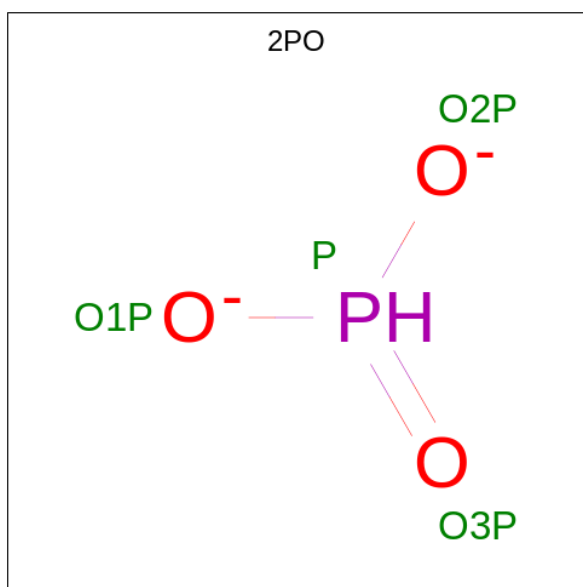
Mol	Chain	Residues	Atoms		AltConf
21	BC	3	Total	Ca	0
			3	3	

- Molecule 22 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
22	EA	1	Total	C	N	O	0
			14	8	1	5	
22	FA	1	Total	C	N	O	0
			14	8	1	5	
22	EB	1	Total	C	N	O	0
			14	8	1	5	
22	FB	1	Total	C	N	O	0
			14	8	1	5	
22	EC	1	Total	C	N	O	0
			14	8	1	5	
22	FC	1	Total	C	N	O	0
			14	8	1	5	

- Molecule 23 is PHOSPHONATE (CCD ID: 2PO) (formula: HO_3P).



Mol	Chain	Residues	Atoms			AltConf
23	EA	1	Total	O	P	0
			4	3	1	
23	FA	1	Total	O	P	0
			4	3	1	
23	AA	1	Total	O	P	0
			4	3	1	
23	AA	1	Total	O	P	0
			4	3	1	
23	AA	1	Total	O	P	0
			4	3	1	
23	BA	1	Total	O	P	0
			4	3	1	
23	BA	1	Total	O	P	0
			4	3	1	
23	EB	1	Total	O	P	0
			4	3	1	
23	FB	1	Total	O	P	0
			4	3	1	
23	AB	1	Total	O	P	0
			4	3	1	
23	AB	1	Total	O	P	0
			4	3	1	
23	AB	1	Total	O	P	0
			4	3	1	
23	BB	1	Total	O	P	0
			4	3	1	
23	BB	1	Total	O	P	0
			4	3	1	

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Mol	Chain	Residues	Atoms			AltConf
23	EC	1	Total	O	P	0
			4	3	1	
23	FC	1	Total	O	P	0
			4	3	1	
23	AC	1	Total	O	P	0
			4	3	1	
23	AC	1	Total	O	P	0
			4	3	1	
23	AC	1	Total	O	P	0
			4	3	1	
23	BC	1	Total	O	P	0
			4	3	1	
23	BC	1	Total	O	P	0
			4	3	1	

- Molecule 24 is CHLORIDE ION (CCD ID: CL) (formula: Cl) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
24	DA	1	Total	Cl	0
			1	1	
24	DB	1	Total	Cl	0
			1	1	
24	DC	1	Total	Cl	0
			1	1	

- Molecule 25 is water.

Mol	Chain	Residues	Atoms		AltConf
25	EA	293	Total	O	0
			293	293	
25	FA	632	Total	O	0
			632	632	
25	DA	167	Total	O	0
			167	167	
25	CA	219	Total	O	0
			219	219	
25	AA	610	Total	O	0
			610	610	
25	BA	275	Total	O	0
			275	275	
25	EB	294	Total	O	0
			294	294	

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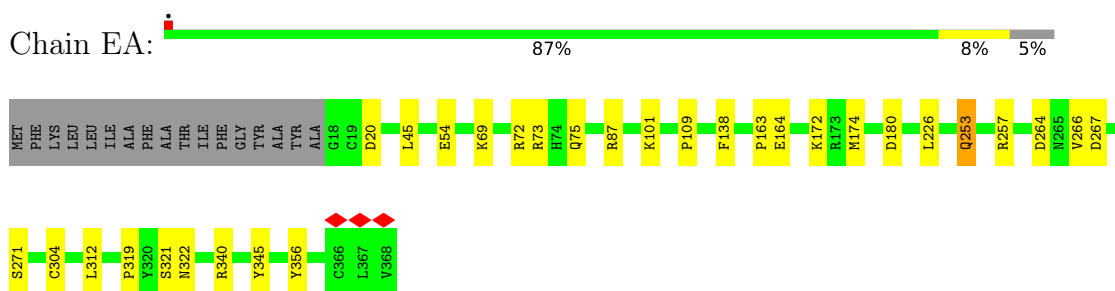
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Mol	Chain	Residues	Atoms		AltConf
25	FB	635	Total 635	O 635	0
25	DB	169	Total 169	O 169	0
25	CB	217	Total 217	O 217	0
25	AB	619	Total 619	O 619	0
25	BB	300	Total 300	O 300	0
25	EC	324	Total 324	O 324	0
25	FC	636	Total 636	O 636	0
25	DC	170	Total 170	O 170	0
25	CC	209	Total 209	O 209	0
25	AC	617	Total 617	O 617	0
25	BC	301	Total 301	O 301	0

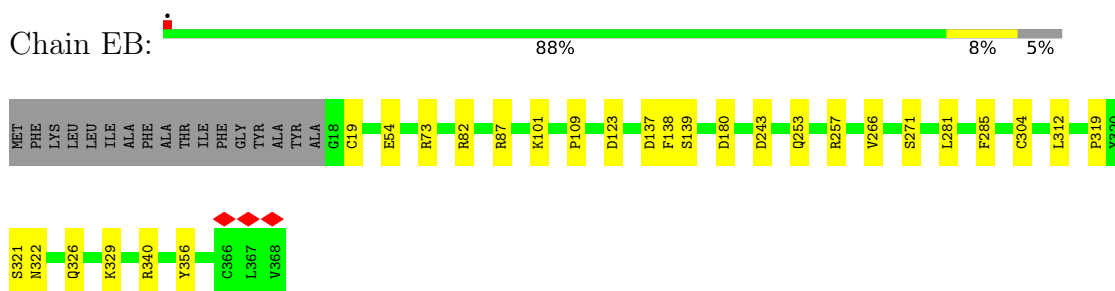
3 Residue-property plots [i](#)

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.

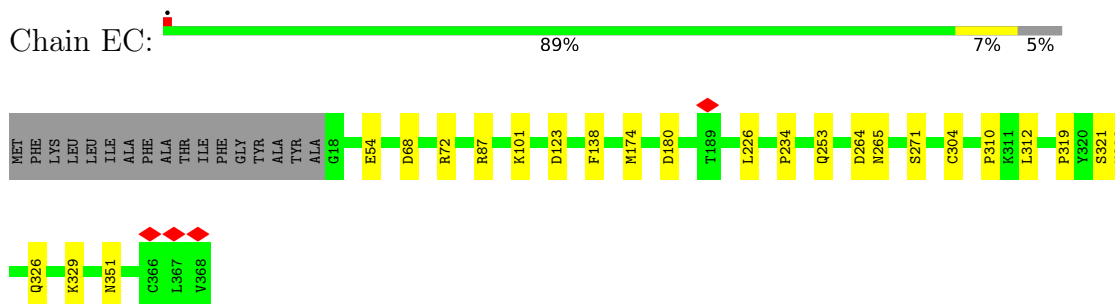
- Molecule 1: OCM5



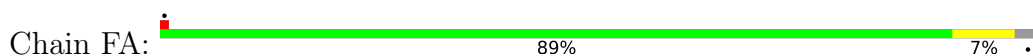
- Molecule 1: OCM5



- Molecule 1: OCM5



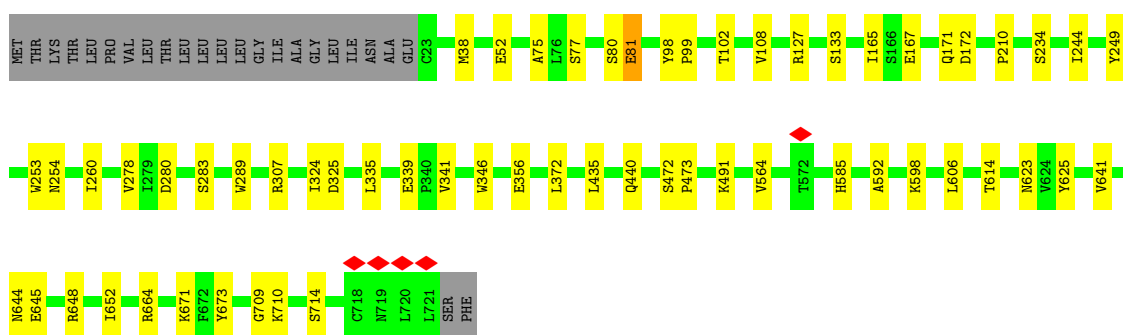
- Molecule 2: OCM6





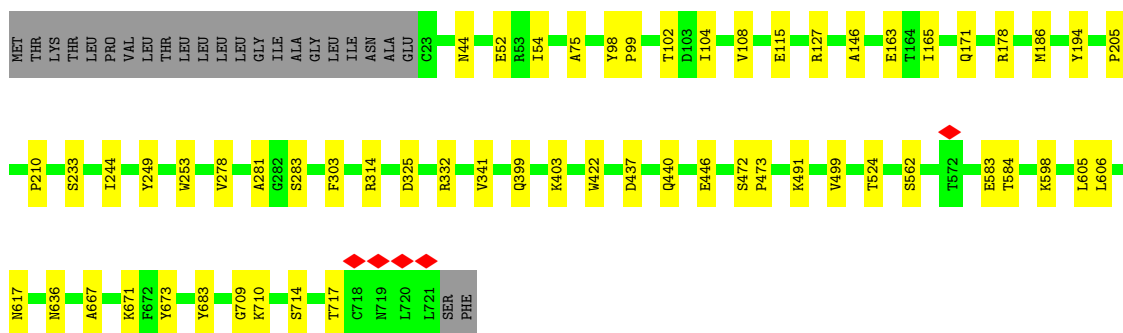
- Molecule 2: OCM6

Chain FB: 88% 8%



- Molecule 2: OCM6

Chain FC: 89% 8%



- Molecule 3: Tubular mastigoneme protein

Chain DA: 82% 10% 8%



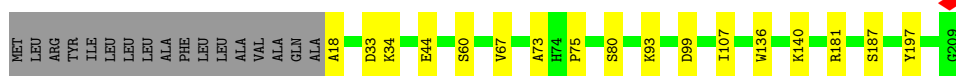
- Molecule 3: Tubular mastigoneme protein

Chain DB: 86% 6% 8%



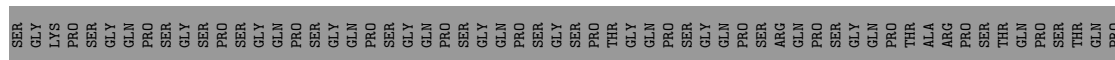
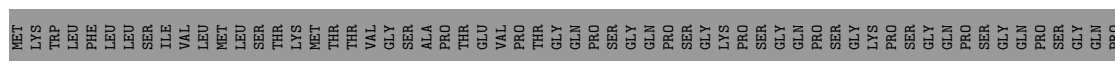
• Molecule 3: Tubular mastigoneme protein

Chain DC: 84% 8% 8%



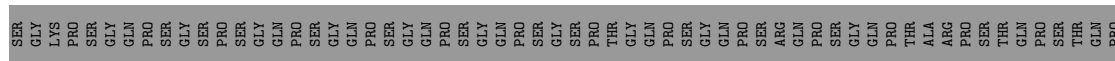
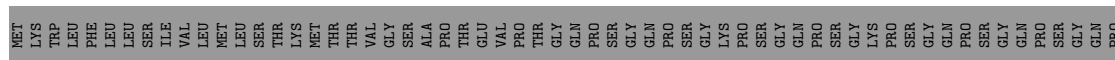
• Molecule 4: OCM3

Chain CA: 60% 5% 35%



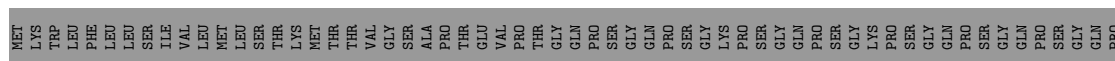
• Molecule 4: OCM3

Chain CB: 60% 5% 35%



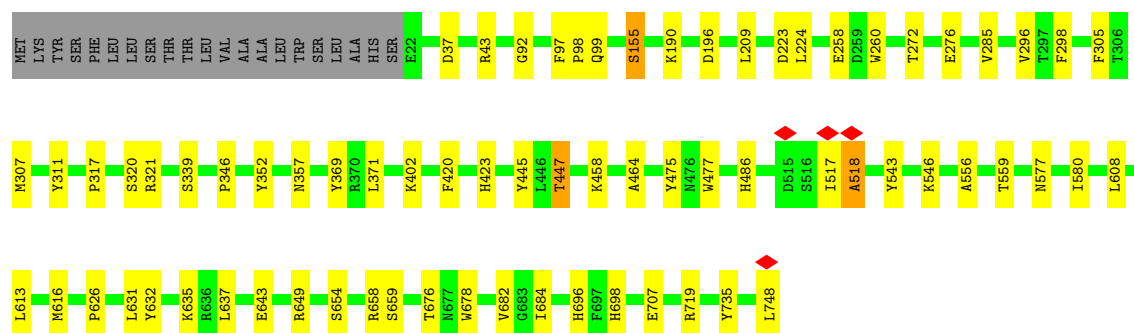
• Molecule 4: OCM3

Chain CC: 60% 5% 35%



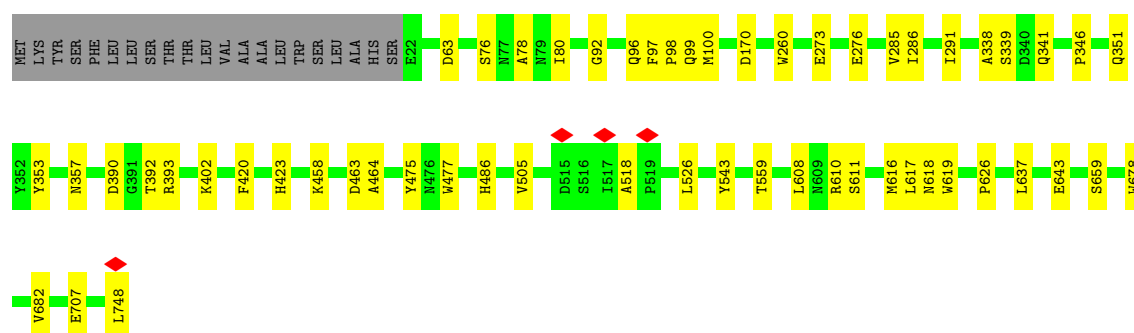
• Molecule 5: Tubular mastigoneme protein

Chain AA: 



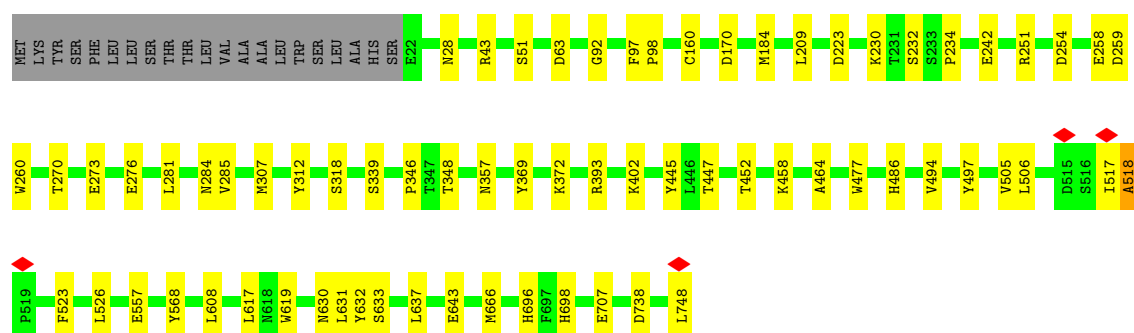
• Molecule 5: Tubular mastigoneme protein

Chain AB: 



• Molecule 5: Tubular mastigoneme protein

Chain AC: 



• Molecule 6: Tubular mastigoneme protein

Chain BA: 





- Molecule 6: Tubular mastigoneme protein

Chain BB: 88% 7% 5%



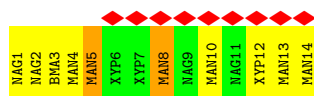
- Molecule 6: Tubular mastigoneme protein

Chain BC: 87% 8% 5%



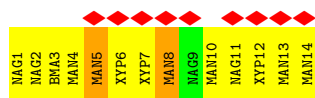
- Molecule 7: beta-D-xylopyranose-(1-2)-beta-D-xylopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)][2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]alpha-D-mannopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)][beta-D-xylopyranose-(1-2)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-2)][alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain aA: 29% 64% 57% 14%

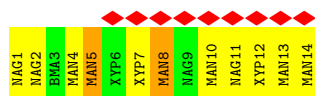


- Molecule 7: beta-D-xylopyranose-(1-2)-beta-D-xylopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)][2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]alpha-D-mannopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)][beta-D-xylopyranose-(1-2)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-2)][alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

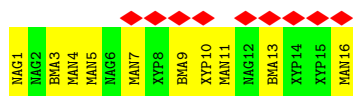
Chain aF: 7% 64% 79% 14%



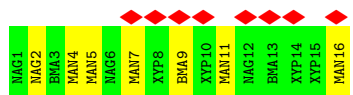
- Molecule 7: beta-D-xylopyranose-(1-2)-beta-D-xylopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)][2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]alpha-D-mannopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)][beta-D-xylopyranose-(1-2)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-2)][alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



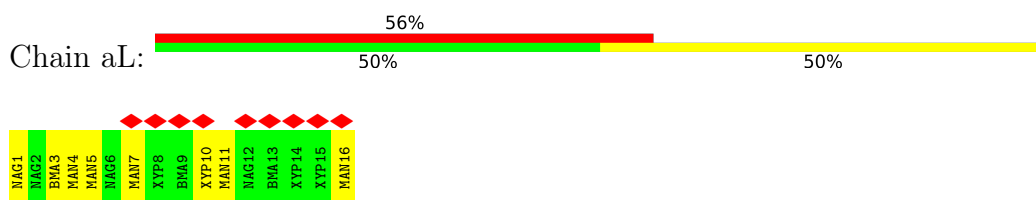
- Molecule 8: alpha-D-mannopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[beta-D-mannopyranose-(1-2)-beta-D-xylopyranose-(1-6)][beta-D-xylopyranose-(1-3)]alpha-D-mannopyranose-(1-3)-[beta-D-mannopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-[beta-D-xylopyranose-(1-3)]alpha-D-mannopyranose-(1-6)][beta-D-xylopyranose-(1-2)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 8: alpha-D-mannopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[beta-D-mannopyranose-(1-2)-beta-D-xylopyranose-(1-6)][beta-D-xylopyranose-(1-3)]alpha-D-mannopyranose-(1-3)-[beta-D-mannopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-[beta-D-xylopyranose-(1-3)]alpha-D-mannopyranose-(1-6)][beta-D-xylopyranose-(1-2)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



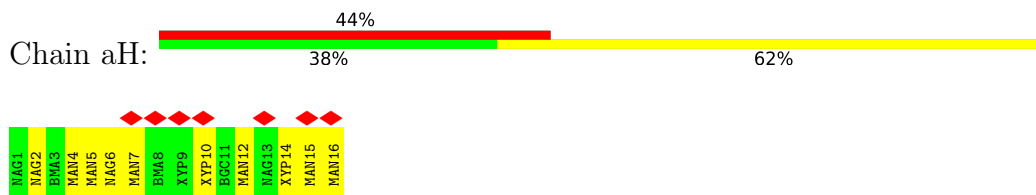
- Molecule 8: alpha-D-mannopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[beta-D-mannopyranose-(1-2)-beta-D-xylopyranose-(1-6)][beta-D-xylopyranose-(1-3)]alpha-D-mannopyranose-(1-3)-[beta-D-mannopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-[beta-D-xylopyranose-(1-3)]alpha-D-mannopyranose-(1-6)][beta-D-xylopyranose-(1-2)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



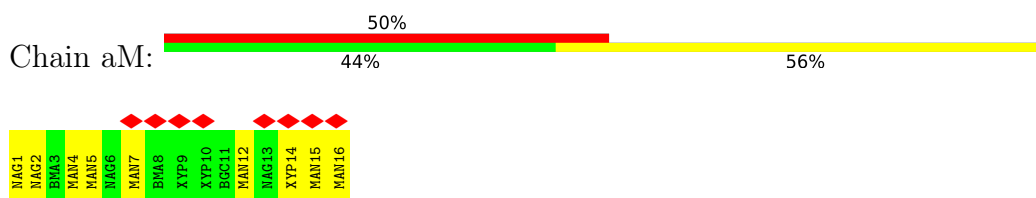
• Molecule 9: alpha-D-mannopyranose-(1-3)-[beta-D-mannopyranose-(1-4)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[beta-D-xylopyranose-(1-2)-beta-D-xylopyranose-(1-6)][beta-D-glucopyranose-(1-3)]alpha-D-mannopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)][beta-D-xylopyranose-(1-2)]alpha-D-mannopyranose-(1-6)-[alpha-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



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



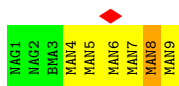
• Molecule 9: alpha-D-mannopyranose-(1-3)-[beta-D-mannopyranose-(1-4)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[beta-D-xylopyranose-(1-2)-beta-D-xylopyranose-(1-6)][beta-D-glucopyranose-(1-3)]alpha-D-mannopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)][beta-D-xylopyranose-(1-2)]alpha-D-mannopyranose-(1-6)-[alpha-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



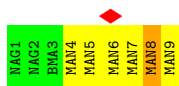
• Molecule 10: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



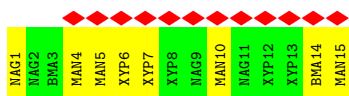
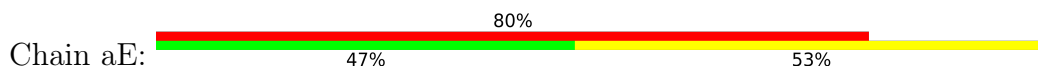
- Molecule 10: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



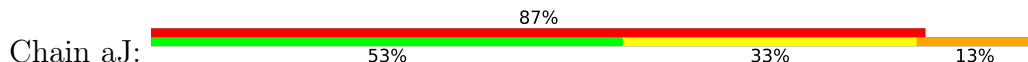
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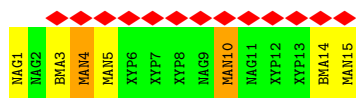


- Molecule 11: beta-D-xylopyranose-(1-2)-beta-D-xylopyranose-(1-6)-[beta-D-xylopyranose-(1-3)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]alpha-D-mannopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-[beta-D-xylopyranose-(1-3)]alpha-D-mannopyranose-(1-6)]beta-D-xylopyranose-(1-2)]alpha-D-mannopyranose-(1-6)-[beta-D-mannopyranose-(1-2)]alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

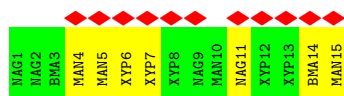
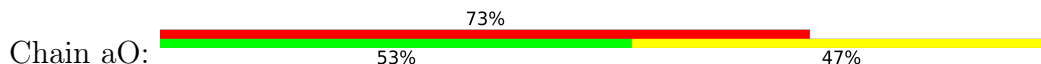


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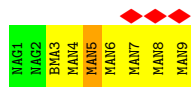
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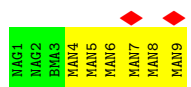
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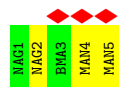
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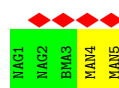
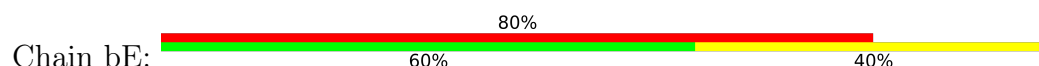
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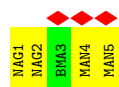
- Molecule 13: alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 13: 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



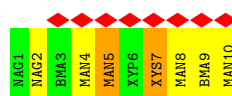
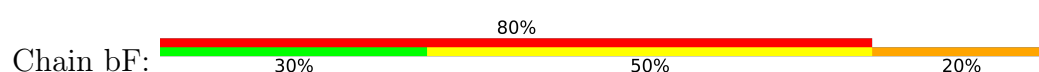
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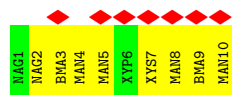
- Molecule 14: beta-D-xylopyranose-(1-6)-alpha-D-mannopyranose-(1-3)-[alpha-D-xylopyranose-(1-2)][alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[beta-D-mannopyranose-(1-2)][alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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



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



- Molecule 15: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-beta-D-xylopyranose



- Molecule 15: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-beta-D-xylopyranose



- Molecule 15: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-beta-D-xylopyranose



- Molecule 16: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-beta-D-xylopyranose



- Molecule 16: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-beta-D-xylopyranose





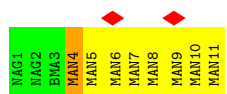
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- Molecule 17: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 17: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]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



- Molecule 17: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]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



- Molecule 17: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]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

se-(1-2)-alpha-D-mannopyranose-(1-6)]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



• Molecule 17: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]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



• Molecule 17: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]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



• Molecule 17: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]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



• Molecule 17: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]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



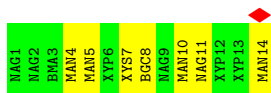
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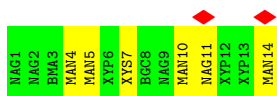
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- Molecule 18: alpha-D-xylopyranose-(1-2)-beta-D-xylopyranose-(1-6)-[beta-D-glucopyranose-(1-3)]|[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]alpha-D-mannopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-[beta-D-xylopyranose-(1-3)]alpha-D-mannopyranose-(1-6)]|[beta-D-xylopyranose-(1-2)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 18: alpha-D-xylopyranose-(1-2)-beta-D-xylopyranose-(1-6)-[beta-D-glucopyranose-(1-3)]|[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]alpha-D-mannopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-[beta-D-xylopyranose-(1-3)]alpha-D-mannopyranose-(1-6)]|[beta-D-xylopyranose-(1-2)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



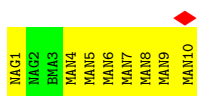
- Molecule 19: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 19: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



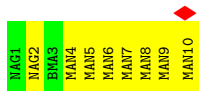
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- Molecule 19: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



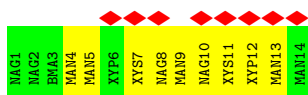
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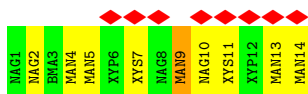
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- Molecule 20: alpha-D-xylopyranose-(1-2)-beta-D-xylopyranose-(1-6)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]alpha-D-mannopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-[alpha-D-xylopyranose-(1-3)]alpha-D-mannopyranose-(1-6)]beta-D-xylopyranose-(1-2)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-2)]alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

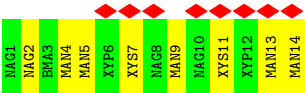


- Molecule 20: alpha-D-xylopyranose-(1-2)-beta-D-xylopyranose-(1-6)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]alpha-D-mannopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-[alpha-D-xylopyranose-(1-3)]alpha-D-mannopyranose-(1-6)]beta-D-xylopyranose-(1-2)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-2)]alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 20: alpha-D-xylopyranose-(1-2)-beta-D-xylopyranose-(1-6)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]alpha-D-mannopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-[alpha-D-xylopyranose-(1-3)]alpha-D-mannopyranose-(1-6)]beta-D-xylopyranose-(1-2)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-2)]alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

e-(1-2)-[alpha-D-xylopyranose-(1-3)]alpha-D-mannopyranose-(1-6)][beta-D-xylopyranose-(1-2)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-2)][alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	104125	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	1200	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	1.519	Depositor
Minimum map value	-0.995	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.055	Depositor
Recommended contour level	0.2	Depositor
Map size (Å)	460.00128, 460.00128, 460.00128	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.89844, 0.89844, 0.89844	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 2PO, MAN, XYS, CL, NAG, CA, BGC, BMA, XYP

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	EA	0.24	0/2733	0.41	0/3708
1	EB	0.24	0/2733	0.42	0/3708
1	EC	0.23	0/2733	0.43	0/3708
2	FA	0.22	0/5484	0.40	0/7488
2	FB	0.23	0/5484	0.42	0/7488
2	FC	0.24	0/5484	0.43	0/7488
3	DA	0.25	0/1439	0.45	0/1947
3	DB	0.27	0/1439	0.46	0/1947
3	DC	0.25	0/1439	0.47	0/1947
4	CA	0.24	0/1776	0.41	0/2413
4	CB	0.24	0/1776	0.45	0/2413
4	CC	0.26	0/1776	0.44	0/2413
5	AA	0.23	0/5841	0.40	0/7967
5	AB	0.24	0/5841	0.43	0/7967
5	AC	0.24	0/5841	0.43	2/7967 (0.0%)
6	BA	0.23	0/2782	0.42	0/3781
6	BB	0.25	0/2782	0.44	0/3781
6	BC	0.25	0/2782	0.44	0/3781
All	All	0.24	0/60165	0.42	2/81912 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
5	AA	0	1
5	AB	0	1
5	AC	0	1
All	All	0	3

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	AC	234	PRO	N-CD-CG	-8.23	93.92	103.80
5	AC	234	PRO	CA-N-CD	-5.62	103.62	111.50

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	AA	518	ALA	Peptide
5	AB	518	ALA	Peptide
5	AC	518	ALA	Peptide

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	EA	2672	0	2469	24	0
1	EB	2672	0	2470	20	0
1	EC	2672	0	2470	18	0
2	FA	5350	0	4914	35	0
2	FB	5350	0	4914	35	0
2	FC	5350	0	4913	41	0
3	DA	1409	0	1268	17	0
3	DB	1409	0	1268	11	0
3	DC	1409	0	1268	14	0
4	CA	1728	0	1530	12	0
4	CB	1728	0	1530	11	0
4	CC	1728	0	1530	9	0
5	AA	5689	0	5214	43	0
5	AB	5689	0	5214	36	0
5	AC	5689	0	5214	44	0
6	BA	2725	0	2484	16	0
6	BB	2725	0	2486	22	0
6	BC	2725	0	2485	22	0
7	aA	160	0	109	2	0
7	aF	160	0	109	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	aK	160	0	109	2	0
8	aB	180	0	117	0	0
8	aG	180	0	117	0	0
8	aL	180	0	117	1	0
9	aC	182	0	127	1	0
9	aH	182	0	127	0	0
9	aM	182	0	127	1	0
10	aD	105	0	88	1	0
10	aI	105	0	88	1	0
10	aN	105	0	88	1	0
11	aE	167	0	98	2	0
11	aJ	167	0	98	2	0
11	aO	167	0	98	1	0
12	bA	105	0	88	0	0
12	bD	105	0	88	1	0
12	bG	105	0	88	0	0
13	bB	61	0	52	0	0
13	bE	61	0	52	0	0
13	bH	61	0	52	0	0
14	bC	112	0	84	0	0
14	bF	112	0	84	1	0
14	bI	112	0	84	0	0
15	cA	42	0	28	0	0
15	cB	42	0	28	0	0
15	cC	42	0	28	0	0
16	dA	75	0	55	0	0
16	dB	75	0	55	0	0
16	dC	75	0	55	1	0
17	eA	127	0	106	0	0
17	eC	127	0	106	2	0
17	eE	127	0	106	0	0
17	fC	127	0	106	1	0
17	fD	127	0	106	0	0
17	fH	127	0	106	0	0
17	fI	127	0	106	1	0
17	fM	127	0	106	3	0
17	fN	127	0	106	1	0
18	eB	158	0	107	1	0
18	eD	158	0	107	0	0
18	eF	158	0	107	0	0
19	fB	116	0	97	0	0
19	fE	116	0	97	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	fG	116	0	97	0	0
19	fJ	116	0	97	1	0
19	fL	116	0	97	0	0
19	fO	116	0	97	1	0
20	fF	158	0	115	2	0
20	fK	158	0	115	1	0
20	fP	158	0	115	0	0
21	AA	7	0	0	0	0
21	AB	7	0	0	0	0
21	AC	7	0	0	0	0
21	BA	3	0	0	0	0
21	BB	3	0	0	1	0
21	BC	3	0	0	0	0
21	CA	1	0	0	0	0
21	CB	1	0	0	0	0
21	CC	1	0	0	0	0
21	EA	2	0	0	1	0
21	EB	1	0	0	0	0
21	EC	1	0	0	0	0
21	FA	6	0	0	0	0
21	FB	6	0	0	0	0
21	FC	6	0	0	0	0
22	EA	14	0	13	1	0
22	EB	14	0	13	1	0
22	EC	14	0	13	1	0
22	FA	14	0	13	0	0
22	FB	14	0	13	0	0
22	FC	14	0	13	0	0
23	AA	12	0	0	0	0
23	AB	12	0	0	0	0
23	AC	12	0	0	0	0
23	BA	8	0	0	0	0
23	BB	8	0	0	0	0
23	BC	8	0	0	0	0
23	EA	4	0	0	0	0
23	EB	4	0	0	0	0
23	EC	4	0	0	0	0
23	FA	4	0	0	0	0
23	FB	4	0	0	0	0
23	FC	4	0	0	0	0
24	DA	1	0	0	0	0
24	DB	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	DC	1	0	0	0	0
25	AA	610	0	0	8	0
25	AB	619	0	0	8	0
25	AC	617	0	0	8	0
25	BA	275	0	0	1	0
25	BB	300	0	0	6	0
25	BC	301	0	0	9	0
25	CA	219	0	0	2	0
25	CB	217	0	0	2	0
25	CC	209	0	0	1	0
25	DA	167	0	0	5	0
25	DB	169	0	0	2	0
25	DC	170	0	0	3	0
25	EA	293	0	0	8	0
25	EB	294	0	0	7	0
25	EC	324	0	0	7	0
25	FA	632	0	0	4	0
25	FB	635	0	0	7	0
25	FC	636	0	0	14	0
All	All	71986	0	58459	415	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 3.

All (415) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:FC:440:GLN:NE2	2:FC:491:LYS:O	2.05	0.89
2:FC:524:THR:HG1	17:fM:4:MAN:HO4	1.17	0.87
4:CB:17:HIS:ND1	25:AB:902:HOH:O	2.09	0.85
2:FB:440:GLN:NE2	2:FB:491:LYS:O	2.11	0.83
2:FA:524:THR:HG1	17:fC:4:MAN:HO4	1.25	0.80
1:EC:253:GLN:HG2	2:FC:104:ILE:HD11	1.64	0.80
2:FC:178:ARG:NH1	25:FC:904:HOH:O	2.13	0.80
1:EA:319:PRO:O	25:EA:501:HOH:O	1.99	0.79
25:FC:903:HOH:O	3:DC:34:LYS:NZ	2.15	0.77
6:BC:133:ASP:OD1	25:BC:501:HOH:O	2.01	0.77
2:FC:446:GLU:OE1	25:FC:901:HOH:O	2.03	0.76
3:DB:86:ASP:HB2	3:DB:93:LYS:HD2	1.65	0.76
5:AA:546:LYS:HD2	5:AA:707:GLU:HG3	1.67	0.75
1:EB:319:PRO:O	25:EB:501:HOH:O	2.06	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:EB:253:GLN:OE1	1:EB:257:ARG:NH1	2.21	0.73
5:AB:463:ASP:OD1	25:AB:901:HOH:O	2.07	0.72
5:AC:92:GLY:O	25:AC:901:HOH:O	2.06	0.72
6:BC:100:GLU:OE2	6:BC:157:ARG:NH2	2.23	0.71
5:AB:92:GLY:O	25:AB:904:HOH:O	2.09	0.71
1:EC:319:PRO:O	25:EC:502:HOH:O	2.07	0.71
6:BB:189:ILE:HG22	6:BB:190:ILE:HD12	1.72	0.70
5:AB:63:ASP:OD1	25:AB:903:HOH:O	2.09	0.69
3:DC:44:GLU:OE2	25:DC:401:HOH:O	2.09	0.69
4:CA:160:ASP:OD1	25:CA:401:HOH:O	2.09	0.69
1:EA:180:ASP:OD2	25:EA:502:HOH:O	2.11	0.69
4:CC:160:ASP:OD1	25:CC:401:HOH:O	2.11	0.69
3:DC:93:LYS:NZ	25:DC:403:HOH:O	2.26	0.69
6:BC:123:GLU:O	25:BC:503:HOH:O	2.11	0.69
3:DA:68:GLN:NE2	25:DA:405:HOH:O	2.27	0.68
6:BC:55:ASP:OD2	25:BC:504:HOH:O	2.12	0.68
6:BA:124:GLU:OE1	25:BA:502:HOH:O	2.11	0.68
1:EB:266:VAL:O	25:EB:502:HOH:O	2.11	0.68
2:FB:280:ASP:OD1	25:FB:901:HOH:O	2.11	0.68
5:AC:506:LEU:HD11	5:AC:523:PHE:HB3	1.76	0.68
1:EC:101:LYS:O	25:EC:503:HOH:O	2.12	0.67
6:BB:124:GLU:OE1	25:BB:502:HOH:O	2.12	0.67
6:BC:100:GLU:HG2	6:BC:108:THR:HG22	1.77	0.67
4:CA:192:GLU:OE2	25:CA:402:HOH:O	2.13	0.67
6:BC:74:PHE:O	25:BC:505:HOH:O	2.13	0.67
2:FA:568:THR:HA	2:FA:646:GLU:HG2	1.77	0.66
2:FC:583:GLU:HG2	2:FC:584:THR:HG23	1.76	0.66
5:AA:99:GLN:O	25:AA:903:HOH:O	2.12	0.66
4:CA:17:HIS:ND1	25:AA:901:HOH:O	2.13	0.66
5:AC:43:ARG:NH1	6:BC:254:ASN:O	2.28	0.66
2:FC:281:ALA:O	25:FC:905:HOH:O	2.14	0.66
5:AA:475:TYR:O	25:AA:902:HOH:O	2.12	0.66
1:EB:101:LYS:O	25:EB:503:HOH:O	2.14	0.66
1:EB:73:ARG:NH2	25:BC:506:HOH:O	2.28	0.65
2:FA:339:GLU:O	25:FA:901:HOH:O	2.14	0.65
5:AA:43:ARG:NH2	25:AA:917:HOH:O	2.30	0.65
3:DA:44:GLU:OE1	25:DA:402:HOH:O	2.15	0.64
5:AA:272:THR:O	5:AA:276:GLU:HG3	1.96	0.64
2:FB:244:ILE:HD11	2:FB:325:ASP:HB2	1.79	0.64
5:AC:170:ASP:OD2	25:AC:903:HOH:O	2.14	0.64
1:EA:101:LYS:O	25:EA:503:HOH:O	2.14	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:BC:125:LEU:O	25:BC:506:HOH:O	2.15	0.64
4:CB:3:ARG:O	25:CB:401:HOH:O	2.15	0.63
6:BC:61:GLU:HG3	6:BC:105:GLN:HB3	1.80	0.63
2:FC:244:ILE:HD11	2:FC:325:ASP:HB2	1.81	0.63
4:CC:66:ALA:HB3	4:CC:79:PRO:HD2	1.82	0.61
3:DB:44:GLU:OE1	25:DB:401:HOH:O	2.16	0.61
5:AC:63:ASP:OD1	25:AC:905:HOH:O	2.16	0.61
1:EC:351:ASN:ND2	25:EC:501:HOH:O	2.07	0.60
6:BB:61:GLU:HG3	6:BB:105:GLN:HB3	1.83	0.60
5:AC:276:GLU:OE1	25:AC:904:HOH:O	2.16	0.60
5:AB:170:ASP:OD1	25:AB:907:HOH:O	2.16	0.60
4:CA:160:ASP:OD1	4:CA:160:ASP:N	2.33	0.60
1:EA:267:ASP:OD2	25:EA:504:HOH:O	2.16	0.59
5:AB:390:ASP:OD1	25:AB:906:HOH:O	2.16	0.59
5:AB:659:SER:HA	11:aJ:1:NAG:H82	1.84	0.59
1:EB:180:ASP:OD2	25:EB:504:HOH:O	2.17	0.59
5:AB:99:GLN:O	25:AB:905:HOH:O	2.16	0.59
2:FA:244:ILE:HD11	2:FA:325:ASP:HB2	1.82	0.59
2:FA:329:ASP:OD2	5:AB:392:THR:OG1	2.20	0.59
1:EA:340:ARG:HD2	1:EA:356:TYR:CZ	2.38	0.59
5:AB:559:THR:HG21	5:AB:682:VAL:HG13	1.84	0.58
6:BA:61:GLU:HG3	6:BA:105:GLN:HB3	1.85	0.58
2:FB:339:GLU:O	25:FB:903:HOH:O	2.16	0.58
2:FA:165:ILE:HD11	3:DA:73:ALA:HB3	1.85	0.58
5:AA:559:THR:HG21	5:AA:682:VAL:HG13	1.84	0.58
4:CA:103:ASP:HB2	4:CA:111:VAL:HG12	1.85	0.57
1:EB:304:CYS:HB2	1:EB:312:LEU:H	1.69	0.57
1:EB:326:GLN:NE2	1:EB:329:LYS:HG2	2.18	0.57
2:FB:341:VAL:HA	5:AC:242:GLU:HG3	1.85	0.57
2:FC:341:VAL:O	25:FC:906:HOH:O	2.17	0.57
1:EC:174:MET:HE3	1:EC:226:LEU:HD22	1.86	0.57
1:EB:54:GLU:HB3	1:EB:87:ARG:HB3	1.85	0.57
6:BA:167:ASP:HB2	6:BA:172:LYS:HG3	1.86	0.57
1:EB:137:ASP:OD1	1:EB:139:SER:OG	2.24	0.56
5:AB:423:HIS:HB2	5:AB:543:TYR:CE2	2.41	0.56
2:FB:75:ALA:HB2	10:aI:8:MAN:H3	1.87	0.56
6:BB:312:GLN:NE2	25:BB:511:HOH:O	2.30	0.56
11:aO:6:XYP:O3	11:aO:7:XYP:O2	2.23	0.56
1:EA:253:GLN:HG2	2:FA:104:ILE:HD11	1.87	0.56
2:FC:44:ASN:HA	2:FC:54:ILE:HD12	1.88	0.55
4:CB:-1:ALA:O	25:CB:402:HOH:O	2.18	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:FC:249:TYR:OH	25:FC:902:HOH:O	2.07	0.55
3:DA:18:ALA:N	3:DA:33:ASP:OD2	2.40	0.55
2:FC:717:THR:HG22	2:FC:717:THR:O	2.06	0.54
2:FC:75:ALA:HB2	10:aN:8:MAN:H3	1.90	0.54
2:FB:254:ASN:ND2	25:FB:933:HOH:O	2.38	0.54
6:BB:123:GLU:O	25:BB:503:HOH:O	2.18	0.54
2:FB:81:GLU:OE1	25:FB:904:HOH:O	2.18	0.54
2:FC:52:GLU:HB3	2:FC:127:ARG:HB3	1.90	0.54
4:CC:22:LEU:HD13	5:AC:209:LEU:HB3	1.89	0.54
4:CC:103:ASP:HB2	4:CC:111:VAL:HG12	1.89	0.54
1:EC:265:ASN:OD1	25:EC:504:HOH:O	2.19	0.53
2:FC:146:ALA:O	2:FC:186:MET:HB2	2.08	0.53
2:FA:63:ASP:HB2	3:DA:121:GLN:HE22	1.73	0.53
2:FA:100:ALA:O	25:FA:902:HOH:O	2.17	0.53
5:AA:654:SER:O	5:AA:658:ARG:HG2	2.09	0.53
1:EC:180:ASP:O	25:EC:505:HOH:O	2.19	0.53
5:AC:160:CYS:SG	5:AC:184:MET:HB3	2.49	0.53
3:DA:108:CYS:O	25:DA:403:HOH:O	2.19	0.52
6:BA:100:GLU:HG2	6:BA:108:THR:HG22	1.91	0.52
5:AA:352:TYR:O	25:AA:904:HOH:O	2.19	0.52
2:FA:606:LEU:HD22	2:FA:667:ALA:HA	1.91	0.52
3:DA:62:ALA:HB3	3:DA:75:PRO:HD2	1.91	0.52
3:DA:140:LYS:HE2	25:DA:421:HOH:O	2.09	0.52
1:EB:123:ASP:OD2	25:EB:505:HOH:O	2.19	0.52
2:FC:399:GLN:O	2:FC:403:LYS:HG3	2.10	0.52
5:AC:339:SER:HA	5:AC:402:LYS:HD2	1.91	0.52
5:AB:98:PRO:HB2	5:AB:100:MET:SD	2.49	0.52
5:AA:339:SER:HA	5:AA:402:LYS:HD2	1.91	0.52
5:AA:321:ARG:NH2	25:AA:947:HOH:O	2.42	0.51
6:BC:267:ASP:OD1	6:BC:270:THR:OG1	2.20	0.51
4:CC:121:THR:OG1	4:CC:123:TRP:NE1	2.39	0.51
5:AA:643:GLU:HB3	6:BA:315:TYR:CE2	2.46	0.51
2:FC:165:ILE:HD11	3:DC:73:ALA:HB3	1.91	0.51
5:AC:260:TRP:CE2	5:AC:285:VAL:HG21	2.46	0.51
1:EA:340:ARG:NH2	25:EA:502:HOH:O	2.44	0.51
25:AC:1400:HOH:O	17:fI:10:MAN:O3	2.10	0.51
11:aE:6:XYP:O3	11:aE:7:XYP:O2	2.27	0.51
2:FA:709:GLY:O	2:FA:710:LYS:HB2	2.11	0.51
3:DA:99:ASP:HB2	3:DA:107:ILE:HG22	1.93	0.51
2:FB:167:GLU:O	2:FB:171:GLN:HG3	2.11	0.51
2:FB:664:ARG:NH2	20:fK:9:MAN:H4	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:EA:138:PHE:CD1	1:EA:322:ASN:HB3	2.46	0.50
2:FB:210:PRO:HG3	2:FB:714:SER:O	2.11	0.50
5:AC:458:LYS:HG2	5:AC:477:TRP:CH2	2.47	0.50
5:AC:346:PRO:HA	6:BC:315:TYR:CE2	2.46	0.50
5:AB:260:TRP:CE2	5:AB:285:VAL:HG21	2.47	0.50
2:FA:44:ASN:HA	2:FA:54:ILE:HD12	1.93	0.50
5:AA:260:TRP:CE2	5:AA:285:VAL:HG21	2.47	0.50
5:AC:643:GLU:HB3	6:BC:315:TYR:CE2	2.47	0.50
2:FA:434:LYS:HB3	2:FA:529:TYR:HB2	1.94	0.50
2:FC:671:LYS:HE2	2:FC:673:TYR:CZ	2.47	0.50
2:FA:277:ASN:O	25:FA:904:HOH:O	2.20	0.49
4:CA:67:TRP:CH2	4:CA:110:THR:HG23	2.46	0.49
2:FC:194:TYR:O	25:FC:907:HOH:O	2.20	0.49
3:DC:140:LYS:HE2	25:DC:420:HOH:O	2.11	0.49
1:EA:72:ARG:NH1	1:EA:75:GLN:HE22	2.10	0.49
2:FB:564:VAL:HG22	2:FB:652:ILE:HG12	1.95	0.49
5:AB:346:PRO:HA	6:BB:315:TYR:CE2	2.47	0.49
2:FA:210:PRO:HG3	2:FA:714:SER:O	2.12	0.49
5:AA:719:ARG:HD2	5:AA:735:TYR:CZ	2.47	0.49
2:FB:165:ILE:HD11	3:DB:73:ALA:HB3	1.93	0.49
5:AC:43:ARG:HG3	6:BC:255:ARG:HB2	1.94	0.49
5:AA:659:SER:HA	11:aE:1:NAG:H82	1.94	0.49
1:EB:266:VAL:HG12	1:EB:285:PHE:HA	1.95	0.49
5:AB:273:GLU:HA	5:AB:276:GLU:HG3	1.94	0.49
5:AA:423:HIS:HB2	5:AA:543:TYR:CE2	2.47	0.49
1:EC:54:GLU:HB3	1:EC:87:ARG:HB3	1.95	0.49
2:FC:683:TYR:CE1	3:DC:34:LYS:HE2	2.48	0.49
1:EC:68:ASP:OD1	1:EC:72:ARG:N	2.46	0.49
5:AA:649:ARG:NH2	5:AA:684:ILE:O	2.37	0.49
5:AB:339:SER:HA	5:AB:402:LYS:HD2	1.93	0.49
25:FC:1519:HOH:O	17:fN:2:NAG:O3	2.14	0.49
4:CA:70:GLU:HG3	4:CA:79:PRO:HG3	1.95	0.48
6:BA:203:ILE:HA	6:BA:312:GLN:HG2	1.94	0.48
3:DB:93:LYS:HG3	25:DB:544:HOH:O	2.13	0.48
7:aK:5:MAN:H3	7:aK:8:MAN:H2	1.56	0.48
1:EC:138:PHE:CD1	1:EC:322:ASN:HB3	2.48	0.48
2:FC:210:PRO:HG3	2:FC:714:SER:O	2.13	0.48
2:FC:499:VAL:HG21	2:FC:605:LEU:HD11	1.94	0.48
5:AC:223:ASP:HA	5:AC:369:TYR:O	2.13	0.48
5:AC:348:THR:HG22	5:AC:666:MET:HE1	1.94	0.48
1:EB:138:PHE:CD1	1:EB:322:ASN:HB3	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:FC:163:GLU:OE1	2:FC:171:GLN:NE2	2.40	0.48
5:AA:37:ASP:OD1	25:AA:905:HOH:O	2.19	0.48
1:EA:174:MET:HE3	1:EA:226:LEU:HD22	1.96	0.48
6:BB:132:ASN:HA	6:BB:135:SER:O	2.13	0.48
4:CC:124:PRO:HG2	4:CC:127:LEU:HG	1.95	0.48
6:BB:189:ILE:HG22	6:BB:190:ILE:CD1	2.42	0.48
5:AC:707:GLU:H	5:AC:707:GLU:CD	2.21	0.48
14:bF:5:MAN:H5	14:bF:7:XYS:H52	1.96	0.48
1:EA:138:PHE:CG	1:EA:322:ASN:HB3	2.49	0.48
1:EA:304:CYS:HB2	1:EA:312:LEU:HB2	1.96	0.48
1:EA:321:SER:HB2	22:EA:402:NAG:H82	1.95	0.48
1:EB:321:SER:HB2	22:EB:401:NAG:H82	1.95	0.48
4:CB:67:TRP:CH2	4:CB:110:THR:HG23	2.49	0.48
1:EB:82:ARG:NH1	25:EB:515:HOH:O	2.32	0.48
1:EB:138:PHE:CG	1:EB:322:ASN:HB3	2.49	0.48
2:FB:671:LYS:HE2	2:FB:673:TYR:CZ	2.49	0.47
1:EC:264:ASP:OD2	25:EC:507:HOH:O	2.20	0.47
1:EC:326:GLN:NE2	1:EC:329:LYS:HG3	2.28	0.47
2:FC:99:PRO:HB3	2:FC:115:GLU:CD	2.39	0.47
6:BC:132:ASN:HA	6:BC:135:SER:O	2.14	0.47
5:AC:505:VAL:HG21	5:AC:617:LEU:HD11	1.95	0.47
5:AB:616:MET:HE2	5:AB:616:MET:HB2	1.80	0.47
1:EC:304:CYS:HB2	1:EC:312:LEU:H	1.80	0.47
5:AA:346:PRO:HA	6:BA:315:TYR:CE2	2.49	0.47
2:FB:644:ASN:O	2:FB:648:ARG:HG3	2.14	0.47
1:EC:123:ASP:OD2	25:EC:506:HOH:O	2.20	0.47
5:AA:224:LEU:HD13	5:AA:371:LEU:HD12	1.97	0.47
4:CB:103:ASP:HB2	4:CB:111:VAL:HG12	1.96	0.47
25:FC:1337:HOH:O	17:fM:2:NAG:O6	2.18	0.47
2:FA:75:ALA:HB2	10:aD:8:MAN:H3	1.96	0.47
4:CB:132:ALA:HB2	5:AB:96:GLN:HG2	1.97	0.47
2:FC:403:LYS:HD3	2:FC:422:TRP:CZ2	2.49	0.47
6:BB:210:ARG:NH2	6:BB:235:ASP:OD2	2.28	0.46
2:FC:606:LEU:HD23	2:FC:667:ALA:HA	1.95	0.46
3:DC:18:ALA:HA	3:DC:33:ASP:OD1	2.15	0.46
2:FA:671:LYS:HE2	2:FA:673:TYR:CZ	2.50	0.46
5:AC:517:ILE:HG22	5:AC:518:ALA:H	1.81	0.46
6:BB:314:LEU:O	6:BB:319:HIS:NE2	2.47	0.46
2:FC:598:LYS:HE2	3:DC:67:VAL:HB	1.97	0.46
4:CC:67:TRP:CH2	4:CC:110:THR:HG23	2.50	0.46
5:AC:630:ASN:HB2	5:AC:632:TYR:CZ	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:BC:207:GLN:NE2	25:BC:514:HOH:O	2.33	0.46
3:DA:86:ASP:HB2	3:DA:93:LYS:CD	2.45	0.46
1:EB:340:ARG:HD2	1:EB:356:TYR:CZ	2.51	0.46
3:DC:181:ARG:HD2	3:DC:197:TYR:CZ	2.50	0.46
5:AA:608:LEU:HB3	5:AA:637:LEU:HD21	1.97	0.46
4:CA:22:LEU:HD13	5:AA:209:LEU:HB3	1.98	0.46
2:FA:162:CYS:SG	2:FA:186:MET:HB3	2.56	0.46
2:FA:206:VAL:O	25:FA:905:HOH:O	2.20	0.46
25:FC:1438:HOH:O	16:DC:2:MAN:O6	2.21	0.46
2:FA:644:ASN:O	2:FA:648:ARG:HG3	2.16	0.45
6:BA:166:GLY:HA3	6:BA:174:LEU:HD21	1.98	0.45
5:AA:613:LEU:HA	5:AA:632:TYR:O	2.17	0.45
2:FB:709:GLY:O	2:FB:710:LYS:HB2	2.16	0.45
3:DB:18:ALA:N	3:DB:33:ASP:OD2	2.49	0.45
1:EC:138:PHE:CG	1:EC:322:ASN:HB3	2.50	0.45
1:EC:319:PRO:HB3	2:FC:636:ASN:HA	1.98	0.45
5:AA:92:GLY:O	25:AA:906:HOH:O	2.21	0.45
6:BB:312:GLN:OE1	6:BB:314:LEU:HB2	2.16	0.45
1:EA:45:LEU:HD21	6:BB:172:LYS:HD2	1.99	0.45
2:FA:403:LYS:HG2	2:FA:422:TRP:CH2	2.52	0.45
3:DA:34:LYS:NZ	25:DA:401:HOH:O	2.14	0.45
2:FA:550:TYR:HD1	20:FF:10:NAG:H82	1.81	0.45
5:AC:698:HIS:NE2	25:AC:902:HOH:O	2.10	0.45
6:BA:212:GLN:HB3	6:BA:308:GLY:O	2.17	0.45
5:AB:707:GLU:CD	5:AB:707:GLU:H	2.24	0.45
1:EC:234:PRO:HG3	1:EC:310:PRO:HB2	1.99	0.45
2:FA:145:ARG:HD2	2:FA:186:MET:HE2	1.98	0.45
2:FB:98:TYR:CG	2:FB:99:PRO:HD2	2.51	0.45
2:FA:98:TYR:CG	2:FA:99:PRO:HD2	2.52	0.45
2:FA:445:TYR:HB3	2:FA:453:ILE:HG23	1.99	0.45
5:AA:458:LYS:HG2	5:AA:477:TRP:CH2	2.52	0.45
1:EC:321:SER:HB2	22:EC:401:NAG:H82	1.99	0.45
5:AC:284:ASN:HD21	17:EC:11:MAN:H4	1.82	0.45
1:EA:73:ARG:NH2	25:BB:513:HOH:O	2.49	0.44
5:AA:223:ASP:HA	5:AA:369:TYR:O	2.18	0.44
5:AA:626:PRO:HD3	5:AA:678:TRP:CD1	2.53	0.44
3:DB:18:ALA:HA	3:DB:33:ASP:OD1	2.16	0.44
5:AC:445:TYR:CE2	5:AC:447:THR:HG23	2.52	0.44
21:EA:404:CA:CA	21:BB:405:CA:CA	1.51	0.44
2:FA:314:ARG:HD3	2:FA:314:ARG:HA	1.70	0.44
2:FB:249:TYR:OH	25:FB:902:HOH:O	2.13	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:FB:372:LEU:HD21	2:FB:435:LEU:HD13	1.99	0.44
2:FC:399:GLN:OE1	25:FC:908:HOH:O	2.21	0.44
2:FC:583:GLU:OE2	25:FC:909:HOH:O	2.21	0.44
5:AC:28:ASN:ND2	5:AC:51:SER:HB3	2.33	0.44
3:DA:86:ASP:HB2	3:DA:93:LYS:HD2	1.99	0.44
5:AC:568:TYR:CZ	5:AC:666:MET:HE3	2.52	0.44
6:BA:172:LYS:HD3	6:BA:343:TYR:CG	2.52	0.44
5:AB:526:LEU:HD21	5:AB:619:TRP:CZ3	2.53	0.44
5:AB:626:PRO:HD3	5:AB:678:TRP:CD1	2.52	0.44
6:BB:61:GLU:OE2	25:BB:504:HOH:O	2.21	0.44
4:CA:64:ASP:HA	4:CA:80:TRP:CZ3	2.53	0.44
2:FA:210:PRO:HG3	2:FA:714:SER:C	2.42	0.44
5:AA:445:TYR:CE2	5:AA:447:THR:HG23	2.53	0.44
6:BB:332:SER:HB3	12:bD:5:MAN:O4	2.18	0.44
7:aA:5:MAN:H3	7:aA:8:MAN:H2	1.76	0.44
2:FC:253:TRP:CE2	2:FC:278:VAL:HG21	2.53	0.44
3:DC:60:SER:HB3	3:DC:80:SER:OG	2.18	0.44
1:EA:264:ASP:HB3	25:EA:606:HOH:O	2.17	0.44
4:CB:71:VAL:HG22	4:CB:77:LEU:HD11	1.99	0.44
3:DC:136:TRP:O	3:DC:140:LYS:HD2	2.17	0.44
4:CA:24:GLU:OE2	5:AA:719:ARG:NH1	2.50	0.43
5:AA:296:VAL:HB	5:AA:311:TYR:CE1	2.53	0.43
18:eB:8:BGC:O6	18:eB:9:NAG:H2	2.18	0.43
2:FB:52:GLU:HB3	2:FB:127:ARG:HB3	2.00	0.43
2:FA:289:TRP:CG	2:FA:307:ARG:HG2	2.52	0.43
2:FC:472:SER:N	2:FC:473:PRO:HD2	2.34	0.43
1:EB:19:CYS:O	25:EB:506:HOH:O	2.21	0.43
5:AB:338:ALA:HB3	5:AB:341:GLN:HG2	2.00	0.43
2:FC:437:ASP:OD2	17:fM:4:MAN:O6	2.31	0.43
5:AA:420:PHE:O	5:AA:543:TYR:HB3	2.18	0.43
2:FB:472:SER:N	2:FB:473:PRO:HD2	2.33	0.43
5:AC:307:MET:HE2	7:aK:1:NAG:H62	2.00	0.43
3:DA:75:PRO:HA	19:fE:6:MAN:O2	2.18	0.43
5:AA:517:ILE:HG22	5:AA:518:ALA:H	1.84	0.43
2:FB:253:TRP:CE2	2:FB:278:VAL:HG21	2.53	0.43
5:AC:494:VAL:HB	5:AC:497:TYR:HE1	1.83	0.43
7:aF:5:MAN:H3	7:aF:8:MAN:H2	1.82	0.43
2:FA:275:PRO:O	2:FA:278:VAL:HG23	2.18	0.43
5:AB:458:LYS:HG2	5:AB:477:TRP:CH2	2.54	0.43
5:AC:284:ASN:ND2	17:eC:11:MAN:H4	2.34	0.43
5:AA:307:MET:HE2	7:aA:1:NAG:H62	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:FB:289:TRP:CG	2:FB:307:ARG:HG2	2.54	0.43
3:DB:99:ASP:HB2	3:DB:107:ILE:HG22	2.00	0.43
2:FC:332:ARG:O	25:FC:910:HOH:O	2.21	0.43
5:AC:464:ALA:HB2	5:AC:486:HIS:CE1	2.53	0.43
5:AC:526:LEU:HD21	5:AC:619:TRP:CZ3	2.54	0.43
6:BC:338:ARG:HD2	6:BC:354:TYR:CZ	2.54	0.43
1:EA:20:ASP:OD1	25:EA:505:HOH:O	2.21	0.43
6:BC:145:THR:HB	25:BC:503:HOH:O	2.19	0.43
6:BA:226:PHE:CG	6:BA:253:PRO:HD2	2.54	0.42
2:FB:356:GLU:OE1	25:FB:906:HOH:O	2.21	0.42
5:AB:286:ILE:HG21	5:AB:291:ILE:HD11	2.01	0.42
4:CA:86:LYS:HD3	4:CA:86:LYS:HA	1.90	0.42
5:AA:97:PHE:CG	5:AA:98:PRO:HD2	2.54	0.42
5:AC:557:GLU:HB2	8:aL:1:NAG:H82	2.00	0.42
9:aM:1:NAG:H61	9:aM:2:NAG:C7	2.49	0.42
5:AB:78:ALA:HB2	5:AB:97:PHE:HB3	2.01	0.42
2:FC:709:GLY:O	2:FC:710:LYS:HB2	2.19	0.42
5:AC:97:PHE:CG	5:AC:98:PRO:HD2	2.54	0.42
3:DA:19:CYS:HA	3:DA:20:PRO:HD2	1.86	0.42
3:DA:136:TRP:O	3:DA:140:LYS:HD2	2.19	0.42
6:BA:238:LEU:HD23	6:BA:238:LEU:HA	1.92	0.42
20:fF:8:NAG:O7	20:fF:12:XYP:O3	2.37	0.42
1:EA:73:ARG:HD2	6:BB:148:TYR:CD1	2.54	0.42
3:DC:75:PRO:HA	19:fO:6:MAN:O2	2.18	0.42
5:AC:230:LYS:HE2	5:AC:232:SER:O	2.19	0.42
2:FA:226:TYR:HA	2:FA:347:HIS:O	2.19	0.42
2:FB:80:SER:OG	25:FB:905:HOH:O	2.19	0.42
2:FB:172:ASP:OD2	2:FB:598:LYS:NZ	2.51	0.42
3:DB:97:ASN:HA	3:DB:107:ILE:HG12	2.02	0.42
5:AB:464:ALA:HB2	5:AB:486:HIS:CE1	2.55	0.42
2:FC:98:TYR:CG	2:FC:99:PRO:HD2	2.55	0.42
3:DB:181:ARG:HD2	3:DB:197:TYR:CZ	2.55	0.42
2:FC:283:SER:HB2	2:FC:314:ARG:HG3	2.02	0.42
5:AC:254:ASP:OD2	5:AC:258:GLU:HB3	2.20	0.42
1:EA:69:LYS:HD3	6:BB:127:PHE:CZ	2.54	0.42
1:EA:163:PRO:O	1:EA:164:GLU:HB2	2.19	0.42
5:AA:155:SER:OG	5:AA:196:ASP:O	2.25	0.42
1:EB:109:PRO:HB3	6:BC:96:PHE:CD2	2.55	0.42
2:FB:606:LEU:HD23	2:FB:614:THR:HG23	2.01	0.42
5:AB:626:PRO:HB3	5:AB:678:TRP:CD2	2.55	0.42
2:FA:440:GLN:OE1	2:FA:491:LYS:O	2.38	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:FB:280:ASP:O	2:FB:283:SER:OG	2.25	0.42
5:AB:610:ARG:HD2	5:AB:611:SER:N	2.35	0.42
5:AA:298:PHE:HA	5:AA:305:PHE:CE2	2.55	0.41
2:FB:623:ASN:HB2	2:FB:625:TYR:CZ	2.54	0.41
4:CB:170:PRO:HG3	4:CB:207:GLN:HA	2.01	0.41
25:FC:971:HOH:O	3:DC:34:LYS:HE3	2.20	0.41
5:AC:393:ARG:O	25:AC:906:HOH:O	2.20	0.41
2:FA:100:ALA:O	2:FA:102:THR:N	2.53	0.41
4:CB:66:ALA:HB3	4:CB:79:PRO:HD2	2.01	0.41
2:FC:205:PRO:HA	2:FC:249:TYR:OH	2.20	0.41
2:FA:221:TYR:CZ	2:FA:313:PRO:HB3	2.54	0.41
4:CB:18:ARG:NH1	4:CB:36:ASN:OD1	2.46	0.41
5:AB:351:GLN:HB2	5:AB:353:TYR:CZ	2.56	0.41
5:AB:420:PHE:O	5:AB:543:TYR:HB3	2.21	0.41
5:AB:608:LEU:HB3	5:AB:637:LEU:HD21	2.03	0.41
5:AC:372:LYS:HE3	25:AC:1103:HOH:O	2.19	0.41
4:CA:66:ALA:HB3	4:CA:79:PRO:HD2	2.02	0.41
6:BA:139:PHE:CZ	6:BA:320:SER:HB3	2.56	0.41
2:FB:260:ILE:HB	2:FB:335:LEU:HD11	2.03	0.41
1:EA:54:GLU:HB3	1:EA:87:ARG:HB3	2.03	0.41
4:CB:33:CYS:HA	4:CB:38:ASN:O	2.20	0.41
2:FC:233:SER:HA	2:FC:303:PHE:CD2	2.55	0.41
9:aC:9:XYP:O3	9:aC:10:XYP:O2	2.38	0.41
11:aJ:4:MAN:H62	11:aJ:10:MAN:H2	1.75	0.41
1:EA:253:GLN:HG3	1:EA:257:ARG:HD2	2.03	0.41
5:AA:635:LYS:HA	5:AA:635:LYS:HD2	1.85	0.41
6:BA:132:ASN:HA	6:BA:135:SER:O	2.21	0.41
2:FB:102:THR:HG22	2:FB:108:VAL:HA	2.03	0.41
2:FC:499:VAL:HG21	2:FC:605:LEU:CD1	2.51	0.41
4:CC:64:ASP:HA	4:CC:80:TRP:CZ3	2.55	0.41
5:AA:577:ASN:HB3	5:AA:580:ILE:HD12	2.02	0.41
1:EB:281:LEU:HD23	1:EB:281:LEU:HA	1.97	0.41
2:FB:585:HIS:CE1	2:FB:592:ALA:HB2	2.54	0.41
5:AB:76:SER:HB2	5:AB:80:ILE:HB	2.03	0.41
1:EA:109:PRO:HB3	6:BB:96:PHE:CD2	2.56	0.41
2:FA:329:ASP:HB3	5:AB:393:ARG:NH2	2.36	0.41
5:AA:190:LYS:HG3	5:AA:258:GLU:HA	2.03	0.41
6:BA:106:ARG:HD3	6:BA:121:TYR:OH	2.21	0.41
5:AA:631:LEU:HD12	5:AA:631:LEU:HA	1.90	0.41
5:AB:475:TYR:O	25:AB:908:HOH:O	2.22	0.41
5:AB:505:VAL:HG21	5:AB:617:LEU:HD11	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:AC:251:ARG:NH1	5:AC:259:ASP:OD2	2.54	0.41
3:DA:181:ARG:HD2	3:DA:197:TYR:CZ	2.56	0.41
5:AA:464:ALA:HB2	5:AA:486:HIS:CE1	2.56	0.41
5:AB:97:PHE:CG	5:AB:98:PRO:HD2	2.56	0.41
2:FC:102:THR:HG22	2:FC:108:VAL:HA	2.02	0.41
5:AC:260:TRP:HB3	5:AC:281:LEU:HD22	2.03	0.41
5:AA:317:PRO:HD2	5:AA:320:SER:HB3	2.02	0.40
6:BA:175:CYS:HB3	6:BA:348:CYS:SG	2.61	0.40
2:FB:641:VAL:O	2:FB:645:GLU:HB2	2.21	0.40
3:DB:75:PRO:HA	19:fJ:6:MAN:O2	2.20	0.40
6:BB:31:SER:HB3	6:BB:37:GLU:OE1	2.21	0.40
3:DC:99:ASP:HB2	3:DC:107:ILE:HG22	2.02	0.40
4:CC:136:TYR:CZ	4:CC:139:PRO:HG2	2.56	0.40
5:AC:608:LEU:HB3	5:AC:637:LEU:HD21	2.03	0.40
6:BC:210:ARG:NH2	6:BC:235:ASP:OD2	2.46	0.40
25:EA:502:HOH:O	6:BB:35:VAL:HG22	2.21	0.40
5:AB:643:GLU:HB3	6:BB:315:TYR:CE2	2.56	0.40
1:EA:172:LYS:HD3	1:EA:345:TYR:CD2	2.56	0.40
3:DA:18:ALA:HA	3:DA:33:ASP:OD1	2.21	0.40
2:FA:32:LYS:HB2	2:FA:32:LYS:HE2	1.91	0.40
5:AA:616:MET:HE1	5:AA:676:THR:HG22	2.02	0.40
2:FB:38:MET:HE1	3:DB:170:PHE:CD2	2.56	0.40
2:FB:324:ILE:HB	2:FB:346:TRP:CD2	2.56	0.40
6:BB:106:ARG:HG3	25:BB:529:HOH:O	2.22	0.40
5:AC:738:ASP:HB3	6:BC:39:TYR:HB3	2.04	0.40
5:AA:556:ALA:O	5:AA:698:HIS:ND1	2.54	0.40
6:BB:238:LEU:HD23	6:BB:238:LEU:HA	1.95	0.40
5:AC:270:THR:OG1	5:AC:273:GLU:HG3	2.22	0.40
5:AC:312:TYR:CD2	5:AC:318:SER:HB3	2.57	0.40
5:AC:631:LEU:HD12	5:AC:631:LEU:HA	1.95	0.40
6:BC:157:ARG:HD2	25:BC:712:HOH:O	2.22	0.40
6:BC:212:GLN:HB3	6:BC:308:GLY:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	EA	349/368 (95%)	345 (99%)	4 (1%)	0	100	100
1	EB	349/368 (95%)	343 (98%)	6 (2%)	0	100	100
1	EC	349/368 (95%)	343 (98%)	6 (2%)	0	100	100
2	FA	697/723 (96%)	677 (97%)	20 (3%)	0	100	100
2	FB	697/723 (96%)	674 (97%)	23 (3%)	0	100	100
2	FC	697/723 (96%)	681 (98%)	16 (2%)	0	100	100
3	DA	190/209 (91%)	181 (95%)	9 (5%)	0	100	100
3	DB	190/209 (91%)	184 (97%)	6 (3%)	0	100	100
3	DC	190/209 (91%)	184 (97%)	6 (3%)	0	100	100
4	CA	225/349 (64%)	218 (97%)	7 (3%)	0	100	100
4	CB	225/349 (64%)	220 (98%)	5 (2%)	0	100	100
4	CC	225/349 (64%)	219 (97%)	6 (3%)	0	100	100
5	AA	725/748 (97%)	705 (97%)	20 (3%)	0	100	100
5	AB	725/748 (97%)	700 (97%)	25 (3%)	0	100	100
5	AC	725/748 (97%)	708 (98%)	17 (2%)	0	100	100
6	BA	346/366 (94%)	332 (96%)	14 (4%)	0	100	100
6	BB	346/366 (94%)	334 (96%)	12 (4%)	0	100	100
6	BC	346/366 (94%)	336 (97%)	10 (3%)	0	100	100
All	All	7596/8289 (92%)	7384 (97%)	212 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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	EA	294/306 (96%)	291 (99%)	3 (1%)	68	79
1	EB	294/306 (96%)	292 (99%)	2 (1%)	76	86
1	EC	294/306 (96%)	293 (100%)	1 (0%)	86	92
2	FA	582/602 (97%)	580 (100%)	2 (0%)	86	92
2	FB	582/602 (97%)	578 (99%)	4 (1%)	76	86
2	FC	582/602 (97%)	580 (100%)	2 (0%)	86	92
3	DA	152/165 (92%)	152 (100%)	0	100	100
3	DB	152/165 (92%)	152 (100%)	0	100	100
3	DC	152/165 (92%)	151 (99%)	1 (1%)	76	86
4	CA	187/287 (65%)	186 (100%)	1 (0%)	81	89
4	CB	187/287 (65%)	186 (100%)	1 (0%)	81	89
4	CC	187/287 (65%)	187 (100%)	0	100	100
5	AA	628/646 (97%)	623 (99%)	5 (1%)	73	83
5	AB	628/646 (97%)	625 (100%)	3 (0%)	81	89
5	AC	628/646 (97%)	623 (99%)	5 (1%)	73	83
6	BA	306/319 (96%)	305 (100%)	1 (0%)	86	92
6	BB	306/319 (96%)	303 (99%)	3 (1%)	68	79
6	BC	306/319 (96%)	303 (99%)	3 (1%)	68	79
All	All	6447/6975 (92%)	6410 (99%)	37 (1%)	76	87

