



wwPDB EM Validation Summary Report i

Nov 22, 2022 – 02:21 AM JST

PDB ID : 7DX8
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 i symbol.

The types of validation reports are described at
<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references](#) ①) were used in the production of this report:

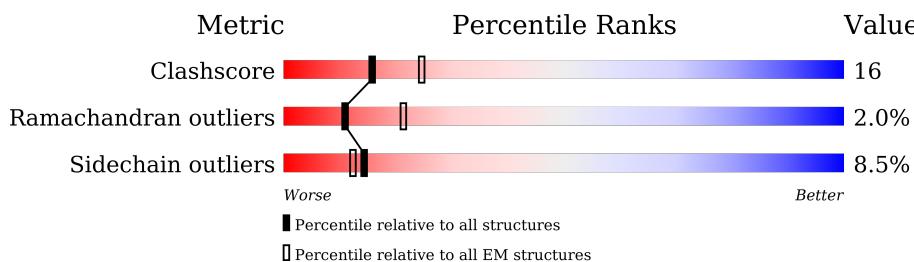
EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.3

1 Overall quality at a glance

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

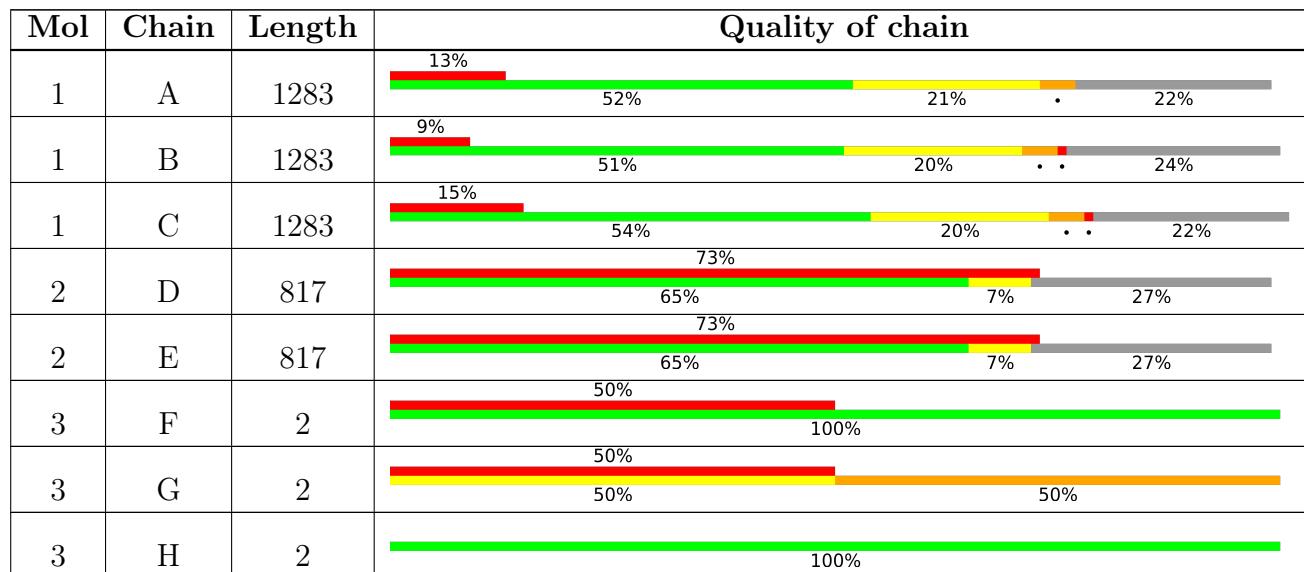
The reported resolution of this entry is 2.90 Å.

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.



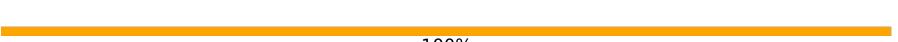
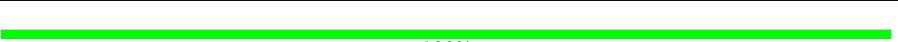
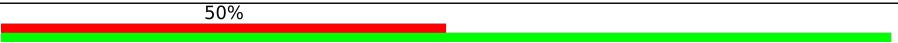
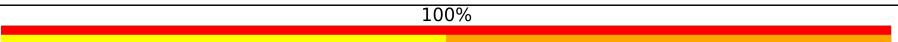
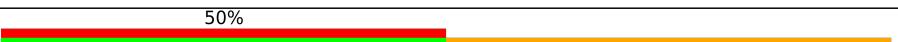
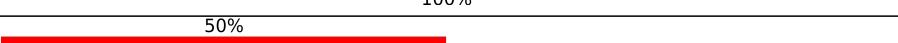
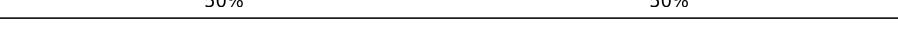
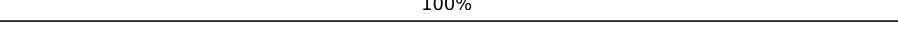
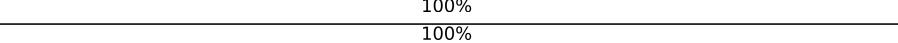
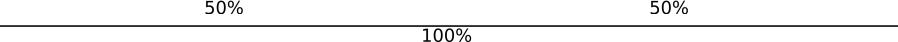
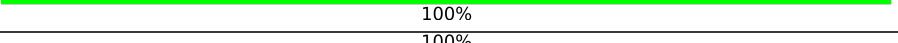
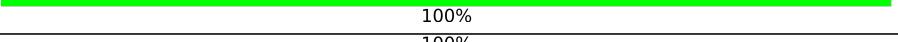
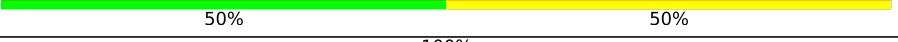
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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



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Mol	Chain	Length	Quality of chain
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	
3	e	2	
3	f	2	
3	g	2	

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

2 Entry composition (i)

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

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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
			Total	C	N	O	S		
2	D	595	4857	3108	804	916	29	0	0
2	E	595	4857	3108	804	916	29	0	0

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

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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-aacetamido-2-deoxy-beta-D-glucopyranose.



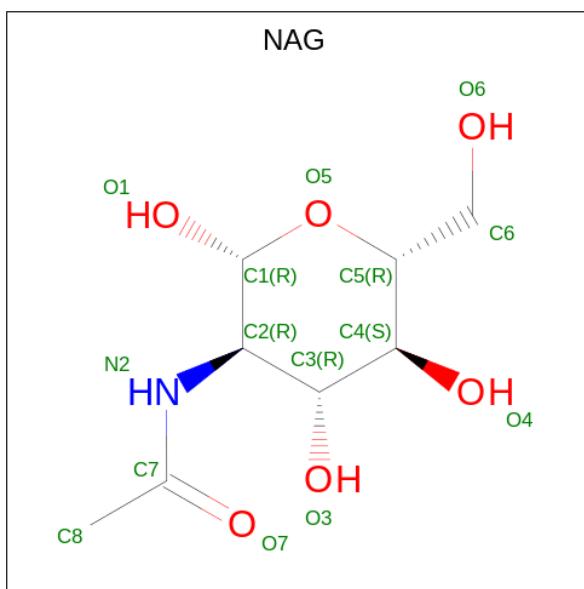
Mol	Chain	Residues	Atoms				AltConf	Trace
3	F	2	Total	C	N	O	0	0
			28	16	2	10		
3	G	2	Total	C	N	O	0	0
			28	16	2	10		
3	H	2	Total	C	N	O	0	0
			28	16	2	10		
3	I	2	Total	C	N	O	0	0
			28	16	2	10		
3	J	2	Total	C	N	O	0	0
			28	16	2	10		
3	K	2	Total	C	N	O	0	0
			28	16	2	10		
3	L	2	Total	C	N	O	0	0
			28	16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

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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 (three-letter code: NAG) (formula: C₈H₁₅NO₆) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
4	A	1	Total 126	C 72	N 9	O 45	0
4	A	1	Total 126	C 72	N 9	O 45	0
4	A	1	Total 126	C 72	N 9	O 45	0
4	A	1	Total 126	C 72	N 9	O 45	0
4	A	1	Total 126	C 72	N 9	O 45	0
4	A	1	Total 126	C 72	N 9	O 45	0
4	A	1	Total 126	C 72	N 9	O 45	0
4	A	1	Total 126	C 72	N 9	O 45	0
4	B	1	Total 140	C 80	N 10	O 50	0
4	B	1	Total 140	C 80	N 10	O 50	0
4	B	1	Total 140	C 80	N 10	O 50	0
4	B	1	Total 140	C 80	N 10	O 50	0
4	B	1	Total 140	C 80	N 10	O 50	0

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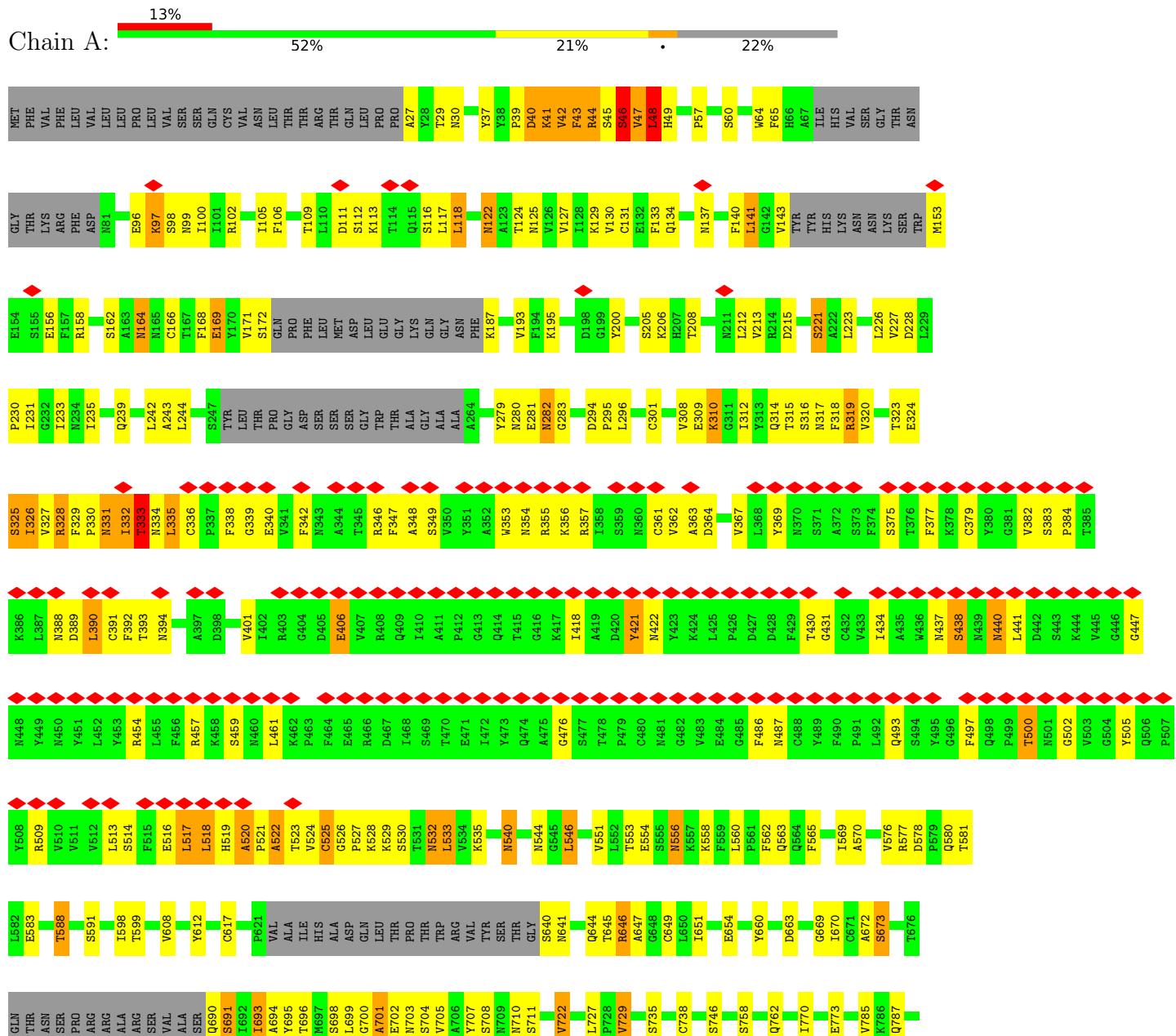
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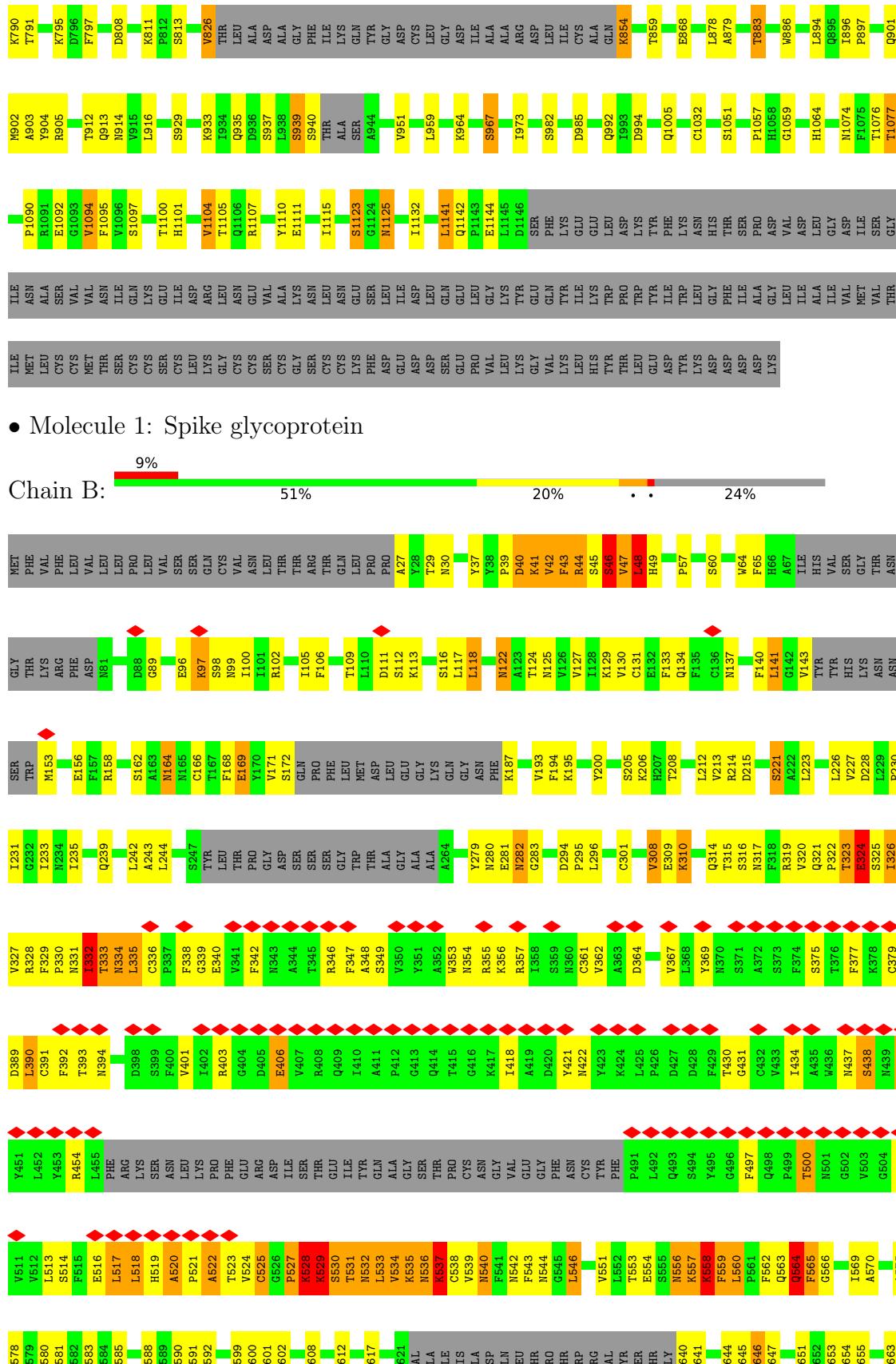
Mol	Chain	Residues	Atoms				AltConf
4	B	1	Total	C	N	O	0
			140	80	10	50	
4	B	1	Total	C	N	O	0
			140	80	10	50	
4	B	1	Total	C	N	O	0
			140	80	10	50	
4	B	1	Total	C	N	O	0
			140	80	10	50	
4	B	1	Total	C	N	O	0
			140	80	10	50	
4	C	1	Total	C	N	O	0
			112	64	8	40	
4	C	1	Total	C	N	O	0
			112	64	8	40	
4	C	1	Total	C	N	O	0
			112	64	8	40	
4	C	1	Total	C	N	O	0
			112	64	8	40	
4	C	1	Total	C	N	O	0
			112	64	8	40	
4	C	1	Total	C	N	O	0
			112	64	8	40	
4	D	1	Total	C	N	O	0
			14	8	1	5	
4	E	1	Total	C	N	O	0
			14	8	1	5	

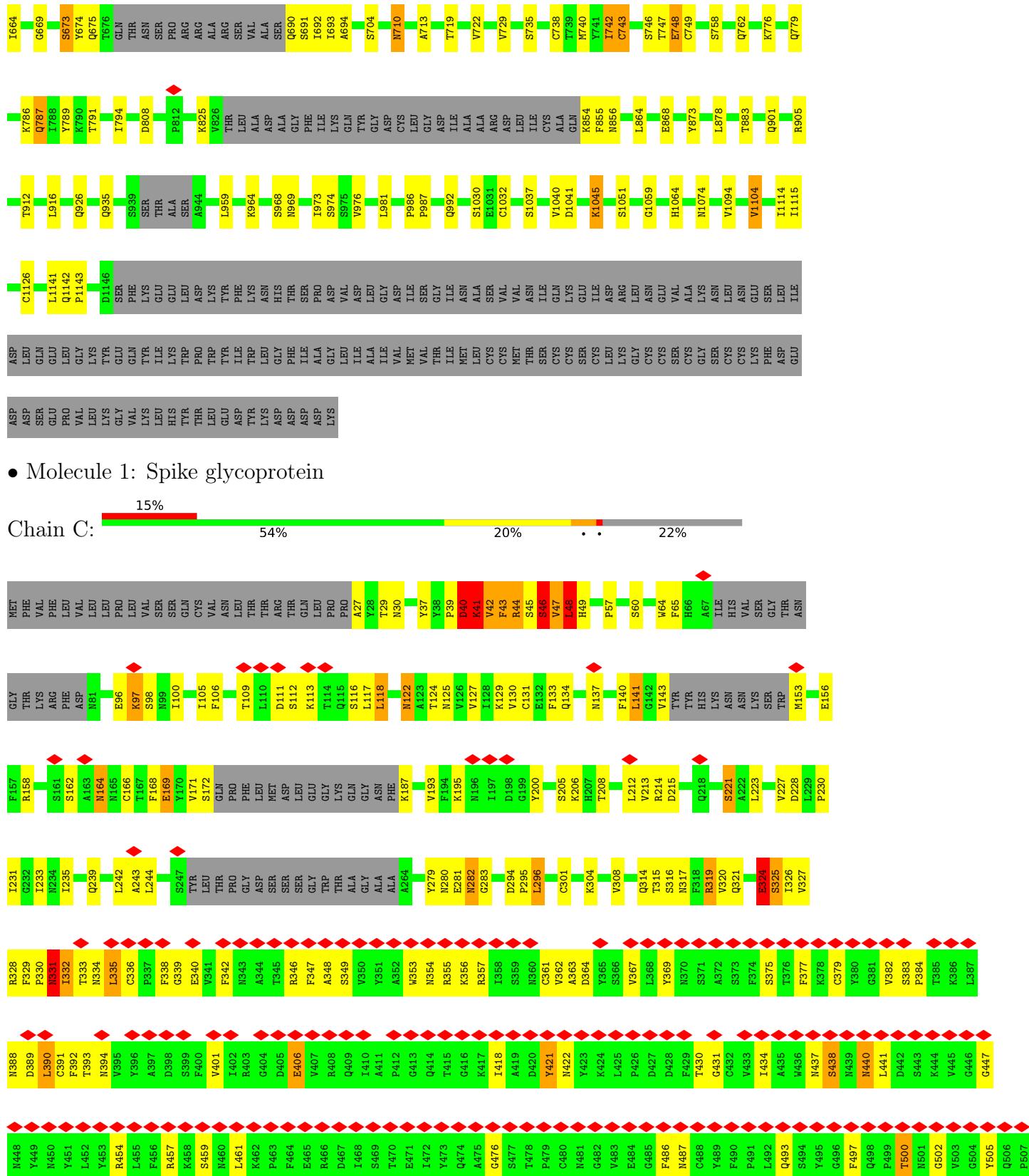
3 Residue-property plots

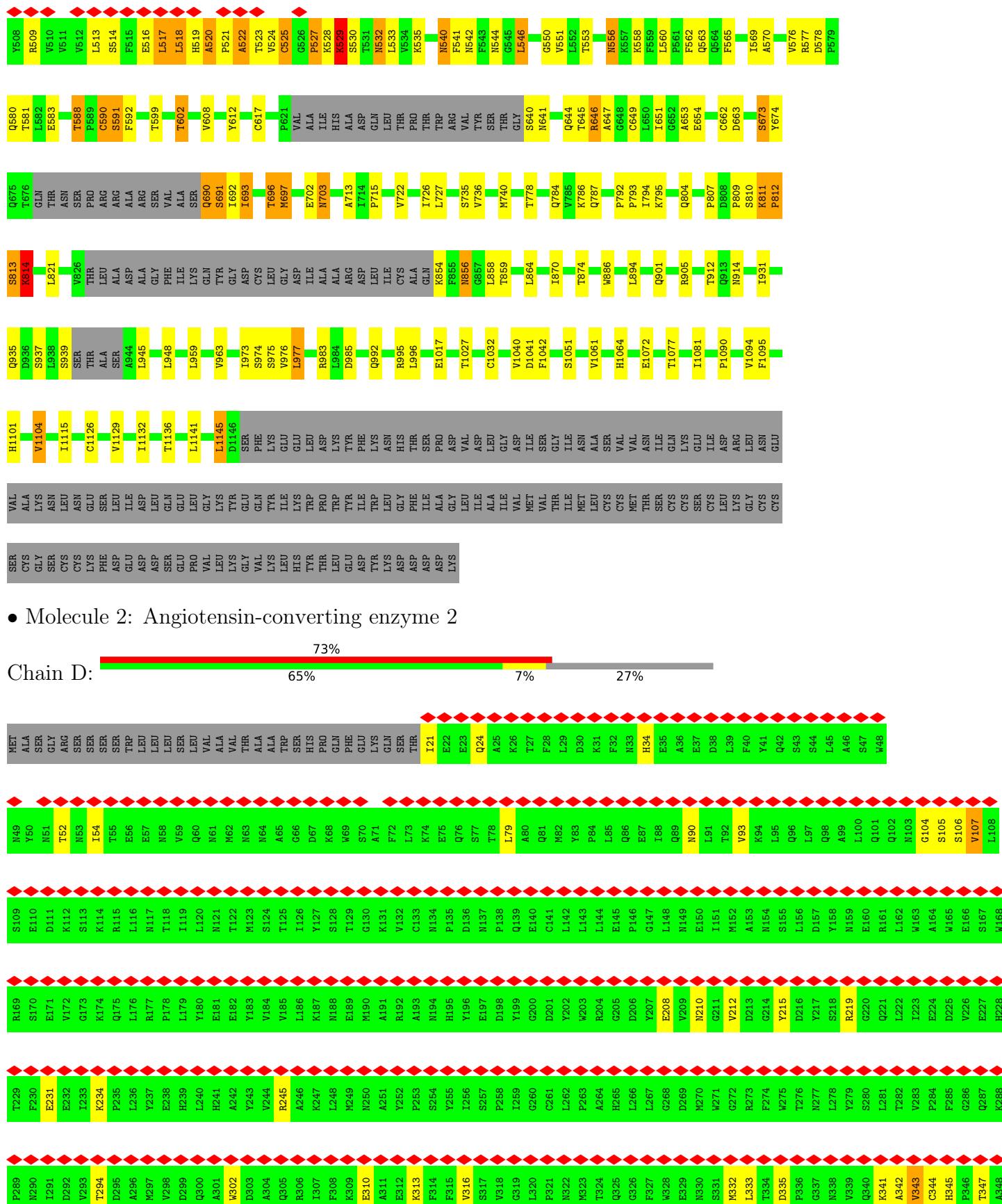
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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



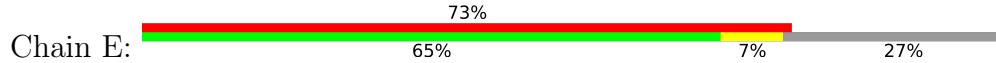






R169	S109	N49	L529	W349
S170	E110	Y50	C530	D350
E171	D111	N51	Q531	L361
E232	E233	V172	T52	A411
K234	K233	G173	SER	A412
V293	I233	K174	SER	A413
T294	K234	K174	SER	K353
D292	N290	R175	I54	G354
N299	V298	P175	SER	G355
D299	H239	P235	SER	D365
D295	Q300	L236	T55	F356
A296	L236	L176	E56	K416
M297	Y237	R177	E57	K417
V298	E238	P178	N58	R357
H239	L240	L179	V59	L418
Q300	A301	L120	Y180	L358
A301	H241	E181	N121	K419
W302	A242	E182	T122	T414
D303	Y243	Y183	M62	T415
A304	V244	V184	N63	D471
R305	R245	V185	N64	D472
B306	A246	L186	G66	Q472
I307	K247	K187	D67	Q473
F308	L248	S123	F68	Q474
K309	M249	E188	N65	Q475
E310	N250	M190	T125	Q476
A311	A251	A191	T126	Q477
E312	Y252	R192	G67	Q478
K313	P253	C193	F72	Q479
F314	S254	N194	L73	Q480
E315	Y255	H195	T129	Q481
V316	I256	Y196	K74	Q482
S317	S257	E197	K75	Q483
K318	P258	D198	E76	Q484
G319	I259	Y199	T77	Q485
L320	G260	G200	E75	Q486
P321	C261	D201	A80	Q487
M322	L262	Y202	C81	Q488
M323	P263	W203	P146	Q489
T324	A264	R204	L144	Q490
Q325	H265	G205	E145	Q491
G326	L266	D206	P146	Q492
F327	L267	Y207	G147	Q493
W328	G268	E208	L148	Q494
E329	D269	V209	M149	Q495
N330	M270	N210	E150	Q496
S331	W271	G211	I151	Q497
M332	G272	V212	M152	Q498
L333	R273	D213	A153	Q499
T334	F274	G214	M154	Q500
D335	W275	Y215	S155	Q501
P336	T276	D216	L156	Q502
G337	N277	Y217	D157	Q503
N338	L278	S218	Y158	Q504
V339	Y279	R219	N159	Q505
C344	A284	E224	A164	Q506
H345	F285	S280	E160	Q507
P346	G286	L281	K161	Q508
T347	Q287	E227	E166	Q509
A348	K288	H228	W168	Q510

- Molecule 2: Angiotensin-converting enzyme 2



N49	L529	W349
E110	Y50	D350
D111	N51	L361
V172	K112	A411
G173	S113	A412
K174	K114	A413
R175	R115	K353
P176	T55	K354
Q175	E56	G355
L176	E57	D365
L116	E57	F356
M117	E57	K416
T118	N58	K417
I119	V59	R357
L120	Q60	L418
Y180	Y181	L358
E181	N121	K419
E182	T122	T414
Y183	M62	T415
M123	N63	D471
E188	N64	D472
S124	G66	Q472
T125	A65	Q473
L126	G66	Q474
K187	D67	Q475
S128	K68	Q476
T129	W69	Q477
E189	T70	Q478
M130	G70	Q479
A191	A71	Q480
K192	F72	Q481
C193	L73	Q482
N194	K74	Q483
H195	E75	Q484
P136	E75	Q485
D136	Q76	Q486
E197	S77	Q487
M137	S77	Q488
C133	A25	Q489
T138	T78	Q490
Q139	L79	Q491
E222	E223	Q492
E223	E224	Q493
Q24	Q24	Q494
THR	THR	Q495
A225	A226	Q496
T226	T227	Q497
V227	V228	Q498
A228	A229	Q499
G229	G230	Q500
H230	H231	Q501
C261	D201	Q502
C262	L262	Q503
L262	Y202	Q504
Y202	M149	Q505
W203	L143	Q506
L143	Y83	Q507
D204	P84	Q508
A264	P84	Q509
E145	L85	Q510
C141	Q81	Q511
L142	M82	Q512
M142	D30	Q513
L143	D30	Q514
K31	K31	Q515
E144	P84	Q516
E145	F32	Q517
C205	F32	Q518
D206	N33	Q519
P146	Q86	Q520
G147	E87	Q521
M147	E87	Q522
L148	I88	Q523
E208	E35	Q524
L148	I88	Q525
M149	A36	Q526
V209	A36	Q527
N210	N90	Q528
G211	L91	Q529
M152	T92	Q530
A153	V93	Q531
D213	V93	Q532
F274	K94	Q533
W275	Y215	Q534
S276	D216	Q535
N277	Y217	Q536
L278	S218	Q537
E224	G220	Q538
S280	G220	Q539
L281	K221	Q540
T282	L222	Q541
V283	I223	Q542
Y279	R219	Q543
N159	A99	Q544
E160	L100	Q545
K161	Q101	Q546
L162	Q102	Q547
W168	N103	Q548

SER	LYS	E539	P469	S409	W349
ARG	ALA	P530	K470	L410	D350
ILE	MET	I531	D471	L411	L351
ASN	ARG	L591	Q472	A412	G352
ASP	GLN	F592			
ALA	ALA				
TYR	TYR	T533	W473	K353	
PHE	PHENYL ALANINE	I534	K474	T414	G354
LEU	LEU	I535	K475	P415	D355
LYS	GLY	I536	K476	K416	F356
VAL	ASN	I537	K477	H417	R357
ASP	ASP	D538	W478	L418	I358
ASN	PRO	I539	E479	K419	L359
SER	SER	I540	M480	S420	M360
ALA	ALA	I541	K481	I421	C361
GLY	GLU	I542	K482	G422	T362
GLU	GLU	I543	E483	L423	K363
GLN	GLN	V604	I484	L424	V364
PRO	ASP	G605	S545	S425	T365
THR	VAL	W606	I546	P426	M366
LEU	ARG	S607	S547	V487	D427
GLY	VAL	T608	T548	V488	F428
PRO	ALA	D609	I549	E489	Q429
PRO	ASN	I610	A550	P490	E360
ASP	GLN	P611	O551	V491	D431
GLN	ASN	P612	O552	P492	N432
PRO	PRO	I613	I553	H493	E433
ASP	SER	A614	I554	D494	T434
ILE	PHE	D615	P655	E495	E375
ASN	TRP	LEU	W616	E496	M376
PRO	PRO	ILE	I617	T496	G377
THR	THR	VAL	I618	Y497	N437
SER	SER	VAL	I619	S502	D382
ASP	ASP	VAL	I620	L503	M383
ILE	PHE	VAL	I621	D499	L439
ALA	GLN	PRO	I622	P500	L440
VAL	TRP	ILE	I623	A501	K441
ASP	ASP	VAL	I624	P502	Q442
ILE	ILE	VAL	I625	C498	F438
LYS	LYS	VAL	I626	F504	A443
VAL	VAL	VAL	I627	L505	L444
PRO	PRO	VAL	I628	H505	T445
ILE	ILE	VAL	I629	P506	V485
VAL	VAL	VAL	I630	A507	Y381
ASP	ASP	VAL	I631	P508	
ILE	ILE	VAL	I632	I509	
VAL	VAL	VAL	I633	V506	
ASP	ASP	VAL	I634	S507	
ILE	ILE	VAL	I635	N508	
VAL	VAL	VAL	I636	D509	
ALA	ALA	VAL	I637	T513	
VAL	VAL	VAL	I638	T449	
ILE	ILE	VAL	I639	R514	
VAL	VAL	VAL	I640	Y454	
ASP	ASP	VAL	I641		
ILE	ILE	VAL	I642		
VAL	VAL	VAL	I643		
ASP	ASP	VAL	I644		
ILE	ILE	VAL	I645		
VAL	VAL	VAL	I646		
ASP	ASP	VAL	I647		
ILE	ILE	VAL	I648		
VAL	VAL	VAL	I649		
ASP	ASP	VAL	I650		
ILE	ILE	VAL	I651		
VAL	VAL	VAL	I652		
ASP	ASP	VAL	I653		
ILE	ILE	VAL	I654		
VAL	VAL	VAL	I655		
ASP	ASP	VAL	I656		
ILE	ILE	VAL	I657		
VAL	VAL	VAL	I658		
ASP	ASP	VAL	I659		
ILE	ILE	VAL	I660		
VAL	VAL	VAL	I661		
ASP	ASP	VAL	I662		
ILE	ILE	VAL	I663		
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VAL	VAL	VAL	I670		
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VAL	VAL	VAL	I679		
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ILE	ILE	VAL	I681		
VAL	VAL	VAL	I682		
ASP	ASP	VAL	I683		
ILE	ILE	VAL	I684		
VAL	VAL	VAL	I685		
ASP	ASP	VAL	I686		
ILE	ILE	VAL	I687		
VAL	VAL	VAL	I688		
ASP	ASP	VAL	I689		
ILE	ILE	VAL	I690		
VAL	VAL	VAL	I691		
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ILE	ILE	VAL	I693		
VAL	VAL	VAL	I694		
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VAL	VAL	VAL	I703		
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VAL	VAL	VAL	I736		
ASP	ASP	VAL	I737		
ILE	ILE	VAL	I738		
VAL	VAL	VAL	I739		
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VAL	VAL	VAL	I751		
ASP	ASP	VAL	I752		
ILE	ILE	VAL	I753		
VAL	VAL	VAL	I754		
ASP	ASP	VAL	I755		
ILE	ILE	VAL	I756		
VAL	VAL	VAL	I757		
ASP	ASP	VAL	I758		
ILE	ILE	VAL	I759		
VAL	VAL	VAL	I760		
ASP	ASP	VAL	I761		
ILE	ILE	VAL	I762		
VAL	VAL	VAL	I763		
ASP	ASP	VAL	I764		
ILE	ILE	VAL	I765		
VAL	VAL	VAL	I766		
ASP	ASP	VAL	I767		
ILE	ILE	VAL	I768		
VAL	VAL	VAL	I769		
ASP	ASP	VAL	I770		
ILE	ILE	VAL	I771		
VAL	VAL	VAL	I772		
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ILE	ILE	VAL	I783		
VAL	VAL	VAL	I784		
ASP	ASP	VAL	I785		
ILE	ILE	VAL	I786		
VAL	VAL	VAL	I787		
ASP	ASP	VAL	I788		
ILE	ILE	VAL	I789		
VAL	VAL	VAL	I790		
ASP	ASP	VAL	I791		
ILE	ILE	VAL	I792		
VAL	VAL	VAL	I793		
ASP	ASP	VAL	I794		
ILE	ILE	VAL	I795		
VAL	VAL	VAL	I796		
ASP	ASP	VAL	I797		
ILE	ILE	VAL	I798		
VAL	VAL	VAL	I799		
ASP	ASP	VAL	I800		
ILE	ILE	VAL	I801		
VAL	VAL	VAL	I802		
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ILE	ILE	VAL	I825		
VAL	VAL	VAL	I826		
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ILE	ILE	VAL	I828		
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VAL	VAL	VAL	I832		
ASP	ASP	VAL	I833		
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VAL	VAL	VAL	I835		
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ILE	ILE	VAL	I849		
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ILE	ILE	VAL	I861		
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ILE	ILE	VAL	I864		
VAL	VAL	VAL	I865		
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ILE	ILE	VAL	I885		
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ASP	ASP	VAL	I887		
ILE	ILE	VAL	I888		
VAL	VAL	VAL	I889		
ASP	ASP	VAL	I890		
ILE	ILE	VAL	I891		
VAL	VAL	VAL	I892		
ASP	ASP	VAL	I893		</

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



MAG1 MAG2

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



The diagram consists of two identical orange rectangular boxes arranged horizontally. Each box has a small red diamond positioned above its top edge. The boxes are labeled "MAG1" and "MAG2" respectively, with "MAG1" positioned to the left of "MAG2".

