



wwPDB EM Validation Summary Report ⓘ

Mar 9, 2026 – 02:17 PM UTC

PDB ID : 7DX8 / pdb_00007dx8
EMDB ID : EMD-30899
Title : Trypsin-digested S protein of SARS-CoV-2 bound with PD of ACE2 in the conformation 2 (2 up RBD and 2 PD bound)
Authors : Yan, R.H.; Zhang, Y.Y.; Li, Y.N.; Ye, F.F.; Guo, Y.Y.; Xia, L.; Zhong, X.Y.; Chi, X.M.; Zhou, Q.
Deposited on : 2021-01-18
Resolution : 2.90 Å(reported)

This is a wwPDB EM 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/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

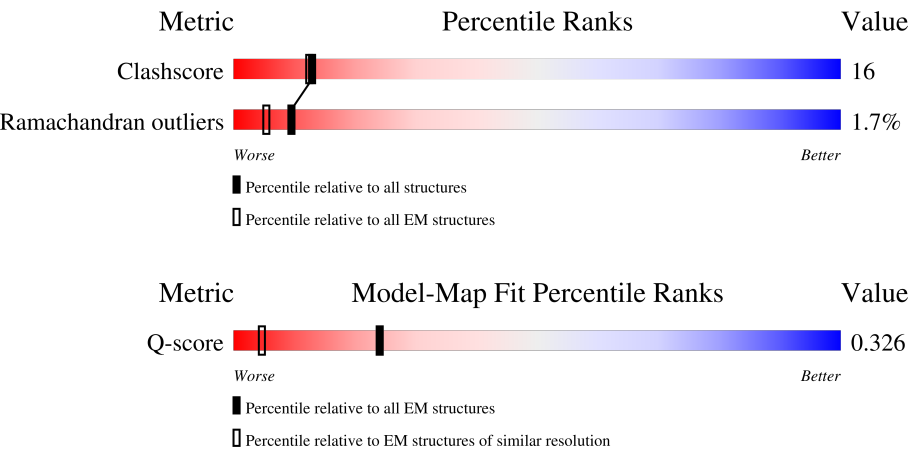
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.90 Å.

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



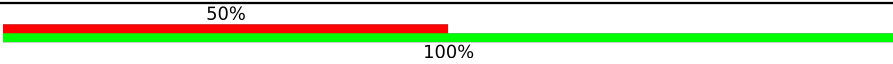
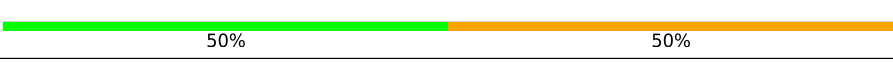
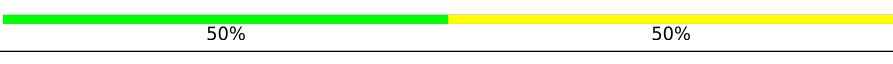
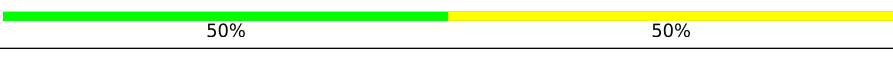
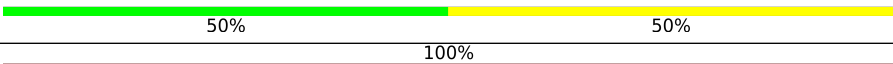
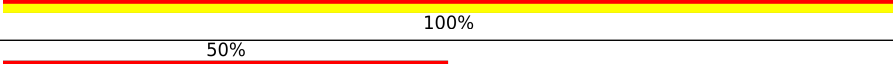
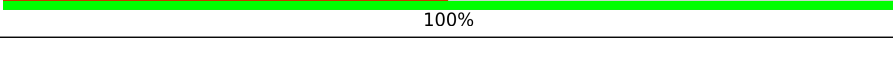
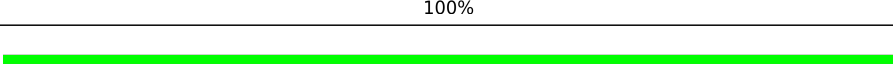
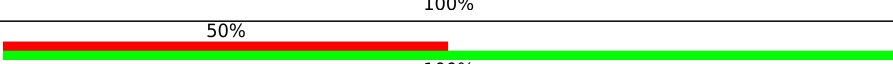
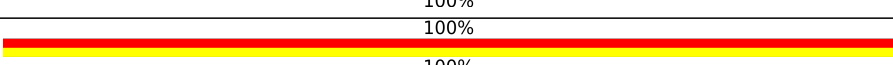
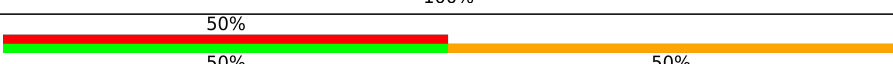
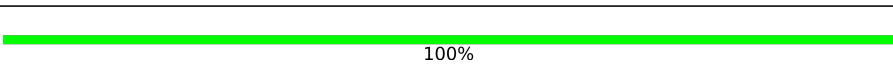
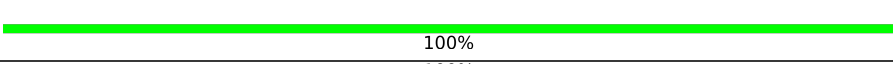
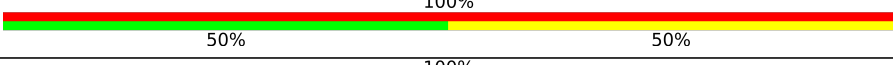
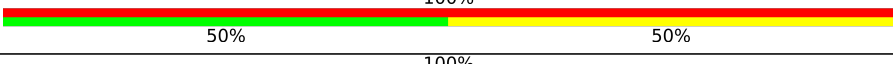
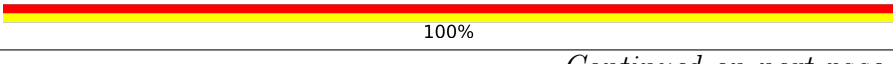
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Q-score	-	25397	13054 (2.40 - 3.40)

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

Mol	Chain	Length	Quality of chain
1	A	1283	13% 57% 20% • 22%
1	B	1283	9% 55% 20% 24%
1	C	1283	15% 57% 20% • 22%
2	D	817	73% 65% 7% 27%
2	E	817	73% 65% 7% 27%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	F	2	
3	G	2	
3	H	2	
3	I	2	
3	J	2	
3	K	2	
3	L	2	
3	M	2	
3	N	2	
3	O	2	
3	P	2	
3	Q	2	
3	R	2	
3	S	2	
3	T	2	
3	U	2	
3	V	2	
3	W	2	
3	X	2	
3	Y	2	
3	Z	2	
3	a	2	
3	b	2	
3	c	2	
3	d	2	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	e	2	100%
3	f	2	100%
3	g	2	100% 50% 50%
3	h	2	100% 50% 50%
3	i	2	100%
3	j	2	100%
3	k	2	100% 50% 50%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 34338 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1007	Total	C	N	O	S	0	0
			7872	5025	1310	1501	36		
1	B	971	Total	C	N	O	S	0	0
			7584	4843	1262	1445	34		
1	C	1006	Total	C	N	O	S	0	0
			7866	5022	1309	1499	36		

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	986	PRO	LYS	engineered mutation	UNP P0DTC2
A	987	PRO	VAL	engineered mutation	UNP P0DTC2
A	1274	LEU	-	expression tag	UNP P0DTC2
A	1275	GLU	-	expression tag	UNP P0DTC2
A	1276	ASP	-	expression tag	UNP P0DTC2
A	1277	TYR	-	expression tag	UNP P0DTC2
A	1278	LYS	-	expression tag	UNP P0DTC2
A	1279	ASP	-	expression tag	UNP P0DTC2
A	1280	ASP	-	expression tag	UNP P0DTC2
A	1281	ASP	-	expression tag	UNP P0DTC2
A	1282	ASP	-	expression tag	UNP P0DTC2
A	1283	LYS	-	expression tag	UNP P0DTC2
B	986	PRO	LYS	engineered mutation	UNP P0DTC2
B	987	PRO	VAL	engineered mutation	UNP P0DTC2
B	1274	LEU	-	expression tag	UNP P0DTC2
B	1275	GLU	-	expression tag	UNP P0DTC2
B	1276	ASP	-	expression tag	UNP P0DTC2
B	1277	TYR	-	expression tag	UNP P0DTC2
B	1278	LYS	-	expression tag	UNP P0DTC2
B	1279	ASP	-	expression tag	UNP P0DTC2
B	1280	ASP	-	expression tag	UNP P0DTC2
B	1281	ASP	-	expression tag	UNP P0DTC2
B	1282	ASP	-	expression tag	UNP P0DTC2
B	1283	LYS	-	expression tag	UNP P0DTC2

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	986	PRO	LYS	engineered mutation	UNP P0DTC2
C	987	PRO	VAL	engineered mutation	UNP P0DTC2
C	1274	LEU	-	expression tag	UNP P0DTC2
C	1275	GLU	-	expression tag	UNP P0DTC2
C	1276	ASP	-	expression tag	UNP P0DTC2
C	1277	TYR	-	expression tag	UNP P0DTC2
C	1278	LYS	-	expression tag	UNP P0DTC2
C	1279	ASP	-	expression tag	UNP P0DTC2
C	1280	ASP	-	expression tag	UNP P0DTC2
C	1281	ASP	-	expression tag	UNP P0DTC2
C	1282	ASP	-	expression tag	UNP P0DTC2
C	1283	LYS	-	expression tag	UNP P0DTC2

- Molecule 2 is a protein called Angiotensin-converting enzyme 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	595	Total	C	N	O	S	0	0
			4857	3108	804	916	29		
2	E	595	Total	C	N	O	S	0	0
			4857	3108	804	916	29		

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-11	MET	-	expression tag	UNP Q9BYF1
D	-10	ALA	-	expression tag	UNP Q9BYF1
D	-9	SER	-	expression tag	UNP Q9BYF1
D	-8	GLY	-	expression tag	UNP Q9BYF1
D	-7	ARG	-	expression tag	UNP Q9BYF1
D	10	TRP	-	insertion	UNP Q9BYF1
D	11	SER	-	insertion	UNP Q9BYF1
D	12	HIS	-	insertion	UNP Q9BYF1
D	13	PRO	-	insertion	UNP Q9BYF1
D	14	GLN	-	insertion	UNP Q9BYF1
D	15	PHE	-	insertion	UNP Q9BYF1
D	16	GLU	-	insertion	UNP Q9BYF1
D	17	LYS	-	insertion	UNP Q9BYF1
E	-11	MET	-	expression tag	UNP Q9BYF1
E	-10	ALA	-	expression tag	UNP Q9BYF1
E	-9	SER	-	expression tag	UNP Q9BYF1
E	-8	GLY	-	expression tag	UNP Q9BYF1
E	-7	ARG	-	expression tag	UNP Q9BYF1

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
E	10	TRP	-	insertion	UNP Q9BYF1
E	11	SER	-	insertion	UNP Q9BYF1
E	12	HIS	-	insertion	UNP Q9BYF1
E	13	PRO	-	insertion	UNP Q9BYF1
E	14	GLN	-	insertion	UNP Q9BYF1
E	15	PHE	-	insertion	UNP Q9BYF1
E	16	GLU	-	insertion	UNP Q9BYF1
E	17	LYS	-	insertion	UNP Q9BYF1

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



Mol	Chain	Residues	Atoms				AltConf	Trace
3	F	2	Total	C	N	O	0	0
			28	16	2	10		
3	G	2	Total	C	N	O	0	0
			28	16	2	10		
3	H	2	Total	C	N	O	0	0
			28	16	2	10		
3	I	2	Total	C	N	O	0	0
			28	16	2	10		
3	J	2	Total	C	N	O	0	0
			28	16	2	10		
3	K	2	Total	C	N	O	0	0
			28	16	2	10		
3	L	2	Total	C	N	O	0	0
			28	16	2	10		
3	M	2	Total	C	N	O	0	0
			28	16	2	10		
3	N	2	Total	C	N	O	0	0
			28	16	2	10		
3	O	2	Total	C	N	O	0	0
			28	16	2	10		
3	P	2	Total	C	N	O	0	0
			28	16	2	10		
3	Q	2	Total	C	N	O	0	0
			28	16	2	10		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf	Trace
3	R	2	Total	C	N	O	0	0
			28	16	2	10		
3	S	2	Total	C	N	O	0	0
			28	16	2	10		
3	T	2	Total	C	N	O	0	0
			28	16	2	10		
3	U	2	Total	C	N	O	0	0
			28	16	2	10		
3	V	2	Total	C	N	O	0	0
			28	16	2	10		
3	W	2	Total	C	N	O	0	0
			28	16	2	10		
3	X	2	Total	C	N	O	0	0
			28	16	2	10		
3	Y	2	Total	C	N	O	0	0
			28	16	2	10		
3	Z	2	Total	C	N	O	0	0
			28	16	2	10		
3	a	2	Total	C	N	O	0	0
			28	16	2	10		
3	b	2	Total	C	N	O	0	0
			28	16	2	10		
3	c	2	Total	C	N	O	0	0
			28	16	2	10		
3	d	2	Total	C	N	O	0	0
			28	16	2	10		
3	e	2	Total	C	N	O	0	0
			28	16	2	10		
3	f	2	Total	C	N	O	0	0
			28	16	2	10		
3	g	2	Total	C	N	O	0	0
			28	16	2	10		
3	h	2	Total	C	N	O	0	0
			28	16	2	10		
3	i	2	Total	C	N	O	0	0
			28	16	2	10		
3	j	2	Total	C	N	O	0	0
			28	16	2	10		
3	k	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$) (labeled as "Ligand of Interest" by depositor).



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

Continued on next page...

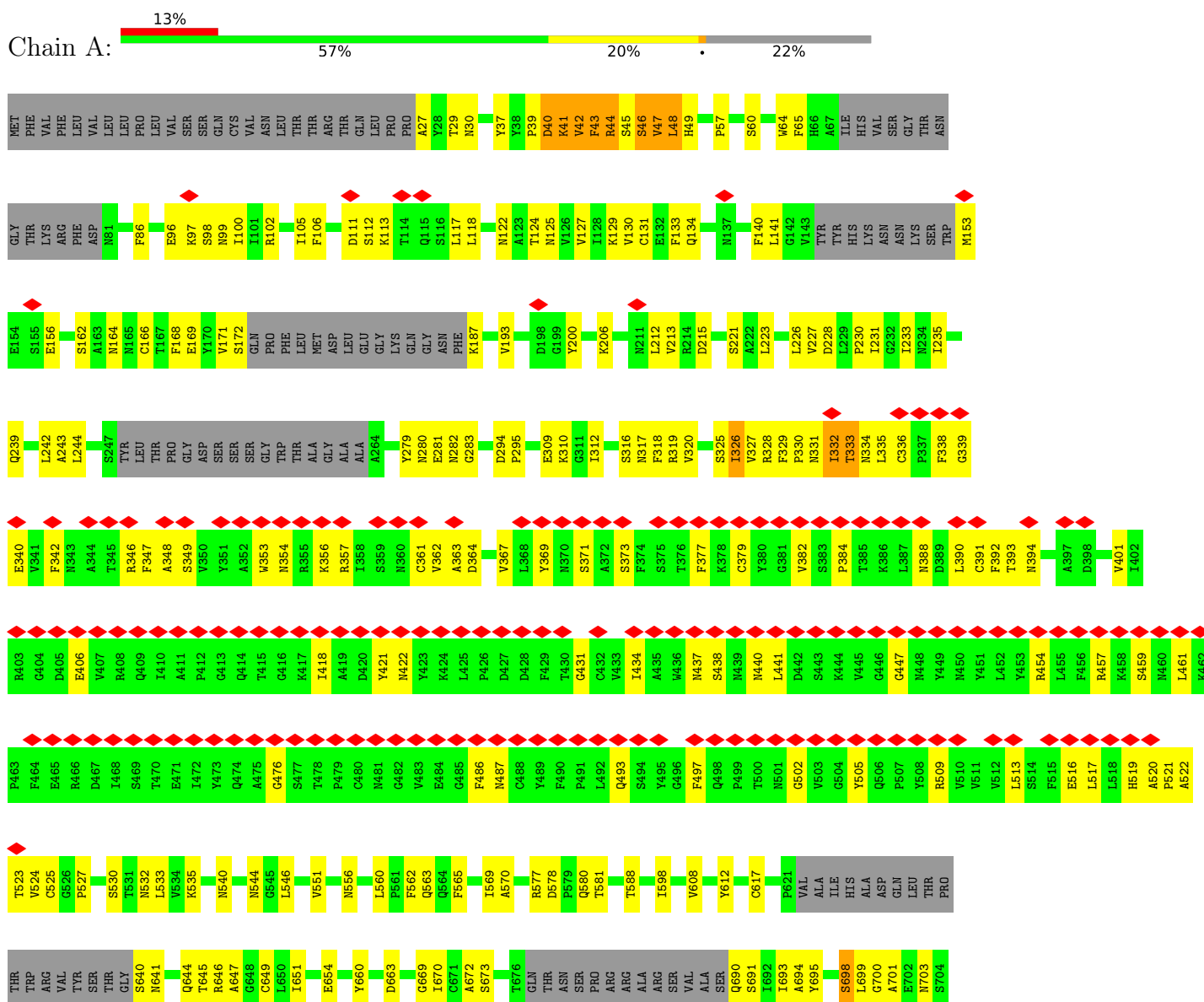
Continued from previous page...

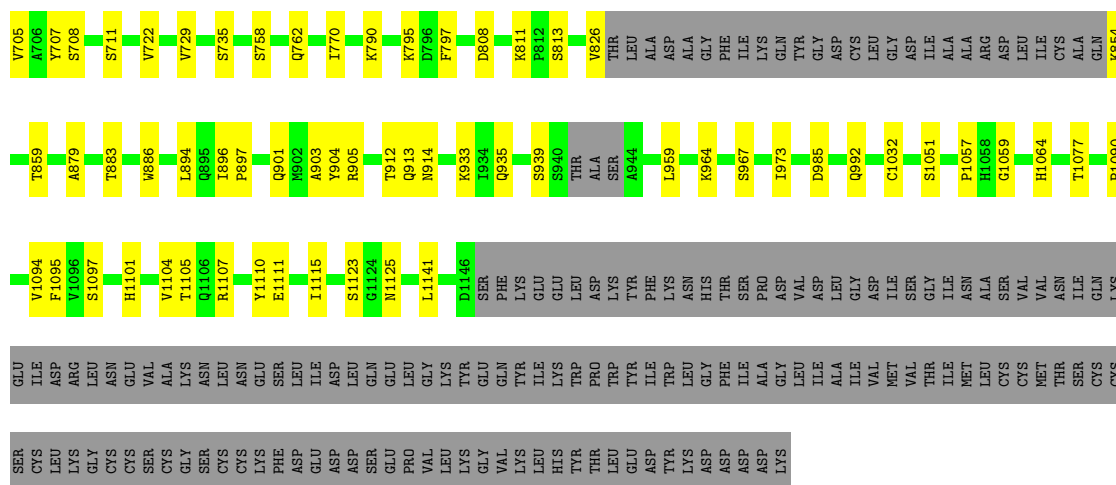
Mol	Chain	Residues	Atoms				AltConf
4	B	1	Total 14	C 8	N 1	O 5	0
4	B	1	Total 14	C 8	N 1	O 5	0
4	B	1	Total 14	C 8	N 1	O 5	0
4	B	1	Total 14	C 8	N 1	O 5	0
4	B	1	Total 14	C 8	N 1	O 5	0
4	C	1	Total 14	C 8	N 1	O 5	0
4	C	1	Total 14	C 8	N 1	O 5	0
4	C	1	Total 14	C 8	N 1	O 5	0
4	C	1	Total 14	C 8	N 1	O 5	0
4	C	1	Total 14	C 8	N 1	O 5	0
4	C	1	Total 14	C 8	N 1	O 5	0
4	C	1	Total 14	C 8	N 1	O 5	0
4	C	1	Total 14	C 8	N 1	O 5	0
4	C	1	Total 14	C 8	N 1	O 5	0
4	D	1	Total 14	C 8	N 1	O 5	0
4	E	1	Total 14	C 8	N 1	O 5	0

3 Residue-property plots

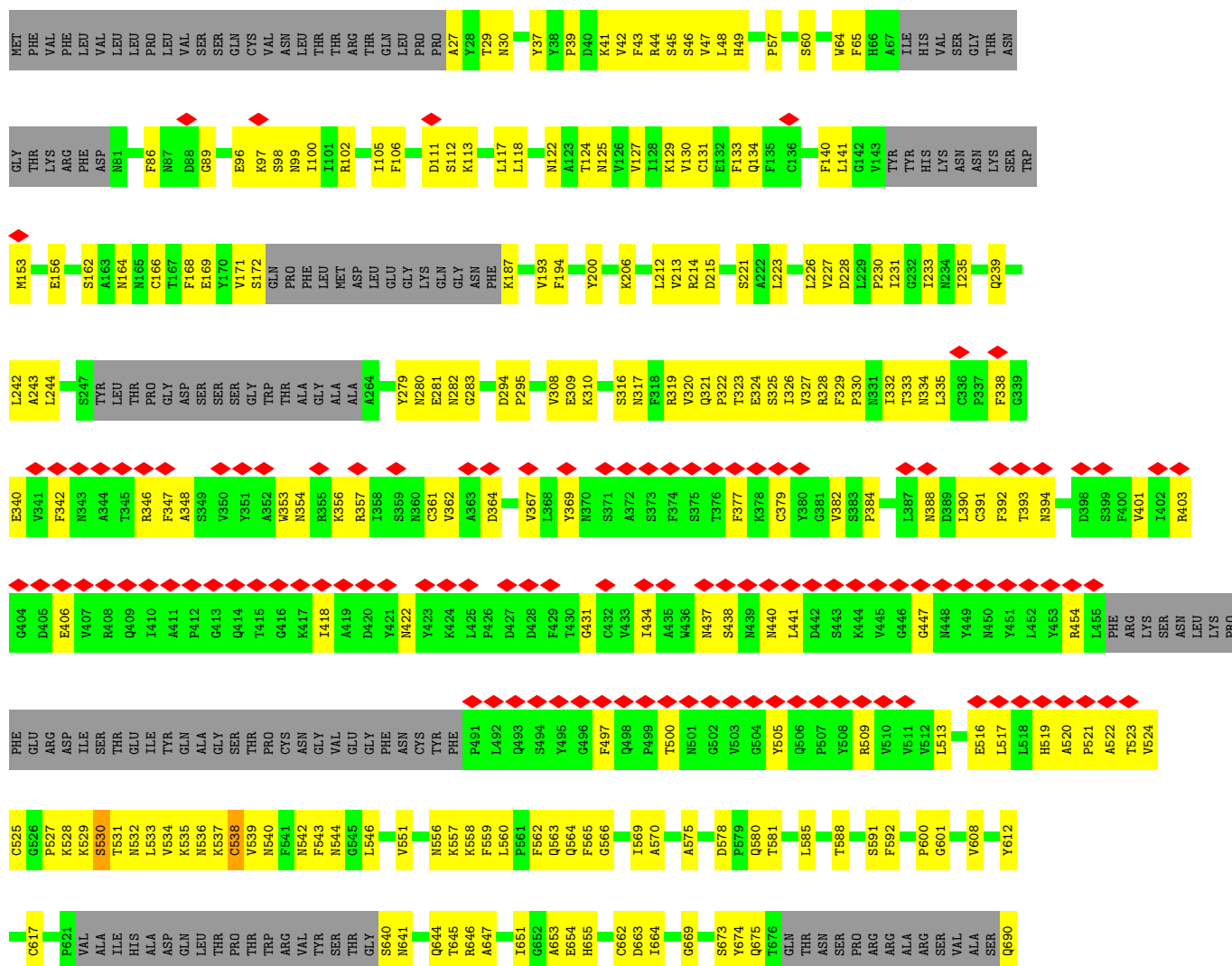
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

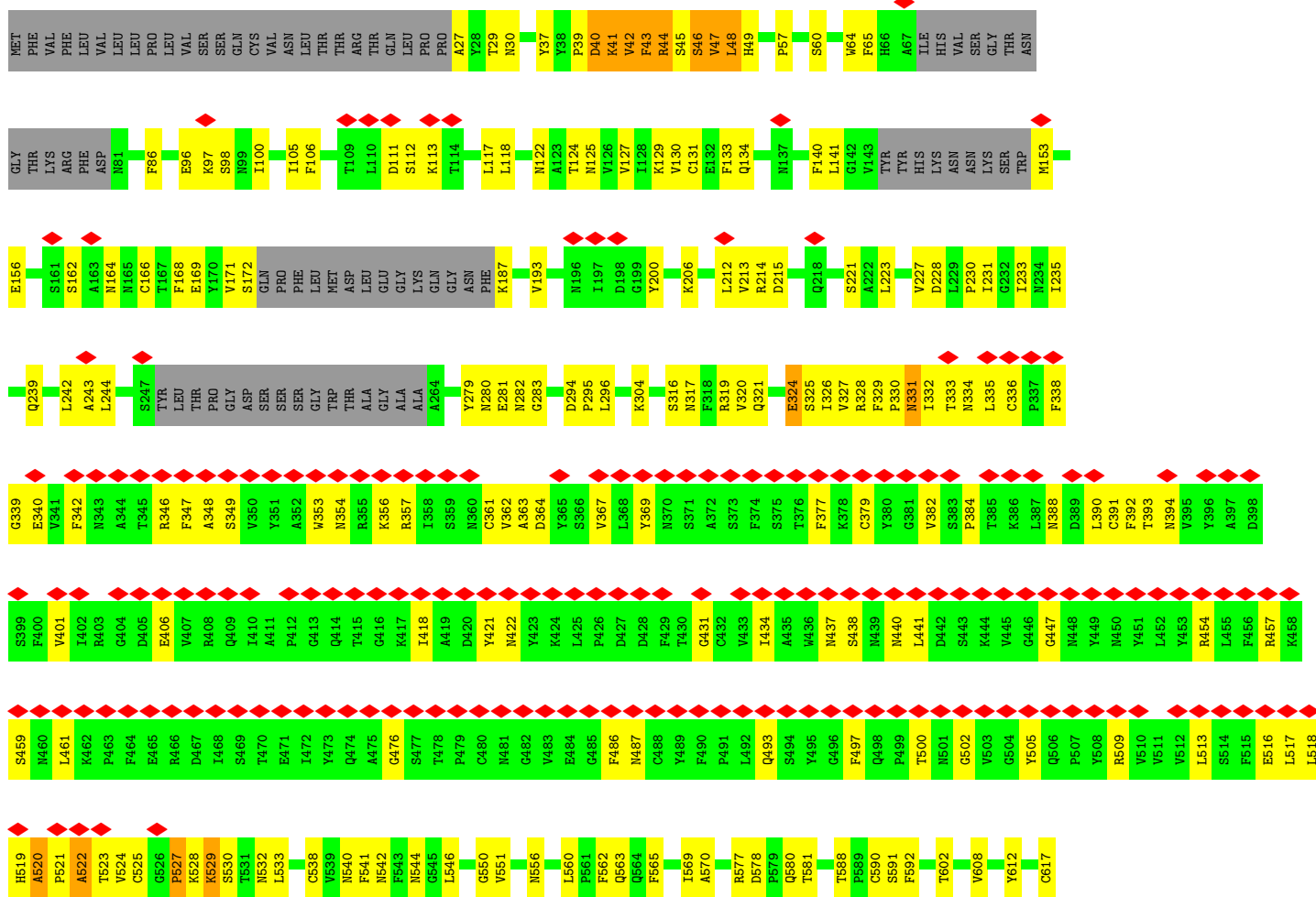
• Molecule 1: Spike glycoprotein

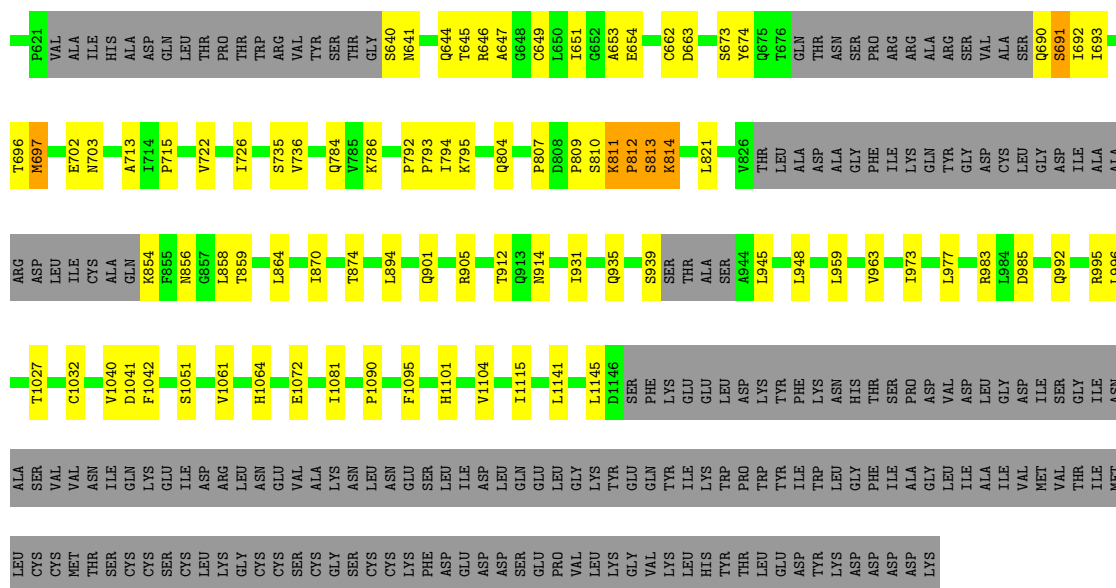




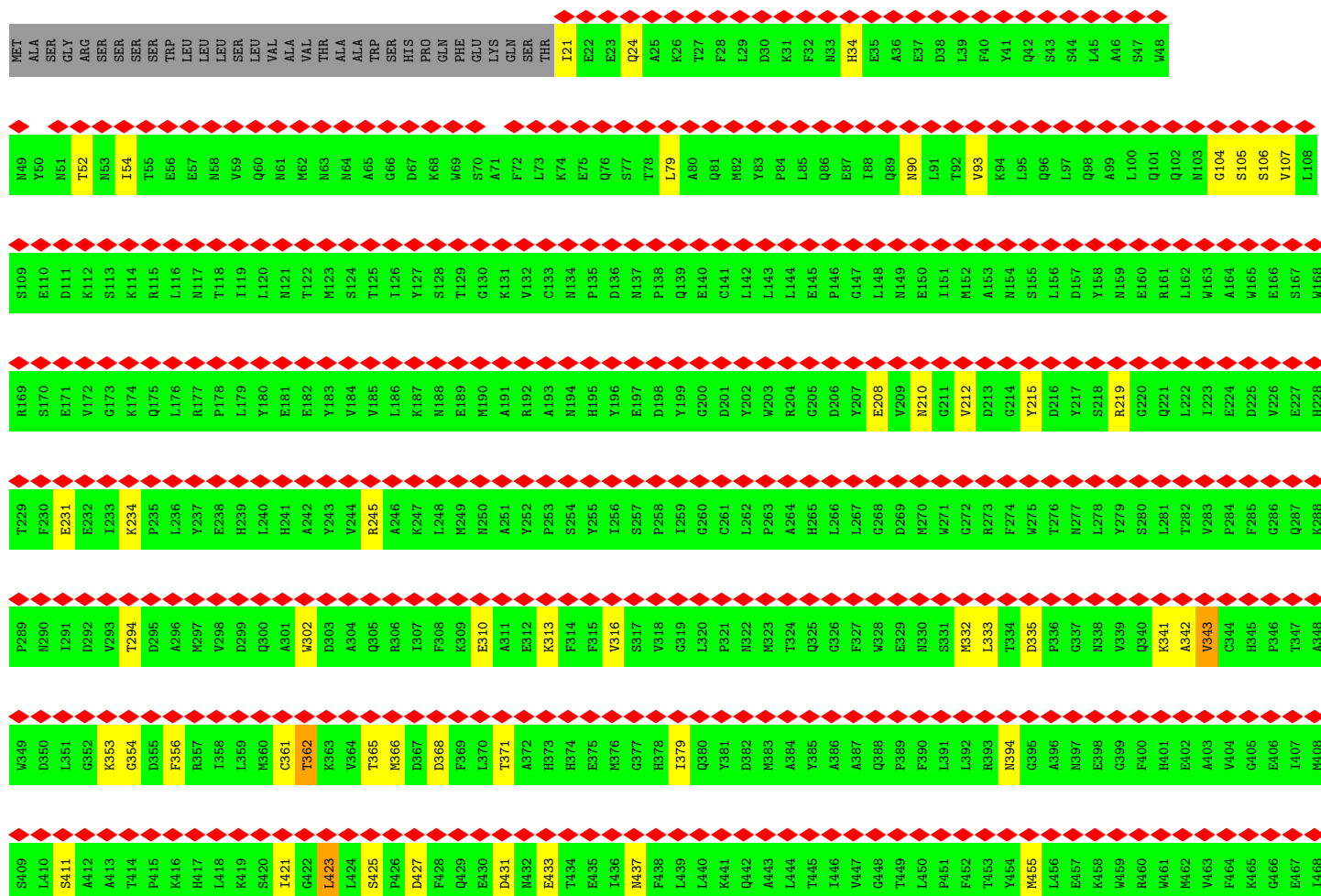
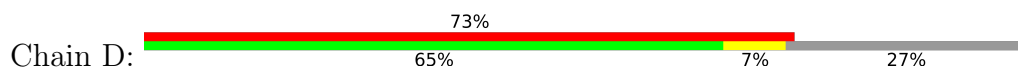
● Molecule 1: Spike glycoprotein





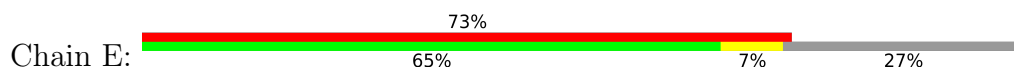


• Molecule 2: Angiotensin-converting enzyme 2



P469	L529	E589	TYR	LYS
K470	C530	P590	ARG	LYS
D471	Q531	P591	ILE	ASN
Q472	L591	L591	GLY	ASN
W473	A532	F592	GLN	LYS
M474	A533	T593	ASP	ALA
K475	K534	W594	PHE	ARG
K476	H535	L595	LEU	ARG
K477	E536	K596	VAL	GLY
W478	G537	D597	LYS	GLU
W479	P538	Q598	ASN	ASP
E479	L539	Q599	GLN	ASN
M480	H540	N599	MET	LEU
K481	K541	K600	ILE	GLU
R482	G542	N601	PHE	LEU
E483	D543	S602	GLY	ALA
I484	I544	F603	GLU	ILE
V485	S545	V604	GLU	GLN
G486	N546	G605	VAL	PRO
V487	W547	W606	THR	THR
V488	T548	S607	VAL	GLY
E489	T549	T608	ALA	PRO
P490	A550	D609	ASN	ASN
V491	G551	W610	LYS	GLN
P492	Q552	S611	PRO	THR
H493	K553	P612	ILE	ASP
D494	L554	Y613	SER	ASP
E495	F555	A614	ILE	VAL
T496	N556	D615	PHE	GLN
Y497	M557	GLN	VAL	ILE
C498	L558	SER	VAL	THR
D499	R559	LYS	ALA	GLY
P500	L560	VAL	PRO	VAL
A501	G561	ARG	LYS	MET
S502	K562	ILE	ASN	GLY
L503	S563	LEU	VAL	VAL
F504	E564	LYS	ASP	ILE
H505	P565	SER	ILE	VAL
V506	W566	LEU	ILE	GLY
S507	T567	GLY	PRO	ILE
N508	L568	ASP	THR	VAL
D509	A569	LYS	GLU	LEU
W510	L570	ALA	VAL	ILE
S511	E571	TRP	LYS	PHE
F512	N572	ASN	THR	GLY
I513	V573	ASP	ILE	ILE
R514	W574	ASN	ARG	ASP
Y515	G575	GLU	MET	ASP
Y516	A576	TYR	THR	ARG
T517	K577	LEU	PHE	ARG
R518	N578	ARG	ARG	SER
T519	M579	SER	SER	SER
L520	N580	VAL	VAL	VAL
Y521	V581	ALA	ALA	ALA
Q522	R582			
F523	P583			
Q524	L584			
F525	L585			
Q526	N586			
E527	Y587			
A528	F588			

• Molecule 2: Angiotensin-converting enzyme 2



MET	M49	S109	R169	T229	P289	W349	S409
ALA	Y50	E110	S170	F230	N289	D350	L410
GLY	M51	D111	E171	E231	I291	L351	S411
ARG	T52	K112	V172	E232	D292	G352	A412
ASP	M53	S113	G173	I233	V293	K353	A413
PHE	I54	K114	K174	K234	T294	G354	T414
ARG	T55	R115	Q175	P235	D295	D355	P415
LEU	E56	L116	L176	L236	A296	F356	K416
ASP	E57	M117	R177	Y237	M297	R357	H417
ASN	M58	T118	P178	E238	V298	L358	L418
SER	V59	I119	L179	H239	D299	L359	K419
LEU	Q60	L120	Y180	L240	Q300	M360	S420
LEU	M61	M121	E181	H241	A301	C361	I421
ALA	M62	T122	E182	A242	W302	T362	G422
GLY	M63	M123	Y183	Y243	D303	K363	L423
ILE	M64	S124	V184	V244	A304	V364	L424
GLN	A65	T125	V185	R245	Q305	T365	S425
THR	G66	I126	L186	A246	R306	M366	A426
PRO	D67	Y127	K187	K247	I307	D367	D427
ASN	K68	S128	M188	L248	F308	D368	F428
GLY	M69	T129	E189	M249	K309	F369	Q429
PHE	S70	G130	M190	N250	E310	L370	E430
LEU	A71	K131	A191	A251	A311	T371	D431
THR	F72	V132	R192	Y252	E312	A372	N432
SER	L73	C133	A193	P253	K313	H373	E433
THR	K74	M134	H194	S254	F314	H374	T434
ILE	E75	P135	H195	Y255	F315	E375	E435
VAL	Q76	D136	V196	I256	V316	M376	I436
THR	S77	M137	E197	S257	S317	G377	M437
GLN	T78	P138	D198	T258	V318	H378	F438
ASP	L79	Q139	Y199	I259	G319	I379	L439
VAL	A80	E140	Q200	G260	L320	Q380	L440
THR	Q81	C141	D201	C261	P321	Y381	K441
GLY	M82	L142	Y202	L262	N322	D382	Q442
ILE	F83	L143	W203	P263	M323	M383	A443
VAL	P84	L144	R204	A264	T324	A384	L444
GLY	L85	E145	G205	H265	Q325	Y385	T445
ILE	Q86	P146	D206	L266	G326	A386	I446
THR	E87	G147	Y207	L267	F327	A387	V447
ASP	T88	L148	E208	G268	W328	Q388	G448
LEU	Q89	M149	V209	D269	E329	P389	T449
ALA	N90	E150	M210	M270	N330	F390	L450
THR	L91	I151	G211	W271	S331	L391	P451
GLY	T92	M152	V212	G272	M332	L392	F452
ILE	V93	A153	D213	R273	L333	R393	T453
ASP	K94	M154	G214	F274	T334	N394	Y454
ARG	Q42	S155	Y215	W275	D335	G395	M455
ASP	S43	L156	D216	T276	P336	A396	L456
THR	S44	D157	Y217	N277	G337	A397	E457
GLY	L45	Y158	S218	L278	N338	E398	K458
ILE	A99	M159	R219	Y279	V339	G399	W459
ASP	L100	E160	Q220	S280	F400	H401	R460
ARG	Q101	R161	Q221	L281	K341	H402	W461
ASP	Q102	L162	L222	T282	A342	E403	M462
THR	M103	W163	I223	V283	V343	A403	V463
GLY	G104	A164	E224	P284	C344	V404	F464
ILE	S105	W165	D225	F285	H345	G405	K465
ASP	S106	E166	V226	G286	P346	E406	G466
ARG	V107	S167	E227	Q287	T347	I407	E467
	L108	W168	H228	K288	A348	M408	I468

