



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 08:08 PM UTC

PDB ID : 4YD9 / pdb_00004yd9
Title : Crystal structure of squid hemocyanin
Authors : Matsuno, A.; Gai, Z.; Kato, K.; Tanaka, Y.; Yao, M.
Deposited on : 2015-02-21
Resolution : 3.00 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

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:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

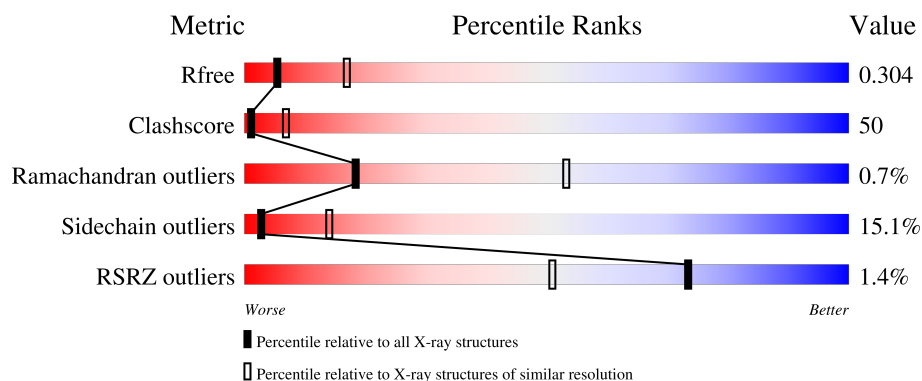
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower 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 electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	2000	
1	D	2000	
1	G	2000	
1	J	2000	
1	M	2000	

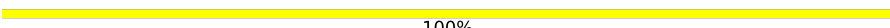
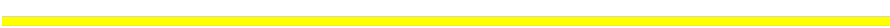
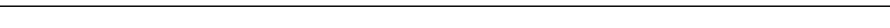
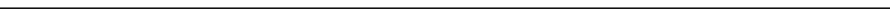
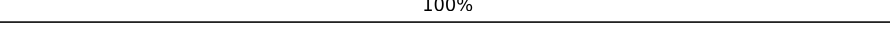
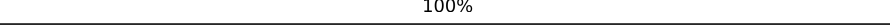
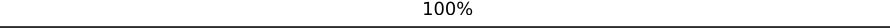
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	P	2000	
1	S	2000	
1	V	2000	
1	Y	2000	
1	b	2000	
2	B	920	
2	E	920	
2	H	920	
2	K	920	
2	N	920	
2	Q	920	
2	T	920	
2	W	920	
2	Z	920	
2	c	920	
3	C	394	
3	F	394	
3	I	394	
3	L	394	
3	O	394	
3	R	394	
3	U	394	
3	X	394	
3	a	394	
3	d	394	

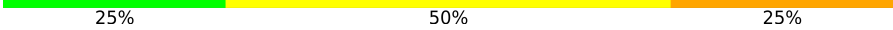
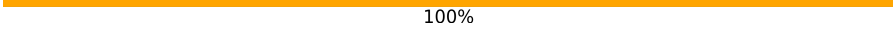
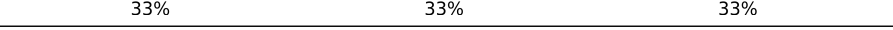
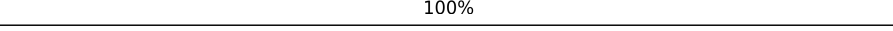
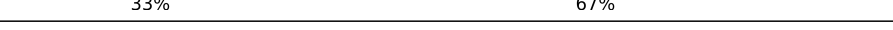
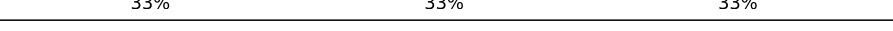
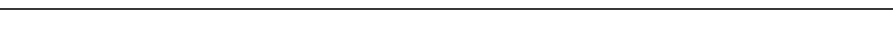
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	1	2	 50% 50%
4	2	2	 50% 50%
4	4	2	 100%
4	6	2	 50% 50%
4	7	2	 100%
4	8	2	 100%
4	9	2	 100%
4	BA	2	 100%
4	HA	2	 50% 50%
4	IA	2	 100%
4	JA	2	 50% 50%
4	MA	2	 100%
4	OA	2	 100%
4	QA	2	 50% 50%
4	RA	2	 50% 50%
4	e	2	 50% 50%
4	f	2	 50% 50%
4	i	2	 100%
4	j	2	 100%
4	m	2	 100%
4	n	2	 100%
4	o	2	 50% 50%
4	p	2	 50% 50%
4	q	2	 100%
4	s	2	 50% 50%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	t	2	 50% 50%
4	u	2	 50% 50%
4	v	2	 100%
4	x	2	 50% 50%
5	AA	4	 25% 50% 25%
5	FA	4	 100%
5	KA	4	 75% 25%
5	PA	4	 25% 25% 50%
5	g	4	 50% 50%
5	l	4	 50% 50%
6	3	3	 33% 33% 33%
6	5	3	 100%
6	CA	3	 33% 67%
6	DA	3	 33% 67%
6	EA	3	 33% 33% 33%
6	GA	3	 33% 67%
6	LA	3	 33% 67%
6	NA	3	 67% 33%
6	h	3	 67% 33%
6	k	3	 33% 67%
6	r	3	 33% 33% 33%
6	w	3	 33% 33% 33%
6	y	3	 100%
7	z	5	 20% 40% 40%
8	0	4	 25% 75%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	NAG	MA	1	-	-	X	-
4	NAG	m	1	-	-	X	-
4	NAG	q	2	-	-	X	-
6	NAG	GA	1	-	-	X	-
6	NAG	GA	2	-	-	X	-
6	NAG	r	1	-	-	X	-
8	NAG	0	2	-	-	X	-
9	CUO	A	5001	-	-	X	-
9	CUO	C	3401[A]	-	-	X	-
9	CUO	C	3401[B]	-	-	X	-
9	CUO	F	3401[A]	-	-	X	-
9	CUO	F	3401[B]	-	-	X	-
9	CUO	I	3401[A]	-	-	X	-
9	CUO	L	3401[A]	-	-	X	-
9	CUO	L	3401[B]	-	-	X	-
9	CUO	M	2105	-	-	X	-
9	CUO	O	3401[A]	-	-	X	-
9	CUO	O	3401[B]	-	-	X	-
9	CUO	R	3401[A]	-	-	X	-
9	CUO	S	2104	-	-	X	-
9	CUO	U	3401[A]	-	-	X	-
9	CUO	U	3401[B]	-	-	X	-
9	CUO	X	3401[A]	-	-	X	-
9	CUO	X	3401[B]	-	-	X	-
9	CUO	a	3401[A]	-	-	X	-
9	CUO	a	3401[B]	-	-	X	-
9	CUO	d	3401[A]	-	-	X	-
9	CUO	d	3401[B]	-	-	X	-

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 261470 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 hemocyanin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1656	Total	C	N	O	S	0	0	0
			13318	8513	2259	2478	68			
1	D	1656	Total	C	N	O	S	0	0	0
			13318	8513	2259	2478	68			
1	G	1656	Total	C	N	O	S	0	0	0
			13318	8513	2259	2478	68			
1	J	1656	Total	C	N	O	S	0	0	0
			13318	8513	2259	2478	68			
1	M	1656	Total	C	N	O	S	0	0	0
			13318	8513	2259	2478	68			
1	P	1656	Total	C	N	O	S	0	0	0
			13318	8513	2259	2478	68			
1	S	1656	Total	C	N	O	S	0	0	0
			13318	8513	2259	2478	68			
1	V	1656	Total	C	N	O	S	0	0	0
			13318	8513	2259	2478	68			
1	Y	1656	Total	C	N	O	S	0	0	0
			13318	8513	2259	2478	68			
1	b	1656	Total	C	N	O	S	0	0	0
			13318	8513	2259	2478	68			

- Molecule 2 is a protein called hemocyanin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	825	Total	C	N	O	S	0	0	0
			6704	4311	1128	1224	41			
2	E	825	Total	C	N	O	S	0	0	0
			6704	4311	1128	1224	41			
2	H	825	Total	C	N	O	S	0	0	0
			6704	4311	1128	1224	41			
2	K	825	Total	C	N	O	S	0	0	0
			6704	4311	1128	1224	41			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	N	825	Total	C	N	O	S	0	0	0
			6704	4311	1128	1224	41			
2	Q	825	Total	C	N	O	S	0	0	0
			6704	4311	1128	1224	41			
2	T	825	Total	C	N	O	S	0	0	0
			6704	4311	1128	1224	41			
2	W	825	Total	C	N	O	S	0	0	0
			6704	4311	1128	1224	41			
2	Z	825	Total	C	N	O	S	0	0	0
			6704	4311	1128	1224	41			
2	c	825	Total	C	N	O	S	0	0	0
			6704	4311	1128	1224	41			

- Molecule 3 is a protein called hemocyanin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	366	Total	C	N	O	S	0	366	0
			5912	3808	994	1076	34			
3	F	366	Total	C	N	O	S	0	366	0
			5912	3808	994	1076	34			
3	I	366	Total	C	N	O	S	0	366	0
			5912	3808	994	1076	34			
3	L	366	Total	C	N	O	S	0	366	0
			5912	3808	994	1076	34			
3	O	366	Total	C	N	O	S	0	366	0
			5912	3808	994	1076	34			
3	R	366	Total	C	N	O	S	0	366	0
			5912	3808	994	1076	34			
3	U	366	Total	C	N	O	S	0	366	0
			5912	3808	994	1076	34			
3	X	366	Total	C	N	O	S	0	366	0
			5912	3808	994	1076	34			
3	a	366	Total	C	N	O	S	0	366	0
			5912	3808	994	1076	34			
3	d	366	Total	C	N	O	S	0	366	0
			5912	3808	994	1076	34			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	e	2	Total 28	C 16	N 2	O 10	0	0	0
4	f	2	Total 28	C 16	N 2	O 10	0	0	0
4	i	2	Total 28	C 16	N 2	O 10	0	0	0
4	j	2	Total 28	C 16	N 2	O 10	0	0	0
4	m	2	Total 28	C 16	N 2	O 10	0	0	0
4	n	2	Total 28	C 16	N 2	O 10	0	0	0
4	o	2	Total 28	C 16	N 2	O 10	0	0	0
4	p	2	Total 28	C 16	N 2	O 10	0	0	0
4	q	2	Total 28	C 16	N 2	O 10	0	0	0
4	s	2	Total 28	C 16	N 2	O 10	0	0	0
4	t	2	Total 28	C 16	N 2	O 10	0	0	0
4	u	2	Total 28	C 16	N 2	O 10	0	0	0
4	v	2	Total 28	C 16	N 2	O 10	0	0	0
4	x	2	Total 28	C 16	N 2	O 10	0	0	0
4	1	2	Total 28	C 16	N 2	O 10	0	0	0
4	2	2	Total 28	C 16	N 2	O 10	0	0	0
4	4	2	Total 28	C 16	N 2	O 10	0	0	0
4	6	2	Total 28	C 16	N 2	O 10	0	0	0
4	7	2	Total 28	C 16	N 2	O 10	0	0	0
4	8	2	Total 28	C 16	N 2	O 10	0	0	0
4	9	2	Total 28	C 16	N 2	O 10	0	0	0
4	BA	2	Total 28	C 16	N 2	O 10	0	0	0

Continued on next page...

Continued from previous page...

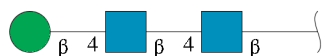
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	HA	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	IA	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	JA	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	MA	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	OA	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	QA	2	Total	C	N	O	0	0	0
			28	16	2	10			
4	RA	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



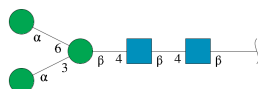
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	g	4	Total	C	N	O	0	0	0
			50	28	2	20			
5	l	4	Total	C	N	O	0	0	0
			50	28	2	20			
5	AA	4	Total	C	N	O	0	0	0
			50	28	2	20			
5	FA	4	Total	C	N	O	0	0	0
			50	28	2	20			
5	KA	4	Total	C	N	O	0	0	0
			50	28	2	20			
5	PA	4	Total	C	N	O	0	0	0
			50	28	2	20			

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



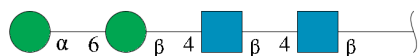
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	h	3	Total	C	N	O	0	0	0
			39	22	2	15			
6	k	3	Total	C	N	O	0	0	0
			39	22	2	15			
6	r	3	Total	C	N	O	0	0	0
			39	22	2	15			
6	w	3	Total	C	N	O	0	0	0
			39	22	2	15			
6	y	3	Total	C	N	O	0	0	0
			39	22	2	15			
6	3	3	Total	C	N	O	0	0	0
			39	22	2	15			
6	5	3	Total	C	N	O	0	0	0
			39	22	2	15			
6	CA	3	Total	C	N	O	0	0	0
			39	22	2	15			
6	DA	3	Total	C	N	O	0	0	0
			39	22	2	15			
6	EA	3	Total	C	N	O	0	0	0
			39	22	2	15			
6	GA	3	Total	C	N	O	0	0	0
			39	22	2	15			
6	LA	3	Total	C	N	O	0	0	0
			39	22	2	15			
6	NA	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 7 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.



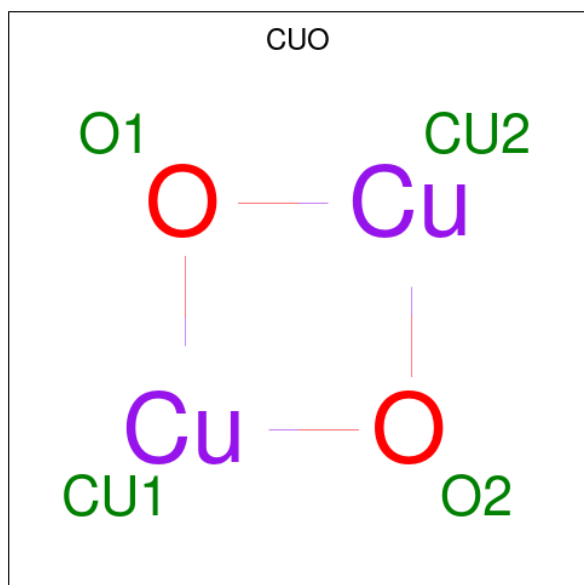
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	z	5	Total	C	N	O	0	0	0
			61	34	2	25			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
8	0	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 9 is CU2-O2 CLUSTER (CCD ID: CUO) (formula: Cu_2O_2).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	Cu	O	0	0
			4	2	2		
9	A	1	Total	Cu	O	0	0
			4	2	2		
9	A	1	Total	Cu	O	0	0
			4	2	2		
9	A	1	Total	Cu	O	0	1
			8	4	4		
9	B	1	Total	Cu	O	0	0
			4	2	2		
9	B	1	Total	Cu	O	0	0
			4	2	2		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	C	1	Total	Cu	O	0	1
			8	4	4		
9	D	1	Total	Cu	O	0	0
			4	2	2		
9	D	1	Total	Cu	O	0	0
			4	2	2		
9	D	1	Total	Cu	O	0	0
			4	2	2		
9	D	1	Total	Cu	O	0	0
			4	2	2		
9	D	1	Total	Cu	O	0	1
			8	4	4		
9	E	1	Total	Cu	O	0	0
			4	2	2		
9	E	1	Total	Cu	O	0	0
			4	2	2		
9	F	1	Total	Cu	O	0	1
			8	4	4		
9	G	1	Total	Cu	O	0	1
			8	4	4		
9	G	1	Total	Cu	O	0	0
			4	2	2		
9	G	1	Total	Cu	O	0	0
			4	2	2		
9	G	1	Total	Cu	O	0	0
			4	2	2		
9	G	1	Total	Cu	O	0	0
			4	2	2		
9	H	1	Total	Cu	O	0	0
			4	2	2		
9	H	1	Total	Cu	O	0	0
			4	2	2		
9	I	1	Total	Cu	O	0	1
			8	4	4		
9	J	1	Total	Cu	O	0	0
			4	2	2		
9	J	1	Total	Cu	O	0	0
			4	2	2		
9	J	1	Total	Cu	O	0	0
			4	2	2		
9	J	1	Total	Cu	O	0	0
			4	2	2		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	J	1	Total 8	Cu 4	O 4	0	1
9	K	1	Total 4	Cu 2	O 2	0	0
9	K	1	Total 4	Cu 2	O 2	0	0
9	L	1	Total 8	Cu 4	O 4	0	1
9	M	1	Total 8	Cu 4	O 4	0	1
9	M	1	Total 4	Cu 2	O 2	0	0
9	M	1	Total 4	Cu 2	O 2	0	0
9	M	1	Total 4	Cu 2	O 2	0	0
9	M	1	Total 4	Cu 2	O 2	0	0
9	M	1	Total 4	Cu 2	O 2	0	0
9	N	1	Total 4	Cu 2	O 2	0	0
9	N	1	Total 4	Cu 2	O 2	0	0
9	O	1	Total 8	Cu 4	O 4	0	1
9	P	1	Total 4	Cu 2	O 2	0	0
9	P	1	Total 4	Cu 2	O 2	0	0
9	P	1	Total 4	Cu 2	O 2	0	0
9	P	1	Total 4	Cu 2	O 2	0	0
9	P	1	Total 8	Cu 4	O 4	0	1
9	Q	1	Total 4	Cu 2	O 2	0	0
9	Q	1	Total 4	Cu 2	O 2	0	0
9	R	1	Total 8	Cu 4	O 4	0	1
9	S	1	Total 8	Cu 4	O 4	0	1

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	S	1	Total 4	Cu 2	O 2	0	0
9	S	1	Total 4	Cu 2	O 2	0	0
9	S	1	Total 4	Cu 2	O 2	0	0
9	S	1	Total 4	Cu 2	O 2	0	0
9	T	1	Total 4	Cu 2	O 2	0	0
9	T	1	Total 4	Cu 2	O 2	0	0
9	U	1	Total 8	Cu 4	O 4	0	1
9	V	1	Total 4	Cu 2	O 2	0	0
9	V	1	Total 4	Cu 2	O 2	0	0
9	V	1	Total 4	Cu 2	O 2	0	0
9	V	1	Total 4	Cu 2	O 2	0	0
9	V	1	Total 8	Cu 4	O 4	0	1
9	W	1	Total 4	Cu 2	O 2	0	0
9	W	1	Total 4	Cu 2	O 2	0	0
9	X	1	Total 8	Cu 4	O 4	0	1
9	Y	1	Total 8	Cu 4	O 4	0	1
9	Y	1	Total 4	Cu 2	O 2	0	0
9	Y	1	Total 4	Cu 2	O 2	0	0
9	Y	1	Total 4	Cu 2	O 2	0	0
9	Y	1	Total 4	Cu 2	O 2	0	0
9	Z	1	Total 4	Cu 2	O 2	0	0

Continued on next page...

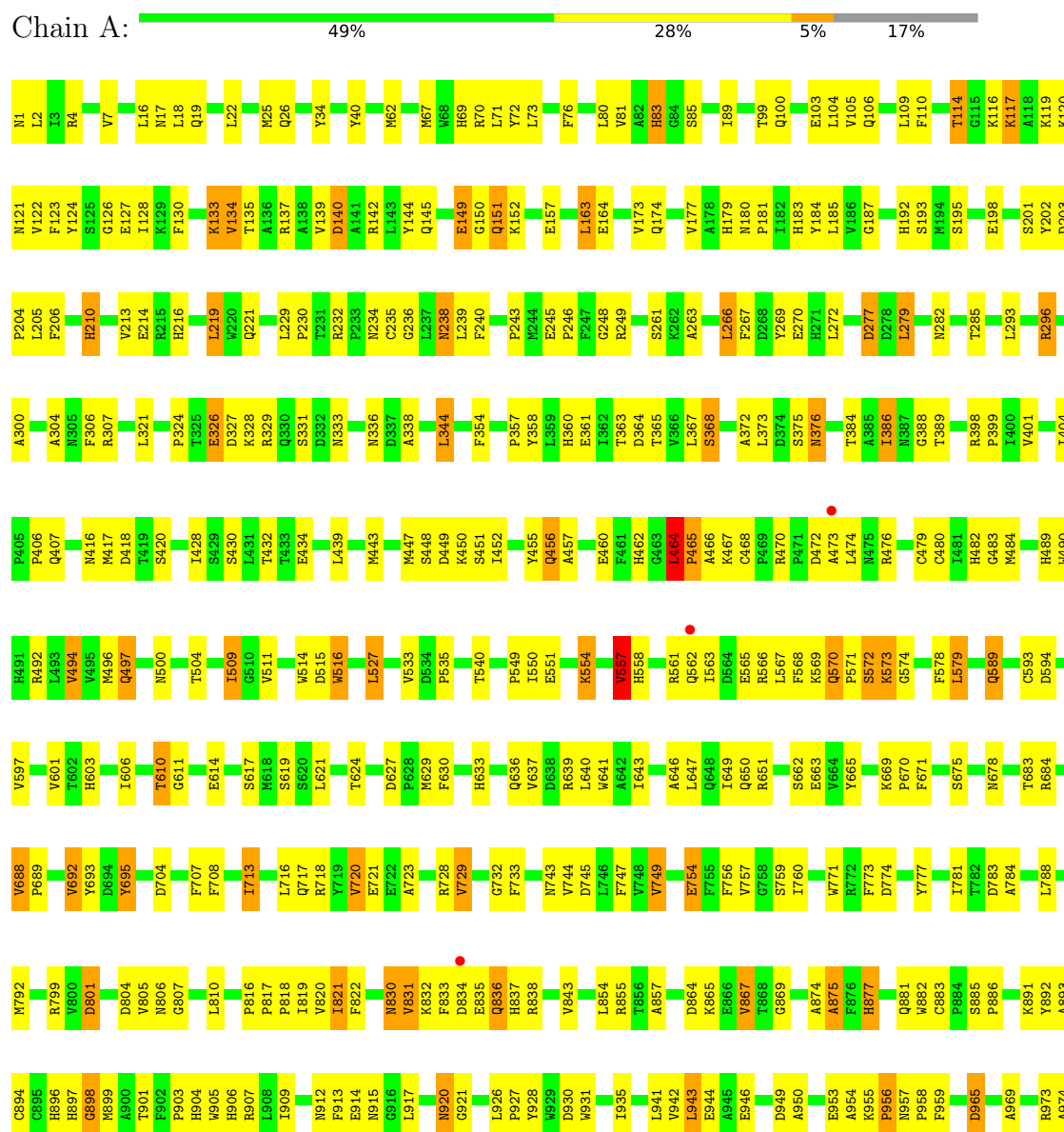
Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	Z	1	Total 4	Cu 2	O 2	0	0
9	a	1	Total 8	Cu 4	O 4	0	1
9	b	1	Total 8	Cu 4	O 4	0	1
9	b	1	Total 4	Cu 2	O 2	0	0
9	b	1	Total 4	Cu 2	O 2	0	0
9	b	1	Total 4	Cu 2	O 2	0	0
9	b	1	Total 4	Cu 2	O 2	0	0
9	c	1	Total 4	Cu 2	O 2	0	0
9	c	1	Total 4	Cu 2	O 2	0	0
9	d	1	Total 8	Cu 4	O 4	0	1

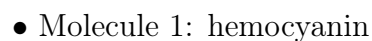
3 Residue-property plots

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 electron 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 dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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: hemocyanin



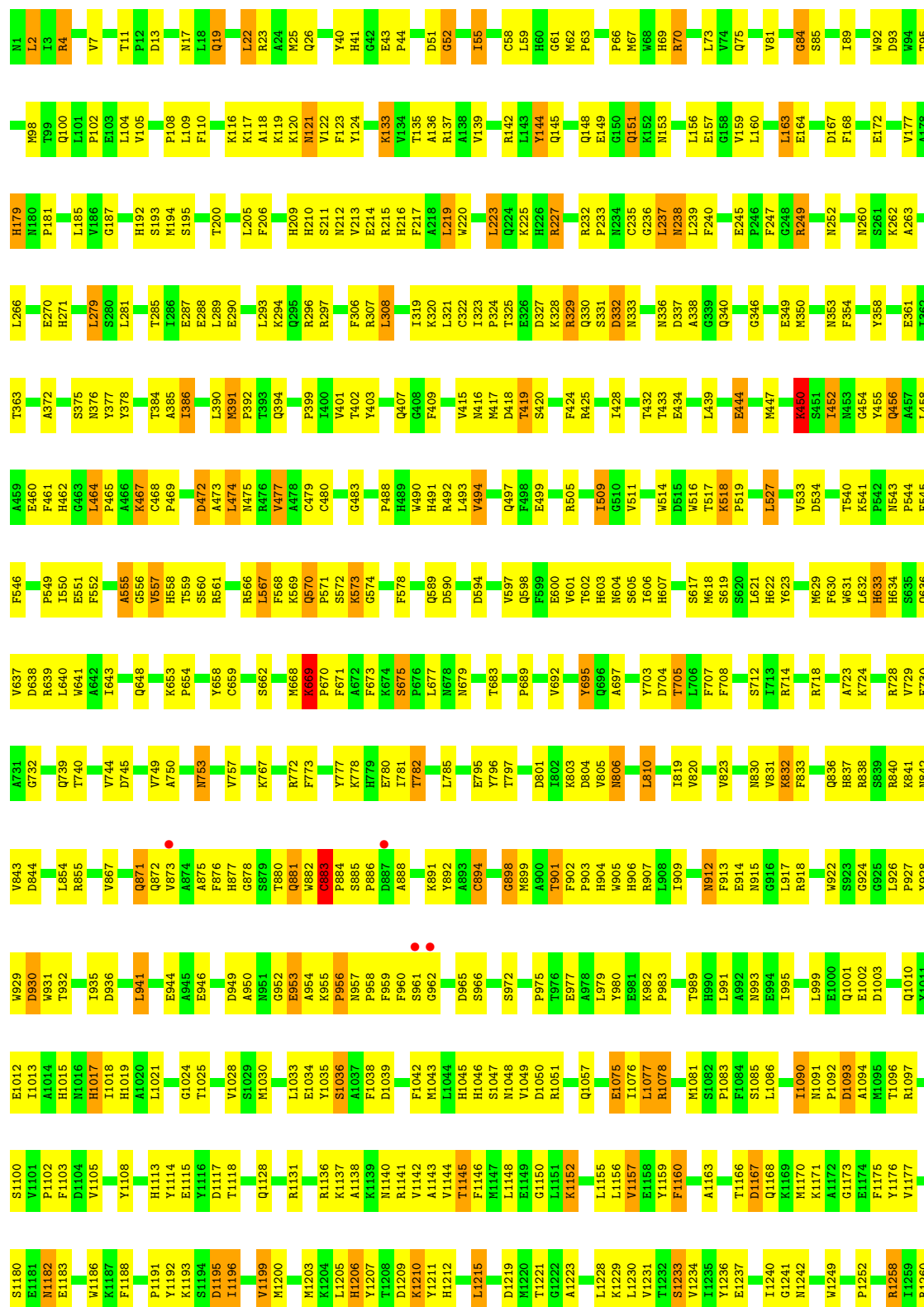
F1384	R1286	V1199	H1113	L1021	E946	N842	V749	S662	P571	H482	P397	T285	S193	I89
E1385	I1290	M1200	D1117	V1022	E947	V843	N753	E663	S572	G483	R398	T286	M194	K96
D1390	V1296	M1203	T1118	G1023	T948	M851	E754	V664	G574	N484	P399	L289	S195	L104
R1391	L1204	L1205	L1121	G1024	D949	R855	V757	M668	F578	P488	V401	R296	T200	V105
T1393	H1206	H1209	N1122	M1030	A950	R855	G758	P670	L579	H489	Q407	R297	D203	L109
Q1394	D1209	P1300	I1126	S1029	E953	K865	S759	F671	L583	W490	G408	R301	P204	F110
E1396	Y1211	S1302	L1129	E1033	A954	E866	I760	F673	F587	L493	D411	A304	F206	G115
L1397	I1217	E1303	L1133	E1034	K955	V867	S766	K674	E588	V494	Q408	R305	L208	K116
M1400	G1305	D1304	I1133	Y1035	N957	Y870	K767	S675	Q589	Q497	W416	F306	H209	K117
H1406	T1306	G1306	H1148	S1036	P958	H877	V771	L677	C593	F498	W417	N316	H210	A118
T1407	M1307	M1308	M1140	A1037	P959	R772	R772	N678	D594	N679	T419	V317	V213	K119
L1408	T1221	S961	V1144	F1042	S961	T880	Y777	N679	D594	P508	R423	R318	E214	K120
F1409	V1144	G962	A963	F1042	G962	W882	Y777	T683	V597	F424	R425	R319	R215	F123
V1410	L1148	A963	I964	H1045	I964	C883	E780	R684	V601	G510	T432	K320	K225	E127
F1411	E1149	S970	S970	H1046	S970	P884	I781	R685	T602	T683	T433	K321	H226	I128
E1412	K1152	T971	S972	M1048	T971	S885	A784	R686	H603	W513	E434	L321	R227	K129
Q1413	K1153	S972	S972	V1049	S972	P886	L785	P689	I606	W514	E435	C322	G228	
T1414	S1154	D1050	P975	D1050	S972	K891	L788	V692	W809	D515	E435	T325	G228	
E1420	L1155	R1051	P975	R1051	P975	Y892	L788	V692	T610	W516	E435	E326	L229	M132
V1421	L1156	P975	P975	P975	P975	A893	L788	V692	S613	T517	L439	R329	P230	K133
H1422	V1157	L979	L979	L979	L979	C894	E795	Y695	W809	K518	W441	R440	T231	X134
F1423	F1160	Y980	Y980	Y980	Y980	C895	Y796	Y695	T610	K518	W441	R440	C235	T135
E1424	I1161	K982	K982	K982	K982	H896	T797	Y703	S613	A442	A442	N333	C235	A136
L1426	K1169	Y988	Y988	Y988	Y988	R897	L798	D704	M618	N438	N438	N336	N238	A137
H1427	P983	P983	P983	P983	P983	R799	R799	T705	W618	E444	E444	D337	L239	A138
E1430	D984	D984	D984	D984	D984	M899	W800	L706	S619	R446	R446	A338	F240	V139
D1438	P985	P985	P985	P985	P985	A900	D801	F707	S620	F446	F446	G339	H241	D140
R1439	G986	G986	G986	G986	G986	T901	I802	F708	L621	D534	D449	Q340	P246	A141
G1436	K1065	K1065	K1065	K1065	K1065	P903	K803	L711	H622	N447	N447	M350	P246	R142
R1437	A1066	A1066	A1066	A1066	A1066	H904	V805	K541	D627	S448	S448	P351	R249	Q145
D1438	Y1067	Y1067	Y1067	Y1067	Y1067	V905	N806	P544	P628	K450	K450	K352	D249	A146
H1440	E1075	E1075	E1075	E1075	E1075	H906	G807	P544	W629	S451	S451	N353	D250	E157
D1446	I1076	I1076	I1076	I1076	I1076	R907	T808	P544	F630	Y455	Y455	Y358	T251	L163
Y1447	L1077	L1077	L1077	L1077	L1077	I909	L810	V720	W631	Q456	Q456	E361	T257	H170
D1451	S997	S997	S997	S997	S997	N915	T813	K724	H633	E460	E460	T362	D258	
L1456	A998	A998	A998	A998	A998	G916	T813	K724	Q636	F461	F461	T363	D259	V173
H1457	L999	L999	L999	L999	L999	L917	P816	R728	V637	H462	H462	T363	N260	Q174
D1462	E1000	E1000	E1000	E1000	E1000	P817	P817	V729	D638	G463	G463	T365	K261	L175
E1470	Q1001	Q1001	Q1001	Q1001	Q1001	P917	P917	F730	R639	H558	H558	L371	A263	V177
Q1472	E1002	E1002	E1002	E1002	E1002	A829	A829	G732	L640	T559	T559	L371	A263	A178
R1473	E1008	E1008	E1008	E1008	E1008	N830	N830	G732	W641	A466	A466	L371	L266	H179
Q1474	E1012	E1012	E1012	E1012	E1012	V831	V831	W736	A642	K467	K467	V383	E270	P181
L1475	I1013	I1013	I1013	I1013	I1013	W929	W929	G737	L643	C468	C468	T384	E270	M180
V1476	A1014	A1014	A1014	A1014	A1014	W931	W931	G737	W644	Q562	Q562	A385	F276	F181
L1477	H1015	H1015	H1015	H1015	H1015	D930	D930	W738	P471	D564	D564	T386	F276	L185
R1478	N1016	N1016	N1016	N1016	N1016	Q836	Q836	Q739	L647	P469	P469	T386	D277	V186
F1479	H1017	H1017	H1017	H1017	H1017	H837	H837	W744	R651	D472	D472	T389	L279	G187
L1479	I1018	I1018	I1018	I1018	I1018	R838	R838	D745	Y658	A473	A473	Q394	S280	G188
F1479	A1020	A1020	A1020	A1020	A1020	V942	V942	V748	Y658	C480	C480	T395	L281	
L1477	A1020	A1020	A1020	A1020	A1020	V942	V942	V748	Y658	L481	L481	I396	N282	H192





• Molecule 1: hemocyanin

Chain J:  47% 31% 5% 17%







LEU	ASN	LEU	LEU	ASP	ASP	PRO	MET	ARG	PRO	PHE	GLY	PHE	ASN	ASN	LYS	THR	THR	ASN	GLN	GLN	HIS	LEU	ALA	ASP	THR	ASP	THR	THR	ASN	SER	ILE	ARG	CYS	PRO	VAL	PRO	ASP	P44	VAL	PHE	VAL	GLY	TYR	GLN	ASN	SER	LEU	ASN	TYR	LYS	PHE	ASP	SER	LEU	SER	PHE	GLY	LEU	SER	ILE	ARG	LEU	ASP	ASP	LEU	GLU
SER	ARG	GLN	SER	HIS	ASP	ARG	VAL	PHE	ALA	GLY	PHE	TRP	LEU	LYS	SER	THR	GLY	ALA	LYS	ALA	SER	ALA	LEU	ASP	VAL	ASN	THR	ILE	HIS	ILE	CYS	VAL	PRO	VAL	ILE	GLY	VAL	GLU	HIS	GLU	ASN	SER	LEU	ASN	CYS	ASP	ASN	ASN	TYR	LYS	PHE	ASP	SER	LEU	SER	PHE	GLY	LEU	SER	ILE	ARG	LEU	ASP	ASP	LEU	GLU

● Molecule 1: hemocyanin

Chain P: 49% 28% 6% 17%

H1046	T971	S885	L788	V692	H603	W514	S420	F306	E164	H83	N1
S1047	S972	K891	G789	Y695	B604	D515	R423	R307	E164	H83	L2
N1048	R973	Y892	V790	G696	S605	W516	R423	L308	Q174	G84	I3
P1049	A974	H896	D791	A697	I606	T517	F424	L321	V177	I89	R4
D1050	A975	A893	M792	F793	H607	P524	I428	P324	A178	T11	T11
R1051	T976	C894	F793	Y703	W609	L527	I428	T326	H179	W92	P12
E977	E977	C895	A794	T705	T610	L527	T432	E326	M180		D13
A978	H896	H897	T796	D704	G611	V533	E435	D327	L185	P102	L16
R979	Y980	H898	T797	T705	G612	D534	E435	K328	V186	E103	L16
E981	G980	M899	L798	F708	S613	D534	L439	R329	G187	L104	N17
N982	X982	A900	R799	F708	S613	D534	L439	R329	V186	V105	L18
P983	P983	T901	W800	R718	M618	T540	M447	Q330	H192	Q106	Q19
D984	D984	H904	D801	K724	L621	K541	S448	D332	V20	H07	V20
K987	K987	W905	L802	K724	H622	K547	S448	D332	H192	P108	S21
H990	H990	H906	D804	R728	Y623	A548	D449	N336	M194	S193	L22
L991	L991	R907	W805	W729	T624	P549	S451	Q340	L109	F110	R23
I995	I995	L908	L810	F730	S625	E551	I452	G345	S196	I111	A24
P996	P996	I909		A731	M629	E551	I452	G345	L197	D112	M25
K1078	K1078	E914	P816	G732	F630	L553	I452	G345	L205	P113	D28
P1079	P1079	N915	P817	F733	W631	K554	Q456	W352	H210	G115	Q35
M1081	M1081	G916	P817	L734	L631	K554	Q456	N353	K116	K117	A36
L1076	L1076	L917	A829	L735	L632	A555	L464	E361	S211	A118	I37
R1077	R1077	L917	N830	M736	H633	G556	L464	E361	N212	K117	A36
K1078	K1078	L917	N830	M736	H633	G556	L464	E361	N212	K117	A36
P1080	P1080	L917	N830	M736	H633	G556	L464	E361	N212	K117	A36
M1081	M1081	L917	N830	M736	H633	G556	L464	E361	N212	K117	A36
S1082	S1082	L917	N830	M736	H633	G556	L464	E361	N212	K117	A36
P1083	P1083	L917	N830	M736	H633	G556	L464	E361	N212	K117	A36
F1084	F1084	L917	N830	M736	H633	G556	L464	E361	N212	K117	A36
S1085	S1085	L917	N830	M736	H633	G556	L464	E361	N212	K117	A36
L1086	L1086	L917	N830	M736	H633	G556	L464	E361	N212	K117	A36
D1089	D1089	L917	N830	M736	H633	G556	L464	E361	N212	K117	A36
I1090	I1090	L917	N830	M736	H633	G556	L464	E361	N212	K117	A36
N1091	N1091	L917	N830	M736	H633	G556	L464	E361	N212	K117	A36
P1092	P1092	L917	N830	M736	H633	G556	L464	E361	N212	K117	A36
D1093	D1093	L917	N830	M736	H633	G556	L464	E361	N212	K117	A36
S1100	S1100	L917	N830	M736	H633	G556	L464	E361	N212	K117	A36
V1101	V1101	L917	N830	M736	H633	G556	L464	E361	N212	K117	A36
P1102	P1102	L917	N830	M736	H633	G556	L464	E361	N212	K117	A36
V1105	V1105	L917	N830	M736	H633	G556	L464	E361	N212	K117	A36
K1109	K1109	L917	N830	M736	H633	G556	L464	E361	N212	K117	A36
H1113	H1113	L917	N830	M736	H633	G556	L464	E361	N212	K117	A36
D1117	D1117	L917	N830	M736	H633	G556	L464	E361	N212	K117	A36
T1118	T1118	L917	N830	M736	H633	G556	L464	E361	N212	K117	A36
L1119	L1119	L917	N830	M736	H633	G556	L464	E361	N212	K117	A36
E1120	E1120	L917	N830	M736	H633	G556	L464	E361	N212	K117	A36
N1121	N1121	L917	N830	M736	H633	G556	L464	E361	N212	K117	A36
L1122	L1122	L917	N830	M736	H633	G556	L464	E361	N212	K117	A36
S1125	S1125	L917	N830	M736	H633	G556	L464	E361	N212	K117	A36
I1126	I1126	L917	N830	M736	H633	G556	L464	E361	N212	K117	A36
A1127	A1127	L917	N830	M736	H633	G556	L464	E361	N212	K117	A36
Q1128	Q1128	L917	N830	M736	H633	G556	L464	E361	N212	K117	A36
L1129	L1129	L917	N830	M736	H633	G556	L464	E361	N212	K117	A36
S1130	S1130	L917	N830	M736	H633	G556	L464	E361	N212	K117	A36
R1131	R1131	L917	N830	M736	H633	G556	L464	E361	N212	K117	A36
E1132	E1132	L917	N830	M736	H633	G556	L464	E361	N212	K117	A36

T1133	K1210	V1308	T1407	R1494	L1615	MET	GLU	ARG	ASP	SER	HIS
N1134	Y1211	H1309	F1411	S1497	K1616	PHE	ASN	LYS	PRO	ARG	ILE
R1135	H1212	T1310	N1498	N1498	L1617	SER	LEU	PRO	ILE	ASN	CYS
K1137	V1213	C1311	T1414	S1499	L1618	LEU	LEU	ASP	PHE	PRO	VAL
	D1219	C1312	T1500	T1500	Q1622	ALA	ALA	GLN	LEU	VAL	ILE
N1140	M1220	L1313	C1417	T1507	R1627	ALA	ARG	LEU	HIS	PHE	GLY
R1141	T1221	H1314	E1420	T1507	Y1628	PHE	GLY	PHE	HIS	ASP	GLY
V1142	G1222	G1315	E1420	S1511	E1629	LYS	SER	ASN	SER	ASN	TYR
A1143	A1223	M1316	V1421	S1511	M1630	ASN	ASP	ASN	THR	ASN	GLN
V1144	E1224	P1317	H1422	V1516	E1631	MET	VAL	ARG	VAL	ASN	GLU
T1145	V1225	V1318	Y1423	V1516	E1631	THR	ALA	TYR	ASP	SER	CYS
	T1226	F1319	E1424	Y1519	M1636	ASP	VAL	LEU	ARG	LEU	ASP
E1149	L1230	P1320	V1425	Y1519	G1637	PRO	PRO	TYR	LEU	ASN	ASN
	K1152	H1321	H1426	H1524	G1637	GLY	GLY	TRP	TRP	TYR	TYR
K1153	S1233	W1322	H1427	Y1525	S1638	ALA	TRP	HIS	ALA	LYS	LYS
L1156	Y1236	R1324	I1430	D1528	I1640	LEU	TRP	ALA	ILE	ASP	ASP
V1157		L1325	W1433	T1529	T1641	ILE	ILE	PHE	GLN	SER	SER
	G1241	L1329	G1436	T1530	Q1642	GLU	GLU	PHE	ASP	LEU	LEU
F1160	N1242	V1330	G1437	E1541	K1643	ALA	PRO	PHE	LEU	PHE	PHE
T1161	F1243	E1331	R1437	E1541	F1645	ALA	ASP	GLU	GLN	GLU	GLU
A1162	R1247	D1332	D1438	I1542	P1646	THR	SER	HIS	ARG	VAL	CYS
A1163	R1248	E1333	V1439	I1543	M1647	GLY	LEU	THR	ARG	LEU	LEU
			H1440	L1544	P1648	LEU	PRO	PHE	LYS	ASP	SER
T1166	R1337	R1337	S1441	D1551	T1649	PRO	GLY	CYS	LEU	LEU	ILE
D1167	G1338	G1338	M1442	D1559	F1652	ALA	ILE	PHE	TYR	ASP	ARG
Q1168	S1251	S1339	D1446	L1559		GLN	ILE	GLU	ASN	LEU	LEU
K1169	P1252	G1340	D1446	H1560	D1656	CYS	ASP	VAL	VAL	ASP	ASP
M1170	S1255	P1344	Y1450	G1561	VAL	ASN	GLU	HIS	ALA	ALA	LEU
K1171		Y1345	Y1450	G1561	GLU	ALA	THR	PHE	PHE	LEU	LEU
G1172	R1258	W1346	F1454	G1562	PHE	ALA	TYR	GLU	GLU	CYS	GLU
E1174	I1259	D1347	F1455	K1563	GLU	GLY	LYS	VAL	VAL	GLU	GLU
F1175	R1260	W1348	L1456	V1568	GLU	SER	HIS	LEU	LEU	SER	ARG
Y1176			H1457	R1569	ASP	ASN	PRO	HIS	ASN	ARG	GLN
V1177	F1266	L1355	H1458	C1573	THR	ILE	LYS	ASN	LEU	LEU	ILE
L1178		P1356		V1574	TRP	HIS	THR	SER	LEU	LEU	SER
G1179	M1271	R1357	V1461	V1574	ARG	THR	ASN	ILE	ASN	ASN	HIS
S1180	E1272	L1358	D1462	P1575	ASP	CYS	GLU	HIS	ASP	ASP	ASP
E1181	S1273		W1465	T1576	VAL	CYS	TRP	SER	PRO	PRO	ARG
N1182	L1274	I1372		G1577	VAL	LEU	ILE	TRP	MET	ARG	PHE
E1183			E1470	I1578	THR	HIS	GLU	ILE	PRO	ALA	ALA
	K1279	P1376	E1470	G1579	SER	GLY	ASN	GLY	PRO	PHE	GLY
W1186	Q1280		L1471	E1580	ALA	MET	PRO	GLY	GLY	ASN	GLY
K1187		G1380	Q1472	E1581	ASN	PRO	PHE	ASN	PRO	ASN	ASN
	R1286		R1473	N1582	ARG	THR	HIS	ASN	ASN	TRP	TRP
		T1369	Y1474	C1583	ILE	PHE	HIS	PRO	LYS	LYS	THR
Y1192	F1293		R1475	G1584	ARG	PRO	GLY	HIS	SER	THR	GLY
K1193		T1393	K1476	A1587	ARG	HIS	LYS	SER	ALA	ALA	GLY
S1194	V1296	Q1394	L1477	W1601	ASN	TRP	ILE	MET	ASN	ASN	ILE
D1195	Q1299	P1395	Y1479	F1603	LYS	ARG	SER	SER	GLN	ALA	LYS
I1196		E1396		D1604	ASP	HIS	PHE	LEU	ASP	HIS	SER
V1199	G1300	N1400	C1483	F1603	LEU	TYR	ASP	LEU	LEU	ASP	ALA
M1200	P1301	R1401	A1485	D1604	SER	LEU	ALA	PHE	THR	THR	PHE
	S1302	Y1402	P1492	R1605	LYS	SER	VAL	ALA	THR	ALA	ALA
M1203	D1304	L1403	M1493	E1614	GLU	LEU	THR	ALA	THR	ALA	THR
D1209	G1305				ASP	VAL	VAL	TYR	ASN	TYR	VAL

• Molecule 1: hemocyanin

Chain S:  50% 27% 6% 17%

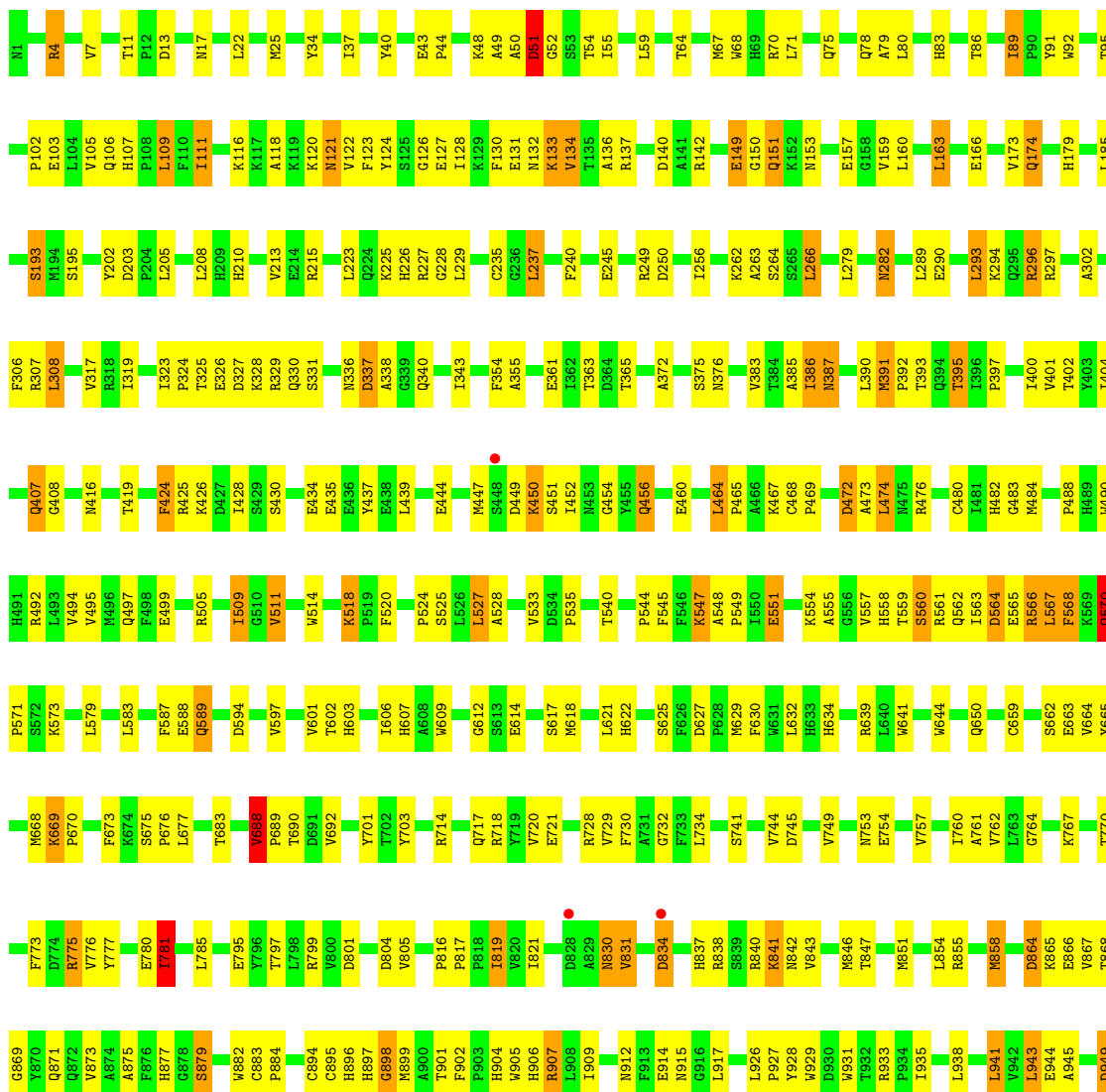
H1	V105	T200	H1	V105	T200
L2	L109	S201	L2	L109	S201
I3	F110	L206	I3	F110	L206
R4	I111	L208	R4	I111	L208
V7	K116	H209	V7	K116	H209
	K117	G210		K117	G210
T11	K118	H211	T11	K118	H211
P12	K119	S211	P12	K119	S211
D13	K120	V213	D13	K120	V213
E14	N121	E214	E14	N121	E214
	N121	R215		N121	R215
N17	V122	Q221	N17	V122	Q221
L16	Y124	H226	L16	Y124	H226
V20	F123	R227	V20	F123	R227
S21	L128	G236	S21	L128	G236
L22	K129	N238	L22	K129	N238
	F130	L239		F130	L239
W25	T135	F240	W25	T135	F240
Y34	A136	H241	Y34	A136	H241
I37	R137	E245	I37	R137	E245
	R142	P246		R142	P246
H41	Q145	F247	H41	Q145	F247
G42	Q148	G248	G42	Q148	G248
E43	E149	R249	E43	E149	R249
P44	G150	D250	P44	G150	D250
	D51	K258		D51	K258
I55	K152	A263	I55	K152	A263
	I55	L266		I55	L266
G61	E157	F267	G61	E157	F267
M62	M161	D277	M62	M161	D277
	E164	D278		E164	D278
W68	Q165	L281	W68	Q165	L281
H69	E166	M284	H69	E166	M284
R70	Q174	T285	R70	Q174	T285
L71	L175	E287	L71	L175	E287
Y72	E176	L288	Y72	E176	L288
L73	H179	L292	L73	H179	L292
V74	L185	R296	V74	L185	R296
Q75	V186	R297	Q75	V186	R297
F76	G187	R301	F76	G187	R301
E77	G188		E77	G188	
	T191			T191	
V81	H192		V81	H192	
A82	S193		A82	S193	
H83	M194		H83	M194	
S85	S195		S85	S195	
I89			I89		
P90			P90		
Y91			Y91		

L1618	G1619	N1620	M1621	Q1622	R1627	M1498	S1499	T1500	L1632	T1633	A1634	V1635	M1636	G1637	S1638	K1639	T1640	T1641	K1643	I1644	L1651	D1656	VAL	GLU	PHE	GLU	GLU	ASP	THR	TRP	ARG	ASP	VAL	VAL	THR	SER	ALA	ASN	ARG	ILE	ARG	ASN	LEU	LYS	ASP	LEU	SER	LYS	GLU	ASP	MET	PHE	SER	LEU
N305	F306	R307	L308	R318	I319	K320	E326	D327	K328	R329	Q330	S331	D332	N336	N353	F354	A355	E361	I362	L364	G363	P471	D472	S473	T393	M391	P392	H489	W490	Q394	R398	F399	I400	V401	T402	Y403	Q407	G408	F409	K410	D411	V415	M416	T419										
S420	R423	F424	I428	T432	E435	F446	K450	S451	I452	Y455	Q456	E460	F461	H462	G463	L464	P465	H482	G483	M484	A485	T486	F487	P488	K589	P571	T393	W490	S572	H491	R492	L493	V494	Q497	N500	T504	R505	K410	D509	G510	V511	W514	Q598	D515										
H516	T517	K518	L523	P524	S525	L526	L527	V533	T540	N543	S451	I452	F545	F546	K547	A548	P549	H557	H558	T559	S560	R561	Q562	L563	D564	E565	R566	L567	F568	K569	P571	T393	W490	S572	H491	R492	L493	V494	Q497	N500	T504	R505	K410	D509	G510	V511	W514	Q598	D515					
V601	T602	H603	T606	V609	S613	E614	P615	M618	L621	H622	Y623	T624	D627	P628	M629	F630	E551	K554	V557	H558	T559	S560	R561	Q562	L563	D564	E565	R566	L567	F568	K569	P571	T393	W490	S572	H491	R492	L493	V494	Q497	N500	T504	R505	K410	D509	G510	V511	W514	Q598	D515				
H686	S687	P688	T689	D691	E696	Y701	T705	F708	S712	I713	Y716	T717	L716	R718	Y719	F720	E721	E722	Q636	V637	T638	R639	S640	R641	A642	T643	L647	R651	G652	K653	P654	Y658	N661	S662	E663	V664	P670	F671	F673	L677	M678	T683	R684	E685	R772									
F773	D774	Y777	E780	I781	T782	L785	L788	M792	E795	I796	T797	L798	R799	W800	D801	L802	D804	W805	N806	G807	T808	R809	L810	H813	P816	R817	P818	T819	V820	D828	V831	K832	F833	D834	E835	Q836	H837	R838	K841	N842	W843	L854	R855	V842	L943	E944	M858	A945						
K865	E866	V867	T868	G869	Y870	Q871	F873	F876	H877	G878	S879	T880	Q881	A888	L889	Q890	K891	C895	H896	R897	G898	N899	F902	P903	H904	N905	R906	R907	L908	L909	F913	E914	N915	G916	L917	N920	L926	P927	Y928	D929	N930	K931	T932	L935	L941	V942	L943	E944	M858	A945				
E946	Y947	T948	D949	A950	E953	A954	K955	N957	P958	S961	G962	A963	T964	T971	S972	P975	T976	E977	A978	L979	Y980	E981	K982	P983	D984	P985	T989	H990	L991	L995	I996	S997	A998	L999	E1000	Q1001	E1002	D1003	F1004	F1007	Y1011	E1012	H1015	N1016	I1017	I1018	H1019	A1020	Y1114	L1021				
T1025	E1026	A1027	V1028	M1030	E1034	Y1035	S1036	H1046	S1047	N1048	V1049	T1051	T1055	W1056	Q1057	A1058	K1051	T1060	Q1061	F1062	R1063	G1064	K1065	P1066	A1067	I1067	I1074	H990	L991	L995	I996	S997	A998	L999	E1000	Q1001	E1002	D1003	F1004	F1007	Y1011	E1012	H1015	N1016	I1017	I1018	H1019	A1020	Y1114	L1021				
E1120	N1121	N1122	I1126	R1131	E1132	T1133	K1137	M1140	T1145	K1152	K1153	S1154	L1155	V1157	F1160	L1161	A1162	A1163	D1164	G1165	T1166	D1167	Q1168	K1169	M1170	K1171	L1172	G1173	F1175	Y1176	G1179	S1180	E1181	M1182	E1183	W1186	R1190	D1195	L1196	M1200	M1203	H1113	Y1114	L1021										
I1217	D1218	T1219	A1223	E1224	V1225	L1228	K1229	L1230	V1231	T1232	S1233	T1234	I1235	Y1236	G1239	R1248	W1249	L1250	S1251	R1258	I1259	R1260	L1263	M1271	R1275	E1284	G1285	R1286	V1296	Q1299	F1300	P1301	D1304	G1305	T1306	V1307	V1308	C1312	L1313	H1314	G1315	F1319												
W1322	H1323	R1324	L1325	S1328	E1331	D1332	E1333	L1334	L1335	A1336	R1337	G1338	S1339	G1340	V1341	W1346	D1347	W1348	F1352	D1353	E1354	R1357	L1358	I1359	A1362	S1367	R1368	T1369	L1370	F1378	K1379	G1380	K1381	I1382	S1383	F1384	E1385	D1390	R1391	D1392	T1393	Q1394	P1395	E1396	L1397	F1398	G1399	L1403						
T1407	L1408	T1414	F1416	V1421	H1422	Y1423	E1424	V1425	L1426	H1427	T1429	I1430	H1431	S1432	W1433	G1436	R1437	D1438	V1439	H1440	M1442	D1446	Y1447	Y1450	F1454	F1455	L1456	N1460	V1461	D1462	W1465	A1466	W1467	Q1469	E1470	R1473	L1477	C1484	A1485	L1486	L1487	L1488	M1489											
W1490	Q1491	M1492	R1494	M1498	S1499	T1500	S1511	T1512	A1513	V1516	L1523	F1532	I1537	K1541	E1541	G1549	F1557	L1558	L1559	S1565	L1566	D1567	V1568	P1574	P1575	I1578	G1579	E1580	E1581	N1582	C1583	S1591	G1594	G1595	E1596	T1597	W1601	D1604	R1605	R1608	L1618	K1617												