- 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



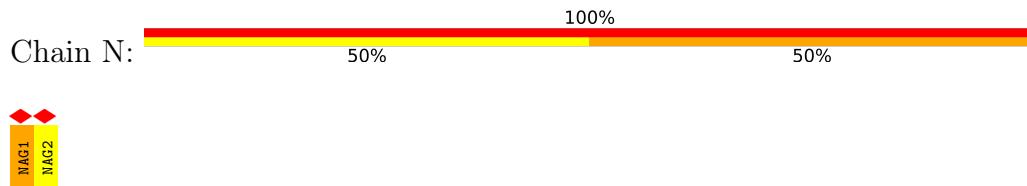
- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- 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



- 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



- 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



- 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 i

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	0.58	0/8048	0.55	0/10947
1	B	0.57	0/7751	0.55	0/10544
1	C	0.58	0/8042	0.54	0/10939
2	D	0.35	0/4994	0.50	0/6785
2	E	0.35	0/4994	0.50	0/6785
All	All	0.52	0/33829	0.54	0/46000

There are no bond length outliers.

There are no bond angle outliers.

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	335	0
1	B	7584	0	7402	364	0
1	C	7866	0	7663	373	0
2	D	4857	0	4624	66	0
2	E	4857	0	4624	67	0
3	F	28	0	25	0	0
3	G	28	0	25	3	0
3	H	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	I	28	0	25	6	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	0	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	0	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
All	All	34338	0	33157	1090	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 1090 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	989/1283 (77%)	876 (89%)	91 (9%)	22 (2%)	6 24
1	B	951/1283 (74%)	823 (86%)	98 (10%)	30 (3%)	4 16
1	C	988/1283 (77%)	866 (88%)	96 (10%)	26 (3%)	5 20
2	D	593/817 (73%)	563 (95%)	28 (5%)	2 (0%)	41 71
2	E	593/817 (73%)	563 (95%)	28 (5%)	2 (0%)	41 71
All	All	4114/5483 (75%)	3691 (90%)	341 (8%)	82 (2%)	11 27

5 of 82 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	A	518	LEU

5.3.2 Protein sidechains [\(i\)](#)

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

entries.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	882/1122 (79%)	776 (88%)	106 (12%)	5 15
1	B	850/1122 (76%)	746 (88%)	104 (12%)	5 15
1	C	881/1122 (78%)	792 (90%)	89 (10%)	7 23
2	D	525/721 (73%)	518 (99%)	7 (1%)	69 90
2	E	525/721 (73%)	518 (99%)	7 (1%)	69 90
All	All	3663/4808 (76%)	3350 (92%)	313 (8%)	14 31

5 of 313 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	301	CYS
1	C	974	SER
1	C	331	ASN
1	C	540	ASN
2	D	344	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 102 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	188	ASN
1	C	703	ASN
2	E	472	GLN
1	C	317	ASN
1	C	540	ASN

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	1,3	14,14,15	0.55	0	17,19,21	0.50	0
3	NAG	F	2	3	14,14,15	0.24	0	17,19,21	0.58	0
3	NAG	G	1	1,3	14,14,15	0.58	1 (7%)	17,19,21	0.56	0
3	NAG	G	2	3	14,14,15	0.30	0	17,19,21	0.46	0
3	NAG	H	1	1,3	14,14,15	0.31	0	17,19,21	0.62	0
3	NAG	H	2	3	14,14,15	0.53	0	17,19,21	0.48	0
3	NAG	I	1	1,3	14,14,15	0.37	0	17,19,21	0.73	0
3	NAG	I	2	3	14,14,15	0.28	0	17,19,21	1.32	2 (11%)
3	NAG	J	1	1,3	14,14,15	0.70	1 (7%)	17,19,21	0.70	0
3	NAG	J	2	3	14,14,15	0.39	0	17,19,21	1.40	3 (17%)
3	NAG	K	1	1,3	14,14,15	0.70	1 (7%)	17,19,21	0.67	0
3	NAG	K	2	3	14,14,15	0.30	0	17,19,21	0.65	0
3	NAG	L	1	1,3	14,14,15	0.25	0	17,19,21	0.69	1 (5%)
3	NAG	L	2	3	14,14,15	0.17	0	17,19,21	0.48	0
3	NAG	M	1	1,3	14,14,15	0.56	0	17,19,21	0.51	0
3	NAG	M	2	3	14,14,15	0.25	0	17,19,21	0.58	0
3	NAG	N	1	1,3	14,14,15	0.57	1 (7%)	17,19,21	0.56	0
3	NAG	N	2	3	14,14,15	0.30	0	17,19,21	0.46	0
3	NAG	O	1	1,3	14,14,15	0.32	0	17,19,21	0.40	0
3	NAG	O	2	3	14,14,15	0.37	0	17,19,21	0.35	0
3	NAG	P	1	1,3	14,14,15	0.35	0	17,19,21	1.14	1 (5%)
3	NAG	P	2	3	14,14,15	0.26	0	17,19,21	0.47	0
3	NAG	Q	1	1,3	14,14,15	0.31	0	17,19,21	0.70	1 (5%)
3	NAG	Q	2	3	14,14,15	0.21	0	17,19,21	0.39	0
3	NAG	R	1	1,3	14,14,15	0.74	1 (7%)	17,19,21	0.91	1 (5%)
3	NAG	R	2	3	14,14,15	0.34	0	17,19,21	0.70	1 (5%)
3	NAG	S	1	1,3	14,14,15	0.22	0	17,19,21	0.44	0
3	NAG	S	2	3	14,14,15	0.27	0	17,19,21	0.38	0
3	NAG	T	1	1,3	14,14,15	0.55	0	17,19,21	0.49	0
3	NAG	T	2	3	14,14,15	0.25	0	17,19,21	0.58	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	U	1	1,3	14,14,15	0.58	1 (7%)	17,19,21	0.56	0
3	NAG	U	2	3	14,14,15	0.29	0	17,19,21	0.46	0
3	NAG	V	1	1,3	14,14,15	0.23	0	17,19,21	1.36	1 (5%)
3	NAG	V	2	3	14,14,15	0.19	0	17,19,21	0.50	0
3	NAG	W	1	1,3	14,14,15	0.54	0	17,19,21	0.70	1 (5%)
3	NAG	W	2	3	14,14,15	0.38	0	17,19,21	0.46	0
3	NAG	X	1	1,3	14,14,15	0.36	0	17,19,21	0.39	0
3	NAG	X	2	3	14,14,15	0.20	0	17,19,21	0.74	0
3	NAG	Y	1	1,3	14,14,15	0.36	0	17,19,21	0.48	0
3	NAG	Y	2	3	14,14,15	0.53	0	17,19,21	1.30	1 (5%)
3	NAG	Z	1	1,3	14,14,15	0.63	1 (7%)	17,19,21	0.43	0
3	NAG	Z	2	3	14,14,15	0.32	0	17,19,21	1.36	2 (11%)
3	NAG	a	1	1,3	14,14,15	0.40	0	17,19,21	0.44	0
3	NAG	a	2	3	14,14,15	0.25	0	17,19,21	0.49	0
3	NAG	b	1	2,3	14,14,15	0.62	1 (7%)	17,19,21	0.73	0
3	NAG	b	2	3	14,14,15	0.54	0	17,19,21	0.36	0
3	NAG	c	1	2,3	14,14,15	0.41	0	17,19,21	0.65	0
3	NAG	c	2	3	14,14,15	0.27	0	17,19,21	0.69	1 (5%)
3	NAG	d	1	2,3	14,14,15	0.30	0	17,19,21	0.62	0
3	NAG	d	2	3	14,14,15	0.30	0	17,19,21	0.63	0
3	NAG	e	1	2,3	14,14,15	0.30	0	17,19,21	0.52	0
3	NAG	e	2	3	14,14,15	0.36	0	17,19,21	0.47	0
3	NAG	f	1	2,3	14,14,15	0.23	0	17,19,21	0.62	0
3	NAG	f	2	3	14,14,15	0.33	0	17,19,21	0.59	1 (5%)
3	NAG	g	1	2,3	14,14,15	0.62	1 (7%)	17,19,21	0.73	0
3	NAG	g	2	3	14,14,15	0.54	0	17,19,21	0.36	0
3	NAG	h	1	2,3	14,14,15	0.42	0	17,19,21	0.65	0
3	NAG	h	2	3	14,14,15	0.27	0	17,19,21	0.70	1 (5%)
3	NAG	i	1	2,3	14,14,15	0.30	0	17,19,21	0.62	0
3	NAG	i	2	3	14,14,15	0.29	0	17,19,21	0.63	0
3	NAG	j	1	2,3	14,14,15	0.31	0	17,19,21	0.51	0
3	NAG	j	2	3	14,14,15	0.36	0	17,19,21	0.47	0
3	NAG	k	1	2,3	14,14,15	0.22	0	17,19,21	0.62	0
3	NAG	k	2	3	14,14,15	0.32	0	17,19,21	0.59	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	1,3	-	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	1,3	-	0/6/23/26	0/1/1/1
3	NAG	G	2	3	-	4/6/23/26	0/1/1/1
3	NAG	H	1	1,3	-	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	1,3	-	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	1,3	-	2/6/23/26	0/1/1/1
3	NAG	J	2	3	-	5/6/23/26	0/1/1/1
3	NAG	K	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	K	2	3	-	3/6/23/26	0/1/1/1
3	NAG	L	1	1,3	-	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	1,3	-	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	1,3	-	0/6/23/26	0/1/1/1
3	NAG	N	2	3	-	4/6/23/26	0/1/1/1
3	NAG	O	1	1,3	-	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	1,3	-	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	1,3	-	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	1,3	-	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	1,3	-	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	1,3	-	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	1,3	-	0/6/23/26	0/1/1/1
3	NAG	U	2	3	-	4/6/23/26	0/1/1/1
3	NAG	V	1	1,3	-	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	1,3	-	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	1,3	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	X	2	3	-	1/6/23/26	0/1/1/1
3	NAG	Y	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	Y	2	3	-	5/6/23/26	0/1/1/1
3	NAG	Z	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	Z	2	3	-	4/6/23/26	0/1/1/1
3	NAG	a	1	1,3	-	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	-	4/6/23/26	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
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	-	4/6/23/26	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

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	R	1	NAG	O5-C1	-2.68	1.39	1.43
3	K	1	NAG	O5-C1	-2.55	1.39	1.43
3	J	1	NAG	O5-C1	-2.33	1.40	1.43
3	b	1	NAG	O5-C1	-2.19	1.40	1.43
3	g	1	NAG	O5-C1	-2.17	1.40	1.43

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	V	1	NAG	C2-N2-C7	4.64	129.52	122.90
3	J	2	NAG	C2-N2-C7	4.43	129.21	122.90
3	Z	2	NAG	C2-N2-C7	4.35	129.10	122.90
3	I	2	NAG	C2-N2-C7	4.29	129.00	122.90
3	Y	2	NAG	C2-N2-C7	4.28	128.99	122.90

There are no chirality outliers.

5 of 120 torsion outliers are listed below:

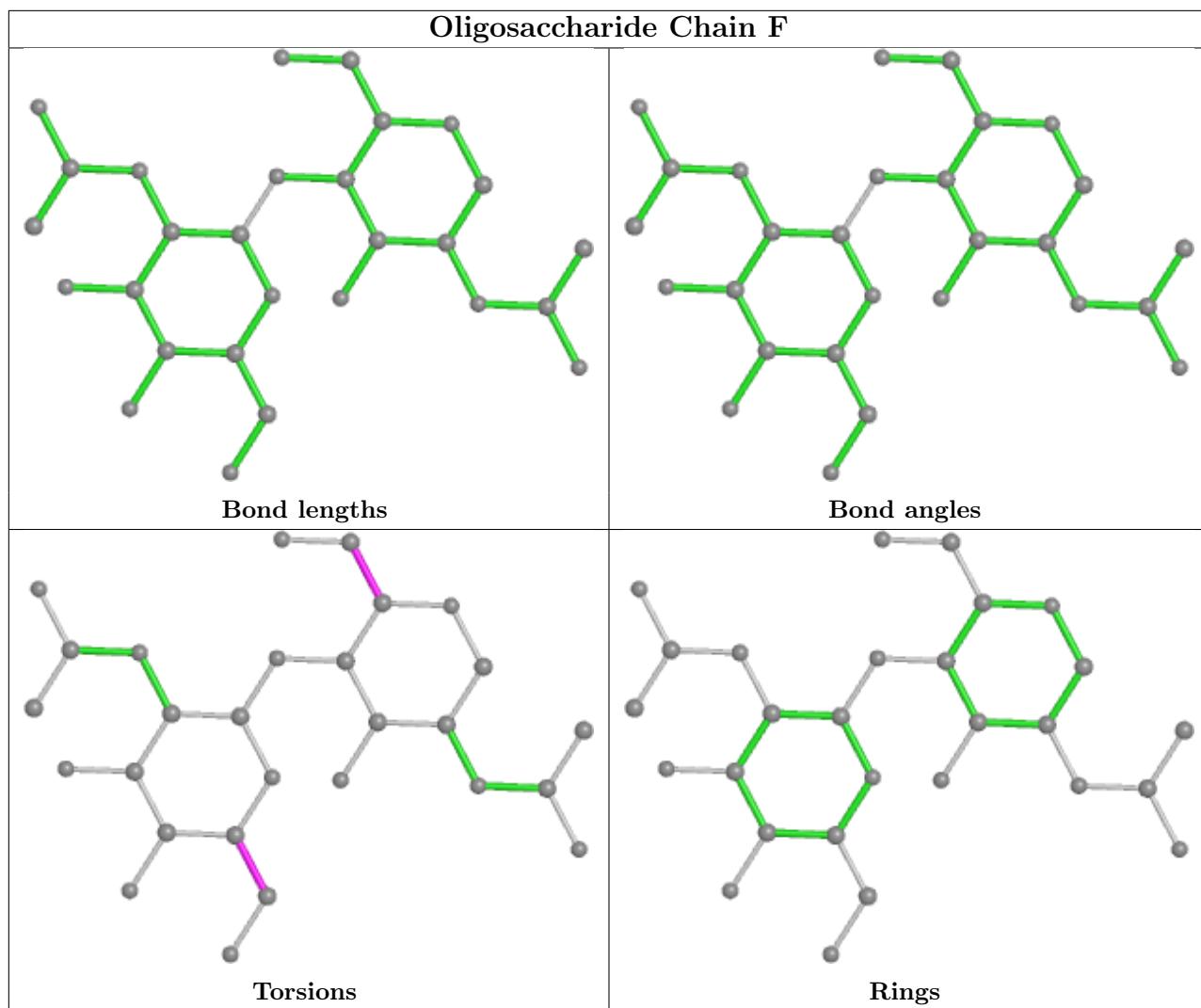
Mol	Chain	Res	Type	Atoms
3	d	1	NAG	C8-C7-N2-C2
3	d	1	NAG	O7-C7-N2-C2
3	d	2	NAG	C3-C2-N2-C7
3	d	2	NAG	C8-C7-N2-C2
3	d	2	NAG	O7-C7-N2-C2

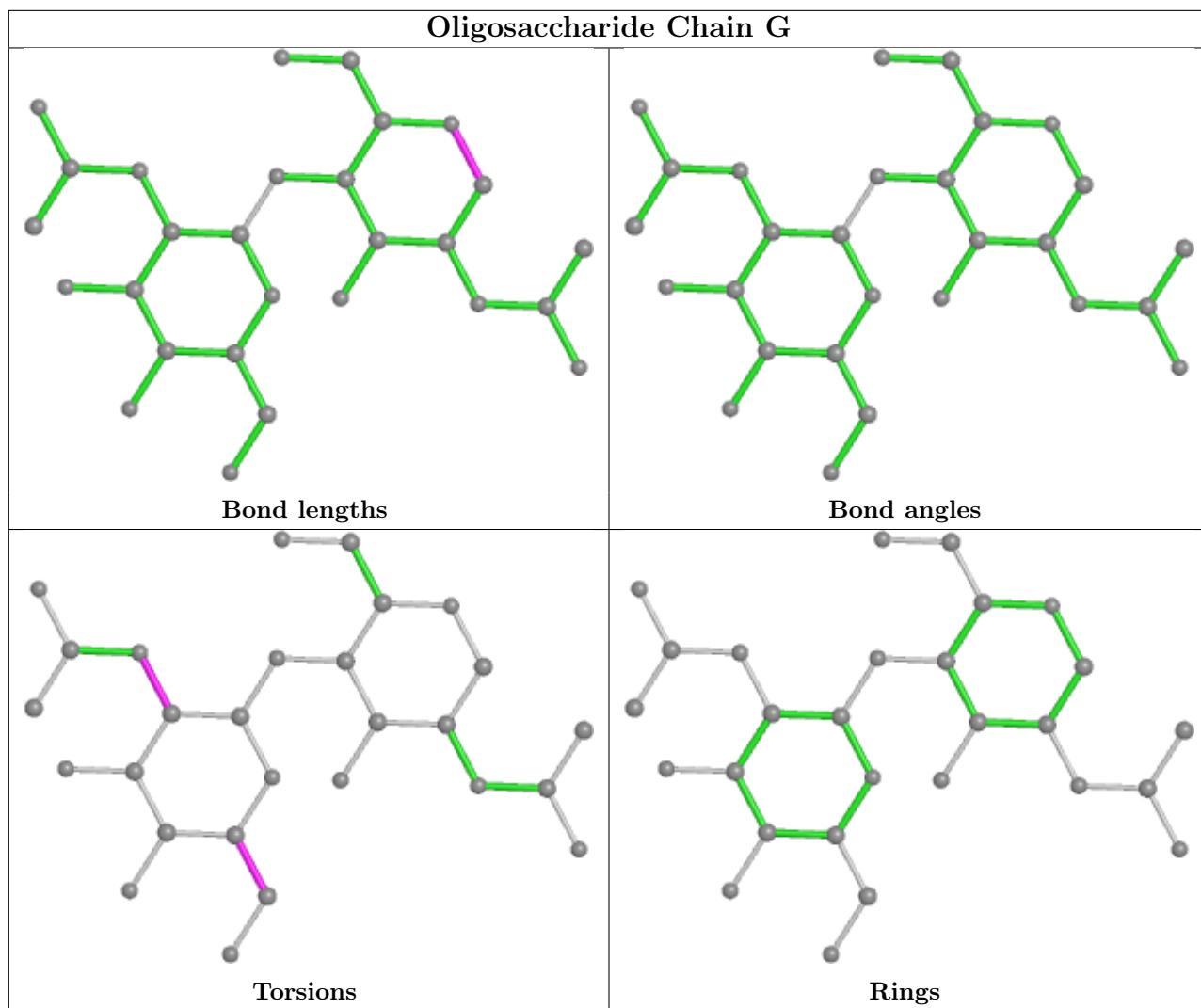
There are no ring outliers.

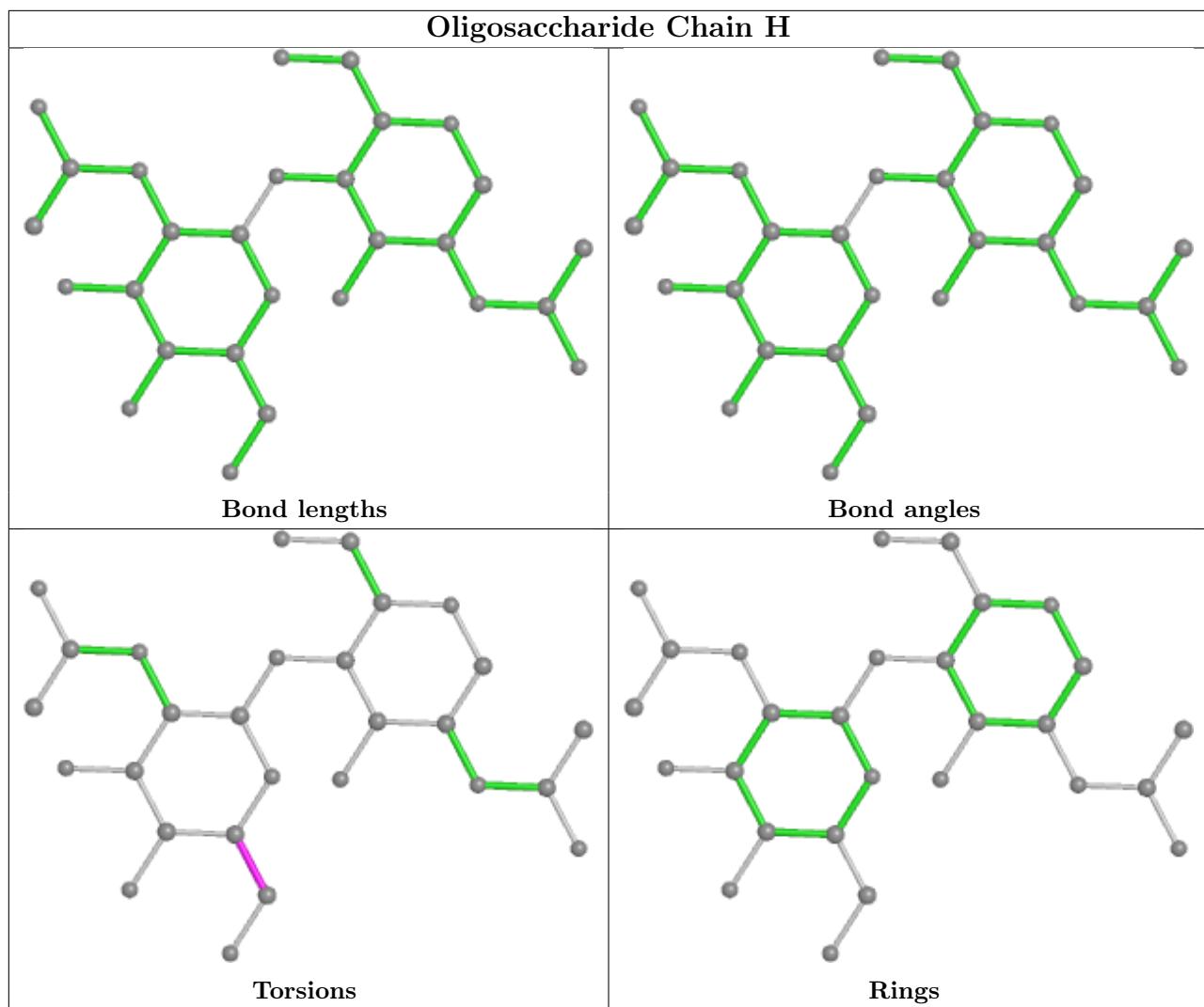
16 monomers are involved in 24 short contacts:

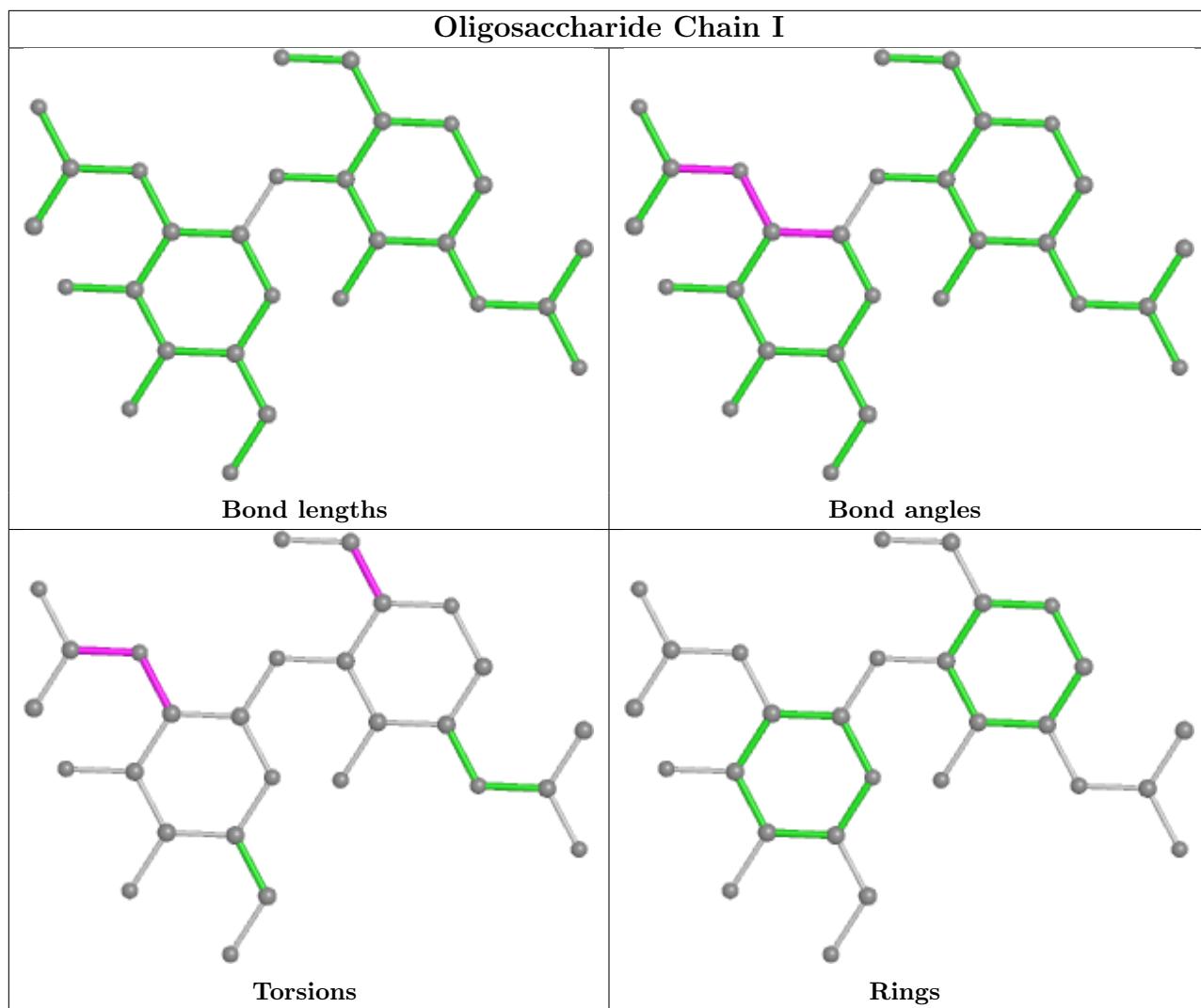
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	N	2	NAG	2	0
3	G	1	NAG	3	0
3	I	1	NAG	4	0
3	R	2	NAG	1	0
3	Z	1	NAG	1	0
3	Z	2	NAG	1	0
3	V	1	NAG	1	0
3	M	1	NAG	2	0
3	J	2	NAG	1	0
3	G	2	NAG	2	0
3	U	1	NAG	4	0
3	R	1	NAG	1	0
3	U	2	NAG	2	0
3	I	2	NAG	6	0
3	Y	2	NAG	1	0
3	N	1	NAG	3	0

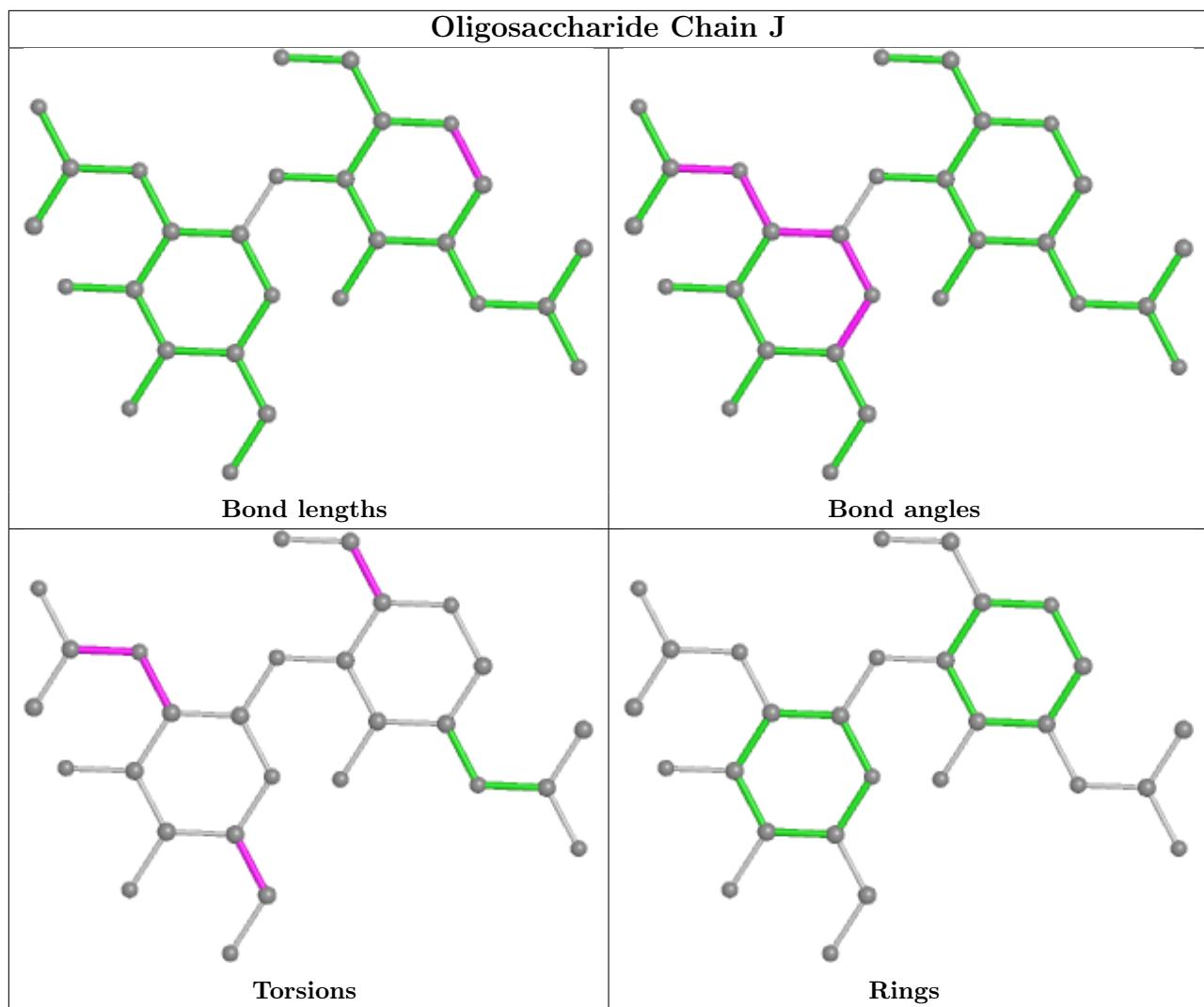
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