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	EA	253	GLN
1	EA	266	VAL
1	EA	271	SER
2	FA	562	SER
2	FA	617	ASN
4	CA	112	CYS
5	AA	155	SER
5	AA	357	ASN
5	AA	447	THR
5	AA	696	HIS
5	AA	748	LEU
6	BA	135	SER
1	EB	243	ASP
1	EB	271	SER

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Mol	Chain	Res	Type
2	FB	77	SER
2	FB	81	GLU
2	FB	133	SER
2	FB	234	SER
4	CB	127	LEU
5	AB	357	ASN
5	AB	618	ASN
5	AB	748	LEU
6	BB	135	SER
6	BB	261	SER
6	BB	298	CYS
1	EC	271	SER
2	FC	562	SER
2	FC	617	ASN
3	DC	187	SER
5	AC	357	ASN
5	AC	452	THR
5	AC	633	SER
5	AC	696	HIS
5	AC	748	LEU
6	BC	261	SER
6	BC	298	CYS
6	BC	299	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (68) such sidechains are listed below:

Mol	Chain	Res	Type
1	EA	198	GLN
1	EA	291	GLN
2	FA	171	GLN
2	FA	201	GLN
2	FA	277	ASN
2	FA	315	ASN
2	FA	492	GLN
2	FA	566	HIS
2	FA	650	ASN
3	DA	32	ASN
3	DA	68	GLN
3	DA	110	ASN
3	DA	192	ASN
4	CA	196	GLN
5	AA	132	GLN

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Mol	Chain	Res	Type
5	AA	322	HIS
5	AA	376	ASN
6	BA	344	ASN
1	EB	149	ASN
1	EB	198	GLN
1	EB	291	GLN
2	FB	215	ASN
2	FB	301	ASN
2	FB	315	ASN
2	FB	492	GLN
2	FB	566	HIS
2	FB	650	ASN
3	DB	192	ASN
4	CB	37	ASN
4	CB	114	ASN
4	CB	162	GLN
5	AB	132	GLN
5	AB	376	ASN
5	AB	539	ASN
6	BB	94	GLN
6	BB	149	HIS
6	BB	153	ASN
6	BB	316	ASN
6	BB	317	GLN
6	BB	344	ASN
1	EC	141	GLN
1	EC	291	GLN
1	EC	294	GLN
2	FC	30	HIS
2	FC	201	GLN
2	FC	215	ASN
2	FC	277	ASN
2	FC	315	ASN
2	FC	440	GLN
2	FC	650	ASN
3	DC	32	ASN
3	DC	110	ASN
4	CC	19	GLN
4	CC	97	ASN
4	CC	117	ASN
4	CC	196	GLN
5	AC	28	ASN

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Mol	Chain	Res	Type
5	AC	46	GLN
5	AC	132	GLN
5	AC	157	HIS
5	AC	284	ASN
5	AC	341	GLN
5	AC	376	ASN
5	AC	539	ASN
6	BC	105	GLN
6	BC	153	ASN
6	BC	316	ASN
6	BC	344	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

558 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	$\# Z > 2$
7	NAG	aA	1	5,7	14,14,15	0.34	0	17,19,21	0.81	0
7	MAN	aA	10	23,7	11,11,12	0.66	0	15,15,17	1.04	2 (13%)
7	NAG	aA	11	7	14,14,15	0.28	0	17,19,21	0.66	0
7	XYP	aA	12	7	9,9,10	1.89	3 (33%)	10,12,14	0.91	0
7	MAN	aA	13	7	11,11,12	0.67	1 (9%)	15,15,17	1.06	1 (6%)
7	MAN	aA	14	7	11,11,12	0.69	0	15,15,17	1.27	3 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	NAG	aA	2	7	14,14,15	0.38	0	17,19,21	0.96	1 (5%)
7	BMA	aA	3	7	11,11,12	0.24	0	15,15,17	0.96	1 (6%)
7	MAN	aA	4	7	11,11,12	1.08	1 (9%)	15,15,17	1.29	3 (20%)
7	MAN	aA	5	7	11,11,12	0.64	0	15,15,17	1.33	3 (20%)
7	XYP	aA	6	7	9,9,10	0.19	0	10,12,14	0.90	0
7	XYP	aA	7	7	9,9,10	0.18	0	10,12,14	0.65	0
7	MAN	aA	8	7	11,11,12	0.79	1 (9%)	15,15,17	1.18	2 (13%)
7	NAG	aA	9	7	14,14,15	0.27	0	17,19,21	0.65	0
8	NAG	aB	1	5,8	14,14,15	0.33	0	17,19,21	0.69	1 (5%)
8	XYP	aB	10	8	9,9,10	0.16	0	10,12,14	0.73	1 (10%)
8	MAN	aB	11	8	11,11,12	0.76	1 (9%)	15,15,17	1.04	1 (6%)
8	NAG	aB	12	8	14,14,15	0.35	0	17,19,21	0.81	0
8	BMA	aB	13	8	11,11,12	0.25	0	15,15,17	0.72	1 (6%)
8	XYP	aB	14	8	9,9,10	0.18	0	10,12,14	0.66	0
8	XYP	aB	15	8	9,9,10	0.17	0	10,12,14	0.61	0
8	MAN	aB	16	8	11,11,12	0.68	0	15,15,17	1.08	2 (13%)
8	NAG	aB	2	8	14,14,15	0.33	0	17,19,21	0.74	0
8	BMA	aB	3	8	11,11,12	0.22	0	15,15,17	0.93	1 (6%)
8	MAN	aB	4	8	11,11,12	0.87	1 (9%)	15,15,17	1.13	2 (13%)
8	MAN	aB	5	8	11,11,12	0.59	0	15,15,17	1.48	3 (20%)
8	NAG	aB	6	8	14,14,15	0.39	0	17,19,21	0.48	0
8	MAN	aB	7	8	11,11,12	0.71	0	15,15,17	1.04	2 (13%)
8	XYP	aB	8	8	9,9,10	0.17	0	10,12,14	0.66	0
8	BMA	aB	9	8	11,11,12	0.28	0	15,15,17	1.35	2 (13%)
9	NAG	aC	1	5,9	14,14,15	0.29	0	17,19,21	0.78	0
9	XYP	aC	10	9	9,9,10	0.17	0	10,12,14	0.68	0
9	BGC	aC	11	9	11,11,12	0.22	0	15,15,17	0.59	0
9	MAN	aC	12	23,9	11,11,12	0.88	1 (9%)	15,15,17	1.28	2 (13%)
9	NAG	aC	13	9	14,14,15	0.30	0	17,19,21	0.89	1 (5%)
9	XYP	aC	14	9	9,9,10	1.78	3 (33%)	10,12,14	1.90	3 (30%)
9	MAN	aC	15	9	11,11,12	0.57	0	15,15,17	1.21	3 (20%)
9	MAN	aC	16	9	11,11,12	0.80	1 (9%)	15,15,17	1.11	2 (13%)
9	NAG	aC	2	9	14,14,15	0.28	0	17,19,21	0.78	0
9	BMA	aC	3	9	11,11,12	0.27	0	15,15,17	0.61	0
9	MAN	aC	4	9	11,11,12	0.94	1 (9%)	15,15,17	1.20	1 (6%)
9	MAN	aC	5	9	11,11,12	0.91	0	15,15,17	1.27	2 (13%)
9	NAG	aC	6	9	14,14,15	0.34	0	17,19,21	0.85	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	MAN	aC	7	9	11,11,12	0.70	0	15,15,17	1.34	3 (20%)
9	BMA	aC	8	9	11,11,12	0.24	0	15,15,17	0.80	0
9	XYP	aC	9	9	9,9,10	0.15	0	10,12,14	0.59	0
10	NAG	aD	1	10,5	14,14,15	0.41	0	17,19,21	0.61	0
10	NAG	aD	2	10	14,14,15	0.40	0	17,19,21	0.78	0
10	BMA	aD	3	10	11,11,12	0.21	0	15,15,17	0.91	1 (6%)
10	MAN	aD	4	10	11,11,12	0.91	1 (9%)	15,15,17	1.16	1 (6%)
10	MAN	aD	5	10	11,11,12	0.85	1 (9%)	15,15,17	1.11	2 (13%)
10	MAN	aD	6	10	11,11,12	0.83	0	15,15,17	1.13	2 (13%)
10	MAN	aD	7	10	11,11,12	0.73	0	15,15,17	1.29	3 (20%)
10	MAN	aD	8	10	11,11,12	0.91	1 (9%)	15,15,17	1.17	2 (13%)
10	MAN	aD	9	10	11,11,12	0.69	0	15,15,17	1.31	2 (13%)
11	NAG	aE	1	5,11	14,14,15	0.30	0	17,19,21	0.67	0
11	MAN	aE	10	23,11	11,11,12	0.93	1 (9%)	15,15,17	0.93	1 (6%)
11	NAG	aE	11	11	14,14,15	0.26	0	17,19,21	0.89	0
11	XYP	aE	12	11	9,9,10	0.19	0	10,12,14	0.67	0
11	XYP	aE	13	11	9,9,10	0.18	0	10,12,14	0.62	0
11	BMA	aE	14	11	11,11,12	0.88	1 (9%)	15,15,17	1.15	2 (13%)
11	MAN	aE	15	11	11,11,12	0.76	0	15,15,17	0.99	1 (6%)
11	NAG	aE	2	11	14,14,15	0.33	0	17,19,21	0.76	0
11	BMA	aE	3	11	11,11,12	0.36	0	15,15,17	0.95	0
11	MAN	aE	4	11	11,11,12	0.84	1 (9%)	15,15,17	1.03	1 (6%)
11	MAN	aE	5	11	11,11,12	0.60	0	15,15,17	1.56	3 (20%)
11	XYP	aE	6	11	9,9,10	0.20	0	10,12,14	0.70	0
11	XYP	aE	7	11	9,9,10	0.18	0	10,12,14	0.60	0
11	XYP	aE	8	11	9,9,10	0.20	0	10,12,14	0.64	0
11	NAG	aE	9	11	14,14,15	0.31	0	17,19,21	0.75	0
7	NAG	aF	1	5,7	14,14,15	0.35	0	17,19,21	0.89	1 (5%)
7	MAN	aF	10	23,7	11,11,12	0.71	0	15,15,17	1.01	1 (6%)
7	NAG	aF	11	7	14,14,15	0.26	0	17,19,21	0.83	1 (5%)
7	XYP	aF	12	7	9,9,10	1.86	3 (33%)	10,12,14	0.92	1 (10%)
7	MAN	aF	13	7	11,11,12	0.60	0	15,15,17	1.08	2 (13%)
7	MAN	aF	14	7	11,11,12	0.81	0	15,15,17	1.19	2 (13%)
7	NAG	aF	2	7	14,14,15	0.37	0	17,19,21	0.81	1 (5%)
7	BMA	aF	3	7	11,11,12	0.22	0	15,15,17	0.81	1 (6%)
7	MAN	aF	4	7	11,11,12	1.02	1 (9%)	15,15,17	1.15	1 (6%)
7	MAN	aF	5	7	11,11,12	0.56	0	15,15,17	1.44	3 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	XYP	aF	6	7	9,9,10	0.19	0	10,12,14	1.00	1 (10%)
7	XYP	aF	7	7	9,9,10	0.17	0	10,12,14	0.72	1 (10%)
7	MAN	aF	8	7	11,11,12	0.81	1 (9%)	15,15,17	1.00	2 (13%)
7	NAG	aF	9	7	14,14,15	0.28	0	17,19,21	0.72	0
8	NAG	aG	1	5,8	14,14,15	0.36	0	17,19,21	0.79	0
8	XYP	aG	10	8	9,9,10	0.17	0	10,12,14	0.65	0
8	MAN	aG	11	8	11,11,12	0.72	0	15,15,17	1.25	1 (6%)
8	NAG	aG	12	8	14,14,15	0.33	0	17,19,21	0.75	0
8	BMA	aG	13	8	11,11,12	0.24	0	15,15,17	0.65	0
8	XYP	aG	14	8	9,9,10	0.19	0	10,12,14	0.68	0
8	XYP	aG	15	8	9,9,10	0.19	0	10,12,14	0.58	0
8	MAN	aG	16	8	11,11,12	0.86	1 (9%)	15,15,17	1.03	1 (6%)
8	NAG	aG	2	8	14,14,15	0.31	0	17,19,21	0.92	1 (5%)
8	BMA	aG	3	8	11,11,12	0.24	0	15,15,17	0.91	0
8	MAN	aG	4	8	11,11,12	0.63	0	15,15,17	1.22	2 (13%)
8	MAN	aG	5	8	11,11,12	0.64	0	15,15,17	1.53	3 (20%)
8	NAG	aG	6	8	14,14,15	0.35	0	17,19,21	0.49	0
8	MAN	aG	7	8	11,11,12	0.63	0	15,15,17	1.23	2 (13%)
8	XYP	aG	8	8	9,9,10	0.17	0	10,12,14	0.63	0
8	BMA	aG	9	8	11,11,12	0.27	0	15,15,17	1.30	3 (20%)
9	NAG	aH	1	5,9	14,14,15	0.35	0	17,19,21	0.79	0
9	XYP	aH	10	9	9,9,10	0.13	0	10,12,14	0.73	1 (10%)
9	BGC	aH	11	9	11,11,12	0.28	0	15,15,17	0.56	0
9	MAN	aH	12	9	11,11,12	1.07	1 (9%)	15,15,17	1.27	3 (20%)
9	NAG	aH	13	9	14,14,15	0.31	0	17,19,21	0.67	0
9	XYP	aH	14	9	9,9,10	1.94	4 (44%)	10,12,14	0.86	1 (10%)
9	MAN	aH	15	9	11,11,12	0.54	0	15,15,17	1.26	3 (20%)
9	MAN	aH	16	9	11,11,12	0.84	1 (9%)	15,15,17	0.89	1 (6%)
9	NAG	aH	2	9	14,14,15	0.34	0	17,19,21	1.04	1 (5%)
9	BMA	aH	3	9	11,11,12	0.26	0	15,15,17	0.66	0
9	MAN	aH	4	9	11,11,12	1.43	1 (9%)	15,15,17	1.32	3 (20%)
9	MAN	aH	5	9	11,11,12	1.02	1 (9%)	15,15,17	1.18	2 (13%)
9	NAG	aH	6	9	14,14,15	0.36	0	17,19,21	0.80	1 (5%)
9	MAN	aH	7	9	11,11,12	0.76	0	15,15,17	1.30	3 (20%)
9	BMA	aH	8	9	11,11,12	0.23	0	15,15,17	0.95	0
9	XYP	aH	9	9	9,9,10	0.17	0	10,12,14	0.67	0
10	NAG	aI	1	10,5	14,14,15	0.42	0	17,19,21	0.73	0
10	NAG	aI	2	10	14,14,15	0.40	0	17,19,21	0.75	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	BMA	aI	3	10	11,11,12	0.22	0	15,15,17	0.79	0
10	MAN	aI	4	10	11,11,12	0.83	1 (9%)	15,15,17	1.26	2 (13%)
10	MAN	aI	5	10	11,11,12	0.69	0	15,15,17	1.09	2 (13%)
10	MAN	aI	6	10	11,11,12	0.69	0	15,15,17	1.17	1 (6%)
10	MAN	aI	7	10	11,11,12	0.72	0	15,15,17	1.31	3 (20%)
10	MAN	aI	8	10	11,11,12	0.86	0	15,15,17	1.27	2 (13%)
10	MAN	aI	9	10	11,11,12	0.81	0	15,15,17	1.25	2 (13%)
11	NAG	aJ	1	5,11	14,14,15	0.38	0	17,19,21	0.75	0
11	MAN	aJ	10	11	11,11,12	0.85	1 (9%)	15,15,17	1.09	1 (6%)
11	NAG	aJ	11	11	14,14,15	0.27	0	17,19,21	0.72	0
11	XYP	aJ	12	11	9,9,10	0.17	0	10,12,14	0.61	0
11	XYP	aJ	13	11	9,9,10	0.18	0	10,12,14	0.67	0
11	BMA	aJ	14	11	11,11,12	0.94	1 (9%)	15,15,17	0.99	2 (13%)
11	MAN	aJ	15	11	11,11,12	0.74	0	15,15,17	1.03	1 (6%)
11	NAG	aJ	2	11	14,14,15	0.32	0	17,19,21	0.62	0
11	BMA	aJ	3	11	11,11,12	0.33	0	15,15,17	0.92	1 (6%)
11	MAN	aJ	4	11	11,11,12	0.99	1 (9%)	15,15,17	1.08	2 (13%)
11	MAN	aJ	5	11	11,11,12	0.62	0	15,15,17	1.42	2 (13%)
11	XYP	aJ	6	11	9,9,10	0.18	0	10,12,14	0.62	0
11	XYP	aJ	7	11	9,9,10	0.20	0	10,12,14	0.58	0
11	XYP	aJ	8	11	9,9,10	0.21	0	10,12,14	0.62	0
11	NAG	aJ	9	11	14,14,15	0.34	0	17,19,21	0.75	0
7	NAG	aK	1	5,7	14,14,15	0.34	0	17,19,21	0.72	0
7	MAN	aK	10	23,7	11,11,12	0.60	0	15,15,17	1.28	2 (13%)
7	NAG	aK	11	7	14,14,15	0.28	0	17,19,21	0.84	1 (5%)
7	XYP	aK	12	7	9,9,10	1.93	3 (33%)	10,12,14	1.13	1 (10%)
7	MAN	aK	13	7	11,11,12	0.72	0	15,15,17	1.04	2 (13%)
7	MAN	aK	14	7	11,11,12	0.73	0	15,15,17	1.08	2 (13%)
7	NAG	aK	2	7	14,14,15	0.40	0	17,19,21	0.80	1 (5%)
7	BMA	aK	3	7	11,11,12	0.19	0	15,15,17	0.72	0
7	MAN	aK	4	7	11,11,12	0.99	1 (9%)	15,15,17	1.08	1 (6%)
7	MAN	aK	5	7	11,11,12	0.62	0	15,15,17	1.26	2 (13%)
7	XYP	aK	6	7	9,9,10	0.17	0	10,12,14	0.94	0
7	XYP	aK	7	7	9,9,10	0.17	0	10,12,14	0.79	1 (10%)
7	MAN	aK	8	7	11,11,12	0.67	0	15,15,17	1.17	3 (20%)
7	NAG	aK	9	7	14,14,15	0.35	0	17,19,21	0.72	0
8	NAG	aL	1	5,8	14,14,15	0.37	0	17,19,21	0.73	0
8	XYP	aL	10	8	9,9,10	0.18	0	10,12,14	0.73	1 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	MAN	aL	11	23,8	11,11,12	0.70	0	15,15,17	1.21	2 (13%)
8	NAG	aL	12	8	14,14,15	0.35	0	17,19,21	0.84	0
8	BMA	aL	13	8	11,11,12	0.25	0	15,15,17	0.65	0
8	XYP	aL	14	8	9,9,10	0.17	0	10,12,14	0.68	0
8	XYP	aL	15	8	9,9,10	0.17	0	10,12,14	0.60	0
8	MAN	aL	16	8	11,11,12	0.73	1 (9%)	15,15,17	0.98	1 (6%)
8	NAG	aL	2	8	14,14,15	0.35	0	17,19,21	0.59	0
8	BMA	aL	3	8	11,11,12	0.22	0	15,15,17	0.97	1 (6%)
8	MAN	aL	4	8	11,11,12	0.77	0	15,15,17	1.31	2 (13%)
8	MAN	aL	5	8	11,11,12	0.66	0	15,15,17	1.46	2 (13%)
8	NAG	aL	6	8	14,14,15	0.39	0	17,19,21	0.71	0
8	MAN	aL	7	8	11,11,12	0.63	0	15,15,17	1.36	3 (20%)
8	XYP	aL	8	8	9,9,10	0.17	0	10,12,14	0.61	0
8	BMA	aL	9	8	11,11,12	0.24	0	15,15,17	0.84	0
9	NAG	aM	1	5,9	14,14,15	0.38	0	17,19,21	0.68	0
9	XYP	aM	10	9	9,9,10	0.16	0	10,12,14	0.62	0
9	BGC	aM	11	9	11,11,12	0.28	0	15,15,17	0.56	0
9	MAN	aM	12	23,9	11,11,12	0.68	0	15,15,17	1.19	2 (13%)
9	NAG	aM	13	9	14,14,15	0.26	0	17,19,21	0.67	0
9	XYP	aM	14	9	9,9,10	1.85	3 (33%)	10,12,14	1.02	1 (10%)
9	MAN	aM	15	9	11,11,12	0.63	0	15,15,17	1.22	2 (13%)
9	MAN	aM	16	9	11,11,12	1.02	1 (9%)	15,15,17	0.83	0
9	NAG	aM	2	9	14,14,15	0.26	0	17,19,21	0.77	0
9	BMA	aM	3	9	11,11,12	0.25	0	15,15,17	0.62	0
9	MAN	aM	4	9	11,11,12	0.87	0	15,15,17	1.23	1 (6%)
9	MAN	aM	5	9	11,11,12	1.10	1 (9%)	15,15,17	1.25	3 (20%)
9	NAG	aM	6	9	14,14,15	0.37	0	17,19,21	0.52	0
9	MAN	aM	7	9	11,11,12	0.53	0	15,15,17	1.30	3 (20%)
9	BMA	aM	8	9	11,11,12	0.23	0	15,15,17	0.61	0
9	XYP	aM	9	9	9,9,10	0.17	0	10,12,14	0.51	0
10	NAG	aN	1	10,5	14,14,15	0.41	0	17,19,21	0.64	0
10	NAG	aN	2	10	14,14,15	0.38	0	17,19,21	0.91	0
10	BMA	aN	3	10	11,11,12	0.23	0	15,15,17	0.72	0
10	MAN	aN	4	10	11,11,12	0.88	0	15,15,17	1.06	2 (13%)
10	MAN	aN	5	10	11,11,12	0.89	1 (9%)	15,15,17	1.10	2 (13%)
10	MAN	aN	6	10	11,11,12	0.91	0	15,15,17	1.22	2 (13%)
10	MAN	aN	7	10	11,11,12	0.61	0	15,15,17	1.34	2 (13%)
10	MAN	aN	8	10	11,11,12	0.88	1 (9%)	15,15,17	1.11	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	MAN	aN	9	10	11,11,12	0.82	0	15,15,17	1.21	2 (13%)
11	NAG	aO	1	5,11	14,14,15	0.33	0	17,19,21	0.80	0
11	MAN	aO	10	11	11,11,12	0.75	0	15,15,17	0.87	0
11	NAG	aO	11	11	14,14,15	0.31	0	17,19,21	1.07	1 (5%)
11	XYP	aO	12	11	9,9,10	0.20	0	10,12,14	0.62	0
11	XYP	aO	13	11	9,9,10	0.19	0	10,12,14	0.62	0
11	BMA	aO	14	11	11,11,12	0.74	0	15,15,17	1.05	1 (6%)
11	MAN	aO	15	11	11,11,12	0.90	1 (9%)	15,15,17	1.08	2 (13%)
11	NAG	aO	2	11	14,14,15	0.37	0	17,19,21	0.62	0
11	BMA	aO	3	11	11,11,12	0.29	0	15,15,17	0.98	0
11	MAN	aO	4	11	11,11,12	0.92	1 (9%)	15,15,17	1.05	1 (6%)
11	MAN	aO	5	11	11,11,12	0.57	0	15,15,17	1.37	2 (13%)
11	XYP	aO	6	11	9,9,10	0.18	0	10,12,14	0.63	0
11	XYP	aO	7	11	9,9,10	0.19	0	10,12,14	0.61	0
11	XYP	aO	8	11	9,9,10	0.19	0	10,12,14	0.67	0
11	NAG	aO	9	11	14,14,15	0.33	0	17,19,21	0.64	0
12	NAG	bA	1	6,12	14,14,15	0.44	0	17,19,21	0.73	0
12	NAG	bA	2	12	14,14,15	0.30	0	17,19,21	0.92	0
12	BMA	bA	3	12	11,11,12	0.25	0	15,15,17	0.79	1 (6%)
12	MAN	bA	4	12	11,11,12	0.89	1 (9%)	15,15,17	1.11	1 (6%)
12	MAN	bA	5	12	11,11,12	0.82	0	15,15,17	1.30	3 (20%)
12	MAN	bA	6	12	11,11,12	0.71	0	15,15,17	1.12	1 (6%)
12	MAN	bA	7	12	11,11,12	0.73	1 (9%)	15,15,17	1.11	2 (13%)
12	MAN	bA	8	12	11,11,12	0.70	0	15,15,17	1.14	2 (13%)
12	MAN	bA	9	12	11,11,12	0.73	0	15,15,17	0.98	0
13	NAG	bB	1	13,6	14,14,15	0.33	0	17,19,21	0.50	0
13	NAG	bB	2	13	14,14,15	0.28	0	17,19,21	0.89	1 (5%)
13	BMA	bB	3	13	11,11,12	0.18	0	15,15,17	0.57	0
13	MAN	bB	4	13	11,11,12	0.78	0	15,15,17	1.24	2 (13%)
13	MAN	bB	5	13	11,11,12	0.69	0	15,15,17	1.26	3 (20%)
14	NAG	bC	1	6,14	14,14,15	0.39	0	17,19,21	0.61	0
14	MAN	bC	10	14	11,11,12	0.79	1 (9%)	15,15,17	0.91	1 (6%)
14	NAG	bC	2	14	14,14,15	0.35	0	17,19,21	0.69	0
14	BMA	bC	3	14	11,11,12	0.23	0	15,15,17	1.13	2 (13%)
14	MAN	bC	4	14	11,11,12	0.92	1 (9%)	15,15,17	1.27	2 (13%)
14	MAN	bC	5	14	11,11,12	0.75	0	15,15,17	1.35	2 (13%)
14	XYP	bC	6	14	9,9,10	0.18	0	10,12,14	0.59	0
14	XYS	bC	7	14	9,9,10	1.93	3 (33%)	10,12,14	0.91	1 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	MAN	bC	8	14,23	11,11,12	0.95	1 (9%)	15,15,17	0.92	1 (6%)
14	BMA	bC	9	14	11,11,12	0.84	1 (9%)	15,15,17	1.07	2 (13%)
12	NAG	bD	1	6,12	14,14,15	0.48	0	17,19,21	0.65	0
12	NAG	bD	2	12	14,14,15	0.35	0	17,19,21	0.84	0
12	BMA	bD	3	12	11,11,12	0.28	0	15,15,17	0.79	1 (6%)
12	MAN	bD	4	12	11,11,12	0.96	1 (9%)	15,15,17	1.17	1 (6%)
12	MAN	bD	5	12	11,11,12	1.03	1 (9%)	15,15,17	1.23	2 (13%)
12	MAN	bD	6	12	11,11,12	0.95	1 (9%)	15,15,17	1.19	2 (13%)
12	MAN	bD	7	12	11,11,12	0.79	1 (9%)	15,15,17	1.05	2 (13%)
12	MAN	bD	8	12	11,11,12	0.74	0	15,15,17	1.14	2 (13%)
12	MAN	bD	9	12	11,11,12	0.75	0	15,15,17	1.12	1 (6%)
13	NAG	bE	1	13,6	14,14,15	0.32	0	17,19,21	0.54	0
13	NAG	bE	2	13	14,14,15	0.31	0	17,19,21	0.68	0
13	BMA	bE	3	13	11,11,12	0.20	0	15,15,17	0.61	0
13	MAN	bE	4	13	11,11,12	0.72	0	15,15,17	1.18	2 (13%)
13	MAN	bE	5	13	11,11,12	0.63	0	15,15,17	1.18	2 (13%)
14	NAG	bF	1	6,14	14,14,15	0.43	0	17,19,21	0.63	0
14	MAN	bF	10	14	11,11,12	0.90	1 (9%)	15,15,17	0.95	1 (6%)
14	NAG	bF	2	14	14,14,15	0.38	0	17,19,21	0.91	1 (5%)
14	BMA	bF	3	14	11,11,12	0.35	0	15,15,17	0.80	0
14	MAN	bF	4	14	11,11,12	0.83	1 (9%)	15,15,17	1.05	2 (13%)
14	MAN	bF	5	14	11,11,12	0.89	0	15,15,17	1.46	2 (13%)
14	XYP	bF	6	14	9,9,10	0.19	0	10,12,14	0.61	0
14	XYS	bF	7	14	9,9,10	1.93	3 (33%)	10,12,14	1.03	1 (10%)
14	MAN	bF	8	14,23	11,11,12	0.79	1 (9%)	15,15,17	1.04	2 (13%)
14	BMA	bF	9	14	11,11,12	1.09	1 (9%)	15,15,17	1.03	2 (13%)
12	NAG	bG	1	6,12	14,14,15	0.45	0	17,19,21	0.75	0
12	NAG	bG	2	12	14,14,15	0.35	0	17,19,21	0.81	0
12	BMA	bG	3	12	11,11,12	0.37	0	15,15,17	0.69	0
12	MAN	bG	4	12	11,11,12	0.81	0	15,15,17	1.30	2 (13%)
12	MAN	bG	5	12	11,11,12	0.87	0	15,15,17	1.27	2 (13%)
12	MAN	bG	6	12	11,11,12	0.79	0	15,15,17	1.14	2 (13%)
12	MAN	bG	7	12	11,11,12	0.82	1 (9%)	15,15,17	1.13	2 (13%)
12	MAN	bG	8	12	11,11,12	0.70	0	15,15,17	1.16	2 (13%)
12	MAN	bG	9	12	11,11,12	0.82	1 (9%)	15,15,17	0.93	1 (6%)
13	NAG	bH	1	13,6	14,14,15	0.35	0	17,19,21	0.60	1 (5%)
13	NAG	bH	2	13	14,14,15	0.29	0	17,19,21	0.79	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	BMA	bH	3	13	11,11,12	0.28	0	15,15,17	0.49	0
13	MAN	bH	4	13	11,11,12	0.85	1 (9%)	15,15,17	1.11	2 (13%)
13	MAN	bH	5	13	11,11,12	0.62	0	15,15,17	1.48	3 (20%)
14	NAG	bI	1	6,14	14,14,15	0.42	0	17,19,21	0.67	0
14	MAN	bI	10	14	11,11,12	0.69	0	15,15,17	1.07	2 (13%)
14	NAG	bI	2	14	14,14,15	0.33	0	17,19,21	0.98	1 (5%)
14	BMA	bI	3	14	11,11,12	0.42	0	15,15,17	1.30	1 (6%)
14	MAN	bI	4	14	11,11,12	0.58	0	15,15,17	1.32	2 (13%)
14	MAN	bI	5	14	11,11,12	0.53	0	15,15,17	1.51	3 (20%)
14	XYP	bI	6	14	9,9,10	0.18	0	10,12,14	0.58	0
14	XYS	bI	7	14	9,9,10	1.92	3 (33%)	10,12,14	1.37	1 (10%)
14	MAN	bI	8	14,23	11,11,12	0.82	1 (9%)	15,15,17	0.92	1 (6%)
14	BMA	bI	9	14	11,11,12	1.01	1 (9%)	15,15,17	0.99	1 (6%)
15	XYP	cA	1	15	9,9,10	0.16	0	10,12,14	0.63	0
15	MAN	cA	2	15	11,11,12	0.80	0	15,15,17	1.49	2 (13%)
15	MAN	cA	3	15	11,11,12	0.96	1 (9%)	15,15,17	1.09	2 (13%)
15	MAN	cA	4	15	11,11,12	0.64	0	15,15,17	1.39	3 (20%)
15	XYP	cB	1	15	9,9,10	0.21	0	10,12,14	0.71	0
15	MAN	cB	2	15	11,11,12	0.99	1 (9%)	15,15,17	1.09	1 (6%)
15	MAN	cB	3	15	11,11,12	0.95	1 (9%)	15,15,17	1.16	2 (13%)
15	MAN	cB	4	15	11,11,12	0.74	0	15,15,17	1.35	2 (13%)
15	XYP	cC	1	15	9,9,10	0.18	0	10,12,14	0.63	0
15	MAN	cC	2	15	11,11,12	0.78	0	15,15,17	1.43	2 (13%)
15	MAN	cC	3	15	11,11,12	0.85	0	15,15,17	1.24	2 (13%)
15	MAN	cC	4	15	11,11,12	0.78	0	15,15,17	1.44	3 (20%)
16	XYP	dA	1	16	9,9,10	0.16	0	10,12,14	0.74	0
16	MAN	dA	2	16	11,11,12	0.73	0	15,15,17	1.27	3 (20%)
16	MAN	dA	3	16	11,11,12	1.21	1 (9%)	15,15,17	1.25	2 (13%)
16	MAN	dA	4	16	11,11,12	1.08	1 (9%)	15,15,17	1.27	2 (13%)
16	MAN	dA	5	16	11,11,12	0.85	1 (9%)	15,15,17	1.22	2 (13%)
16	MAN	dA	6	16	11,11,12	0.94	1 (9%)	15,15,17	1.05	2 (13%)
16	MAN	dA	7	16	11,11,12	0.66	0	15,15,17	1.27	3 (20%)
16	XYP	dB	1	16	9,9,10	0.20	0	10,12,14	0.67	0
16	MAN	dB	2	16	11,11,12	0.96	1 (9%)	15,15,17	1.18	2 (13%)
16	MAN	dB	3	16	11,11,12	1.06	1 (9%)	15,15,17	1.31	2 (13%)
16	MAN	dB	4	16	11,11,12	0.87	1 (9%)	15,15,17	1.31	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
16	MAN	dB	5	16	11,11,12	0.63	0	15,15,17	1.22	2 (13%)
16	MAN	dB	6	16	11,11,12	0.99	1 (9%)	15,15,17	1.01	1 (6%)
16	MAN	dB	7	16	11,11,12	0.72	0	15,15,17	1.23	2 (13%)
16	XYP	dC	1	16	9,9,10	0.15	0	10,12,14	0.65	0
16	MAN	dC	2	16	11,11,12	0.92	1 (9%)	15,15,17	1.11	2 (13%)
16	MAN	dC	3	16	11,11,12	1.02	1 (9%)	15,15,17	1.24	2 (13%)
16	MAN	dC	4	16	11,11,12	0.95	1 (9%)	15,15,17	1.35	3 (20%)
16	MAN	dC	5	16	11,11,12	0.75	0	15,15,17	1.30	2 (13%)
16	MAN	dC	6	16	11,11,12	0.93	1 (9%)	15,15,17	1.12	2 (13%)
16	MAN	dC	7	16	11,11,12	0.86	1 (9%)	15,15,17	1.07	1 (6%)
17	NAG	eA	1	17,1	14,14,15	0.40	0	17,19,21	0.81	1 (5%)
17	MAN	eA	10	17	11,11,12	0.77	1 (9%)	15,15,17	1.13	2 (13%)
17	MAN	eA	11	17	11,11,12	0.77	0	15,15,17	1.20	2 (13%)
17	NAG	eA	2	17	14,14,15	0.38	0	17,19,21	0.72	0
17	BMA	eA	3	17	11,11,12	0.25	0	15,15,17	0.72	0
17	MAN	eA	4	17	11,11,12	0.57	0	15,15,17	1.23	2 (13%)
17	MAN	eA	5	17	11,11,12	0.82	1 (9%)	15,15,17	1.02	1 (6%)
17	MAN	eA	6	17	11,11,12	0.67	0	15,15,17	1.00	2 (13%)
17	MAN	eA	7	17	11,11,12	0.76	0	15,15,17	1.30	3 (20%)
17	MAN	eA	8	17	11,11,12	1.00	1 (9%)	15,15,17	1.03	2 (13%)
17	MAN	eA	9	17	11,11,12	0.83	0	15,15,17	1.20	2 (13%)
18	NAG	eB	1	18,1	14,14,15	0.36	0	17,19,21	0.80	1 (5%)
18	MAN	eB	10	18	11,11,12	0.69	0	15,15,17	1.10	2 (13%)
18	NAG	eB	11	18	14,14,15	0.33	0	17,19,21	1.12	2 (11%)
18	XYP	eB	12	18	9,9,10	0.18	0	10,12,14	0.66	0
18	XYP	eB	13	18	9,9,10	0.16	0	10,12,14	0.63	0
18	MAN	eB	14	18	11,11,12	0.82	1 (9%)	15,15,17	1.14	2 (13%)
18	NAG	eB	2	18	14,14,15	0.31	0	17,19,21	0.76	0
18	BMA	eB	3	18	11,11,12	0.24	0	15,15,17	0.69	0
18	MAN	eB	4	18	11,11,12	0.98	0	15,15,17	1.25	1 (6%)
18	MAN	eB	5	18	11,11,12	1.00	1 (9%)	15,15,17	1.19	2 (13%)
18	XYP	eB	6	18	9,9,10	0.16	0	10,12,14	0.65	0
18	XYS	eB	7	18	9,9,10	1.85	3 (33%)	10,12,14	0.93	1 (10%)
18	BGC	eB	8	18	11,11,12	0.42	0	15,15,17	0.67	0
18	NAG	eB	9	18	14,14,15	0.32	0	17,19,21	0.61	0
17	NAG	eC	1	17,1	14,14,15	0.41	0	17,19,21	0.62	0
17	MAN	eC	10	17	11,11,12	0.70	0	15,15,17	1.19	3 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	MAN	eC	11	17	11,11,12	0.69	0	15,15,17	1.08	1 (6%)
17	NAG	eC	2	17	14,14,15	0.38	0	17,19,21	0.71	0
17	BMA	eC	3	17	11,11,12	0.25	0	15,15,17	0.92	1 (6%)
17	MAN	eC	4	17	11,11,12	0.69	0	15,15,17	1.13	2 (13%)
17	MAN	eC	5	17	11,11,12	0.97	1 (9%)	15,15,17	1.02	2 (13%)
17	MAN	eC	6	17	11,11,12	0.63	0	15,15,17	1.37	3 (20%)
17	MAN	eC	7	17	11,11,12	0.69	0	15,15,17	1.33	3 (20%)
17	MAN	eC	8	17	11,11,12	1.02	1 (9%)	15,15,17	1.07	2 (13%)
17	MAN	eC	9	17	11,11,12	0.71	0	15,15,17	1.19	2 (13%)
18	NAG	eD	1	18,1	14,14,15	0.37	0	17,19,21	0.59	0
18	MAN	eD	10	18,23	11,11,12	0.70	0	15,15,17	1.15	2 (13%)
18	NAG	eD	11	18	14,14,15	0.36	0	17,19,21	0.93	1 (5%)
18	XYP	eD	12	18	9,9,10	0.15	0	10,12,14	0.64	0
18	XYP	eD	13	18	9,9,10	0.17	0	10,12,14	0.61	0
18	MAN	eD	14	18	11,11,12	0.87	1 (9%)	15,15,17	1.08	2 (13%)
18	NAG	eD	2	18	14,14,15	0.39	0	17,19,21	0.68	0
18	BMA	eD	3	18	11,11,12	0.21	0	15,15,17	0.77	0
18	MAN	eD	4	18	11,11,12	0.89	0	15,15,17	1.52	3 (20%)
18	MAN	eD	5	18	11,11,12	0.99	1 (9%)	15,15,17	1.32	3 (20%)
18	XYP	eD	6	18	9,9,10	0.17	0	10,12,14	0.61	0
18	XYS	eD	7	18	9,9,10	1.84	3 (33%)	10,12,14	0.99	0
18	BGC	eD	8	18	11,11,12	0.23	0	15,15,17	0.73	1 (6%)
18	NAG	eD	9	18	14,14,15	0.33	0	17,19,21	0.56	0
17	NAG	eE	1	17,1	14,14,15	0.40	0	17,19,21	0.65	0
17	MAN	eE	10	17	11,11,12	0.80	0	15,15,17	1.05	1 (6%)
17	MAN	eE	11	17	11,11,12	0.80	1 (9%)	15,15,17	1.06	2 (13%)
17	NAG	eE	2	17	14,14,15	0.35	0	17,19,21	0.74	0
17	BMA	eE	3	17	11,11,12	0.29	0	15,15,17	0.89	1 (6%)
17	MAN	eE	4	17	11,11,12	0.68	0	15,15,17	1.14	2 (13%)
17	MAN	eE	5	17	11,11,12	0.95	1 (9%)	15,15,17	1.10	2 (13%)
17	MAN	eE	6	17	11,11,12	0.74	0	15,15,17	1.09	2 (13%)
17	MAN	eE	7	17	11,11,12	0.71	0	15,15,17	1.27	2 (13%)
17	MAN	eE	8	17	11,11,12	0.99	1 (9%)	15,15,17	0.99	1 (6%)
17	MAN	eE	9	17	11,11,12	0.73	0	15,15,17	1.15	2 (13%)
18	NAG	eF	1	18,1	14,14,15	0.38	0	17,19,21	0.62	0
18	MAN	eF	10	18	11,11,12	0.66	0	15,15,17	1.14	2 (13%)
18	NAG	eF	11	18	14,14,15	0.36	0	17,19,21	0.92	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	XYP	eF	12	18	9,9,10	0.19	0	10,12,14	0.64	0
18	XYP	eF	13	18	9,9,10	0.16	0	10,12,14	0.63	0
18	MAN	eF	14	18	11,11,12	0.81	1 (9%)	15,15,17	1.03	2 (13%)
18	NAG	eF	2	18	14,14,15	0.31	0	17,19,21	0.56	0
18	BMA	eF	3	18	11,11,12	0.20	0	15,15,17	0.68	0
18	MAN	eF	4	18	11,11,12	0.91	0	15,15,17	1.54	3 (20%)
18	MAN	eF	5	18	11,11,12	1.02	1 (9%)	15,15,17	1.23	2 (13%)
18	XYP	eF	6	18	9,9,10	0.16	0	10,12,14	0.60	0
18	XYS	eF	7	18	9,9,10	1.93	3 (33%)	10,12,14	0.77	0
18	BGC	eF	8	18	11,11,12	0.29	0	15,15,17	0.72	0
18	NAG	eF	9	18	14,14,15	0.30	0	17,19,21	0.58	0
19	NAG	fB	1	19,2	14,14,15	0.40	0	17,19,21	0.75	1 (5%)
19	MAN	fB	10	19	11,11,12	0.76	1 (9%)	15,15,17	0.98	2 (13%)
19	NAG	fB	2	19	14,14,15	0.31	0	17,19,21	1.24	1 (5%)
19	BMA	fB	3	19	11,11,12	0.25	0	15,15,17	0.73	0
19	MAN	fB	4	19	11,11,12	0.97	1 (9%)	15,15,17	1.08	2 (13%)
19	MAN	fB	5	19	11,11,12	0.79	0	15,15,17	1.07	1 (6%)
19	MAN	fB	6	19	11,11,12	0.78	0	15,15,17	1.20	2 (13%)
19	MAN	fB	7	19	11,11,12	0.81	1 (9%)	15,15,17	1.33	2 (13%)
19	MAN	fB	8	19	11,11,12	0.83	1 (9%)	15,15,17	1.25	3 (20%)
19	MAN	fB	9	19	11,11,12	0.81	1 (9%)	15,15,17	1.07	2 (13%)
17	NAG	fC	1	17,2	14,14,15	0.41	0	17,19,21	0.75	0
17	MAN	fC	10	17	11,11,12	0.91	1 (9%)	15,15,17	1.07	2 (13%)
17	MAN	fC	11	17	11,11,12	0.68	0	15,15,17	1.05	2 (13%)
17	NAG	fC	2	17	14,14,15	0.40	0	17,19,21	0.81	0
17	BMA	fC	3	17	11,11,12	0.26	0	15,15,17	0.96	0
17	MAN	fC	4	17	11,11,12	0.72	0	15,15,17	1.46	2 (13%)
17	MAN	fC	5	17	11,11,12	0.84	1 (9%)	15,15,17	1.10	1 (6%)
17	MAN	fC	6	17	11,11,12	0.67	0	15,15,17	1.02	2 (13%)
17	MAN	fC	7	17	11,11,12	0.82	1 (9%)	15,15,17	1.08	1 (6%)
17	MAN	fC	8	17	11,11,12	0.79	1 (9%)	15,15,17	1.12	2 (13%)
17	MAN	fC	9	17	11,11,12	0.61	0	15,15,17	1.26	3 (20%)
17	NAG	fD	1	17,2	14,14,15	0.31	0	17,19,21	0.81	0
17	MAN	fD	10	17	11,11,12	0.73	0	15,15,17	1.21	2 (13%)
17	MAN	fD	11	17	11,11,12	0.96	1 (9%)	15,15,17	1.25	1 (6%)
17	NAG	fD	2	17	14,14,15	0.37	0	17,19,21	0.57	0
17	BMA	fD	3	17	11,11,12	0.27	0	15,15,17	0.75	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	MAN	fD	4	17	11,11,12	0.77	0	15,15,17	1.32	3 (20%)
17	MAN	fD	5	17	11,11,12	0.76	0	15,15,17	0.96	1 (6%)
17	MAN	fD	6	17	11,11,12	0.74	0	15,15,17	1.25	1 (6%)
17	MAN	fD	7	17	11,11,12	1.08	2 (18%)	15,15,17	1.11	1 (6%)
17	MAN	fD	8	17	11,11,12	0.76	0	15,15,17	1.20	2 (13%)
17	MAN	fD	9	17	11,11,12	0.73	0	15,15,17	1.16	3 (20%)
19	NAG	fE	1	19,2	14,14,15	0.36	0	17,19,21	0.57	0
19	MAN	fE	10	19	11,11,12	0.79	1 (9%)	15,15,17	0.97	1 (6%)
19	NAG	fE	2	19	14,14,15	0.32	0	17,19,21	0.58	0
19	BMA	fE	3	19	11,11,12	0.28	0	15,15,17	0.82	0
19	MAN	fE	4	19	11,11,12	0.86	0	15,15,17	1.31	3 (20%)
19	MAN	fE	5	19	11,11,12	0.89	1 (9%)	15,15,17	1.22	2 (13%)
19	MAN	fE	6	19	11,11,12	0.92	1 (9%)	15,15,17	1.02	2 (13%)
19	MAN	fE	7	19	11,11,12	0.77	0	15,15,17	1.25	2 (13%)
19	MAN	fE	8	19	11,11,12	0.81	1 (9%)	15,15,17	1.26	2 (13%)
19	MAN	fE	9	19	11,11,12	0.80	0	15,15,17	1.01	1 (6%)
20	NAG	fF	1	20,2	14,14,15	0.31	0	17,19,21	0.68	0
20	NAG	fF	10	20	14,14,15	0.32	0	17,19,21	0.75	0
20	XYS	fF	11	20	9,9,10	2.09	4 (44%)	10,12,14	1.04	1 (10%)
20	XYP	fF	12	20	9,9,10	0.17	0	10,12,14	0.65	0
20	MAN	fF	13	20	11,11,12	0.85	1 (9%)	15,15,17	1.03	2 (13%)
20	MAN	fF	14	20	11,11,12	0.73	0	15,15,17	0.92	0
20	NAG	fF	2	20	14,14,15	0.36	0	17,19,21	0.89	0
20	BMA	fF	3	20	11,11,12	0.16	0	15,15,17	0.88	0
20	MAN	fF	4	20	11,11,12	0.77	0	15,15,17	1.18	2 (13%)
20	MAN	fF	5	20	11,11,12	0.69	0	15,15,17	1.22	2 (13%)
20	XYP	fF	6	20	9,9,10	0.17	0	10,12,14	0.64	0
20	XYS	fF	7	20	9,9,10	1.89	3 (33%)	10,12,14	1.47	1 (10%)
20	NAG	fF	8	20	14,14,15	0.38	0	17,19,21	0.48	0
20	MAN	fF	9	20	11,11,12	0.80	1 (9%)	15,15,17	1.02	1 (6%)
19	NAG	fG	1	19,2	14,14,15	0.41	0	17,19,21	0.73	1 (5%)
19	MAN	fG	10	19	11,11,12	0.77	1 (9%)	15,15,17	1.04	1 (6%)
19	NAG	fG	2	19	14,14,15	0.33	0	17,19,21	0.93	0
19	BMA	fG	3	19	11,11,12	0.29	0	15,15,17	0.72	0
19	MAN	fG	4	19	11,11,12	0.91	1 (9%)	15,15,17	1.16	1 (6%)
19	MAN	fG	5	19	11,11,12	0.87	1 (9%)	15,15,17	1.29	1 (6%)
19	MAN	fG	6	19	11,11,12	0.82	0	15,15,17	1.23	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	MAN	fG	7	19	11,11,12	0.89	1 (9%)	15,15,17	1.32	3 (20%)
19	MAN	fG	8	19	11,11,12	0.93	1 (9%)	15,15,17	1.14	2 (13%)
19	MAN	fG	9	19	11,11,12	0.82	1 (9%)	15,15,17	1.03	1 (6%)
17	NAG	fH	1	17,2	14,14,15	0.50	0	17,19,21	0.93	0
17	MAN	fH	10	17	11,11,12	0.90	1 (9%)	15,15,17	1.10	1 (6%)
17	MAN	fH	11	17	11,11,12	0.67	0	15,15,17	1.09	2 (13%)
17	NAG	fH	2	17	14,14,15	0.39	0	17,19,21	0.53	0
17	BMA	fH	3	17	11,11,12	0.28	0	15,15,17	0.75	0
17	MAN	fH	4	17	11,11,12	0.73	0	15,15,17	1.24	2 (13%)
17	MAN	fH	5	17	11,11,12	1.12	1 (9%)	15,15,17	1.01	1 (6%)
17	MAN	fH	6	17	11,11,12	0.64	0	15,15,17	1.19	2 (13%)
17	MAN	fH	7	17	11,11,12	1.03	1 (9%)	15,15,17	1.11	1 (6%)
17	MAN	fH	8	17	11,11,12	0.74	0	15,15,17	1.10	2 (13%)
17	MAN	fH	9	17	11,11,12	0.56	0	15,15,17	1.21	2 (13%)
17	NAG	fI	1	17,2	14,14,15	0.35	0	17,19,21	0.79	0
17	MAN	fI	10	17	11,11,12	0.75	0	15,15,17	1.15	2 (13%)
17	MAN	fI	11	17	11,11,12	1.04	1 (9%)	15,15,17	1.04	2 (13%)
17	NAG	fI	2	17	14,14,15	0.40	0	17,19,21	0.48	0
17	BMA	fI	3	17	11,11,12	0.28	0	15,15,17	0.79	0
17	MAN	fI	4	17	11,11,12	0.72	0	15,15,17	1.24	3 (20%)
17	MAN	fI	5	17	11,11,12	0.95	1 (9%)	15,15,17	1.04	1 (6%)
17	MAN	fI	6	17	11,11,12	0.64	0	15,15,17	1.27	2 (13%)
17	MAN	fI	7	17	11,11,12	0.90	0	15,15,17	1.44	2 (13%)
17	MAN	fI	8	17	11,11,12	0.86	1 (9%)	15,15,17	1.11	2 (13%)
17	MAN	fI	9	17	11,11,12	0.84	1 (9%)	15,15,17	1.04	2 (13%)
19	NAG	fJ	1	19,2	14,14,15	0.36	0	17,19,21	0.67	1 (5%)
19	MAN	fJ	10	19	11,11,12	0.92	1 (9%)	15,15,17	0.99	1 (6%)
19	NAG	fJ	2	19	14,14,15	0.34	0	17,19,21	0.51	0
19	BMA	fJ	3	19	11,11,12	0.24	0	15,15,17	0.80	0
19	MAN	fJ	4	19	11,11,12	0.85	0	15,15,17	1.31	2 (13%)
19	MAN	fJ	5	19	11,11,12	0.93	1 (9%)	15,15,17	1.12	2 (13%)
19	MAN	fJ	6	19	11,11,12	0.85	1 (9%)	15,15,17	1.14	2 (13%)
19	MAN	fJ	7	19	11,11,12	0.95	1 (9%)	15,15,17	1.28	1 (6%)
19	MAN	fJ	8	19	11,11,12	0.90	1 (9%)	15,15,17	1.12	1 (6%)
19	MAN	fJ	9	19	11,11,12	0.87	1 (9%)	15,15,17	1.09	1 (6%)
20	NAG	fK	1	20,2	14,14,15	0.34	0	17,19,21	0.78	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	NAG	fK	10	20	14,14,15	0.32	0	17,19,21	0.89	1 (5%)
20	XYS	fK	11	20	9,9,10	1.99	4 (44%)	10,12,14	1.59	1 (10%)
20	XYP	fK	12	20	9,9,10	0.17	0	10,12,14	0.66	0
20	MAN	fK	13	20	11,11,12	0.58	0	15,15,17	1.15	2 (13%)
20	MAN	fK	14	20	11,11,12	0.66	0	15,15,17	0.98	2 (13%)
20	NAG	fK	2	20	14,14,15	0.36	0	17,19,21	0.97	1 (5%)
20	BMA	fK	3	20	11,11,12	0.22	0	15,15,17	0.75	0
20	MAN	fK	4	20	11,11,12	0.89	1 (9%)	15,15,17	1.12	2 (13%)
20	MAN	fK	5	20	11,11,12	0.55	0	15,15,17	1.16	1 (6%)
20	XYP	fK	6	20	9,9,10	0.17	0	10,12,14	0.64	0
20	XYS	fK	7	20	9,9,10	1.94	3 (33%)	10,12,14	1.20	1 (10%)
20	NAG	fK	8	20	14,14,15	0.41	0	17,19,21	0.59	0
20	MAN	fK	9	20,23	11,11,12	0.70	0	15,15,17	1.11	1 (6%)
19	NAG	fL	1	19,2	14,14,15	0.41	0	17,19,21	0.57	0
19	MAN	fL	10	19	11,11,12	0.75	0	15,15,17	1.00	2 (13%)
19	NAG	fL	2	19	14,14,15	0.34	0	17,19,21	1.16	1 (5%)
19	BMA	fL	3	19	11,11,12	0.21	0	15,15,17	0.62	0
19	MAN	fL	4	19	11,11,12	0.85	1 (9%)	15,15,17	1.33	2 (13%)
19	MAN	fL	5	19	11,11,12	0.94	1 (9%)	15,15,17	1.19	1 (6%)
19	MAN	fL	6	19	11,11,12	0.80	0	15,15,17	1.34	2 (13%)
19	MAN	fL	7	19	11,11,12	0.95	1 (9%)	15,15,17	1.44	3 (20%)
19	MAN	fL	8	19	11,11,12	1.14	1 (9%)	15,15,17	1.19	2 (13%)
19	MAN	fL	9	19	11,11,12	0.83	1 (9%)	15,15,17	1.03	1 (6%)
17	NAG	fM	1	17,2	14,14,15	0.55	0	17,19,21	0.83	0
17	MAN	fM	10	17	11,11,12	0.68	0	15,15,17	1.45	3 (20%)
17	MAN	fM	11	17	11,11,12	0.73	0	15,15,17	1.17	2 (13%)
17	NAG	fM	2	17	14,14,15	0.37	0	17,19,21	1.03	1 (5%)
17	BMA	fM	3	17	11,11,12	0.29	0	15,15,17	0.85	0
17	MAN	fM	4	17	11,11,12	0.73	0	15,15,17	1.48	3 (20%)
17	MAN	fM	5	17	11,11,12	0.85	1 (9%)	15,15,17	1.16	1 (6%)
17	MAN	fM	6	17	11,11,12	0.58	0	15,15,17	1.26	2 (13%)
17	MAN	fM	7	17	11,11,12	1.00	1 (9%)	15,15,17	1.11	2 (13%)
17	MAN	fM	8	17	11,11,12	0.86	1 (9%)	15,15,17	1.13	1 (6%)
17	MAN	fM	9	17	11,11,12	0.73	0	15,15,17	1.12	2 (13%)
17	NAG	fN	1	17,2	14,14,15	0.31	0	17,19,21	0.86	0
17	MAN	fN	10	17	11,11,12	0.76	0	15,15,17	1.20	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	MAN	fN	11	17	11,11,12	0.95	1 (9%)	15,15,17	1.23	2 (13%)
17	NAG	fN	2	17	14,14,15	0.36	0	17,19,21	0.67	0
17	BMA	fN	3	17	11,11,12	0.27	0	15,15,17	0.85	1 (6%)
17	MAN	fN	4	17	11,11,12	0.84	1 (9%)	15,15,17	1.21	2 (13%)
17	MAN	fN	5	17	11,11,12	0.78	0	15,15,17	1.05	2 (13%)
17	MAN	fN	6	17	11,11,12	0.68	0	15,15,17	1.19	1 (6%)
17	MAN	fN	7	17	11,11,12	0.86	0	15,15,17	1.30	2 (13%)
17	MAN	fN	8	17	11,11,12	0.85	0	15,15,17	1.27	2 (13%)
17	MAN	fN	9	17	11,11,12	0.75	1 (9%)	15,15,17	1.08	2 (13%)
19	NAG	fO	1	19,2	14,14,15	0.44	0	17,19,21	0.48	0
19	MAN	fO	10	19	11,11,12	0.83	1 (9%)	15,15,17	1.04	2 (13%)
19	NAG	fO	2	19	14,14,15	0.34	0	17,19,21	0.65	0
19	BMA	fO	3	19	11,11,12	0.32	0	15,15,17	0.73	0
19	MAN	fO	4	19	11,11,12	0.90	0	15,15,17	1.29	3 (20%)
19	MAN	fO	5	19	11,11,12	1.05	1 (9%)	15,15,17	1.11	2 (13%)
19	MAN	fO	6	19	11,11,12	0.91	1 (9%)	15,15,17	1.15	2 (13%)
19	MAN	fO	7	19	11,11,12	0.82	1 (9%)	15,15,17	1.27	2 (13%)
19	MAN	fO	8	19	11,11,12	0.67	0	15,15,17	1.18	2 (13%)
19	MAN	fO	9	19	11,11,12	0.84	1 (9%)	15,15,17	1.02	1 (6%)
20	NAG	fP	1	20,2	14,14,15	0.38	0	17,19,21	0.67	0
20	NAG	fP	10	20	14,14,15	0.36	0	17,19,21	0.80	0
20	XYS	fP	11	20	9,9,10	1.99	3 (33%)	10,12,14	1.27	2 (20%)
20	XYP	fP	12	20	9,9,10	0.20	0	10,12,14	0.66	0
20	MAN	fP	13	20	11,11,12	0.77	1 (9%)	15,15,17	1.07	1 (6%)
20	MAN	fP	14	20	11,11,12	0.71	1 (9%)	15,15,17	0.99	1 (6%)
20	NAG	fP	2	20	14,14,15	0.36	0	17,19,21	0.79	1 (5%)
20	BMA	fP	3	20	11,11,12	0.22	0	15,15,17	0.87	0
20	MAN	fP	4	20	11,11,12	0.74	0	15,15,17	1.17	3 (20%)
20	MAN	fP	5	20	11,11,12	0.63	0	15,15,17	1.33	3 (20%)
20	XYP	fP	6	20	9,9,10	0.17	0	10,12,14	0.62	0
20	XYS	fP	7	20	9,9,10	1.90	3 (33%)	10,12,14	1.12	1 (10%)
20	NAG	fP	8	20	14,14,15	0.34	0	17,19,21	0.70	0
20	MAN	fP	9	20,23	11,11,12	0.67	0	15,15,17	1.09	1 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	aA	1	5,7	-	0/6/23/26	0/1/1/1
7	MAN	aA	10	23,7	-	0/2/19/22	0/1/1/1
7	NAG	aA	11	7	-	0/6/23/26	0/1/1/1
7	XYP	aA	12	7	-	-	0/1/1/1
7	MAN	aA	13	7	-	0/2/19/22	0/1/1/1
7	MAN	aA	14	7	-	2/2/19/22	0/1/1/1
7	NAG	aA	2	7	-	0/6/23/26	0/1/1/1
7	BMA	aA	3	7	-	0/2/19/22	0/1/1/1
7	MAN	aA	4	7	-	0/2/19/22	0/1/1/1
7	MAN	aA	5	7	-	0/2/19/22	0/1/1/1
7	XYP	aA	6	7	-	-	0/1/1/1
7	XYP	aA	7	7	-	-	0/1/1/1
7	MAN	aA	8	7	-	0/2/19/22	0/1/1/1
7	NAG	aA	9	7	-	0/6/23/26	0/1/1/1
8	NAG	aB	1	5,8	-	0/6/23/26	0/1/1/1
8	XYP	aB	10	8	-	-	0/1/1/1
8	MAN	aB	11	8	-	0/2/19/22	0/1/1/1
8	NAG	aB	12	8	-	2/6/23/26	0/1/1/1
8	BMA	aB	13	8	-	0/2/19/22	0/1/1/1
8	XYP	aB	14	8	-	-	0/1/1/1
8	XYP	aB	15	8	-	-	0/1/1/1
8	MAN	aB	16	8	-	0/2/19/22	0/1/1/1
8	NAG	aB	2	8	-	2/6/23/26	0/1/1/1
8	BMA	aB	3	8	-	0/2/19/22	0/1/1/1
8	MAN	aB	4	8	-	0/2/19/22	0/1/1/1
8	MAN	aB	5	8	-	0/2/19/22	0/1/1/1
8	NAG	aB	6	8	-	0/6/23/26	0/1/1/1
8	MAN	aB	7	8	-	2/2/19/22	0/1/1/1
8	XYP	aB	8	8	-	-	0/1/1/1
8	BMA	aB	9	8	-	0/2/19/22	0/1/1/1
9	NAG	aC	1	5,9	-	0/6/23/26	0/1/1/1
9	XYP	aC	10	9	-	-	0/1/1/1
9	BGC	aC	11	9	-	1/2/19/22	0/1/1/1
9	MAN	aC	12	23,9	-	0/2/19/22	0/1/1/1
9	NAG	aC	13	9	-	0/6/23/26	0/1/1/1
9	XYP	aC	14	9	-	-	0/1/1/1
9	MAN	aC	15	9	-	0/2/19/22	0/1/1/1
9	MAN	aC	16	9	-	0/2/19/22	0/1/1/1
9	NAG	aC	2	9	-	0/6/23/26	0/1/1/1
9	BMA	aC	3	9	-	0/2/19/22	0/1/1/1
9	MAN	aC	4	9	-	0/2/19/22	0/1/1/1
9	MAN	aC	5	9	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	NAG	aC	6	9	-	2/6/23/26	0/1/1/1
9	MAN	aC	7	9	-	0/2/19/22	0/1/1/1
9	BMA	aC	8	9	-	0/2/19/22	0/1/1/1
9	XYP	aC	9	9	-	-	0/1/1/1
10	NAG	aD	1	10,5	-	0/6/23/26	0/1/1/1
10	NAG	aD	2	10	-	0/6/23/26	0/1/1/1
10	BMA	aD	3	10	-	0/2/19/22	0/1/1/1
10	MAN	aD	4	10	-	0/2/19/22	0/1/1/1
10	MAN	aD	5	10	-	1/2/19/22	0/1/1/1
10	MAN	aD	6	10	-	0/2/19/22	0/1/1/1
10	MAN	aD	7	10	-	2/2/19/22	0/1/1/1
10	MAN	aD	8	10	-	2/2/19/22	0/1/1/1
10	MAN	aD	9	10	-	0/2/19/22	0/1/1/1
11	NAG	aE	1	5,11	-	0/6/23/26	0/1/1/1
11	MAN	aE	10	23,11	-	0/2/19/22	0/1/1/1
11	NAG	aE	11	11	-	3/6/23/26	0/1/1/1
11	XYP	aE	12	11	-	-	0/1/1/1
11	XYP	aE	13	11	-	-	0/1/1/1
11	BMA	aE	14	11	-	0/2/19/22	0/1/1/1
11	MAN	aE	15	11	-	2/2/19/22	0/1/1/1
11	NAG	aE	2	11	-	0/6/23/26	0/1/1/1
11	BMA	aE	3	11	-	0/2/19/22	0/1/1/1
11	MAN	aE	4	11	-	2/2/19/22	0/1/1/1
11	MAN	aE	5	11	-	2/2/19/22	0/1/1/1
11	XYP	aE	6	11	-	-	0/1/1/1
11	XYP	aE	7	11	-	-	0/1/1/1
11	XYP	aE	8	11	-	-	0/1/1/1
11	NAG	aE	9	11	-	2/6/23/26	0/1/1/1
7	NAG	aF	1	5,7	-	0/6/23/26	0/1/1/1
7	MAN	aF	10	23,7	-	1/2/19/22	0/1/1/1
7	NAG	aF	11	7	-	0/6/23/26	0/1/1/1
7	XYP	aF	12	7	-	-	0/1/1/1
7	MAN	aF	13	7	-	0/2/19/22	0/1/1/1
7	MAN	aF	14	7	-	2/2/19/22	0/1/1/1
7	NAG	aF	2	7	-	0/6/23/26	0/1/1/1
7	BMA	aF	3	7	-	0/2/19/22	0/1/1/1
7	MAN	aF	4	7	-	1/2/19/22	0/1/1/1
7	MAN	aF	5	7	-	0/2/19/22	0/1/1/1
7	XYP	aF	6	7	-	-	0/1/1/1
7	XYP	aF	7	7	-	-	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	MAN	aF	8	7	-	0/2/19/22	0/1/1/1
7	NAG	aF	9	7	-	0/6/23/26	0/1/1/1
8	NAG	aG	1	5,8	-	0/6/23/26	0/1/1/1
8	XYP	aG	10	8	-	-	0/1/1/1
8	MAN	aG	11	8	-	0/2/19/22	0/1/1/1
8	NAG	aG	12	8	-	0/6/23/26	0/1/1/1
8	BMA	aG	13	8	-	0/2/19/22	0/1/1/1
8	XYP	aG	14	8	-	-	0/1/1/1
8	XYP	aG	15	8	-	-	0/1/1/1
8	MAN	aG	16	8	-	0/2/19/22	0/1/1/1
8	NAG	aG	2	8	-	0/6/23/26	0/1/1/1
8	BMA	aG	3	8	-	0/2/19/22	0/1/1/1
8	MAN	aG	4	8	-	0/2/19/22	0/1/1/1
8	MAN	aG	5	8	-	0/2/19/22	0/1/1/1
8	NAG	aG	6	8	-	0/6/23/26	0/1/1/1
8	MAN	aG	7	8	-	0/2/19/22	0/1/1/1
8	XYP	aG	8	8	-	-	0/1/1/1
8	BMA	aG	9	8	-	0/2/19/22	0/1/1/1
9	NAG	aH	1	5,9	-	0/6/23/26	0/1/1/1
9	XYP	aH	10	9	-	-	0/1/1/1
9	BGC	aH	11	9	-	2/2/19/22	0/1/1/1
9	MAN	aH	12	9	-	2/2/19/22	0/1/1/1
9	NAG	aH	13	9	-	0/6/23/26	0/1/1/1
9	XYP	aH	14	9	-	-	0/1/1/1
9	MAN	aH	15	9	-	1/2/19/22	0/1/1/1
9	MAN	aH	16	9	-	0/2/19/22	0/1/1/1
9	NAG	aH	2	9	-	0/6/23/26	0/1/1/1
9	BMA	aH	3	9	-	1/2/19/22	0/1/1/1
9	MAN	aH	4	9	-	2/2/19/22	0/1/1/1
9	MAN	aH	5	9	-	1/2/19/22	0/1/1/1
9	NAG	aH	6	9	-	2/6/23/26	0/1/1/1
9	MAN	aH	7	9	-	0/2/19/22	0/1/1/1
9	BMA	aH	8	9	-	0/2/19/22	0/1/1/1
9	XYP	aH	9	9	-	-	0/1/1/1
10	NAG	aI	1	10,5	-	2/6/23/26	0/1/1/1
10	NAG	aI	2	10	-	0/6/23/26	0/1/1/1
10	BMA	aI	3	10	-	0/2/19/22	0/1/1/1
10	MAN	aI	4	10	-	0/2/19/22	0/1/1/1
10	MAN	aI	5	10	-	1/2/19/22	0/1/1/1
10	MAN	aI	6	10	-	2/2/19/22	0/1/1/1
10	MAN	aI	7	10	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	MAN	aI	8	10	-	0/2/19/22	0/1/1/1
10	MAN	aI	9	10	-	0/2/19/22	0/1/1/1
11	NAG	aJ	1	5,11	-	0/6/23/26	0/1/1/1
11	MAN	aJ	10	11	-	0/2/19/22	0/1/1/1
11	NAG	aJ	11	11	-	3/6/23/26	0/1/1/1
11	XYP	aJ	12	11	-	-	0/1/1/1
11	XYP	aJ	13	11	-	-	0/1/1/1
11	BMA	aJ	14	11	-	0/2/19/22	0/1/1/1
11	MAN	aJ	15	11	-	1/2/19/22	0/1/1/1
11	NAG	aJ	2	11	-	0/6/23/26	0/1/1/1
11	BMA	aJ	3	11	-	0/2/19/22	0/1/1/1
11	MAN	aJ	4	11	-	1/2/19/22	0/1/1/1
11	MAN	aJ	5	11	-	0/2/19/22	0/1/1/1
11	XYP	aJ	6	11	-	-	0/1/1/1
11	XYP	aJ	7	11	-	-	0/1/1/1
11	XYP	aJ	8	11	-	-	0/1/1/1
11	NAG	aJ	9	11	-	2/6/23/26	0/1/1/1
7	NAG	aK	1	5,7	-	0/6/23/26	0/1/1/1
7	MAN	aK	10	23,7	-	0/2/19/22	0/1/1/1
7	NAG	aK	11	7	-	0/6/23/26	0/1/1/1
7	XYP	aK	12	7	-	-	0/1/1/1
7	MAN	aK	13	7	-	0/2/19/22	0/1/1/1
7	MAN	aK	14	7	-	0/2/19/22	0/1/1/1
7	NAG	aK	2	7	-	0/6/23/26	0/1/1/1
7	BMA	aK	3	7	-	0/2/19/22	0/1/1/1
7	MAN	aK	4	7	-	0/2/19/22	0/1/1/1
7	MAN	aK	5	7	-	2/2/19/22	0/1/1/1
7	XYP	aK	6	7	-	-	0/1/1/1
7	XYP	aK	7	7	-	-	0/1/1/1
7	MAN	aK	8	7	-	0/2/19/22	0/1/1/1
7	NAG	aK	9	7	-	0/6/23/26	0/1/1/1
8	NAG	aL	1	5,8	-	0/6/23/26	0/1/1/1
8	XYP	aL	10	8	-	-	0/1/1/1
8	MAN	aL	11	23,8	-	0/2/19/22	0/1/1/1
8	NAG	aL	12	8	-	0/6/23/26	0/1/1/1
8	BMA	aL	13	8	-	0/2/19/22	0/1/1/1
8	XYP	aL	14	8	-	-	0/1/1/1
8	XYP	aL	15	8	-	-	0/1/1/1
8	MAN	aL	16	8	-	0/2/19/22	0/1/1/1
8	NAG	aL	2	8	-	2/6/23/26	0/1/1/1
8	BMA	aL	3	8	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	MAN	aL	4	8	-	0/2/19/22	0/1/1/1
8	MAN	aL	5	8	-	0/2/19/22	0/1/1/1
8	NAG	aL	6	8	-	0/6/23/26	0/1/1/1
8	MAN	aL	7	8	-	0/2/19/22	0/1/1/1
8	XYP	aL	8	8	-	-	0/1/1/1
8	BMA	aL	9	8	-	0/2/19/22	0/1/1/1
9	NAG	aM	1	5,9	-	0/6/23/26	0/1/1/1
9	XYP	aM	10	9	-	-	0/1/1/1
9	BGC	aM	11	9	-	1/2/19/22	0/1/1/1
9	MAN	aM	12	23,9	-	0/2/19/22	0/1/1/1
9	NAG	aM	13	9	-	2/6/23/26	0/1/1/1
9	XYP	aM	14	9	-	-	0/1/1/1
9	MAN	aM	15	9	-	0/2/19/22	0/1/1/1
9	MAN	aM	16	9	-	1/2/19/22	0/1/1/1
9	NAG	aM	2	9	-	0/6/23/26	0/1/1/1
9	BMA	aM	3	9	-	0/2/19/22	0/1/1/1
9	MAN	aM	4	9	-	0/2/19/22	0/1/1/1
9	MAN	aM	5	9	-	2/2/19/22	0/1/1/1
9	NAG	aM	6	9	-	0/6/23/26	0/1/1/1
9	MAN	aM	7	9	-	0/2/19/22	0/1/1/1
9	BMA	aM	8	9	-	0/2/19/22	0/1/1/1
9	XYP	aM	9	9	-	-	0/1/1/1
10	NAG	aN	1	10,5	-	0/6/23/26	0/1/1/1
10	NAG	aN	2	10	-	0/6/23/26	0/1/1/1
10	BMA	aN	3	10	-	0/2/19/22	0/1/1/1
10	MAN	aN	4	10	-	0/2/19/22	0/1/1/1
10	MAN	aN	5	10	-	1/2/19/22	0/1/1/1
10	MAN	aN	6	10	-	0/2/19/22	0/1/1/1
10	MAN	aN	7	10	-	2/2/19/22	0/1/1/1
10	MAN	aN	8	10	-	2/2/19/22	0/1/1/1
10	MAN	aN	9	10	-	0/2/19/22	0/1/1/1
11	NAG	aO	1	5,11	-	0/6/23/26	0/1/1/1
11	MAN	aO	10	11	-	0/2/19/22	0/1/1/1
11	NAG	aO	11	11	-	3/6/23/26	0/1/1/1
11	XYP	aO	12	11	-	-	0/1/1/1
11	XYP	aO	13	11	-	-	0/1/1/1
11	BMA	aO	14	11	-	0/2/19/22	0/1/1/1
11	MAN	aO	15	11	-	0/2/19/22	0/1/1/1
11	NAG	aO	2	11	-	0/6/23/26	0/1/1/1
11	BMA	aO	3	11	-	0/2/19/22	0/1/1/1
11	MAN	aO	4	11	-	2/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	MAN	aO	5	11	-	2/2/19/22	0/1/1/1
11	XYP	aO	6	11	-	-	0/1/1/1
11	XYP	aO	7	11	-	-	0/1/1/1
11	XYP	aO	8	11	-	-	0/1/1/1
11	NAG	aO	9	11	-	0/6/23/26	0/1/1/1
12	NAG	bA	1	6,12	-	0/6/23/26	0/1/1/1
12	NAG	bA	2	12	-	0/6/23/26	0/1/1/1
12	BMA	bA	3	12	-	0/2/19/22	0/1/1/1
12	MAN	bA	4	12	-	0/2/19/22	0/1/1/1
12	MAN	bA	5	12	-	0/2/19/22	0/1/1/1
12	MAN	bA	6	12	-	2/2/19/22	0/1/1/1
12	MAN	bA	7	12	-	2/2/19/22	0/1/1/1
12	MAN	bA	8	12	-	2/2/19/22	0/1/1/1
12	MAN	bA	9	12	-	2/2/19/22	0/1/1/1
13	NAG	bB	1	13,6	-	0/6/23/26	0/1/1/1
13	NAG	bB	2	13	-	0/6/23/26	0/1/1/1
13	BMA	bB	3	13	-	1/2/19/22	0/1/1/1
13	MAN	bB	4	13	-	1/2/19/22	0/1/1/1
13	MAN	bB	5	13	-	0/2/19/22	0/1/1/1
14	NAG	bC	1	6,14	-	0/6/23/26	0/1/1/1
14	MAN	bC	10	14	-	2/2/19/22	0/1/1/1
14	NAG	bC	2	14	-	0/6/23/26	0/1/1/1
14	BMA	bC	3	14	-	0/2/19/22	0/1/1/1
14	MAN	bC	4	14	-	2/2/19/22	0/1/1/1
14	MAN	bC	5	14	-	0/2/19/22	0/1/1/1
14	XYP	bC	6	14	-	-	0/1/1/1
14	XYS	bC	7	14	-	-	0/1/1/1
14	MAN	bC	8	14,23	-	0/2/19/22	0/1/1/1
14	BMA	bC	9	14	-	0/2/19/22	0/1/1/1
12	NAG	bD	1	6,12	-	0/6/23/26	0/1/1/1
12	NAG	bD	2	12	-	0/6/23/26	0/1/1/1
12	BMA	bD	3	12	-	0/2/19/22	0/1/1/1
12	MAN	bD	4	12	-	0/2/19/22	0/1/1/1
12	MAN	bD	5	12	-	0/2/19/22	0/1/1/1
12	MAN	bD	6	12	-	2/2/19/22	0/1/1/1
12	MAN	bD	7	12	-	0/2/19/22	0/1/1/1
12	MAN	bD	8	12	-	0/2/19/22	0/1/1/1
12	MAN	bD	9	12	-	2/2/19/22	0/1/1/1
13	NAG	bE	1	13,6	-	0/6/23/26	0/1/1/1
13	NAG	bE	2	13	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	BMA	bE	3	13	-	1/2/19/22	0/1/1/1
13	MAN	bE	4	13	-	2/2/19/22	0/1/1/1
13	MAN	bE	5	13	-	0/2/19/22	0/1/1/1
14	NAG	bF	1	6,14	-	0/6/23/26	0/1/1/1
14	MAN	bF	10	14	-	1/2/19/22	0/1/1/1
14	NAG	bF	2	14	-	0/6/23/26	0/1/1/1
14	BMA	bF	3	14	-	0/2/19/22	0/1/1/1
14	MAN	bF	4	14	-	2/2/19/22	0/1/1/1
14	MAN	bF	5	14	-	0/2/19/22	0/1/1/1
14	XYP	bF	6	14	-	-	0/1/1/1
14	XYS	bF	7	14	-	-	0/1/1/1
14	MAN	bF	8	14,23	-	0/2/19/22	0/1/1/1
14	BMA	bF	9	14	-	0/2/19/22	0/1/1/1
12	NAG	bG	1	6,12	-	0/6/23/26	0/1/1/1
12	NAG	bG	2	12	-	0/6/23/26	0/1/1/1
12	BMA	bG	3	12	-	0/2/19/22	0/1/1/1
12	MAN	bG	4	12	-	0/2/19/22	0/1/1/1
12	MAN	bG	5	12	-	0/2/19/22	0/1/1/1
12	MAN	bG	6	12	-	0/2/19/22	0/1/1/1
12	MAN	bG	7	12	-	0/2/19/22	0/1/1/1
12	MAN	bG	8	12	-	0/2/19/22	0/1/1/1
12	MAN	bG	9	12	-	0/2/19/22	0/1/1/1
13	NAG	bH	1	13,6	-	0/6/23/26	0/1/1/1
13	NAG	bH	2	13	-	0/6/23/26	0/1/1/1
13	BMA	bH	3	13	-	2/2/19/22	0/1/1/1
13	MAN	bH	4	13	-	1/2/19/22	0/1/1/1
13	MAN	bH	5	13	-	2/2/19/22	0/1/1/1
14	NAG	bI	1	6,14	-	0/6/23/26	0/1/1/1
14	MAN	bI	10	14	-	2/2/19/22	0/1/1/1
14	NAG	bI	2	14	-	1/6/23/26	0/1/1/1
14	BMA	bI	3	14	-	0/2/19/22	0/1/1/1
14	MAN	bI	4	14	-	2/2/19/22	0/1/1/1
14	MAN	bI	5	14	-	0/2/19/22	0/1/1/1
14	XYP	bI	6	14	-	-	0/1/1/1
14	XYS	bI	7	14	-	-	0/1/1/1
14	MAN	bI	8	14,23	-	0/2/19/22	0/1/1/1
14	BMA	bI	9	14	-	0/2/19/22	0/1/1/1
15	XYP	cA	1	15	-	-	0/1/1/1
15	MAN	cA	2	15	-	0/2/19/22	0/1/1/1
15	MAN	cA	3	15	-	0/2/19/22	0/1/1/1
15	MAN	cA	4	15	-	2/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	XYP	cB	1	15	-	-	0/1/1/1
15	MAN	cB	2	15	-	0/2/19/22	0/1/1/1
15	MAN	cB	3	15	-	1/2/19/22	0/1/1/1
15	MAN	cB	4	15	-	0/2/19/22	0/1/1/1
15	XYP	cC	1	15	-	-	0/1/1/1
15	MAN	cC	2	15	-	0/2/19/22	0/1/1/1
15	MAN	cC	3	15	-	0/2/19/22	0/1/1/1
15	MAN	cC	4	15	-	0/2/19/22	0/1/1/1
16	XYP	dA	1	16	-	-	0/1/1/1
16	MAN	dA	2	16	-	0/2/19/22	0/1/1/1
16	MAN	dA	3	16	-	1/2/19/22	0/1/1/1
16	MAN	dA	4	16	-	1/2/19/22	0/1/1/1
16	MAN	dA	5	16	-	0/2/19/22	0/1/1/1
16	MAN	dA	6	16	-	2/2/19/22	0/1/1/1
16	MAN	dA	7	16	-	1/2/19/22	0/1/1/1
16	XYP	dB	1	16	-	-	0/1/1/1
16	MAN	dB	2	16	-	0/2/19/22	0/1/1/1
16	MAN	dB	3	16	-	2/2/19/22	0/1/1/1
16	MAN	dB	4	16	-	0/2/19/22	0/1/1/1
16	MAN	dB	5	16	-	0/2/19/22	0/1/1/1
16	MAN	dB	6	16	-	2/2/19/22	0/1/1/1
16	MAN	dB	7	16	-	0/2/19/22	0/1/1/1
16	XYP	dC	1	16	-	-	0/1/1/1
16	MAN	dC	2	16	-	2/2/19/22	0/1/1/1
16	MAN	dC	3	16	-	2/2/19/22	0/1/1/1
16	MAN	dC	4	16	-	0/2/19/22	0/1/1/1
16	MAN	dC	5	16	-	0/2/19/22	0/1/1/1
16	MAN	dC	6	16	-	2/2/19/22	0/1/1/1
16	MAN	dC	7	16	-	1/2/19/22	0/1/1/1
17	NAG	eA	1	17,1	-	0/6/23/26	0/1/1/1
17	MAN	eA	10	17	-	0/2/19/22	0/1/1/1
17	MAN	eA	11	17	-	0/2/19/22	0/1/1/1
17	NAG	eA	2	17	-	0/6/23/26	0/1/1/1
17	BMA	eA	3	17	-	0/2/19/22	0/1/1/1
17	MAN	eA	4	17	-	0/2/19/22	0/1/1/1
17	MAN	eA	5	17	-	1/2/19/22	0/1/1/1
17	MAN	eA	6	17	-	0/2/19/22	0/1/1/1
17	MAN	eA	7	17	-	2/2/19/22	0/1/1/1
17	MAN	eA	8	17	-	1/2/19/22	0/1/1/1
17	MAN	eA	9	17	-	0/2/19/22	0/1/1/1
18	NAG	eB	1	18,1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	MAN	eB	10	18	-	0/2/19/22	0/1/1/1
18	NAG	eB	11	18	-	3/6/23/26	0/1/1/1
18	XYP	eB	12	18	-	-	0/1/1/1
18	XYP	eB	13	18	-	-	0/1/1/1
18	MAN	eB	14	18	-	2/2/19/22	0/1/1/1
18	NAG	eB	2	18	-	0/6/23/26	0/1/1/1
18	BMA	eB	3	18	-	0/2/19/22	0/1/1/1
18	MAN	eB	4	18	-	0/2/19/22	0/1/1/1
18	MAN	eB	5	18	-	0/2/19/22	0/1/1/1
18	XYP	eB	6	18	-	-	0/1/1/1
18	XYS	eB	7	18	-	-	0/1/1/1
18	BGC	eB	8	18	-	2/2/19/22	0/1/1/1
18	NAG	eB	9	18	-	0/6/23/26	0/1/1/1
17	NAG	eC	1	17,1	-	0/6/23/26	0/1/1/1
17	MAN	eC	10	17	-	0/2/19/22	0/1/1/1
17	MAN	eC	11	17	-	0/2/19/22	0/1/1/1
17	NAG	eC	2	17	-	2/6/23/26	0/1/1/1
17	BMA	eC	3	17	-	0/2/19/22	0/1/1/1
17	MAN	eC	4	17	-	0/2/19/22	0/1/1/1
17	MAN	eC	5	17	-	1/2/19/22	0/1/1/1
17	MAN	eC	6	17	-	0/2/19/22	0/1/1/1
17	MAN	eC	7	17	-	0/2/19/22	0/1/1/1
17	MAN	eC	8	17	-	0/2/19/22	0/1/1/1
17	MAN	eC	9	17	-	2/2/19/22	0/1/1/1
18	NAG	eD	1	18,1	-	0/6/23/26	0/1/1/1
18	MAN	eD	10	18,23	-	0/2/19/22	0/1/1/1
18	NAG	eD	11	18	-	0/6/23/26	0/1/1/1
18	XYP	eD	12	18	-	-	0/1/1/1
18	XYP	eD	13	18	-	-	0/1/1/1
18	MAN	eD	14	18	-	2/2/19/22	0/1/1/1
18	NAG	eD	2	18	-	0/6/23/26	0/1/1/1
18	BMA	eD	3	18	-	0/2/19/22	0/1/1/1
18	MAN	eD	4	18	-	0/2/19/22	0/1/1/1
18	MAN	eD	5	18	-	0/2/19/22	0/1/1/1
18	XYP	eD	6	18	-	-	0/1/1/1
18	XYS	eD	7	18	-	-	0/1/1/1
18	BGC	eD	8	18	-	2/2/19/22	0/1/1/1
18	NAG	eD	9	18	-	0/6/23/26	0/1/1/1
17	NAG	eE	1	17,1	-	0/6/23/26	0/1/1/1
17	MAN	eE	10	17	-	0/2/19/22	0/1/1/1
17	MAN	eE	11	17	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	NAG	eE	2	17	-	1/6/23/26	0/1/1/1
17	BMA	eE	3	17	-	0/2/19/22	0/1/1/1
17	MAN	eE	4	17	-	0/2/19/22	0/1/1/1
17	MAN	eE	5	17	-	2/2/19/22	0/1/1/1
17	MAN	eE	6	17	-	0/2/19/22	0/1/1/1
17	MAN	eE	7	17	-	0/2/19/22	0/1/1/1
17	MAN	eE	8	17	-	1/2/19/22	0/1/1/1
17	MAN	eE	9	17	-	1/2/19/22	0/1/1/1
18	NAG	eF	1	18,1	-	0/6/23/26	0/1/1/1
18	MAN	eF	10	18	-	0/2/19/22	0/1/1/1
18	NAG	eF	11	18	-	0/6/23/26	0/1/1/1
18	XYP	eF	12	18	-	-	0/1/1/1
18	XYP	eF	13	18	-	-	0/1/1/1
18	MAN	eF	14	18	-	2/2/19/22	0/1/1/1
18	NAG	eF	2	18	-	0/6/23/26	0/1/1/1
18	BMA	eF	3	18	-	0/2/19/22	0/1/1/1
18	MAN	eF	4	18	-	0/2/19/22	0/1/1/1
18	MAN	eF	5	18	-	0/2/19/22	0/1/1/1
18	XYP	eF	6	18	-	-	0/1/1/1
18	XYS	eF	7	18	-	-	0/1/1/1
18	BGC	eF	8	18	-	0/2/19/22	0/1/1/1
18	NAG	eF	9	18	-	0/6/23/26	0/1/1/1
19	NAG	fB	1	19,2	-	0/6/23/26	0/1/1/1
19	MAN	fB	10	19	-	2/2/19/22	0/1/1/1
19	NAG	fB	2	19	-	1/6/23/26	0/1/1/1
19	BMA	fB	3	19	-	0/2/19/22	0/1/1/1
19	MAN	fB	4	19	-	0/2/19/22	0/1/1/1
19	MAN	fB	5	19	-	2/2/19/22	0/1/1/1
19	MAN	fB	6	19	-	0/2/19/22	0/1/1/1
19	MAN	fB	7	19	-	2/2/19/22	0/1/1/1
19	MAN	fB	8	19	-	0/2/19/22	0/1/1/1
19	MAN	fB	9	19	-	1/2/19/22	0/1/1/1
17	NAG	fC	1	17,2	-	1/6/23/26	0/1/1/1
17	MAN	fC	10	17	-	0/2/19/22	0/1/1/1
17	MAN	fC	11	17	-	2/2/19/22	0/1/1/1
17	NAG	fC	2	17	-	0/6/23/26	0/1/1/1
17	BMA	fC	3	17	-	0/2/19/22	0/1/1/1
17	MAN	fC	4	17	-	0/2/19/22	0/1/1/1
17	MAN	fC	5	17	-	0/2/19/22	0/1/1/1
17	MAN	fC	6	17	-	0/2/19/22	0/1/1/1
17	MAN	fC	7	17	-	2/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	MAN	fC	8	17	-	0/2/19/22	0/1/1/1
17	MAN	fC	9	17	-	1/2/19/22	0/1/1/1
17	NAG	fD	1	17,2	-	2/6/23/26	0/1/1/1
17	MAN	fD	10	17	-	0/2/19/22	0/1/1/1
17	MAN	fD	11	17	-	0/2/19/22	0/1/1/1
17	NAG	fD	2	17	-	0/6/23/26	0/1/1/1
17	BMA	fD	3	17	-	0/2/19/22	0/1/1/1
17	MAN	fD	4	17	-	0/2/19/22	0/1/1/1
17	MAN	fD	5	17	-	0/2/19/22	0/1/1/1
17	MAN	fD	6	17	-	0/2/19/22	0/1/1/1
17	MAN	fD	7	17	-	0/2/19/22	0/1/1/1
17	MAN	fD	8	17	-	2/2/19/22	0/1/1/1
17	MAN	fD	9	17	-	2/2/19/22	0/1/1/1
19	NAG	fE	1	19,2	-	2/6/23/26	0/1/1/1
19	MAN	fE	10	19	-	2/2/19/22	0/1/1/1
19	NAG	fE	2	19	-	0/6/23/26	0/1/1/1
19	BMA	fE	3	19	-	0/2/19/22	0/1/1/1
19	MAN	fE	4	19	-	0/2/19/22	0/1/1/1
19	MAN	fE	5	19	-	0/2/19/22	0/1/1/1
19	MAN	fE	6	19	-	0/2/19/22	0/1/1/1
19	MAN	fE	7	19	-	0/2/19/22	0/1/1/1
19	MAN	fE	8	19	-	2/2/19/22	0/1/1/1
19	MAN	fE	9	19	-	0/2/19/22	0/1/1/1
20	NAG	fF	1	20,2	-	0/6/23/26	0/1/1/1
20	NAG	fF	10	20	-	0/6/23/26	0/1/1/1
20	XYS	fF	11	20	-	-	0/1/1/1
20	XYP	fF	12	20	-	-	0/1/1/1
20	MAN	fF	13	20	-	0/2/19/22	0/1/1/1
20	MAN	fF	14	20	-	0/2/19/22	0/1/1/1
20	NAG	fF	2	20	-	0/6/23/26	0/1/1/1
20	BMA	fF	3	20	-	0/2/19/22	0/1/1/1
20	MAN	fF	4	20	-	0/2/19/22	0/1/1/1
20	MAN	fF	5	20	-	0/2/19/22	0/1/1/1
20	XYP	fF	6	20	-	-	0/1/1/1
20	XYS	fF	7	20	-	-	0/1/1/1
20	NAG	fF	8	20	-	0/6/23/26	0/1/1/1
20	MAN	fF	9	20	-	0/2/19/22	0/1/1/1
19	NAG	fG	1	19,2	-	0/6/23/26	0/1/1/1
19	MAN	fG	10	19	-	2/2/19/22	0/1/1/1
19	NAG	fG	2	19	-	3/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	BMA	fG	3	19	-	0/2/19/22	0/1/1/1
19	MAN	fG	4	19	-	0/2/19/22	0/1/1/1
19	MAN	fG	5	19	-	2/2/19/22	0/1/1/1
19	MAN	fG	6	19	-	0/2/19/22	0/1/1/1
19	MAN	fG	7	19	-	2/2/19/22	0/1/1/1
19	MAN	fG	8	19	-	1/2/19/22	0/1/1/1
19	MAN	fG	9	19	-	1/2/19/22	0/1/1/1
17	NAG	fH	1	17,2	-	2/6/23/26	0/1/1/1
17	MAN	fH	10	17	-	0/2/19/22	0/1/1/1
17	MAN	fH	11	17	-	0/2/19/22	0/1/1/1
17	NAG	fH	2	17	-	0/6/23/26	0/1/1/1
17	BMA	fH	3	17	-	0/2/19/22	0/1/1/1
17	MAN	fH	4	17	-	2/2/19/22	0/1/1/1
17	MAN	fH	5	17	-	0/2/19/22	0/1/1/1
17	MAN	fH	6	17	-	0/2/19/22	0/1/1/1
17	MAN	fH	7	17	-	2/2/19/22	0/1/1/1
17	MAN	fH	8	17	-	2/2/19/22	0/1/1/1
17	MAN	fH	9	17	-	2/2/19/22	0/1/1/1
17	NAG	fI	1	17,2	-	1/6/23/26	0/1/1/1
17	MAN	fI	10	17	-	0/2/19/22	0/1/1/1
17	MAN	fI	11	17	-	0/2/19/22	0/1/1/1
17	NAG	fI	2	17	-	0/6/23/26	0/1/1/1
17	BMA	fI	3	17	-	0/2/19/22	0/1/1/1
17	MAN	fI	4	17	-	2/2/19/22	0/1/1/1
17	MAN	fI	5	17	-	0/2/19/22	0/1/1/1
17	MAN	fI	6	17	-	0/2/19/22	0/1/1/1
17	MAN	fI	7	17	-	0/2/19/22	0/1/1/1
17	MAN	fI	8	17	-	0/2/19/22	0/1/1/1
17	MAN	fI	9	17	-	2/2/19/22	0/1/1/1
19	NAG	fJ	1	19,2	-	2/6/23/26	0/1/1/1
19	MAN	fJ	10	19	-	0/2/19/22	0/1/1/1
19	NAG	fJ	2	19	-	0/6/23/26	0/1/1/1
19	BMA	fJ	3	19	-	0/2/19/22	0/1/1/1
19	MAN	fJ	4	19	-	0/2/19/22	0/1/1/1
19	MAN	fJ	5	19	-	0/2/19/22	0/1/1/1
19	MAN	fJ	6	19	-	0/2/19/22	0/1/1/1
19	MAN	fJ	7	19	-	2/2/19/22	0/1/1/1
19	MAN	fJ	8	19	-	0/2/19/22	0/1/1/1
19	MAN	fJ	9	19	-	2/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	NAG	fK	1	20,2	-	0/6/23/26	0/1/1/1
20	NAG	fK	10	20	-	0/6/23/26	0/1/1/1
20	XYS	fK	11	20	-	-	0/1/1/1
20	XYP	fK	12	20	-	-	0/1/1/1
20	MAN	fK	13	20	-	0/2/19/22	0/1/1/1
20	MAN	fK	14	20	-	1/2/19/22	0/1/1/1
20	NAG	fK	2	20	-	0/6/23/26	0/1/1/1
20	BMA	fK	3	20	-	0/2/19/22	0/1/1/1
20	MAN	fK	4	20	-	0/2/19/22	0/1/1/1
20	MAN	fK	5	20	-	0/2/19/22	0/1/1/1
20	XYP	fK	6	20	-	-	0/1/1/1
20	XYS	fK	7	20	-	-	0/1/1/1
20	NAG	fK	8	20	-	2/6/23/26	0/1/1/1
20	MAN	fK	9	20,23	-	0/2/19/22	0/1/1/1
19	NAG	fL	1	19,2	-	0/6/23/26	0/1/1/1
19	MAN	fL	10	19	-	0/2/19/22	0/1/1/1
19	NAG	fL	2	19	-	1/6/23/26	0/1/1/1
19	BMA	fL	3	19	-	0/2/19/22	0/1/1/1
19	MAN	fL	4	19	-	0/2/19/22	0/1/1/1
19	MAN	fL	5	19	-	0/2/19/22	0/1/1/1
19	MAN	fL	6	19	-	0/2/19/22	0/1/1/1
19	MAN	fL	7	19	-	2/2/19/22	0/1/1/1
19	MAN	fL	8	19	-	2/2/19/22	0/1/1/1
19	MAN	fL	9	19	-	2/2/19/22	0/1/1/1
17	NAG	fM	1	17,2	-	0/6/23/26	0/1/1/1
17	MAN	fM	10	17	-	1/2/19/22	0/1/1/1
17	MAN	fM	11	17	-	0/2/19/22	0/1/1/1
17	NAG	fM	2	17	-	0/6/23/26	0/1/1/1
17	BMA	fM	3	17	-	0/2/19/22	0/1/1/1
17	MAN	fM	4	17	-	1/2/19/22	0/1/1/1
17	MAN	fM	5	17	-	0/2/19/22	0/1/1/1
17	MAN	fM	6	17	-	2/2/19/22	0/1/1/1
17	MAN	fM	7	17	-	0/2/19/22	0/1/1/1
17	MAN	fM	8	17	-	2/2/19/22	0/1/1/1
17	MAN	fM	9	17	-	0/2/19/22	0/1/1/1
17	NAG	fN	1	17,2	-	2/6/23/26	0/1/1/1
17	MAN	fN	10	17	-	0/2/19/22	0/1/1/1
17	MAN	fN	11	17	-	0/2/19/22	0/1/1/1
17	NAG	fN	2	17	-	0/6/23/26	0/1/1/1
17	BMA	fN	3	17	-	0/2/19/22	0/1/1/1
17	MAN	fN	4	17	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	MAN	fN	5	17	-	2/2/19/22	0/1/1/1
17	MAN	fN	6	17	-	0/2/19/22	0/1/1/1
17	MAN	fN	7	17	-	0/2/19/22	0/1/1/1
17	MAN	fN	8	17	-	0/2/19/22	0/1/1/1
17	MAN	fN	9	17	-	2/2/19/22	0/1/1/1
19	NAG	fO	1	19,2	-	2/6/23/26	0/1/1/1
19	MAN	fO	10	19	-	0/2/19/22	0/1/1/1
19	NAG	fO	2	19	-	0/6/23/26	0/1/1/1
19	BMA	fO	3	19	-	0/2/19/22	0/1/1/1
19	MAN	fO	4	19	-	0/2/19/22	0/1/1/1
19	MAN	fO	5	19	-	0/2/19/22	0/1/1/1
19	MAN	fO	6	19	-	0/2/19/22	0/1/1/1
19	MAN	fO	7	19	-	1/2/19/22	0/1/1/1
19	MAN	fO	8	19	-	2/2/19/22	0/1/1/1
19	MAN	fO	9	19	-	0/2/19/22	0/1/1/1
20	NAG	fP	1	20,2	-	0/6/23/26	0/1/1/1
20	NAG	fP	10	20	-	0/6/23/26	0/1/1/1
20	XYS	fP	11	20	-	-	0/1/1/1
20	XYP	fP	12	20	-	-	0/1/1/1
20	MAN	fP	13	20	-	0/2/19/22	0/1/1/1
20	MAN	fP	14	20	-	0/2/19/22	0/1/1/1
20	NAG	fP	2	20	-	0/6/23/26	0/1/1/1
20	BMA	fP	3	20	-	0/2/19/22	0/1/1/1
20	MAN	fP	4	20	-	0/2/19/22	0/1/1/1
20	MAN	fP	5	20	-	0/2/19/22	0/1/1/1
20	XYP	fP	6	20	-	-	0/1/1/1
20	XYS	fP	7	20	-	-	0/1/1/1
20	NAG	fP	8	20	-	0/6/23/26	0/1/1/1
20	MAN	fP	9	20,23	-	0/2/19/22	0/1/1/1