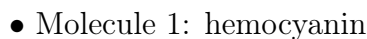
[illegible]

- Molecule 1: hemocyanin

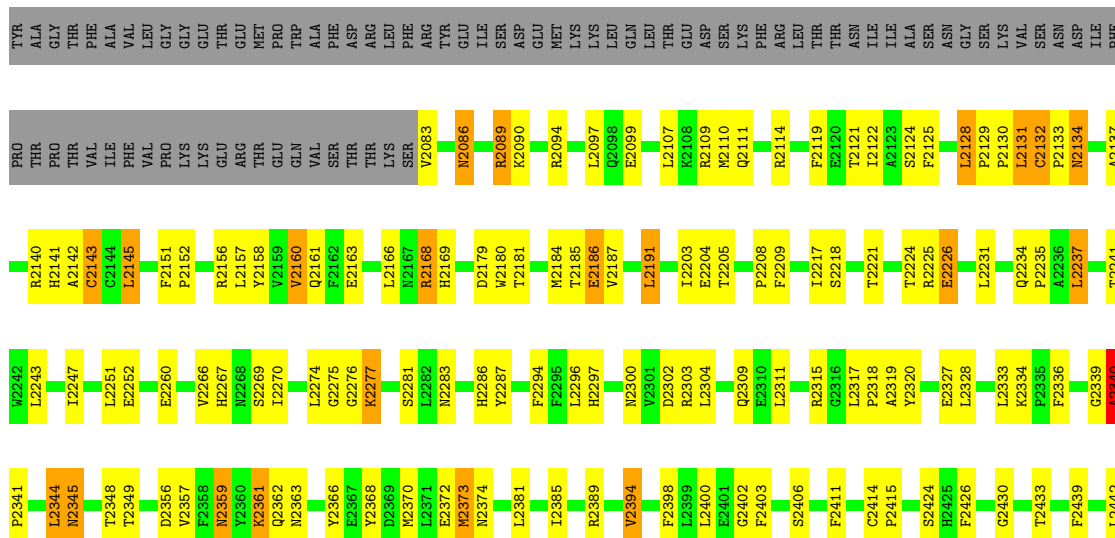
Chain V:

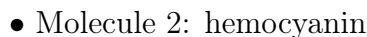


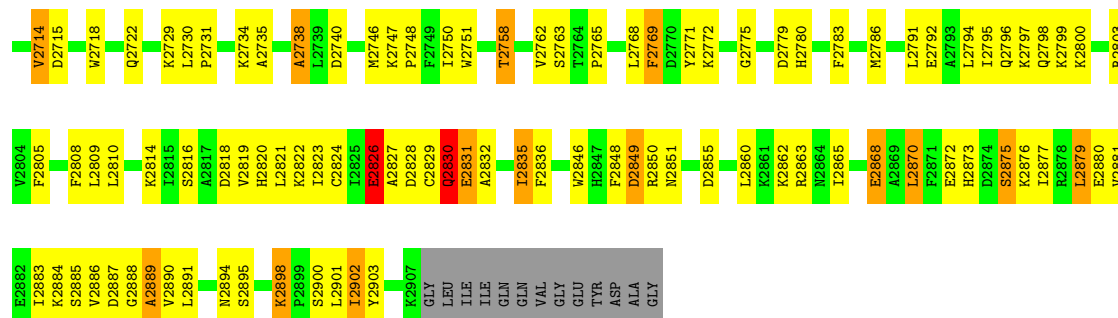
E1396	C1311	R1190	F1103	E1012	L926	V848	V757	M688	E565	A473	T365	D250	Q145	G84
L1397	C1312	P1191	D1104	I1013	P927	V848	V757	K669	R566	L474	T371	D258	E166	S85
N1400	L1313	Y1192	V1105	H1015	P928	N852	G758	P670	L567	R475	A372	K259	D167	L87
R1401	H1314	D1195	Y1108	N1016	Q929	A853	I760	A672	F568	G483	S375	N260	H170	Y91
L1403	M1315	I1196	H1113	H1017	D930	L854	K767	F673	K569	T486	K376	K262	E171	W92
Y1404	P1317	T1197	Y1114	I1018	W931	R855	K767	K674	E172	T486	K376	K262	E172	D93
	V1318			H1019	T932			S675	Q570		Y377	S264	V173	W94
T1407	F1319	M1200	T1118	A1020	I935	A859	W771	P676	D575		A385	S264	Q174	
F1411	P1320		L1021	V1022	I935	A860	R772	L677	F578	H489	A385	L266	V177	M98
T1414	H1321	M1203	L1119	G1023	L941	F981	F773	W678	L579	W490	I386	L266	A178	T99
D1415	L1322	V1213	L1121	G1024	E946	A862	D774	M679	L579	H491	I386	L266	H179	Q100
F1416	H1323		L1121	G1024	E946	A863	W776	T683	Q589	L493	M391	H271	M180	
C1417	R1324	T1221	E1026	A1027	Y947	R865	Y777	A694	C593	V494	P392	D277	P181	E103
	V1325		E1027	D1028	T948	E866			C593	Q497	T393	D278	I182	L104
T1421	L1326	D1227	R1135	S1029	D949	V867	I781	S687	D594	Q497	Q394	L279	H183	V105
H1422	V1327	K1229	R1136	S1030	A950		A784	P689	V597	E499	R398	L281	Y184	L109
Y1423	L1328	L1230	K1137	M1030	N951	Y870	L785	T690	T602	I509	P399	N282	V186	
E1424	E1331	V1231	Q871			Q872	L788	D691	H603	G510	I400	T285	G187	T114
V1425	T1232	T1232	T880	I1041	K955			V692	H604	V511	T402		F190	K115
H1427	V1236	Y1236	Q881	H1045	P958	W882	E795	Q696	S605	W514	Q407	L289	S193	K117
N1428	E1245	E1245	V882	H1046	F959	V882	Y796		I606	D515	G408	R296	M194	A118
T1429	G1246	G1246	C883	H1047	P960	C883	T797	W703		W516		R297	S195	K119
I1430	R1247	R1247	P884	H1048	S961	P884	L798	D704	W609	T517	D411	N305	T200	V122
W1433	S1339	I1250	R885	N1049	I964	S885	R799	T705	T610	T517	W412	F306	S201	F124
D1438	G1340	I1250	P886	V1049	D965	P886	W800	L706	G611	L527	N413	N307	Y202	S125
	V1341		A888	R1051	P967	A888	I802	F707	G612		M414	R307		
M1442	Y1345	I1253	K891	T1055	S972	K891	K803	G709	S619	T531	W415	L308	L205	G126
D1446	D1347	R1258	Y892	W1056	S972	Y892	D804	G710	H622	Y532	N416	N316	F207	K133
Y1447	W1348	I1259	A893	L1059	A974	A893	R806	S712	Y623	D534	M417		L208	V134
	V1349		C894		P975	C894	G807	R713	T624		D418	L321	L321	T135
F1454	E1354	L1263	H896	R1063	T976	H896	L810	E715	M629	T540	L422	I323	H209	A136
L1455	L1355	E1284	H897	G1064	E977	H897	P817	L716	W631	K541	R493	I323	H210	R137
H1457	P1356	G1285	C898	L1065	A978	C898	P818	Q717	F630	P542	F424	P324	S211	
H1458	R1357	R1286	M899	A1070	L979	M899	R818	R718	L632	F546	L439	E326	N212	V139
S1459	L1358		A900		Y980	A900	R819	Y719	L632	K547	E444	D327	E214	D140
N1460	I1359	I1290	T901		E981	T901	V823	W720	H633	A548		K328	R215	A141
V1461			H904	E1075	K987	H904		E721	V637	A548	E444	R329	H216	R142
W1465	Y1365	F1293	W905	L1076	Y988	W905	T826	E722	D638	P649	S448	Q330	F217	L143
	T1369		H906	L1077	T989	H906	R827		R639	I550	D449	Q330	W220	Y144
E1470	I1372	Q1299	R907	R1078	T989	R907	D828	V729	L640	E551	K450	D332	Q221	Q145
L1471	P1301	C1300	L909	P1083	L991	L909	N830	W736	F552	L553	Q456	N336	A222	A146
R1473	S1302	S1302	N912	L1086	I995	N912	W831	G737	A642	K554		Q340	L223	S147
Y1474	I1382	S1302	F913	L1086	L999	F913	R832	I738	I643	A555	H462	Q340	H226	E149
R1475	I1382	S1302	E914	L1090	L999	E914	F833	Q739	G556	G556	G463	M350	H226	G150
K1476	I1387	D1304	N915	N1091	Q1001	N915	D834	Q739	V557	L464	L464	P357	C235	Q151
L1477	G1305	G1305	G916	P1092	Q1001	G916	E835	Q836	C659	H558	P465	P357	C235	K152
S1478	T1306	T1306	L917	D1093	F1007	L917	Q836	D745	D466	S560	K467	E361	Q236	N153
Y1479	D1392	V1308	R918	D1093	E1008	R918	R841	L746	S662	R561	C468	E361	N238	E157
			R1097	R1097	E1008	R1097	R841	F747	S662	G562	P469	I362	N238	
					Y1011	Y1011	R843	V748	V664	I563	T363	T363	L239	L163
										D564	D472	D364		E164





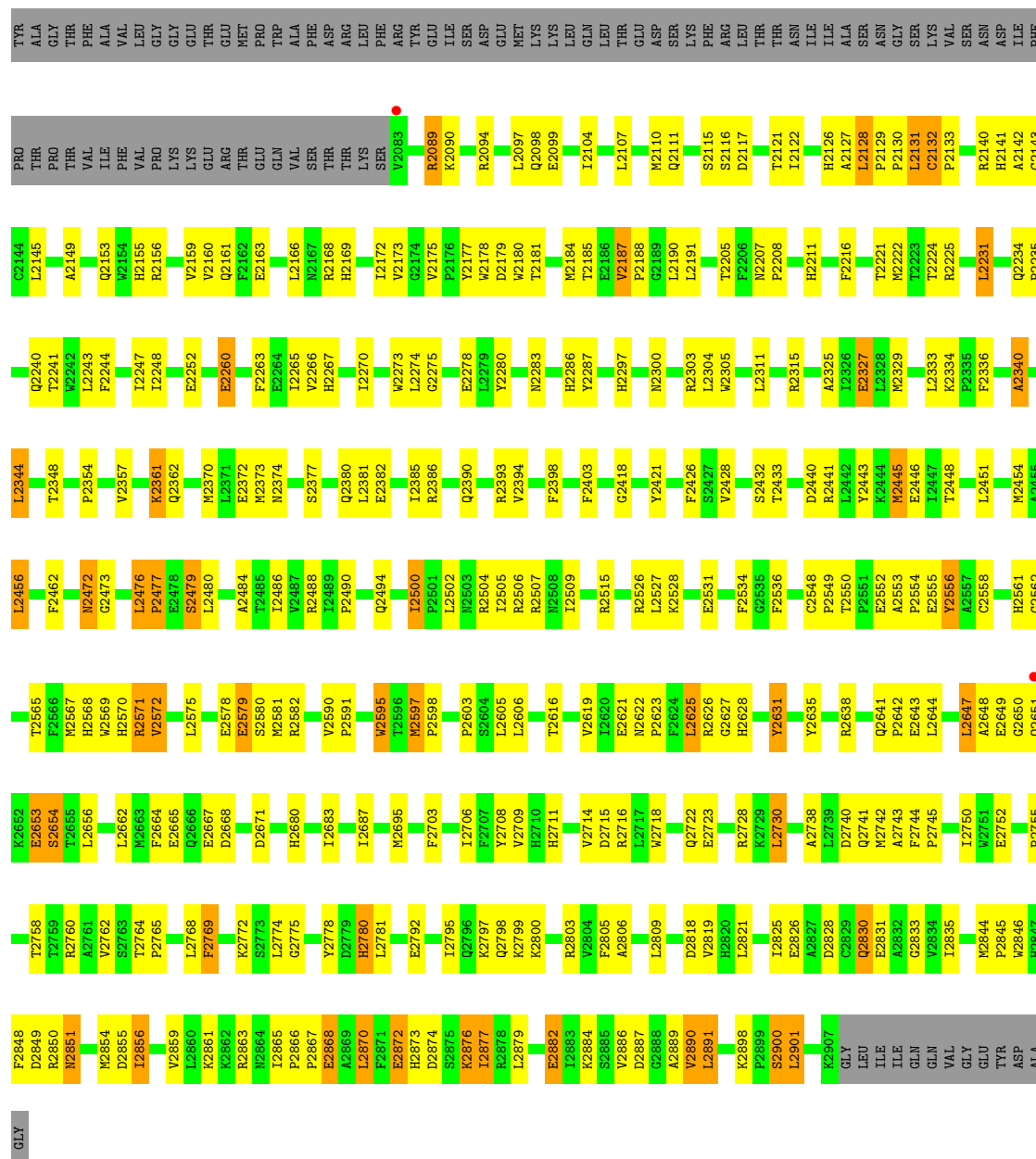






• Molecule 2: hemocyanin

Chain N: 55% 30% 5% 10%



- Molecule 2: hemocyanin

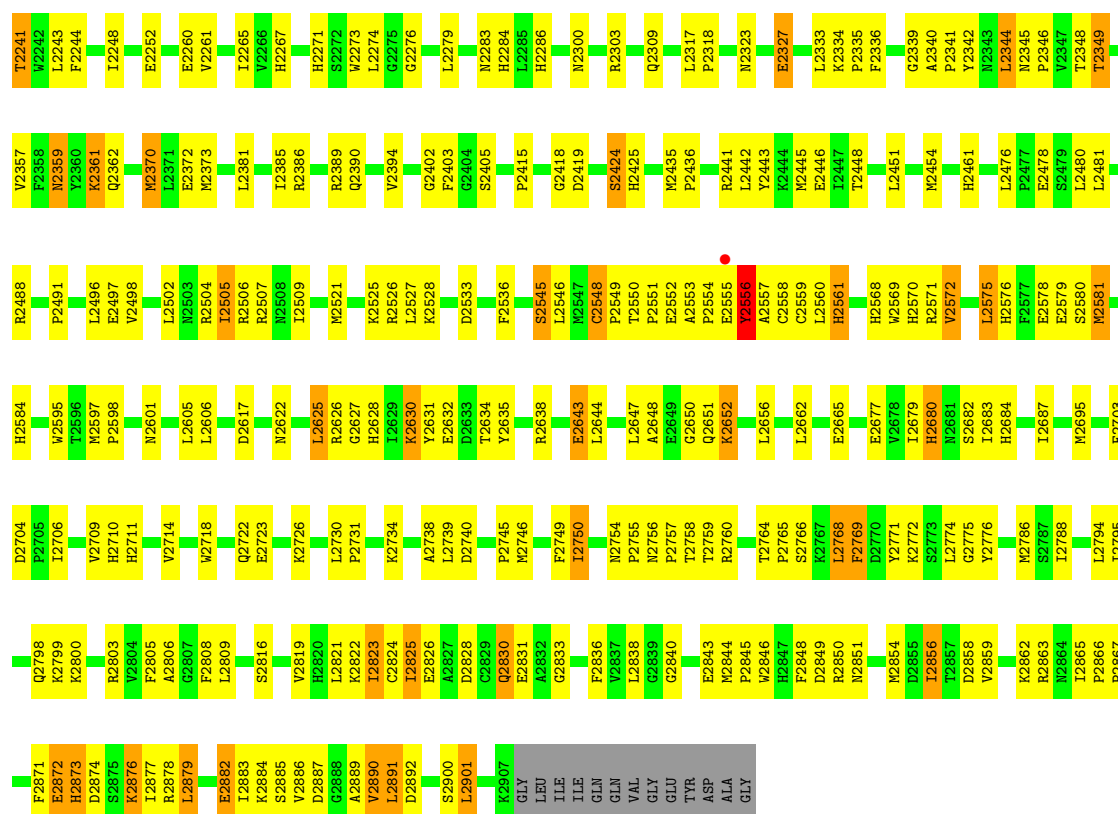
Chain Q:  56% 28% 5% 10%

TYR	PRO	H2141	Q2240	H2373		P2598		R2803	V2681
ALA	THR	A2142	T2241	N2374		S2599		V2604	E2882
GLY	PRO	C2143	W2242	S2377		D2600		F2805	I2883
THR	THR	C2144	L2243	S2377		L2502		F2806	I2884
PHE	VAL	L2145	F2244	Q2380		R2503		F2707	S2885
ALA	ILE	A2149	L2249	T2385		R2504		H2711	V2886
VAL	PHE	R2156	A2250	T2385		L2509		H2811	D2687
LEU	VAL	R2156	E2252	Q2390		R2515		K2814	Q2888
GLY	GLY	V2160	E2252	Q2390		R2515		L2815	A2889
GLY	LYS	Q2161	E2260	D2392		S2522		S2816	V2890
THR	GLU	Q2161	V2261	R2393		K2525		L2816	S2895
GLU	ARG	L2166	H2267	V2394		R2526		L2821	K2898
THR	THR	R2167	H2267	F2395		L2629		K2822	P2899
PRO	GLU	H2168	H2267	F2395		L2630		L2823	S2900
TRP	GLN	H2169	I2270	F2398		K2528		K2824	L2901
ALA	VAL	H2169	I2270	F2398		F2536		L2825	L2902
PHE	SER	L2172	L2274	G2402		T2635		E2826	V2903
ASP	THR	V2173	H2286	F2403		V2636		C2829	I2904
ARG	THR	V2173	Y2287	F2411		T2637		Q2830	A2904
LEU	LYS	D2179	L2296	F2411		E2643		E2831	P2905
PHE	ARG	W2180	H2297	D2419		L2644		A2832	A2906
TYR	TYR	T2181	H2297	F2426		F2645		G2833	K2907
GLU	GLU	W2184	N2300	F2426		A2646		G2840	GLY
ILE	ILE	T2185	N2300	R2441		L2647		E2843	LEU
SER	ASP	V2187	R2303	R2441		A2648		E2843	ILE
GLU	GLU	L2097	R2303	M2445		L2648		E2843	GLN
LYS	LYS	Q2098	Q2309	E2446		E2651		E2846	VAL
LEU	LYS	E2099	E2310	I2447		S2654		H2847	GLY
GLN	LEU	T2104	E2310	T2448		V2660		F2848	
LEU	LEU	L2107	T2205	D2449		L2661		R2849	
THR	THR	K2108	N2207	L2451		L2662		R2850	
GLU	ASP	R2109	P2208	L2451		M2663		N2851	
SER	SER	R2114	F2209	K2457		F2664		M2854	
LYS	LYS	S2115	H2210	F2462		E2665		D2855	
PHE	PHE	S2116	H2211	F2462		D2668		L2856	
ARG	ARG	D2117	F2216	T2466		Y2669		T2857	
LEU	LEU	S2217	S2217	R2571		E2673		D2858	
THR	THR	E2120	S2219	V2572		E2677		V2859	
ASN	ASN	S2124	E2220	L2575		E2677		K2861	
ILE	ILE	A2127	M2222	E2578		H2680		R2862	
ALA	ALA	L2128	R2225	L2476		E2678		P2867	
SER	SER	P2129	E2225	E2475		H2684		E2868	
ASN	ASN	P2130	V2227	L2480		Y2685		A2869	
GLY	GLY	L2131	Q2362	I2486		L2686		L2870	
SER	SER	C2132	Q2362	V2487		I2687		F2871	
LYS	LYS	P2133	L2231	V2590		K2692		S2875	
VAL	VAL	M2134	Q2234	V2593		K2692		K2876	
SER	SER	P2235	P2235	V2594		M2695		S2876	
ASN	ASN	A2137	L2237	W2595		I2877		I2877	
ILE	ILE	R2140	L2237	T2596		M2699		L2878	
PHE	PHE	R2140	E2372	M2597		F2700		L2879	

- Molecule 2: hemocyanin

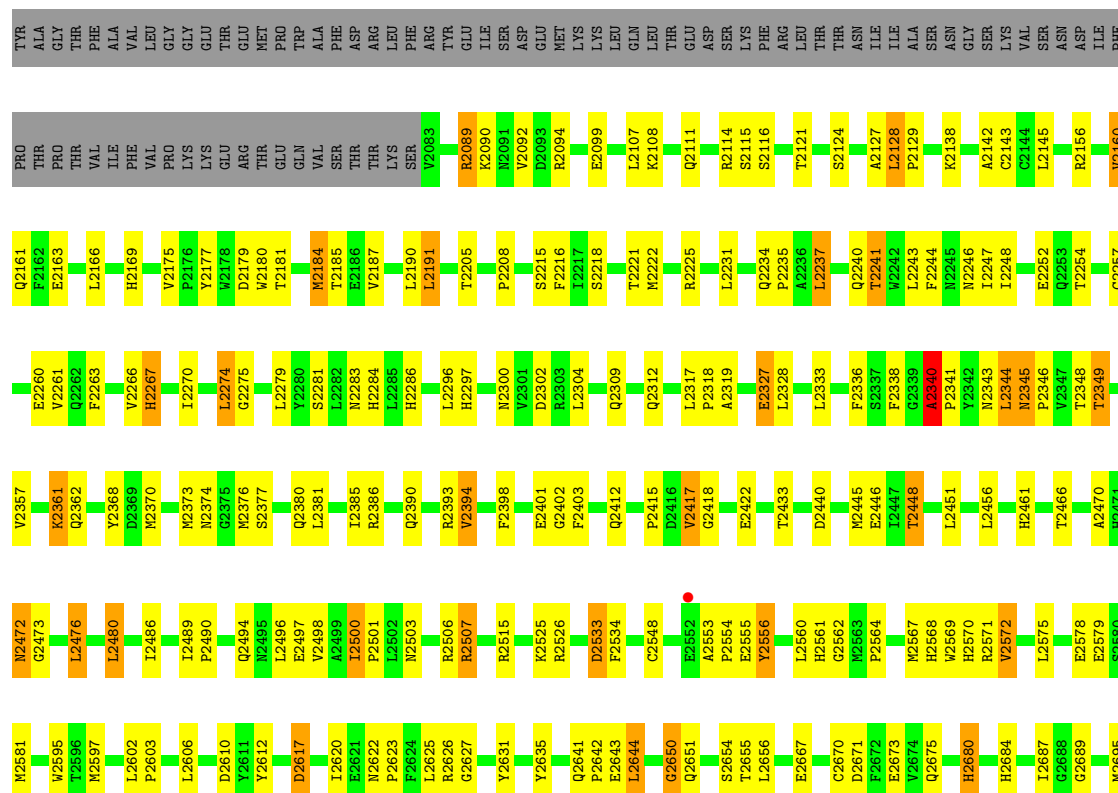
Chain T:  55% 30% 5% 10%

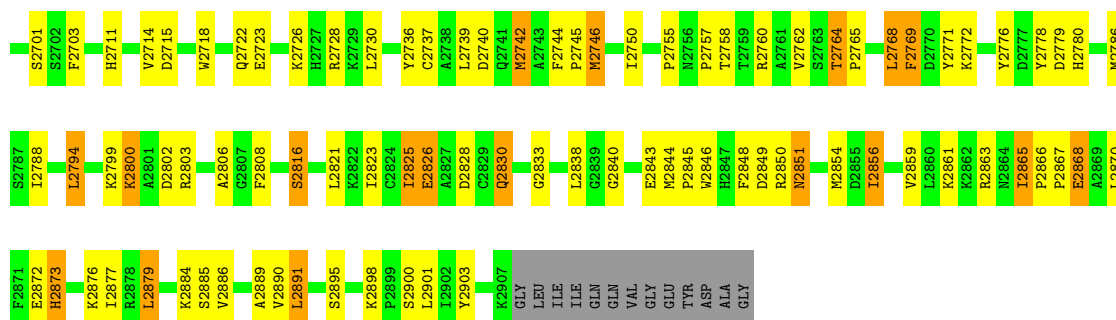
TYR	PRO	C2143	N2207	TYR	PRO	H2141	Q2240	TYR	PRO
ALA	THR	C2144	P2208	ALA	THR	A2142	A2142	ALA	THR
GLY	PRO	L2145	F2208	GLY	PRO	C2143	C2143	GLY	PRO
THR	THR	R2156	S2215	THR	THR	L2145	L2145	THR	THR
ALA	ILE	V2160	F2216	ALA	ILE	R2156	R2156	ALA	ILE
VAL	PHE	Q2161	I2217	VAL	PHE	V2160	V2160	VAL	PHE
LEU	VAL	Q2161	S2218	LEU	VAL	Q2161	Q2161	LEU	VAL
GLY	VAL	F2162	A2235	GLY	VAL	F2162	F2162	GLY	VAL
GLY	LYS	E2163	L2237	GLY	LYS	E2163	E2163	GLY	LYS
THR	GLU	L2166	R2225	THR	GLU	L2166	L2166	THR	GLU
GLU	ARG	R2167	L2231	GLU	ARG	R2167	R2167	GLU	ARG
THR	THR	R2168	F2232	THR	THR	R2168	R2168	THR	THR
PRO	GLU	H2169	Q2234	PRO	GLU	H2169	H2169	PRO	GLU
GLY	GLN	L2172	Q2235	GLY	GLN	L2172	L2172	GLY	GLN
TRP	VAL	V2173	P2235	TRP	VAL	V2173	V2173	TRP	VAL
ALA	SER	C2174	L2237	ALA	SER	C2174	C2174	ALA	SER
PHE	THR	G2176	H2238	PHE	THR	G2176	G2176	PHE	THR
ASP	THR	F2177	K2239	ASP	THR	F2177	F2177	ASP	THR
ARG	LYS	W2178	H2141	ARG	LYS	W2178	W2178	ARG	LYS
LEU	SER	D2180	A2142	LEU	SER	D2180	D2180	LEU	SER
TYR	TYR	T2181		TYR	TYR	T2181		TYR	TYR
GLU	GLU	M2184		GLU	GLU	M2184		GLU	GLU
ILE	ILE	T2185		ILE	ILE	T2185		ILE	ILE
SER	ASP	E2186		SER	ASP	E2186		SER	ASP
GLU	GLU	L2191		GLU	GLU	L2191		GLU	GLU
LYS	LYS	T2201		LYS	LYS	T2201		LYS	LYS
LEU	GLN	G2202		LEU	GLN	G2202		LEU	GLN
THR	THR	I2203		THR	THR	I2203		THR	THR
GLU	ASP	N2207		GLU	ASP	N2207		GLU	ASP
ASP	SER	P2208		ASP	SER	P2208		ASP	SER
SER	LYS	S2215		SER	LYS	S2215		SER	LYS
PHE	PHE	I2210		PHE	PHE	I2210		PHE	PHE
ARG	ARG	Q2111		ARG	ARG	Q2111		ARG	ARG
LEU	LEU	K2112		LEU	LEU	K2112		LEU	LEU
THR	THR	D2113		THR	THR	D2113		THR	THR
ASN	ASN	S2115		ASN	ASN	S2115		ASN	ASN
ILE	ILE	S2116		ILE	ILE	S2116		ILE	ILE
ALA	ALA	D2117		ALA	ALA	D2117		ALA	ALA
SER	SER	A2127		SER	SER	A2127		SER	SER
ASN	ASN	L2128		ASN	ASN	L2128		ASN	ASN
GLY	GLY	P2129		GLY	GLY	P2129		GLY	GLY
LYS	LYS	P2130		LYS	LYS	P2130		LYS	LYS
VAL	VAL	L2131		VAL	VAL	L2131		VAL	VAL
SER	SER	C2132		SER	SER	C2132		SER	SER
ASN	ASN	P2133		ASN	ASN	P2133		ASN	ASN
ASP	ASP	R2140		ASP	ASP	R2140		ASP	ASP
ILE	ILE	H2141		ILE	ILE	H2141		ILE	ILE
PHE	PHE	A2142		PHE	PHE	A2142		PHE	PHE



Chain W:

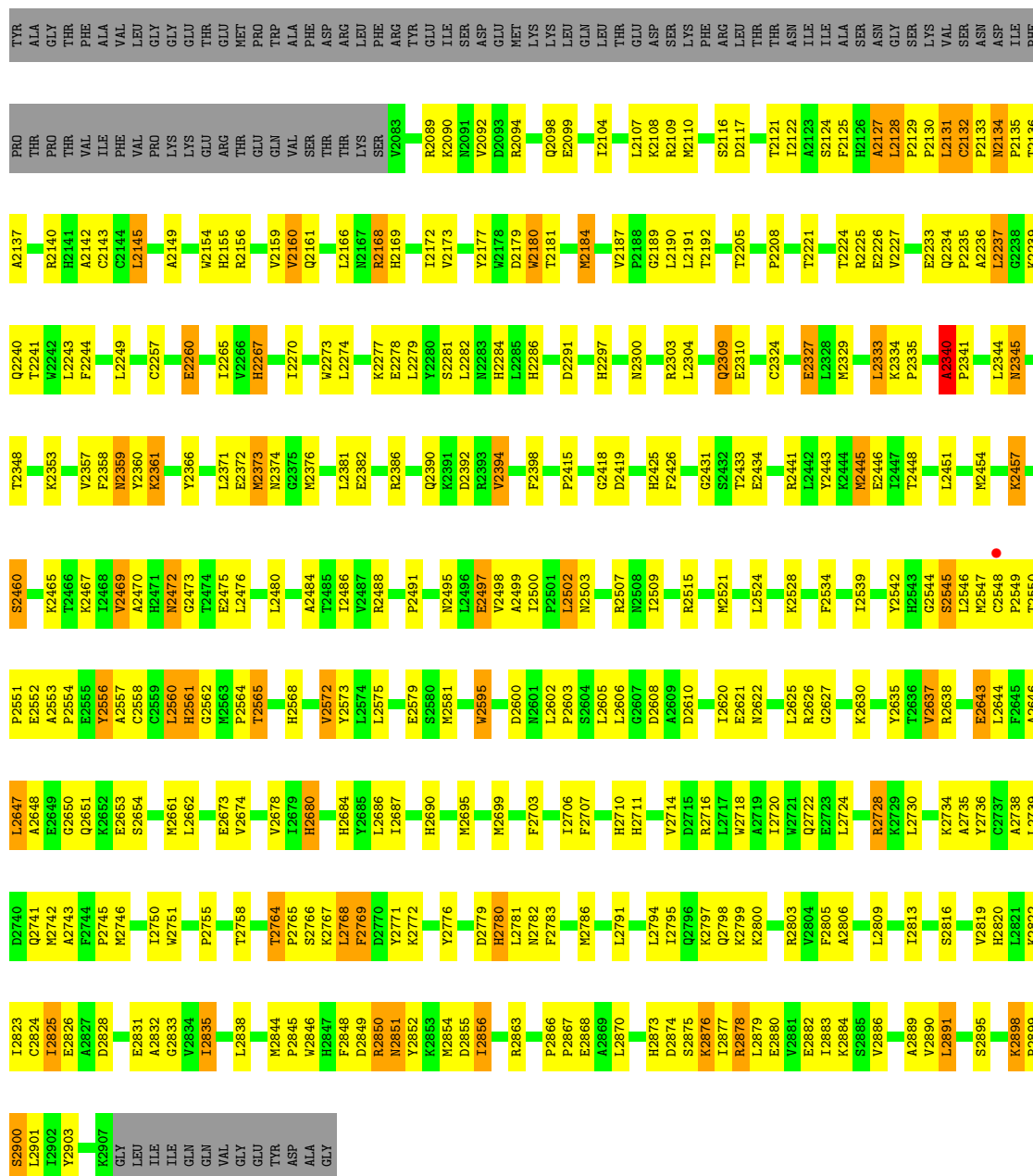
58% 27% 5% 10%





• Molecule 2: hemocyanin

Chain Z: 53% 31% 6% 10%



• Molecule 2: hemocyanin

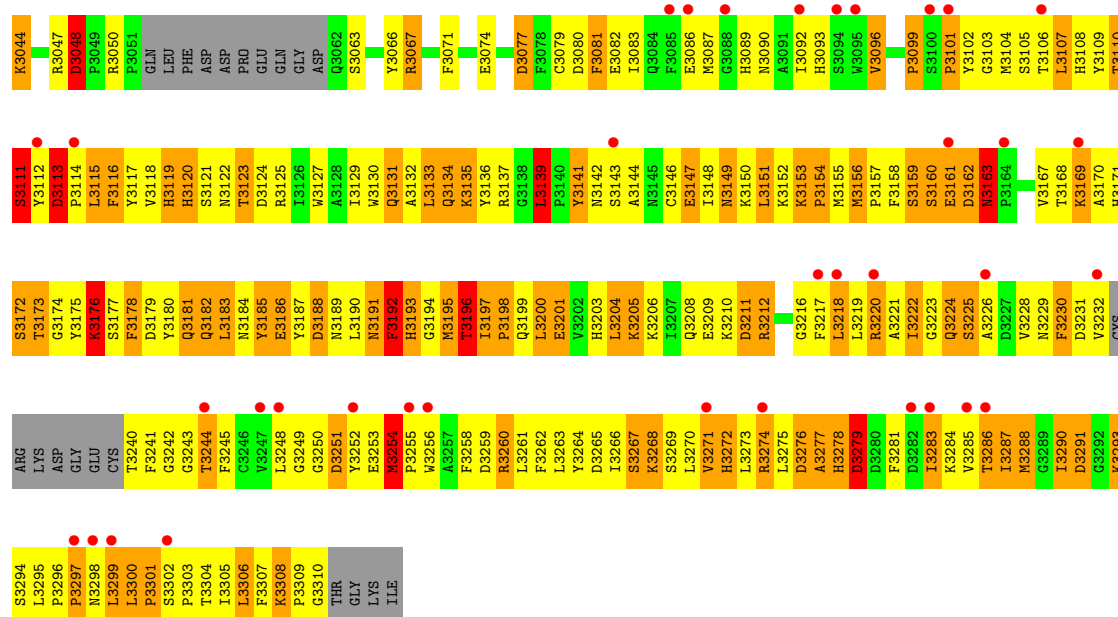
Chain c:  55% 29% 6% 10%

TYR	ALA	GLY	THR	PHE	VAL	LEU	GLY	GLY	GLY	THR	GLU	THR	MET	PRO	TRP	ALA	PHE	ASP	ARG	LEU	PHE	ARG	GLY	ILE	SER	ASP	GLU	MET	LYS	LYS	LEU	GLN	LEU	LEU	THR	GLU	ASP	SER	LYS	PHE	ARG	LEU	THR	THR	ASN	ILE	ILE	ALA	SER	ASN	ASP	ILE	PHE
PRO	THR	THR	THR	VAL	ILE	PHE	VAL	PHO	PHO	LYS	GLY	ARG	THR	THR	GLN	VAL	SER	THR	THR	LYS	SER	V2083	B2069	K2090	L2097	Q2098	E2099	L2107	M2110	Q2111	R2114	S2115	S2116	E2120	T2121	A2123	S2124	A2127	L2128	P2129	L2131	C2132	P2133	R2140	H2141	A2142	C2143	L2145					
A2149	Q2153	V2160	L2166	H2167	H2169	D2179	W2180	M2184	L2185	E2186	V2187	F2188	G2189	L2190	L2191	T2192	I2203	P2208	Q2212	T2221	L2326	E2327	L2333	K2334	F2336	L2344	N2345	T2348	K2361	Y2368	D2369	M2370	L2371	E2372	M2373	N2374	G2375	M2376	L2381	Q2390	I2265	V2266	H2267										
L2400	G2404	S2405	S2406	F2411	G2418	F2426	L2429	G2430	G2431	S2432	L2433	E2434	F2439	Y2443	M2444	E2445	T2447	T2448	L2451	Q2452	H2461	F2462	V2469	A2470	H2471	N2472	G2473	T2474	L2475	L2476	P2477	L2480	I2486	V2487	R2488	L2489	P2490	P2491	N2495	L2496	E2497	V2498	A2499	I2500									
P2501	L2502	N2503	R2504	L2505	R2506	R2507	L2508	L2509	R2515	D2516	V2517	M2521	L2524	L2525	L2539	G2544	S2545	L2546	M2547	C2548	P2549	T2550	E2552	A2553	P2554	E2555	L2556	A2557	C2558	L2560	H2561	G2562	M2563	P2564	T2565	F2566	H2567	H2568	W2569	H2570	R2571	V2572	Y2573	L2574	L2575	E2578	S2579	L2580	H2581	V2590	P2591		
W2595	T2596	M2597	R2598	S2599	L2602	P2603	S2604	L2605	L2606	G2607	D2608	A2609	D2610	V2615	T2616	L2620	E2621	N2622	L2625	R2626	G2627	R2628	L2629	K2630	Y2631	R2638	E2639	T2640	E2643	L2644	F2645	A2646	L2647	A2648	E2649	Q2650	R2651	K2652	E2653	S2654	T2655	L2656	F2657	K2658	M2661	L2662	Y2669	C2670	E2677				
H2680	I2683	H2684	Y2685	L2686	L2687	M2695	H2778	H2780	L2781	N2782	M2786	S2787	L2788	L2791	Q2798	K2799	K2800	A2801	D2802	A2806	G2807	L2808	L2809	L2810	H2811	D2818	L2823	E2826	A2827	D2828	Q2830	L2838	G2839	E2841	W2846	H2847	F2848	R2849	N2851	W2854	D2855	L2856	T2857	D2858									
L2768	F2769	D2770	Y2771	K2772	S2773	L2774	Y2778	H2780	L2781	N2782	M2786	S2787	L2788	L2791	Q2798	K2799	K2800	A2801	D2802	A2806	G2807	L2808	L2809	L2810	H2811	D2818	L2823	E2826	A2827	D2828	Q2830	L2838	G2839	E2841	W2846	H2847	F2848	R2849	N2851	W2854	D2855	L2856	T2857	D2858									
V2859	L2860	K2861	K2862	R2863	N2864	L2865	P2866	P2867	P2868	P2869	D2874	S2875	K2876	L2877	R2878	L2879	E2882	L2883	K2884	S2885	V2886	D2887	G2888	A2889	T2890	L2891	D2892	F2893	N2894	K2898	P2899	S2900	L2901	T2902	Y2903	K2907	GLY	LEU	ILE	ILE	GLN	VAL	GLY	GLY	TYR	ASP	ALA	GLY					

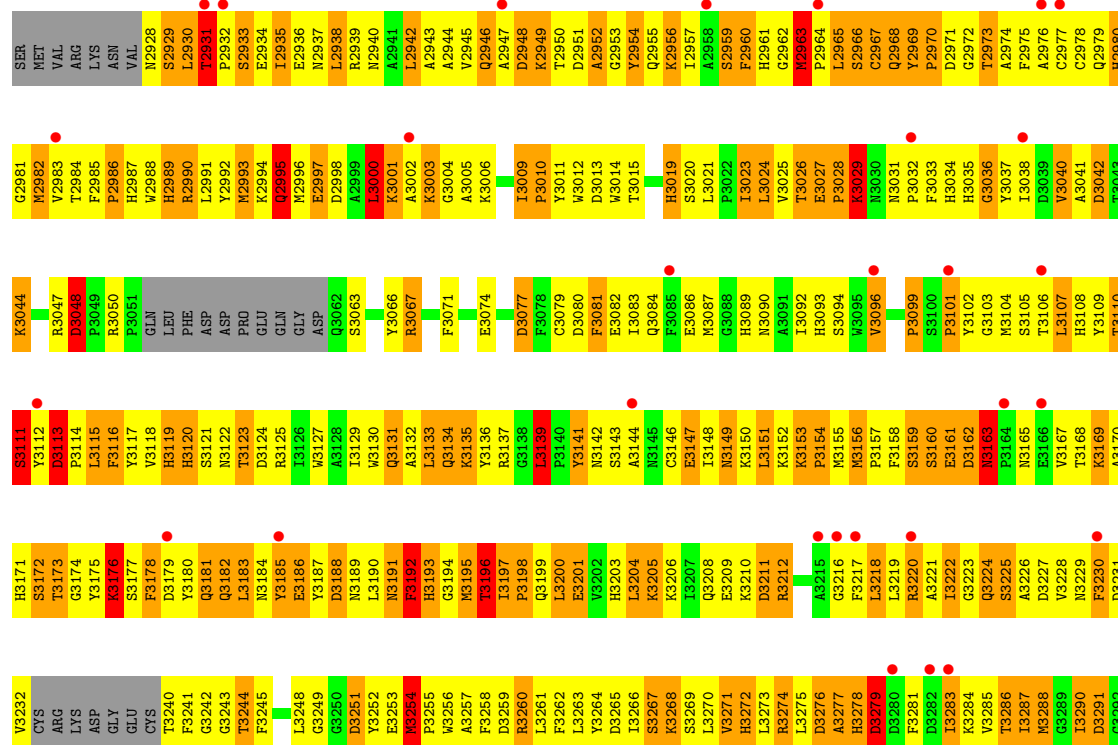
• Molecule 3: hemocyanin

Chain C:  12% 14% 44% 31% 7%

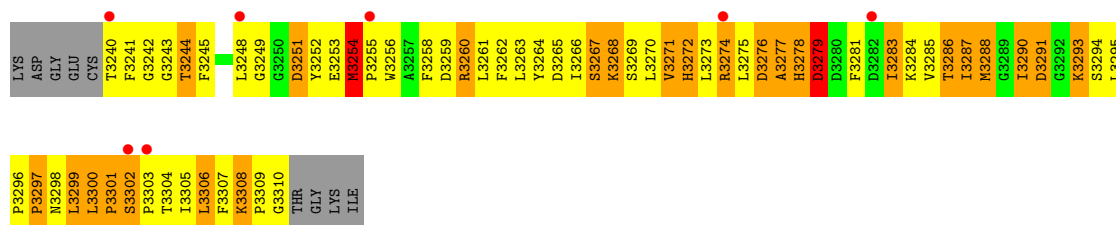
SER	MET	VAL	ARG	LYS	ASN	VAL	N2928	S2929	L2930	T2931	P2932	S2933	E2934	L2935	E2936	L2937	L2938	R2939	N2940	A2941	L2942	A2943	A2944	V2945	Q2946	A2947	D2948	K2949	T2950	L2951	D2952	K2953	W2954	Q2955	K2956	L2957	A2958	S2959	F2960	H2961	G2962	K2963	P2964	L2965	S2966	C2967	Q2968	Y2969	P2970	D2971	G2972	T2973	A2974	F2975	A2976	C2977	C2978	Q2979	H2980
G2981	M2982	V2983	T2984	F2985	P2986	H2987	W2988	H2989	R2990	L2991	Y2992	M2993	K2994	Q2995	E2996	E2997	D2998	A2999	L3000	K3001	A3002	K3003	G3004	A3005	K3006	I3009	P3010	Y3011	K3012	D3013	W3014	T3015	H3019	S3020	L3021	F3022	I3023	L3024	H3025	T3026	E3027	P3028	K3029	N3030	N3031	P3032	F3033	H3034	G3035	T3036	Y3037	I3038	D3039	V3040	A3041	Q3042	T3043		



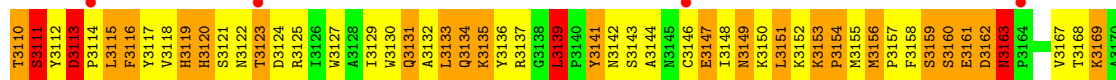
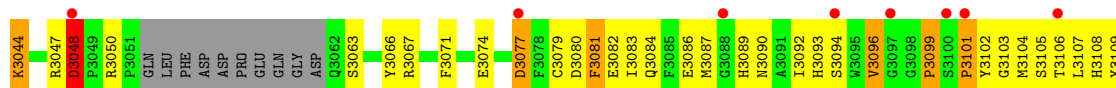
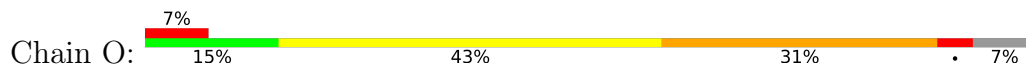
• Molecule 3: hemocyanin



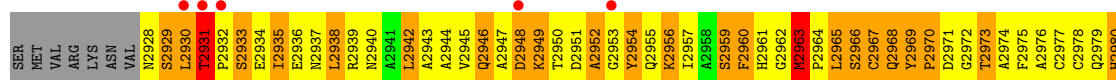
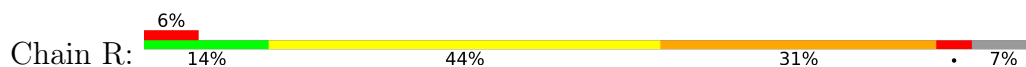
• Molecule 3: hemocyanin

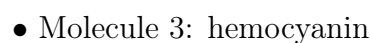


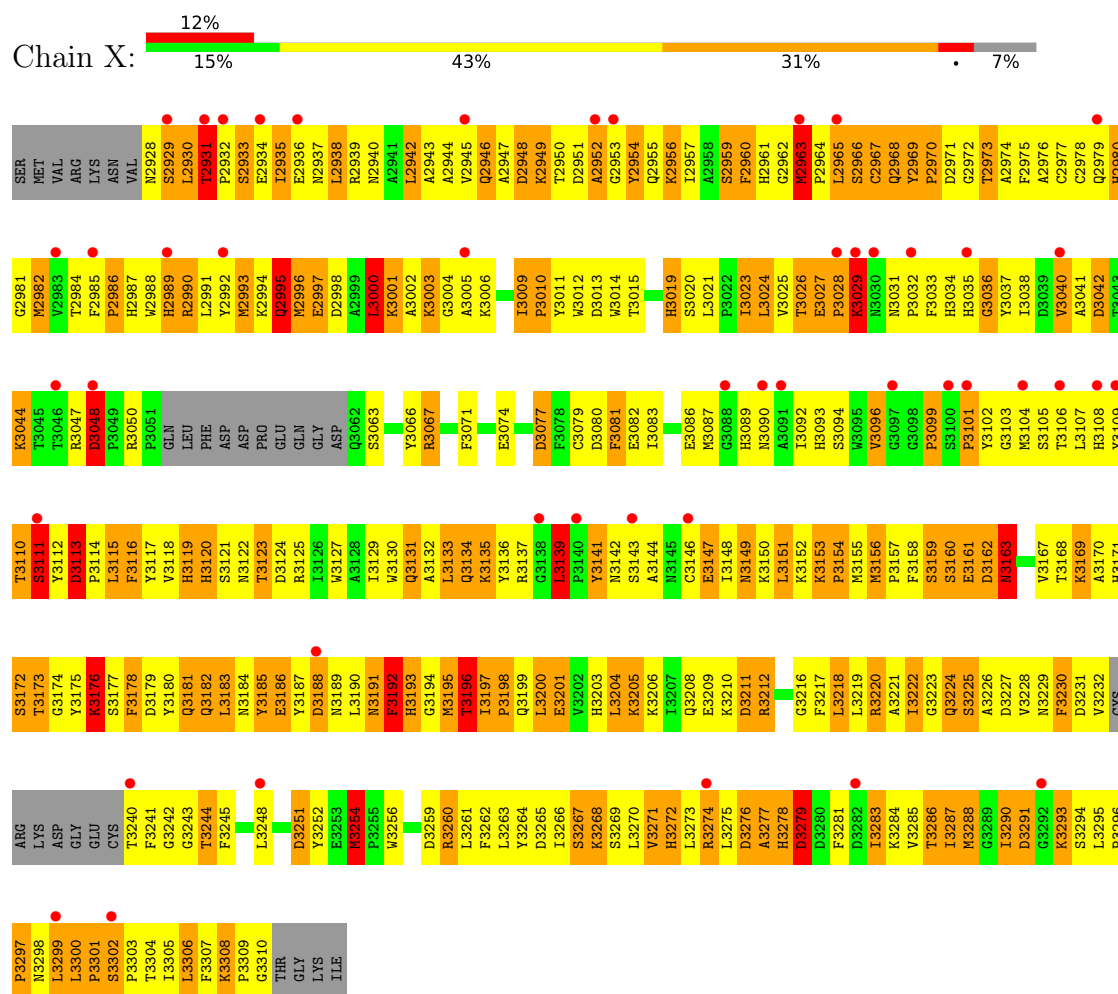
• Molecule 3: hemocyanin



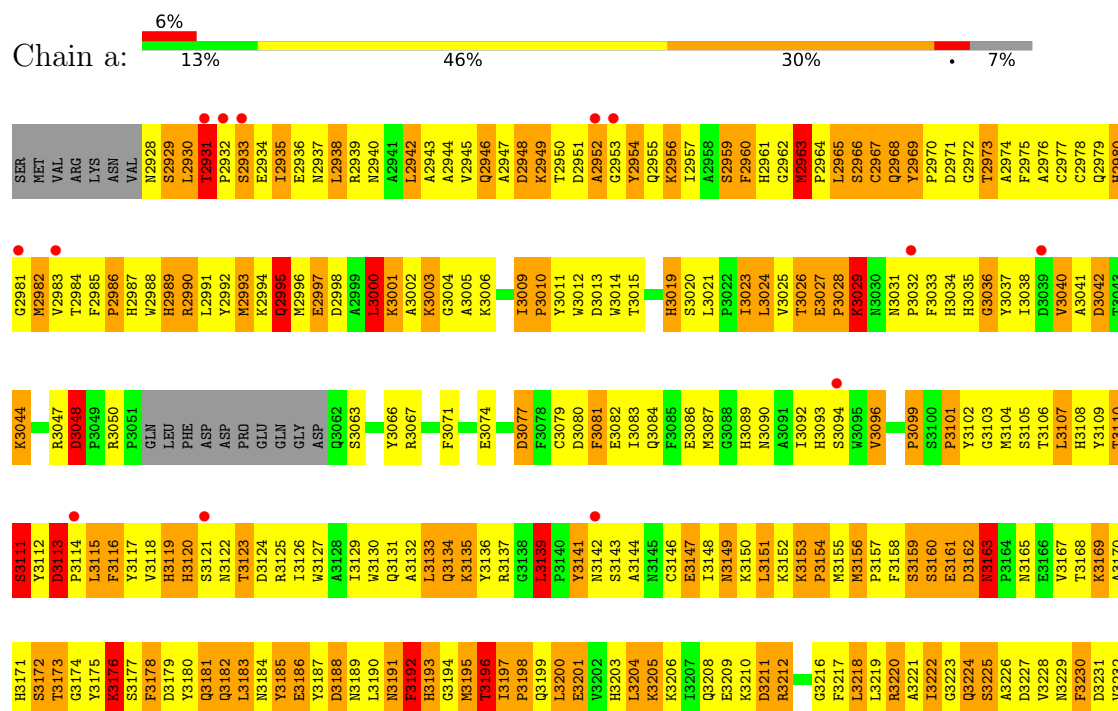
• Molecule 3: hemocyanin

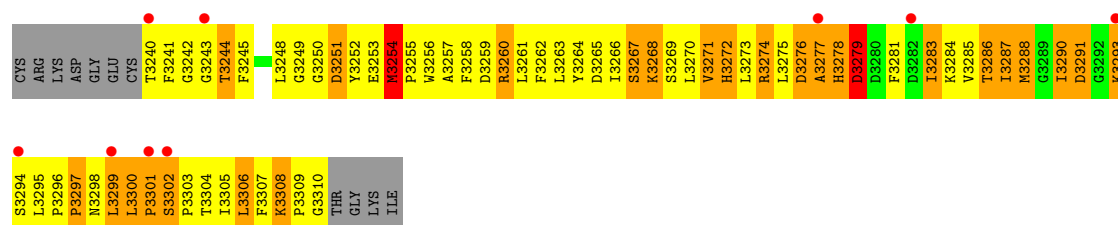




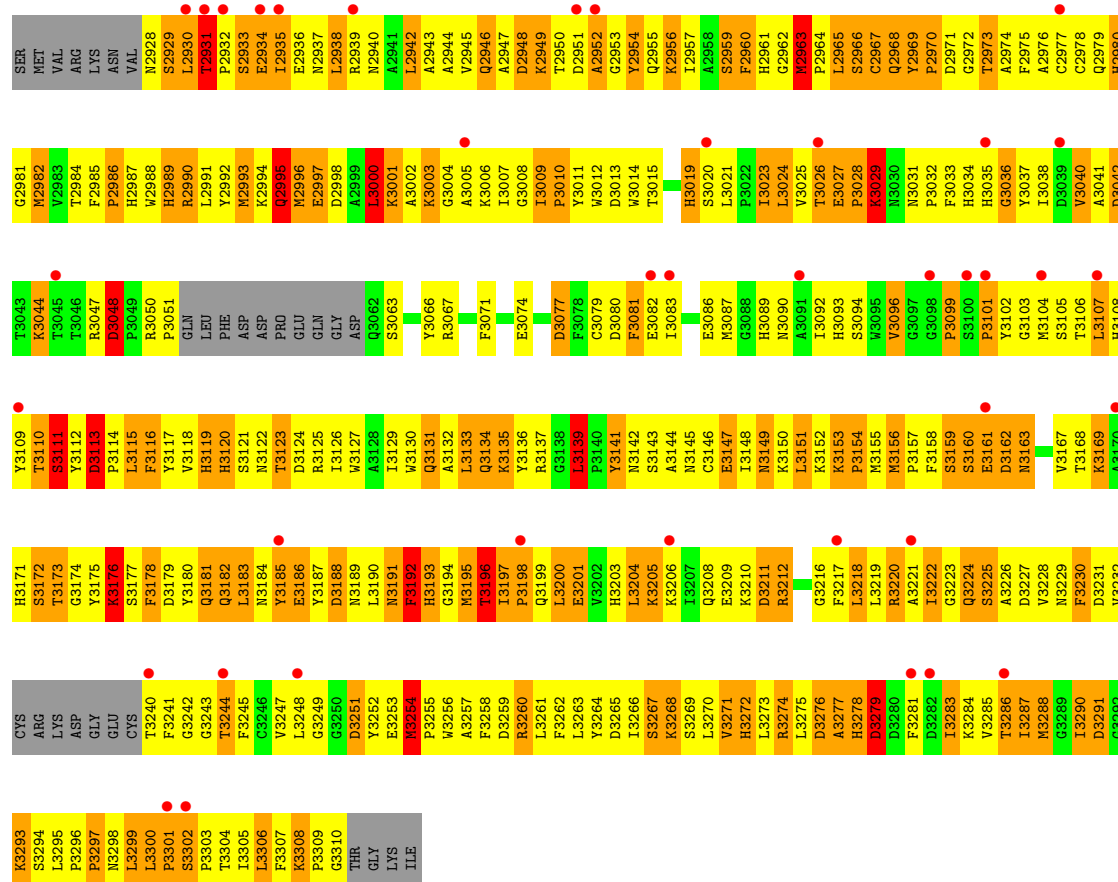


• Molecule 3: hemocyanin





• Molecule 3: hemocyanin



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



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





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

Chain i:  100%



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

Chain j:  100%



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

Chain m:  100%



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

Chain n:  100%



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

Chain o:  50% 50%



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

Chain p:  50% 50%



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

Chain q:  100%

MAG1
MAG2

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

Chain s:  50% 50%

MAG1
MAG2

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

Chain t:  50% 50%

MAG1
MAG2

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

Chain u:  50% 50%

MAG1
MAG2

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

Chain v:  100%

MAG1
MAG2

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

Chain x:  50% 50%

MAG1
MAG2

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

Chain 1:  50% 50%



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

Chain 2:  50% 50%



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

Chain 4:  100%



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

Chain 6:  50% 50%



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

Chain 7:  100%



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

Chain 8:  100%



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

Chain 9:  100%



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

Chain BA:  100%

MAG1
MAG2

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

Chain HA:  50% 50%

MAG1
MAG2

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

Chain IA:  100%

MAG1
MAG2

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

Chain JA:  50% 50%

MAG1
MAG2

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

Chain MA:  100%

MAG1
MAG2

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

Chain OA:  100%

MAG1
MAG2

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

Chain QA:  50% 50%



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



- Molecule 5: 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 5: 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



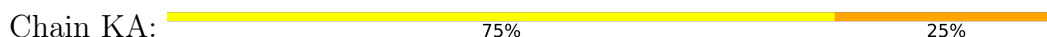
- Molecule 5: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 5: 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 5: 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 5: 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 PA: 



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

Chain h: 

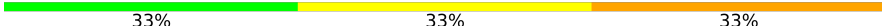


- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain k: 

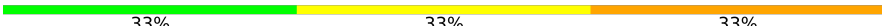


- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain r: 

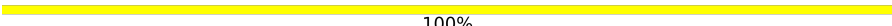


- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain w: 

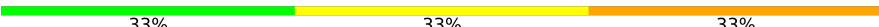


- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain y: 



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

Chain 3: 



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

Chain 5:

100%



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

Chain CA:

33%

67%



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

Chain DA:

33%

67%



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

Chain EA:

33%

33%

33%



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

Chain GA:

33%

67%



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

Chain LA:

33%

67%

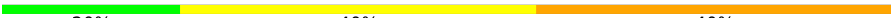


- Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain NA:  67% 33%

MAG1
MAG2
BMA3

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

Chain z:  20% 40% 40%

MAG1
MAG2
BMA3
MAN4
MAN5

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

Chain 0:  25% 75%

MAG1
MAG2
BMA3
MAN4

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	171.37Å 538.66Å 310.92Å 90.00° 104.09° 90.00°	Depositor
Resolution (Å)	49.10 – 3.00 49.10 – 3.00	Depositor EDS
% Data completeness (in resolution range)	98.9 (49.10-3.00) 89.6 (49.10-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.74 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.274 , 0.303 0.275 , 0.304	Depositor DCC
R_{free} test set	53588 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	64.8	Xtriage
Anisotropy	0.538	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 48.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	0.055 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	261470	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.47% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.37	0/13698	0.89	40/18607 (0.2%)
1	D	0.37	0/13698	0.89	21/18607 (0.1%)
1	G	0.37	1/13698 (0.0%)	0.86	27/18607 (0.1%)
1	J	0.37	0/13698	0.87	22/18607 (0.1%)
1	M	0.35	0/13698	0.87	32/18607 (0.2%)
1	P	0.36	1/13698 (0.0%)	0.86	34/18607 (0.2%)
1	S	0.36	0/13698	0.86	32/18607 (0.2%)
1	V	0.36	0/13698	0.85	33/18607 (0.2%)
1	Y	0.34	0/13698	0.84	21/18607 (0.1%)
1	b	0.35	0/13698	0.87	26/18607 (0.1%)
2	B	0.34	0/6909	0.85	12/9383 (0.1%)
2	E	0.35	0/6909	0.87	17/9383 (0.2%)
2	H	0.35	0/6909	0.84	14/9383 (0.1%)
2	K	0.35	0/6909	0.85	13/9383 (0.1%)
2	N	0.35	0/6909	0.84	9/9383 (0.1%)
2	Q	0.34	0/6909	0.83	11/9383 (0.1%)
2	T	0.34	0/6909	0.82	9/9383 (0.1%)
2	W	0.33	0/6909	0.84	18/9383 (0.2%)
2	Z	0.33	0/6909	0.84	13/9383 (0.1%)
2	c	0.33	0/6909	0.82	9/9383 (0.1%)
3	C	1.08	36/6100 (0.6%)	1.39	120/8282 (1.4%)
3	F	1.08	36/6100 (0.6%)	1.40	120/8282 (1.4%)
3	I	1.08	34/6100 (0.6%)	1.40	120/8282 (1.4%)
3	L	1.08	36/6100 (0.6%)	1.39	120/8282 (1.4%)
3	O	1.08	36/6100 (0.6%)	1.39	120/8282 (1.4%)
3	R	1.08	36/6100 (0.6%)	1.40	120/8282 (1.4%)
3	U	1.08	36/6100 (0.6%)	1.40	122/8282 (1.5%)
3	X	1.08	38/6100 (0.6%)	1.40	116/8282 (1.4%)
3	a	1.08	34/6100 (0.6%)	1.39	120/8282 (1.4%)
3	d	1.08	38/6100 (0.6%)	1.40	122/8282 (1.5%)
All	All	0.60	362/267070 (0.1%)	1.01	1613/362720 (0.4%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	D	0	3
1	G	0	1
1	J	0	2
1	M	0	1
1	S	0	3
1	Y	0	1
1	b	0	2
2	B	0	1
2	K	0	3
2	N	0	1
2	Q	0	1
2	T	0	2
2	W	0	1
2	Z	0	2
2	c	0	1
3	C	0	4
3	F	0	4
3	I	0	4
3	L	0	4
3	O	0	4
3	R	0	4
3	U	0	4
3	X	0	4
3	a	0	4
3	d	0	4
All	All	0	67

The worst 5 of 362 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	a	3296[A]	PRO	C-N	6.78	1.41	1.33
3	a	3296[B]	PRO	C-N	6.78	1.41	1.33
3	O	3296[A]	PRO	C-N	6.77	1.41	1.33
3	O	3296[B]	PRO	C-N	6.77	1.41	1.33
3	L	3296[A]	PRO	C-N	6.76	1.41	1.33

The worst 5 of 1613 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	464	LEU	CA-C-N	-16.02	99.82	119.84
1	D	464	LEU	C-N-CA	-16.02	99.82	119.84
1	J	883	CYS	CA-C-N	-12.76	103.89	119.84
1	J	883	CYS	C-N-CA	-12.76	103.89	119.84
1	b	464	LEU	CA-C-N	-12.27	104.50	119.84

There are no chirality outliers.

