



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 4, 2023 – 06:37 PM EDT

PDB ID : 6OM1
Title : Crystal structure of an atypical integrin
Authors : Wang, J.C.; Springer, T.A.
Deposited on : 2019-04-17
Resolution : 2.66 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 : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.35.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.35.1

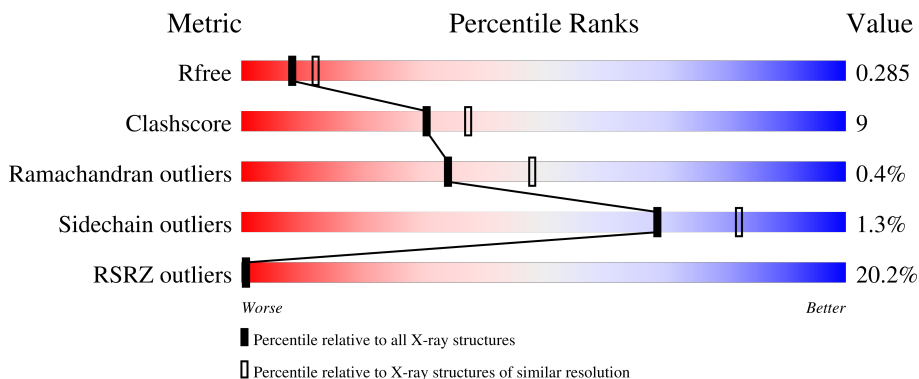
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.66 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}	130704	1332 (2.68-2.64)
Clashscore	141614	1374 (2.68-2.64)
Ramachandran outliers	138981	1349 (2.68-2.64)
Sidechain outliers	138945	1349 (2.68-2.64)
RSRZ outliers	127900	1318 (2.68-2.64)

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
10	NAG	C	601	-	-	-	X
10	NAG	C	626	-	-	-	X
10	NAG	F	501	-	-	-	X
10	NAG	G	2023	-	-	-	X
10	NAG	G	2024	-	-	-	X
12	EDO	C	629	-	-	-	X
3	NAG	I	1	-	-	-	X
3	NAG	I	2	-	-	X	-
3	BMA	I	3	-	-	X	-
3	MAN	I	4	-	-	-	X
3	BMA	Q	3	-	-	X	-
6	NAG	M	2	-	-	-	X
6	NAG	T	1	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	NAG	T	2	-	-	-	X
6	NAG	Z	2	-	-	-	X
6	NAG	e	1	-	-	-	X
6	NAG	e	2	-	-	-	X
6	NAG	g	2	-	-	-	X
7	BMA	R	3	-	-	X	-
7	BMA	W	3	-	-	X	-

2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 57933 atoms, of which 27345 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 Integrin alpha-V.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	592	8954	2905	4374	776	878	21	0	0	0
1	C	595	9011	2918	4409	780	883	21	0	0	0
1	E	593	8984	2905	4399	778	881	21	0	0	0
1	G	596	9006	2922	4395	783	885	21	0	0	0

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	400	GLY	-	insertion	UNP P06756
A	401	CYS	MET	engineered mutation	UNP P06756
A	596	THR	-	expression tag	UNP P06756
A	597	GLY	-	expression tag	UNP P06756
A	598	GLY	-	expression tag	UNP P06756
A	599	LEU	-	expression tag	UNP P06756
C	400	GLY	-	insertion	UNP P06756
C	401	CYS	MET	engineered mutation	UNP P06756
C	596	THR	-	expression tag	UNP P06756
C	597	GLY	-	expression tag	UNP P06756
C	598	GLY	-	expression tag	UNP P06756
C	599	LEU	-	expression tag	UNP P06756
E	400	GLY	-	insertion	UNP P06756
E	401	CYS	MET	engineered mutation	UNP P06756
E	596	THR	-	expression tag	UNP P06756
E	597	GLY	-	expression tag	UNP P06756
E	598	GLY	-	expression tag	UNP P06756
E	599	LEU	-	expression tag	UNP P06756
G	400	GLY	-	insertion	UNP P06756
G	401	CYS	MET	engineered mutation	UNP P06756
G	596	THR	-	expression tag	UNP P06756

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Chain	Residue	Modelled	Actual	Comment	Reference
G	597	GLY	-	expression tag	UNP P06756
G	598	GLY	-	expression tag	UNP P06756
G	599	LEU	-	expression tag	UNP P06756

- Molecule 2 is a protein called Integrin beta-8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
2	B	333	Total	C	H	N	O	S	0	0	0
			5068	1658	2455	447	491	17			
2	D	312	Total	C	H	N	O	S	0	0	0
			4742	1559	2291	416	462	14			
2	F	332	Total	C	H	N	O	S	0	0	0
			5069	1648	2470	448	488	15			
2	H	336	Total	C	H	N	O	S	0	0	0
			5181	1667	2552	453	491	18			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	259	CYS	VAL	engineered mutation	UNP P26012
D	259	CYS	VAL	engineered mutation	UNP P26012
F	259	CYS	VAL	engineered mutation	UNP P26012
H	259	CYS	VAL	engineered mutation	UNP P26012

- Molecule 3 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.



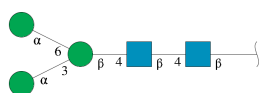
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	I	4	Total	C	N	O	0	0	0
			50	28	2	20			
3	K	4	Total	C	N	O	0	0	0
			50	28	2	20			
3	O	4	Total	C	N	O	0	0	0
			50	28	2	20			
3	Q	4	Total	C	N	O	0	0	0
			50	28	2	20			

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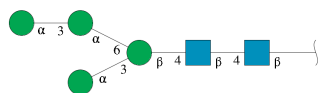
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	S	4	Total	C	N	O	0	0	0
			50	28	2	20			
3	a	4	Total	C	N	O	0	0	0
			50	28	2	20			
3	d	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 4 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.



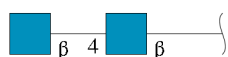
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	J	5	Total	C	N	O	0	0	0
			61	34	2	25			
4	U	5	Total	C	N	O	0	0	0
			61	34	2	25			
4	X	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



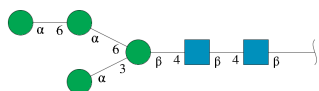
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	L	6	Total	C	N	O	0	0	0
			72	40	2	30			

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



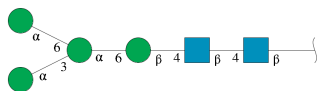
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	M	2	Total	C	N	O	0	0	0
			28	16	2	10			
6	N	2	Total	C	N	O	0	0	0
			28	16	2	10			
6	T	2	Total	C	N	O	0	0	0
			28	16	2	10			
6	V	2	Total	C	N	O	0	0	0
			28	16	2	10			
6	Y	2	Total	C	N	O	0	0	0
			28	16	2	10			
6	Z	2	Total	C	N	O	0	0	0
			28	16	2	10			
6	e	2	Total	C	N	O	0	0	0
			28	16	2	10			
6	f	2	Total	C	N	O	0	0	0
			28	16	2	10			
6	g	2	Total	C	N	O	0	0	0
			28	16	2	10			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	P	6	Total	C	N	O	0	0	0
			72	40	2	30			
7	R	6	Total	C	N	O	0	0	0
			72	40	2	30			
7	W	6	Total	C	N	O	0	0	0
			72	40	2	30			

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



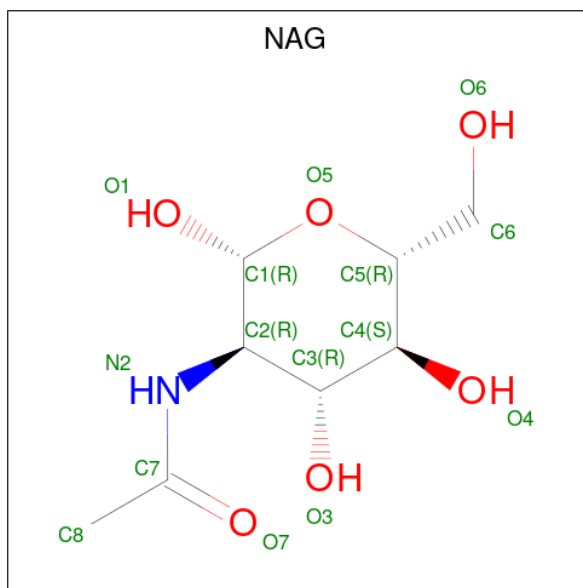
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
8	b	6	72	40	2	30	0	0	0

- Molecule 9 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-beta-D-mannopyranos e-(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
			Total	C	N	O			
9	c	4	50	28	2	20	0	0	0

- Molecule 10 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
10	A	1	14	8	1	5	0	0
10	B	1	14	8	1	5	0	0
10	C	1	14	8	1	5	0	0
10	C	1	14	8	1	5	0	0

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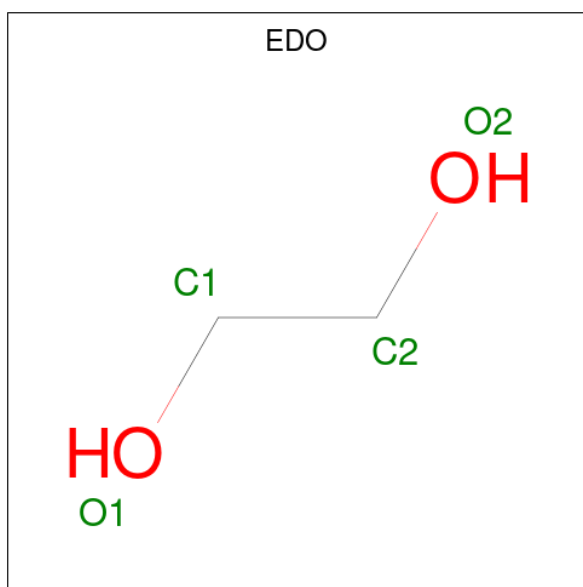
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	D	1	Total	C	N	O	0	0
			14	8	1	5		
10	D	1	Total	C	N	O	0	0
			14	8	1	5		
10	E	1	Total	C	N	O	0	0
			14	8	1	5		
10	E	1	Total	C	N	O	0	0
			14	8	1	5		
10	F	1	Total	C	N	O	0	0
			14	8	1	5		
10	F	1	Total	C	N	O	0	0
			14	8	1	5		
10	G	1	Total	C	N	O	0	0
			14	8	1	5		
10	G	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 11 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	4	Total	Ca	0	0
			4	4		
11	B	1	Total	Ca	0	0
			1	1		
11	C	4	Total	Ca	0	0
			4	4		
11	D	1	Total	Ca	0	0
			1	1		
11	E	4	Total	Ca	0	0
			4	4		
11	F	1	Total	Ca	0	0
			1	1		
11	G	4	Total	Ca	0	0
			4	4		
11	H	1	Total	Ca	0	0
			1	1		

- Molecule 12 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).

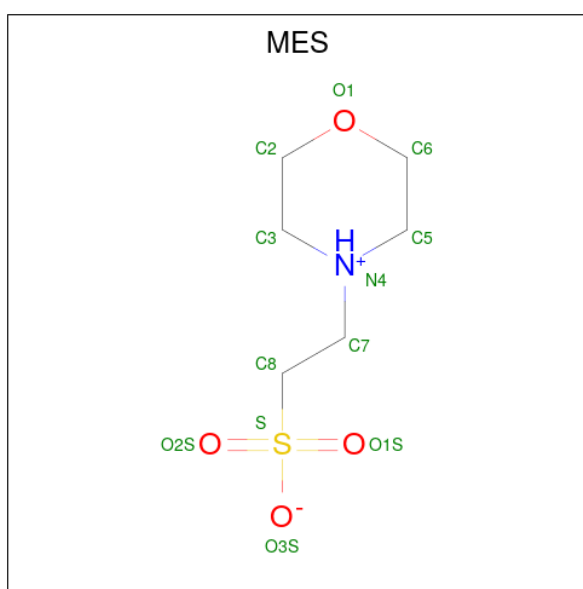


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	A	1	Total C O 4 2 2	0	0
12	B	1	Total C O 4 2 2	0	0
12	B	1	Total C O 4 2 2	0	0
12	C	1	Total C O 4 2 2	0	0
12	C	1	Total C O 4 2 2	0	0
12	C	1	Total C O 4 2 2	0	0
12	E	1	Total C O 4 2 2	0	0
12	F	1	Total C O 4 2 2	0	0
12	G	1	Total C O 4 2 2	0	0
12	G	1	Total C O 4 2 2	0	0
12	G	1	Total C O 4 2 2	0	0
12	G	1	Total C O 4 2 2	0	0
12	H	1	Total C O 4 2 2	0	0

- Molecule 13 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	B	1	Total Mg 1 1	0	0
13	D	1	Total Mg 1 1	0	0
13	F	1	Total Mg 1 1	0	0
13	H	1	Total Mg 1 1	0	0

- Molecule 14 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C₆H₁₃NO₄S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	B	1	Total C N O S 12 6 1 4 1	0	0
14	D	1	Total C N O S 12 6 1 4 1	0	0
14	F	1	Total C N O S 12 6 1 4 1	0	0
14	H	1	Total C N O S 12 6 1 4 1	0	0

- Molecule 15 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	A	137	Total O 137 137	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	B	25	Total O 25 25	0	0
15	C	108	Total O 108 108	0	0
15	D	14	Total O 14 14	0	0
15	E	47	Total O 47 47	0	0
15	F	23	Total O 23 23	0	0
15	G	62	Total O 62 62	0	0
15	H	15	Total O 15 15	0	0

SEQUENCE-PLOTS INFOmissingINFO

3 Data and refinement statistics i

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	144.24Å 55.07Å 175.07Å 90.37° 107.00° 90.01°	Depositor
Resolution (Å)	48.07 – 2.66 48.07 – 2.60	Depositor EDS
% Data completeness (in resolution range)	95.6 (48.07-2.66) 95.3 (48.07-2.60)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.99 (at 2.61Å)	Xtrriage
Refinement program	PHENIX (1.14_3260: ???)	Depositor
R, R_{free}	0.248 , 0.280 0.254 , 0.285	Depositor DCC
R_{free} test set	2001 reflections (1.32%)	wwPDB-VP
Wilson B-factor (Å ²)	79.1	Xtrriage
Anisotropy	0.201	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 75.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.015 for -h,k,-l	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	57933	wwPDB-VP
Average B, all atoms (Å ²)	118.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.76% 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.

4 Model quality [i](#)

4.1 Standard geometry [i](#)

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

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	0.27	0/4681	0.46	0/6332
1	C	0.26	0/4704	0.46	0/6367
1	E	0.26	0/4687	0.45	0/6343
1	G	0.26	0/4713	0.45	0/6377
2	B	0.25	0/2662	0.42	0/3600
2	D	0.25	0/2497	0.42	0/3378
2	F	0.25	0/2650	0.41	0/3587
2	H	0.25	0/2679	0.44	0/3621
All	All	0.26	0/29273	0.44	0/39605

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

4.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4580	4374	4429	64	1
1	C	4602	4409	4450	60	2
1	E	4585	4399	4427	82	0
1	G	4611	4395	4458	61	0
2	B	2613	2455	2600	65	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	2451	2291	2431	51	0
2	F	2599	2470	2580	48	0
2	H	2629	2552	2615	54	0
3	I	50	0	43	11	1
3	K	50	0	43	2	0
3	O	50	0	43	2	0
3	Q	50	0	43	10	0
3	S	50	0	43	1	0
3	a	50	0	43	0	0
3	d	50	0	43	0	0
4	J	61	0	52	0	0
4	U	61	0	52	1	0
4	X	61	0	52	1	0
5	L	72	0	61	8	0
6	M	28	0	25	1	0
6	N	28	0	25	0	0
6	T	28	0	25	2	0
6	V	28	0	25	1	0
6	Y	28	0	25	4	0
6	Z	28	0	25	1	0
6	e	28	0	25	0	0
6	f	28	0	25	0	0
6	g	28	0	25	0	0
7	P	72	0	61	1	0
7	R	72	0	61	7	0
7	W	72	0	61	7	0
8	b	72	0	61	0	0
9	c	50	0	43	0	0
10	A	14	0	13	0	0
10	B	14	0	13	0	0
10	C	28	0	26	1	0
10	D	28	0	26	3	0
10	E	28	0	26	1	0
10	F	28	0	26	1	0
10	G	28	0	26	3	0
11	A	4	0	0	0	0
11	B	1	0	0	0	0
11	C	4	0	0	0	0
11	D	1	0	0	0	0
11	E	4	0	0	0	0
11	F	1	0	0	0	0
11	G	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	H	1	0	0	0	0
12	A	4	0	6	0	0
12	B	8	0	12	0	0
12	C	12	0	18	0	0
12	E	4	0	6	0	0
12	F	4	0	6	0	0
12	G	16	0	24	2	0
12	H	4	0	6	0	0
13	B	1	0	0	0	0
13	D	1	0	0	0	0
13	F	1	0	0	0	0
13	H	1	0	0	0	0
14	B	12	0	13	3	0
14	D	12	0	13	3	0
14	F	12	0	13	4	0
14	H	12	0	13	2	0
15	A	137	0	0	3	1
15	B	25	0	0	5	0
15	C	108	0	0	4	1
15	D	14	0	0	1	0
15	E	47	0	0	3	0
15	F	23	0	0	1	0
15	G	62	0	0	3	1
15	H	15	0	0	2	1
All	All	30588	27345	29306	512	4

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 9.

The worst 5 of 512 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:325:GLU:HG2	2:D:327:LYS:HE2	1.26	1.12
3:I:2:NAG:O3	3:I:3:BMA:O5	1.78	1.02
2:B:66:ILE:HB	2:B:67:PRO:HD3	1.44	0.98
2:H:352:ASN:HB3	2:H:406:ALA:HB1	1.44	0.97
7:R:2:NAG:H61	7:R:3:BMA:H2	1.56	0.87

All (4) 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)
15:A:809:HOH:O	15:C:731:HOH:O[1_545]	2.01	0.19
15:G:2123:HOH:O	15:H:603:HOH:O[1_565]	2.07	0.13
1:A:530:ARG:O	1:C:417:LYS:NZ[1_545]	2.08	0.12
1:C:491:LYS:NZ	3:I:3:BMA:O6[1_565]	2.19	0.01

4.3 Torsion angles [i](#)

4.3.1 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	584/599 (98%)	550 (94%)	31 (5%)	3 (0%)	29	43
1	C	589/599 (98%)	556 (94%)	32 (5%)	1 (0%)	47	64
1	E	587/599 (98%)	538 (92%)	48 (8%)	1 (0%)	47	64
1	G	590/599 (98%)	546 (92%)	43 (7%)	1 (0%)	47	64
2	B	322/456 (71%)	290 (90%)	28 (9%)	4 (1%)	13	19
2	D	298/456 (65%)	266 (89%)	29 (10%)	3 (1%)	15	23
2	F	323/456 (71%)	288 (89%)	35 (11%)	0	100	100
2	H	326/456 (72%)	293 (90%)	31 (10%)	2 (1%)	25	37
All	All	3619/4220 (86%)	3327 (92%)	277 (8%)	15 (0%)	34	48

5 of 15 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	400	GLY
2	B	326	SER
1	A	596	THR
2	B	72	ILE
2	B	175	ASP

4.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	485/489 (99%)	479 (99%)	6 (1%)	71	84
1	C	487/489 (100%)	480 (99%)	7 (1%)	67	81
1	E	485/489 (99%)	479 (99%)	6 (1%)	71	84
1	G	488/489 (100%)	480 (98%)	8 (2%)	62	78
2	B	296/402 (74%)	293 (99%)	3 (1%)	76	86
2	D	277/402 (69%)	275 (99%)	2 (1%)	84	91
2	F	292/402 (73%)	290 (99%)	2 (1%)	84	91
2	H	296/402 (74%)	291 (98%)	5 (2%)	60	77
All	All	3106/3564 (87%)	3067 (99%)	39 (1%)	69	82

5 of 39 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	275	TYR
2	H	124	LEU
1	G	401	CYS
1	G	475	ASN
2	H	353	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	180	HIS
2	D	294	ASN
2	H	383	ASN

4.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

4.5 Carbohydrates [i](#)

95 monosaccharides are modelled in this entry.

There are no bond length outliers.

There are no bond angle outliers.

