



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 02:23 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 Full wwPDB EM Validation 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:

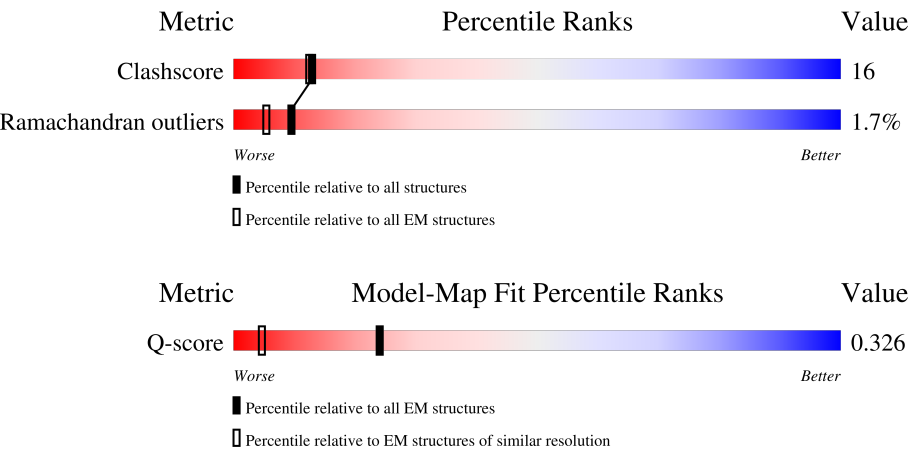
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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.



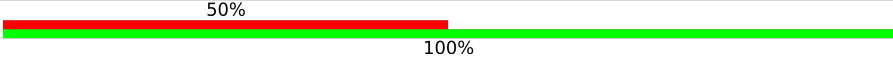
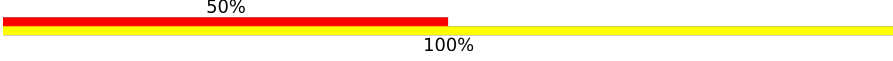
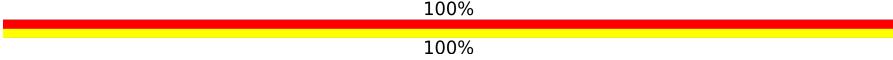
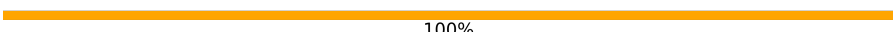
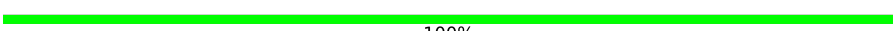
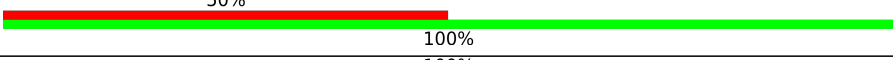
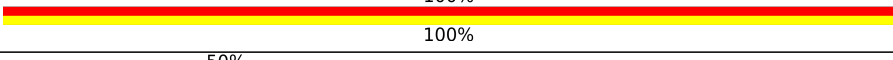
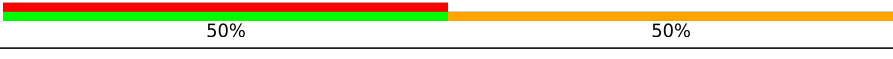
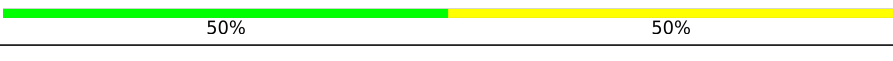
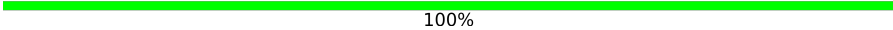
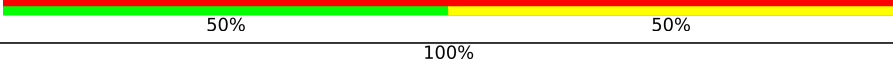
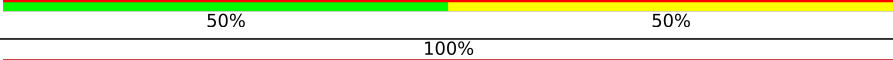
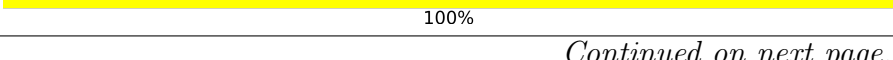
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Q-score	-	25397	13054 (2.40 - 3.40)

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%

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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	

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

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

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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
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

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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-acetamido-2-deoxy-beta-D-glucopyranose.