5 of 67 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	464	LEU	Peptide
1	A	982	LYS	Peptide
2	B	2127	ALA	Peptide
3	C	3113[A]	ASP	Mainchain
3	C	3113[B]	ASP	Mainchain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	13318	0	12755	476	1
1	D	13318	0	12755	482	0
1	G	13318	0	12754	503	0
1	J	13318	0	12755	508	0
1	M	13318	0	12755	448	0
1	P	13318	0	12755	450	0
1	S	13318	0	12755	451	0
1	V	13318	0	12755	448	0
1	Y	13318	0	12744	528	0
1	b	13318	0	12754	452	1
2	B	6704	0	6445	213	0
2	E	6704	0	6445	245	0
2	H	6704	0	6445	243	0
2	K	6704	0	6445	218	0
2	N	6704	0	6445	203	0
2	Q	6704	0	6445	218	0
2	T	6704	0	6445	221	0
2	W	6704	0	6445	226	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	Z	6704	0	6444	238	0
2	c	6704	0	6445	224	0
3	C	5912	0	5607	2341	0
3	F	5912	0	5599	2386	0
3	I	5912	0	5601	2460	0
3	L	5912	0	5604	2354	0
3	O	5912	0	5604	2061	0
3	R	5912	0	5598	2438	0
3	U	5912	0	5612	2074	0
3	X	5912	0	5598	2059	0
3	a	5912	0	5594	2398	0
3	d	5912	0	5608	2177	0
4	1	28	0	25	1	0
4	2	28	0	25	1	0
4	4	28	0	25	0	0
4	6	28	0	25	2	0
4	7	28	0	25	6	0
4	8	28	0	25	0	0
4	9	28	0	25	2	0
4	BA	28	0	25	5	0
4	HA	28	0	25	6	0
4	IA	28	0	25	0	0
4	JA	28	0	25	2	0
4	MA	28	0	25	9	0
4	OA	28	0	25	2	0
4	QA	28	0	25	4	0
4	RA	28	0	25	1	0
4	e	28	0	25	0	0
4	f	28	0	25	2	0
4	i	28	0	25	3	0
4	j	28	0	25	4	0
4	m	28	0	25	9	0
4	n	28	0	25	1	0
4	o	28	0	25	3	0
4	p	28	0	25	0	0
4	q	28	0	25	7	0
4	s	28	0	25	2	0
4	t	28	0	25	1	0
4	u	28	0	25	6	0
4	v	28	0	25	2	0
4	x	28	0	25	0	0
5	AA	50	0	43	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	FA	50	0	43	2	0
5	KA	50	0	43	1	0
5	PA	50	0	43	1	0
5	g	50	0	43	0	0
5	l	50	0	43	2	0
6	3	39	0	34	3	0
6	5	39	0	34	2	0
6	CA	39	0	34	3	0
6	DA	39	0	34	2	0
6	EA	39	0	34	1	0
6	GA	39	0	34	9	0
6	LA	39	0	34	5	0
6	NA	39	0	34	3	0
6	h	39	0	34	1	0
6	k	39	0	34	4	0
6	r	39	0	34	8	0
6	w	39	0	34	2	0
6	y	39	0	34	0	0
7	z	61	0	52	2	0
8	0	50	0	43	8	0
9	A	24	0	0	2	0
9	B	8	0	0	0	0
9	C	8	0	0	7	0
9	D	24	0	0	2	0
9	E	8	0	0	0	0
9	F	8	0	0	7	0
9	G	24	0	0	1	0
9	H	8	0	0	0	0
9	I	8	0	0	6	0
9	J	24	0	0	2	0
9	K	8	0	0	0	0
9	L	8	0	0	7	0
9	M	24	0	0	3	0
9	N	8	0	0	0	0
9	O	8	0	0	10	0
9	P	24	0	0	0	0
9	Q	8	0	0	0	0
9	R	8	0	0	6	0
9	S	24	0	0	3	0
9	T	8	0	0	1	0
9	U	8	0	0	10	0
9	V	24	0	0	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	W	8	0	0	1	0
9	X	8	0	0	10	0
9	Y	24	0	0	3	0
9	Z	8	0	0	0	0
9	a	8	0	0	7	0
9	b	24	0	0	1	0
9	c	8	0	0	0	0
9	d	8	0	0	10	0
All	All	261470	0	249531	25303	1

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 50.

The worst 5 of 25303 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:2975[B]:PHE:CD1	3:a:3107[B]:LEU:HD11	1.20	1.69
3:F:2969[B]:TYR:HD1	3:a:2961[B]:HIS:CG	1.09	1.68
3:C:3079[B]:CYS:CB	3:L:3161[B]:GLU:HG2	1.22	1.65
3:C:2982[B]:MET:SD	3:L:3156[B]:MET:HB2	1.37	1.64
3:F:2970[B]:PRO:HD3	3:a:2989[B]:HIS:CD2	1.23	1.64

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1:ASN:N	1:b:887:ASP:OD1[1_455]	2.19	0.01

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1654/2000 (83%)	1552 (94%)	89 (5%)	13 (1%)	16	50
1	D	1654/2000 (83%)	1541 (93%)	100 (6%)	13 (1%)	16	50
1	G	1654/2000 (83%)	1560 (94%)	78 (5%)	16 (1%)	12	45
1	J	1654/2000 (83%)	1537 (93%)	103 (6%)	14 (1%)	16	50
1	M	1654/2000 (83%)	1569 (95%)	73 (4%)	12 (1%)	18	53
1	P	1654/2000 (83%)	1562 (94%)	78 (5%)	14 (1%)	16	50
1	S	1654/2000 (83%)	1581 (96%)	64 (4%)	9 (0%)	24	60
1	V	1654/2000 (83%)	1570 (95%)	68 (4%)	16 (1%)	12	45
1	Y	1654/2000 (83%)	1580 (96%)	66 (4%)	8 (0%)	24	60
1	b	1654/2000 (83%)	1564 (95%)	80 (5%)	10 (1%)	21	56
2	B	823/920 (90%)	778 (94%)	40 (5%)	5 (1%)	21	56
2	E	823/920 (90%)	781 (95%)	34 (4%)	8 (1%)	12	45
2	H	823/920 (90%)	787 (96%)	33 (4%)	3 (0%)	30	65
2	K	823/920 (90%)	778 (94%)	37 (4%)	8 (1%)	12	45
2	N	823/920 (90%)	789 (96%)	32 (4%)	2 (0%)	43	76
2	Q	823/920 (90%)	787 (96%)	32 (4%)	4 (0%)	24	60
2	T	823/920 (90%)	794 (96%)	22 (3%)	7 (1%)	14	48
2	W	823/920 (90%)	791 (96%)	28 (3%)	4 (0%)	24	60
2	Z	823/920 (90%)	797 (97%)	23 (3%)	3 (0%)	30	65
2	c	823/920 (90%)	791 (96%)	29 (4%)	3 (0%)	30	65
3	C	720/394 (183%)	666 (92%)	48 (7%)	6 (1%)	16	50
3	F	720/394 (183%)	666 (92%)	48 (7%)	6 (1%)	16	50
3	I	720/394 (183%)	666 (92%)	48 (7%)	6 (1%)	16	50
3	L	720/394 (183%)	666 (92%)	48 (7%)	6 (1%)	16	50
3	O	720/394 (183%)	666 (92%)	48 (7%)	6 (1%)	16	50
3	R	720/394 (183%)	666 (92%)	48 (7%)	6 (1%)	16	50
3	U	720/394 (183%)	666 (92%)	48 (7%)	6 (1%)	16	50
3	X	720/394 (183%)	666 (92%)	48 (7%)	6 (1%)	16	50
3	a	720/394 (183%)	666 (92%)	48 (7%)	6 (1%)	16	50
3	d	720/394 (183%)	666 (92%)	48 (7%)	6 (1%)	16	50
All	All	31970/33140 (96%)	30149 (94%)	1589 (5%)	232 (1%)	18	53

5 of 232 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1196	ILE
1	D	695	TYR
1	D	1196	ILE
1	G	331	SER
1	G	1086	LEU

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 X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1429/1738 (82%)	1263 (88%)	166 (12%)	5	23
1	D	1429/1738 (82%)	1249 (87%)	180 (13%)	4	20
1	G	1429/1738 (82%)	1242 (87%)	187 (13%)	4	19
1	J	1429/1738 (82%)	1246 (87%)	183 (13%)	4	19
1	M	1429/1738 (82%)	1269 (89%)	160 (11%)	6	24
1	P	1429/1738 (82%)	1245 (87%)	184 (13%)	4	19
1	S	1429/1738 (82%)	1241 (87%)	188 (13%)	4	18
1	V	1429/1738 (82%)	1249 (87%)	180 (13%)	4	20
1	Y	1429/1738 (82%)	1243 (87%)	186 (13%)	4	19
1	b	1429/1738 (82%)	1265 (88%)	164 (12%)	5	24
2	B	731/814 (90%)	654 (90%)	77 (10%)	6	27
2	E	731/814 (90%)	651 (89%)	80 (11%)	6	26
2	H	731/814 (90%)	631 (86%)	100 (14%)	3	17
2	K	731/814 (90%)	649 (89%)	82 (11%)	6	24
2	N	731/814 (90%)	646 (88%)	85 (12%)	5	23
2	Q	731/814 (90%)	650 (89%)	81 (11%)	6	25
2	T	731/814 (90%)	653 (89%)	78 (11%)	6	26
2	W	731/814 (90%)	655 (90%)	76 (10%)	7	28
2	Z	731/814 (90%)	639 (87%)	92 (13%)	4	20
2	c	731/814 (90%)	641 (88%)	90 (12%)	4	21

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	636/343 (185%)	412 (65%)	224 (35%)	0	1
3	F	636/343 (185%)	412 (65%)	224 (35%)	0	1
3	I	636/343 (185%)	410 (64%)	226 (36%)	0	1
3	L	636/343 (185%)	412 (65%)	224 (35%)	0	1
3	O	636/343 (185%)	412 (65%)	224 (35%)	0	1
3	R	636/343 (185%)	412 (65%)	224 (35%)	0	1
3	U	636/343 (185%)	412 (65%)	224 (35%)	0	1
3	X	636/343 (185%)	412 (65%)	224 (35%)	0	1
3	a	636/343 (185%)	412 (65%)	224 (35%)	0	1
3	d	636/343 (185%)	412 (65%)	224 (35%)	0	1
All	All	27960/28950 (97%)	23099 (83%)	4861 (17%)	3	10

5 of 4861 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	X	3001[A]	LYS
2	c	2548	CYS
3	X	3205[B]	LYS
3	X	2997[A]	GLU
3	a	2929[B]	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 420 such sidechains are listed below:

Mol	Chain	Res	Type
1	P	897	HIS
2	T	2741	GLN
1	b	1394	GLN
1	P	1280	GLN
1	S	562	GLN

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 ⓘ

130 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	$\# Z > 2$
8	NAG	0	1	8,1	14,14,15	0.75	1 (7%)	17,19,21	1.50	2 (11%)
8	NAG	0	2	8	14,14,15	0.53	0	17,19,21	1.52	4 (23%)
8	BMA	0	3	8	11,11,12	0.23	0	15,15,17	1.75	3 (20%)
8	MAN	0	4	8	11,11,12	0.31	0	15,15,17	0.83	1 (6%)
4	NAG	1	1	4,1	14,14,15	0.45	0	17,19,21	1.00	1 (5%)
4	NAG	1	2	4	14,14,15	0.44	0	17,19,21	1.15	2 (11%)
4	NAG	2	1	2,4	14,14,15	1.14	1 (7%)	17,19,21	1.42	2 (11%)
4	NAG	2	2	4	14,14,15	0.33	0	17,19,21	0.69	0
6	NAG	3	1	6,1	14,14,15	1.04	1 (7%)	17,19,21	1.44	2 (11%)
6	NAG	3	2	6	14,14,15	0.42	0	17,19,21	0.76	0
6	BMA	3	3	6	11,11,12	0.25	0	15,15,17	0.55	0
4	NAG	4	1	4,1	14,14,15	0.77	1 (7%)	17,19,21	1.25	2 (11%)
4	NAG	4	2	4	14,14,15	0.41	0	17,19,21	1.17	3 (17%)
6	NAG	5	1	6,1	14,14,15	0.74	0	17,19,21	1.28	1 (5%)
6	NAG	5	2	6	14,14,15	0.30	0	17,19,21	1.03	1 (5%)
6	BMA	5	3	6	11,11,12	0.27	0	15,15,17	1.24	2 (13%)
4	NAG	6	1	4,1	14,14,15	0.97	1 (7%)	17,19,21	1.95	2 (11%)
4	NAG	6	2	4	14,14,15	0.43	0	17,19,21	1.15	2 (11%)
4	NAG	7	1	2,4	14,14,15	0.86	1 (7%)	17,19,21	1.46	2 (11%)
4	NAG	7	2	4	14,14,15	0.43	0	17,19,21	1.08	2 (11%)
4	NAG	8	1	4,1	14,14,15	1.00	1 (7%)	17,19,21	1.88	2 (11%)
4	NAG	8	2	4	14,14,15	0.40	0	17,19,21	0.70	1 (5%)
4	NAG	9	1	4,1	14,14,15	0.96	1 (7%)	17,19,21	1.35	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	9	2	4	14,14,15	0.28	0	17,19,21	0.77	1 (5%)
5	NAG	AA	1	5,1	14,14,15	0.69	0	17,19,21	1.18	3 (17%)
5	NAG	AA	2	5	14,14,15	0.42	0	17,19,21	0.89	1 (5%)
5	BMA	AA	3	5	11,11,12	0.29	0	15,15,17	1.74	3 (20%)
5	MAN	AA	4	5	11,11,12	0.23	0	15,15,17	0.43	0
4	NAG	BA	1	4,1	14,14,15	0.75	1 (7%)	17,19,21	1.34	2 (11%)
4	NAG	BA	2	4	14,14,15	0.57	0	17,19,21	1.12	1 (5%)
6	NAG	CA	1	2,6	14,14,15	1.12	1 (7%)	17,19,21	1.55	2 (11%)
6	NAG	CA	2	6	14,14,15	0.33	0	17,19,21	0.95	1 (5%)
6	BMA	CA	3	6	11,11,12	0.22	0	15,15,17	0.56	0
6	NAG	DA	1	6,1	14,14,15	0.80	1 (7%)	17,19,21	1.17	1 (5%)
6	NAG	DA	2	6	14,14,15	0.31	0	17,19,21	1.22	2 (11%)
6	BMA	DA	3	6	11,11,12	0.25	0	15,15,17	0.88	1 (6%)
6	NAG	EA	1	6,1	14,14,15	0.84	1 (7%)	17,19,21	1.37	2 (11%)
6	NAG	EA	2	6	14,14,15	0.36	0	17,19,21	2.22	4 (23%)
6	BMA	EA	3	6	11,11,12	0.22	0	15,15,17	0.70	0
5	NAG	FA	1	5,1	14,14,15	0.82	1 (7%)	17,19,21	1.37	2 (11%)
5	NAG	FA	2	5	14,14,15	0.50	0	17,19,21	0.91	1 (5%)
5	BMA	FA	3	5	11,11,12	0.59	0	15,15,17	1.26	2 (13%)
5	MAN	FA	4	5	11,11,12	0.21	0	15,15,17	1.09	1 (6%)
6	NAG	GA	1	6,1	14,14,15	0.75	1 (7%)	17,19,21	1.33	1 (5%)
6	NAG	GA	2	6	14,14,15	0.43	0	17,19,21	1.15	2 (11%)
6	BMA	GA	3	6	11,11,12	0.31	0	15,15,17	0.86	0
4	NAG	HA	1	2,4	14,14,15	0.72	1 (7%)	17,19,21	1.20	1 (5%)
4	NAG	HA	2	4	14,14,15	0.31	0	17,19,21	0.57	0
4	NAG	IA	1	4,1	14,14,15	0.85	1 (7%)	17,19,21	1.52	2 (11%)
4	NAG	IA	2	4	14,14,15	0.54	0	17,19,21	0.93	1 (5%)
4	NAG	JA	1	4,1	14,14,15	0.85	1 (7%)	17,19,21	1.24	1 (5%)
4	NAG	JA	2	4	14,14,15	0.35	0	17,19,21	0.77	0
5	NAG	KA	1	5,1	14,14,15	0.75	0	17,19,21	1.88	5 (29%)
5	NAG	KA	2	5	14,14,15	0.38	0	17,19,21	1.31	2 (11%)
5	BMA	KA	3	5	11,11,12	0.29	0	15,15,17	1.29	1 (6%)
5	MAN	KA	4	5	11,11,12	0.41	0	15,15,17	1.70	2 (13%)
6	NAG	LA	1	6,1	14,14,15	1.06	1 (7%)	17,19,21	2.37	4 (23%)
6	NAG	LA	2	6	14,14,15	0.46	0	17,19,21	1.15	2 (11%)
6	BMA	LA	3	6	11,11,12	0.21	0	15,15,17	0.64	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	MA	1	2,4	14,14,15	1.06	1 (7%)	17,19,21	2.42	3 (17%)
4	NAG	MA	2	4	14,14,15	0.33	0	17,19,21	1.73	3 (17%)
6	NAG	NA	1	6,1	14,14,15	0.76	1 (7%)	17,19,21	1.01	1 (5%)
6	NAG	NA	2	6	14,14,15	0.37	0	17,19,21	0.84	0
6	BMA	NA	3	6	11,11,12	0.24	0	15,15,17	0.86	1 (6%)
4	NAG	OA	1	4,1	14,14,15	1.27	1 (7%)	17,19,21	1.60	2 (11%)
4	NAG	OA	2	4	14,14,15	0.54	0	17,19,21	0.99	1 (5%)
5	NAG	PA	1	5,1	14,14,15	0.67	0	17,19,21	1.14	1 (5%)
5	NAG	PA	2	5	14,14,15	0.37	0	17,19,21	0.94	1 (5%)
5	BMA	PA	3	5	11,11,12	0.60	0	15,15,17	2.08	4 (26%)
5	MAN	PA	4	5	11,11,12	0.26	0	15,15,17	0.74	0
4	NAG	QA	1	4,1	14,14,15	0.57	0	17,19,21	2.46	5 (29%)
4	NAG	QA	2	4	14,14,15	0.24	0	17,19,21	0.68	0
4	NAG	RA	1	2,4	14,14,15	1.22	1 (7%)	17,19,21	2.17	2 (11%)
4	NAG	RA	2	4	14,14,15	0.45	0	17,19,21	0.72	0
4	NAG	e	1	4,1	14,14,15	0.64	0	17,19,21	1.68	4 (23%)
4	NAG	e	2	4	14,14,15	0.34	0	17,19,21	0.49	0
4	NAG	f	1	4,1	14,14,15	0.97	1 (7%)	17,19,21	1.43	2 (11%)
4	NAG	f	2	4	14,14,15	0.25	0	17,19,21	1.00	1 (5%)
5	NAG	g	1	5,1	14,14,15	0.61	0	17,19,21	1.53	2 (11%)
5	NAG	g	2	5	14,14,15	0.52	0	17,19,21	1.04	0
5	BMA	g	3	5	11,11,12	0.47	0	15,15,17	1.99	4 (26%)
5	MAN	g	4	5	11,11,12	0.24	0	15,15,17	0.57	0
6	NAG	h	1	6,1	14,14,15	0.66	0	17,19,21	1.15	3 (17%)
6	NAG	h	2	6	14,14,15	0.57	0	17,19,21	1.10	1 (5%)
6	BMA	h	3	6	11,11,12	0.25	0	15,15,17	1.02	2 (13%)
4	NAG	i	1	2,4	14,14,15	1.15	1 (7%)	17,19,21	1.23	2 (11%)
4	NAG	i	2	4	14,14,15	0.44	0	17,19,21	0.88	1 (5%)
4	NAG	j	1	4,1	14,14,15	1.08	1 (7%)	17,19,21	1.66	2 (11%)
4	NAG	j	2	4	14,14,15	0.50	0	17,19,21	1.35	3 (17%)
6	NAG	k	1	6,1	14,14,15	0.85	1 (7%)	17,19,21	1.11	1 (5%)
6	NAG	k	2	6	14,14,15	0.28	0	17,19,21	0.67	1 (5%)
6	BMA	k	3	6	11,11,12	0.25	0	15,15,17	0.44	0
5	NAG	l	1	5,1	14,14,15	0.69	0	17,19,21	1.21	1 (5%)
5	NAG	l	2	5	14,14,15	0.27	0	17,19,21	0.58	0
5	BMA	l	3	5	11,11,12	0.27	0	15,15,17	0.72	0
5	MAN	l	4	5	11,11,12	0.27	0	15,15,17	0.85	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	m	1	4,1	14,14,15	0.39	0	17,19,21	0.93	1 (5%)
4	NAG	m	2	4	14,14,15	0.37	0	17,19,21	0.88	1 (5%)
4	NAG	n	1	2,4	14,14,15	0.52	0	17,19,21	1.59	3 (17%)
4	NAG	n	2	4	14,14,15	0.39	0	17,19,21	0.99	1 (5%)
4	NAG	o	1	4,1	14,14,15	0.61	0	17,19,21	1.02	1 (5%)
4	NAG	o	2	4	14,14,15	0.45	0	17,19,21	1.06	1 (5%)
4	NAG	p	1	4	14,14,15	0.95	1 (7%)	17,19,21	1.94	4 (23%)
4	NAG	p	2	4	14,14,15	0.32	0	17,19,21	0.64	0
4	NAG	q	1	4,1	14,14,15	0.56	0	17,19,21	1.19	2 (11%)
4	NAG	q	2	4	14,14,15	0.51	0	17,19,21	0.88	1 (5%)
6	NAG	r	1	6,1	14,14,15	0.73	1 (7%)	17,19,21	1.75	3 (17%)
6	NAG	r	2	6	14,14,15	0.59	0	17,19,21	1.01	0
6	BMA	r	3	6	11,11,12	0.23	0	15,15,17	0.54	0
4	NAG	s	1	2,4	14,14,15	0.85	1 (7%)	17,19,21	1.24	2 (11%)
4	NAG	s	2	4	14,14,15	0.34	0	17,19,21	0.75	0
4	NAG	t	1	4,1	14,14,15	0.68	0	17,19,21	1.51	3 (17%)
4	NAG	t	2	4	14,14,15	0.32	0	17,19,21	0.49	0
4	NAG	u	1	4,1	14,14,15	0.89	1 (7%)	17,19,21	1.68	3 (17%)
4	NAG	u	2	4	14,14,15	0.33	0	17,19,21	0.77	0
4	NAG	v	1	4,1	14,14,15	0.59	0	17,19,21	1.12	1 (5%)
4	NAG	v	2	4	14,14,15	0.36	0	17,19,21	0.95	1 (5%)
6	NAG	w	1	6,1	14,14,15	0.75	1 (7%)	17,19,21	1.89	4 (23%)
6	NAG	w	2	6	14,14,15	0.43	0	17,19,21	1.16	2 (11%)
6	BMA	w	3	6	11,11,12	0.30	0	15,15,17	0.70	0
4	NAG	x	1	2,4	14,14,15	0.50	0	17,19,21	0.94	0
4	NAG	x	2	4	14,14,15	0.51	0	17,19,21	1.00	1 (5%)
6	NAG	y	1	6,1	14,14,15	0.92	1 (7%)	17,19,21	1.17	1 (5%)
6	NAG	y	2	6	14,14,15	0.34	0	17,19,21	1.91	3 (17%)
6	BMA	y	3	6	11,11,12	0.22	0	15,15,17	1.11	2 (13%)
7	NAG	z	1	7,1	14,14,15	1.15	1 (7%)	17,19,21	2.12	3 (17%)
7	NAG	z	2	7	14,14,15	0.58	0	17,19,21	1.56	3 (17%)
7	BMA	z	3	7	11,11,12	0.45	0	15,15,17	2.53	5 (33%)
7	MAN	z	4	7	11,11,12	0.41	0	15,15,17	1.89	4 (26%)
7	MAN	z	5	7	11,11,12	0.22	0	15,15,17	0.49	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.
'-' means no outliers of that kind were identified.

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

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	EA	1	6,1	-	2/6/23/26	0/1/1/1
6	NAG	EA	2	6	-	0/6/23/26	0/1/1/1
6	BMA	EA	3	6	-	0/2/19/22	0/1/1/1
5	NAG	FA	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	FA	2	5	-	0/6/23/26	0/1/1/1
5	BMA	FA	3	5	-	0/2/19/22	0/1/1/1
5	MAN	FA	4	5	-	0/2/19/22	0/1/1/1
6	NAG	GA	1	6,1	-	5/6/23/26	0/1/1/1
6	NAG	GA	2	6	-	0/6/23/26	0/1/1/1
6	BMA	GA	3	6	-	0/2/19/22	0/1/1/1
4	NAG	HA	1	2,4	-	5/6/23/26	0/1/1/1
4	NAG	HA	2	4	-	0/6/23/26	0/1/1/1
4	NAG	IA	1	4,1	-	4/6/23/26	0/1/1/1
4	NAG	IA	2	4	-	4/6/23/26	0/1/1/1
4	NAG	JA	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	JA	2	4	-	4/6/23/26	0/1/1/1
5	NAG	KA	1	5,1	-	4/6/23/26	0/1/1/1
5	NAG	KA	2	5	-	0/6/23/26	0/1/1/1
5	BMA	KA	3	5	-	0/2/19/22	0/1/1/1
5	MAN	KA	4	5	-	0/2/19/22	0/1/1/1
6	NAG	LA	1	6,1	-	4/6/23/26	0/1/1/1
6	NAG	LA	2	6	-	2/6/23/26	0/1/1/1
6	BMA	LA	3	6	-	0/2/19/22	0/1/1/1
4	NAG	MA	1	2,4	-	5/6/23/26	0/1/1/1
4	NAG	MA	2	4	-	1/6/23/26	0/1/1/1
6	NAG	NA	1	6,1	-	4/6/23/26	0/1/1/1
6	NAG	NA	2	6	-	3/6/23/26	0/1/1/1
6	BMA	NA	3	6	-	0/2/19/22	0/1/1/1
4	NAG	OA	1	4,1	-	6/6/23/26	0/1/1/1
4	NAG	OA	2	4	-	4/6/23/26	0/1/1/1
5	NAG	PA	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	PA	2	5	-	0/6/23/26	0/1/1/1
5	BMA	PA	3	5	-	0/2/19/22	0/1/1/1
5	MAN	PA	4	5	-	0/2/19/22	0/1/1/1
4	NAG	QA	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	QA	2	4	-	0/6/23/26	0/1/1/1
4	NAG	RA	1	2,4	-	4/6/23/26	0/1/1/1
4	NAG	RA	2	4	-	2/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

The worst 5 of 33 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	OA	1	NAG	C1-C2	4.47	1.58	1.52
4	2	1	NAG	C1-C2	4.11	1.57	1.52
4	i	1	NAG	C1-C2	4.08	1.57	1.52
4	RA	1	NAG	C1-C2	4.06	1.57	1.52
7	z	1	NAG	C1-C2	3.99	1.57	1.52

The worst 5 of 205 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	LA	1	NAG	C1-O5-C5	8.10	123.04	112.19
4	MA	1	NAG	C1-O5-C5	8.02	122.94	112.19
4	QA	1	NAG	C2-N2-C7	-7.79	112.46	122.90
4	RA	1	NAG	C1-O5-C5	7.46	122.19	112.19
7	z	1	NAG	C1-O5-C5	7.17	121.79	112.19

There are no chirality outliers.

5 of 239 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	e	1	NAG	C8-C7-N2-C2
4	e	1	NAG	O7-C7-N2-C2
4	f	1	NAG	C1-C2-N2-C7
4	i	1	NAG	C1-C2-N2-C7
4	j	1	NAG	C3-C2-N2-C7

There are no ring outliers.

78 monomers are involved in 141 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	o	1	NAG	3	0
4	RA	1	NAG	1	0
4	MA	1	NAG	7	0
6	NA	2	NAG	2	0
6	5	2	NAG	2	0
6	CA	1	NAG	2	0
6	GA	3	BMA	2	0
4	RA	2	NAG	1	0
4	s	1	NAG	2	0
5	l	3	BMA	1	0
4	n	1	NAG	1	0
4	MA	2	NAG	5	0
4	HA	2	NAG	2	0
4	9	2	NAG	1	0
4	v	2	NAG	2	0
6	DA	1	NAG	2	0
4	u	1	NAG	6	0
4	t	1	NAG	1	0
4	m	2	NAG	4	0
6	EA	1	NAG	1	0
6	LA	3	BMA	1	0
6	w	1	NAG	2	0
4	j	2	NAG	3	0
6	NA	1	NAG	3	0
5	FA	3	BMA	1	0
6	CA	2	NAG	3	0
6	GA	2	NAG	9	0
4	9	1	NAG	2	0
4	1	1	NAG	1	0
4	QA	1	NAG	4	0
6	5	3	BMA	1	0
6	h	2	NAG	1	0
4	JA	1	NAG	2	0

Continued on next page...

Continued from previous page...

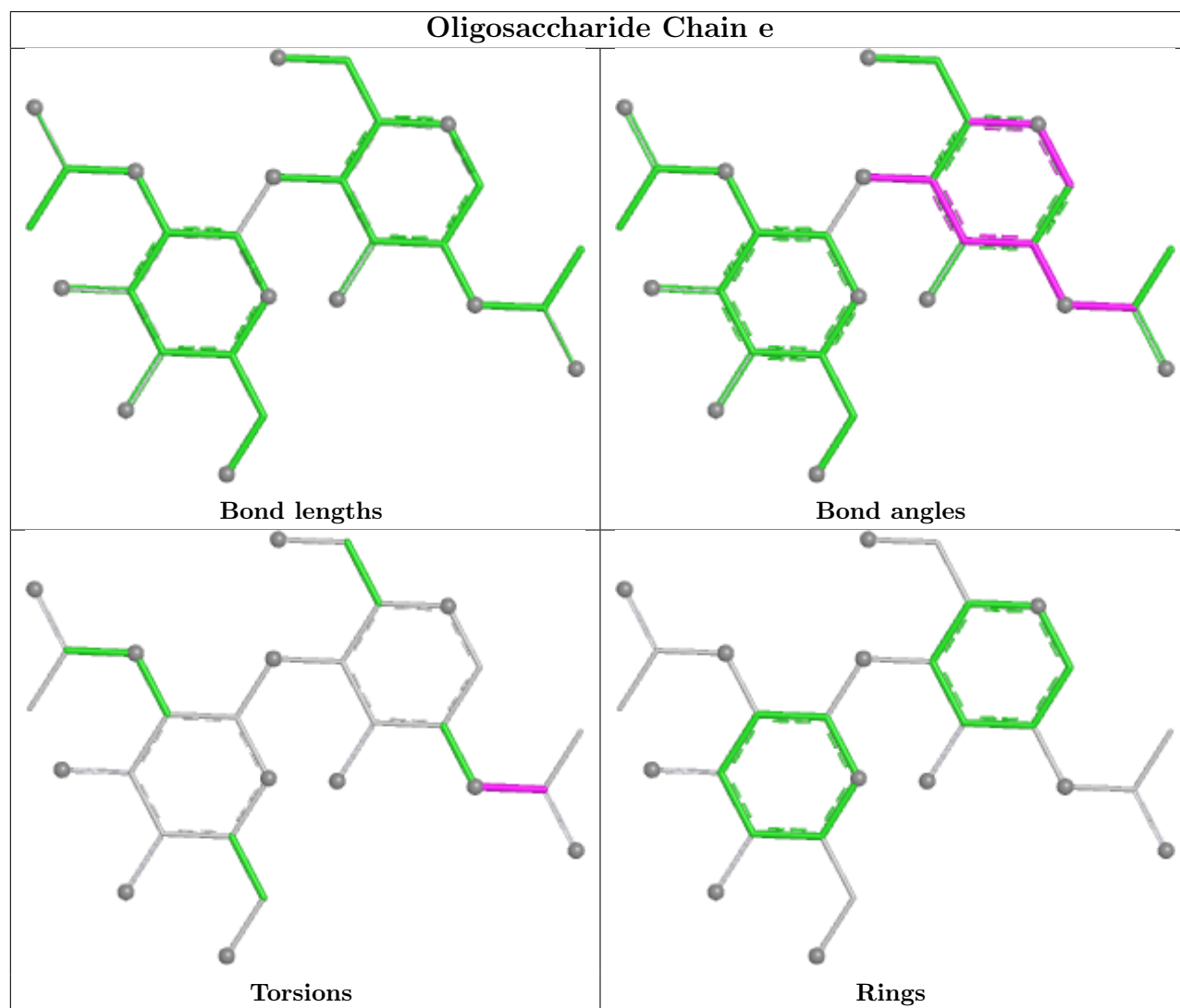
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	r	1	NAG	8	0
6	DA	2	NAG	2	0
4	q	1	NAG	3	0
5	l	1	NAG	1	0
4	i	1	NAG	3	0
4	6	1	NAG	2	0
6	k	1	NAG	4	0
4	OA	1	NAG	2	0
7	z	4	MAN	2	0
8	0	1	NAG	6	0
4	i	2	NAG	1	0
5	l	4	MAN	1	0
5	l	2	NAG	1	0
4	q	2	NAG	7	0
4	2	1	NAG	1	0
6	GA	1	NAG	7	0
8	0	2	NAG	8	0
6	5	1	NAG	1	0
4	v	1	NAG	1	0
8	0	3	BMA	1	0
4	JA	2	NAG	1	0
4	BA	2	NAG	3	0
7	z	3	BMA	2	0
4	BA	1	NAG	3	0
4	HA	1	NAG	4	0
4	OA	2	NAG	1	0
6	LA	1	NAG	3	0
5	FA	1	NAG	1	0
5	PA	1	NAG	1	0
5	FA	4	MAN	1	0
6	r	2	NAG	3	0
4	7	1	NAG	6	0
4	m	1	NAG	9	0
4	f	1	NAG	2	0
5	KA	1	NAG	1	0
4	n	2	NAG	1	0
6	3	2	NAG	1	0
4	7	2	NAG	6	0
6	k	2	NAG	1	0
6	LA	2	NAG	5	0
5	FA	2	NAG	1	0
4	j	1	NAG	4	0

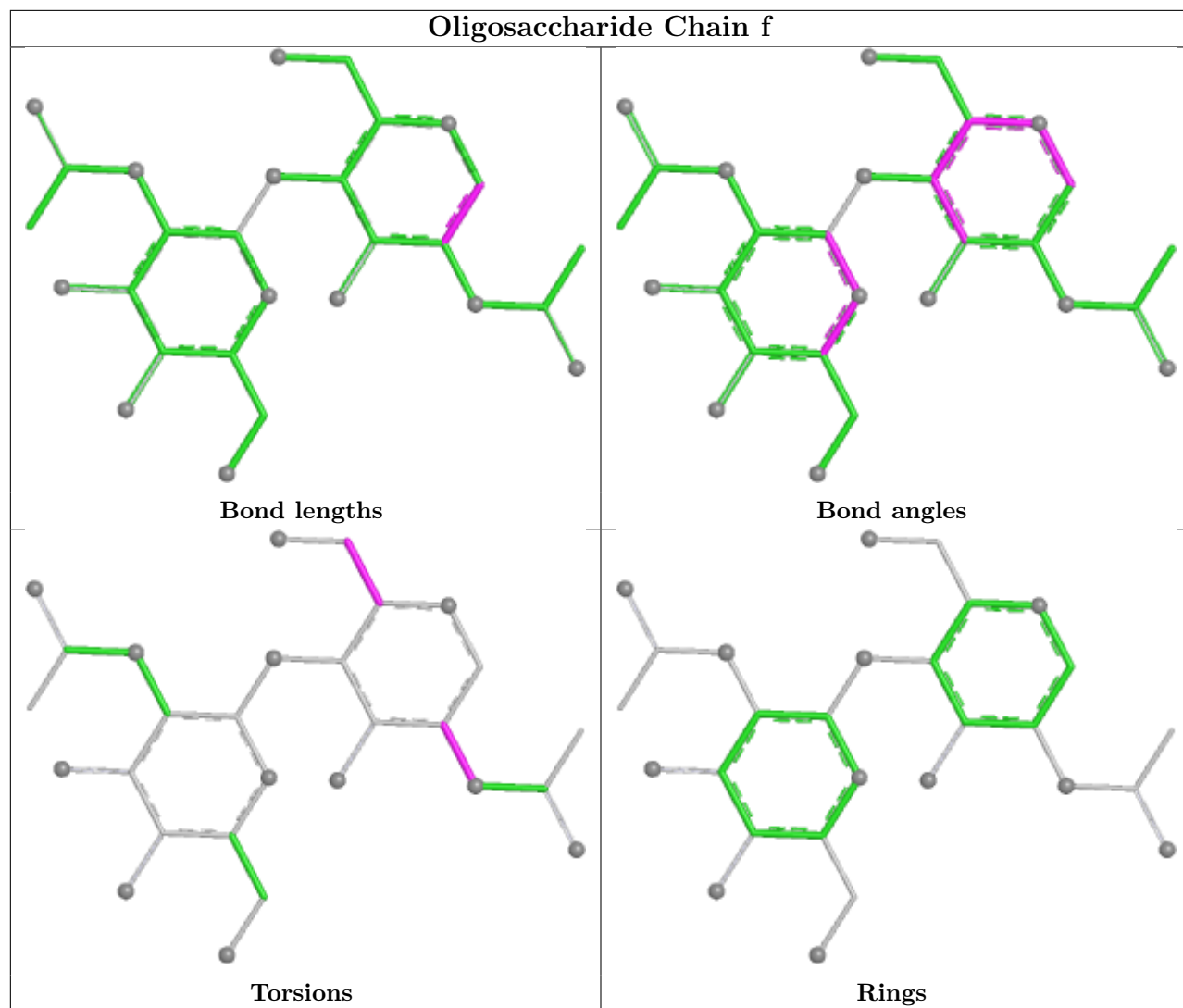
Continued on next page...

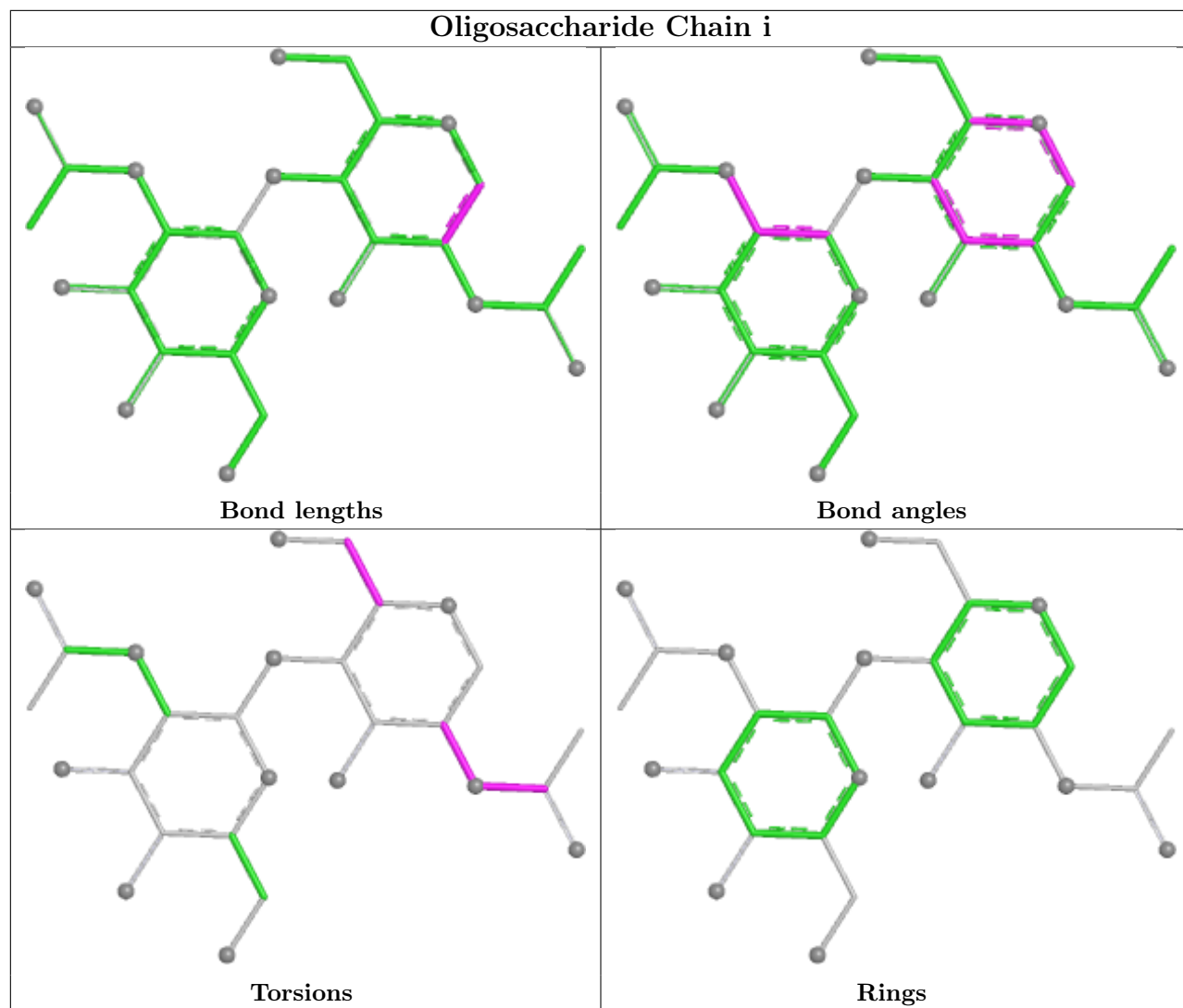
Continued from previous page...

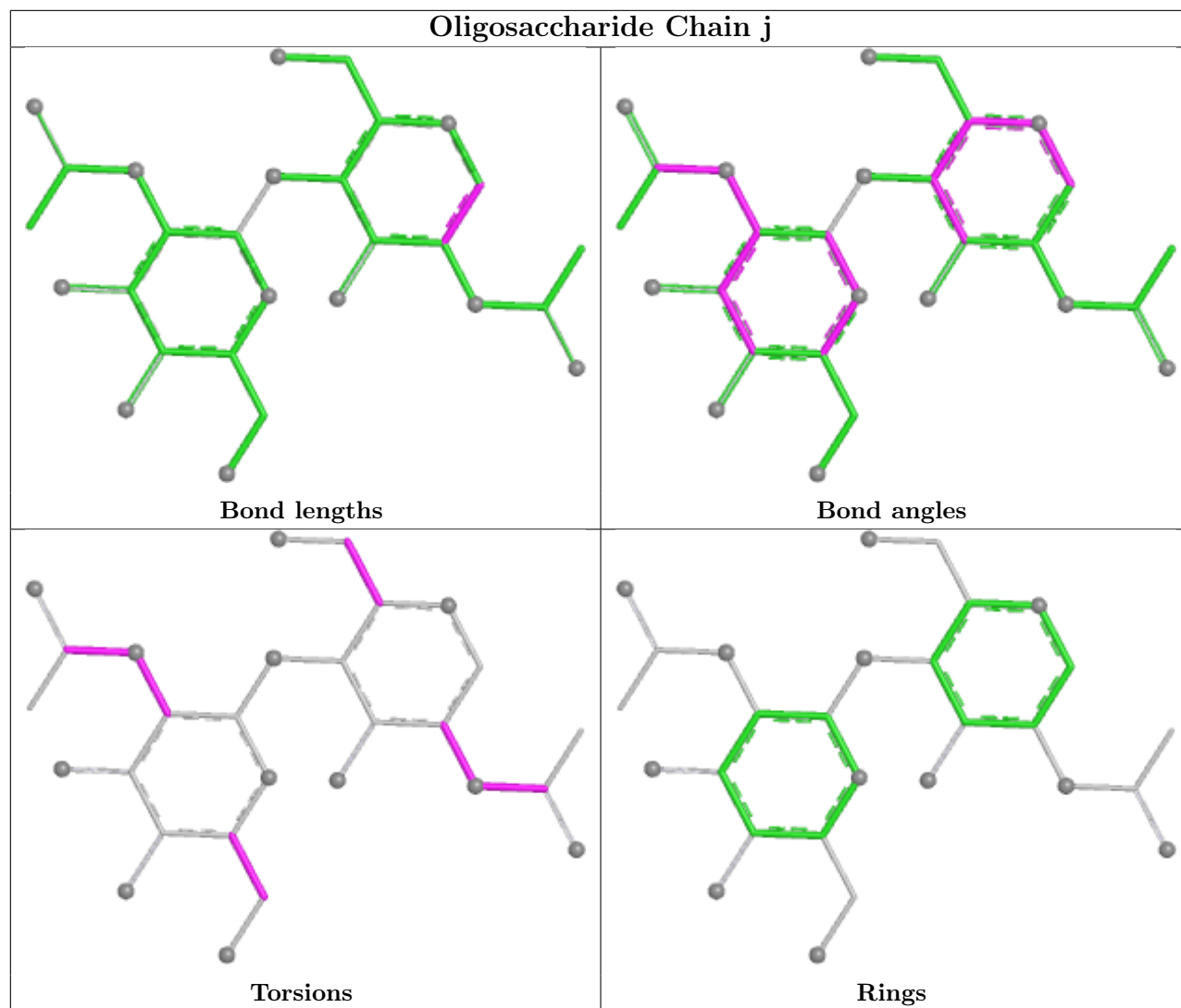
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	3	1	NAG	3	0
5	AA	1	NAG	1	0
5	PA	2	NAG	1	0

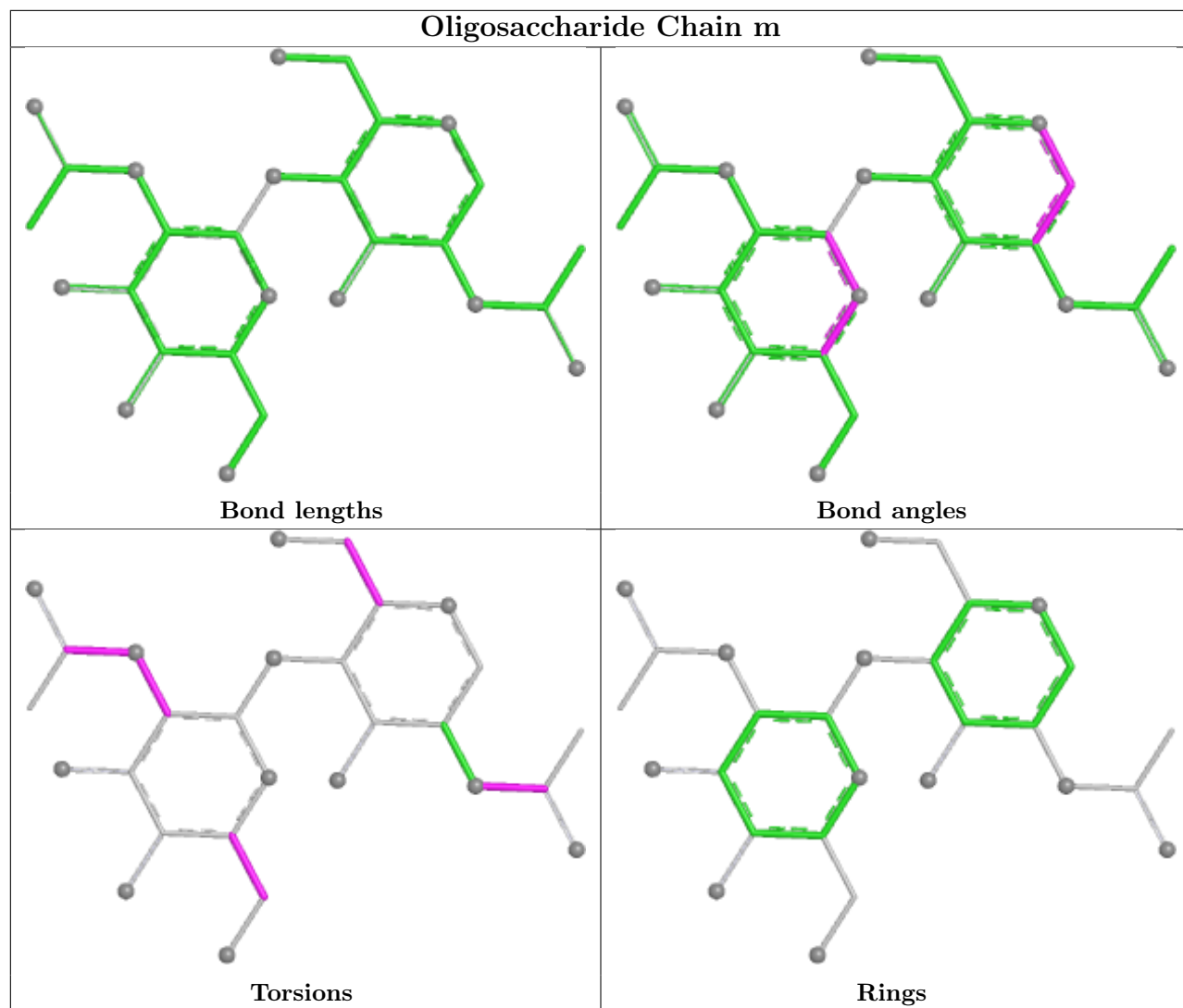
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