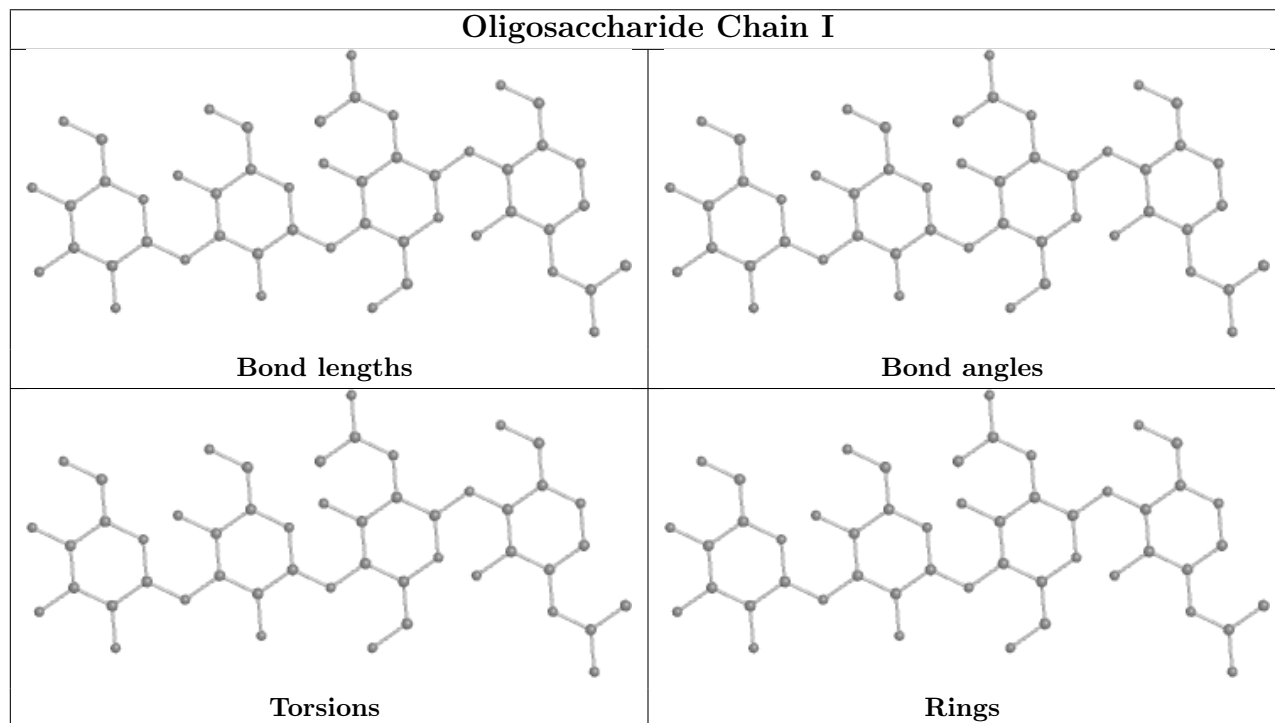
There are no chirality outliers.

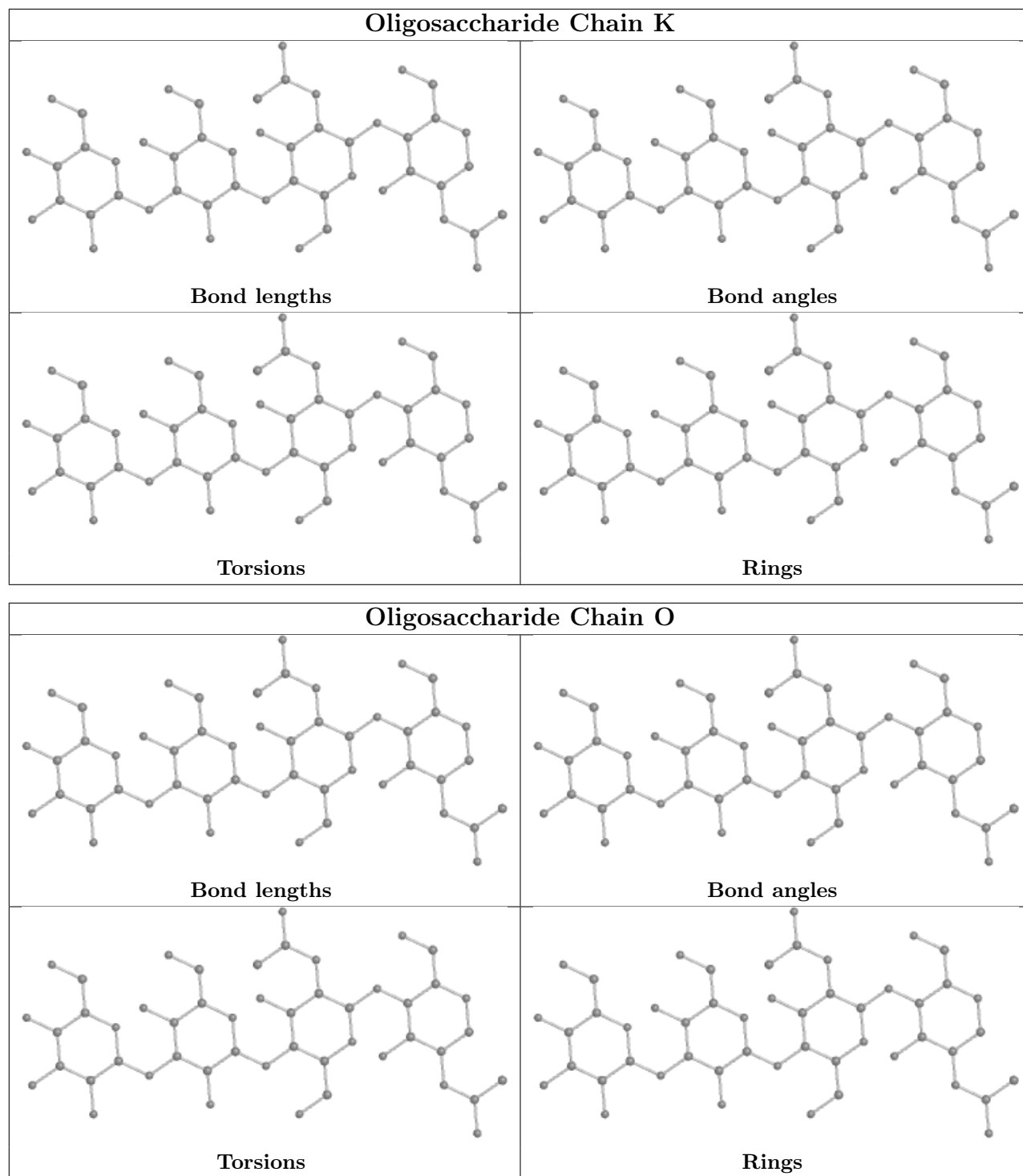
There are no torsion outliers.

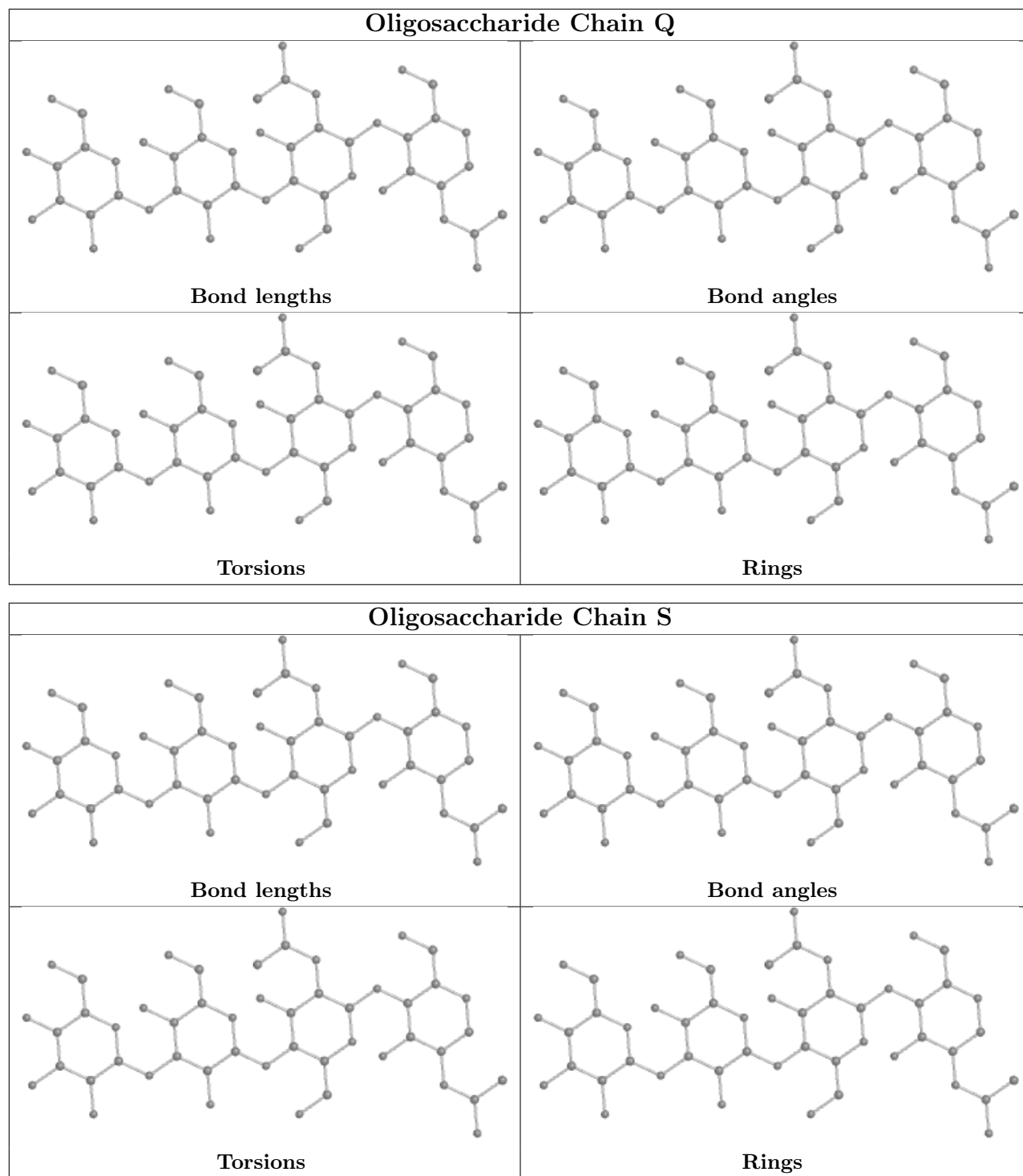
There are no ring outliers.

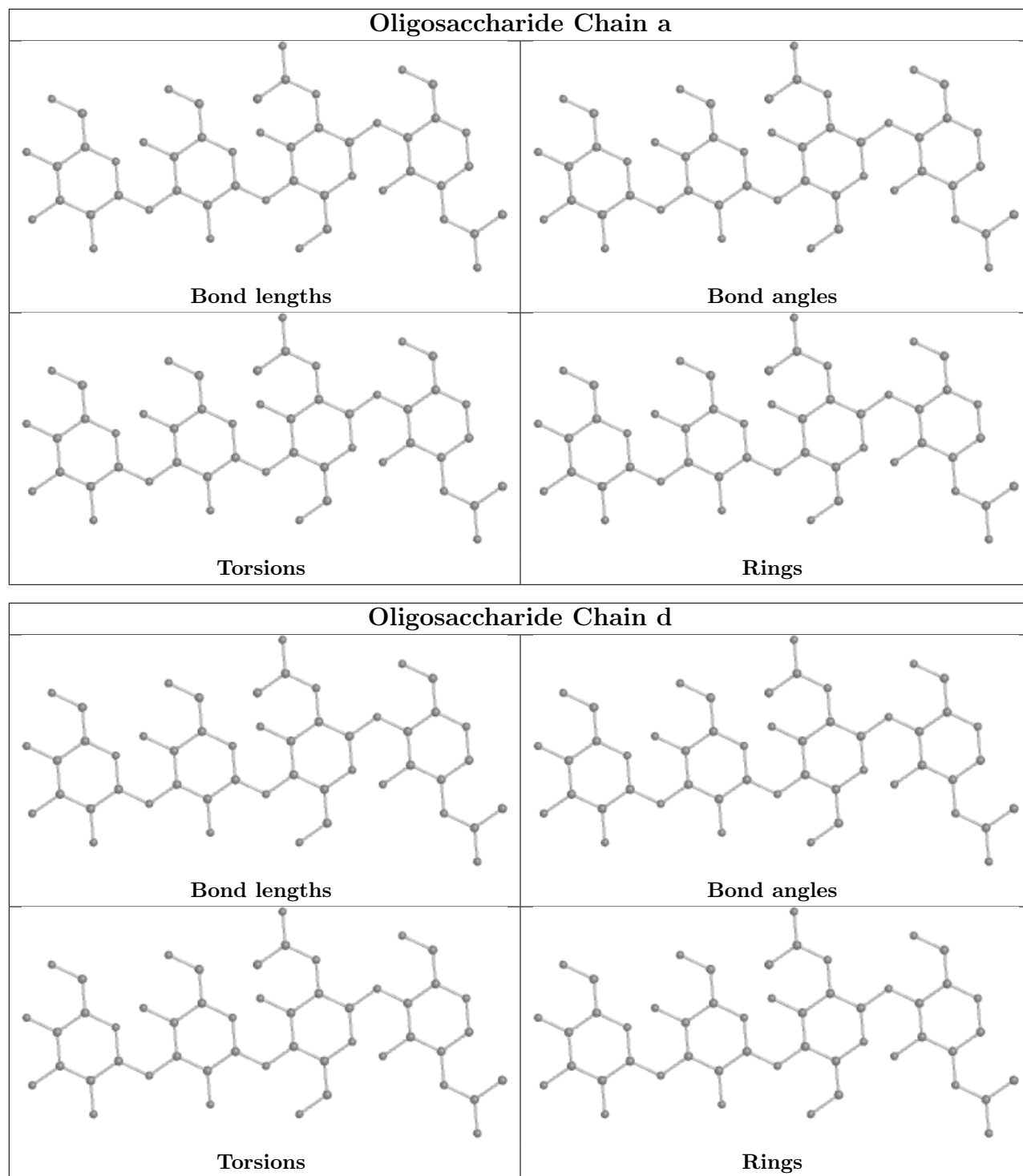
No monomer is involved in short contacts.

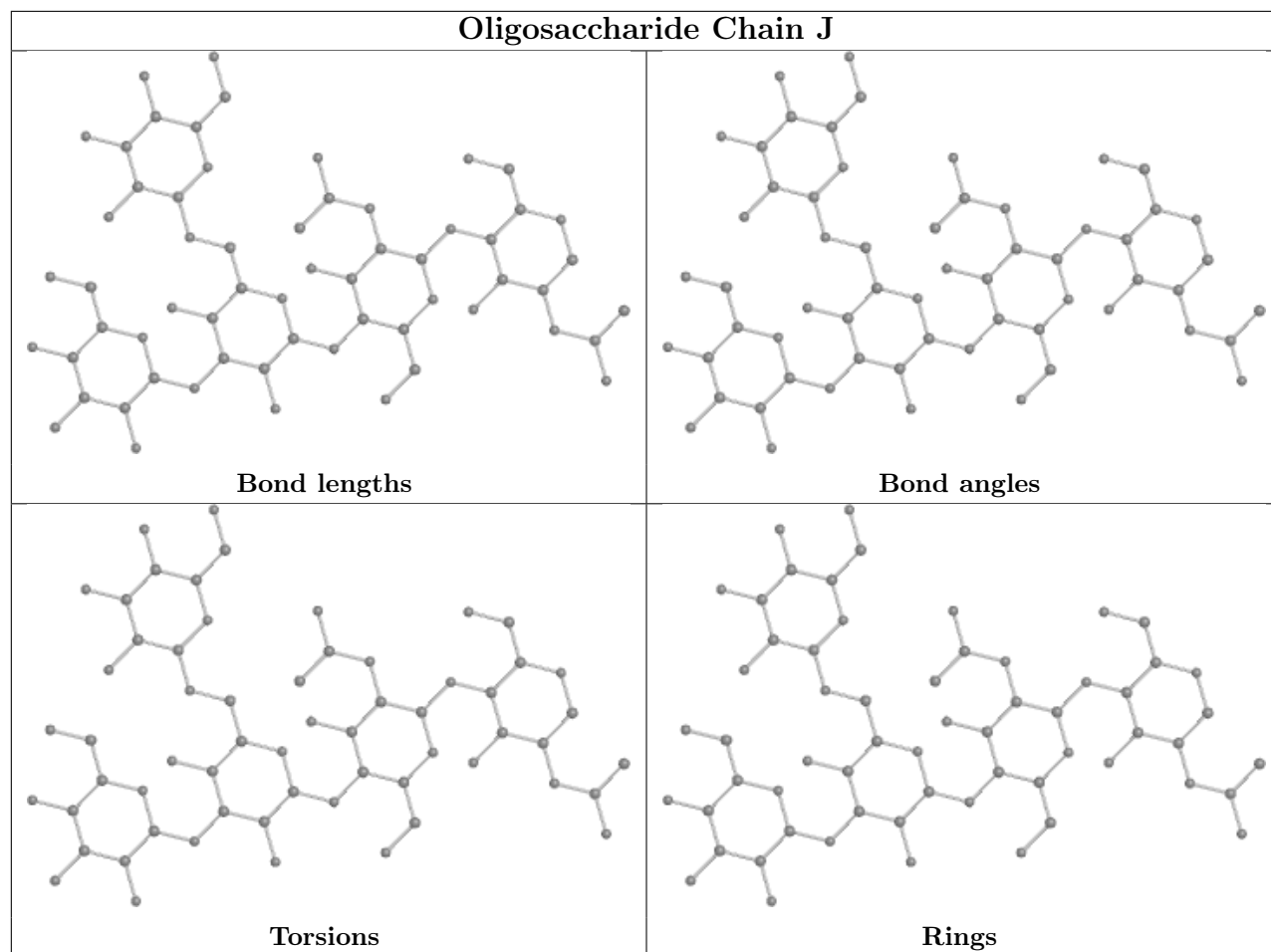
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