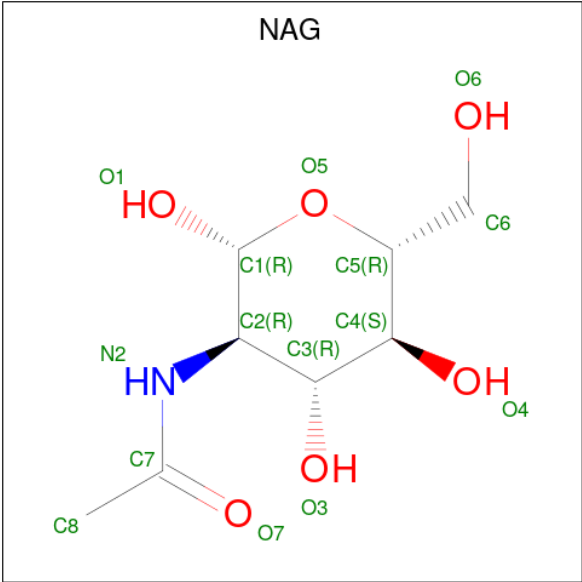
Mol	Chain	Residues	Atoms				AltConf	Trace
3	F	2	Total	C	N	O	0	0
			28	16	2	10		
3	G	2	Total	C	N	O	0	0
			28	16	2	10		
3	H	2	Total	C	N	O	0	0
			28	16	2	10		
3	I	2	Total	C	N	O	0	0
			28	16	2	10		
3	J	2	Total	C	N	O	0	0
			28	16	2	10		
3	K	2	Total	C	N	O	0	0
			28	16	2	10		
3	L	2	Total	C	N	O	0	0
			28	16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

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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 (CCD ID: NAG) (formula: C₈H₁₅NO₆) (labeled as "Ligand of Interest" by depositor).