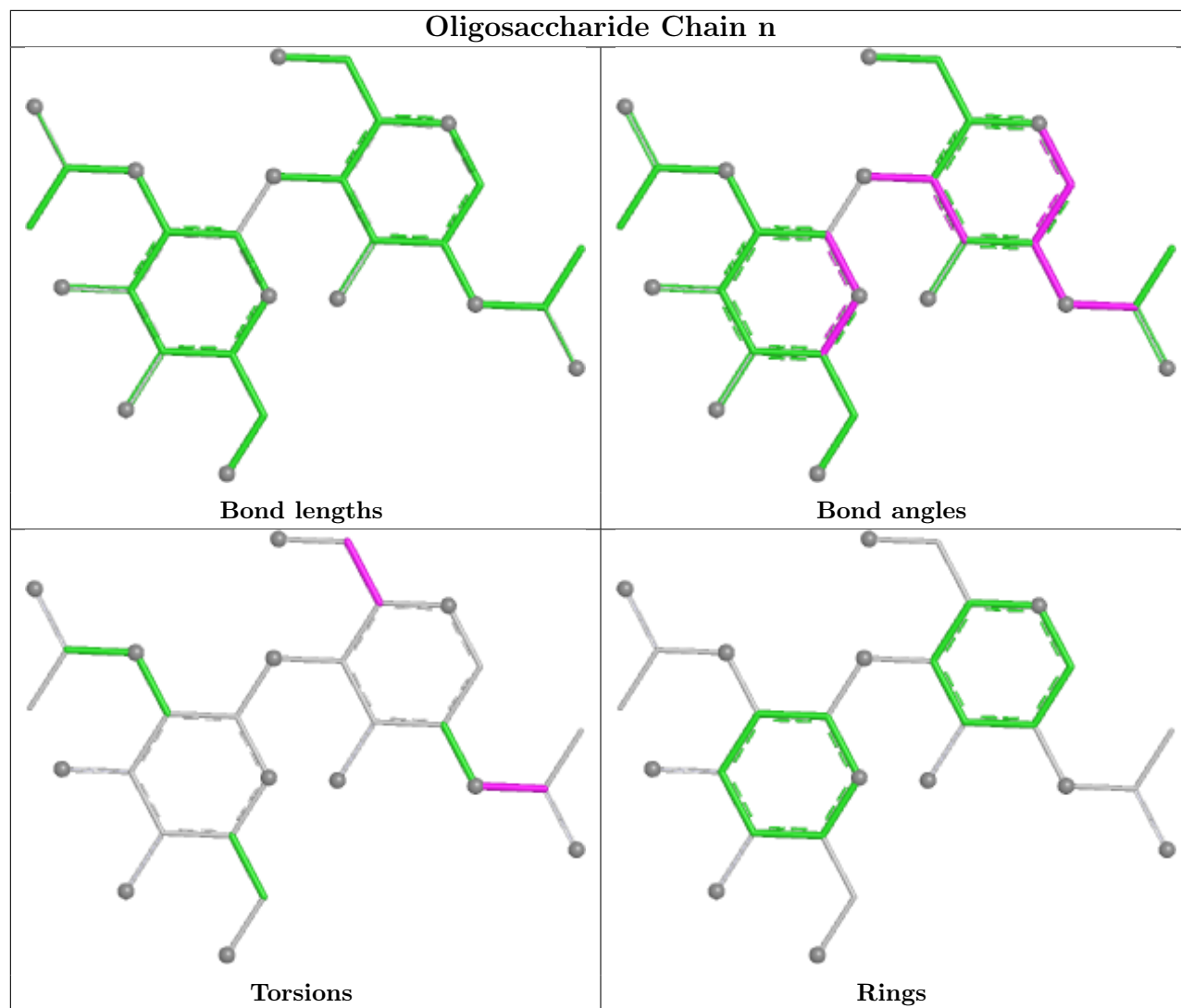


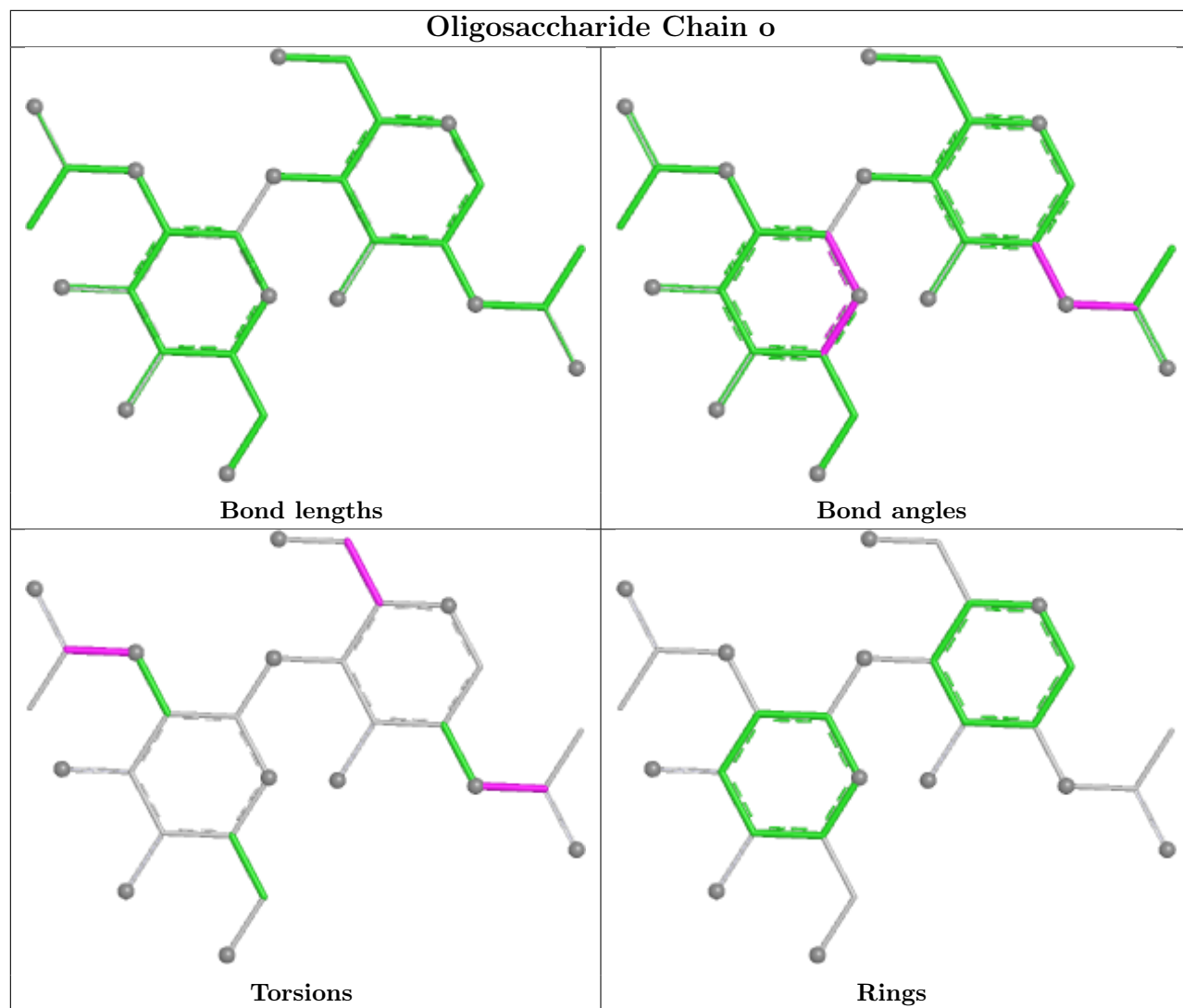


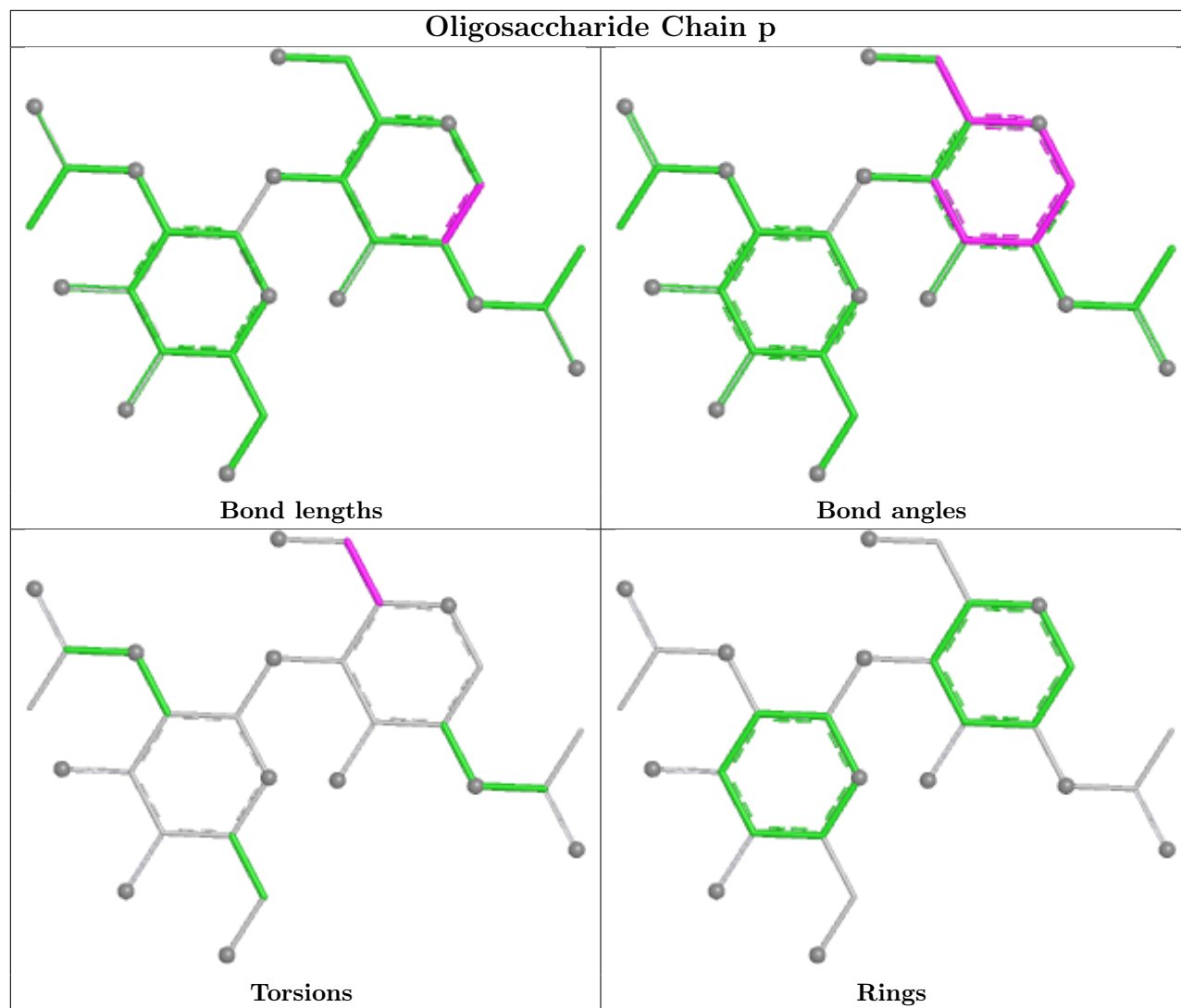


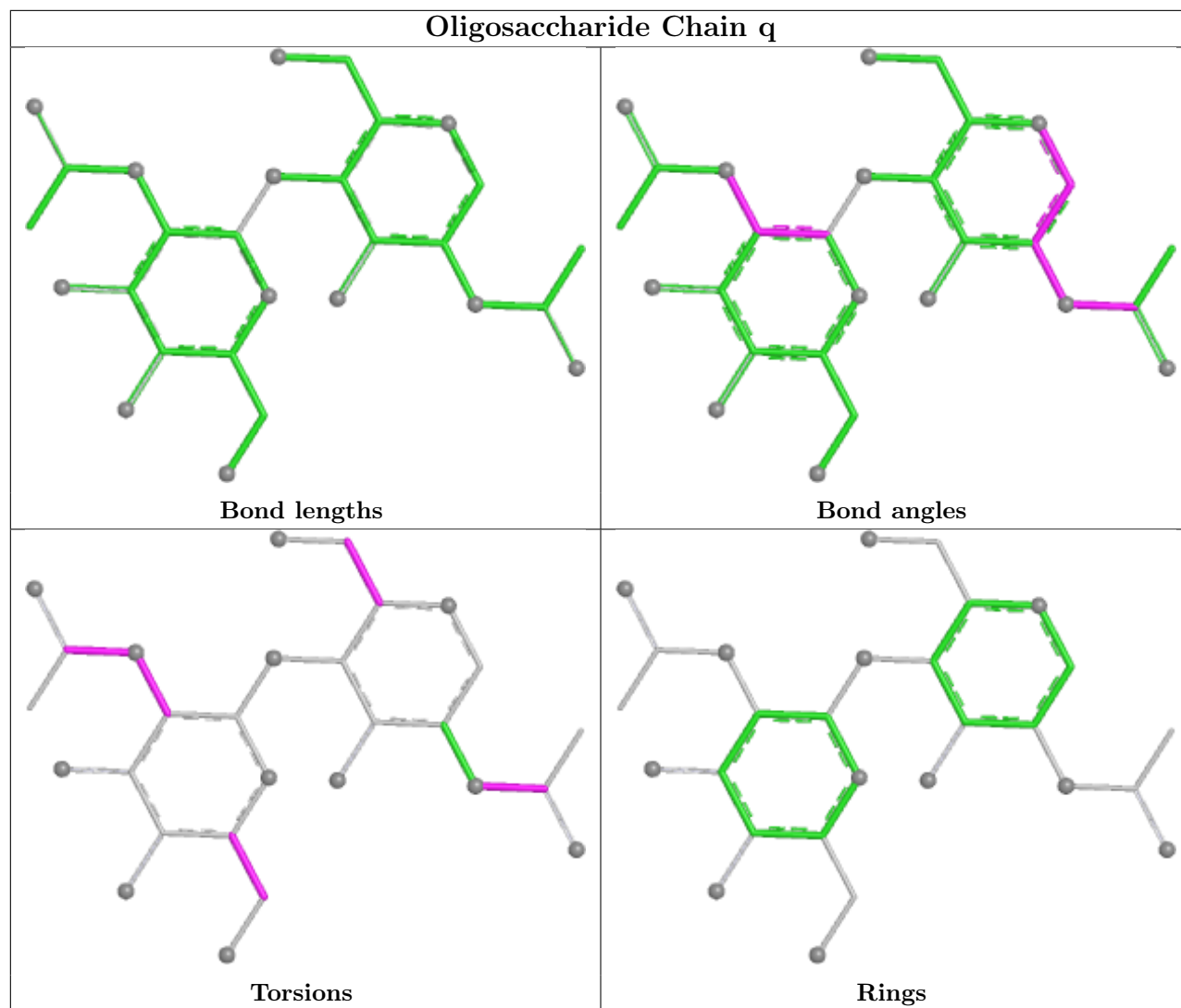


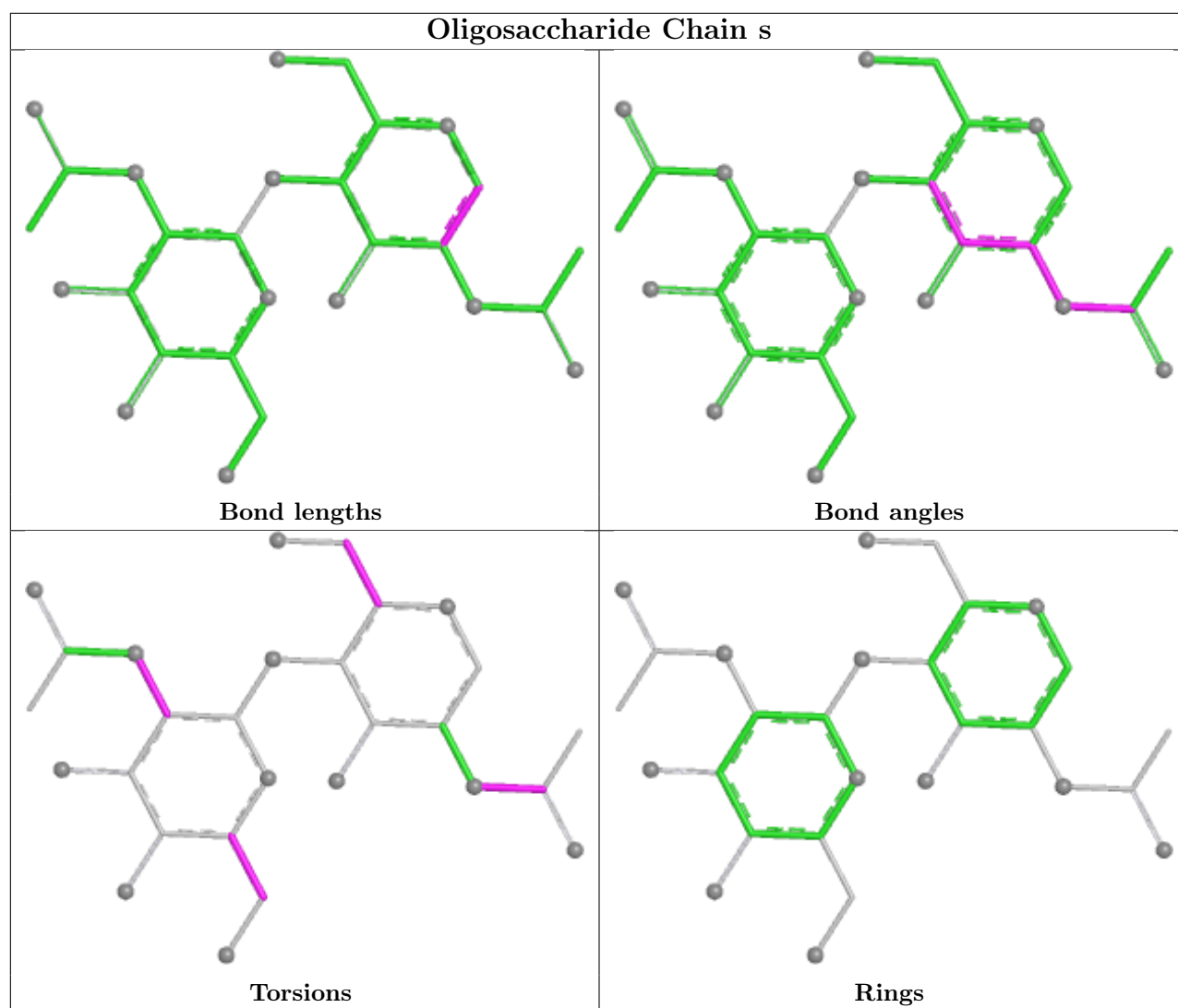


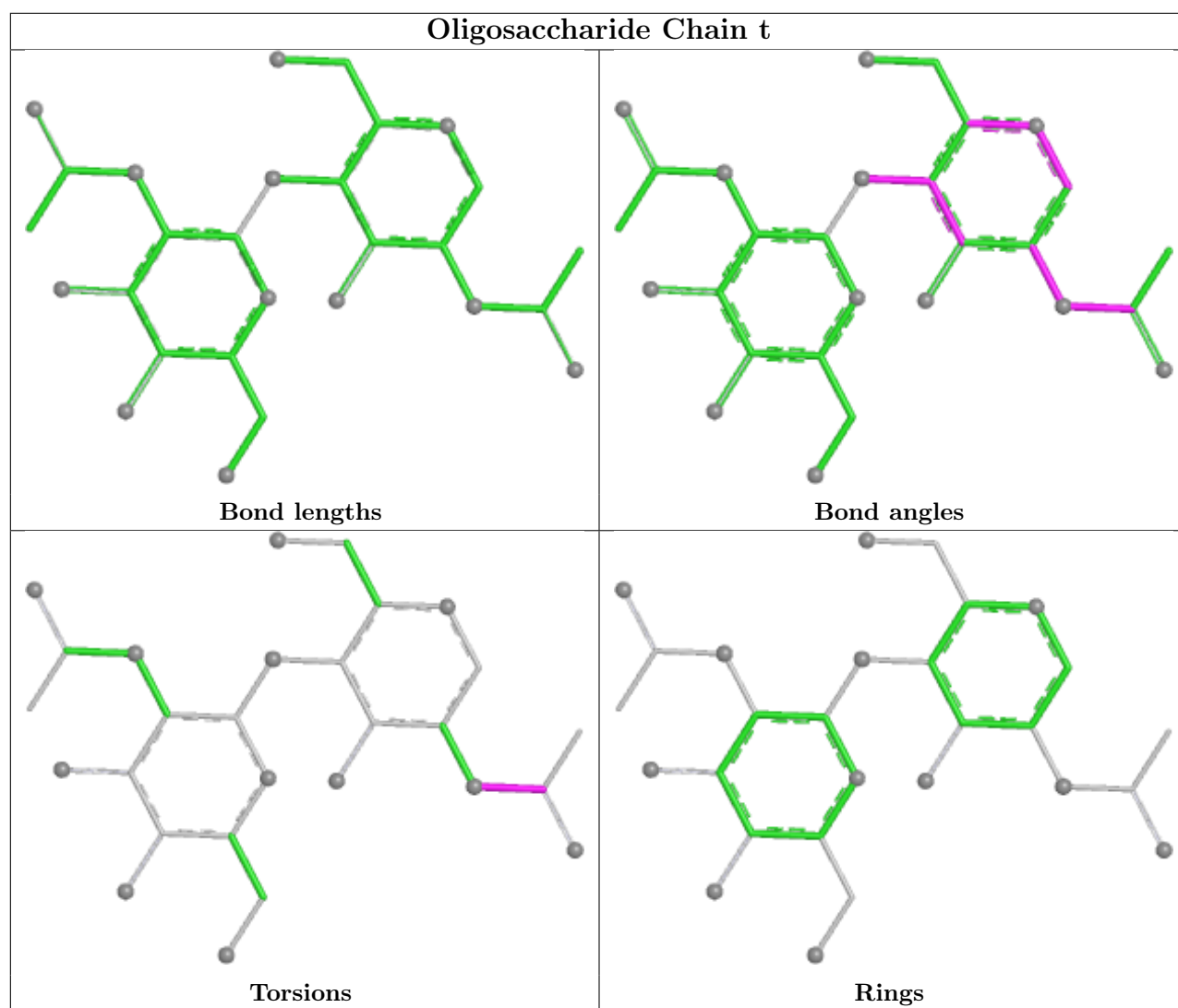


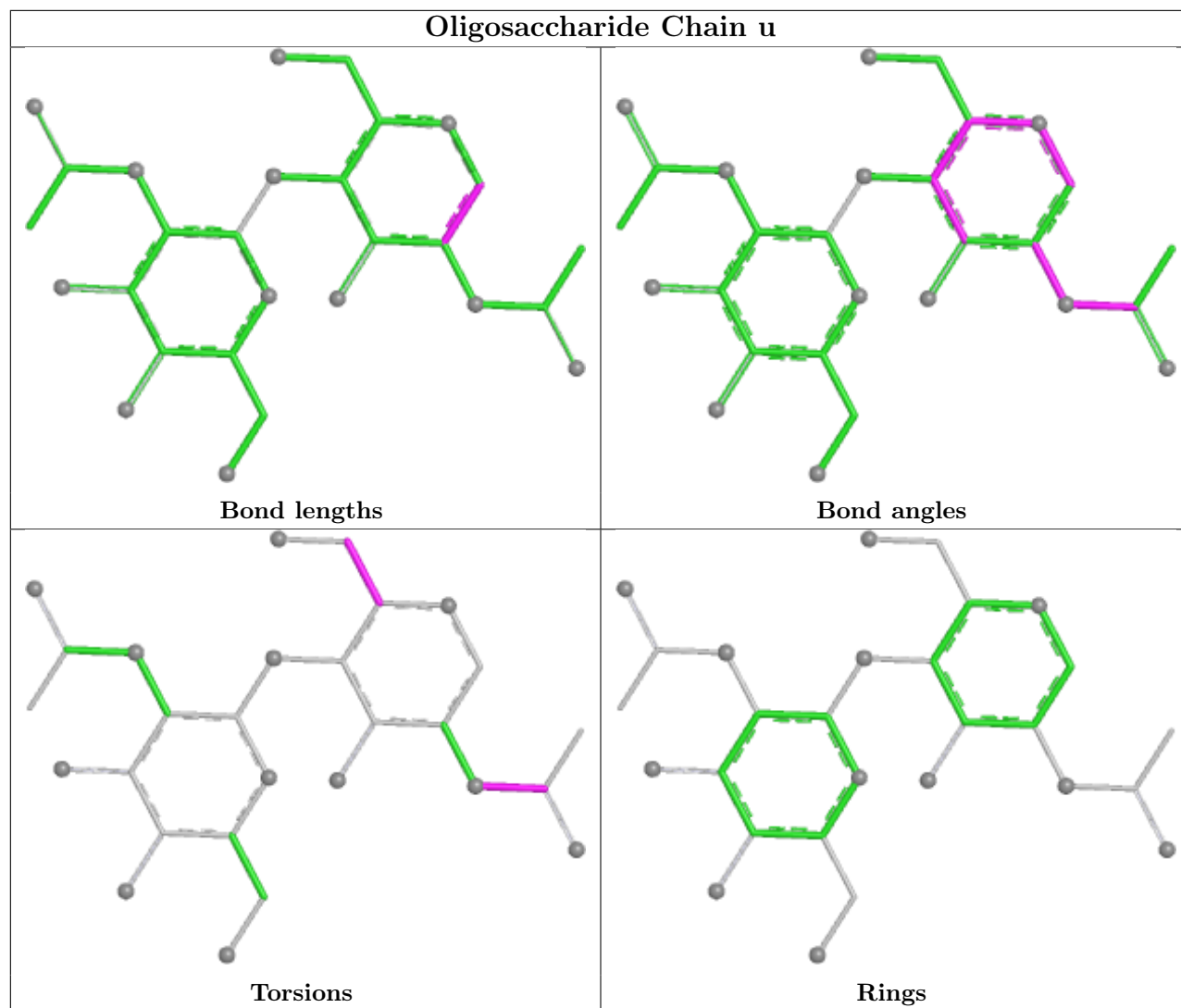


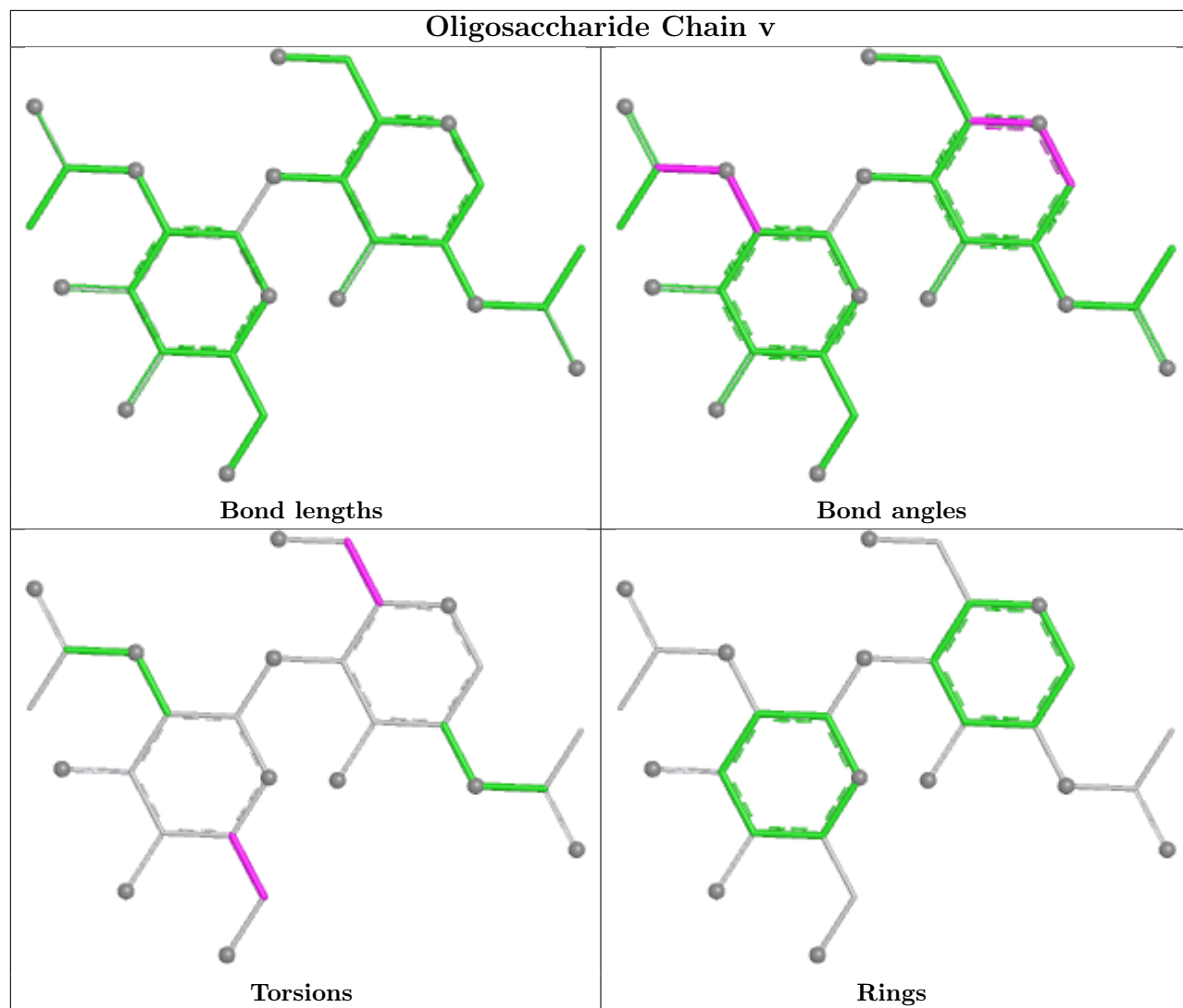


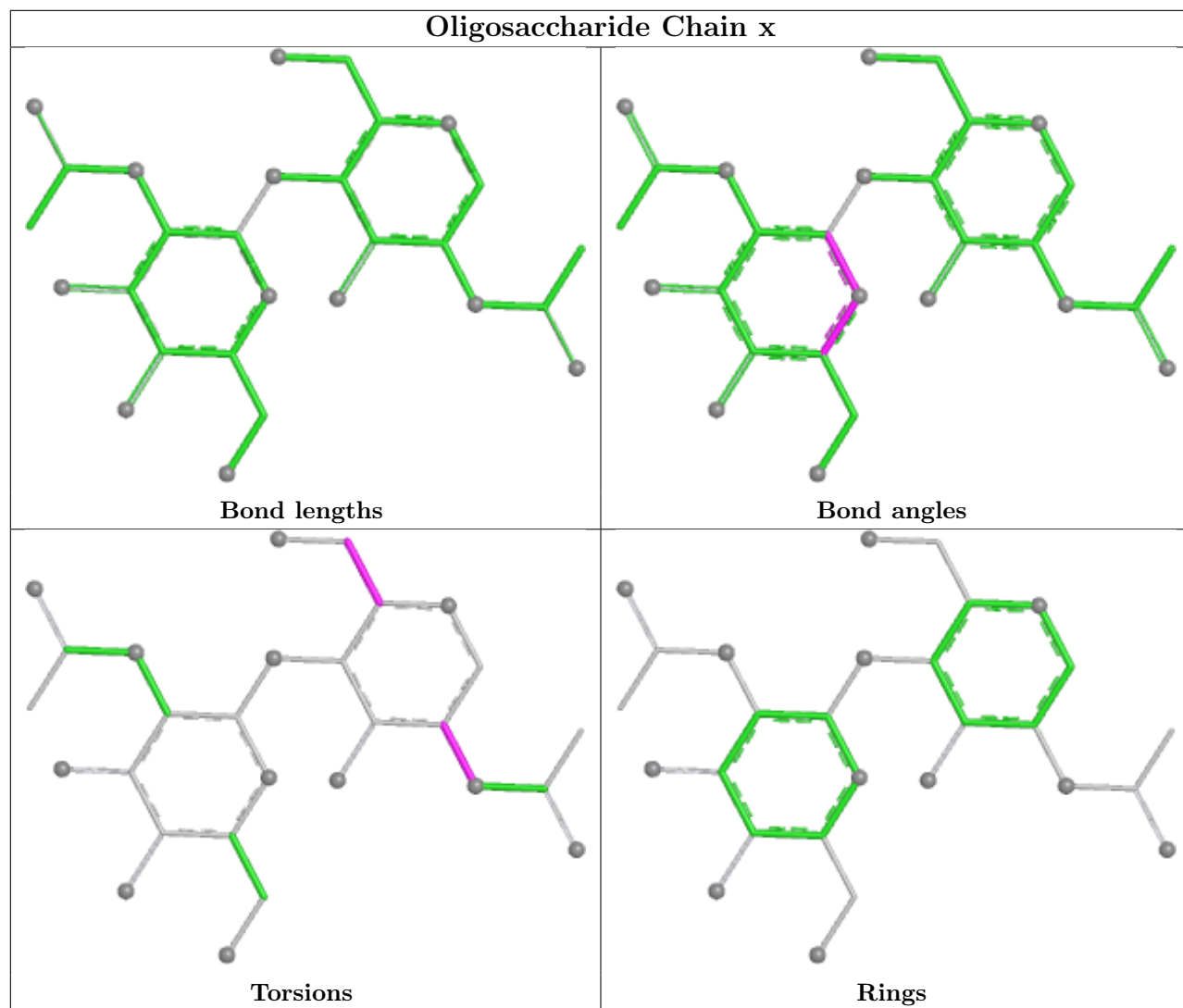


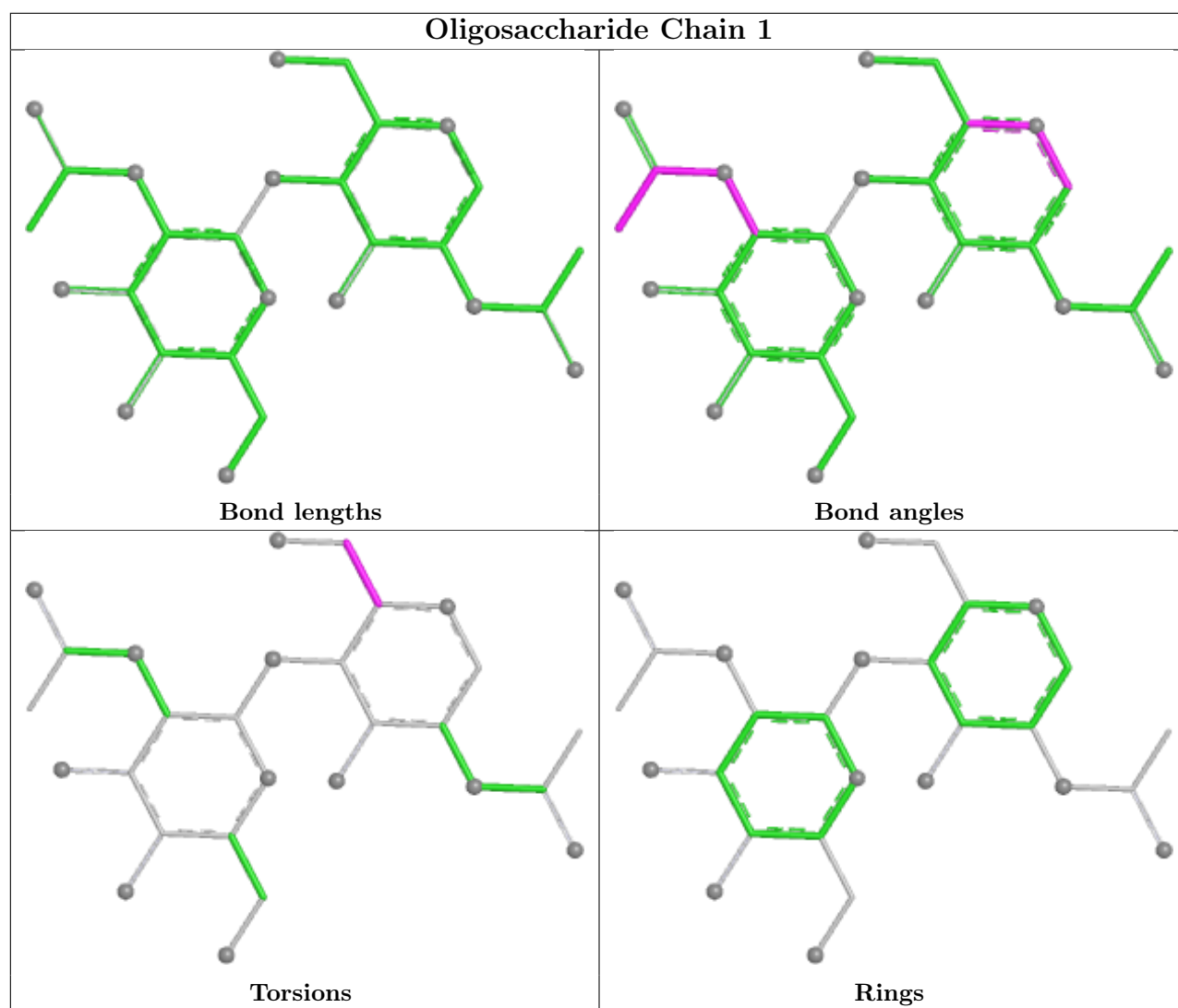


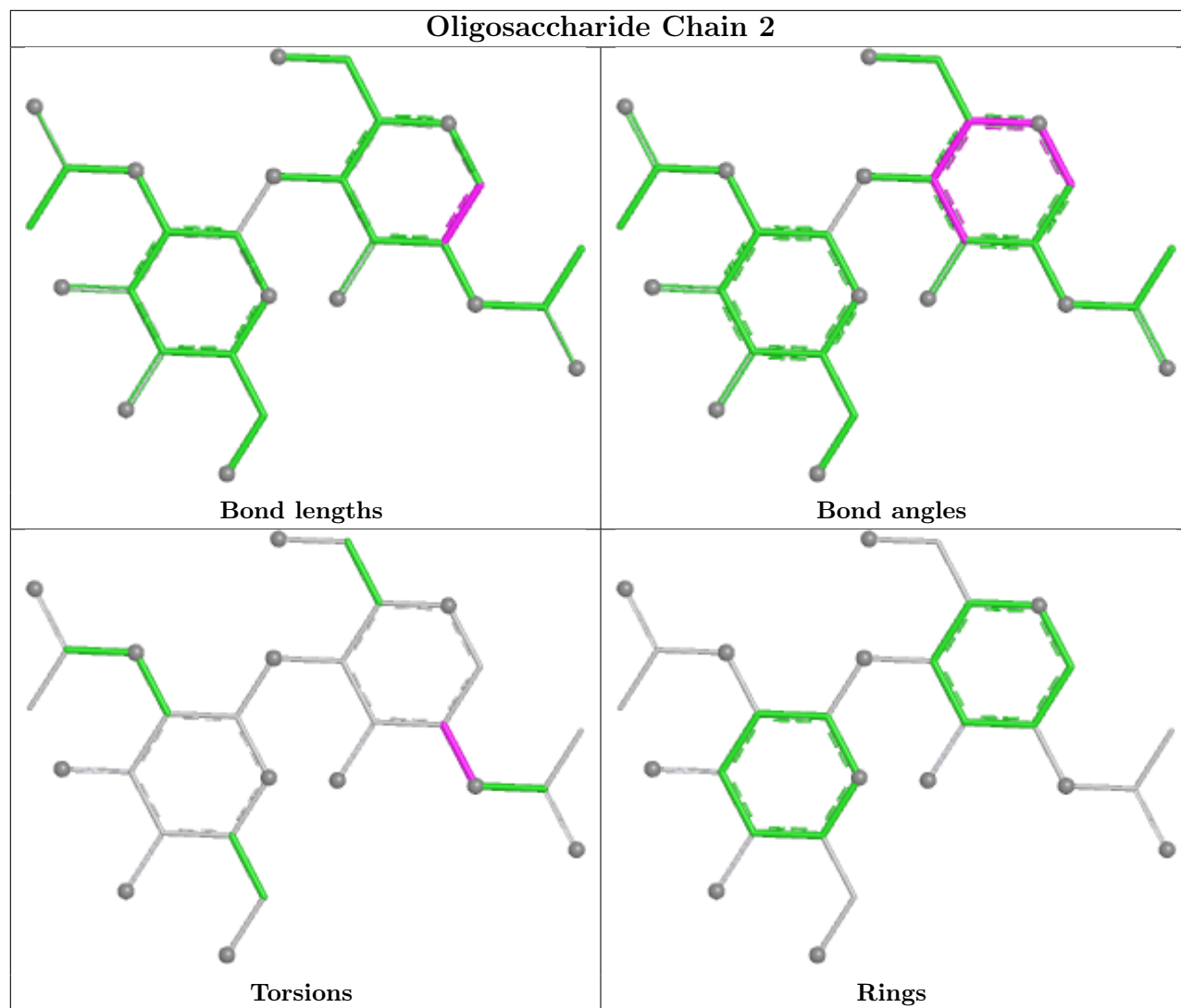


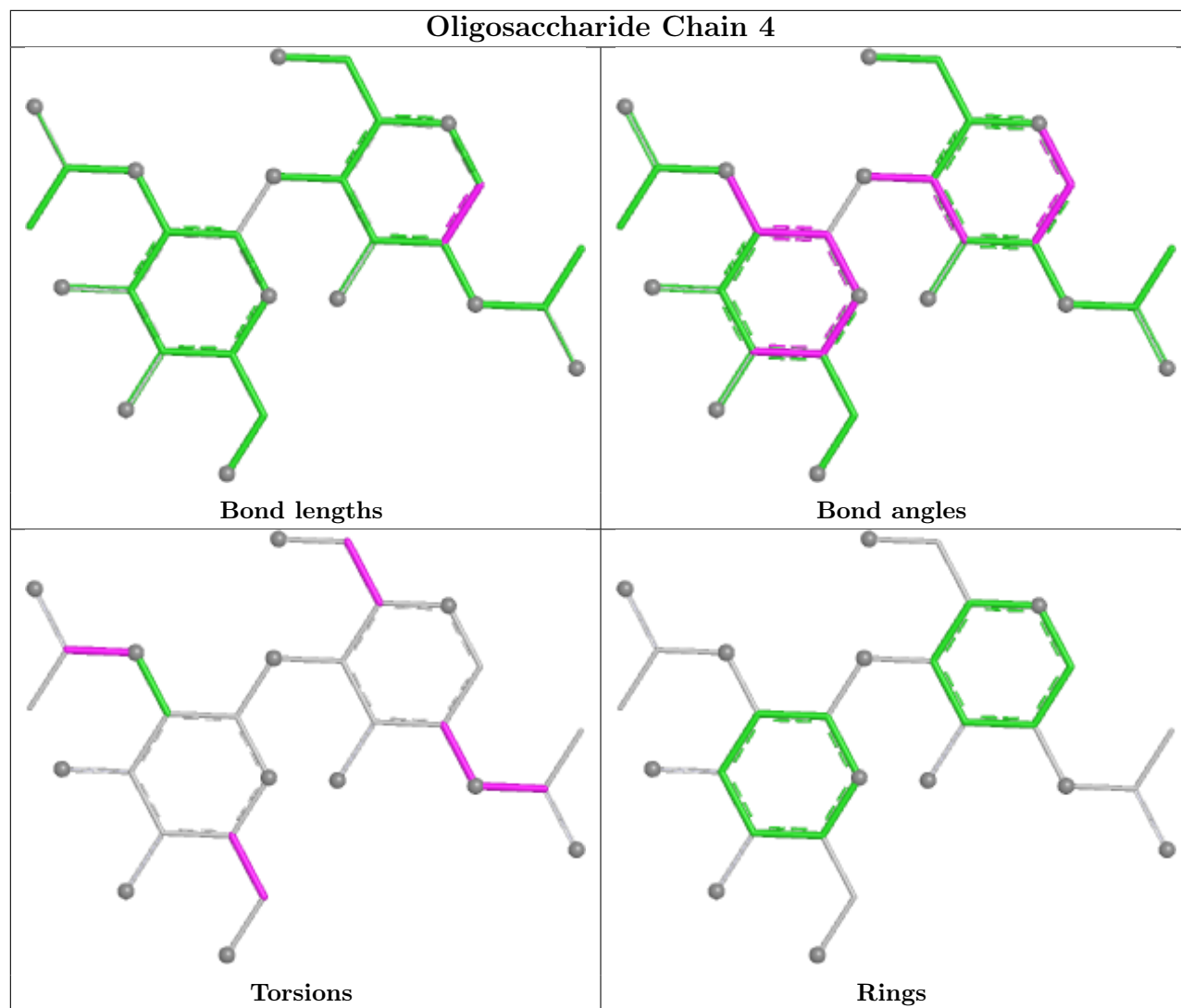


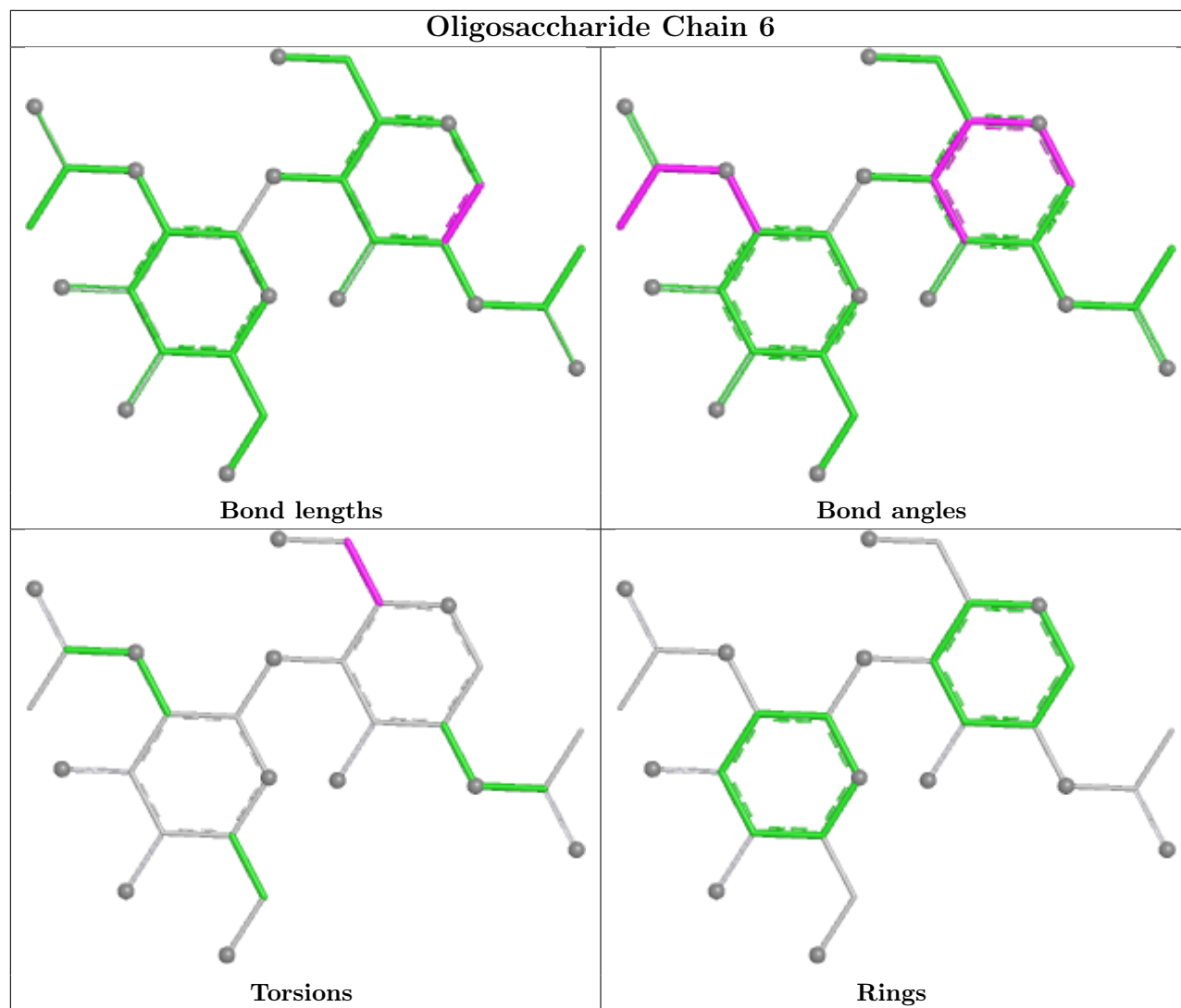


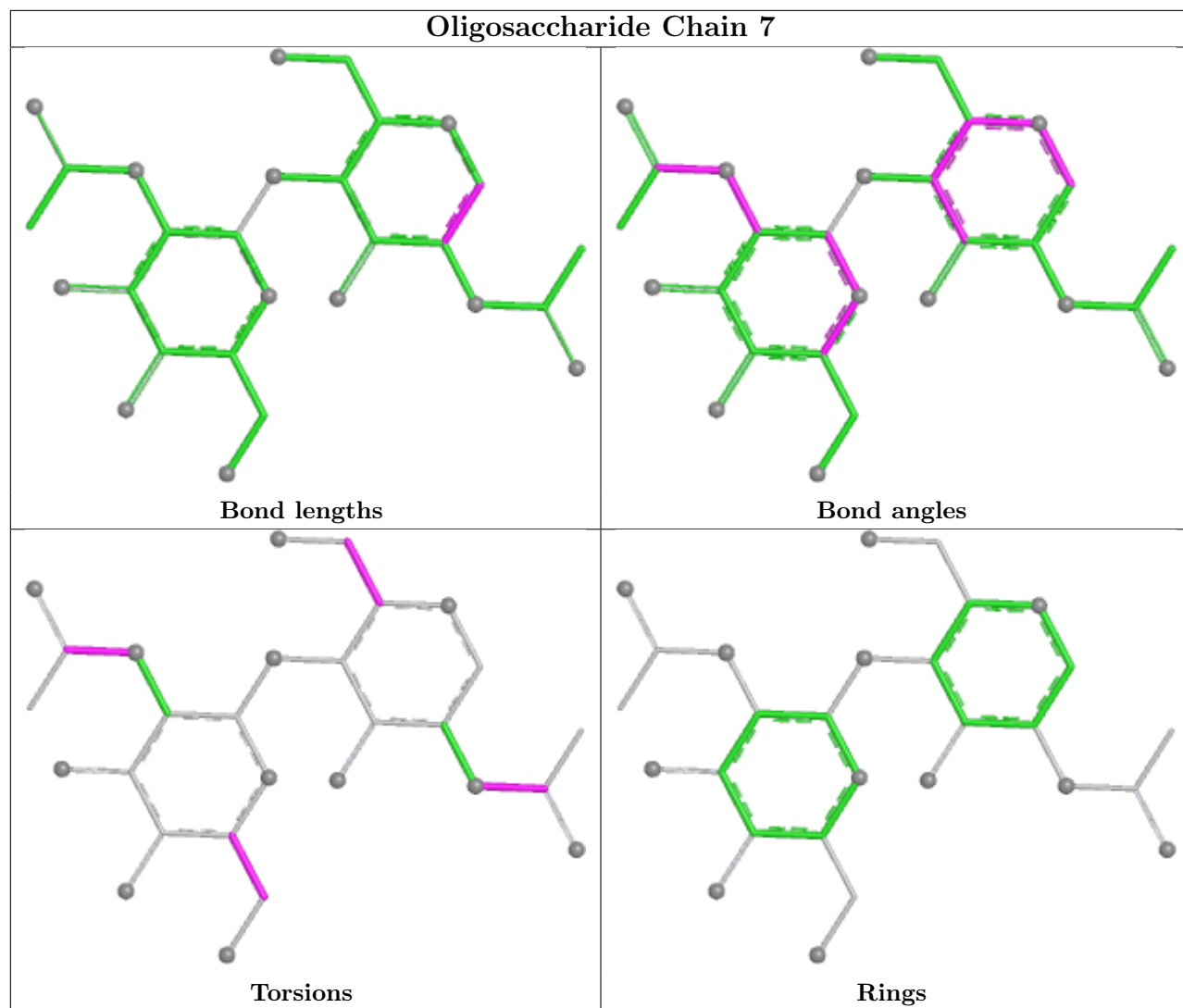


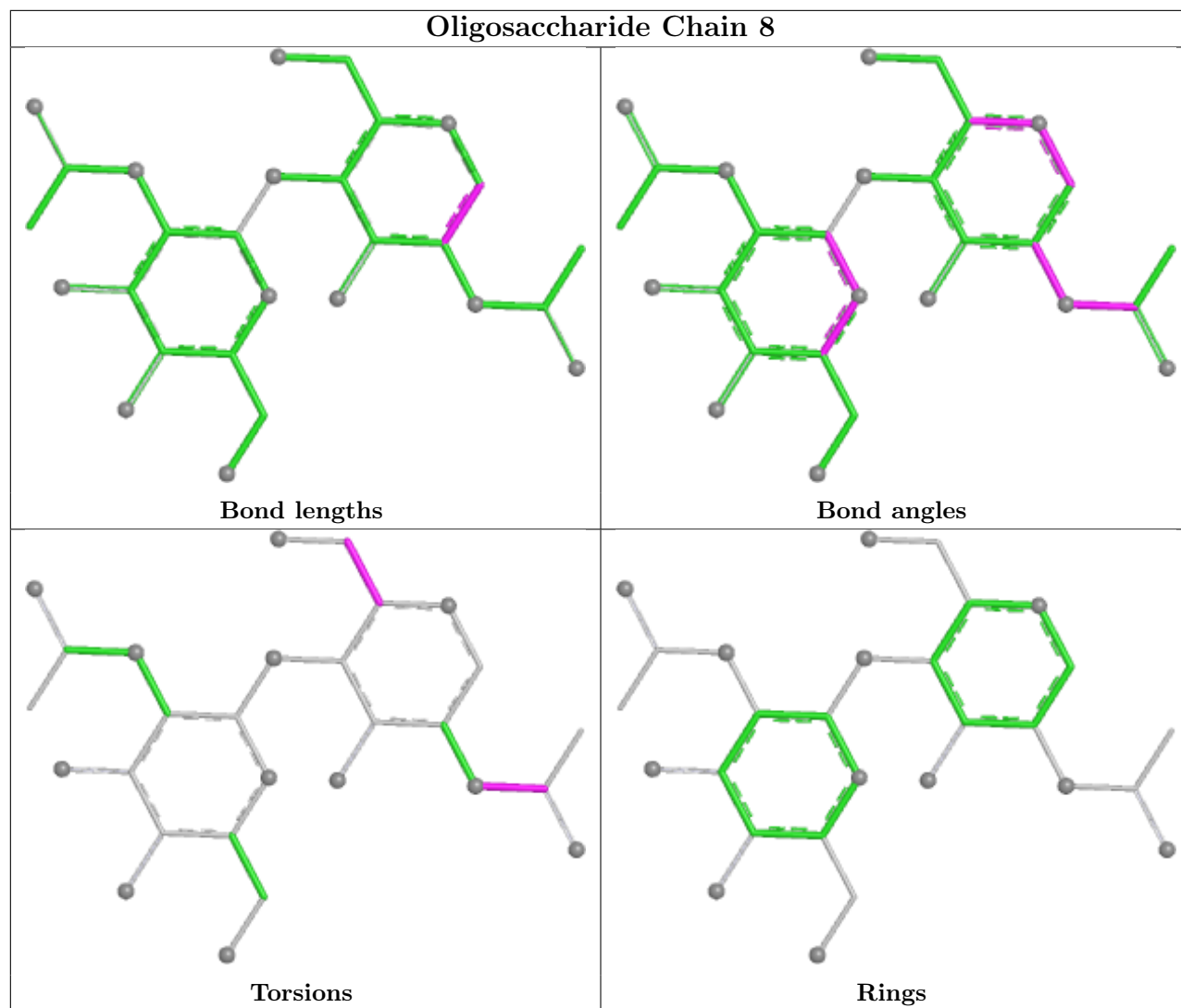


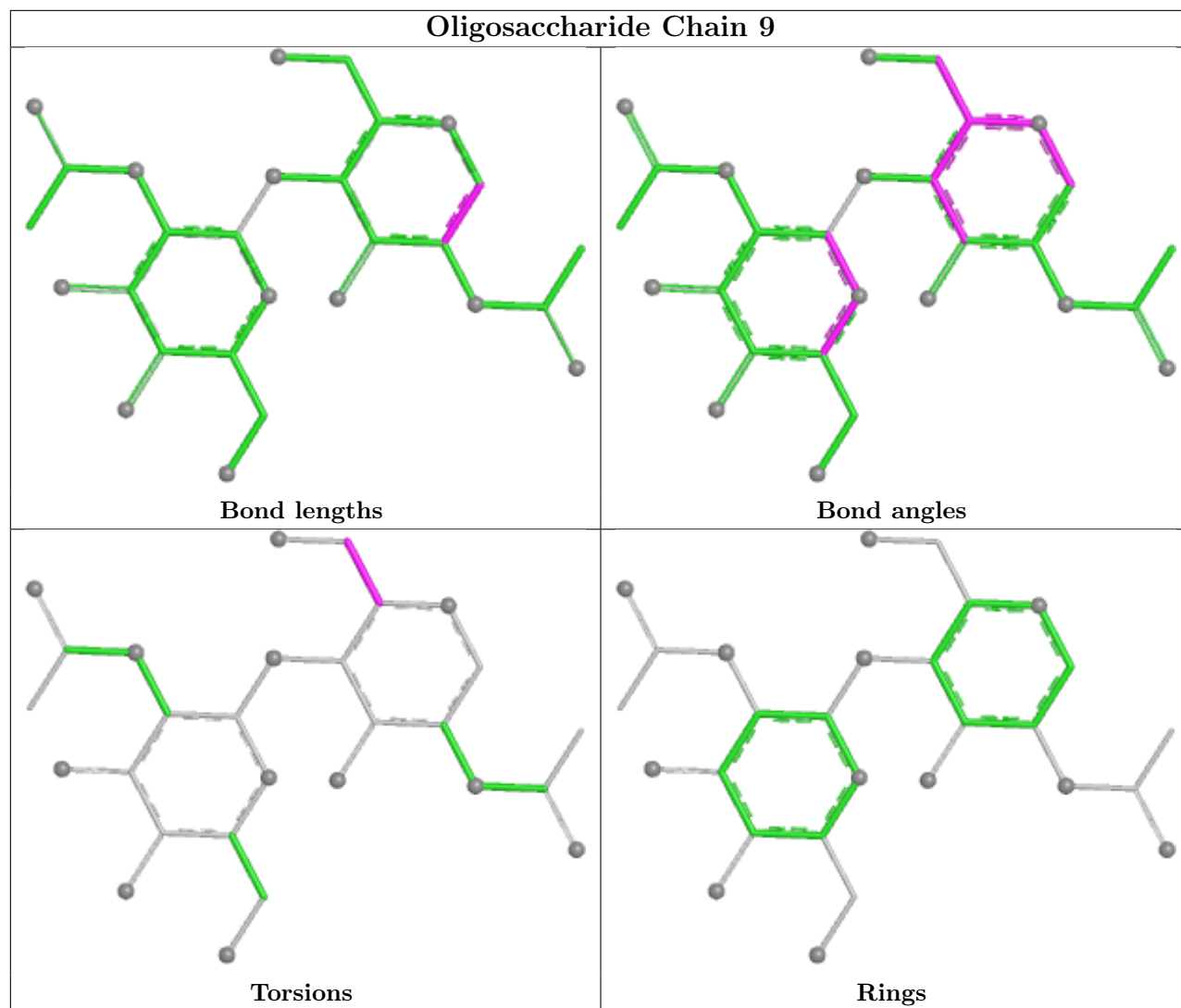


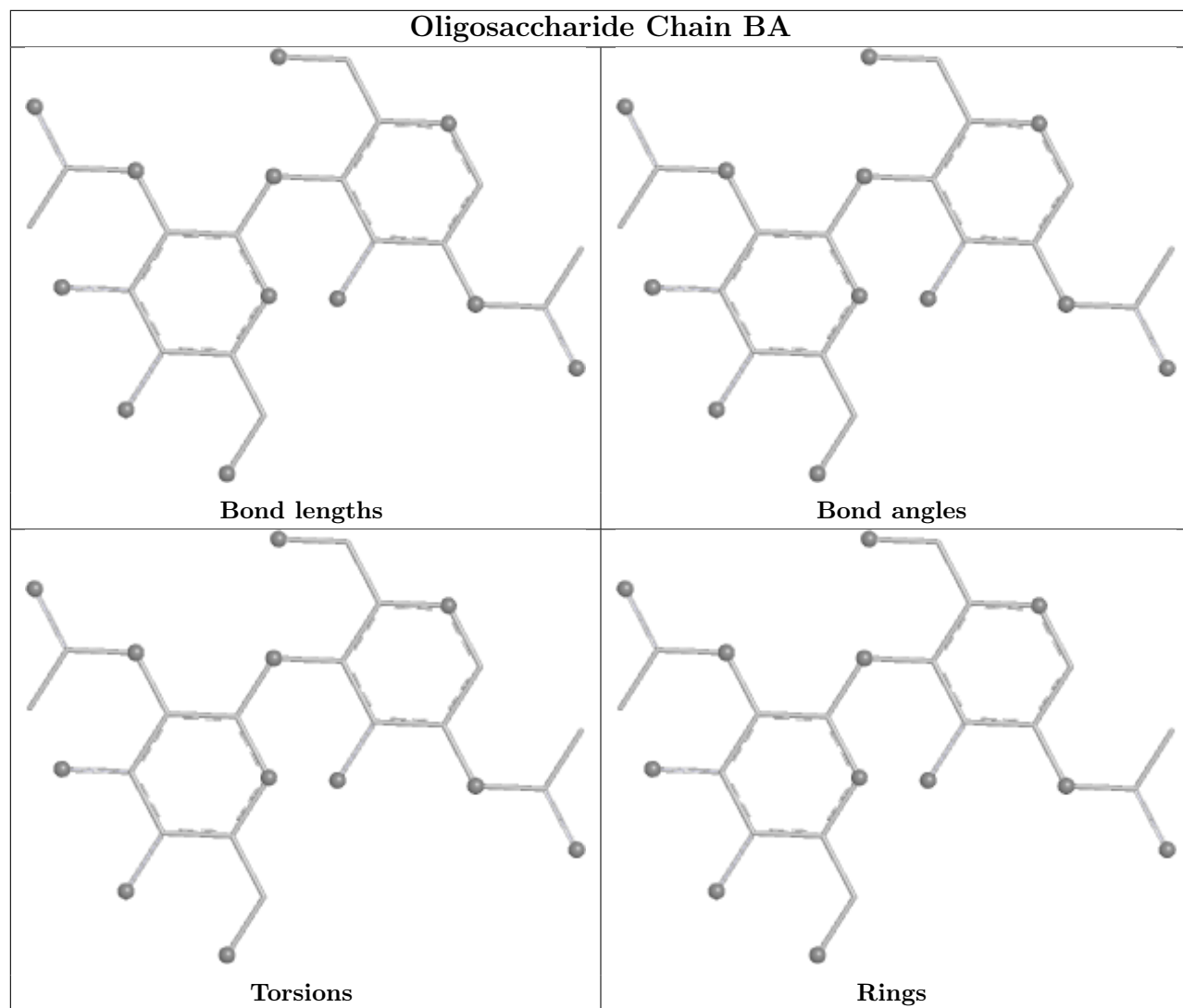


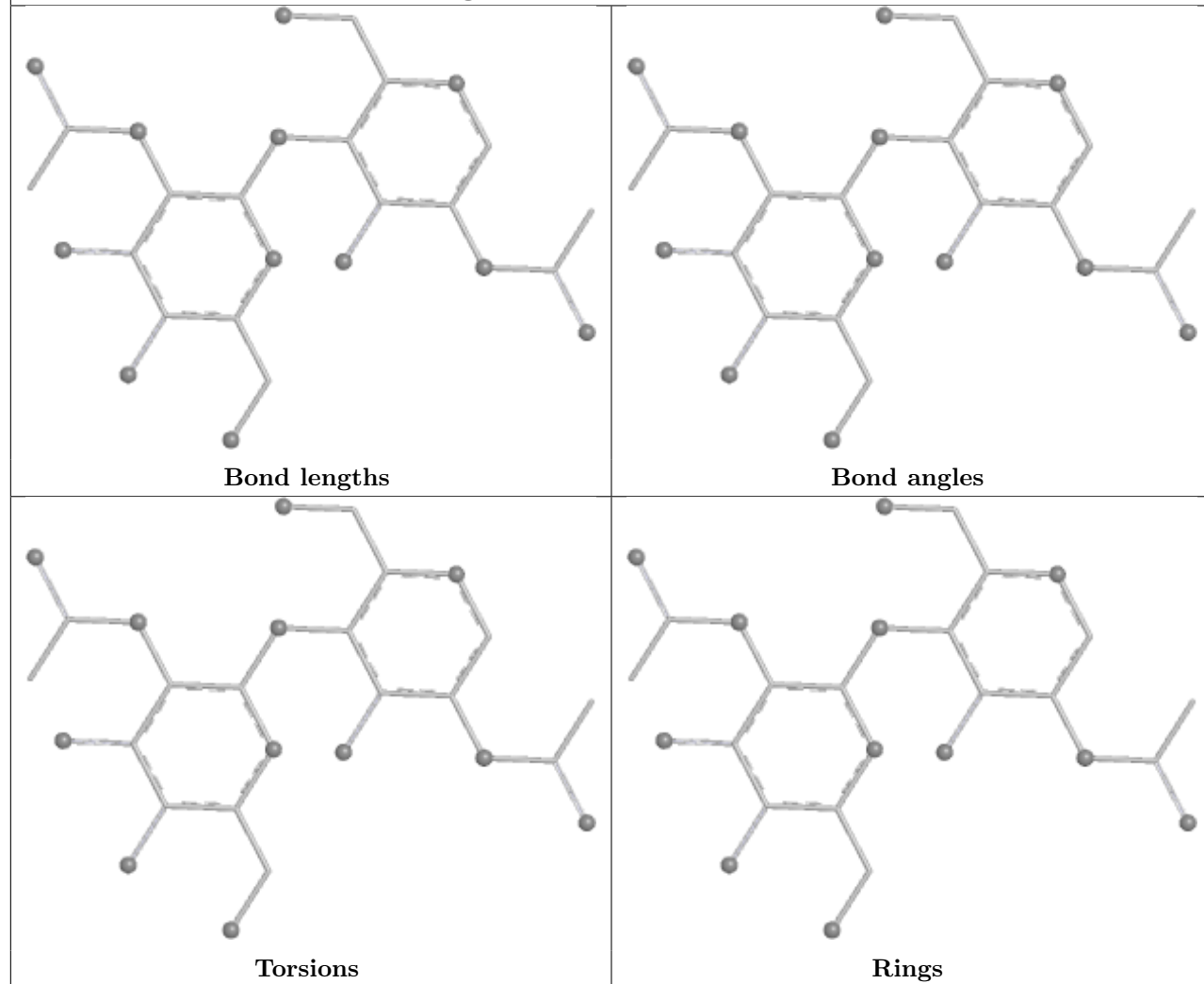