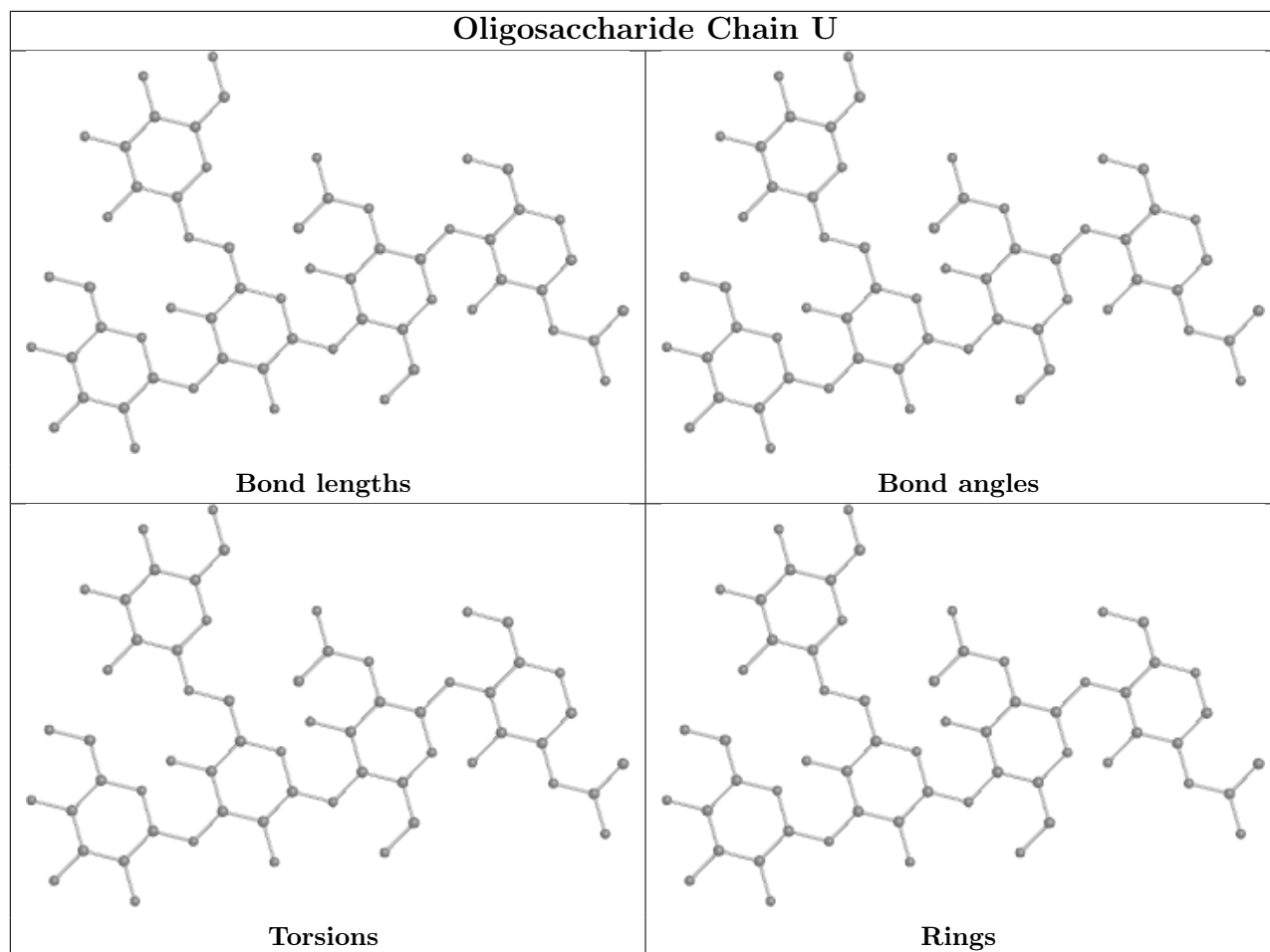


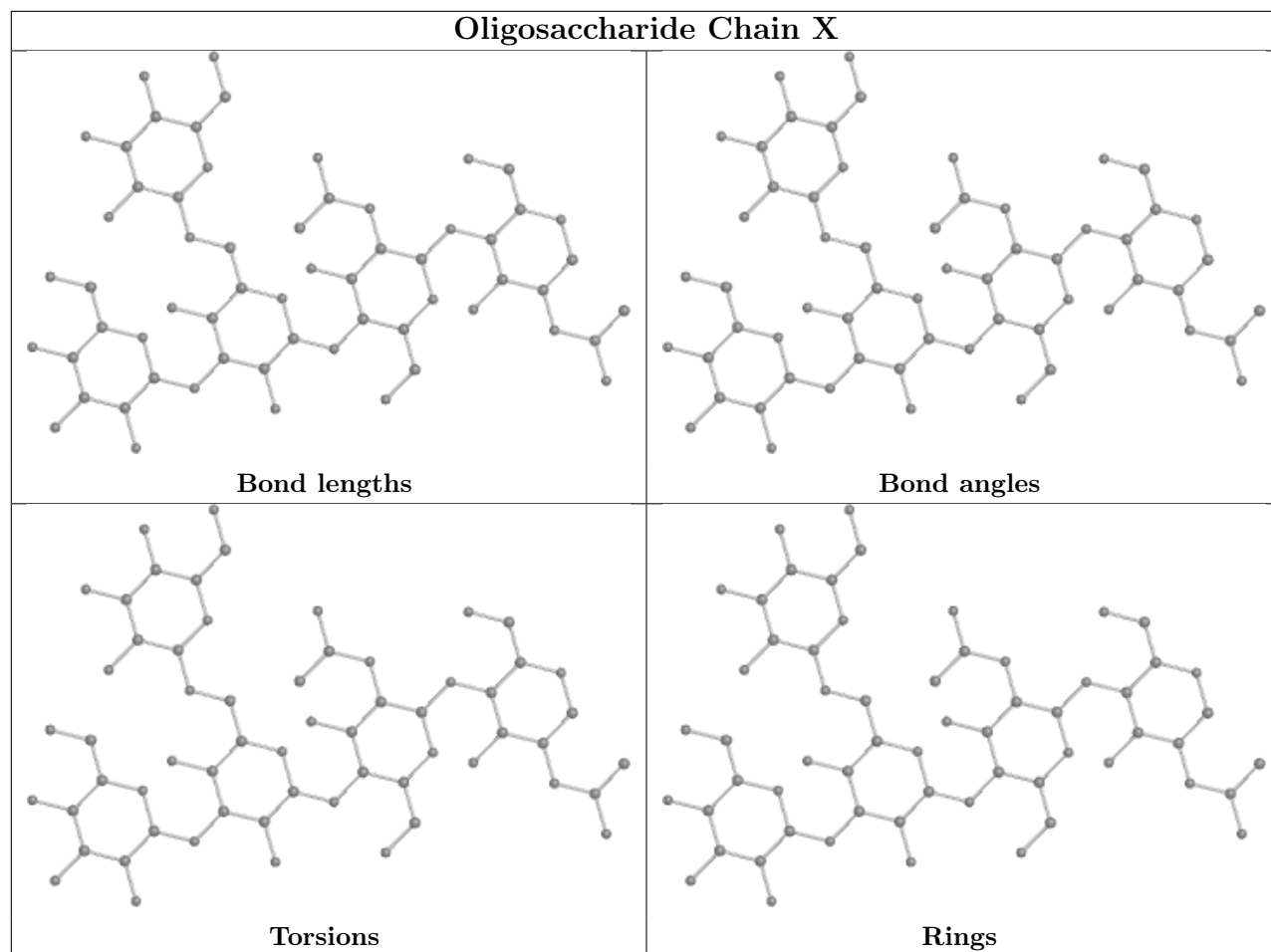


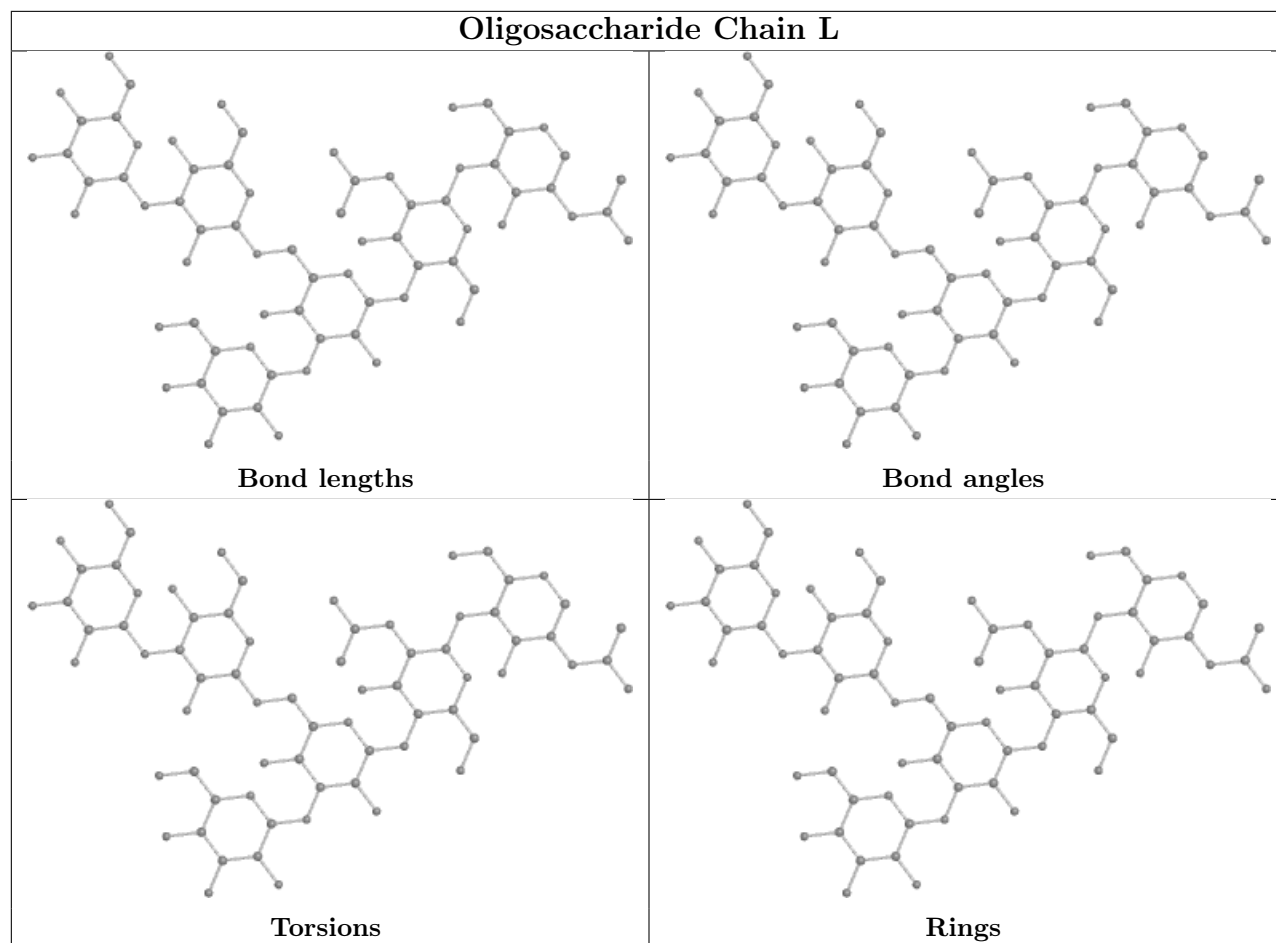


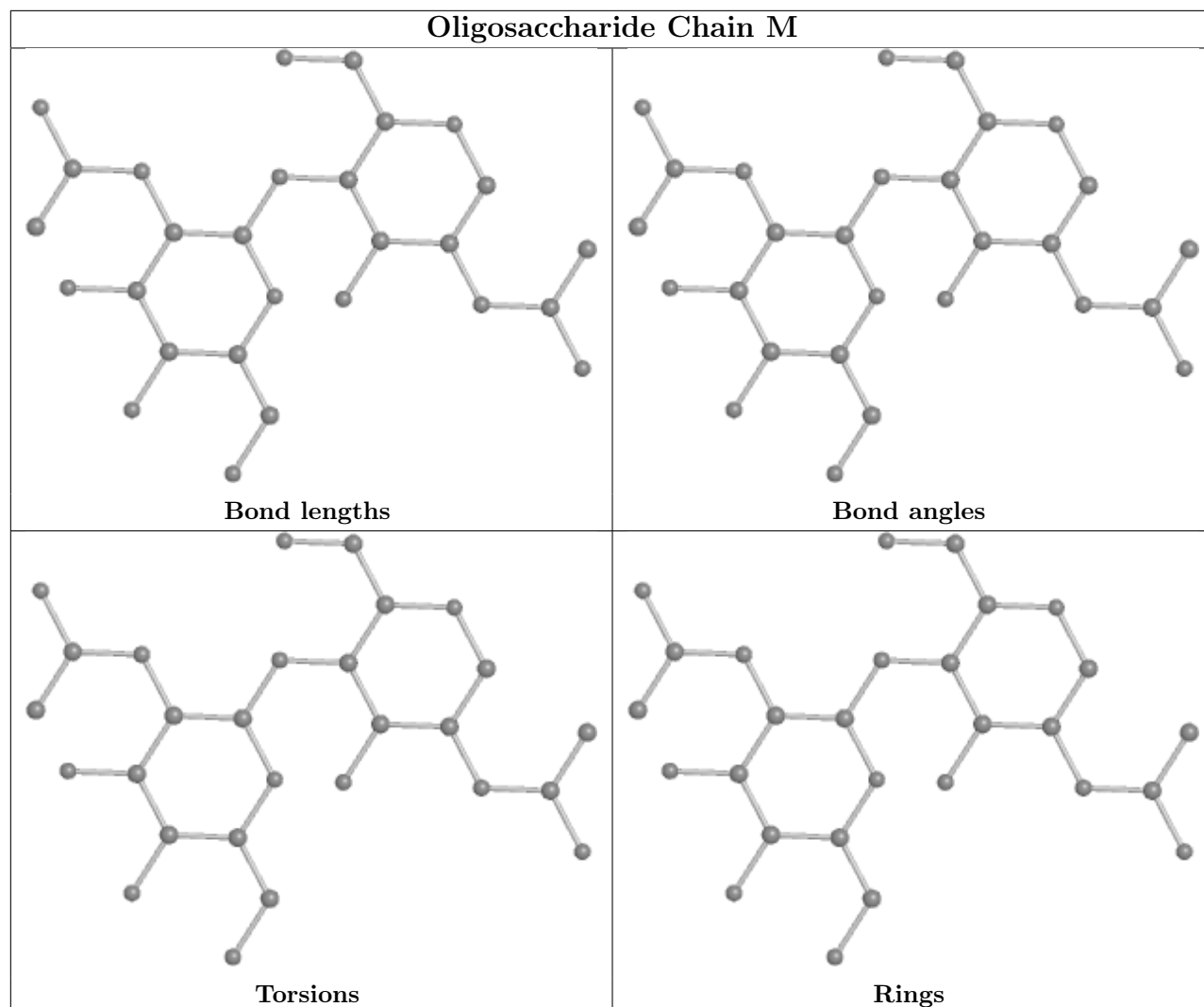


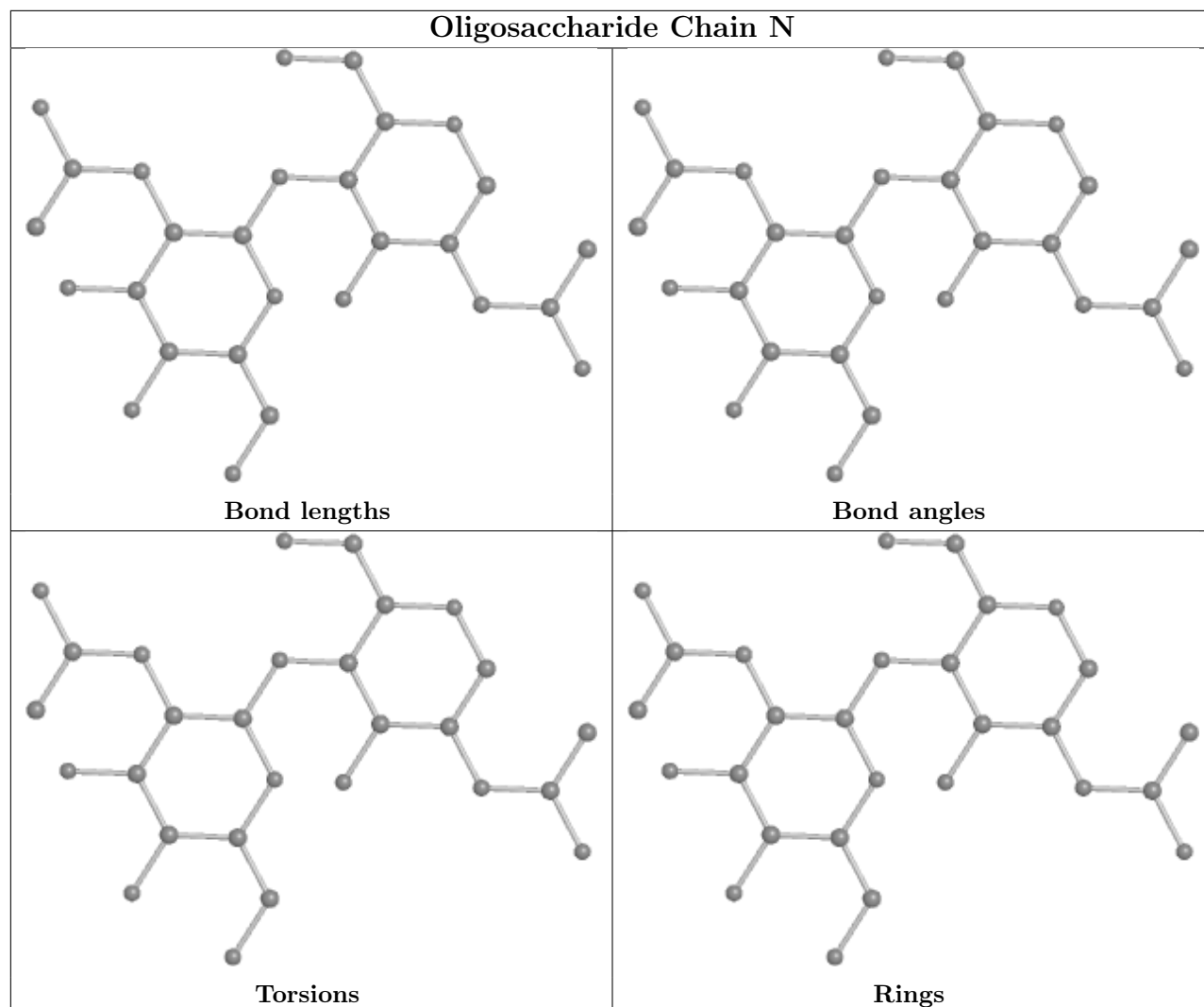


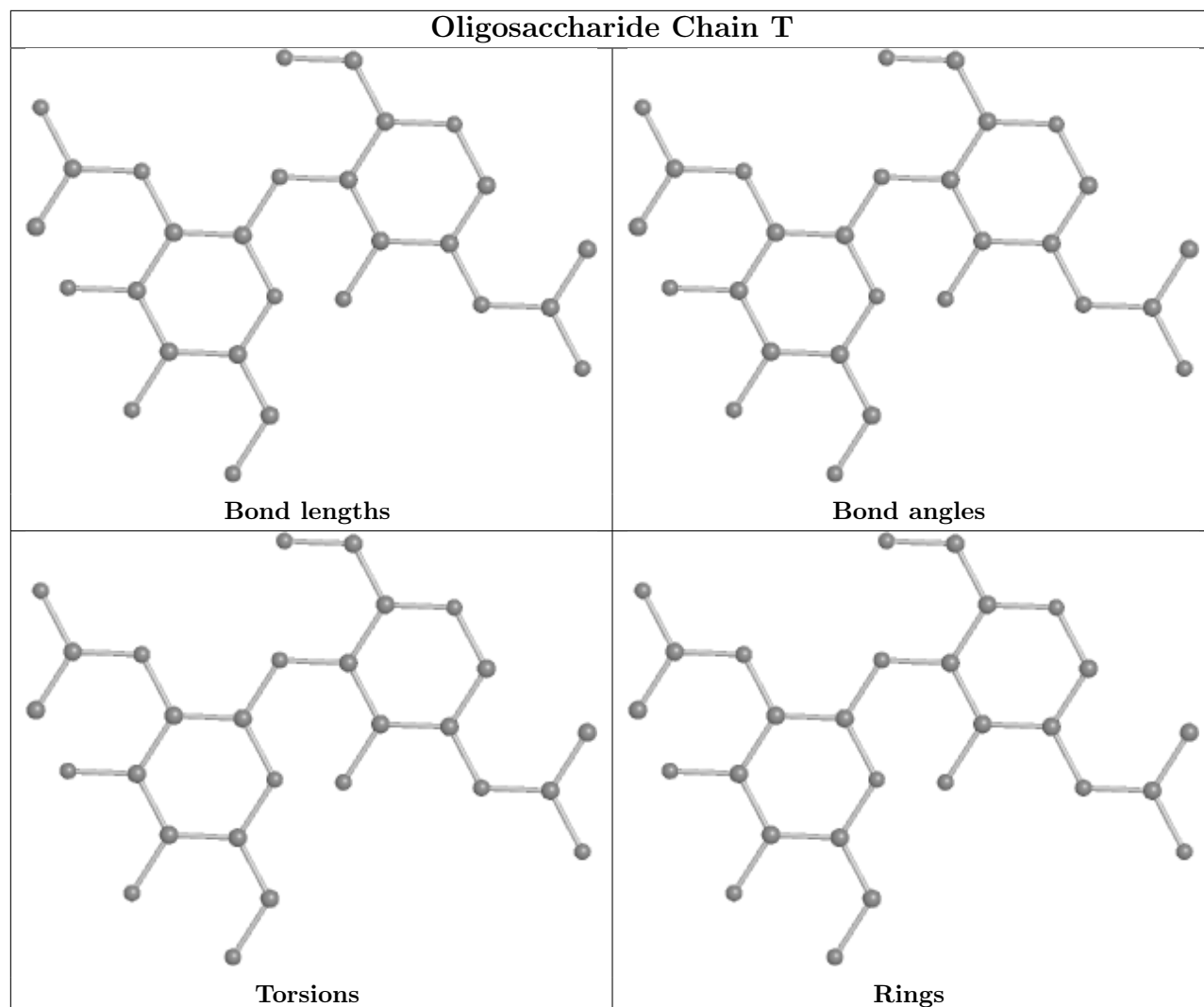


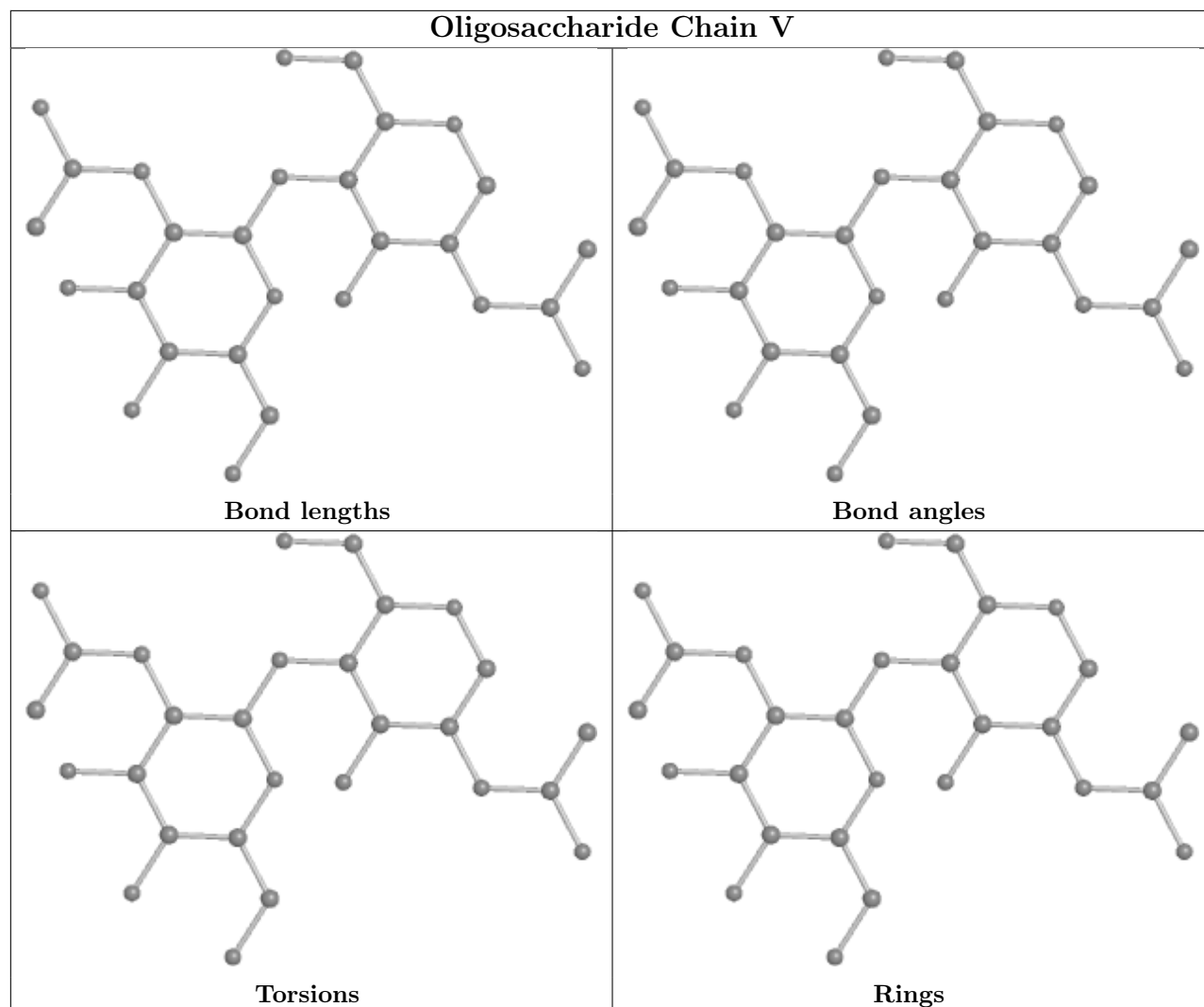


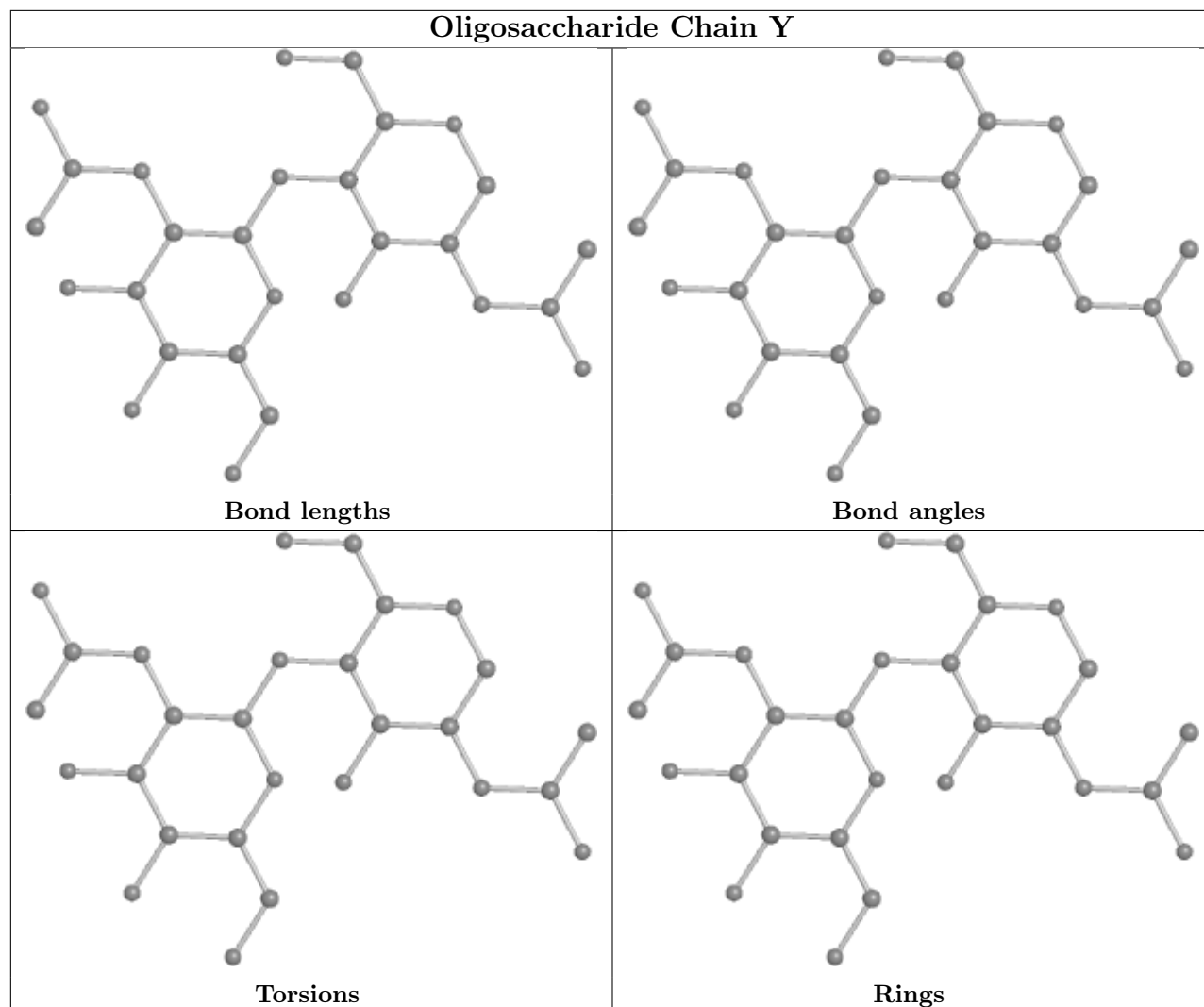