L529	C530	Q531	A532	A533	K534	H535	E536	G537	P538	L539	H540	K541	C542	D543	I544	S545	N546	S547	T548	E549	A550	G551	Q552	K553	L554	F555	N556	M557	L558	R559	L560	G561	K562	S563	E564	P565	W566	T567	L568	A569	L570	E571	N572	V573	V574	G575	A576	K577	N578	M579	N580	V581	R582	P583	L584	L585	N586	Y587	F588
E589	P590	L591	F592	T593	W594	L595	K596	D597	Q598	N599	K600	N601	S602	F603	V604	G605	W606	S607	T608	D609	W610	S611	P612	Y613	A614	D615	GLN	SER	ILE	LYS	VAL	ARG	ILE	SER	LEU	LYS	SER	ALA	TYR	TRP	ASN	ASP	ASN	GLU	TYR	PHE	ARG	SER	VAL	ALA									
TYR	ALA	MET	ARG	GLN	TYR	PHE	LEU	VAL	LYS	ASN	GLN	MET	ILE	PHE	GLY	GLU	ASP	VAL	GLY	ASN	LYS	PRO	ARG	ILE	SER	PHE	ASN	PHE	VAL	ALA	LYS	ASN	VAL	SER	ILE	ASP	ILE	VAL	GLU	VAL	LYS	PHE	THR	GLY	ILE	ARG	MET	SER	ASP	ARG									
SER	ARG	ILE	ASN	ASP	ALA	ARG	GLY	ASN	ASP	ASN	SER	LEU	GLU	PHE	ILE	GLY	GLN	PRO	THR	LEU	GLY	PRO	ASN	GLN	LYS	PRO	THR	ILE	SER	PHE	VAL	GLN	THR	ASN	VAL	GLY	ILE	VAL	GLY	ILE	LEU	PHE	THR	GLY	ILE	ARG	ASP	ARG											
LYS	LYS	LYS	ASN	ALA	ARG	SER	GLY	GLU	ASN	PRO	TYR	ALA	SER	ILE	SER	LYS	ASN	ASN	GLY	PHE	GLN	ASN	THR	ASP	VAL	GLN	THR	SER	PHE	VAL	GLY	VAL	ILE	VAL	GLY	ILE	VAL	GLY	ILE	LEU	PHE	THR	GLY	ILE	ARG	ASP	ARG												

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



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



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



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



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

Chain J:  50% 50%



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

Chain K:  50% 50%



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

Chain L:  50% 50%

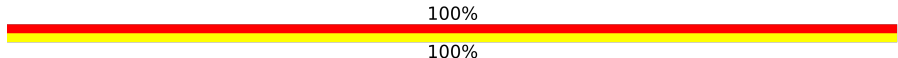


- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:  50% 50%



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

Chain N:  100% 100%



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

Chain O:  50% 100%



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

Chain P:  50% 50%



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

Chain Q:  50% 50%



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

Chain R:  100%



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

Chain S:  100%

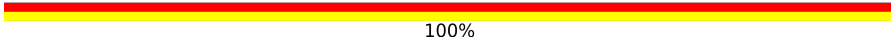


- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain T:  50% 100%



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

Chain U:  100% 100%



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

Chain V:  50% 50% 50%



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

Chain W:



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

Chain X:



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

Chain Y:



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

Chain Z:



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

Chain a:



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

Chain b:



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



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



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



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



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



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



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



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



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



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	208455	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.198	Depositor
Minimum map value	-0.105	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.018	Depositor
Map size (Å)	313.056, 313.056, 313.056	wwPDB
Map dimensions	288, 288, 288	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.087, 1.087, 1.087	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.52	1/8048 (0.0%)	0.62	2/10947 (0.0%)
1	B	0.51	0/7751	0.63	4/10544 (0.0%)
1	C	0.52	0/8042	0.61	3/10939 (0.0%)
2	D	0.30	0/4994	0.54	1/6785 (0.0%)
2	E	0.30	0/4994	0.54	1/6785 (0.0%)
All	All	0.46	1/33829 (0.0%)	0.60	11/46000 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	698	SER	CA-C	-6.55	1.44	1.52

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	538	CYS	N-CA-C	-6.36	100.89	110.24
1	C	538	CYS	N-CA-C	-6.21	100.85	110.10
2	D	362	THR	N-CA-C	6.02	119.33	109.76
2	E	362	THR	N-CA-C	6.01	119.32	109.76
1	B	86	PHE	CA-C-N	5.88	132.77	121.54

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7872	0	7668	341	0
1	B	7584	0	7402	369	0
1	C	7866	0	7663	378	0
2	D	4857	0	4624	68	0
2	E	4857	0	4624	69	0
3	F	28	0	25	0	0
3	G	28	0	25	3	0
3	H	28	0	25	0	0
3	I	28	0	25	1	0
3	J	28	0	25	1	0
3	K	28	0	25	0	0
3	L	28	0	25	0	0
3	M	28	0	25	2	0
3	N	28	0	25	3	0
3	O	28	0	25	0	0
3	P	28	0	25	0	0
3	Q	28	0	25	0	0
3	R	28	0	25	1	0
3	S	28	0	25	0	0
3	T	28	0	25	0	0
3	U	28	0	25	4	0
3	V	28	0	25	1	0
3	W	28	0	25	0	0
3	X	28	0	25	0	0
3	Y	28	0	25	1	0
3	Z	28	0	25	2	0
3	a	28	0	25	0	0
3	b	28	0	25	0	0
3	c	28	0	25	0	0
3	d	28	0	25	6	0
3	e	28	0	25	0	0
3	f	28	0	25	0	0
3	g	28	0	25	0	0
3	h	28	0	25	0	0
3	i	28	0	25	5	0
3	j	28	0	25	0	0
3	k	28	0	25	0	0
4	A	126	0	117	4	0
4	B	140	0	129	8	0
4	C	112	0	104	4	0
4	D	14	0	13	0	0
4	E	14	0	13	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	34338	0	33157	1112	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 16.

The worst 5 of 1112 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:654:GLU:HG3	1:C:693:ILE:CG2	1.37	1.50
4:B:1409:NAG:O4	4:B:1410:NAG:C1	1.63	1.46
1:A:230:PRO:CB	1:C:521:PRO:HG2	1.47	1.44
1:A:703:ASN:HB2	1:B:787:GLN:OE1	1.28	1.28
1:A:486:PHE:CE1	2:D:79:LEU:HD22	1.75	1.21

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	324/1283 (25%)	258 (80%)	51 (16%)	15 (5%)	2	7
1	B	131/1283 (10%)	124 (95%)	7 (5%)	0	100	100
1	C	988/1283 (77%)	866 (88%)	96 (10%)	26 (3%)	4	17
2	D	593/817 (73%)	563 (95%)	28 (5%)	2 (0%)	36	65
2	E	585/817 (72%)	555 (95%)	28 (5%)	2 (0%)	36	65
All	All	2621/5483 (48%)	2366 (90%)	210 (8%)	45 (2%)	9	26

5 of 45 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	48	LEU
1	A	331	ASN
1	A	332	ILE
1	A	333	THR
1	C	48	LEU

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

64 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	$\# Z > 2$
3	NAG	F	1	3,1	14,14,15	0.53	0	17,19,21	0.52	0
3	NAG	F	2	3	14,14,15	0.23	0	17,19,21	0.61	0
3	NAG	G	1	3,1	14,14,15	0.55	0	17,19,21	0.58	0
3	NAG	G	2	3	14,14,15	0.30	0	17,19,21	0.48	0
3	NAG	H	1	3,1	14,14,15	0.30	0	17,19,21	0.64	1 (5%)
3	NAG	H	2	3	14,14,15	0.53	0	17,19,21	0.49	0
3	NAG	I	1	3,1	14,14,15	0.36	0	17,19,21	0.74	0
3	NAG	I	2	3	14,14,15	0.29	0	17,19,21	1.40	2 (11%)
3	NAG	J	1	3,1	14,14,15	0.67	1 (7%)	17,19,21	0.71	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	J	2	3	14,14,15	0.42	0	17,19,21	1.49	3 (17%)
3	NAG	K	1	3,1	14,14,15	0.66	1 (7%)	17,19,21	0.68	0
3	NAG	K	2	3	14,14,15	0.28	0	17,19,21	0.68	0
3	NAG	L	1	3,1	14,14,15	0.25	0	17,19,21	0.71	1 (5%)
3	NAG	L	2	3	14,14,15	0.17	0	17,19,21	0.50	0
3	NAG	M	1	3,1	14,14,15	0.54	0	17,19,21	0.52	0
3	NAG	M	2	3	14,14,15	0.25	0	17,19,21	0.60	0
3	NAG	N	1	3,1	14,14,15	0.54	0	17,19,21	0.58	0
3	NAG	N	2	3	14,14,15	0.30	0	17,19,21	0.47	0
3	NAG	O	1	3,1	14,14,15	0.31	0	17,19,21	0.42	0
3	NAG	O	2	3	14,14,15	0.39	0	17,19,21	0.37	0
3	NAG	P	1	3,1	14,14,15	0.37	0	17,19,21	1.17	1 (5%)
3	NAG	P	2	3	14,14,15	0.25	0	17,19,21	0.49	0
3	NAG	Q	1	3,1	14,14,15	0.30	0	17,19,21	0.72	1 (5%)
3	NAG	Q	2	3	14,14,15	0.21	0	17,19,21	0.41	0
3	NAG	R	1	3,1	14,14,15	0.70	1 (7%)	17,19,21	0.91	1 (5%)
3	NAG	R	2	3	14,14,15	0.36	0	17,19,21	0.73	1 (5%)
3	NAG	S	1	3,1	14,14,15	0.21	0	17,19,21	0.45	0
3	NAG	S	2	3	14,14,15	0.28	0	17,19,21	0.39	0
3	NAG	T	1	3,1	14,14,15	0.52	0	17,19,21	0.51	0
3	NAG	T	2	3	14,14,15	0.25	0	17,19,21	0.60	0
3	NAG	U	1	3,1	14,14,15	0.55	0	17,19,21	0.58	0
3	NAG	U	2	3	14,14,15	0.29	0	17,19,21	0.48	0
3	NAG	V	1	3,1	14,14,15	0.23	0	17,19,21	1.44	2 (11%)
3	NAG	V	2	3	14,14,15	0.19	0	17,19,21	0.52	0
3	NAG	W	1	3,1	14,14,15	0.51	0	17,19,21	0.72	1 (5%)
3	NAG	W	2	3	14,14,15	0.40	0	17,19,21	0.48	0
3	NAG	X	1	3,1	14,14,15	0.37	0	17,19,21	0.40	0
3	NAG	X	2	3	14,14,15	0.20	0	17,19,21	0.77	0
3	NAG	Y	1	3,1	14,14,15	0.36	0	17,19,21	0.49	0
3	NAG	Y	2	3	14,14,15	0.57	0	17,19,21	1.37	2 (11%)
3	NAG	Z	1	3,1	14,14,15	0.61	0	17,19,21	0.45	0
3	NAG	Z	2	3	14,14,15	0.33	0	17,19,21	1.44	2 (11%)
3	NAG	a	1	3,1	14,14,15	0.38	0	17,19,21	0.46	0
3	NAG	a	2	3	14,14,15	0.25	0	17,19,21	0.51	0
3	NAG	b	1	2,3	14,14,15	0.59	1 (7%)	17,19,21	0.74	0
3	NAG	b	2	3	14,14,15	0.56	0	17,19,21	0.38	0
3	NAG	c	1	2,3	14,14,15	0.40	0	17,19,21	0.67	0
3	NAG	c	2	3	14,14,15	0.28	0	17,19,21	0.71	1 (5%)
3	NAG	d	1	2,3	14,14,15	0.29	0	17,19,21	0.56	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	d	2	3	14,14,15	0.31	0	17,19,21	0.58	0
3	NAG	e	1	2,3	14,14,15	0.31	0	17,19,21	0.54	0
3	NAG	e	2	3	14,14,15	0.36	0	17,19,21	0.49	0
3	NAG	f	1	2,3	14,14,15	0.23	0	17,19,21	0.63	0
3	NAG	f	2	3	14,14,15	0.35	0	17,19,21	0.60	1 (5%)
3	NAG	g	1	2,3	14,14,15	0.59	1 (7%)	17,19,21	0.74	0
3	NAG	g	2	3	14,14,15	0.55	0	17,19,21	0.38	0
3	NAG	h	1	2,3	14,14,15	0.41	0	17,19,21	0.67	0
3	NAG	h	2	3	14,14,15	0.28	0	17,19,21	0.72	1 (5%)
3	NAG	i	1	2,3	14,14,15	0.29	0	17,19,21	0.57	0
3	NAG	i	2	3	14,14,15	0.29	0	17,19,21	0.58	0
3	NAG	j	1	2,3	14,14,15	0.31	0	17,19,21	0.53	0
3	NAG	j	2	3	14,14,15	0.37	0	17,19,21	0.49	0
3	NAG	k	1	2,3	14,14,15	0.22	0	17,19,21	0.63	0
3	NAG	k	2	3	14,14,15	0.33	0	17,19,21	0.60	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	F	1	3,1	-	1/6/23/26	0/1/1/1
3	NAG	F	2	3	-	2/6/23/26	0/1/1/1
3	NAG	G	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	G	2	3	-	3/6/23/26	0/1/1/1
3	NAG	H	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	H	2	3	-	2/6/23/26	0/1/1/1
3	NAG	I	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	I	2	3	-	4/6/23/26	0/1/1/1
3	NAG	J	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	J	2	3	-	6/6/23/26	0/1/1/1
3	NAG	K	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	K	2	3	-	4/6/23/26	0/1/1/1
3	NAG	L	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	L	2	3	-	0/6/23/26	0/1/1/1
3	NAG	M	1	3,1	-	1/6/23/26	0/1/1/1
3	NAG	M	2	3	-	2/6/23/26	0/1/1/1
3	NAG	N	1	3,1	-	0/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	N	2	3	-	3/6/23/26	0/1/1/1
3	NAG	O	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	O	2	3	-	1/6/23/26	0/1/1/1
3	NAG	P	1	3,1	-	1/6/23/26	0/1/1/1
3	NAG	P	2	3	-	0/6/23/26	0/1/1/1
3	NAG	Q	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	Q	2	3	-	3/6/23/26	0/1/1/1
3	NAG	R	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	R	2	3	-	3/6/23/26	0/1/1/1
3	NAG	S	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	S	2	3	-	2/6/23/26	0/1/1/1
3	NAG	T	1	3,1	-	1/6/23/26	0/1/1/1
3	NAG	T	2	3	-	2/6/23/26	0/1/1/1
3	NAG	U	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	U	2	3	-	3/6/23/26	0/1/1/1
3	NAG	V	1	3,1	-	6/6/23/26	0/1/1/1
3	NAG	V	2	3	-	2/6/23/26	0/1/1/1
3	NAG	W	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	W	2	3	-	2/6/23/26	0/1/1/1
3	NAG	X	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	X	2	3	-	2/6/23/26	0/1/1/1
3	NAG	Y	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	Y	2	3	-	6/6/23/26	0/1/1/1
3	NAG	Z	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	Z	2	3	-	5/6/23/26	0/1/1/1
3	NAG	a	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	a	2	3	-	2/6/23/26	0/1/1/1
3	NAG	b	1	2,3	-	2/6/23/26	0/1/1/1
3	NAG	b	2	3	-	2/6/23/26	0/1/1/1
3	NAG	c	1	2,3	-	2/6/23/26	0/1/1/1
3	NAG	c	2	3	-	2/6/23/26	0/1/1/1
3	NAG	d	1	2,3	-	2/6/23/26	0/1/1/1
3	NAG	d	2	3	-	3/6/23/26	0/1/1/1
3	NAG	e	1	2,3	-	0/6/23/26	0/1/1/1
3	NAG	e	2	3	-	0/6/23/26	0/1/1/1
3	NAG	f	1	2,3	-	0/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	f	2	3	-	2/6/23/26	0/1/1/1
3	NAG	g	1	2,3	-	2/6/23/26	0/1/1/1
3	NAG	g	2	3	-	2/6/23/26	0/1/1/1
3	NAG	h	1	2,3	-	2/6/23/26	0/1/1/1
3	NAG	h	2	3	-	2/6/23/26	0/1/1/1
3	NAG	i	1	2,3	-	2/6/23/26	0/1/1/1
3	NAG	i	2	3	-	3/6/23/26	0/1/1/1
3	NAG	j	1	2,3	-	0/6/23/26	0/1/1/1
3	NAG	j	2	3	-	0/6/23/26	0/1/1/1
3	NAG	k	1	2,3	-	0/6/23/26	0/1/1/1
3	NAG	k	2	3	-	2/6/23/26	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	R	1	NAG	O5-C1	-2.54	1.39	1.43
3	K	1	NAG	O5-C1	-2.41	1.39	1.43
3	J	1	NAG	O5-C1	-2.21	1.40	1.43
3	b	1	NAG	O5-C1	-2.07	1.40	1.43
3	g	1	NAG	O5-C1	-2.05	1.40	1.43

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	V	1	NAG	C2-N2-C7	4.94	129.52	122.90
3	J	2	NAG	C2-N2-C7	4.71	129.21	122.90
3	Z	2	NAG	C2-N2-C7	4.62	129.10	122.90
3	I	2	NAG	C2-N2-C7	4.56	129.00	122.90
3	Y	2	NAG	C2-N2-C7	4.55	128.99	122.90

There are no chirality outliers.

5 of 121 torsion outliers are listed below:

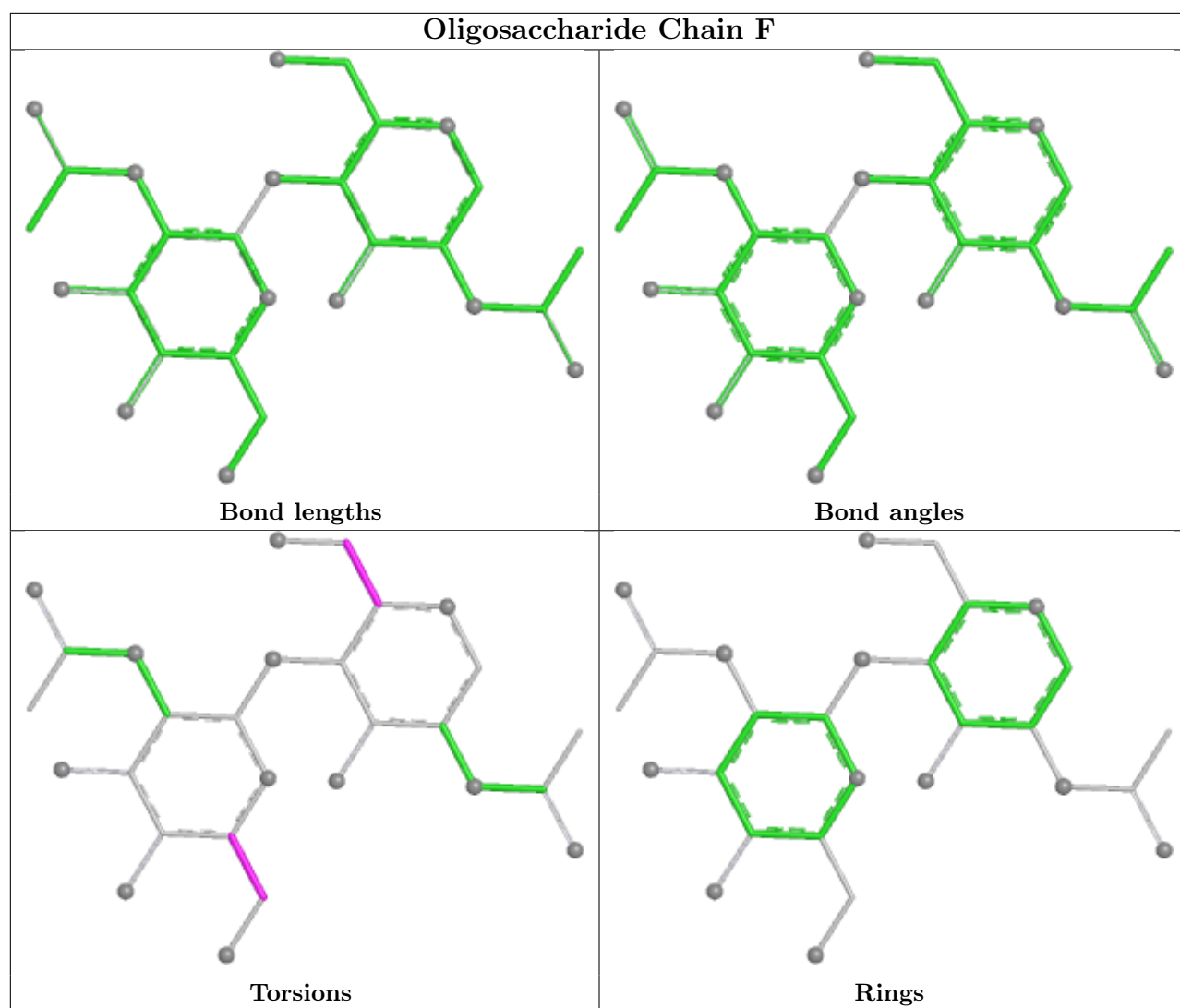
Mol	Chain	Res	Type	Atoms
3	d	1	NAG	C8-C7-N2-C2
3	d	1	NAG	O7-C7-N2-C2
3	d	2	NAG	C3-C2-N2-C7
3	d	2	NAG	C8-C7-N2-C2
3	d	2	NAG	O7-C7-N2-C2

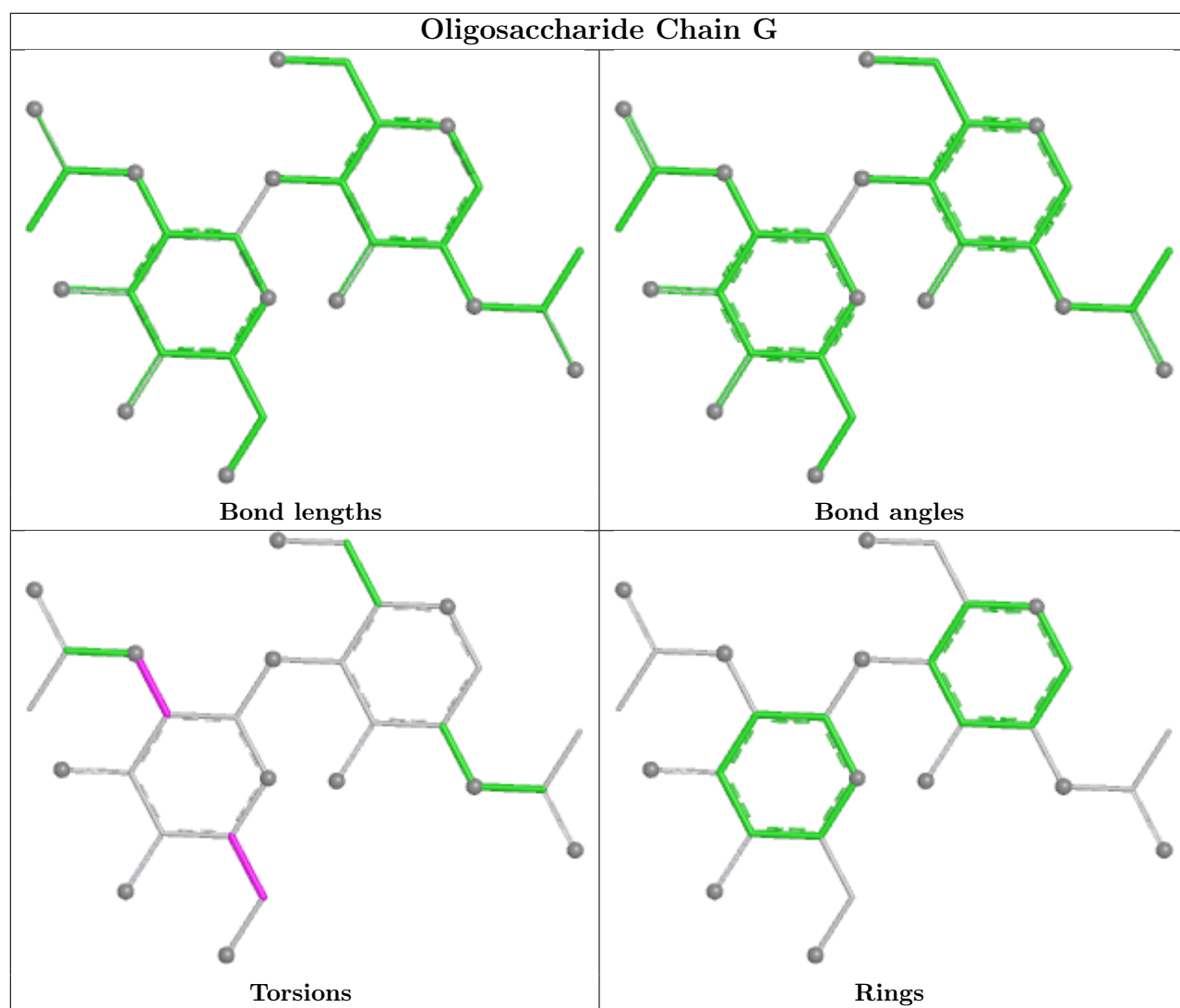
There are no ring outliers.

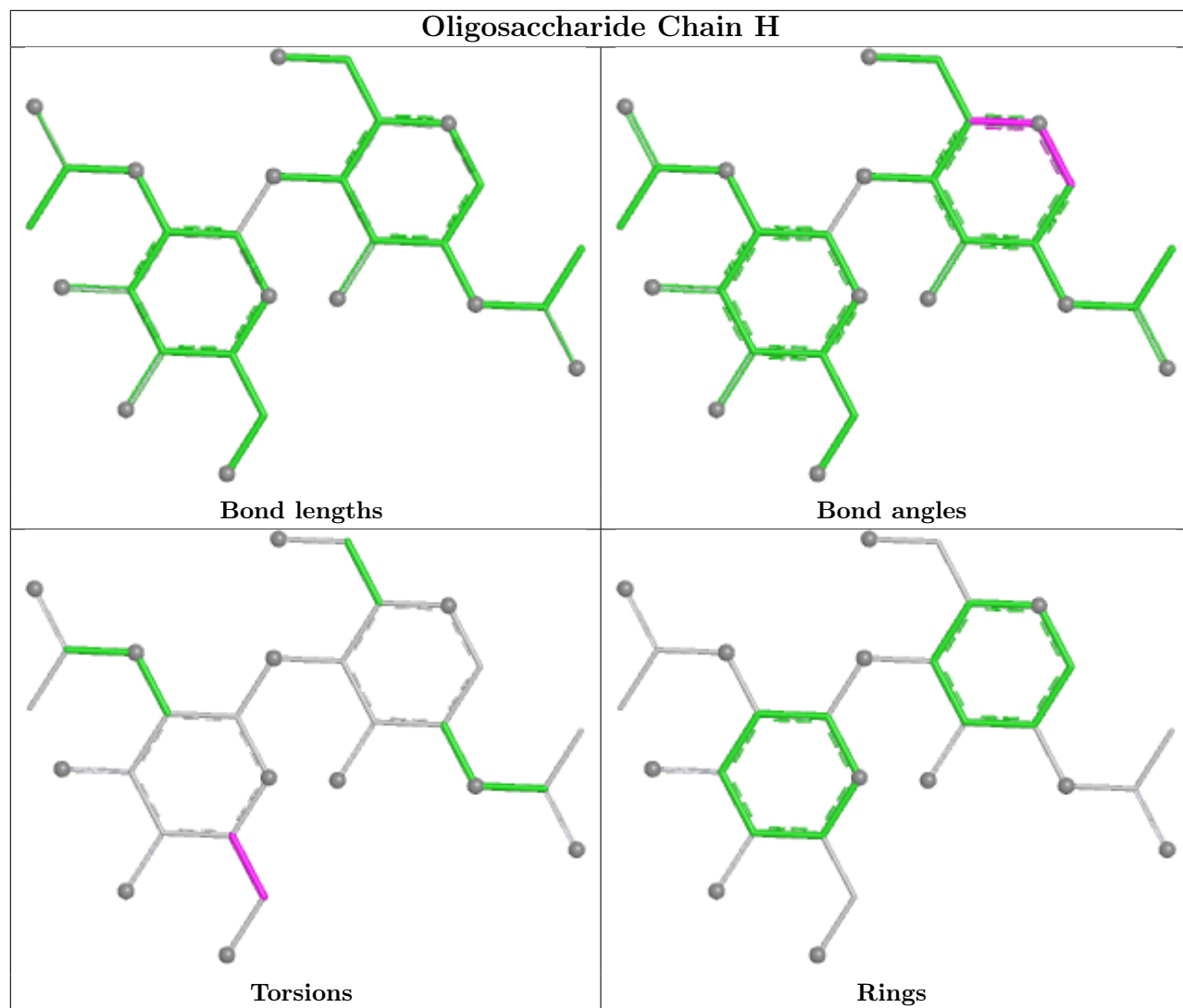
19 monomers are involved in 30 short contacts:

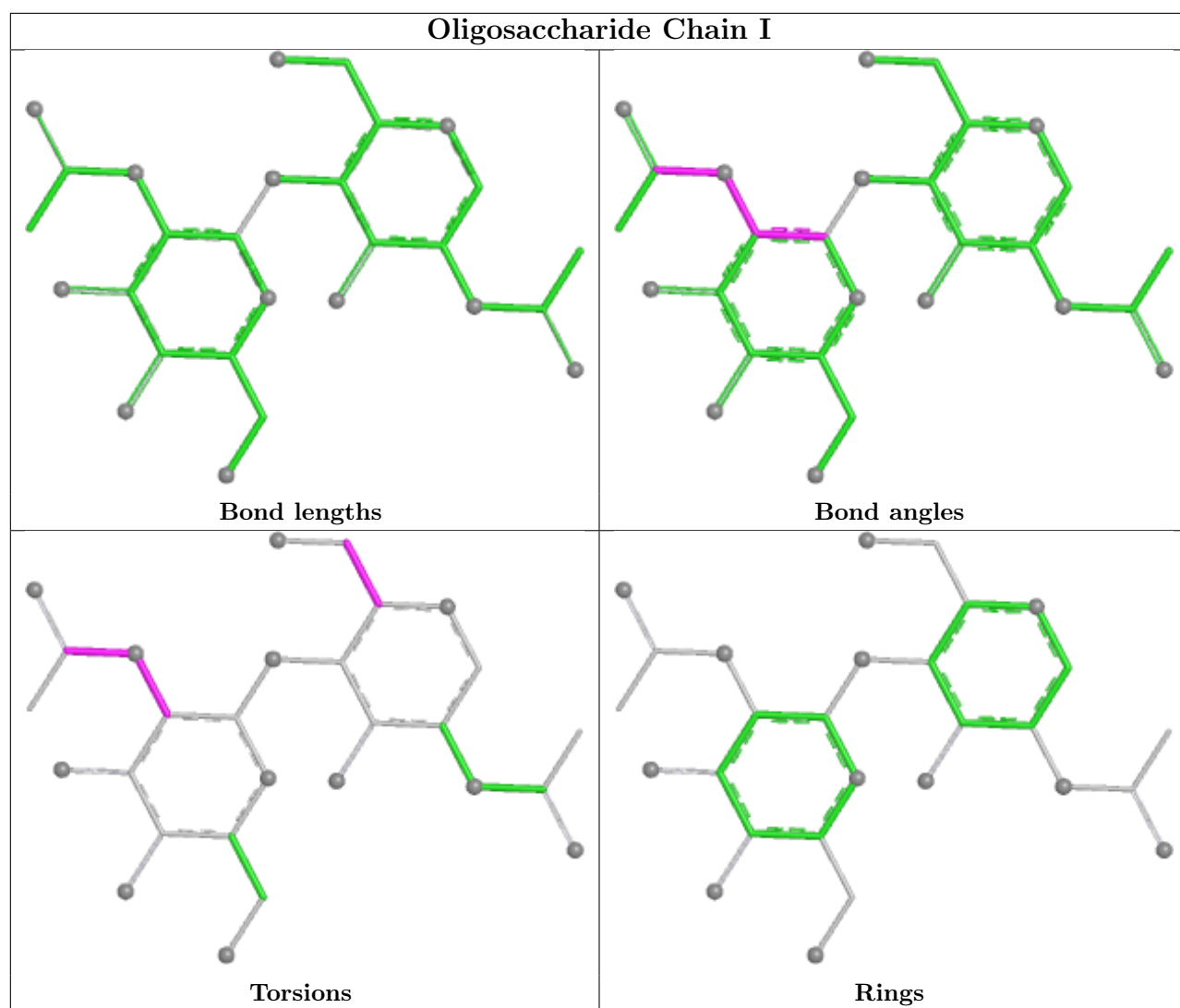
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	U	2	NAG	2	0
3	N	2	NAG	2	0
3	G	1	NAG	3	0
3	J	2	NAG	1	0
3	I	2	NAG	1	0
3	G	2	NAG	2	0
3	M	1	NAG	2	0
3	U	1	NAG	4	0
3	V	1	NAG	1	0
3	R	1	NAG	1	0
3	d	1	NAG	4	0
3	i	1	NAG	4	0
3	R	2	NAG	1	0
3	i	2	NAG	5	0
3	Z	1	NAG	1	0
3	Z	2	NAG	1	0
3	Y	2	NAG	1	0
3	d	2	NAG	6	0
3	N	1	NAG	3	0

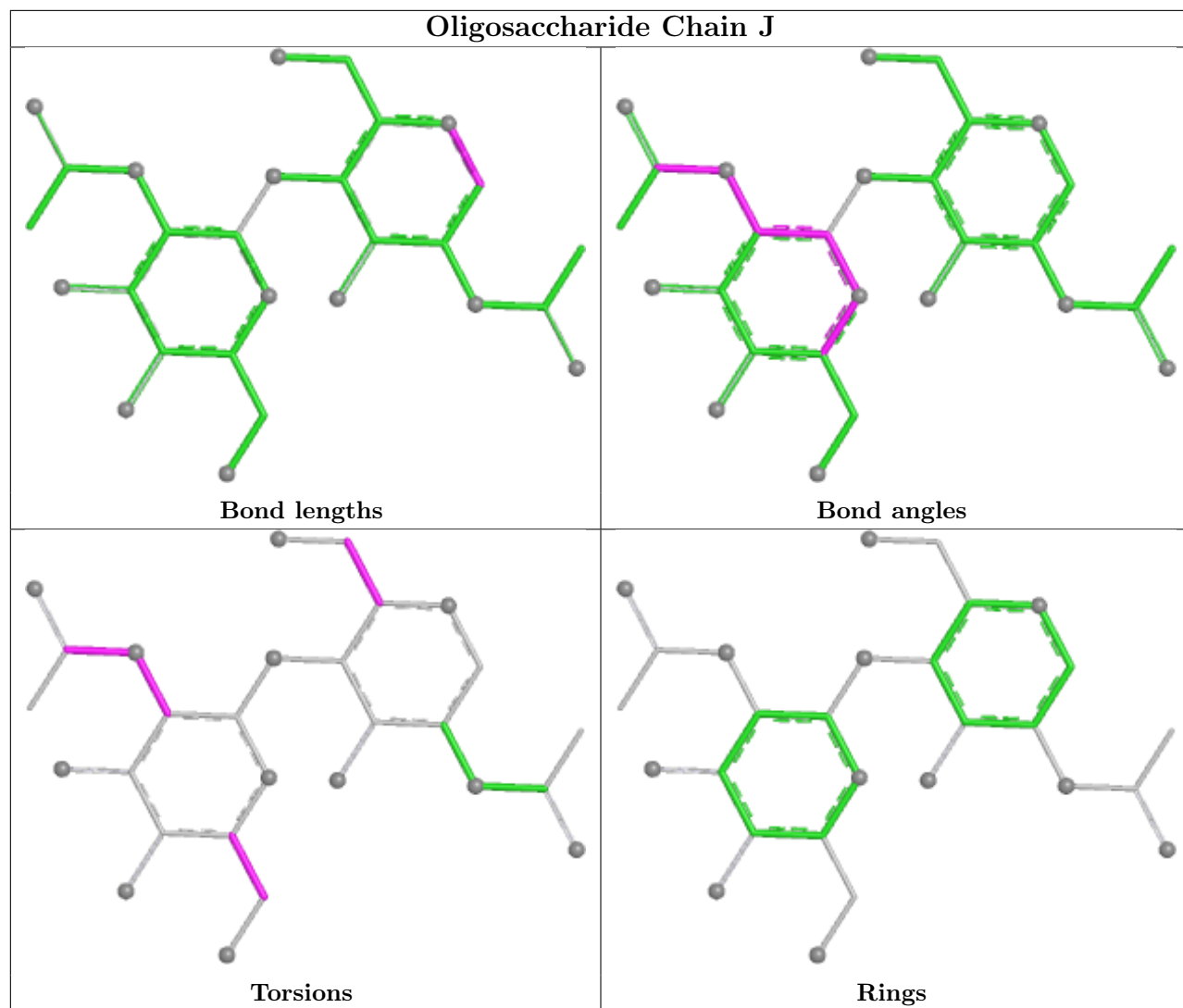
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