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

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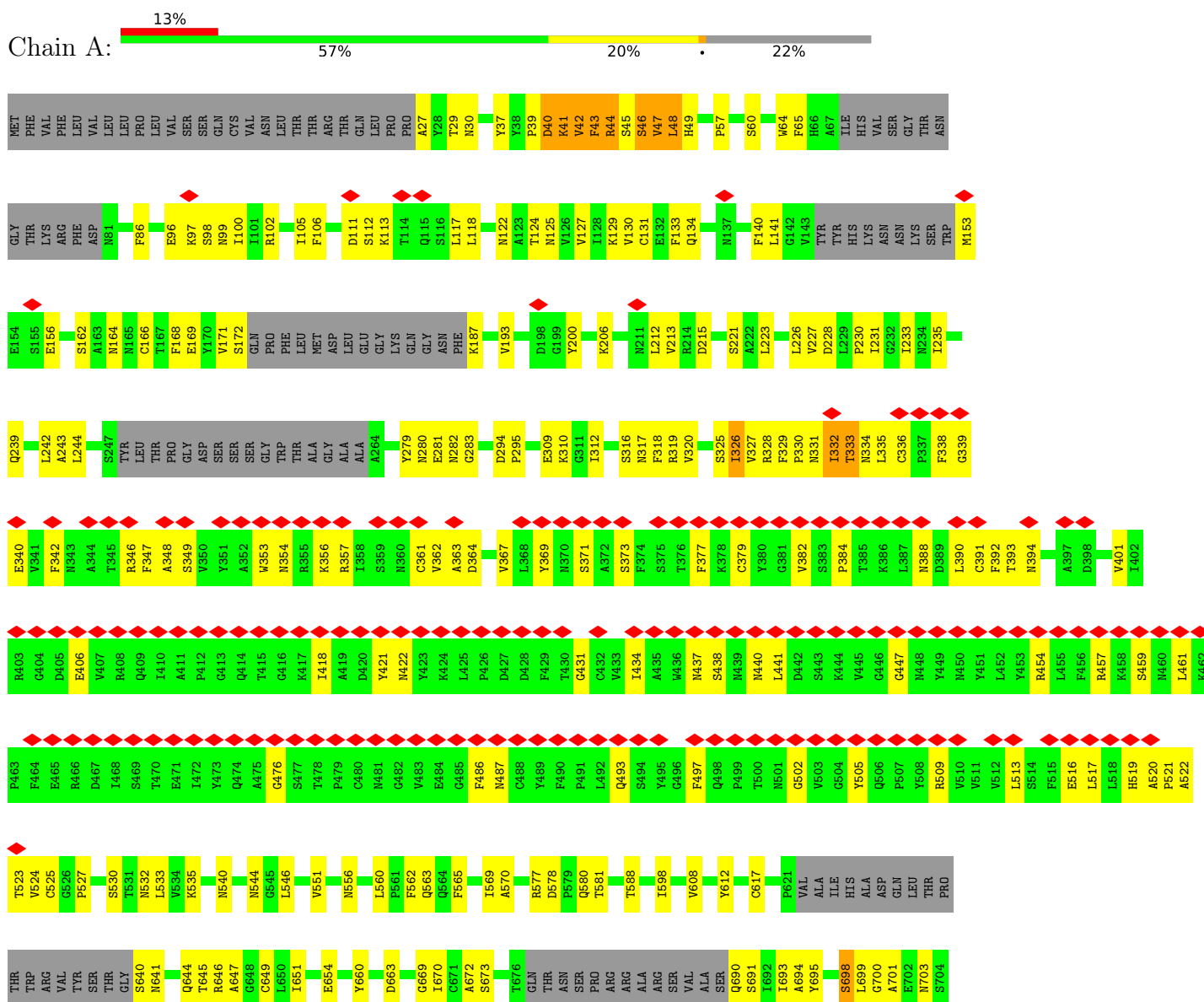
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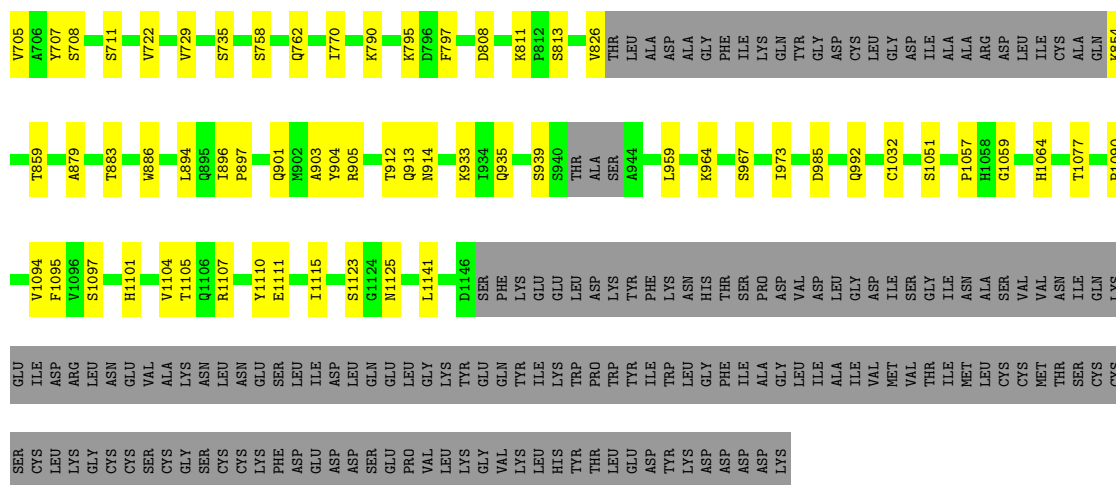
Mol	Chain	Residues	Atoms				AltConf
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4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