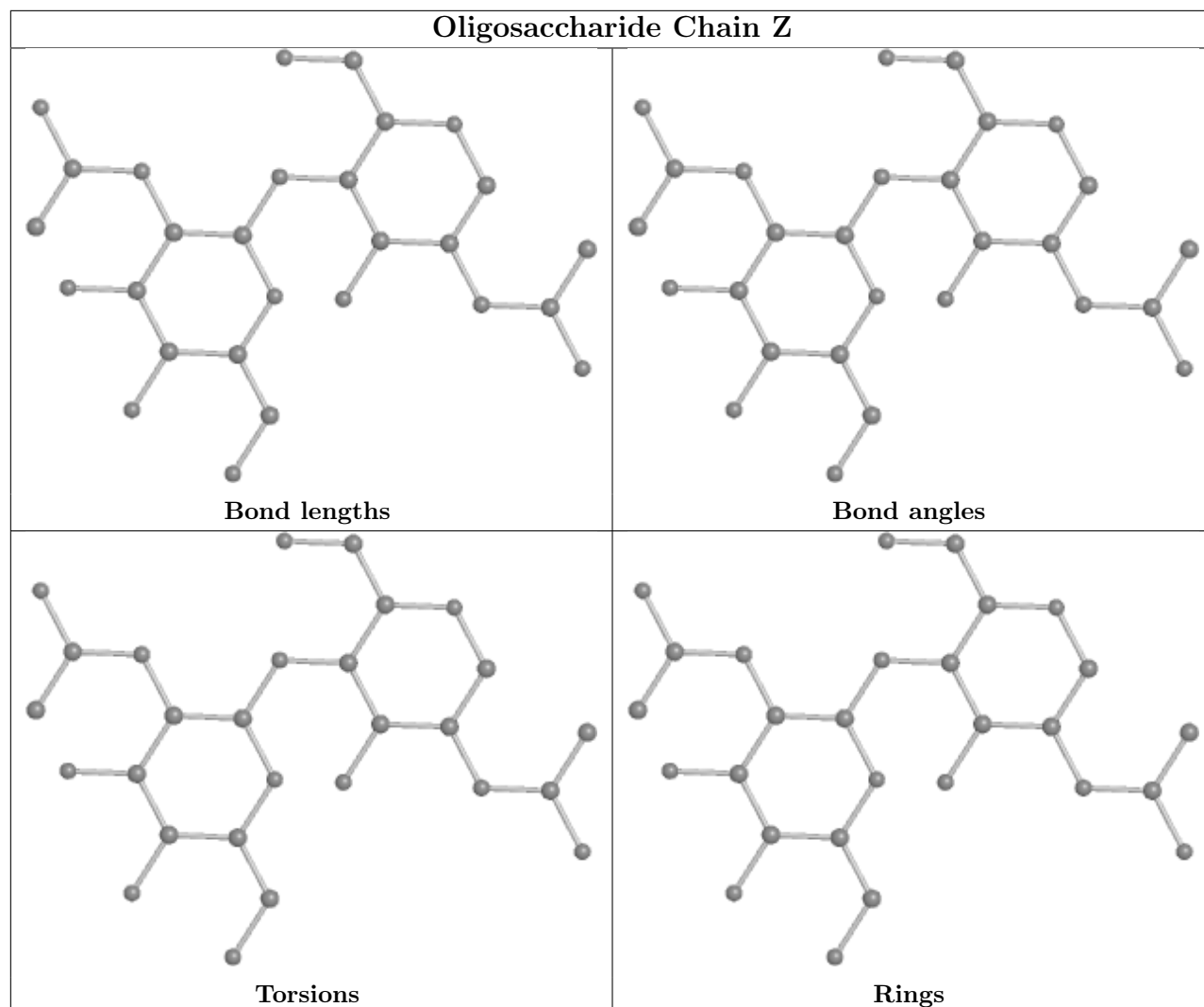


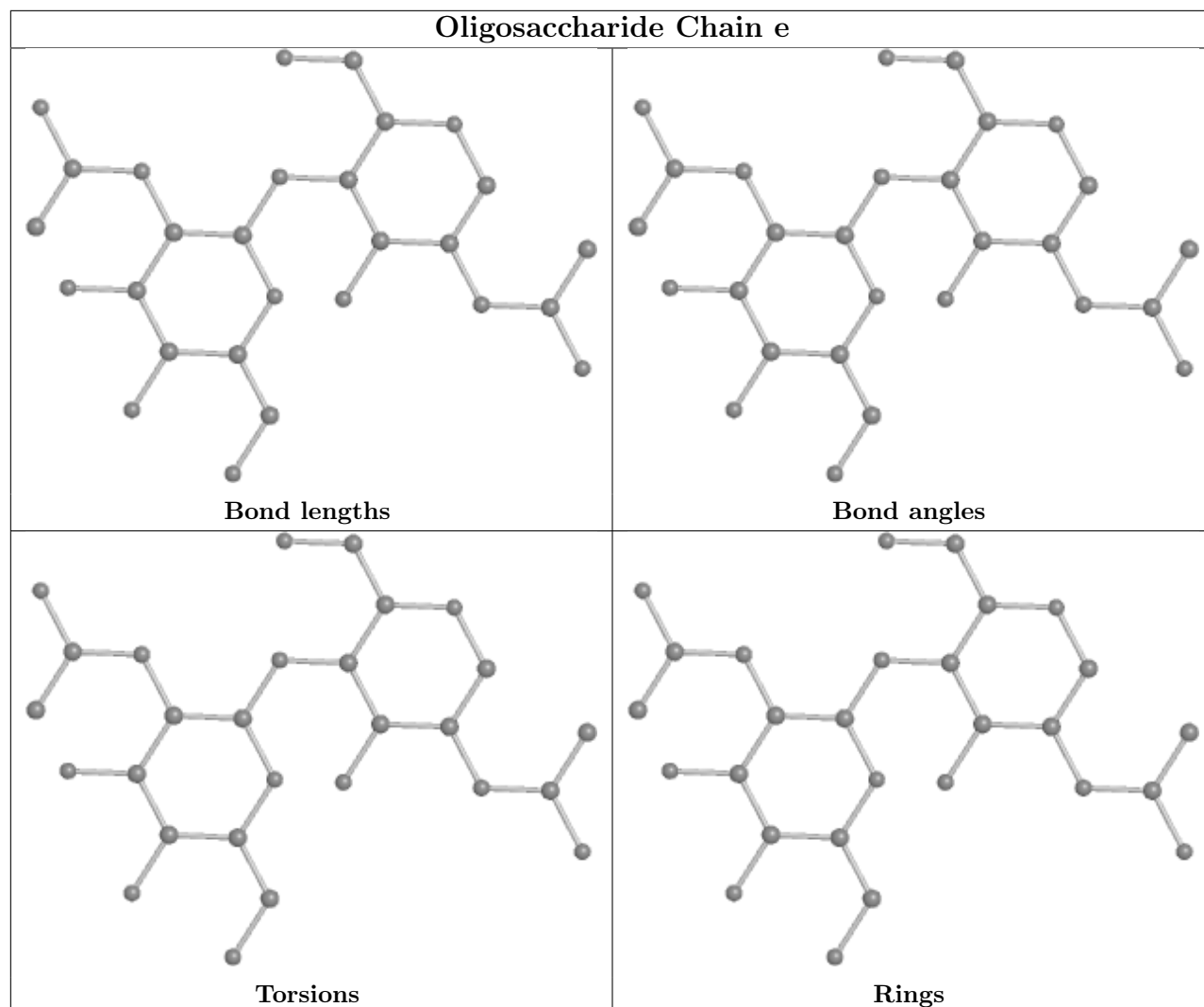


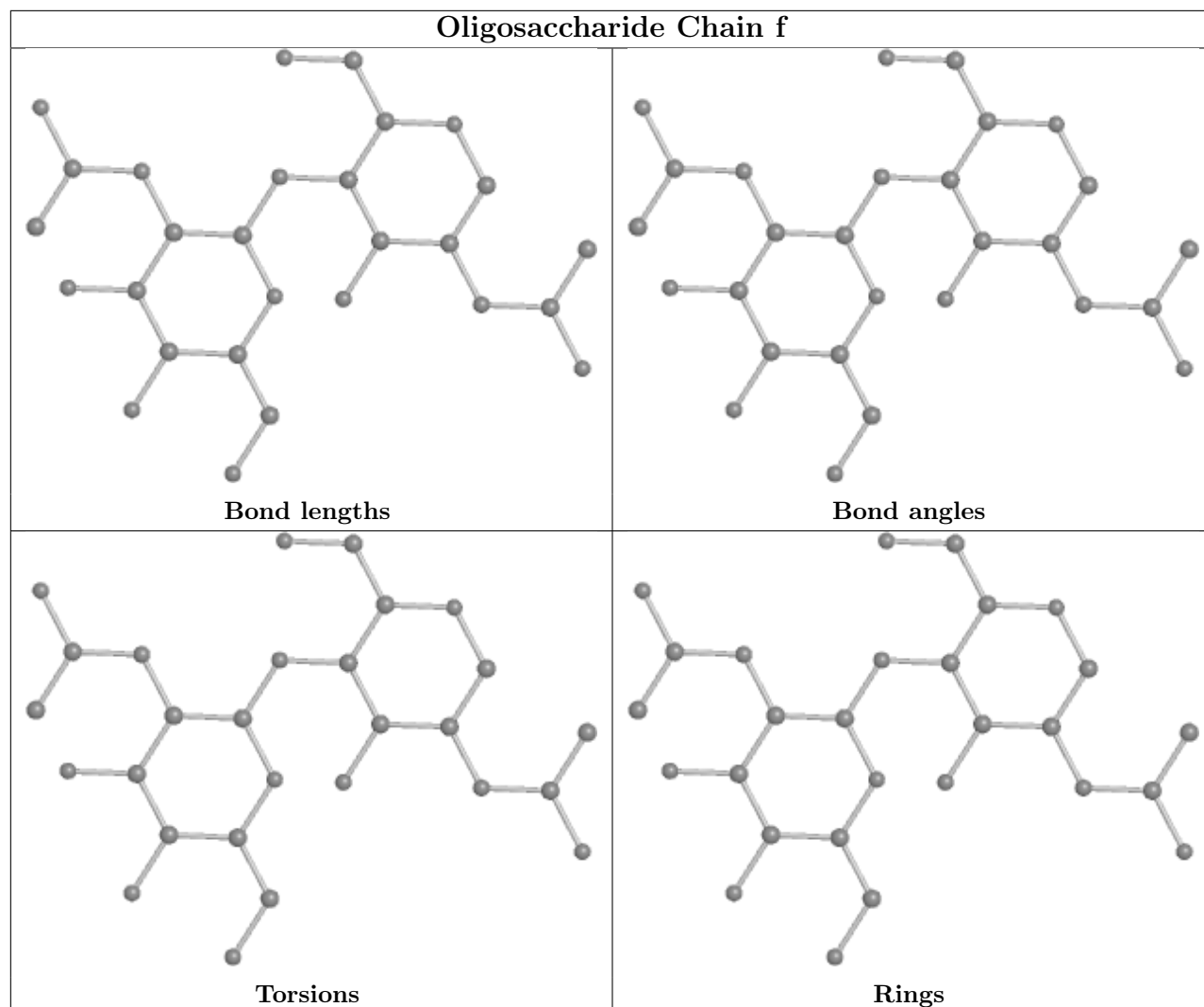


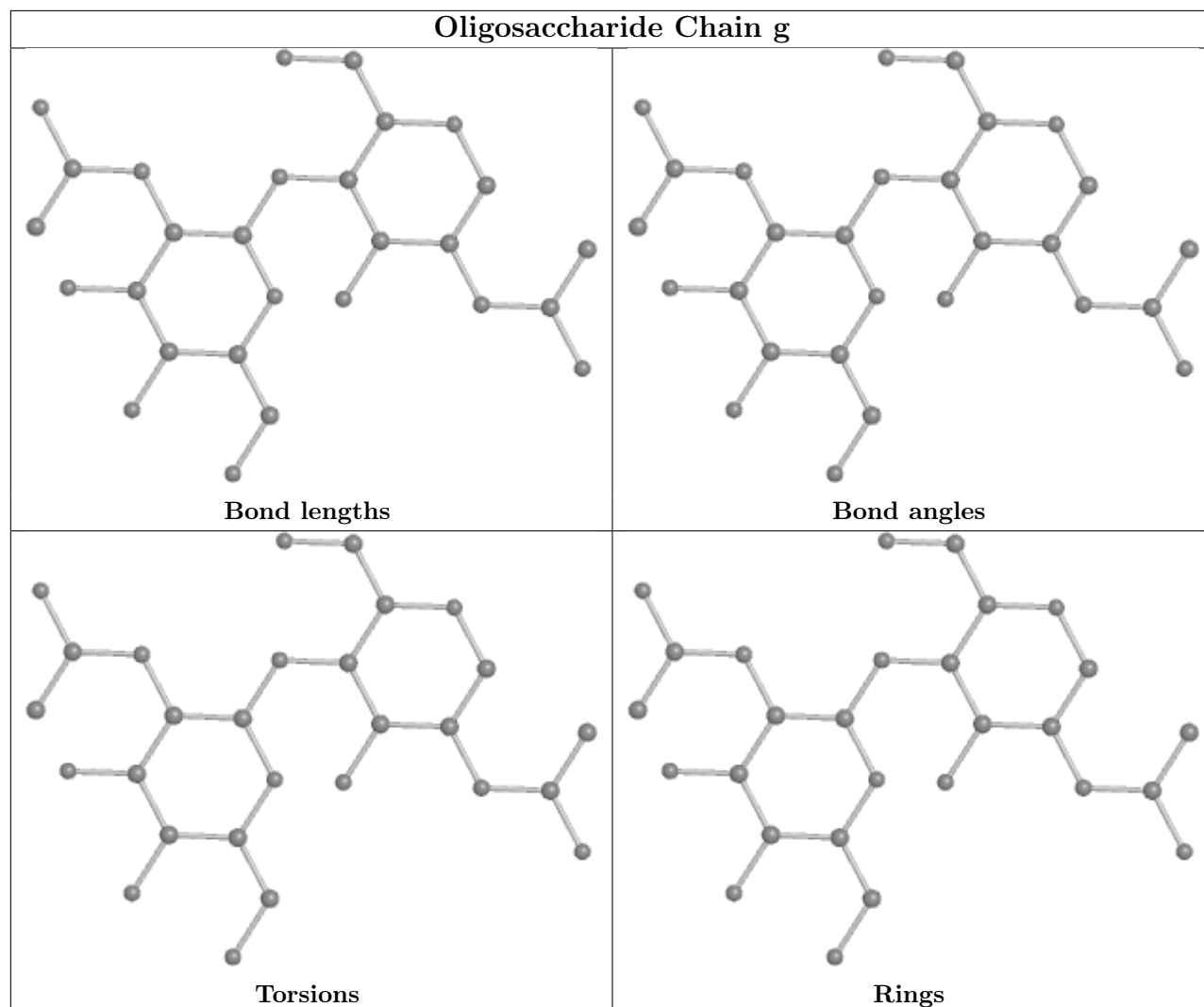


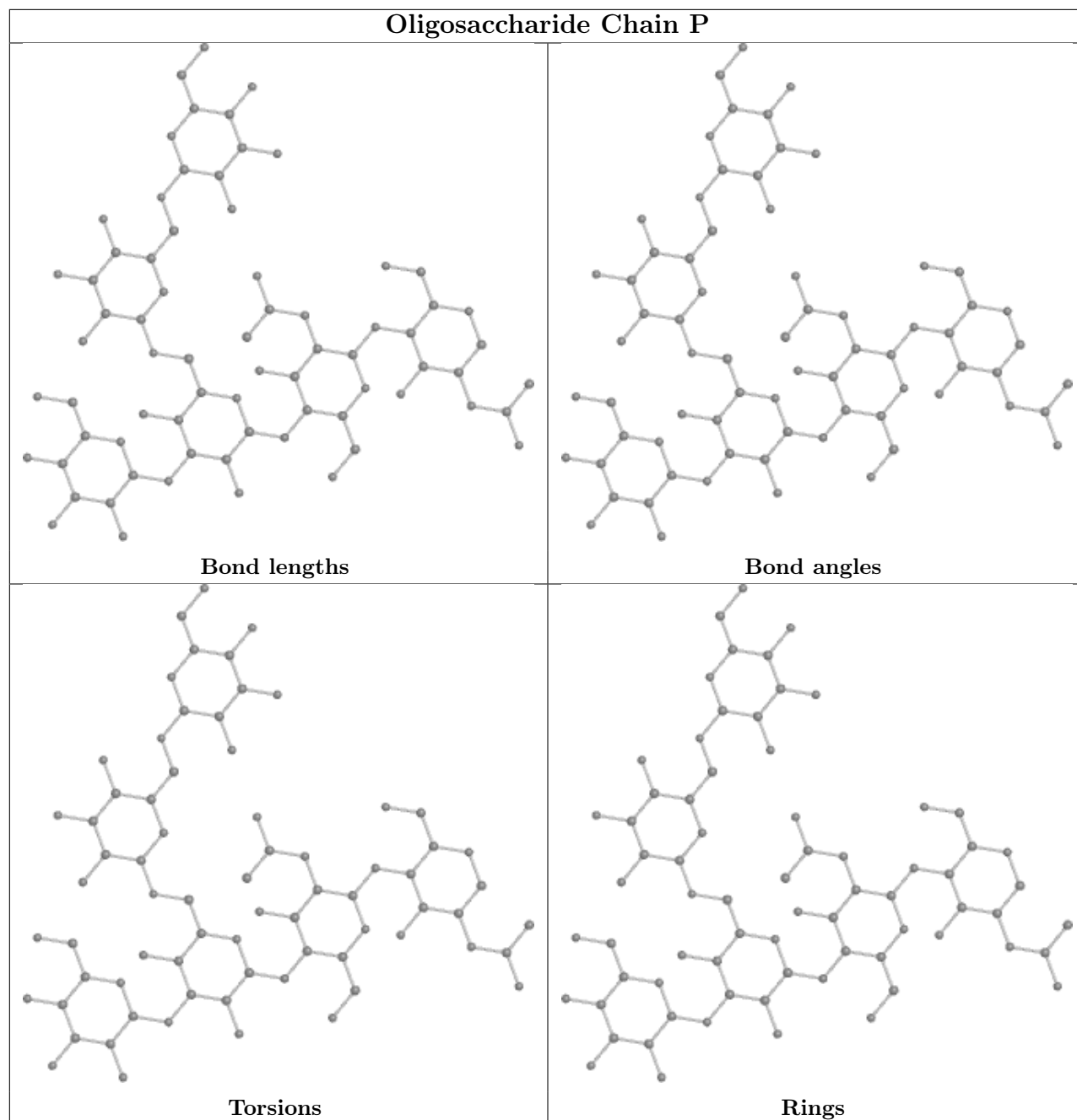


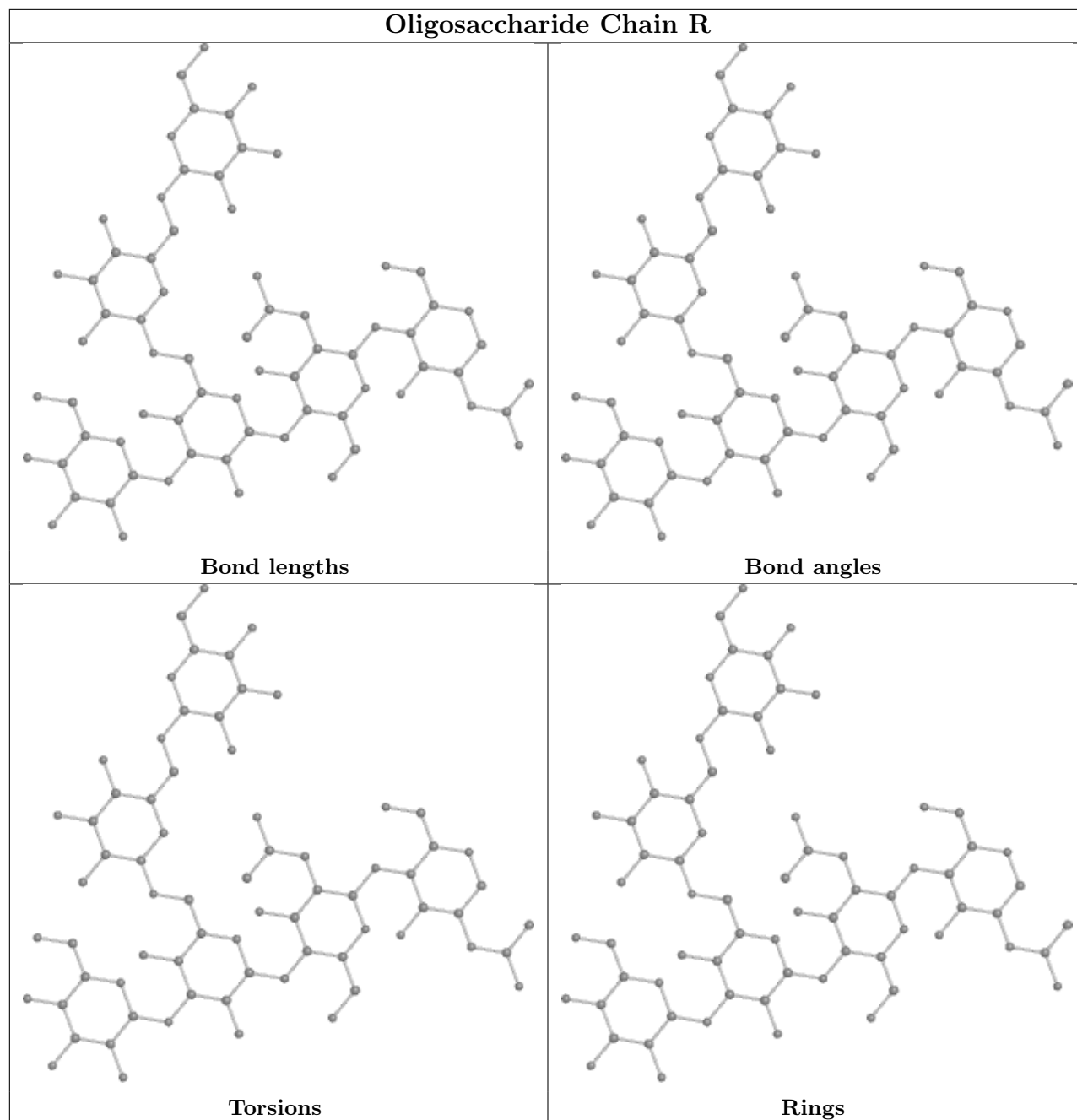


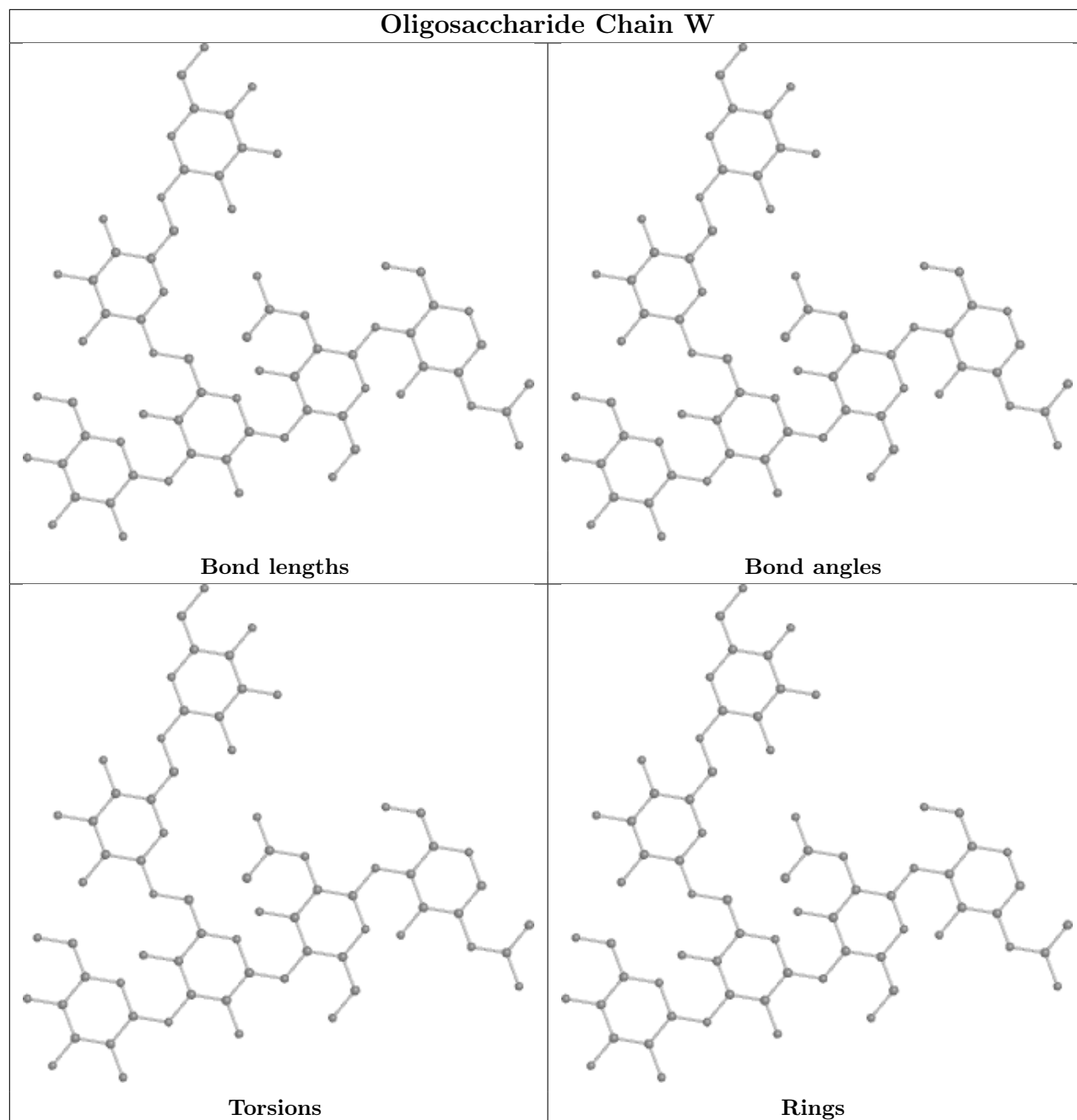


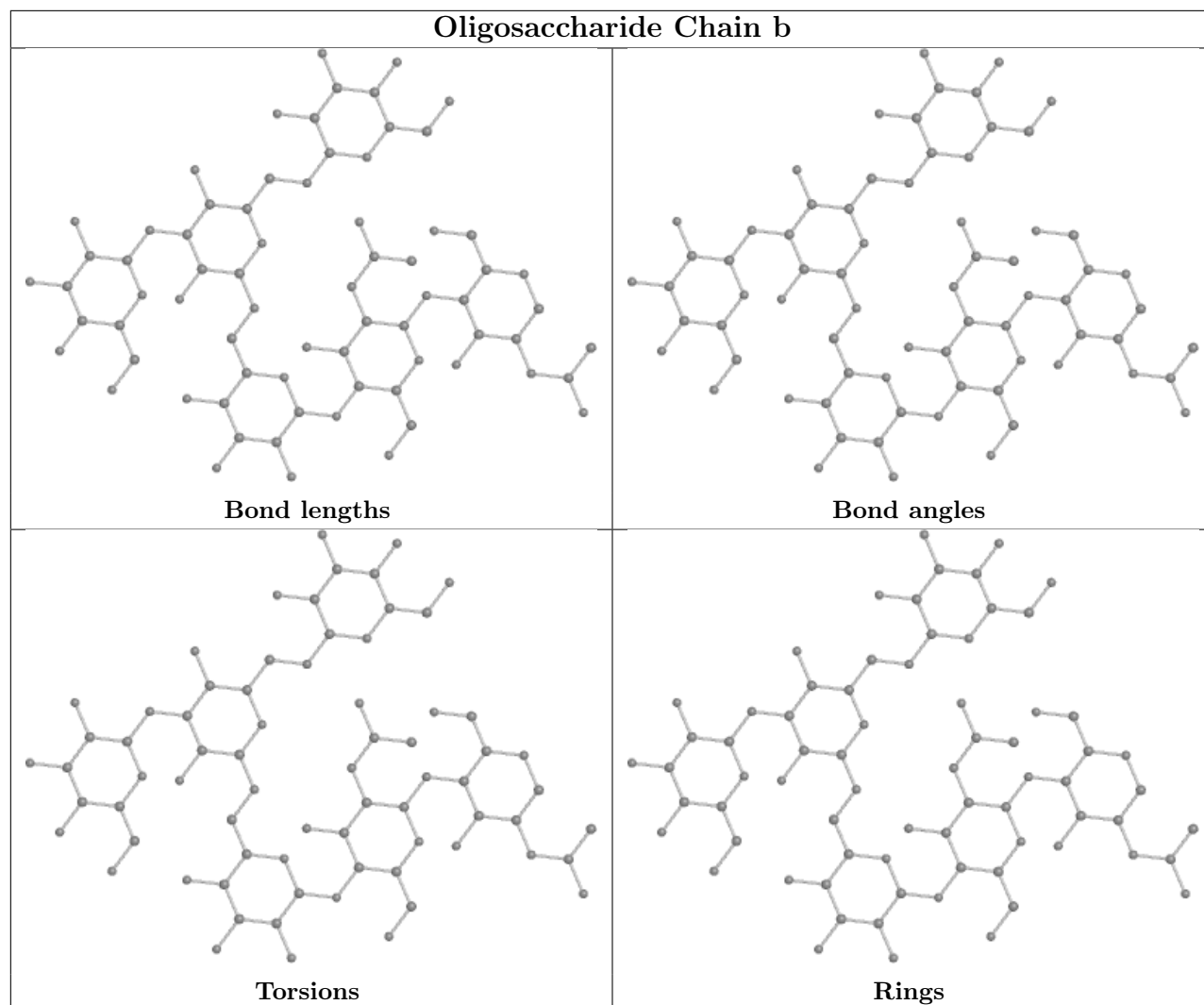