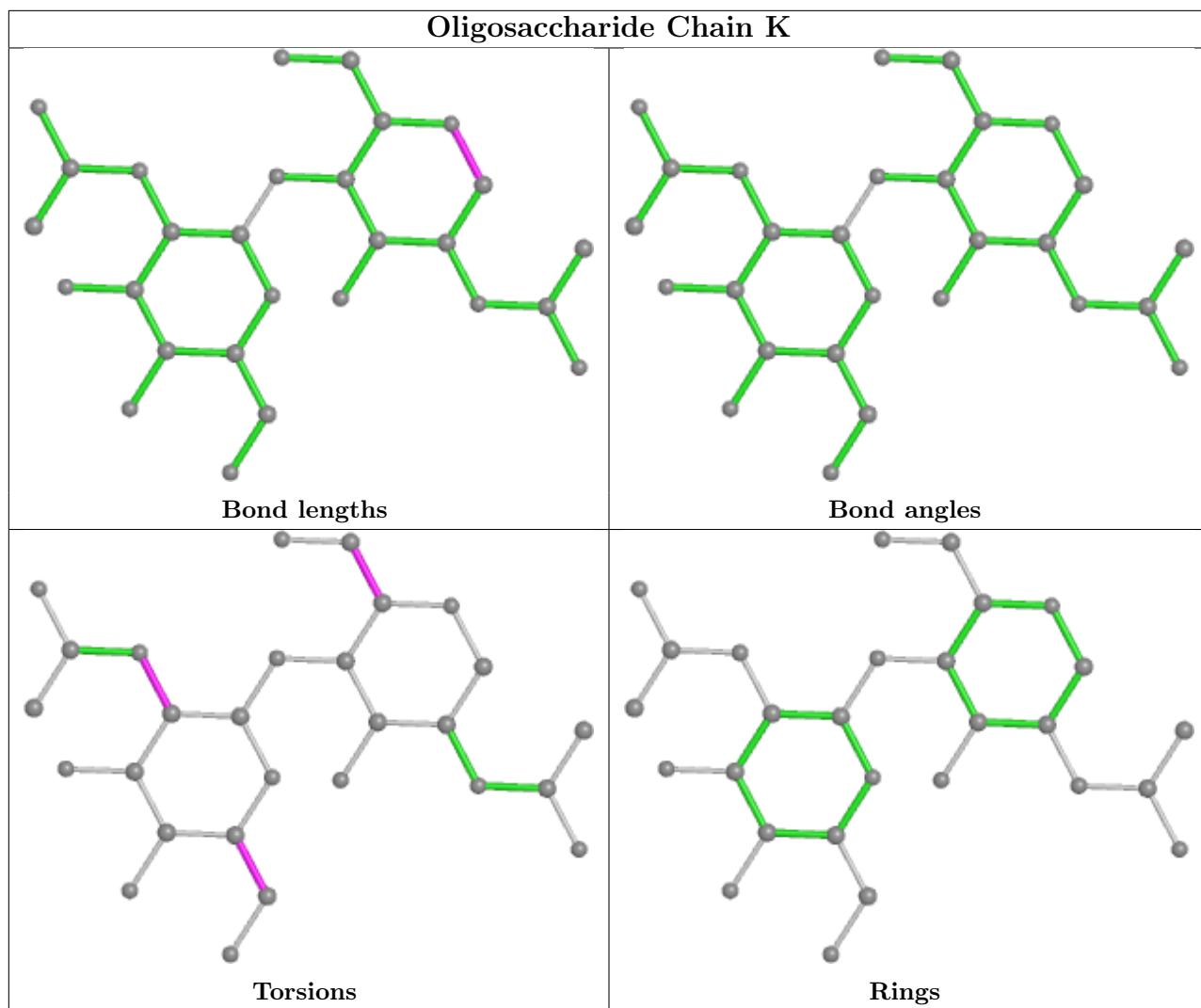


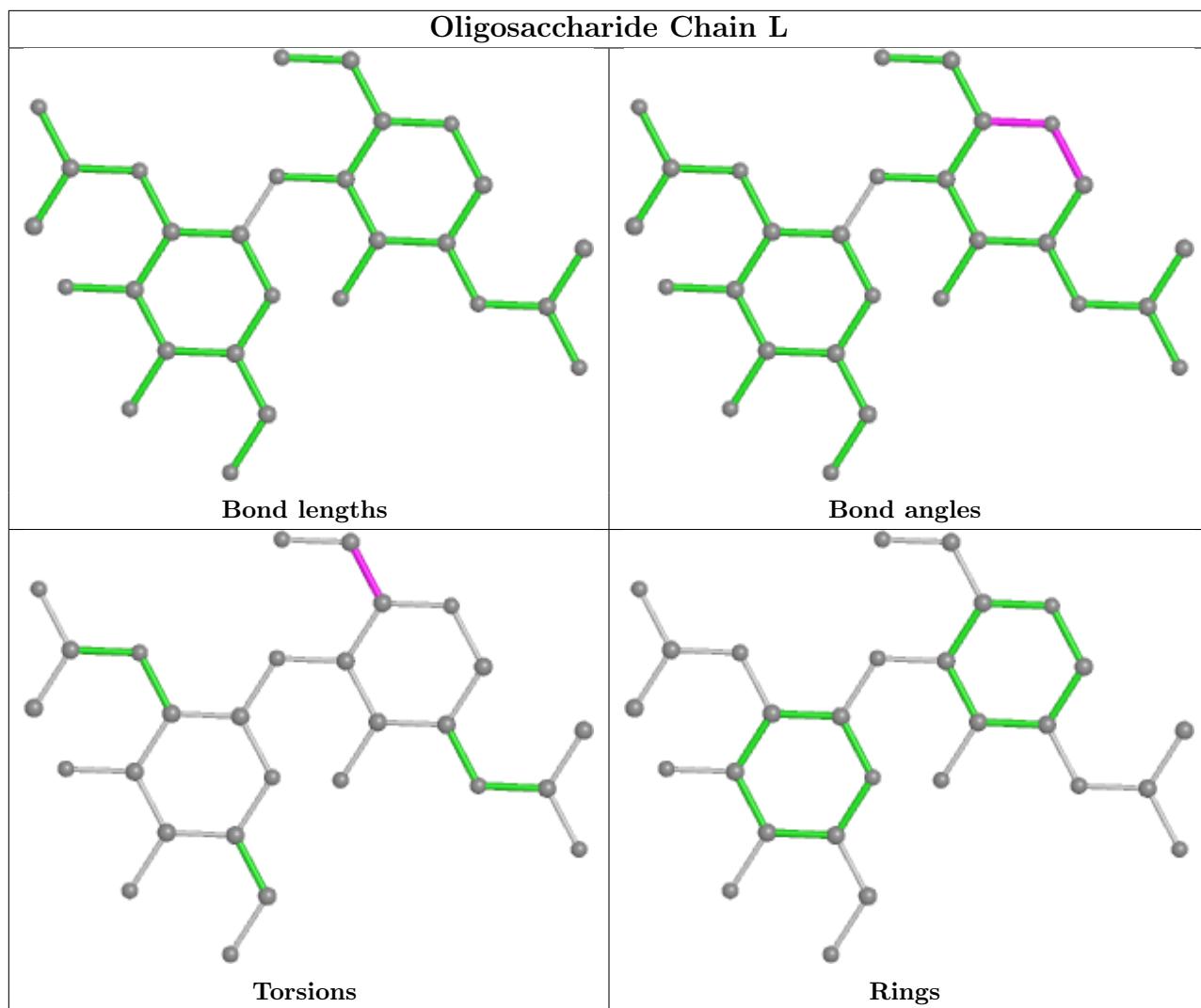


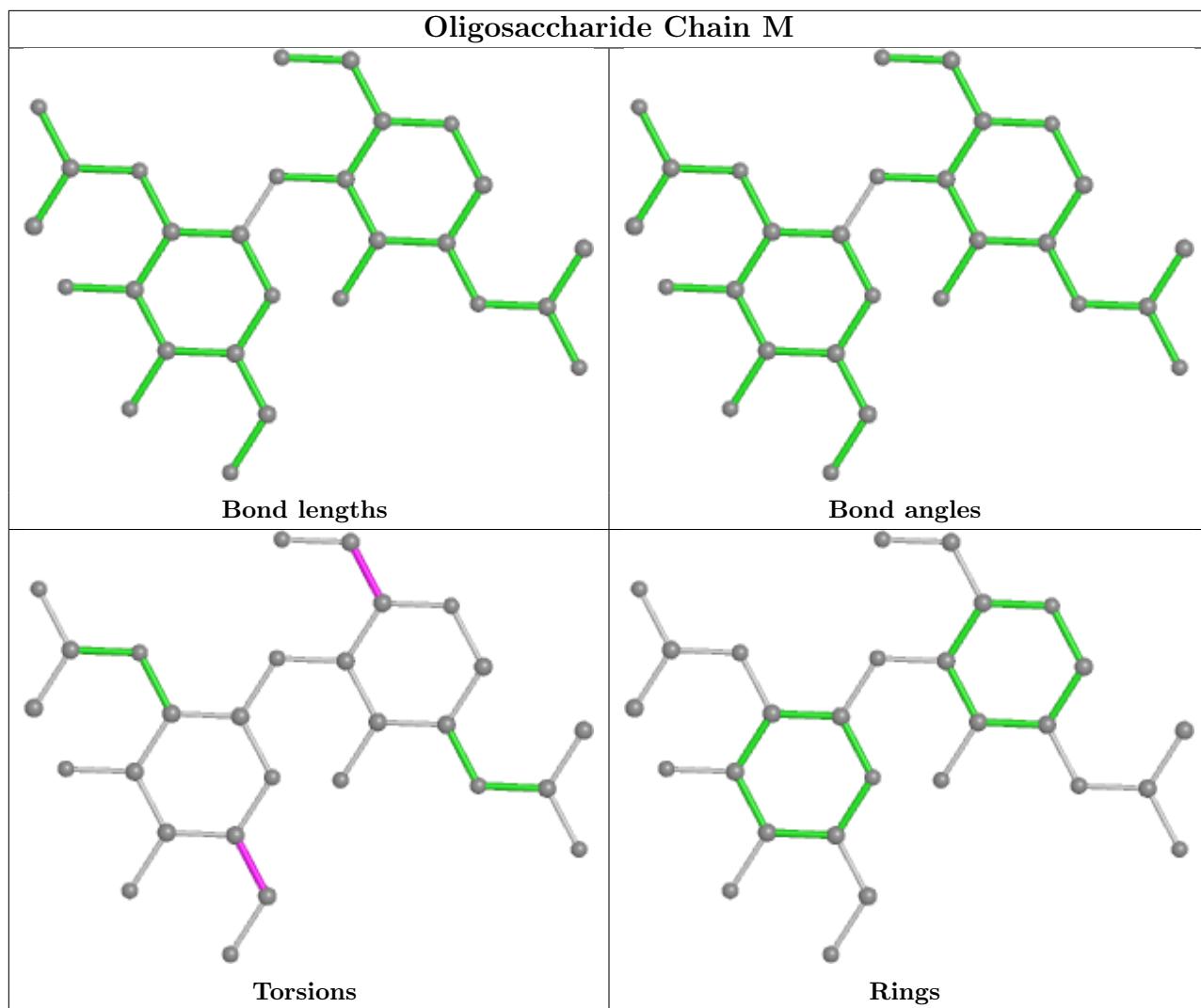


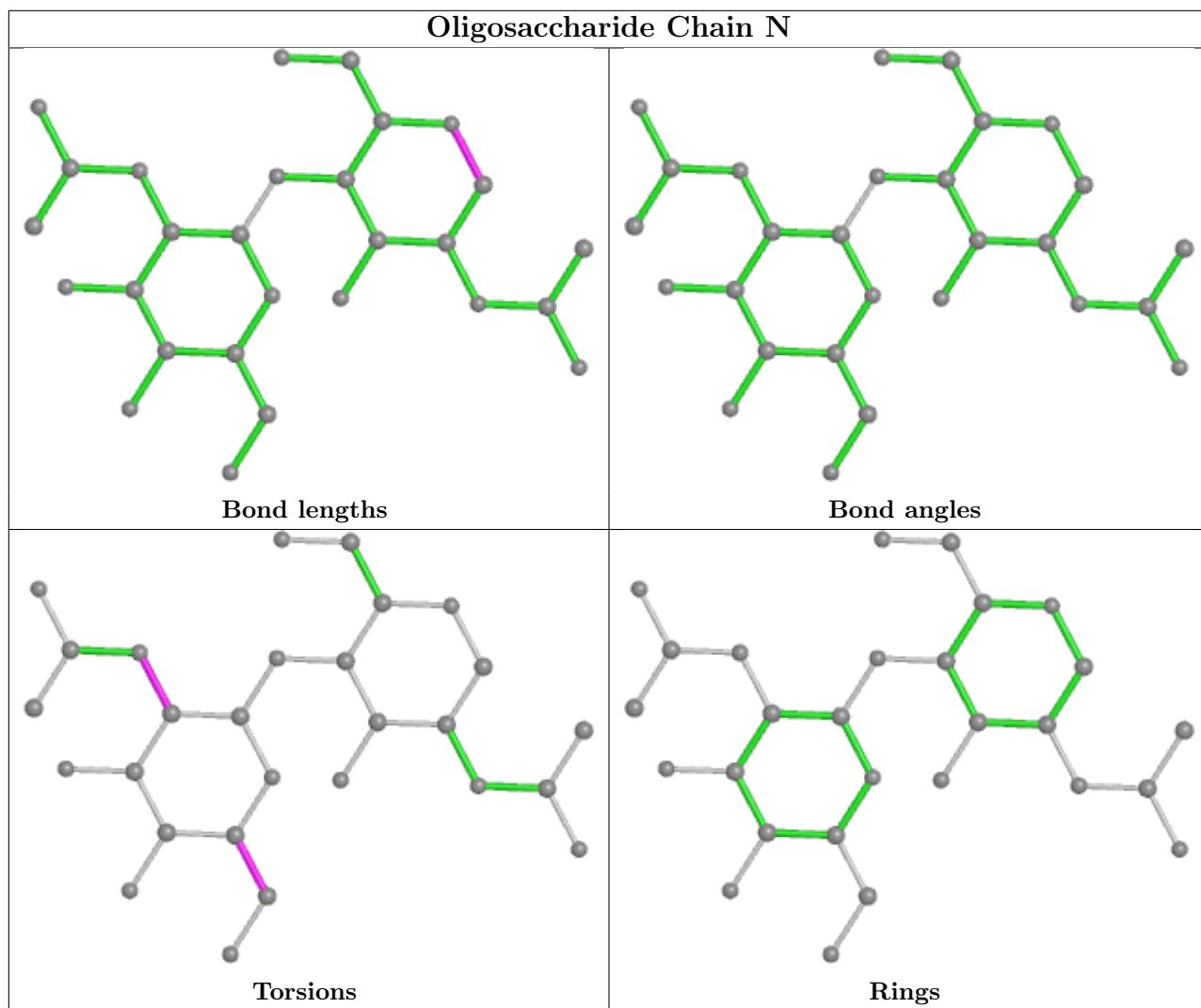


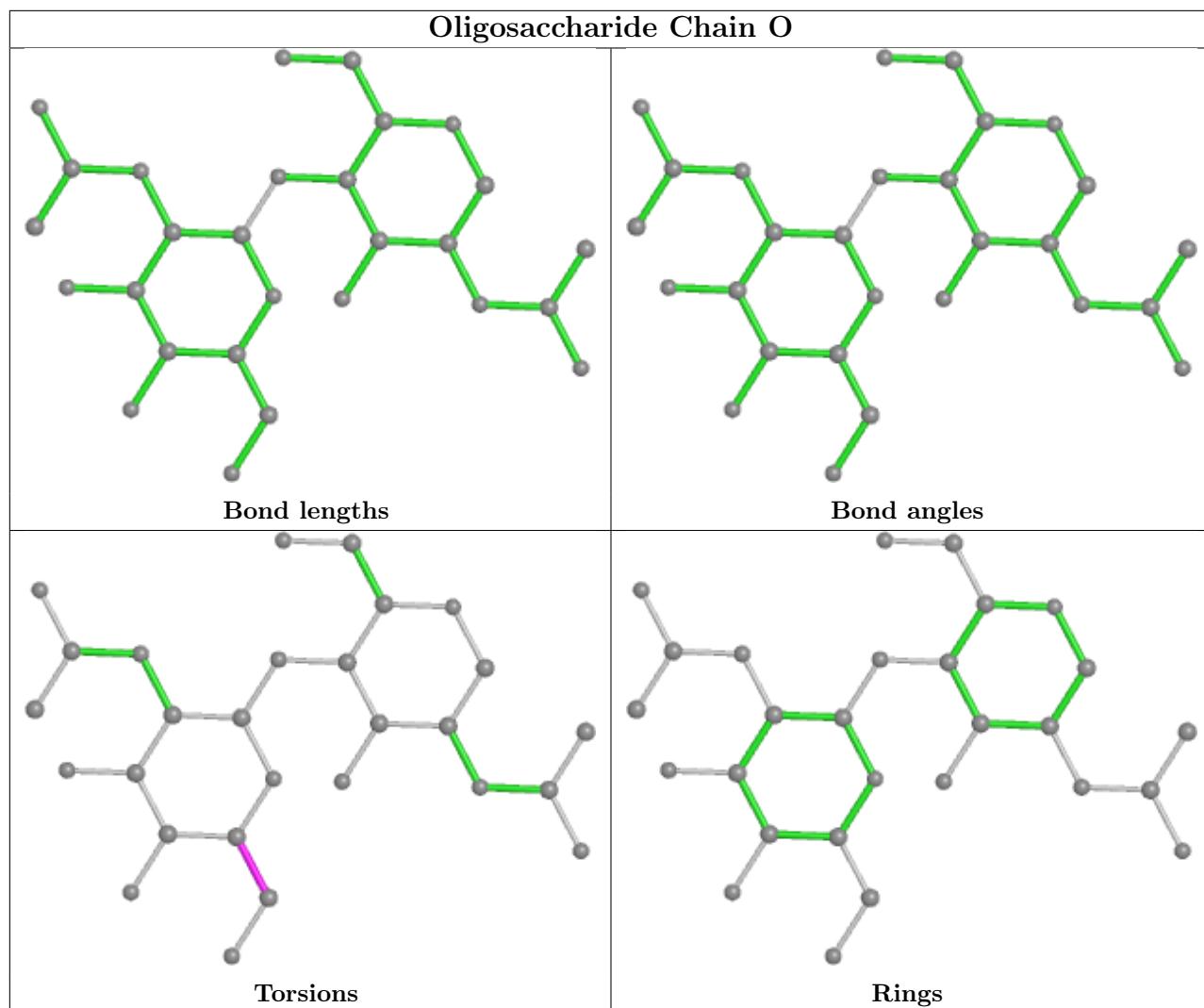


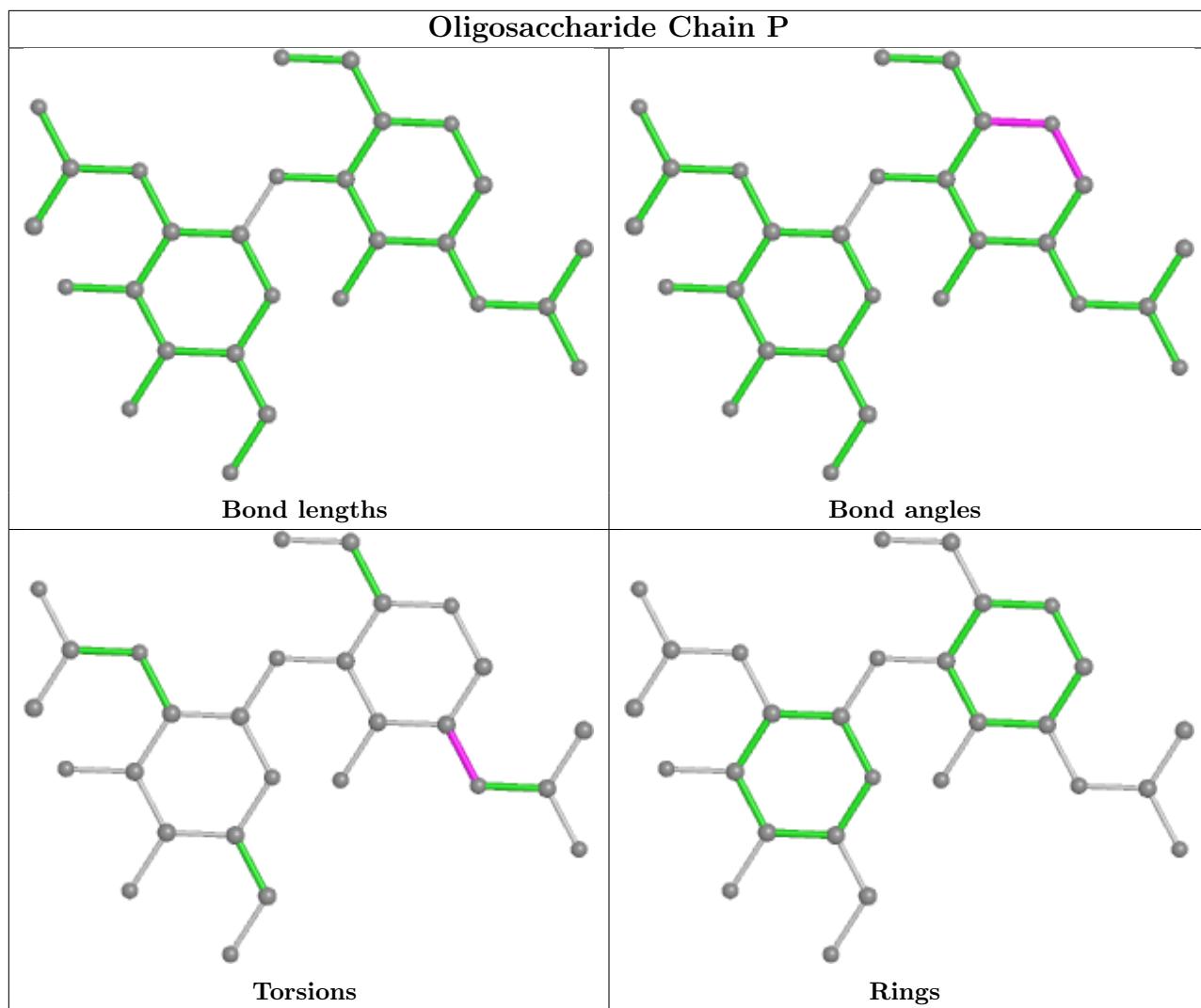


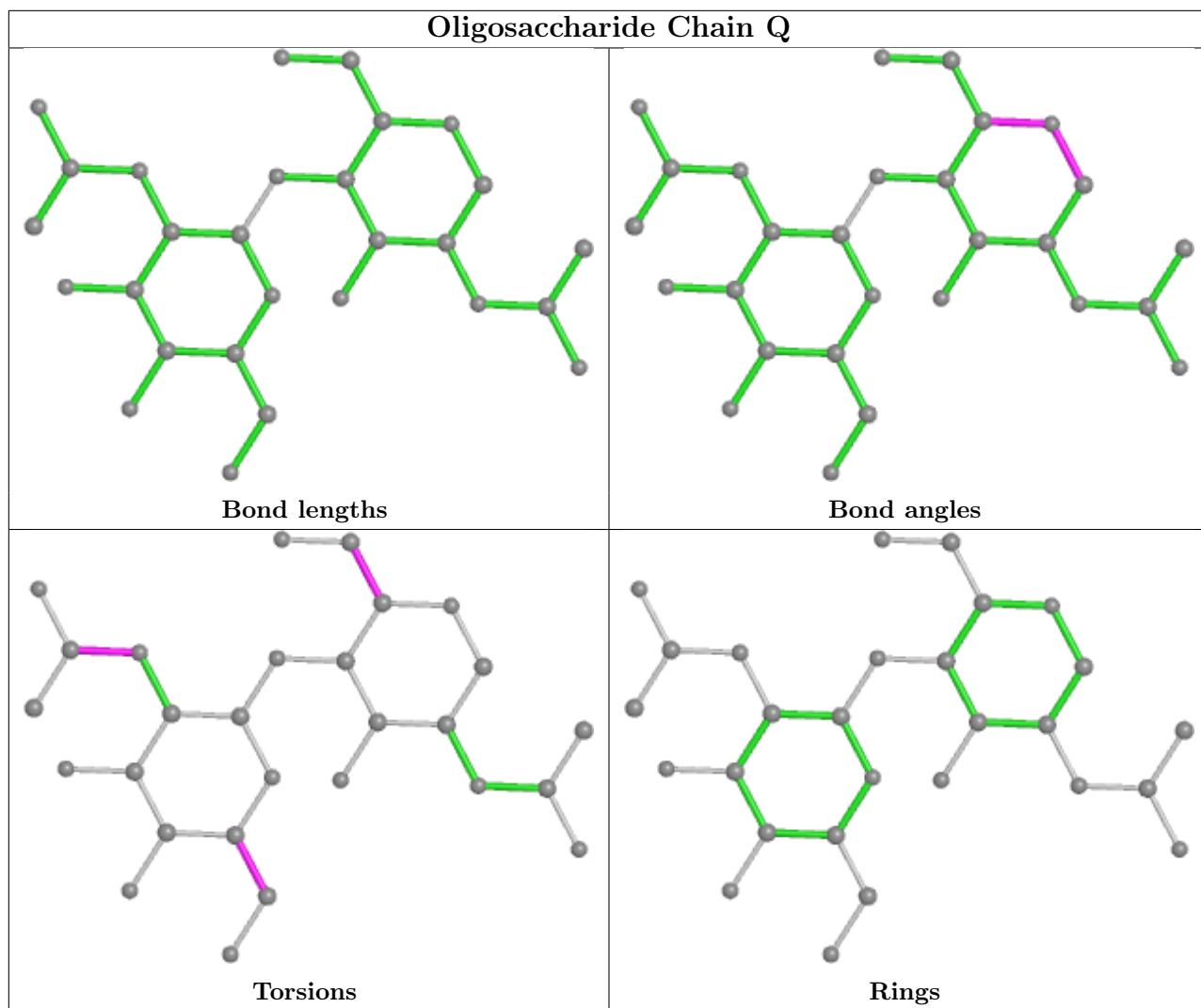


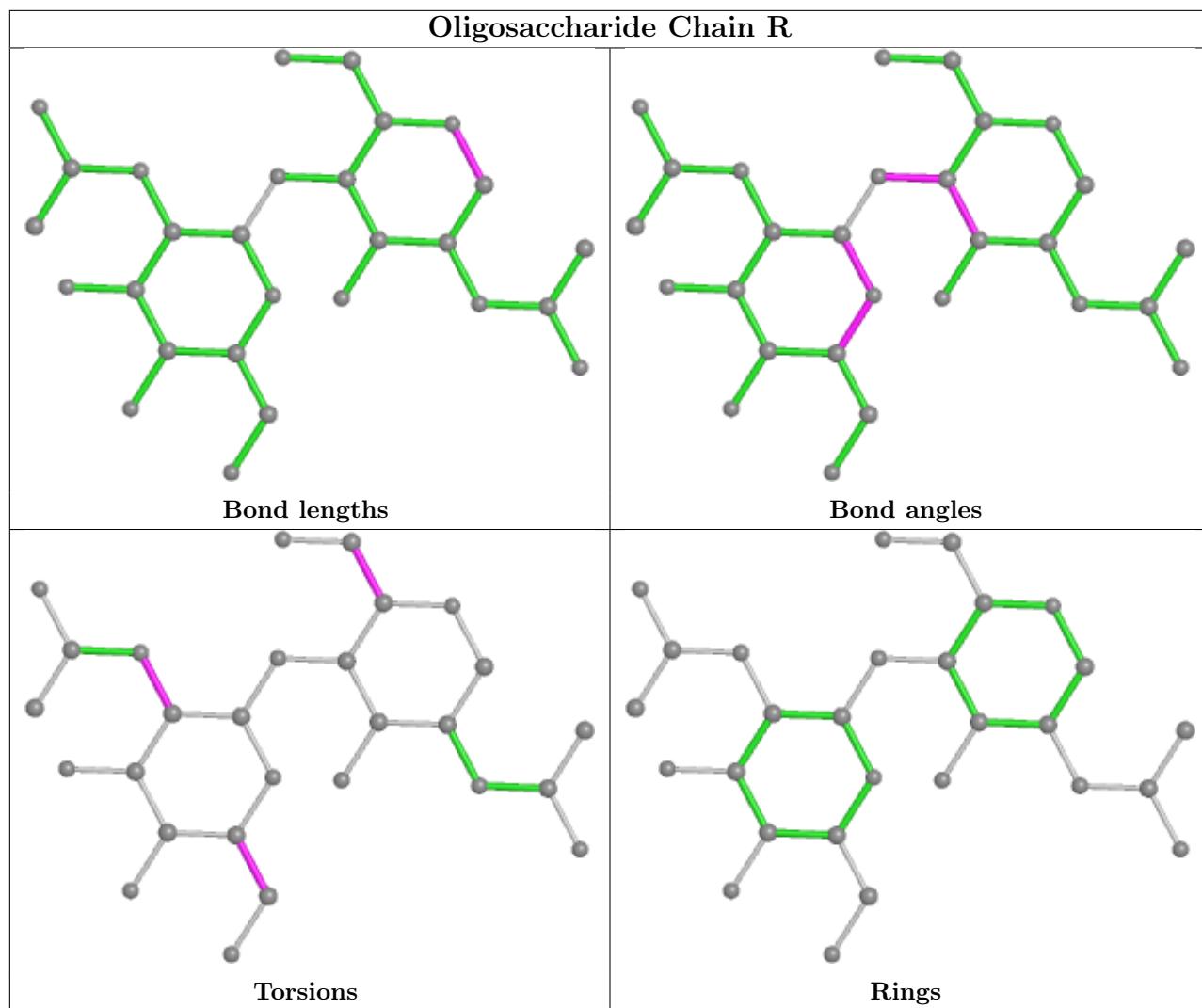


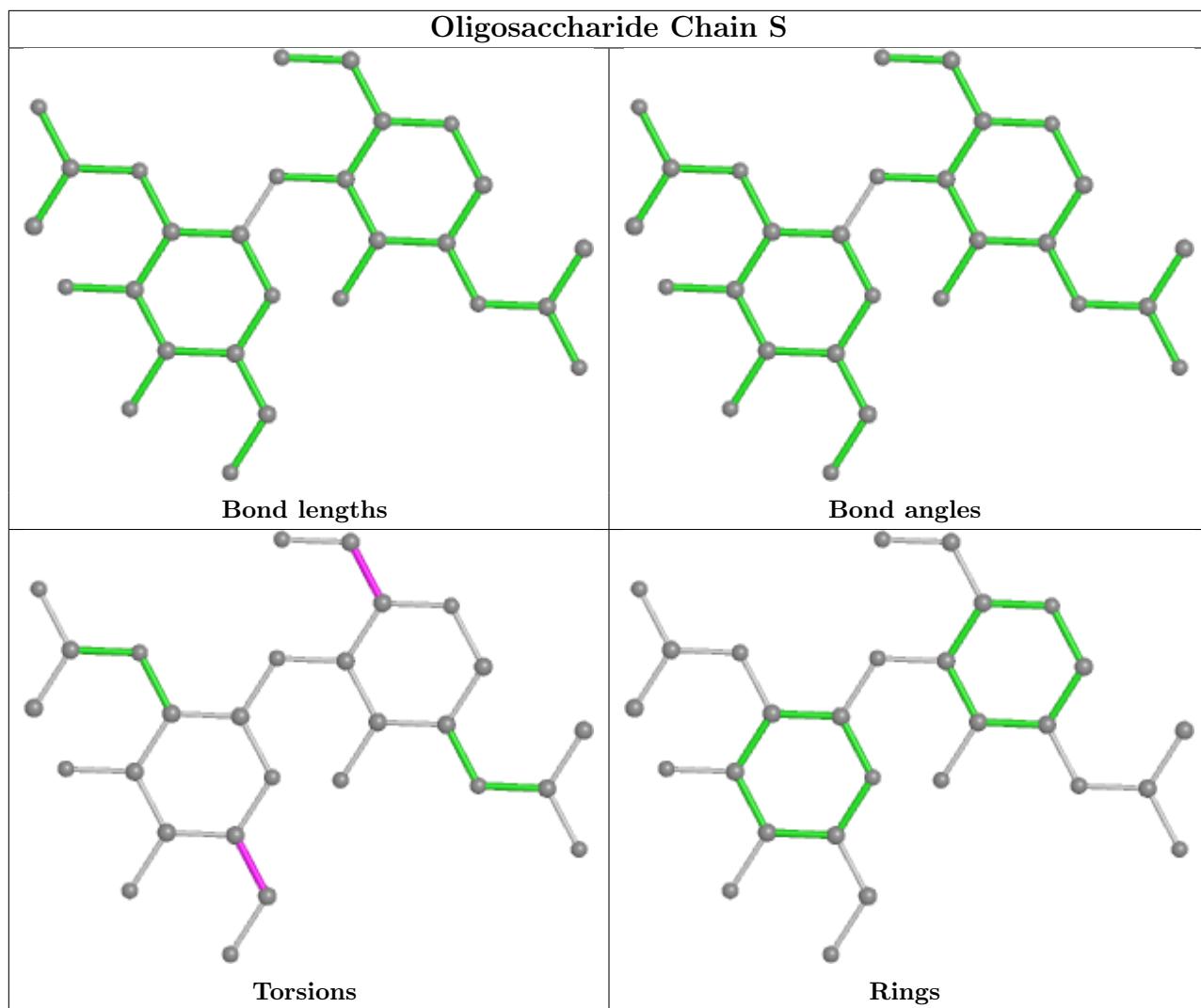


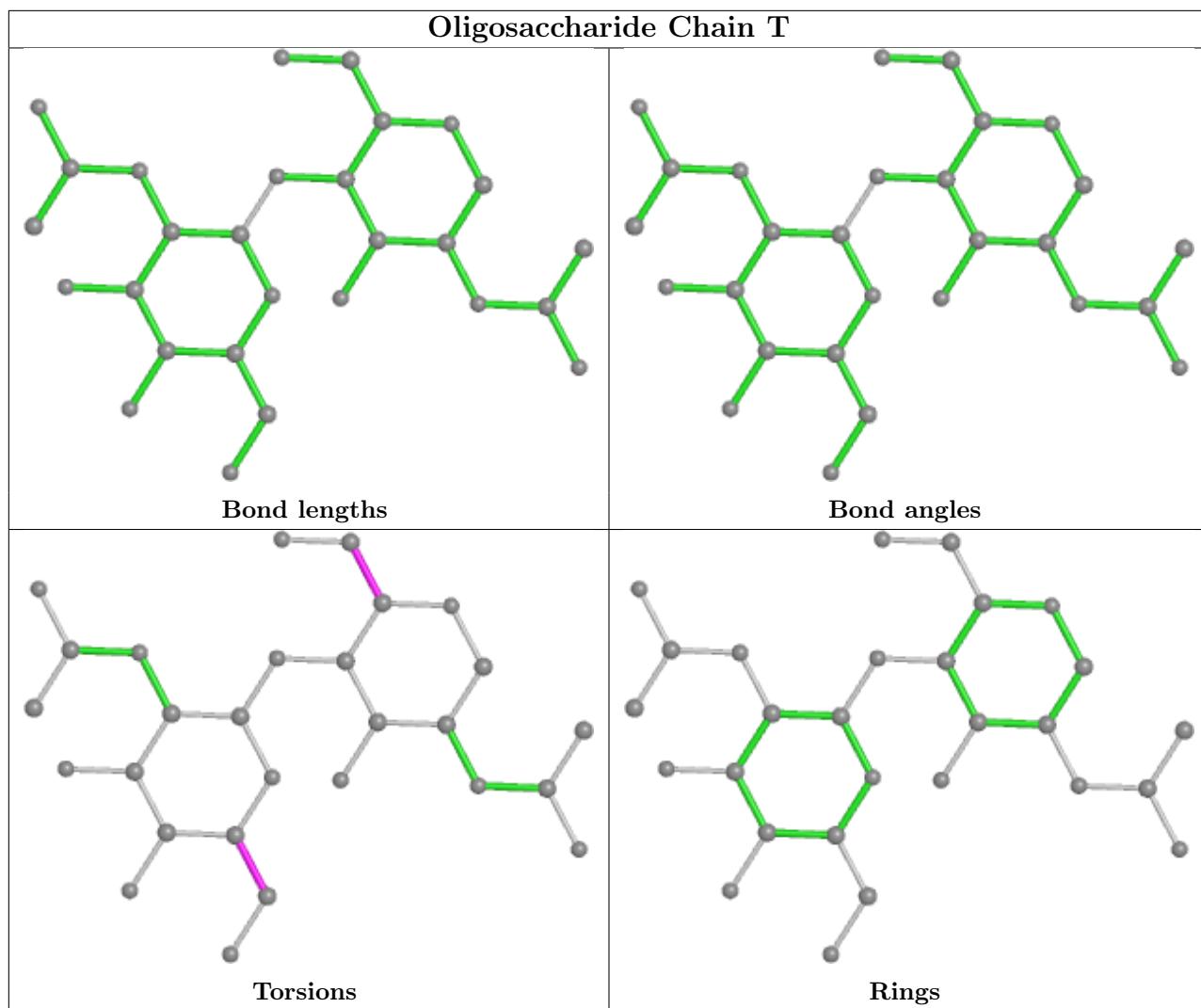


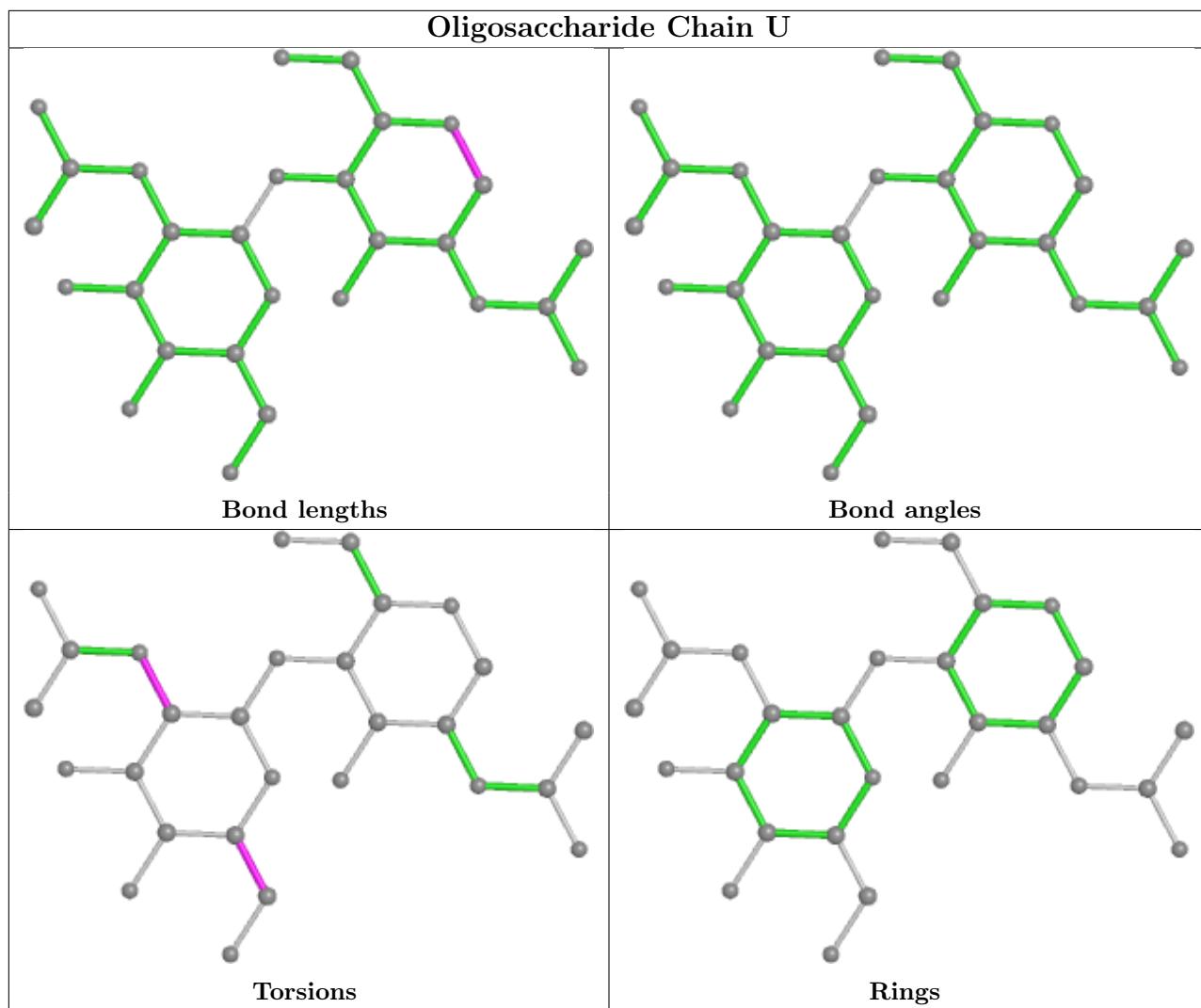


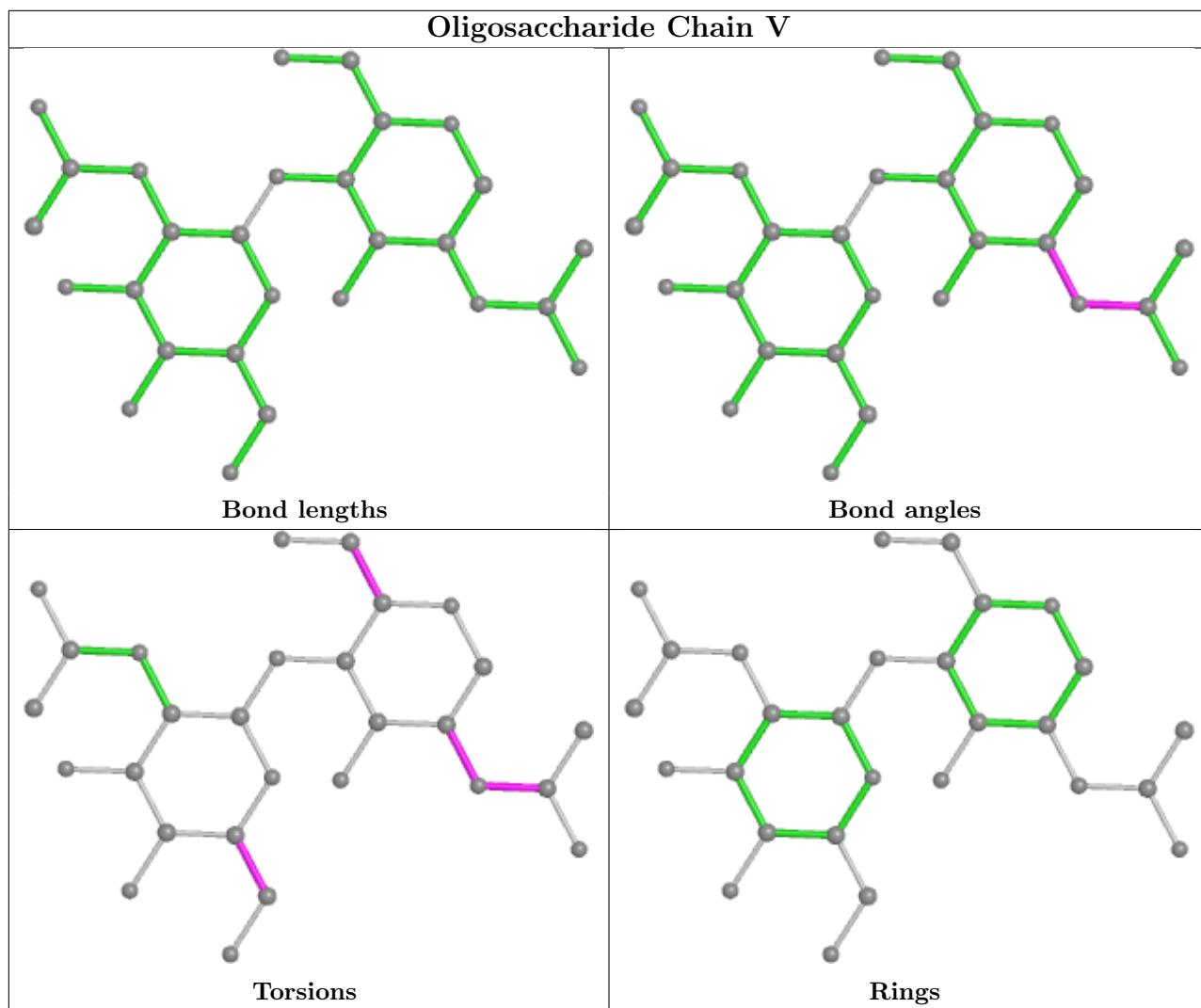


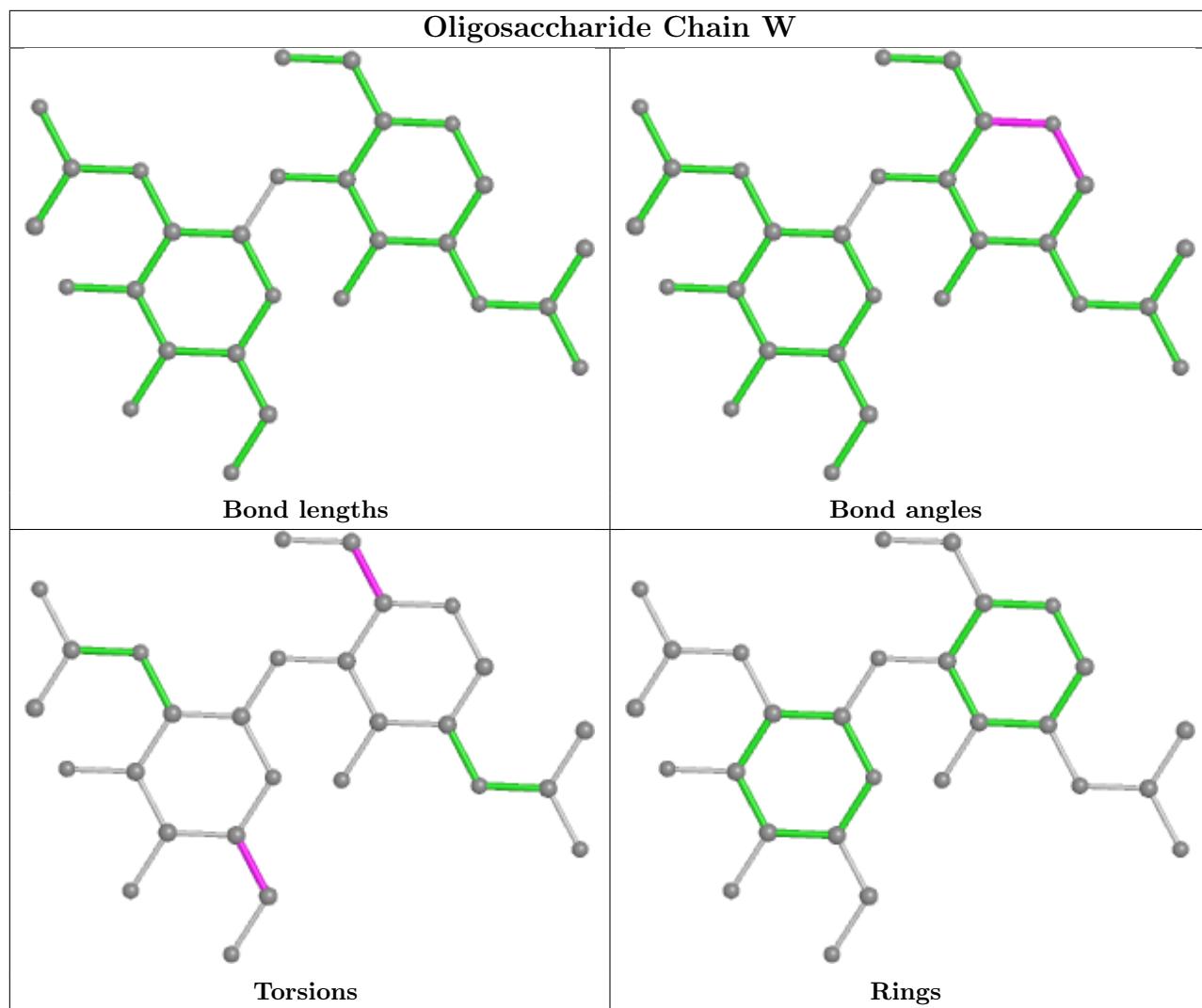


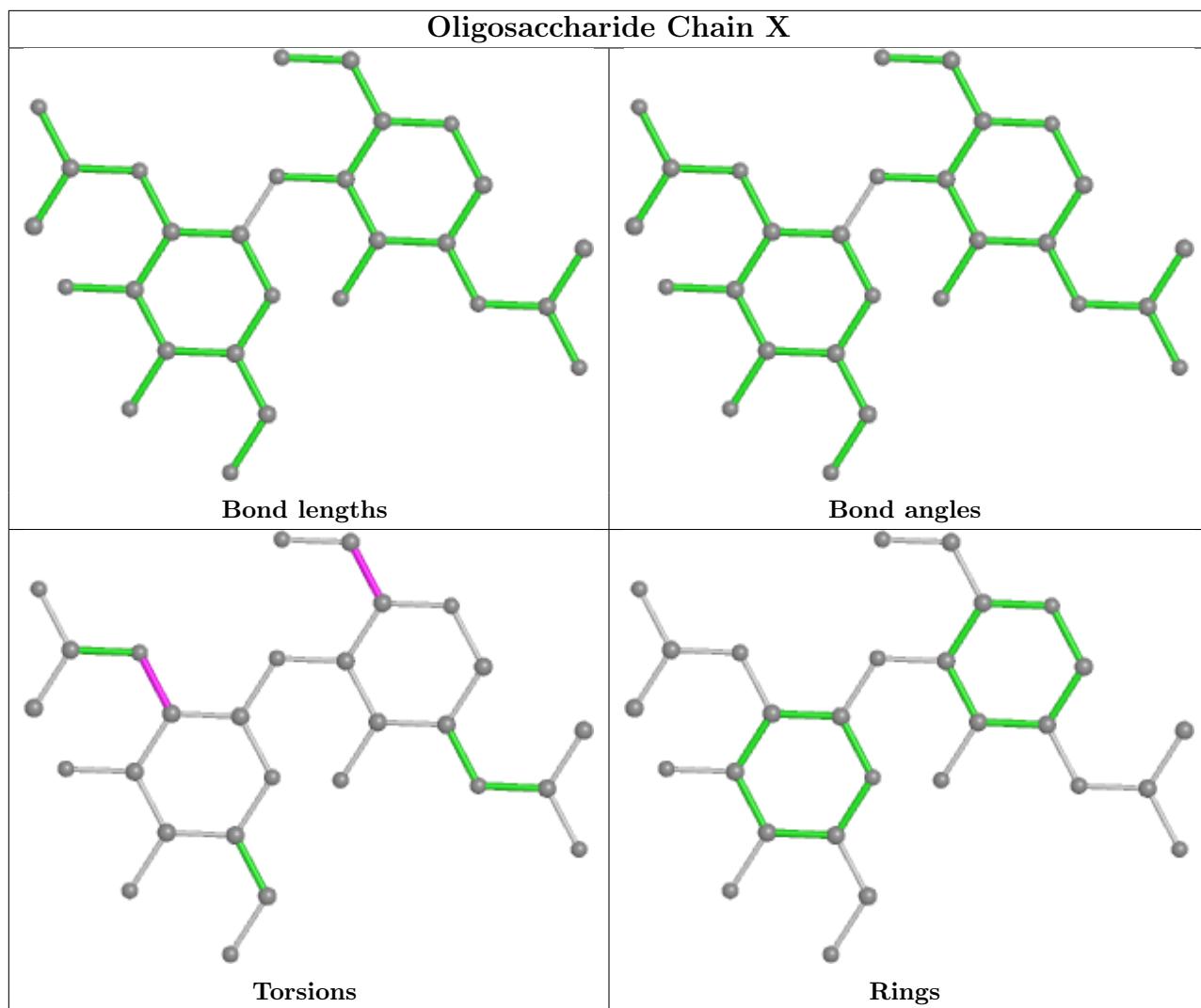


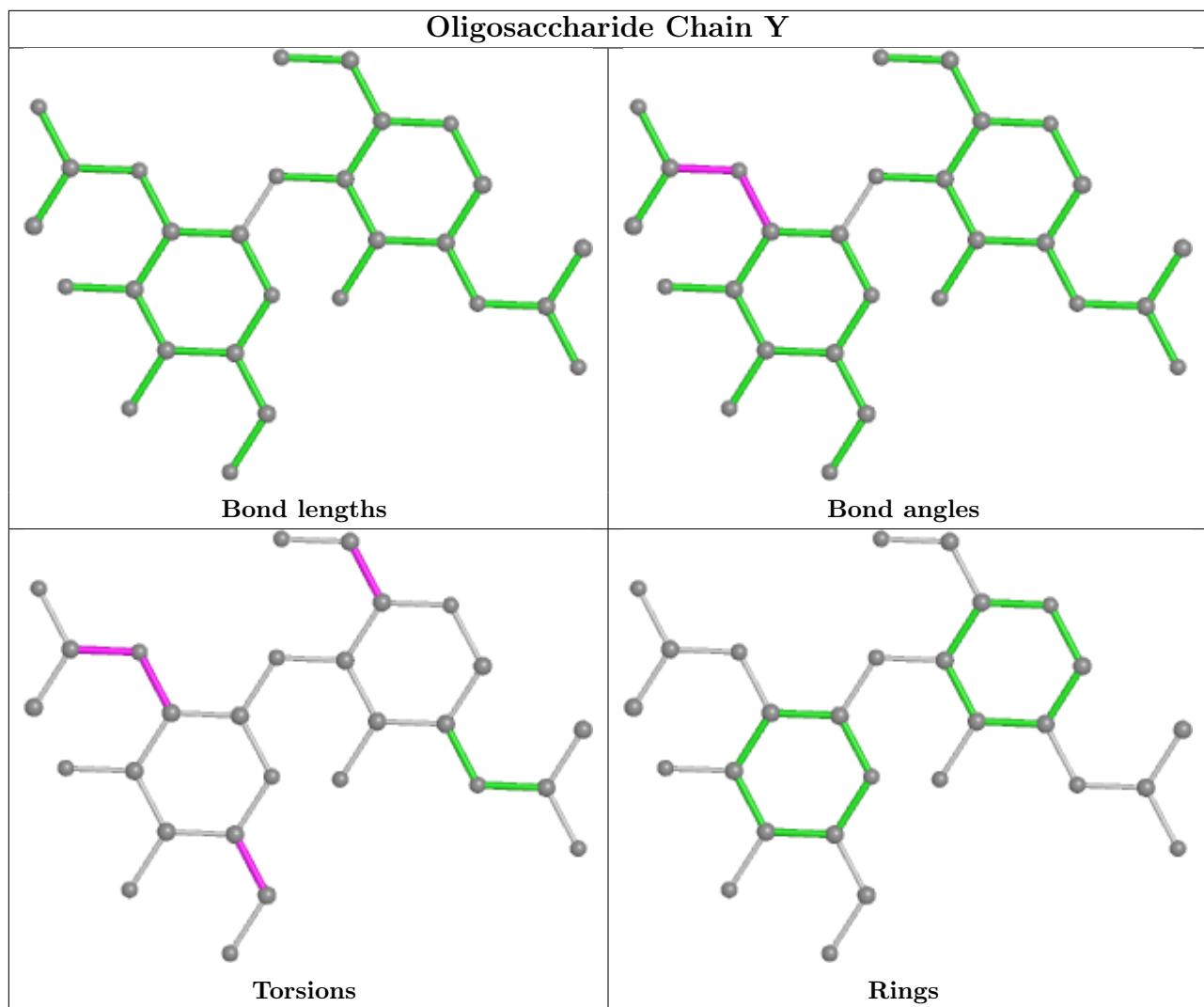


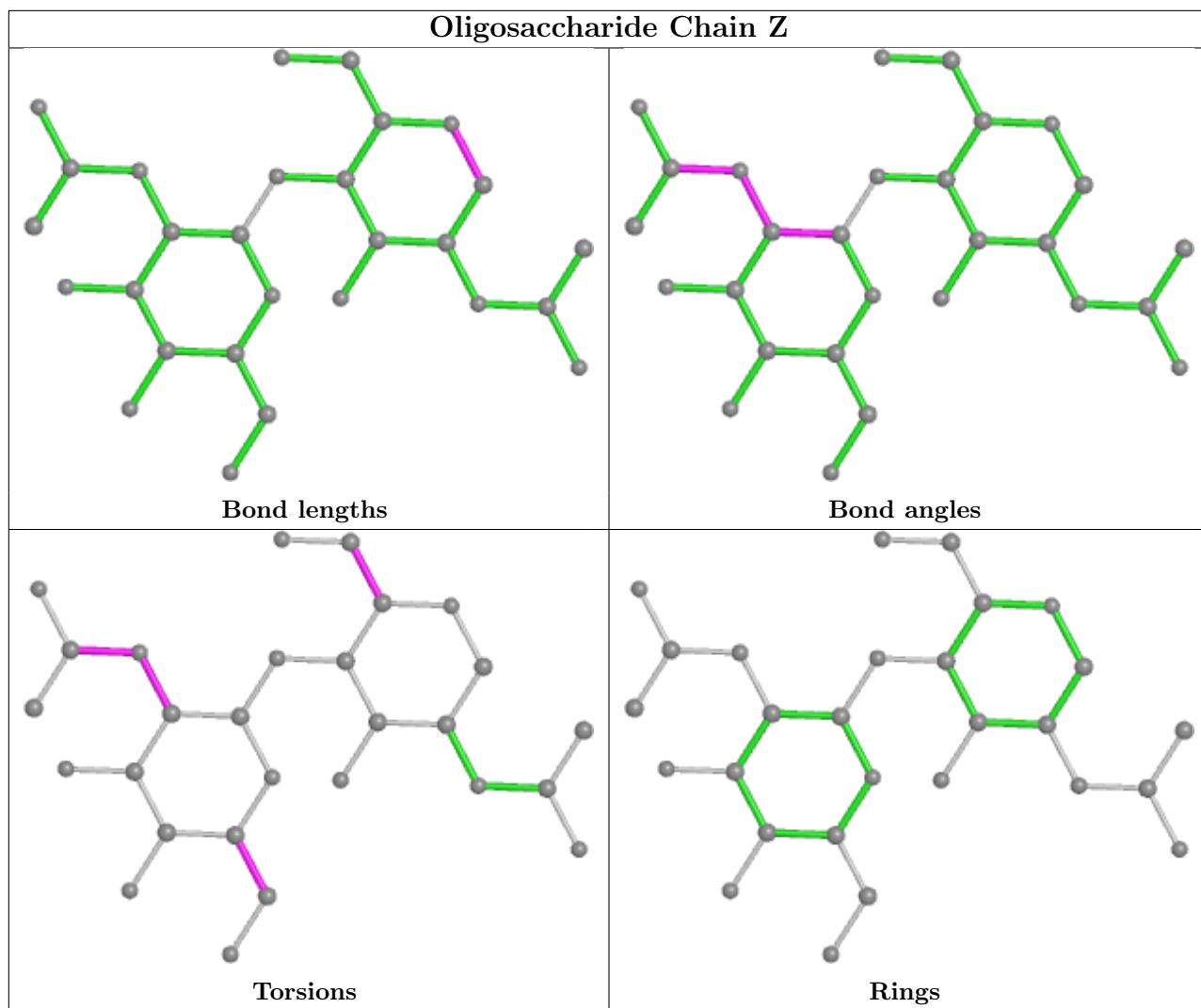


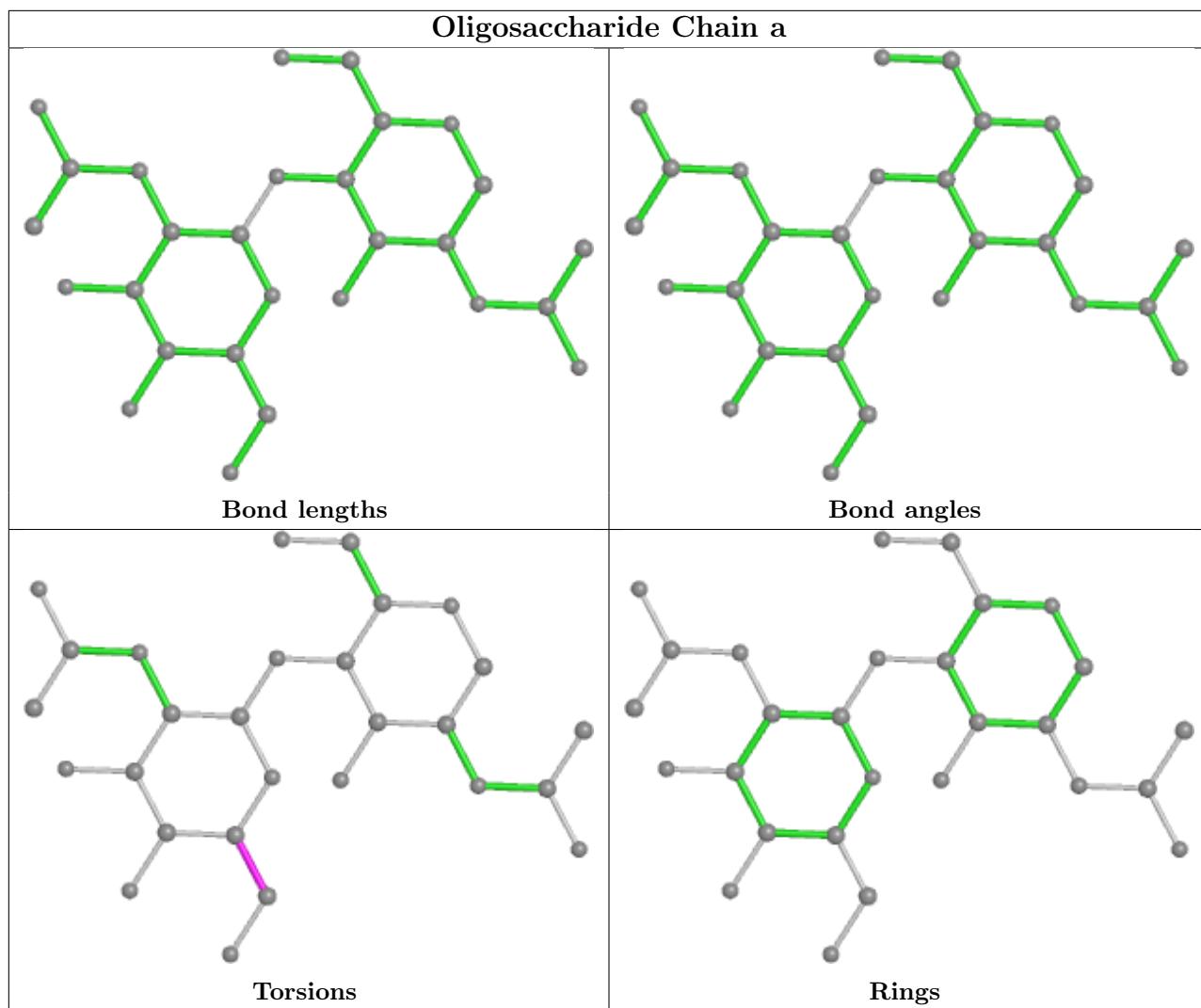


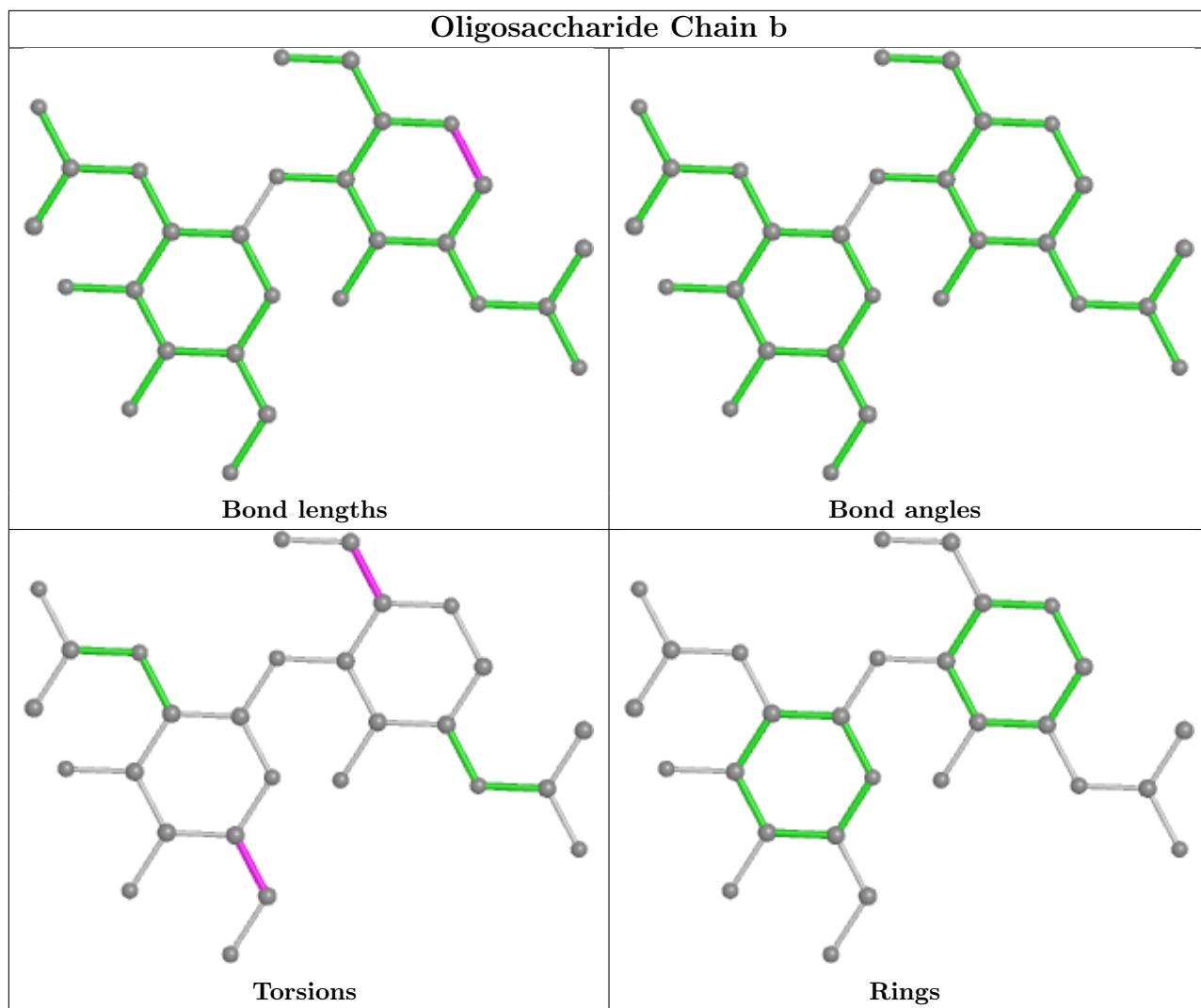


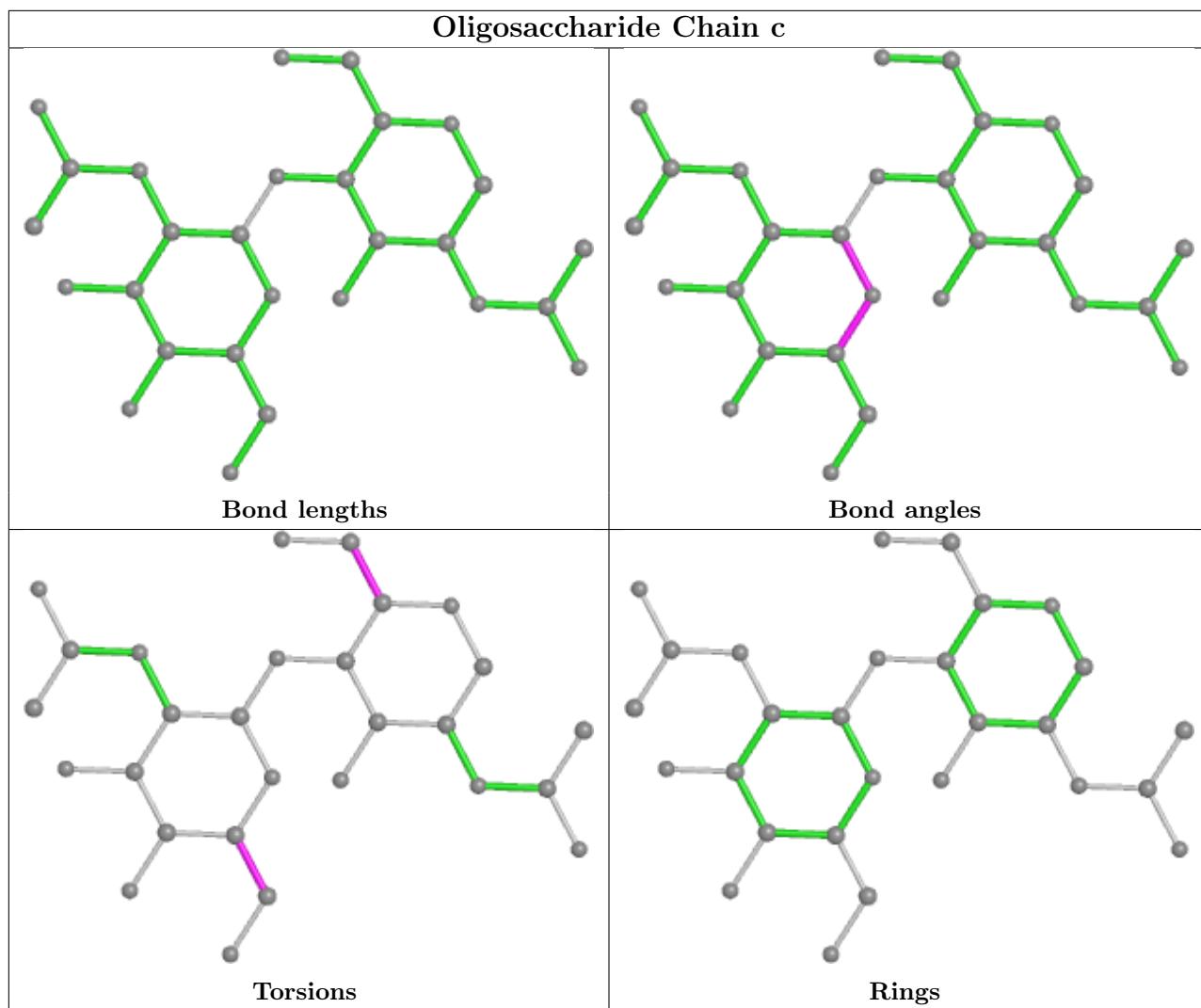


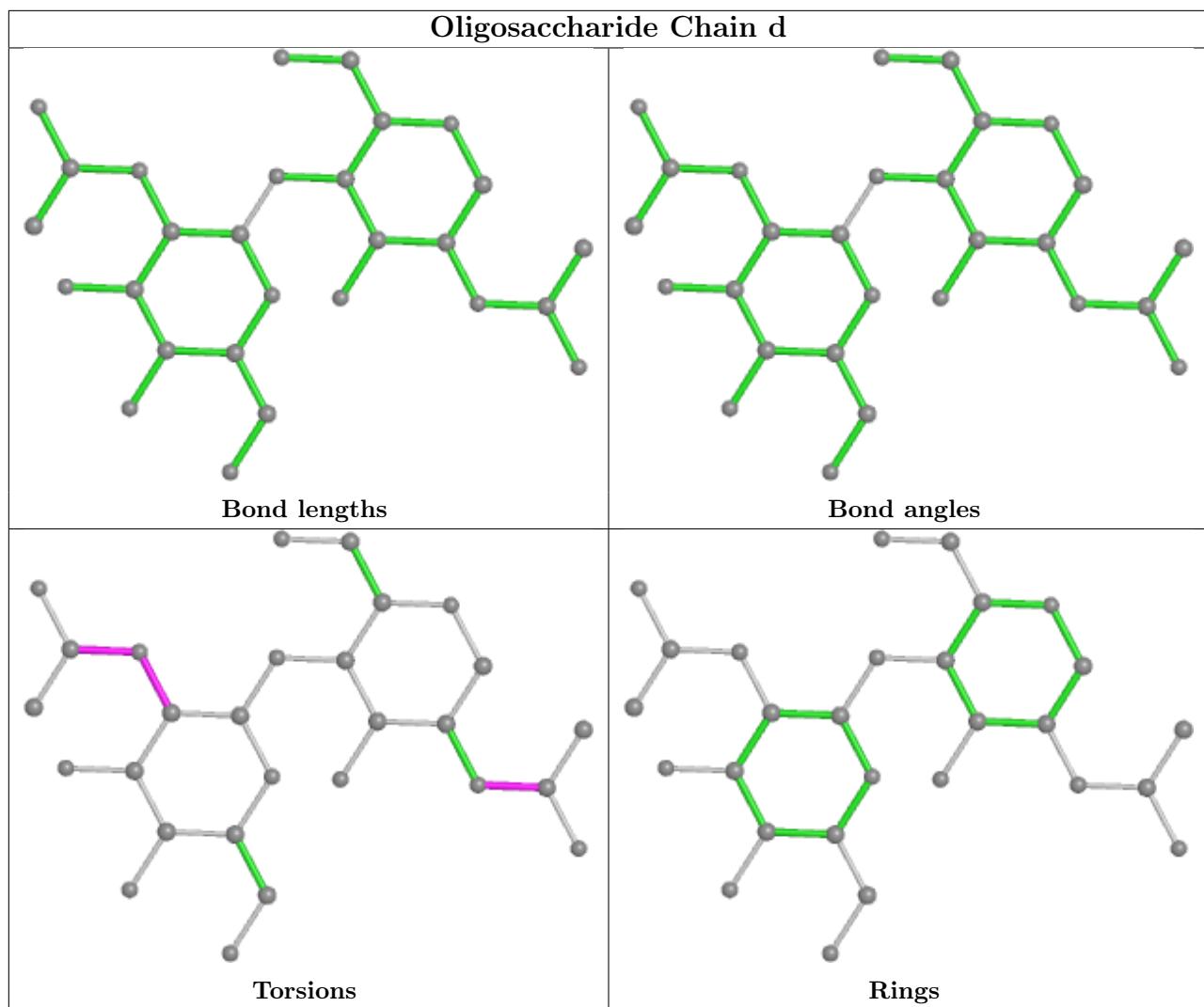


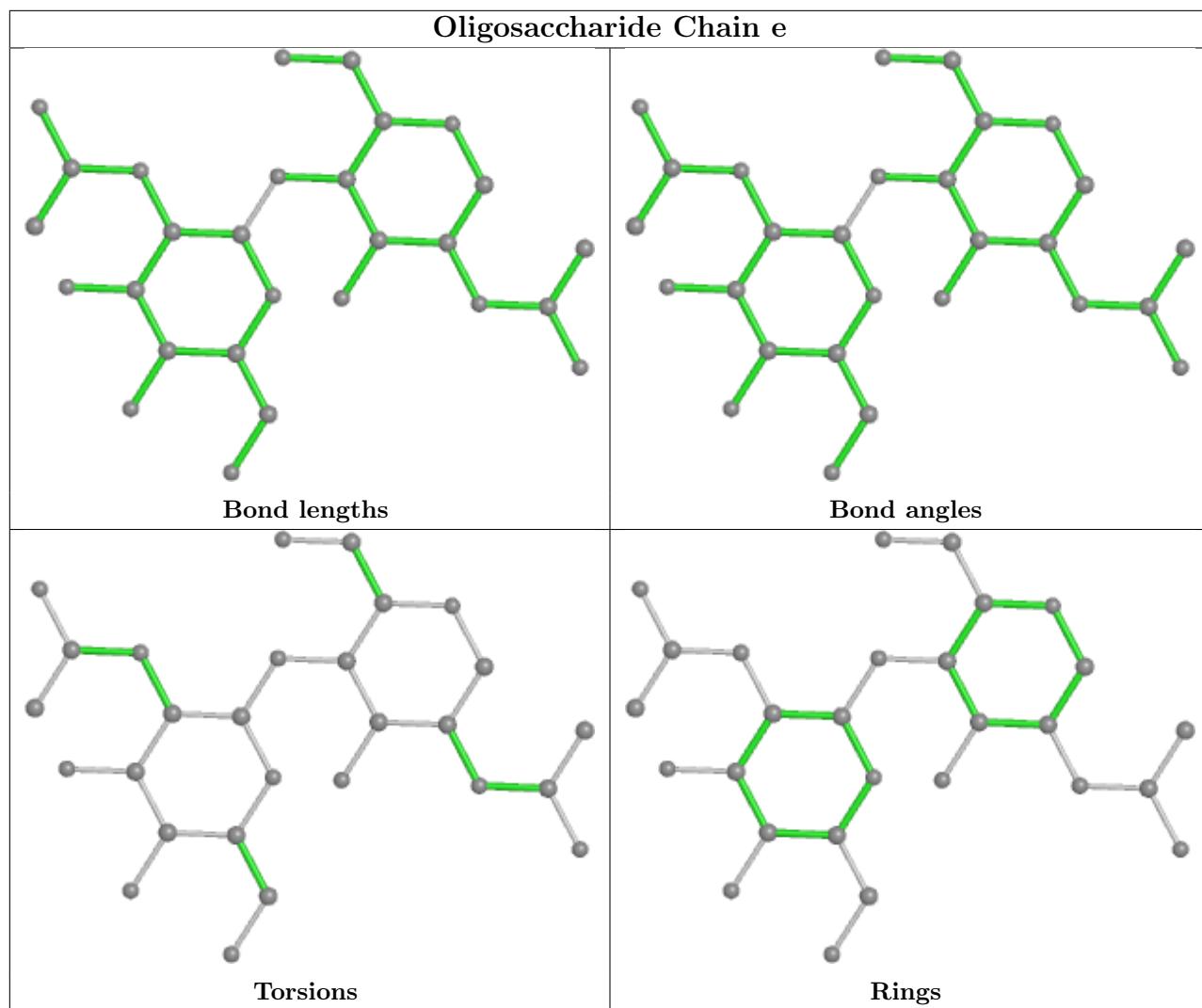


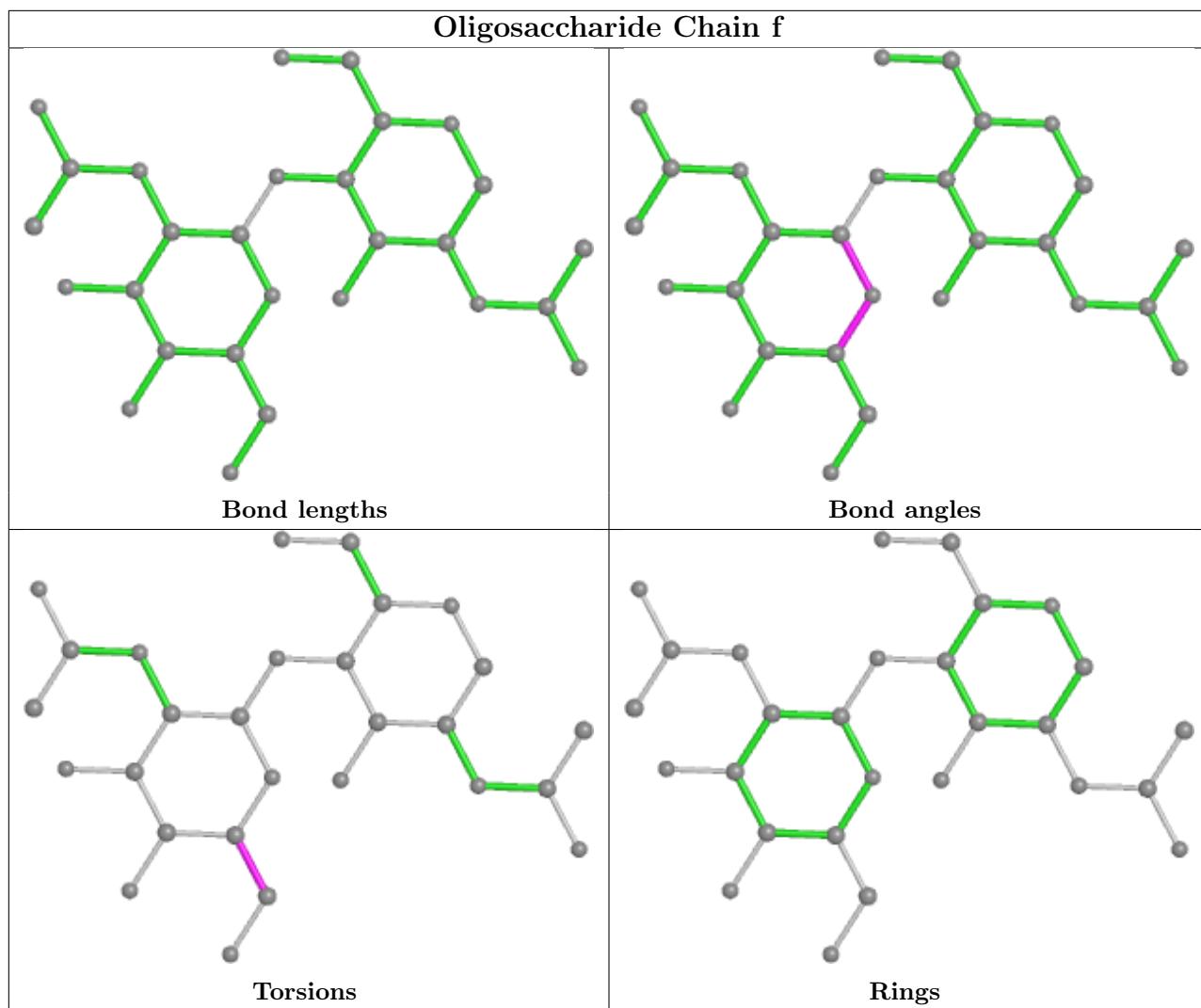


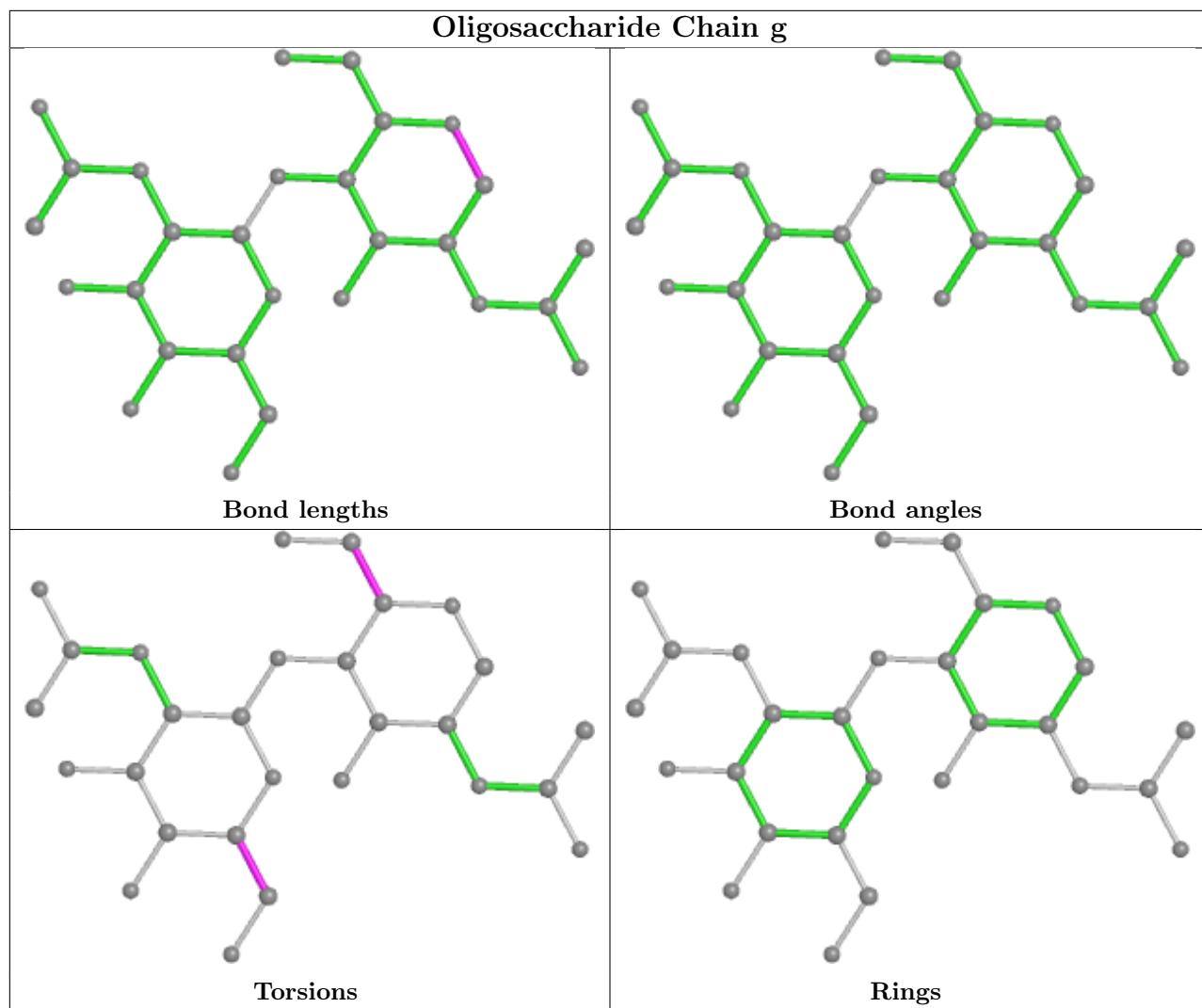


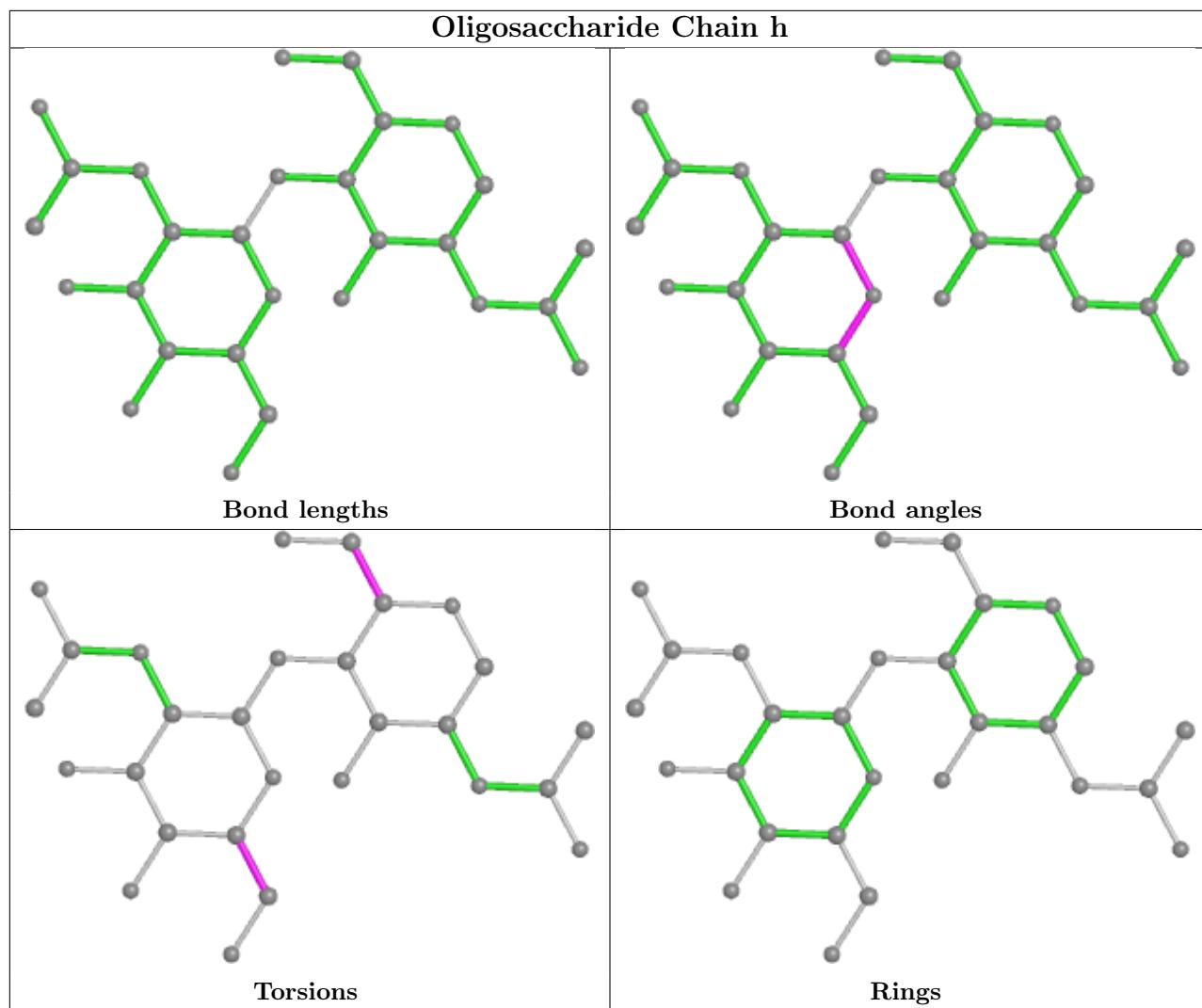


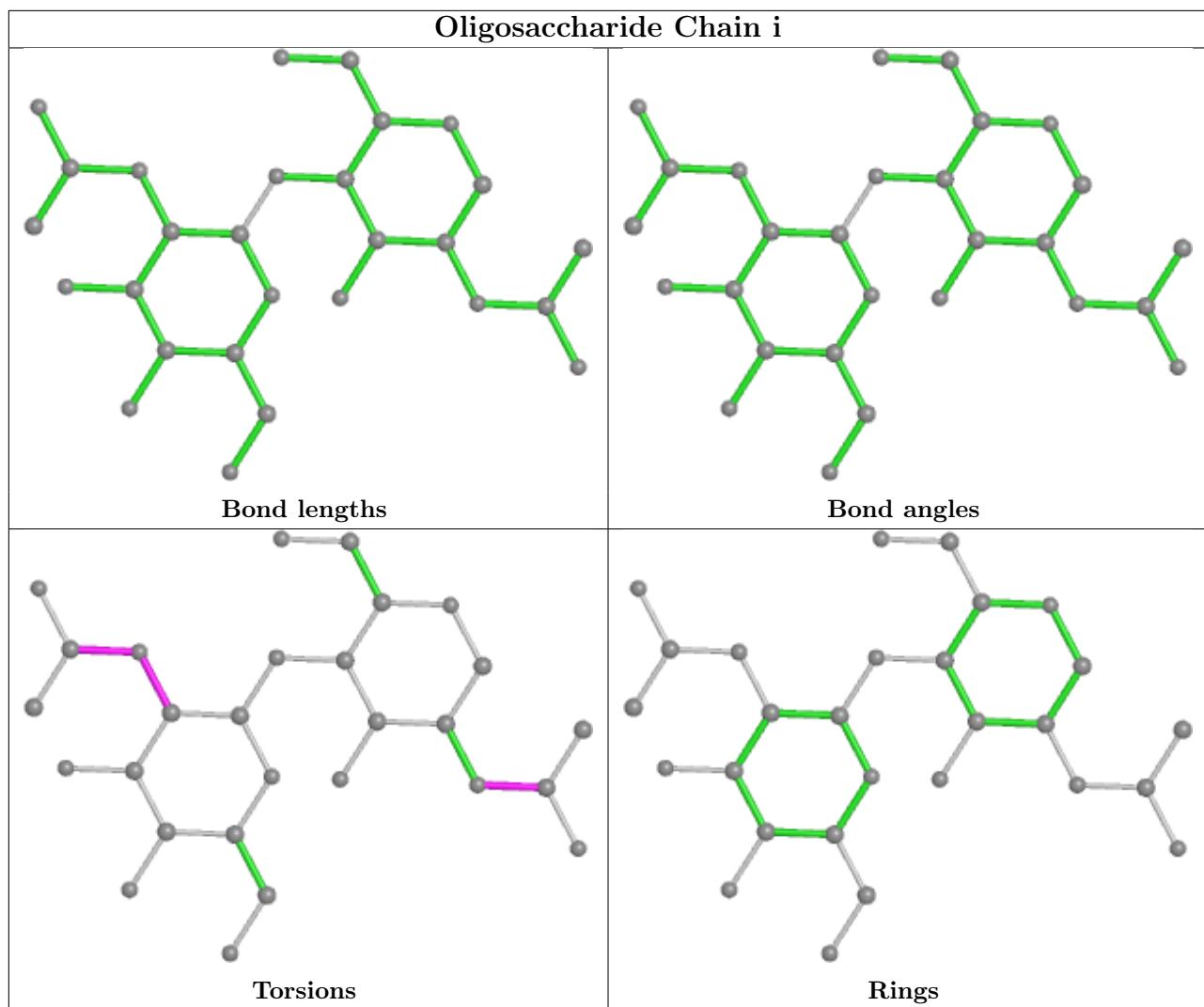


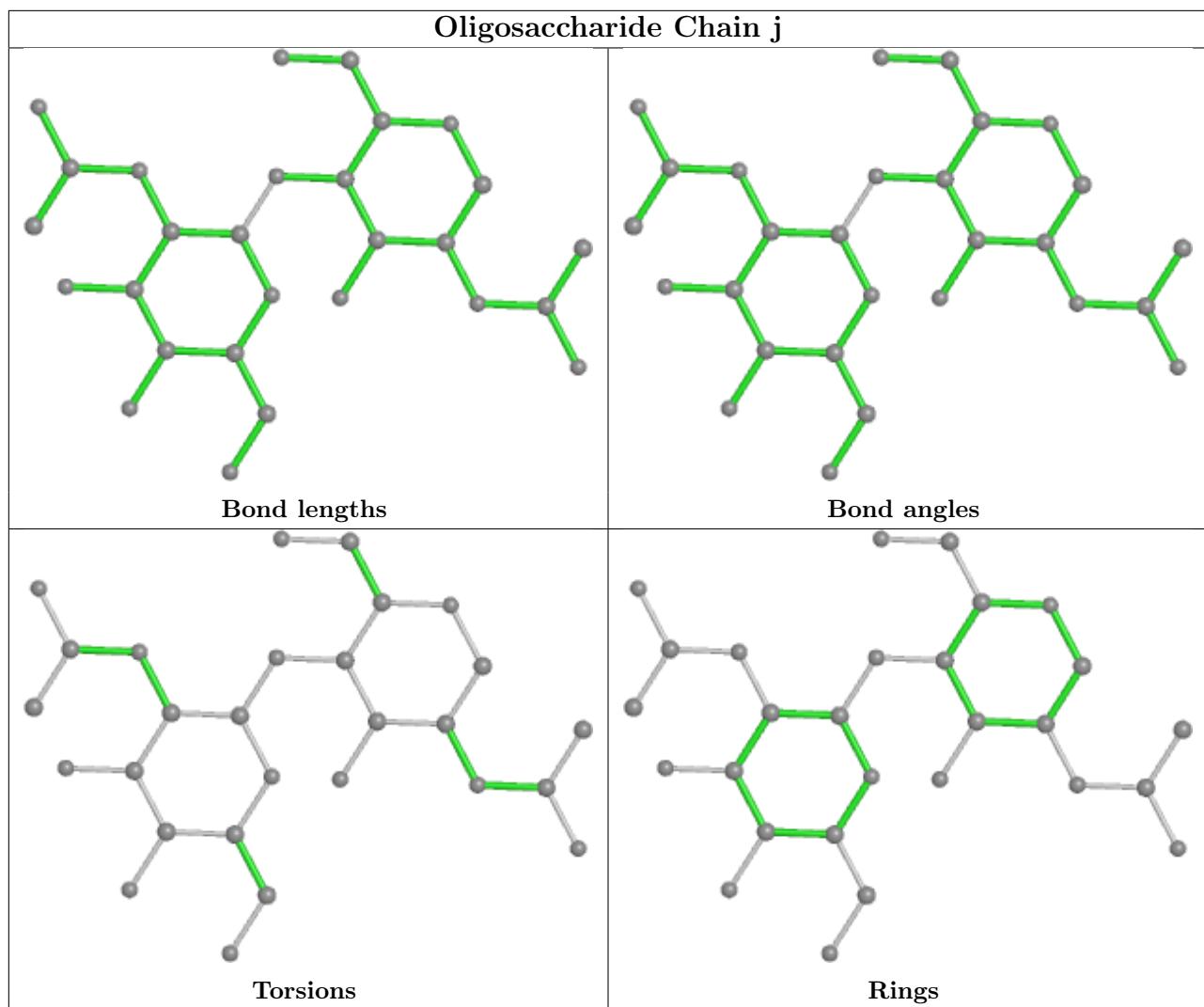


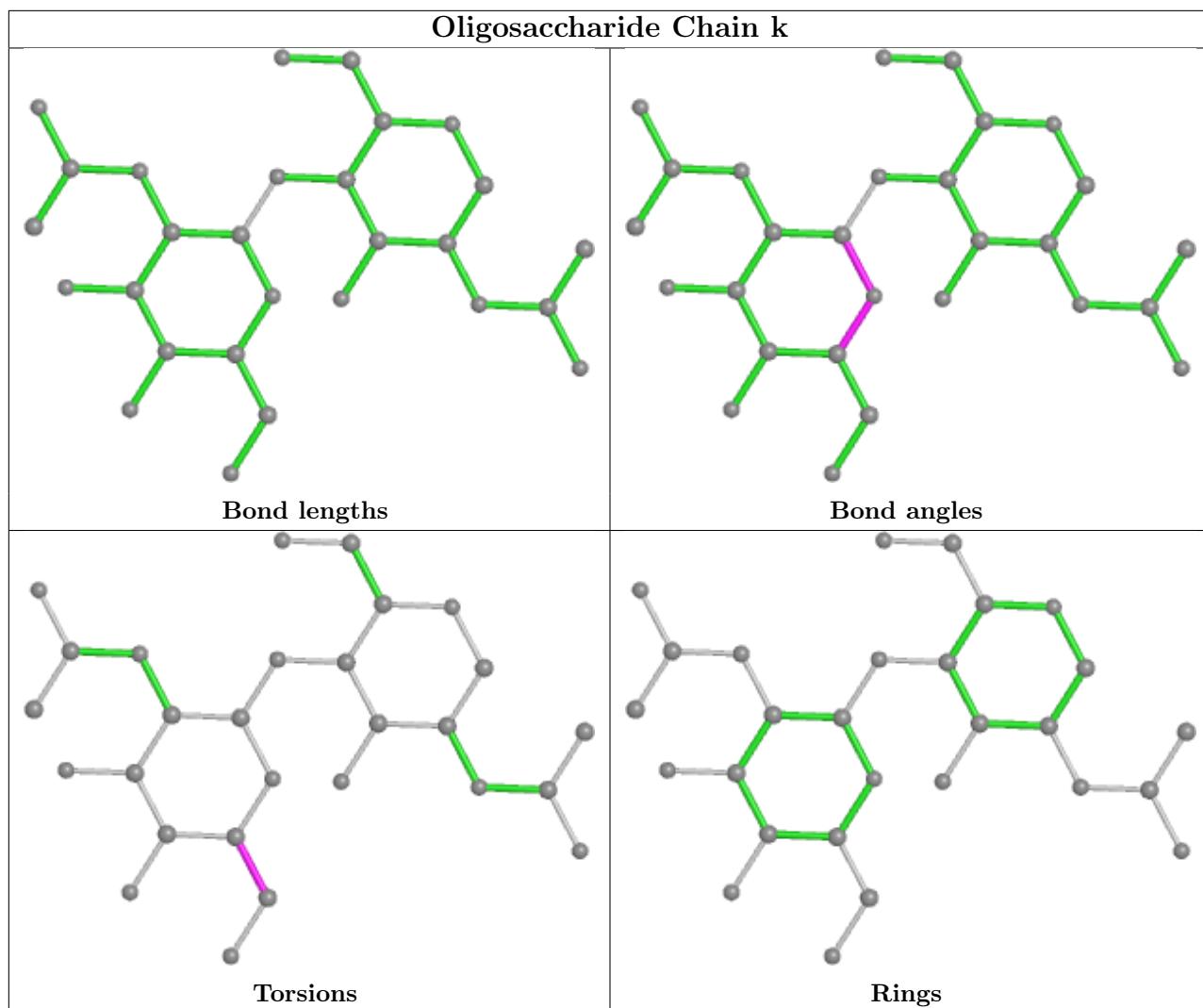












5.6 Ligand geometry (i)

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	B	1406	1	14,14,15	0.29	0	17,19,21	0.38	0