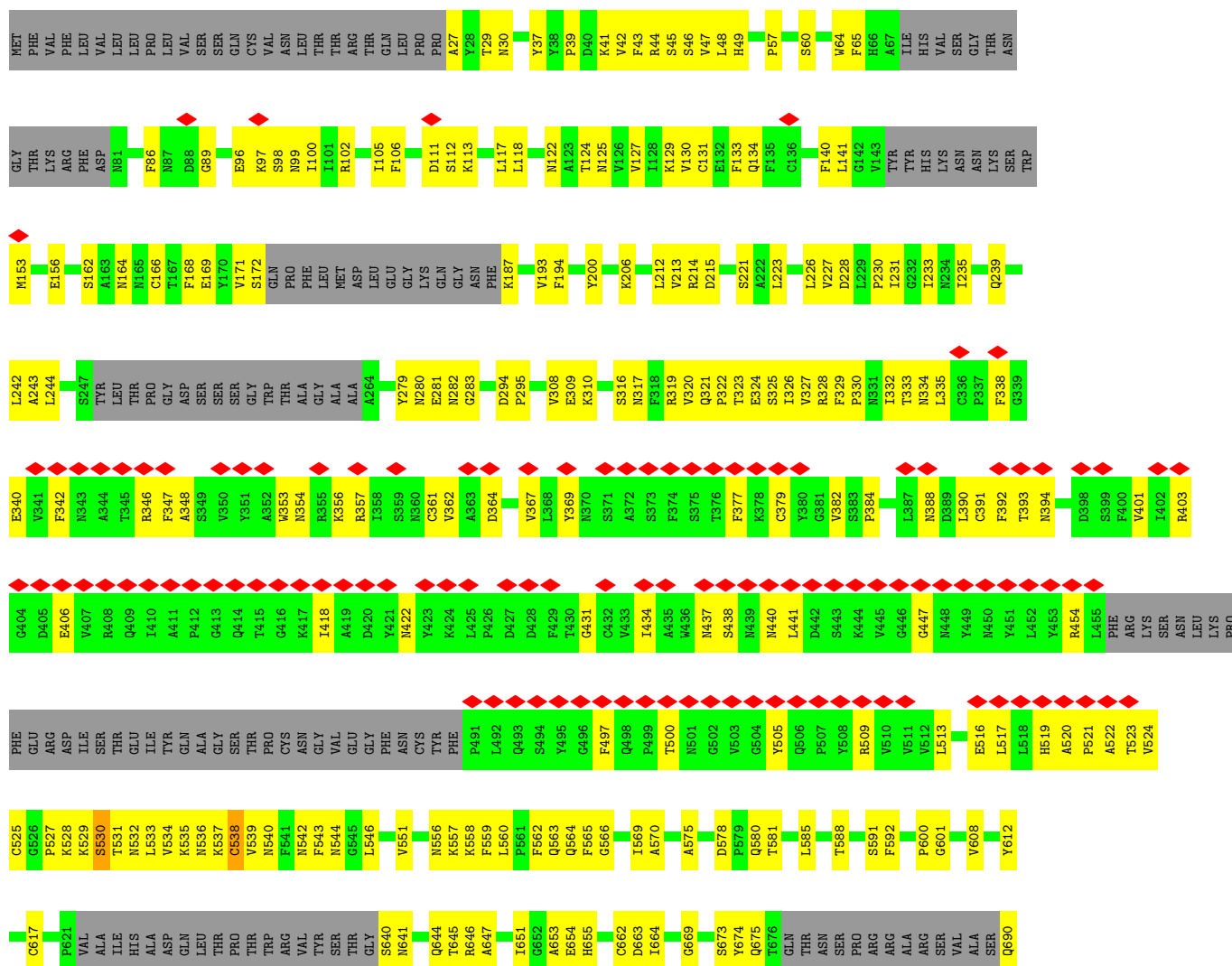
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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