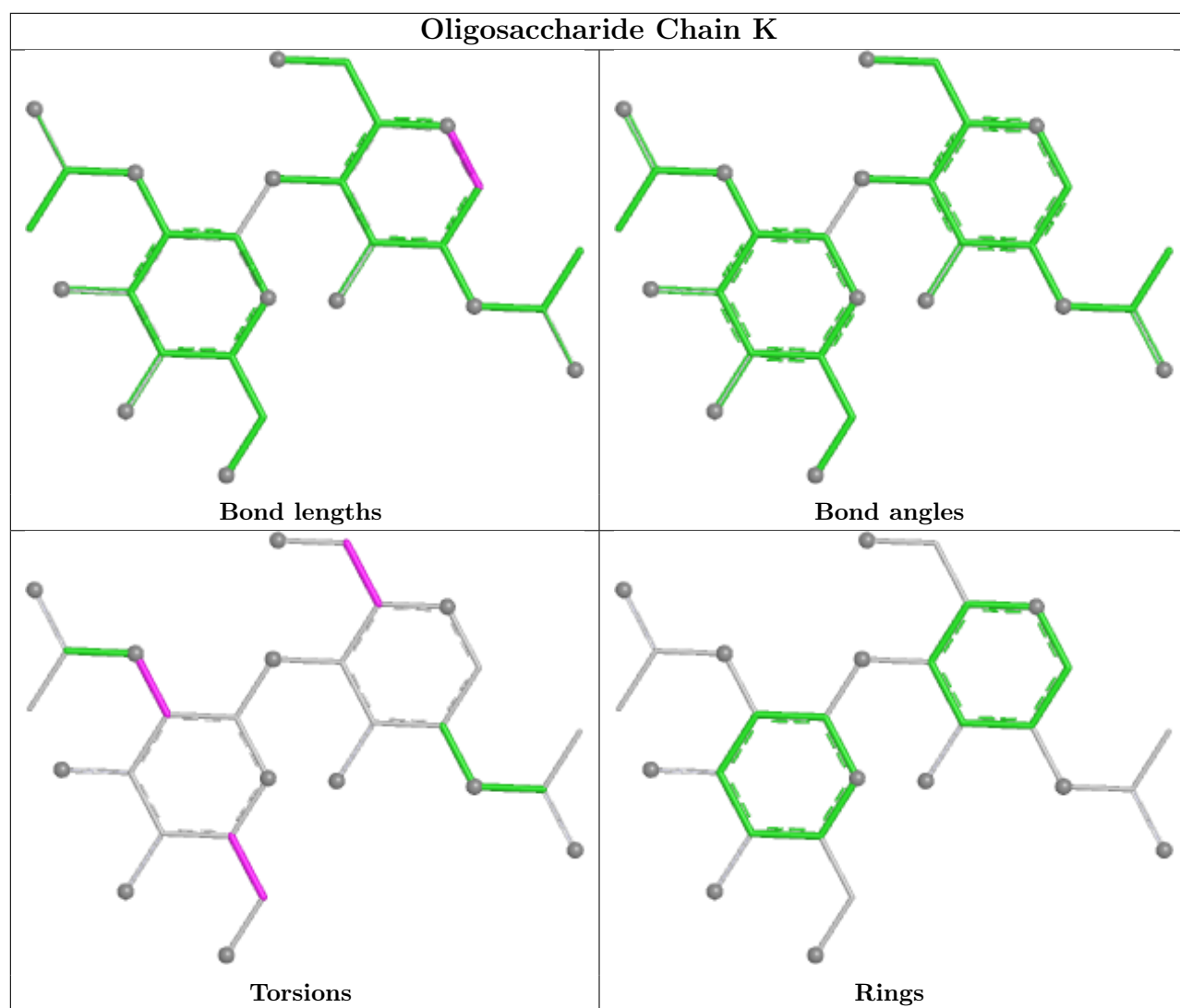


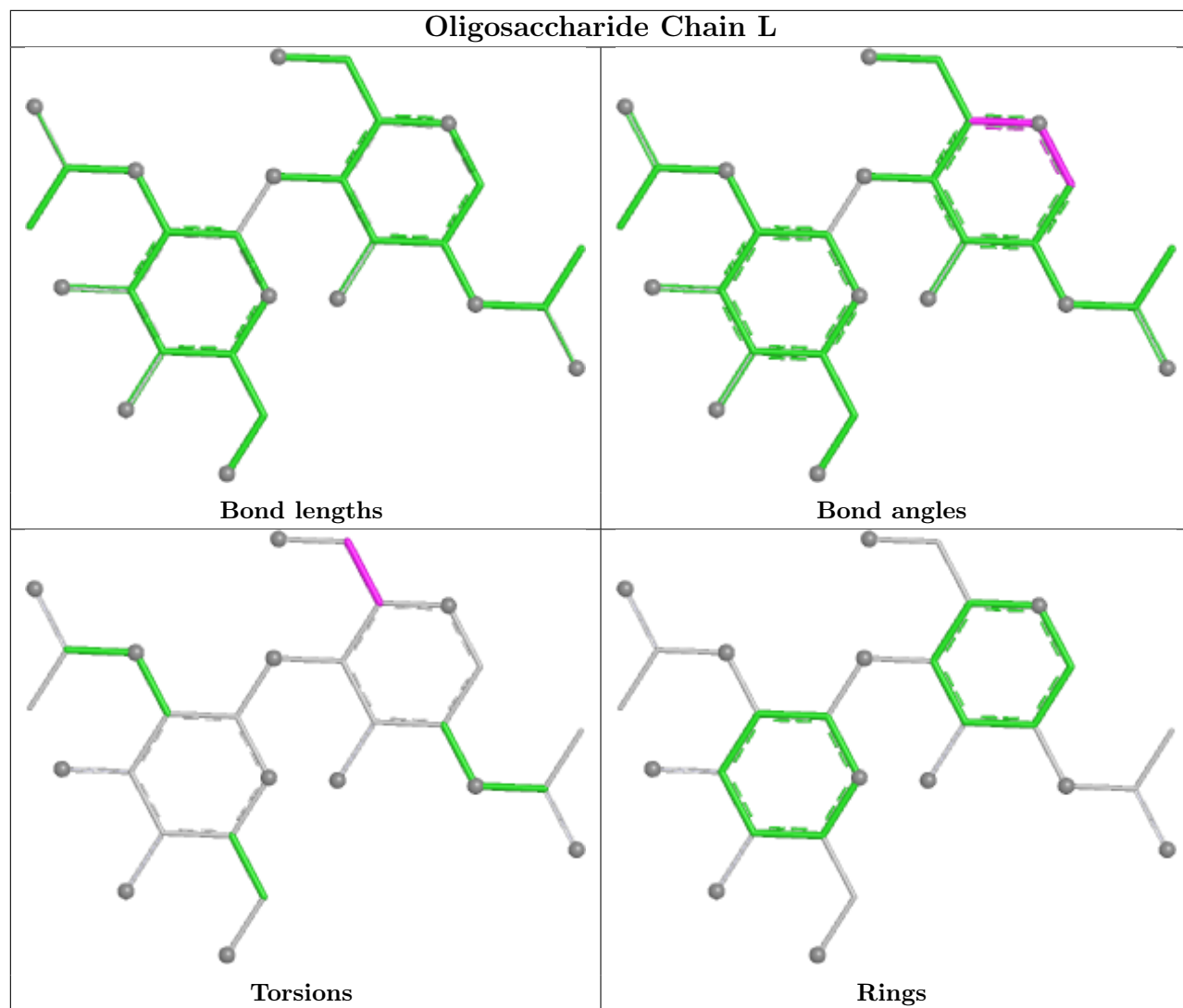


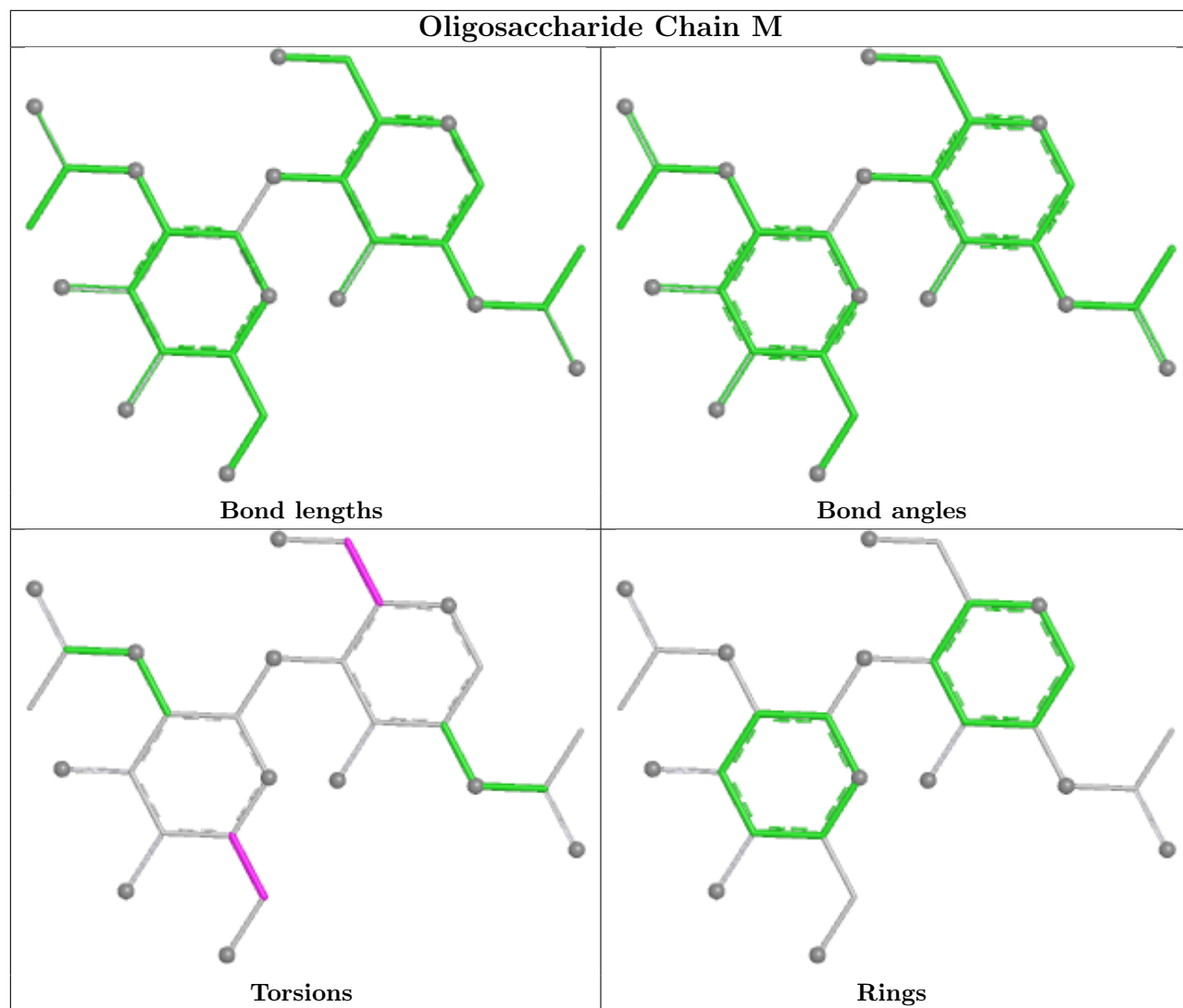


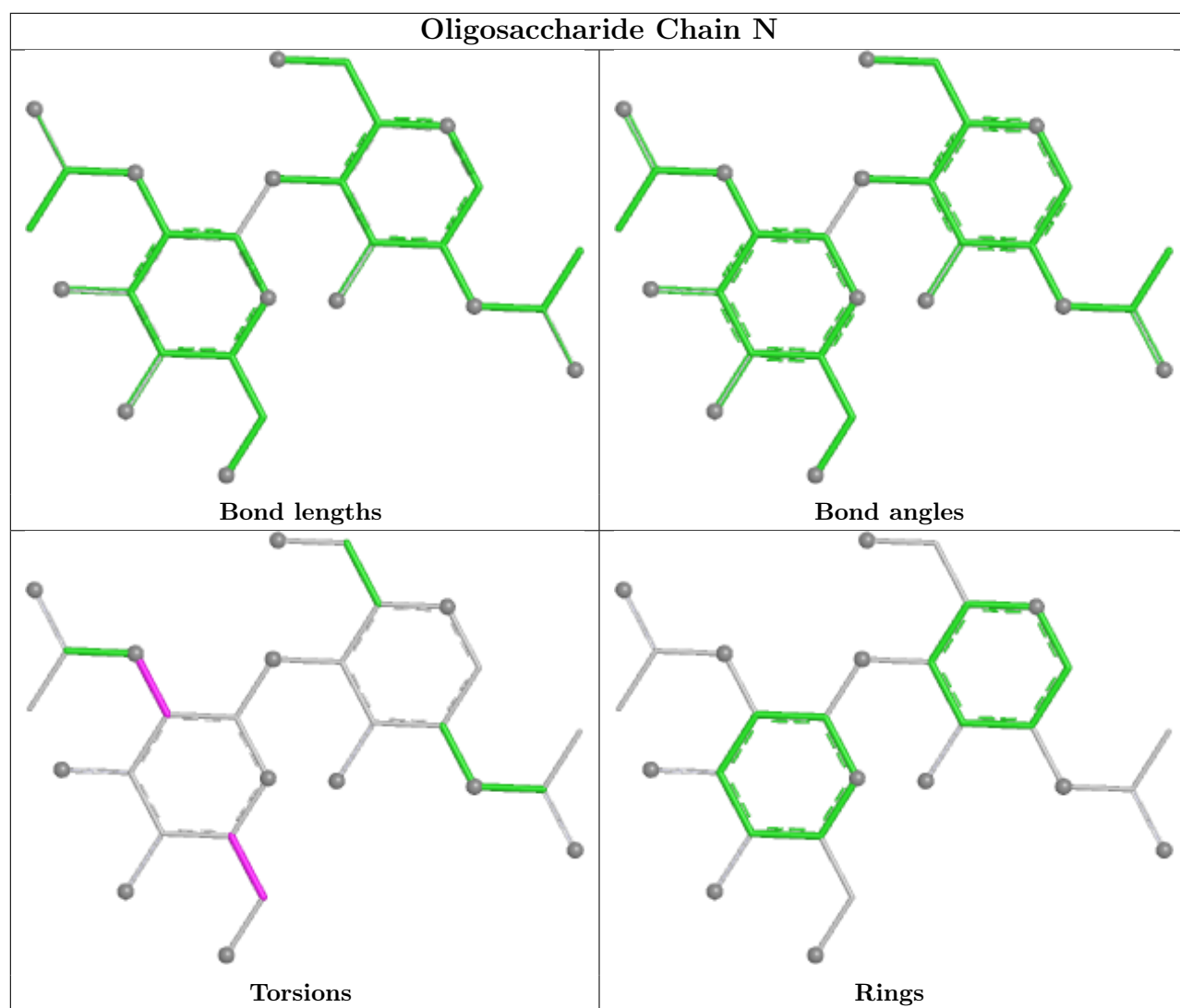


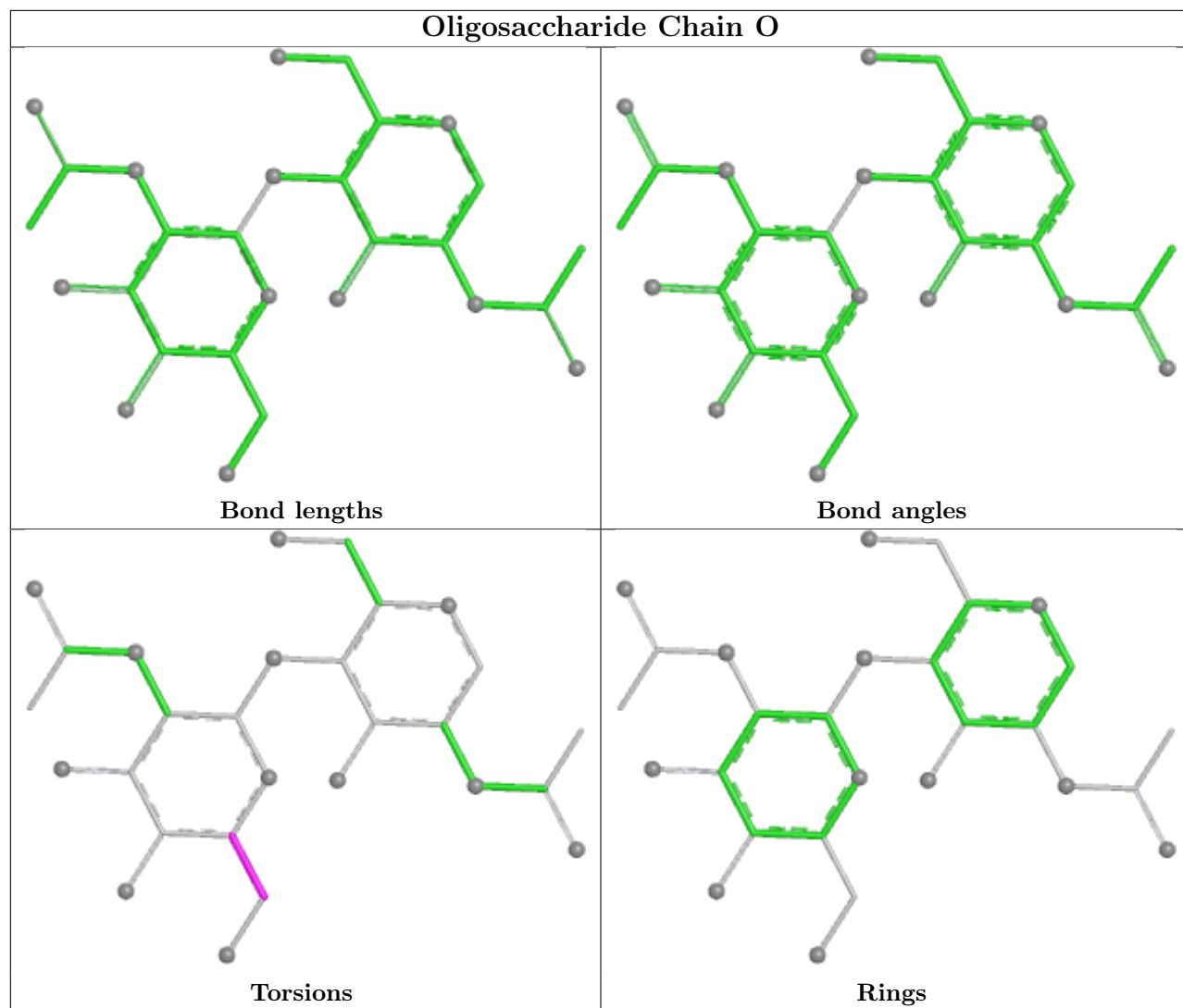


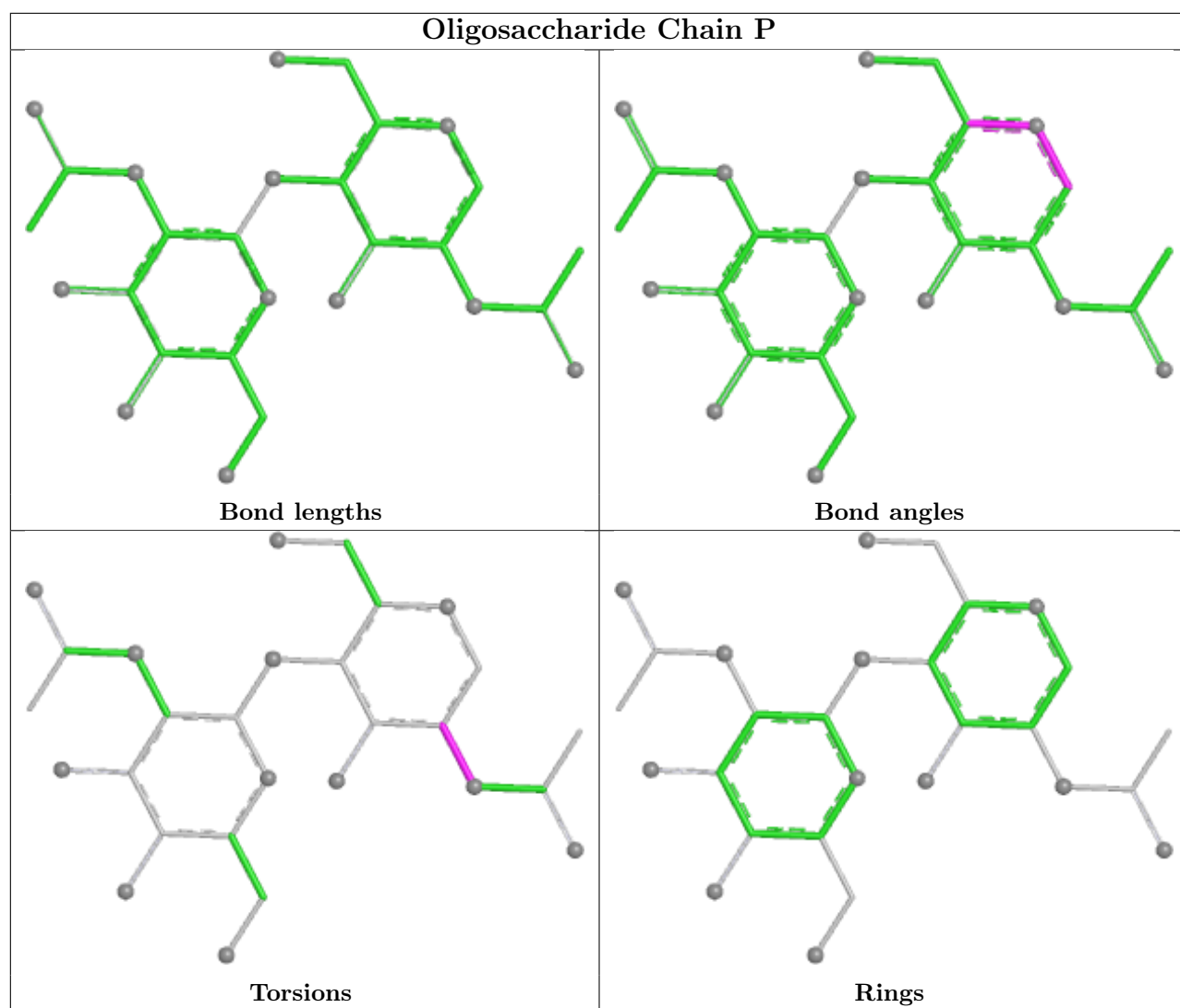


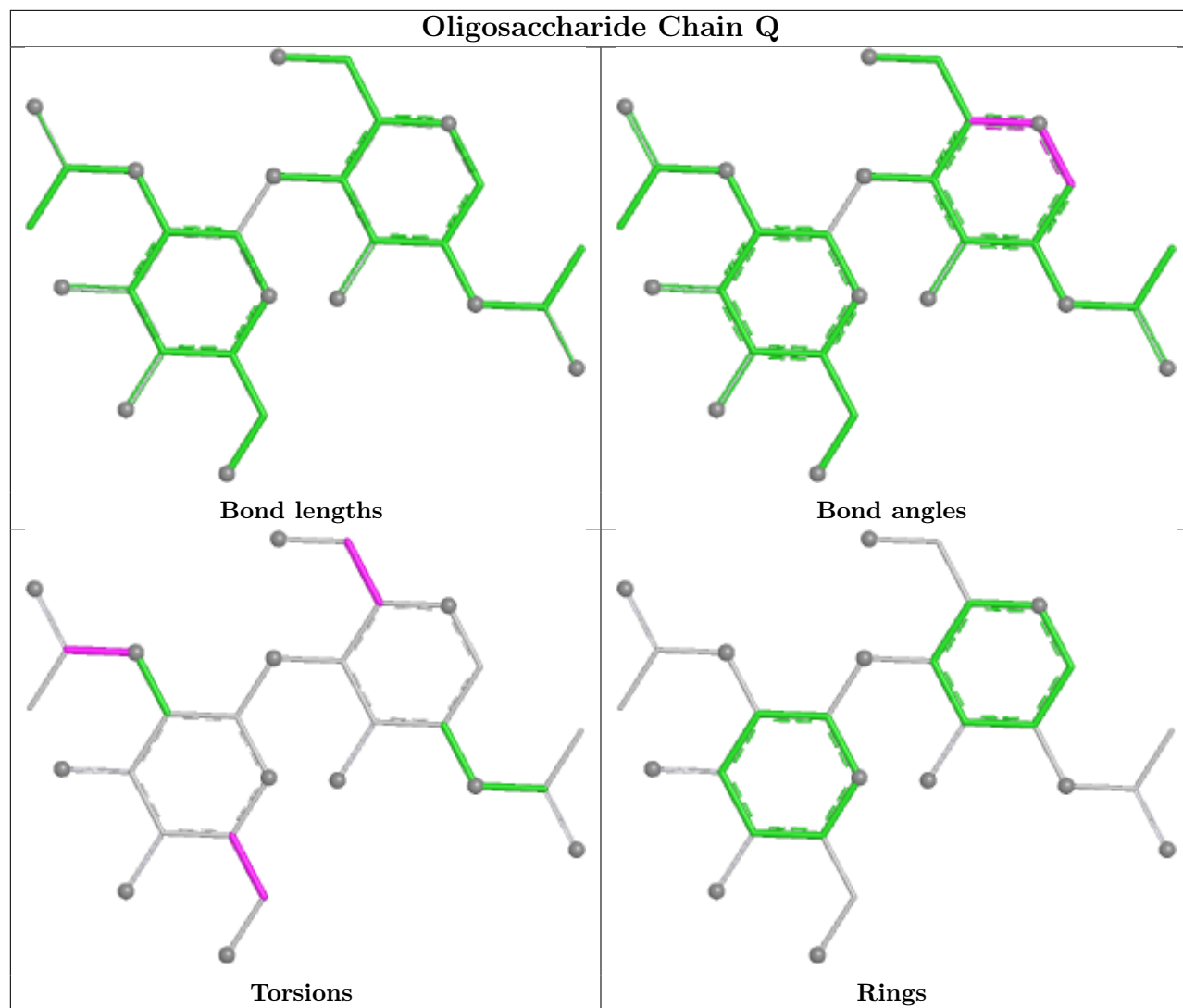


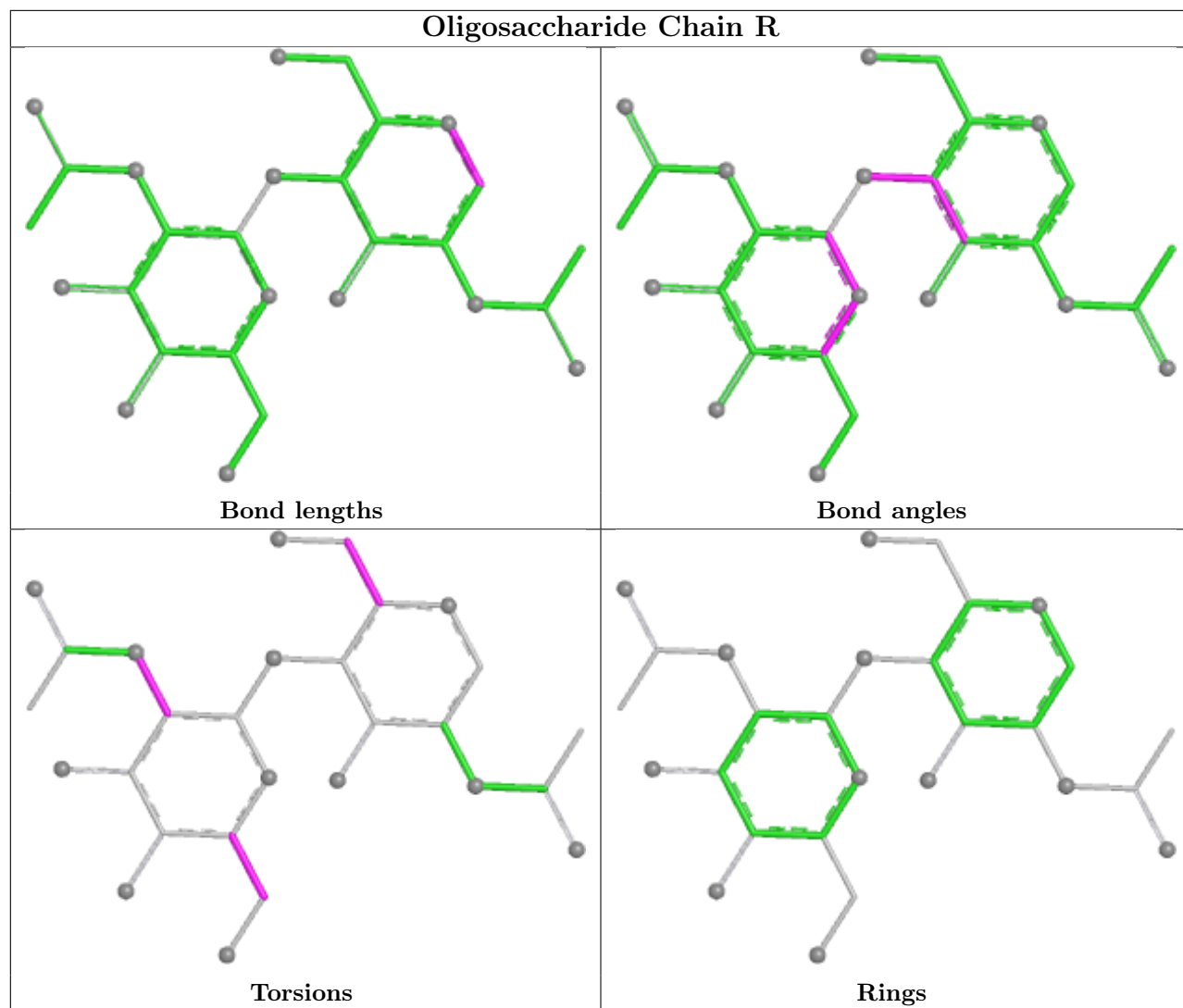


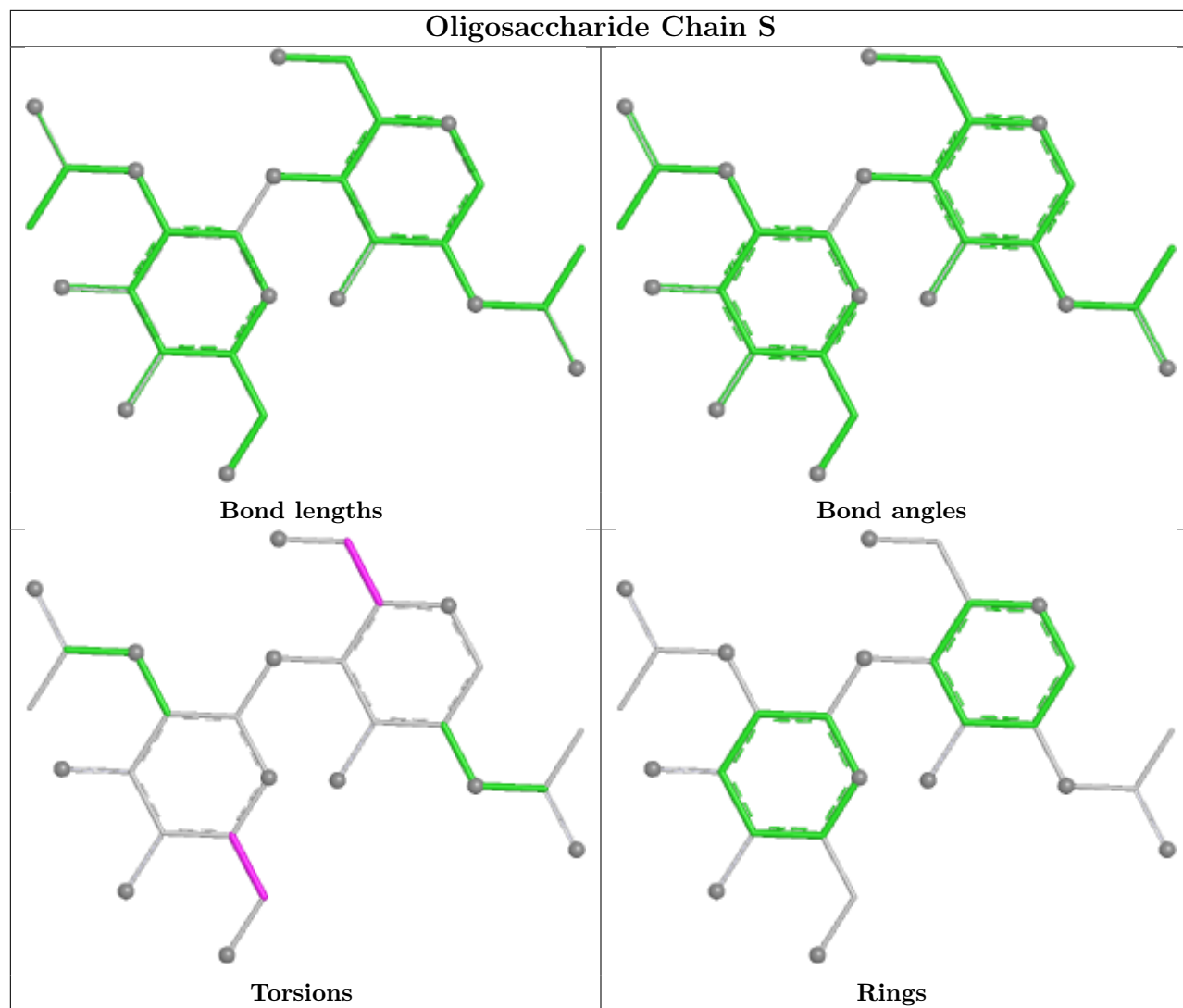


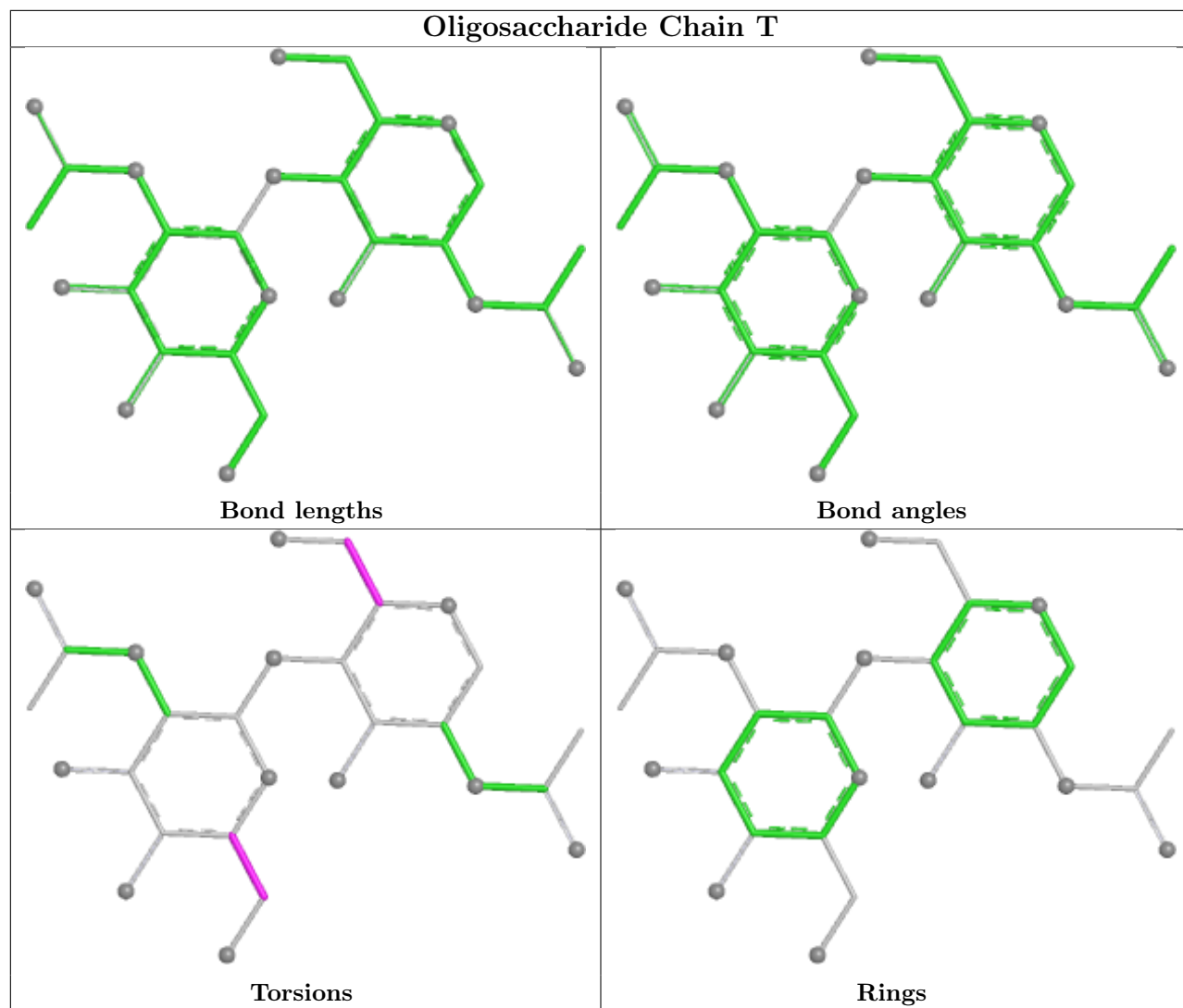


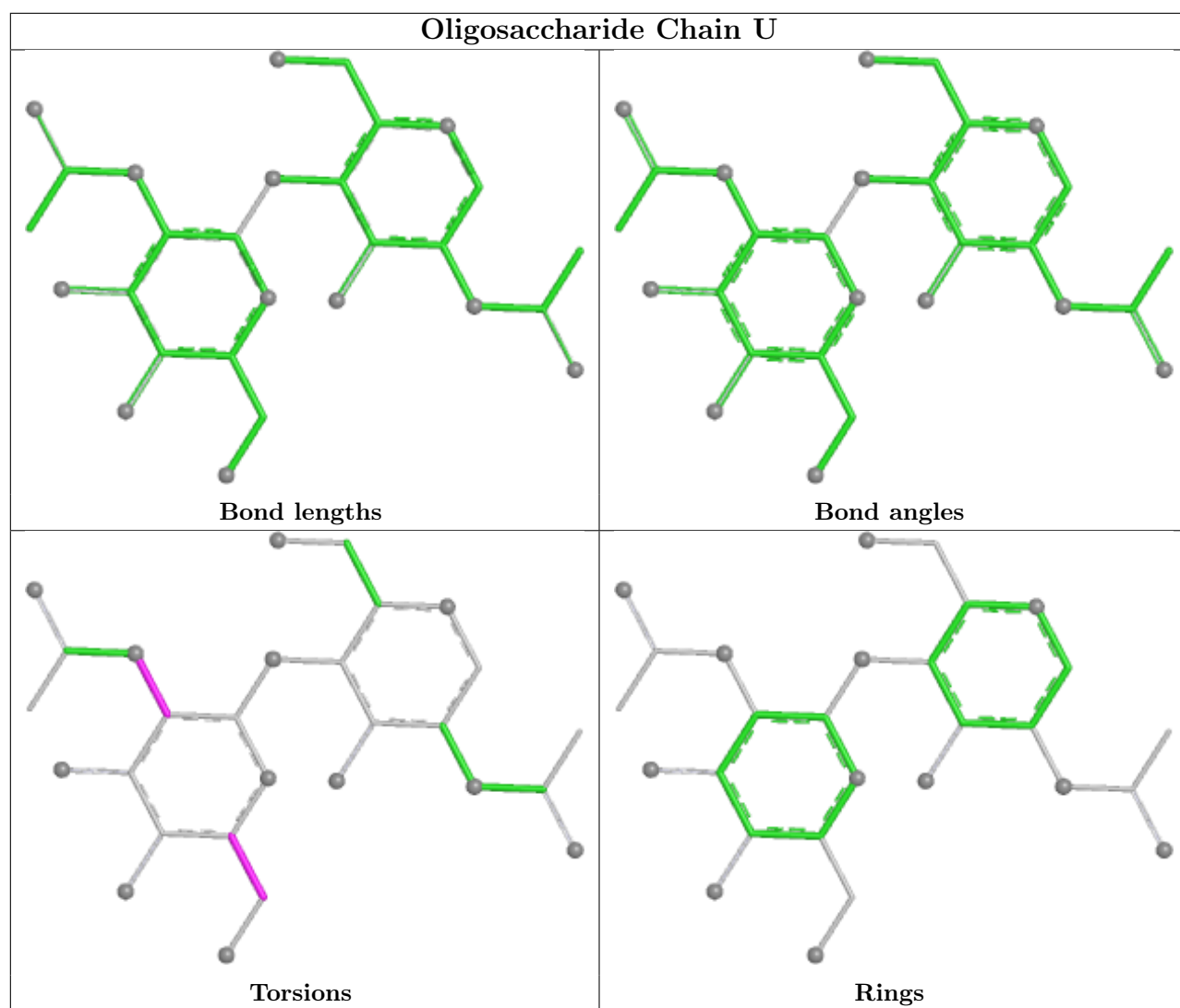


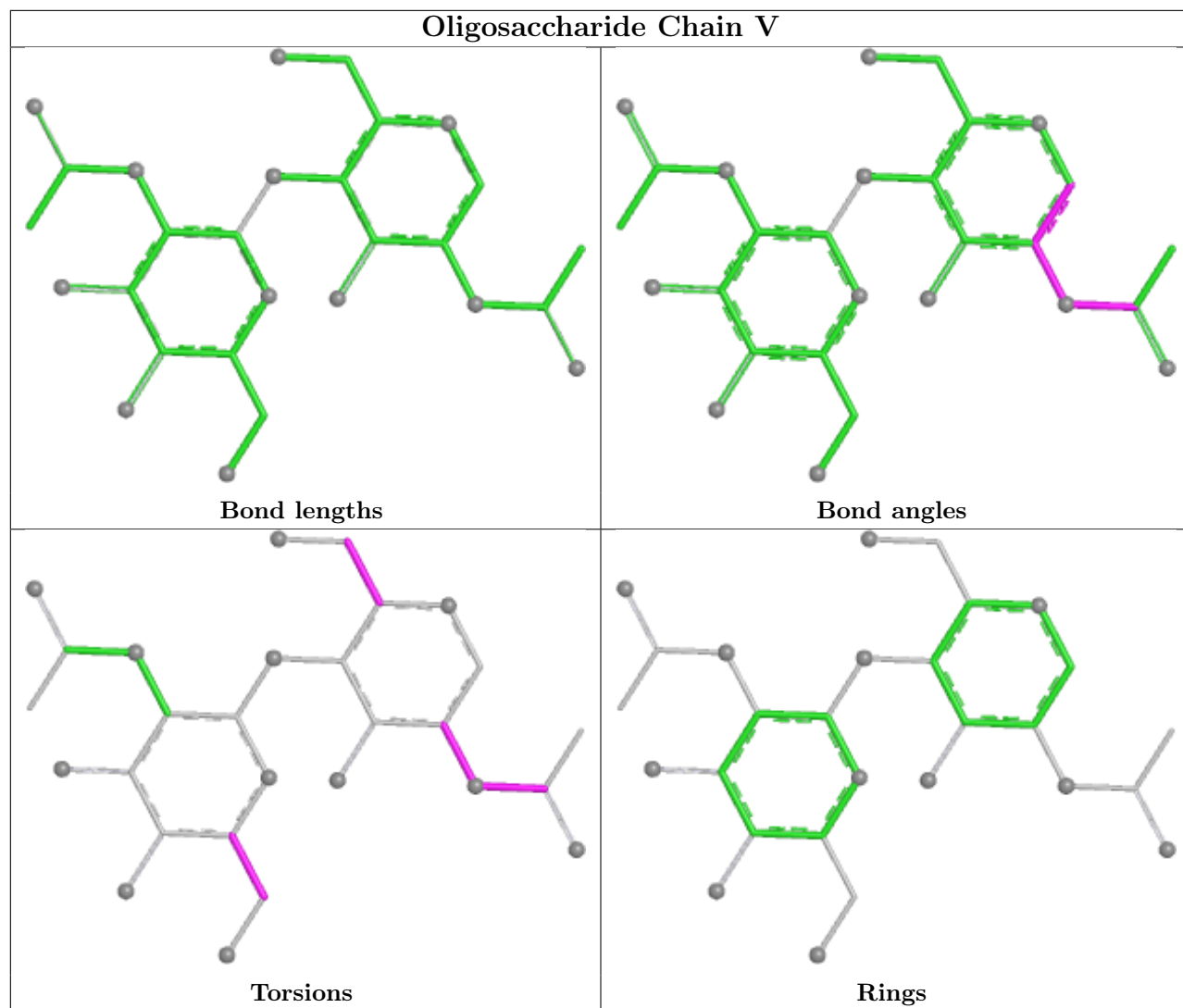


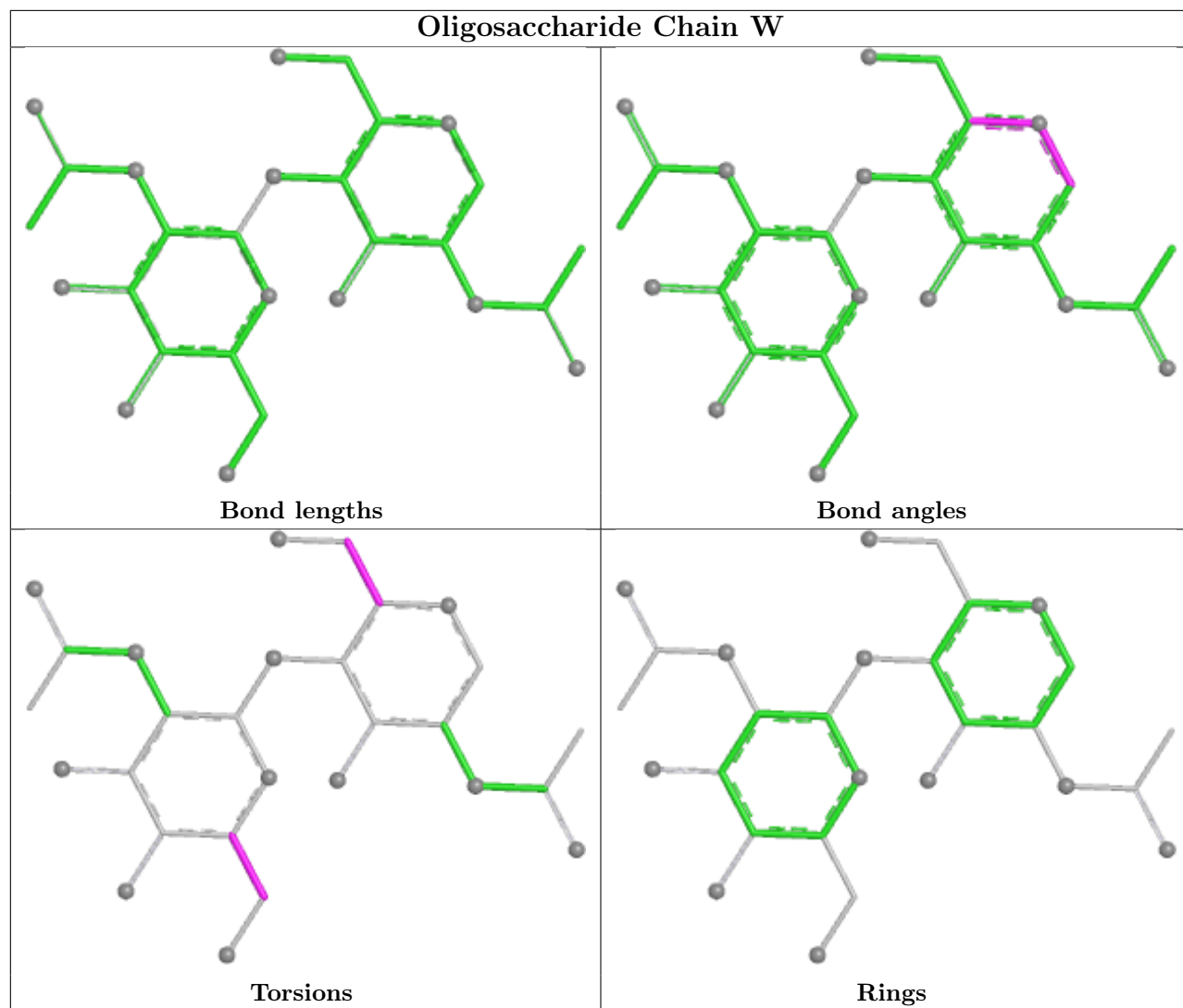


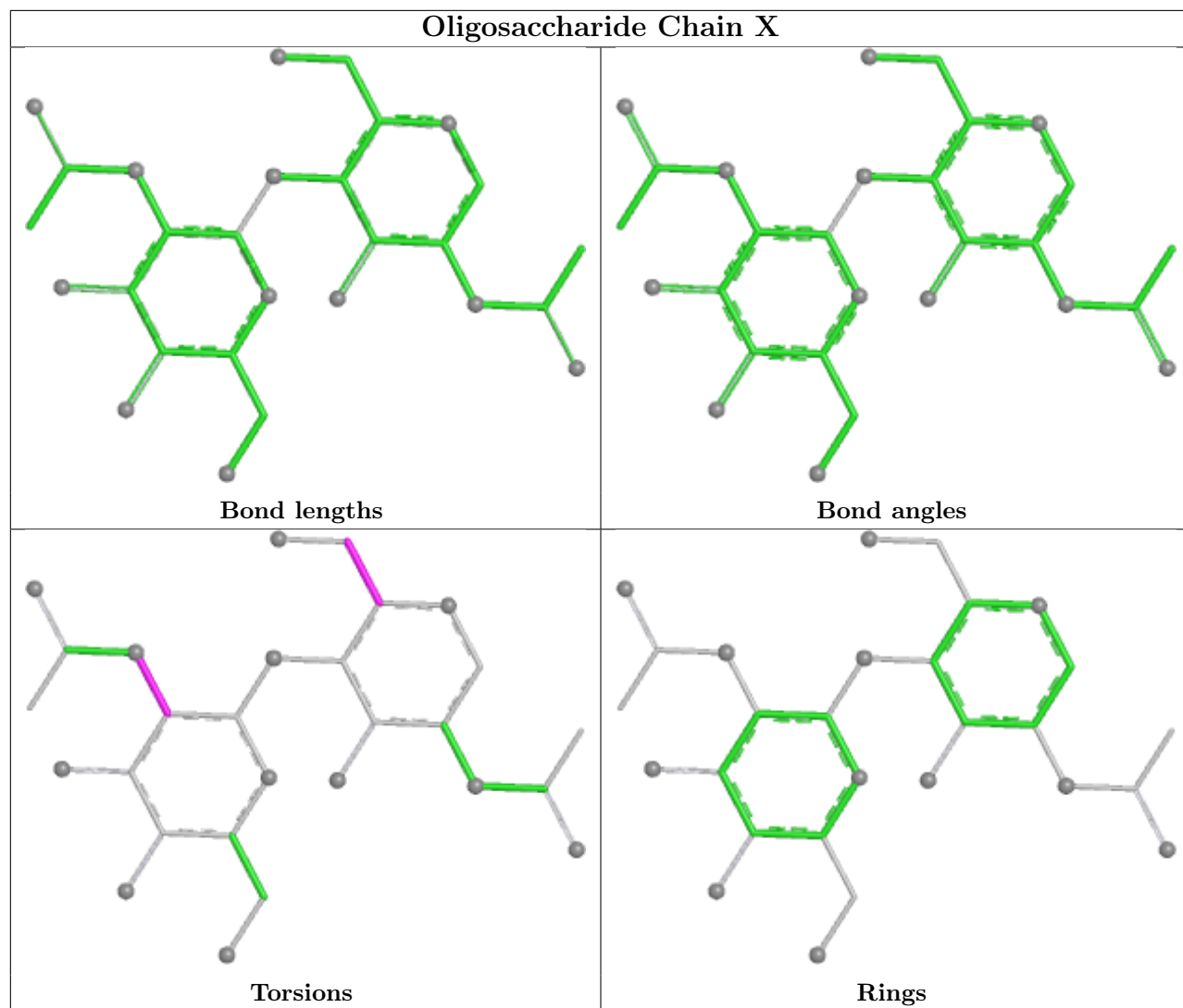


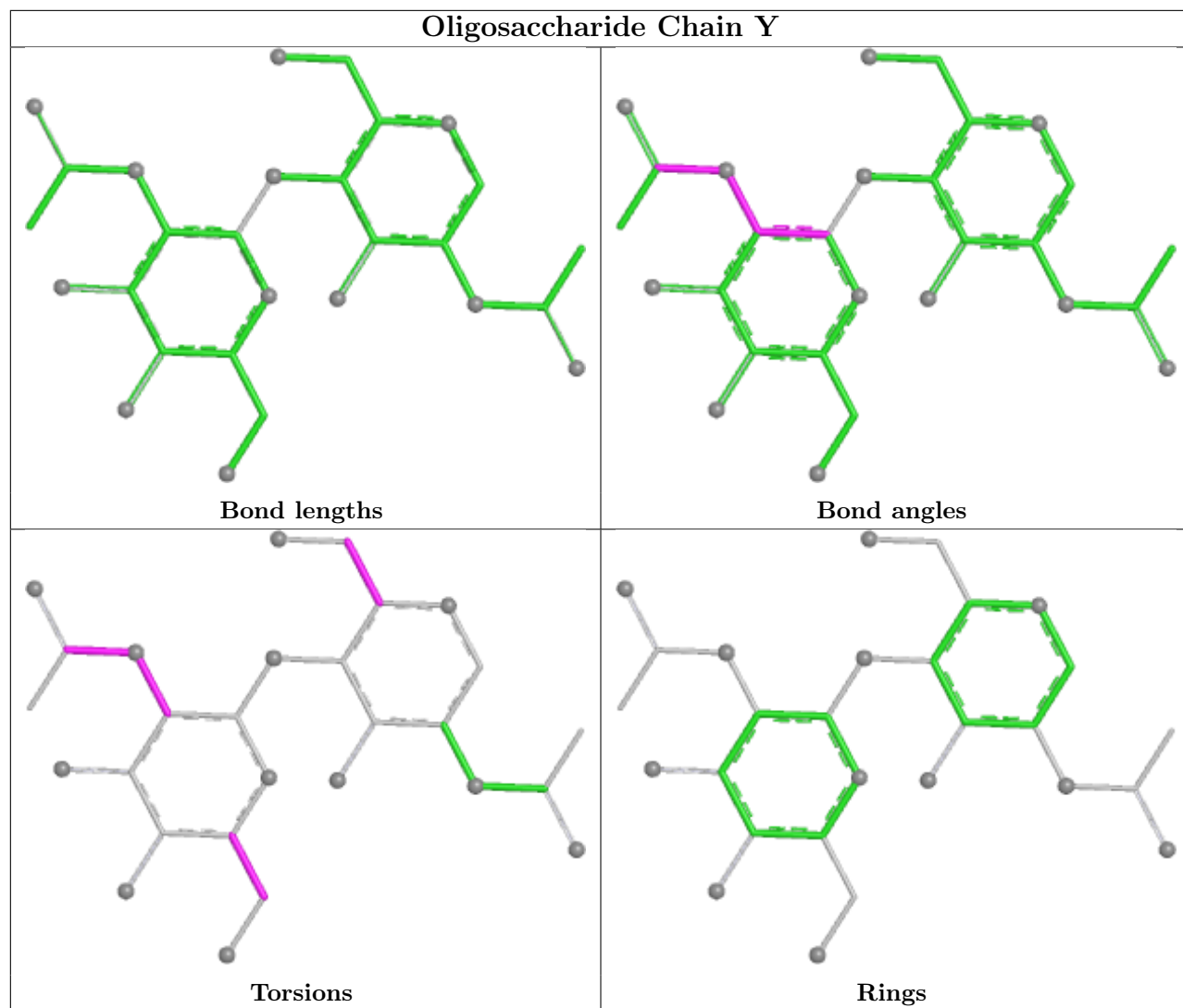


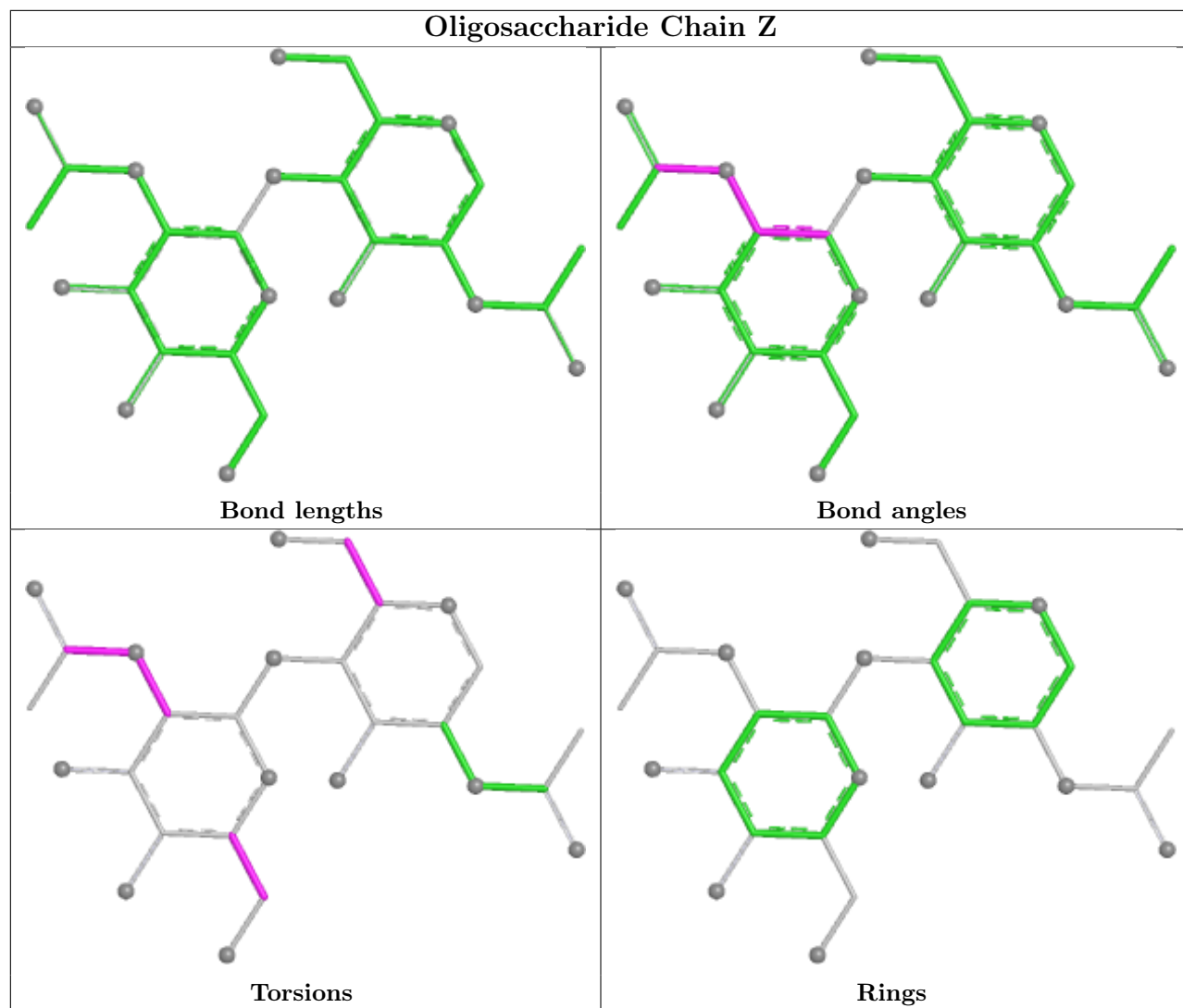


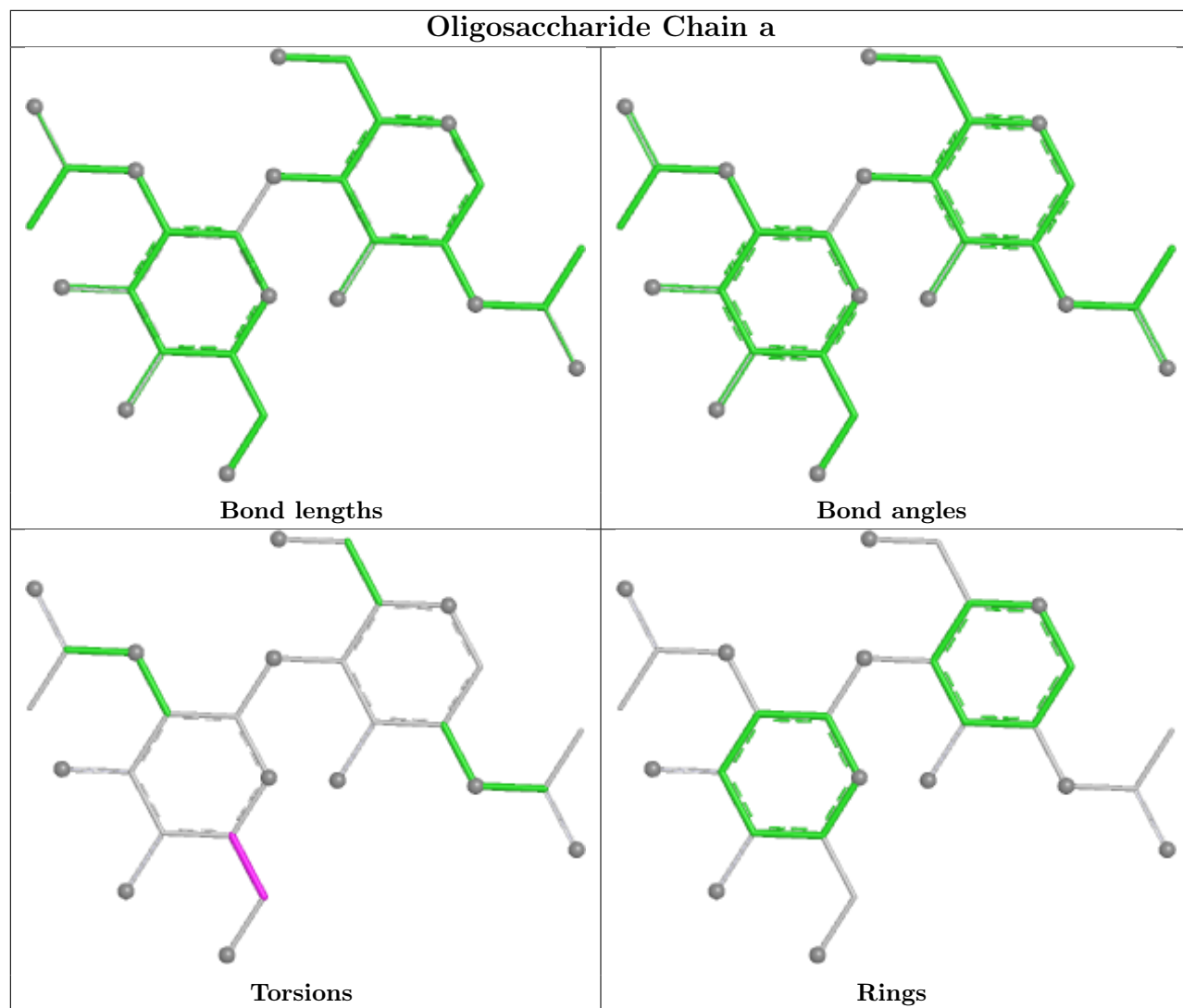


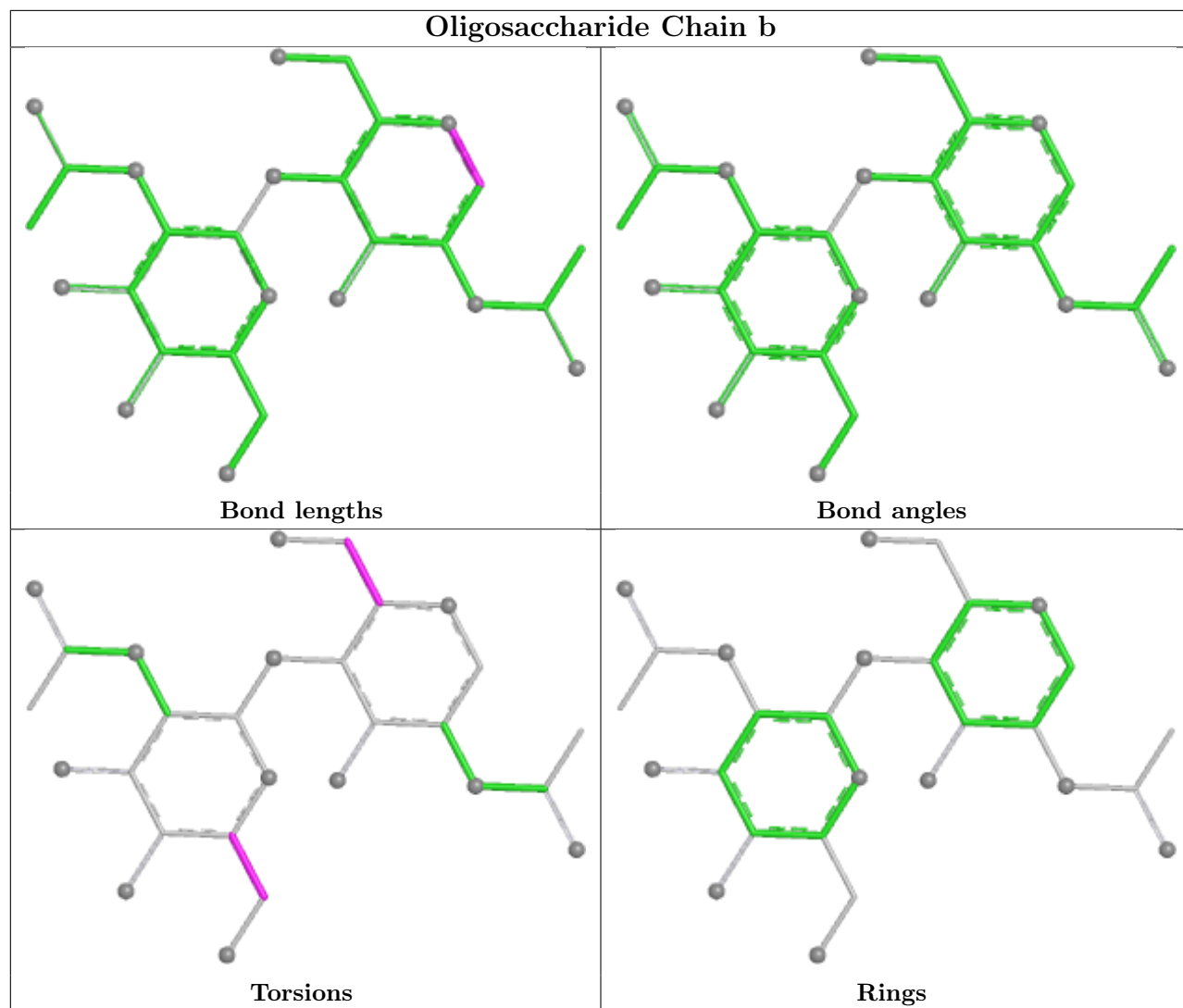


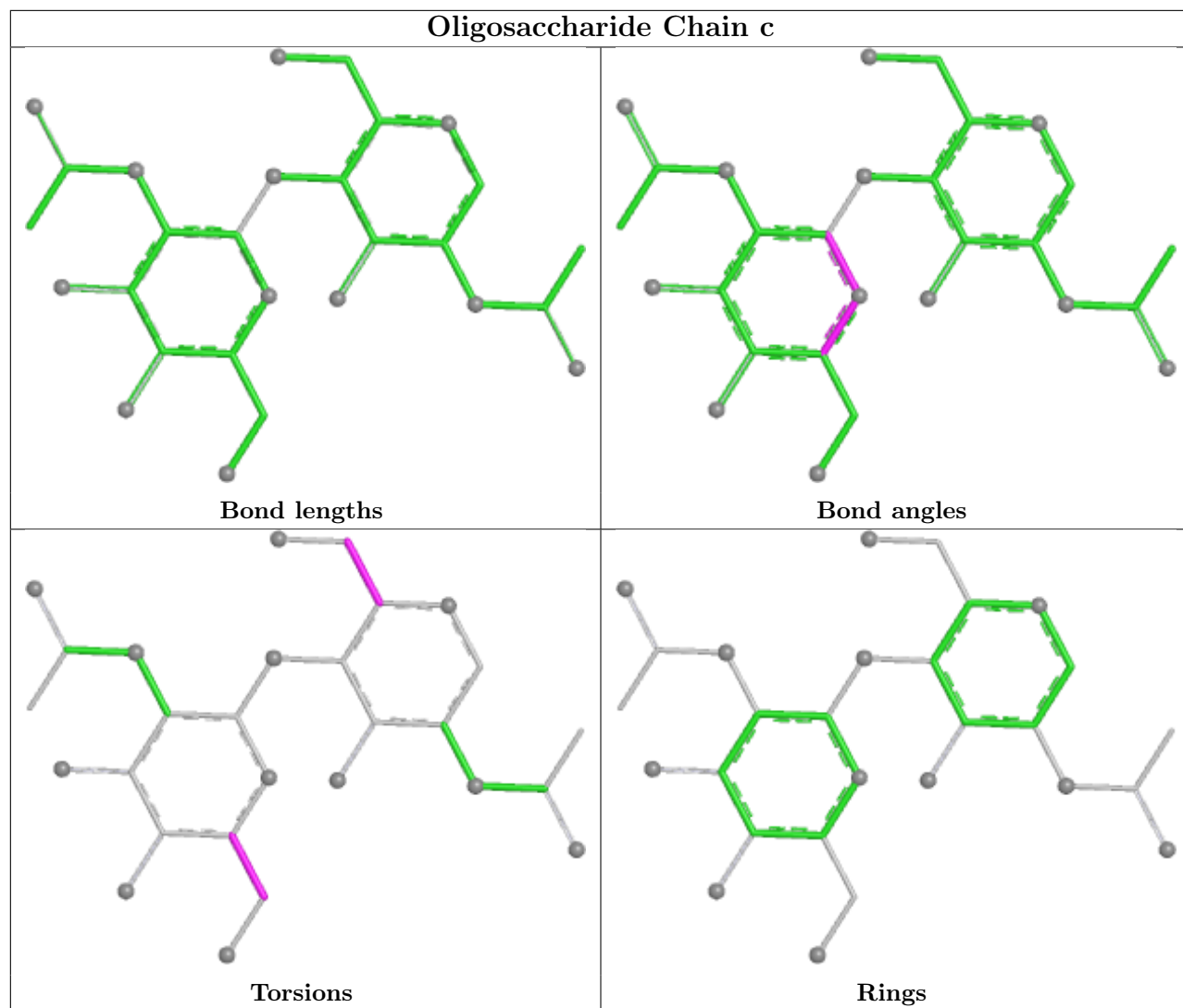


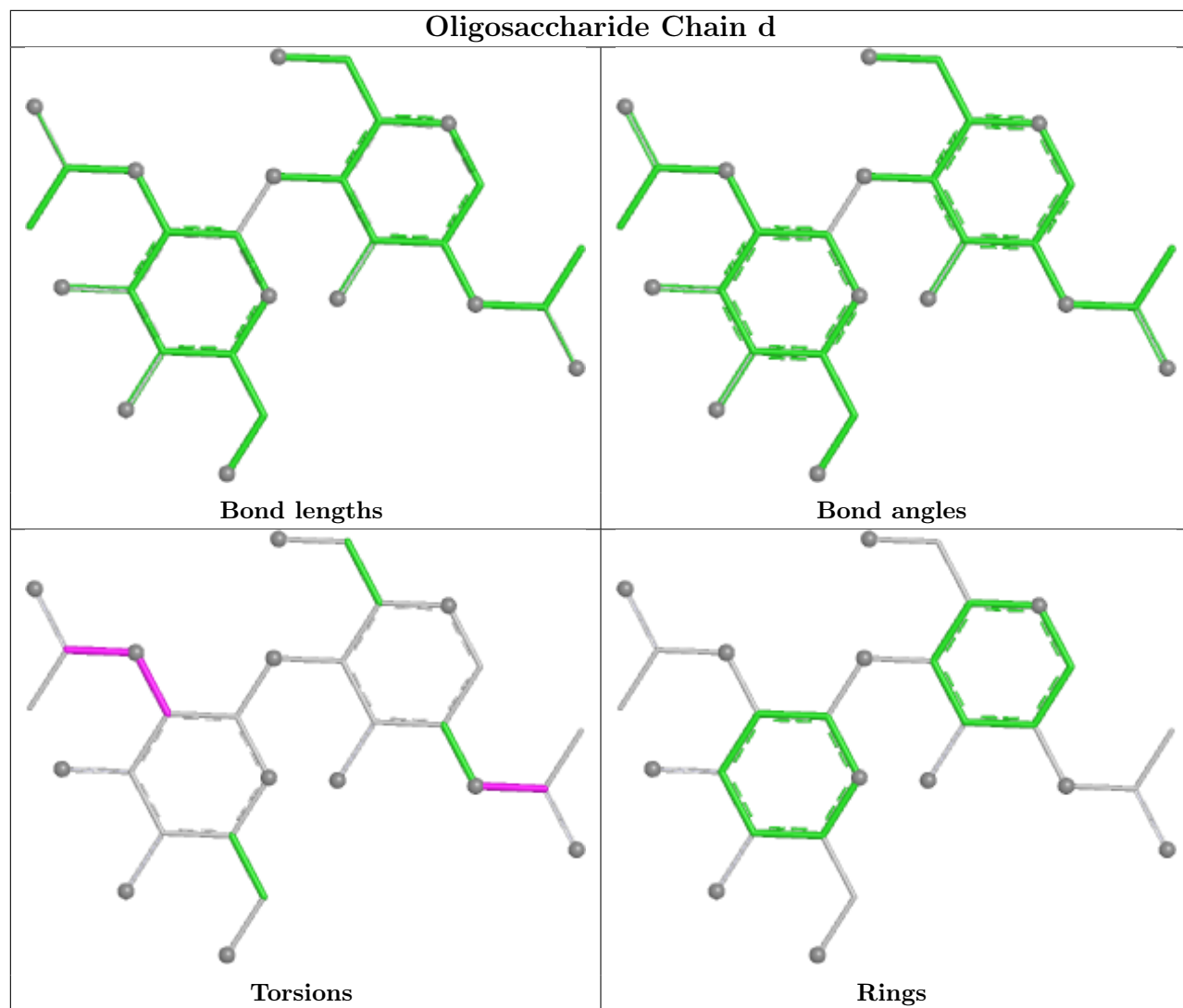


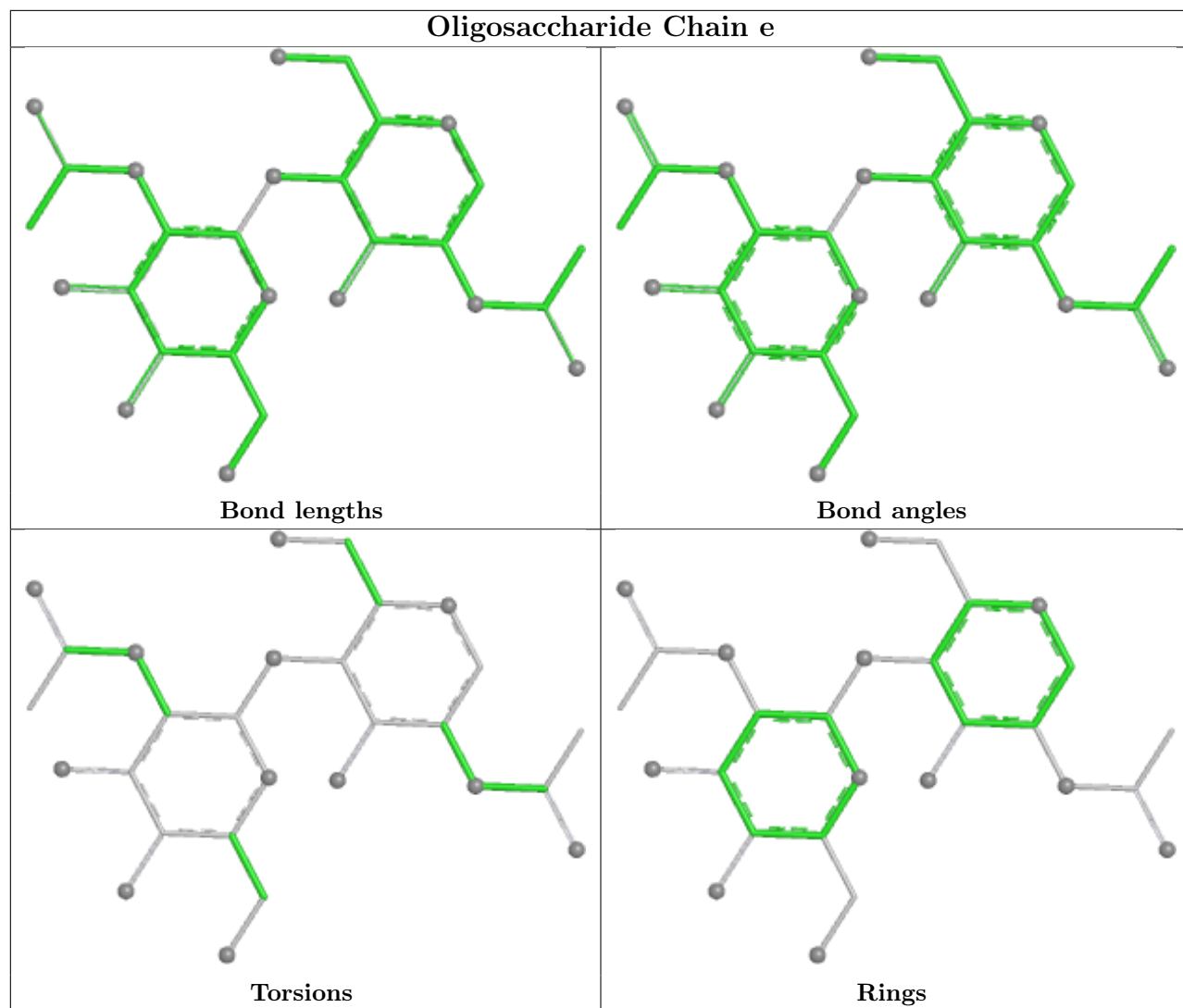


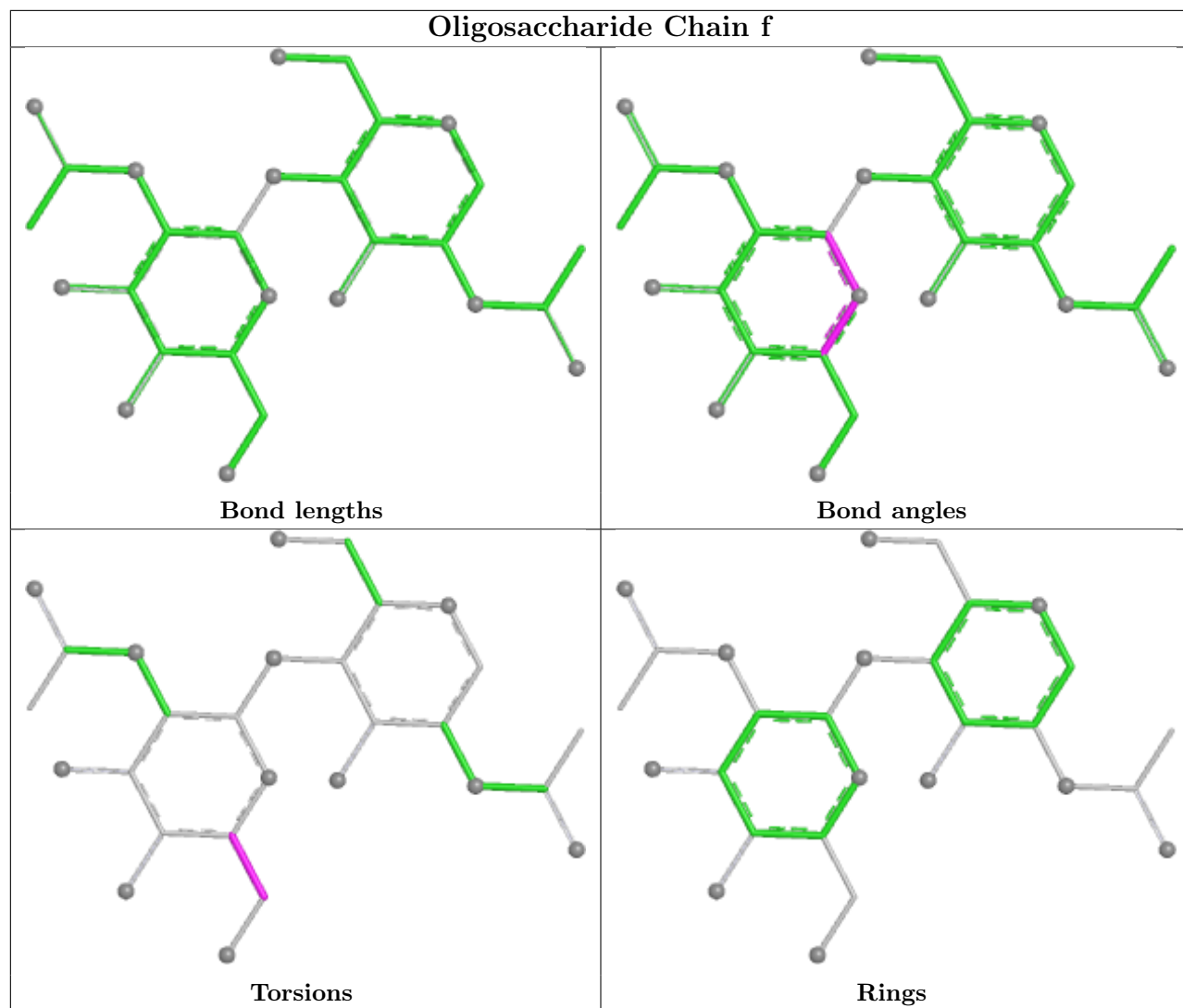


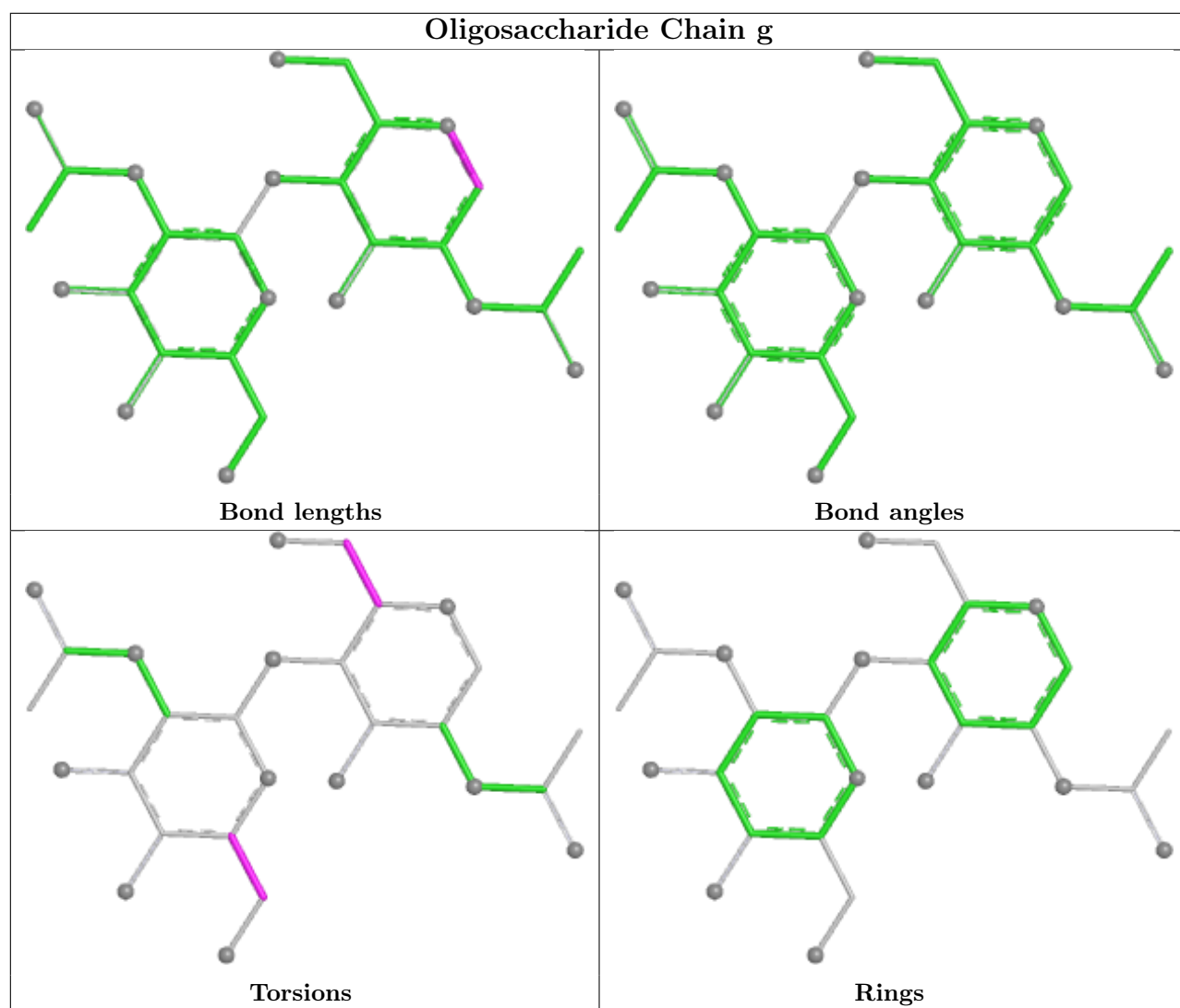


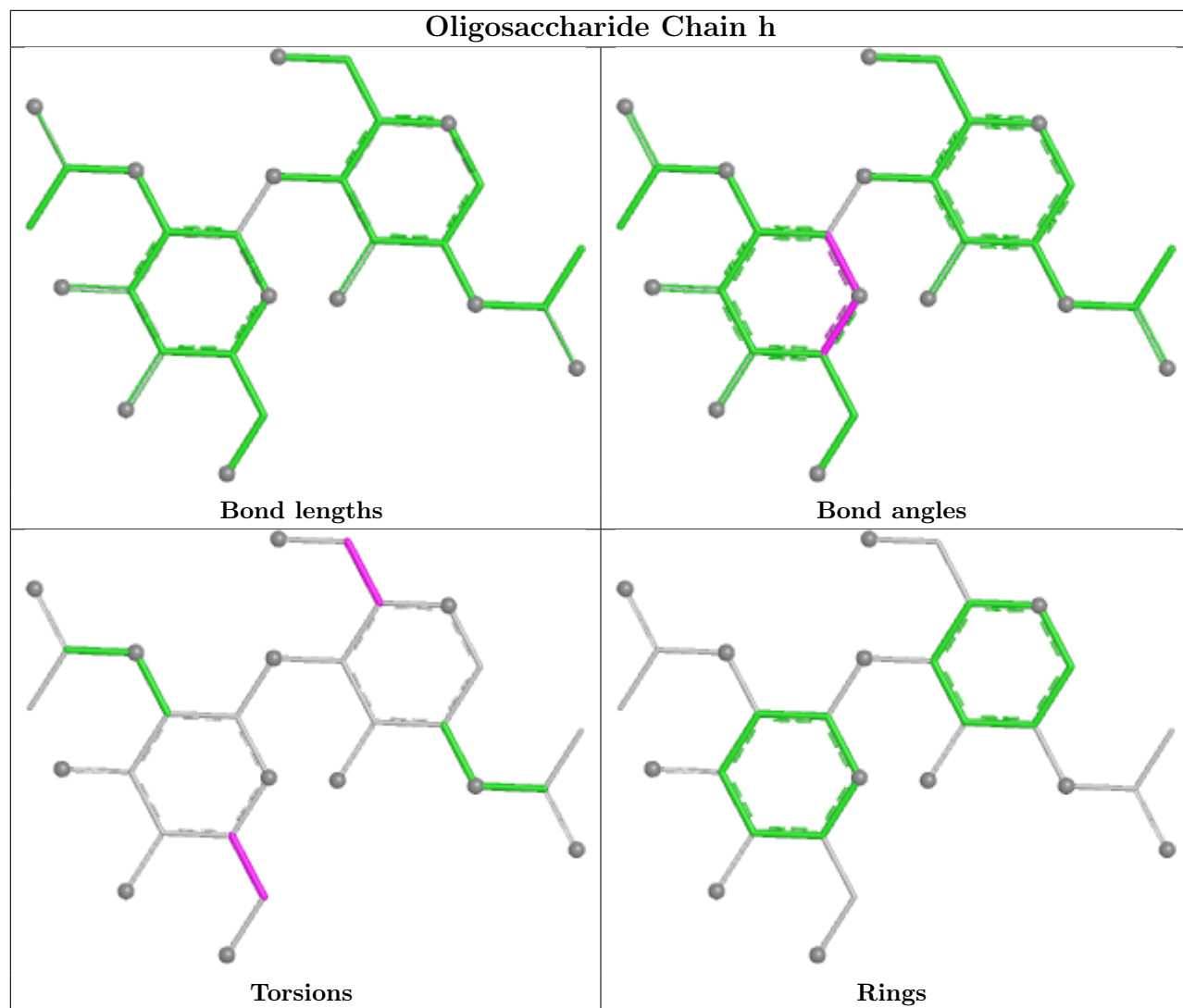


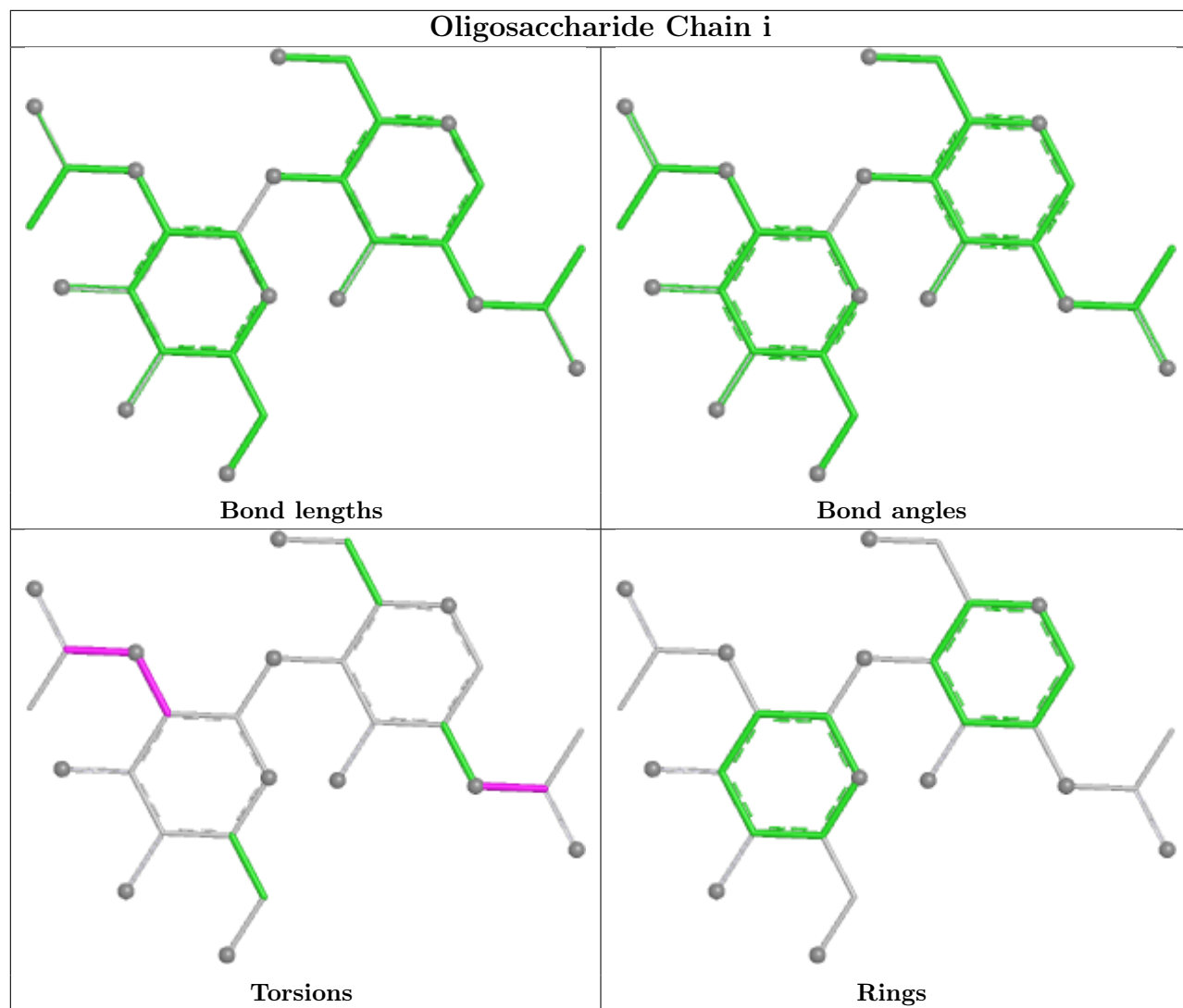


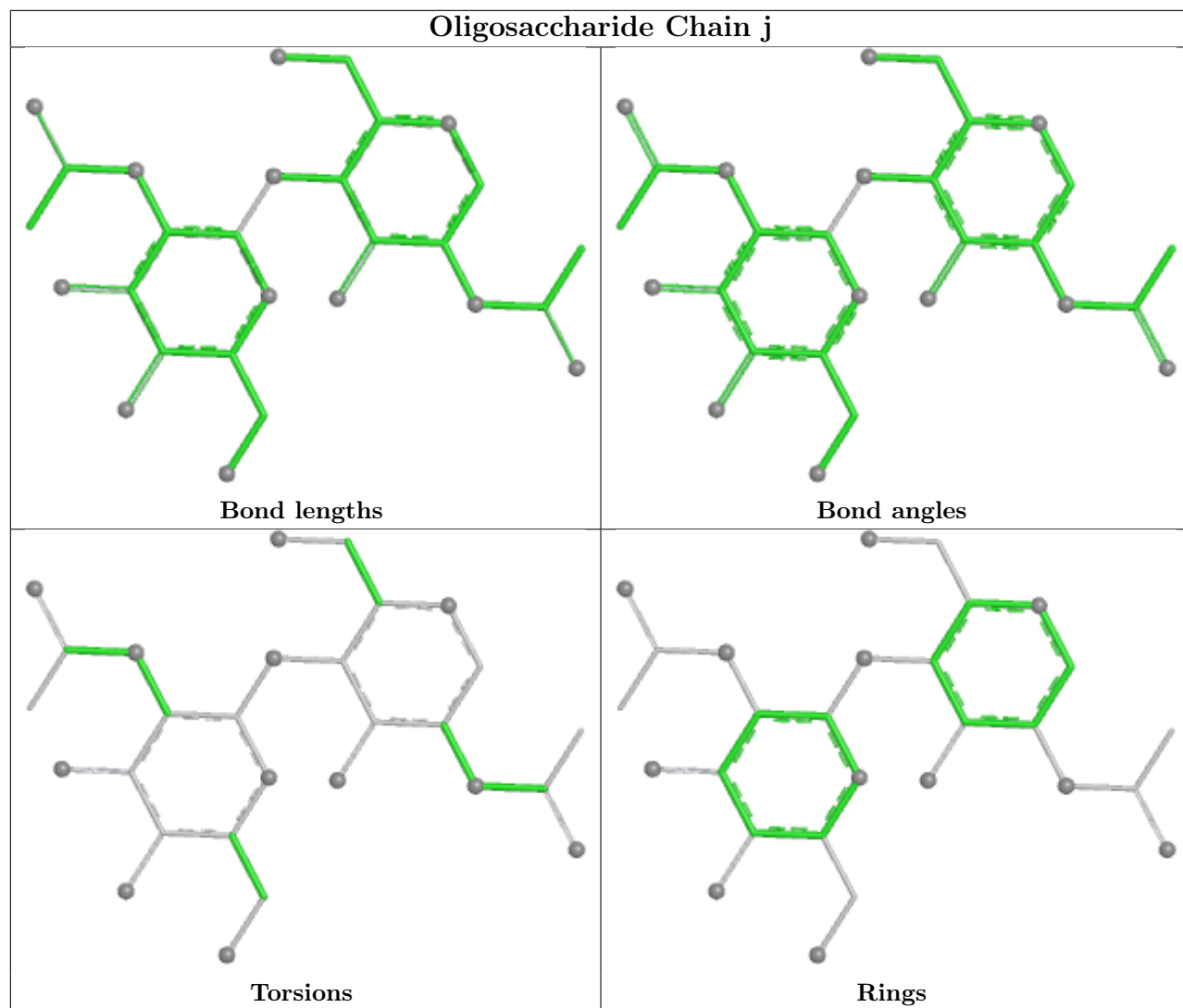


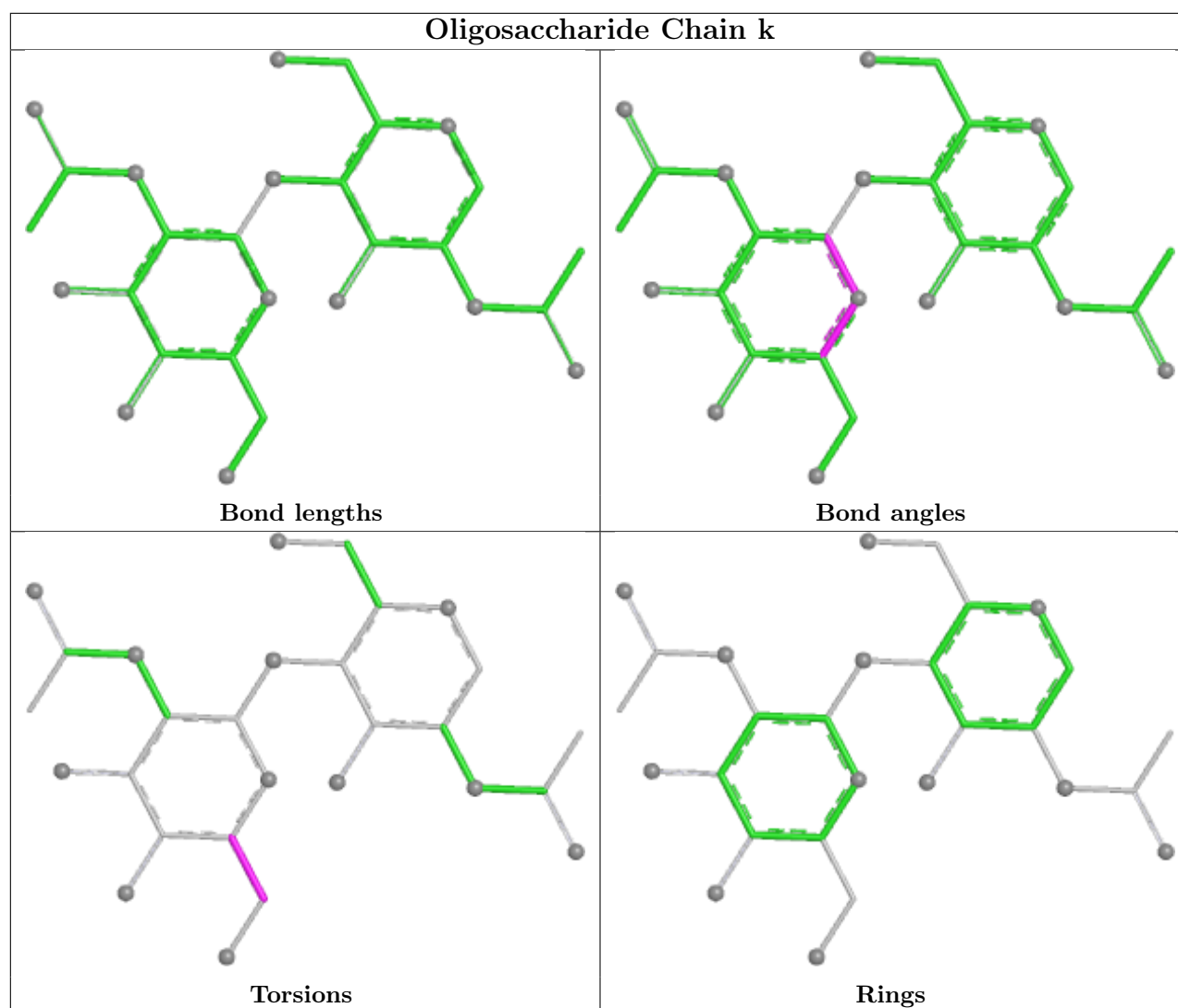












5.6 Ligand geometry [i](#)

29 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	$\# Z > 2$
4	NAG	A	1401	1	14,14,15	0.32	0	17,19,21	0.35	0
4	NAG	C	1408	1	14,14,15	0.32	0	17,19,21	0.40	0
4	NAG	B	1401	1	14,14,15	0.32	0	17,19,21	0.35	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	B	1405	1	14,14,15	0.60	0	17,19,21	1.33	2 (11%)
4	NAG	A	1409	1	14,14,15	0.50	0	17,19,21	0.37	0
4	NAG	C	1405	1	14,14,15	0.60	0	17,19,21	1.35	2 (11%)
4	NAG	C	1404	1	14,14,15	0.50	0	17,19,21	0.55	0
4	NAG	B	1402	1	14,14,15	0.20	0	17,19,21	0.67	0
4	NAG	A	1403	1	14,14,15	0.19	0	17,19,21	0.43	0