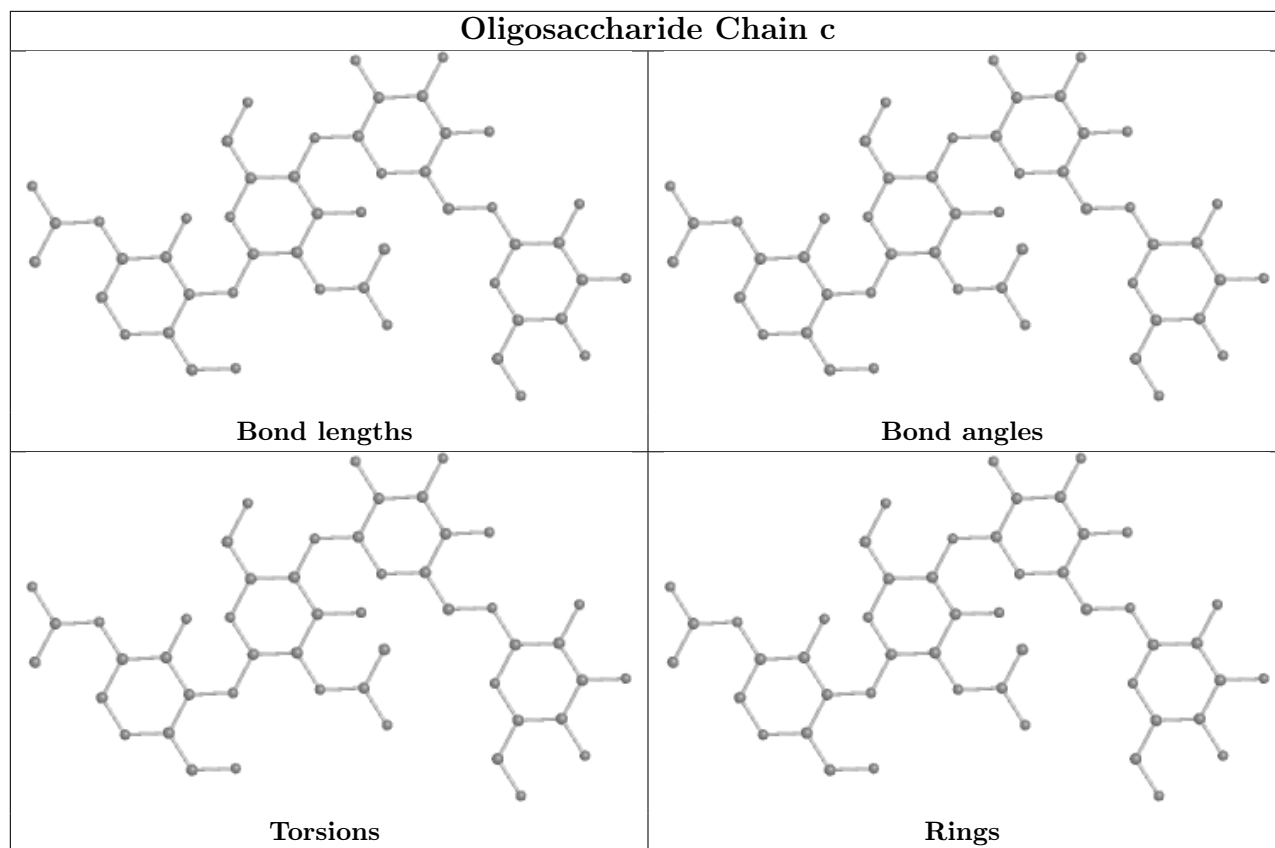












4.6 Ligand geometry [i](#)

Of 53 ligands modelled in this entry, 24 are monoatomic - leaving 29 for Mogul analysis.

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.

No monomer is involved in short contacts.

4.7 Other polymers [i](#)

There are no such residues in this entry.