All (195) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	fP	11	XYS	O5-C1	4.13	1.50	1.42
20	fF	11	XYS	O5-C1	4.13	1.50	1.42
9	aH	4	MAN	O5-C1	-4.07	1.37	1.43
20	fK	11	XYS	O5-C1	4.03	1.50	1.42
14	bF	7	XYS	O5-C1	3.99	1.50	1.42
20	fF	7	XYS	O5-C1	3.91	1.50	1.42
18	eF	7	XYS	O5-C1	3.91	1.50	1.42
14	bC	7	XYS	O5-C1	3.90	1.50	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	bI	7	XYS	O5-C1	3.89	1.50	1.42
20	fK	7	XYS	O5-C1	3.88	1.50	1.42
9	aH	14	XYP	O5-C1	3.87	1.50	1.42
20	fP	7	XYS	O5-C1	3.87	1.50	1.42
7	aK	12	XYP	O5-C1	3.87	1.50	1.42
7	aA	12	XYP	O5-C1	3.83	1.50	1.42
18	eB	7	XYS	O5-C1	3.79	1.50	1.42
7	aF	12	XYP	O5-C1	3.78	1.50	1.42
18	eD	7	XYS	O5-C1	3.68	1.50	1.42
9	aM	14	XYP	O5-C1	3.62	1.49	1.42
9	aC	14	XYP	O5-C1	3.56	1.49	1.42
17	fH	5	MAN	O5-C1	-3.34	1.38	1.43
14	bF	9	BMA	O5-C1	-3.30	1.38	1.43
16	dA	3	MAN	O5-C1	-3.22	1.38	1.43
20	fF	11	XYS	O5-C5	3.05	1.48	1.42
19	fL	8	MAN	O5-C1	-3.03	1.38	1.43
11	aJ	4	MAN	O5-C1	-3.01	1.38	1.43
14	bI	9	BMA	O5-C1	-2.96	1.39	1.43
16	dA	4	MAN	O5-C1	-2.93	1.39	1.43
17	eC	8	MAN	O5-C1	-2.91	1.39	1.43
14	bC	7	XYS	O5-C5	2.89	1.48	1.42
14	bF	7	XYS	O5-C5	2.87	1.48	1.42
16	dB	6	MAN	O5-C1	-2.84	1.39	1.43
18	eF	7	XYS	O5-C5	2.83	1.48	1.42
20	fP	11	XYS	O5-C5	2.83	1.48	1.42
20	fK	7	XYS	O5-C5	2.81	1.48	1.42
17	fD	11	MAN	O5-C1	-2.81	1.39	1.43
17	eE	8	MAN	O5-C1	-2.81	1.39	1.43
9	aM	16	MAN	O5-C1	-2.80	1.39	1.43
19	fO	5	MAN	O5-C1	-2.79	1.39	1.43
20	fK	11	XYS	O5-C5	2.78	1.48	1.42
7	aK	4	MAN	O5-C1	-2.78	1.39	1.43
7	aF	12	XYP	O5-C5	2.76	1.48	1.42
7	aF	4	MAN	O5-C1	-2.76	1.39	1.43
17	fH	7	MAN	O5-C1	-2.75	1.39	1.43
16	dB	3	MAN	O5-C1	-2.74	1.39	1.43
14	bC	8	MAN	O5-C1	-2.74	1.39	1.43
7	aK	12	XYP	O5-C5	2.73	1.48	1.42
17	eA	8	MAN	O5-C1	-2.72	1.39	1.43
14	bI	7	XYS	O5-C5	2.72	1.48	1.42
9	aH	12	MAN	O5-C1	-2.72	1.39	1.43
16	dC	3	MAN	O5-C1	-2.71	1.39	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	eC	5	MAN	O5-C1	-2.70	1.39	1.43
18	eB	5	MAN	O5-C1	-2.70	1.39	1.43
17	fI	11	MAN	O5-C1	-2.70	1.39	1.43
11	aO	4	MAN	O5-C1	-2.70	1.39	1.43
20	fF	7	XYS	O5-C5	2.69	1.48	1.42
20	fP	7	XYS	O5-C5	2.66	1.48	1.42
18	eD	7	XYS	O5-C5	2.66	1.48	1.42
9	aH	14	XYP	O5-C5	2.66	1.48	1.42
9	aM	14	XYP	O5-C5	2.65	1.48	1.42
14	bC	4	MAN	O5-C1	-2.64	1.39	1.43
19	fJ	7	MAN	O5-C1	-2.64	1.39	1.43
17	fM	7	MAN	O5-C1	-2.63	1.39	1.43
16	dC	6	MAN	O5-C1	-2.62	1.39	1.43
17	eE	5	MAN	O5-C1	-2.62	1.39	1.43
9	aC	14	XYP	O5-C5	2.62	1.48	1.42
19	fB	4	MAN	O5-C1	-2.60	1.39	1.43
7	aA	4	MAN	O5-C1	-2.60	1.39	1.43
19	fL	7	MAN	O5-C1	-2.60	1.39	1.43
18	eB	7	XYS	O5-C5	2.59	1.47	1.42
7	aA	12	XYP	O5-C5	2.59	1.47	1.42
11	aO	15	MAN	O5-C1	-2.58	1.39	1.43
16	dA	6	MAN	O5-C1	-2.57	1.39	1.43
14	bF	4	MAN	O5-C1	-2.56	1.39	1.43
19	fE	6	MAN	O5-C1	-2.56	1.39	1.43
9	aH	5	MAN	O5-C1	-2.55	1.39	1.43
17	fC	10	MAN	O5-C1	-2.54	1.39	1.43
20	fF	11	XYS	C2-C3	-2.53	1.48	1.52
19	fJ	5	MAN	O5-C1	-2.52	1.39	1.43
15	cB	2	MAN	O5-C1	-2.51	1.39	1.43
17	fM	8	MAN	O5-C1	-2.50	1.39	1.43
10	aN	5	MAN	O5-C1	-2.50	1.39	1.43
20	fF	13	MAN	O5-C1	-2.49	1.39	1.43
10	aD	8	MAN	O5-C1	-2.48	1.39	1.43
12	bD	5	MAN	O5-C1	-2.47	1.39	1.43
10	aN	8	MAN	O5-C1	-2.44	1.39	1.43
19	fJ	10	MAN	O5-C1	-2.43	1.39	1.43
19	fG	7	MAN	O5-C1	-2.43	1.39	1.43
17	fH	10	MAN	O5-C1	-2.43	1.39	1.43
20	fK	4	MAN	O5-C1	-2.42	1.39	1.43
18	eF	5	MAN	O5-C1	-2.39	1.39	1.43
9	aC	12	MAN	O5-C1	-2.39	1.39	1.43
11	aE	14	BMA	O5-C1	-2.39	1.39	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	fG	8	MAN	O5-C1	-2.39	1.39	1.43
9	aH	16	MAN	O5-C1	-2.38	1.39	1.43
9	aM	14	XYP	C2-C3	-2.38	1.49	1.52
11	aE	10	MAN	O5-C1	-2.38	1.39	1.43
17	fI	5	MAN	O5-C1	-2.36	1.39	1.43
19	fO	6	MAN	O5-C1	-2.36	1.39	1.43
19	fG	4	MAN	O5-C1	-2.35	1.40	1.43
18	eF	14	MAN	O5-C1	-2.35	1.40	1.43
10	aD	5	MAN	O5-C1	-2.35	1.40	1.43
14	bC	9	BMA	O5-C1	-2.35	1.40	1.43
15	cB	3	MAN	O5-C1	-2.34	1.40	1.43
18	eD	14	MAN	O5-C1	-2.34	1.40	1.43
9	aH	14	XYP	C2-C3	-2.34	1.49	1.52
9	aC	4	MAN	O5-C1	-2.34	1.40	1.43
10	aD	4	MAN	O5-C1	-2.32	1.40	1.43
15	cA	3	MAN	O5-C1	-2.32	1.40	1.43
11	aJ	14	BMA	O5-C1	-2.31	1.40	1.43
8	aB	4	MAN	O5-C1	-2.30	1.40	1.43
9	aM	5	MAN	O5-C1	-2.30	1.40	1.43
17	fC	5	MAN	O5-C1	-2.29	1.40	1.43
8	aG	16	MAN	O5-C1	-2.29	1.40	1.43
7	aK	12	XYP	C2-C3	-2.28	1.49	1.52
17	fI	9	MAN	O5-C1	-2.28	1.40	1.43
18	eF	7	XYS	C2-C3	-2.28	1.49	1.52
7	aF	8	MAN	O5-C1	-2.28	1.40	1.43
13	bH	4	MAN	O5-C1	-2.27	1.40	1.43
12	bD	4	MAN	O5-C1	-2.27	1.40	1.43
12	bG	9	MAN	O5-C1	-2.26	1.40	1.43
16	dC	2	MAN	O5-C1	-2.26	1.40	1.43
7	aA	12	XYP	C2-C3	-2.25	1.49	1.52
18	eD	5	MAN	O5-C1	-2.25	1.40	1.43
19	fE	5	MAN	O5-C1	-2.24	1.40	1.43
19	fJ	8	MAN	O5-C1	-2.23	1.40	1.43
16	dB	2	MAN	O5-C1	-2.23	1.40	1.43
19	fB	8	MAN	O5-C1	-2.23	1.40	1.43
17	eA	10	MAN	O5-C1	-2.22	1.40	1.43
7	aA	8	MAN	O5-C1	-2.22	1.40	1.43
17	fN	11	MAN	O5-C1	-2.21	1.40	1.43
20	fK	7	XYS	C2-C3	-2.20	1.49	1.52
16	dA	5	MAN	O5-C1	-2.20	1.40	1.43
12	bD	6	MAN	O5-C1	-2.20	1.40	1.43
16	dC	4	MAN	O5-C1	-2.19	1.40	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	fB	7	MAN	O5-C1	-2.18	1.40	1.43
11	aE	4	MAN	O5-C1	-2.18	1.40	1.43
14	bI	8	MAN	O5-C1	-2.17	1.40	1.43
17	fN	4	MAN	O5-C1	-2.17	1.40	1.43
17	eE	11	MAN	O5-C1	-2.17	1.40	1.43
14	bF	8	MAN	O5-C1	-2.16	1.40	1.43
16	dC	7	MAN	O5-C1	-2.16	1.40	1.43
19	fE	10	MAN	O5-C1	-2.15	1.40	1.43
19	fE	8	MAN	O5-C1	-2.15	1.40	1.43
18	eB	14	MAN	O5-C1	-2.15	1.40	1.43
19	fJ	6	MAN	O5-C1	-2.14	1.40	1.43
20	fP	11	XYS	C2-C3	-2.14	1.49	1.52
9	aC	16	MAN	O5-C1	-2.12	1.40	1.43
14	bF	10	MAN	O5-C1	-2.12	1.40	1.43
19	fB	10	MAN	O5-C1	-2.12	1.40	1.43
11	aJ	10	MAN	O5-C1	-2.12	1.40	1.43
9	aC	14	XYP	C2-C3	-2.12	1.49	1.52
17	fD	7	MAN	O5-C1	-2.12	1.40	1.43
19	fL	4	MAN	O5-C1	-2.12	1.40	1.43
19	fL	5	MAN	O5-C1	-2.10	1.40	1.43
10	aI	4	MAN	O5-C1	-2.10	1.40	1.43
12	bA	7	MAN	O5-C1	-2.09	1.40	1.43
20	fK	11	XYS	C2-C3	-2.09	1.49	1.52
20	fK	11	XYS	C4-C3	-2.08	1.49	1.52
19	fO	9	MAN	O5-C1	-2.08	1.40	1.43
20	fP	13	MAN	O5-C1	-2.08	1.40	1.43
19	fO	10	MAN	O5-C1	-2.08	1.40	1.43
20	fF	7	XYS	C4-C3	-2.08	1.49	1.52
18	eD	7	XYS	C2-C3	-2.07	1.49	1.52
20	fP	7	XYS	C2-C3	-2.07	1.49	1.52
14	bC	10	MAN	O5-C1	-2.07	1.40	1.43
17	fC	7	MAN	O5-C1	-2.07	1.40	1.43
17	fC	8	MAN	O5-C1	-2.07	1.40	1.43
7	aF	12	XYP	C2-C3	-2.07	1.49	1.52
19	fO	7	MAN	O5-C1	-2.07	1.40	1.43
19	fG	10	MAN	O5-C1	-2.07	1.40	1.43
9	aH	14	XYP	C4-C3	-2.07	1.49	1.52
19	fG	5	MAN	O5-C1	-2.06	1.40	1.43
8	aL	16	MAN	O5-C1	-2.06	1.40	1.43
18	eB	7	XYS	C2-C3	-2.05	1.49	1.52
12	bD	7	MAN	O5-C1	-2.04	1.40	1.43
19	fL	9	MAN	O5-C1	-2.04	1.40	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	fB	9	MAN	O5-C1	-2.04	1.40	1.43
17	fI	8	MAN	O5-C1	-2.04	1.40	1.43
8	aB	11	MAN	O5-C1	-2.03	1.40	1.43
12	bG	7	MAN	O5-C1	-2.03	1.40	1.43
14	bC	7	XYS	C2-C3	-2.03	1.49	1.52
14	bF	7	XYS	C2-C3	-2.03	1.49	1.52
12	bA	4	MAN	O5-C1	-2.03	1.40	1.43
19	fJ	9	MAN	O5-C1	-2.02	1.40	1.43
17	fD	7	MAN	C2-C3	2.02	1.55	1.52
14	bI	7	XYS	C2-C3	-2.01	1.49	1.52
19	fG	9	MAN	O5-C1	-2.01	1.40	1.43
17	fN	9	MAN	O5-C1	-2.01	1.40	1.43
20	fP	14	MAN	O5-C1	-2.01	1.40	1.43
16	dB	4	MAN	O5-C1	-2.01	1.40	1.43
17	eA	5	MAN	O5-C1	-2.01	1.40	1.43
20	fF	9	MAN	O5-C1	-2.01	1.40	1.43
20	fF	11	XYS	C4-C3	-2.00	1.49	1.52
17	fM	5	MAN	O5-C1	-2.00	1.40	1.43
7	aA	13	MAN	O5-C1	-2.00	1.40	1.43