4	NAG	E	901	2	14,14,15	0.38	0	17,19,21	0.62	1 (5%)
4	NAG	D	901	2	14,14,15	0.38	0	17,19,21	0.61	1 (5%)
4	NAG	A	1404	1	14,14,15	0.50	0	17,19,21	0.55	0
4	NAG	A	1405	1	14,14,15	0.59	0	17,19,21	1.34	2 (11%)
4	NAG	C	1407	1	14,14,15	0.24	0	17,19,21	0.51	0
4	NAG	B	1404	1	14,14,15	0.50	0	17,19,21	0.54	0
4	NAG	A	1407	1	14,14,15	0.24	0	17,19,21	0.51	0
4	NAG	B	1407	1	14,14,15	0.25	0	17,19,21	0.52	0
4	NAG	B	1406	1	14,14,15	0.28	0	17,19,21	0.40	0
4	NAG	A	1406	1	14,14,15	0.28	0	17,19,21	0.39	0
4	NAG	C	1403	1	14,14,15	0.19	0	17,19,21	0.44	0
4	NAG	C	1402	1	14,14,15	0.21	0	17,19,21	0.66	0
4	NAG	B	1409	1	14,14,15	0.42	0	17,19,21	1.15	2 (11%)
4	NAG	B	1410	-	14,14,15	0.36	0	17,19,21	0.43	0
4	NAG	A	1402	1	14,14,15	0.21	0	17,19,21	0.66	0
4	NAG	C	1406	1	14,14,15	0.28	0	17,19,21	0.41	0
4	NAG	A	1408	1	14,14,15	0.32	0	17,19,21	0.39	0
4	NAG	B	1403	1	14,14,15	0.19	0	17,19,21	0.44	0
4	NAG	B	1408	1	14,14,15	0.33	0	17,19,21	0.40	0
4	NAG	C	1401	1	14,14,15	0.32	0	17,19,21	0.36	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
4	NAG	A	1401	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1408	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1401	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1405	1	-	6/6/23/26	0/1/1/1
4	NAG	A	1409	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1405	1	-	6/6/23/26	0/1/1/1
4	NAG	C	1404	1	-	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	B	1402	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1403	1	-	2/6/23/26	0/1/1/1
4	NAG	E	901	2	-	2/6/23/26	0/1/1/1
4	NAG	D	901	2	-	2/6/23/26	0/1/1/1
4	NAG	A	1404	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1405	1	-	6/6/23/26	0/1/1/1