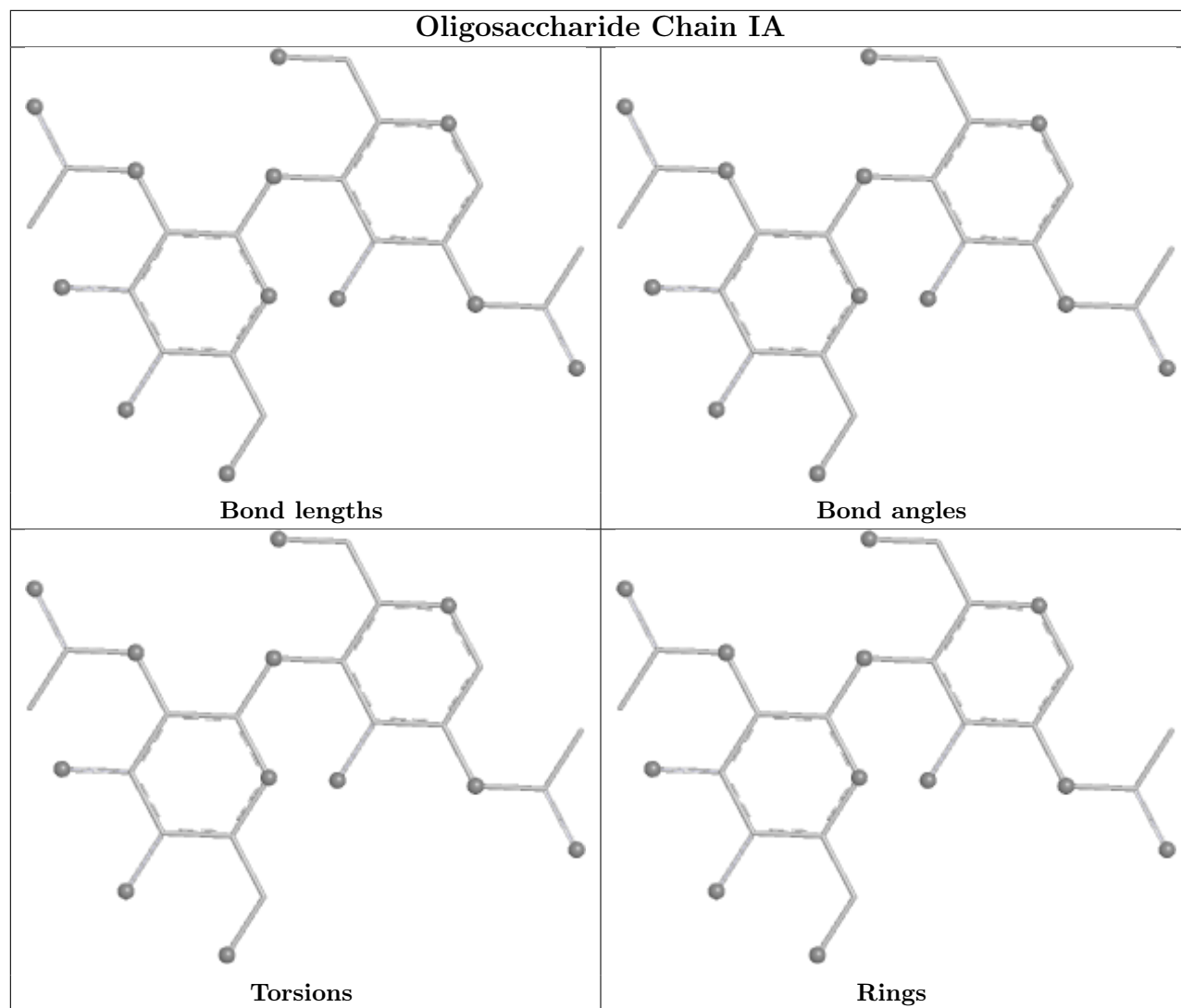


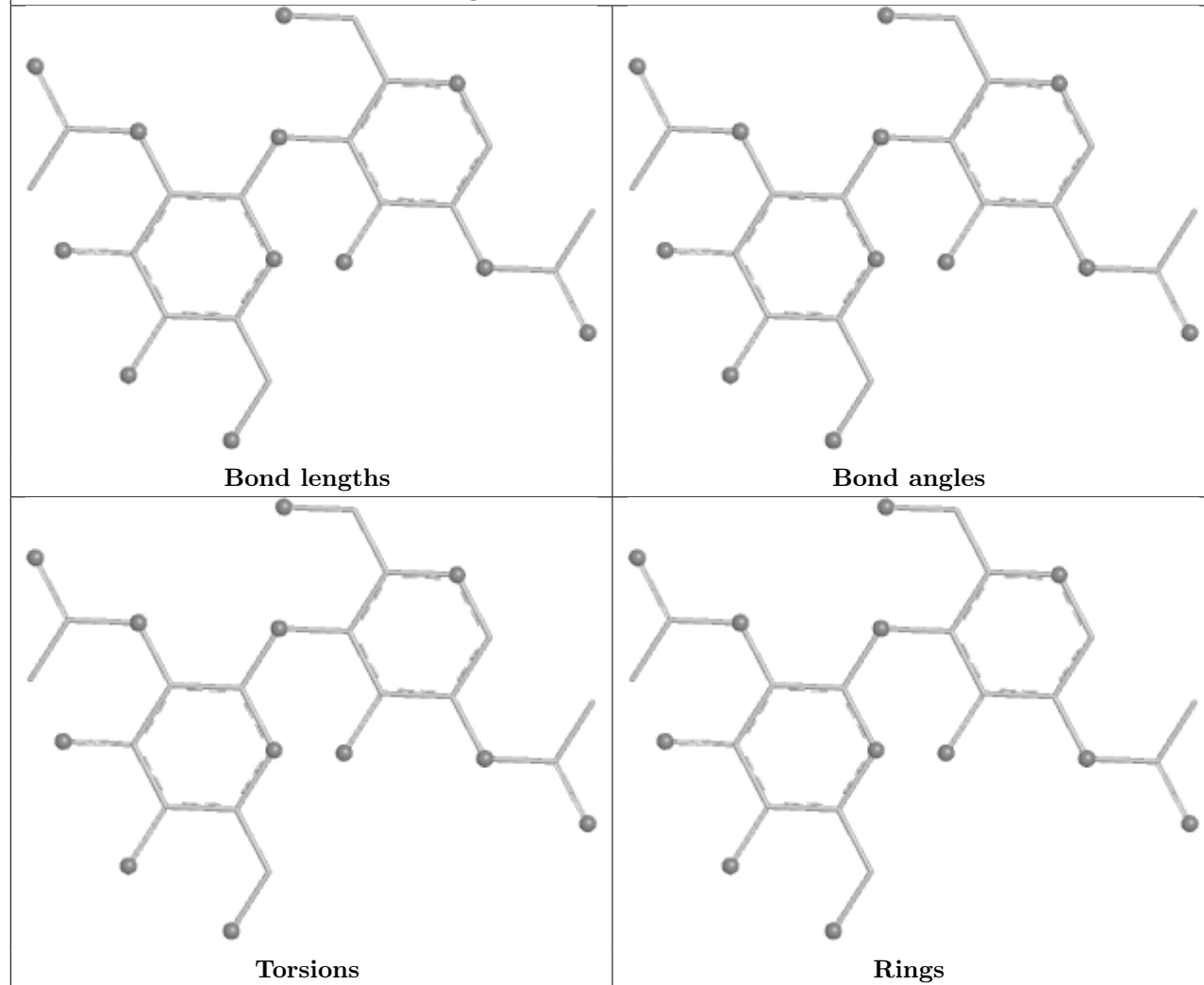


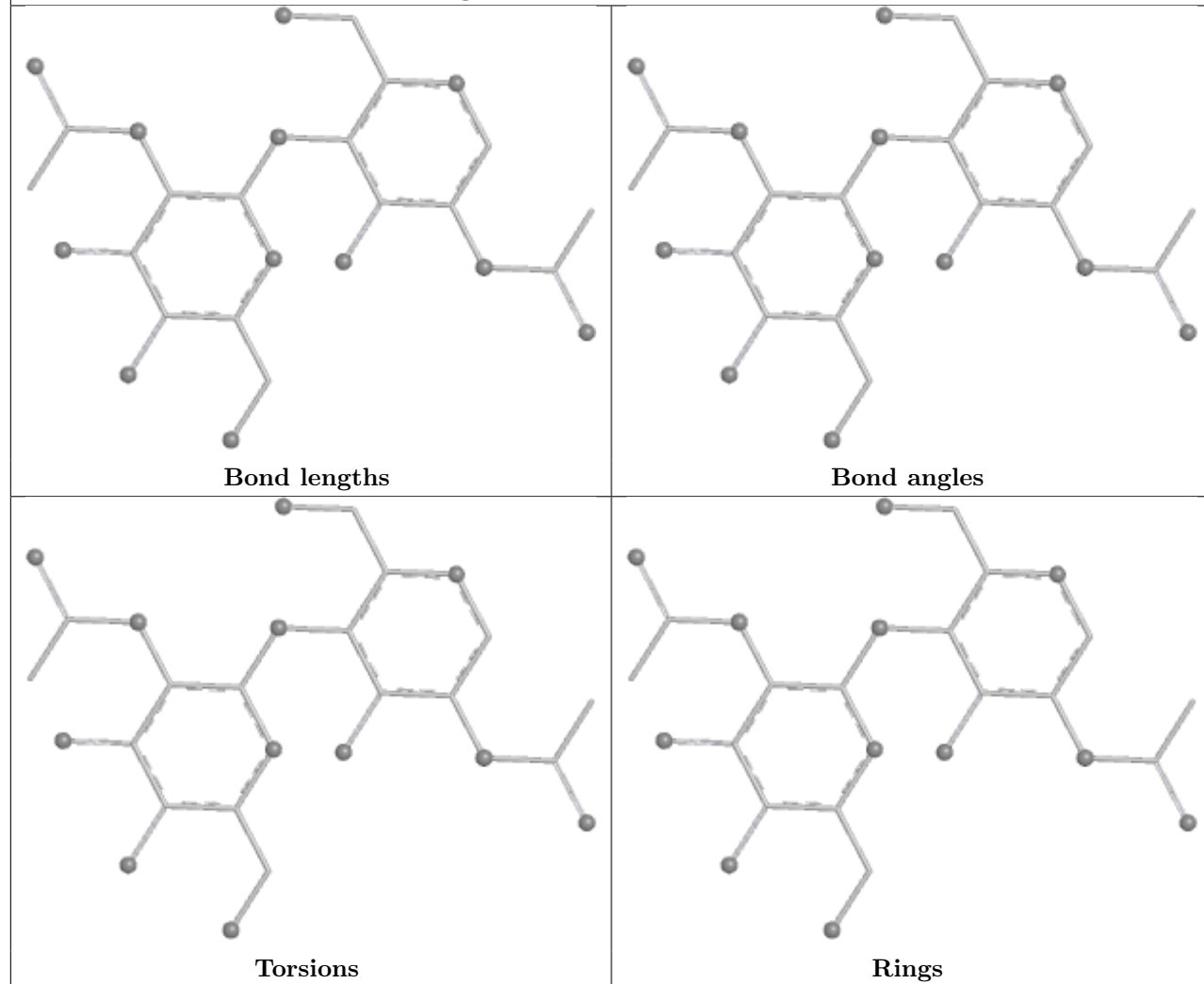
Oligosaccharide Chain BA

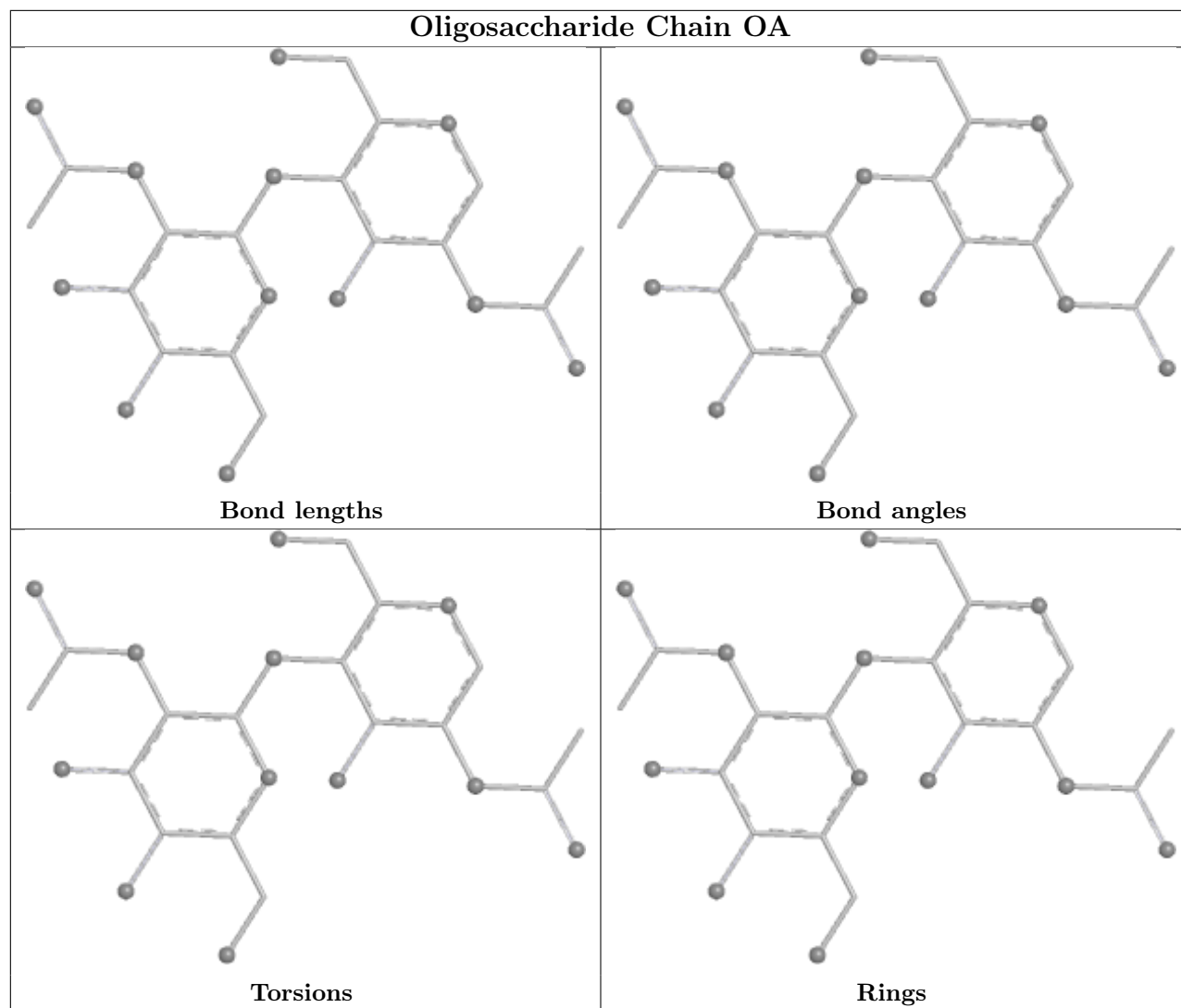
Oligosaccharide Chain HA

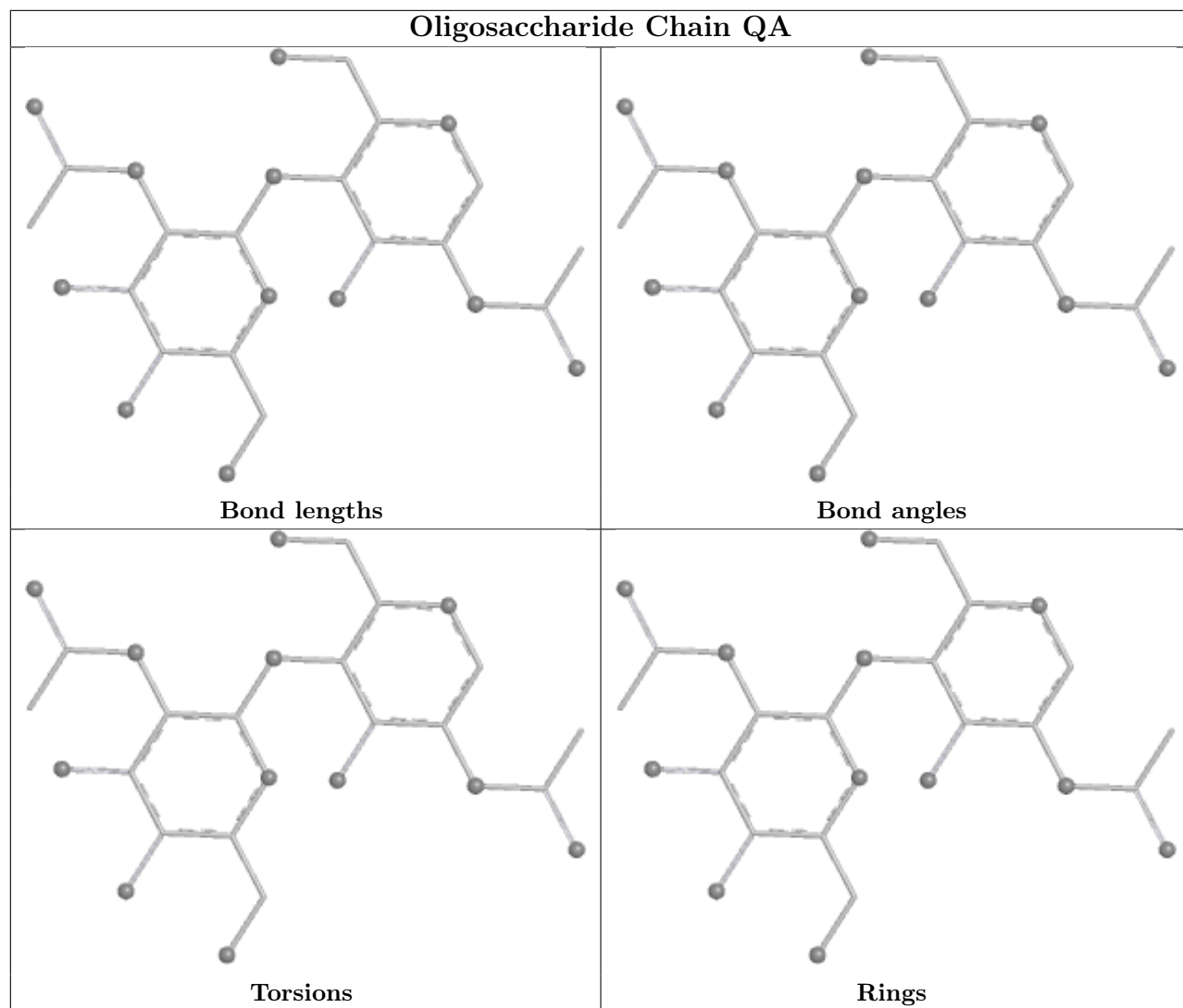
Oligosaccharide Chain IA

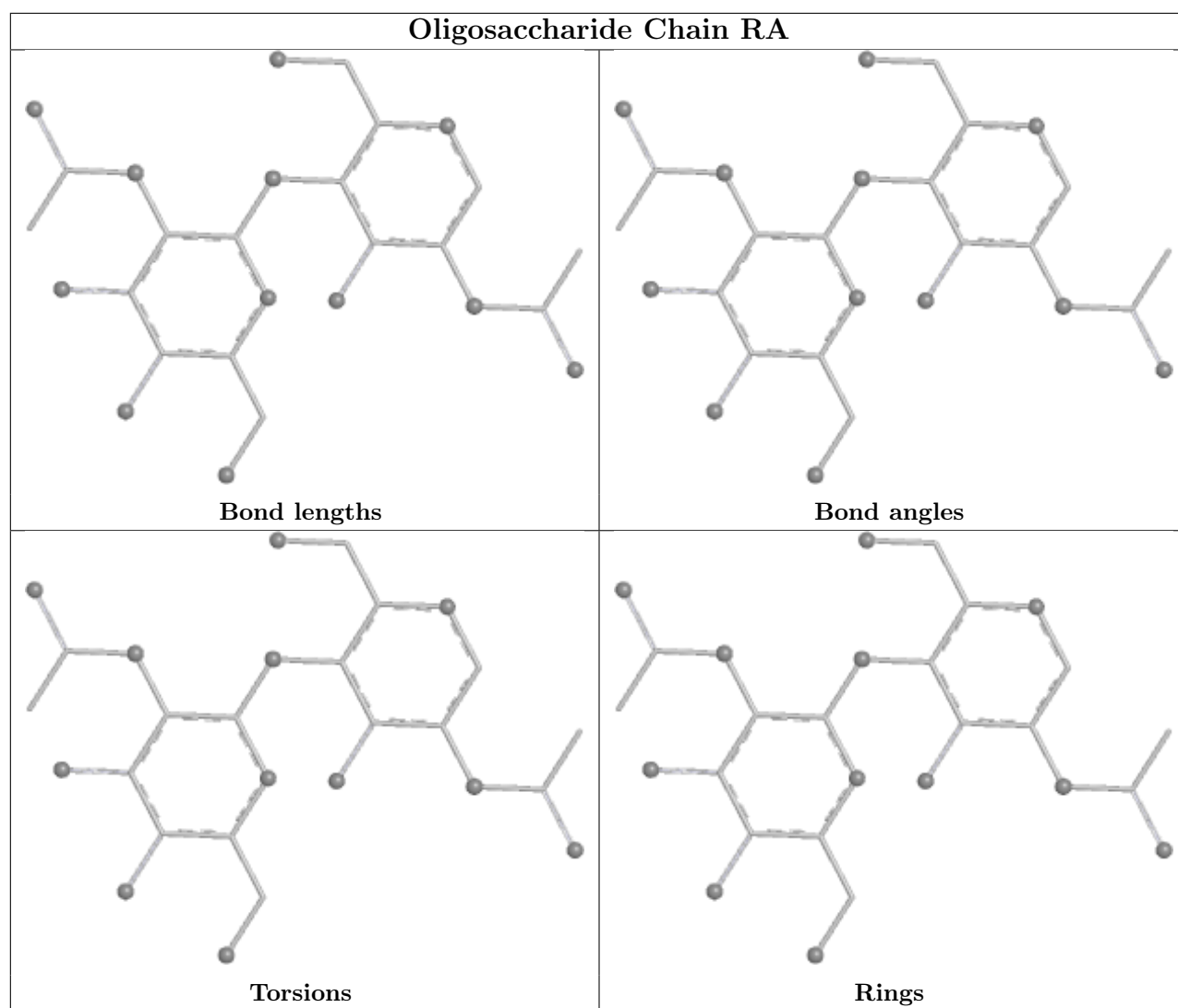


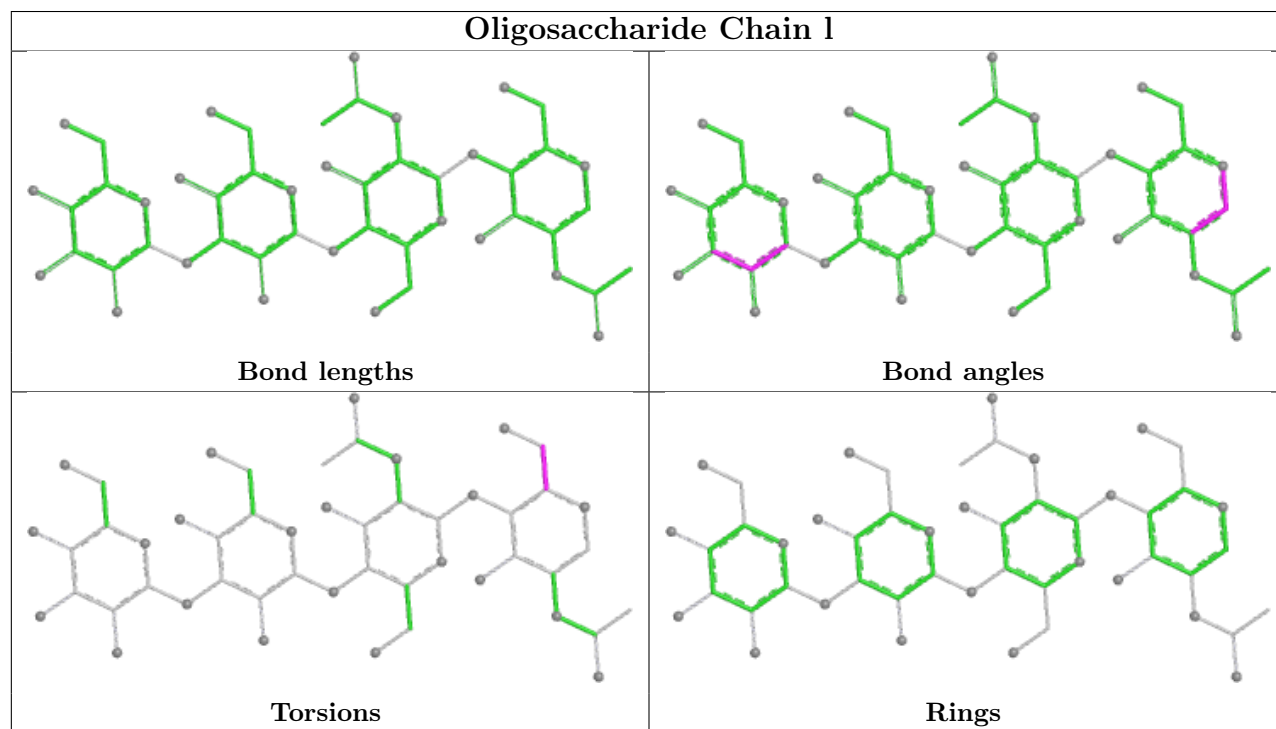
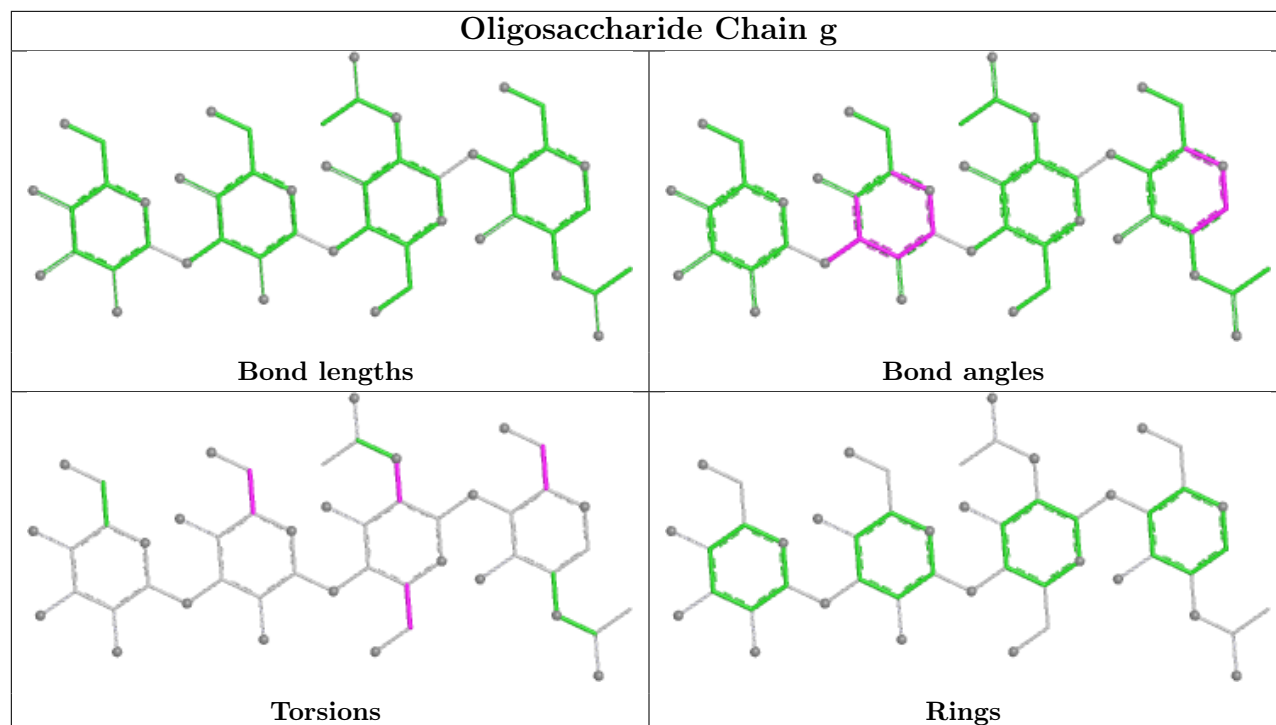
Oligosaccharide Chain JA

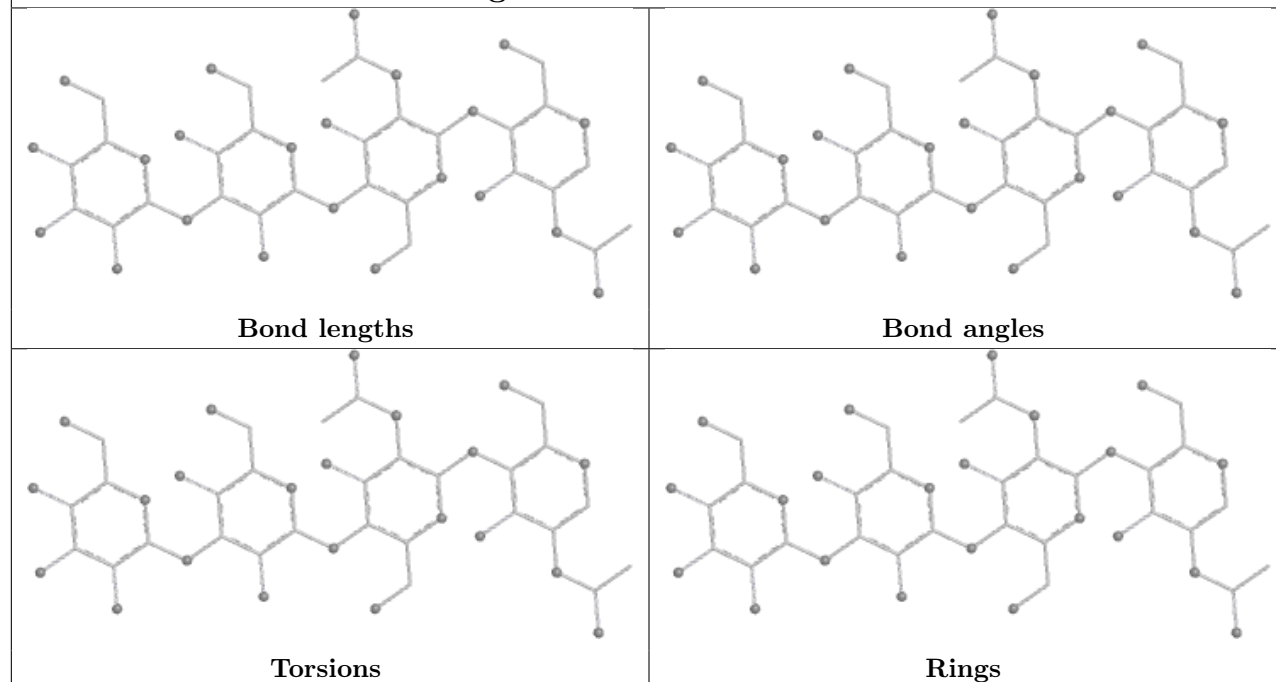
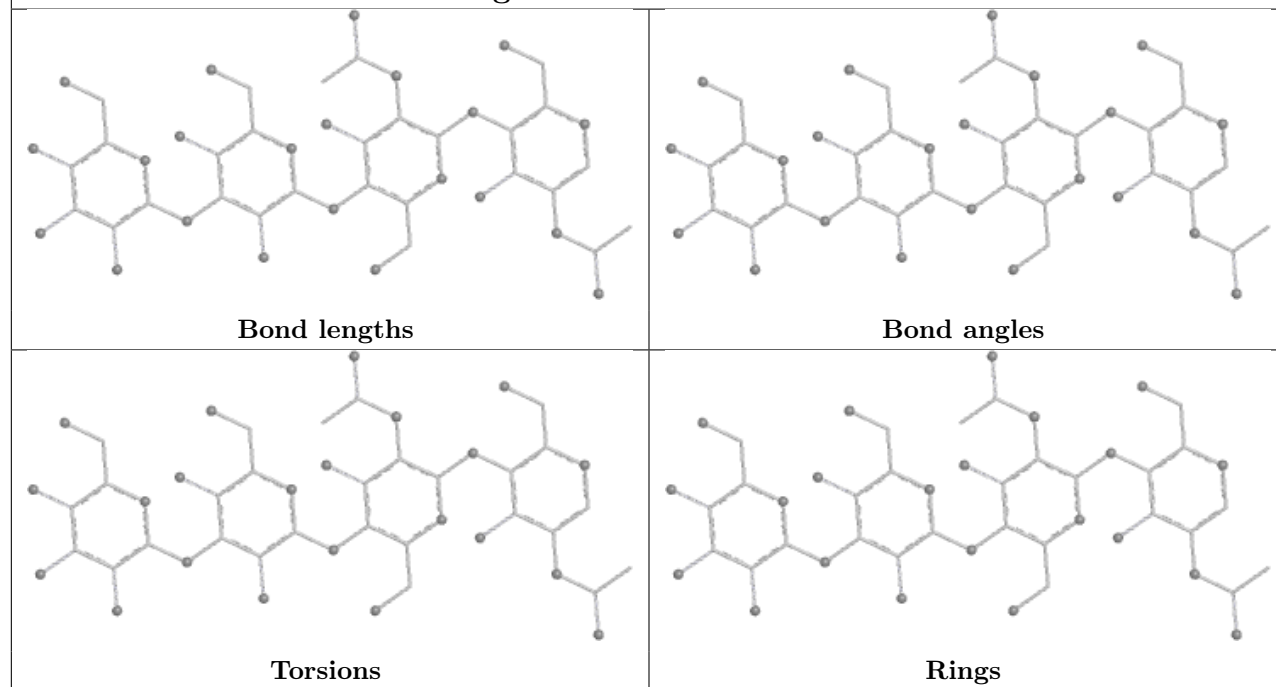
Oligosaccharide Chain MA

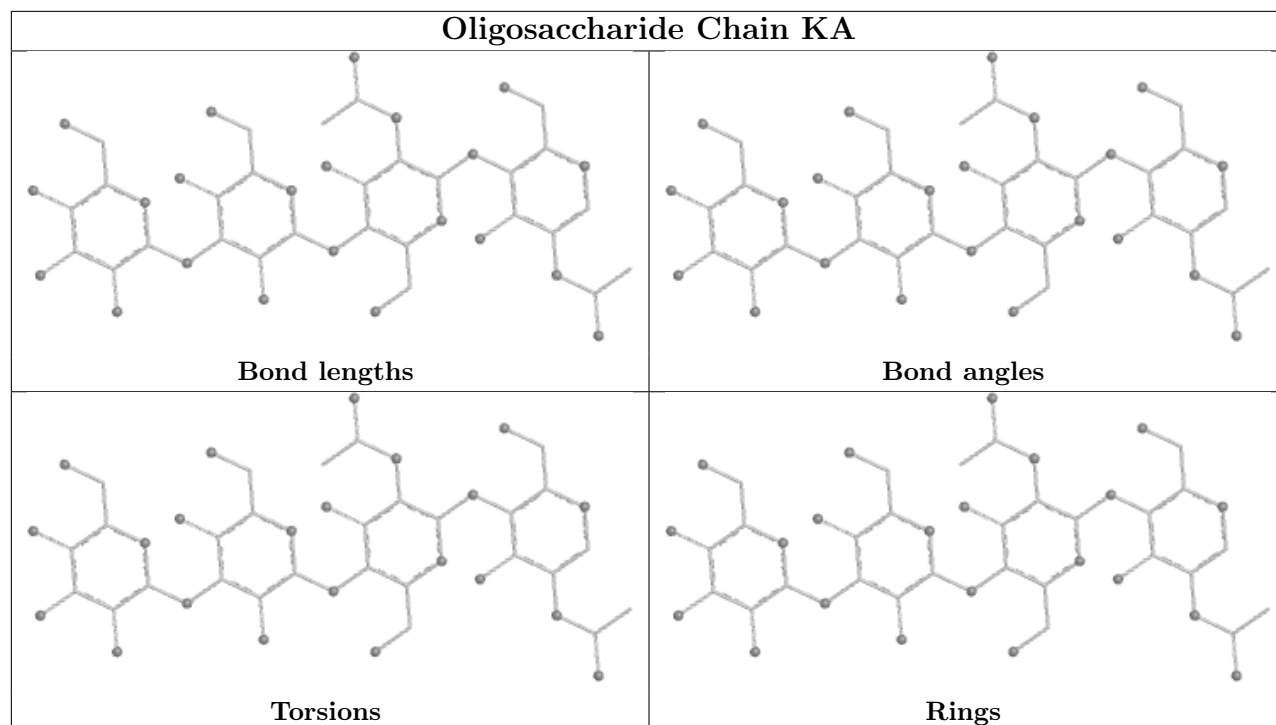
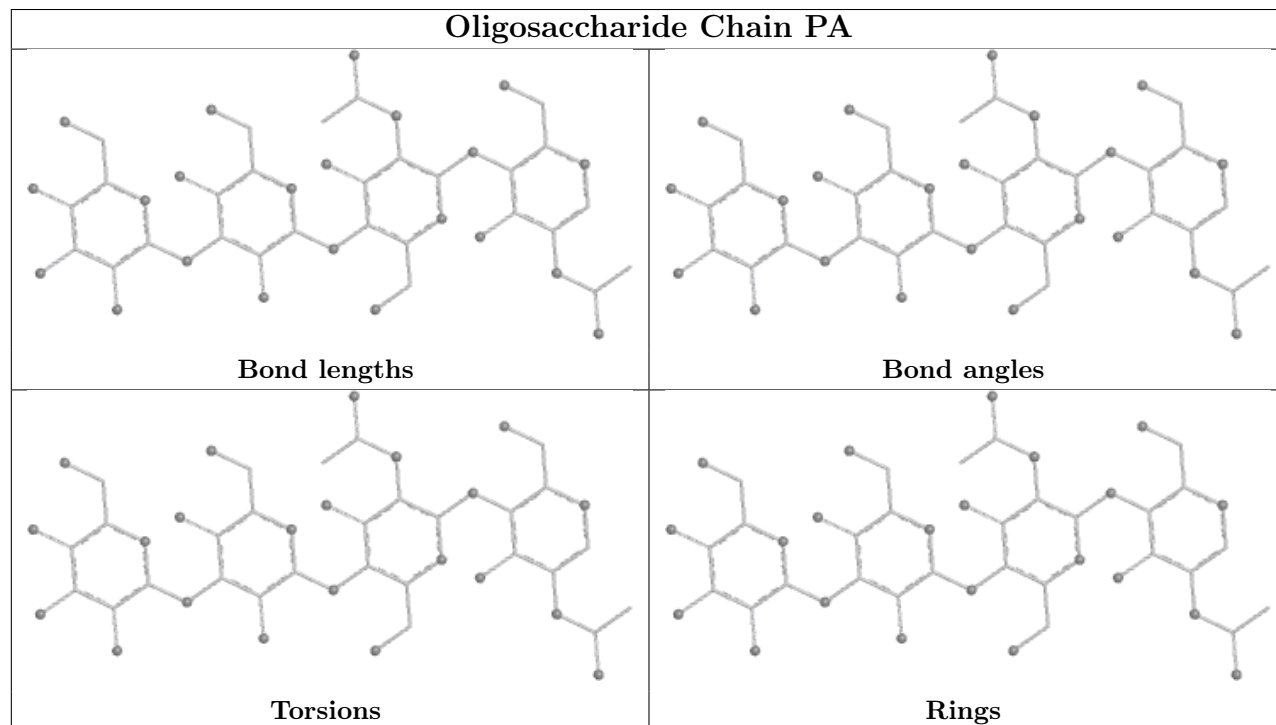


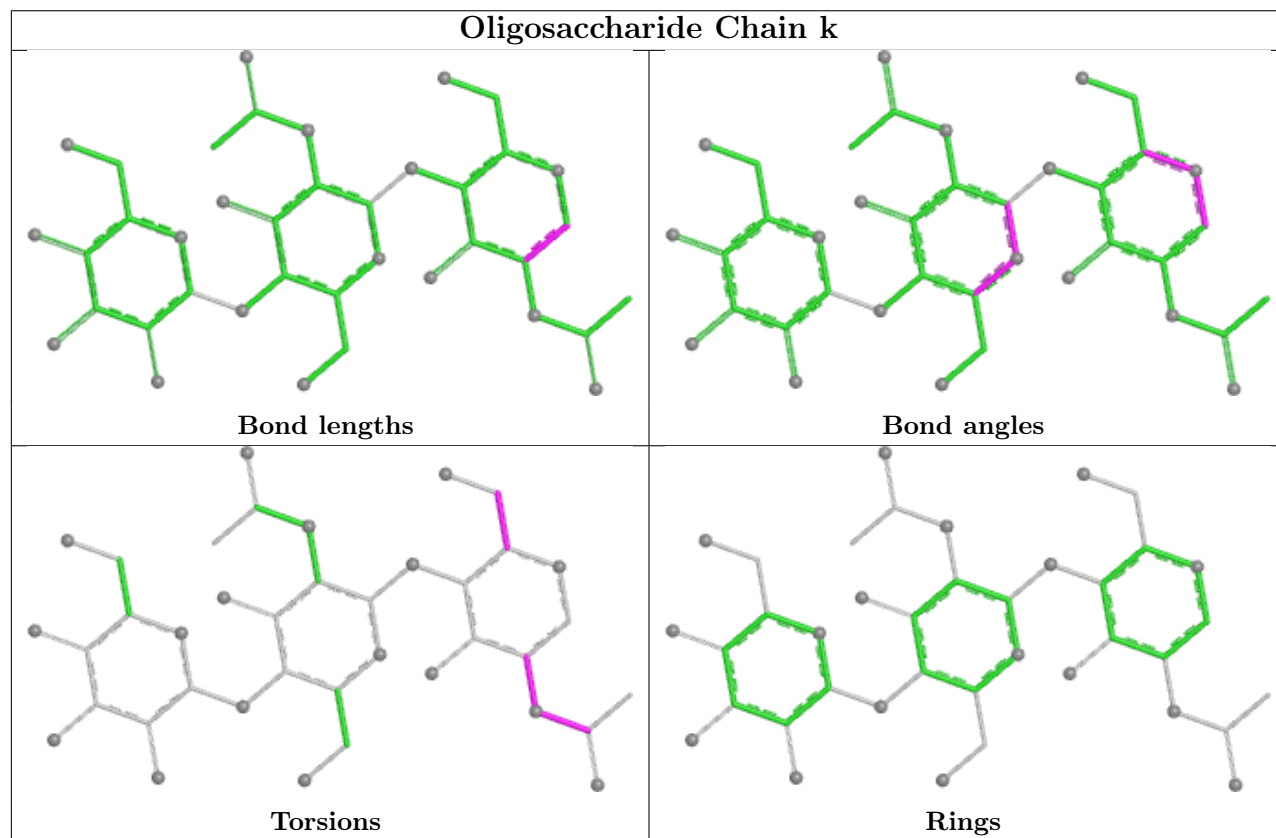
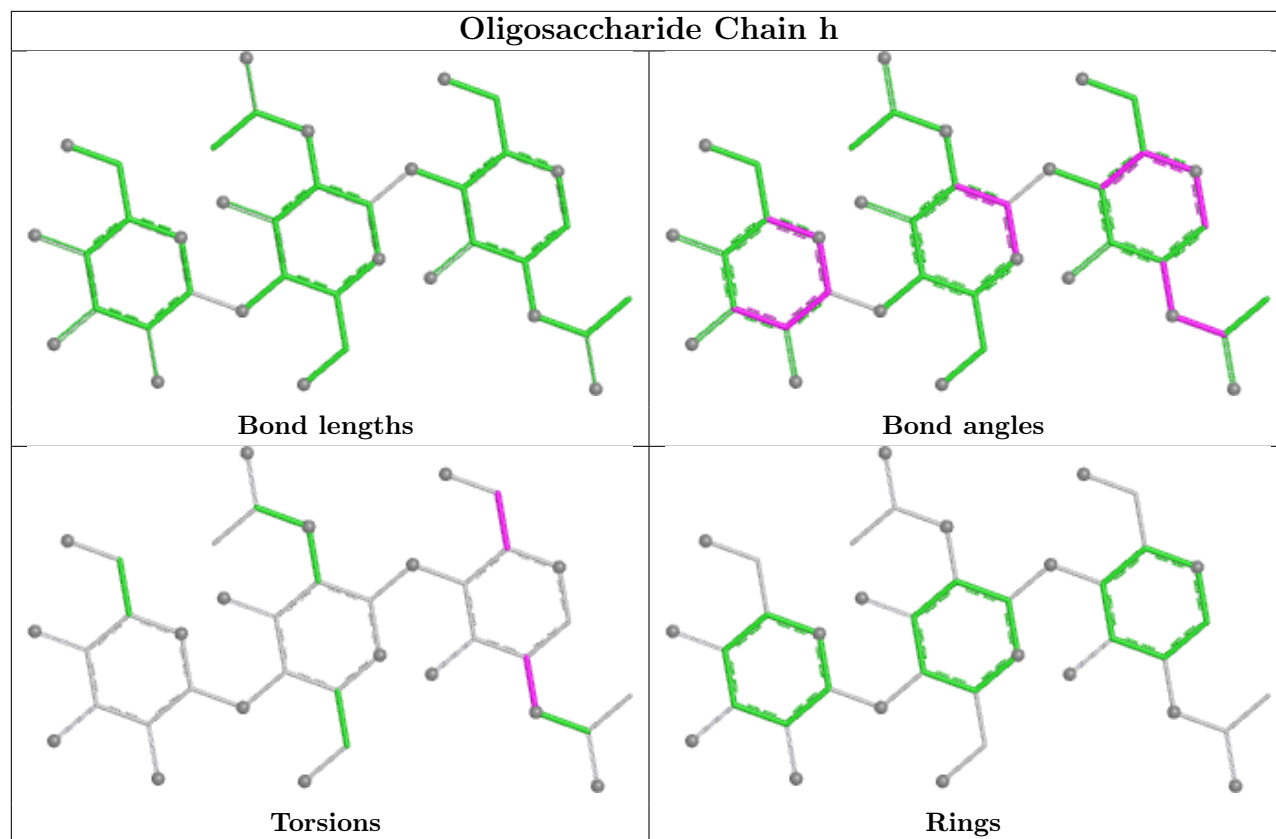
Oligosaccharide Chain QA