4	NAG	A	1408	1	14,14,15	0.30	0	17,19,21	0.38	0
4	NAG	A	1409	1	14,14,15	0.52	0	17,19,21	0.36	0
4	NAG	C	1402	1	14,14,15	0.21	0	17,19,21	0.63	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	A	1407	1	14,14,15	0.23	0	17,19,21	0.49	0
4	NAG	B	1403	1	14,14,15	0.20	0	17,19,21	0.42	0
4	NAG	A	1401	1	14,14,15	0.31	0	17,19,21	0.33	0
4	NAG	C	1405	1	14,14,15	0.57	0	17,19,21	1.26	1 (5%)
4	NAG	C	1407	1	14,14,15	0.24	0	17,19,21	0.49	0
4	NAG	E	901	2	14,14,15	0.38	0	17,19,21	0.60	1 (5%)
4	NAG	A	1403	1	14,14,15	0.20	0	17,19,21	0.41	0
4	NAG	B	1410	-	14,14,15	0.35	0	17,19,21	0.41	0
4	NAG	B	1402	1	14,14,15	0.20	0	17,19,21	0.64	0
4	NAG	C	1401	1	14,14,15	0.30	0	17,19,21	0.34	0
4	NAG	D	901	2	14,14,15	0.38	0	17,19,21	0.60	1 (5%)
4	NAG	B	1404	1	14,14,15	0.47	0	17,19,21	0.53	0
4	NAG	C	1406	1	14,14,15	0.30	0	17,19,21	0.39	0
4	NAG	B	1401	1	14,14,15	0.31	0	17,19,21	0.33	0
4	NAG	A	1405	1	14,14,15	0.55	0	17,19,21	1.26	1 (5%)
4	NAG	B	1408	1	14,14,15	0.31	0	17,19,21	0.39	0
4	NAG	C	1404	1	14,14,15	0.48	0	17,19,21	0.54	0
4	NAG	C	1408	1	14,14,15	0.30	0	17,19,21	0.38	0
4	NAG	A	1404	1	14,14,15	0.47	0	17,19,21	0.54	0
4	NAG	B	1409	1	14,14,15	0.41	0	17,19,21	1.15	2 (11%)
4	NAG	A	1406	1	14,14,15	0.29	0	17,19,21	0.38	0
4	NAG	B	1405	1	14,14,15	0.57	0	17,19,21	1.26	1 (5%)
4	NAG	B	1407	1	14,14,15	0.24	0	17,19,21	0.49	0