4	NAG	C	1407	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1404	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1407	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1407	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1406	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1406	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1403	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1402	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1409	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1410	-	-	0/6/23/26	0/1/1/1
4	NAG	A	1402	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1406	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1408	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1403	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1408	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1401	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	1405	NAG	C2-N2-C7	4.61	129.08	122.90
4	A	1405	NAG	C2-N2-C7	4.59	129.05	122.90
4	B	1405	NAG	C2-N2-C7	4.57	129.02	122.90
4	B	1409	NAG	C8-C7-N2	2.32	119.97	116.12
4	B	1409	NAG	C2-N2-C7	-2.17	120.00	122.90

There are no chirality outliers.

5 of 60 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1406	NAG	O5-C5-C6-O6
4	B	1406	NAG	O5-C5-C6-O6
4	C	1406	NAG	O5-C5-C6-O6
4	A	1402	NAG	O5-C5-C6-O6
4	A	1404	NAG	O5-C5-C6-O6

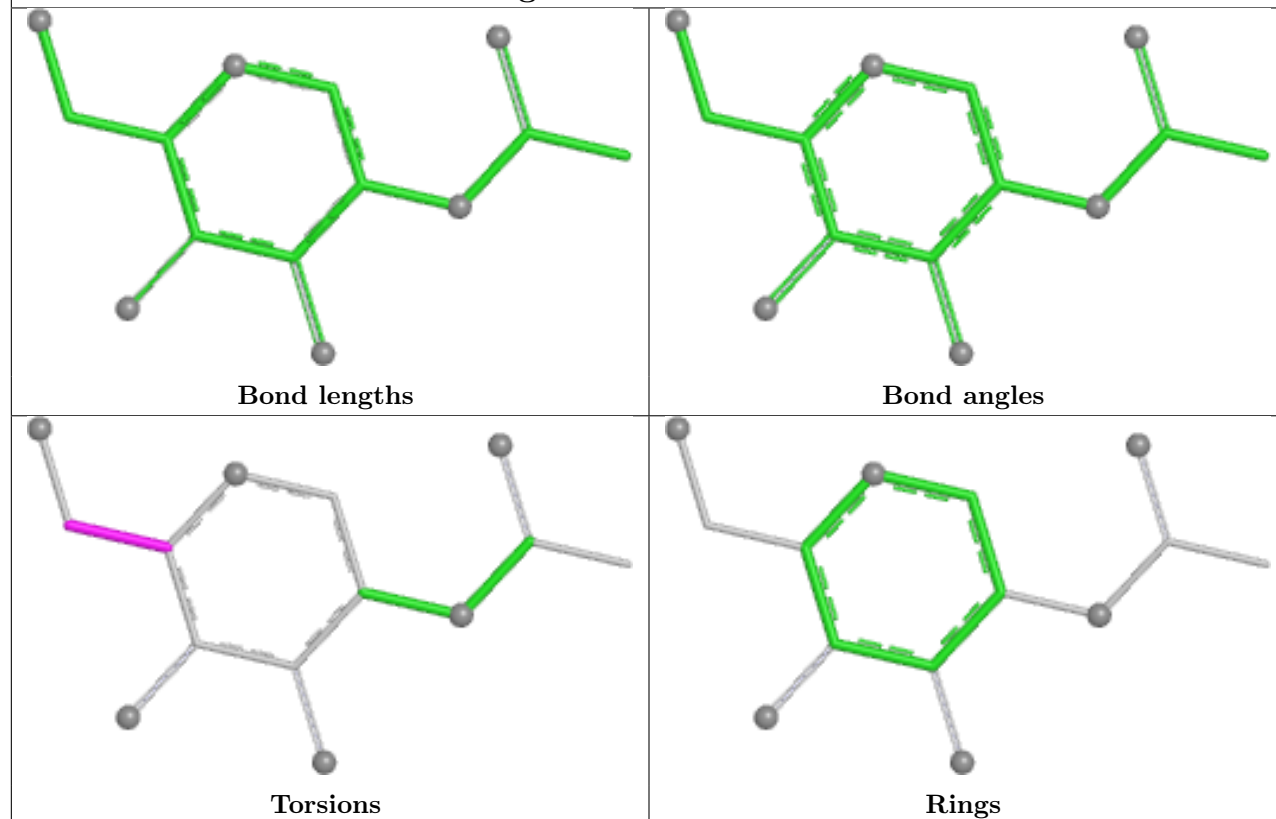
There are no ring outliers.

8 monomers are involved in 16 short contacts:

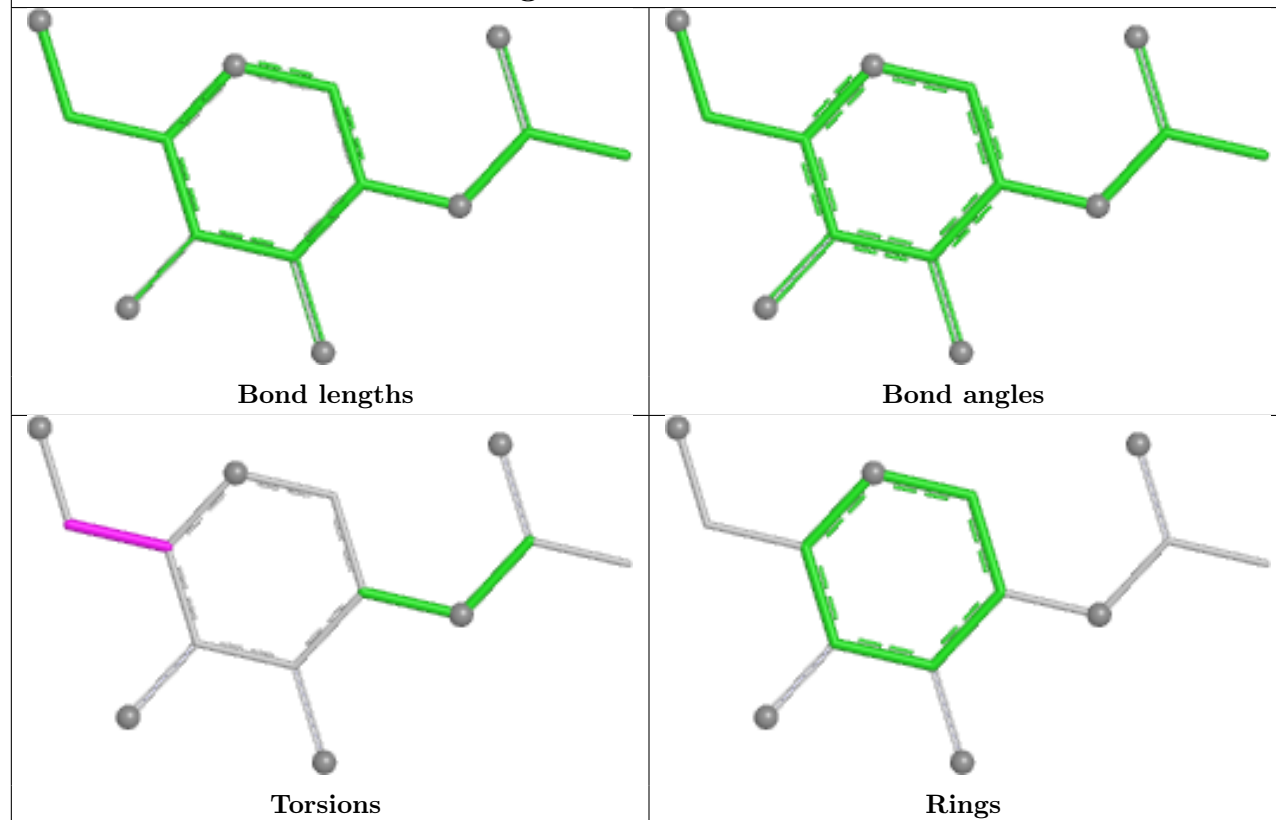
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1405	NAG	1	0
4	C	1405	NAG	1	0
4	B	1402	NAG	3	0
4	A	1405	NAG	1	0
4	C	1402	NAG	3	0
4	B	1409	NAG	4	0
4	B	1410	NAG	4	0
4	A	1402	NAG	3	0

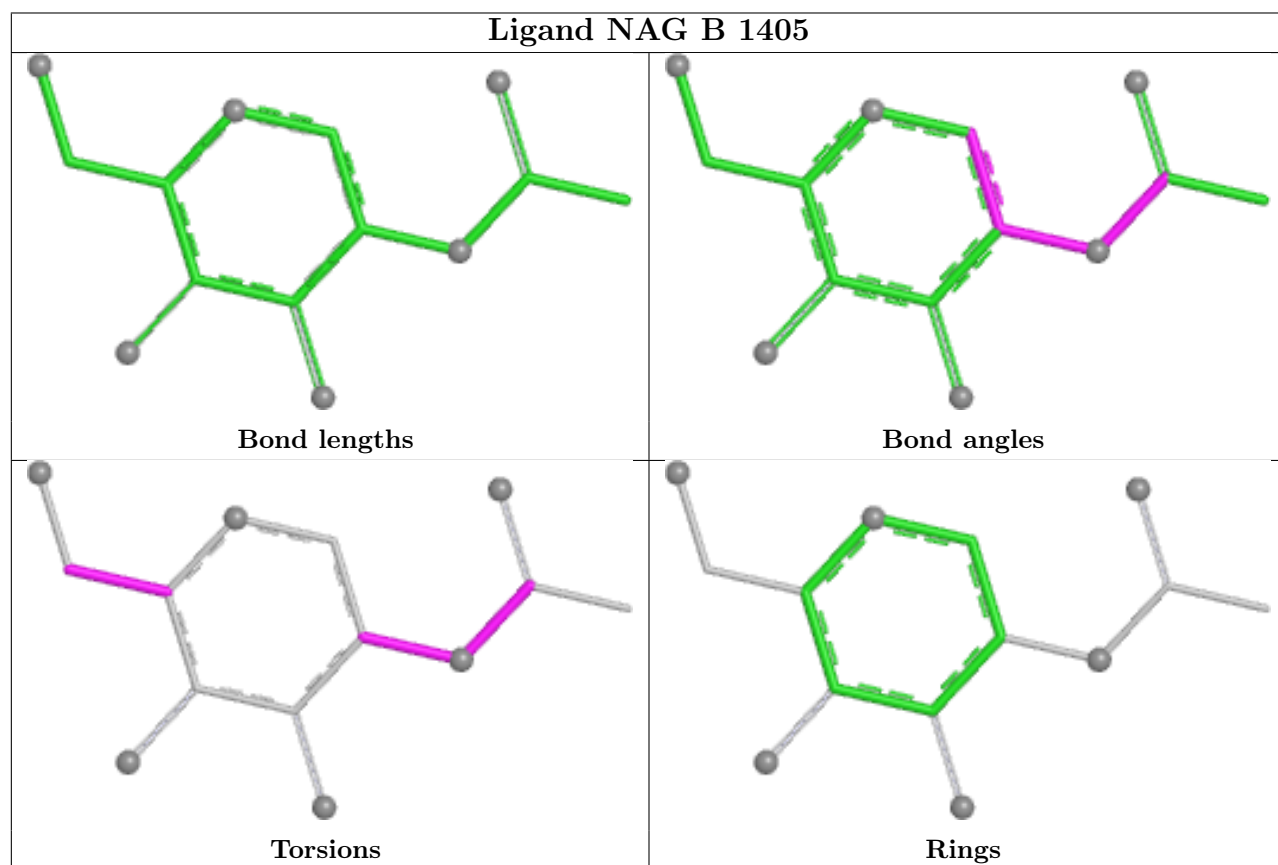
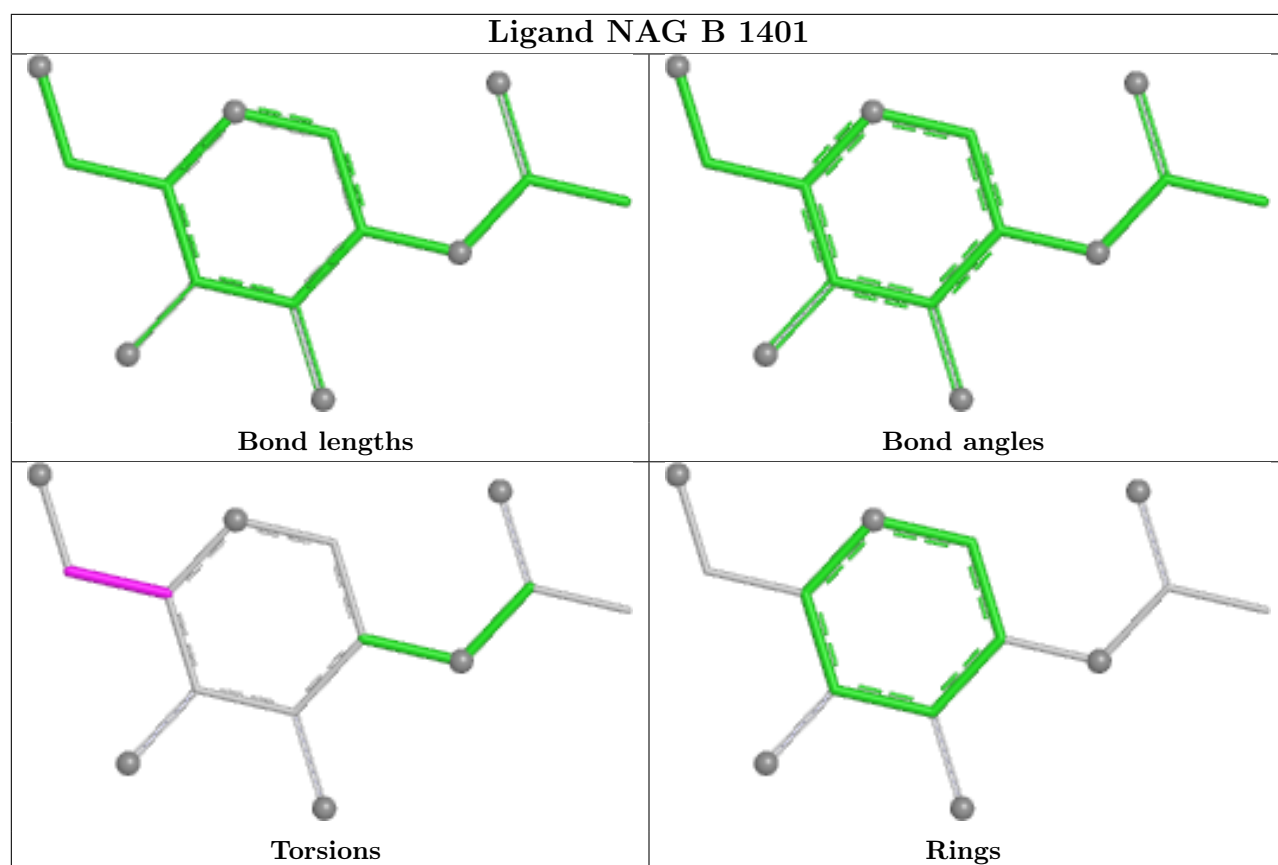
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