4.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

5 Fit of model and data [i](#)

5.1 Protein, DNA and RNA chains [i](#)

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	592/599 (98%)	0.83	34 (5%) 23 20	49, 78, 135, 172	0
1	C	595/599 (99%)	0.98	61 (10%) 6 4	50, 78, 148, 197	0
1	E	593/599 (98%)	1.18	106 (17%) 1 1	62, 100, 158, 204	0
1	G	596/599 (99%)	1.31	118 (19%) 1 1	72, 104, 152, 190	0
2	B	333/456 (73%)	1.31	79 (23%) 0 0	61, 122, 165, 244	0
2	D	312/456 (68%)	1.85	114 (36%) 0 0	58, 133, 178, 237	0
2	F	332/456 (72%)	1.57	91 (27%) 0 0	67, 128, 174, 206	0
2	H	336/456 (73%)	1.95	142 (42%) 0 0	75, 135, 181, 249	0
All	All	3689/4220 (87%)	1.29	745 (20%) 1 1	49, 101, 165, 249	0

The worst 5 of 745 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	358	TYR	10.7
2	D	135	MET	10.6
2	D	95	LEU	9.5
1	E	570	ALA	9.1
1	C	553	LEU	9.1

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

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

5.3 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
6	NAG	e	2	14/15	0.38	0.52	157,165,176,176	0
8	MAN	b	4	11/12	0.41	0.27	157,161,164,165	0
8	MAN	b	6	11/12	0.41	0.40	155,160,164,164	0
3	MAN	I	4	11/12	0.44	0.53	187,189,190,191	0
4	MAN	U	5	11/12	0.47	0.39	140,143,149,151	0
6	NAG	M	2	14/15	0.60	0.69	153,159,169,172	0
3	NAG	I	2	14/15	0.61	0.39	169,174,179,181	0
6	NAG	f	2	14/15	0.65	0.29	165,166,177,178	0
7	MAN	P	4	11/12	0.66	0.20	133,136,141,141	0
3	MAN	a	4	11/12	0.66	0.30	149,157,160,165	0
6	NAG	g	2	14/15	0.66	0.45	161,168,174,175	0
8	MAN	b	5	11/12	0.68	0.38	156,159,161,163	0
8	BMA	b	3	11/12	0.70	0.18	144,148,156,159	0
3	NAG	S	1	14/15	0.70	0.26	94,108,115,116	0
3	BMA	I	3	11/12	0.71	0.24	142,178,189,201	0
7	BMA	P	3	11/12	0.72	0.19	106,117,127,130	0
3	MAN	Q	4	11/12	0.73	0.27	142,144,145,147	0
6	NAG	M	1	14/15	0.73	0.31	115,130,138,144	0
6	NAG	T	1	14/15	0.74	0.48	146,163,166,171	0
7	BMA	W	3	11/12	0.74	0.18	110,118,123,126	0
6	NAG	N	1	14/15	0.75	0.30	127,151,154,156	0
3	BMA	Q	3	11/12	0.75	0.37	136,142,143,143	0
7	MAN	P	5	11/12	0.75	0.29	133,135,139,142	0
6	NAG	e	1	14/15	0.75	0.44	128,147,150,156	0
8	NAG	b	2	14/15	0.76	0.29	141,145,153,156	0
3	NAG	I	1	14/15	0.76	0.41	122,139,150,159	0
6	NAG	Z	2	14/15	0.76	0.45	143,150,154,157	0
6	NAG	g	1	14/15	0.76	0.24	126,146,152,161	0
3	BMA	d	3	11/12	0.76	0.18	120,127,133,135	0
9	BMA	c	3	11/12	0.76	0.19	94,100,106,110	0
6	NAG	Y	2	14/15	0.77	0.27	135,140,144,148	0
3	MAN	S	4	11/12	0.77	0.17	78,96,105,106	0
7	MAN	R	5	11/12	0.77	0.28	130,131,134,135	0
5	BMA	L	3	11/12	0.77	0.15	104,108,115,118	0
6	NAG	T	2	14/15	0.77	0.48	175,180,185,186	0
5	MAN	L	4	11/12	0.78	0.22	123,128,133,135	0
4	MAN	X	5	11/12	0.78	0.18	130,134,141,142	0
5	MAN	L	5	11/12	0.79	0.22	124,131,133,134	0
3	BMA	S	3	11/12	0.79	0.14	108,111,118,121	0
9	MAN	c	4	11/12	0.79	0.20	109,113,116,117	0

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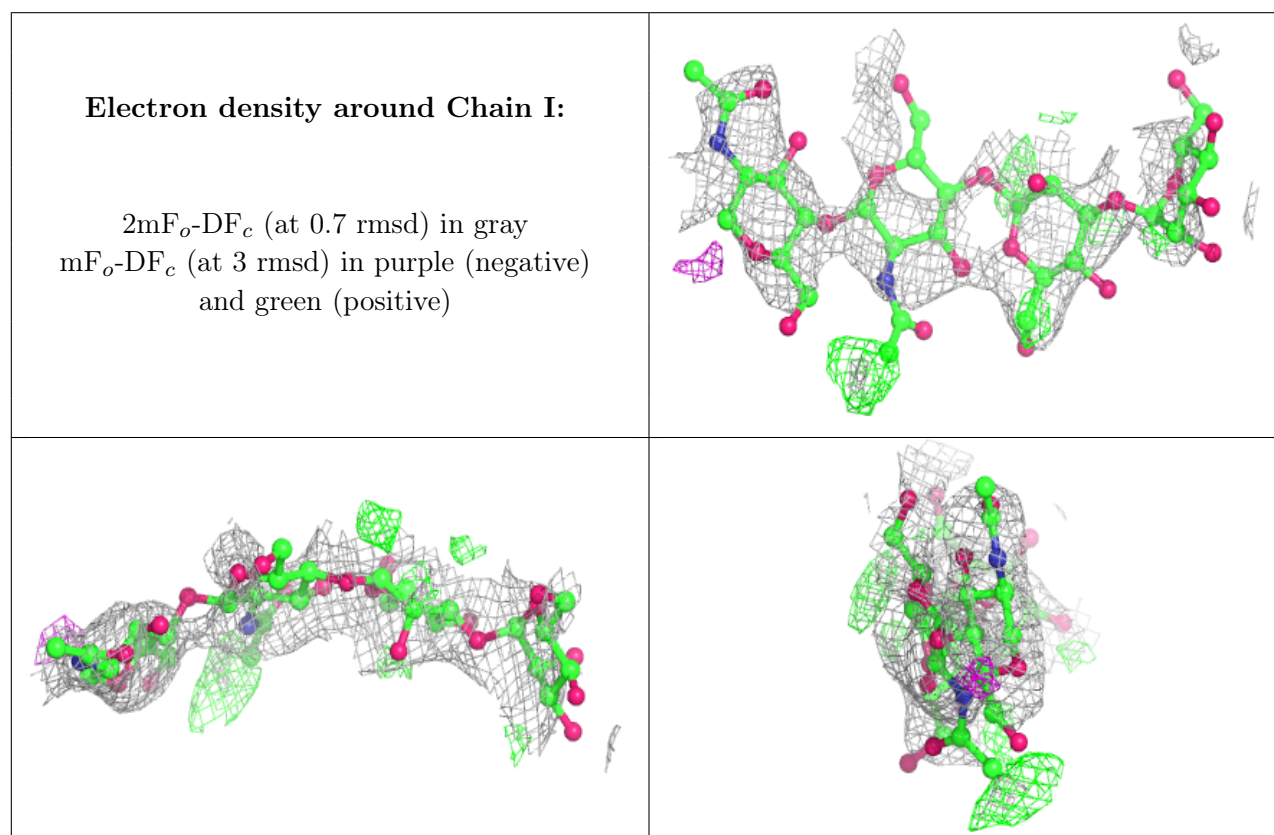
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
7	MAN	R	4	11/12	0.80	0.18	111,113,124,128	0
7	MAN	W	5	11/12	0.80	0.16	92,109,119,121	0
7	BMA	R	3	11/12	0.80	0.14	98,103,109,111	0
4	BMA	U	3	11/12	0.81	0.22	113,124,133,137	0
4	MAN	U	4	11/12	0.81	0.29	136,144,147,149	0
3	NAG	K	2	14/15	0.82	0.30	116,122,125,131	0
4	BMA	J	3	11/12	0.82	0.16	119,125,127,128	0
3	NAG	Q	2	14/15	0.82	0.27	110,118,130,138	0
7	MAN	P	6	11/12	0.83	0.17	128,130,134,136	0
3	BMA	O	3	11/12	0.83	0.18	143,144,150,150	0
7	MAN	W	6	11/12	0.83	0.18	113,118,122,126	0
3	BMA	a	3	11/12	0.83	0.16	126,133,138,142	0
5	MAN	L	6	11/12	0.83	0.15	101,106,114,116	0
3	BMA	K	3	11/12	0.84	0.21	115,122,125,126	0
7	NAG	W	1	14/15	0.84	0.19	62,77,80,86	0
3	MAN	d	4	11/12	0.84	0.16	124,127,130,130	0
6	NAG	N	2	14/15	0.84	0.25	154,157,161,164	0
8	NAG	b	1	14/15	0.85	0.20	87,107,115,129	0
3	MAN	O	4	11/12	0.85	0.27	148,149,151,152	0
5	NAG	L	2	14/15	0.85	0.19	80,84,88,96	0
4	MAN	J	5	11/12	0.85	0.15	111,114,116,118	0
3	NAG	d	2	14/15	0.85	0.18	136,141,150,150	0
7	MAN	W	4	11/12	0.85	0.17	116,120,127,129	0
3	NAG	Q	1	14/15	0.85	0.16	65,79,89,105	0
3	NAG	O	2	14/15	0.85	0.21	130,134,142,148	0
7	MAN	R	6	11/12	0.86	0.16	114,117,125,127	0
6	NAG	V	2	14/15	0.86	0.29	114,121,128,130	0
6	NAG	f	1	14/15	0.86	0.22	143,159,177,178	0
3	NAG	K	1	14/15	0.86	0.15	82,94,109,110	0
6	NAG	Z	1	14/15	0.86	0.40	124,136,138,139	0
4	NAG	X	1	14/15	0.86	0.18	87,106,114,114	0
4	MAN	X	4	11/12	0.86	0.18	108,111,114,116	0
4	BMA	X	3	11/12	0.87	0.17	106,117,121,125	0
9	NAG	c	1	14/15	0.87	0.17	56,67,71,75	0
3	NAG	d	1	14/15	0.87	0.21	97,120,127,128	0
3	NAG	S	2	14/15	0.87	0.21	116,119,124,130	0
3	NAG	O	1	14/15	0.88	0.27	102,124,127,132	0
4	NAG	J	2	14/15	0.88	0.20	99,105,115,120	0
4	MAN	J	4	11/12	0.89	0.17	131,137,142,142	0
7	NAG	W	2	14/15	0.89	0.16	70,84,91,100	0
4	NAG	X	2	14/15	0.89	0.15	117,120,122,124	0
6	NAG	V	1	14/15	0.90	0.26	93,106,119,120	0

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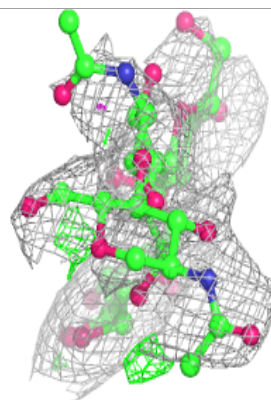
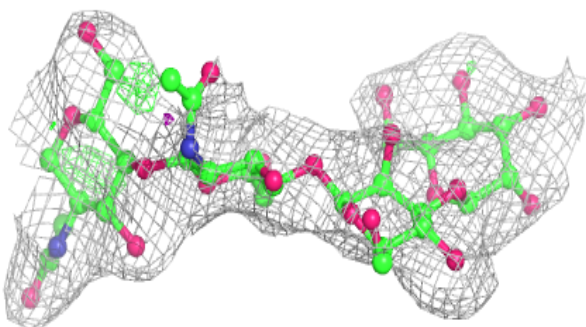
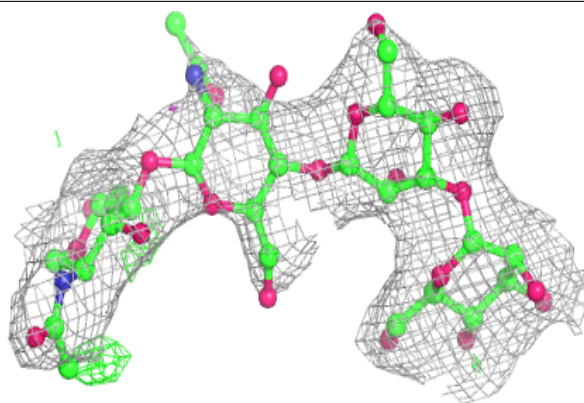
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	NAG	a	2	14/15	0.90	0.20	89,99,106,115	0
6	NAG	Y	1	14/15	0.90	0.26	106,129,133,138	0
4	NAG	U	2	14/15	0.90	0.23	81,86,96,102	0
3	MAN	K	4	11/12	0.90	0.17	75,91,104,105	0
7	NAG	R	2	14/15	0.91	0.14	63,76,83,90	0
4	NAG	J	1	14/15	0.92	0.19	52,70,78,84	0
7	NAG	P	2	14/15	0.92	0.18	87,93,97,101	0
9	NAG	c	2	14/15	0.92	0.15	58,74,83,91	0
3	NAG	a	1	14/15	0.92	0.25	62,81,89,90	0
7	NAG	R	1	14/15	0.92	0.20	46,58,68,71	0
7	NAG	P	1	14/15	0.93	0.13	55,75,81,82	0
5	NAG	L	1	14/15	0.94	0.15	51,60,67,76	0
4	NAG	U	1	14/15	0.94	0.23	53,69,82,82	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.

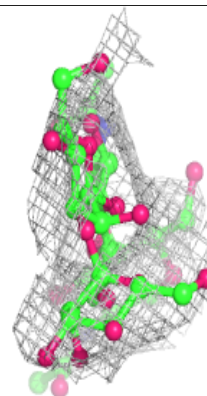
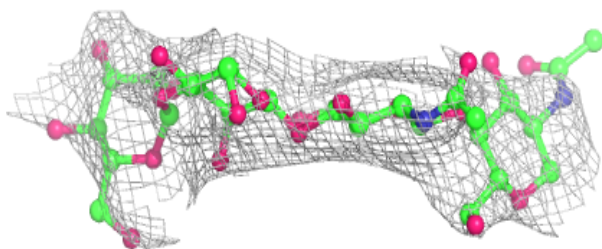
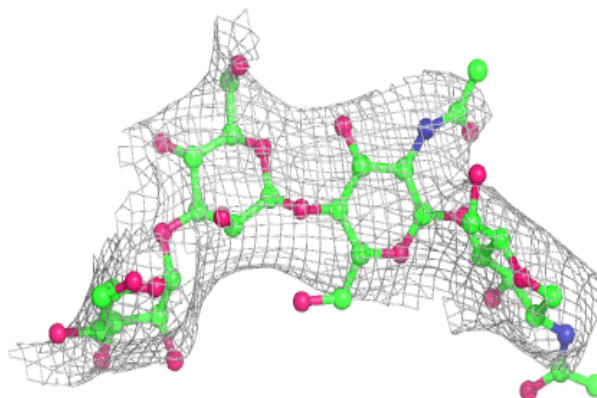


Electron density around Chain K:

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

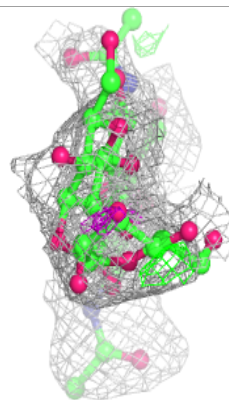
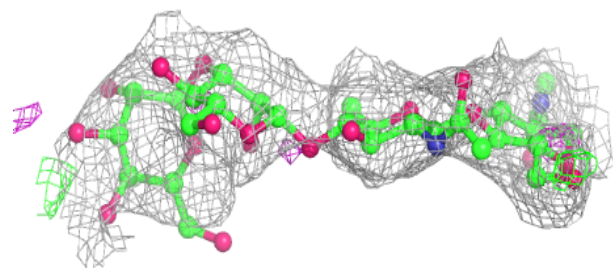
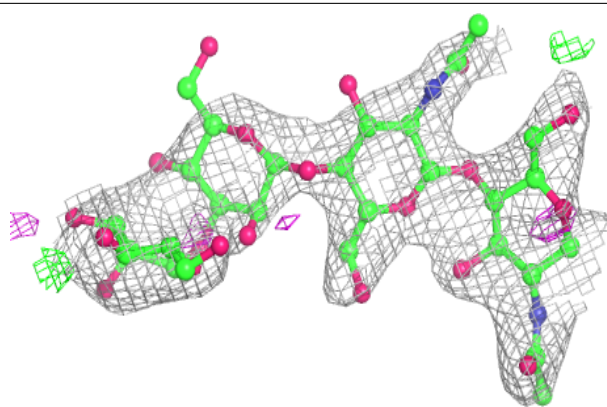
**Electron density around Chain O:**

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

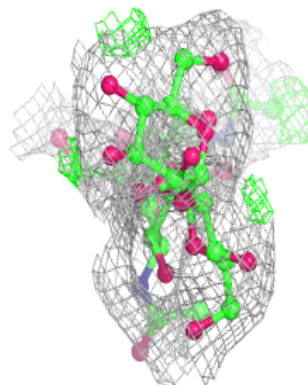
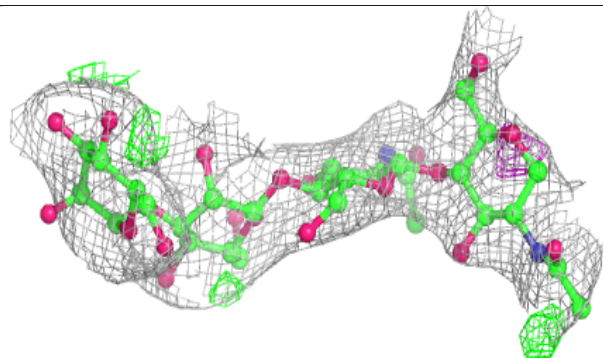
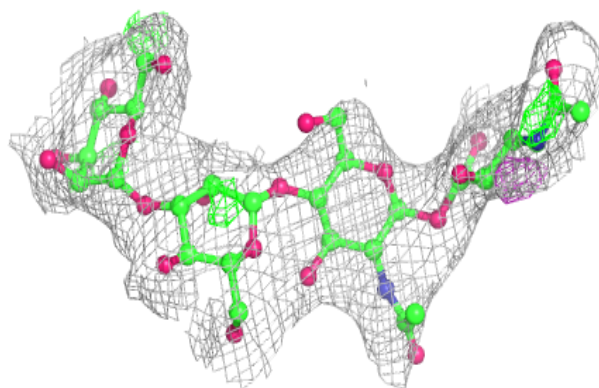


Electron density around Chain Q:

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

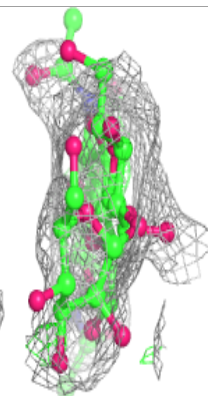
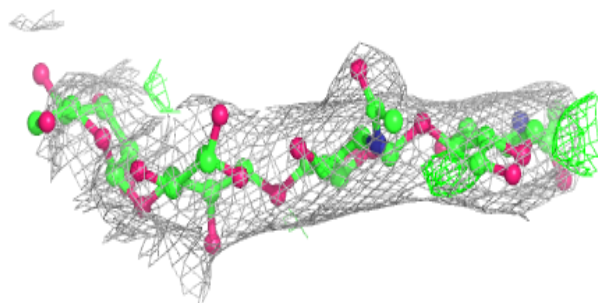
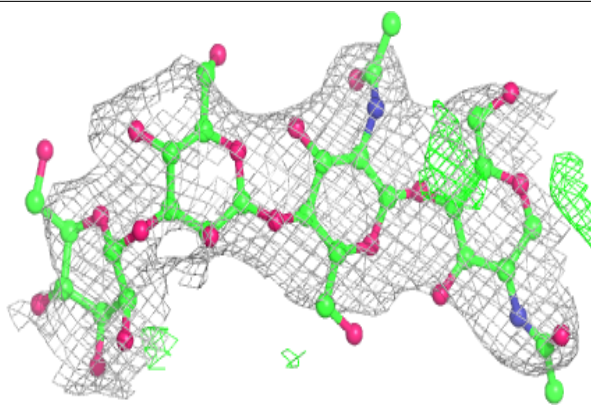
**Electron density around Chain S:**

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

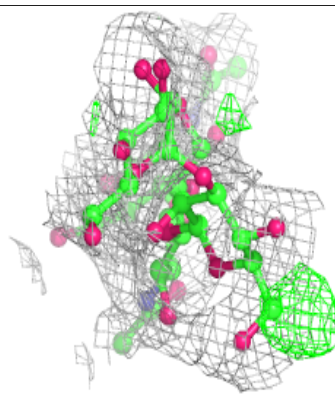
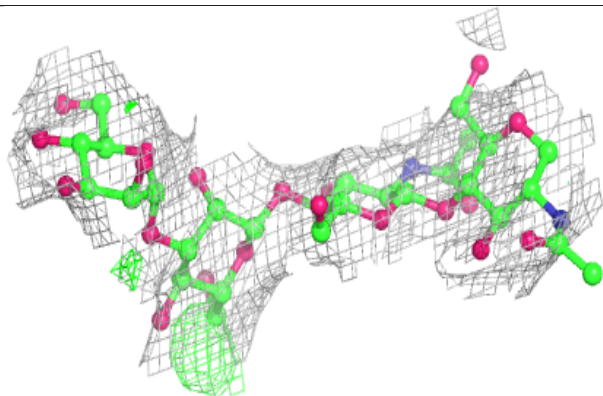
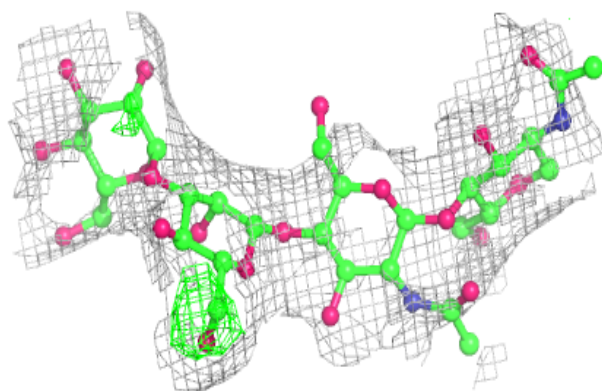