All (629) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	cA	2	MAN	C1-O5-C5	4.65	118.49	112.19
17	fC	4	MAN	C1-O5-C5	4.45	118.22	112.19
8	aG	5	MAN	C1-O5-C5	4.32	118.04	112.19
8	aB	5	MAN	C1-O5-C5	4.25	117.95	112.19
17	fM	10	MAN	C1-O5-C5	4.08	117.72	112.19
11	aE	5	MAN	C1-O5-C5	4.08	117.72	112.19
15	cC	2	MAN	C1-O5-C5	4.06	117.69	112.19
10	aN	7	MAN	C1-O5-C5	4.03	117.65	112.19
14	bI	5	MAN	C1-O5-C5	4.01	117.63	112.19
20	fF	7	XYS	C1-C2-C3	3.96	114.54	109.67
10	aI	4	MAN	C1-O5-C5	3.89	117.46	112.19
19	fB	7	MAN	C1-O5-C5	3.88	117.45	112.19
11	aJ	5	MAN	C1-O5-C5	3.88	117.45	112.19
17	fM	4	MAN	C1-O5-C5	3.87	117.43	112.19
17	fD	6	MAN	C1-O5-C5	3.83	117.39	112.19
20	fK	11	XYS	C1-C2-C3	3.80	114.33	109.67
8	aL	5	MAN	C1-O5-C5	3.79	117.32	112.19
19	fL	4	MAN	C1-O5-C5	3.75	117.27	112.19
16	dC	5	MAN	C1-O5-C5	3.73	117.25	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	fG	5	MAN	C1-O5-C5	3.72	117.24	112.19
7	aF	5	MAN	C1-O5-C5	3.71	117.22	112.19
19	fJ	7	MAN	C1-O5-C5	3.68	117.18	112.19
20	fP	5	MAN	C1-O5-C5	3.67	117.16	112.19
17	fH	4	MAN	C1-O5-C5	3.66	117.15	112.19
19	fO	7	MAN	C1-O5-C5	3.65	117.14	112.19
10	aI	7	MAN	C1-O5-C5	3.64	117.12	112.19
15	cA	4	MAN	C1-O5-C5	3.64	117.12	112.19
19	fL	7	MAN	C1-O5-C5	3.63	117.11	112.19
16	dA	3	MAN	C1-O5-C5	3.62	117.10	112.19
14	bI	7	XYS	C1-C2-C3	3.62	114.11	109.67
13	bH	5	MAN	C1-O5-C5	3.61	117.08	112.19
13	bB	4	MAN	C1-O5-C5	3.60	117.08	112.19
9	aC	12	MAN	C1-O5-C5	3.59	117.06	112.19
17	eA	4	MAN	C1-O5-C5	3.58	117.05	112.19
14	bI	3	BMA	C1-C2-C3	3.58	114.06	109.67
9	aC	14	XYP	C5-C4-C3	3.52	114.00	109.67
17	fI	6	MAN	C1-O5-C5	3.49	116.92	112.19
17	fD	11	MAN	C1-O5-C5	3.49	116.92	112.19
19	fL	6	MAN	C1-O5-C5	3.48	116.91	112.19
16	dC	3	MAN	C1-O5-C5	3.46	116.88	112.19
19	fL	5	MAN	C1-O5-C5	3.46	116.88	112.19
16	dB	3	MAN	C1-O5-C5	3.46	116.88	112.19
17	eC	6	MAN	C1-O5-C5	3.45	116.87	112.19
7	aA	5	MAN	C1-O5-C5	3.45	116.87	112.19
17	fN	6	MAN	C1-O5-C5	3.45	116.86	112.19
16	dA	5	MAN	C1-O5-C5	3.45	116.86	112.19
14	bC	5	MAN	C1-O5-C5	3.44	116.86	112.19
19	fB	8	MAN	C1-O5-C5	3.43	116.84	112.19
10	aD	4	MAN	C1-O5-C5	3.42	116.83	112.19
17	fD	8	MAN	C1-O5-C5	3.41	116.81	112.19
9	aC	5	MAN	C1-O5-C5	3.40	116.80	112.19
17	fC	9	MAN	C1-O5-C5	3.37	116.76	112.19
19	fG	6	MAN	C1-O5-C5	3.37	116.75	112.19
14	bI	4	MAN	C1-O5-C5	3.36	116.74	112.19
7	aK	10	MAN	C1-O5-C5	3.35	116.73	112.19
11	aO	5	MAN	C1-O5-C5	3.35	116.73	112.19
8	aG	11	MAN	C1-O5-C5	3.35	116.73	112.19
19	fG	7	MAN	C1-O5-C5	3.34	116.72	112.19
20	fK	5	MAN	C1-O5-C5	3.33	116.71	112.19
8	aG	7	MAN	C1-O5-C5	3.33	116.71	112.19
18	eF	4	MAN	O5-C1-C2	3.30	115.87	110.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	fJ	6	MAN	C1-O5-C5	3.29	116.64	112.19
9	aC	14	XYP	C4-C3-C2	3.28	114.82	110.92
19	fO	6	MAN	C1-O5-C5	3.28	116.63	112.19
9	aM	7	MAN	C1-O5-C5	3.27	116.62	112.19
15	cC	4	MAN	C1-O5-C5	3.27	116.62	112.19
16	dA	7	MAN	C1-O5-C5	3.23	116.57	112.19
17	eC	7	MAN	C1-O5-C5	3.22	116.56	112.19
12	bG	5	MAN	C1-O5-C5	3.20	116.53	112.19
10	aD	9	MAN	C1-O5-C5	3.20	116.53	112.19
17	eE	5	MAN	C1-O5-C5	3.20	116.53	112.19
12	bA	5	MAN	C1-O5-C5	3.20	116.52	112.19
18	eD	4	MAN	O5-C1-C2	3.18	115.69	110.77
19	fJ	4	MAN	C1-O5-C5	3.18	116.50	112.19
16	dA	4	MAN	C1-O5-C5	3.17	116.48	112.19
17	eC	9	MAN	C1-O5-C5	3.16	116.48	112.19
17	fH	9	MAN	C1-O5-C5	3.16	116.48	112.19
12	bD	6	MAN	C1-O5-C5	3.16	116.47	112.19
10	aI	8	MAN	C1-O5-C5	3.14	116.45	112.19
15	cB	4	MAN	C1-O5-C5	3.14	116.45	112.19
16	dB	4	MAN	C1-O5-C5	3.13	116.43	112.19
8	aL	11	MAN	C1-O5-C5	3.12	116.42	112.19
17	fN	7	MAN	C1-O5-C5	3.12	116.42	112.19
14	bC	4	MAN	C1-O5-C5	3.12	116.41	112.19
16	dC	4	MAN	C1-O5-C5	3.11	116.41	112.19
16	dB	5	MAN	C1-O5-C5	3.11	116.40	112.19
9	aH	15	MAN	C1-O5-C5	3.09	116.38	112.19
17	eE	7	MAN	C1-O5-C5	3.09	116.38	112.19
10	aN	8	MAN	C1-O5-C5	3.07	116.35	112.19
8	aL	7	MAN	C1-O5-C5	3.07	116.35	112.19
20	fP	13	MAN	C1-O5-C5	3.07	116.34	112.19
17	fM	9	MAN	C1-O5-C5	3.06	116.34	112.19
8	aG	9	BMA	C1-C2-C3	3.06	113.42	109.67
15	cC	2	MAN	O5-C1-C2	3.05	115.48	110.77
17	fI	7	MAN	C1-O5-C5	3.05	116.32	112.19
8	aG	2	NAG	C1-O5-C5	3.04	116.31	112.19
19	fO	4	MAN	C1-O5-C5	3.04	116.31	112.19
17	fM	4	MAN	O5-C1-C2	3.04	115.46	110.77
10	aI	8	MAN	O2-C2-C3	-3.03	104.06	110.14
20	fF	5	MAN	C1-O5-C5	3.03	116.30	112.19
17	fD	10	MAN	C1-O5-C5	3.02	116.29	112.19
17	eE	4	MAN	C1-O5-C5	3.02	116.28	112.19
17	eC	4	MAN	C1-O5-C5	3.02	116.28	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	fL	8	MAN	C1-O5-C5	3.01	116.28	112.19
17	fH	10	MAN	C1-O5-C5	3.01	116.28	112.19
9	aH	4	MAN	C1-O5-C5	3.01	116.27	112.19
17	fH	6	MAN	C1-O5-C5	3.01	116.27	112.19
12	bA	6	MAN	C1-O5-C5	3.00	116.26	112.19
10	aN	9	MAN	C1-O5-C5	2.99	116.25	112.19
19	fE	7	MAN	C1-O5-C5	2.99	116.24	112.19
17	fM	11	MAN	C1-O5-C5	2.98	116.24	112.19
8	aB	9	BMA	C1-O5-C5	2.98	116.23	112.19
10	aD	6	MAN	C1-O5-C5	2.98	116.23	112.19
19	fE	8	MAN	C1-O5-C5	2.98	116.23	112.19
9	aH	5	MAN	C1-O5-C5	2.97	116.22	112.19
17	fC	10	MAN	C1-O5-C5	2.97	116.22	112.19
17	fN	11	MAN	C1-O5-C5	2.96	116.21	112.19
19	fB	6	MAN	C1-O5-C5	2.96	116.20	112.19
19	fO	8	MAN	C1-O5-C5	2.96	116.20	112.19
20	fK	13	MAN	C1-O5-C5	2.95	116.19	112.19
9	aM	15	MAN	C1-O5-C5	2.95	116.18	112.19
17	eC	11	MAN	C1-O5-C5	2.94	116.18	112.19
16	dA	2	MAN	C1-O5-C5	2.94	116.18	112.19
12	bG	8	MAN	C1-O5-C5	2.94	116.17	112.19
17	fN	10	MAN	C1-O5-C5	2.94	116.17	112.19
9	aH	2	NAG	C1-O5-C5	2.93	116.16	112.19
19	fE	4	MAN	C1-O5-C5	2.93	116.16	112.19
8	aB	9	BMA	C1-C2-C3	2.92	113.26	109.67
13	bE	5	MAN	C1-O5-C5	2.92	116.15	112.19
14	bF	5	MAN	C1-O5-C5	2.92	116.15	112.19
12	bG	6	MAN	C1-O5-C5	2.92	116.14	112.19
10	aD	7	MAN	C1-O5-C5	2.91	116.14	112.19
17	fH	11	MAN	C1-O5-C5	2.91	116.14	112.19
7	aA	14	MAN	C1-O5-C5	2.90	116.12	112.19
10	aI	9	MAN	C1-O5-C5	2.89	116.11	112.19
20	fP	11	XYS	C1-C2-C3	2.89	113.22	109.67
10	aI	6	MAN	C1-O5-C5	2.89	116.11	112.19
17	eA	7	MAN	C1-O5-C5	2.87	116.08	112.19
18	eB	11	NAG	C2-N2-C7	-2.87	118.82	122.90
19	fG	4	MAN	C1-O5-C5	2.85	116.05	112.19
17	fD	4	MAN	C1-O5-C5	2.84	116.05	112.19
11	aE	5	MAN	O5-C1-C2	2.84	115.15	110.77
8	aL	4	MAN	O2-C2-C3	-2.83	104.46	110.14
8	aB	16	MAN	C1-O5-C5	2.83	116.03	112.19
10	aD	8	MAN	C1-O5-C5	2.83	116.03	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	aN	4	MAN	C1-O5-C5	2.83	116.03	112.19
17	fN	4	MAN	O2-C2-C3	-2.83	104.47	110.14
17	eE	9	MAN	C1-O5-C5	2.82	116.02	112.19
17	eA	11	MAN	C1-O5-C5	2.82	116.01	112.19
18	eB	5	MAN	C1-O5-C5	2.82	116.01	112.19
19	fB	4	MAN	C1-O5-C5	2.81	116.00	112.19
13	bB	5	MAN	C1-O5-C5	2.80	115.99	112.19
9	aM	12	MAN	C1-O5-C5	2.79	115.97	112.19
17	fN	8	MAN	C1-O5-C5	2.79	115.97	112.19
15	cC	4	MAN	O5-C1-C2	2.78	115.07	110.77
9	aM	5	MAN	C1-O5-C5	2.78	115.96	112.19
11	aJ	10	MAN	O2-C2-C3	-2.78	104.56	110.14
11	aJ	4	MAN	C1-O5-C5	2.78	115.96	112.19
17	fD	9	MAN	C1-O5-C5	2.77	115.95	112.19
17	fC	8	MAN	C1-O5-C5	2.77	115.95	112.19
9	aC	15	MAN	C1-O5-C5	2.77	115.94	112.19
16	dC	6	MAN	C1-O5-C5	2.77	115.94	112.19
15	cB	2	MAN	C1-O5-C5	2.77	115.94	112.19
12	bG	7	MAN	C1-O5-C5	2.76	115.94	112.19
17	fI	4	MAN	C1-O5-C5	2.76	115.93	112.19
17	eA	10	MAN	C1-O5-C5	2.75	115.92	112.19
13	bH	5	MAN	O5-C1-C2	2.75	115.01	110.77
9	aH	7	MAN	O2-C2-C3	-2.75	104.64	110.14
9	aH	4	MAN	O2-C2-C3	-2.74	104.64	110.14
19	fE	6	MAN	C1-O5-C5	2.74	115.91	112.19
19	fL	9	MAN	C1-O5-C5	2.74	115.90	112.19
13	bH	4	MAN	C1-O5-C5	2.73	115.90	112.19
19	fJ	9	MAN	C1-O5-C5	2.73	115.90	112.19
7	aA	2	NAG	C1-O5-C5	2.73	115.89	112.19
17	eA	9	MAN	C1-O5-C5	2.73	115.89	112.19
8	aB	4	MAN	O2-C2-C3	-2.73	104.66	110.14
18	eD	5	MAN	C1-O5-C5	2.73	115.89	112.19
17	fM	6	MAN	C1-O5-C5	2.73	115.89	112.19
20	fK	7	XYS	C1-C2-C3	2.73	113.02	109.67
16	dB	3	MAN	O2-C2-C3	-2.72	104.69	110.14
17	fC	11	MAN	C1-O5-C5	2.72	115.88	112.19
19	fL	6	MAN	O5-C1-C2	2.71	114.96	110.77
14	bF	5	MAN	O5-C1-C2	2.71	114.96	110.77
16	dB	4	MAN	O5-C1-C2	2.71	114.96	110.77
17	fI	4	MAN	O2-C2-C3	-2.71	104.71	110.14
17	eC	8	MAN	C1-O5-C5	2.71	115.86	112.19
18	eB	4	MAN	O5-C1-C2	2.71	114.95	110.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	fP	9	MAN	C1-O5-C5	2.71	115.86	112.19
19	fO	5	MAN	C1-O5-C5	2.71	115.86	112.19
14	bI	2	NAG	C1-O5-C5	2.70	115.86	112.19
19	fJ	5	MAN	C1-O5-C5	2.70	115.85	112.19
17	eC	10	MAN	C1-O5-C5	2.70	115.85	112.19
7	aA	10	MAN	C1-O5-C5	2.69	115.84	112.19
17	fI	10	MAN	C1-O5-C5	2.69	115.84	112.19
17	fM	10	MAN	O2-C2-C3	-2.69	104.75	110.14
16	dA	2	MAN	O5-C1-C2	2.68	114.91	110.77
7	aK	13	MAN	C1-O5-C5	2.68	115.82	112.19
15	cA	4	MAN	O5-C1-C2	2.67	114.90	110.77
16	dB	7	MAN	C1-O5-C5	2.67	115.81	112.19
8	aL	4	MAN	C1-O5-C5	2.66	115.80	112.19
7	aF	5	MAN	O5-C1-C2	2.66	114.87	110.77
19	fL	7	MAN	O2-C2-C3	-2.65	104.82	110.14
10	aD	9	MAN	O5-C1-C2	2.65	114.87	110.77
17	fM	2	NAG	C1-O5-C5	2.65	115.79	112.19
20	fK	9	MAN	C1-O5-C5	2.65	115.79	112.19
9	aM	12	MAN	O2-C2-C3	-2.65	104.83	110.14
17	fM	5	MAN	C1-O5-C5	2.65	115.78	112.19
17	fI	7	MAN	O5-C1-C2	2.65	114.86	110.77
8	aG	4	MAN	C1-O5-C5	2.64	115.78	112.19
8	aL	7	MAN	O5-C1-C2	2.64	114.85	110.77
19	fB	5	MAN	C1-O5-C5	2.64	115.76	112.19
12	bA	7	MAN	C1-O5-C5	2.63	115.76	112.19
18	eD	11	NAG	C1-O5-C5	2.63	115.76	112.19
16	dC	4	MAN	O5-C1-C2	2.63	114.83	110.77
20	fF	13	MAN	C1-O5-C5	2.63	115.75	112.19
7	aF	13	MAN	C1-O5-C5	2.63	115.75	112.19
17	fC	5	MAN	C1-O5-C5	2.62	115.75	112.19
13	bH	4	MAN	O2-C2-C3	-2.62	104.88	110.14
15	cC	3	MAN	C1-O5-C5	2.62	115.74	112.19
16	dB	2	MAN	C1-O5-C5	2.62	115.74	112.19
17	fN	4	MAN	C1-O5-C5	2.62	115.74	112.19
10	aD	5	MAN	O2-C2-C3	-2.62	104.90	110.14
17	eA	7	MAN	O2-C2-C3	-2.62	104.90	110.14
17	fN	9	MAN	C1-O5-C5	2.61	115.73	112.19
15	cA	3	MAN	C1-O5-C5	2.61	115.73	112.19
16	dB	2	MAN	O5-C1-C2	2.61	114.80	110.77
11	aE	14	BMA	O2-C2-C3	-2.61	104.91	110.14
12	bD	4	MAN	C1-O5-C5	2.61	115.72	112.19
13	bE	4	MAN	C1-O5-C5	2.60	115.72	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	eA	5	MAN	C1-O5-C5	2.60	115.72	112.19
10	aN	5	MAN	O2-C2-C3	-2.60	104.93	110.14
11	aJ	5	MAN	O2-C2-C3	-2.60	104.94	110.14
7	aA	13	MAN	C1-O5-C5	2.60	115.71	112.19
10	aD	7	MAN	O2-C2-C3	-2.59	104.94	110.14
14	bI	8	MAN	O2-C2-C3	-2.59	104.94	110.14
9	aM	5	MAN	O2-C2-C3	-2.59	104.95	110.14
7	aA	8	MAN	C1-O5-C5	2.59	115.70	112.19
16	dB	5	MAN	O2-C2-C3	-2.59	104.96	110.14
17	fD	4	MAN	O2-C2-C3	-2.57	104.98	110.14
16	dC	6	MAN	O2-C2-C3	-2.57	104.99	110.14
11	aO	5	MAN	O5-C1-C2	2.57	114.73	110.77
17	eE	10	MAN	C1-O5-C5	2.57	115.67	112.19
9	aC	16	MAN	C1-O5-C5	2.56	115.67	112.19
12	bG	4	MAN	C1-O5-C5	2.56	115.67	112.19
7	aK	12	XYP	C5-C4-C3	2.56	112.82	109.67
18	eD	14	MAN	C1-O5-C5	2.56	115.66	112.19
18	eB	14	MAN	O2-C2-C3	-2.56	105.01	110.14
16	dA	6	MAN	O2-C2-C3	-2.56	105.02	110.14
14	bF	9	BMA	O2-C2-C3	-2.55	105.02	110.14
8	aG	5	MAN	O2-C2-C3	-2.55	105.02	110.14
9	aC	16	MAN	O2-C2-C3	-2.55	105.02	110.14
18	eD	10	MAN	C1-O5-C5	2.55	115.65	112.19
16	dA	3	MAN	O2-C2-C3	-2.55	105.03	110.14
18	eF	5	MAN	C1-O5-C5	2.55	115.64	112.19
8	aG	7	MAN	O2-C2-C3	-2.54	105.04	110.14
12	bD	8	MAN	C1-O5-C5	2.54	115.63	112.19
12	bD	5	MAN	C1-O5-C5	2.54	115.63	112.19
12	bG	5	MAN	O5-C1-C2	2.54	114.68	110.77
9	aM	14	XYP	C5-C4-C3	2.54	112.78	109.67
7	aK	5	MAN	C1-O5-C5	2.53	115.63	112.19
10	aD	8	MAN	O2-C2-C3	-2.53	105.06	110.14
20	fP	4	MAN	C1-O5-C5	2.53	115.62	112.19
17	fH	6	MAN	O2-C2-C3	-2.53	105.07	110.14
9	aC	7	MAN	O5-C1-C2	2.53	114.67	110.77
19	fE	10	MAN	O2-C2-C3	-2.53	105.08	110.14
7	aF	14	MAN	C1-O5-C5	2.52	115.61	112.19
17	fM	7	MAN	C1-O5-C5	2.52	115.61	112.19
9	aC	14	XYP	C1-C2-C3	2.52	112.76	109.67
19	fG	7	MAN	O2-C2-C3	-2.51	105.10	110.14
20	fK	10	NAG	C2-N2-C7	-2.51	119.33	122.90
16	dB	6	MAN	O2-C2-C3	-2.51	105.12	110.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	fC	6	MAN	O2-C2-C3	-2.51	105.12	110.14
18	eB	14	MAN	C1-O5-C5	2.50	115.59	112.19
19	fE	5	MAN	C1-O5-C5	2.50	115.59	112.19
19	fO	9	MAN	C1-O5-C5	2.50	115.59	112.19
17	fN	10	MAN	O2-C2-C3	-2.50	105.12	110.14
17	eC	5	MAN	C1-O5-C5	2.50	115.58	112.19
12	bD	5	MAN	O5-C1-C2	2.50	114.62	110.77
20	fF	4	MAN	O2-C2-C3	-2.49	105.14	110.14
20	fP	7	XYS	C1-C2-C3	2.49	112.73	109.67
14	bI	5	MAN	O2-C2-C3	-2.49	105.14	110.14
13	bB	2	NAG	C1-O5-C5	2.49	115.57	112.19
17	fI	11	MAN	C1-O5-C5	2.49	115.56	112.19
14	bI	5	MAN	O5-C1-C2	2.49	114.61	110.77
14	bC	9	BMA	C1-O5-C5	2.49	115.56	112.19
17	eE	8	MAN	C1-O5-C5	2.49	115.56	112.19
10	aN	6	MAN	C1-O5-C5	2.49	115.56	112.19
18	eF	11	NAG	C2-N2-C7	-2.49	119.36	122.90
9	aH	12	MAN	O2-C2-C3	-2.48	105.16	110.14
11	aE	4	MAN	C1-O5-C5	2.48	115.56	112.19
12	bA	5	MAN	O2-C2-C3	-2.48	105.18	110.14
20	fK	2	NAG	C1-O5-C5	2.47	115.54	112.19
19	fL	10	MAN	O2-C2-C3	-2.47	105.19	110.14
7	aF	10	MAN	C1-O5-C5	2.47	115.53	112.19
7	aK	11	NAG	C1-O5-C5	2.46	115.53	112.19
13	bH	5	MAN	O2-C2-C3	-2.46	105.20	110.14
11	aJ	15	MAN	C1-O5-C5	2.46	115.53	112.19
17	fN	8	MAN	O2-C2-C3	-2.46	105.21	110.14
15	cB	4	MAN	O5-C1-C2	2.46	114.56	110.77
17	fC	7	MAN	C1-O5-C5	2.46	115.52	112.19
17	fH	7	MAN	C1-O5-C5	2.45	115.52	112.19
17	fC	4	MAN	O5-C1-C2	2.45	114.55	110.77
16	dB	7	MAN	O5-C1-C2	2.45	114.55	110.77
9	aM	7	MAN	O2-C2-C3	-2.45	105.23	110.14
12	bA	7	MAN	O2-C2-C3	-2.44	105.24	110.14
8	aB	11	MAN	C1-O5-C5	2.44	115.50	112.19
17	eA	8	MAN	C1-O5-C5	2.44	115.50	112.19
8	aL	7	MAN	O2-C2-C3	-2.44	105.25	110.14
13	bB	5	MAN	O2-C2-C3	-2.44	105.25	110.14
17	fI	9	MAN	C1-O5-C5	2.44	115.50	112.19
10	aN	9	MAN	O5-C1-C2	2.42	114.51	110.77
7	aF	6	XYP	O2-C2-C3	2.42	114.99	110.14
18	eF	14	MAN	O2-C2-C3	-2.42	105.29	110.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	fJ	8	MAN	C1-O5-C5	2.42	115.47	112.19
12	bD	7	MAN	O2-C2-C3	-2.42	105.29	110.14
17	eC	6	MAN	O5-C1-C2	2.42	114.51	110.77
17	fC	6	MAN	C1-O5-C5	2.42	115.47	112.19
10	aI	9	MAN	O5-C1-C2	2.42	114.50	110.77
9	aH	7	MAN	O5-C1-C2	2.42	114.50	110.77
18	eB	11	NAG	C1-O5-C5	2.42	115.47	112.19
15	cC	4	MAN	O2-C2-C3	-2.41	105.30	110.14
7	aK	13	MAN	O2-C2-C3	-2.41	105.31	110.14
19	fE	8	MAN	O5-C1-C2	2.41	114.49	110.77
19	fL	2	NAG	C3-C4-C5	2.41	114.53	110.24
17	fI	8	MAN	C1-O5-C5	2.40	115.45	112.19
17	fH	11	MAN	O2-C2-C3	-2.40	105.33	110.14
20	fK	4	MAN	O2-C2-C3	-2.40	105.33	110.14
19	fG	9	MAN	C1-O5-C5	2.40	115.45	112.19
14	bC	7	XYS	C1-C2-C3	2.40	112.62	109.67
16	dC	3	MAN	O2-C2-C3	-2.40	105.33	110.14
8	aG	5	MAN	O5-C1-C2	2.40	114.47	110.77
16	dC	5	MAN	O2-C2-C3	-2.40	105.33	110.14
14	bC	4	MAN	O5-C1-C2	2.40	114.47	110.77
17	eE	6	MAN	O2-C2-C3	-2.40	105.34	110.14
9	aM	4	MAN	O5-C1-C2	2.40	114.47	110.77
11	aE	14	BMA	C1-C2-C3	-2.39	106.72	109.67
17	eE	6	MAN	C1-O5-C5	2.39	115.43	112.19
20	fP	11	XYS	C5-O5-C1	2.39	115.20	111.52
18	eF	4	MAN	C1-O5-C5	2.39	115.42	112.19
14	bC	9	BMA	O2-C2-C3	-2.38	105.36	110.14
19	fE	7	MAN	O2-C2-C3	-2.38	105.37	110.14
18	eB	1	NAG	O5-C5-C6	2.38	110.93	107.20
17	fN	3	BMA	C1-C2-C3	2.38	112.59	109.67
7	aK	8	MAN	C1-O5-C5	2.38	115.41	112.19
12	bA	5	MAN	O5-C1-C2	2.37	114.44	110.77
18	eD	14	MAN	O2-C2-C3	-2.37	105.38	110.14
10	aI	5	MAN	O2-C2-C3	-2.37	105.38	110.14
17	fM	8	MAN	C1-O5-C5	2.37	115.41	112.19
17	fD	4	MAN	O5-C1-C2	2.37	114.43	110.77
15	cA	2	MAN	O5-C1-C2	2.37	114.43	110.77
11	aO	4	MAN	O2-C2-C3	-2.37	105.40	110.14
17	eE	9	MAN	O2-C2-C3	-2.37	105.40	110.14
11	aO	15	MAN	O2-C2-C3	-2.37	105.40	110.14
18	eD	4	MAN	C1-O5-C5	2.37	115.40	112.19
19	fE	9	MAN	C1-O5-C5	2.36	115.39	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	fB	1	NAG	C2-N2-C7	-2.36	119.54	122.90
10	aI	5	MAN	C1-O5-C5	2.36	115.39	112.19
20	fF	4	MAN	C1-O5-C5	2.36	115.39	112.19
7	aK	14	MAN	C1-O5-C5	2.36	115.39	112.19
17	fD	7	MAN	C1-O5-C5	2.36	115.39	112.19
9	aC	6	NAG	C1-O5-C5	2.36	115.39	112.19
10	aN	6	MAN	O5-C1-C2	2.36	114.41	110.77
7	aK	4	MAN	O2-C2-C3	-2.35	105.42	110.14
9	aC	7	MAN	O2-C2-C3	-2.35	105.44	110.14
12	bD	7	MAN	C1-O5-C5	2.34	115.37	112.19
17	fM	6	MAN	O2-C2-C3	-2.34	105.45	110.14
12	bG	4	MAN	O5-C1-C2	2.34	114.38	110.77
16	dA	4	MAN	O5-C1-C2	2.34	114.38	110.77
19	fL	10	MAN	C1-O5-C5	2.34	115.36	112.19
19	fO	10	MAN	O2-C2-C3	-2.33	105.47	110.14
8	aL	5	MAN	O2-C2-C3	-2.33	105.47	110.14
17	eA	10	MAN	O2-C2-C3	-2.32	105.48	110.14
9	aC	13	NAG	C1-O5-C5	2.32	115.34	112.19
19	fB	6	MAN	O5-C1-C2	2.32	114.35	110.77
14	bI	10	MAN	O2-C2-C3	-2.32	105.49	110.14
14	bC	5	MAN	O5-C1-C2	2.32	114.35	110.77
17	eC	6	MAN	O2-C2-C3	-2.32	105.50	110.14
19	fE	5	MAN	O2-C2-C3	-2.31	105.50	110.14
8	aB	5	MAN	O5-C1-C2	2.31	114.34	110.77
17	eE	11	MAN	C1-O5-C5	2.31	115.32	112.19
13	bH	2	NAG	C1-O5-C5	2.31	115.32	112.19
19	fB	10	MAN	C1-O5-C5	2.31	115.32	112.19
7	aK	5	MAN	O5-C1-C2	2.30	114.33	110.77
11	aJ	14	BMA	O2-C2-C3	-2.30	105.53	110.14
16	dA	5	MAN	O2-C2-C3	-2.30	105.53	110.14
17	fN	5	MAN	C1-O5-C5	2.30	115.31	112.19
19	fB	7	MAN	O2-C2-C3	-2.30	105.53	110.14
9	aC	12	MAN	O2-C2-C3	-2.30	105.53	110.14
7	aK	14	MAN	O2-C2-C3	-2.30	105.54	110.14
19	fG	10	MAN	C1-O5-C5	2.29	115.30	112.19
10	aI	7	MAN	O5-C1-C2	2.29	114.31	110.77
12	bG	6	MAN	O2-C2-C3	-2.29	105.55	110.14
17	eE	11	MAN	O2-C2-C3	-2.29	105.55	110.14
7	aA	5	MAN	O2-C2-C3	-2.29	105.55	110.14
13	bB	4	MAN	O2-C2-C3	-2.29	105.55	110.14
16	dC	2	MAN	C1-O5-C5	2.29	115.29	112.19
7	aF	12	XYP	C5-C4-C3	2.29	112.48	109.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	eE	4	MAN	O2-C2-C3	-2.29	105.56	110.14
12	bA	8	MAN	C1-O5-C5	2.29	115.29	112.19
9	aH	15	MAN	O2-C2-C3	-2.28	105.56	110.14
17	fD	5	MAN	C1-O5-C5	2.28	115.29	112.19
14	bF	8	MAN	O2-C2-C3	-2.28	105.56	110.14
7	aF	8	MAN	O2-C2-C3	-2.28	105.56	110.14
20	fP	5	MAN	O2-C2-C3	-2.28	105.57	110.14
19	fO	10	MAN	C1-O5-C5	2.28	115.28	112.19
15	cB	3	MAN	C1-O5-C5	2.28	115.28	112.19
10	aD	5	MAN	C1-O5-C5	2.28	115.28	112.19
16	dA	7	MAN	O2-C2-C3	-2.28	105.58	110.14
19	fE	4	MAN	O2-C2-C3	-2.28	105.58	110.14
19	fJ	6	MAN	O2-C2-C3	-2.27	105.58	110.14
17	eC	9	MAN	O2-C2-C3	-2.27	105.58	110.14
17	fM	10	MAN	O5-C1-C2	2.27	114.28	110.77
8	aB	7	MAN	O2-C2-C3	-2.27	105.59	110.14
10	aN	4	MAN	O2-C2-C3	-2.27	105.59	110.14
12	bD	9	MAN	C1-O5-C5	2.27	115.27	112.19
17	eE	5	MAN	O2-C2-C3	-2.27	105.59	110.14
17	fI	6	MAN	O2-C2-C3	-2.27	105.60	110.14
19	fJ	10	MAN	O2-C2-C3	-2.27	105.60	110.14
12	bA	3	BMA	C1-O5-C5	2.27	115.26	112.19
10	aN	5	MAN	C1-O5-C5	2.27	115.26	112.19
11	aE	15	MAN	O2-C2-C3	-2.27	105.60	110.14
7	aA	4	MAN	O2-C2-C3	-2.26	105.60	110.14
9	aC	7	MAN	C1-O5-C5	2.26	115.26	112.19
20	fP	2	NAG	C1-O5-C5	2.26	115.26	112.19
17	eC	7	MAN	O2-C2-C3	-2.26	105.60	110.14
17	fH	8	MAN	O2-C2-C3	-2.26	105.61	110.14
19	fG	8	MAN	C1-O5-C5	2.26	115.26	112.19
19	fE	6	MAN	O2-C2-C3	-2.26	105.61	110.14
15	cC	3	MAN	O2-C2-C3	-2.26	105.61	110.14
18	eB	10	MAN	O2-C2-C3	-2.26	105.61	110.14
16	dC	7	MAN	C1-O5-C5	2.26	115.25	112.19
19	fB	10	MAN	O2-C2-C3	-2.26	105.61	110.14
17	eA	8	MAN	O2-C2-C3	-2.26	105.62	110.14
11	aE	5	MAN	O2-C2-C3	-2.26	105.62	110.14
12	bA	4	MAN	C1-O5-C5	2.26	115.25	112.19
18	eF	5	MAN	O2-C2-C3	-2.25	105.62	110.14
12	bD	3	BMA	C1-O5-C5	2.25	115.24	112.19
8	aB	7	MAN	C1-O5-C5	2.25	115.24	112.19
14	bF	4	MAN	C1-O5-C5	2.25	115.24	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	fO	7	MAN	O2-C2-C3	-2.25	105.63	110.14
17	eA	1	NAG	C1-O5-C5	2.25	115.24	112.19
10	aN	7	MAN	O2-C2-C3	-2.25	105.64	110.14
14	bI	9	BMA	O2-C2-C3	-2.24	105.64	110.14
7	aK	8	MAN	O5-C1-C2	2.24	114.23	110.77
17	eC	3	BMA	C1-C2-C3	2.24	112.42	109.67
10	aD	3	BMA	O5-C1-C2	2.24	114.23	110.77
17	eC	7	MAN	O5-C1-C2	2.24	114.23	110.77
17	fH	9	MAN	O2-C2-C3	-2.24	105.65	110.14
11	aO	11	NAG	C2-N2-C7	2.24	126.09	122.90
19	fB	2	NAG	C2-N2-C7	2.23	126.08	122.90
7	aA	8	MAN	O2-C2-C3	-2.23	105.67	110.14
9	aH	12	MAN	O5-C1-C2	2.23	114.21	110.77
17	fC	9	MAN	O2-C2-C3	-2.23	105.67	110.14
12	bA	8	MAN	O2-C2-C3	-2.22	105.68	110.14
17	eC	5	MAN	O2-C2-C3	-2.22	105.69	110.14
9	aH	5	MAN	O2-C2-C3	-2.22	105.69	110.14
20	fP	14	MAN	C1-O5-C5	2.22	115.20	112.19
20	fK	13	MAN	O2-C2-C3	-2.22	105.70	110.14
7	aF	1	NAG	C2-N2-C7	-2.22	119.75	122.90
10	aD	7	MAN	O5-C1-C2	2.21	114.19	110.77
14	bF	9	BMA	C1-O5-C5	2.21	115.19	112.19
17	fH	8	MAN	C1-O5-C5	2.21	115.19	112.19
9	aH	16	MAN	O2-C2-C3	-2.21	105.70	110.14
19	fJ	4	MAN	O5-C1-C2	2.21	114.19	110.77
19	fB	9	MAN	O2-C2-C3	-2.21	105.71	110.14
14	bC	3	BMA	C1-C2-C3	2.21	112.38	109.67
7	aF	5	MAN	O2-C2-C3	-2.21	105.71	110.14
7	aK	10	MAN	O2-C2-C3	-2.21	105.71	110.14
14	bC	10	MAN	O2-C2-C3	-2.21	105.71	110.14
20	fK	14	MAN	O2-C2-C3	-2.21	105.72	110.14
7	aF	3	BMA	C1-O5-C5	2.20	115.18	112.19
17	fM	9	MAN	O2-C2-C3	-2.20	105.73	110.14
7	aA	14	MAN	O2-C2-C3	-2.20	105.73	110.14
19	fL	7	MAN	O5-C1-C2	2.19	114.16	110.77
8	aL	16	MAN	O2-C2-C3	-2.19	105.75	110.14
14	bF	4	MAN	O2-C2-C3	-2.19	105.75	110.14
16	dC	2	MAN	O5-C1-C2	2.19	114.15	110.77
17	eC	10	MAN	O2-C2-C3	-2.19	105.75	110.14
7	aK	7	XYP	C1-C2-C3	2.19	112.36	109.67
17	eA	4	MAN	O2-C2-C3	-2.19	105.75	110.14
20	fF	11	XYS	C5-O5-C1	2.19	114.89	111.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	fD	10	MAN	O5-C1-C2	2.19	114.15	110.77
9	aH	12	MAN	C1-O5-C5	2.19	115.16	112.19
17	eC	8	MAN	O2-C2-C3	-2.19	105.76	110.14
9	aC	15	MAN	O2-C2-C3	-2.19	105.76	110.14
14	bC	8	MAN	O2-C2-C3	-2.19	105.76	110.14
15	cA	4	MAN	O2-C2-C3	-2.19	105.76	110.14
7	aF	14	MAN	O2-C2-C3	-2.18	105.76	110.14
17	fC	11	MAN	O2-C2-C3	-2.18	105.77	110.14
8	aB	5	MAN	O2-C2-C3	-2.18	105.77	110.14
20	fP	5	MAN	O5-C1-C2	2.18	114.13	110.77
12	bG	7	MAN	O2-C2-C3	-2.18	105.77	110.14
17	eA	6	MAN	O2-C2-C3	-2.18	105.78	110.14
18	eD	10	MAN	O2-C2-C3	-2.17	105.78	110.14
8	aL	11	MAN	O2-C2-C3	-2.17	105.79	110.14
11	aO	15	MAN	C1-O5-C5	2.17	115.13	112.19
17	fM	4	MAN	O2-C2-C3	-2.17	105.79	110.14
7	aF	13	MAN	O2-C2-C3	-2.17	105.79	110.14
17	eC	4	MAN	O2-C2-C3	-2.17	105.80	110.14
17	fI	10	MAN	O2-C2-C3	-2.17	105.80	110.14
17	fN	9	MAN	O2-C2-C3	-2.17	105.80	110.14
13	bE	5	MAN	O2-C2-C3	-2.16	105.81	110.14
17	eA	6	MAN	C1-O5-C5	2.16	115.12	112.19
18	eF	10	MAN	O2-C2-C3	-2.16	105.81	110.14
18	eD	8	BGC	C1-C2-C3	2.16	112.32	109.67
9	aH	15	MAN	O5-C1-C2	2.16	114.10	110.77
17	fC	8	MAN	O2-C2-C3	-2.16	105.82	110.14
9	aC	5	MAN	O2-C2-C3	-2.16	105.82	110.14
18	eF	14	MAN	C1-O5-C5	2.15	115.11	112.19
7	aA	14	MAN	O5-C1-C2	2.15	114.09	110.77
17	fH	5	MAN	C1-O5-C5	2.15	115.11	112.19
17	eA	11	MAN	O5-C1-C2	2.15	114.09	110.77
11	aE	10	MAN	O2-C2-C3	-2.15	105.83	110.14
7	aA	10	MAN	O2-C2-C3	-2.15	105.83	110.14
20	fK	4	MAN	C1-O5-C5	2.15	115.10	112.19
14	bF	7	XYS	C1-C2-C3	2.15	112.30	109.67
9	aM	15	MAN	O5-C1-C2	2.15	114.08	110.77
18	eD	5	MAN	O2-C2-C3	-2.14	105.84	110.14
19	fG	8	MAN	O5-C1-C2	2.14	114.08	110.77
20	fF	5	MAN	O5-C1-C2	2.14	114.07	110.77
8	aG	4	MAN	O2-C2-C3	-2.14	105.85	110.14
11	aJ	14	BMA	C1-C2-C3	-2.14	107.04	109.67
18	eF	4	MAN	C3-C4-C5	-2.13	106.43	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	fG	6	MAN	O5-C1-C2	2.13	114.06	110.77
12	bD	6	MAN	O2-C2-C3	-2.13	105.87	110.14
11	aJ	4	MAN	O2-C2-C3	-2.13	105.87	110.14
17	fM	11	MAN	O2-C2-C3	-2.13	105.87	110.14
18	eB	7	XYS	C1-C2-C3	2.13	112.28	109.67
11	aO	14	BMA	O2-C2-C3	-2.13	105.87	110.14
17	eE	7	MAN	O2-C2-C3	-2.13	105.88	110.14
14	bF	8	MAN	C1-O5-C5	2.12	115.07	112.19
7	aF	4	MAN	O2-C2-C3	-2.12	105.88	110.14
16	dA	2	MAN	O2-C2-C3	-2.12	105.88	110.14
8	aB	1	NAG	O5-C5-C6	2.12	110.53	107.20
9	aC	4	MAN	O5-C1-C2	2.12	114.05	110.77
7	aF	11	NAG	C1-O5-C5	2.12	115.07	112.19
20	fK	14	MAN	C1-O5-C5	2.12	115.06	112.19
19	fE	4	MAN	O5-C1-C2	2.12	114.04	110.77
14	bI	10	MAN	C1-O5-C5	2.12	115.06	112.19
13	bB	5	MAN	O5-C1-C2	2.12	114.04	110.77
19	fO	8	MAN	O5-C1-C2	2.12	114.04	110.77
17	fI	11	MAN	O2-C2-C3	-2.12	105.90	110.14
7	aA	5	MAN	O5-C1-C2	2.12	114.04	110.77
14	bF	10	MAN	O2-C2-C3	-2.12	105.90	110.14
17	fD	9	MAN	O5-C1-C2	2.12	114.04	110.77
8	aB	10	XYP	C1-C2-C3	2.11	112.26	109.67
8	aL	10	XYP	C1-C2-C3	2.11	112.26	109.67
8	aG	16	MAN	O2-C2-C3	-2.11	105.91	110.14
16	dC	4	MAN	O2-C2-C3	-2.11	105.91	110.14
17	eA	7	MAN	O5-C1-C2	2.11	114.03	110.77
18	eB	10	MAN	C1-O5-C5	2.11	115.05	112.19
19	fB	9	MAN	C1-O5-C5	2.11	115.05	112.19
17	fI	9	MAN	O2-C2-C3	-2.11	105.91	110.14
9	aC	15	MAN	O5-C1-C2	2.11	114.02	110.77
8	aB	3	BMA	O5-C5-C6	2.11	110.51	107.20
7	aF	8	MAN	C1-O5-C5	2.10	115.04	112.19
8	aL	3	BMA	O5-C5-C6	2.10	110.50	107.20
18	eD	5	MAN	C3-C4-C5	-2.10	106.49	110.24
19	fO	4	MAN	O2-C2-C3	-2.10	105.94	110.14
19	fO	6	MAN	O2-C2-C3	-2.09	105.94	110.14
19	fL	8	MAN	O5-C1-C2	2.09	114.00	110.77
18	eF	10	MAN	C1-O5-C5	2.09	115.03	112.19
19	fJ	1	NAG	C1-O5-C5	2.09	115.03	112.19
17	fN	7	MAN	O5-C1-C2	2.09	113.99	110.77
17	fI	4	MAN	O5-C1-C2	2.09	113.99	110.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	fC	10	MAN	O2-C2-C3	-2.09	105.96	110.14
9	aH	10	XYP	C1-C2-C3	2.08	112.23	109.67
15	cB	3	MAN	O5-C1-C2	2.08	113.98	110.77
7	aF	7	XYP	C1-C2-C3	2.08	112.22	109.67
7	aA	4	MAN	O5-C1-C2	2.08	113.98	110.77
9	aM	7	MAN	O5-C1-C2	2.08	113.97	110.77
14	bF	2	NAG	C1-O5-C5	2.08	115.00	112.19
19	fL	4	MAN	O2-C2-C3	-2.07	105.98	110.14
8	aB	4	MAN	C1-O5-C5	2.07	115.00	112.19
8	aB	13	BMA	O5-C5-C6	2.07	110.45	107.20
19	fO	5	MAN	O2-C2-C3	-2.07	105.99	110.14
12	bD	8	MAN	O5-C1-C2	2.07	113.97	110.77
17	fN	11	MAN	O5-C1-C2	2.07	113.97	110.77
14	bI	4	MAN	O2-C2-C3	-2.07	105.99	110.14
17	fH	4	MAN	O2-C2-C3	-2.07	105.99	110.14
9	aH	7	MAN	C1-O5-C5	2.07	115.00	112.19
13	bE	4	MAN	O5-C1-C2	2.07	113.96	110.77
7	aF	2	NAG	C1-O5-C5	2.07	114.99	112.19
20	fP	4	MAN	O5-C1-C2	2.06	113.96	110.77
17	eC	10	MAN	O5-C1-C2	2.06	113.95	110.77
17	fI	8	MAN	O2-C2-C3	-2.06	106.01	110.14
19	fO	4	MAN	O5-C1-C2	2.06	113.95	110.77
9	aH	6	NAG	C2-N2-C7	-2.06	119.97	122.90
19	fJ	5	MAN	O5-C1-C2	2.06	113.94	110.77
13	bH	1	NAG	O5-C5-C6	2.05	110.42	107.20
17	fM	7	MAN	O2-C2-C3	-2.05	106.03	110.14
15	cA	3	MAN	O2-C2-C3	-2.05	106.03	110.14
17	fN	5	MAN	O2-C2-C3	-2.05	106.03	110.14
9	aH	14	XYP	C1-C2-C3	2.05	112.19	109.67
10	aD	6	MAN	O2-C2-C3	-2.05	106.03	110.14
16	dA	7	MAN	O5-C1-C2	2.04	113.93	110.77
19	fG	1	NAG	C2-N2-C7	-2.04	119.99	122.90
10	aI	7	MAN	O2-C2-C3	-2.04	106.04	110.14
12	bG	9	MAN	C1-O5-C5	2.04	114.96	112.19
7	aK	2	NAG	C1-O5-C5	2.04	114.96	112.19
7	aA	4	MAN	C1-C2-C3	2.04	112.17	109.67
18	eD	4	MAN	C3-C4-C5	-2.04	106.60	110.24
11	aJ	3	BMA	C1-C2-C3	2.03	112.17	109.67
9	aH	4	MAN	O5-C5-C6	-2.03	104.02	107.20
20	fF	9	MAN	C1-O5-C5	2.03	114.95	112.19
17	fC	9	MAN	O5-C1-C2	2.03	113.91	110.77
17	eA	9	MAN	O2-C2-C3	-2.03	106.07	110.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	fI	5	MAN	C1-O5-C5	2.03	114.94	112.19
19	fB	8	MAN	O5-C1-C2	2.03	113.90	110.77
18	eB	5	MAN	O2-C2-C3	-2.03	106.08	110.14
19	fB	4	MAN	O2-C2-C3	-2.03	106.08	110.14
20	fF	13	MAN	O2-C2-C3	-2.02	106.08	110.14
17	fD	8	MAN	O2-C2-C3	-2.02	106.09	110.14
19	fB	8	MAN	O2-C2-C3	-2.02	106.09	110.14
16	dA	6	MAN	C1-O5-C5	2.02	114.93	112.19
19	fG	7	MAN	O5-C1-C2	2.02	113.89	110.77
8	aB	16	MAN	O2-C2-C3	-2.02	106.10	110.14
8	aG	9	BMA	C1-O5-C5	2.02	114.92	112.19
7	aK	8	MAN	O2-C2-C3	-2.02	106.10	110.14
10	aN	8	MAN	O2-C2-C3	-2.02	106.10	110.14
12	bG	8	MAN	O2-C2-C3	-2.01	106.10	110.14
17	fD	9	MAN	O2-C2-C3	-2.01	106.11	110.14
9	aM	5	MAN	C1-C2-C3	-2.01	107.19	109.67
17	eE	3	BMA	C1-O5-C5	2.01	114.92	112.19
7	aA	3	BMA	C1-O5-C5	2.01	114.92	112.19
8	aG	9	BMA	O5-C5-C6	2.01	110.36	107.20
20	fP	4	MAN	O2-C2-C3	-2.01	106.11	110.14
10	aI	4	MAN	O2-C2-C3	-2.01	106.12	110.14
14	bC	3	BMA	C3-C4-C5	-2.00	106.66	110.24

There are no chirality outliers.

All (241) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	aE	11	NAG	C8-C7-N2-C2
11	aE	11	NAG	O7-C7-N2-C2
11	aJ	11	NAG	C3-C2-N2-C7
11	aJ	11	NAG	C8-C7-N2-C2
11	aJ	11	NAG	O7-C7-N2-C2
11	aO	11	NAG	C1-C2-N2-C7
11	aO	11	NAG	C8-C7-N2-C2
11	aO	11	NAG	O7-C7-N2-C2
19	fO	1	NAG	C8-C7-N2-C2
12	bA	8	MAN	O5-C5-C6-O6
10	aI	6	MAN	O5-C5-C6-O6
14	bC	4	MAN	C4-C5-C6-O6
11	aO	4	MAN	C4-C5-C6-O6
13	bE	4	MAN	O5-C5-C6-O6
17	fH	9	MAN	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
19	fE	10	MAN	O5-C5-C6-O6
14	bF	4	MAN	C4-C5-C6-O6
11	aE	9	NAG	C8-C7-N2-C2
19	fO	1	NAG	O7-C7-N2-C2
13	bH	3	BMA	O5-C5-C6-O6
10	aI	6	MAN	C4-C5-C6-O6
17	fH	9	MAN	C4-C5-C6-O6
11	aO	5	MAN	O5-C5-C6-O6
16	dC	3	MAN	O5-C5-C6-O6
19	fB	10	MAN	O5-C5-C6-O6
10	aD	8	MAN	C4-C5-C6-O6
19	fE	10	MAN	C4-C5-C6-O6
19	fG	10	MAN	C4-C5-C6-O6
11	aE	4	MAN	O5-C5-C6-O6
11	aE	15	MAN	O5-C5-C6-O6
14	bI	4	MAN	O5-C5-C6-O6
18	eB	8	BGC	O5-C5-C6-O6
11	aO	5	MAN	C4-C5-C6-O6
19	fB	10	MAN	C4-C5-C6-O6
19	fG	10	MAN	O5-C5-C6-O6
19	fJ	7	MAN	C4-C5-C6-O6
10	aD	8	MAN	O5-C5-C6-O6
11	aO	4	MAN	O5-C5-C6-O6
14	bC	4	MAN	O5-C5-C6-O6
16	dB	3	MAN	O5-C5-C6-O6
17	fM	8	MAN	C4-C5-C6-O6
8	aB	12	NAG	C8-C7-N2-C2
11	aE	9	NAG	O7-C7-N2-C2
19	fE	1	NAG	C8-C7-N2-C2
19	fE	1	NAG	O7-C7-N2-C2
9	aH	4	MAN	O5-C5-C6-O6
14	bF	4	MAN	O5-C5-C6-O6
16	dC	6	MAN	O5-C5-C6-O6
17	eE	5	MAN	O5-C5-C6-O6
12	bA	8	MAN	C4-C5-C6-O6
17	fD	1	NAG	C4-C5-C6-O6
11	aE	11	NAG	C1-C2-N2-C7
14	bC	10	MAN	O5-C5-C6-O6
19	fJ	7	MAN	O5-C5-C6-O6
11	aE	15	MAN	C4-C5-C6-O6
13	bH	3	BMA	C4-C5-C6-O6
17	eC	2	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
17	fN	1	NAG	C4-C5-C6-O6
17	fC	11	MAN	C4-C5-C6-O6
18	eB	8	BGC	C4-C5-C6-O6
17	fM	8	MAN	O5-C5-C6-O6
16	dB	3	MAN	C4-C5-C6-O6
16	dC	6	MAN	C4-C5-C6-O6
10	aD	7	MAN	O5-C5-C6-O6
8	aB	12	NAG	O7-C7-N2-C2
19	fJ	1	NAG	C8-C7-N2-C2
19	fJ	1	NAG	O7-C7-N2-C2
7	aK	5	MAN	O5-C5-C6-O6
16	dA	6	MAN	O5-C5-C6-O6
9	aH	4	MAN	C4-C5-C6-O6
17	fI	4	MAN	O5-C5-C6-O6
18	eF	14	MAN	O5-C5-C6-O6
10	aN	7	MAN	C4-C5-C6-O6
14	bC	10	MAN	C4-C5-C6-O6
17	eC	9	MAN	C4-C5-C6-O6
17	fM	6	MAN	C4-C5-C6-O6
19	fL	9	MAN	C4-C5-C6-O6
7	aF	14	MAN	O5-C5-C6-O6
9	aC	11	BGC	O5-C5-C6-O6
13	bH	5	MAN	C4-C5-C6-O6
10	aD	7	MAN	C4-C5-C6-O6
8	aB	7	MAN	O5-C5-C6-O6
11	aJ	9	NAG	C8-C7-N2-C2
12	bD	9	MAN	O5-C5-C6-O6
17	fD	1	NAG	O5-C5-C6-O6
9	aH	11	BGC	O5-C5-C6-O6
17	eC	5	MAN	O5-C5-C6-O6
18	eD	8	BGC	O5-C5-C6-O6
13	bE	4	MAN	C4-C5-C6-O6
17	fC	11	MAN	O5-C5-C6-O6
19	fO	8	MAN	O5-C5-C6-O6
17	fI	4	MAN	C4-C5-C6-O6
7	aA	14	MAN	O5-C5-C6-O6
12	bA	9	MAN	O5-C5-C6-O6
19	fB	5	MAN	O5-C5-C6-O6
16	dA	6	MAN	C4-C5-C6-O6
16	dC	3	MAN	C4-C5-C6-O6
18	eF	14	MAN	C4-C5-C6-O6
12	bA	7	MAN	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
17	eC	2	NAG	O5-C5-C6-O6
17	fN	1	NAG	O5-C5-C6-O6
7	aF	14	MAN	C4-C5-C6-O6
7	aK	5	MAN	C4-C5-C6-O6
19	fO	8	MAN	C4-C5-C6-O6
17	fD	8	MAN	O5-C5-C6-O6
7	aA	14	MAN	C4-C5-C6-O6
17	fN	5	MAN	O5-C5-C6-O6
17	fC	7	MAN	C4-C5-C6-O6
17	fH	7	MAN	C4-C5-C6-O6
10	aN	8	MAN	O5-C5-C6-O6
17	eC	9	MAN	O5-C5-C6-O6
19	fG	5	MAN	C4-C5-C6-O6
10	aN	7	MAN	O5-C5-C6-O6
18	eB	14	MAN	O5-C5-C6-O6
17	fD	8	MAN	C4-C5-C6-O6
13	bH	5	MAN	O5-C5-C6-O6
17	fM	6	MAN	O5-C5-C6-O6
19	fL	9	MAN	O5-C5-C6-O6
16	dA	3	MAN	O5-C5-C6-O6
11	aJ	9	NAG	O7-C7-N2-C2
17	fD	9	MAN	O5-C5-C6-O6
11	aE	4	MAN	C4-C5-C6-O6
17	fN	5	MAN	C4-C5-C6-O6
17	fD	9	MAN	C4-C5-C6-O6
18	eB	14	MAN	C4-C5-C6-O6
19	fL	7	MAN	O5-C5-C6-O6
9	aH	12	MAN	O5-C5-C6-O6
19	fG	2	NAG	C4-C5-C6-O6
10	aI	5	MAN	O5-C5-C6-O6
13	bB	3	BMA	O5-C5-C6-O6
12	bD	9	MAN	C4-C5-C6-O6
15	cA	4	MAN	C4-C5-C6-O6
17	fH	1	NAG	C4-C5-C6-O6
17	fH	8	MAN	C4-C5-C6-O6
18	eB	11	NAG	C4-C5-C6-O6
13	bH	4	MAN	O5-C5-C6-O6
17	fI	9	MAN	O5-C5-C6-O6
8	aB	7	MAN	C4-C5-C6-O6
14	bI	10	MAN	C4-C5-C6-O6
10	aN	5	MAN	O5-C5-C6-O6
8	aB	2	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
19	fG	7	MAN	O5-C5-C6-O6
9	aM	13	NAG	C4-C5-C6-O6
17	fI	9	MAN	C4-C5-C6-O6
9	aM	11	BGC	O5-C5-C6-O6
11	aJ	4	MAN	O5-C5-C6-O6
13	bB	4	MAN	O5-C5-C6-O6
17	eE	5	MAN	C4-C5-C6-O6
10	aD	5	MAN	O5-C5-C6-O6
17	eA	5	MAN	O5-C5-C6-O6
17	fI	1	NAG	C4-C5-C6-O6
18	eD	8	BGC	C4-C5-C6-O6
11	aJ	15	MAN	O5-C5-C6-O6
17	fH	4	MAN	C4-C5-C6-O6
17	fN	9	MAN	C4-C5-C6-O6
19	fL	7	MAN	C4-C5-C6-O6
17	fN	9	MAN	O5-C5-C6-O6
16	dB	6	MAN	O5-C5-C6-O6
19	fG	5	MAN	O5-C5-C6-O6
8	aL	2	NAG	C4-C5-C6-O6
19	fG	7	MAN	C4-C5-C6-O6
19	fG	9	MAN	O5-C5-C6-O6
14	bI	4	MAN	C4-C5-C6-O6
17	fC	7	MAN	O5-C5-C6-O6
16	dC	7	MAN	O5-C5-C6-O6
19	fE	8	MAN	O5-C5-C6-O6
19	fB	5	MAN	C4-C5-C6-O6
16	dC	2	MAN	O5-C5-C6-O6
11	aE	5	MAN	C4-C5-C6-O6
16	dB	6	MAN	C4-C5-C6-O6
12	bA	9	MAN	C4-C5-C6-O6
16	dC	2	MAN	C4-C5-C6-O6
12	bA	7	MAN	C4-C5-C6-O6
15	cA	4	MAN	O5-C5-C6-O6
17	fH	7	MAN	O5-C5-C6-O6
9	aM	5	MAN	C4-C5-C6-O6
19	fE	8	MAN	C4-C5-C6-O6
20	fK	8	NAG	C8-C7-N2-C2
17	fH	8	MAN	O5-C5-C6-O6
14	bI	10	MAN	O5-C5-C6-O6
9	aC	6	NAG	C8-C7-N2-C2
10	aI	1	NAG	C8-C7-N2-C2
17	eE	2	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
16	dA	7	MAN	O5-C5-C6-O6
19	fJ	9	MAN	C4-C5-C6-O6
10	aI	1	NAG	O7-C7-N2-C2
17	fH	1	NAG	O5-C5-C6-O6
9	aM	16	MAN	O5-C5-C6-O6
17	fC	9	MAN	O5-C5-C6-O6
14	bF	10	MAN	O5-C5-C6-O6
17	fH	4	MAN	O5-C5-C6-O6
9	aH	11	BGC	C4-C5-C6-O6
20	fK	8	NAG	O7-C7-N2-C2
20	fK	14	MAN	C4-C5-C6-O6
9	aC	6	NAG	O7-C7-N2-C2
19	fB	2	NAG	C3-C2-N2-C7
19	fG	2	NAG	C3-C2-N2-C7
9	aH	15	MAN	C4-C5-C6-O6
16	dA	4	MAN	C4-C5-C6-O6
17	fM	10	MAN	O5-C5-C6-O6
9	aH	12	MAN	C4-C5-C6-O6
19	fB	7	MAN	C4-C5-C6-O6
18	eD	14	MAN	C4-C5-C6-O6
12	bA	6	MAN	C4-C5-C6-O6
11	aE	5	MAN	O5-C5-C6-O6
10	aN	8	MAN	C4-C5-C6-O6
19	fB	7	MAN	O5-C5-C6-O6
17	eA	7	MAN	O5-C5-C6-O6
9	aH	6	NAG	C8-C7-N2-C2
19	fB	9	MAN	C4-C5-C6-O6
19	fO	7	MAN	C4-C5-C6-O6
18	eD	14	MAN	O5-C5-C6-O6
19	fG	2	NAG	O5-C5-C6-O6
9	aH	3	BMA	O5-C5-C6-O6
13	bE	3	BMA	O5-C5-C6-O6
8	aL	2	NAG	O5-C5-C6-O6
17	fC	1	NAG	C4-C5-C6-O6
12	bD	6	MAN	C4-C5-C6-O6
18	eB	11	NAG	O5-C5-C6-O6
19	fG	8	MAN	C4-C5-C6-O6
17	eA	8	MAN	O5-C5-C6-O6
17	eE	8	MAN	C4-C5-C6-O6
18	eB	11	NAG	C8-C7-N2-C2
17	eA	7	MAN	C4-C5-C6-O6
19	fL	8	MAN	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
8	aB	2	NAG	O5-C5-C6-O6
12	bA	6	MAN	O5-C5-C6-O6
9	aM	5	MAN	O5-C5-C6-O6
12	bD	6	MAN	O5-C5-C6-O6
9	aH	6	NAG	O7-C7-N2-C2
9	aM	13	NAG	O5-C5-C6-O6
9	aH	5	MAN	C4-C5-C6-O6
19	fL	2	NAG	C3-C2-N2-C7
19	fL	8	MAN	C4-C5-C6-O6
17	eE	9	MAN	C4-C5-C6-O6
7	aF	10	MAN	C4-C5-C6-O6
7	aF	4	MAN	C4-C5-C6-O6
15	cB	3	MAN	O5-C5-C6-O6
19	fJ	9	MAN	O5-C5-C6-O6
17	fM	4	MAN	C4-C5-C6-O6
14	bI	2	NAG	C4-C5-C6-O6

There are no ring outliers.