Ligand NAG A 1401

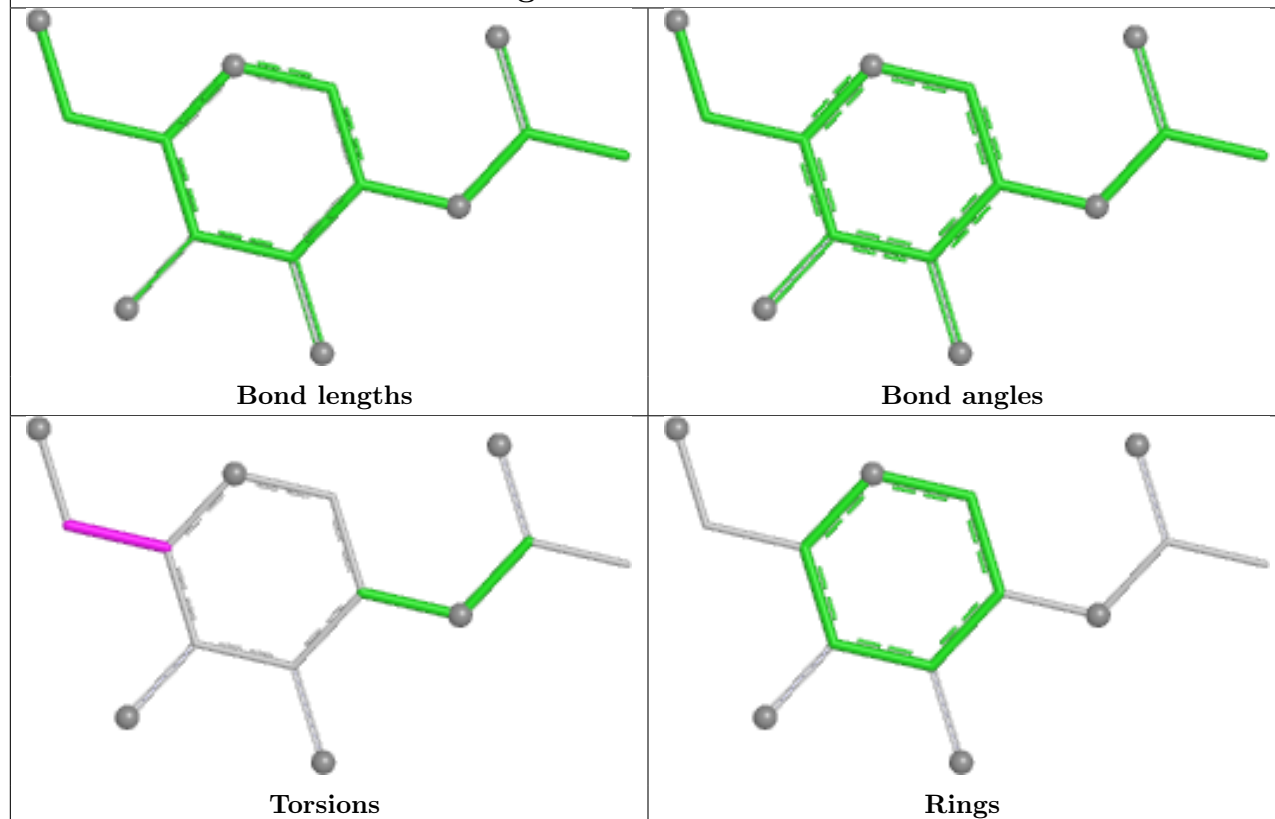


Ligand NAG C 1408

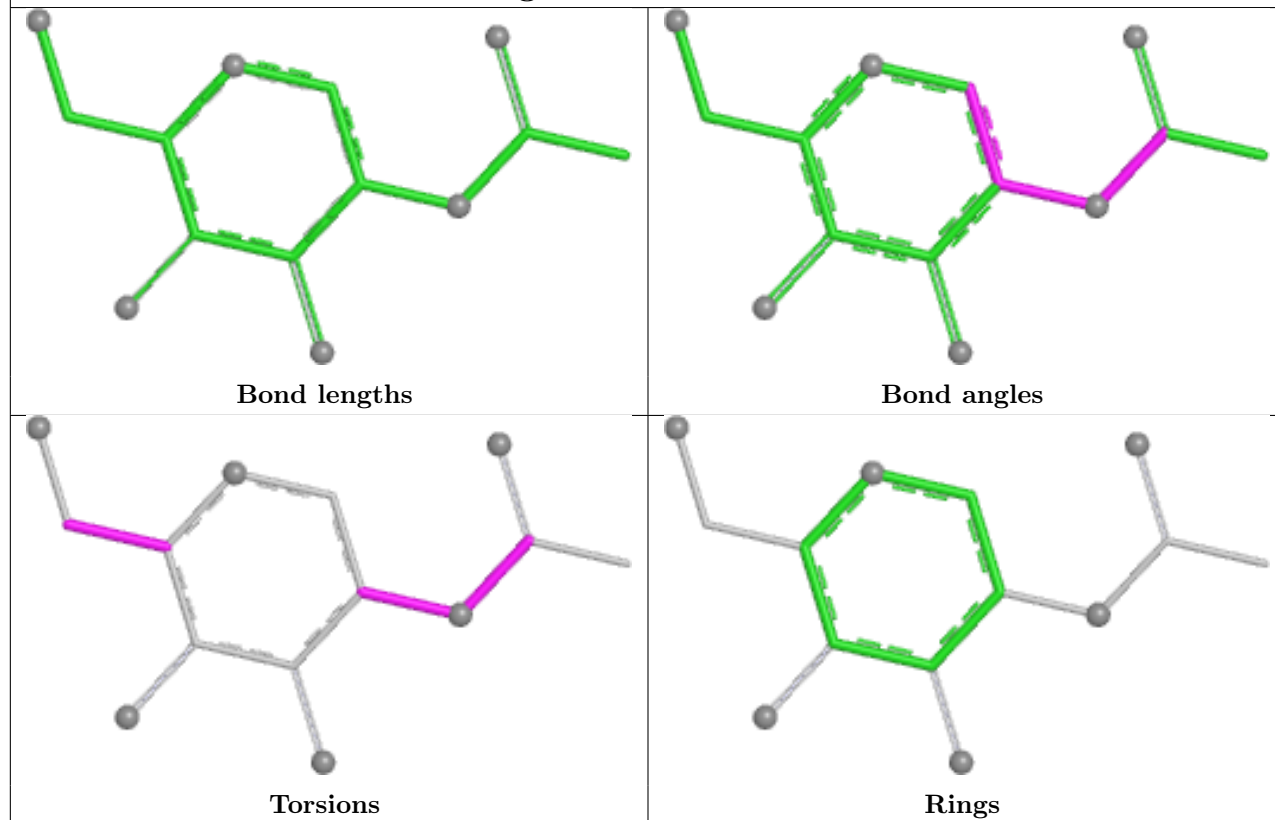




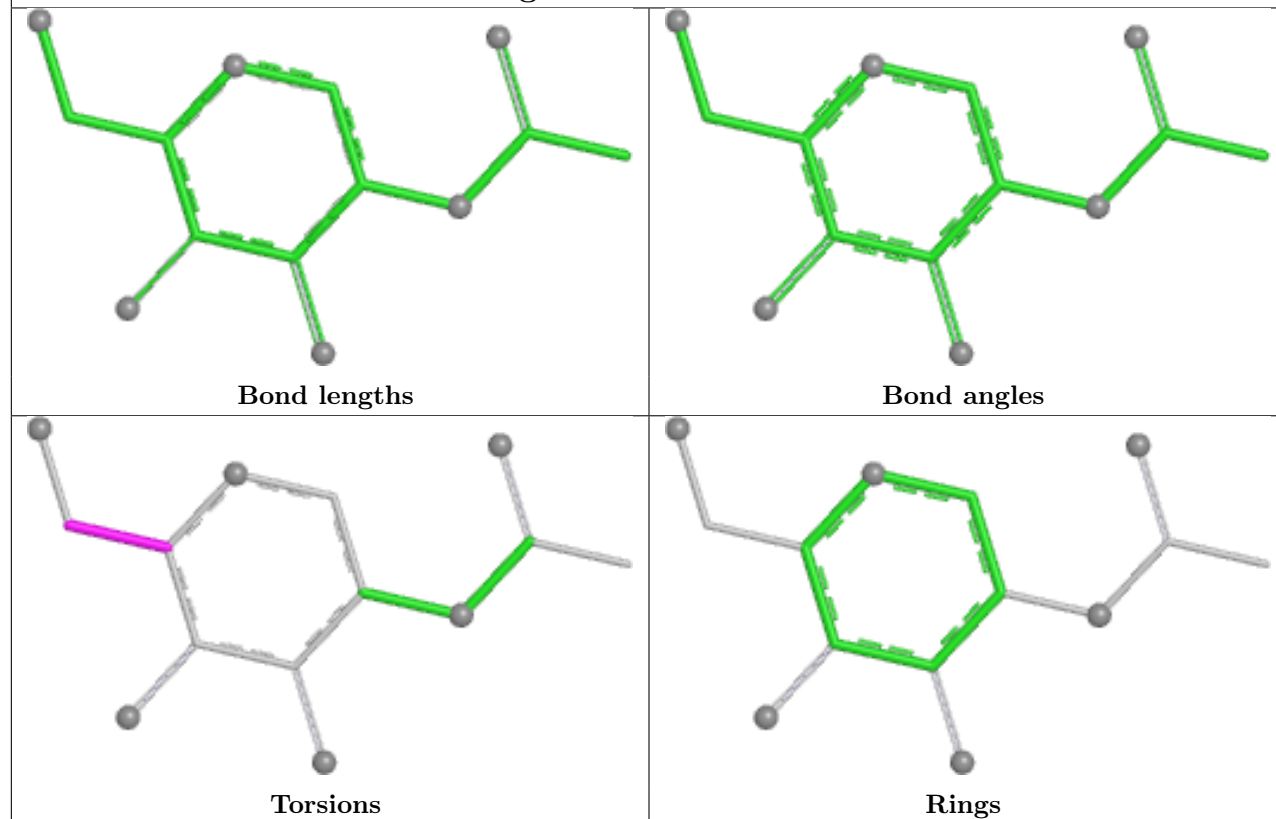
Ligand NAG A 1409



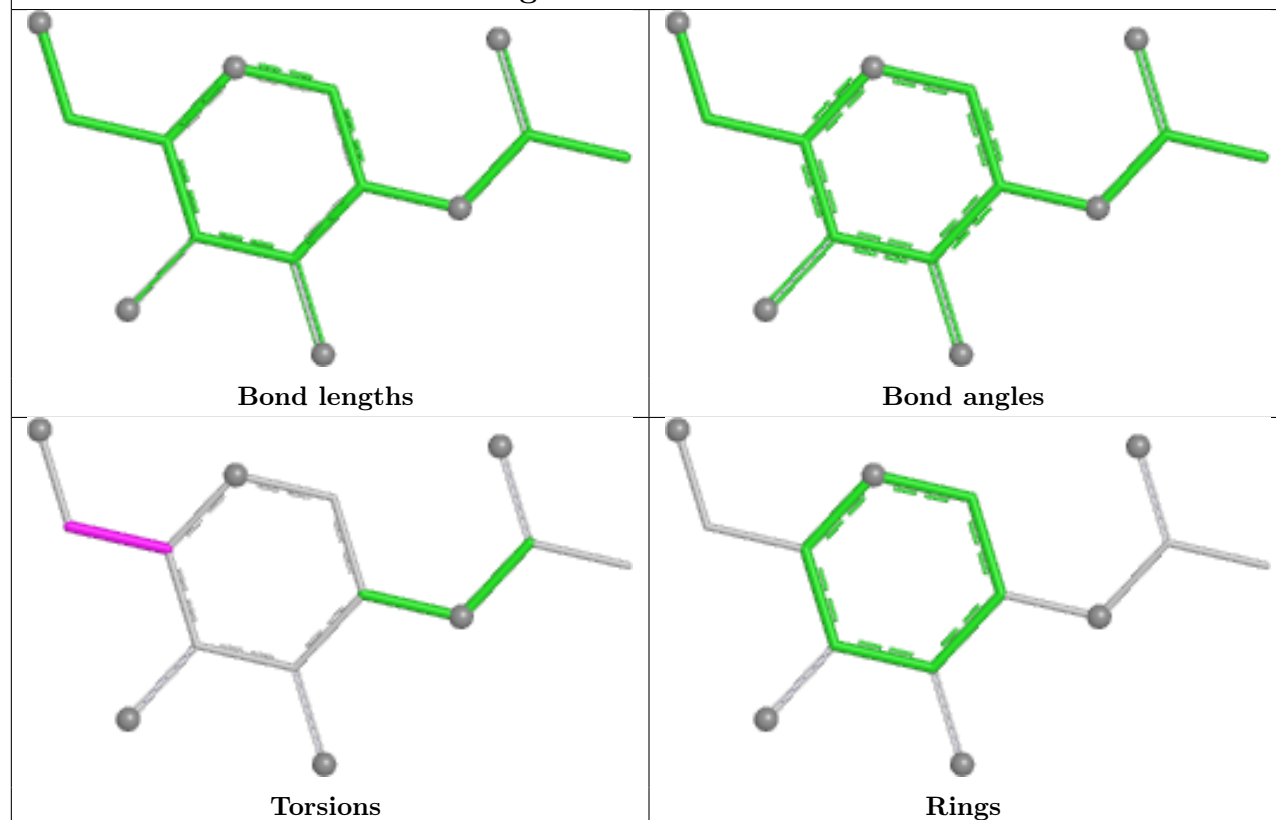
Ligand NAG C 1405



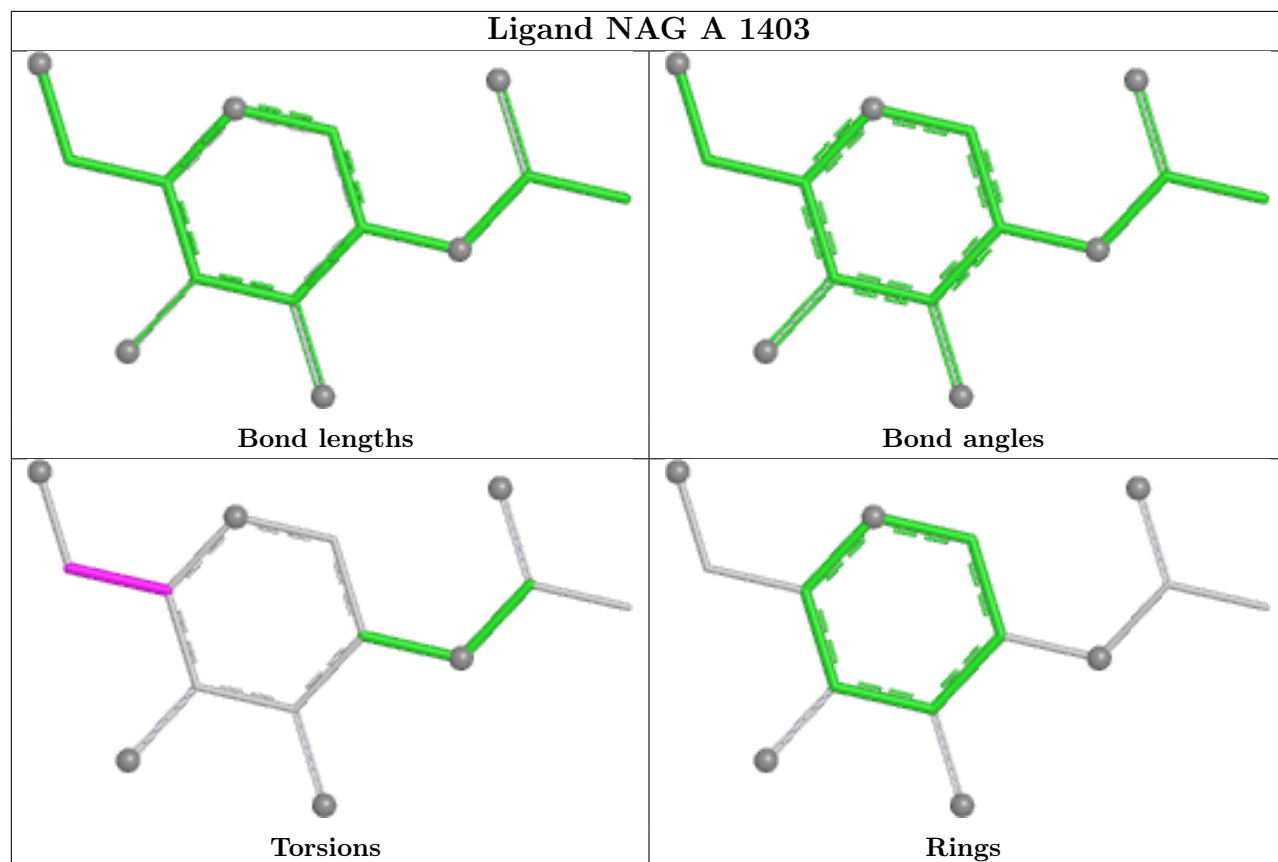
Ligand NAG C 1404



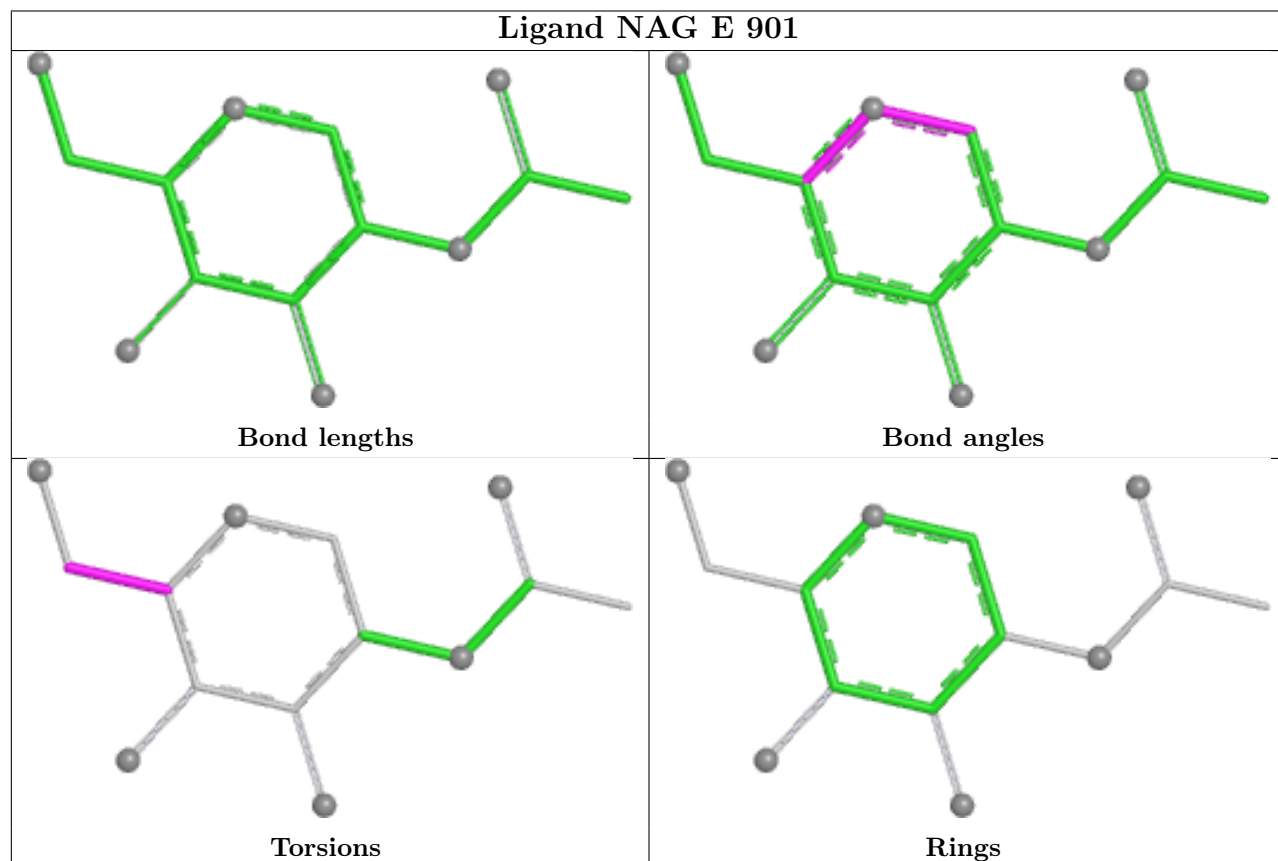
Ligand NAG B 1402

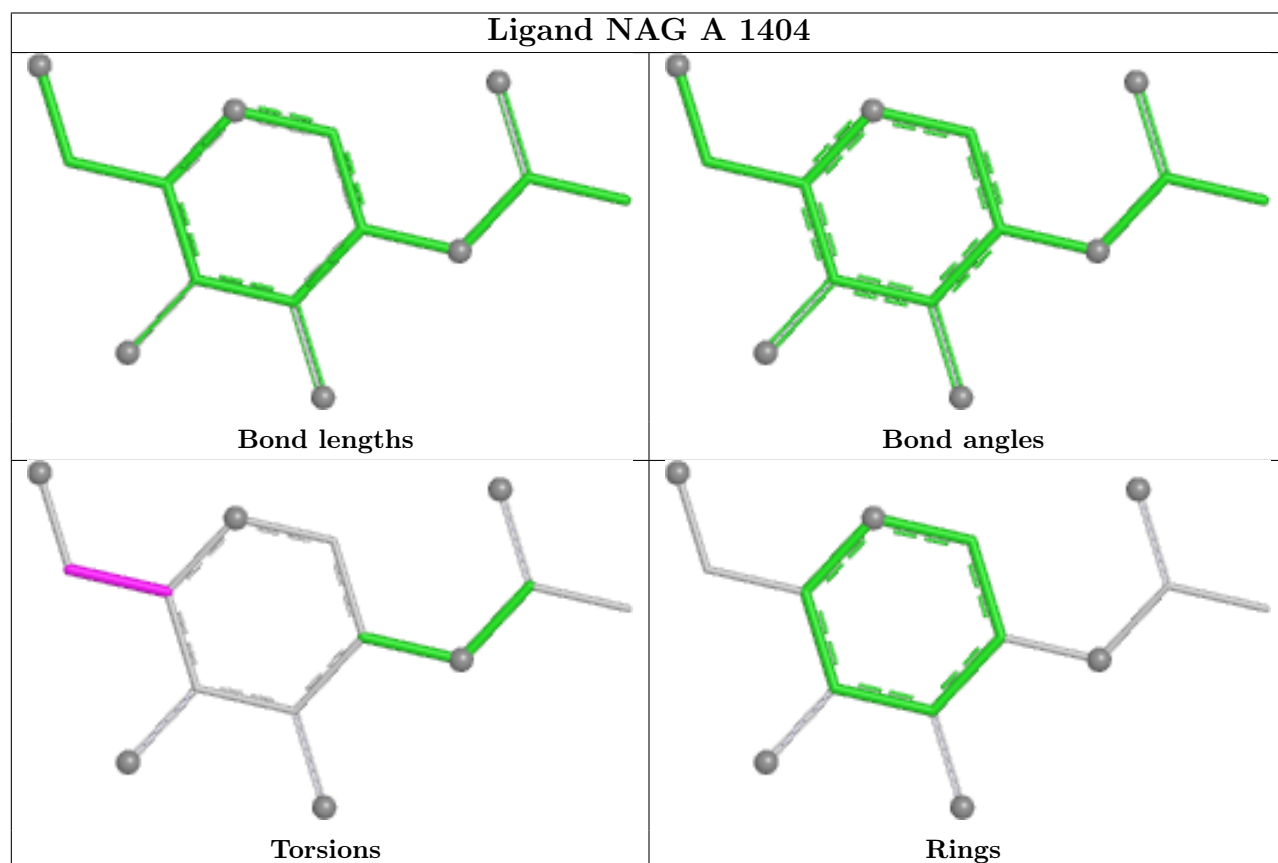
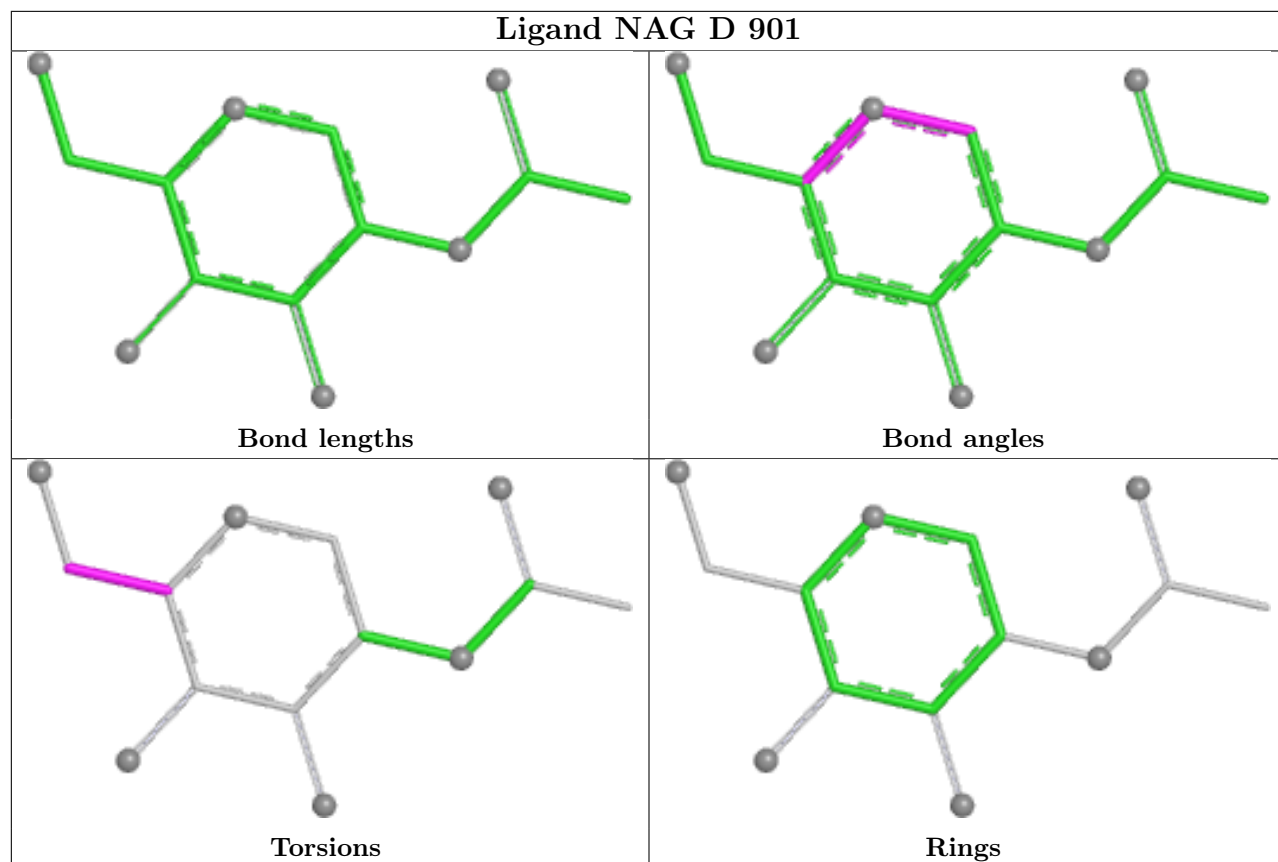