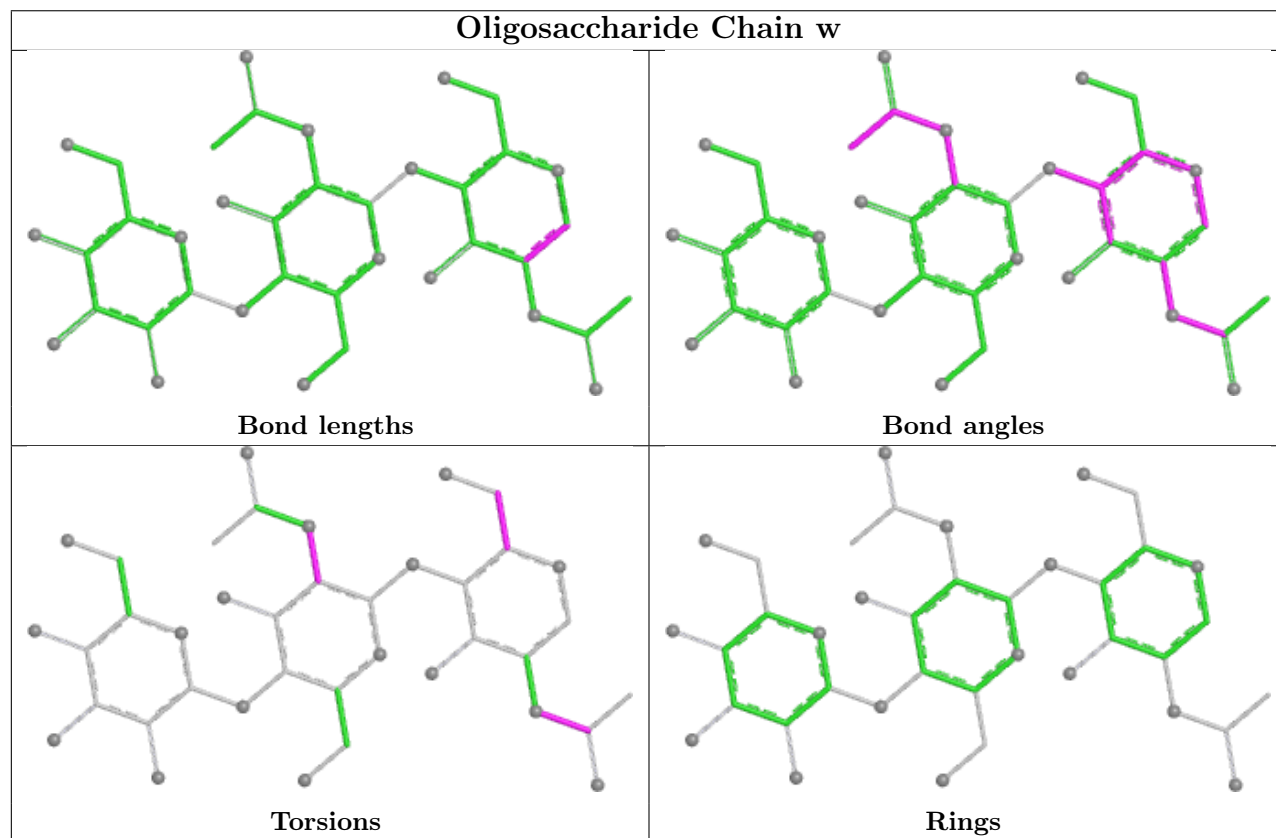
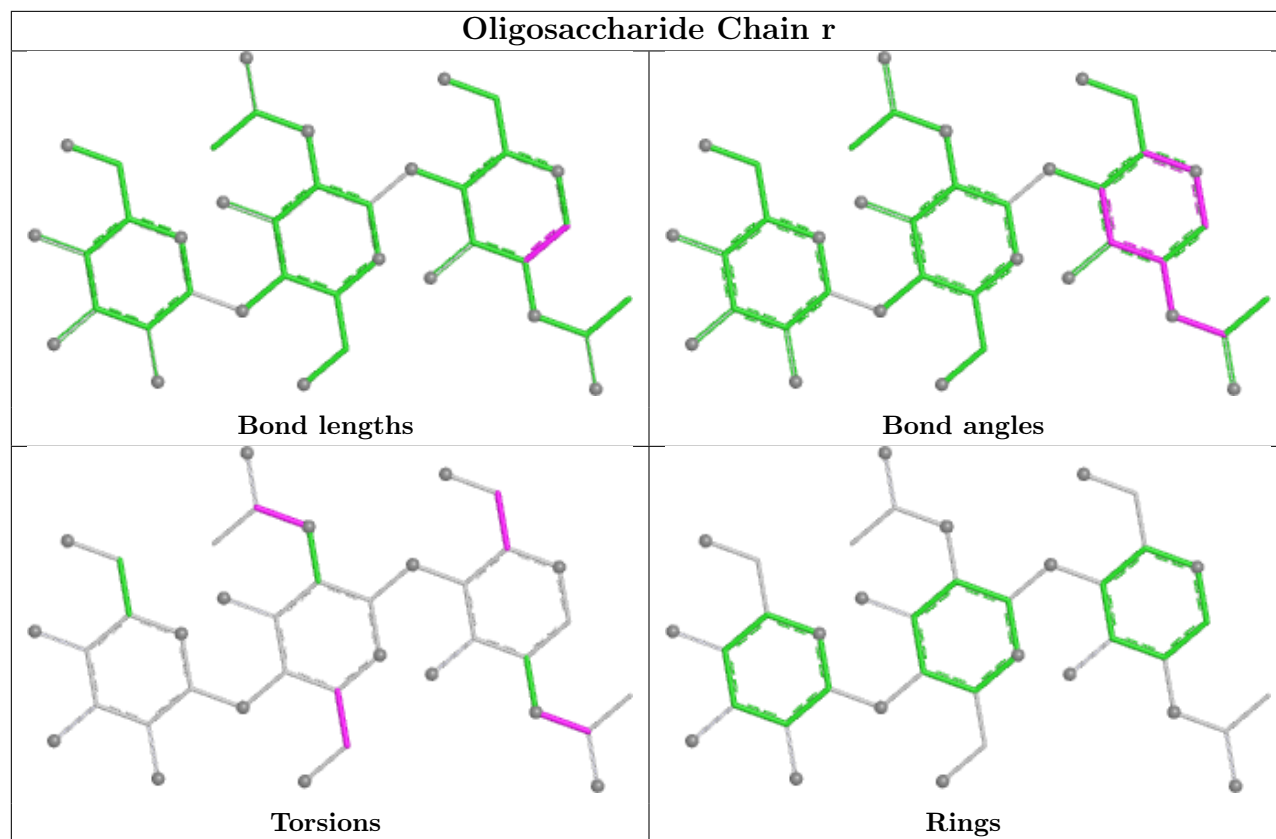


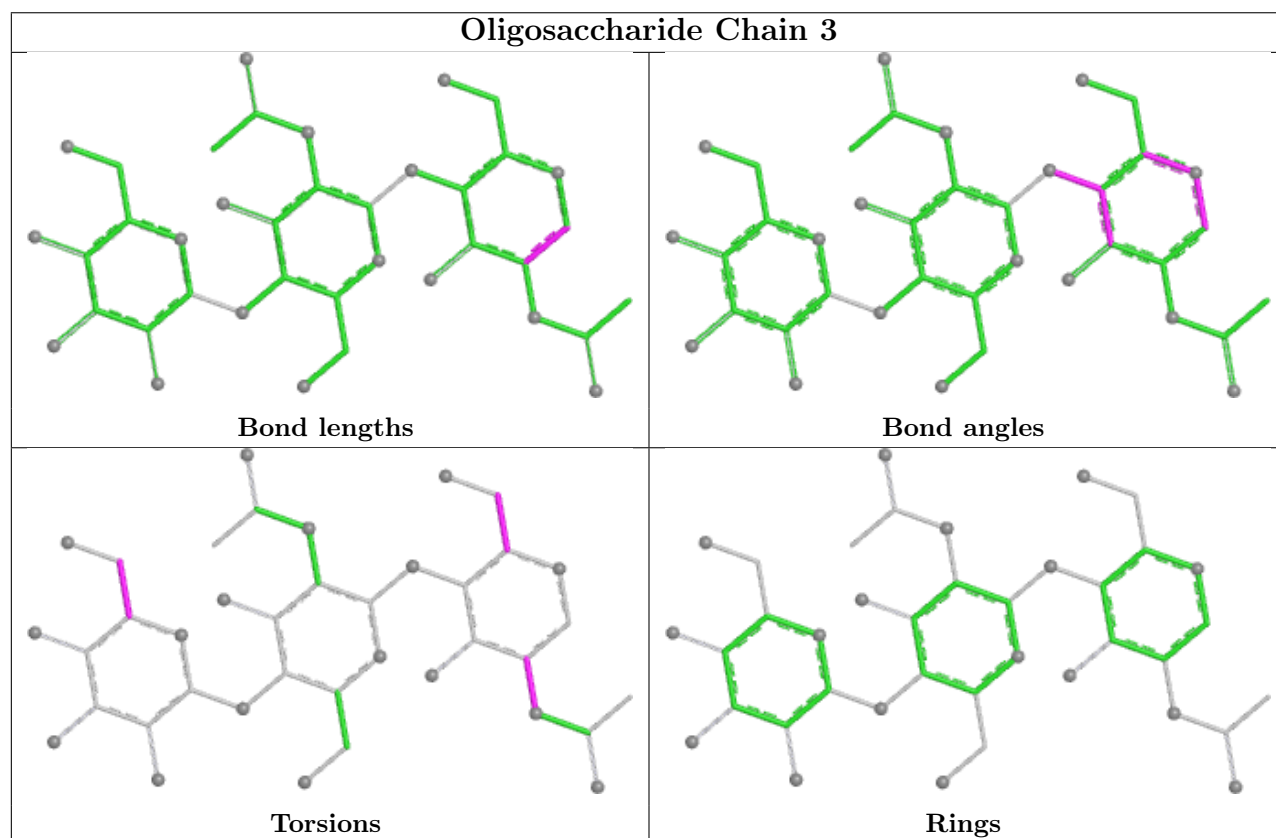
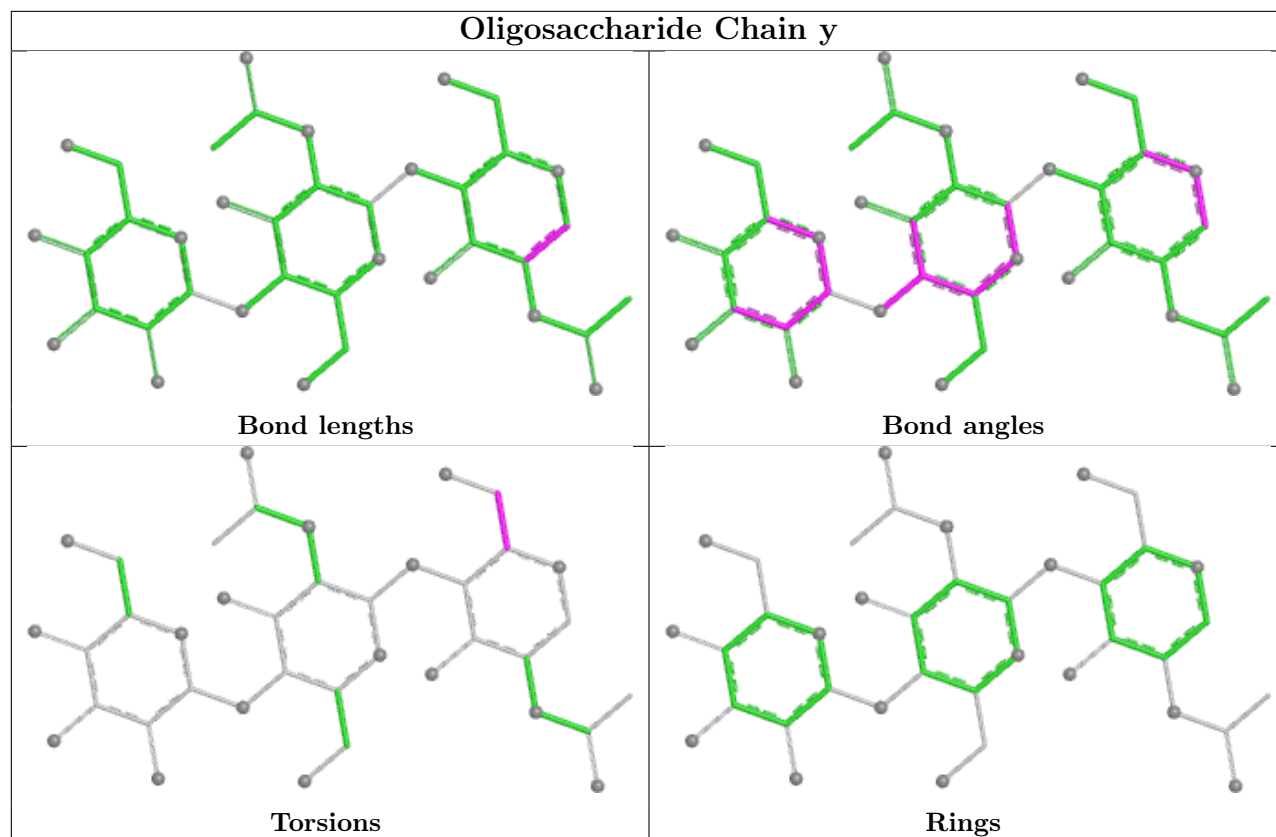


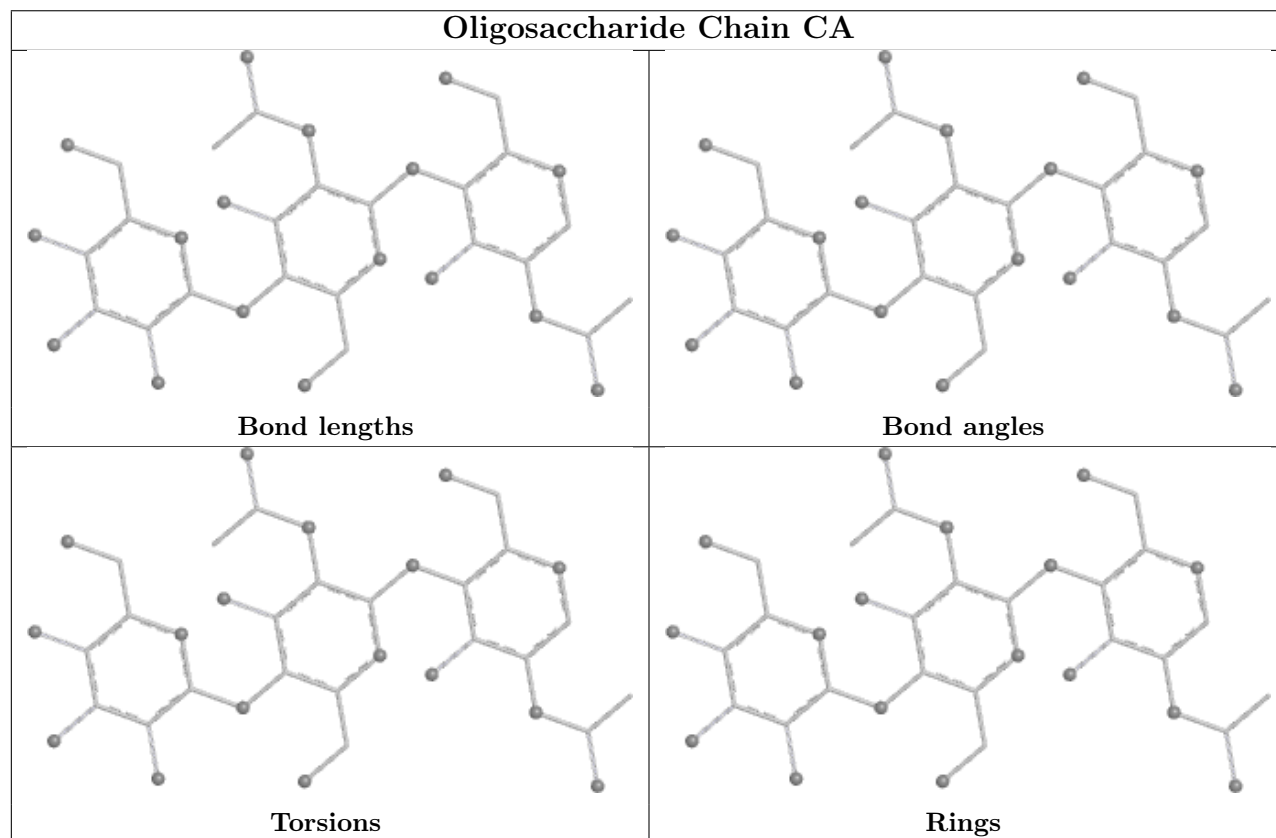
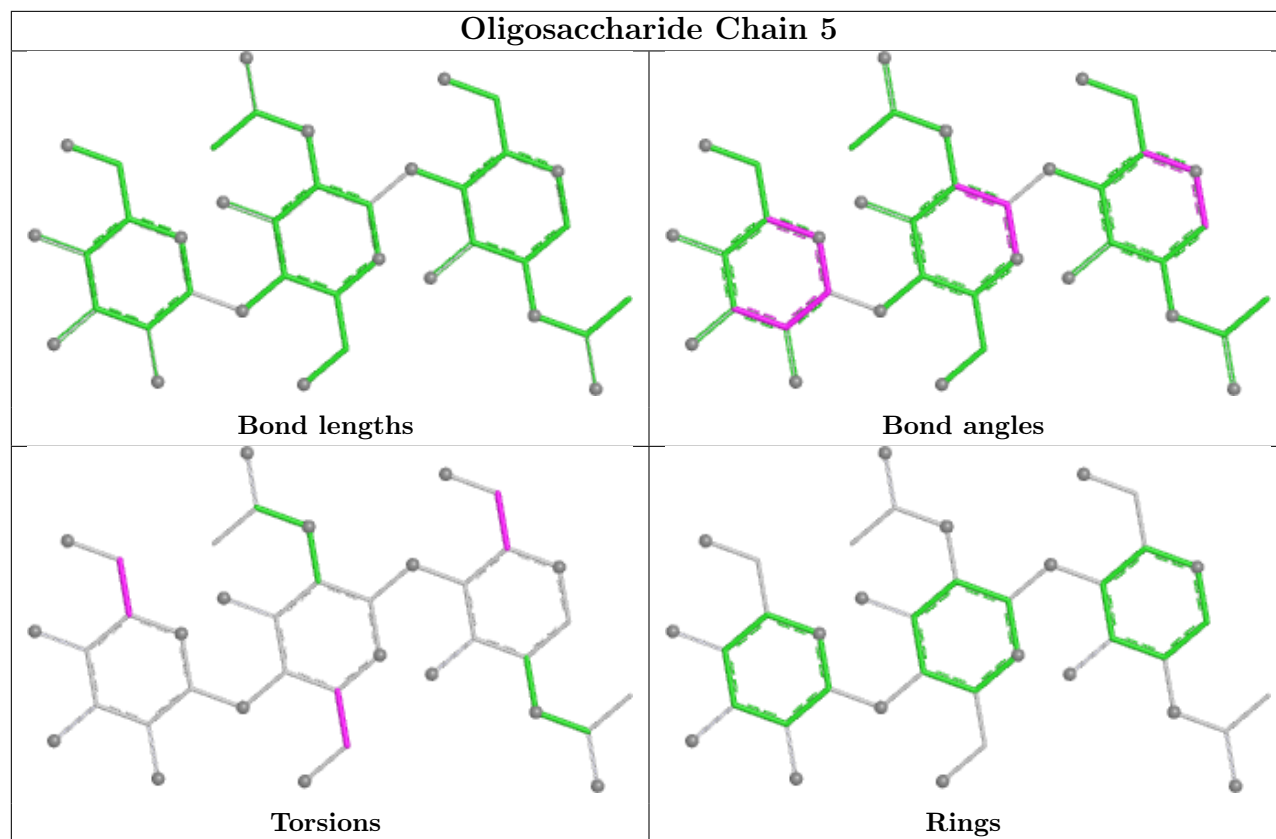
Oligosaccharide Chain AA**Oligosaccharide Chain FA**

Oligosaccharide Chain KA**Oligosaccharide Chain PA**

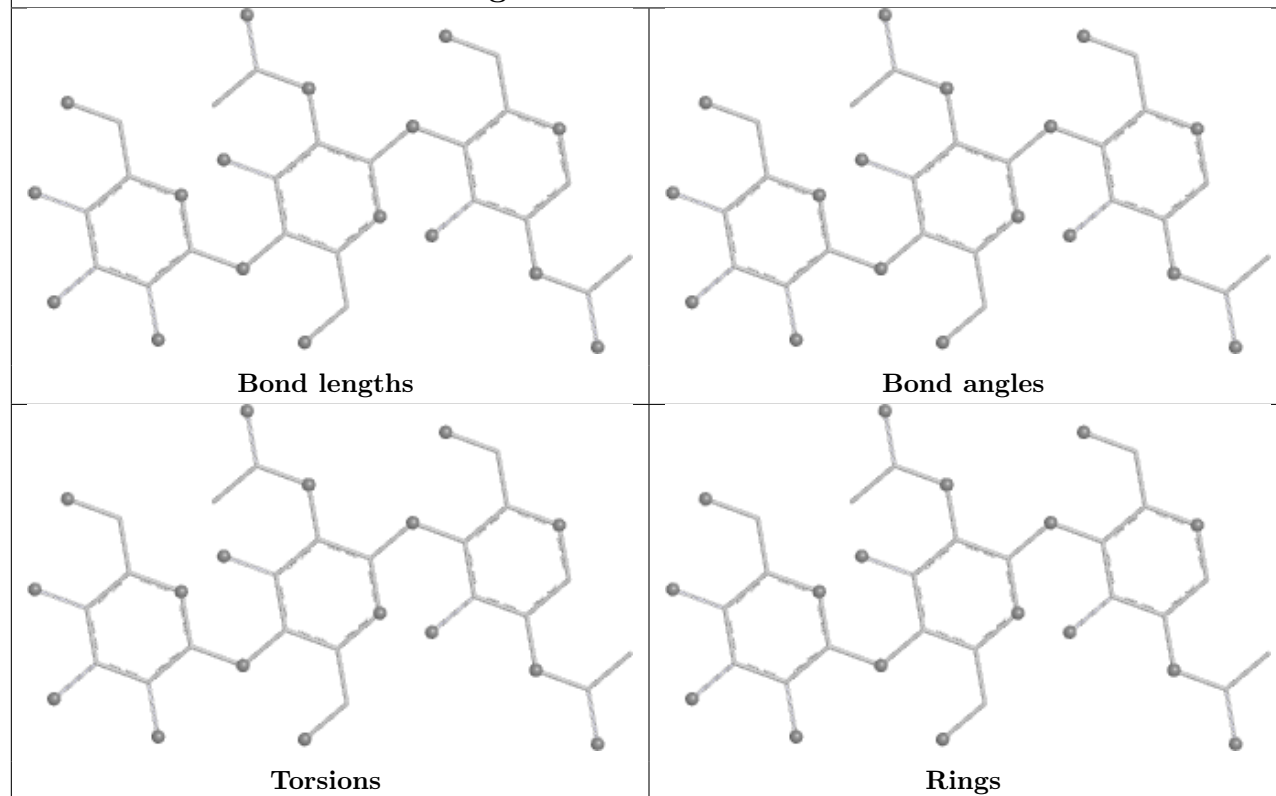




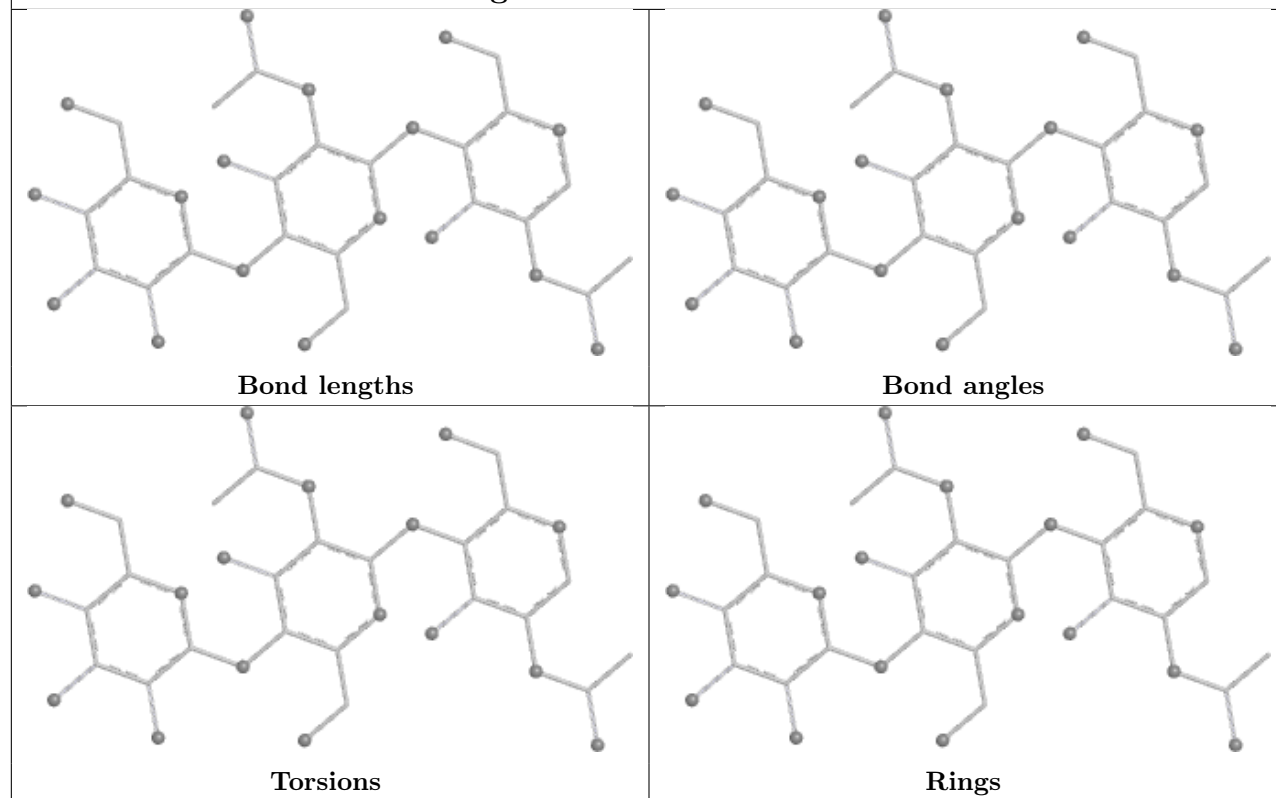




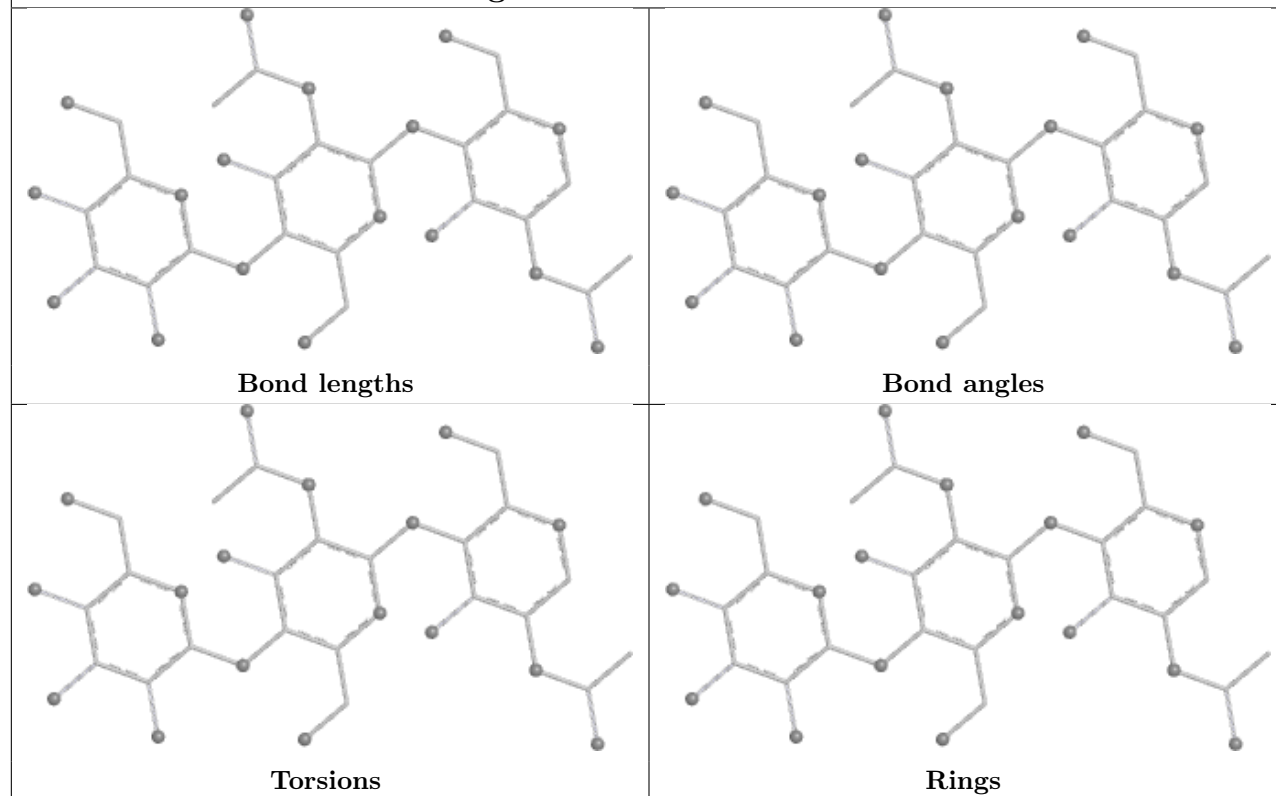
Oligosaccharide Chain DA



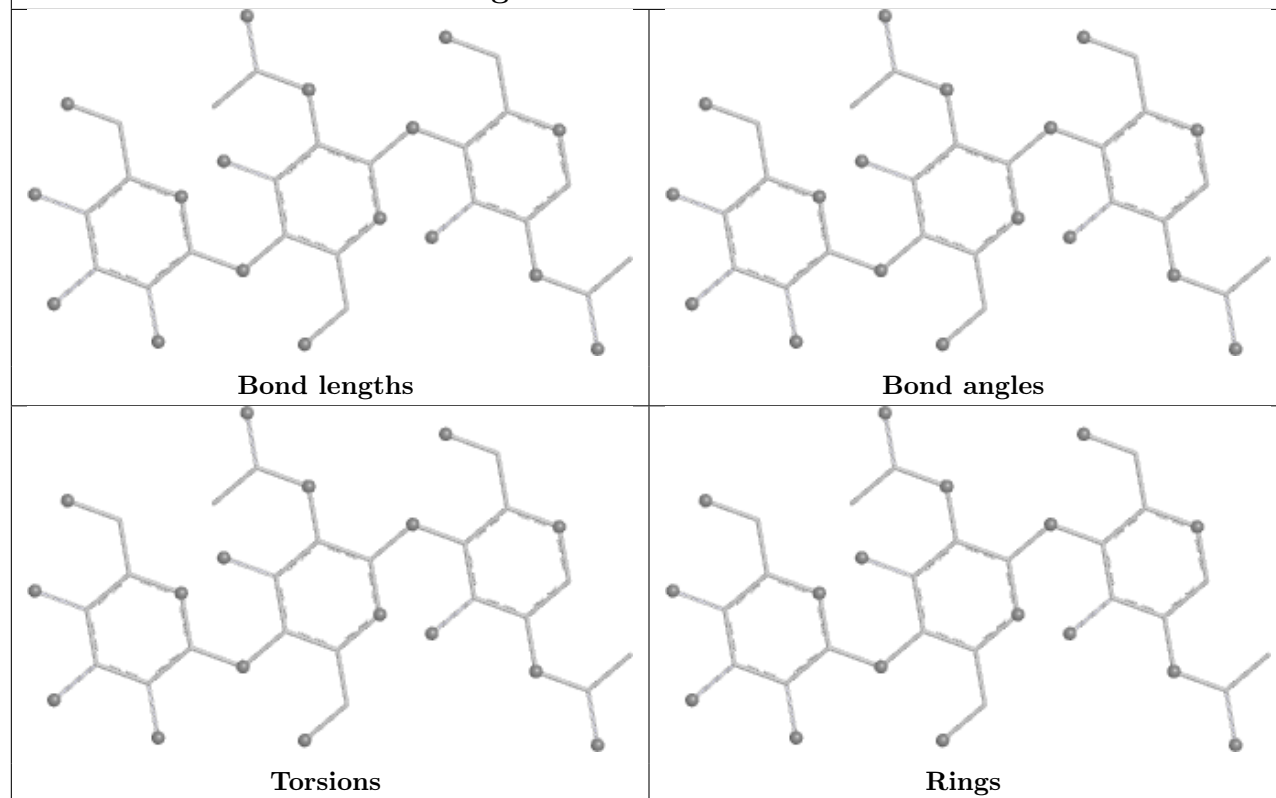
Oligosaccharide Chain EA



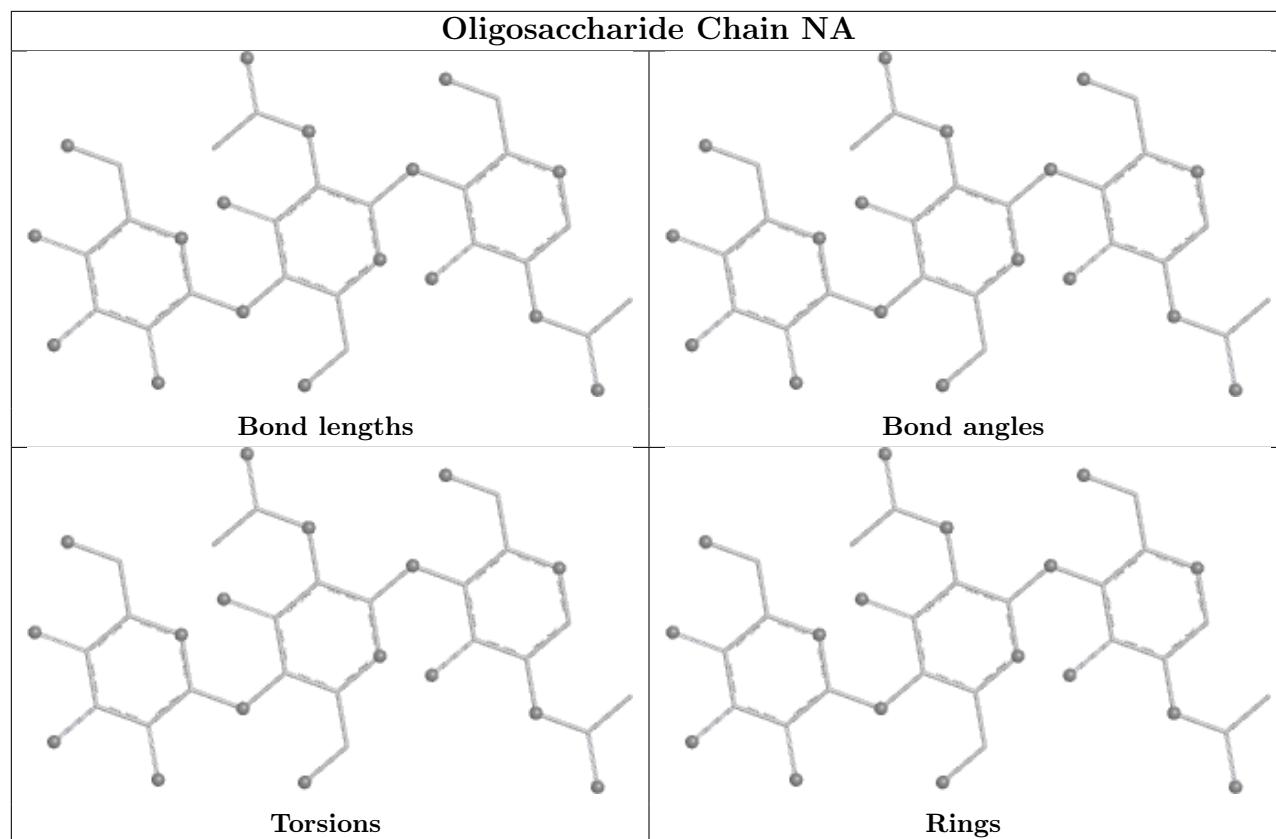
Oligosaccharide Chain GA



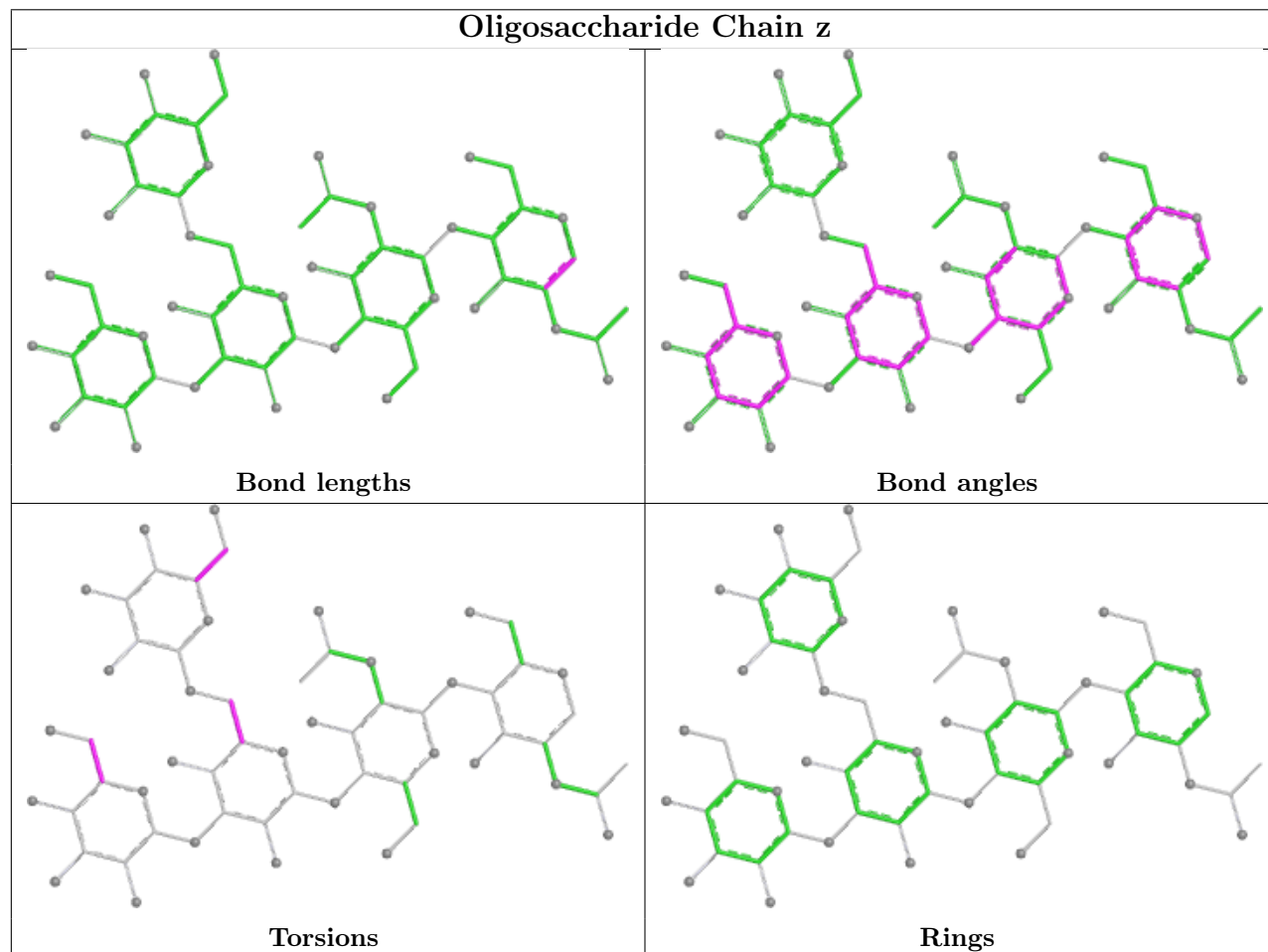
Oligosaccharide Chain LA

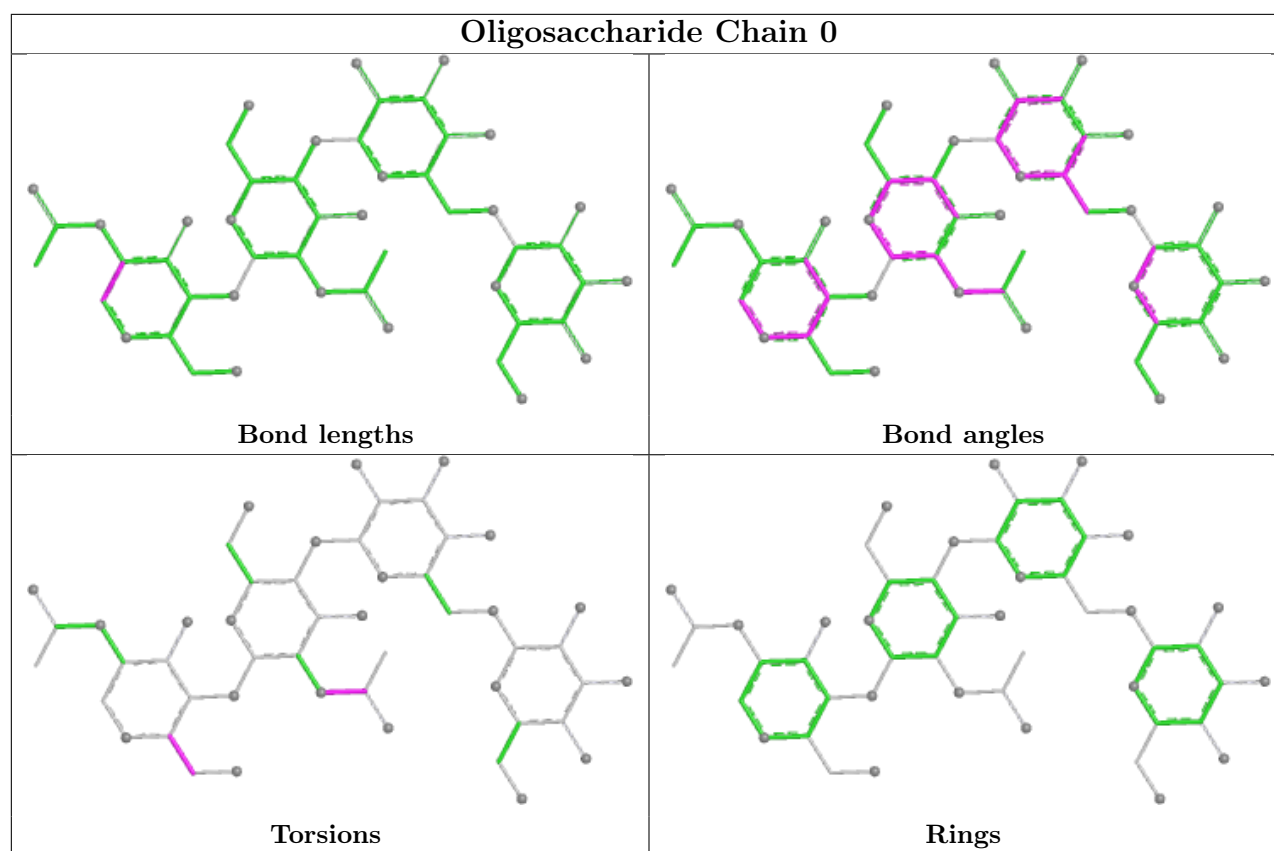


Oligosaccharide Chain NA



Oligosaccharide Chain z





5.6 Ligand geometry [i](#)

100 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
9	CUO	J	5001	1	0,4,4	-	-	-		
9	CUO	A	5005[C]	-	0,4,4	-	-	-		
9	CUO	P	5003	1	0,4,4	-	-	-		
9	CUO	J	5005[C]	-	0,4,4	-	-	-		
9	CUO	D	5004	1	0,4,4	-	-	-		
9	CUO	P	5005[D]	-	0,4,4	-	-	-		
9	CUO	D	5002	1	0,4,4	-	-	-		
9	CUO	X	3401[A]	3	0,4,4	-	-	-		
9	CUO	V	5003	1	0,4,4	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	CUO	S	2105	1	0,4,4	-	-	-		
9	CUO	U	3401[B]	3	0,4,4	-	-	-		
9	CUO	P	5001	1	0,4,4	-	-	-		
9	CUO	L	3401[A]	3	0,4,4	-	-	-		
9	CUO	F	3401[A]	3	0,4,4	-	-	-		
9	CUO	O	3401[B]	3	0,4,4	-	-	-		
9	CUO	a	3401[B]	3	0,4,4	-	-	-		
9	CUO	R	3401[B]	3	0,4,4	-	-	-		
9	CUO	A	5004	1	0,4,4	-	-	-		
9	CUO	I	3401[A]	3	0,4,4	-	-	-		
9	CUO	A	5001	1	0,4,4	-	-	-		
9	CUO	M	2101[C]	-	0,4,4	-	-	-		
9	CUO	Q	3001	2	0,4,4	-	-	-		
9	CUO	S	2103	1	0,4,4	-	-	-		
9	CUO	V	5001	1	0,4,4	-	-	-		
9	CUO	J	5003	1	0,4,4	-	-	-		
9	CUO	N	3001	2	0,4,4	-	-	-		
9	CUO	J	5002	1	0,4,4	-	-	-		
9	CUO	Y	2101[D]	-	0,4,4	-	-	-		
9	CUO	B	3002	2	0,4,4	-	-	-		
9	CUO	J	5004	1	0,4,4	-	-	-		
9	CUO	K	3001	2	0,4,4	-	-	-		
9	CUO	d	3401[B]	3	0,4,4	-	-	-		
9	CUO	X	3401[B]	3	0,4,4	-	-	-		
9	CUO	V	5002	1	0,4,4	-	-	-		
9	CUO	V	5004	1	0,4,4	-	-	-		
9	CUO	D	5005[D]	-	0,4,4	-	-	-		
9	CUO	Y	2101[C]	-	0,4,4	-	-	-		
9	CUO	C	3401[A]	3	0,4,4	-	-	-		
9	CUO	L	3401[B]	3	0,4,4	-	-	-		
9	CUO	P	5005[C]	-	0,4,4	-	-	-		
9	CUO	F	3401[B]	3	0,4,4	-	-	-		
9	CUO	B	3001	2	0,4,4	-	-	-		
9	CUO	Y	2105	1	0,4,4	-	-	-		
9	CUO	D	5001	1	0,4,4	-	-	-		
9	CUO	M	2103	1	0,4,4	-	-	-		
9	CUO	D	5005[C]	-	0,4,4	-	-	-		
9	CUO	A	5002	1	0,4,4	-	-	-		
9	CUO	S	2102	1	0,4,4	-	-	-		
9	CUO	Y	2104	1	0,4,4	-	-	-		
9	CUO	T	3002	2	0,4,4	-	-	-		
9	CUO	D	5003	1	0,4,4	-	-	-		
9	CUO	G	2105	1	0,4,4	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	CUO	Z	3001	2	0,4,4	-	-	-		
9	CUO	V	5005[D]	-	0,4,4	-	-	-		
9	CUO	H	3001	2	0,4,4	-	-	-		
9	CUO	H	3002	2	0,4,4	-	-	-		
9	CUO	V	5005[C]	-	0,4,4	-	-	-		
9	CUO	U	3401[A]	3	0,4,4	-	-	-		
9	CUO	b	2102	1	0,4,4	-	-	-		
9	CUO	Y	2102	1	0,4,4	-	-	-		
9	CUO	S	2104	1	0,4,4	-	-	-		
9	CUO	M	2104	1	0,4,4	-	-	-		
9	CUO	O	3401[A]	3	0,4,4	-	-	-		
9	CUO	N	3002	2	0,4,4	-	-	-		
9	CUO	W	3002	2	0,4,4	-	-	-		
9	CUO	a	3401[A]	3	0,4,4	-	-	-		
9	CUO	R	3401[A]	3	0,4,4	-	-	-		
9	CUO	M	2102	1	0,4,4	-	-	-		
9	CUO	b	2105	1	0,4,4	-	-	-		
9	CUO	W	3001	2	0,4,4	-	-	-		
9	CUO	P	5002	1	0,4,4	-	-	-		
9	CUO	c	3002	2	0,4,4	-	-	-		
9	CUO	I	3401[B]	3	0,4,4	-	-	-		
9	CUO	J	5005[D]	-	0,4,4	-	-	-		
9	CUO	K	3002	2	0,4,4	-	-	-		
9	CUO	A	5003	1	0,4,4	-	-	-		
9	CUO	d	3401[A]	3	0,4,4	-	-	-		
9	CUO	E	3002	2	0,4,4	-	-	-		
9	CUO	T	3001	2	0,4,4	-	-	-		
9	CUO	G	2102	1	0,4,4	-	-	-		
9	CUO	Z	3002	2	0,4,4	-	-	-		
9	CUO	Q	3002	2	0,4,4	-	-	-		
9	CUO	b	2101[D]	-	0,4,4	-	-	-		
9	CUO	M	2101[D]	-	0,4,4	-	-	-		
9	CUO	b	2103	1	0,4,4	-	-	-		
9	CUO	Y	2103	1	0,4,4	-	-	-		
9	CUO	G	2101[D]	-	0,4,4	-	-	-		
9	CUO	S	2101[D]	-	0,4,4	-	-	-		
9	CUO	E	3001	2	0,4,4	-	-	-		
9	CUO	b	2101[C]	-	0,4,4	-	-	-		
9	CUO	C	3401[B]	3	0,4,4	-	-	-		
9	CUO	P	5004	1	0,4,4	-	-	-		
9	CUO	G	2103	1	0,4,4	-	-	-		
9	CUO	b	2104	1	0,4,4	-	-	-		
9	CUO	G	2101[C]	-	0,4,4	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	CUO	A	5005[D]	-	0,4,4	-	-	-		
9	CUO	S	2101[C]	-	0,4,4	-	-	-		
9	CUO	M	2105	1	0,4,4	-	-	-		
9	CUO	c	3001	2	0,4,4	-	-	-		
9	CUO	G	2104	1	0,4,4	-	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	CUO	J	5001	1	-	-	0/1/1/1
9	CUO	A	5005[C]	-	-	-	0/1/1/1
9	CUO	P	5003	1	-	-	0/1/1/1
9	CUO	J	5005[C]	-	-	-	0/1/1/1
9	CUO	D	5004	1	-	-	0/1/1/1
9	CUO	P	5005[D]	-	-	-	0/1/1/1
9	CUO	D	5002	1	-	-	0/1/1/1
9	CUO	X	3401[A]	3	-	-	0/1/1/1
9	CUO	V	5003	1	-	-	0/1/1/1
9	CUO	S	2105	1	-	-	0/1/1/1
9	CUO	U	3401[B]	3	-	-	0/1/1/1
9	CUO	P	5001	1	-	-	0/1/1/1
9	CUO	L	3401[A]	3	-	-	0/1/1/1
9	CUO	F	3401[A]	3	-	-	0/1/1/1
9	CUO	O	3401[B]	3	-	-	0/1/1/1
9	CUO	a	3401[B]	3	-	-	0/1/1/1
9	CUO	R	3401[B]	3	-	-	0/1/1/1
9	CUO	A	5004	1	-	-	0/1/1/1
9	CUO	I	3401[A]	3	-	-	0/1/1/1
9	CUO	A	5001	1	-	-	0/1/1/1
9	CUO	M	2101[C]	-	-	-	0/1/1/1
9	CUO	Q	3001	2	-	-	0/1/1/1
9	CUO	S	2103	1	-	-	0/1/1/1
9	CUO	V	5001	1	-	-	0/1/1/1
9	CUO	J	5003	1	-	-	0/1/1/1
9	CUO	N	3001	2	-	-	0/1/1/1
9	CUO	J	5002	1	-	-	0/1/1/1
9	CUO	Y	2101[D]	-	-	-	0/1/1/1
9	CUO	B	3002	2	-	-	0/1/1/1
9	CUO	J	5004	1	-	-	0/1/1/1
9	CUO	K	3001	2	-	-	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	CUO	d	3401[B]	3	-	-	0/1/1/1
9	CUO	X	3401[B]	3	-	-	0/1/1/1
9	CUO	V	5002	1	-	-	0/1/1/1
9	CUO	V	5004	1	-	-	0/1/1/1
9	CUO	D	5005[D]	-	-	-	0/1/1/1
9	CUO	Y	2101[C]	-	-	-	0/1/1/1
9	CUO	C	3401[A]	3	-	-	0/1/1/1
9	CUO	L	3401[B]	3	-	-	0/1/1/1
9	CUO	P	5005[C]	-	-	-	0/1/1/1
9	CUO	F	3401[B]	3	-	-	0/1/1/1
9	CUO	B	3001	2	-	-	0/1/1/1
9	CUO	Y	2105	1	-	-	0/1/1/1
9	CUO	D	5001	1	-	-	0/1/1/1
9	CUO	M	2103	1	-	-	0/1/1/1
9	CUO	D	5005[C]	-	-	-	0/1/1/1
9	CUO	A	5002	1	-	-	0/1/1/1
9	CUO	S	2102	1	-	-	0/1/1/1
9	CUO	Y	2104	1	-	-	0/1/1/1
9	CUO	T	3002	2	-	-	0/1/1/1
9	CUO	D	5003	1	-	-	0/1/1/1
9	CUO	G	2105	1	-	-	0/1/1/1
9	CUO	Z	3001	2	-	-	0/1/1/1
9	CUO	V	5005[D]	-	-	-	0/1/1/1
9	CUO	H	3001	2	-	-	0/1/1/1
9	CUO	H	3002	2	-	-	0/1/1/1
9	CUO	V	5005[C]	-	-	-	0/1/1/1
9	CUO	U	3401[A]	3	-	-	0/1/1/1
9	CUO	b	2102	1	-	-	0/1/1/1
9	CUO	Y	2102	1	-	-	0/1/1/1
9	CUO	S	2104	1	-	-	0/1/1/1
9	CUO	M	2104	1	-	-	0/1/1/1
9	CUO	O	3401[A]	3	-	-	0/1/1/1
9	CUO	N	3002	2	-	-	0/1/1/1
9	CUO	W	3002	2	-	-	0/1/1/1
9	CUO	a	3401[A]	3	-	-	0/1/1/1
9	CUO	R	3401[A]	3	-	-	0/1/1/1
9	CUO	M	2102	1	-	-	0/1/1/1
9	CUO	b	2105	1	-	-	0/1/1/1
9	CUO	W	3001	2	-	-	0/1/1/1
9	CUO	P	5002	1	-	-	0/1/1/1
9	CUO	c	3002	2	-	-	0/1/1/1
9	CUO	I	3401[B]	3	-	-	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	CUO	J	5005[D]	-	-	-	0/1/1/1
9	CUO	K	3002	2	-	-	0/1/1/1
9	CUO	A	5003	1	-	-	0/1/1/1
9	CUO	d	3401[A]	3	-	-	0/1/1/1
9	CUO	E	3002	2	-	-	0/1/1/1
9	CUO	T	3001	2	-	-	0/1/1/1
9	CUO	G	2102	1	-	-	0/1/1/1
9	CUO	Z	3002	2	-	-	0/1/1/1
9	CUO	Q	3002	2	-	-	0/1/1/1
9	CUO	b	2101[D]	-	-	-	0/1/1/1
9	CUO	M	2101[D]	-	-	-	0/1/1/1
9	CUO	b	2103	1	-	-	0/1/1/1
9	CUO	Y	2103	1	-	-	0/1/1/1
9	CUO	G	2101[D]	-	-	-	0/1/1/1
9	CUO	S	2101[D]	-	-	-	0/1/1/1
9	CUO	E	3001	2	-	-	0/1/1/1
9	CUO	b	2101[C]	-	-	-	0/1/1/1
9	CUO	C	3401[B]	3	-	-	0/1/1/1
9	CUO	P	5004	1	-	-	0/1/1/1
9	CUO	G	2103	1	-	-	0/1/1/1
9	CUO	b	2104	1	-	-	0/1/1/1
9	CUO	G	2101[C]	-	-	-	0/1/1/1
9	CUO	A	5005[D]	-	-	-	0/1/1/1
9	CUO	S	2101[C]	-	-	-	0/1/1/1
9	CUO	M	2105	1	-	-	0/1/1/1
9	CUO	c	3001	2	-	-	0/1/1/1
9	CUO	G	2104	1	-	-	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

38 monomers are involved in 101 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	J	5001	CUO	1	0
9	D	5004	CUO	1	0
9	X	3401[A]	CUO	5	0
9	V	5003	CUO	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	U	3401[B]	CUO	5	0
9	L	3401[A]	CUO	5	0
9	F	3401[A]	CUO	5	0
9	O	3401[B]	CUO	5	0
9	a	3401[B]	CUO	2	0
9	R	3401[B]	CUO	1	0
9	I	3401[A]	CUO	5	0
9	A	5001	CUO	2	0
9	J	5002	CUO	1	0
9	d	3401[B]	CUO	5	0
9	X	3401[B]	CUO	5	0
9	V	5004	CUO	1	0
9	C	3401[A]	CUO	5	0
9	L	3401[B]	CUO	2	0
9	F	3401[B]	CUO	2	0
9	Y	2105	CUO	1	0
9	D	5001	CUO	1	0
9	S	2102	CUO	1	0
9	Y	2104	CUO	1	0
9	T	3002	CUO	1	0
9	U	3401[A]	CUO	5	0
9	Y	2102	CUO	1	0
9	S	2104	CUO	2	0
9	M	2104	CUO	1	0
9	O	3401[A]	CUO	5	0
9	W	3002	CUO	1	0
9	a	3401[A]	CUO	5	0
9	R	3401[A]	CUO	5	0
9	b	2105	CUO	1	0
9	I	3401[B]	CUO	1	0
9	d	3401[A]	CUO	5	0
9	C	3401[B]	CUO	2	0
9	M	2105	CUO	2	0
9	G	2104	CUO	1	0