43 monomers are involved in 34 short contacts:

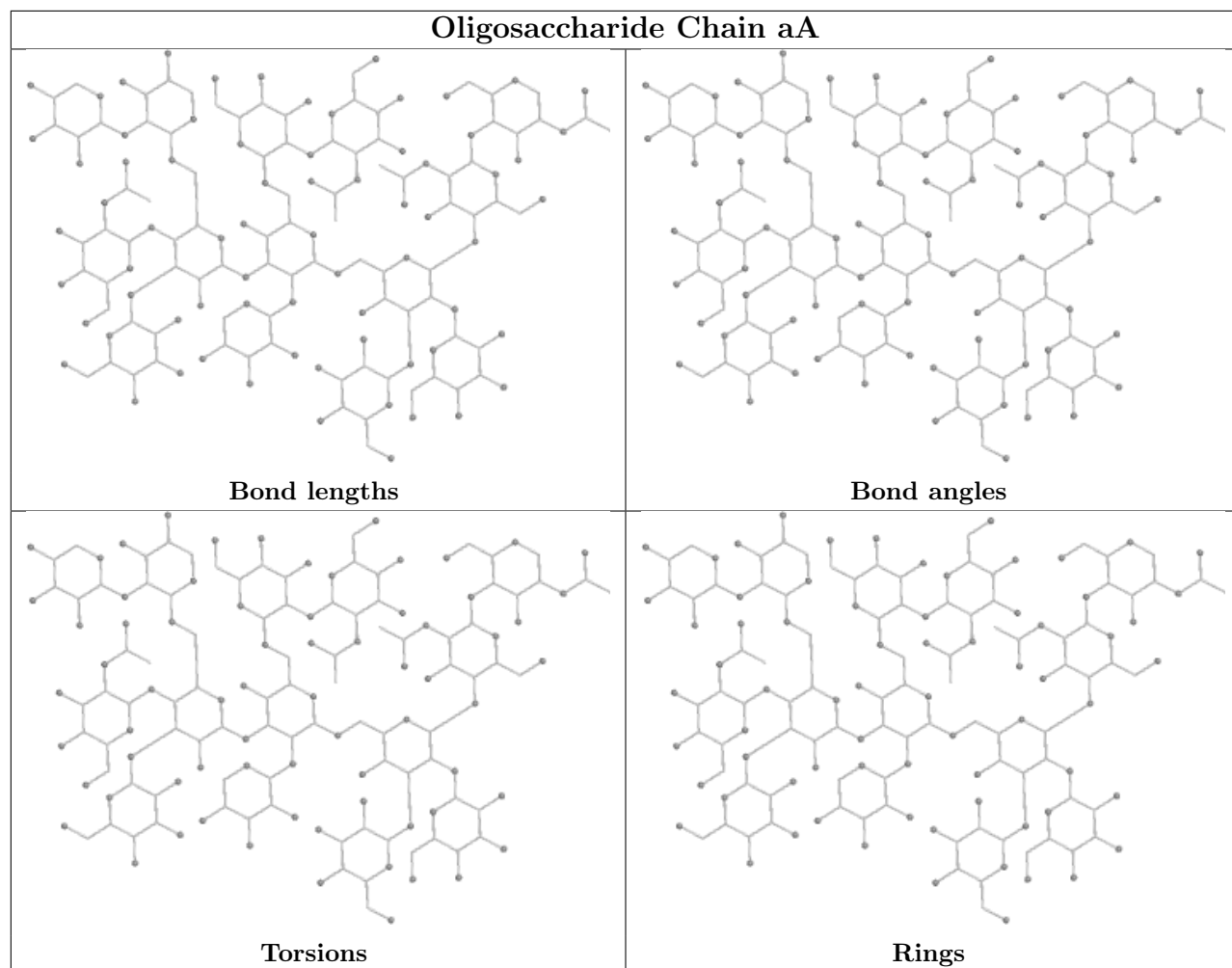
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	aM	1	NAG	1	0
8	aL	1	NAG	1	0
20	fF	12	XYP	1	0
11	aJ	1	NAG	1	0
20	fF	10	NAG	1	0
20	fK	9	MAN	1	0
10	aD	8	MAN	1	0
7	aA	8	MAN	1	0
17	eC	11	MAN	2	0
11	aO	7	XYP	1	0
11	aE	6	XYP	1	0
7	aK	8	MAN	1	0
18	eB	8	BGC	1	0
11	aJ	4	MAN	1	0
11	aO	6	XYP	1	0
10	aN	8	MAN	1	0
17	fN	2	NAG	1	0
17	fM	4	MAN	2	0
11	aE	7	XYP	1	0
19	fO	6	MAN	1	0
19	fE	6	MAN	1	0

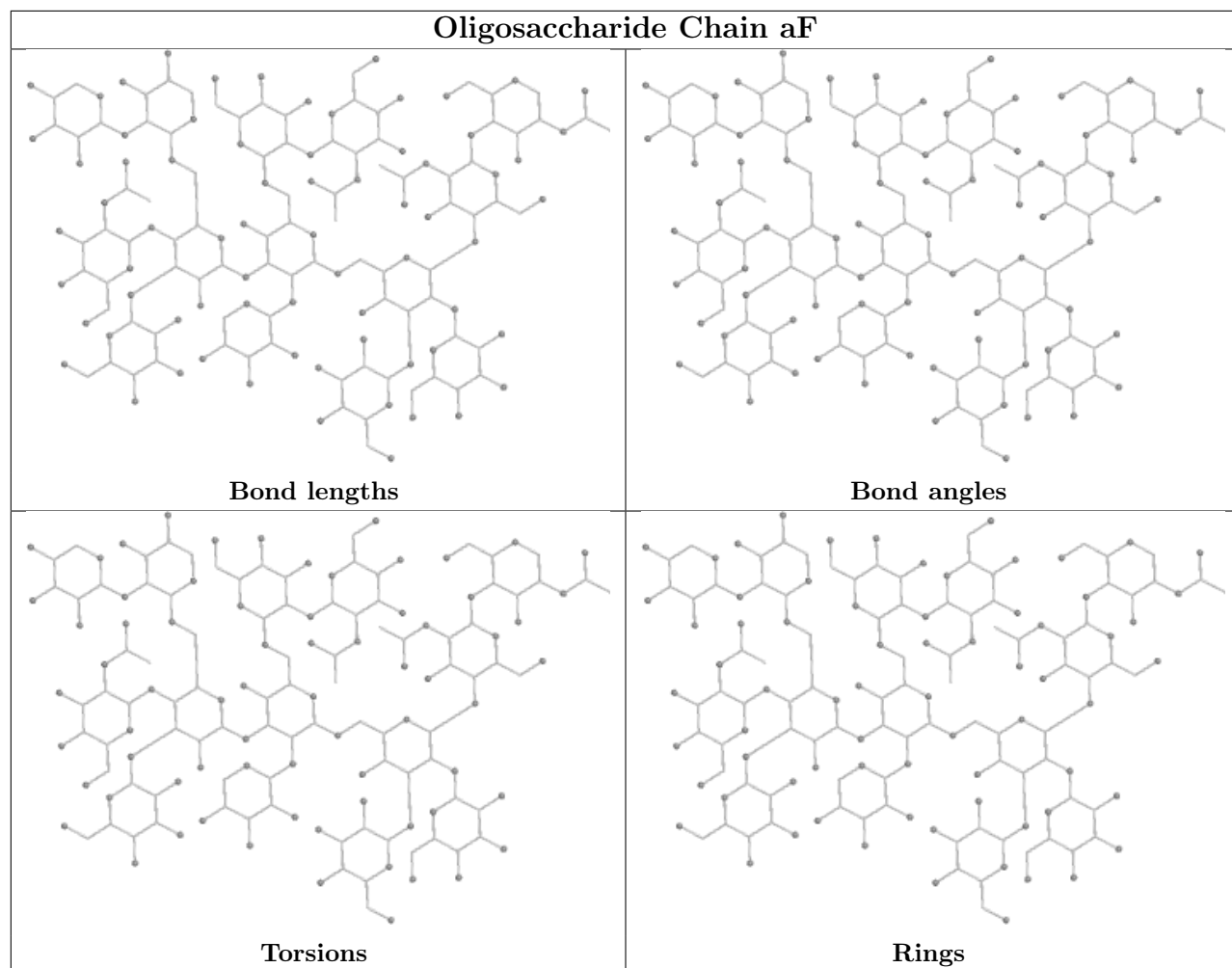
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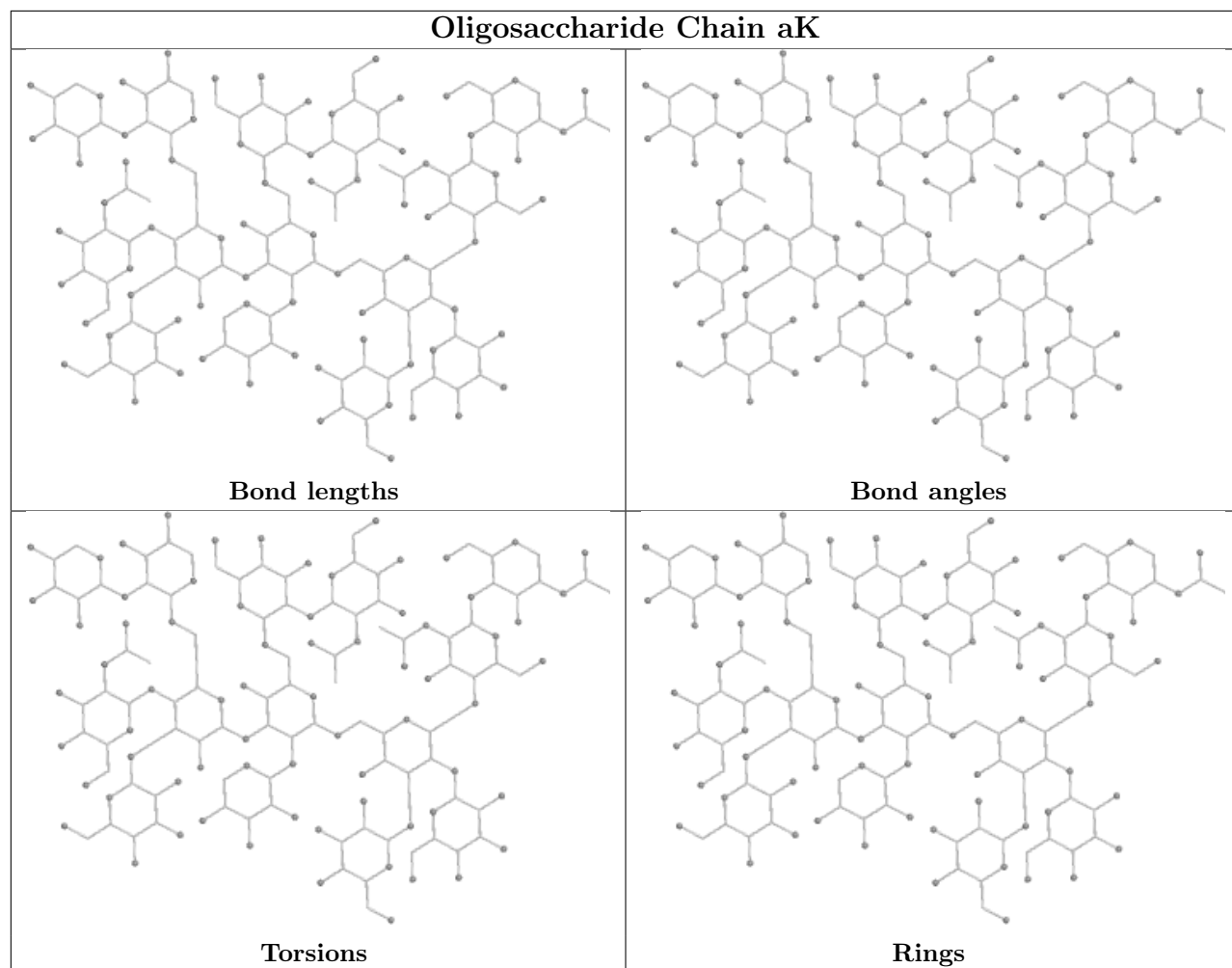
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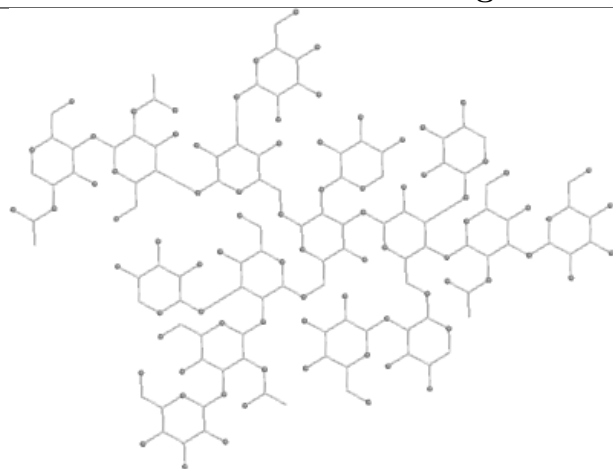
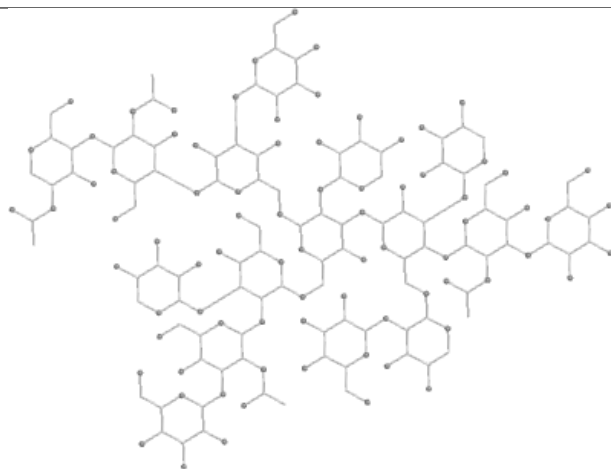
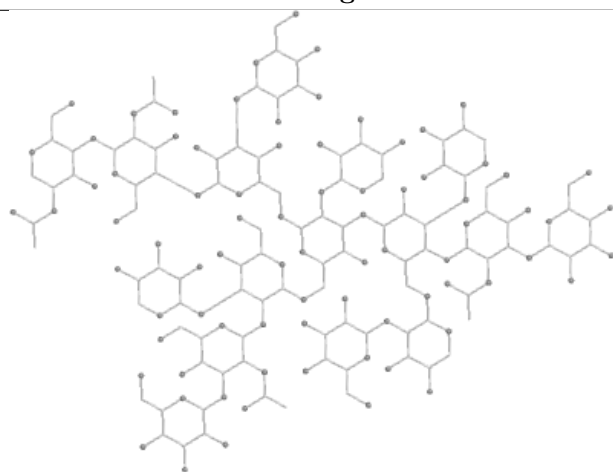
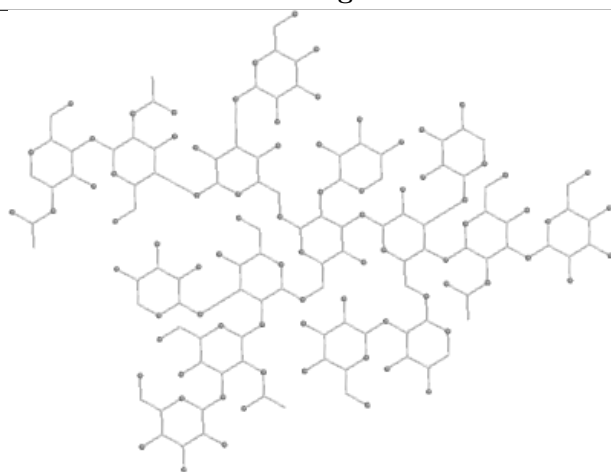
Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	bF	7	XYS	1	0
17	fI	10	MAN	1	0
7	aF	8	MAN	1	0
17	fM	2	NAG	1	0
17	fC	4	MAN	1	0
14	bF	5	MAN	1	0
9	aC	9	XYP	1	0
11	aJ	10	MAN	1	0
9	aM	2	NAG	1	0
10	aI	8	MAN	1	0
18	eB	9	NAG	1	0
16	dC	2	MAN	1	0
12	bD	5	MAN	1	0
7	aF	5	MAN	1	0
7	aA	1	NAG	1	0
20	fF	8	NAG	1	0
7	aK	1	NAG	1	0
9	aC	10	XYP	1	0
7	aA	5	MAN	1	0
19	fJ	6	MAN	1	0
11	aE	1	NAG	1	0
7	aK	5	MAN	1	0

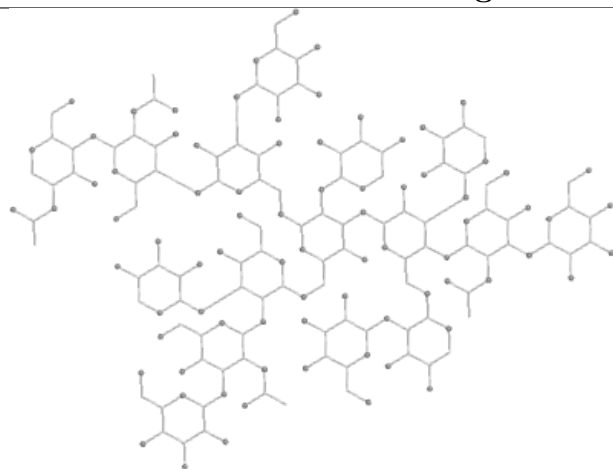
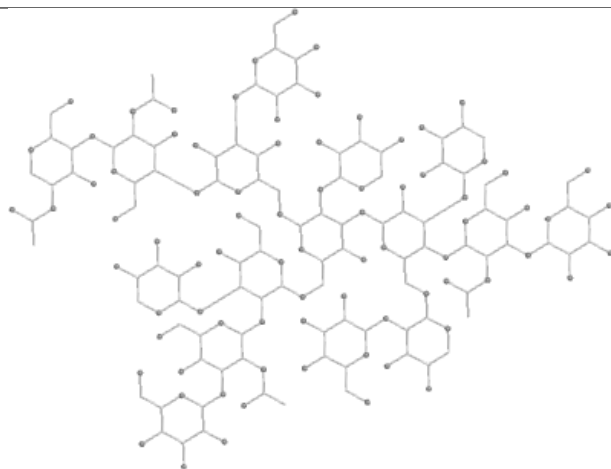
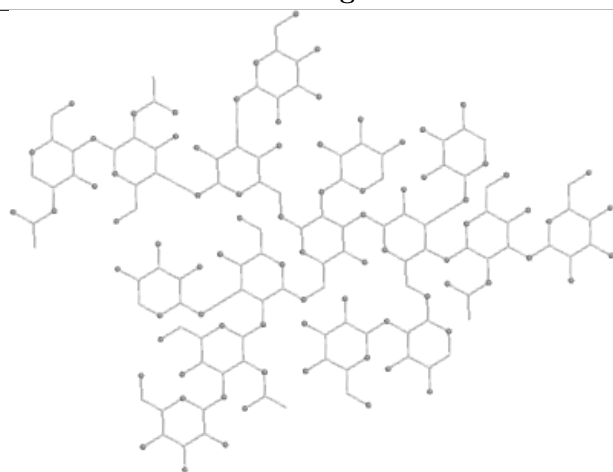
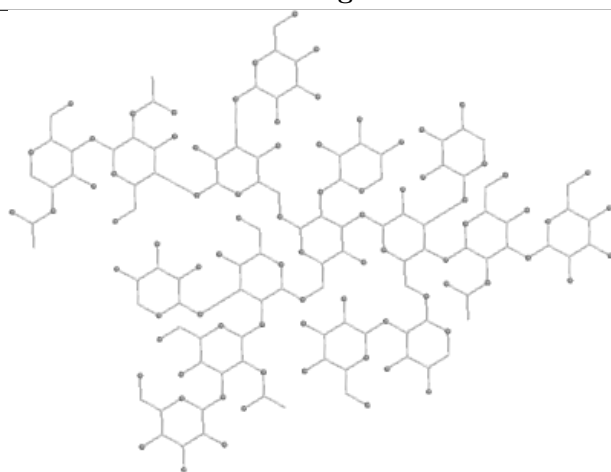
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

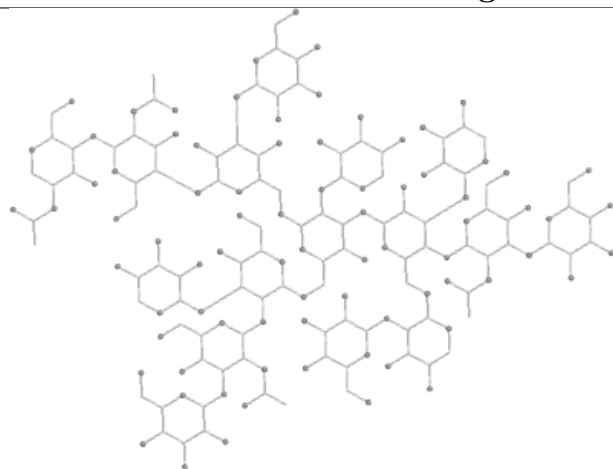
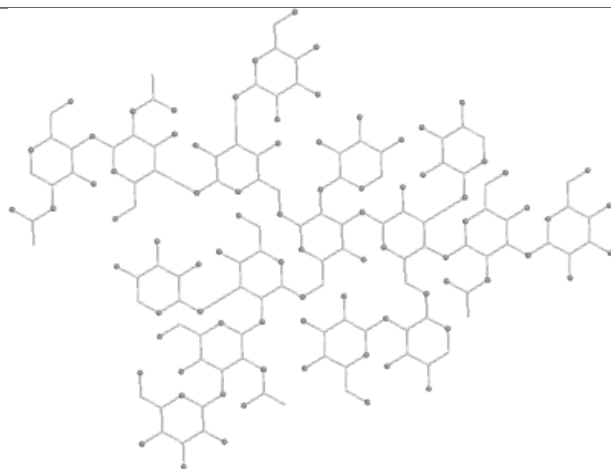
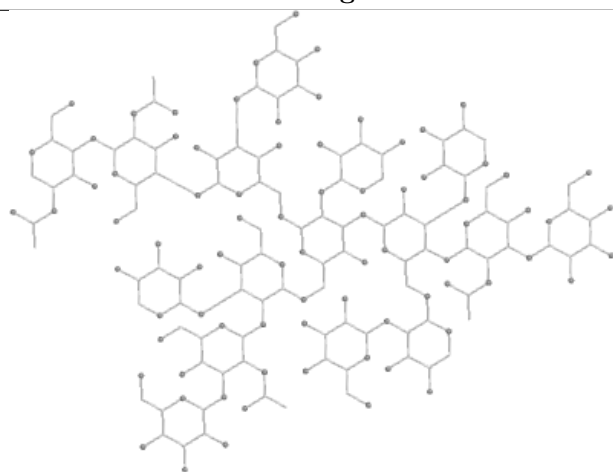
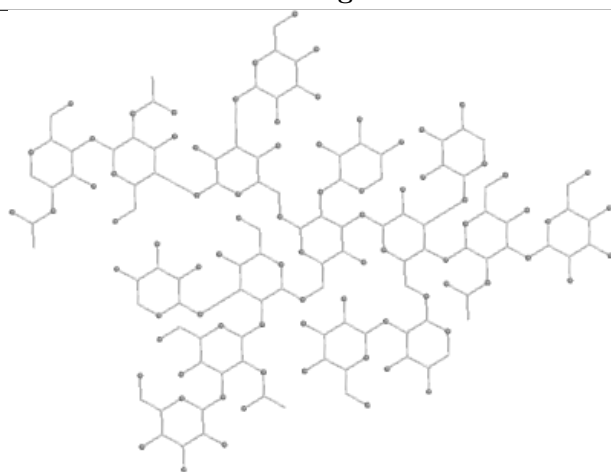


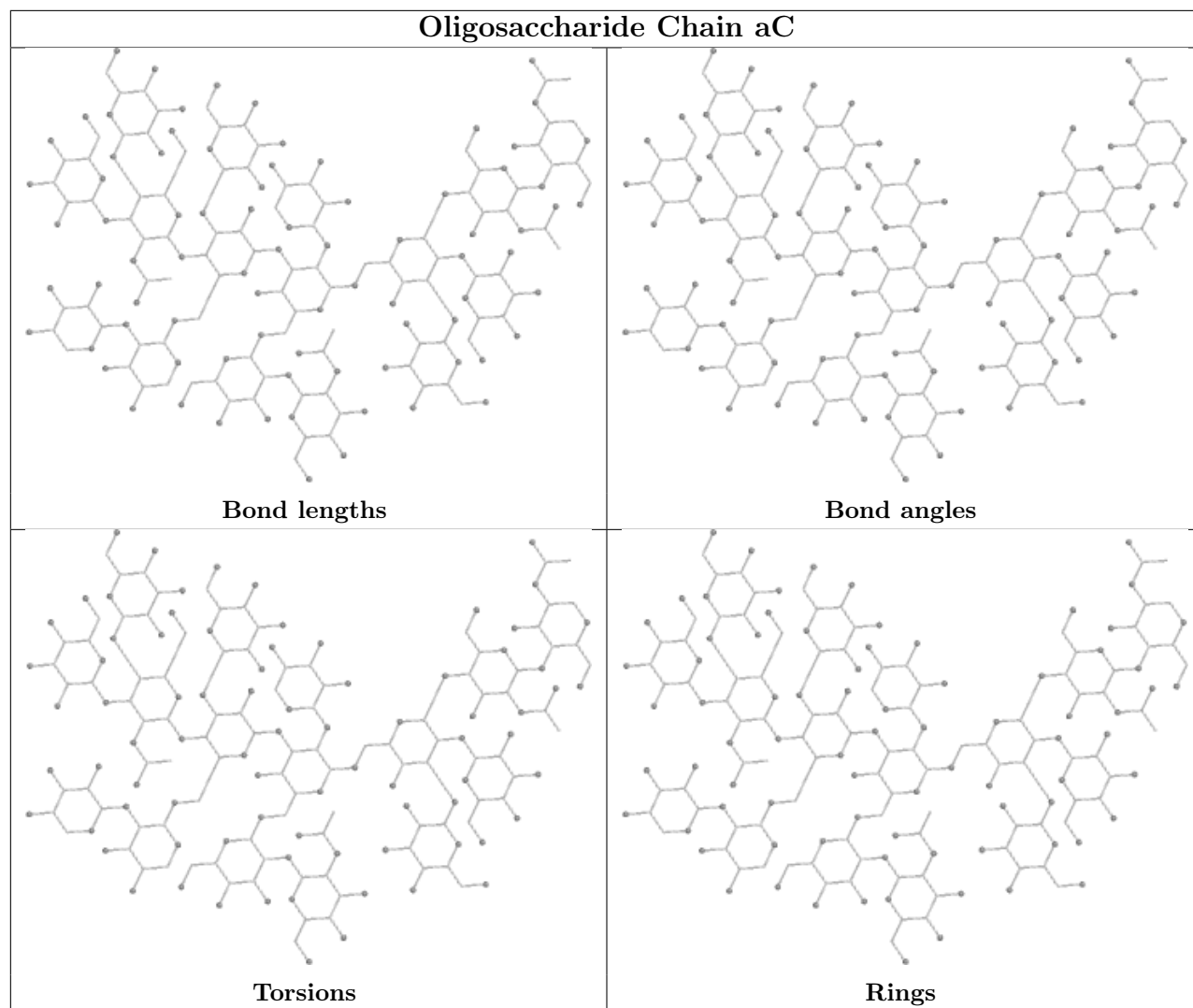


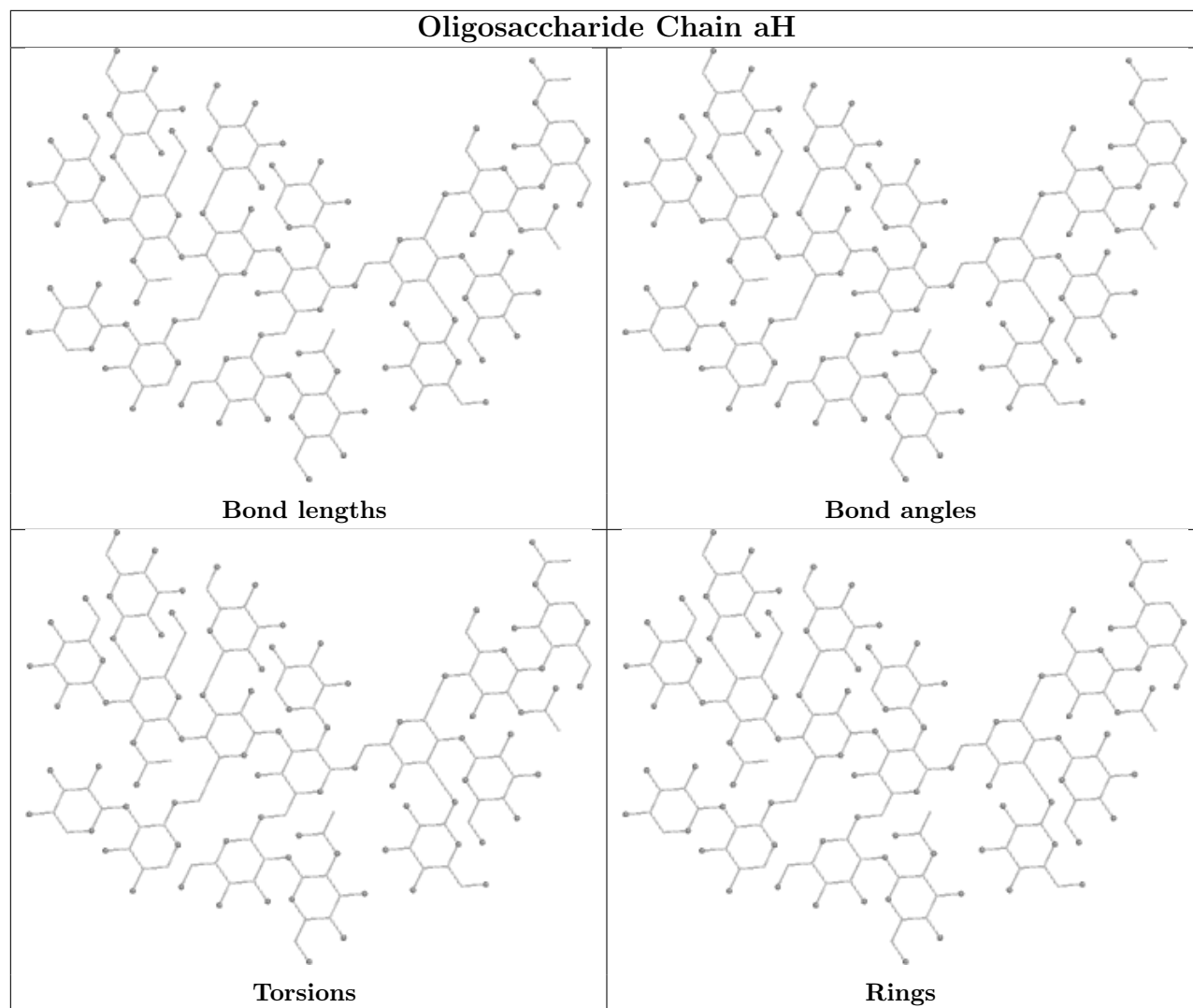


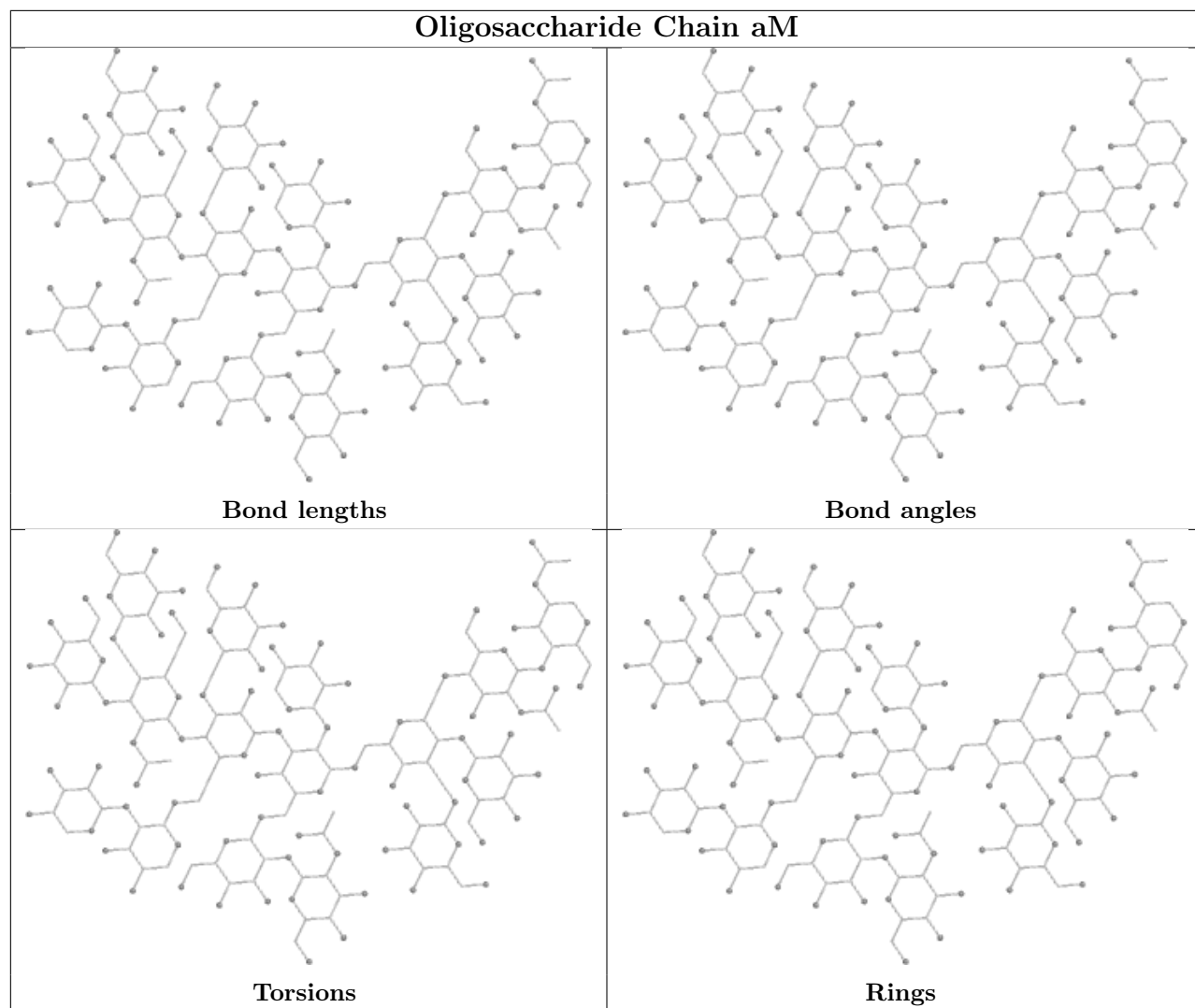
Oligosaccharide Chain aB**Bond lengths****Bond angles****Torsions****Rings**

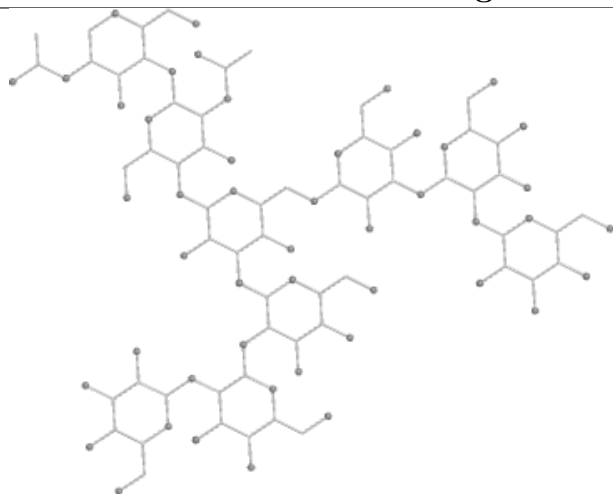
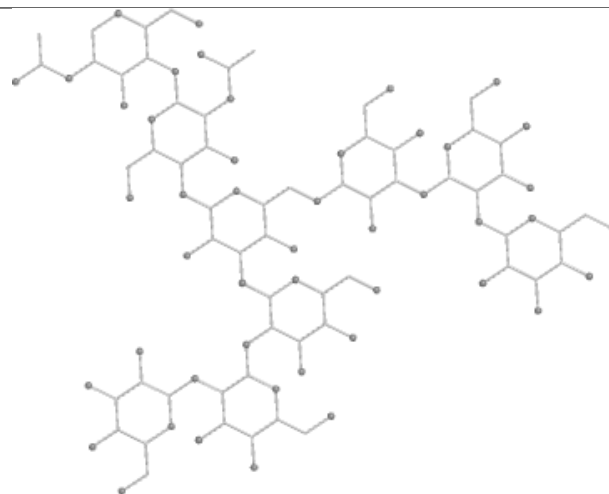
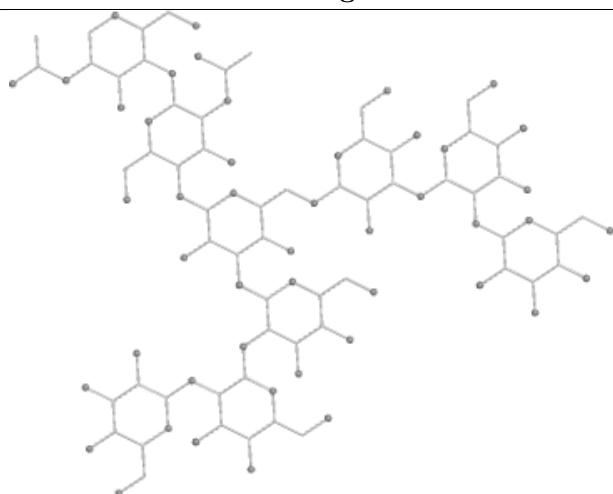
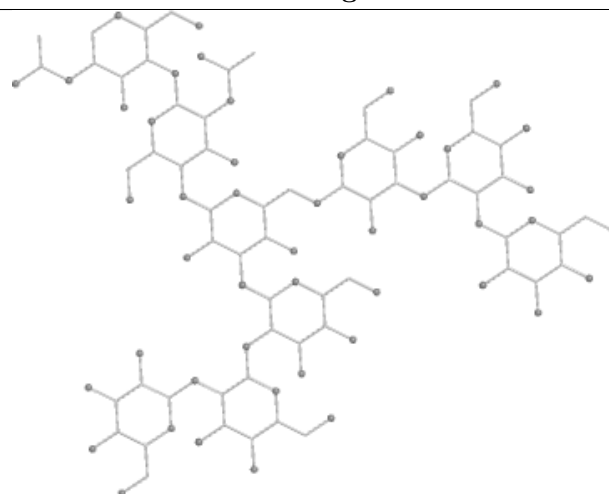
Oligosaccharide Chain aG**Bond lengths****Bond angles****Torsions****Rings**

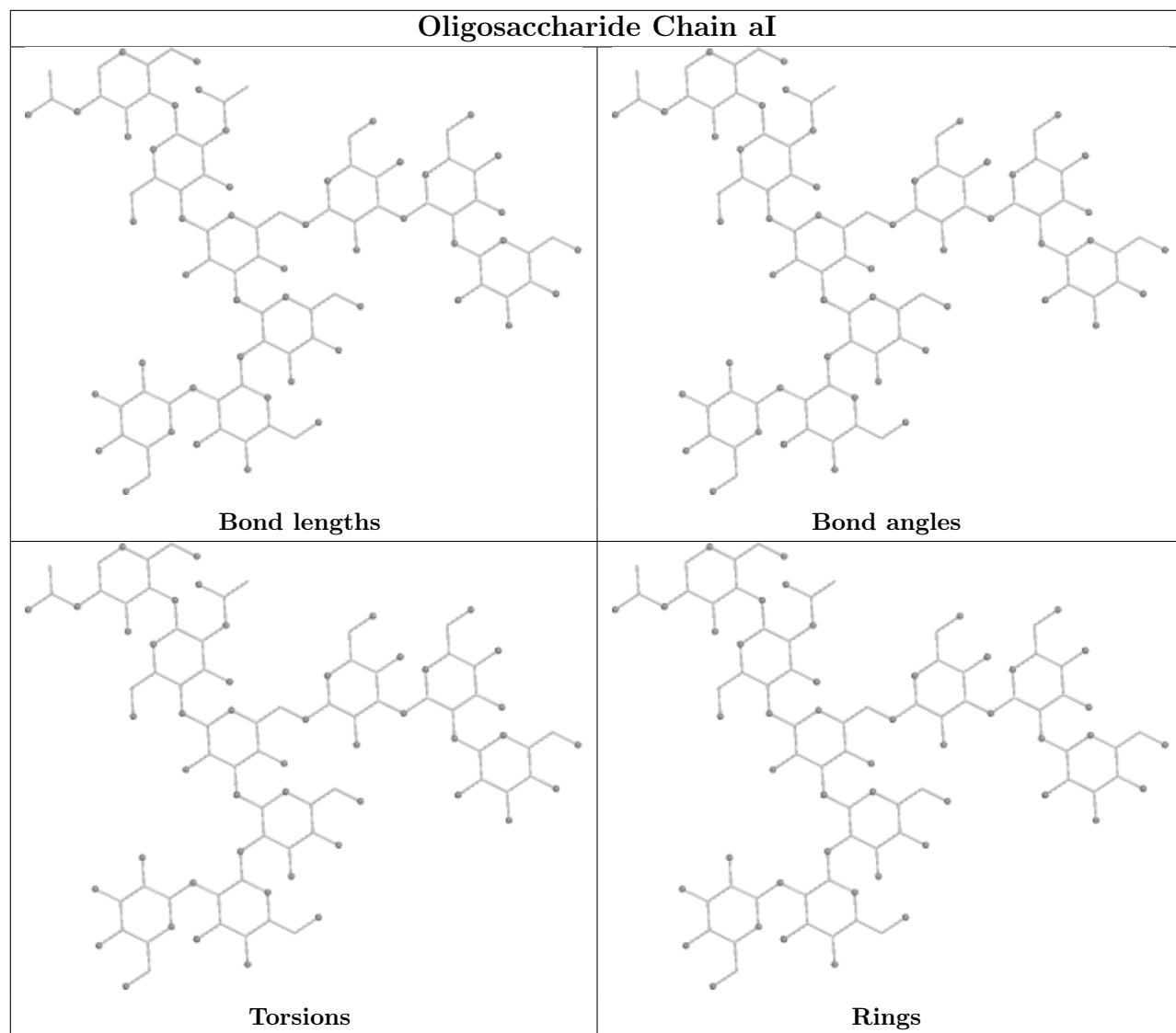
Oligosaccharide Chain aL**Bond lengths****Bond angles****Torsions****Rings**

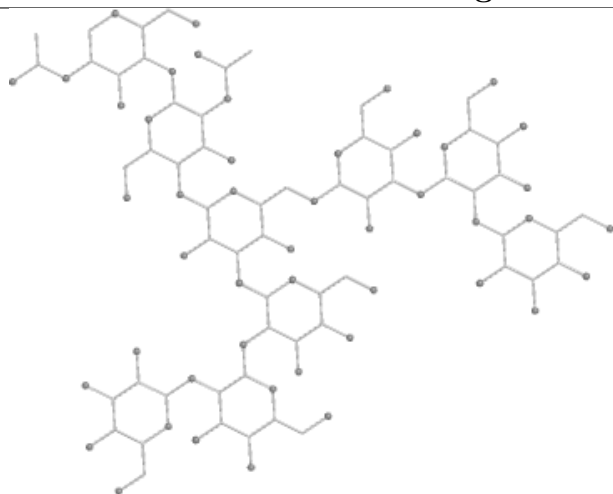
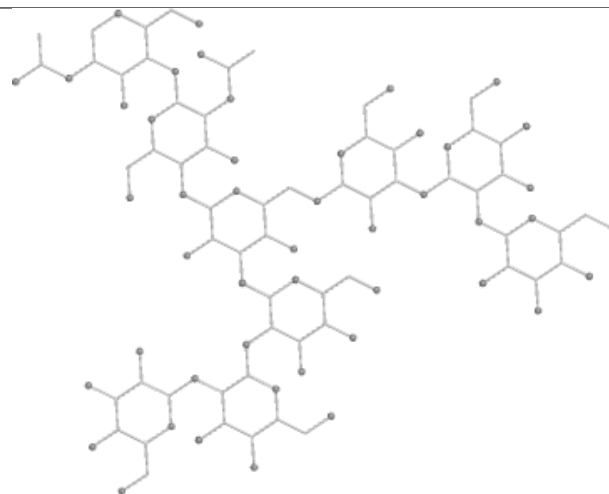
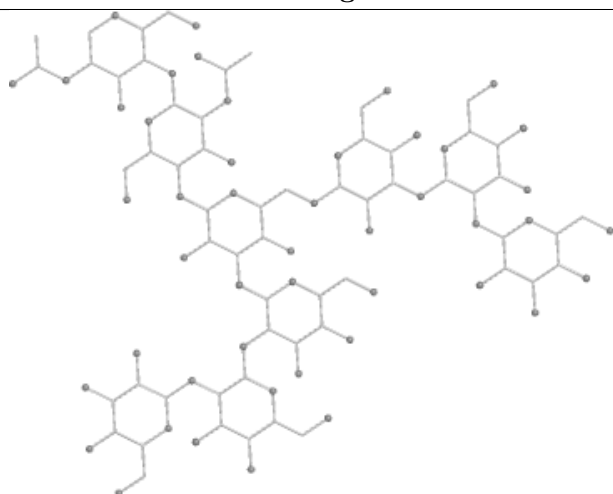
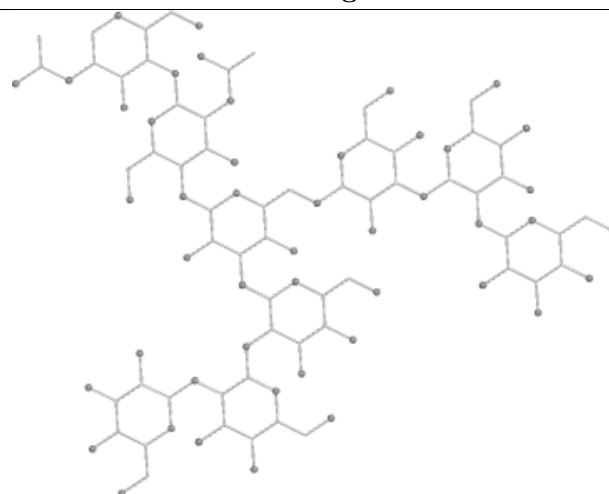


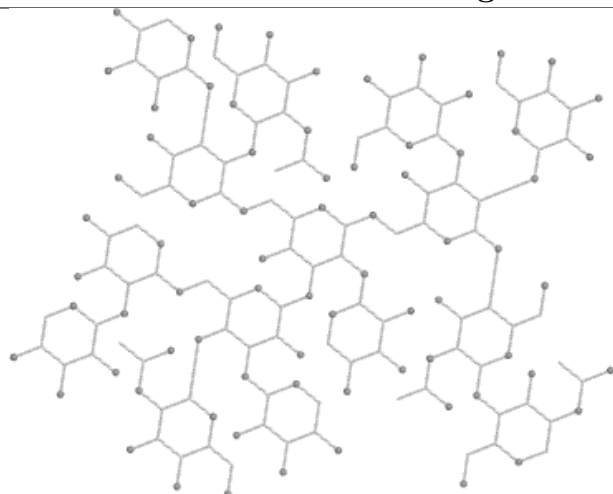
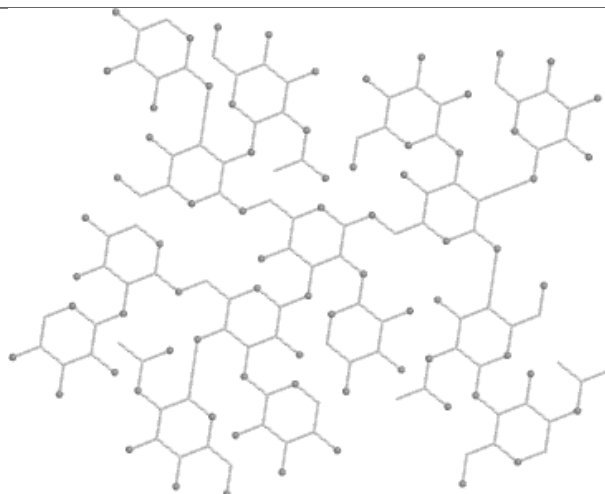
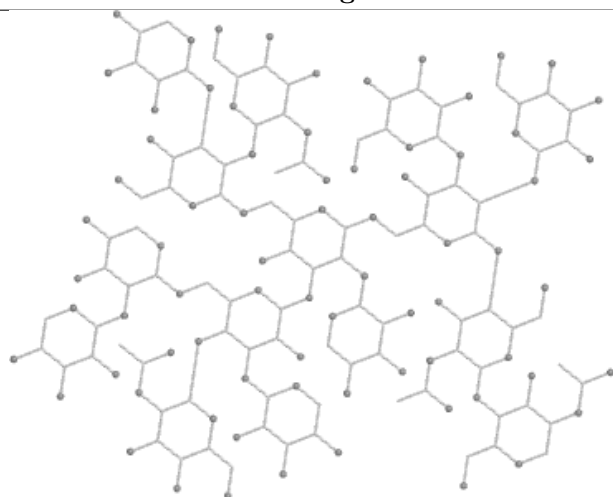
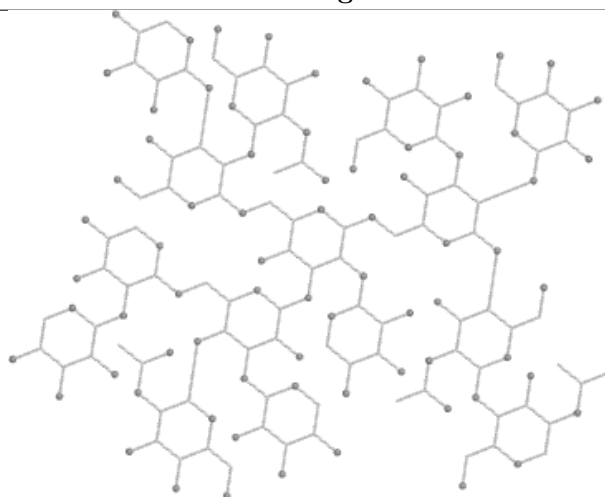


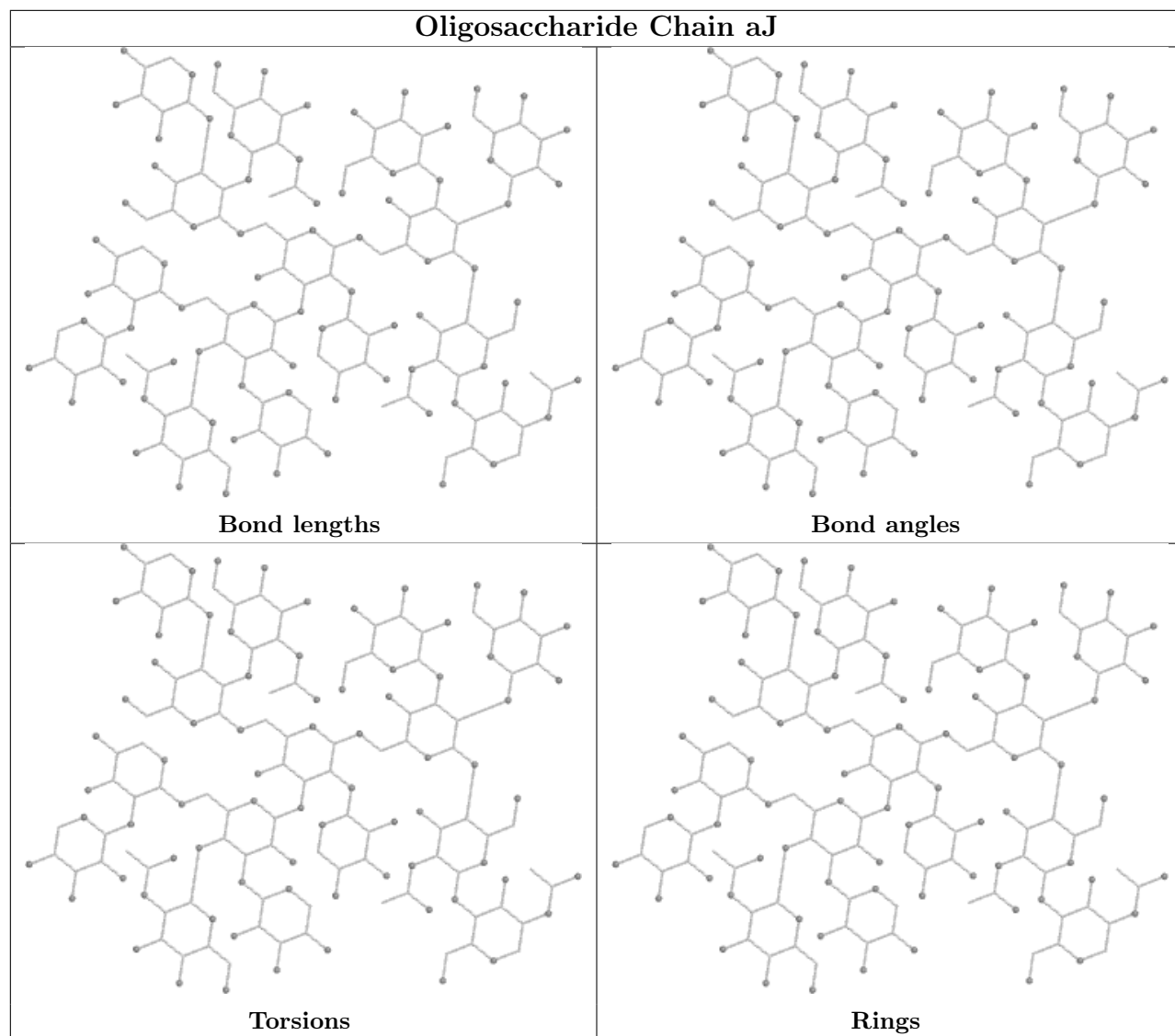


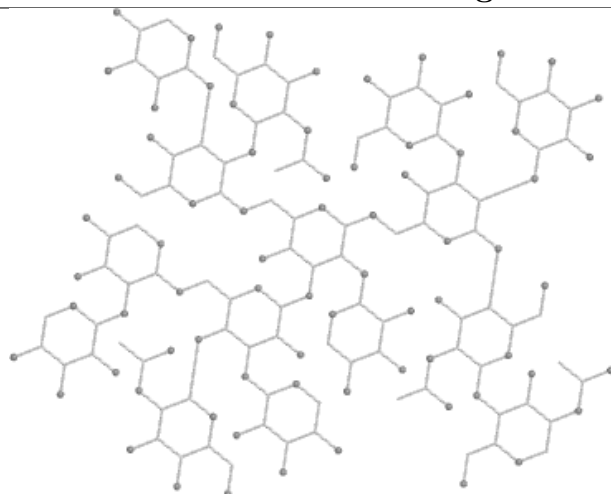
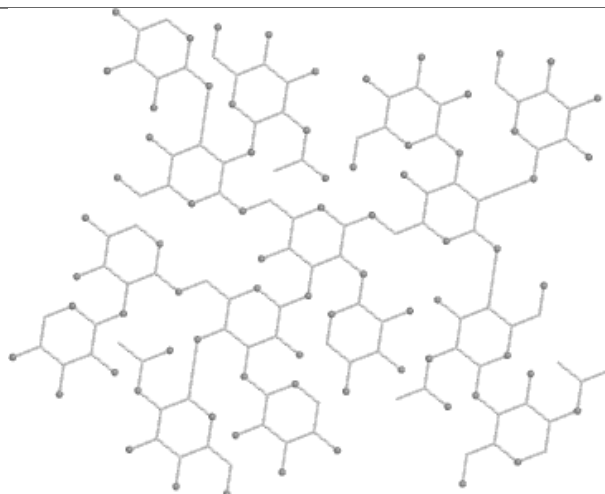
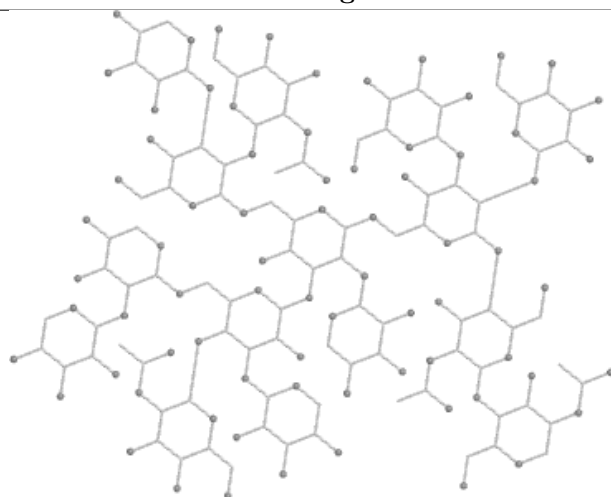
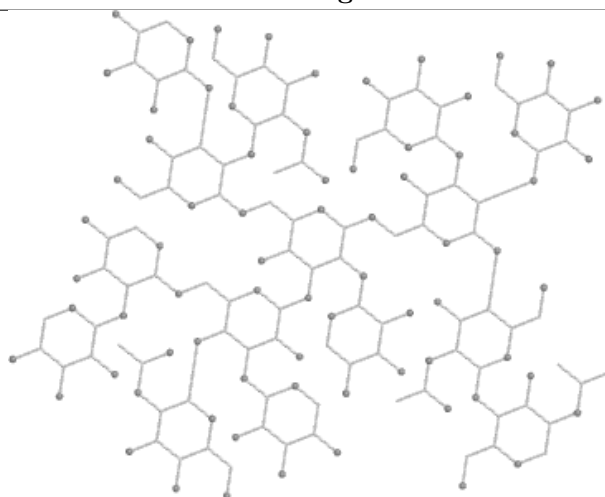
Oligosaccharide Chain aD**Bond lengths****Bond angles****Torsions****Rings**

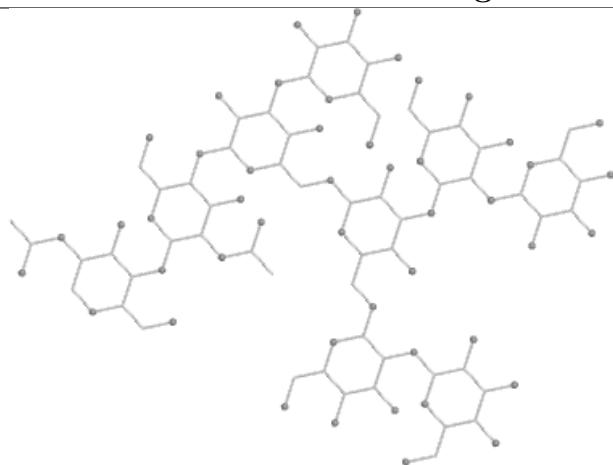
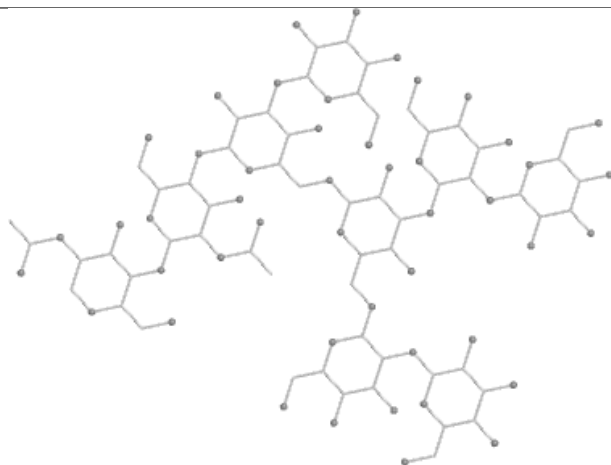
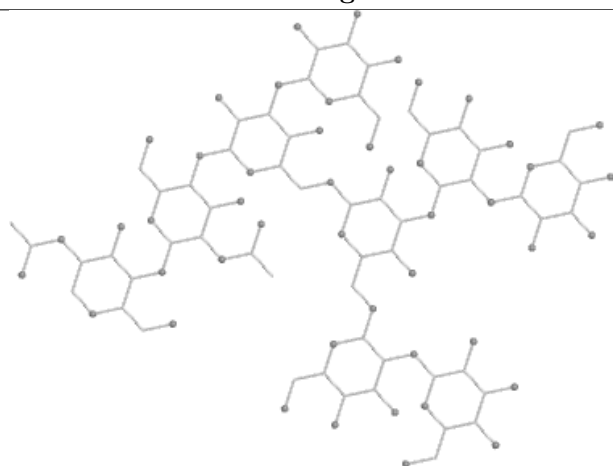
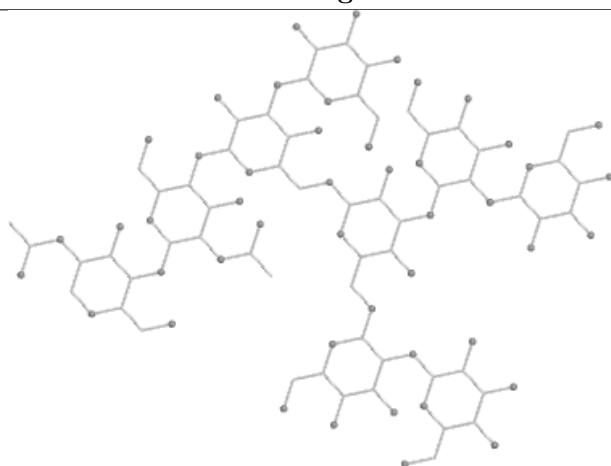


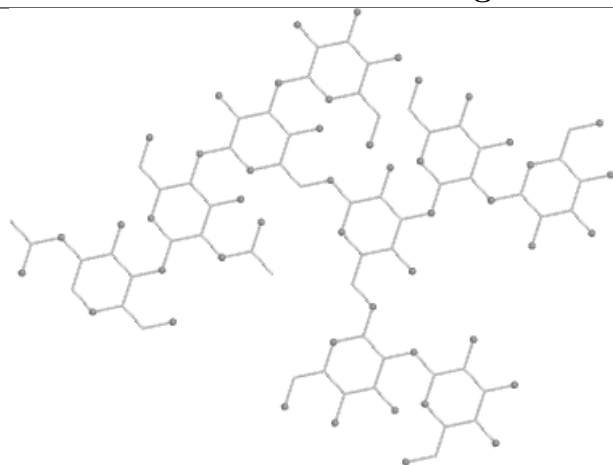
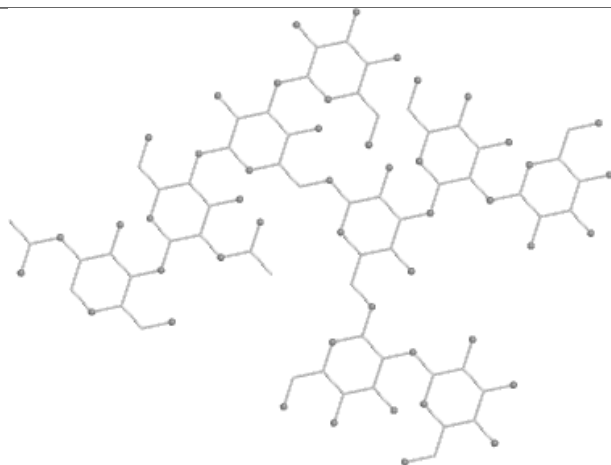
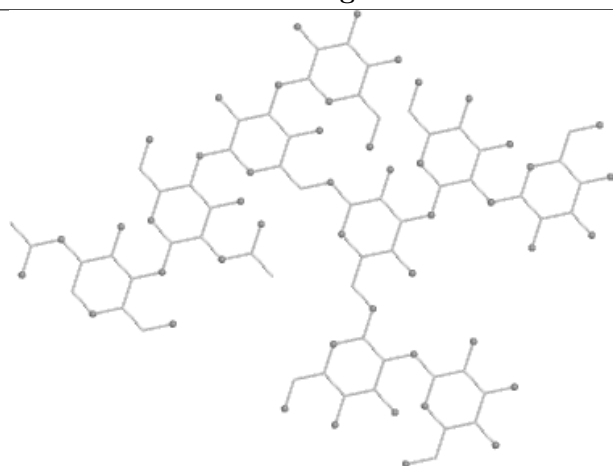
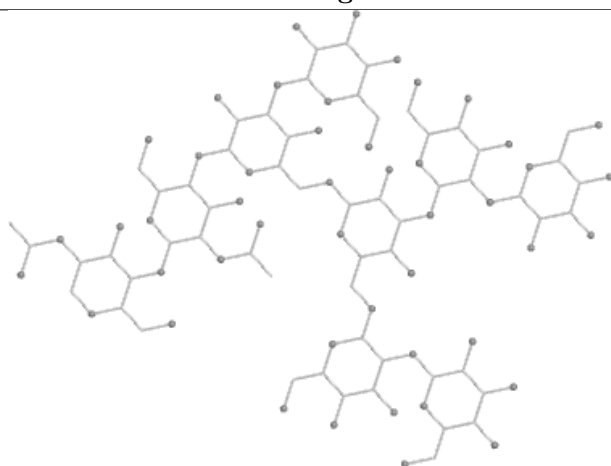
Oligosaccharide Chain aN**Bond lengths****Bond angles****Torsions****Rings**

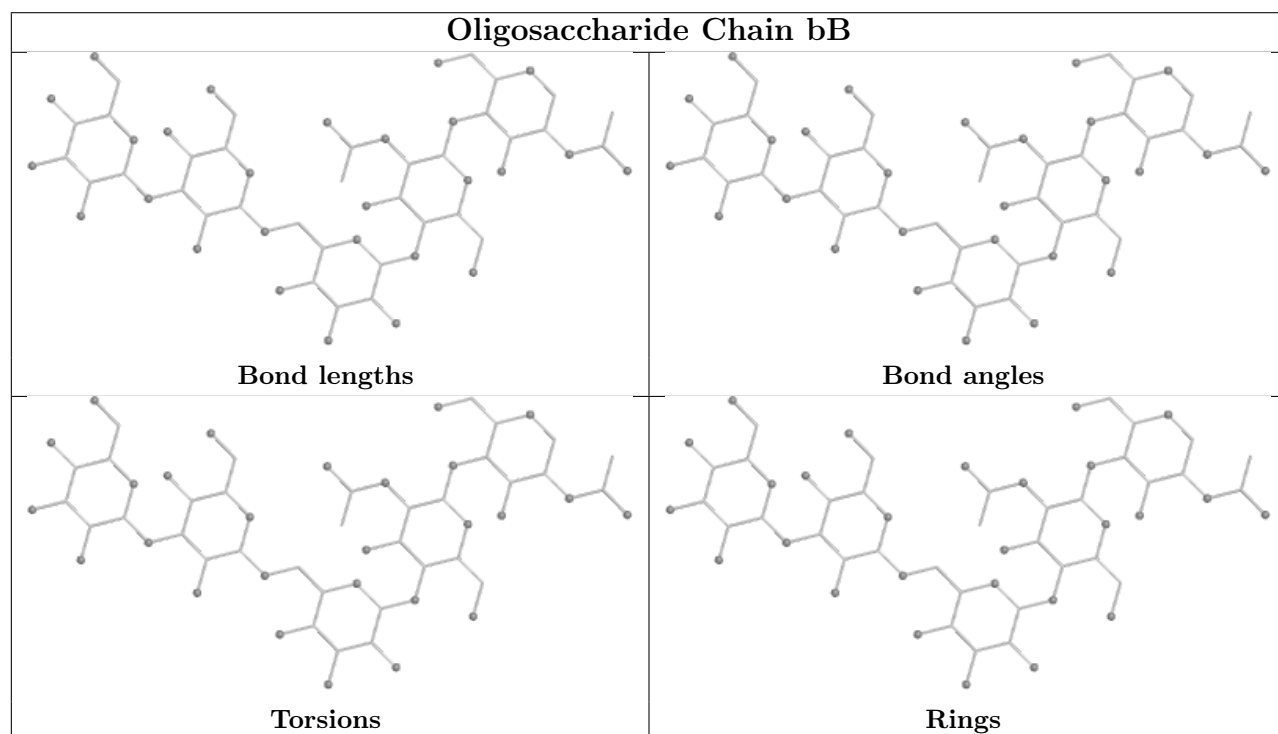
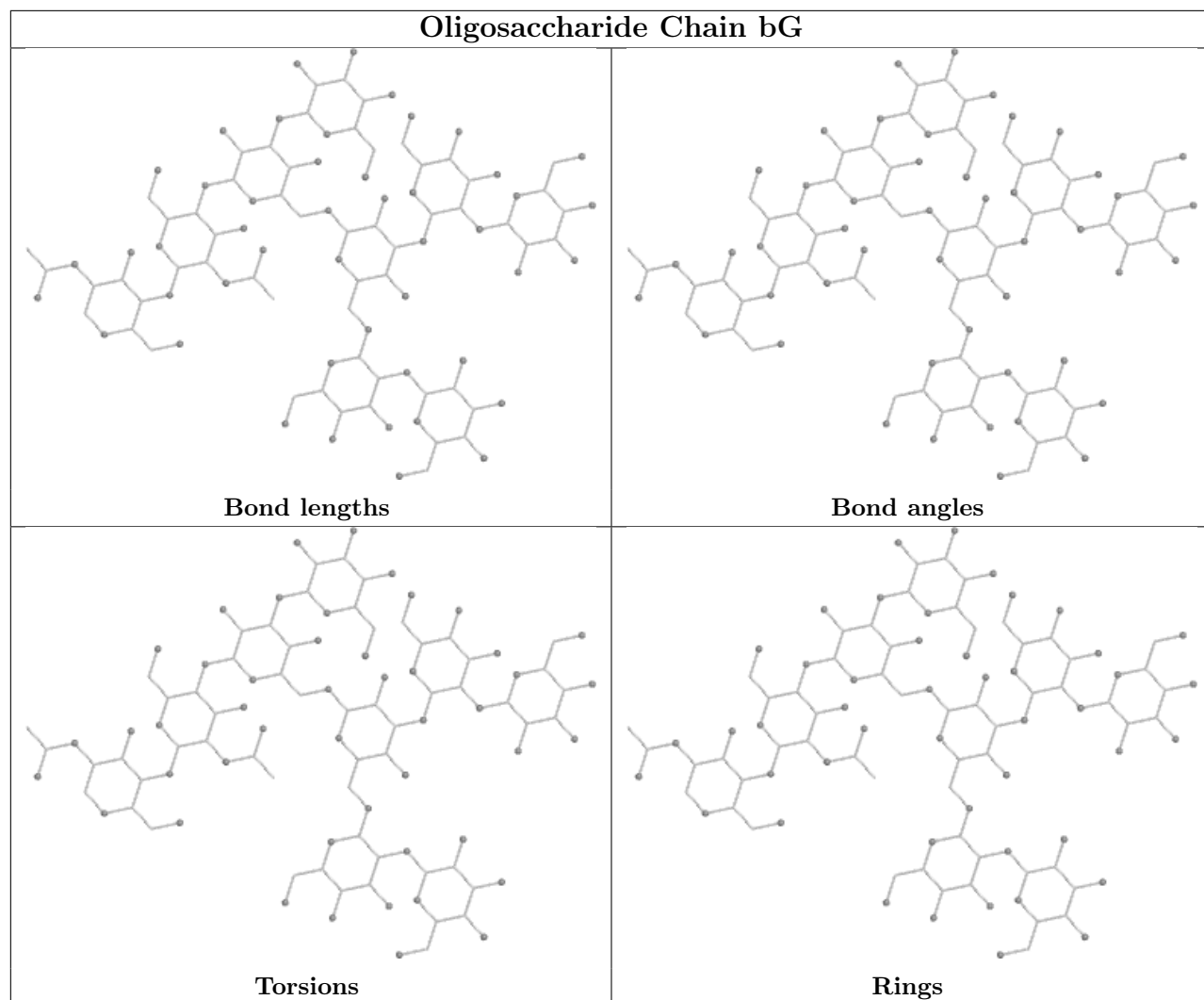
Oligosaccharide Chain aE**Bond lengths****Bond angles****Torsions****Rings**