4	NAG	A	1402	1	14,14,15	0.21	0	17,19,21	0.64	0
4	NAG	C	1403	1	14,14,15	0.20	0	17,19,21	0.42	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	B	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	A	1409	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1402	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1407	1	-	1/6/23/26	0/1/1/1
4	NAG	B	1403	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1401	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1405	1	-	5/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	C	1407	1	-	1/6/23/26	0/1/1/1
4	NAG	E	901	2	-	2/6/23/26	0/1/1/1
4	NAG	A	1403	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1410	-	-	0/6/23/26	0/1/1/1
4	NAG	B	1402	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1401	1	-	2/6/23/26	0/1/1/1
4	NAG	D	901	2	-	2/6/23/26	0/1/1/1
4	NAG	B	1404	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1406	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1401	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1405	1	-	5/6/23/26	0/1/1/1
4	NAG	B	1408	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1404	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1408	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1404	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1409	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1406	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1405	1	-	5/6/23/26	0/1/1/1
4	NAG	B	1407	1	-	1/6/23/26	0/1/1/1
4	NAG	A	1402	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1403	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	1405	NAG	C2-N2-C7	4.34	129.08	122.90
4	A	1405	NAG	C2-N2-C7	4.32	129.05	122.90
4	B	1405	NAG	C2-N2-C7	4.29	129.02	122.90
4	B	1409	NAG	C8-C7-N2	2.29	119.97	116.10
4	E	901	NAG	C1-O5-C5	2.09	115.02	112.19

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

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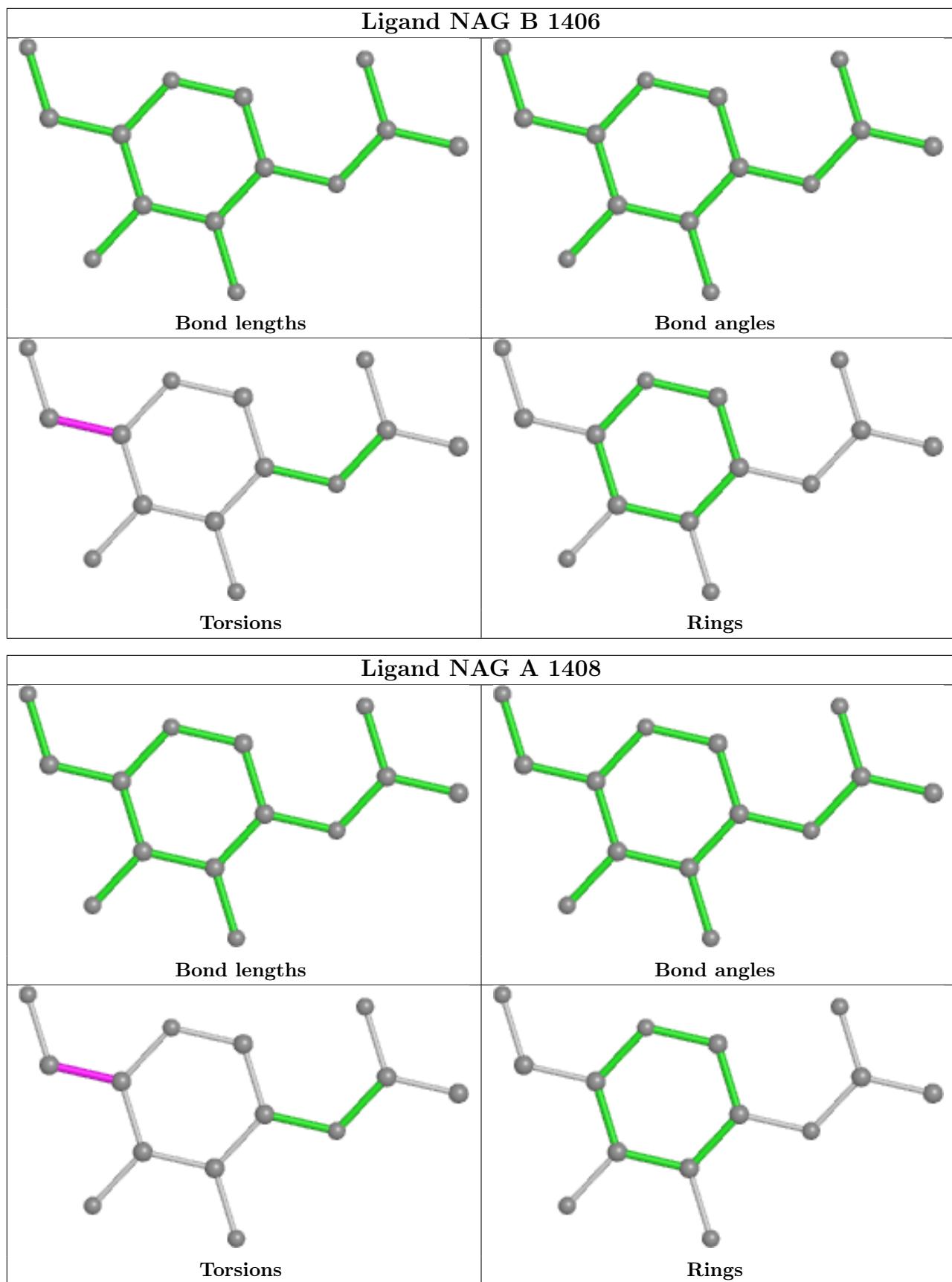
Mol	Chain	Res	Type	Atoms
4	B	1406	NAG	O5-C5-C6-O6
4	C	1406	NAG	O5-C5-C6-O6
4	A	1401	NAG	O5-C5-C6-O6
4	B	1401	NAG	O5-C5-C6-O6

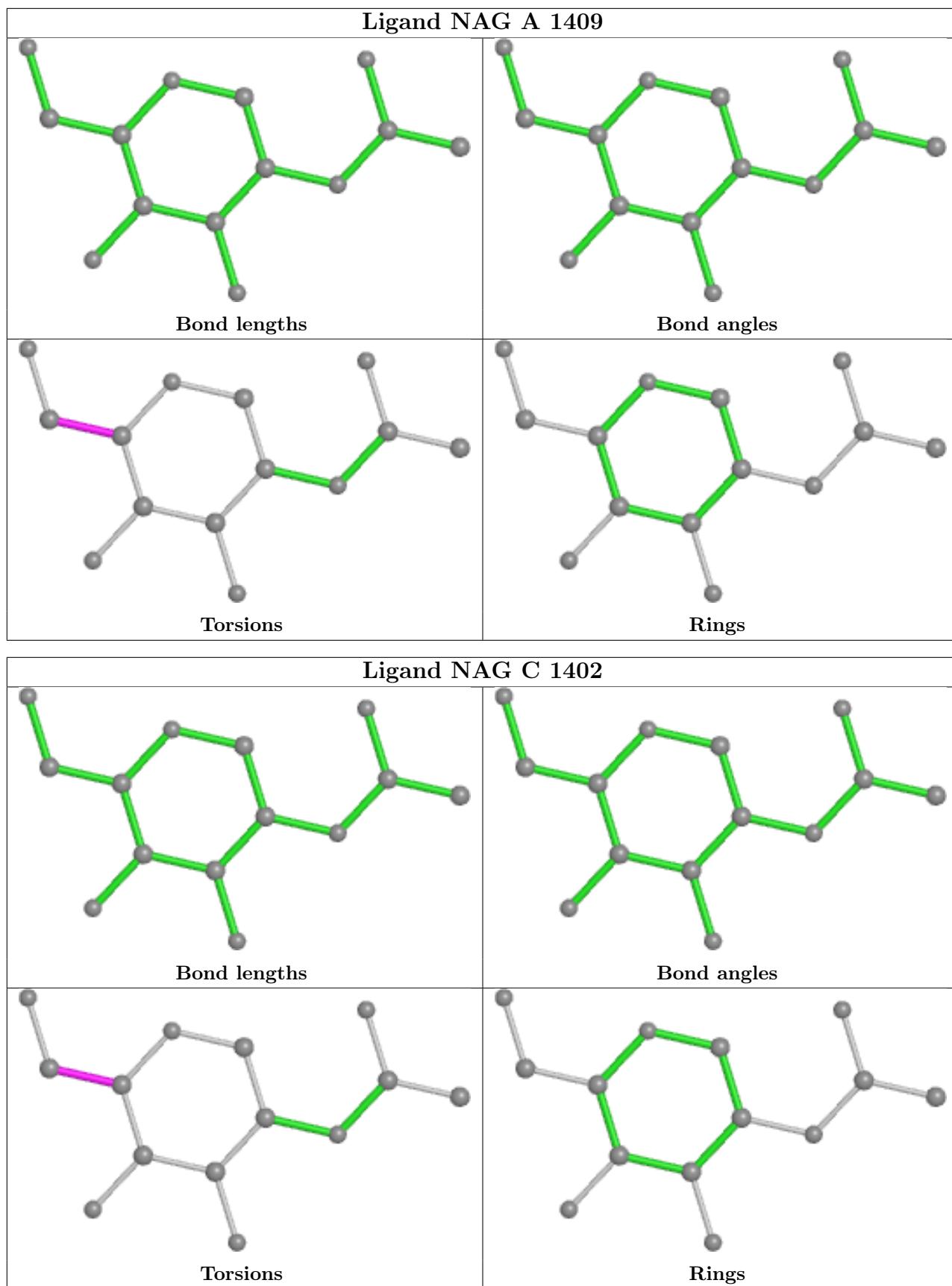
There are no ring outliers.

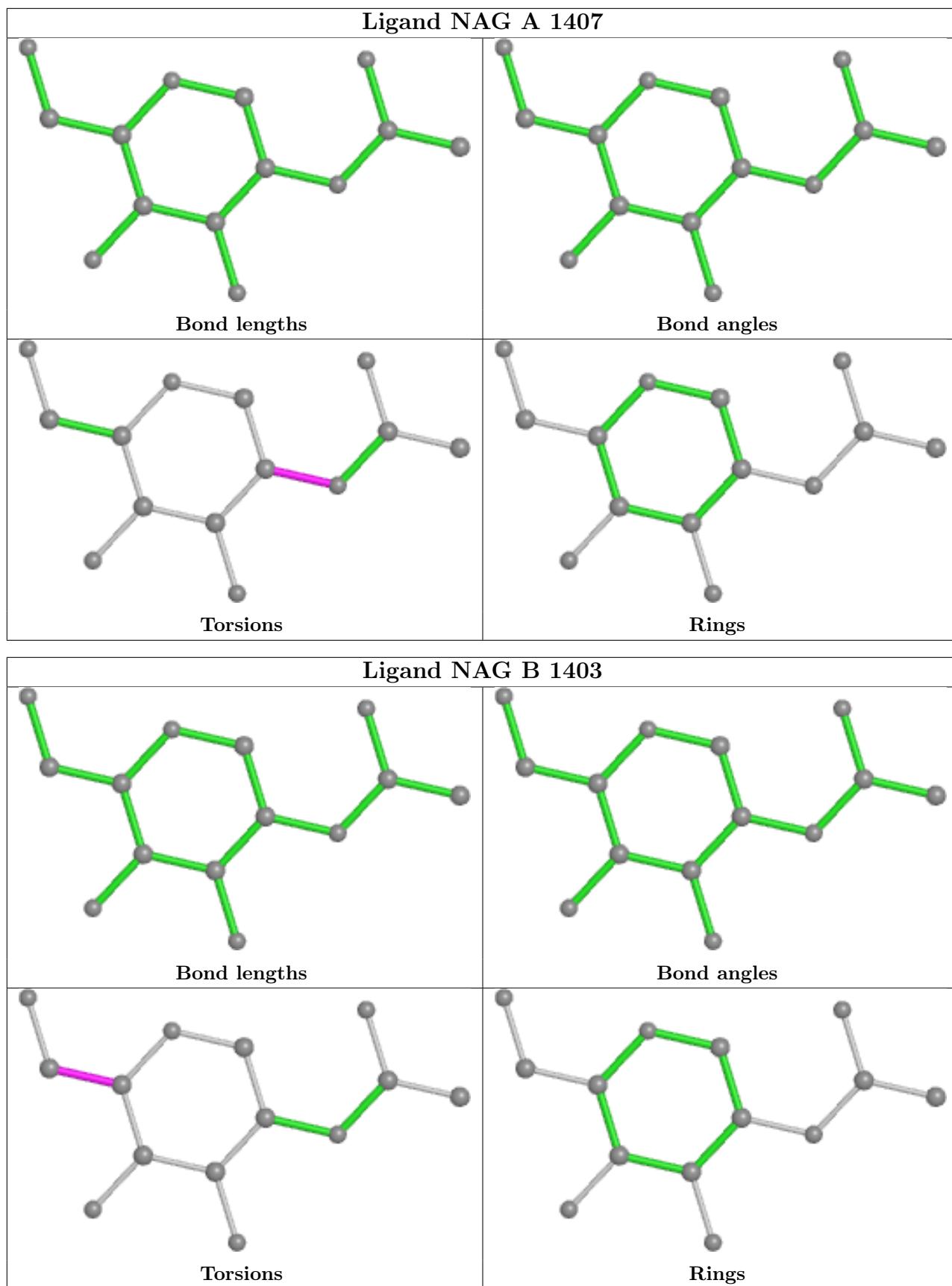
8 monomers are involved in 16 short contacts:

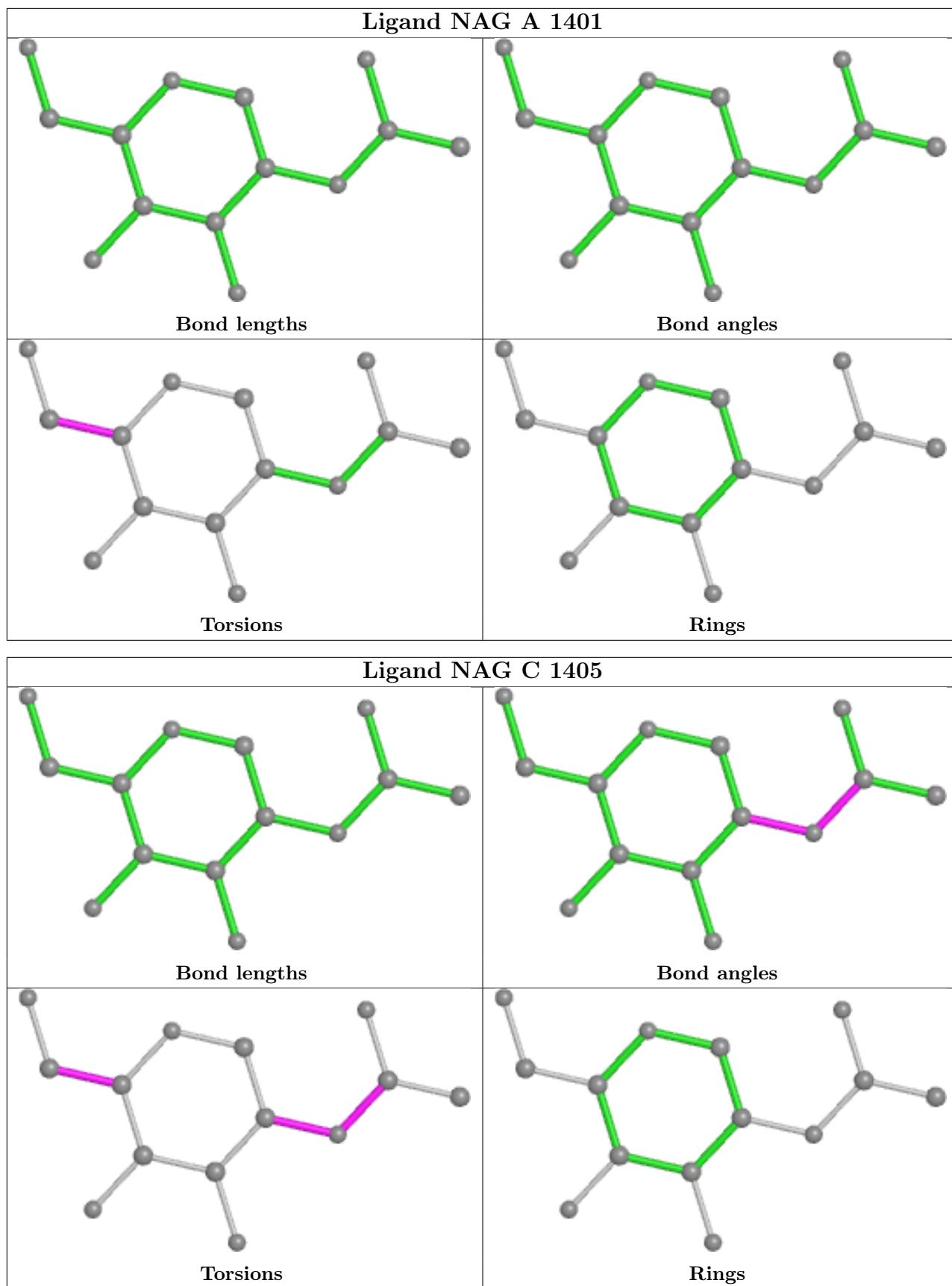
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	1402	NAG	3	0
4	C	1405	NAG	1	0
4	B	1410	NAG	4	0
4	B	1402	NAG	3	0
4	A	1405	NAG	1	0
4	B	1409	NAG	4	0
4	B	1405	NAG	1	0
4	A	1402	NAG	3	0

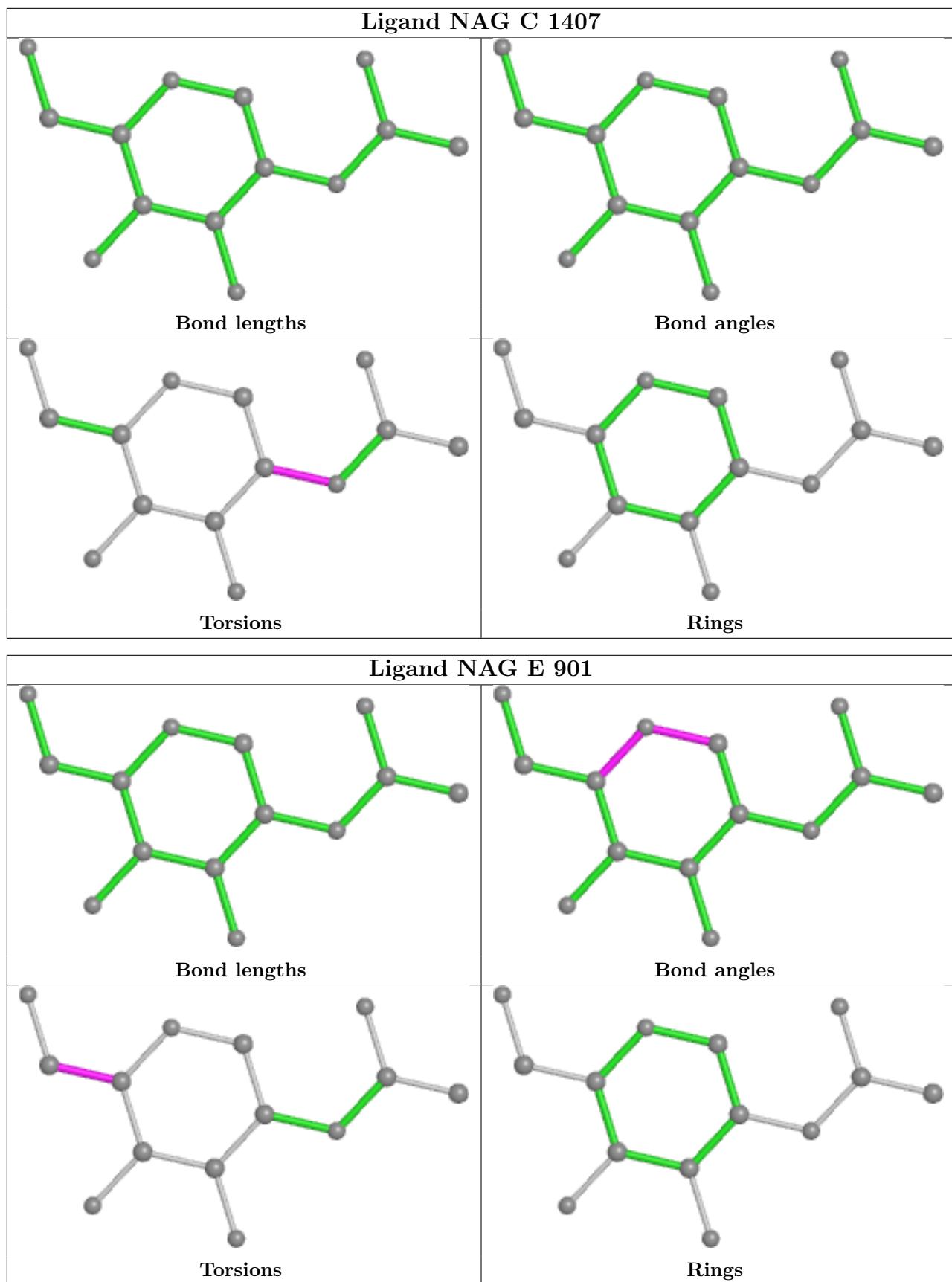
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

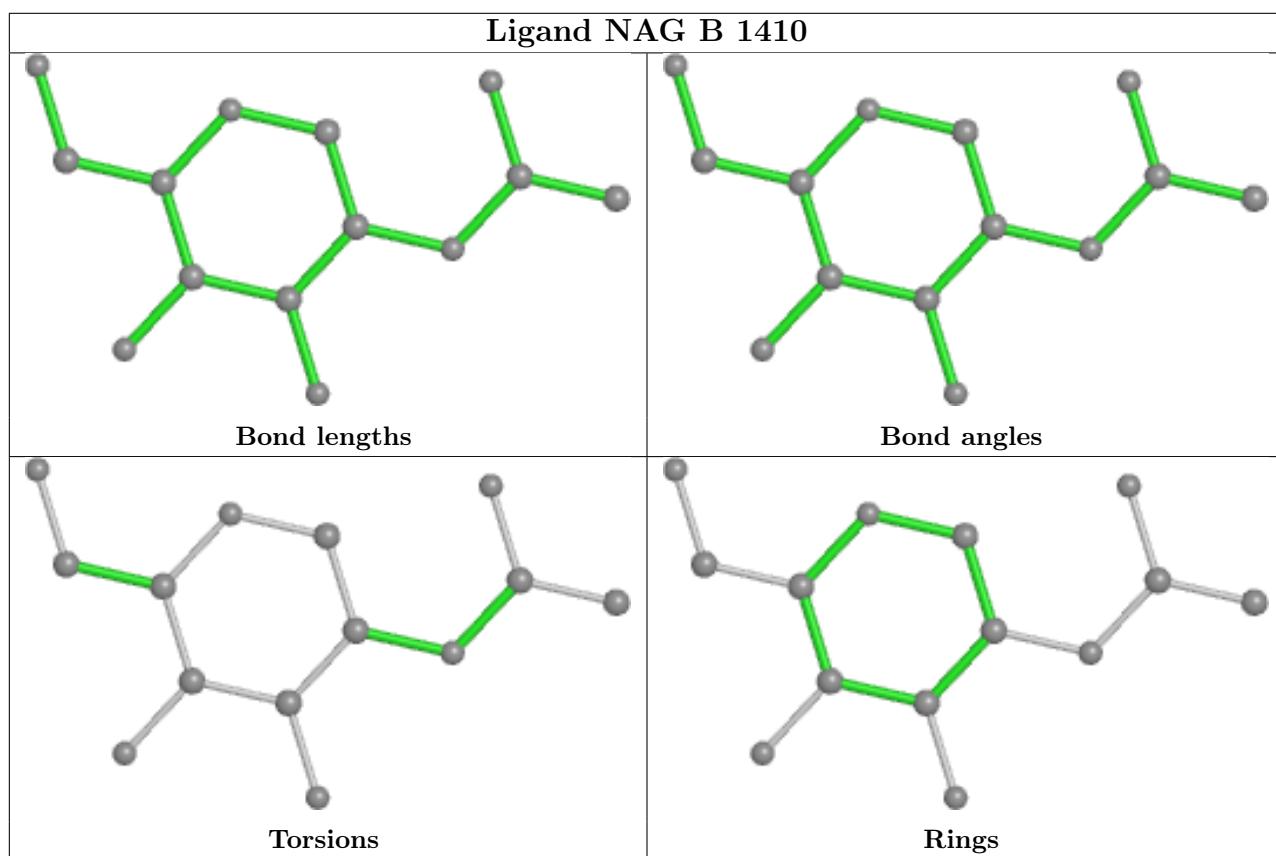
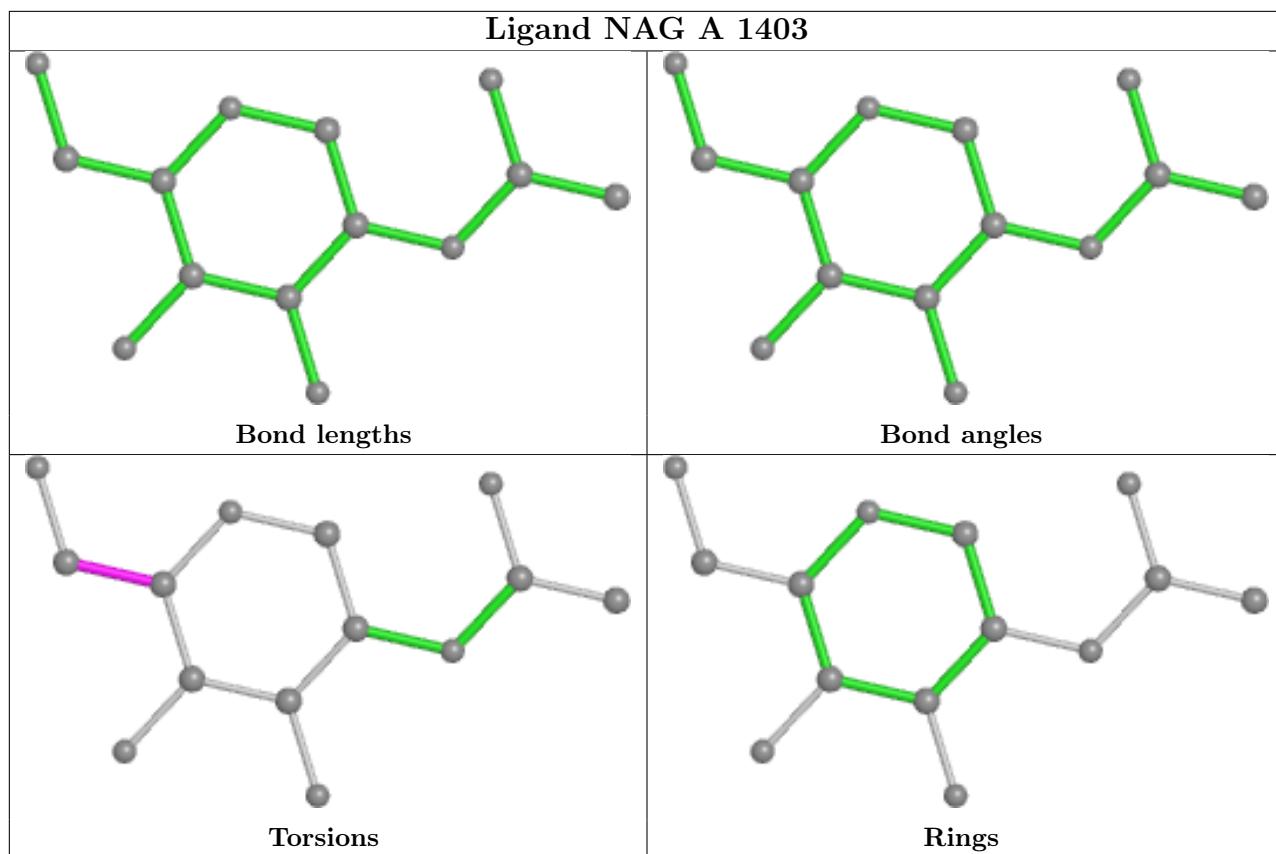