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 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	1656/2000 (82%)	-0.43	6 (0%) 88 76	36, 70, 118, 164	0
1	D	1656/2000 (82%)	-0.44	10 (0%) 85 69	37, 67, 114, 176	0
1	G	1656/2000 (82%)	-0.46	6 (0%) 88 76	31, 68, 109, 152	0
1	J	1656/2000 (82%)	-0.46	5 (0%) 90 79	30, 64, 119, 162	0
1	M	1656/2000 (82%)	-0.59	6 (0%) 88 76	29, 56, 109, 157	0
1	P	1656/2000 (82%)	-0.66	10 (0%) 85 69	27, 53, 97, 176	0
1	S	1656/2000 (82%)	-0.58	5 (0%) 90 79	31, 60, 108, 164	0
1	V	1656/2000 (82%)	-0.66	4 (0%) 91 83	26, 55, 105, 154	0
1	Y	1656/2000 (82%)	-0.50	3 (0%) 91 83	31, 66, 112, 160	0
1	b	1656/2000 (82%)	-0.58	7 (0%) 88 76	30, 60, 105, 161	0
2	B	825/920 (89%)	-0.68	0 100 100	32, 57, 101, 140	0
2	E	825/920 (89%)	-0.65	2 (0%) 91 83	30, 59, 106, 137	0
2	H	825/920 (89%)	-0.55	2 (0%) 91 83	31, 63, 112, 147	0
2	K	825/920 (89%)	-0.59	0 100 100	34, 60, 101, 158	0
2	N	825/920 (89%)	-0.80	2 (0%) 91 83	21, 46, 92, 135	0
2	Q	825/920 (89%)	-0.80	1 (0%) 92 86	26, 49, 100, 134	0
2	T	825/920 (89%)	-0.73	1 (0%) 92 86	30, 53, 93, 137	0
2	W	825/920 (89%)	-0.75	1 (0%) 92 86	25, 53, 99, 129	0
2	Z	825/920 (89%)	-0.76	1 (0%) 92 86	25, 52, 95, 130	0
2	c	825/920 (89%)	-0.71	2 (0%) 91 83	26, 55, 103, 135	0
3	C	366/394 (92%)	0.97	49 (13%) 7 4	34, 45, 49, 55	366 (100%)
3	F	366/394 (92%)	0.76	30 (8%) 17 9	28, 39, 44, 54	366 (100%)
3	I	366/394 (92%)	0.72	28 (7%) 19 10	29, 39, 46, 56	366 (100%)
3	L	366/394 (92%)	0.84	30 (8%) 17 9	32, 44, 49, 53	366 (100%)

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
3	O	366/394 (92%)	0.76	29 (7%) 18 10	26, 37, 47, 53	366 (100%)
3	R	366/394 (92%)	0.68	23 (6%) 26 13	29, 39, 45, 55	366 (100%)
3	U	366/394 (92%)	0.74	27 (7%) 20 10	26, 37, 47, 51	366 (100%)
3	X	366/394 (92%)	1.27	47 (12%) 7 5	39, 51, 56, 58	366 (100%)
3	a	366/394 (92%)	0.69	22 (6%) 27 14	27, 38, 44, 48	366 (100%)
3	d	366/394 (92%)	1.13	39 (10%) 11 6	41, 49, 53, 56	366 (100%)
All	All	28470/33140 (85%)	-0.41	398 (1%) 73 51	21, 56, 106, 176	3660 (12%)

The worst 5 of 398 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	X	3282[A]	ASP	6.6
3	F	3216[A]	GLY	6.3
3	X	3088[A]	GLY	5.9
3	O	3101[A]	PRO	5.8
3	X	3108[A]	HIS	5.8

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	NAG	e	1	14/15	-	-	62,79,86,94	0
4	NAG	e	2	14/15	-	-	69,83,96,102	0
4	NAG	f	1	14/15	-	-	88,95,105,109	0
4	NAG	f	2	14/15	-	-	106,116,123,129	0
4	NAG	i	1	14/15	-	-	59,68,91,95	0
4	NAG	i	2	14/15	-	-	84,92,107,111	0
4	NAG	j	1	14/15	-	-	59,67,76,76	0
4	NAG	j	2	14/15	-	-	49,57,73,79	0
4	NAG	m	1	14/15	-	-	77,91,99,104	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	NAG	m	2	14/15	-	-	80,95,108,108	0
4	NAG	n	1	14/15	-	-	67,77,90,98	0
4	NAG	n	2	14/15	-	-	72,91,105,110	0
4	NAG	o	1	14/15	-	-	61,73,85,88	0
4	NAG	o	2	14/15	-	-	43,67,86,87	0
4	NAG	p	1	14/15	-	-	47,61,75,75	0
4	NAG	p	2	14/15	-	-	54,72,84,88	0
4	NAG	q	1	14/15	-	-	56,67,78,80	0
4	NAG	q	2	14/15	-	-	80,88,92,93	0
4	NAG	s	1	14/15	-	-	71,77,85,90	0
4	NAG	s	2	14/15	-	-	89,102,108,116	0
4	NAG	t	1	14/15	-	-	53,69,82,85	0
4	NAG	t	2	14/15	-	-	50,90,102,103	0
4	NAG	u	1	14/15	-	-	73,78,87,92	0
4	NAG	u	2	14/15	-	-	86,100,114,132	0
4	NAG	v	1	14/15	-	-	64,80,91,91	0
4	NAG	v	2	14/15	-	-	82,97,104,106	0
4	NAG	x	1	14/15	-	-	80,94,105,105	0
4	NAG	x	2	14/15	-	-	104,115,125,125	0
4	NAG	1	1	14/15	-	-	88,96,102,103	0
4	NAG	1	2	14/15	-	-	91,104,121,126	0
4	NAG	2	1	14/15	-	-	41,56,75,80	0
4	NAG	2	2	14/15	-	-	53,71,87,100	0
4	NAG	4	1	14/15	-	-	57,70,74,80	0
4	NAG	4	2	14/15	-	-	78,96,107,116	0
4	NAG	6	1	14/15	-	-	74,81,89,91	0
4	NAG	6	2	14/15	-	-	49,73,85,91	0
4	NAG	7	1	14/15	-	-	57,70,83,84	0
4	NAG	7	2	14/15	-	-	69,83,101,104	0
4	NAG	8	1	14/15	-	-	57,62,72,81	0
4	NAG	8	2	14/15	-	-	64,84,98,101	0
4	NAG	9	1	14/15	-	-	87,95,100,108	0
4	NAG	9	2	14/15	-	-	73,97,113,113	0
4	NAG	BA	1	14/15	-	-	80,84,96,97	0
4	NAG	BA	2	14/15	-	-	62,82,95,101	0
6	NAG	GA	2	14/15	0.91	0.13	88,108,127,131	0
5	BMA	KA	3	11/12	0.92	0.07	79,99,114,127	0
4	NAG	MA	2	14/15	0.92	0.09	84,93,116,127	0
4	NAG	IA	2	14/15	0.93	0.10	75,89,96,100	0
5	NAG	FA	2	14/15	0.94	0.10	74,88,101,105	0
6	NAG	EA	2	14/15	0.94	0.08	70,82,98,108	0
5	NAG	KA	1	14/15	0.94	0.08	60,66,76,78	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	NAG	LA	2	14/15	0.94	0.10	76,89,100,104	0
6	BMA	LA	3	11/12	0.94	0.09	101,110,119,119	0
6	NAG	NA	2	14/15	0.94	0.10	61,80,101,112	0
4	NAG	QA	2	14/15	0.95	0.08	97,115,121,125	0
5	NAG	PA	2	14/15	0.95	0.07	72,80,89,91	0
4	NAG	RA	1	14/15	0.95	0.12	75,83,99,108	0
4	NAG	RA	2	14/15	0.95	0.07	83,92,102,114	0
5	NAG	g	1	14/15	-	-	57,79,95,97	0
5	NAG	g	2	14/15	-	-	99,105,109,109	0
5	BMA	g	3	11/12	-	-	110,124,133,139	0
5	MAN	g	4	11/12	-	-	103,117,133,133	0
5	NAG	l	1	14/15	-	-	52,57,72,76	0
5	NAG	l	2	14/15	-	-	69,84,96,97	0
5	BMA	l	3	11/12	-	-	98,113,119,128	0
5	MAN	l	4	11/12	-	-	114,118,122,128	0
5	NAG	AA	1	14/15	-	-	61,71,75,75	0
5	NAG	AA	2	14/15	-	-	87,92,98,104	0
5	BMA	AA	3	11/12	-	-	112,120,124,127	0
5	MAN	AA	4	11/12	-	-	114,125,132,145	0
6	BMA	GA	3	11/12	0.95	0.09	130,136,142,143	0
4	NAG	MA	1	14/15	0.95	0.10	69,77,85,86	0
5	BMA	FA	3	11/12	-	-	85,101,110,113	0
5	MAN	FA	4	11/12	-	-	94,107,126,132	0
4	NAG	HA	1	14/15	0.95	0.08	56,63,83,93	0
5	NAG	KA	2	14/15	0.95	0.07	67,81,92,93	0
6	NAG	GA	1	14/15	0.96	0.09	79,97,106,109	0
5	MAN	KA	4	11/12	-	-	87,103,122,135	0
6	NAG	EA	1	14/15	0.96	0.07	46,58,71,75	0
4	NAG	OA	1	14/15	0.96	0.09	57,70,80,85	0
5	BMA	PA	3	11/12	-	-	96,97,104,125	0
5	MAN	PA	4	11/12	-	-	107,112,125,133	0
6	NAG	h	1	14/15	-	-	85,93,112,115	0
6	NAG	h	2	14/15	-	-	84,94,107,114	0
6	BMA	h	3	11/12	-	-	108,114,120,126	0
6	NAG	k	1	14/15	-	-	71,83,92,99	0
6	NAG	k	2	14/15	-	-	88,104,119,123	0
6	BMA	k	3	11/12	-	-	110,119,126,133	0
6	NAG	r	1	14/15	-	-	79,88,107,112	0
6	NAG	r	2	14/15	-	-	84,91,98,102	0
6	BMA	r	3	11/12	-	-	111,120,128,129	0
6	NAG	w	1	14/15	-	-	78,100,106,118	0
6	NAG	w	2	14/15	-	-	88,104,108,111	0

Continued on next page...

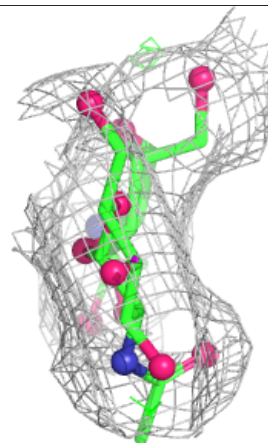
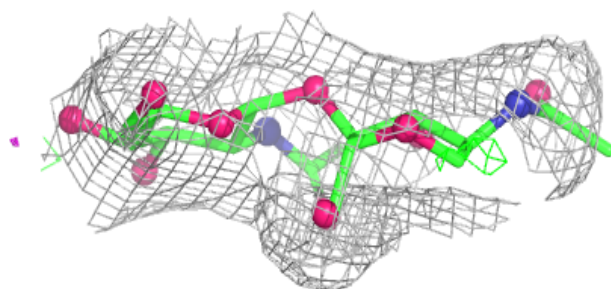
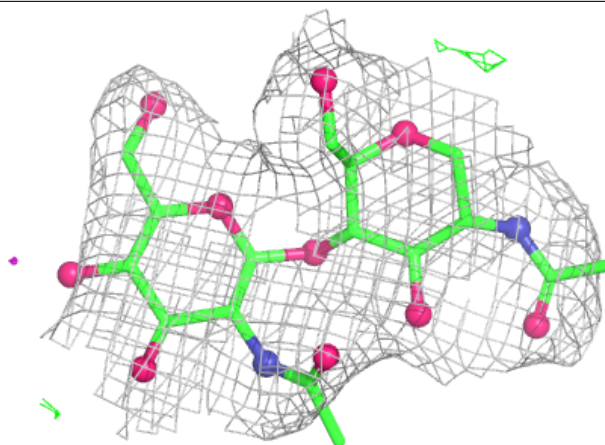
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	BMA	w	3	11/12	-	-	107,110,117,128	0
6	NAG	y	1	14/15	-	-	52,67,74,75	0
6	NAG	y	2	14/15	-	-	65,83,94,109	0
6	BMA	y	3	11/12	-	-	102,116,123,123	0
6	NAG	3	1	14/15	-	-	46,67,81,90	0
6	NAG	3	2	14/15	-	-	61,82,96,102	0
6	BMA	3	3	11/12	-	-	114,119,149,149	0
6	NAG	5	1	14/15	-	-	52,60,70,76	0
6	NAG	5	2	14/15	-	-	61,77,95,103	0
6	BMA	5	3	11/12	-	-	98,114,124,127	0
6	NAG	CA	1	14/15	-	-	59,71,83,91	0
6	NAG	CA	2	14/15	-	-	88,97,115,124	0
6	BMA	CA	3	11/12	-	-	96,123,130,130	0
6	NAG	DA	1	14/15	-	-	50,66,77,82	0
6	NAG	DA	2	14/15	-	-	78,91,95,98	0
6	BMA	DA	3	11/12	-	-	82,103,108,108	0
4	NAG	IA	1	14/15	0.97	0.07	51,66,83,92	0
4	NAG	HA	2	14/15	0.97	0.07	71,82,95,107	0
6	BMA	EA	3	11/12	-	-	104,115,132,134	0
6	NAG	LA	1	14/15	0.97	0.07	78,87,93,98	0
4	NAG	JA	1	14/15	0.97	0.05	70,80,88,90	0
4	NAG	OA	2	14/15	0.97	0.08	55,73,85,91	0
6	NAG	NA	1	14/15	0.97	0.07	56,62,71,72	0
4	NAG	JA	2	14/15	0.97	0.05	82,92,100,100	0
5	NAG	PA	1	14/15	0.98	0.06	62,72,77,78	0
4	NAG	QA	1	14/15	0.98	0.07	97,107,114,118	0
5	NAG	FA	1	14/15	0.98	0.06	49,68,77,78	0
6	BMA	NA	3	11/12	-	-	102,117,134,138	0
7	NAG	z	1	14/15	-	-	79,85,93,96	0
7	NAG	z	2	14/15	-	-	92,105,121,128	0
7	BMA	z	3	11/12	-	-	124,134,140,150	0
7	MAN	z	4	11/12	-	-	135,140,150,154	0
7	MAN	z	5	11/12	-	-	121,135,151,154	0
8	NAG	0	1	14/15	-	-	60,67,72,81	0
8	NAG	0	2	14/15	-	-	58,78,82,90	0
8	BMA	0	3	11/12	-	-	97,112,128,130	0
8	MAN	0	4	11/12	-	-	94,114,123,126	0

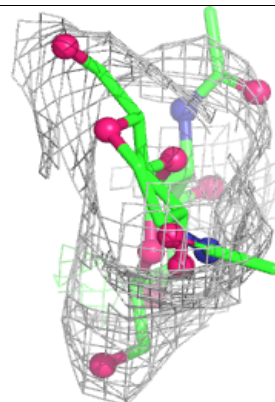
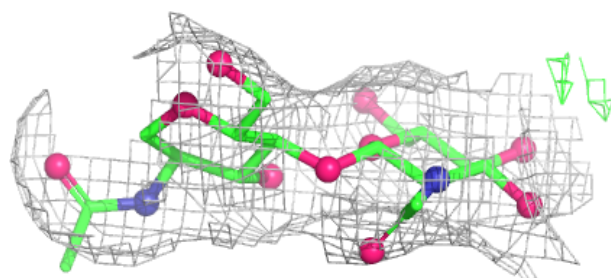
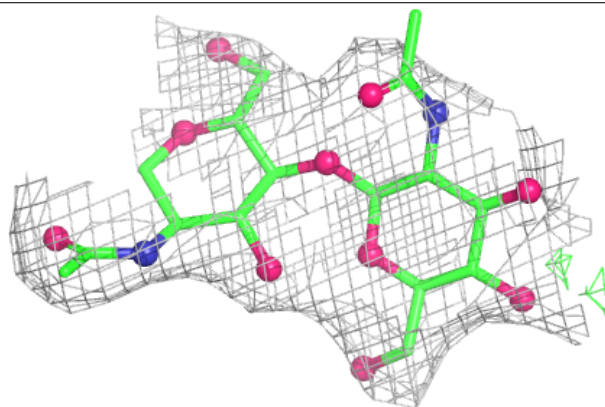
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain e:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

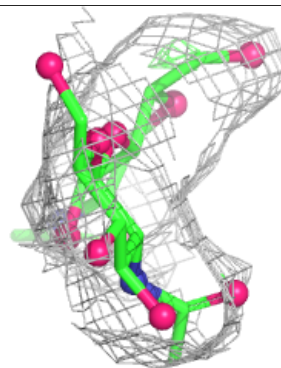
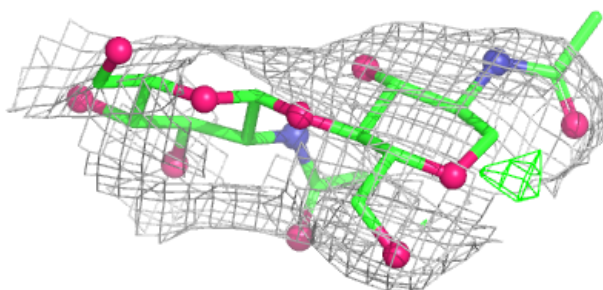
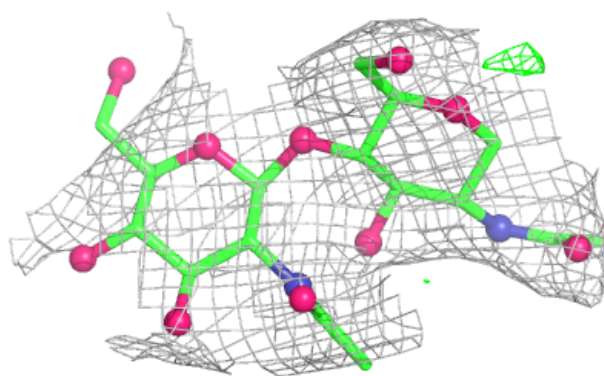
**Electron density around Chain f:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

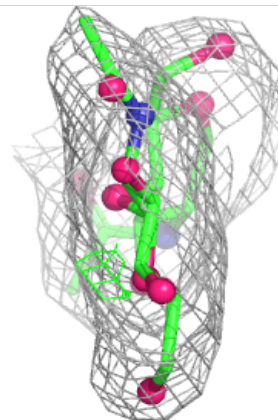
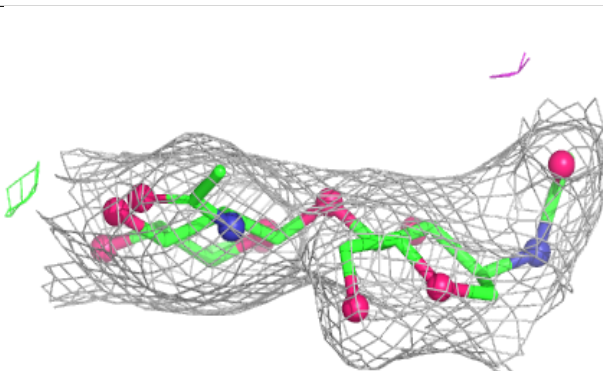
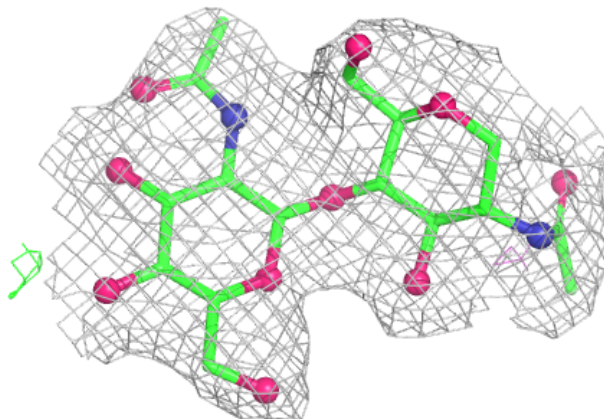


Electron density around Chain i:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

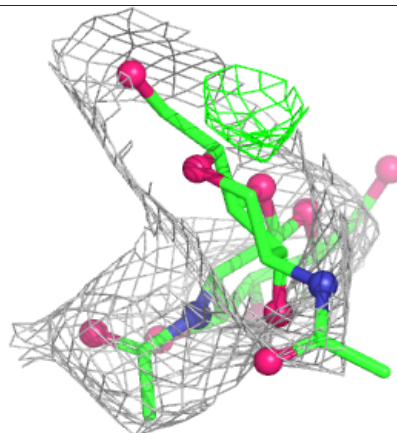
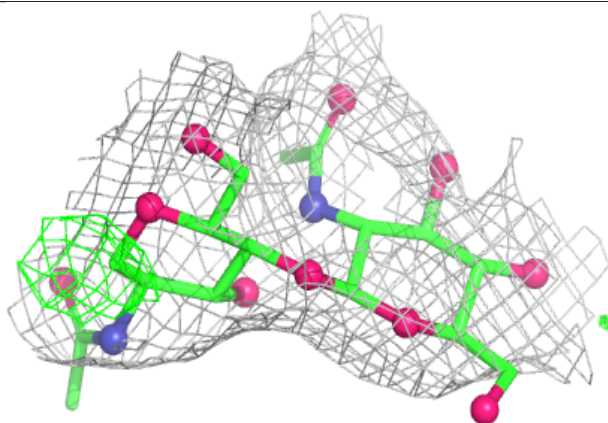
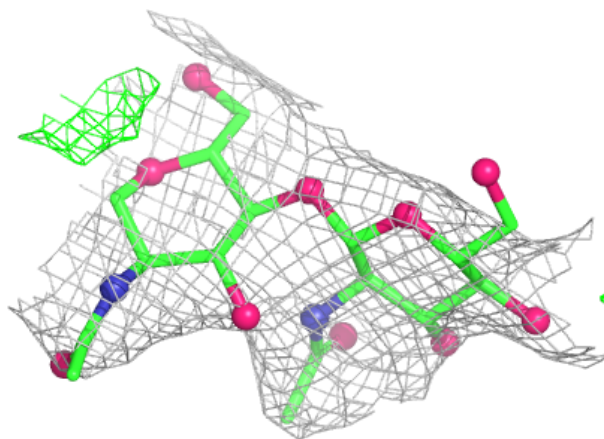
**Electron density around Chain j:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



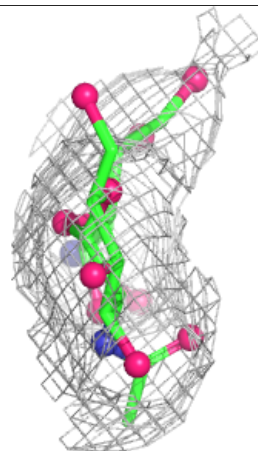
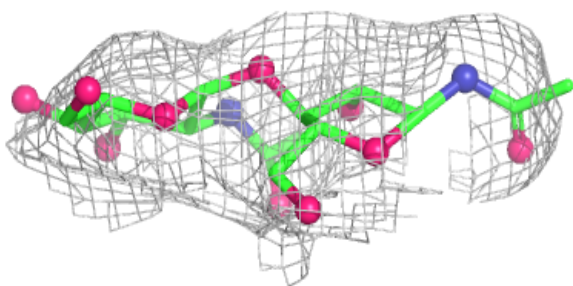
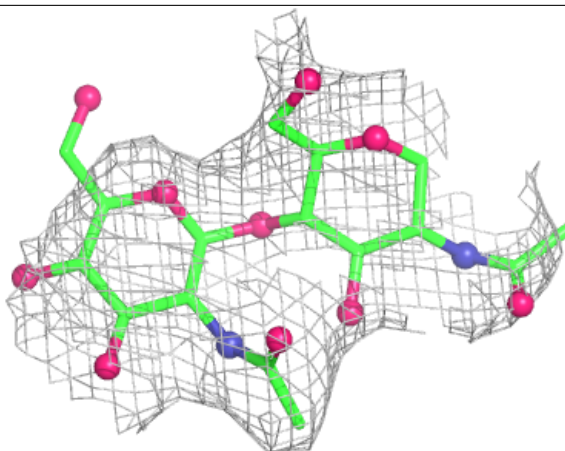
Electron density around Chain m:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



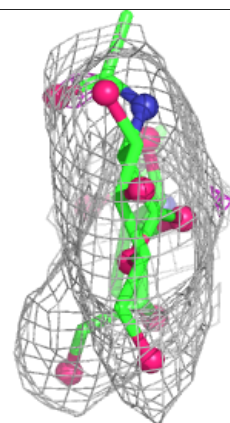
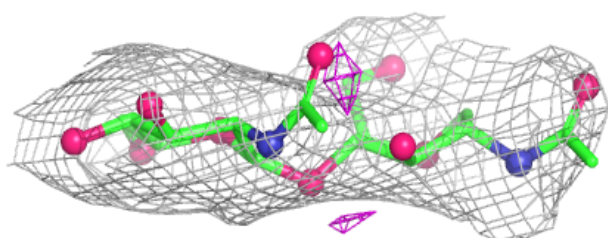
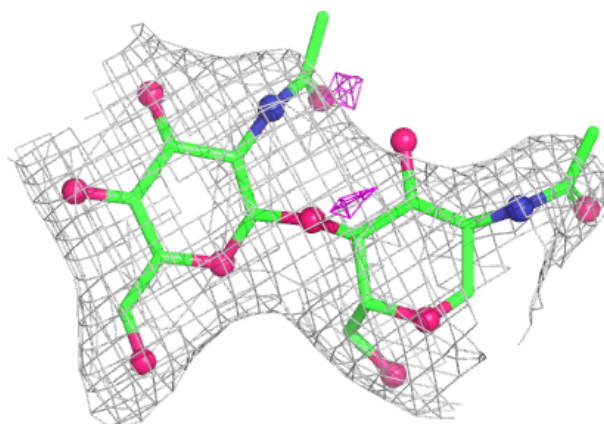
Electron density around Chain n:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

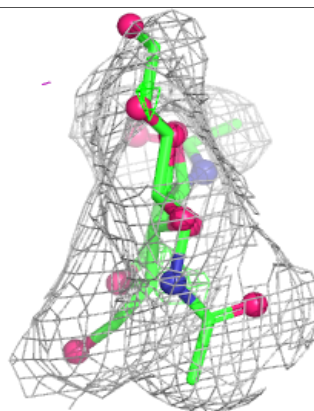
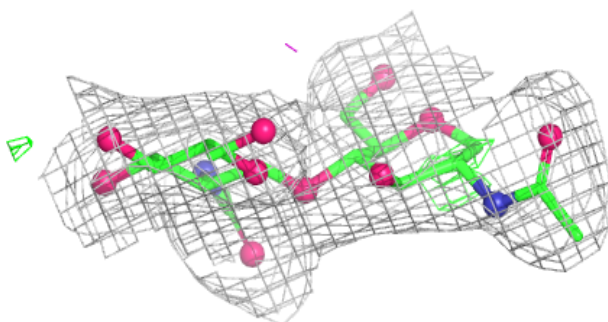
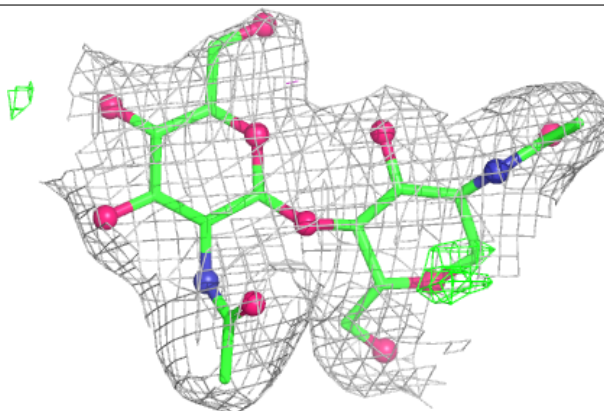


Electron density around Chain o:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

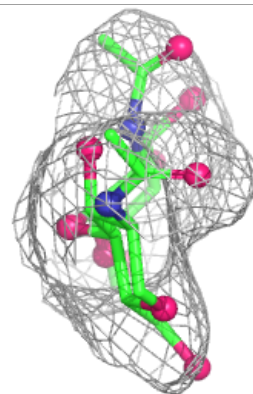
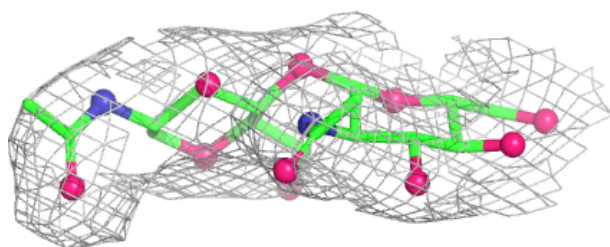
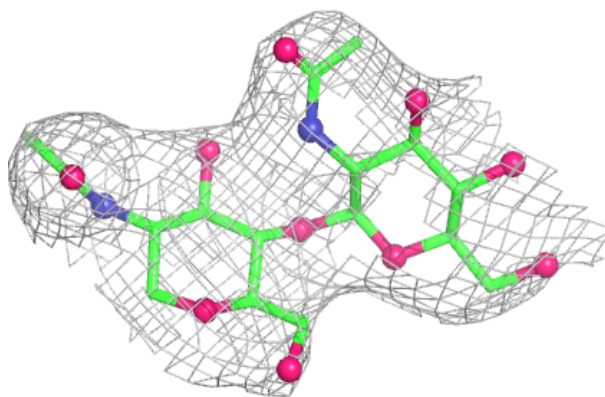
**Electron density around Chain p:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



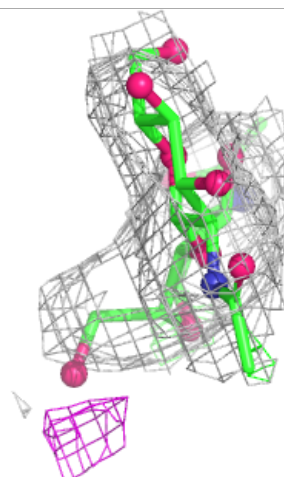
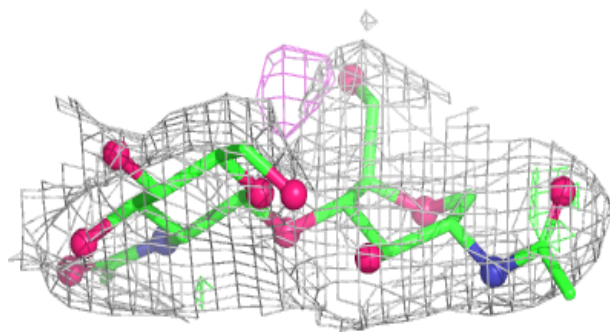
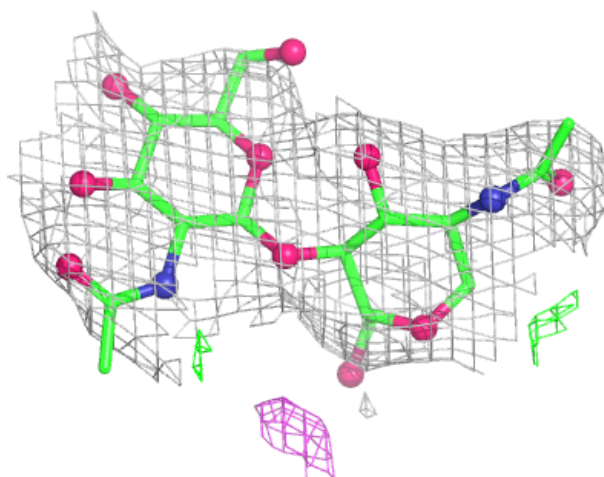
Electron density around Chain q:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



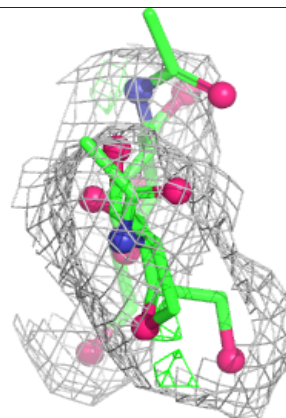
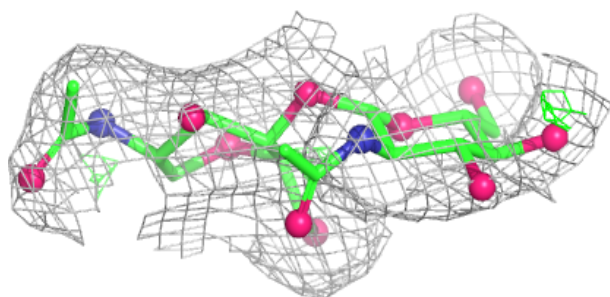
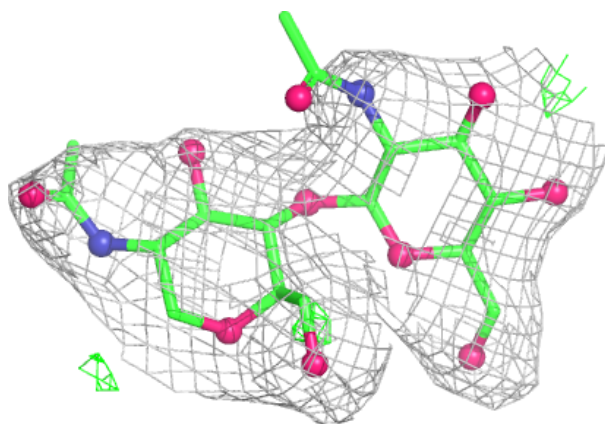
Electron density around Chain s:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



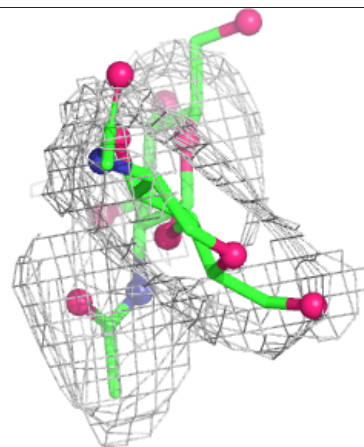
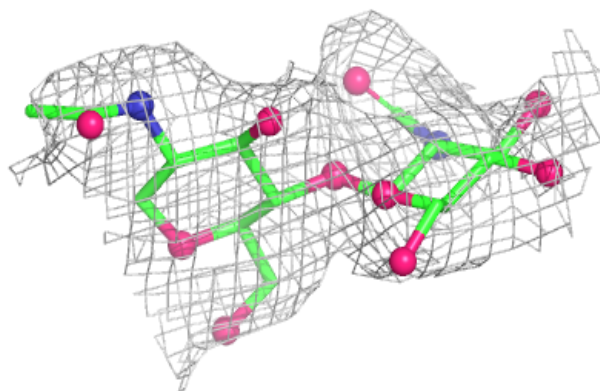
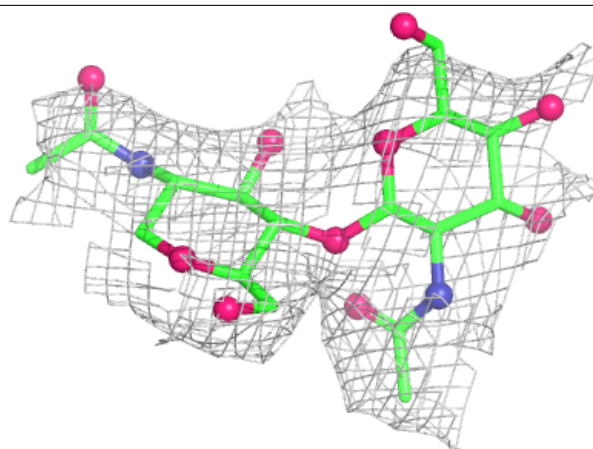
Electron density around Chain t:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

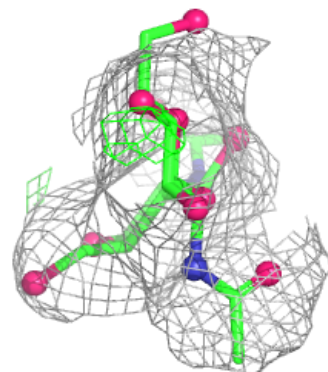
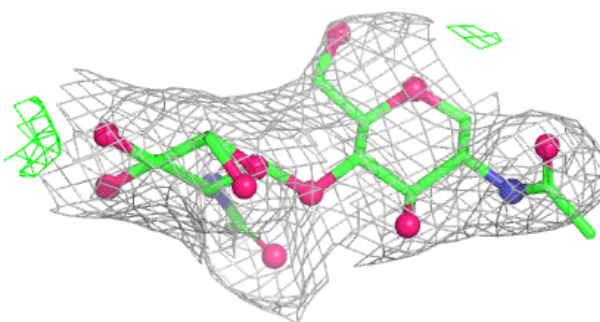
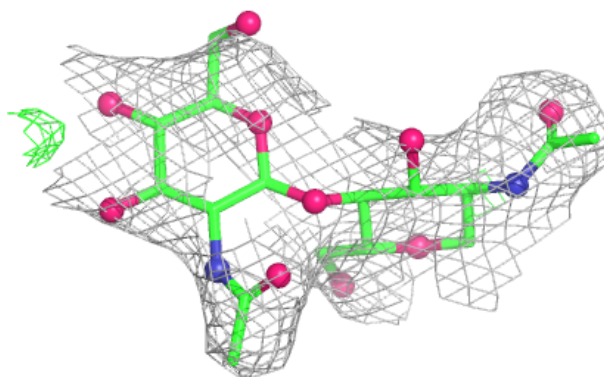


Electron density around Chain u:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

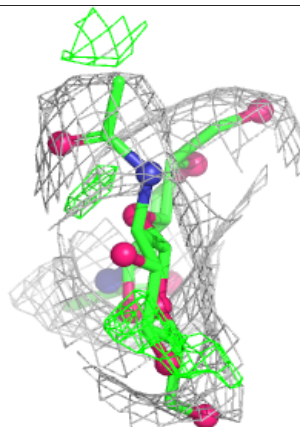
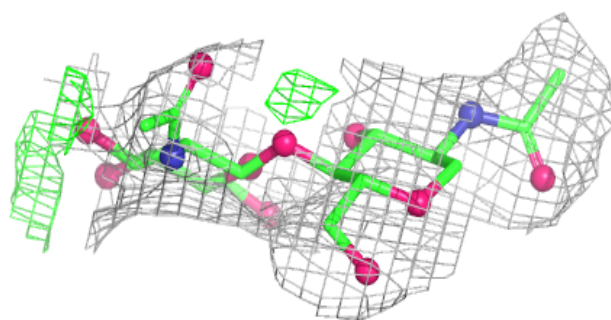
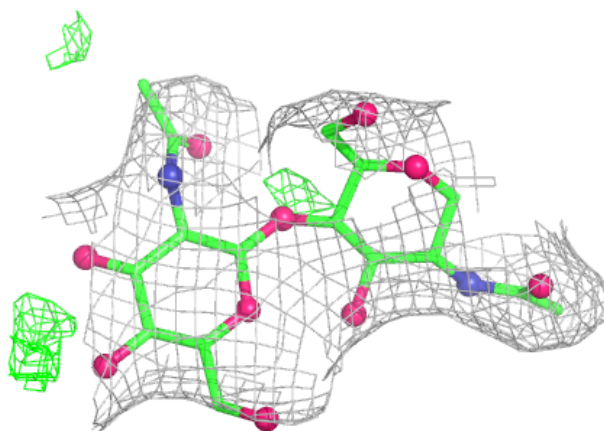
**Electron density around Chain v:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



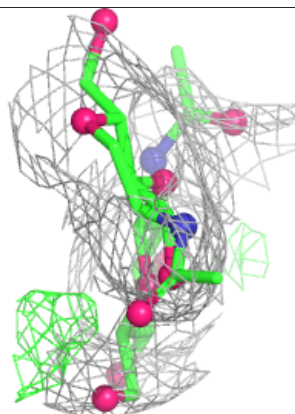
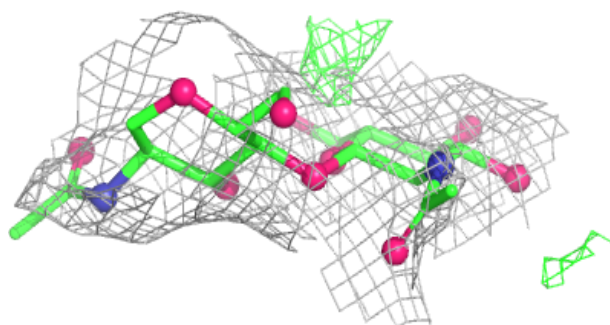
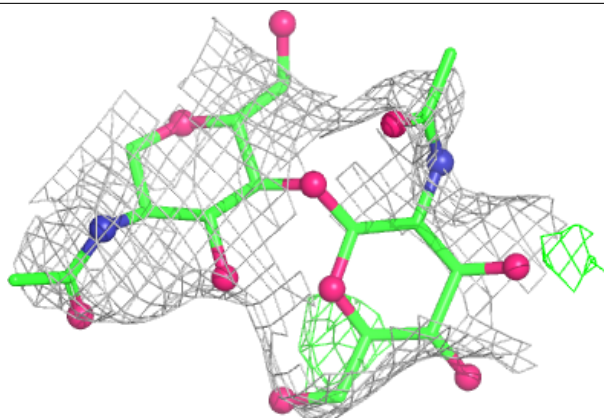
Electron density around Chain x:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

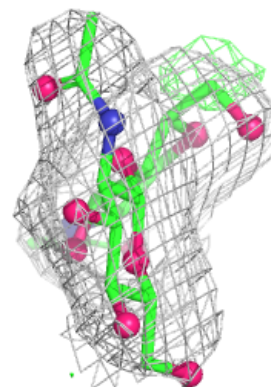
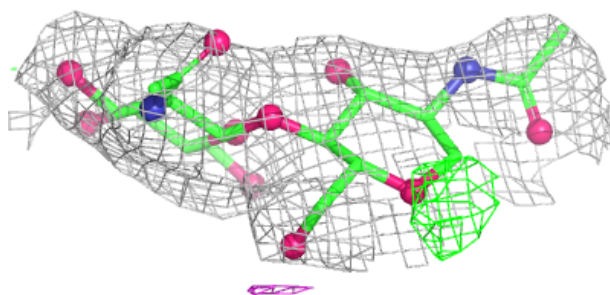
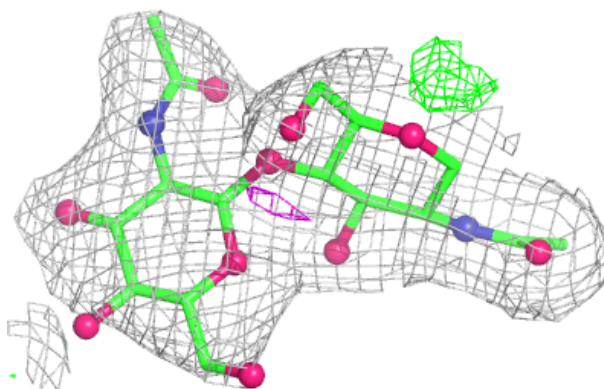


Electron density around Chain 1:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

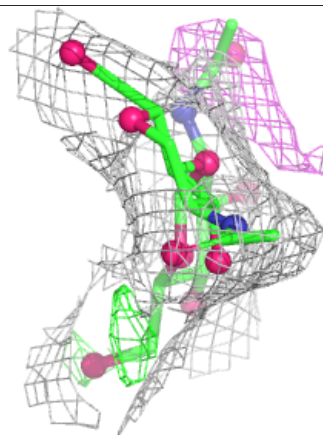
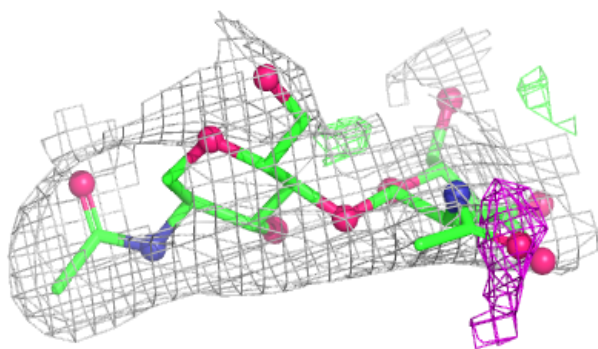
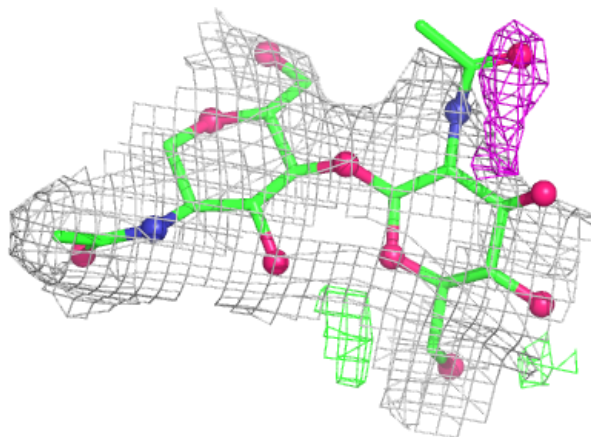
**Electron density around Chain 2:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

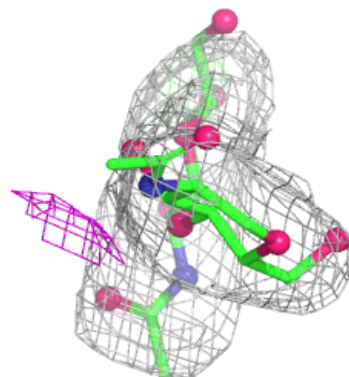
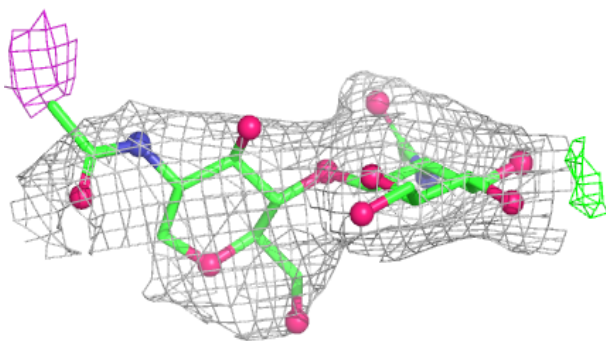
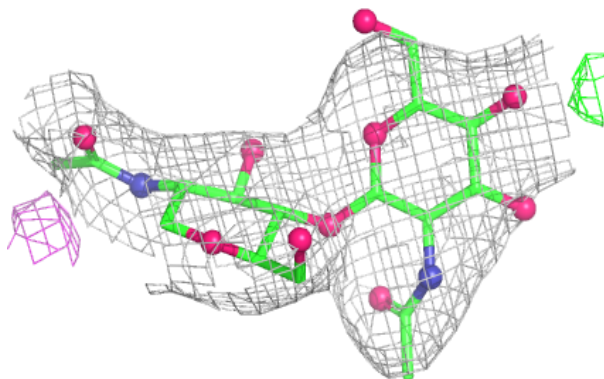


Electron density around Chain 4:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

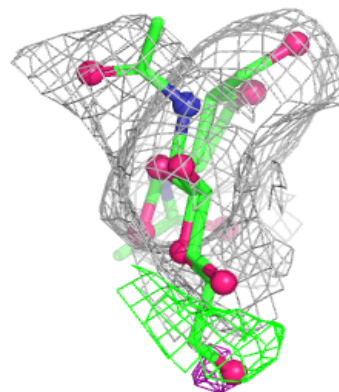
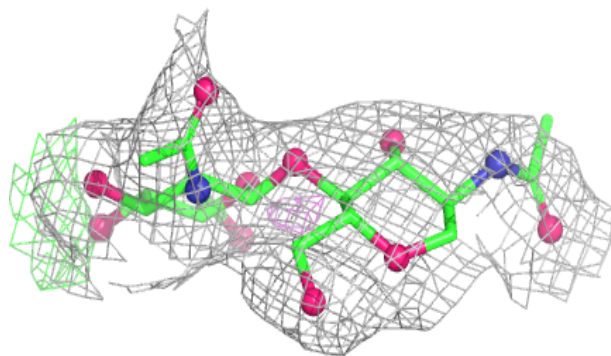
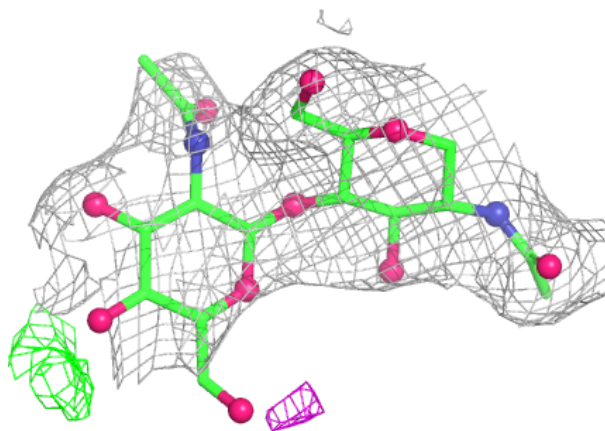
**Electron density around Chain 6:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



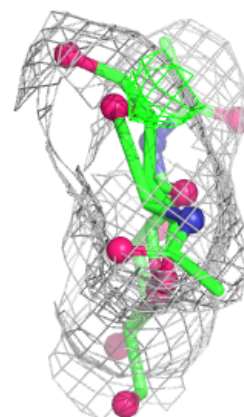
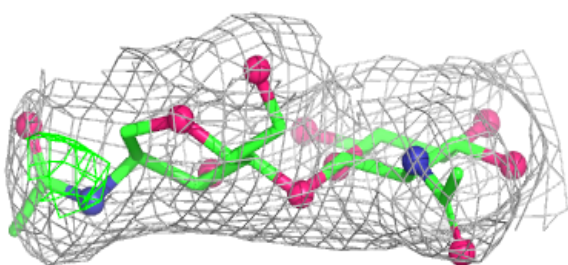
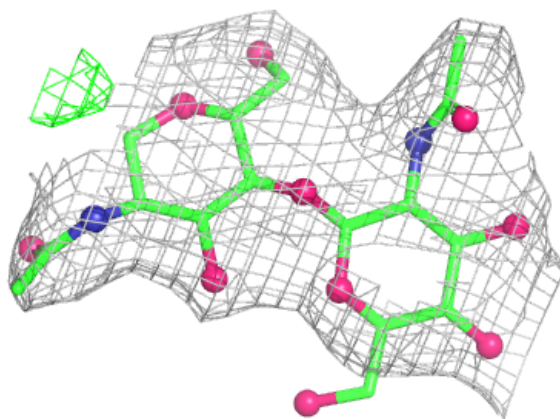
Electron density around Chain 7:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

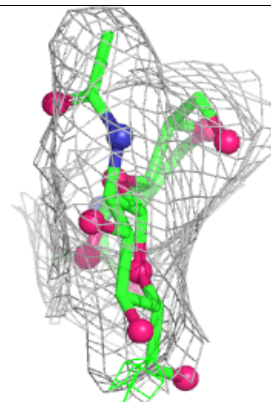
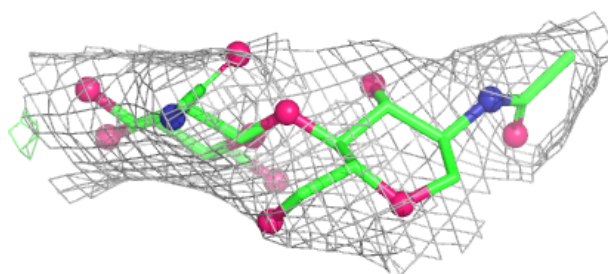
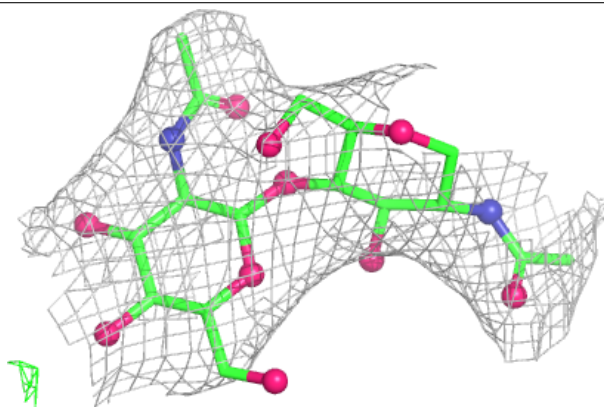


Electron density around Chain 8:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

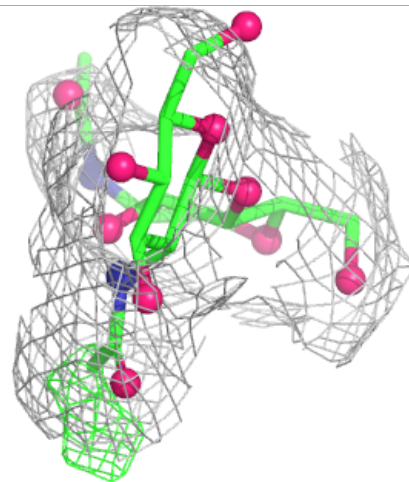
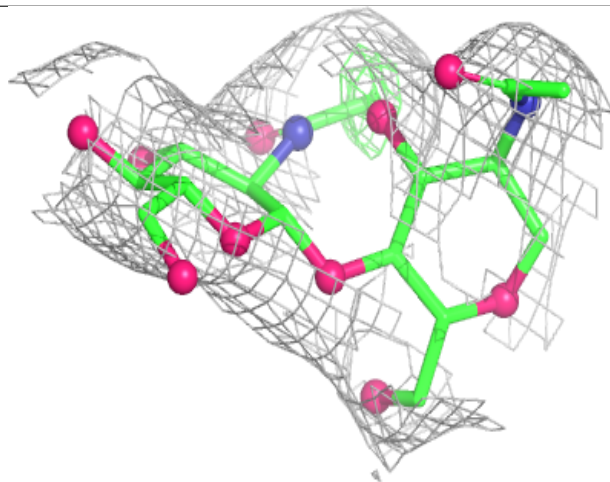
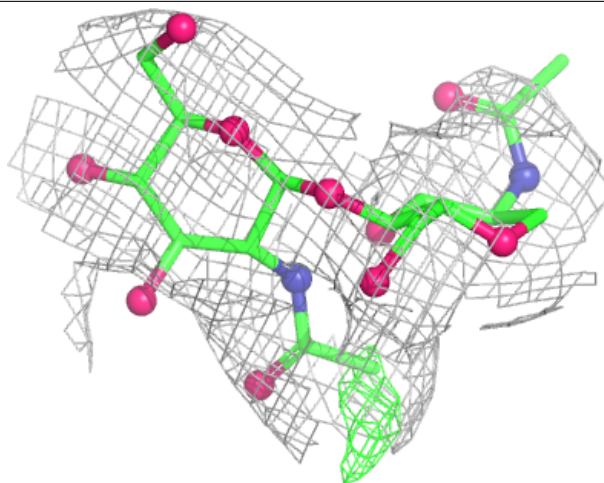
**Electron density around Chain 9:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



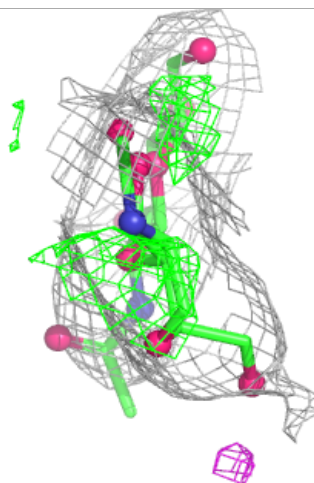
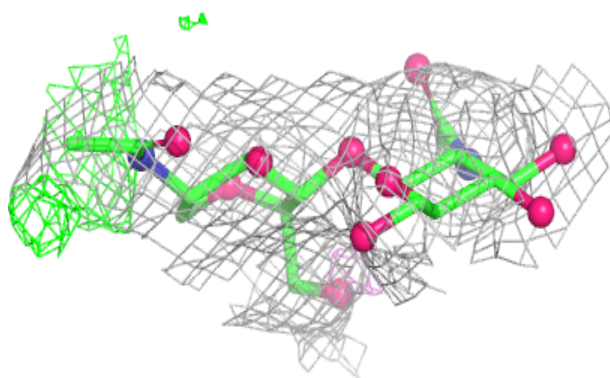
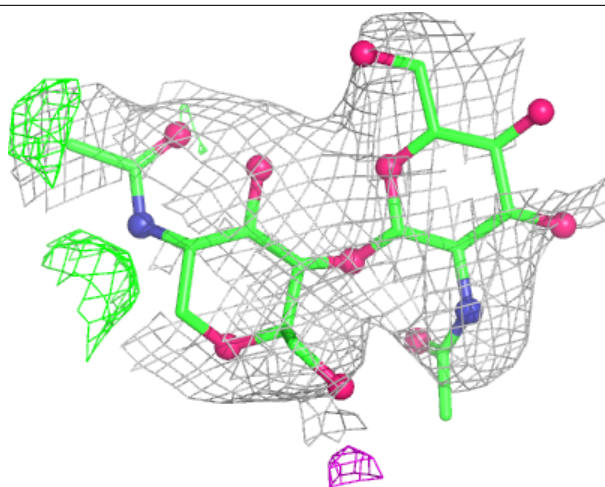
Electron density around Chain BA:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