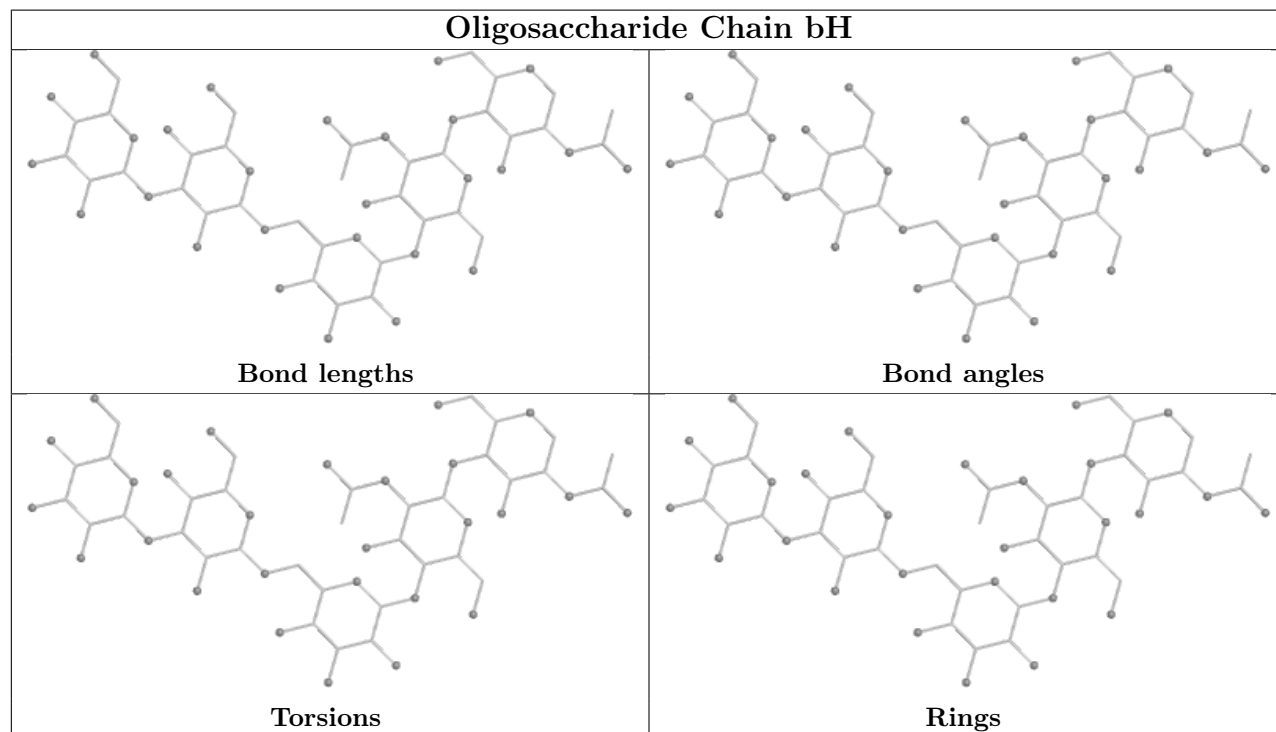
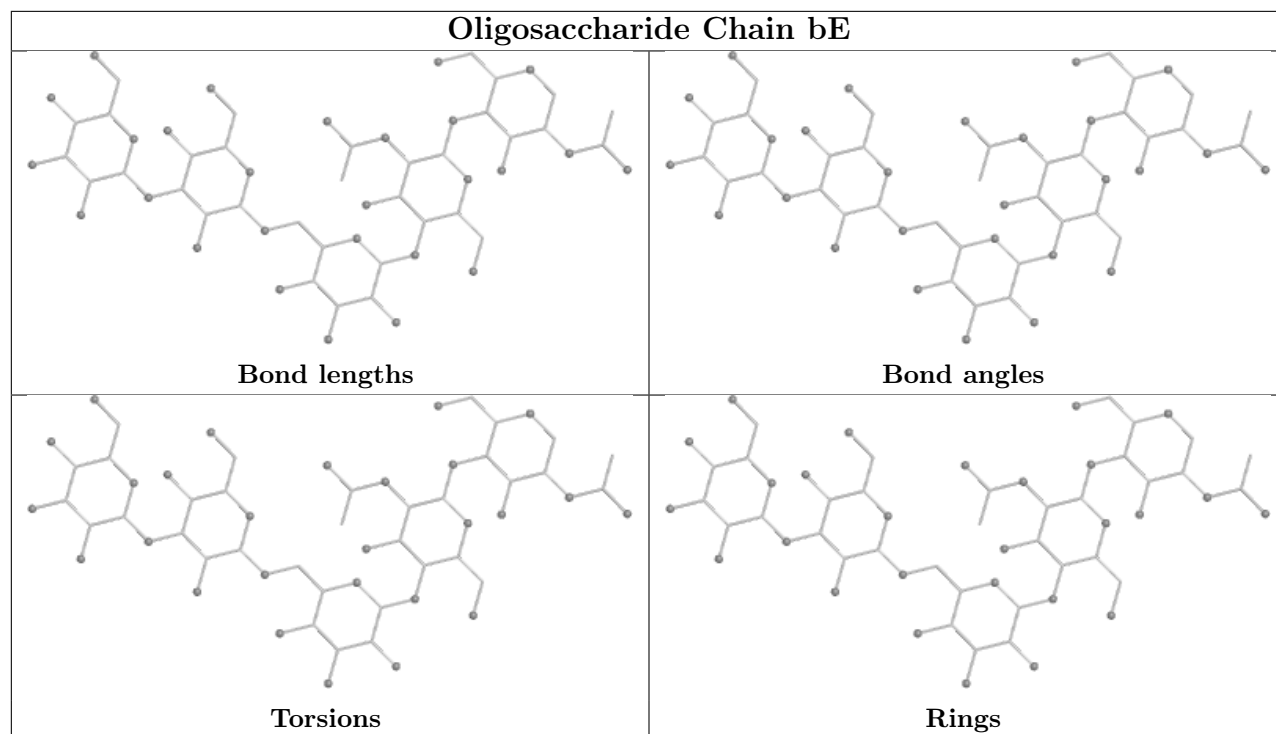


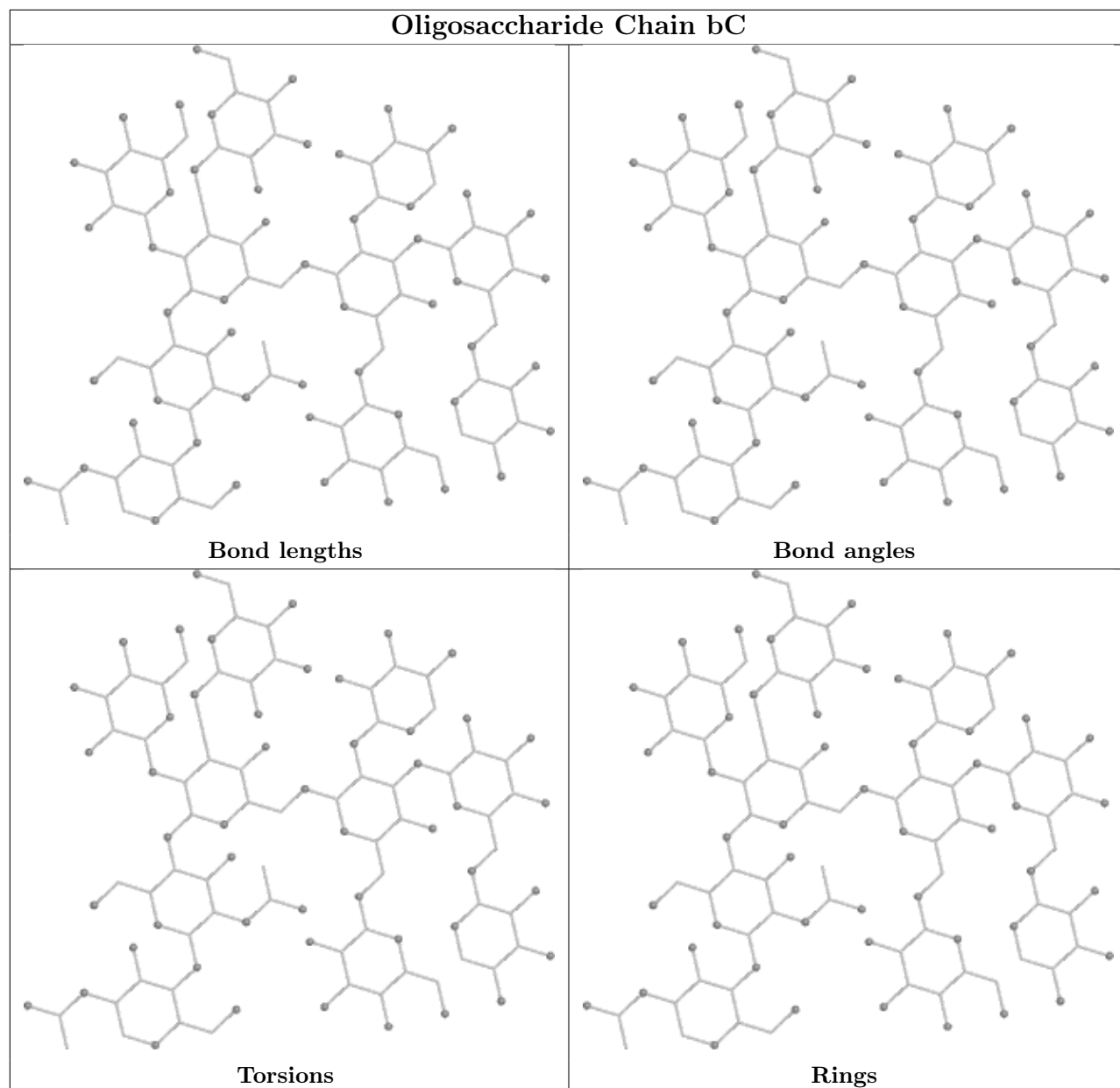
Oligosaccharide Chain aO**Bond lengths****Bond angles****Torsions****Rings**

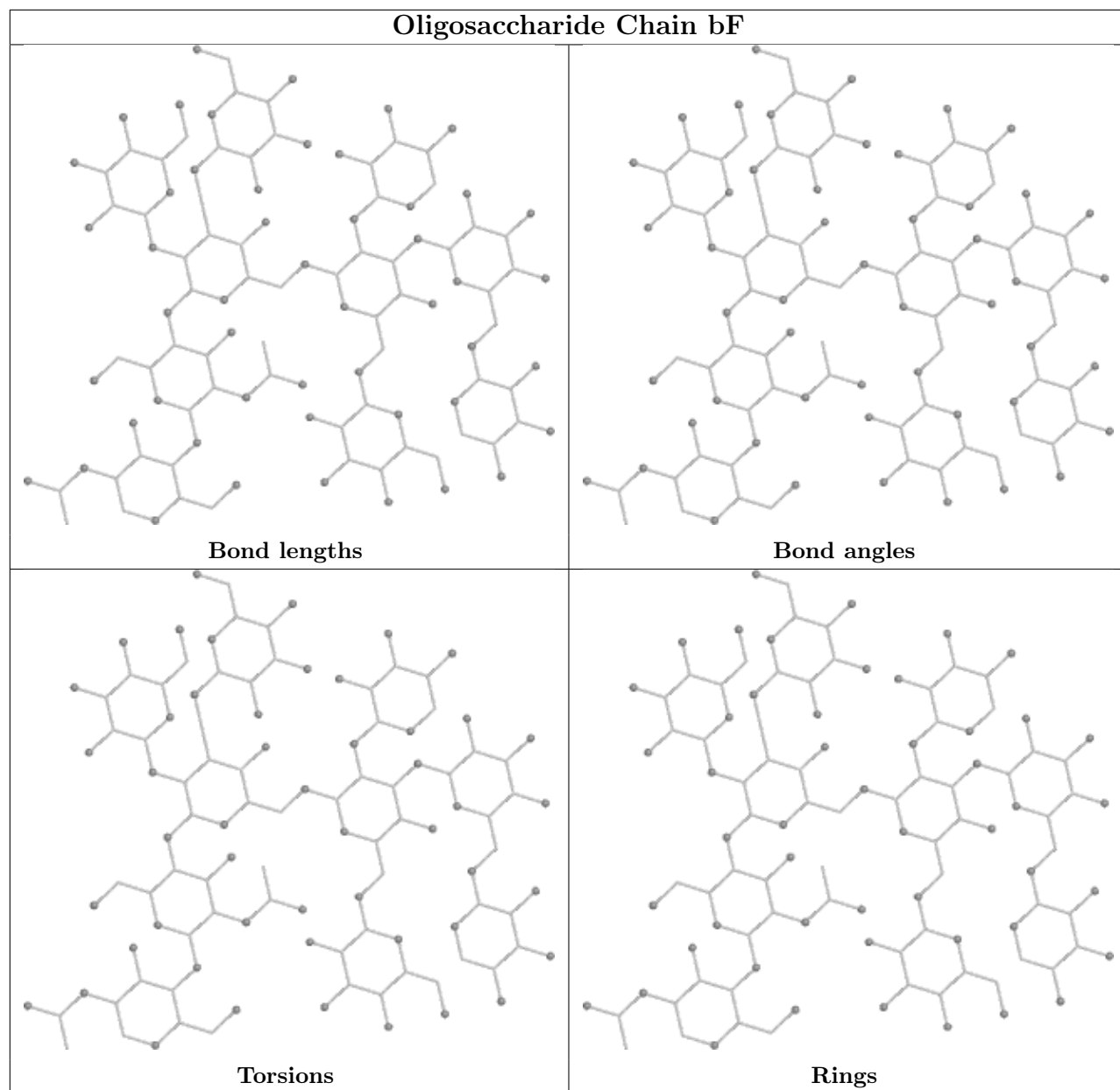
Oligosaccharide Chain bA**Bond lengths****Bond angles****Torsions****Rings**

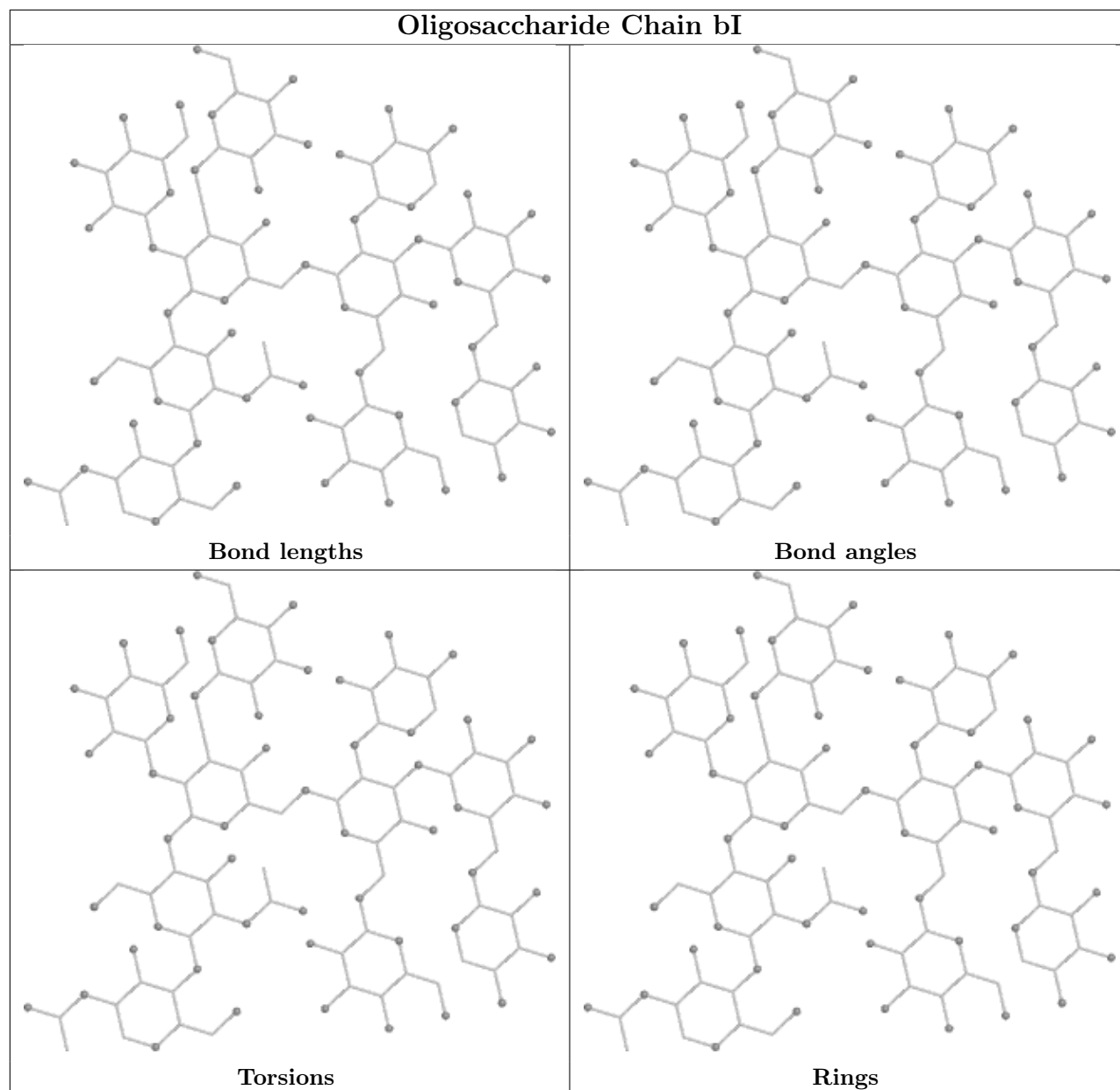
Oligosaccharide Chain bD**Bond lengths****Bond angles****Torsions****Rings**

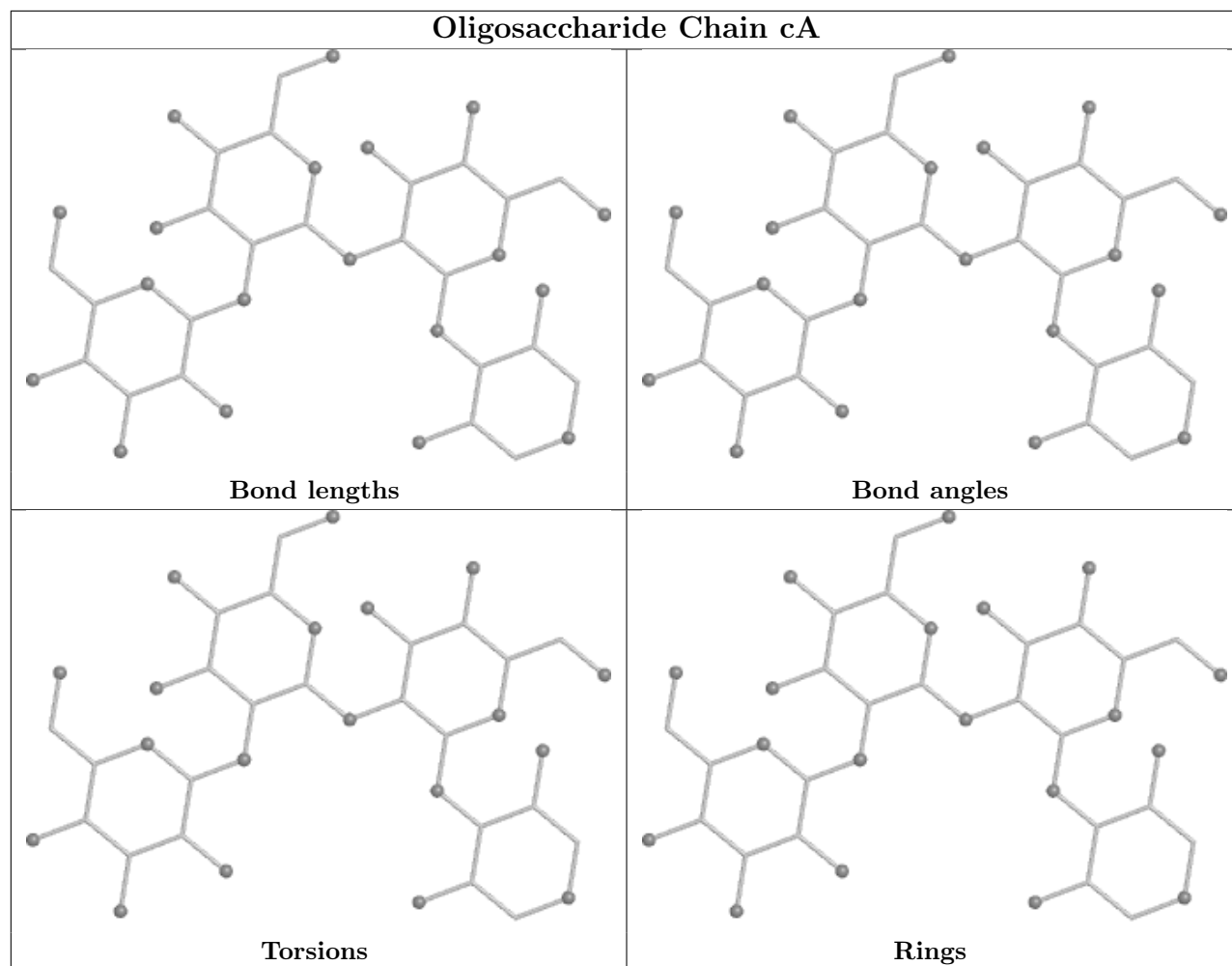


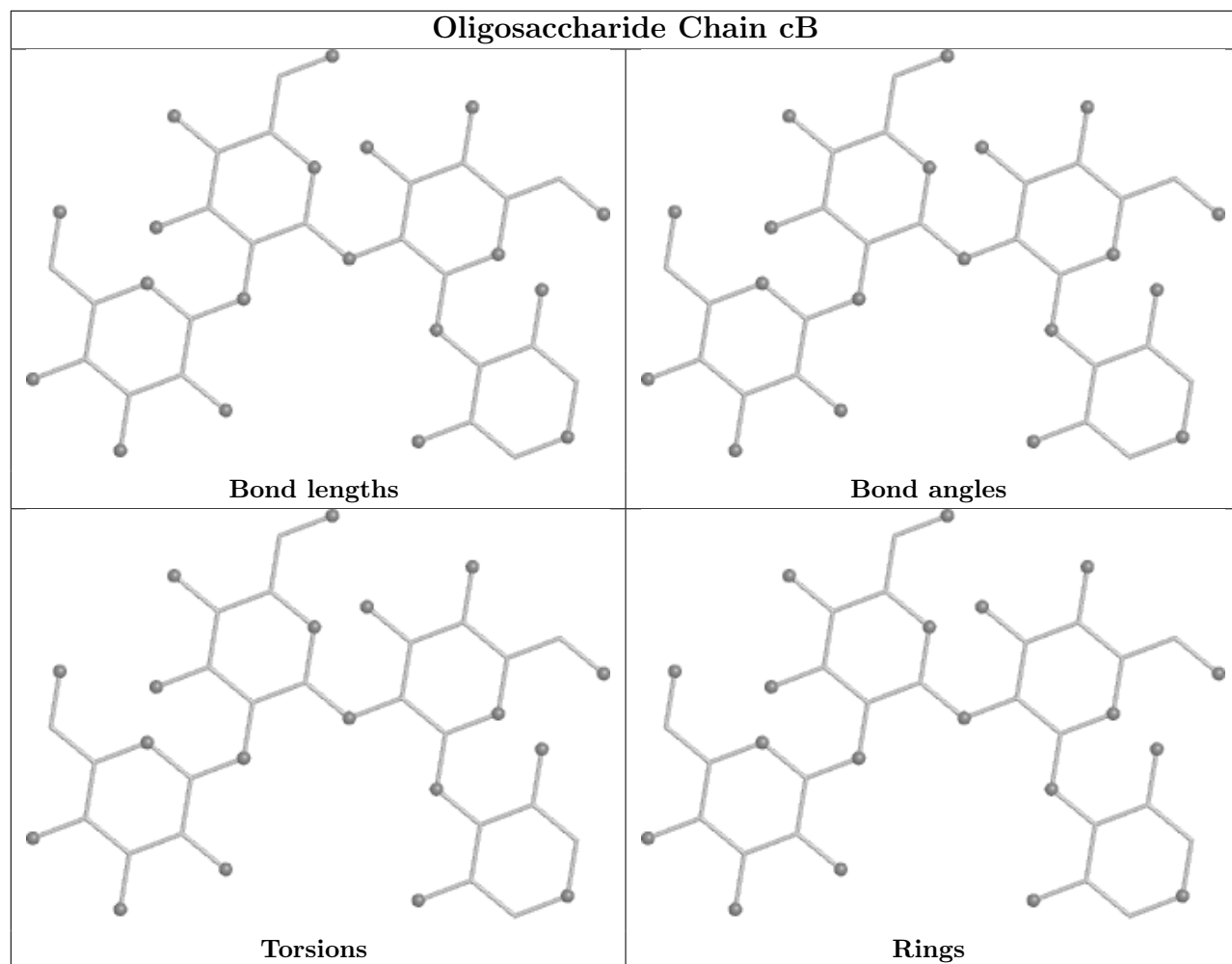


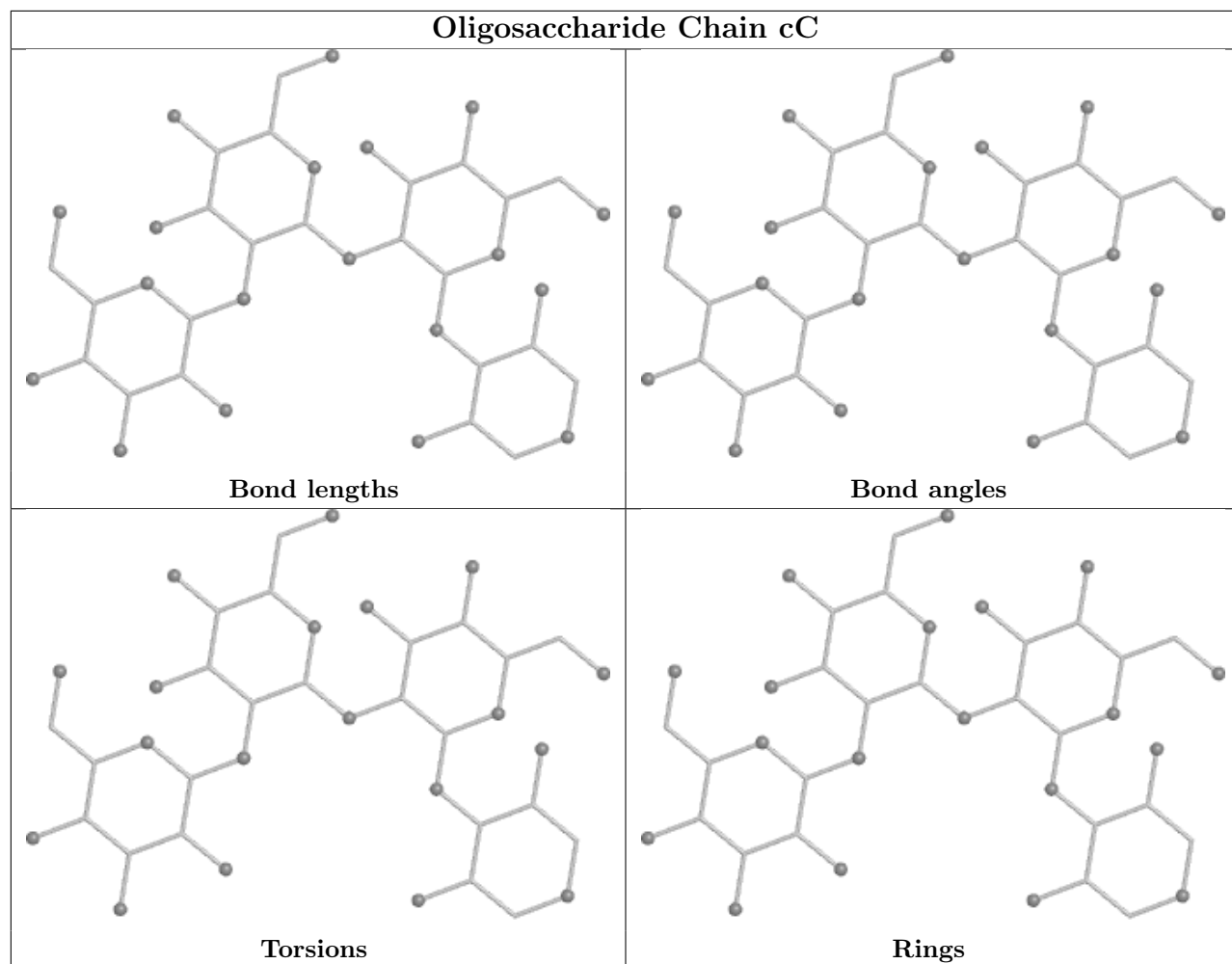


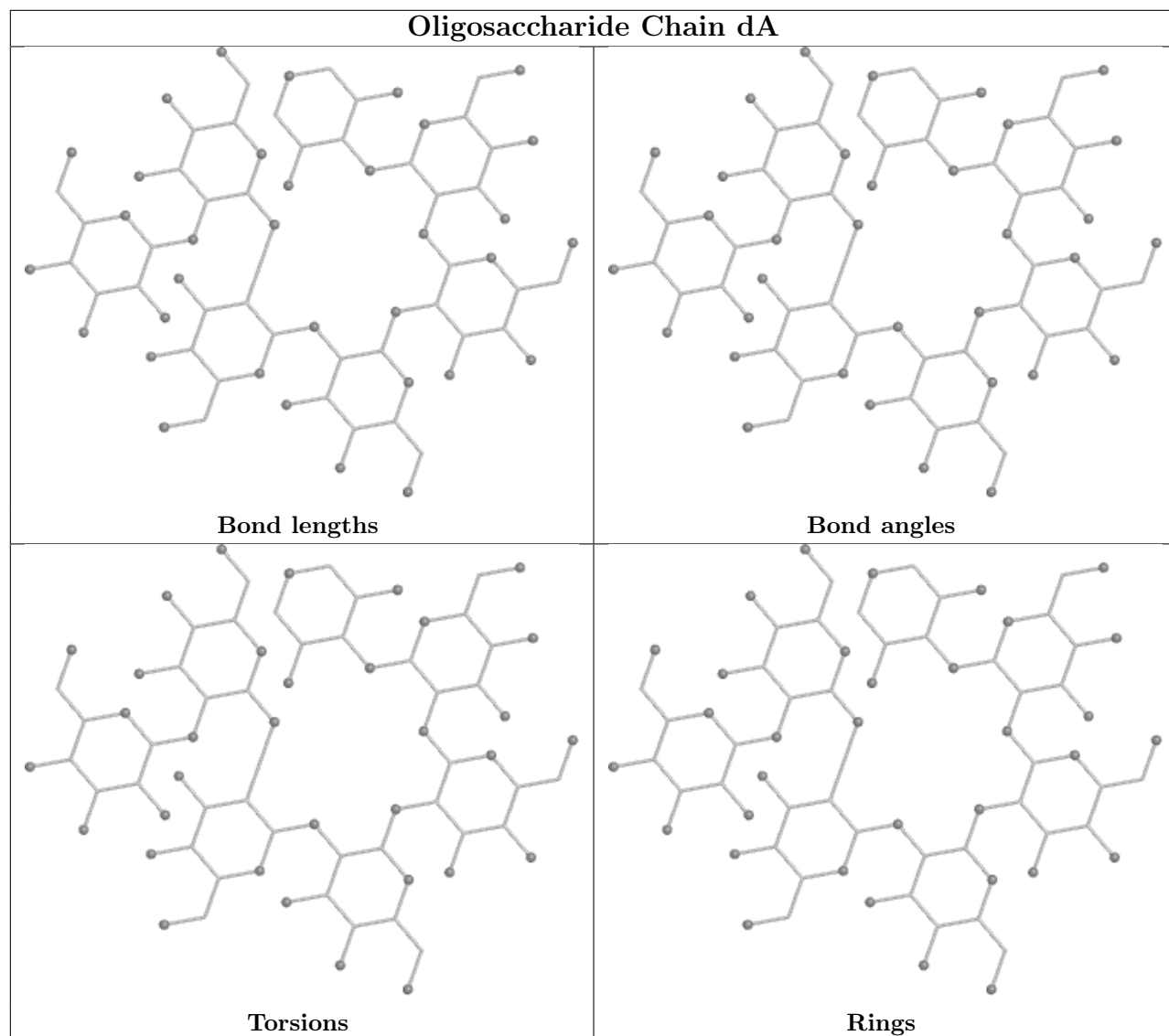


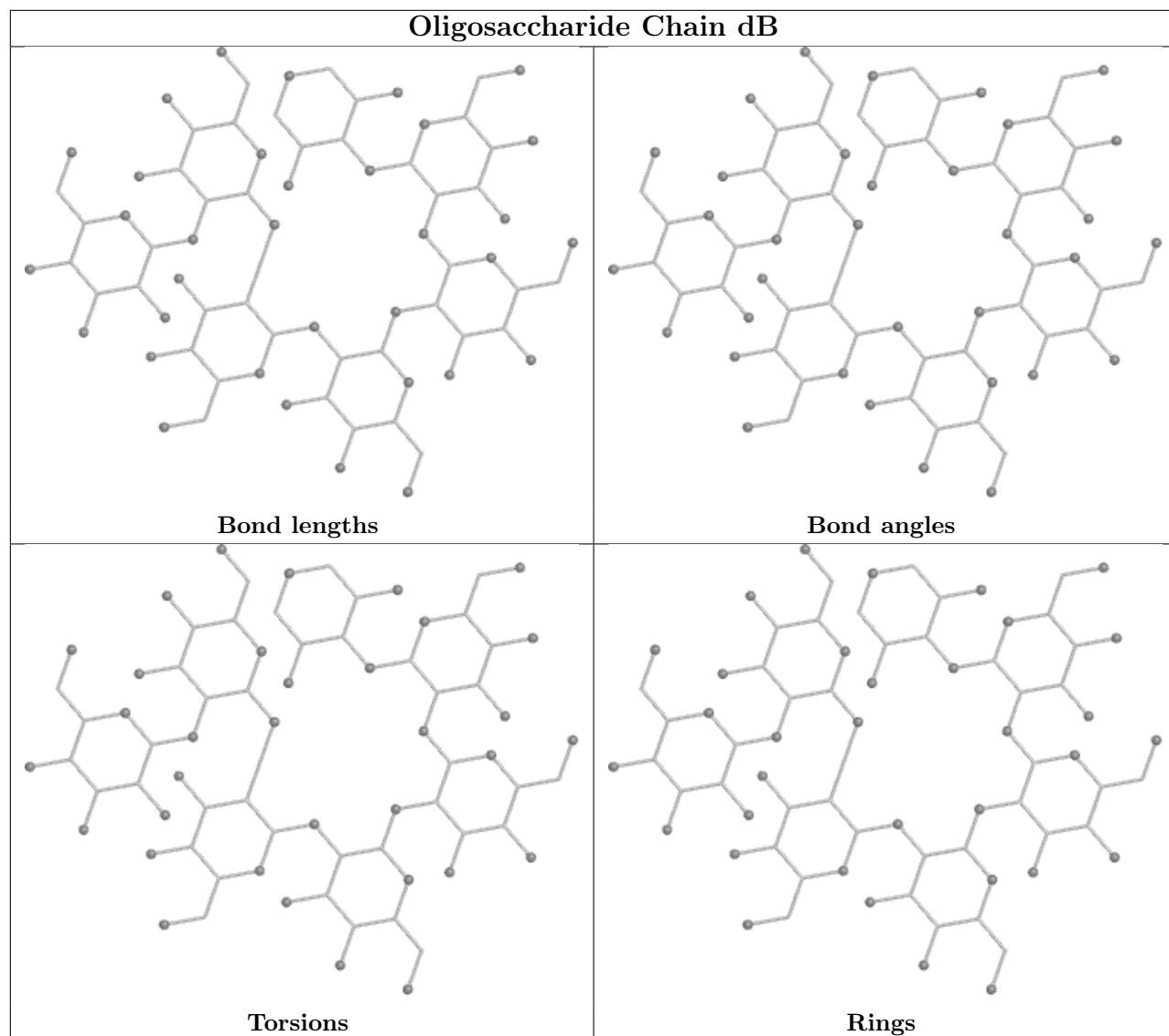


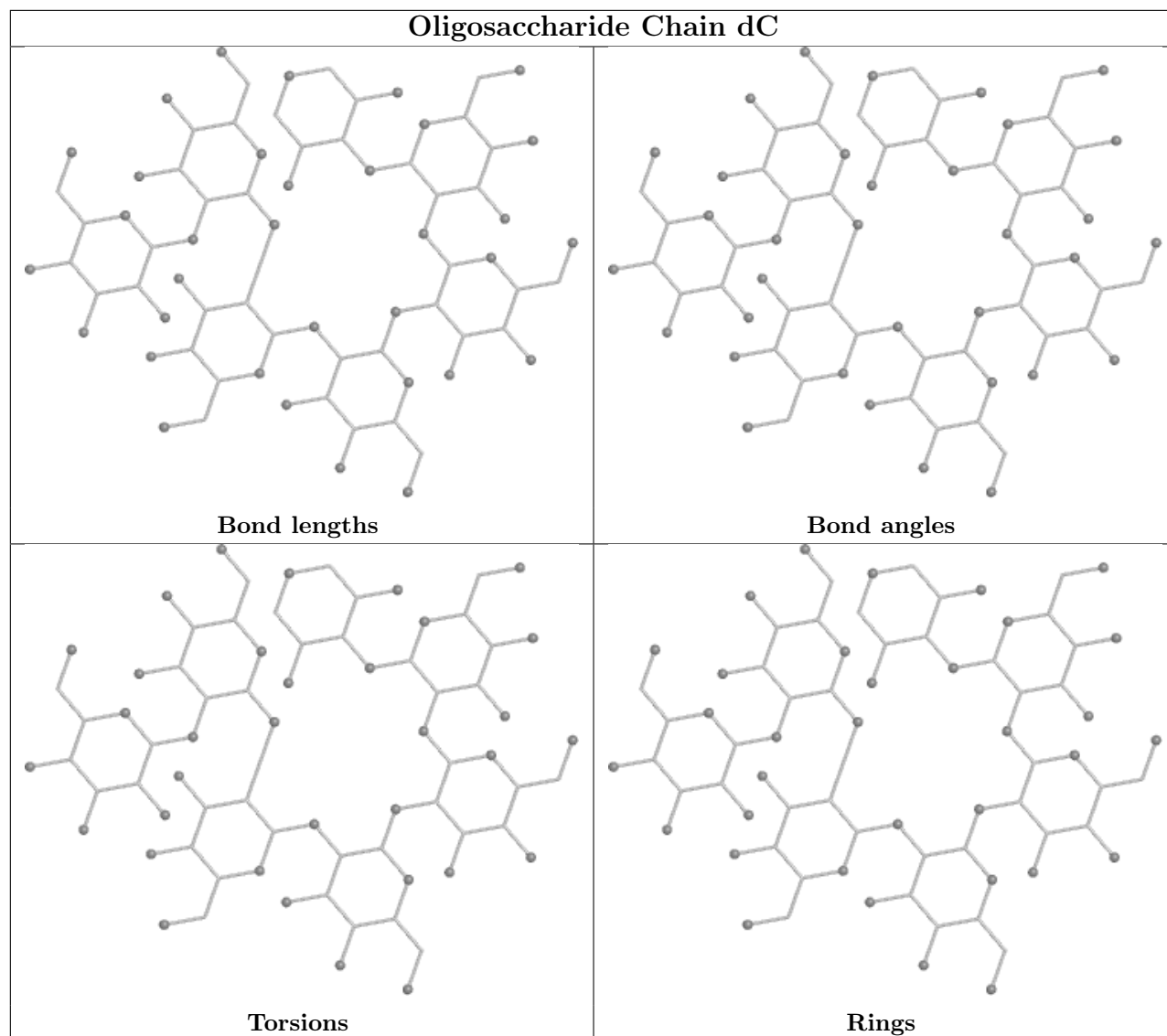


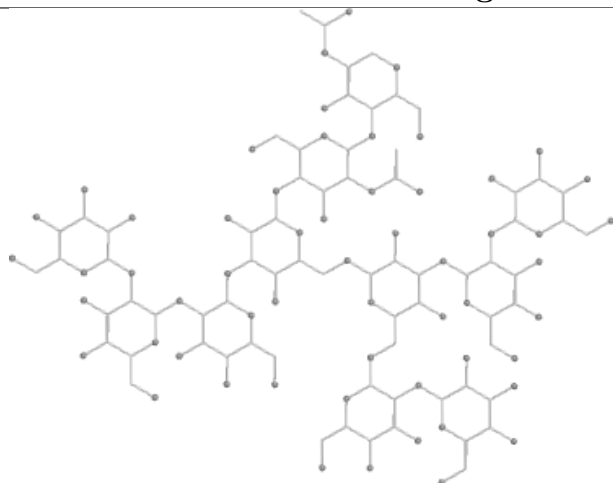
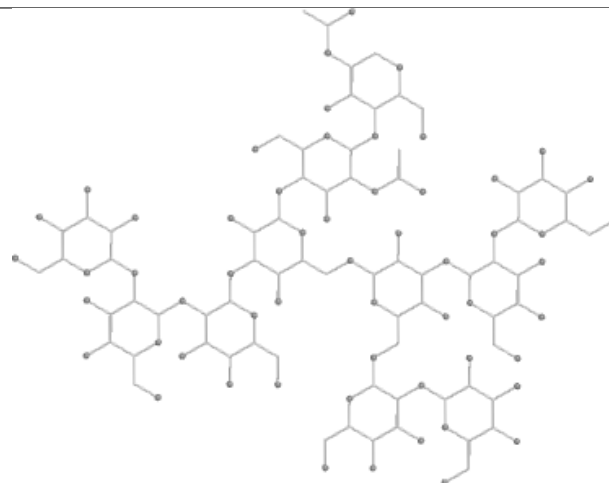
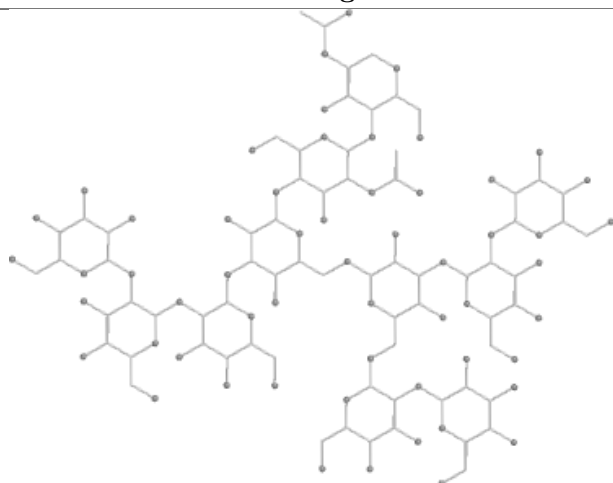
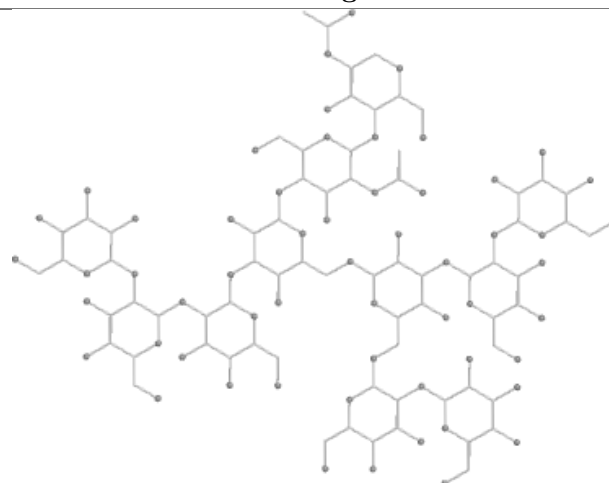


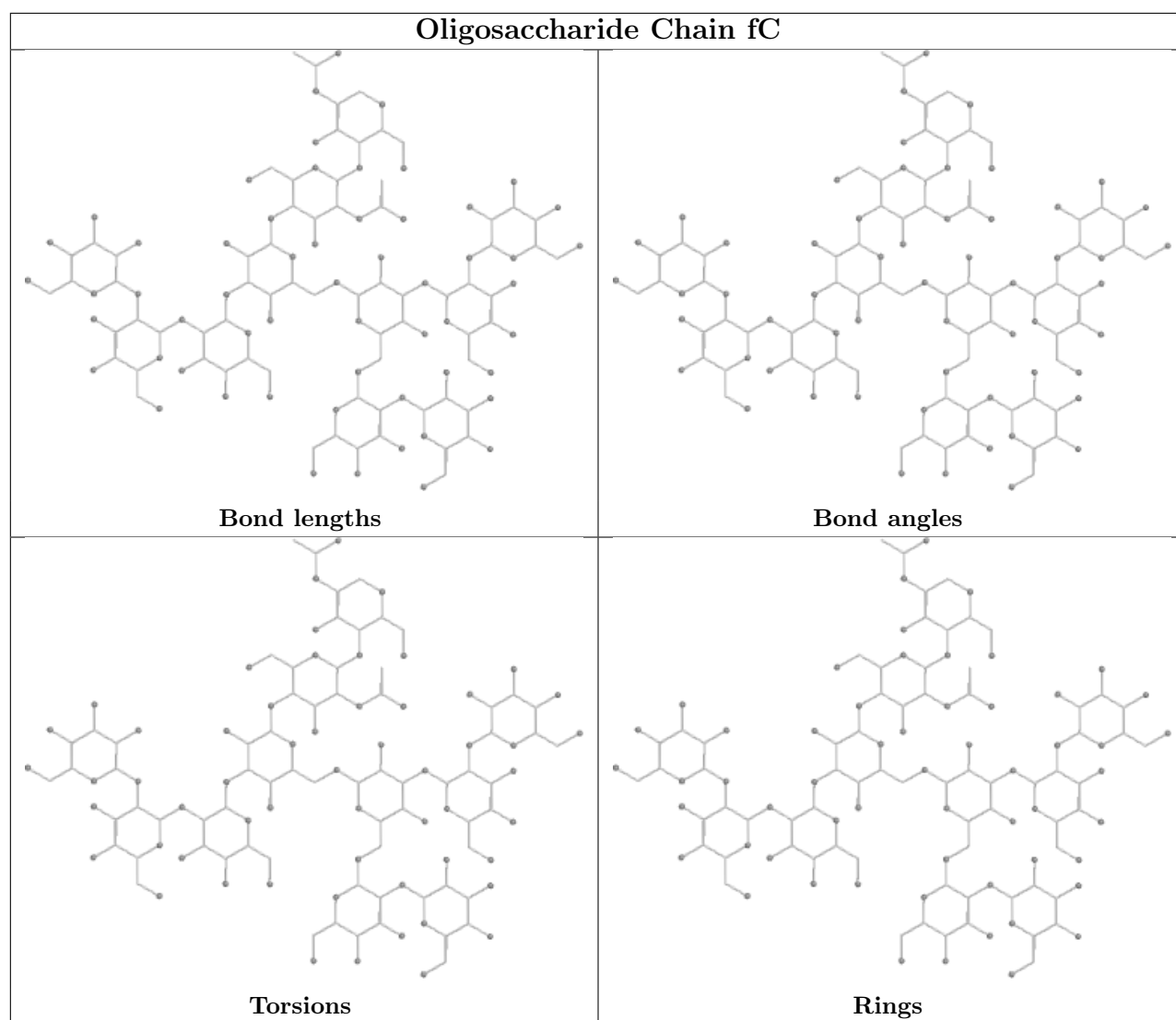


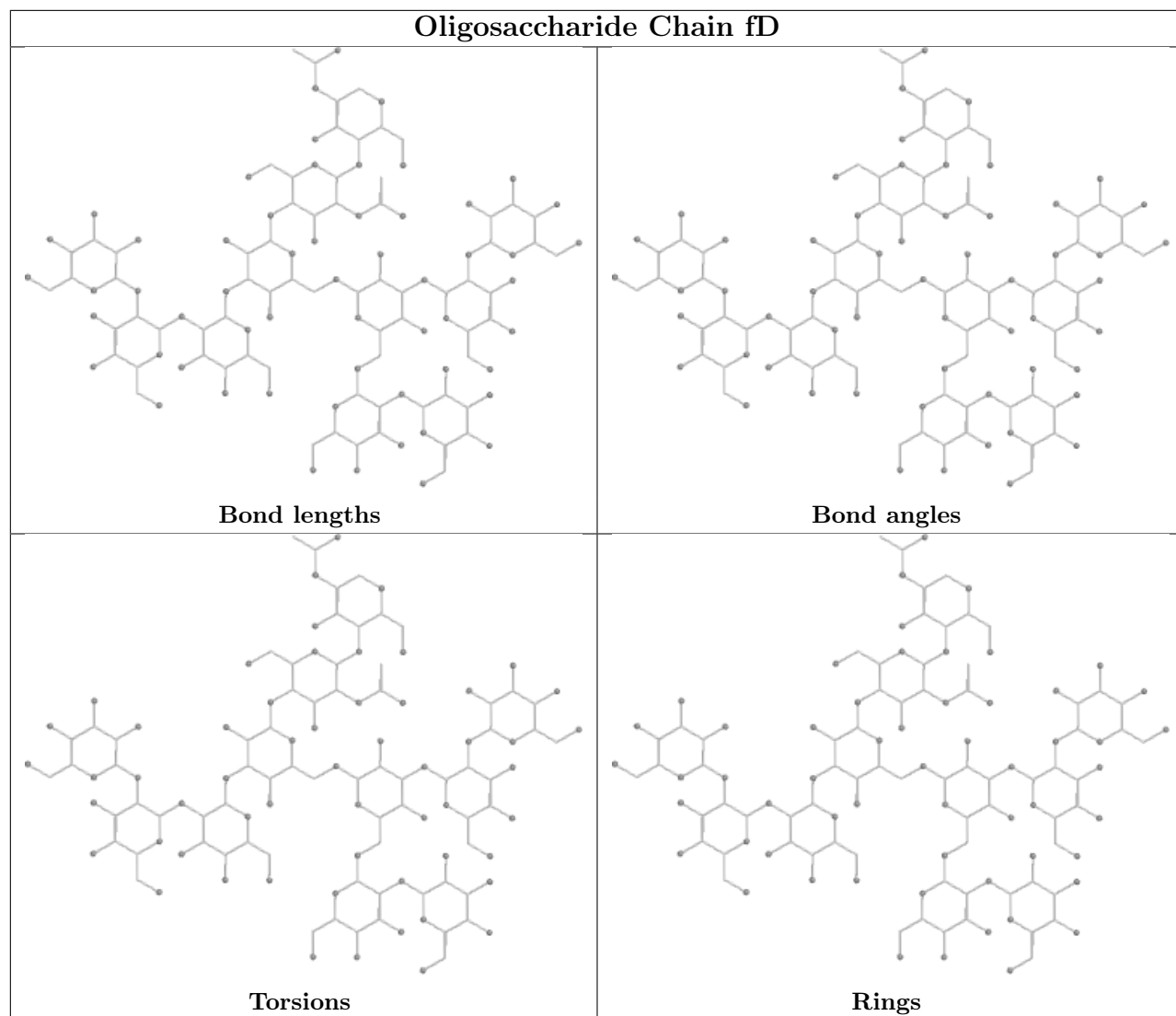


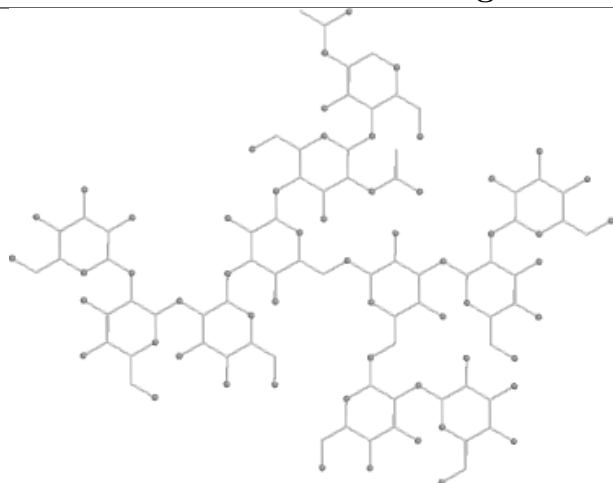
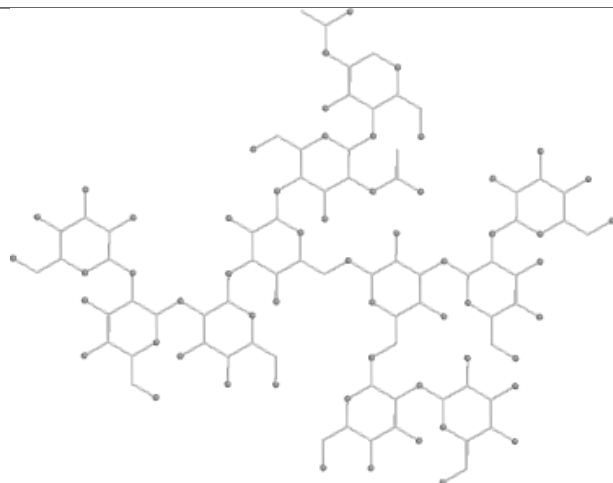
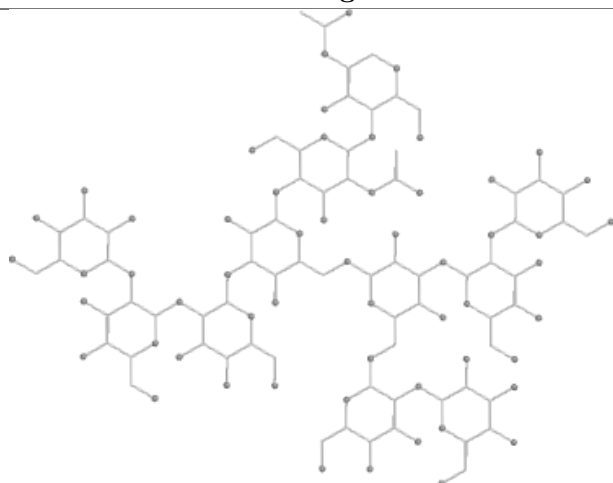
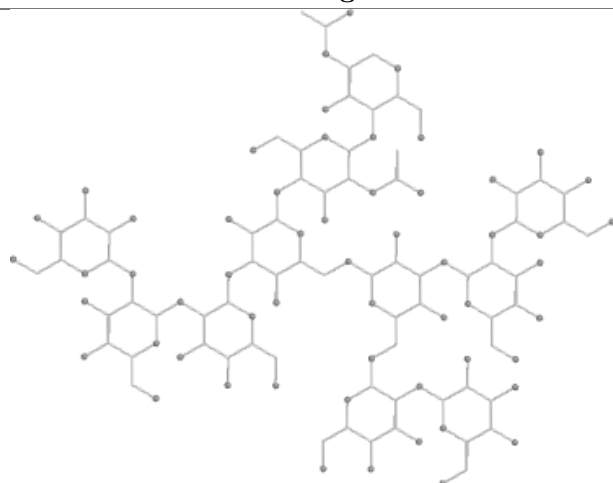


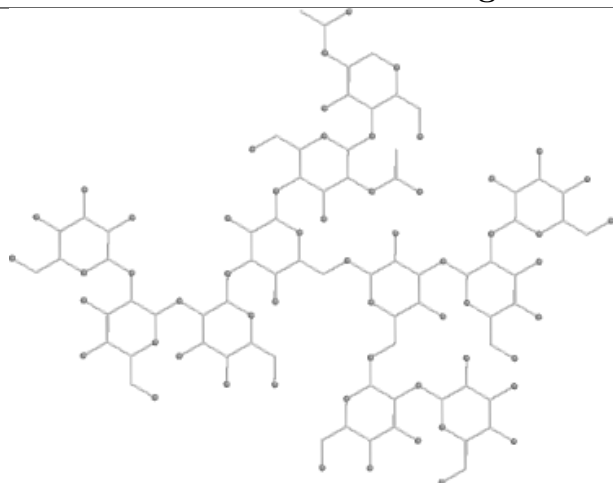
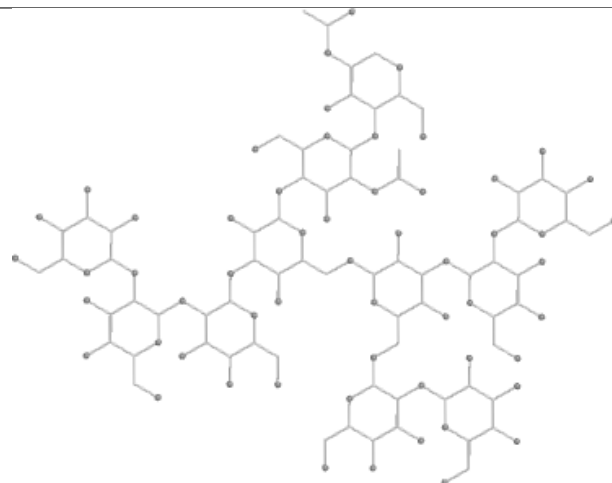
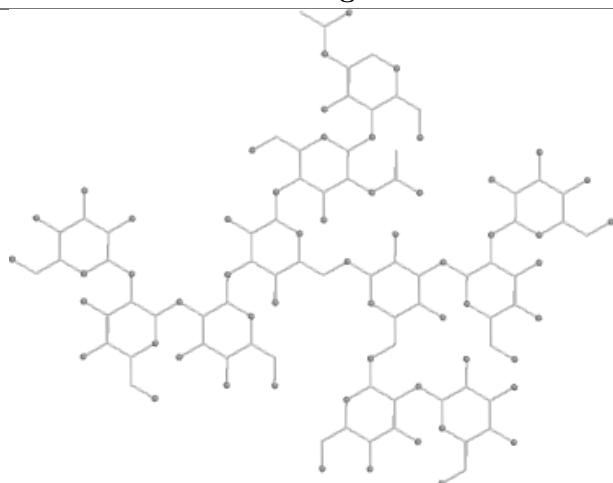
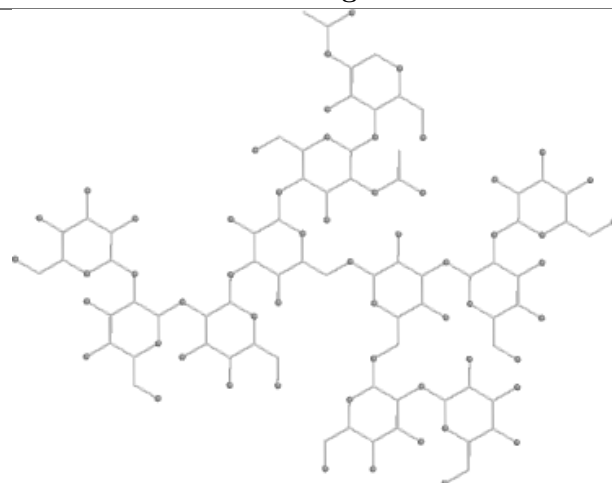


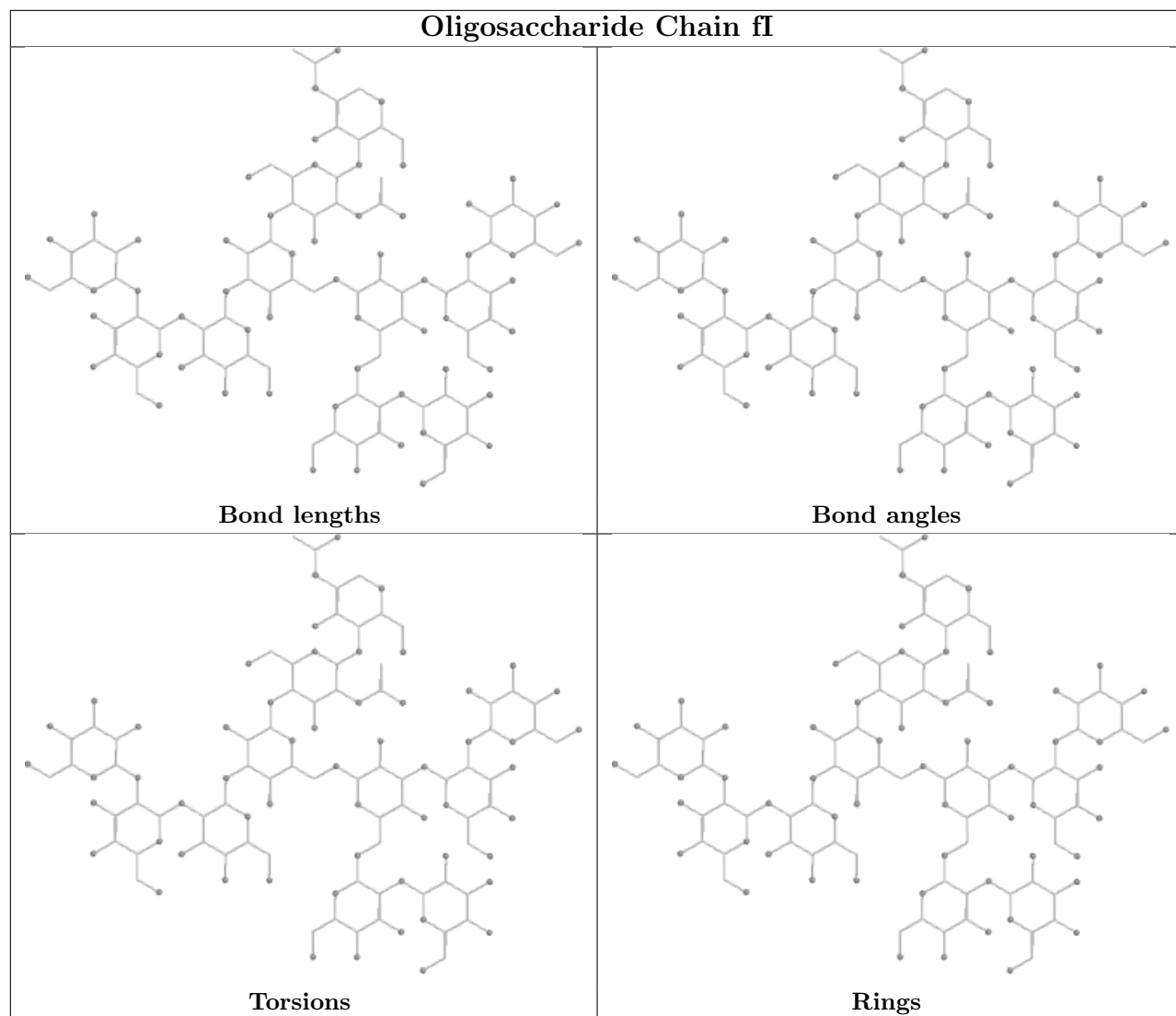
Oligosaccharide Chain eA**Bond lengths****Bond angles****Torsions****Rings**