Ligand NAG A 1403

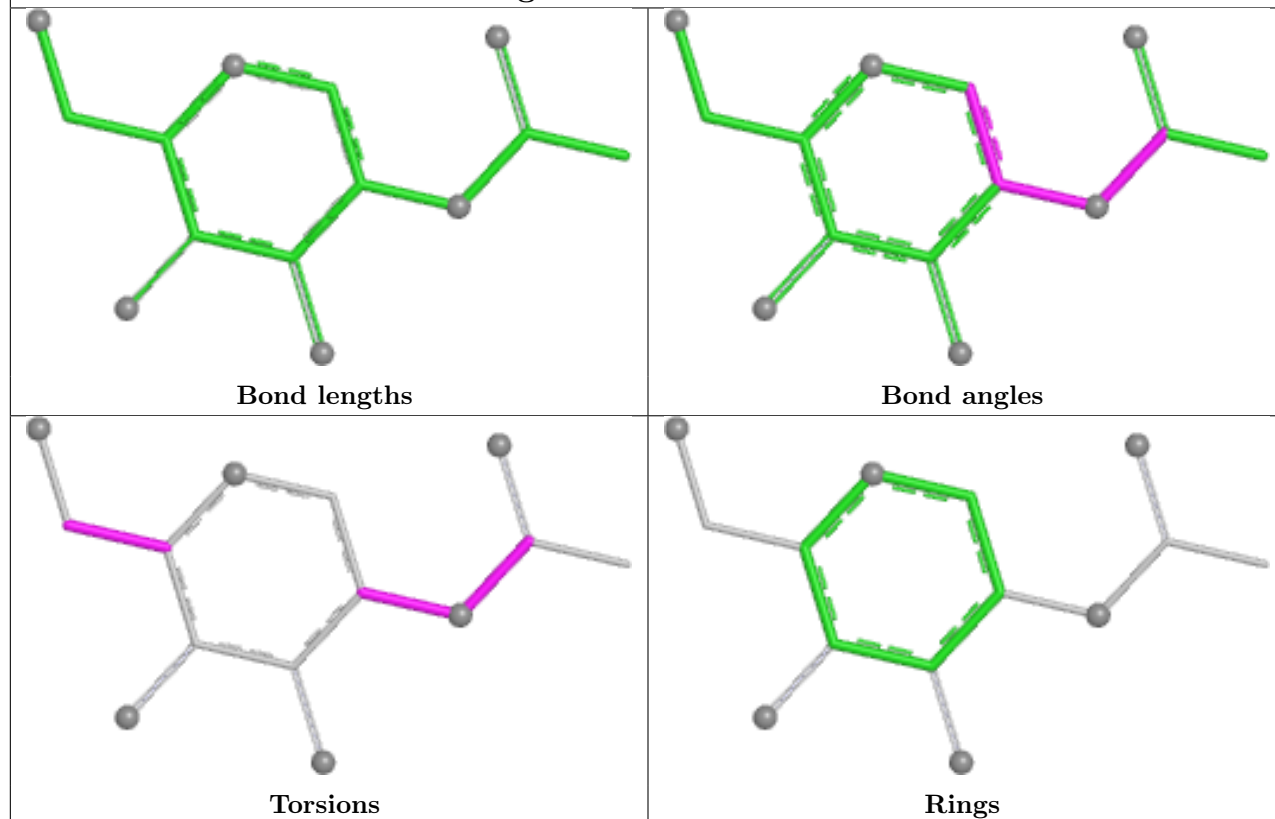


Ligand NAG E 901

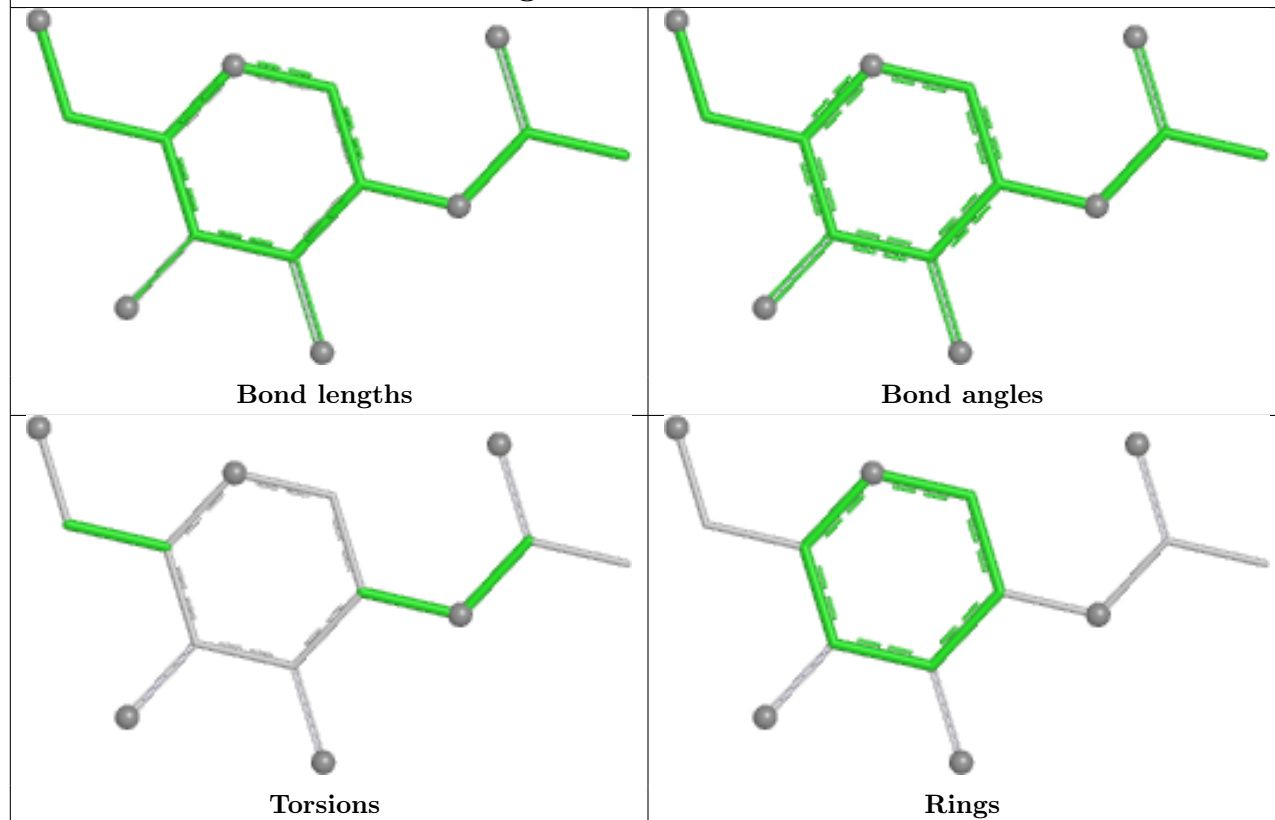




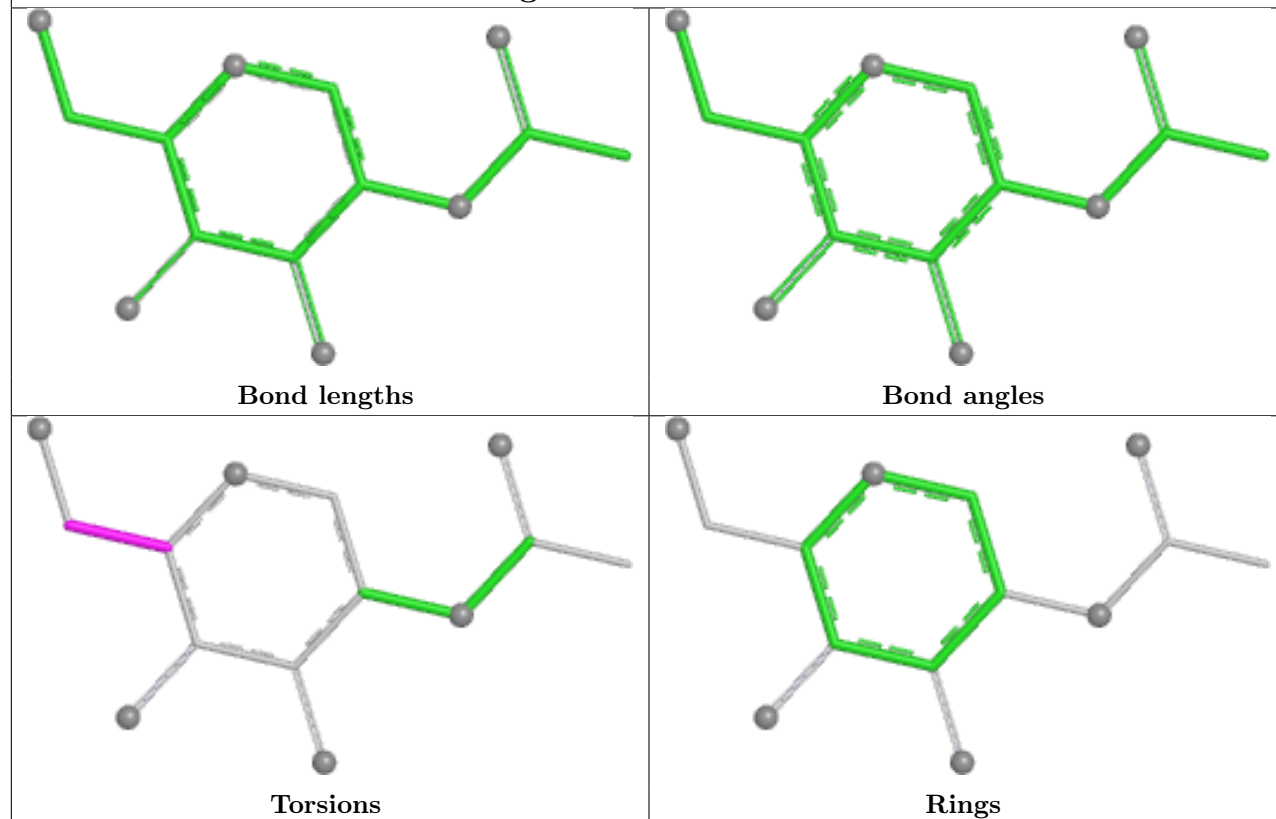
Ligand NAG A 1405



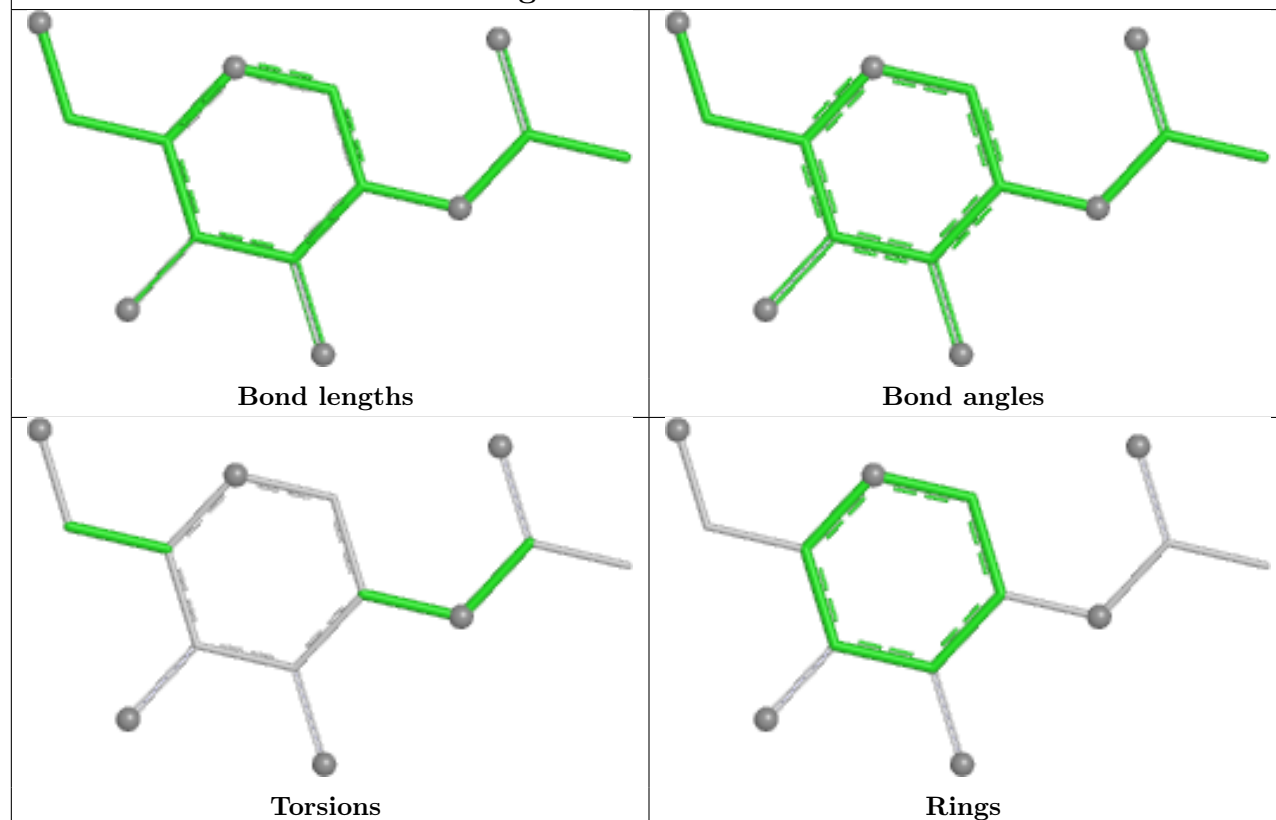
Ligand NAG C 1407

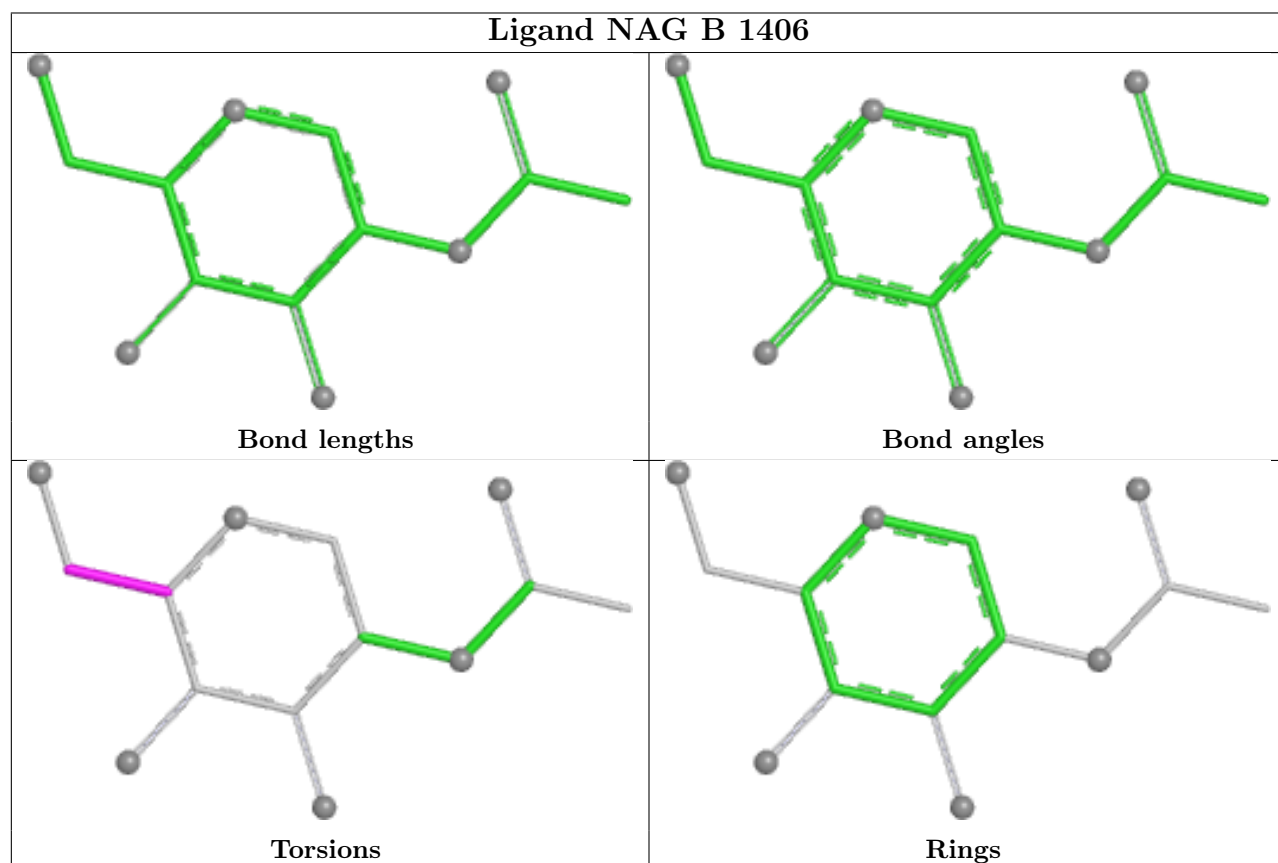
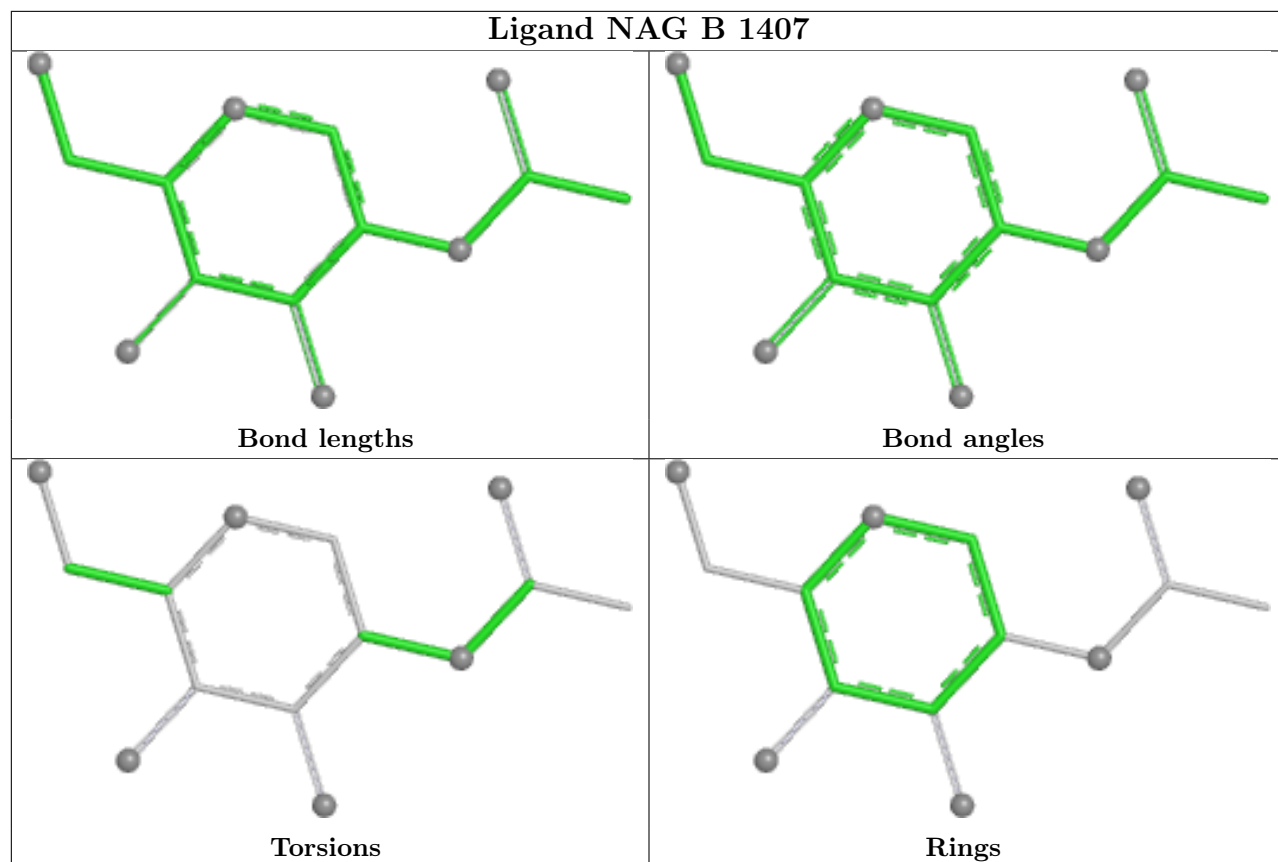