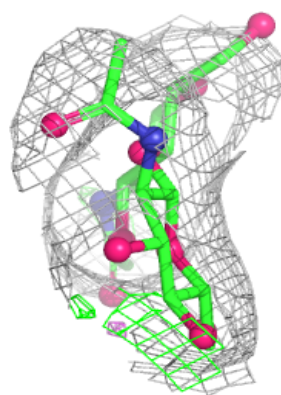
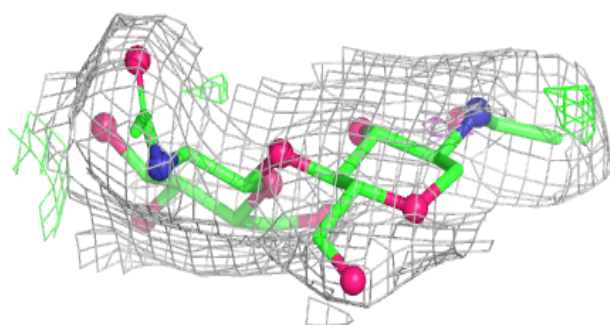
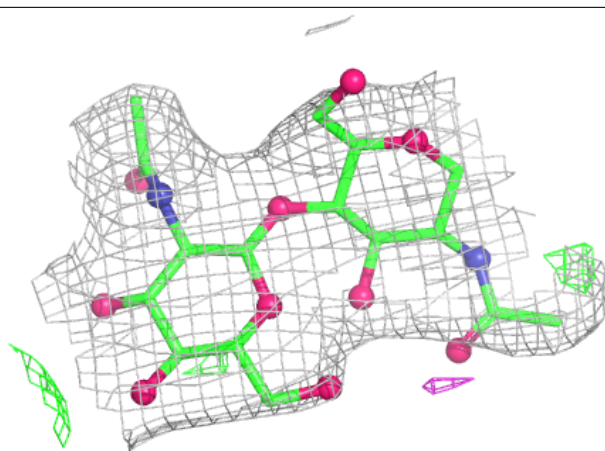
Electron density around Chain HA:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



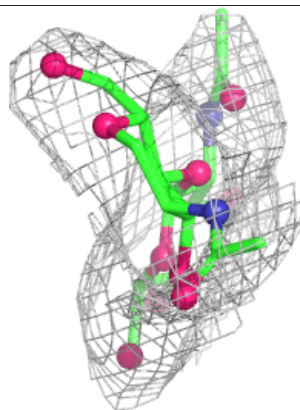
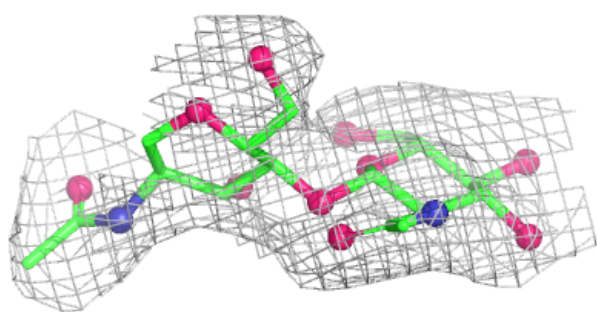
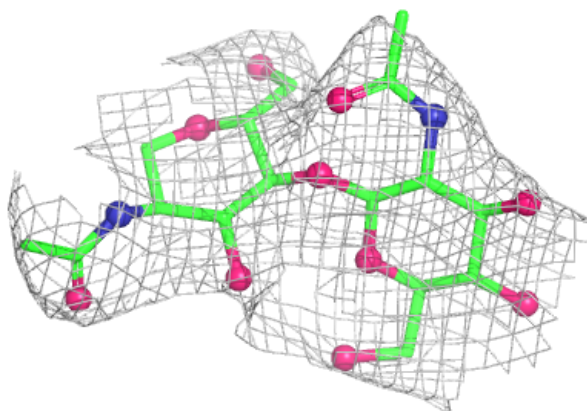
Electron density around Chain IA:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

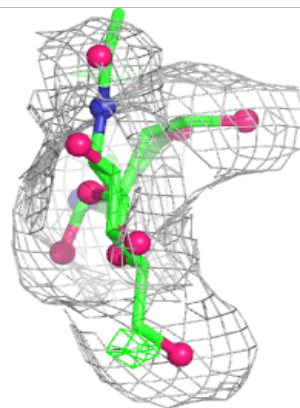
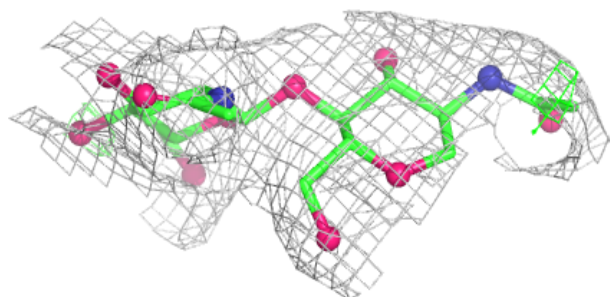
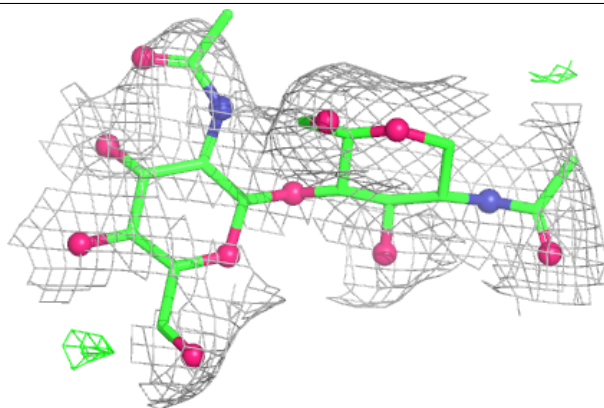


Electron density around Chain JA:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

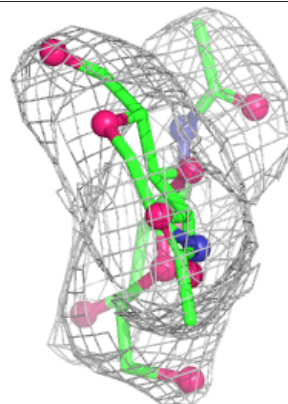
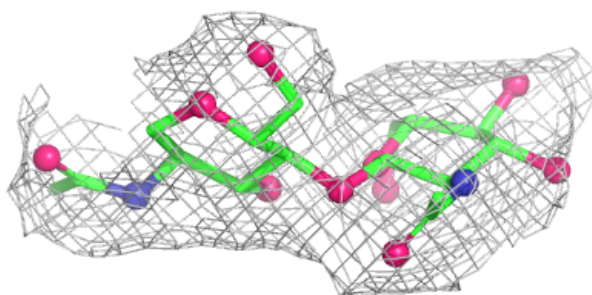
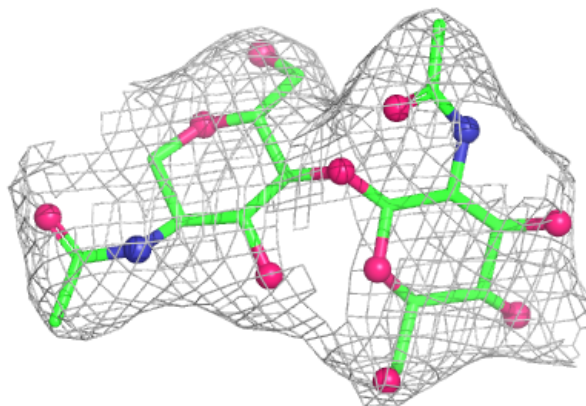
**Electron density around Chain MA:**

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



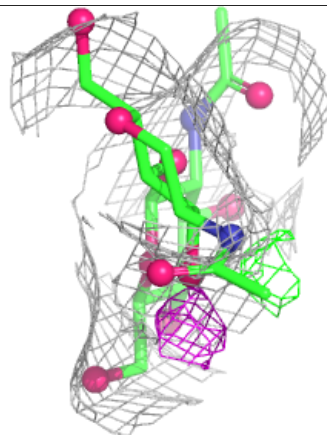
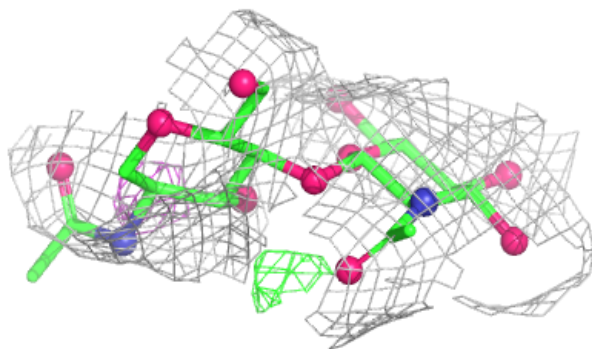
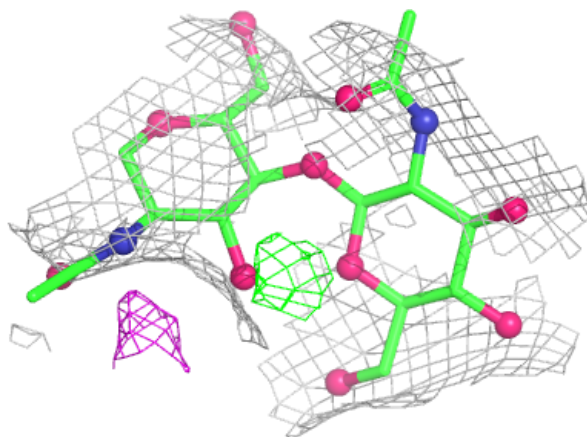
Electron density around Chain OA:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



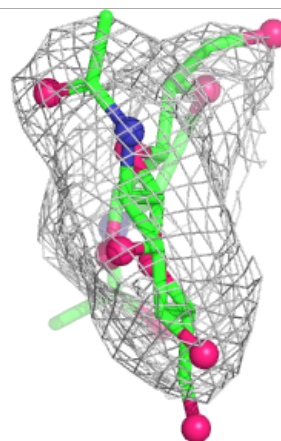
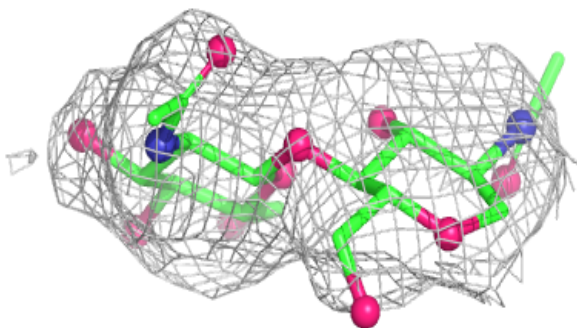
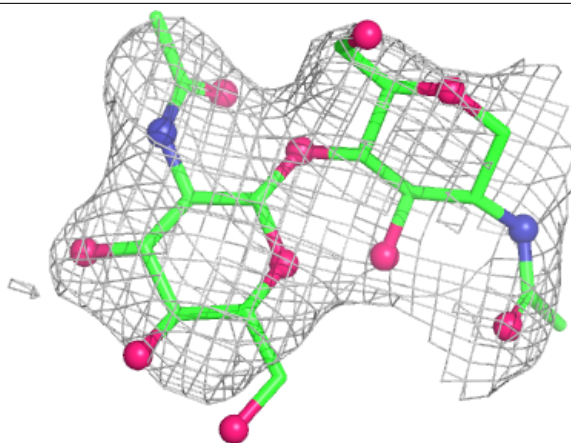
Electron density around Chain QA:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



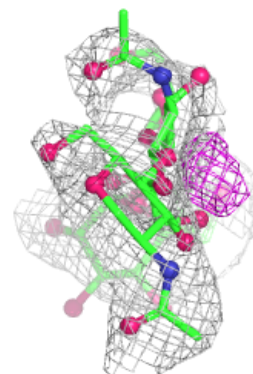
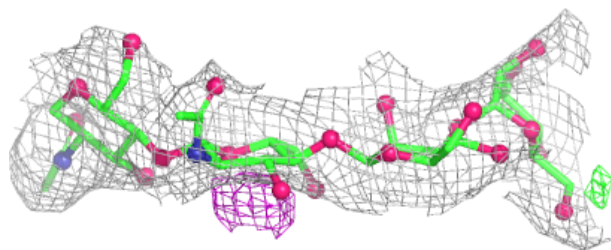
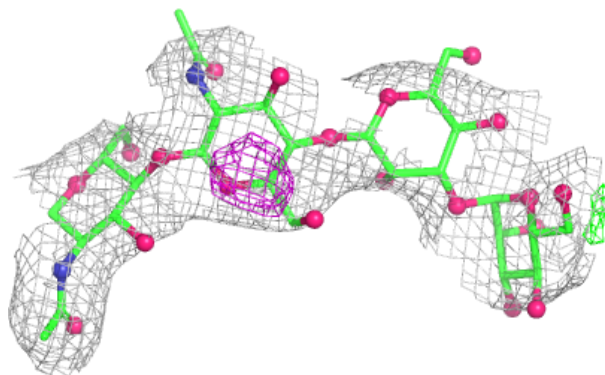
Electron density around Chain RA:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

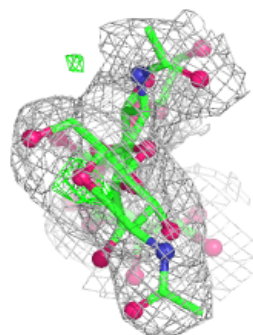
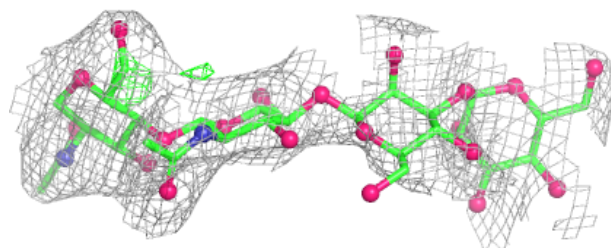
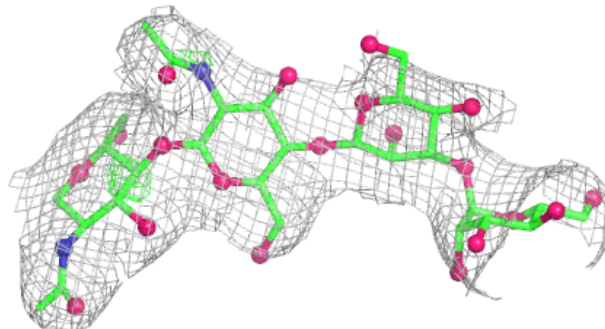


Electron density around Chain g:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

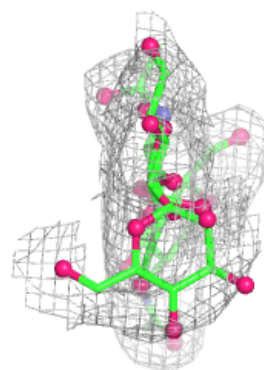
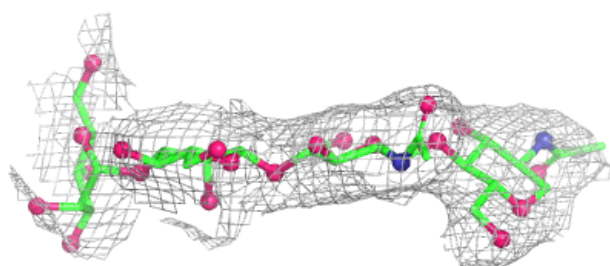
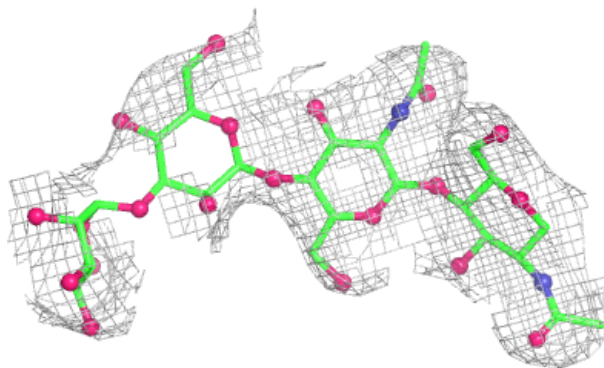
**Electron density around Chain l:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

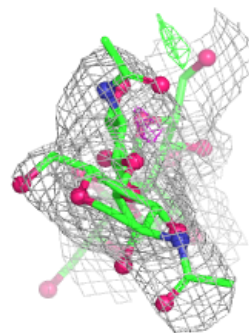
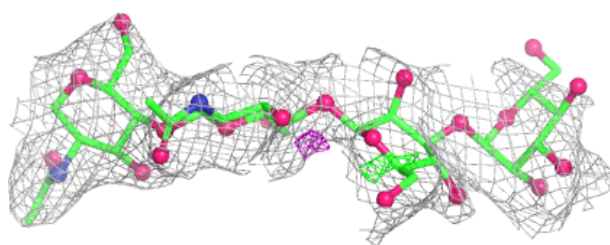
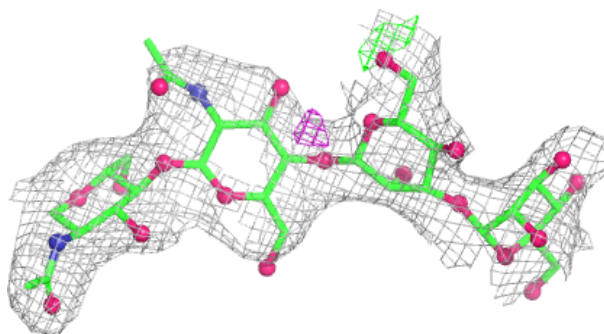


Electron density around Chain AA:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

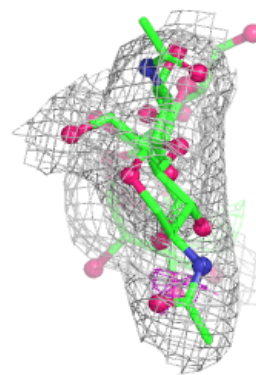
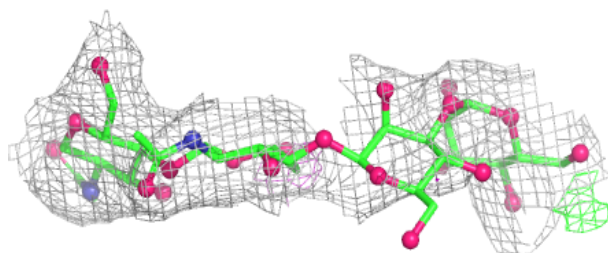
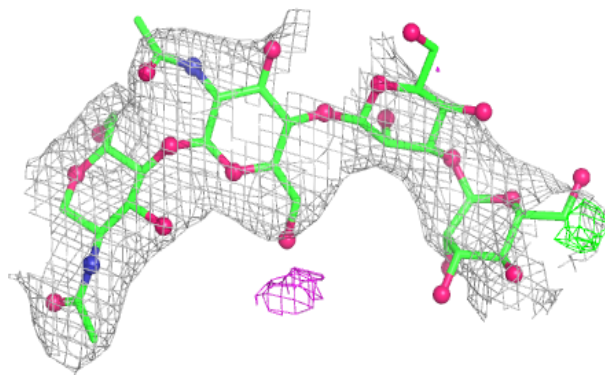
**Electron density around Chain FA:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

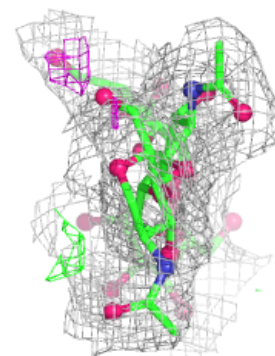
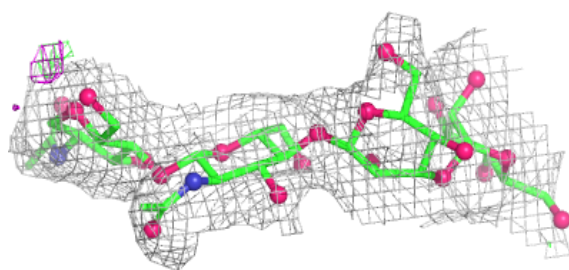
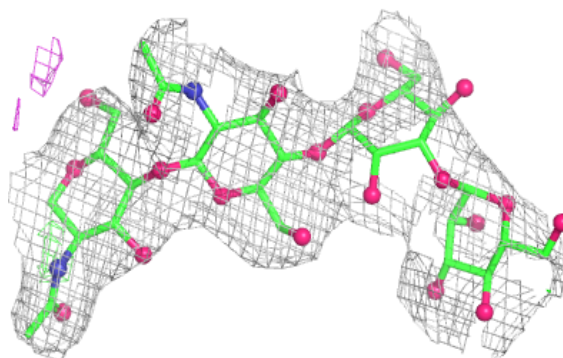


Electron density around Chain KA:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

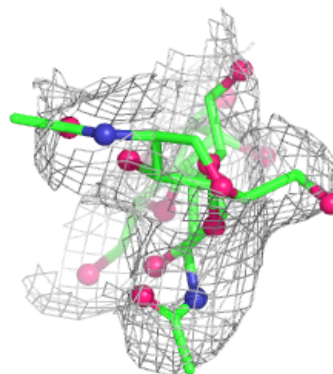
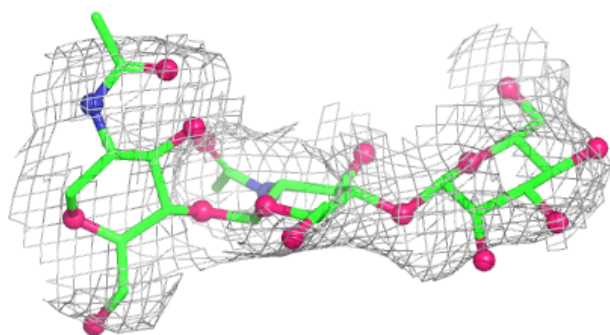
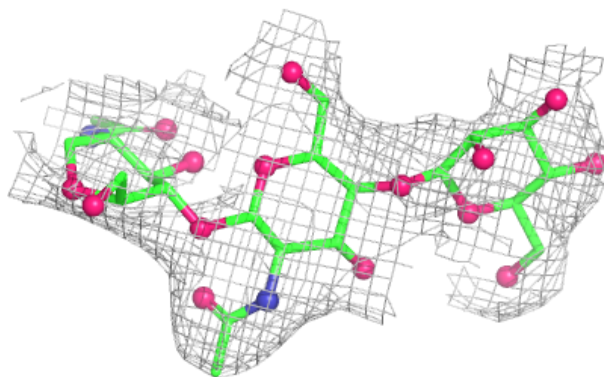
**Electron density around Chain PA:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

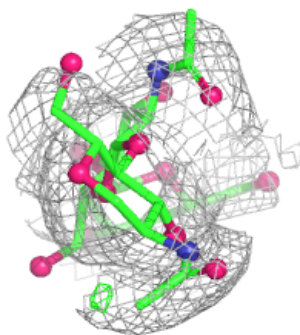
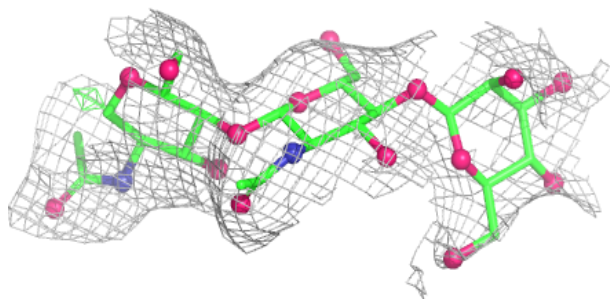
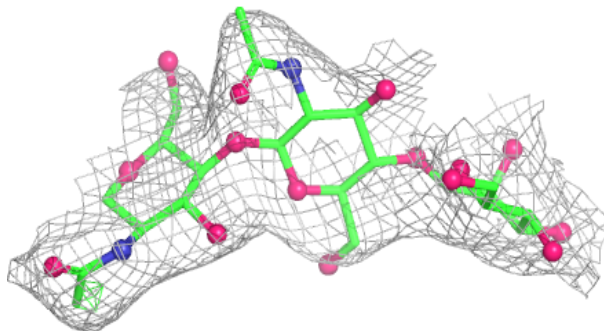


Electron density around Chain h:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

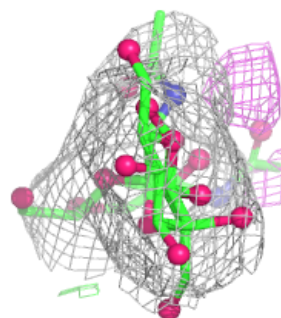
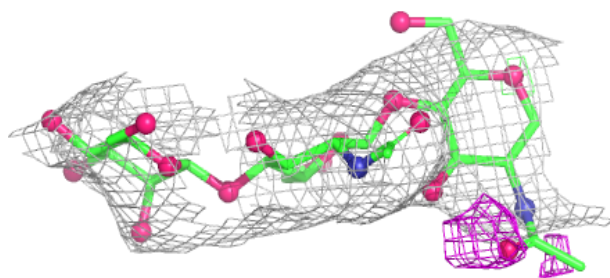
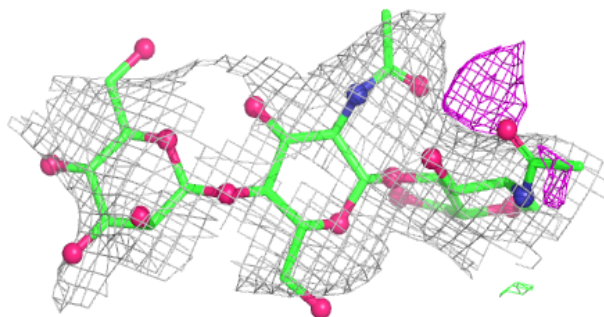
**Electron density around Chain k:**

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

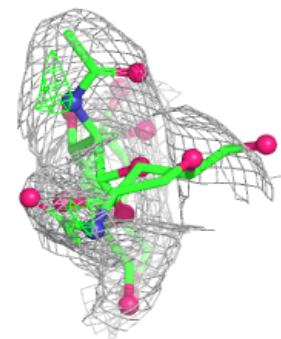
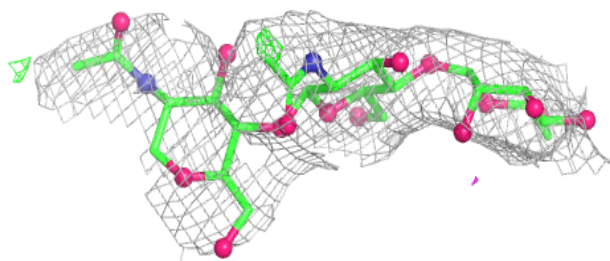
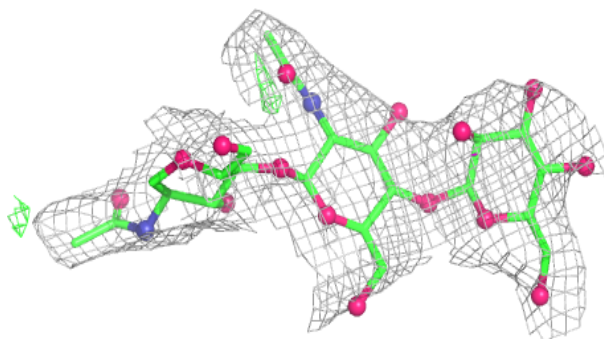


Electron density around Chain r:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

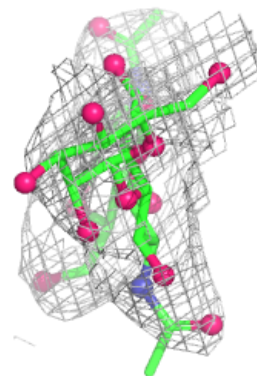
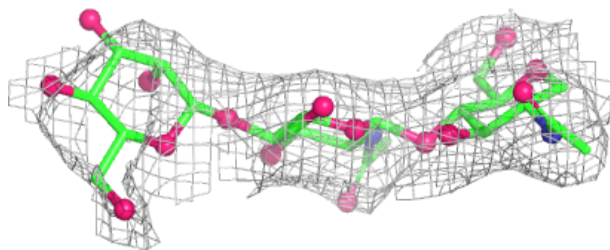
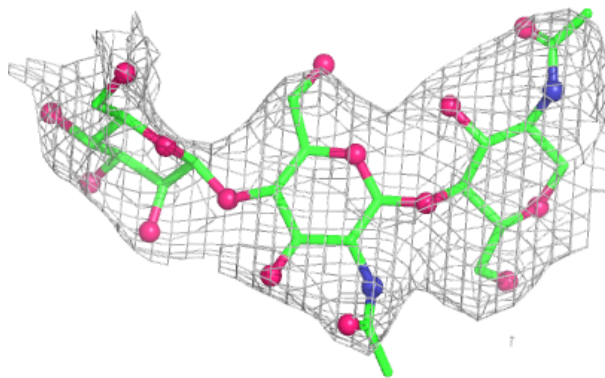
**Electron density around Chain w:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

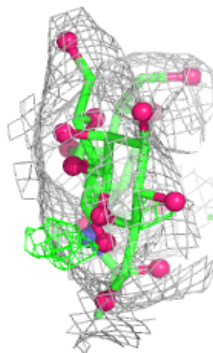
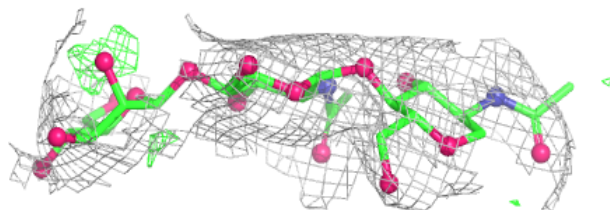
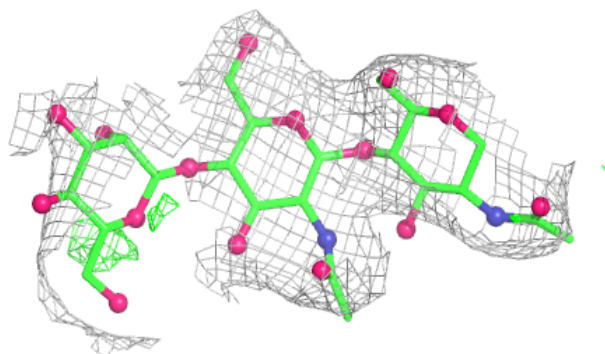


Electron density around Chain y:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

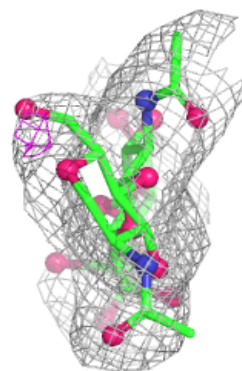
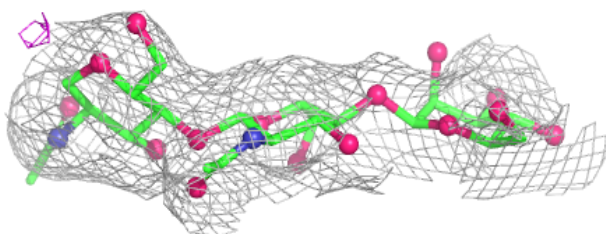
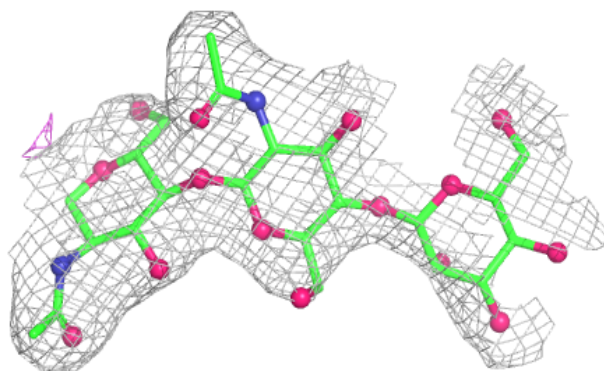
**Electron density around Chain 3:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



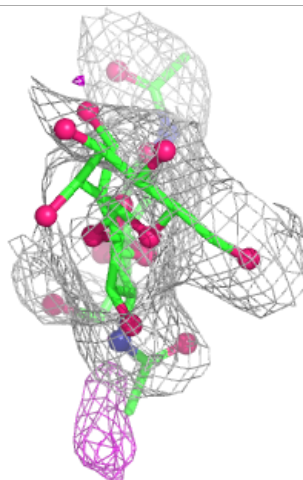
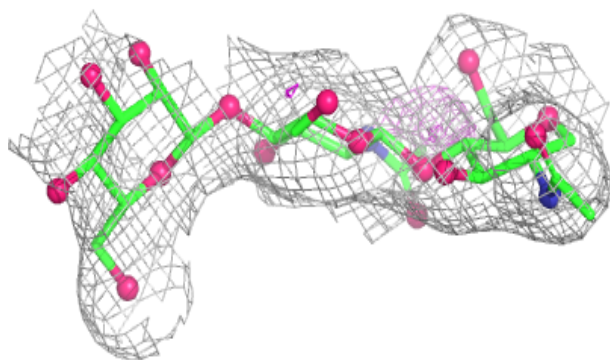
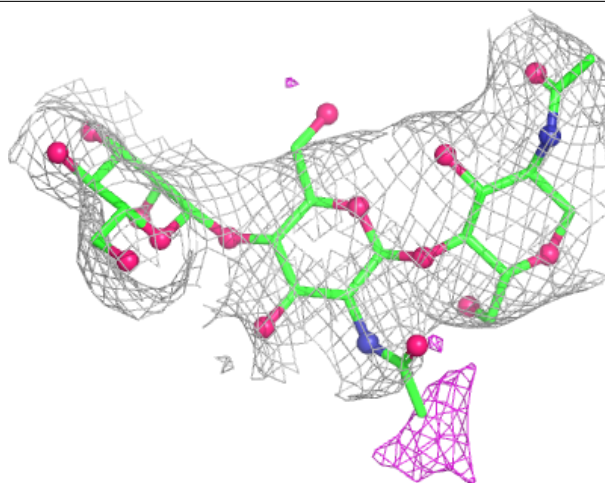
Electron density around Chain 5:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



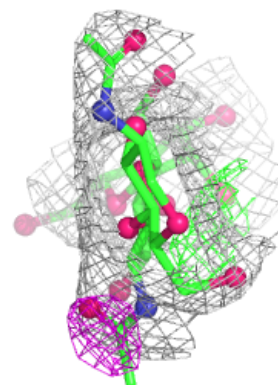
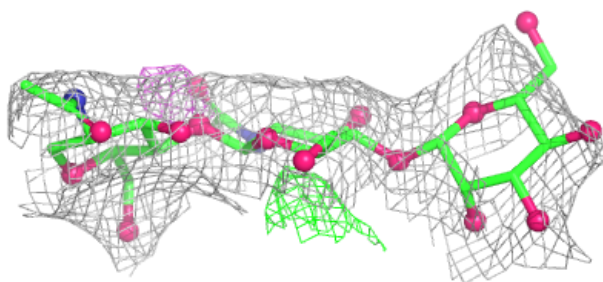
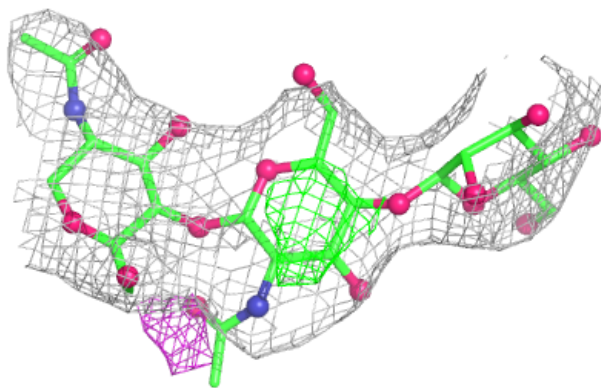
Electron density around Chain CA:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



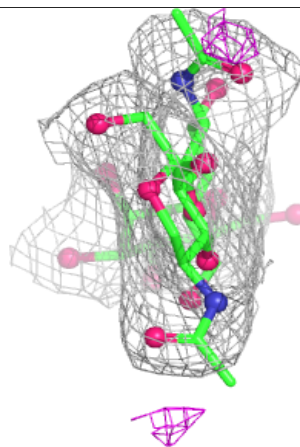
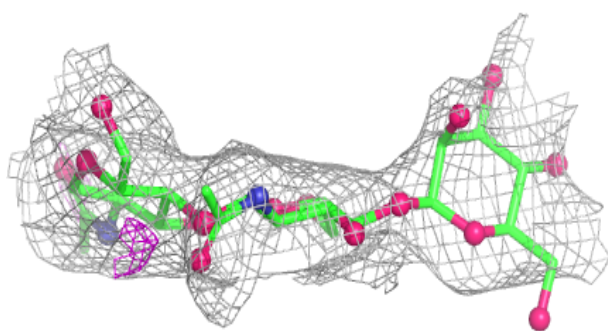
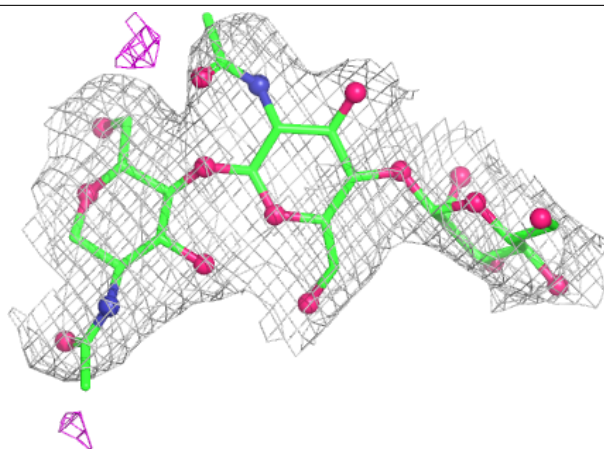
Electron density around Chain DA:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

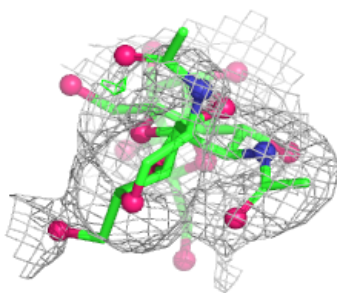
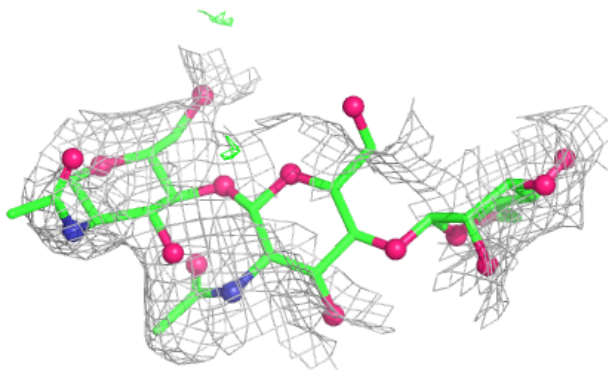
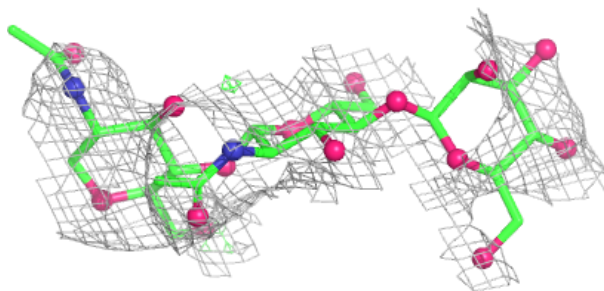


Electron density around Chain EA:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

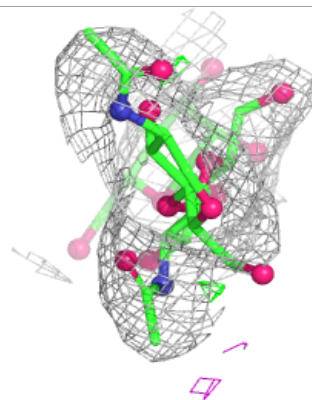
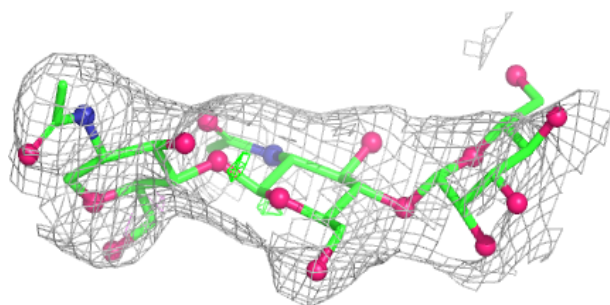
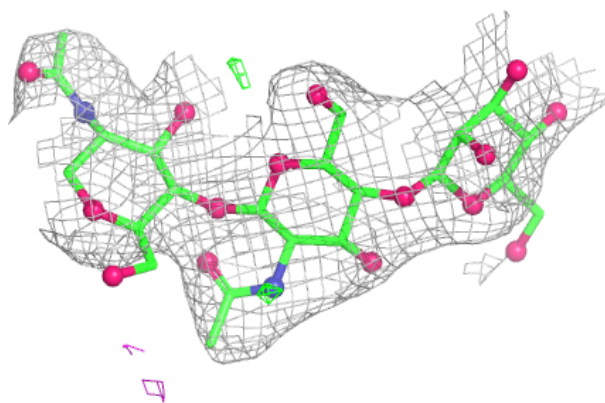
**Electron density around Chain GA:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

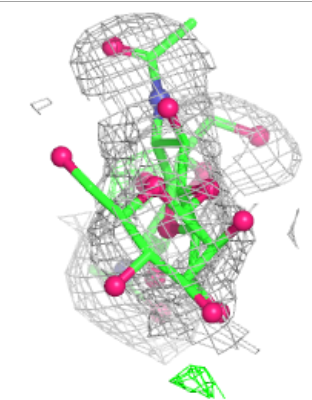
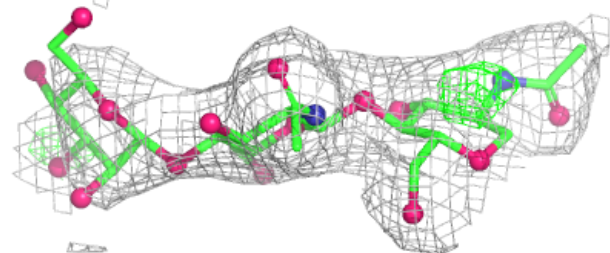
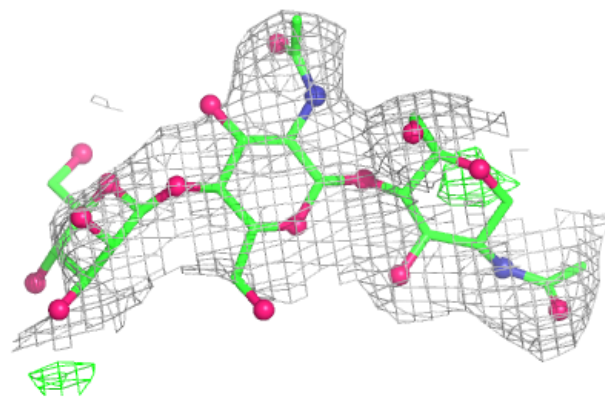


Electron density around Chain LA:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

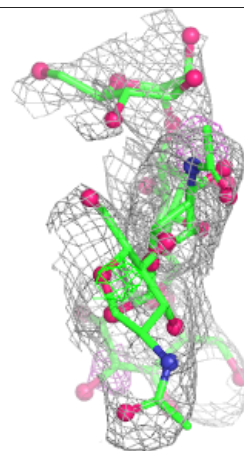
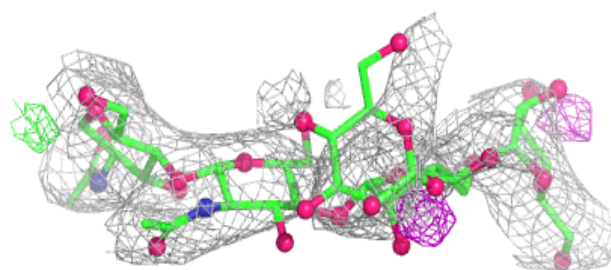
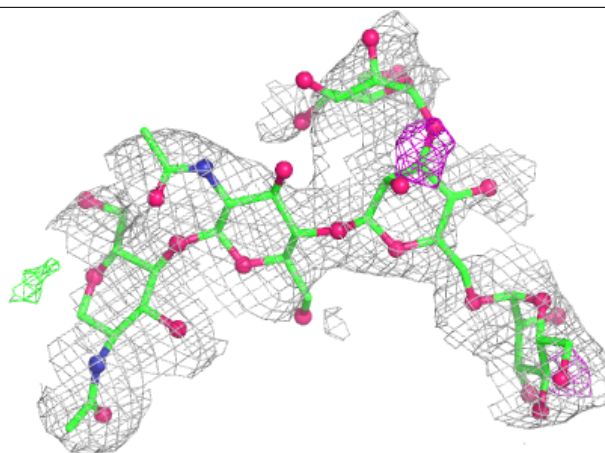
**Electron density around Chain NA:**

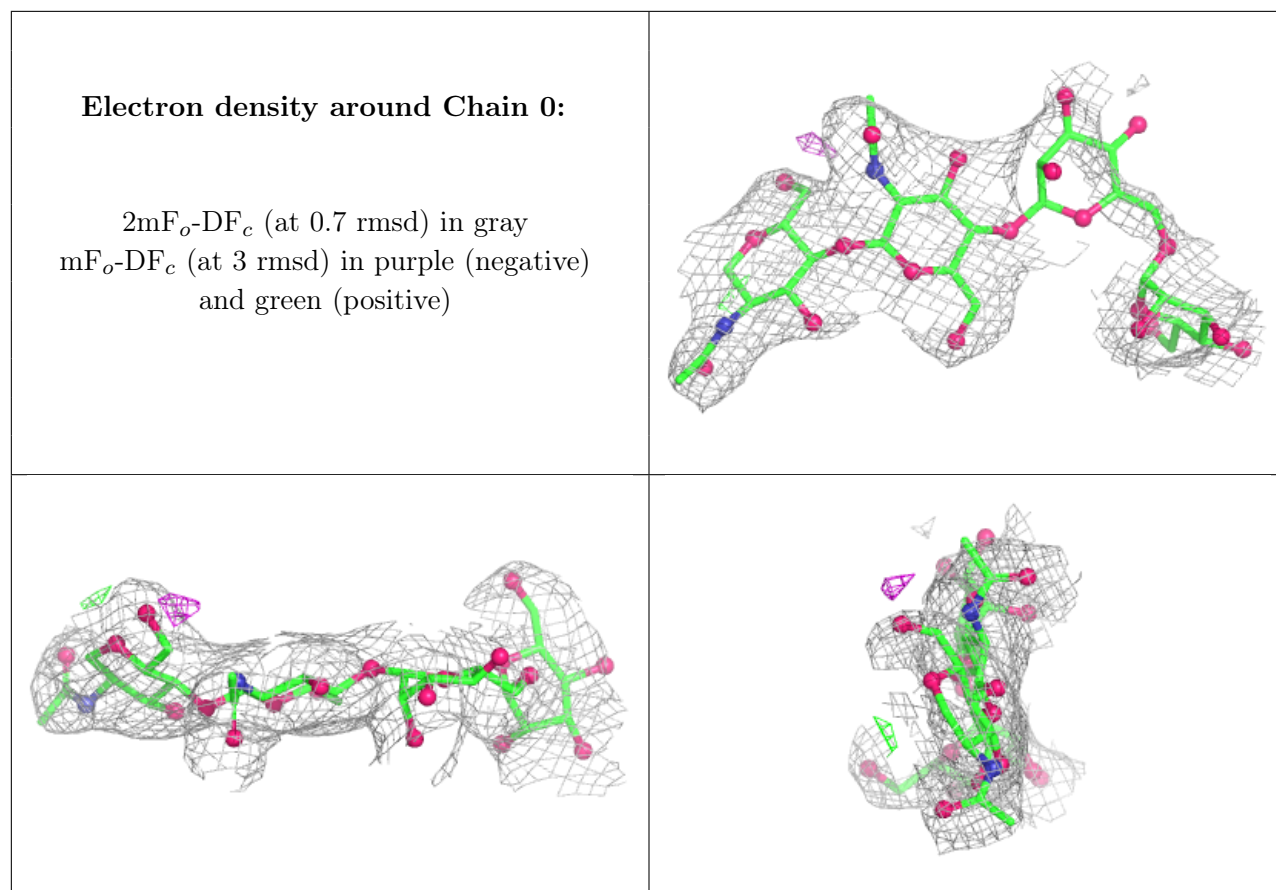
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain z:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)





6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
9	CUO	P	5005[C]	4/4	0.93	0.20	114,114,114,114	4
9	CUO	P	5005[D]	4/4	0.93	0.20	114,114,114,114	4
9	CUO	b	2101[C]	4/4	0.94	0.12	106,106,106,106	4
9	CUO	b	2101[D]	4/4	0.94	0.12	106,106,106,106	4
9	CUO	J	5005[C]	4/4	0.95	0.12	98,98,98,98	4
9	CUO	J	5005[D]	4/4	0.95	0.12	98,98,98,98	4
9	CUO	D	5005[C]	4/4	0.95	0.12	109,109,109,109	4
9	CUO	D	5005[D]	4/4	0.95	0.12	109,109,109,109	4
9	CUO	U	3401[A]	4/4	0.95	0.17	81,81,81,81	4
9	CUO	U	3401[B]	4/4	0.95	0.17	81,81,81,81	4
9	CUO	X	3401[A]	4/4	0.95	0.12	121,121,121,121	4
9	CUO	X	3401[B]	4/4	0.95	0.12	121,121,121,121	4
9	CUO	G	2101[C]	4/4	0.95	0.10	104,104,104,104	4

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
9	CUO	G	2101[D]	4/4	0.95	0.10	104,104,104,104	4
9	CUO	O	3401[A]	4/4	0.96	0.11	85,85,85,85	4
9	CUO	O	3401[B]	4/4	0.96	0.11	85,85,85,85	4
9	CUO	C	3401[A]	4/4	0.96	0.09	99,99,99,99	4
9	CUO	C	3401[B]	4/4	0.96	0.09	99,99,99,99	4
9	CUO	S	2101[C]	4/4	0.96	0.12	94,94,94,94	4
9	CUO	S	2101[D]	4/4	0.96	0.12	94,94,94,94	4
9	CUO	I	3401[A]	4/4	0.96	0.11	84,84,84,84	4
9	CUO	I	3401[B]	4/4	0.96	0.11	84,84,84,84	4
9	CUO	F	3401[A]	4/4	0.96	0.12	86,86,86,86	4
9	CUO	F	3401[B]	4/4	0.96	0.12	86,86,86,86	4
9	CUO	Y	2101[C]	4/4	0.96	0.10	99,99,99,99	4
9	CUO	Y	2101[D]	4/4	0.96	0.10	99,99,99,99	4
9	CUO	M	2101[C]	4/4	0.96	0.10	103,103,103,103	4
9	CUO	M	2101[D]	4/4	0.96	0.10	103,103,103,103	4
9	CUO	L	3401[A]	4/4	0.97	0.09	100,100,100,100	4
9	CUO	L	3401[B]	4/4	0.97	0.09	100,100,100,100	4
9	CUO	A	5005[C]	4/4	0.97	0.10	95,95,95,95	4
9	CUO	A	5005[D]	4/4	0.97	0.10	95,95,95,95	4
9	CUO	a	3401[A]	4/4	0.97	0.10	85,85,85,85	4
9	CUO	a	3401[B]	4/4	0.97	0.10	85,85,85,85	4
9	CUO	V	5005[C]	4/4	0.97	0.14	113,113,113,113	4
9	CUO	V	5005[D]	4/4	0.97	0.14	113,113,113,113	4
9	CUO	d	3401[A]	4/4	0.97	0.12	111,111,111,111	4
9	CUO	d	3401[B]	4/4	0.97	0.12	111,111,111,111	4
9	CUO	J	5003	4/4	0.98	0.07	89,96,96,103	0
9	CUO	M	2104	4/4	0.98	0.07	58,70,74,76	0
9	CUO	R	3401[A]	4/4	0.98	0.06	84,84,84,84	4
9	CUO	R	3401[B]	4/4	0.98	0.06	84,84,84,84	4
9	CUO	A	5002	4/4	0.98	0.09	55,75,89,91	0
9	CUO	G	2104	4/4	0.98	0.09	58,85,92,97	0
9	CUO	S	2104	4/4	0.98	0.07	74,79,82,87	0
9	CUO	N	3002	4/4	0.99	0.05	48,51,70,74	0
9	CUO	D	5002	4/4	0.99	0.08	51,60,82,85	0
9	CUO	G	2105	4/4	0.99	0.04	58,60,66,69	0
9	CUO	P	5001	4/4	0.99	0.05	36,38,56,71	0
9	CUO	P	5002	4/4	0.99	0.06	56,59,75,82	0
9	CUO	P	5003	4/4	0.99	0.07	45,54,76,83	0
9	CUO	P	5004	4/4	0.99	0.06	40,48,67,68	0
9	CUO	H	3001	4/4	0.99	0.06	58,60,72,78	0
9	CUO	H	3002	4/4	0.99	0.04	67,79,83,84	0
9	CUO	Q	3001	4/4	0.99	0.07	37,43,64,70	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
9	CUO	Q	3002	4/4	0.99	0.04	53,62,64,73	0
9	CUO	D	5003	4/4	0.99	0.04	60,62,67,79	0
9	CUO	A	5003	4/4	0.99	0.04	79,87,89,89	0
9	CUO	J	5001	4/4	0.99	0.07	49,52,60,69	0
9	CUO	J	5002	4/4	0.99	0.05	53,56,80,83	0
9	CUO	S	2102	4/4	0.99	0.06	54,65,85,90	0
9	CUO	S	2103	4/4	0.99	0.07	49,52,72,80	0
9	CUO	B	3001	4/4	0.99	0.08	49,55,75,88	0
9	CUO	S	2105	4/4	0.99	0.05	45,45,62,71	0
9	CUO	T	3001	4/4	0.99	0.05	44,59,84,85	0
9	CUO	T	3002	4/4	0.99	0.06	52,69,74,84	0
9	CUO	J	5004	4/4	0.99	0.05	49,58,62,63	0
9	CUO	E	3001	4/4	0.99	0.06	55,55,80,85	0
9	CUO	V	5001	4/4	0.99	0.08	39,39,64,66	0
9	CUO	V	5002	4/4	0.99	0.07	50,61,67,72	0
9	CUO	V	5003	4/4	0.99	0.07	66,79,89,90	0
9	CUO	V	5004	4/4	0.99	0.05	44,50,62,65	0
9	CUO	B	3002	4/4	0.99	0.06	57,58,80,91	0
9	CUO	K	3001	4/4	0.99	0.04	57,73,73,80	0
9	CUO	W	3001	4/4	0.99	0.08	37,41,72,78	0
9	CUO	W	3002	4/4	0.99	0.05	58,62,70,77	0
9	CUO	K	3002	4/4	0.99	0.06	52,69,75,79	0
9	CUO	A	5004	4/4	0.99	0.06	51,60,67,70	0
9	CUO	A	5001	4/4	0.99	0.07	70,73,87,92	0
9	CUO	D	5001	4/4	0.99	0.07	64,68,95,98	0
9	CUO	Y	2102	4/4	0.99	0.06	59,67,69,83	0
9	CUO	Y	2103	4/4	0.99	0.10	58,65,82,85	0
9	CUO	Y	2104	4/4	0.99	0.06	69,75,80,100	0
9	CUO	Y	2105	4/4	0.99	0.05	47,59,61,62	0
9	CUO	Z	3001	4/4	0.99	0.07	46,54,67,69	0
9	CUO	Z	3002	4/4	0.99	0.07	48,68,69,72	0
9	CUO	G	2102	4/4	0.99	0.04	57,62,65,70	0
9	CUO	M	2102	4/4	0.99	0.05	41,52,59,63	0
9	CUO	M	2103	4/4	0.99	0.05	50,59,66,68	0
9	CUO	G	2103	4/4	0.99	0.07	49,58,62,73	0
9	CUO	b	2102	4/4	0.99	0.06	60,63,73,78	0
9	CUO	b	2103	4/4	0.99	0.06	55,59,71,73	0
9	CUO	b	2104	4/4	0.99	0.08	60,75,83,94	0
9	CUO	b	2105	4/4	0.99	0.04	54,57,68,74	0
9	CUO	c	3001	4/4	0.99	0.07	48,56,77,80	0
9	CUO	c	3002	4/4	0.99	0.05	70,71,79,80	0
9	CUO	M	2105	4/4	0.99	0.06	48,60,61,62	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
9	CUO	N	3001	4/4	0.99	0.06	36,39,74,80	0
9	CUO	D	5004	4/4	1.00	0.04	52,54,59,62	0
9	CUO	E	3002	4/4	1.00	0.04	57,61,67,68	0

6.5 Other polymers [i](#)

There are no such residues in this entry.