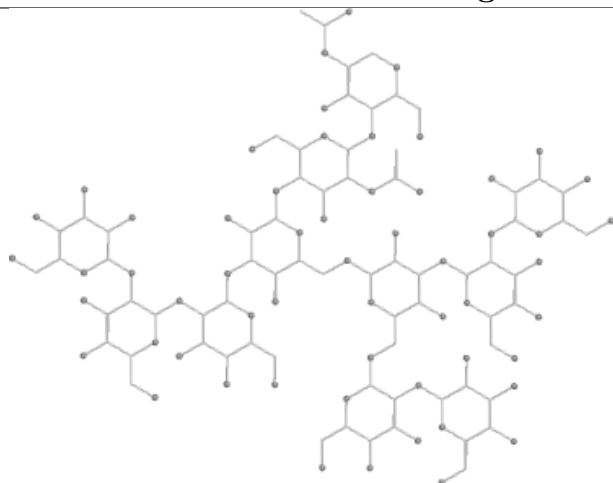
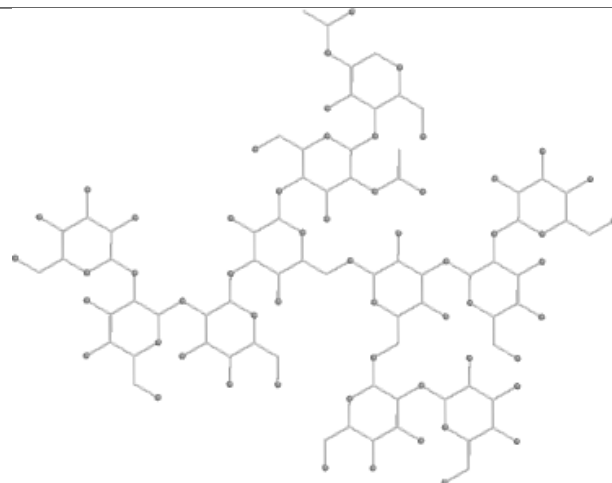
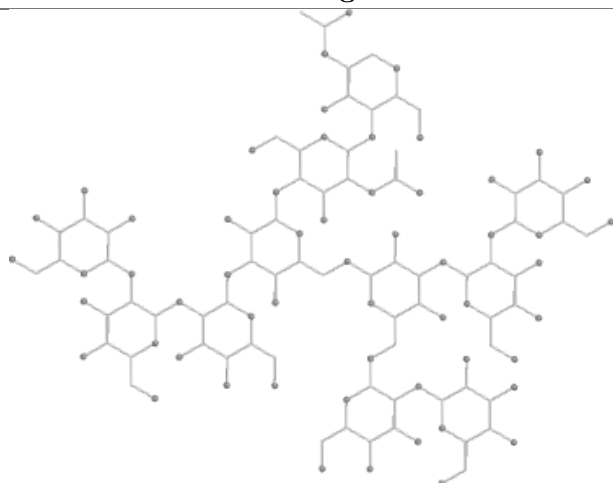
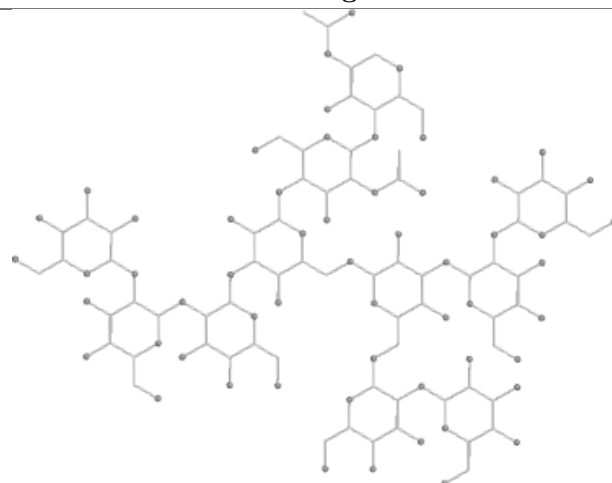


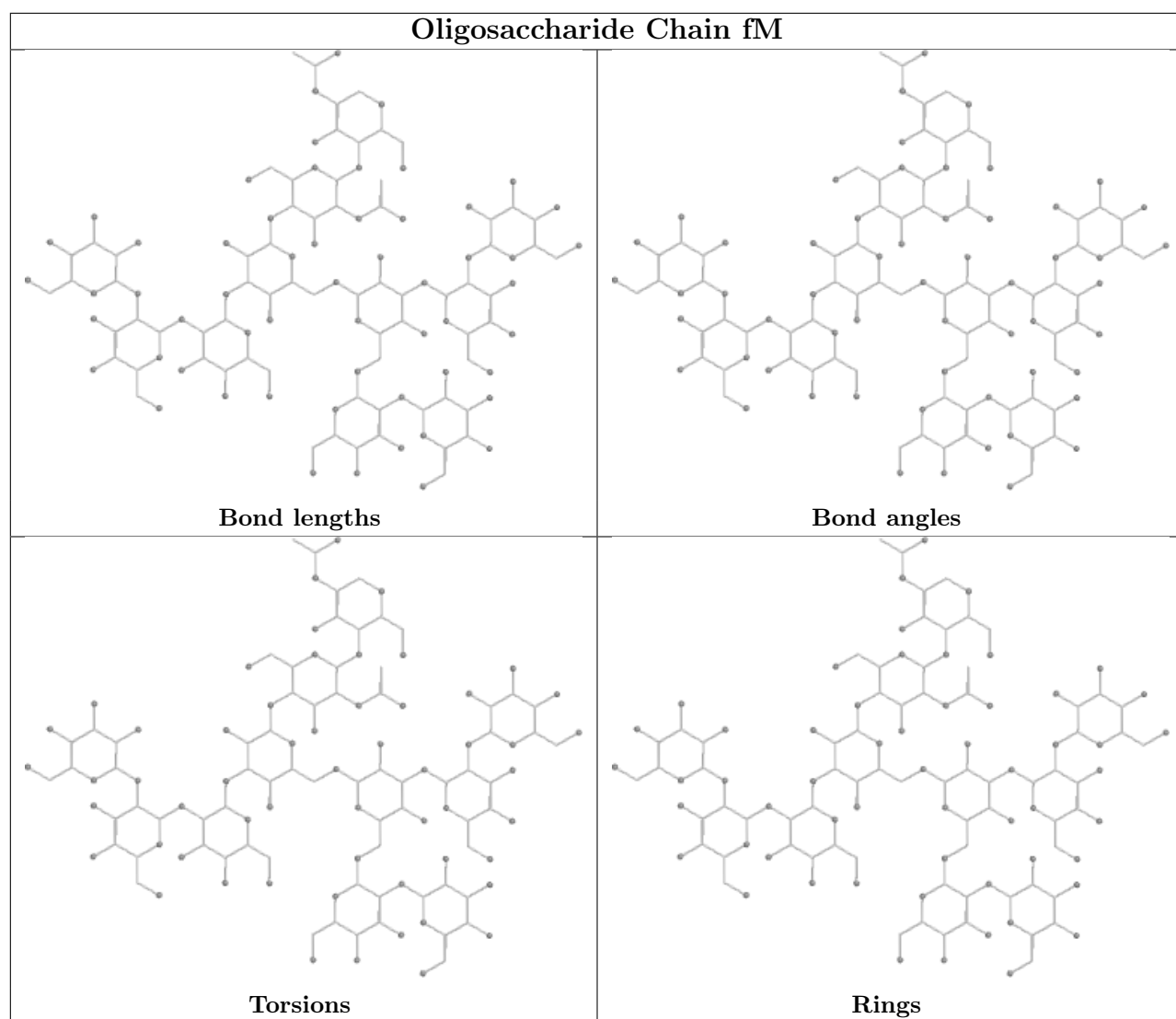


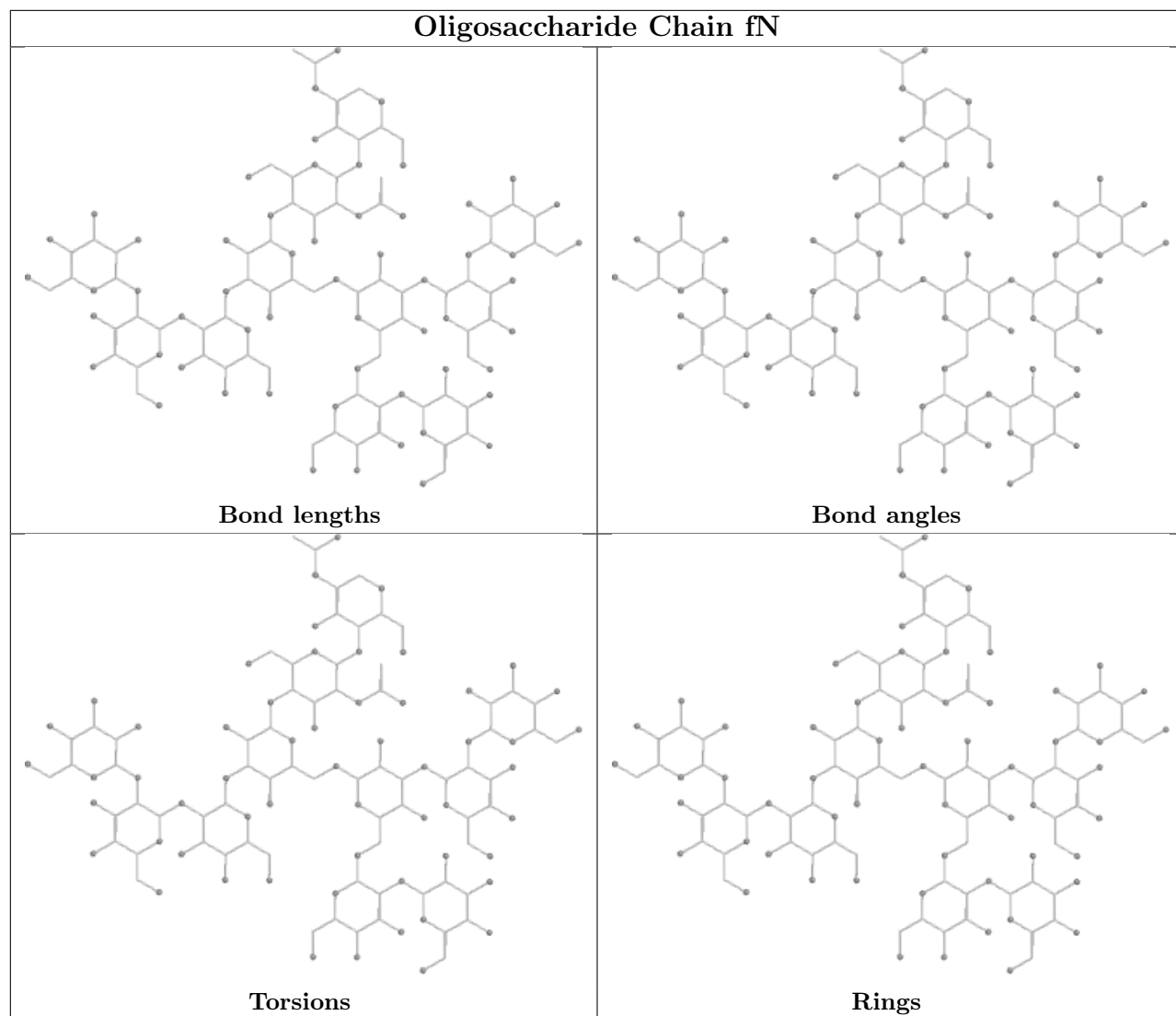
Oligosaccharide Chain eC**Bond lengths****Bond angles****Torsions****Rings**

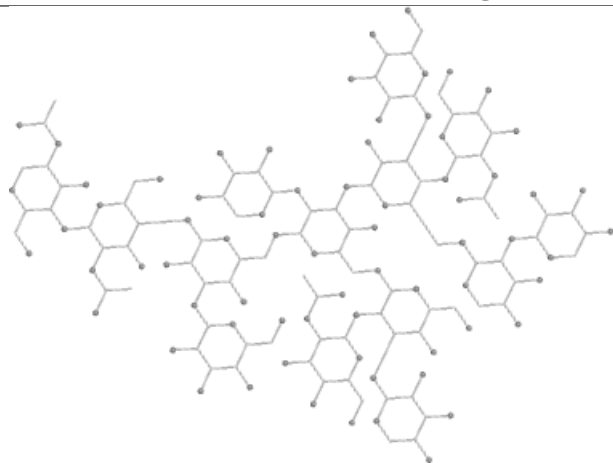
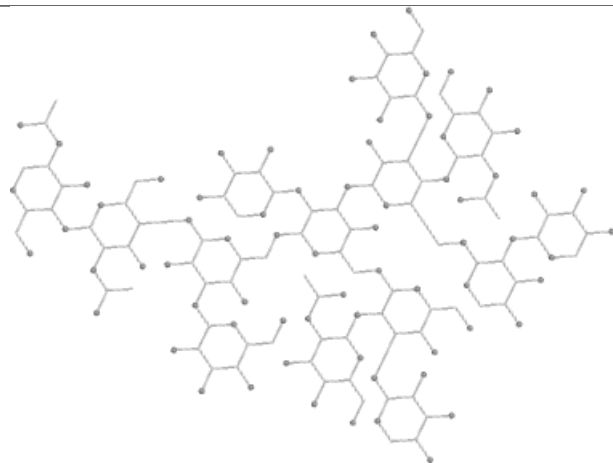
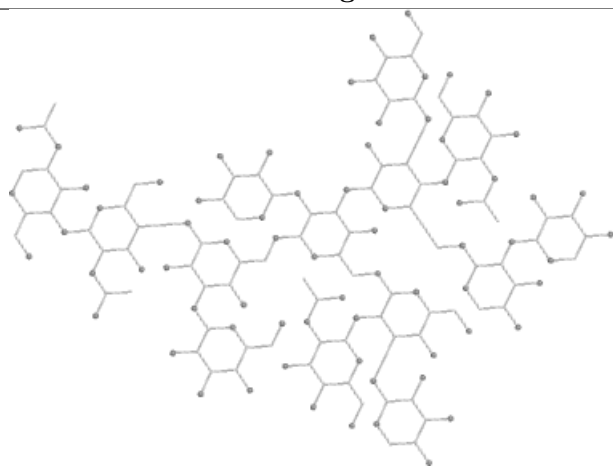
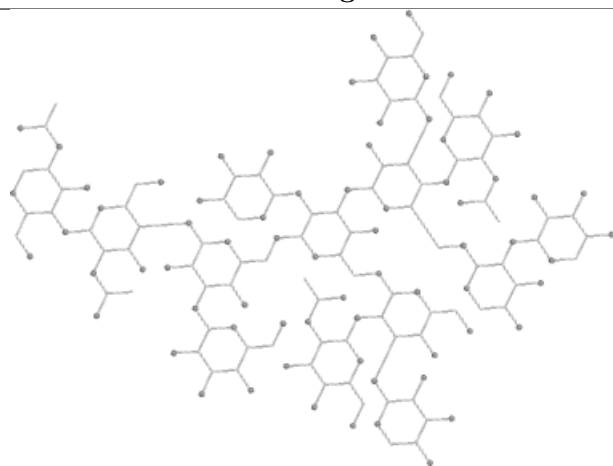
Oligosaccharide Chain fH**Bond lengths****Bond angles****Torsions****Rings**

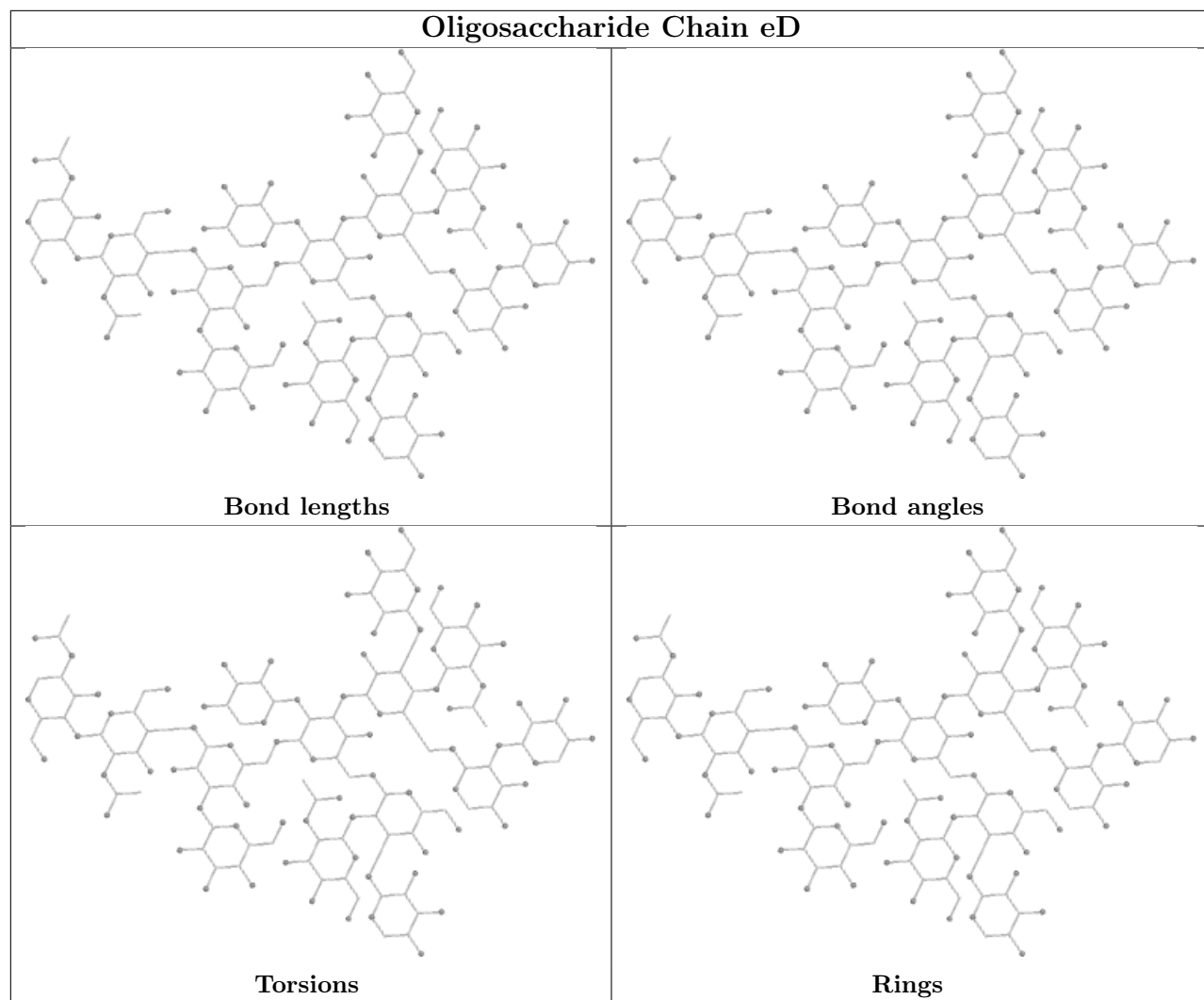


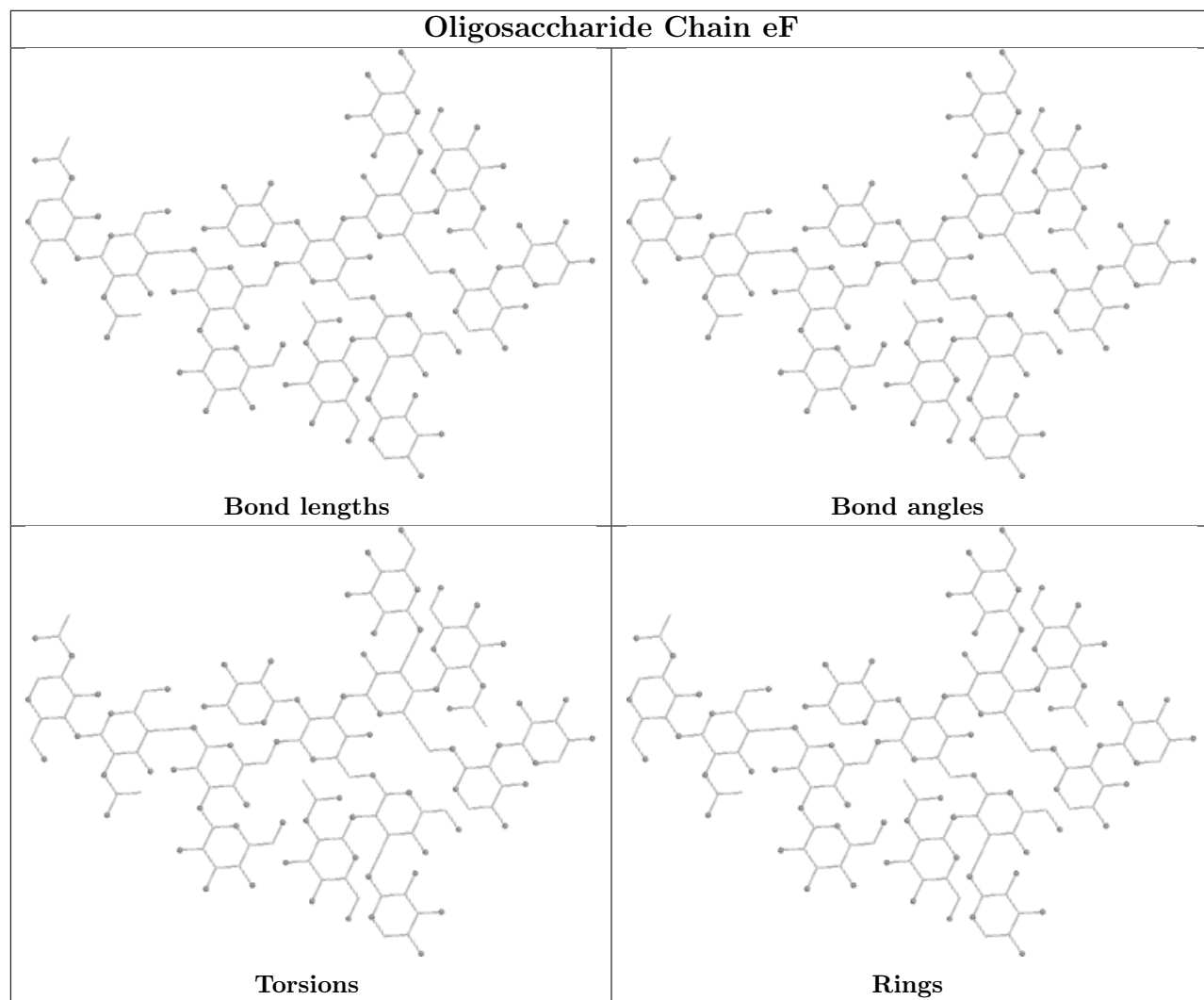
Oligosaccharide Chain eE**Bond lengths****Bond angles****Torsions****Rings**

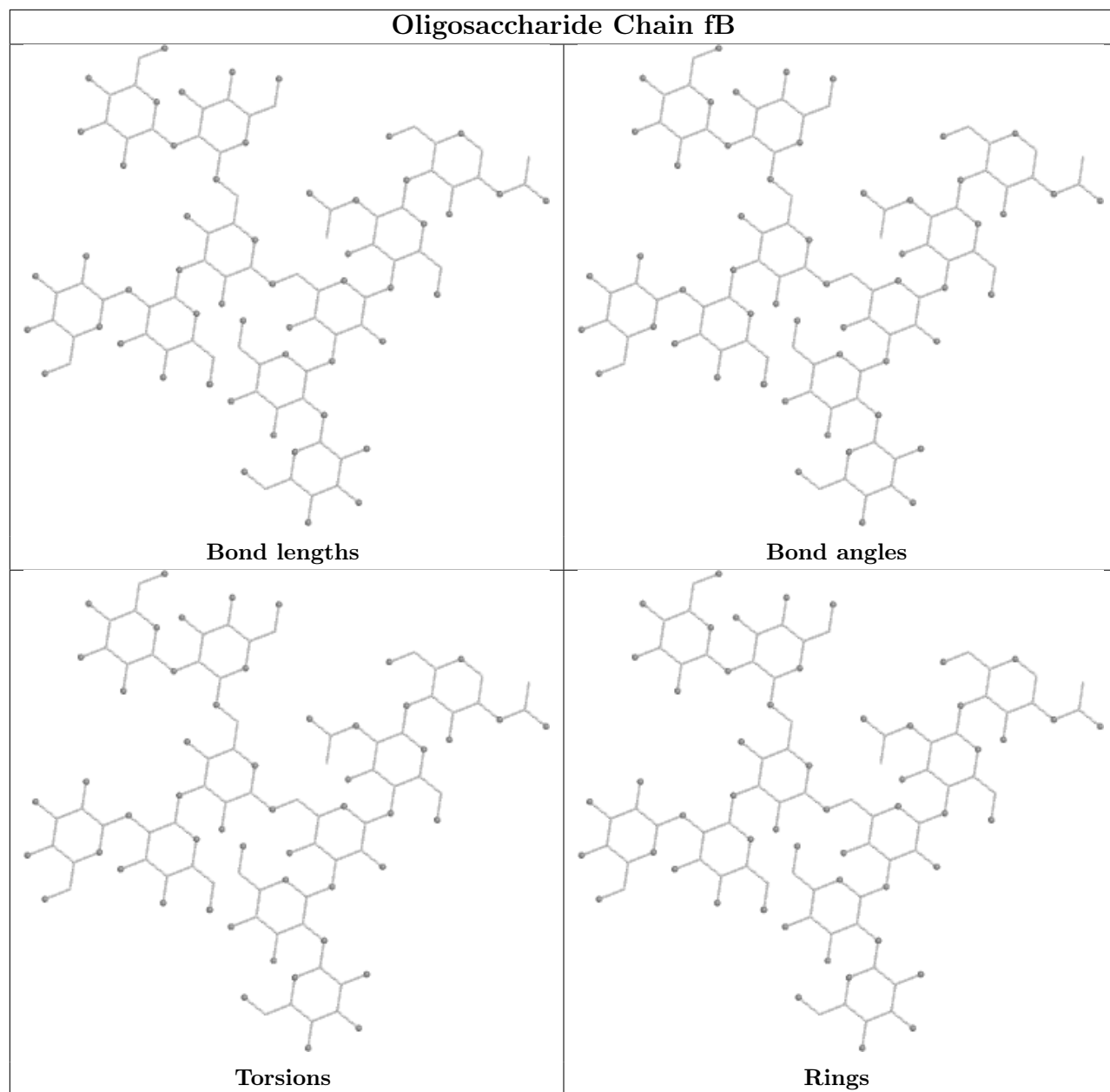


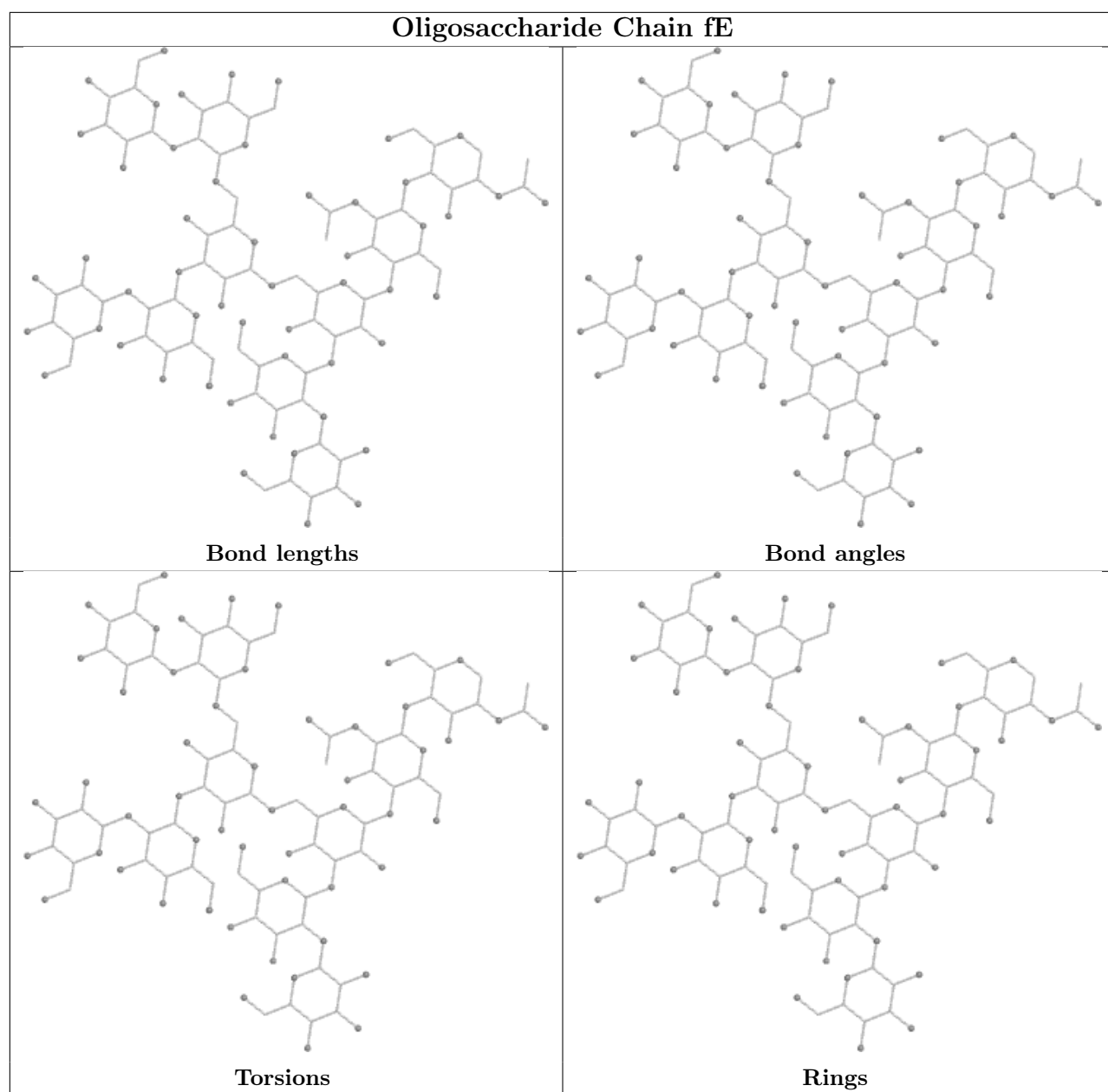


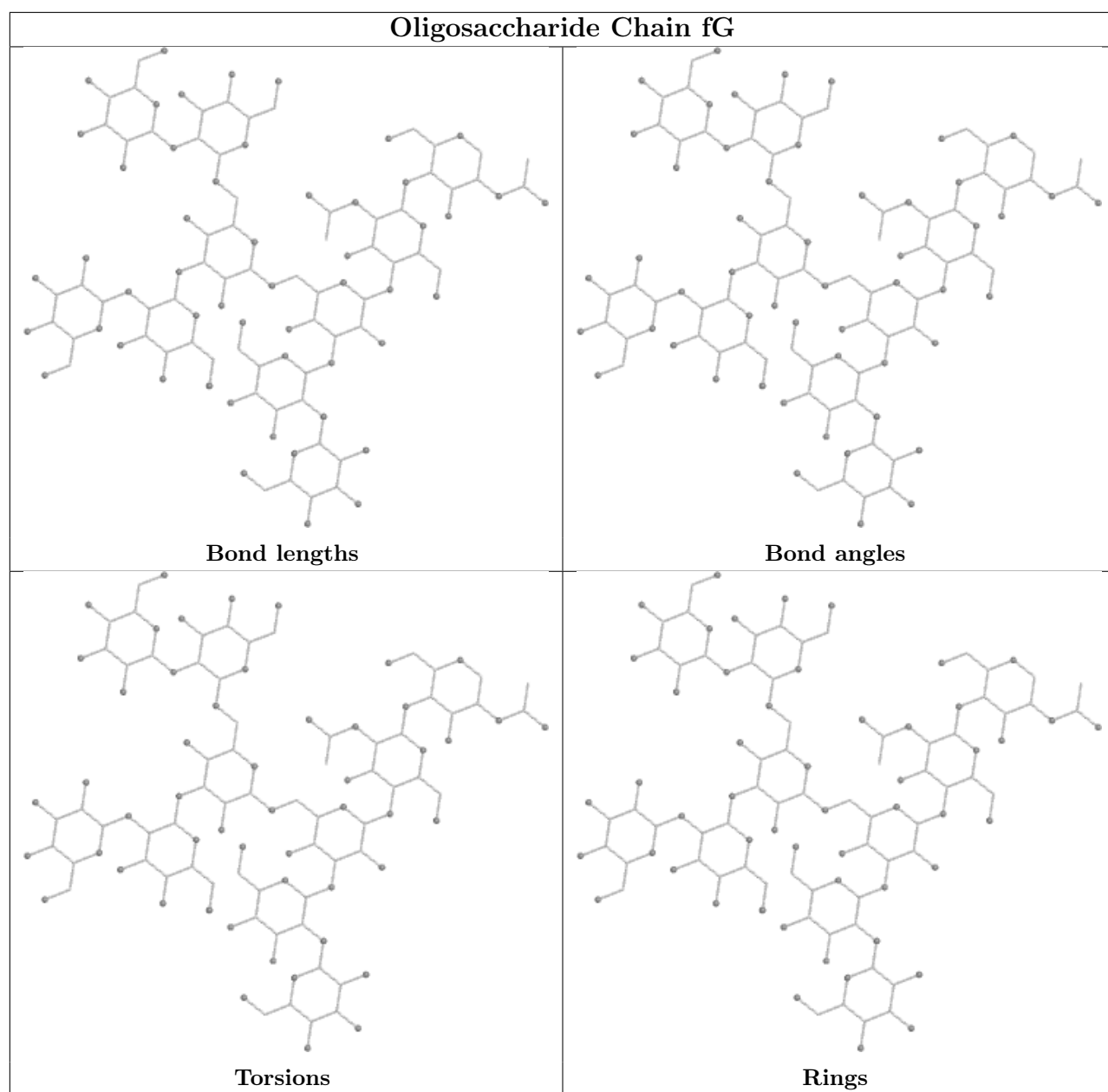
Oligosaccharide Chain eB**Bond lengths****Bond angles****Torsions****Rings**

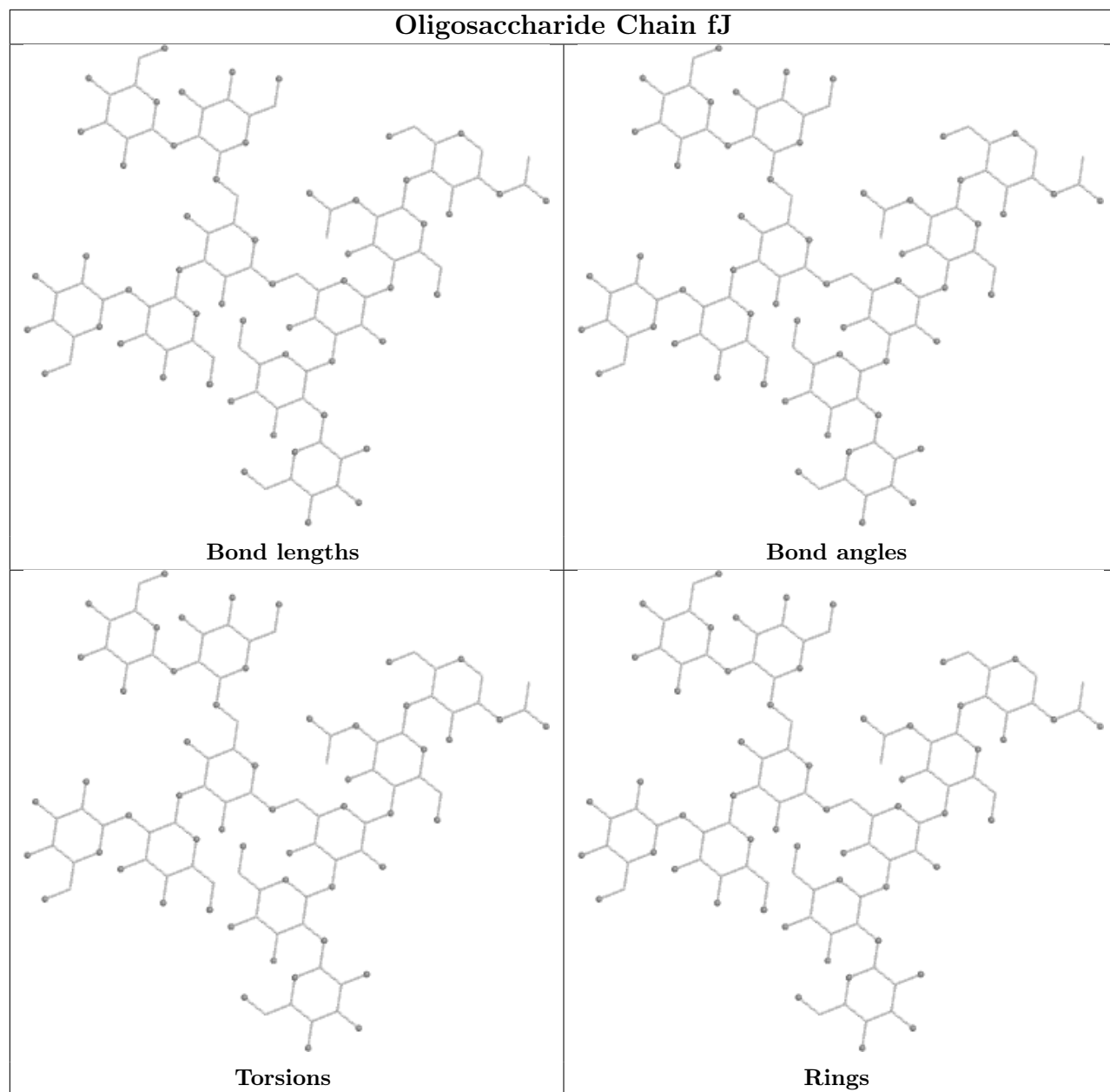


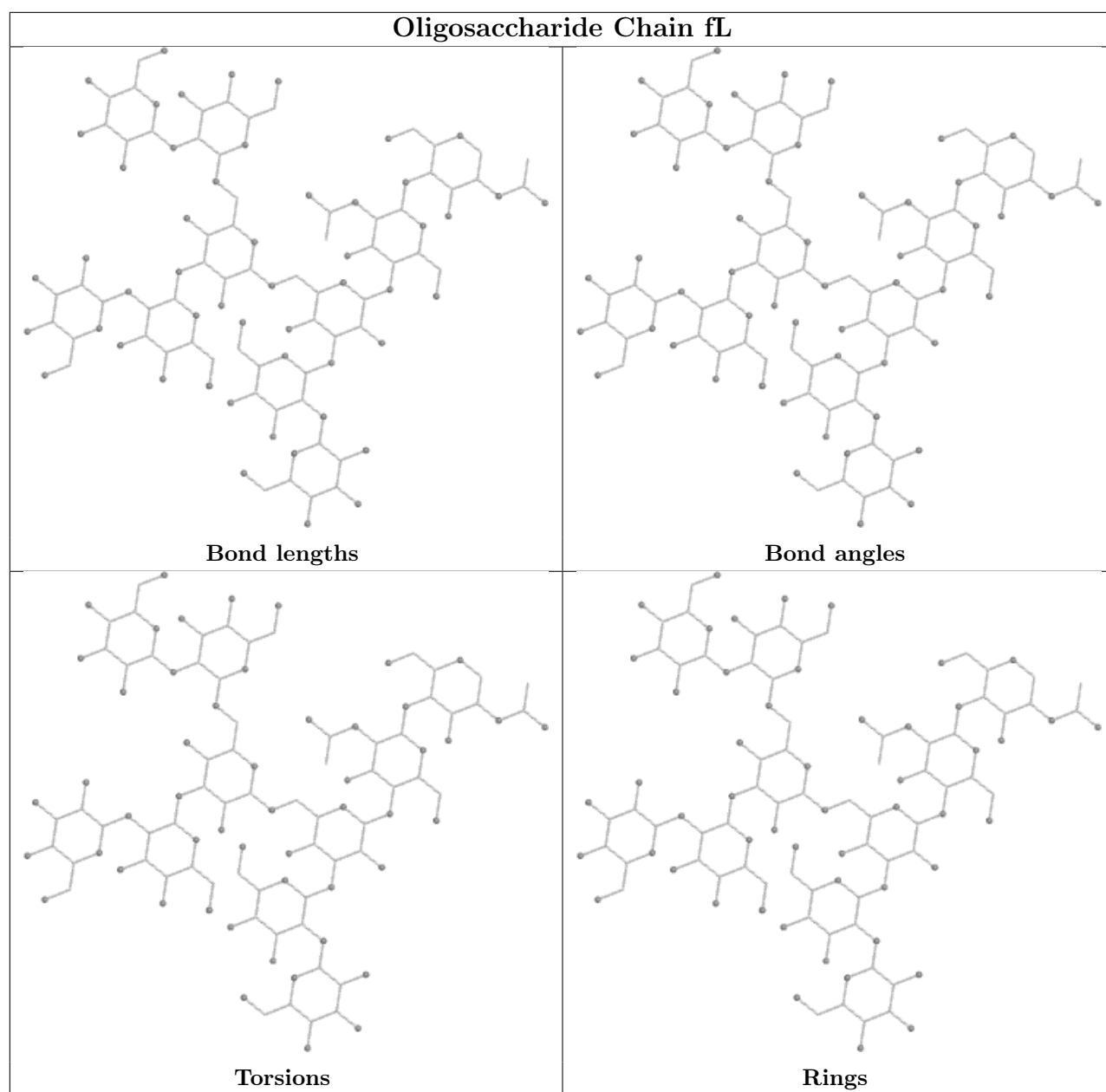


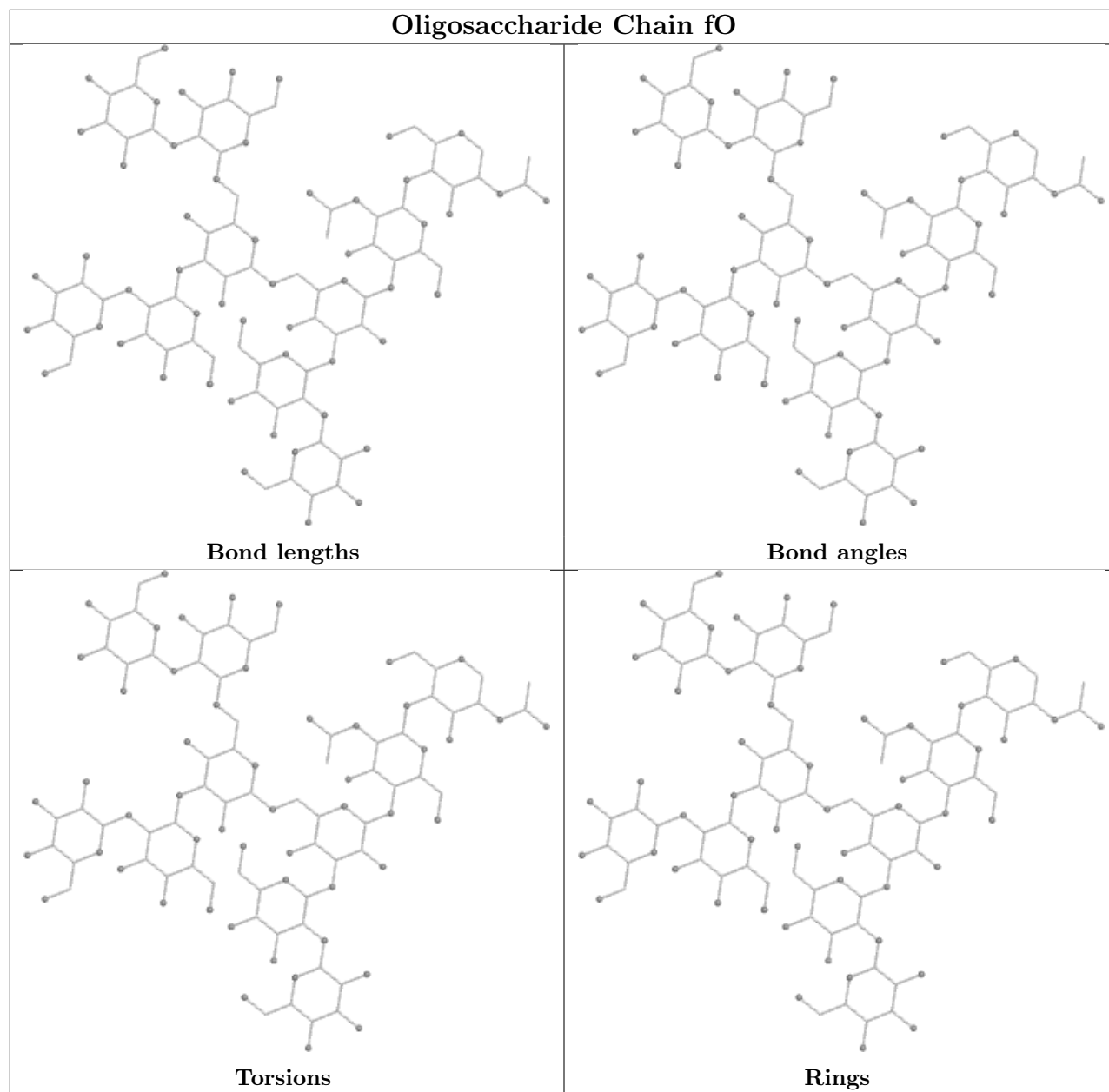


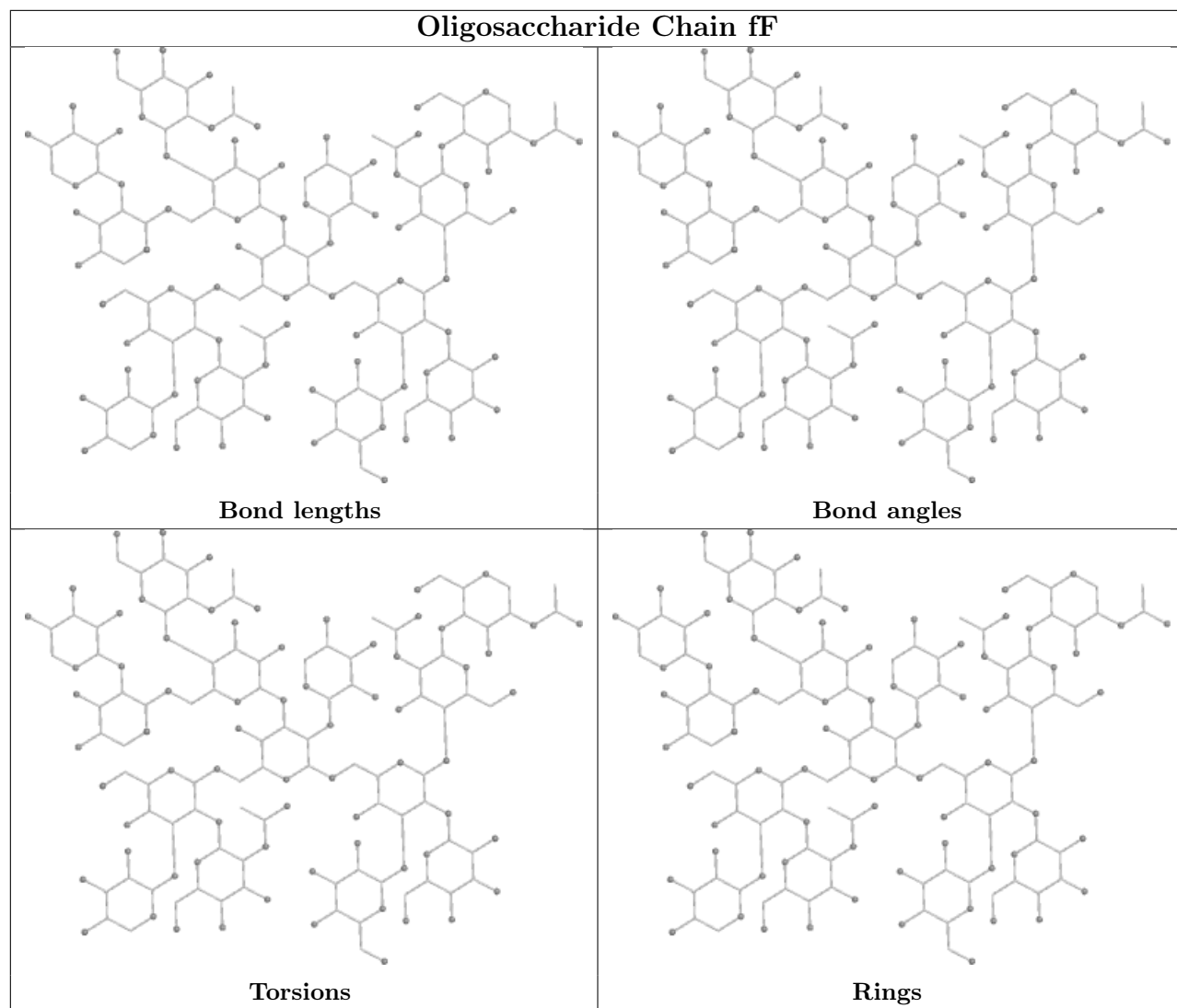


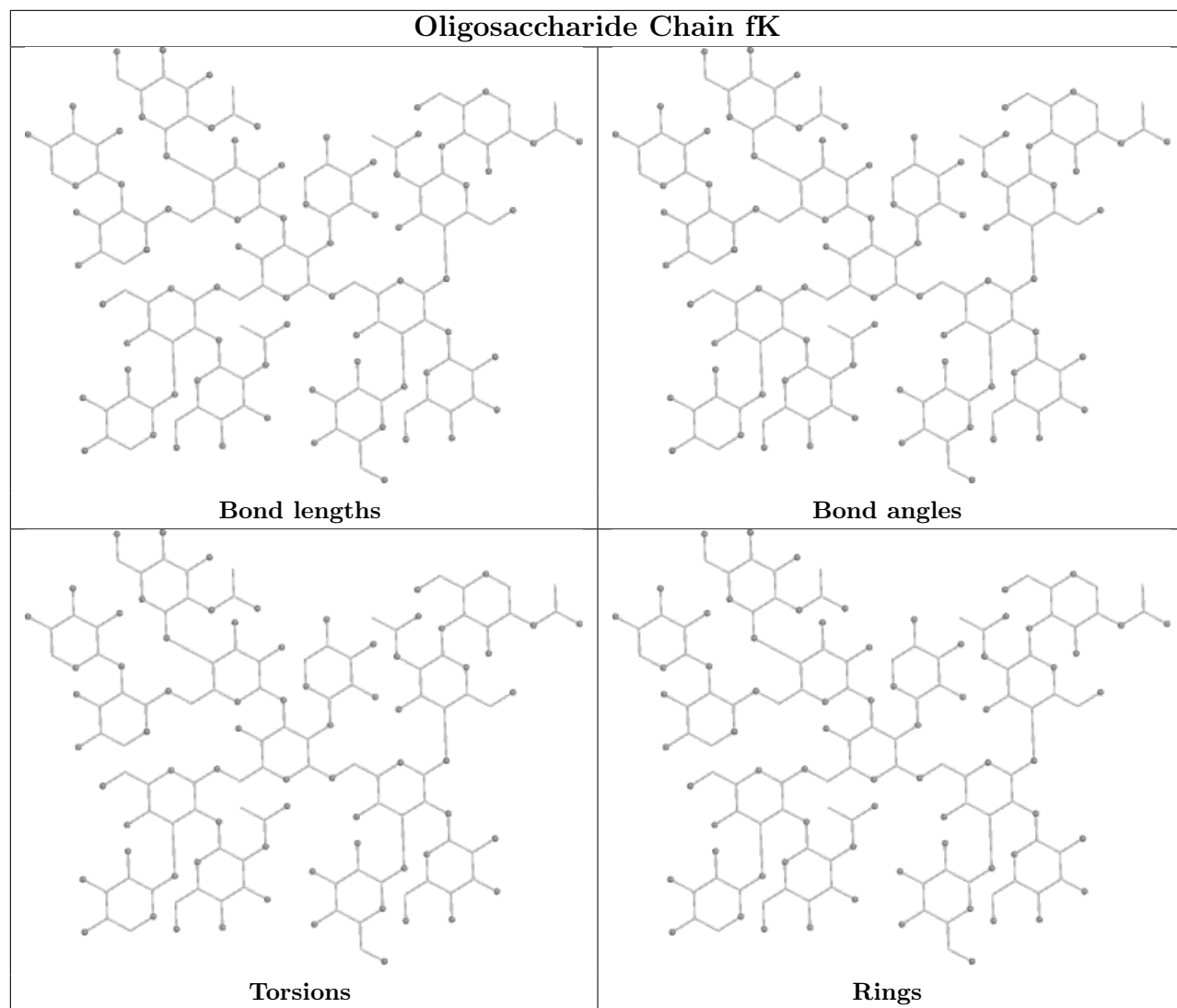


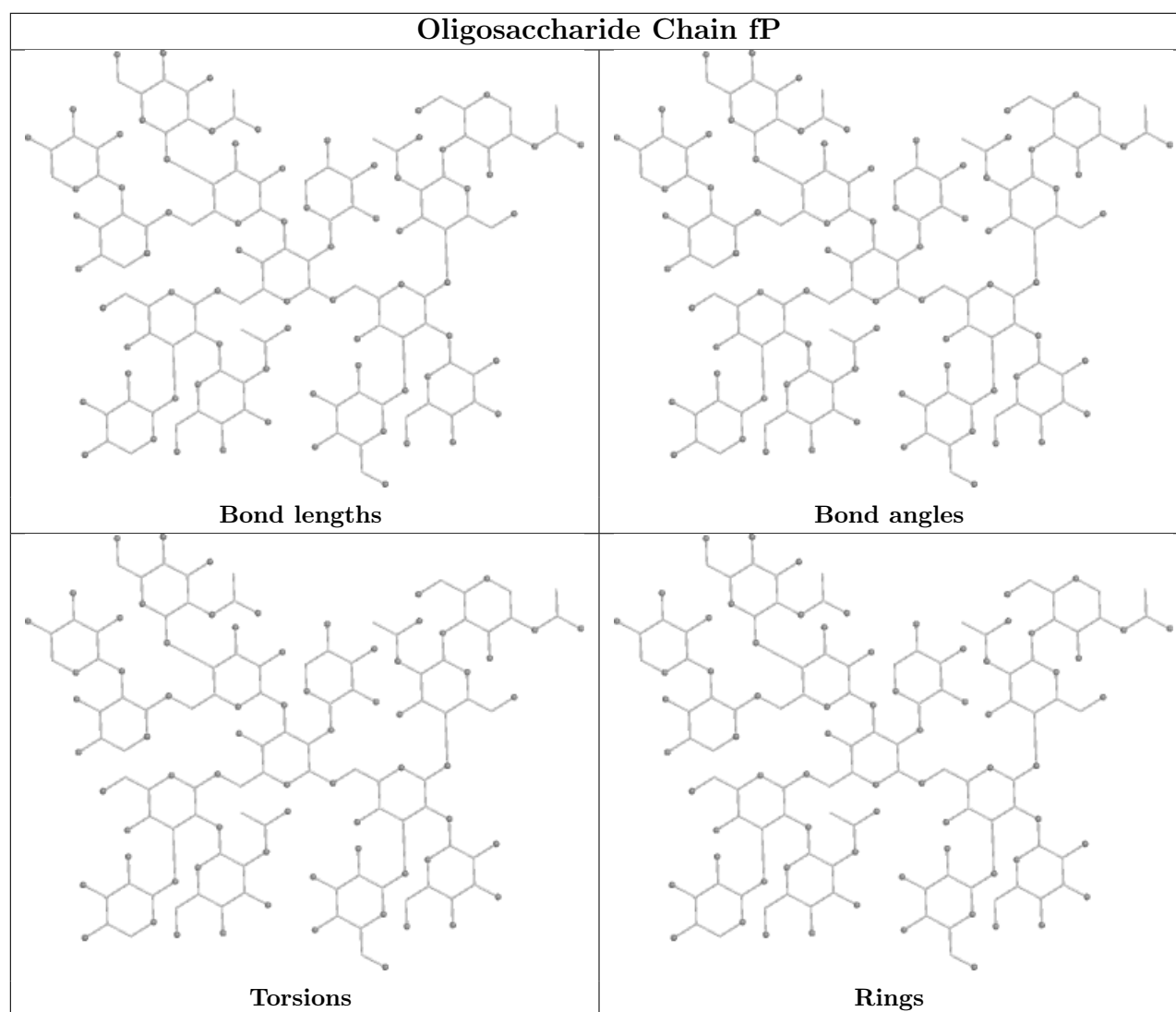












5.6 Ligand geometry [i](#)

Of 85 ligands modelled in this entry, 58 are monoatomic - leaving 27 for Mogul analysis.

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	$\# Z > 2$
22	NAG	FA	801	2	14,14,15	0.37	0	17,19,21	0.63	0
22	NAG	FB	801	2	14,14,15	0.34	0	17,19,21	0.81	0
23	2PO	FC	802	20	0,3,3	-	-	0,3,3	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	2PO	FB	802	20	0,3,3	-	-	0,3,3	-	-
22	NAG	FC	801	2	14,14,15	0.35	0	17,19,21	0.64	0
23	2PO	AC	802	8	0,3,3	-	-	0,3,3	-	-
23	2PO	EA	403	-	0,3,3	-	-	0,3,3	-	-
23	2PO	BA	401	21,11	0,3,3	-	-	0,3,3	-	-
23	2PO	BC	401	21	0,3,3	-	-	0,3,3	-	-
23	2PO	BA	402	14	0,3,3	-	-	0,3,3	-	-
23	2PO	AC	803	9	0,3,3	-	-	0,3,3	-	-
22	NAG	EA	402	1	14,14,15	0.39	0	17,19,21	1.04	1 (5%)
23	2PO	EC	402	-	0,3,3	-	-	0,3,3	-	-
23	2PO	EB	402	18	0,3,3	-	-	0,3,3	-	-
22	NAG	EB	401	1	14,14,15	0.34	0	17,19,21	1.03	1 (5%)
23	2PO	AA	803	9	0,3,3	-	-	0,3,3	-	-
22	NAG	EC	401	1	14,14,15	0.31	0	17,19,21	0.88	1 (5%)
23	2PO	AC	801	7	0,3,3	-	-	0,3,3	-	-
23	2PO	BB	401	21	0,3,3	-	-	0,3,3	-	-
23	2PO	AB	802	-	0,3,3	-	-	0,3,3	-	-
23	2PO	BC	402	14	0,3,3	-	-	0,3,3	-	-
23	2PO	FA	802	-	0,3,3	-	-	0,3,3	-	-
23	2PO	AB	803	-	0,3,3	-	-	0,3,3	-	-
23	2PO	AA	801	7	0,3,3	-	-	0,3,3	-	-
23	2PO	BB	402	14	0,3,3	-	-	0,3,3	-	-
23	2PO	AA	802	-	0,3,3	-	-	0,3,3	-	-
23	2PO	AB	801	7	0,3,3	-	-	0,3,3	-	-

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
22	NAG	EB	401	1	-	0/6/23/26	0/1/1/1
22	NAG	FA	801	2	-	0/6/23/26	0/1/1/1
22	NAG	FB	801	2	-	0/6/23/26	0/1/1/1
22	NAG	FC	801	2	-	0/6/23/26	0/1/1/1
22	NAG	EA	402	1	-	1/6/23/26	0/1/1/1
22	NAG	EC	401	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
22	EA	402	NAG	C1-O5-C5	3.44	116.85	112.19
22	EB	401	NAG	C1-O5-C5	2.96	116.20	112.19
22	EC	401	NAG	C1-O5-C5	2.72	115.88	112.19

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	EA	402	NAG	C4-C5-C6-O6

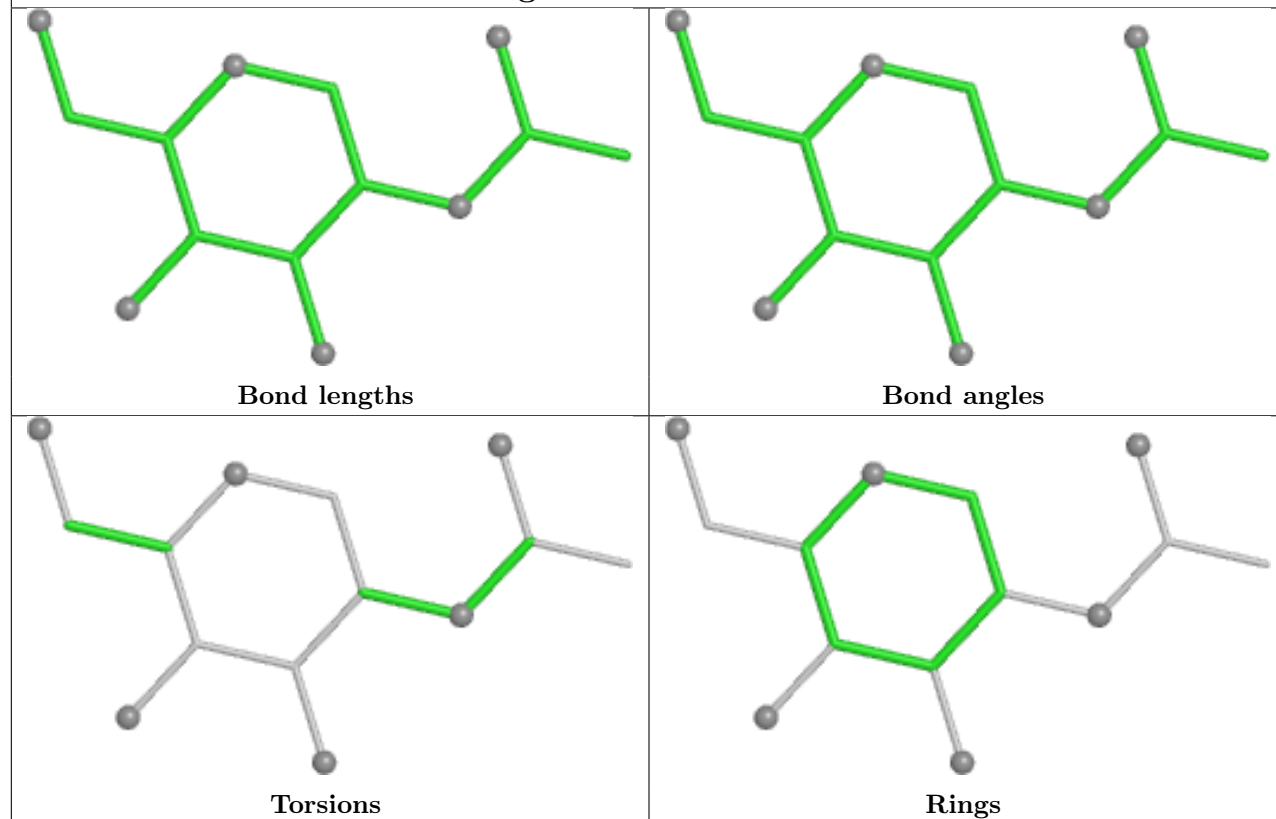
There are no ring outliers.