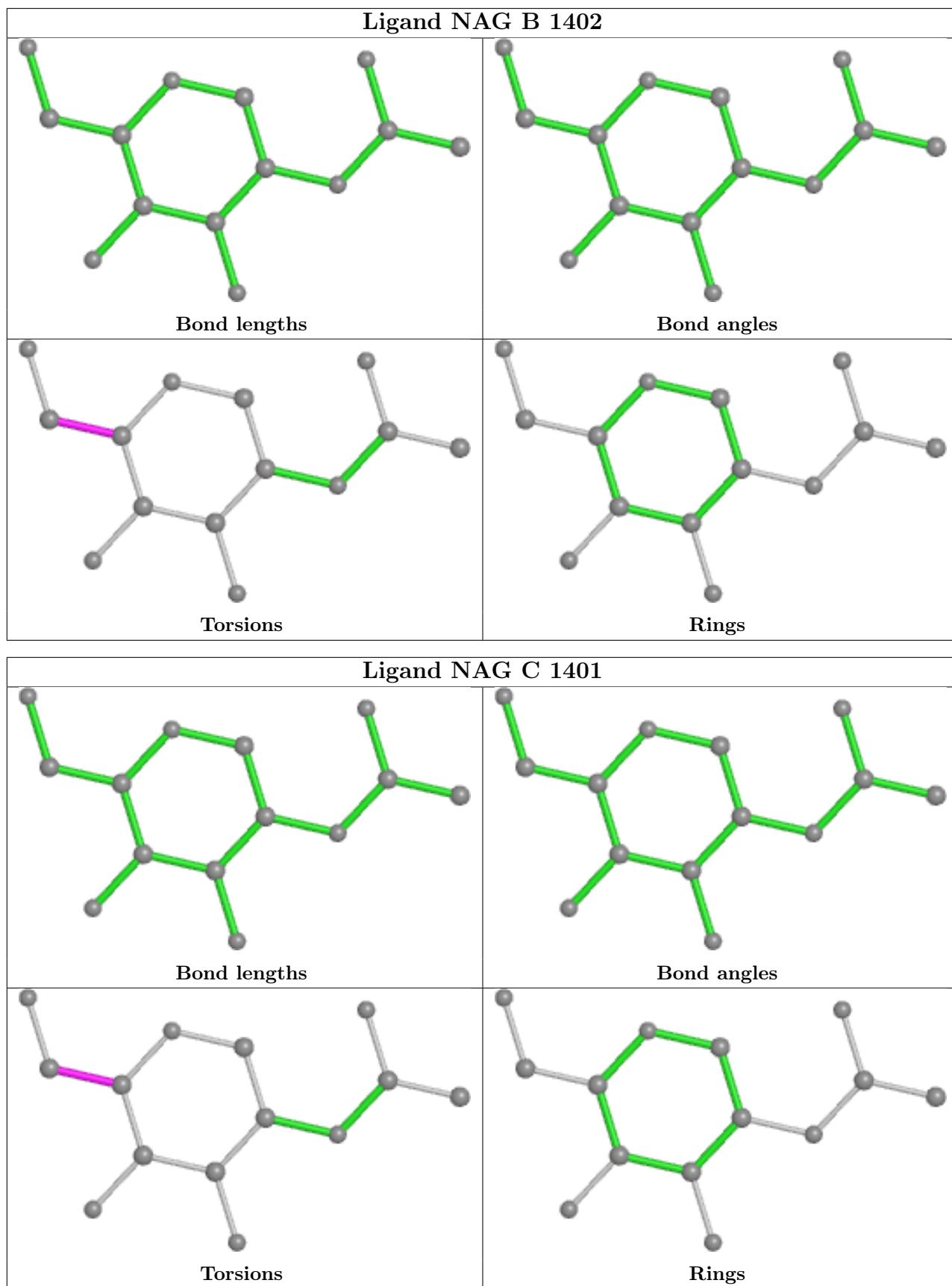


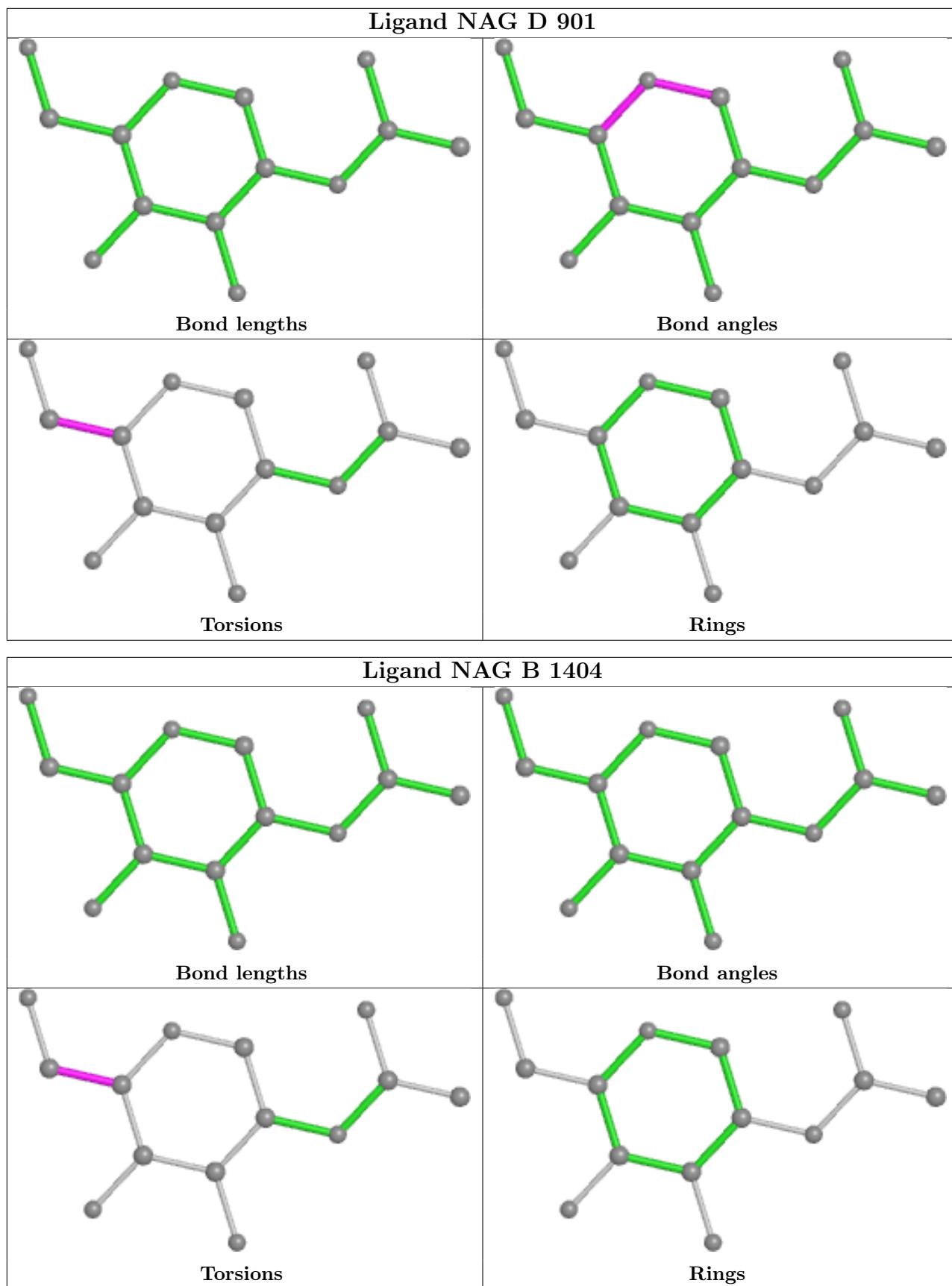


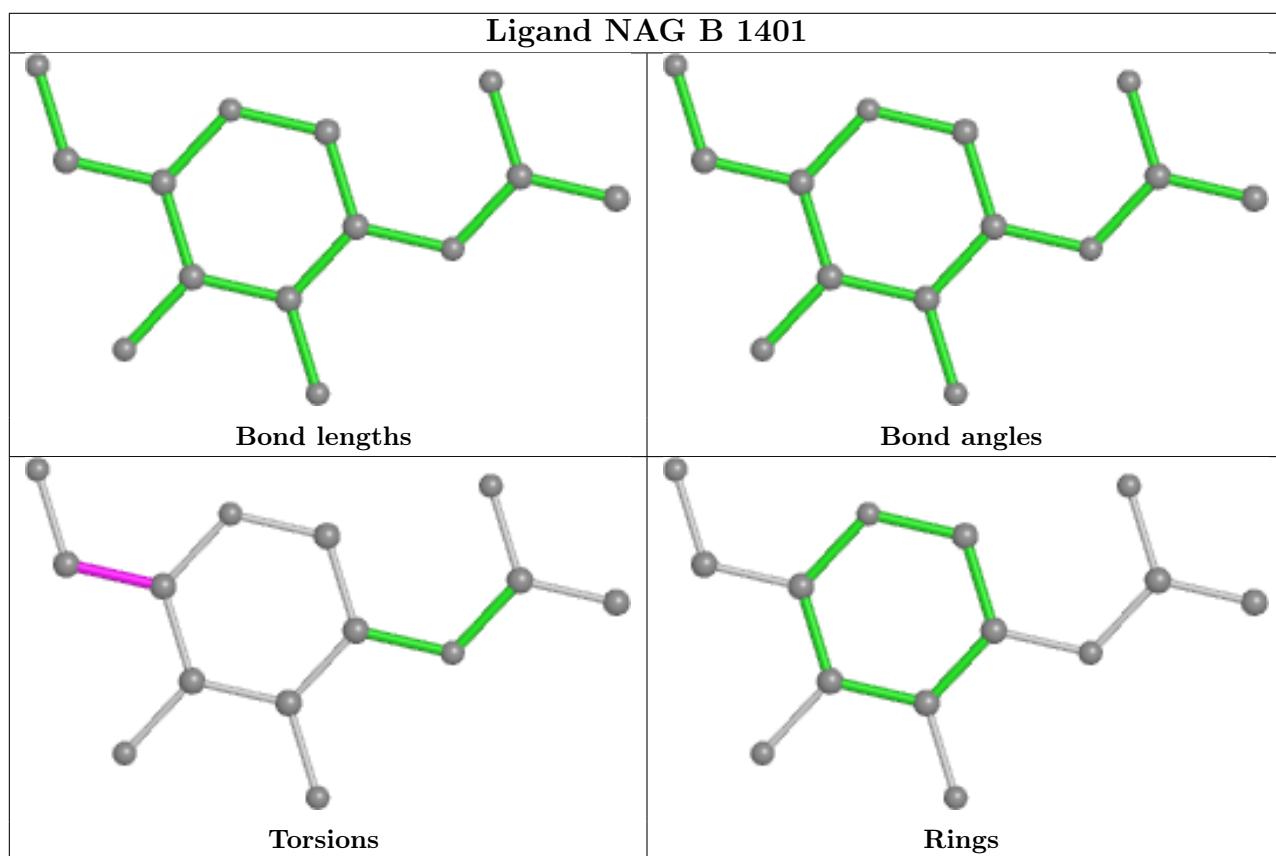
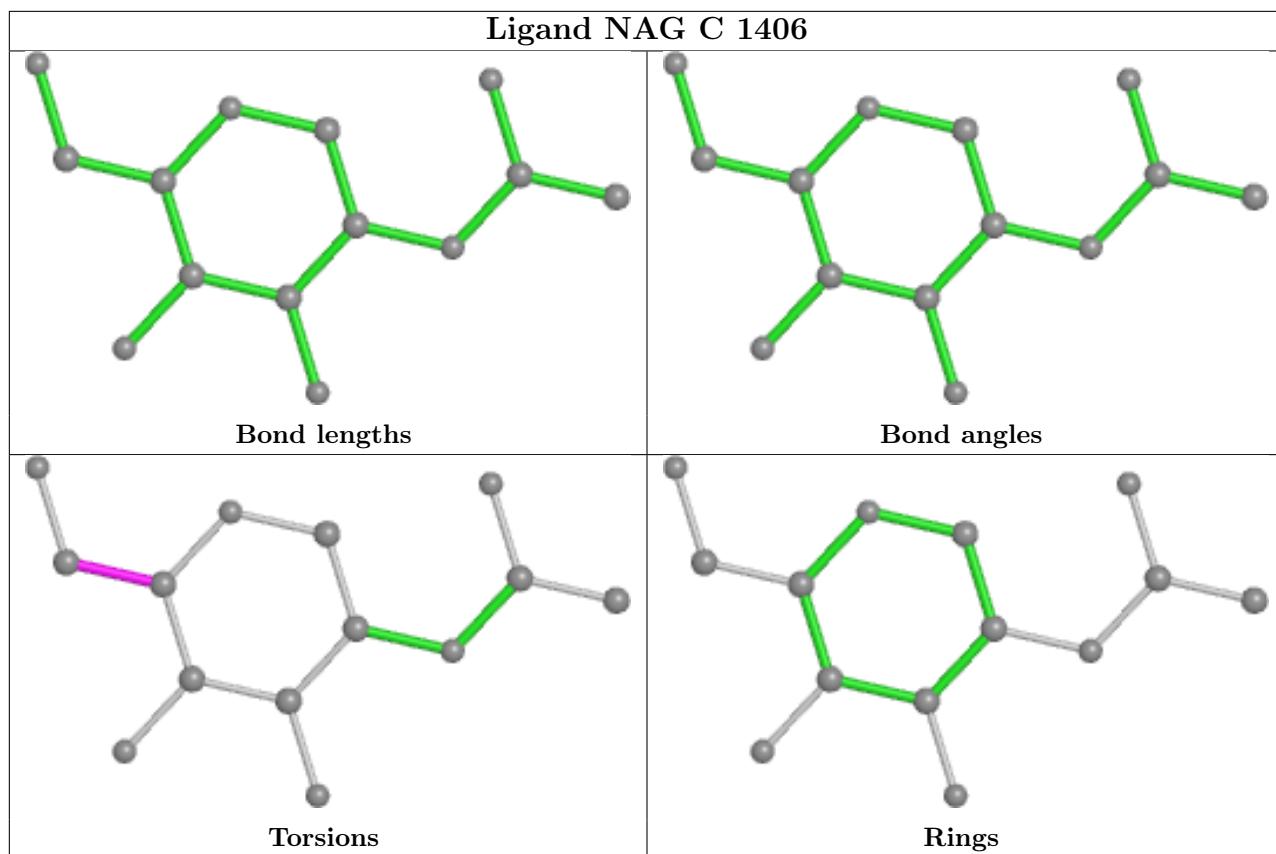


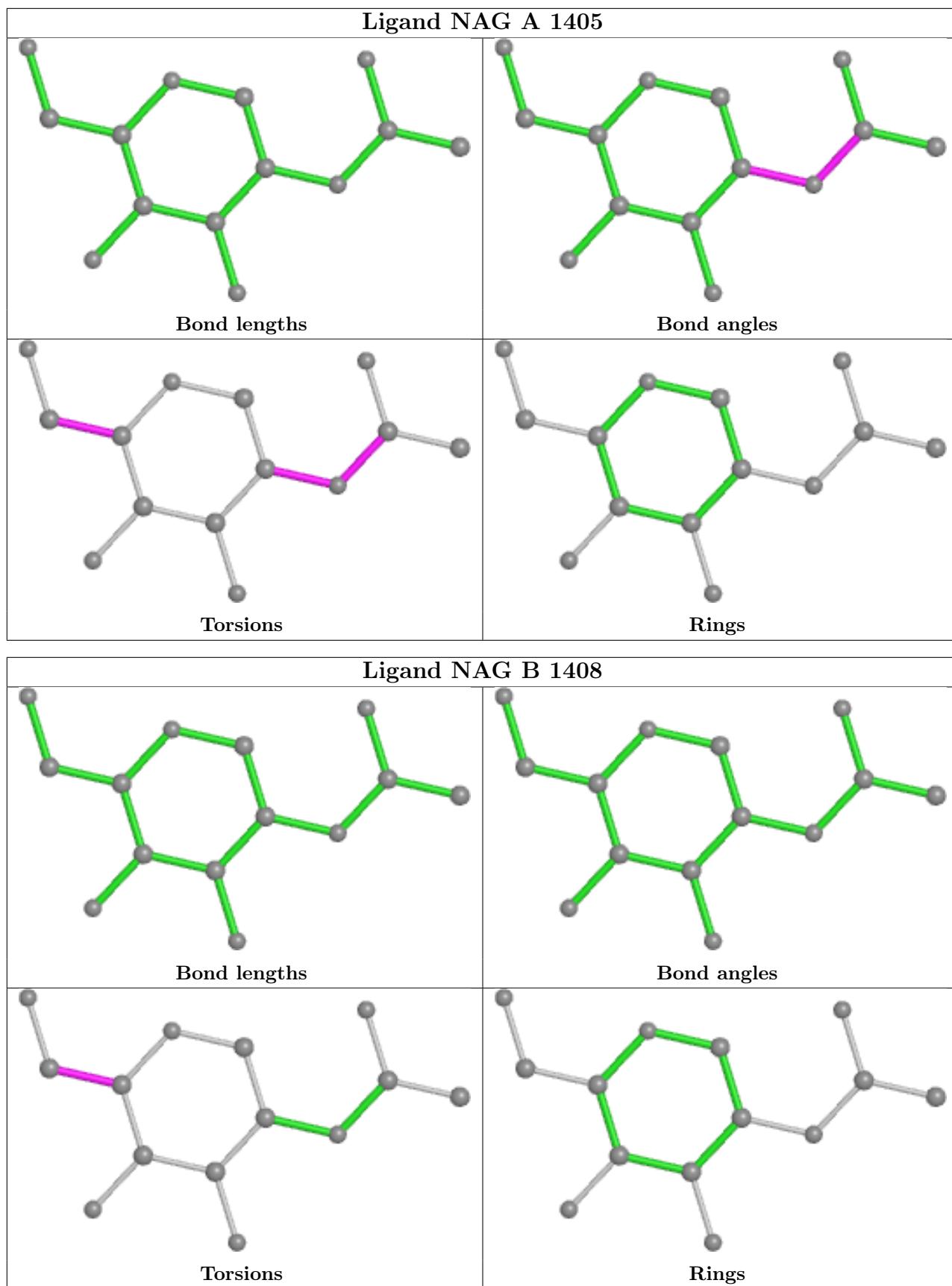


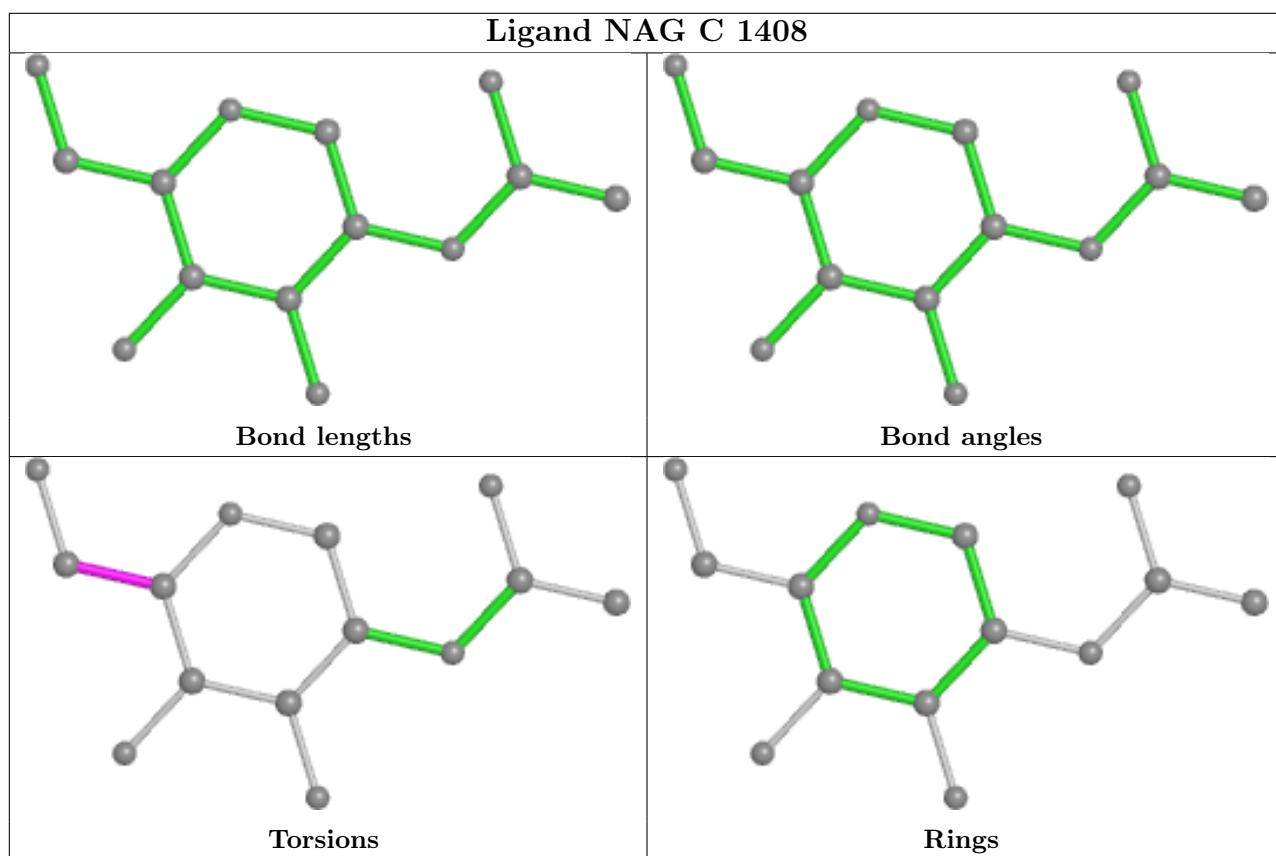
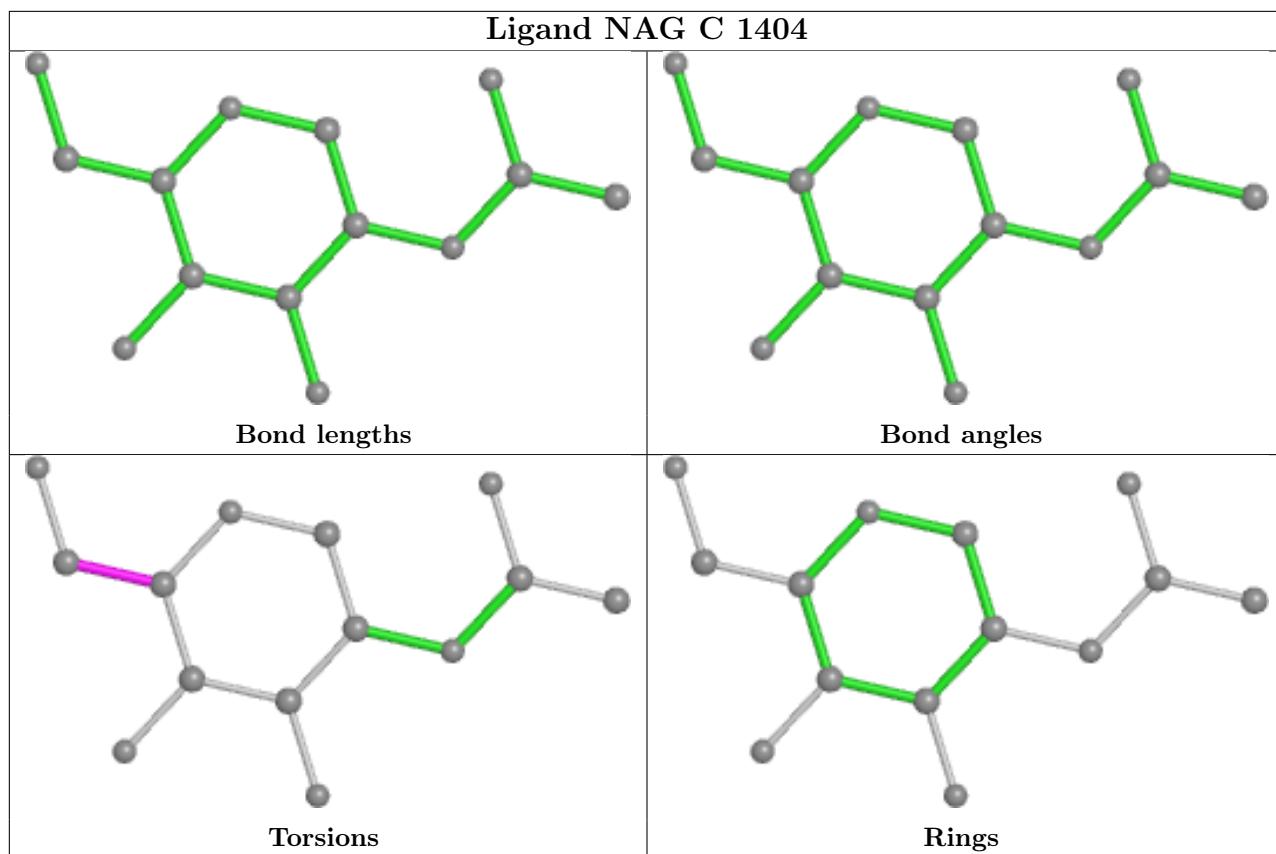