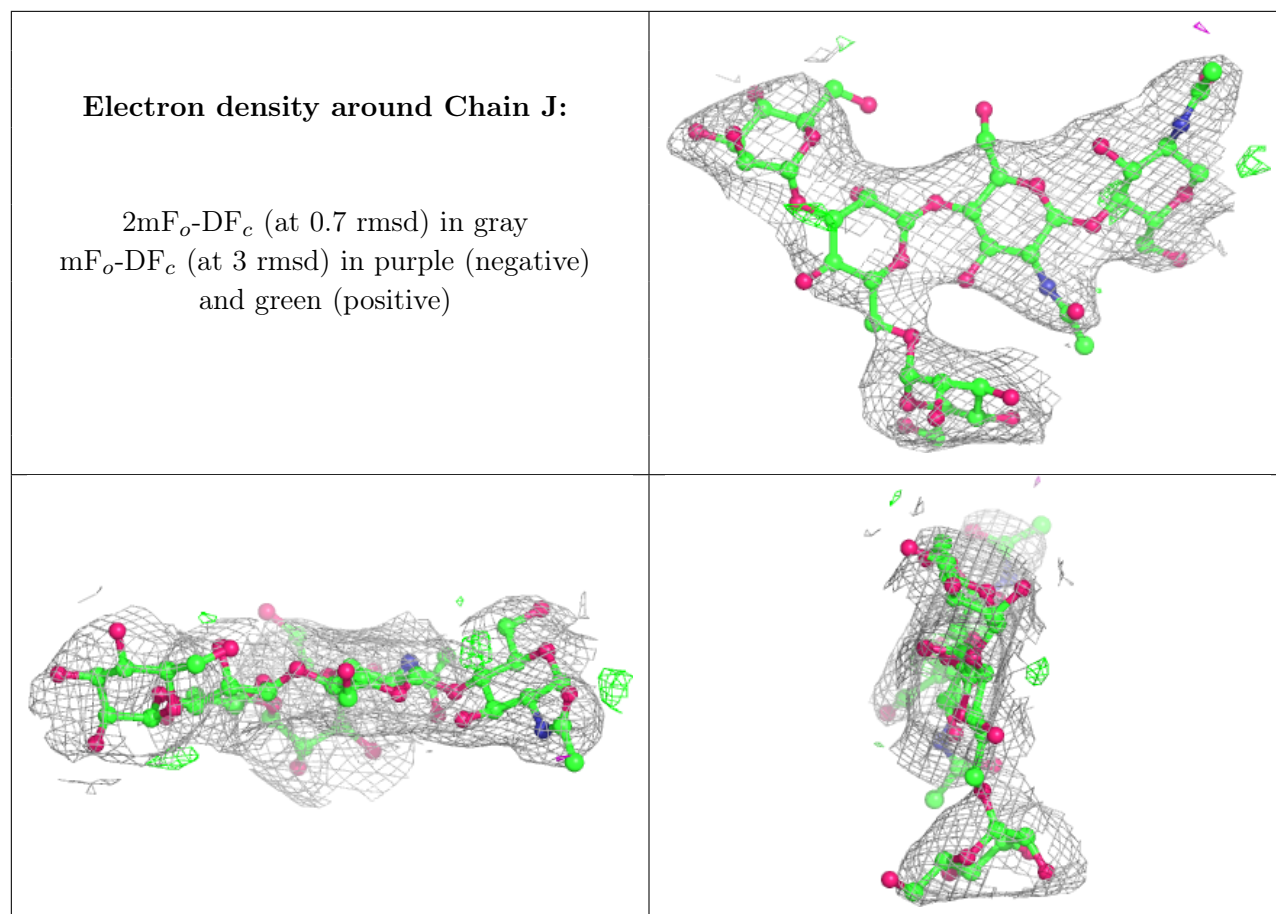
Electron density around Chain a:

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

**Electron density around Chain d:**

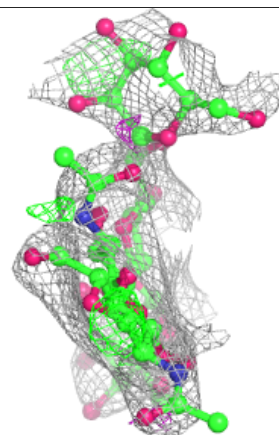
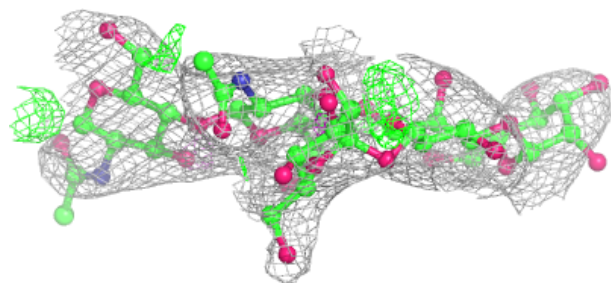
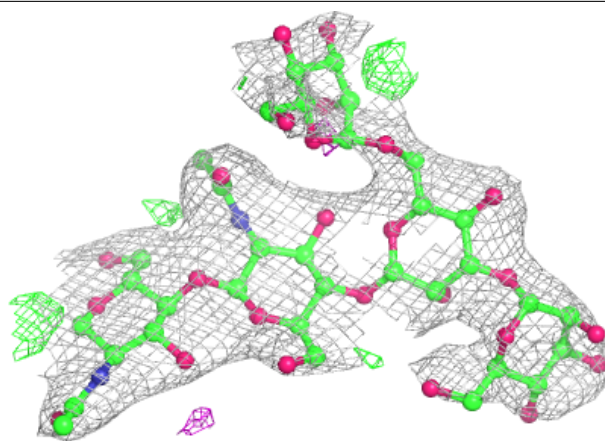
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





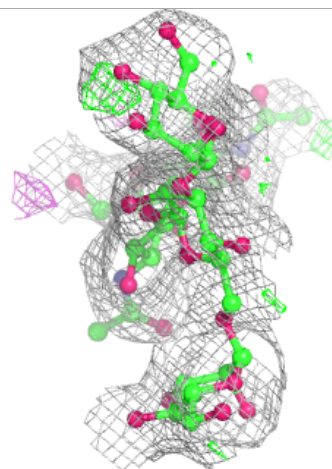
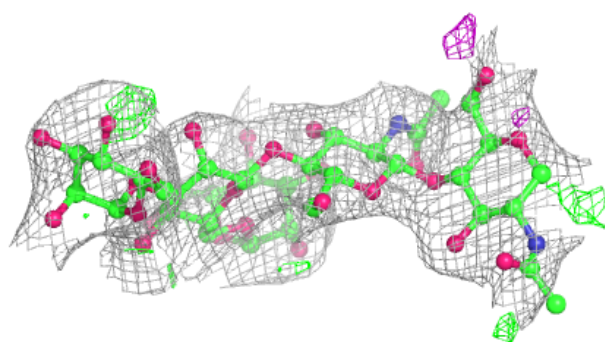
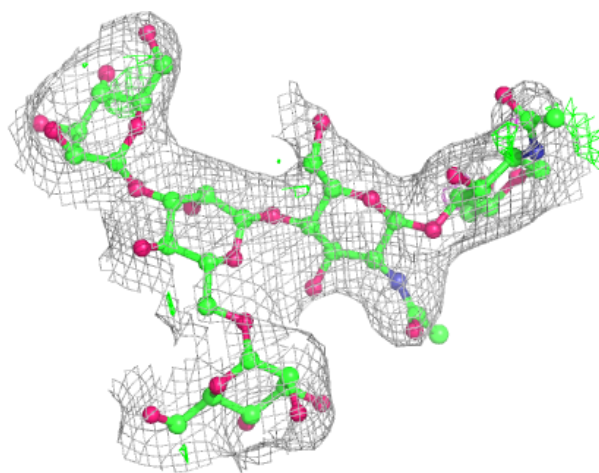
Electron density around Chain U:

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



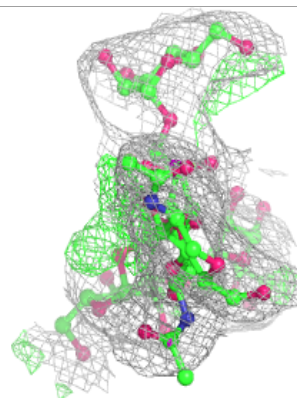
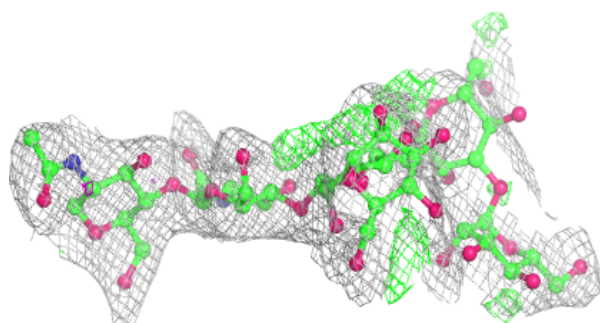
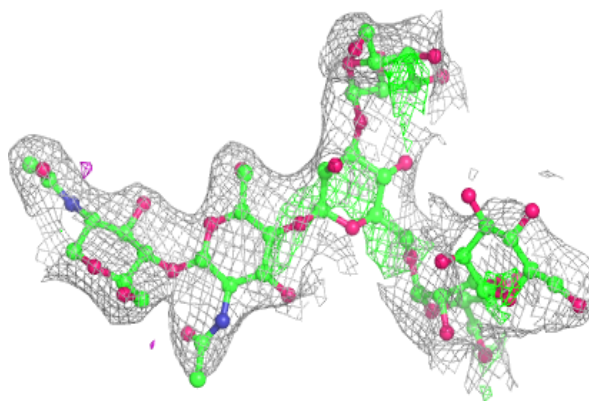
Electron density around Chain X:

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

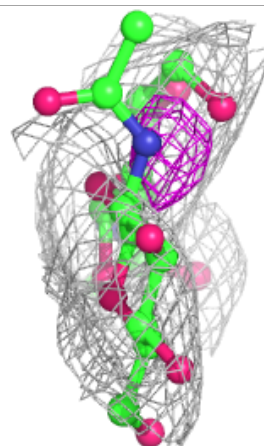
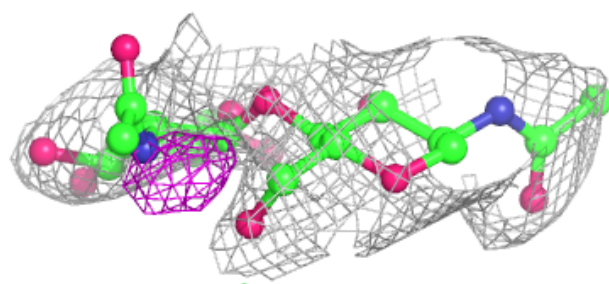
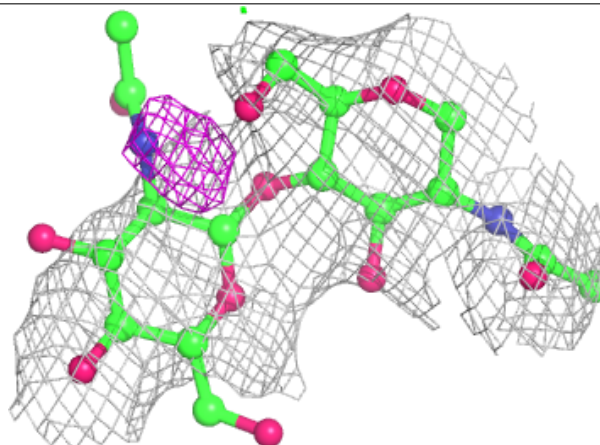


Electron density around Chain L:

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

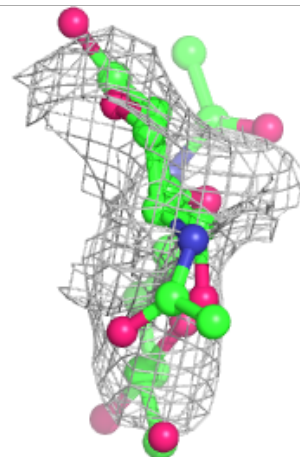
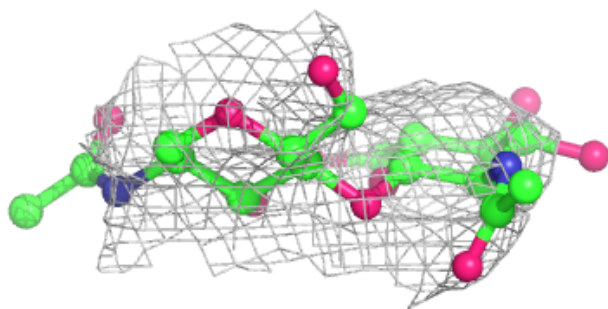
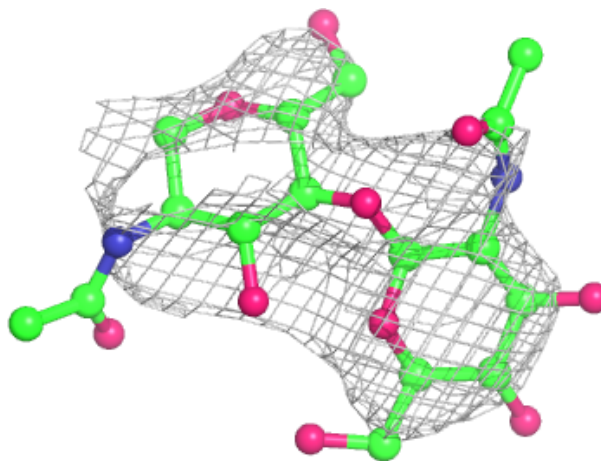
**Electron density around Chain M:**

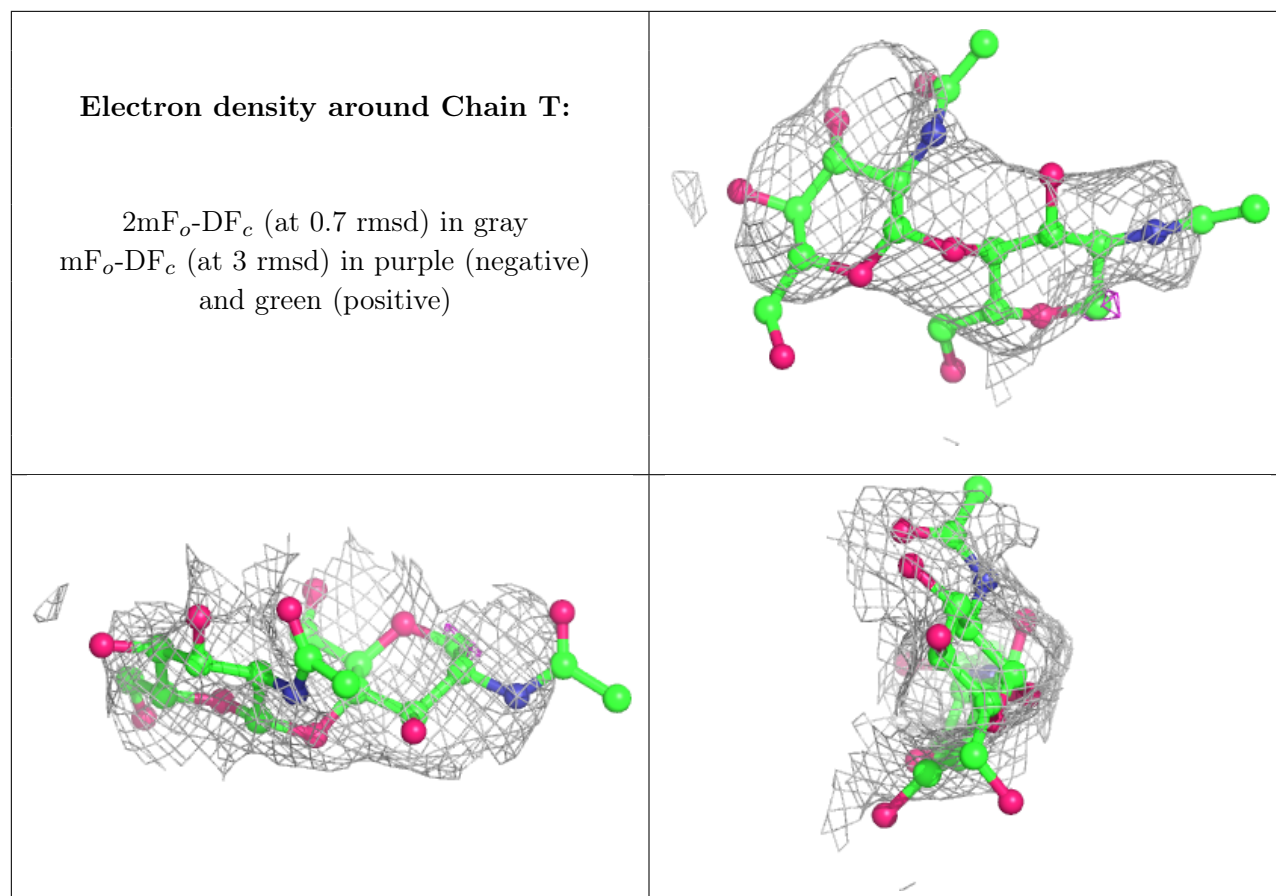
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain N:

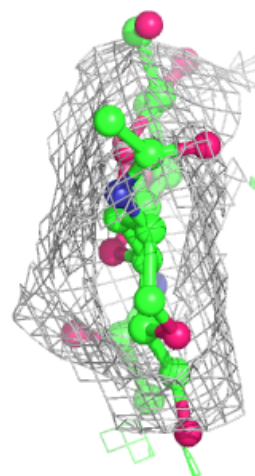
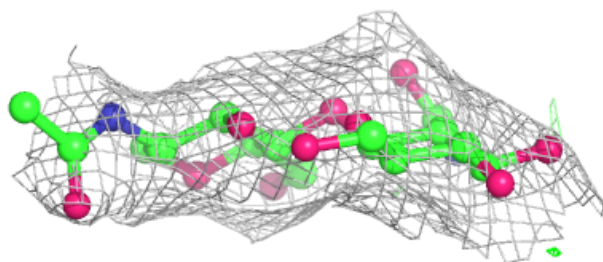
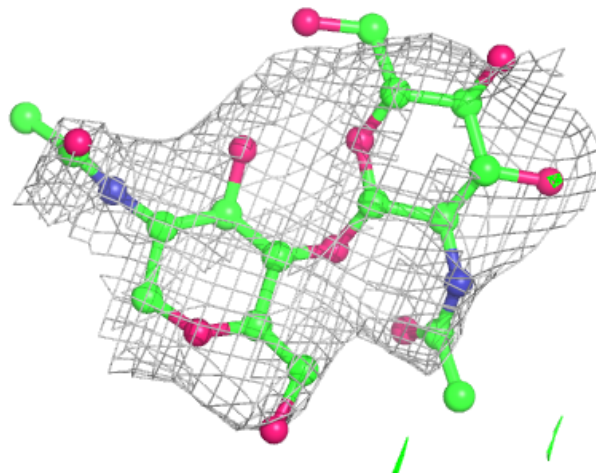
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





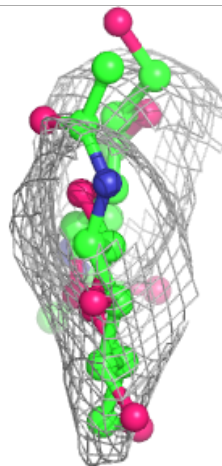
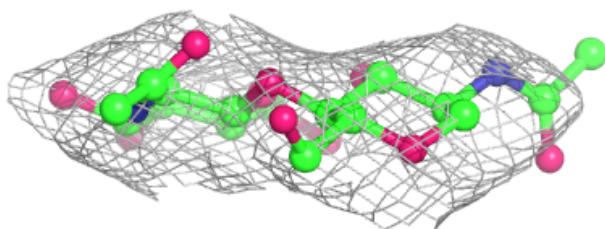
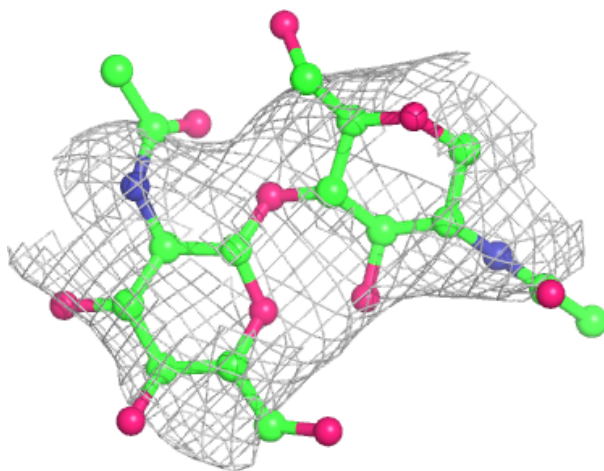
Electron density around Chain V:

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



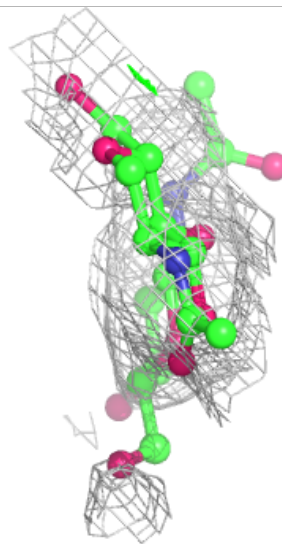
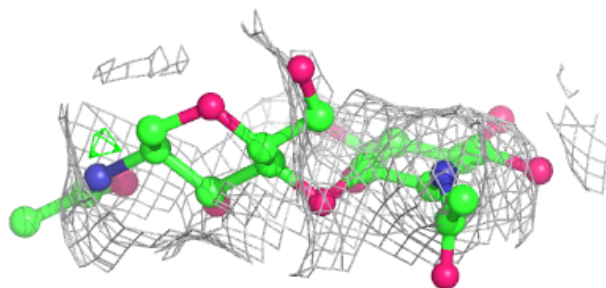
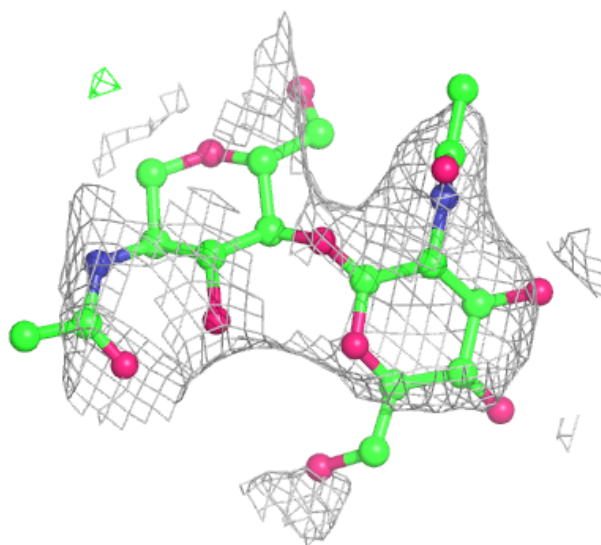
Electron density around Chain Y:

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



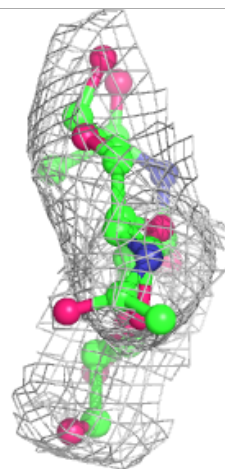
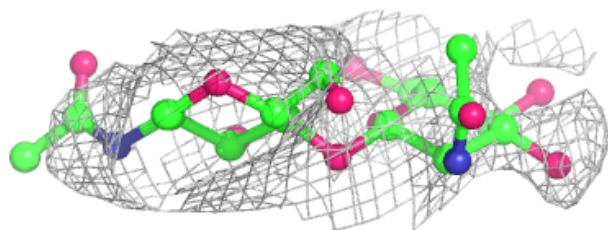
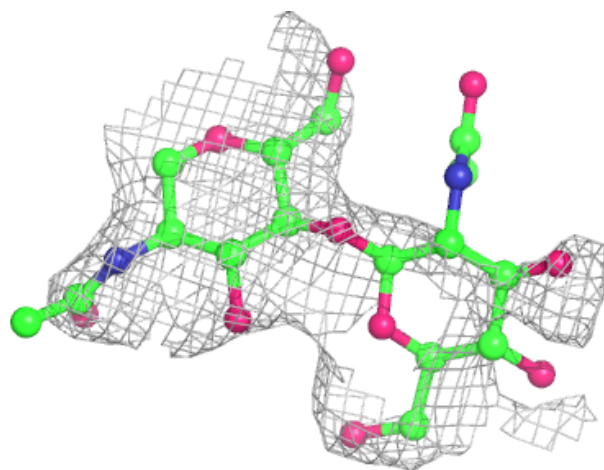
Electron density around Chain Z:

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



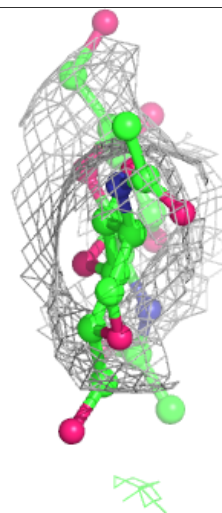
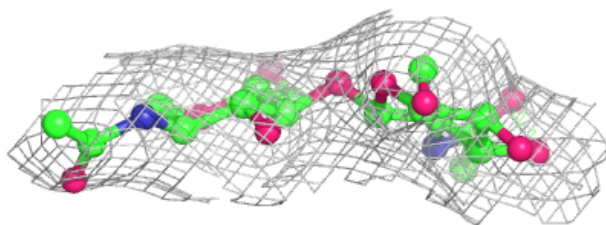
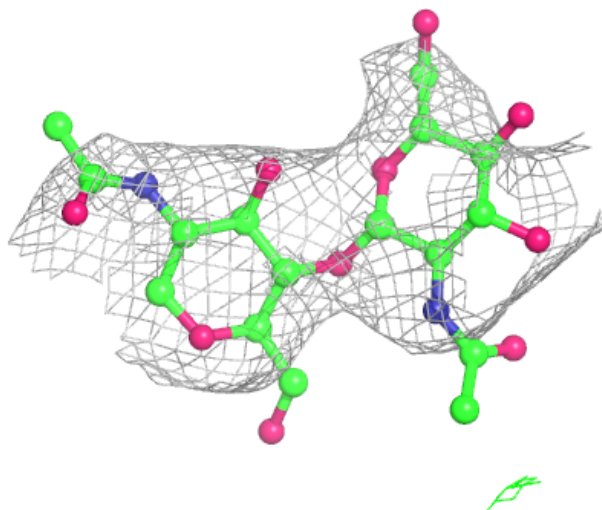
Electron density around Chain e:

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



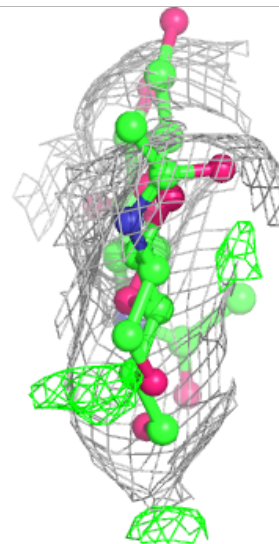
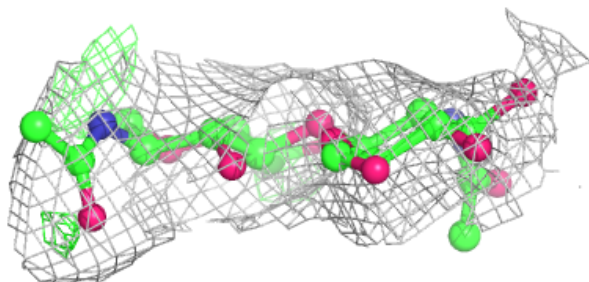
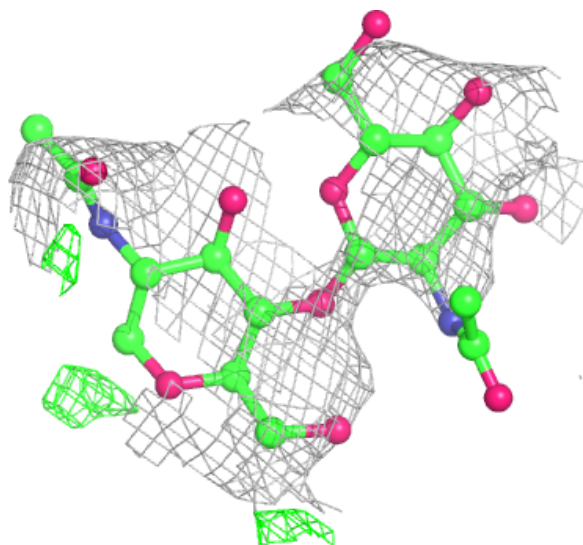
Electron density around Chain f:

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



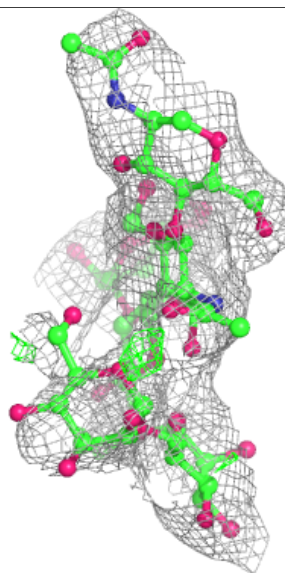
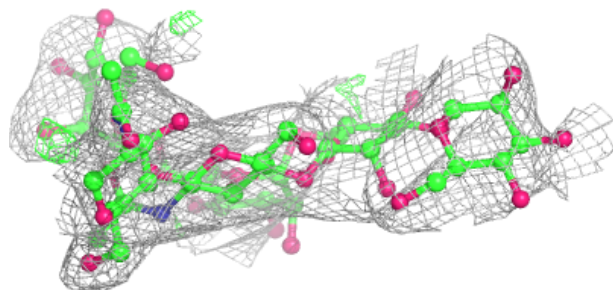
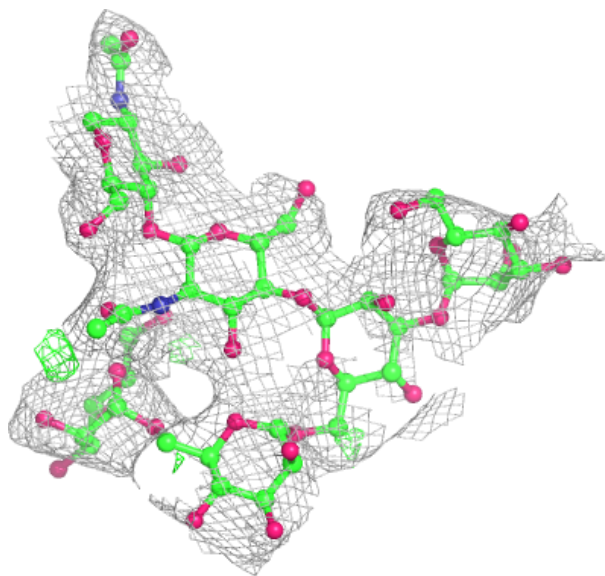
Electron density around Chain g:

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



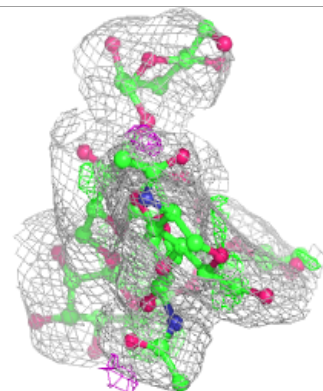
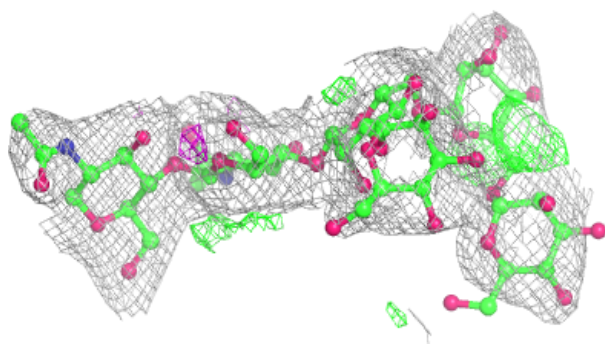
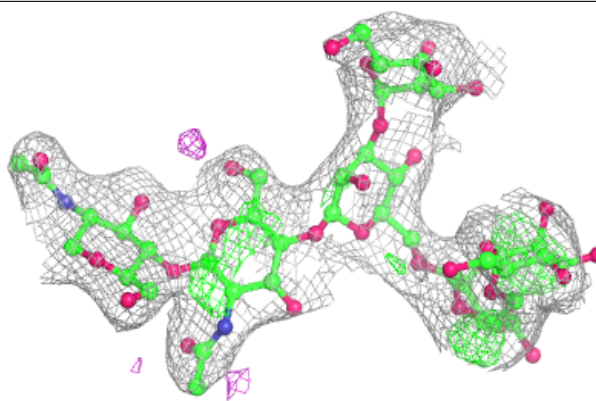
Electron density around Chain P:

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

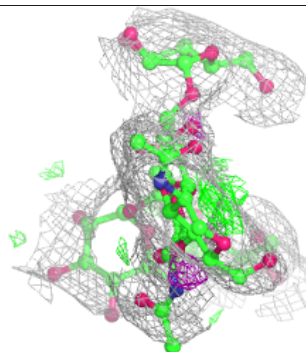
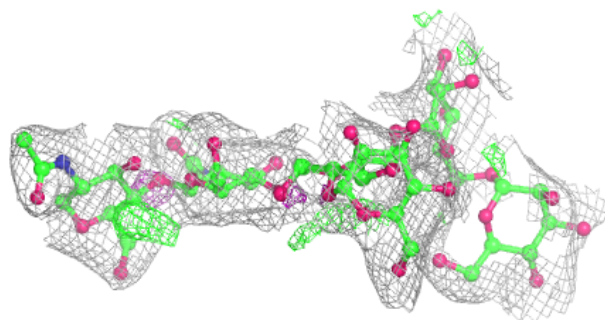
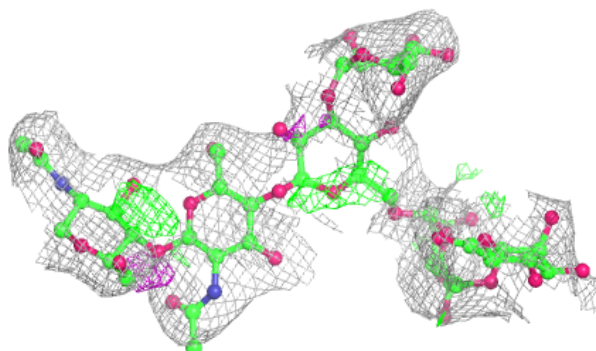


Electron density around Chain R:

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

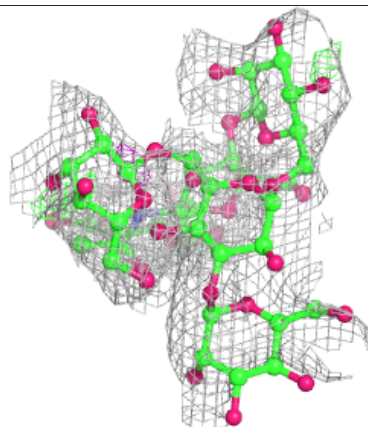
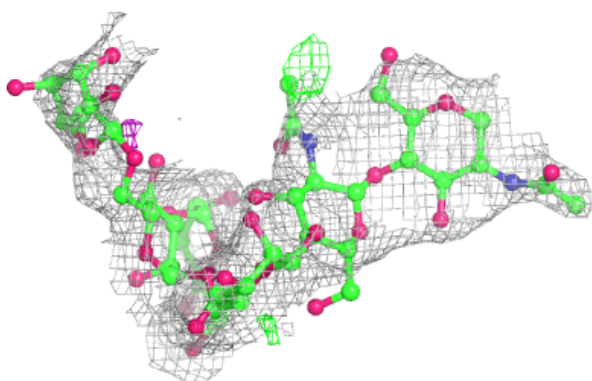
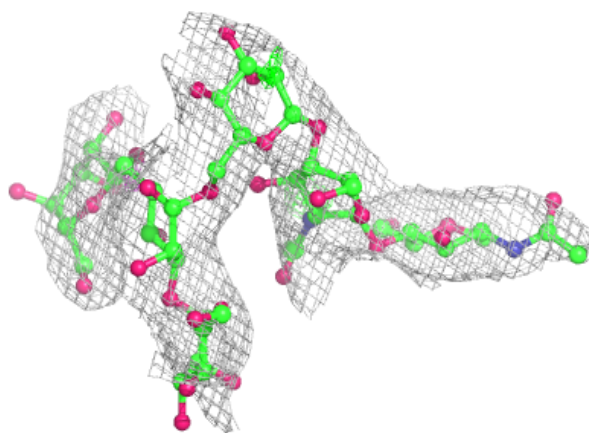
**Electron density around Chain W:**

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

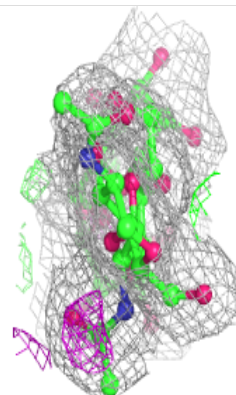
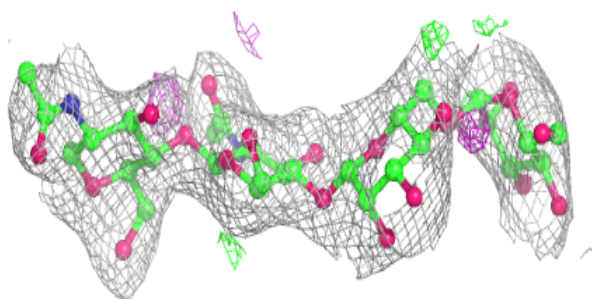
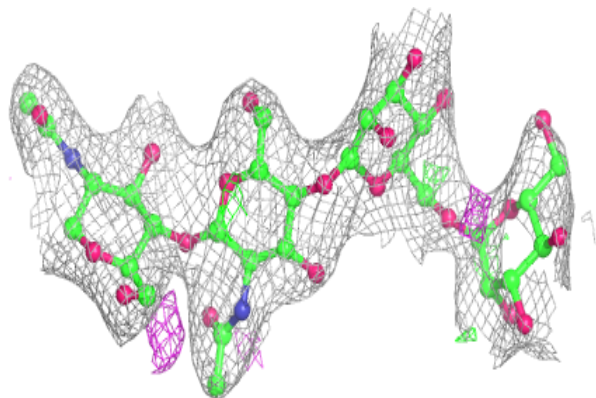


Electron density around Chain b:

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

**Electron density around Chain c:**

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



5.4 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
10	NAG	F	501	14/15	0.38	0.68	125,142,159,163	0
10	NAG	G	2023	14/15	0.52	0.55	125,140,148,155	0
12	EDO	F	509	4/4	0.57	0.36	95,97,98,99	0
10	NAG	G	2024	14/15	0.60	0.44	140,153,166,169	0
12	EDO	G	2027	4/4	0.62	0.31	84,86,89,91	0
12	EDO	C	628	4/4	0.69	0.12	86,88,93,97	0
12	EDO	G	2028	4/4	0.69	0.22	85,88,89,90	0
10	NAG	D	501	14/15	0.71	0.30	134,158,162,162	0
11	CA	B	2002	1/1	0.73	0.16	77,77,77,77	0
12	EDO	A	625	4/4	0.73	0.19	80,82,82,83	0
12	EDO	G	2026	4/4	0.76	0.32	88,89,92,94	0
12	EDO	C	629	4/4	0.76	0.43	85,85,85,86	0
10	NAG	E	624	14/15	0.76	0.25	111,128,144,145	0
10	NAG	C	601	14/15	0.77	0.45	111,129,131,131	0
10	NAG	A	601	14/15	0.77	0.28	95,105,115,118	0
12	EDO	C	627	4/4	0.77	0.18	89,90,90,92	0
10	NAG	B	2005	14/15	0.78	0.38	103,123,133,135	0
10	NAG	C	626	14/15	0.79	0.46	113,129,138,138	0
12	EDO	B	2012	4/4	0.80	0.21	82,83,84,85	0
10	NAG	F	502	14/15	0.81	0.43	118,136,146,146	0
12	EDO	H	509	4/4	0.83	0.22	95,98,102,105	0
13	MG	F	505	1/1	0.83	0.11	82,82,82,82	0
10	NAG	D	502	14/15	0.84	0.40	118,133,138,141	0
14	MES	D	507	12/12	0.87	0.17	82,91,100,100	0
14	MES	F	510	12/12	0.87	0.24	89,99,109,111	0
12	EDO	G	2025	4/4	0.88	0.21	78,80,80,80	0
12	EDO	E	625	4/4	0.88	0.18	58,59,63,67	0
11	CA	D	504	1/1	0.90	0.10	60,60,60,60	0
11	CA	E	603	1/1	0.90	0.10	84,84,84,84	0
13	MG	B	2001	1/1	0.90	0.06	57,57,57,57	0
13	MG	D	503	1/1	0.91	0.06	66,66,66,66	0
11	CA	G	2002	1/1	0.91	0.10	61,61,61,61	0
11	CA	G	2001	1/1	0.92	0.10	82,82,82,82	0
14	MES	B	2014	12/12	0.94	0.22	73,103,110,111	0
14	MES	H	510	12/12	0.94	0.23	75,89,91,91	0
12	EDO	B	2013	4/4	0.95	0.43	62,65,66,68	0
11	CA	E	604	1/1	0.95	0.14	98,98,98,98	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
11	CA	G	2003	1/1	0.95	0.07	63,63,63,63	0
11	CA	G	2004	1/1	0.95	0.07	83,83,83,83	0
11	CA	F	506	1/1	0.95	0.08	53,53,53,53	0
11	CA	C	605	1/1	0.95	0.10	58,58,58,58	0
11	CA	A	606	1/1	0.96	0.14	61,61,61,61	0
11	CA	A	607	1/1	0.96	0.13	54,54,54,54	0
11	CA	E	602	1/1	0.96	0.09	82,82,82,82	0
11	CA	A	609	1/1	0.96	0.13	55,55,55,55	0
10	NAG	E	601	14/15	0.96	0.32	20,20,20,20	0
11	CA	C	604	1/1	0.97	0.11	69,69,69,69	0
13	MG	H	505	1/1	0.97	0.03	60,60,60,60	0
11	CA	E	605	1/1	0.97	0.11	102,102,102,102	0
11	CA	C	602	1/1	0.98	0.15	62,62,62,62	0
11	CA	C	603	1/1	0.98	0.08	56,56,56,56	0
11	CA	H	506	1/1	0.98	0.11	68,68,68,68	0
11	CA	A	608	1/1	0.98	0.14	44,44,44,44	0

5.5 Other polymers [i](#)

There are no such residues in this entry.