3 monomers are involved in 3 short contacts:

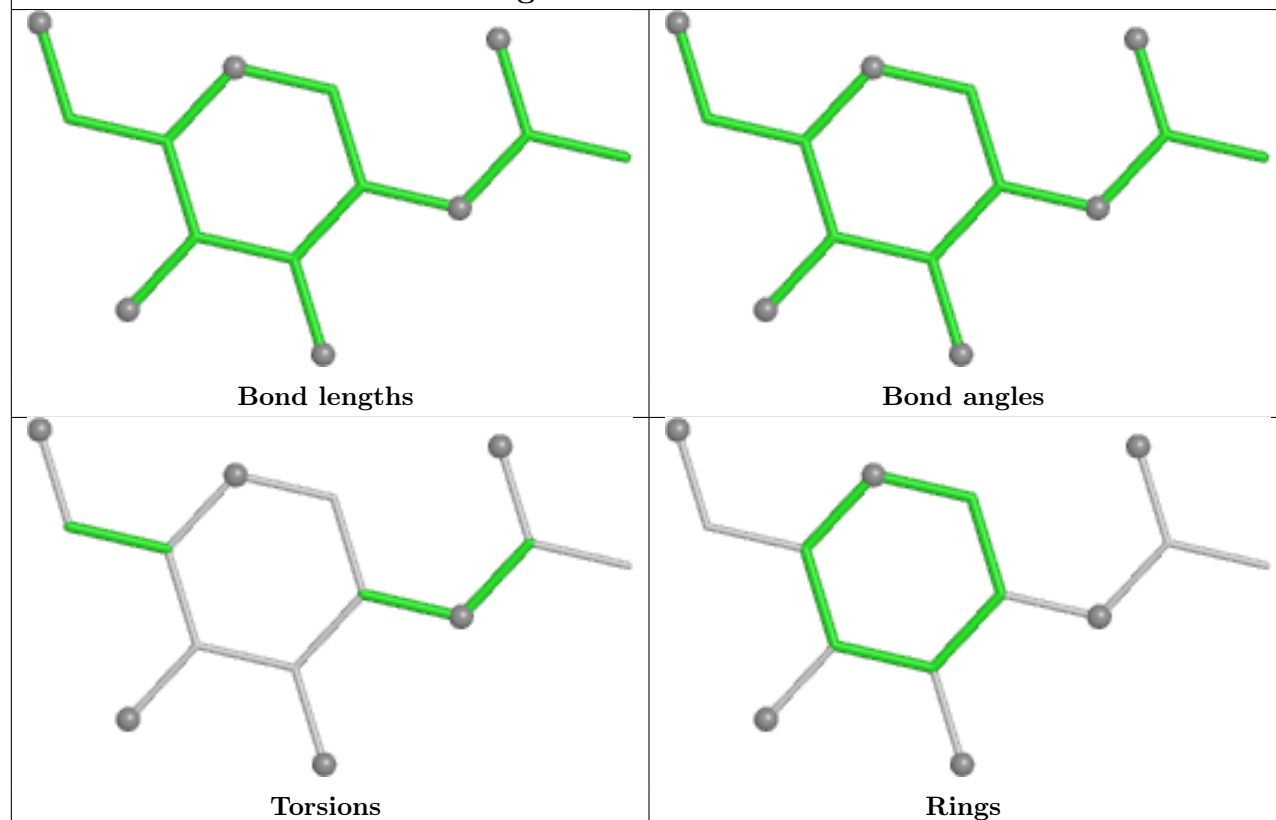
Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	EA	402	NAG	1	0
22	EB	401	NAG	1	0
22	EC	401	NAG	1	0

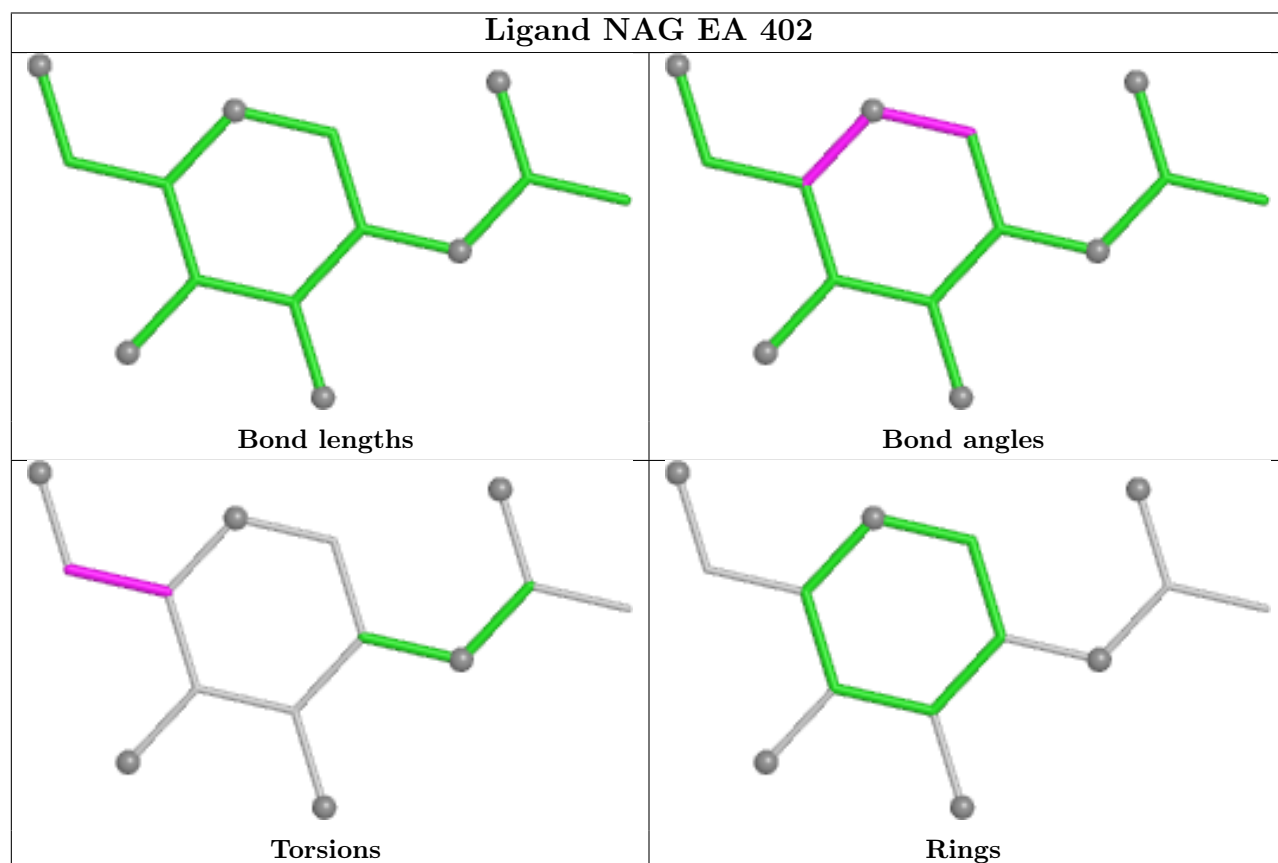
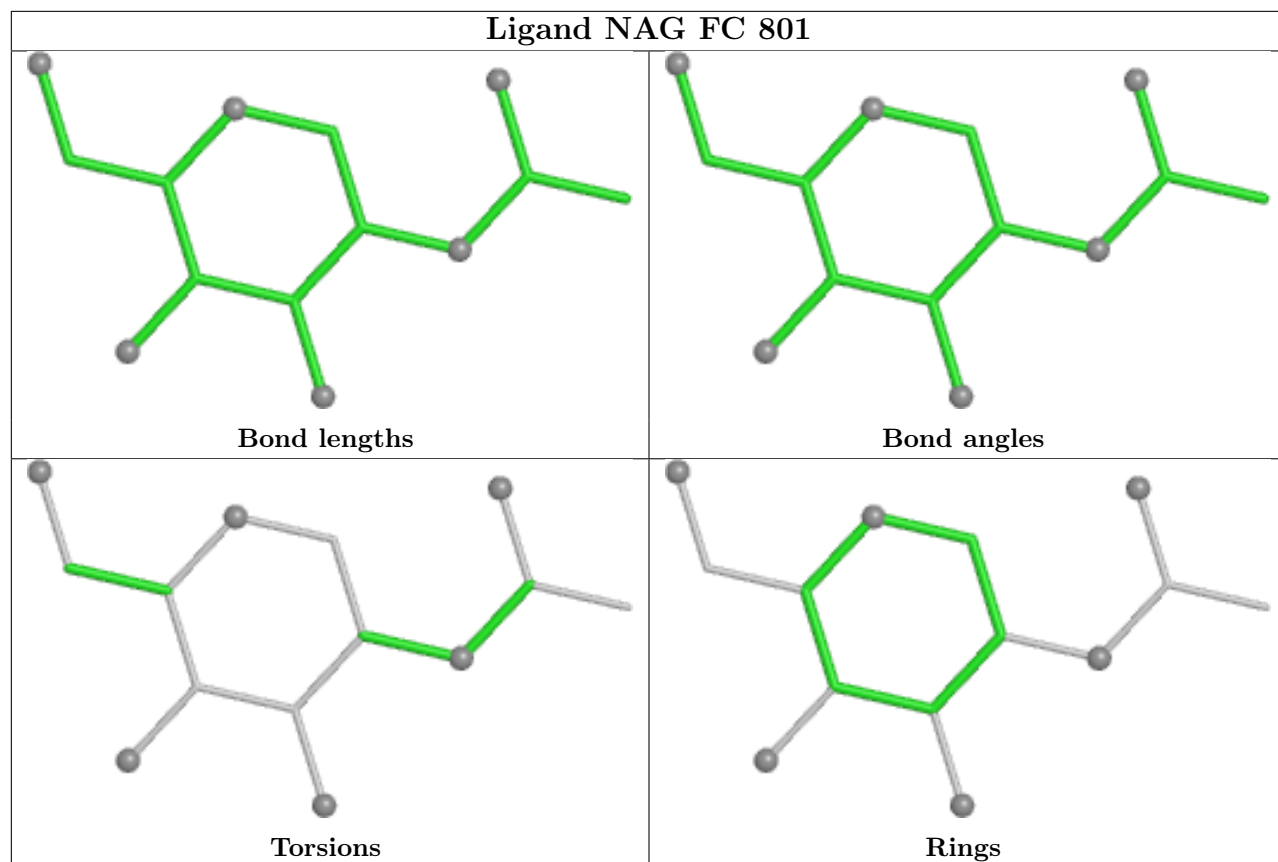
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

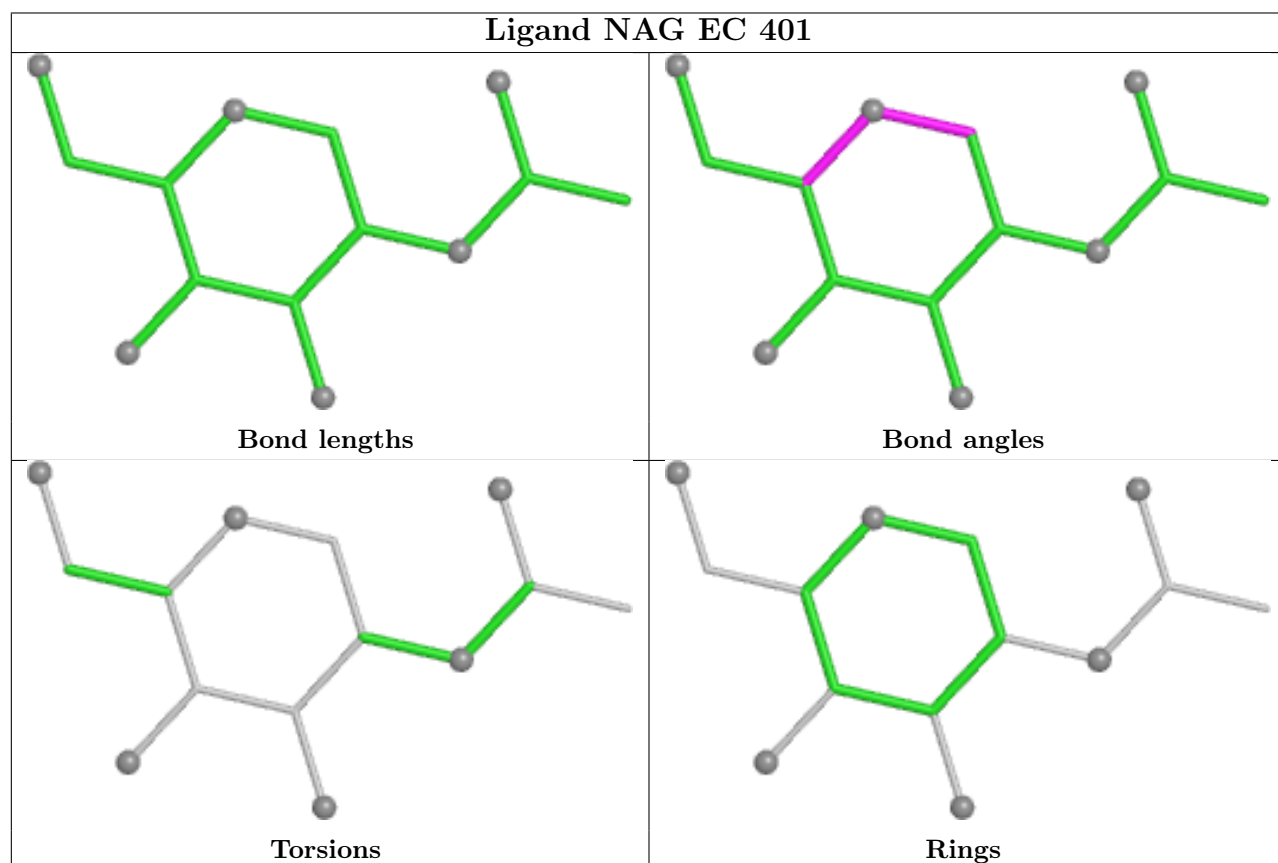
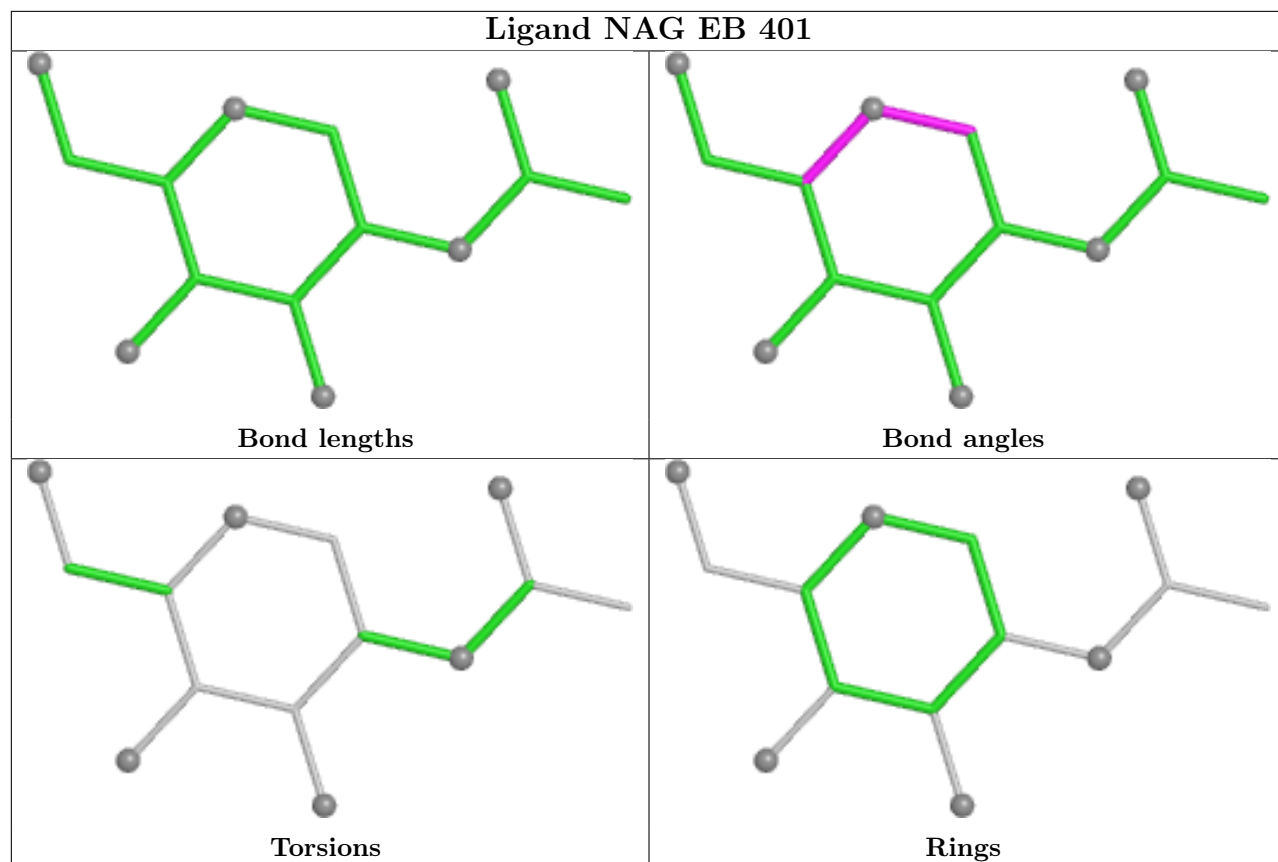
Ligand NAG FA 801



Ligand NAG FB 801







5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

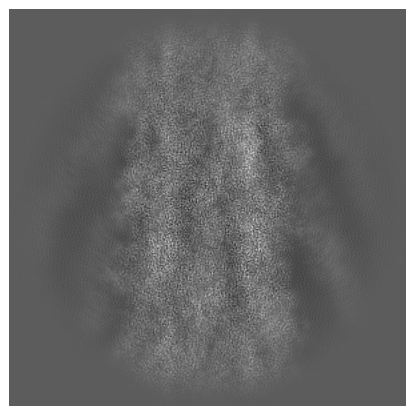
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-64106. These allow visual inspection of the internal detail of the map and identification of artifacts.

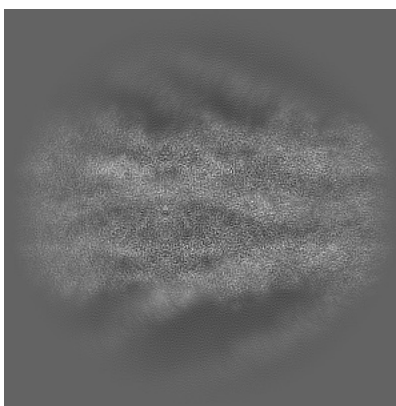
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

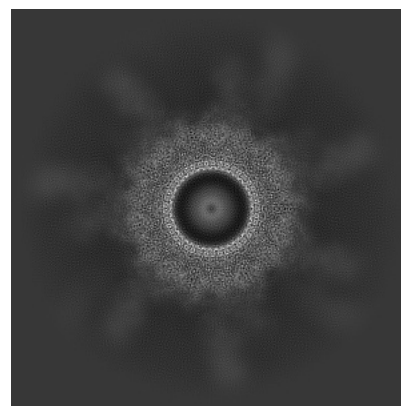
6.1.1 Primary map



X

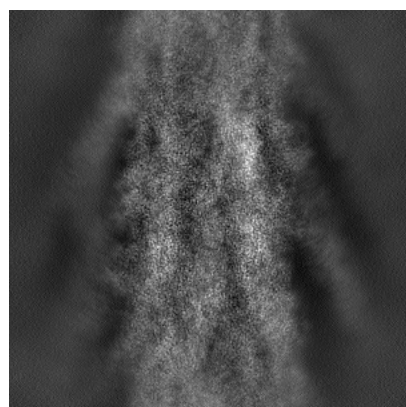


Y

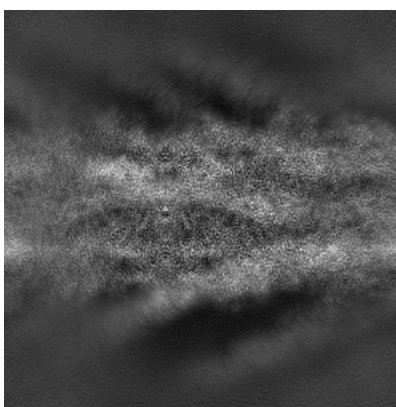


Z

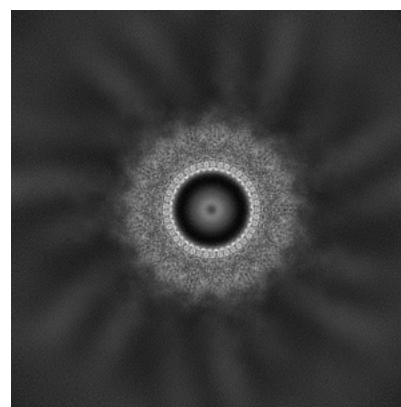
6.1.2 Raw map



X



Y

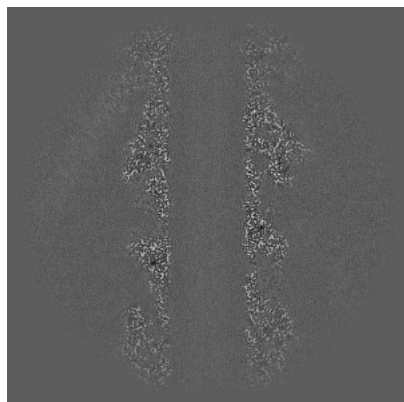


Z

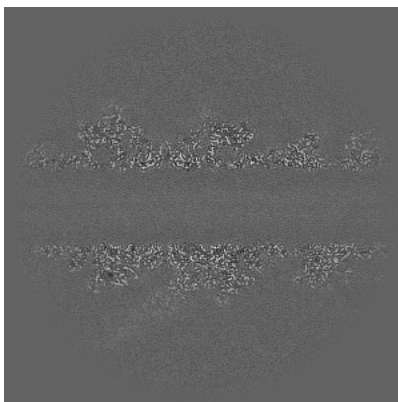
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

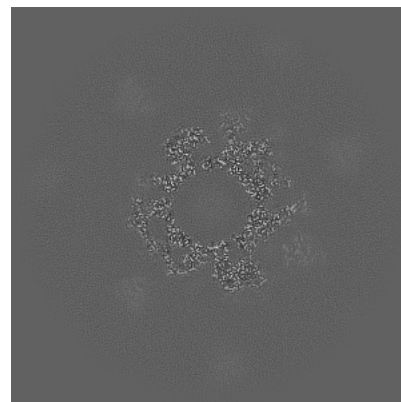
6.2.1 Primary map



X Index: 256

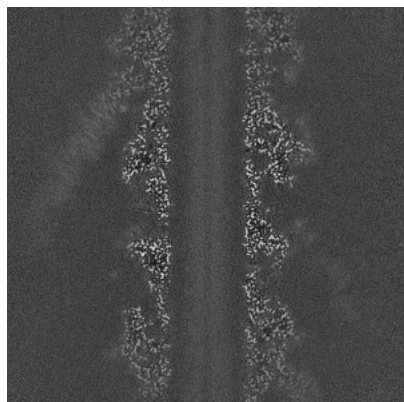


Y Index: 256

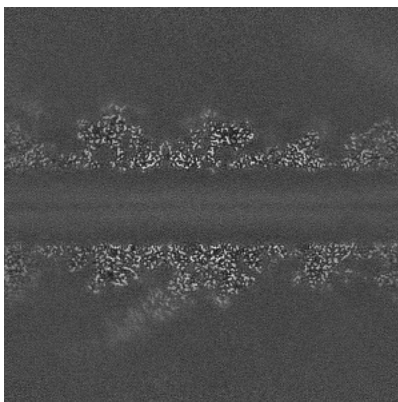


Z Index: 256

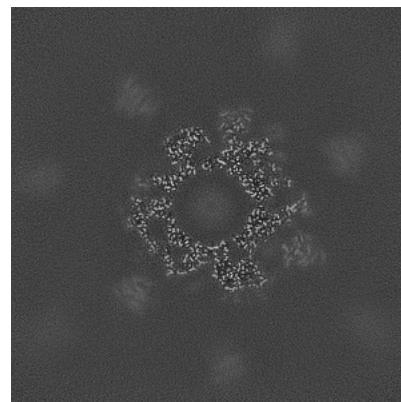
6.2.2 Raw map



X Index: 256



Y Index: 256

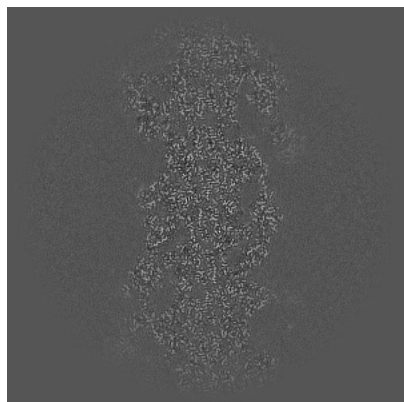


Z Index: 256

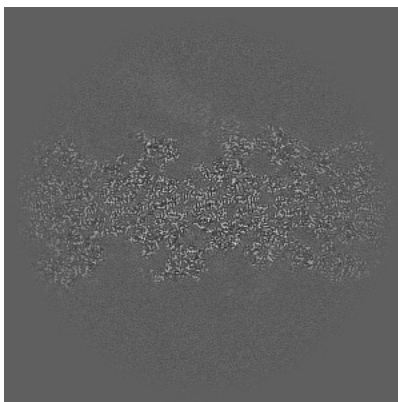
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

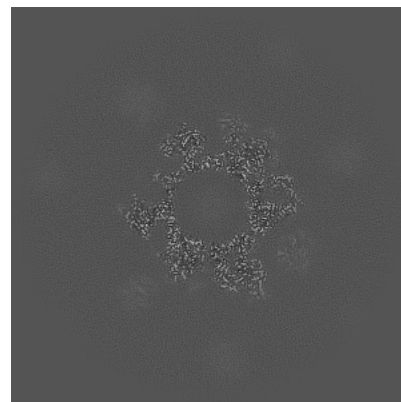
6.3.1 Primary map



X Index: 204

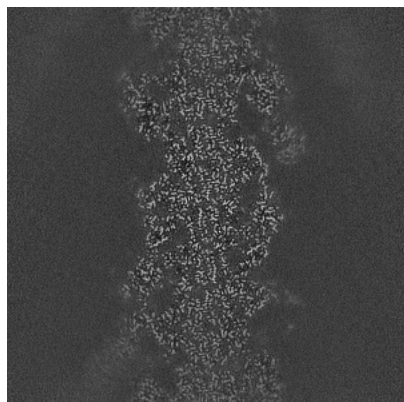


Y Index: 204

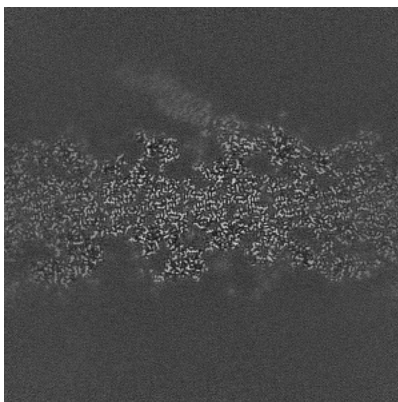


Z Index: 266

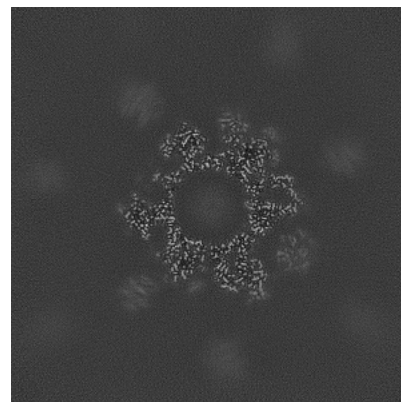
6.3.2 Raw map



X Index: 204



Y Index: 204

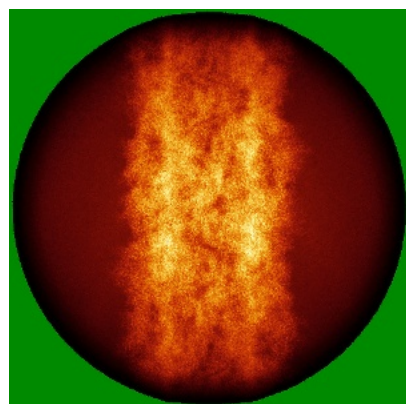


Z Index: 266

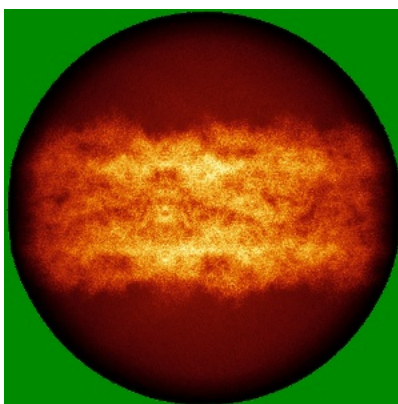
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

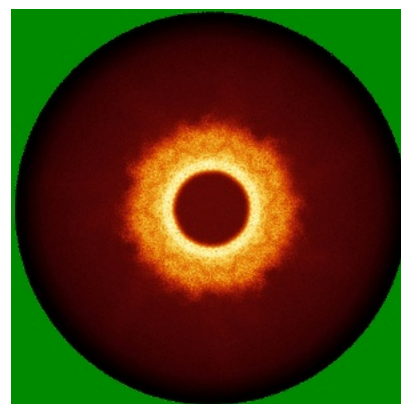
6.4.1 Primary map



X

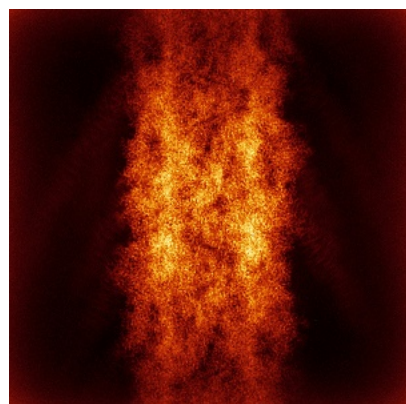


Y

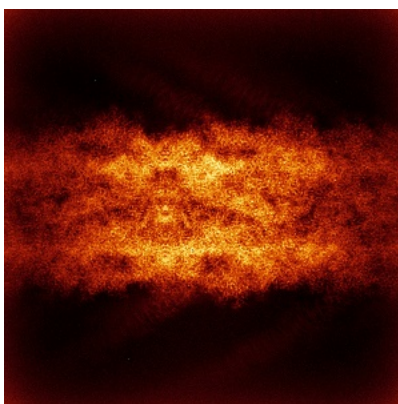


Z

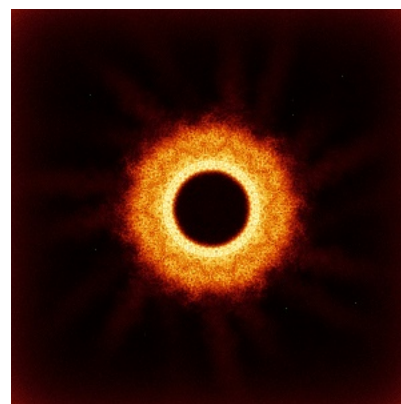
6.4.2 Raw map



X



Y

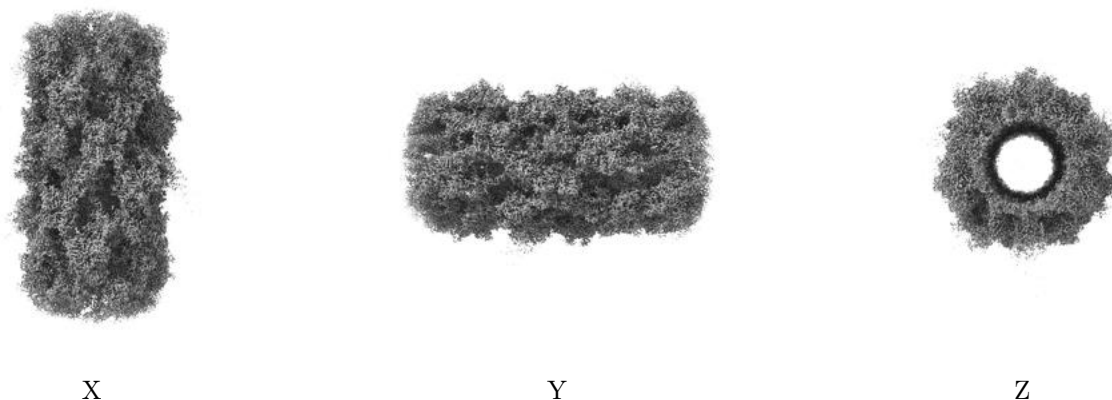


Z

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.

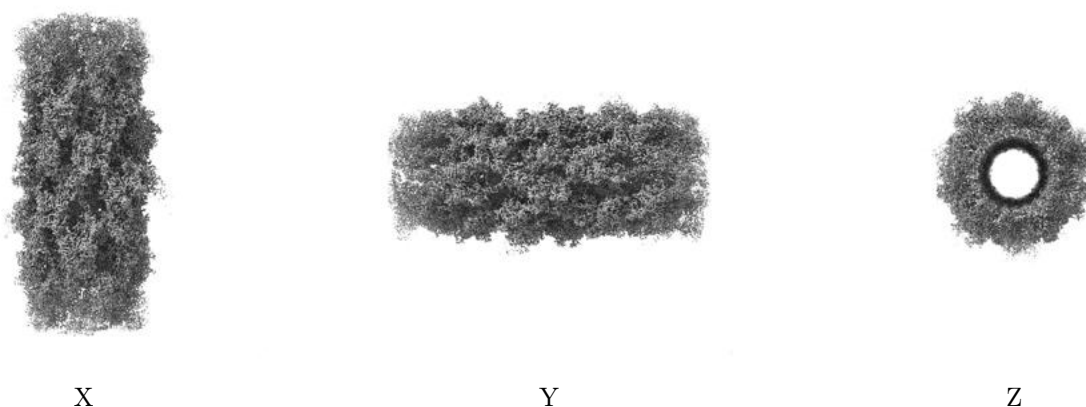
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.2. 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



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.

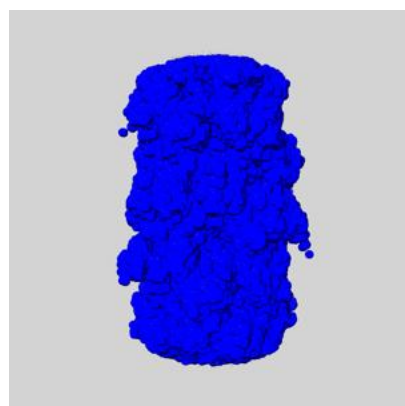
6.6 Mask visualisation [i](#)

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

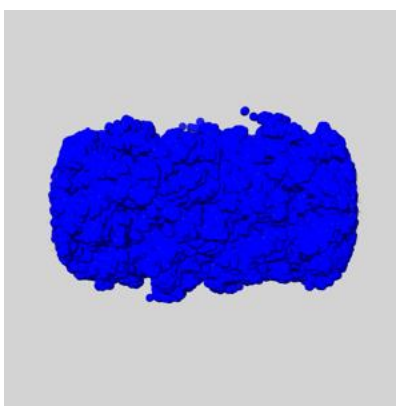
A mask typically either:

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

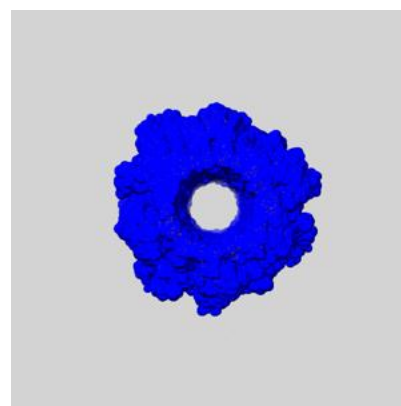
6.6.1 emd_64106_msk_1.map [i](#)



X



Y

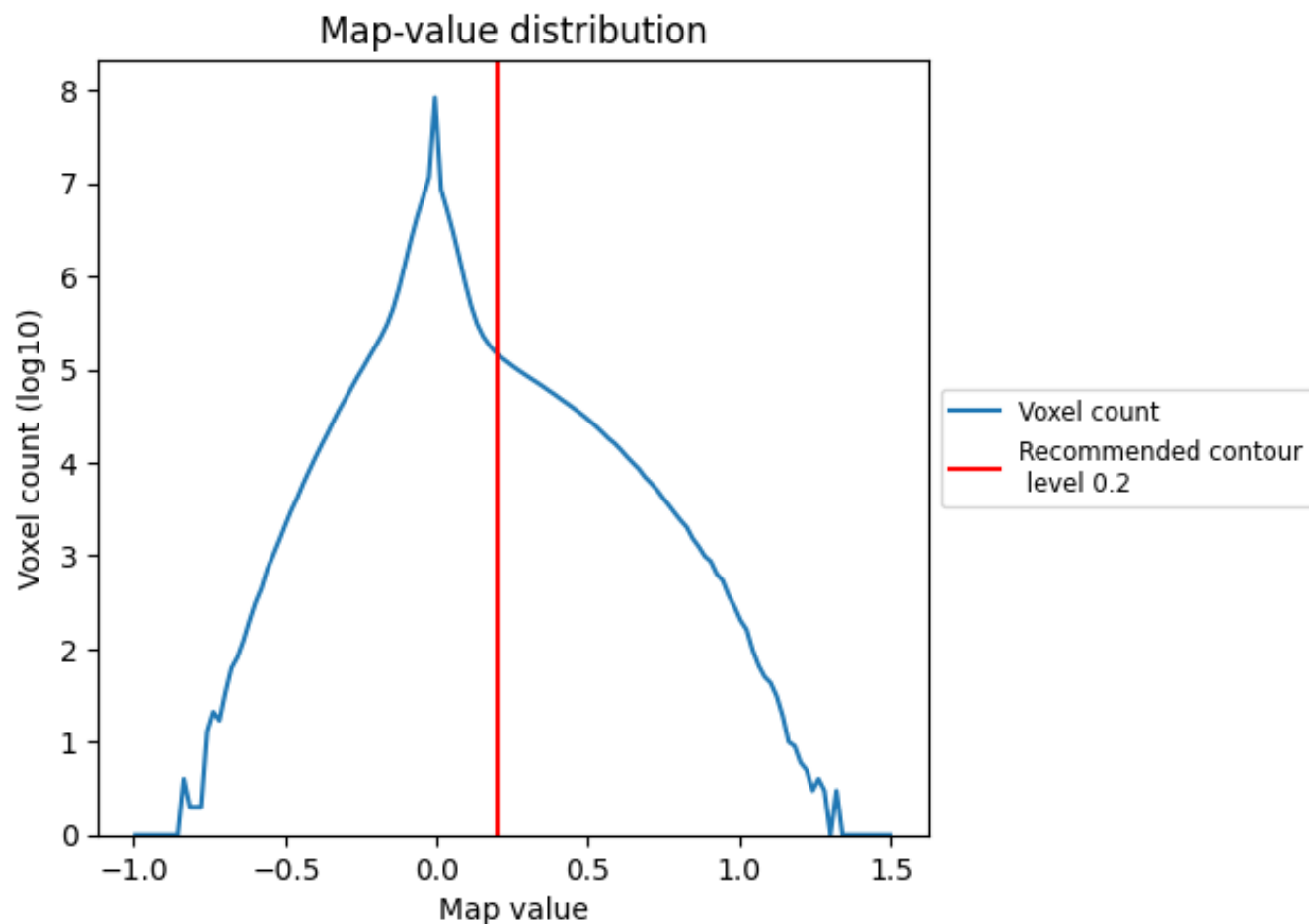


Z

7 Map analysis [i](#)

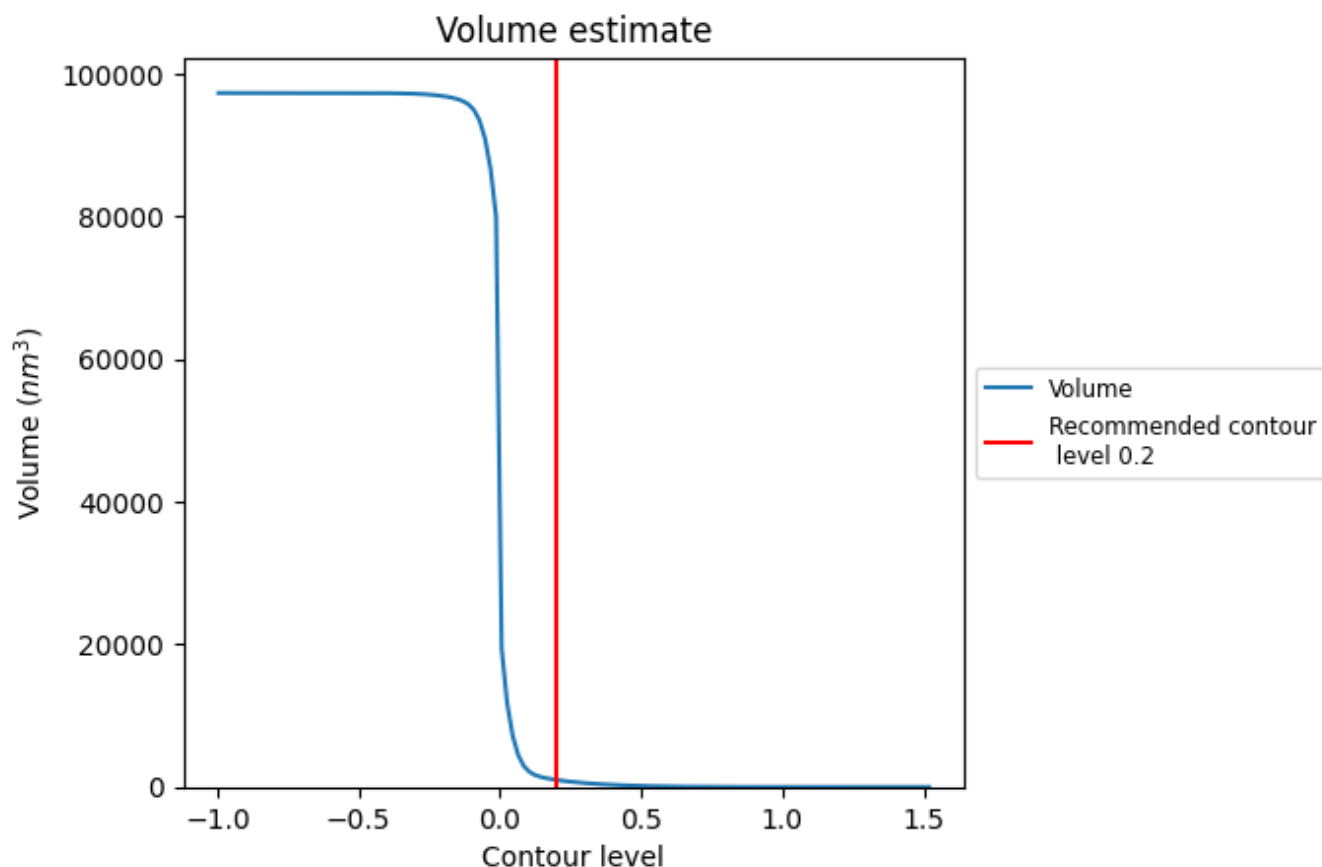
This section contains the results of statistical analysis of the map.

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.

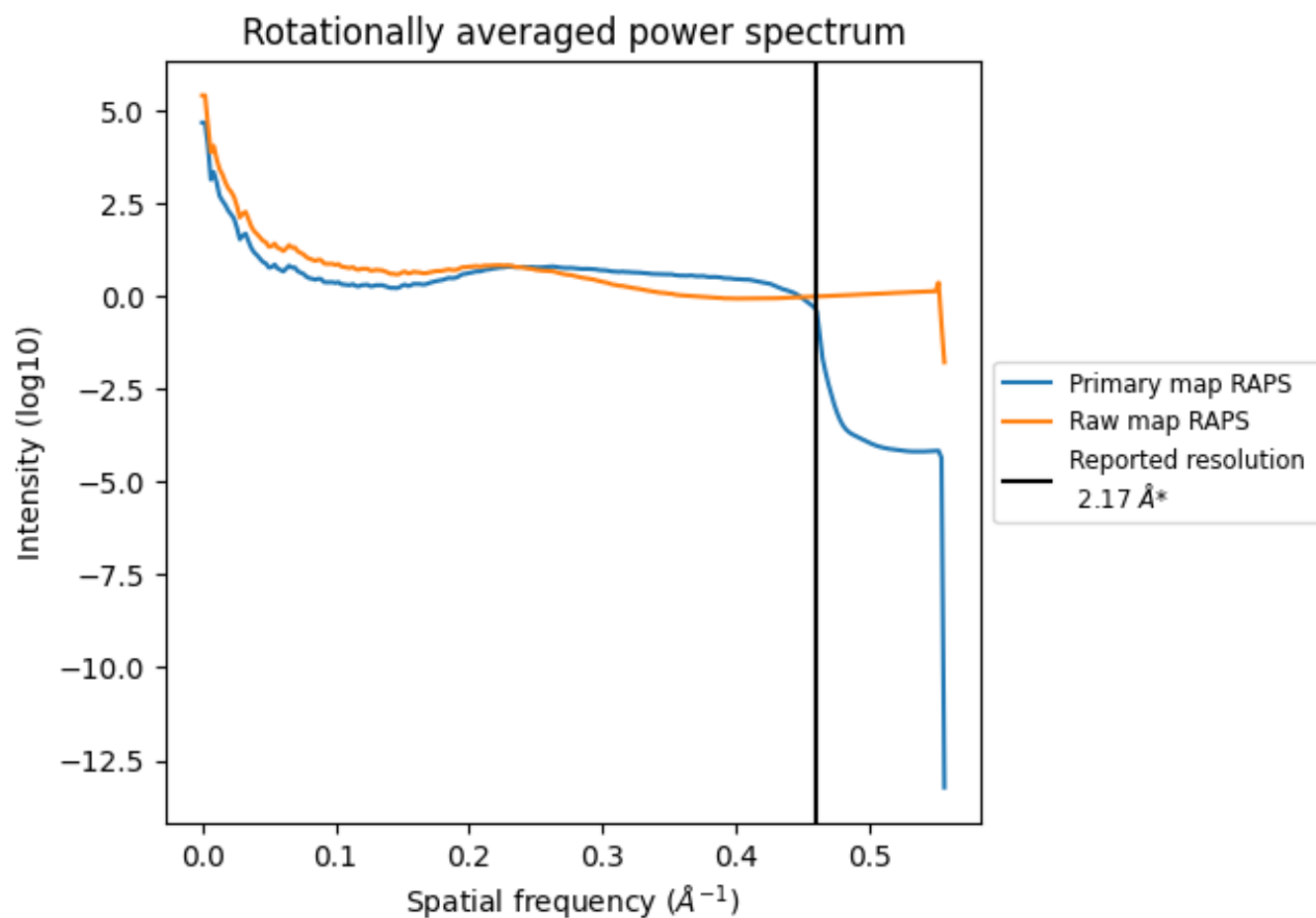
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 984 nm^3 ; this corresponds to an approximate mass of 889 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 ⓘ

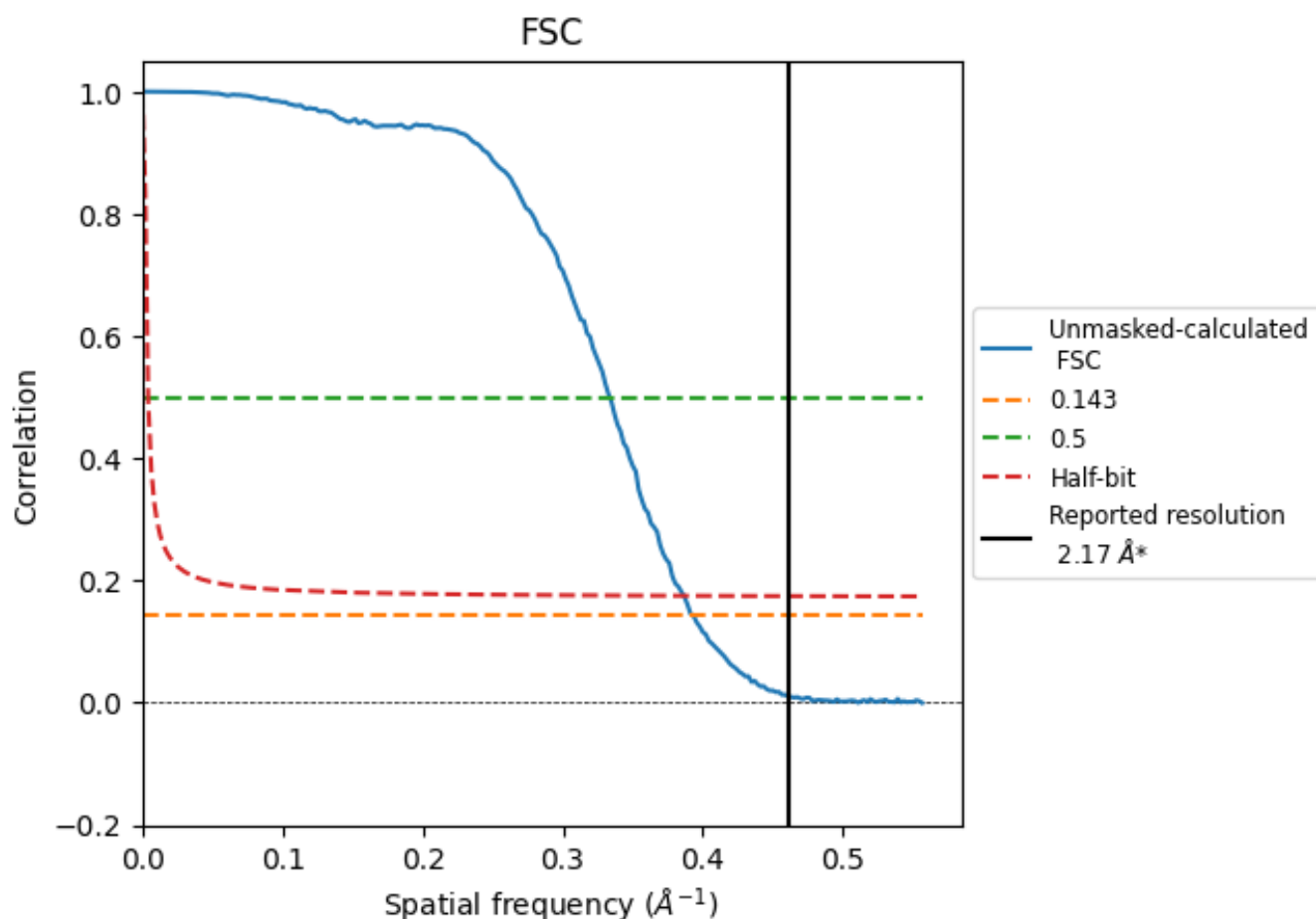


*Reported resolution corresponds to spatial frequency of 0.461 Å⁻¹

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 $0.461 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

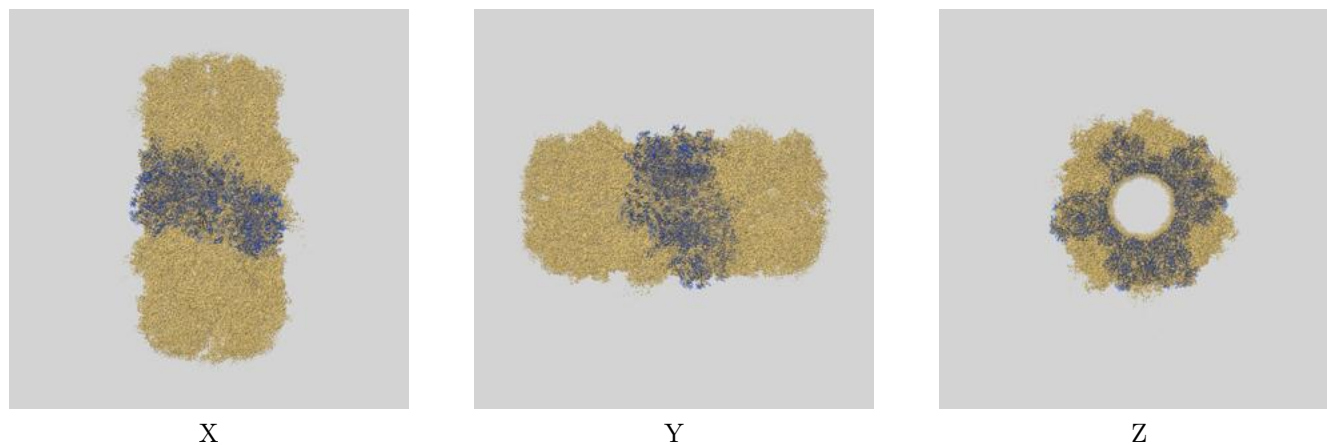
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.17	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	2.55	3.00	2.59

*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 2.55 differs from the reported value 2.17 by more than 10 %

9 Map-model fit [i](#)

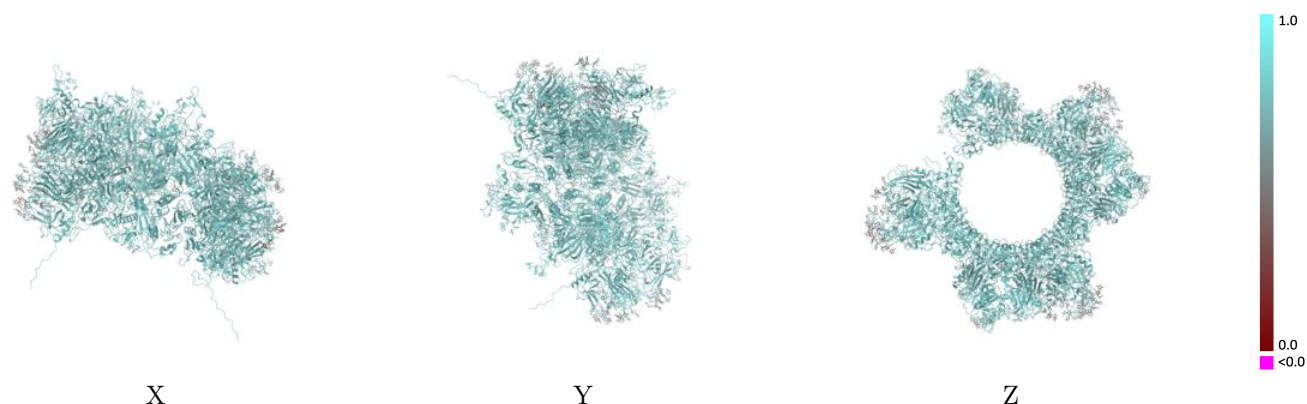
This section contains information regarding the fit between EMDB map EMD-64106 and PDB model 9UFE. Per-residue inclusion information can be found in section 3 on page 19.

9.1 Map-model overlay [i](#)



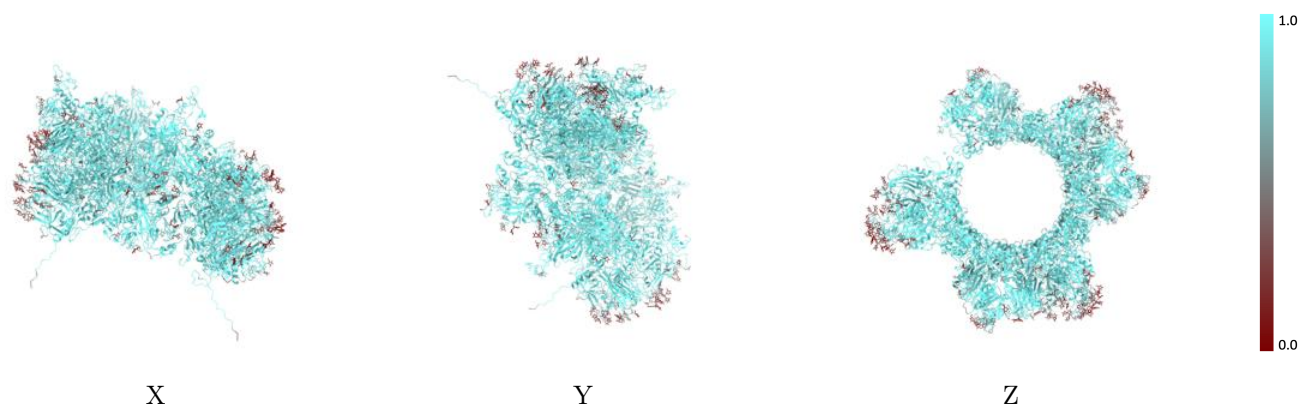
The images above show the 3D surface view of the map at the recommended contour level 0.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



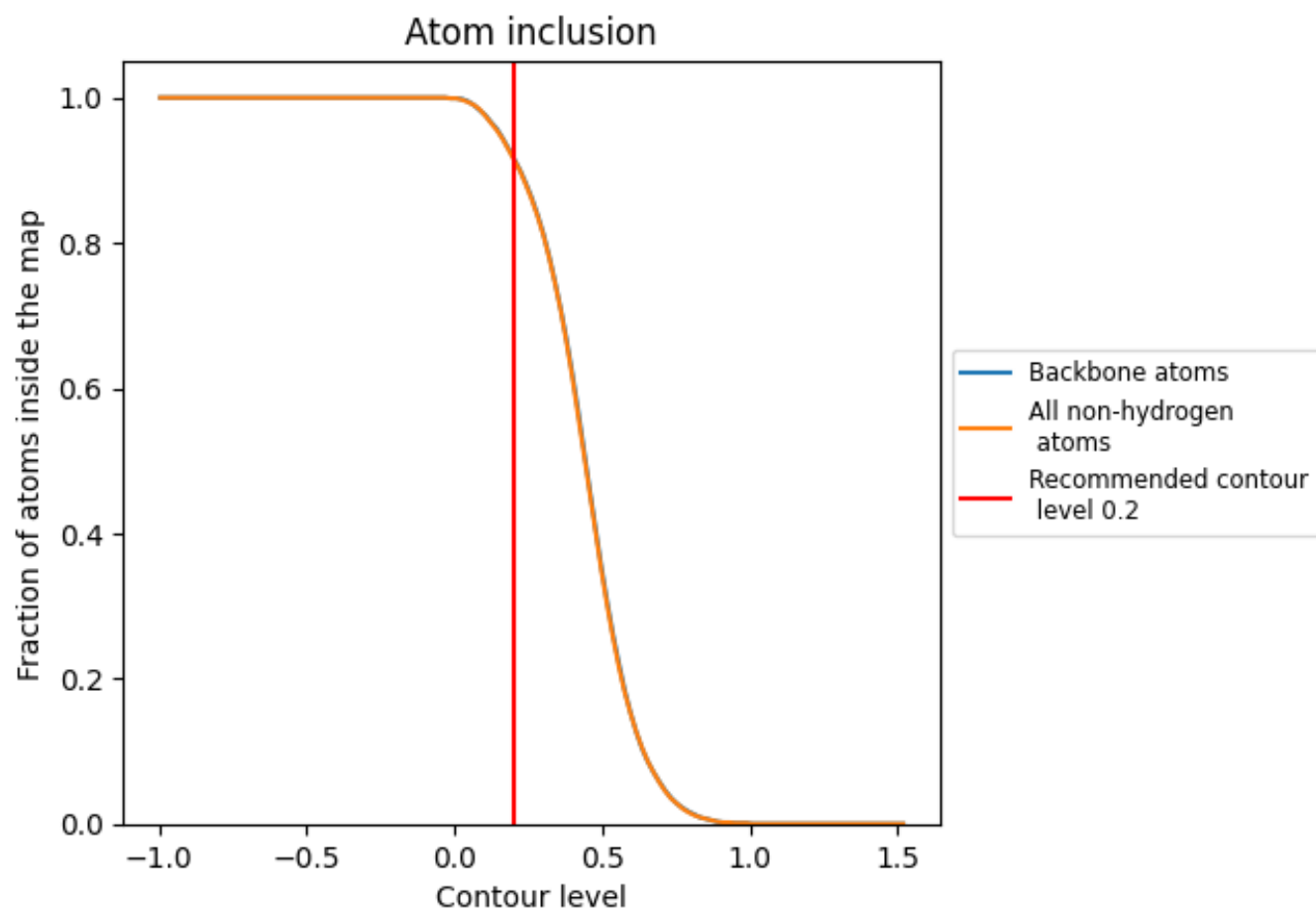
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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](#)



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 (0.2).

9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 92% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9160	 0.7350
AA	 0.9580	 0.7470
AB	 0.9580	 0.7460
AC	 0.9560	 0.7460
BA	 0.9550	 0.7480
BB	 0.9550	 0.7510
BC	 0.9610	 0.7490
CA	 0.9540	 0.7490
CB	 0.9510	 0.7480
CC	 0.9510	 0.7480
DA	 0.9630	 0.7540
DB	 0.9660	 0.7520
DC	 0.9670	 0.7510
EA	 0.9490	 0.7450
EB	 0.9440	 0.7420
EC	 0.9440	 0.7420
FA	 0.9460	 0.7430
FB	 0.9520	 0.7420
FC	 0.9540	 0.7440
aA	 0.3940	 0.5650
aB	 0.4720	 0.5700
aC	 0.4230	 0.5910
aD	 0.8670	 0.7100
aE	 0.2220	 0.5220
aF	 0.3750	 0.5480
aG	 0.4610	 0.5710
aH	 0.4400	 0.5930
aI	 0.8290	 0.7110
aJ	 0.2280	 0.5380
aK	 0.3500	 0.5780
aL	 0.4330	 0.5560
aM	 0.4340	 0.6030
aN	 0.8380	 0.7110
aO	 0.2340	 0.5270
bA	 0.7140	 0.7050



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Chain	Atom inclusion	Q-score
bB	 0.3280	 0.6010
bC	 0.3570	 0.5770
bD	 0.7710	 0.6960
bE	 0.3280	 0.5830
bF	 0.3300	 0.5670
bG	 0.7810	 0.7000
bH	 0.3440	 0.6040
bI	 0.3570	 0.5410
cA	 0.9290	 0.7110
cB	 0.9290	 0.7170
cC	 0.9290	 0.7220
dA	 0.7870	 0.6860
dB	 0.7730	 0.6860
dC	 0.8270	 0.6990
eA	 0.7240	 0.6880
eB	 0.7470	 0.6880
eC	 0.6770	 0.6950
eD	 0.7530	 0.6820
eE	 0.6610	 0.6840
eF	 0.7340	 0.6770
fB	 0.8450	 0.7140
fC	 0.7320	 0.6960
fD	 0.9050	 0.7250
fE	 0.7840	 0.6920
fF	 0.3990	 0.5870
fG	 0.8530	 0.7040
fH	 0.7170	 0.6780
fI	 0.8660	 0.7130
fJ	 0.8100	 0.6930
fK	 0.4050	 0.5960
fL	 0.8970	 0.7010
fM	 0.7790	 0.6890
fN	 0.8580	 0.7180
fO	 0.7930	 0.6930
fP	 0.3730	 0.6040