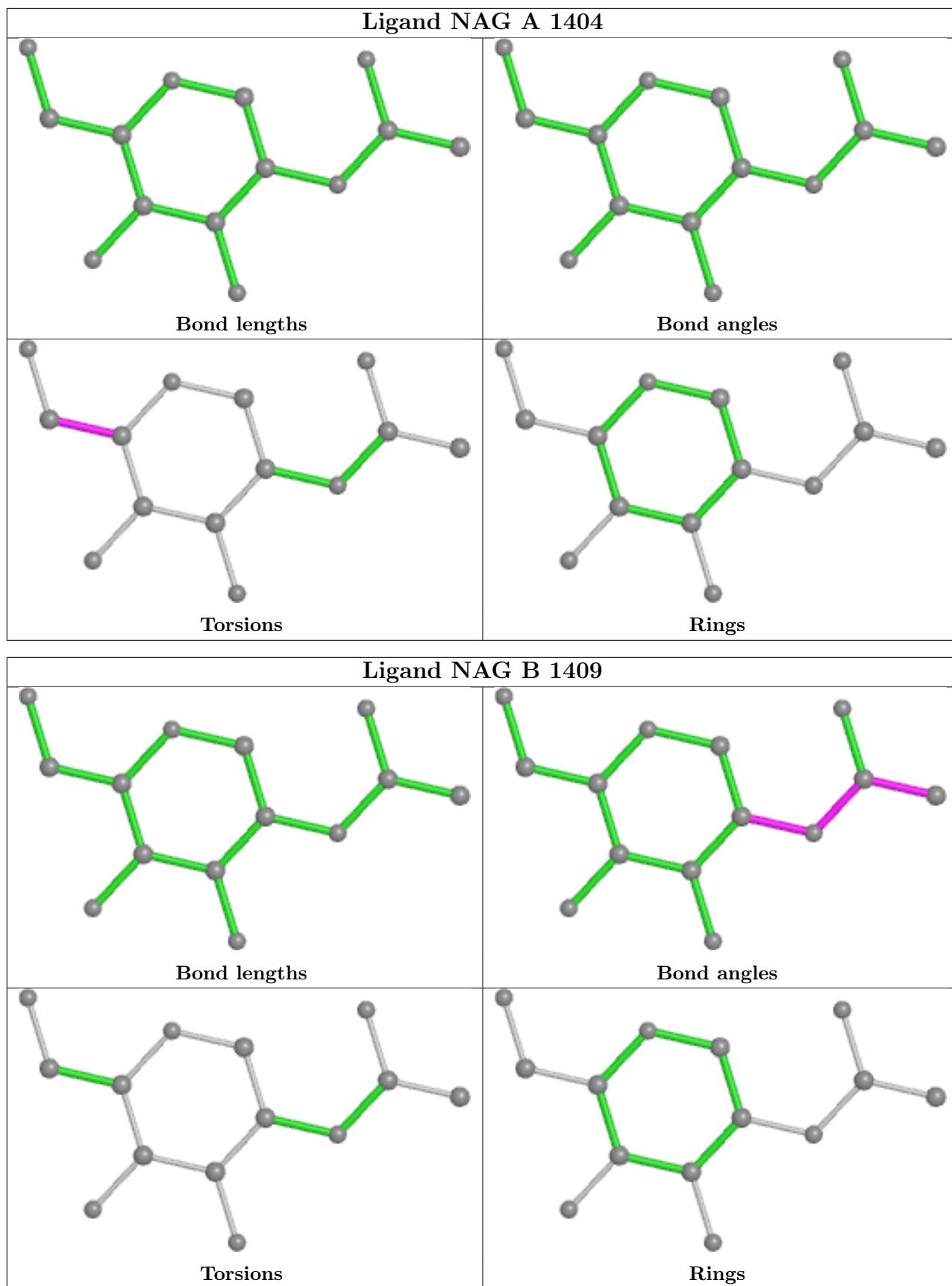


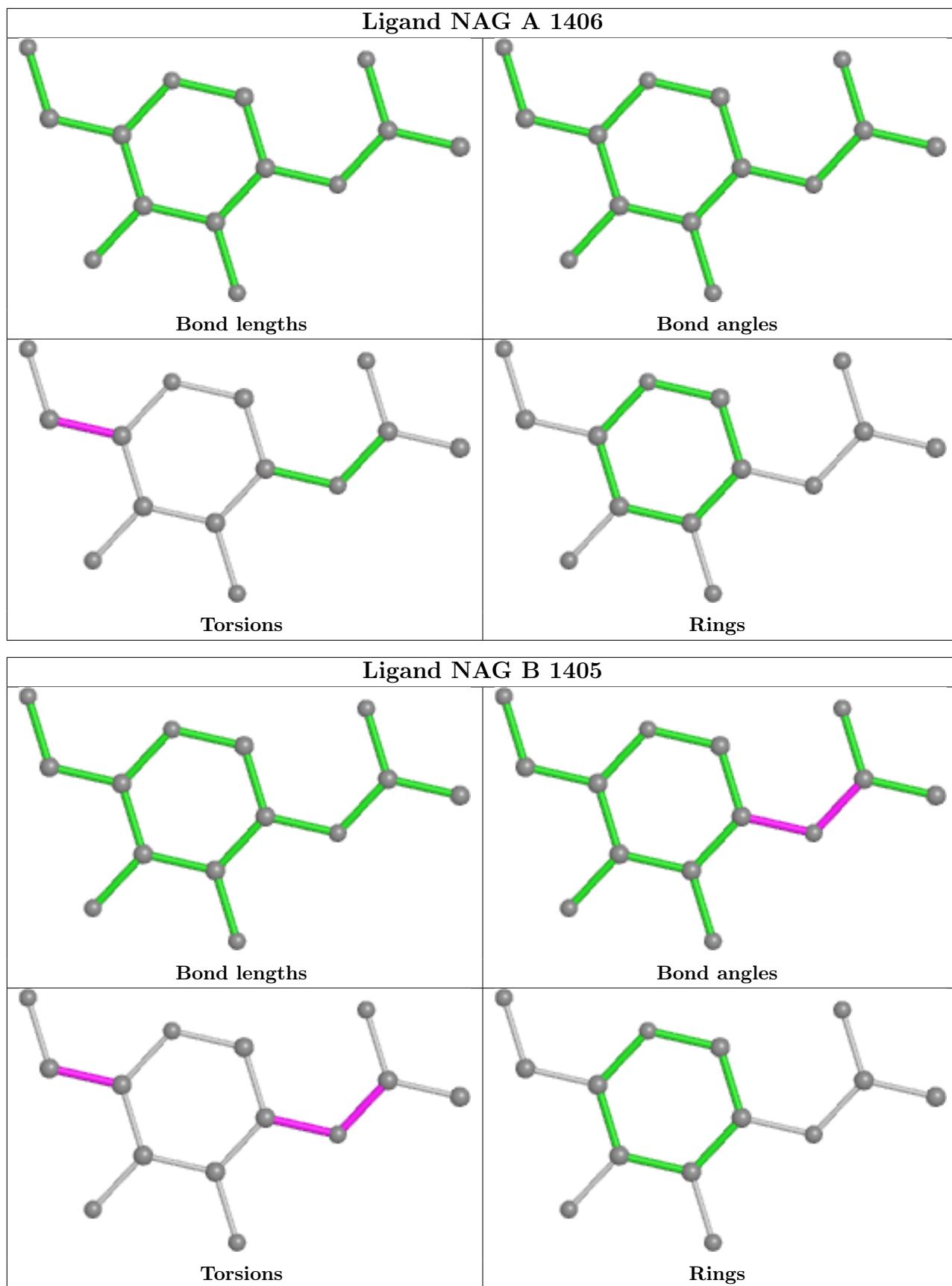


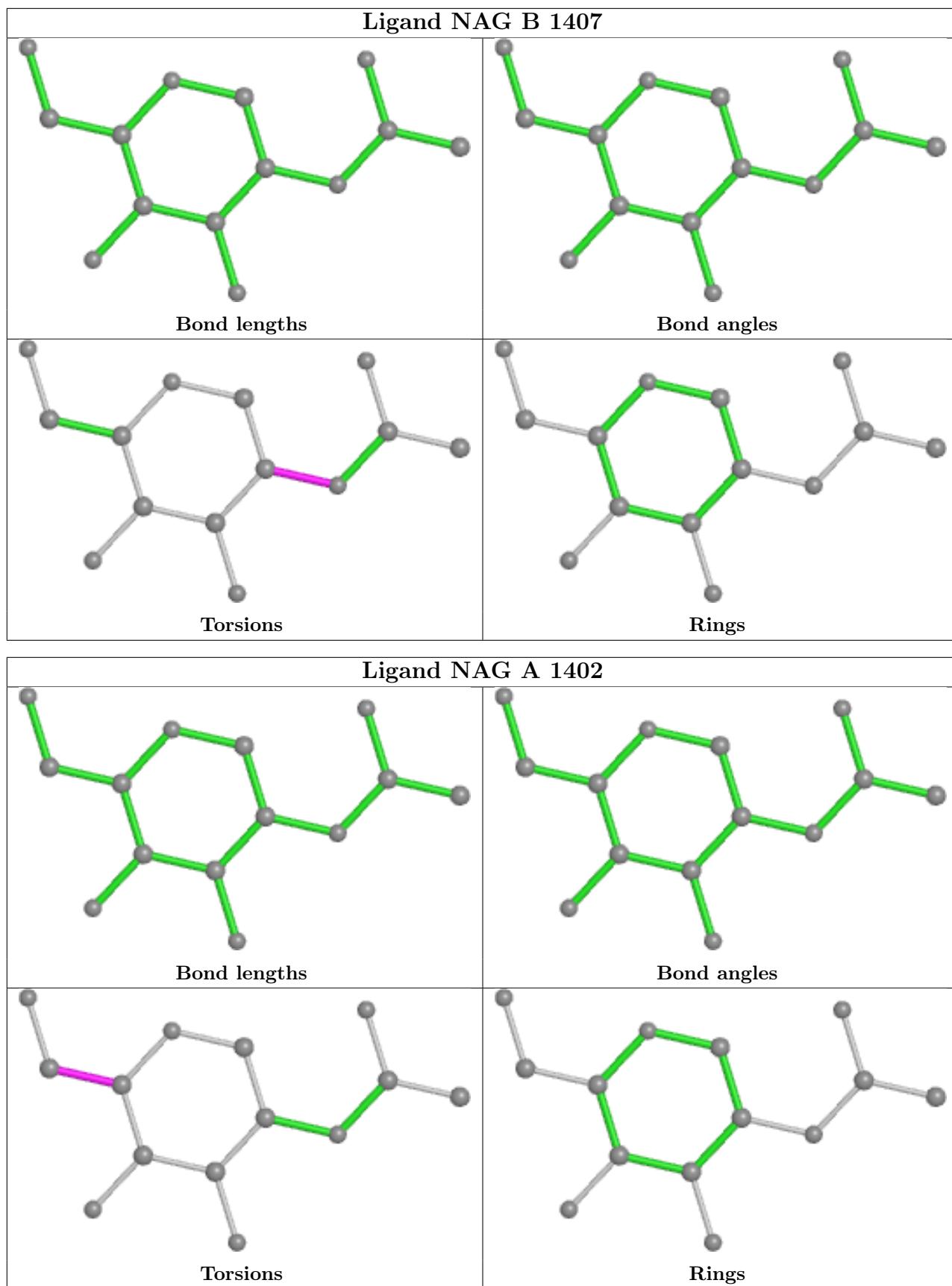


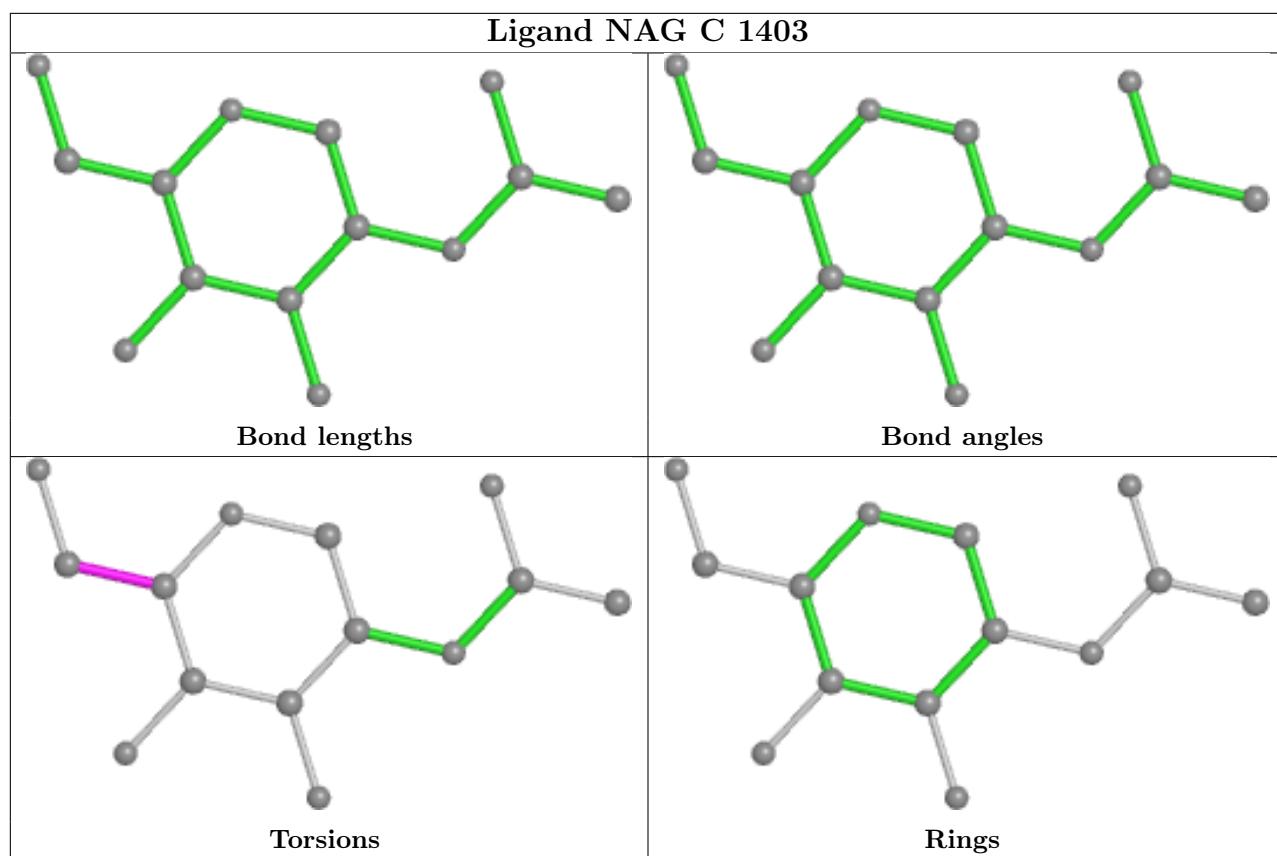












5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [\(i\)](#)

There are no chain breaks in this entry.

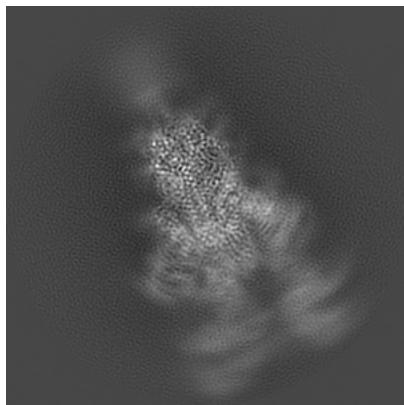
6 Map visualisation i

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.

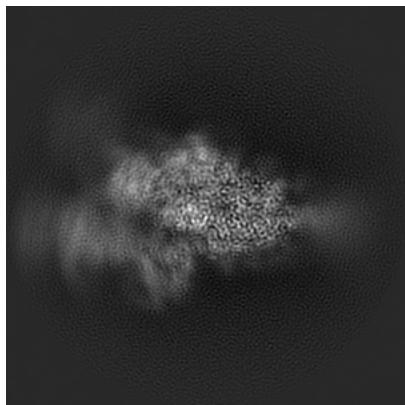
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections i

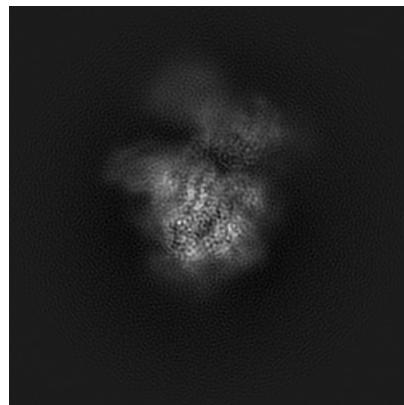
6.1.1 Primary map



X



Y

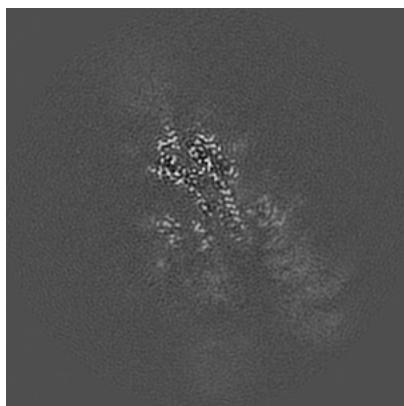


Z

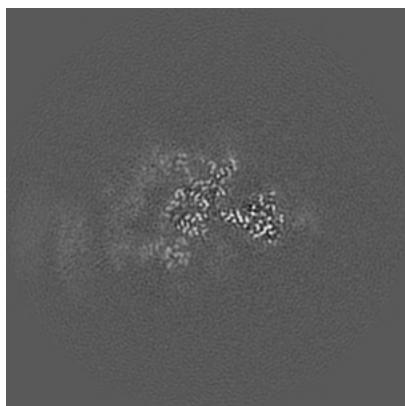
The images above show the map projected in three orthogonal directions.

6.2 Central slices i

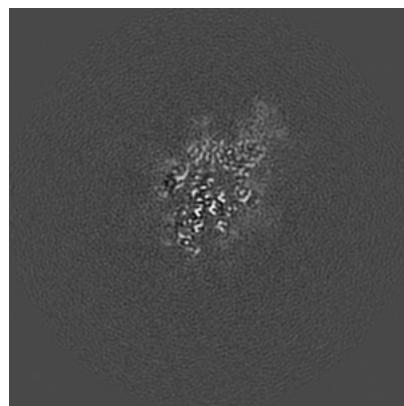
6.2.1 Primary map



X Index: 144



Y Index: 144

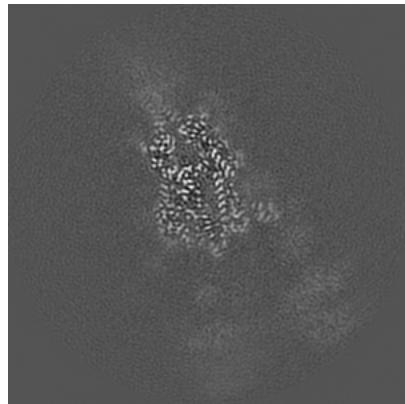


Z Index: 144

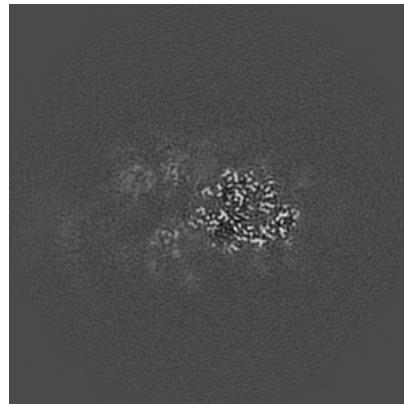
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [\(i\)](#)

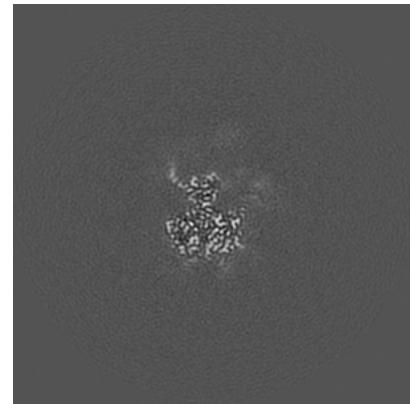
6.3.1 Primary map



X Index: 132



Y Index: 133

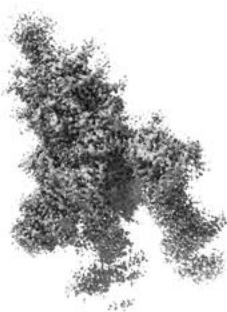


Z Index: 167

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

6.4 Orthogonal surface views [\(i\)](#)

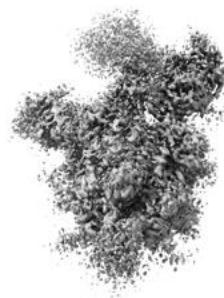
6.4.1 Primary map



X



Y



Z

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.

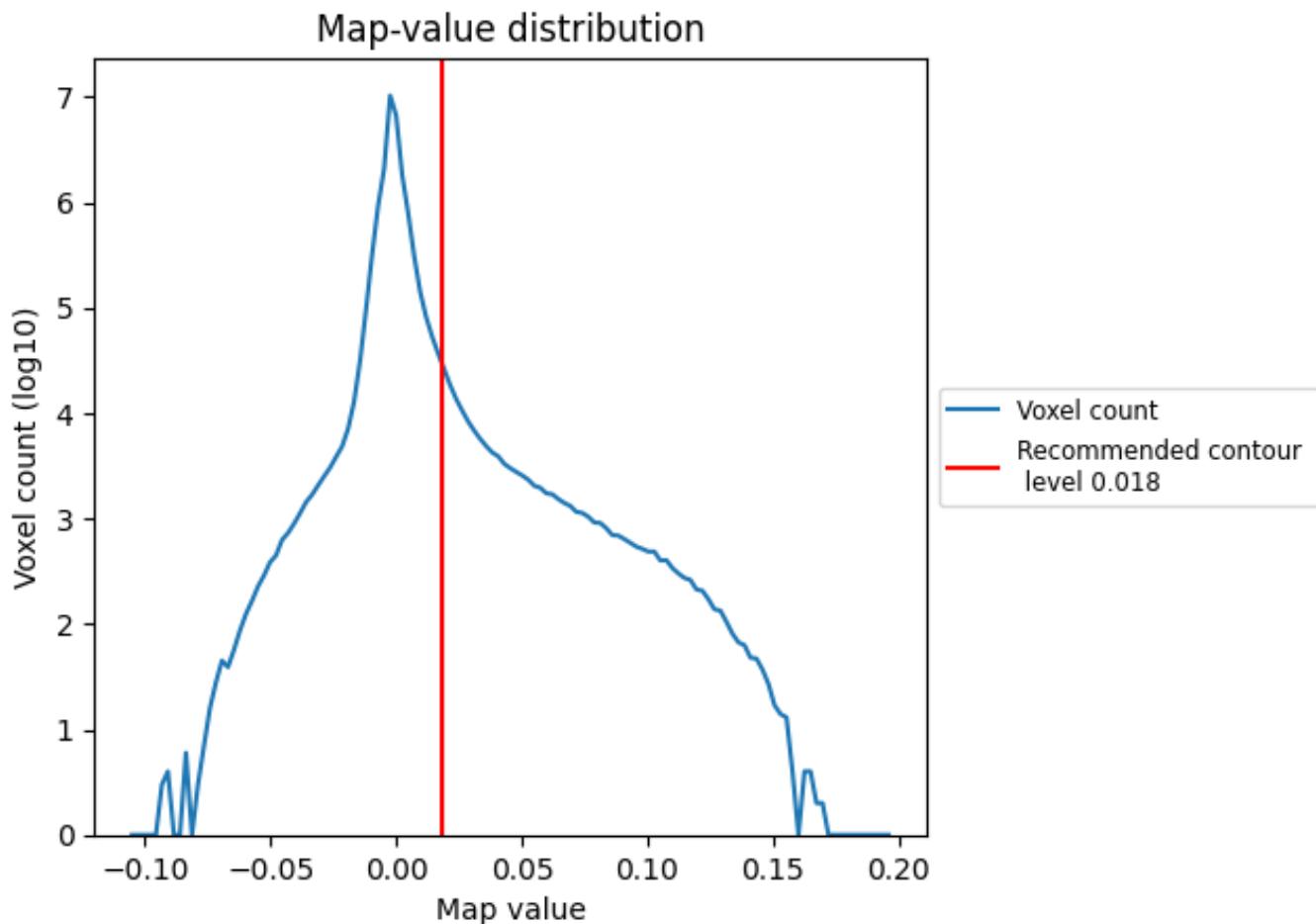
6.5 Mask visualisation

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

7 Map analysis (i)

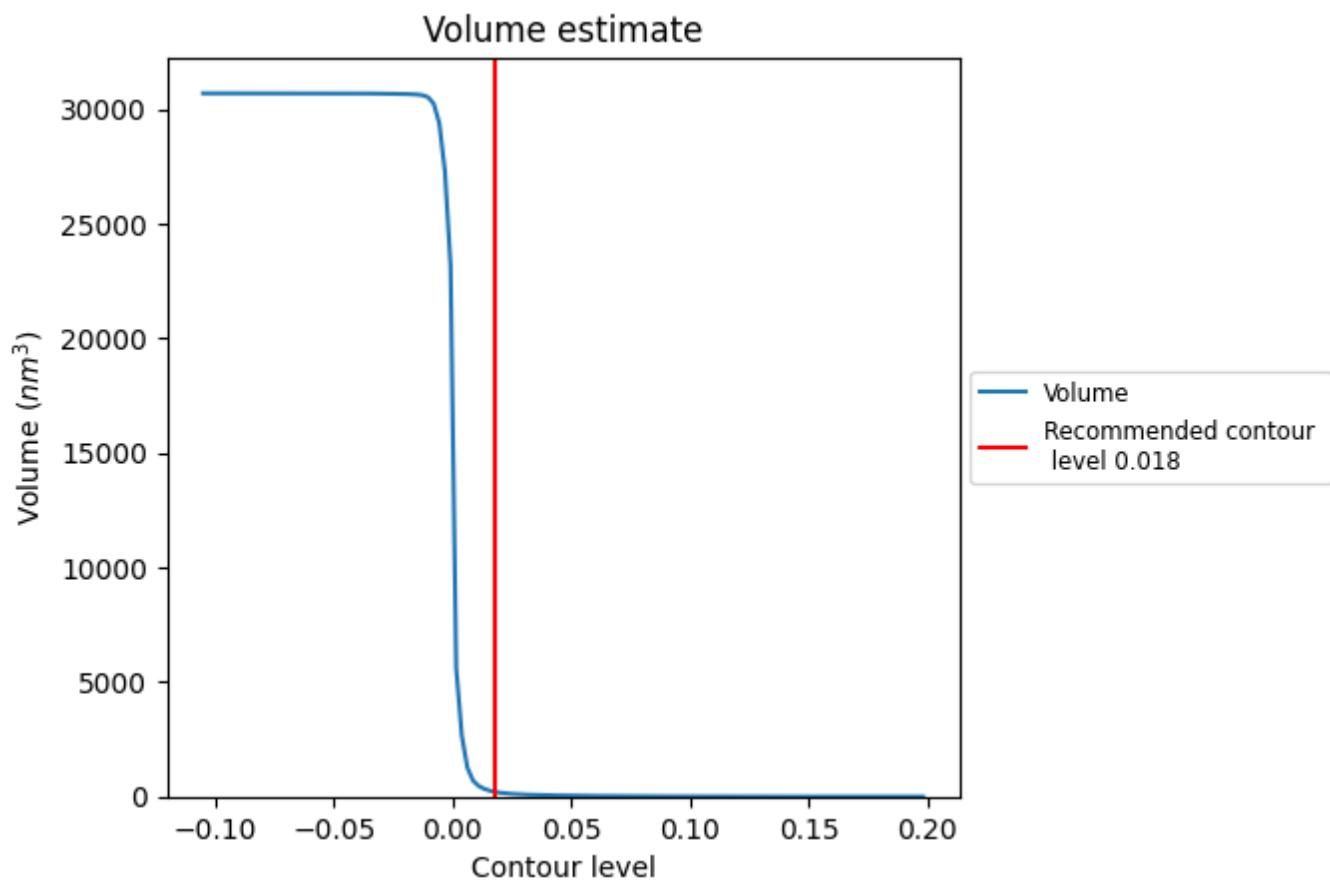
This section contains the results of statistical analysis of the map.

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.

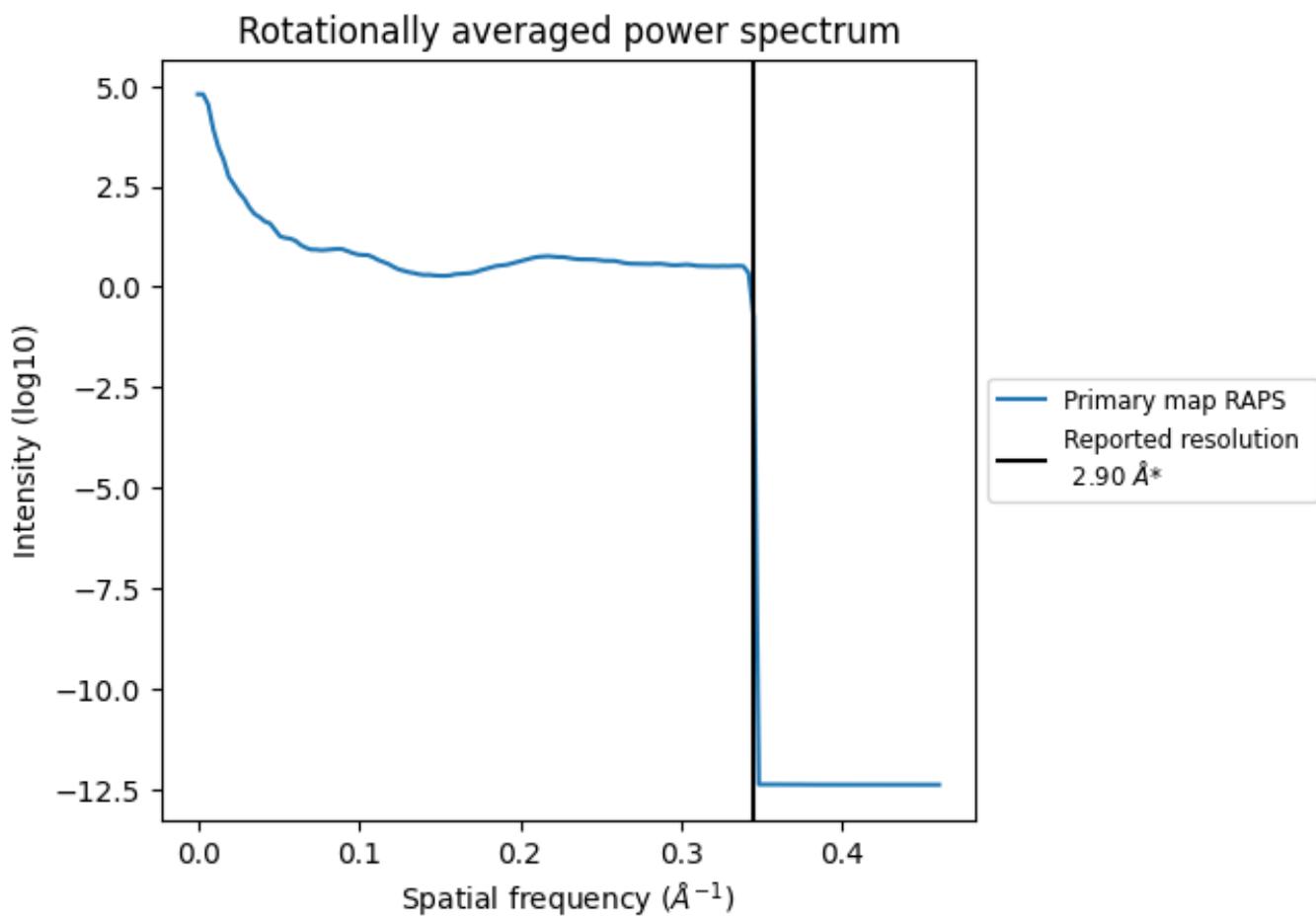
7.2 Volume estimate (i)



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 [\(i\)](#)



*Reported resolution corresponds to spatial frequency of 0.345 \AA^{-1}

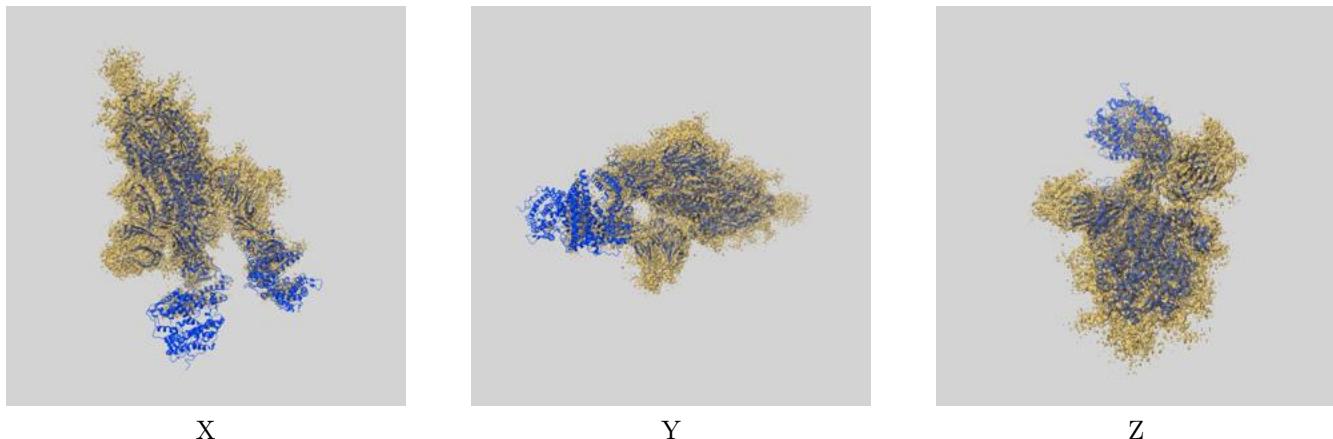
8 Fourier-Shell correlation [i](#)

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

9 Map-model fit (i)

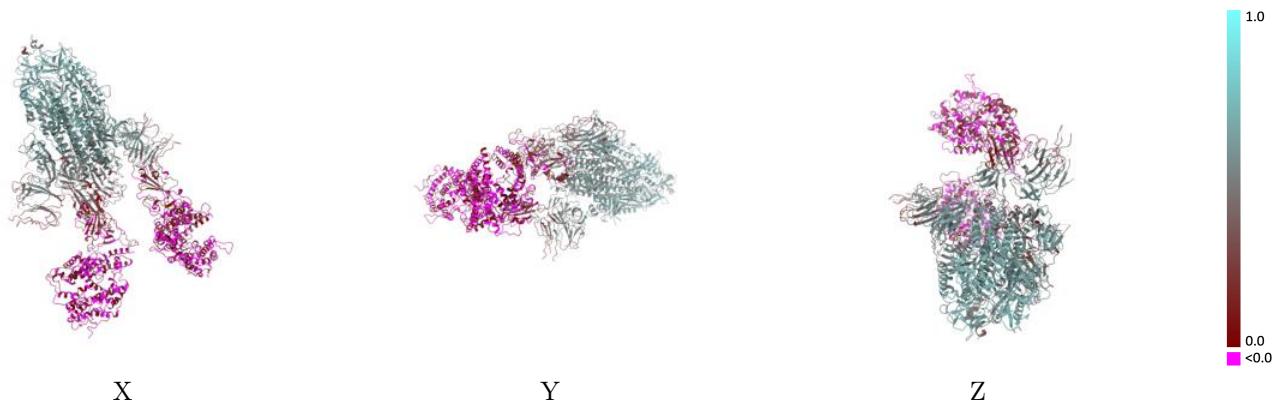
This section contains information regarding the fit between EMDB map EMD-30899 and PDB model 7DX8. Per-residue inclusion information can be found in section 3 on page 11.

9.1 Map-model overlay (i)



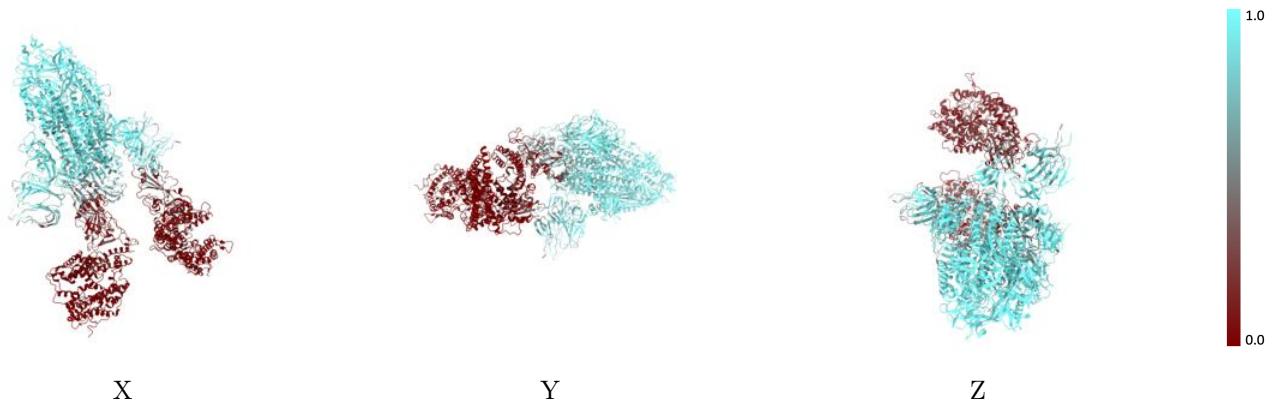
The images above show the 3D surface view of the map at the recommended contour level 0.018 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



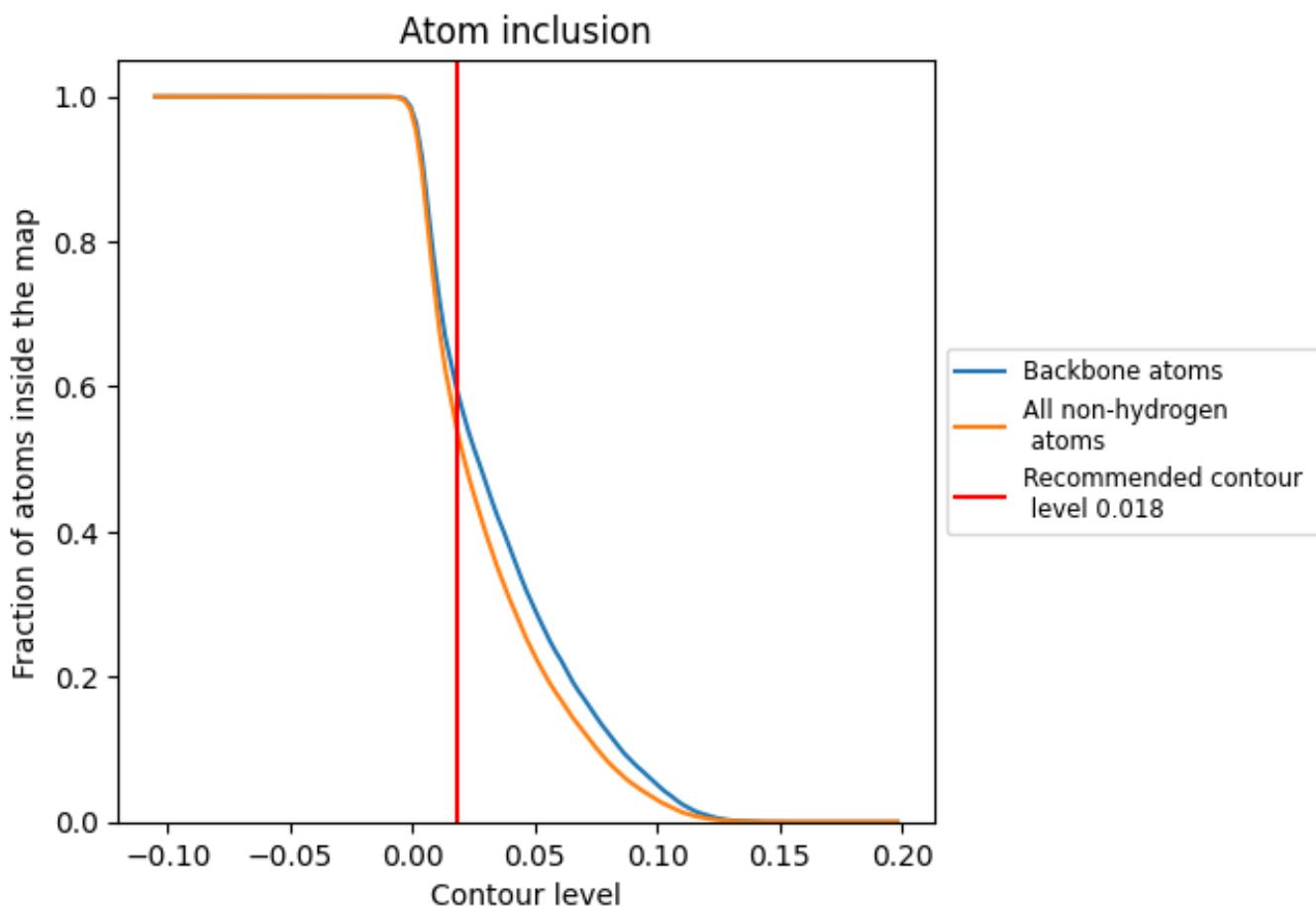
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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	0.7549	0.4550
B	0.7953	0.4820
C	0.7388	0.4400
D	0.0272	0.0150
E	0.0130	0.0070
F	0.5000	0.2070
G	0.2857	0.2920
H	0.9286	0.5270
I	0.8214	0.3920
J	0.6786	0.4650
K	0.8571	0.4920
L	0.7857	0.3800
M	0.4286	0.1450
N	0.1071	0.0750
O	0.6429	0.2710
P	0.8929	0.4990
Q	0.7857	0.3950
R	0.7500	0.4590
S	0.7500	0.3730
T	0.4286	0.2830
U	0.0714	-0.0220
V	0.6429	0.3330
W	0.8571	0.5040
X	0.7500	0.4480
Y	0.6429	0.3680
Z	0.8214	0.4550
a	0.7500	0.4460
b	0.0357	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



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