Ligand NAG B 1404

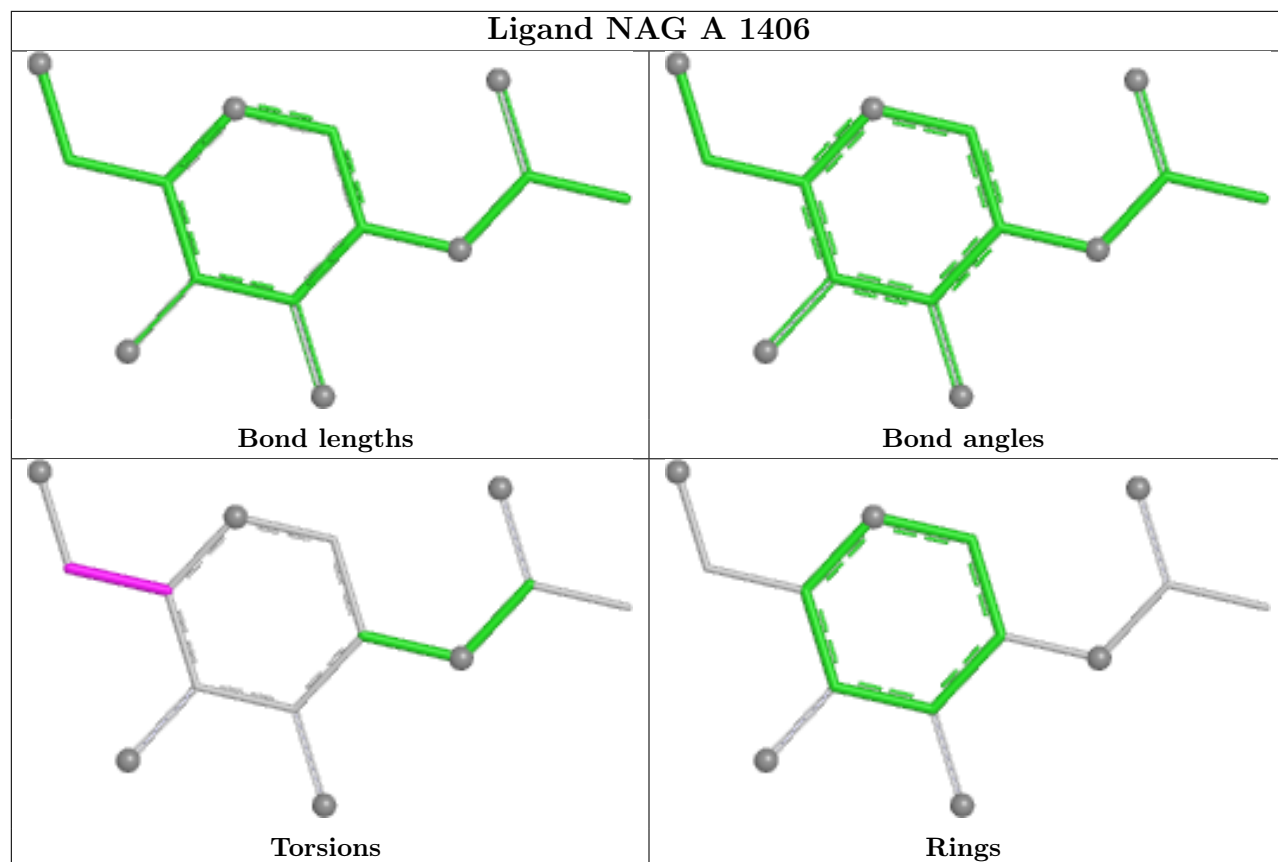


Ligand NAG A 1407

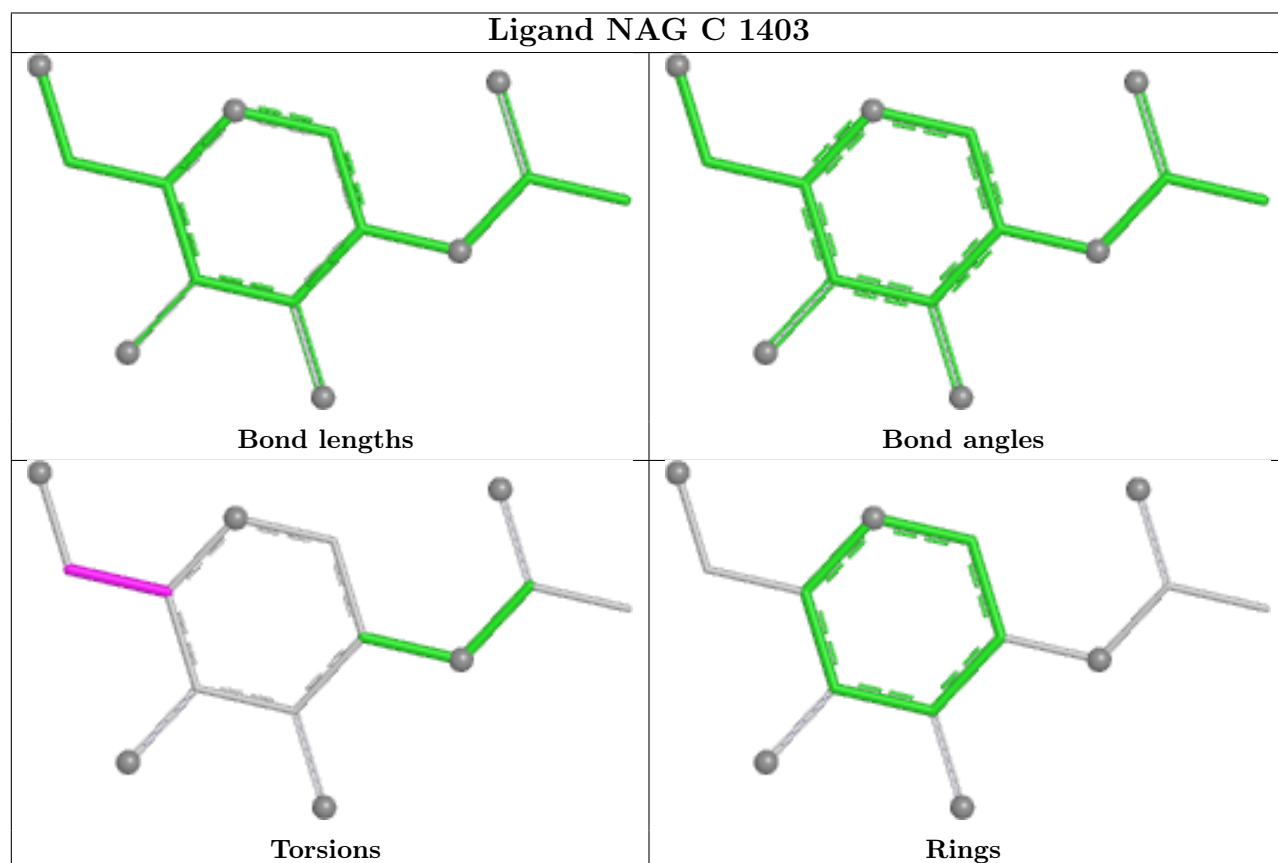




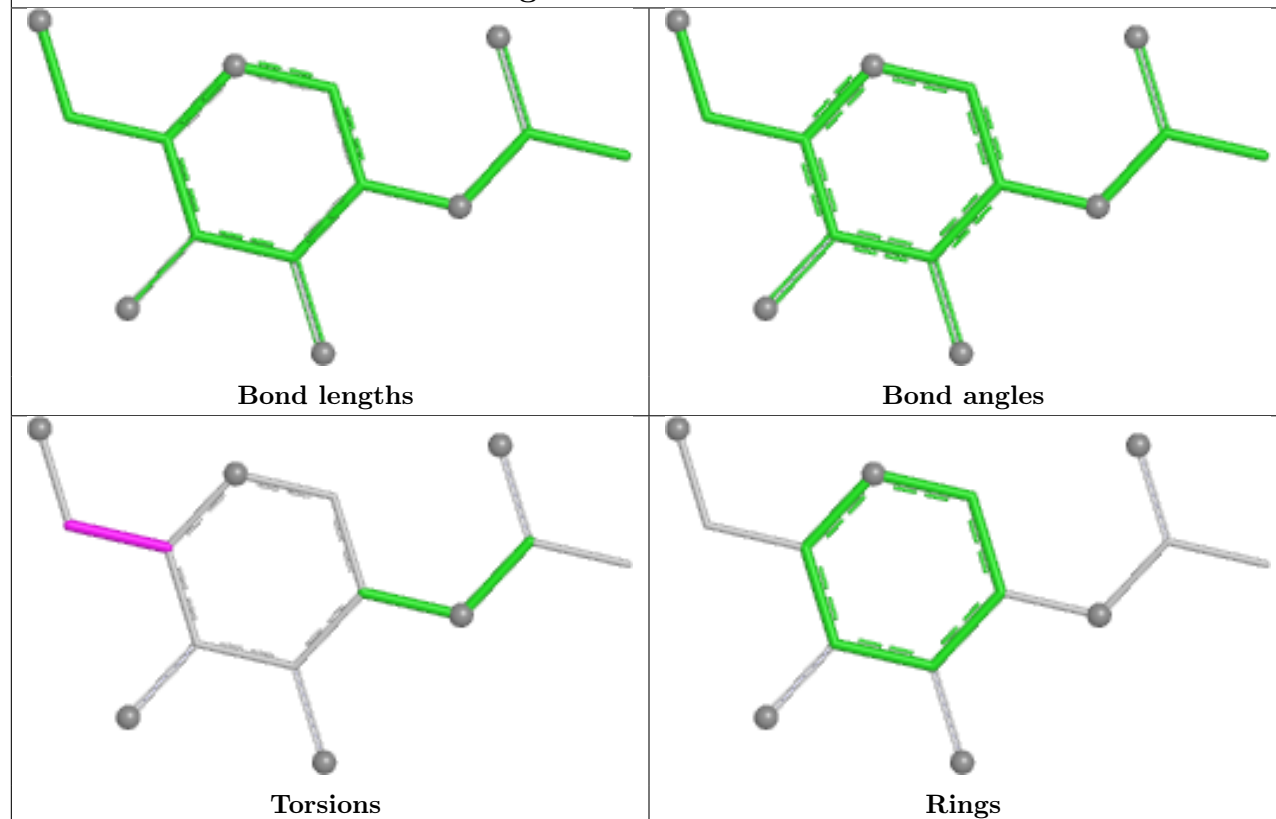
Ligand NAG A 1406



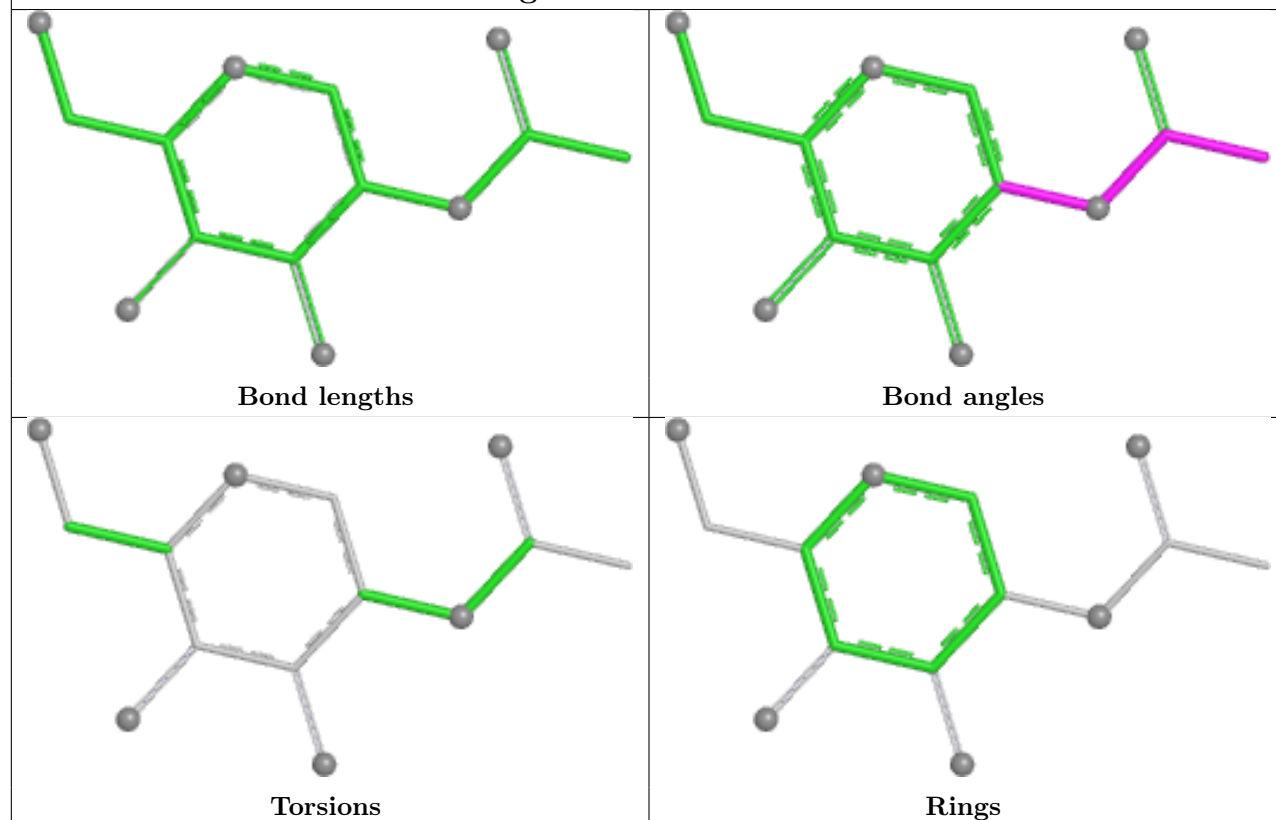
Ligand NAG C 1403



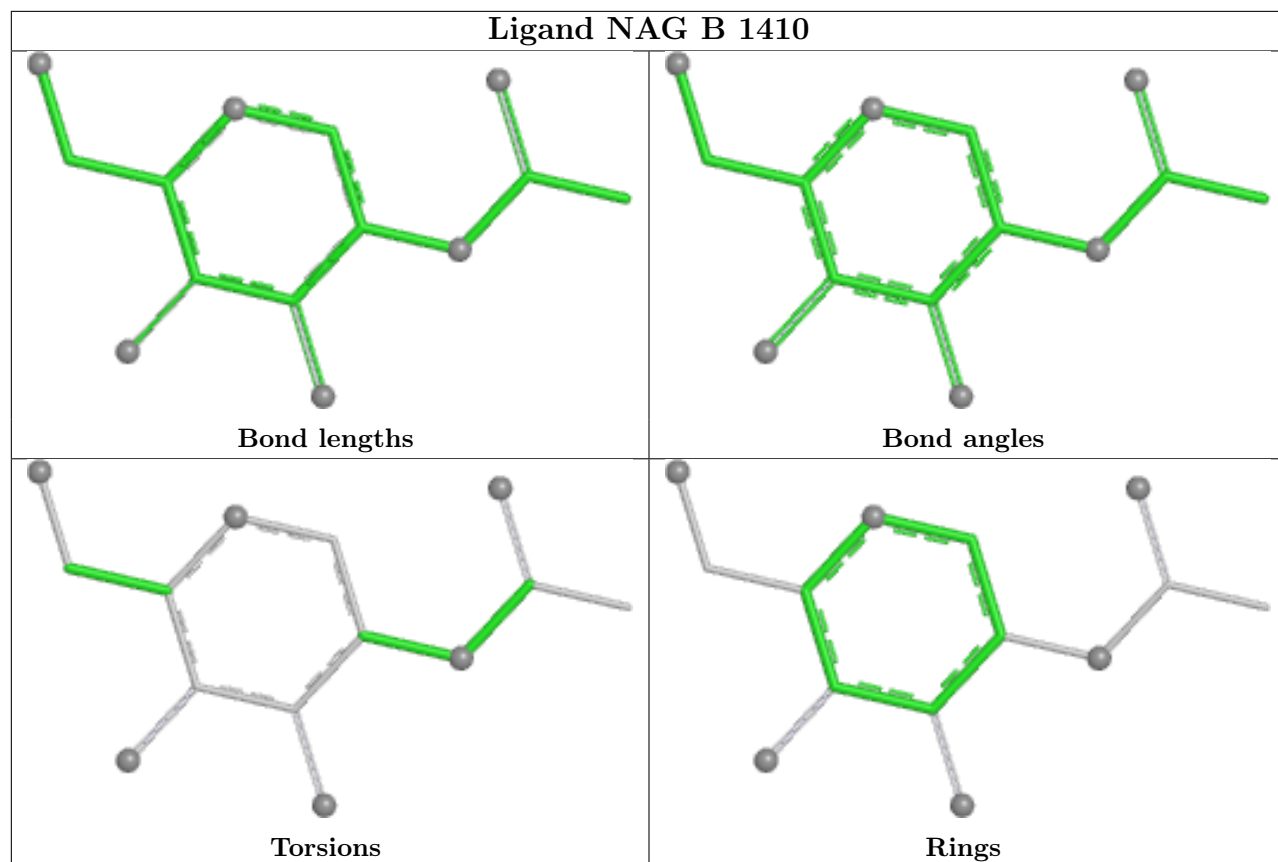
Ligand NAG C 1402



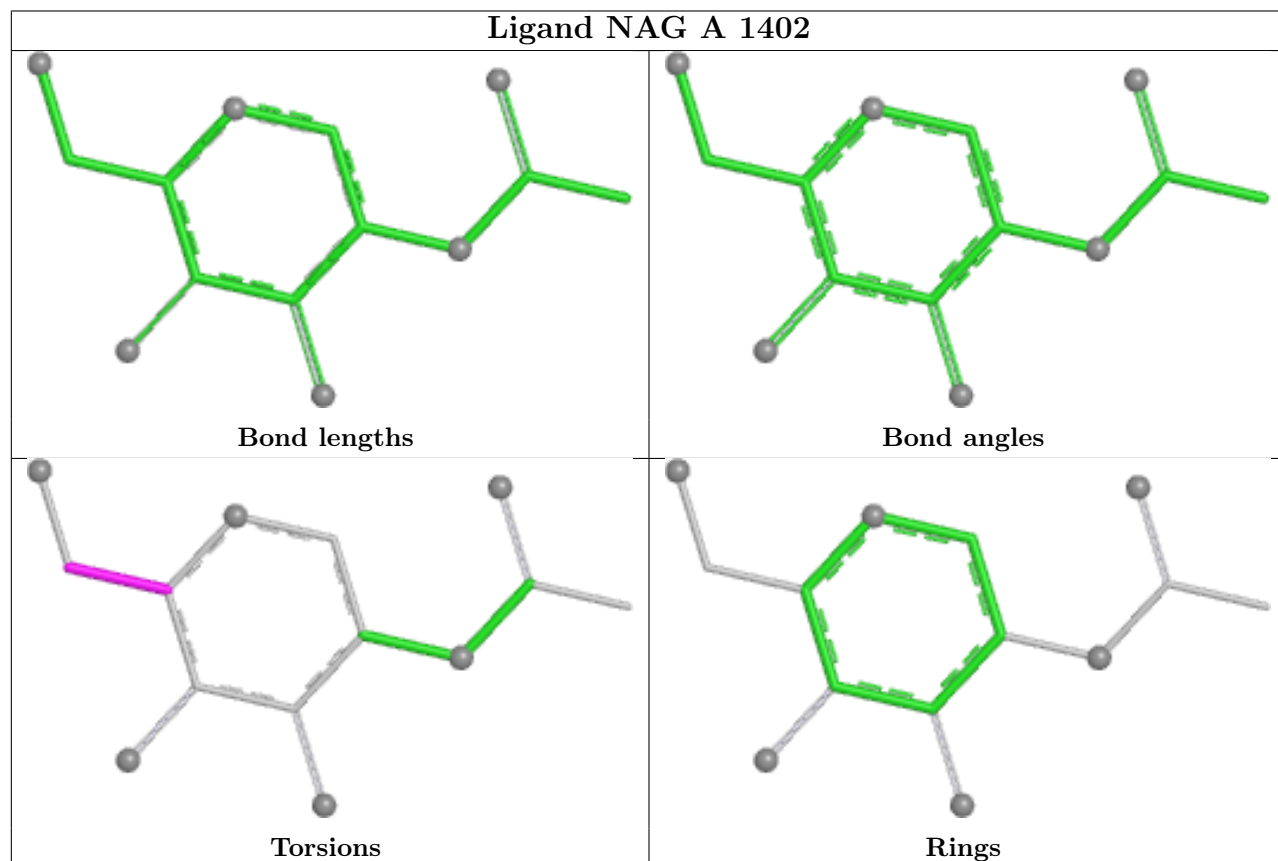
Ligand NAG B 1409



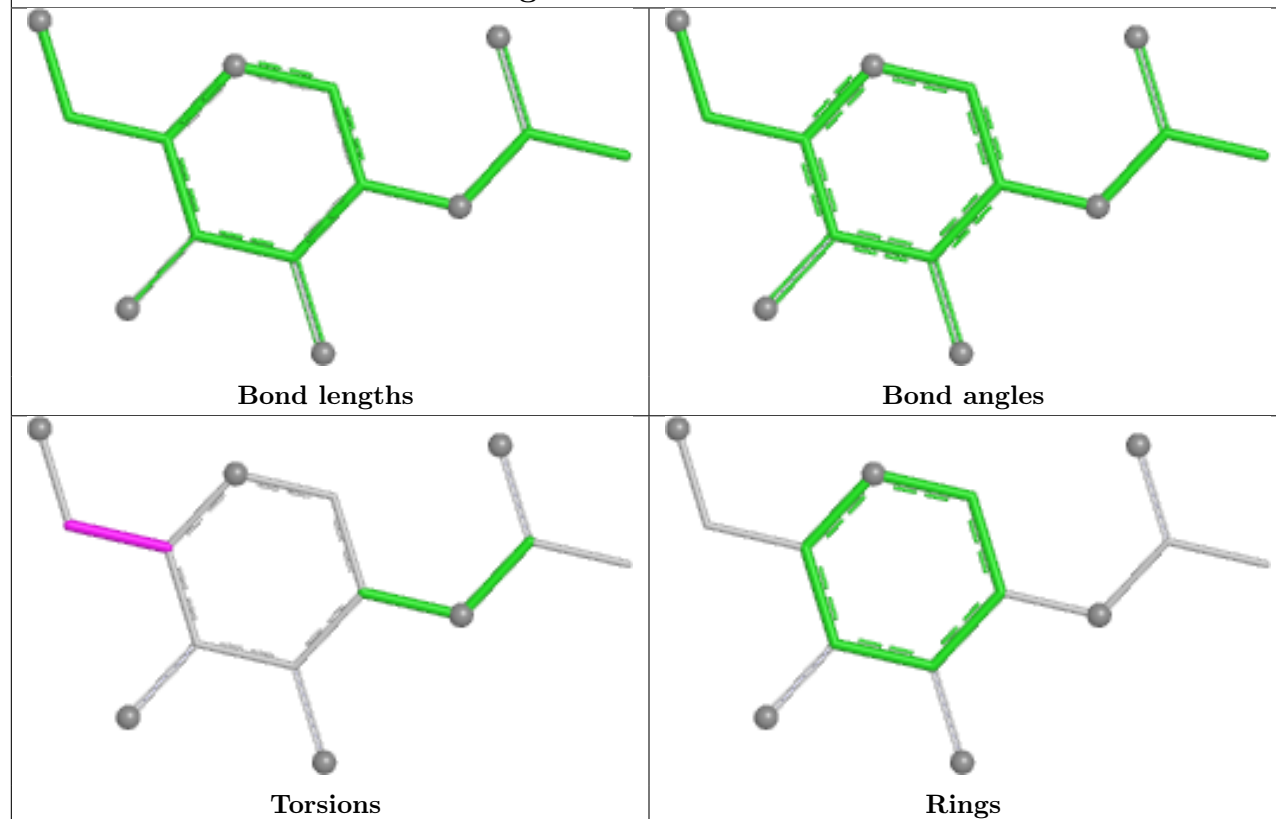
Ligand NAG B 1410



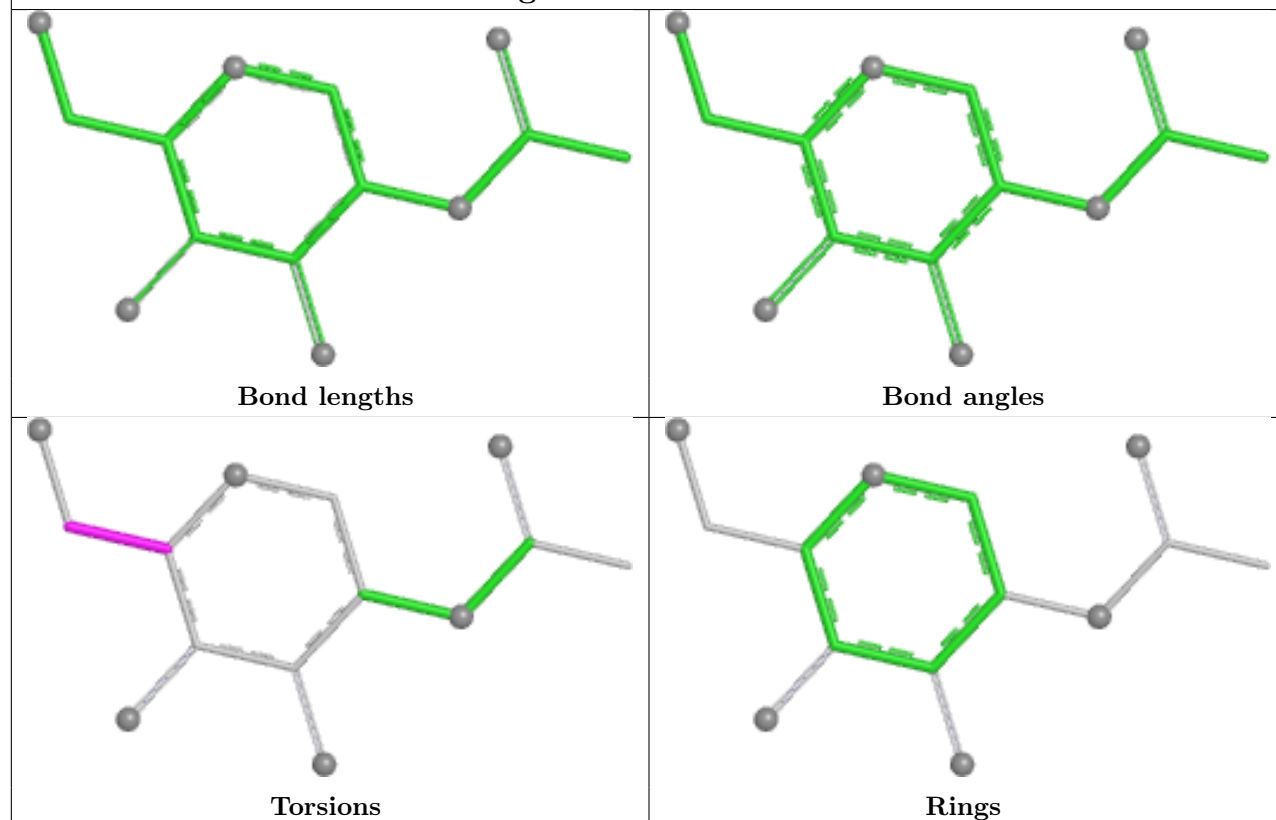
Ligand NAG A 1402



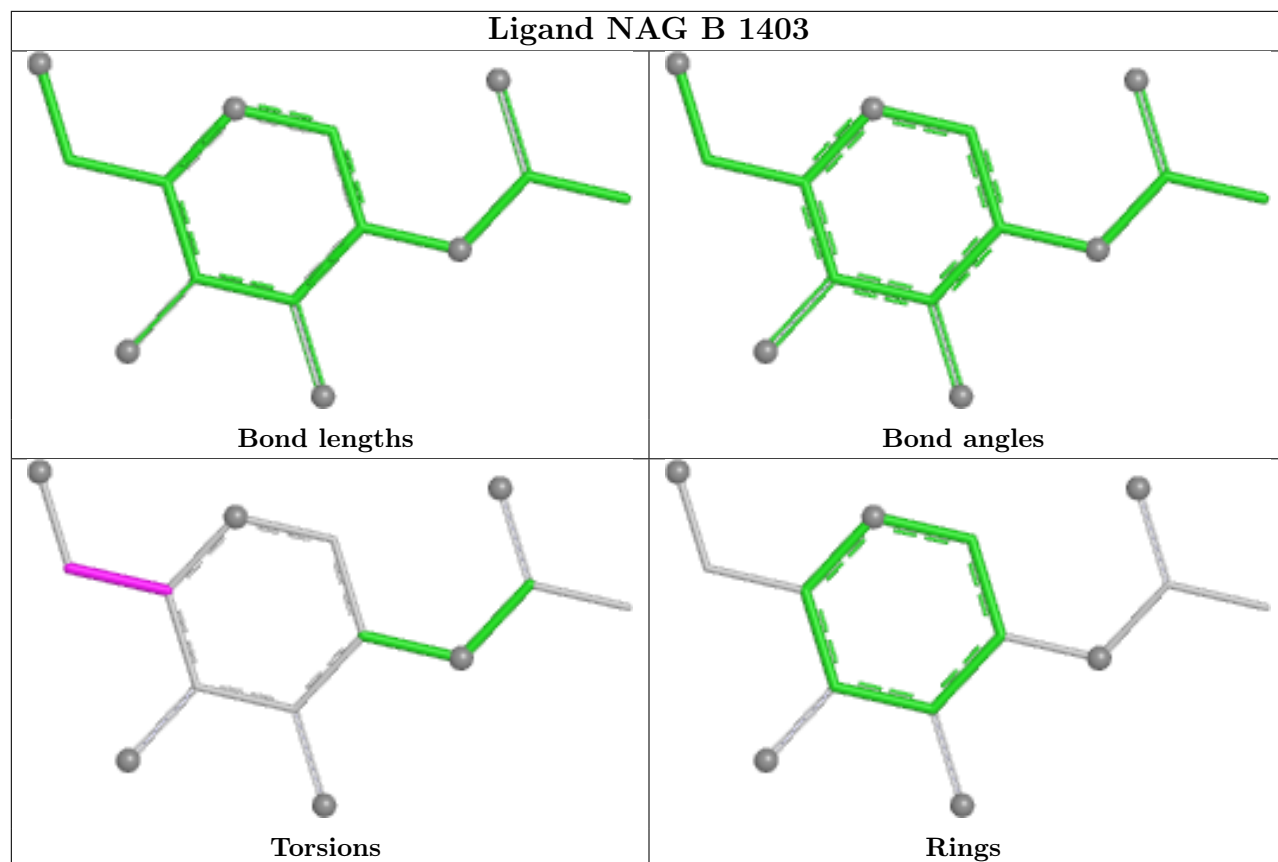
Ligand NAG C 1406



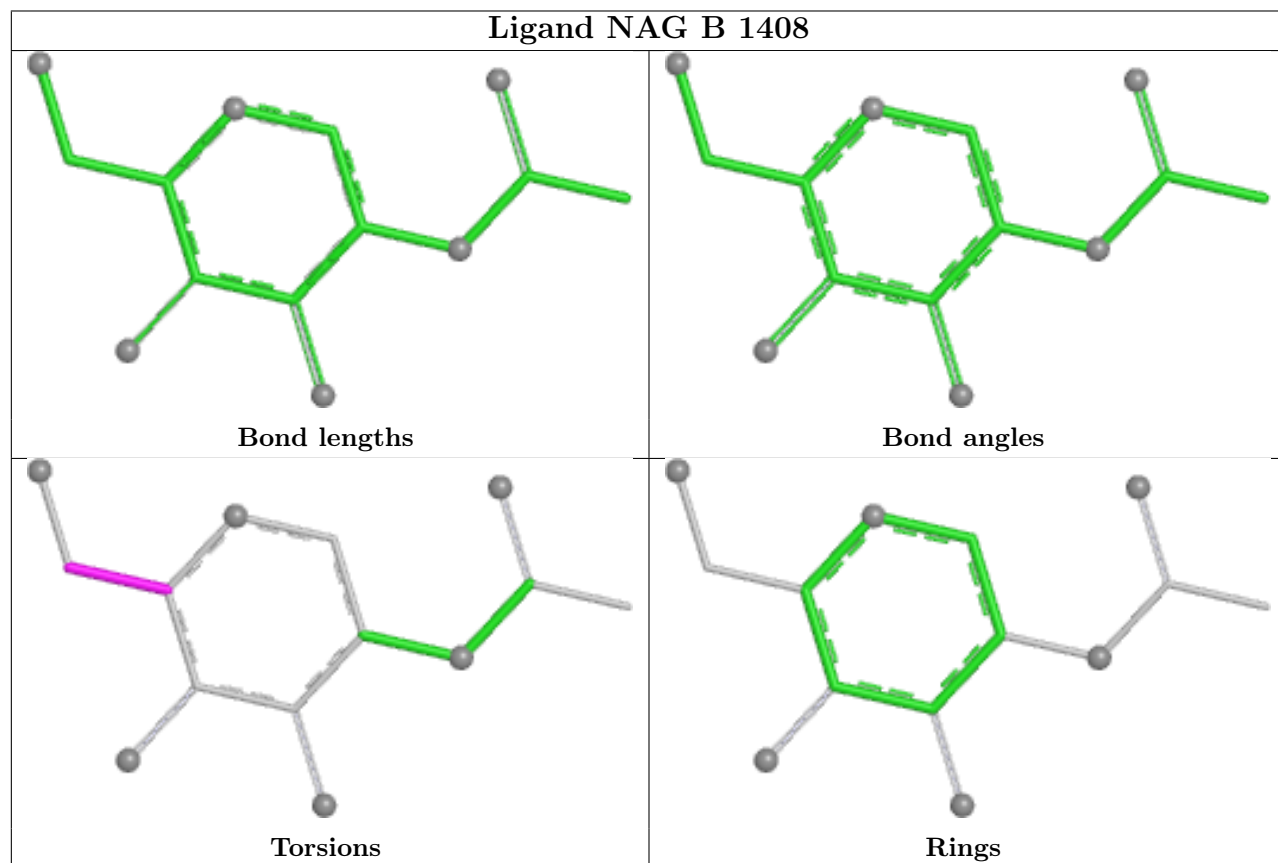
Ligand NAG A 1408

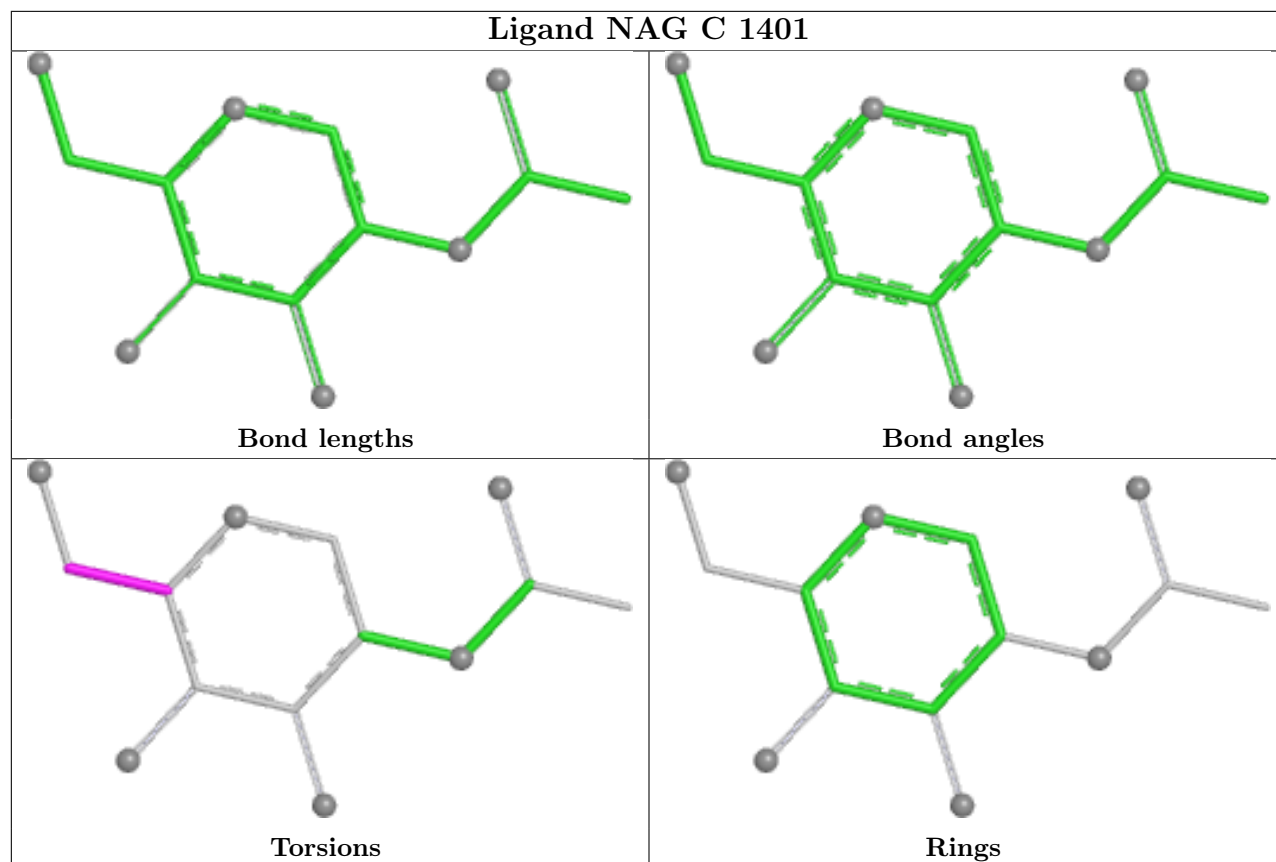


Ligand NAG B 1403



Ligand NAG B 1408





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

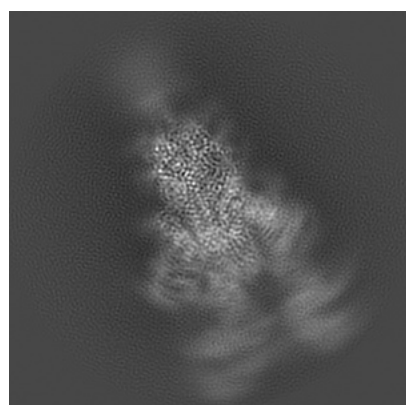
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-30899. These allow visual inspection of the internal detail of the map and identification of artifacts.

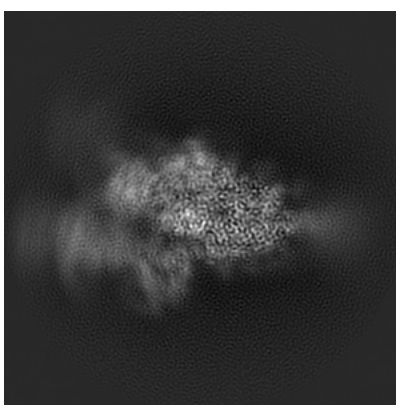
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

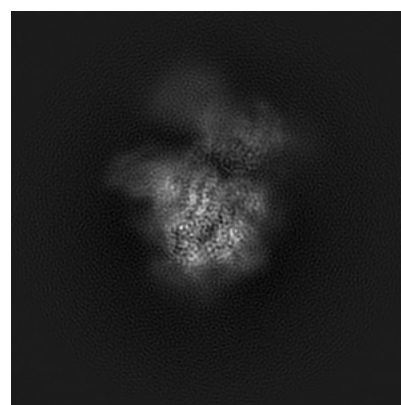
6.1.1 Primary map



X



Y

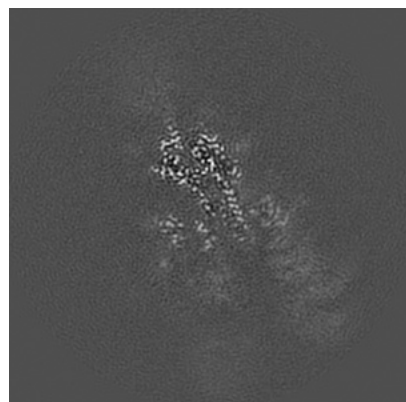


Z

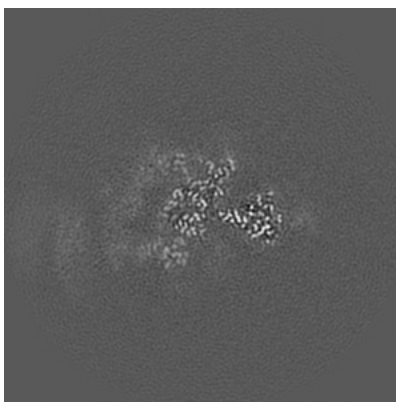
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

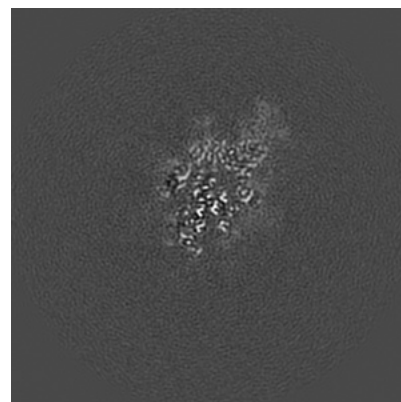
6.2.1 Primary map



X Index: 144



Y Index: 144

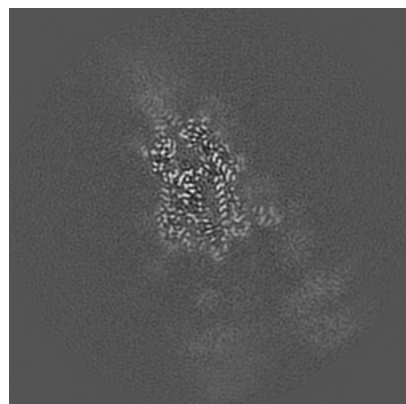


Z Index: 144

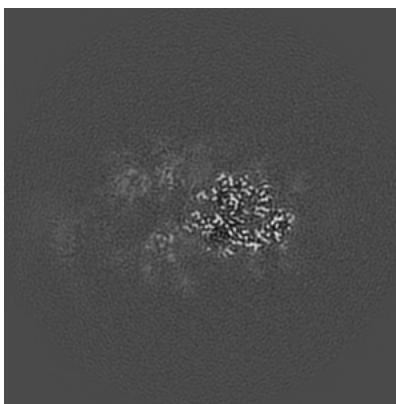
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

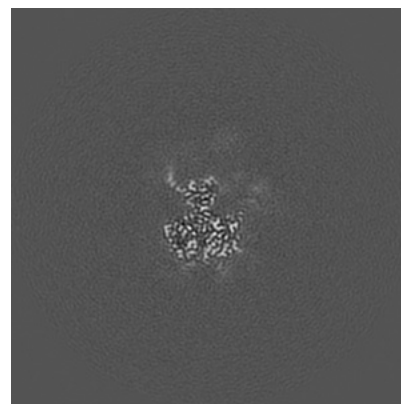
6.3.1 Primary map



X Index: 132



Y Index: 133

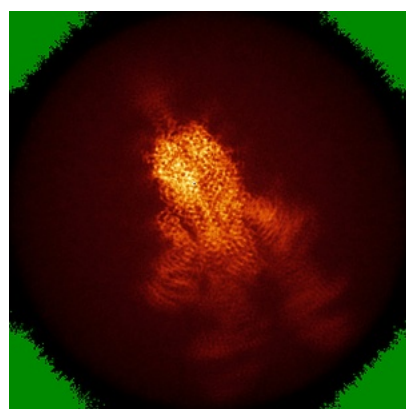


Z Index: 167

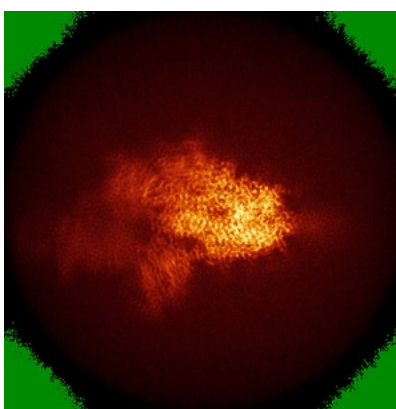
The images above show the largest variance slices of the map in three orthogonal directions.

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

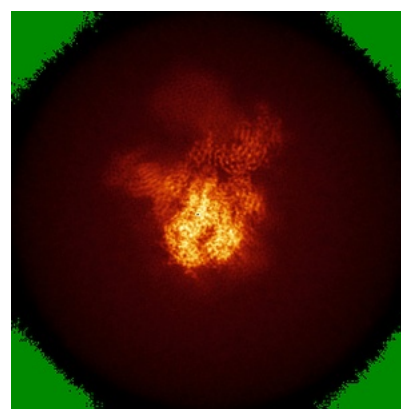
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.018. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

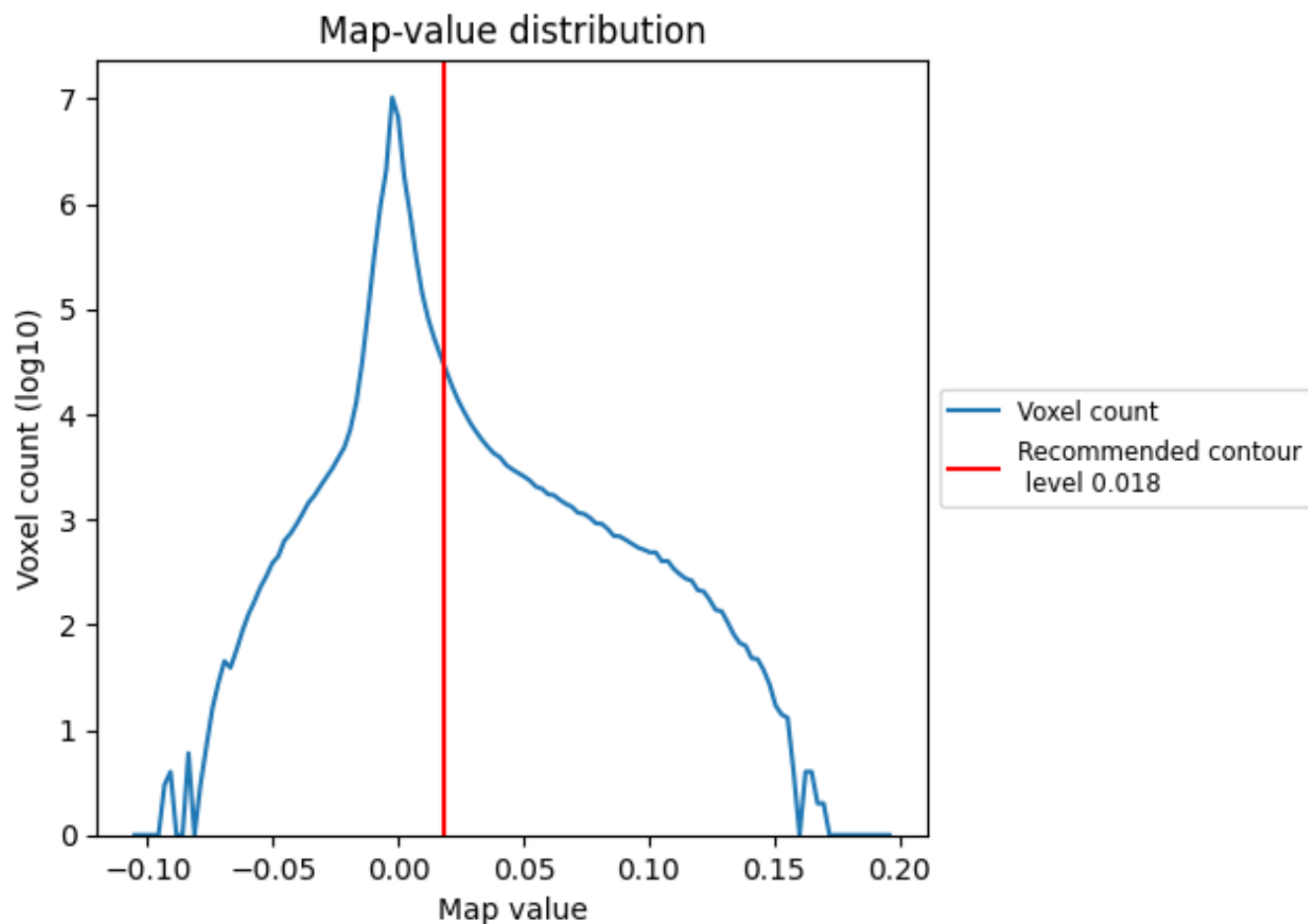
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

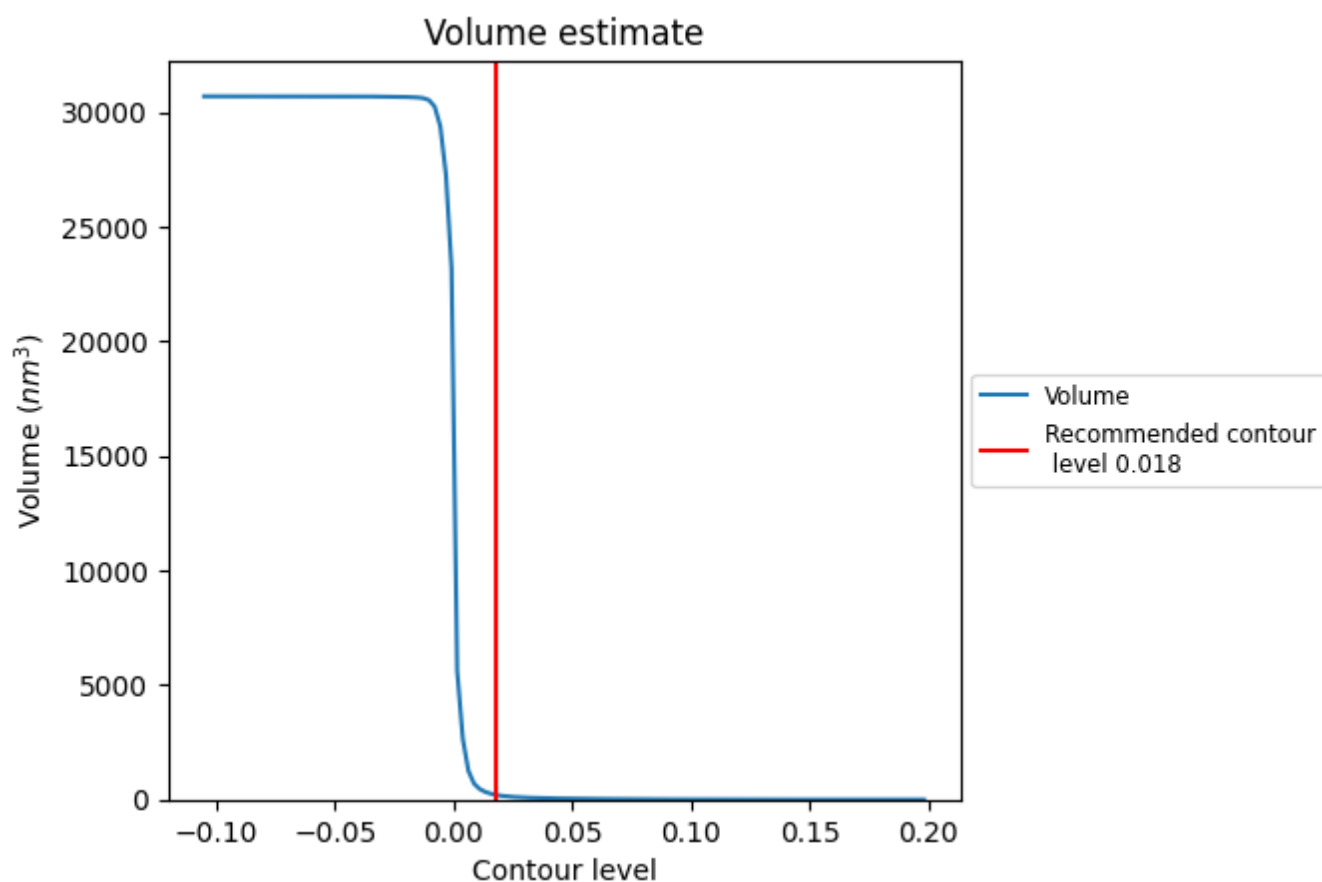
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

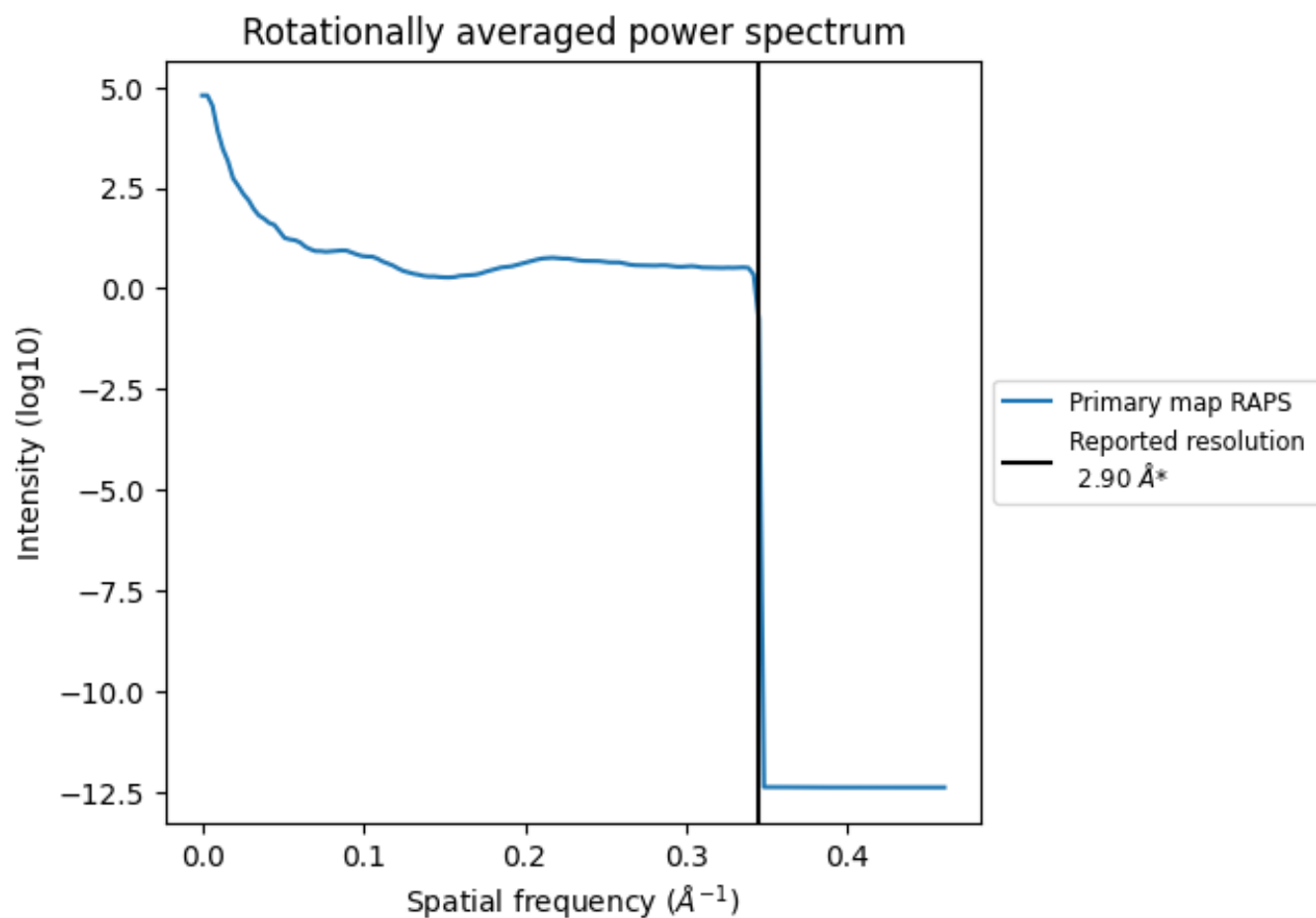
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 204 nm^3 ; this corresponds to an approximate mass of 184 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.345 Å⁻¹

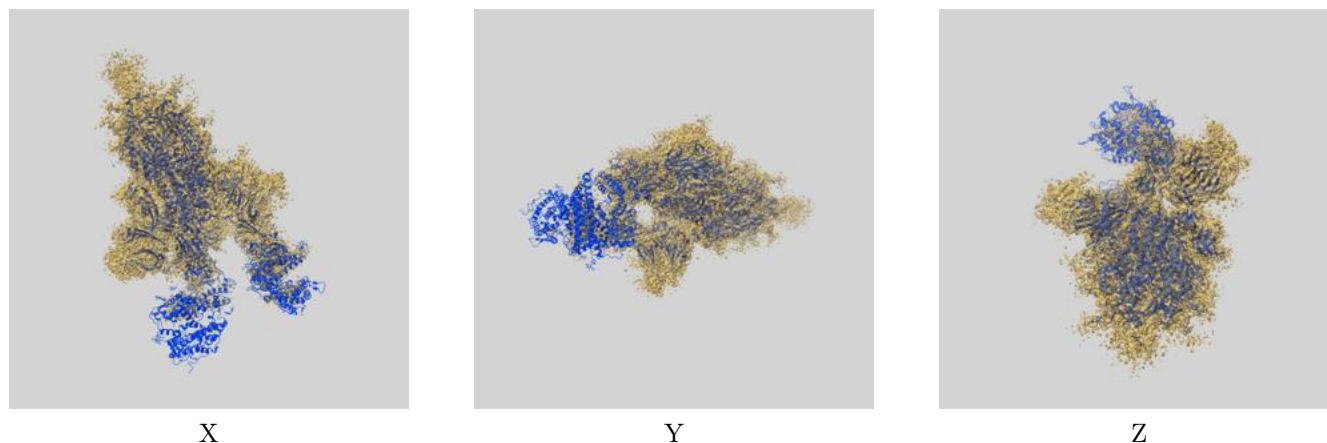
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

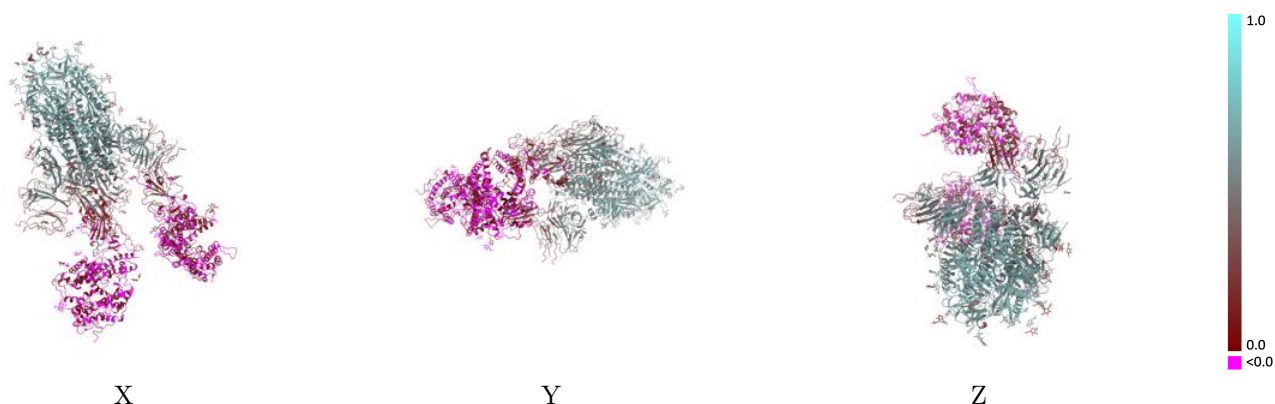
This section contains information regarding the fit between EMDB map EMD-30899 and PDB model 7DX8. Per-residue inclusion information can be found in [section 3](#) on [page 11](#).

9.1 Map-model overlay [i](#)



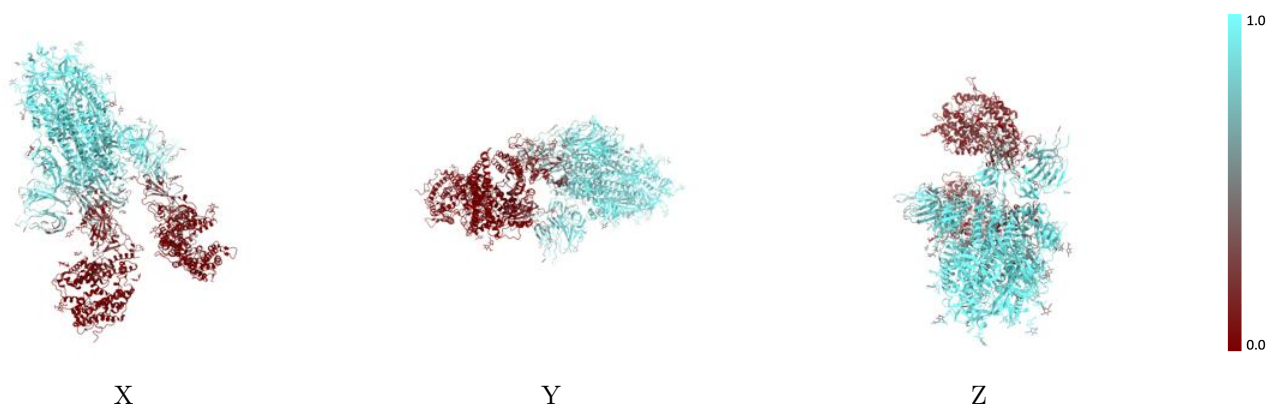
The images above show the 3D surface view of the map at the recommended contour level 0.018 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



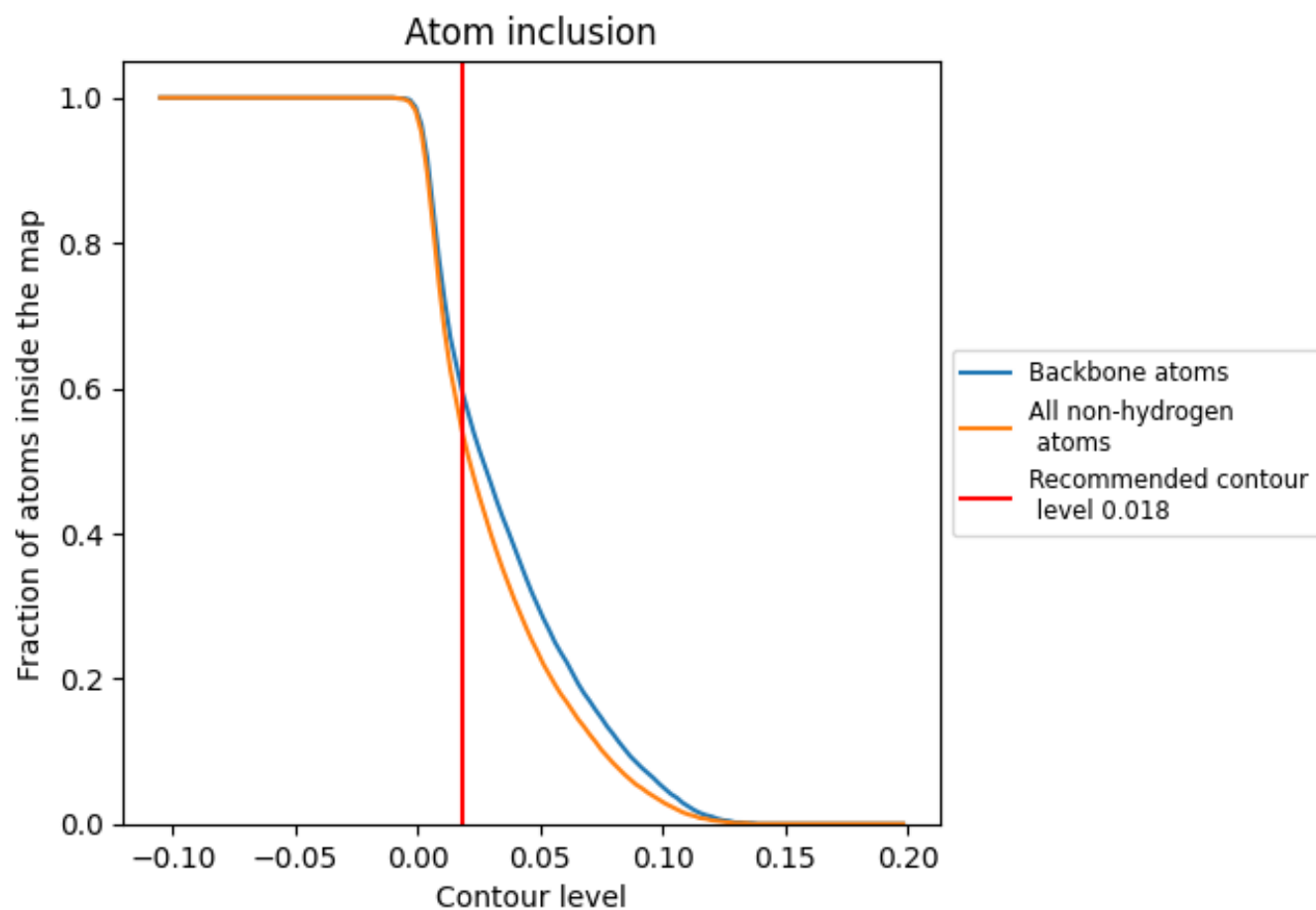
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.018).

9.4 Atom inclusion [i](#)



At the recommended contour level, 60% of all backbone atoms, 54% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.018) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5440	 0.3260
A	 0.7550	 0.4550
B	 0.7950	 0.4820
C	 0.7390	 0.4400
D	 0.0270	 0.0150
E	 0.0130	 0.0070
F	 0.5000	 0.2070
G	 0.2860	 0.2920
H	 0.9290	 0.5270
I	 0.8210	 0.3920
J	 0.6790	 0.4650
K	 0.8570	 0.4920
L	 0.7860	 0.3800
M	 0.4290	 0.1450
N	 0.1070	 0.0750
O	 0.6430	 0.2710
P	 0.8930	 0.4990
Q	 0.7860	 0.3950
R	 0.7500	 0.4590
S	 0.7500	 0.3730
T	 0.4290	 0.2830
U	 0.0710	 -0.0220
V	 0.6430	 0.3340
W	 0.8570	 0.5040
X	 0.7500	 0.4480
Y	 0.6430	 0.3680
Z	 0.8210	 0.4550
a	 0.7500	 0.4460
b	 0.0360	 0.0860
c	 0.0000	 -0.0140
d	 0.0000	 0.0290
e	 0.0000	 0.0820
f	 0.0000	 -0.0280
g	 0.0000	 -0.0920
h	 0.0000	 0.0400



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
i	 0.0000	 0.1070
j	 0.0000	 -0.0520
k	 0.0000	 0.0290