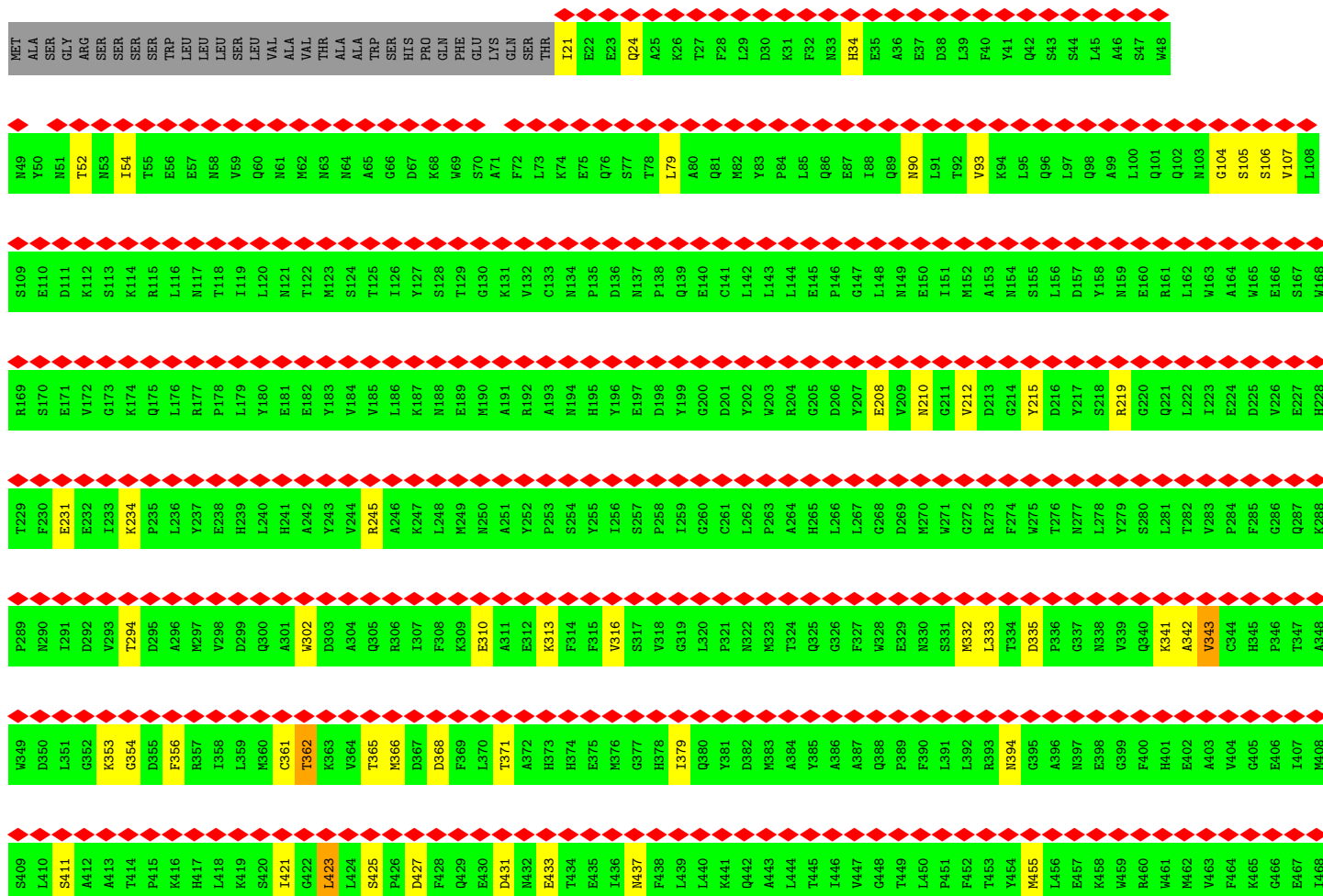
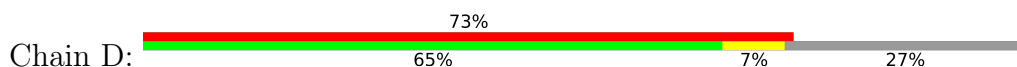


• Molecule 1: Spike glycoprotein



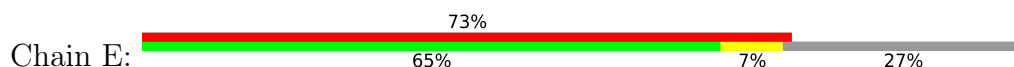


- Molecule 2: Angiotensin-converting enzyme 2



P469	L529	E589	TYR	LYS
K470	C530	P590	ARG	LYS
D471	Q531	P591	ILE	LYS
Q472	L591	L591	ASN	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	N599	GLN	ASN
M480	H540	K600	MET	LEU
K481	K541	N601	ILE	LEU
R482	C542	S602	PHE	LEU
E483	D543	F603	GLY	ALA
I484	I544	V604	GLU	ILE
V485	S545	G605	GLU	GLN
G486	N546	W606	VAL	PRO
V487	S547	S607	ARG	GLY
V488	T548	T608	ALA	PRO
E489	D549	D609	ASN	PRO
P490	A550	W610	LEU	ASN
V491	G551	S611	PRO	PRO
P492	Q552	P612	THR	THR
H493	K553	Y613	ILE	ASP
D494	L554	A614	SER	ASP
E495	F555	D615	LEU	VAL
T496	N556	GLN	PHE	GLN
Y497	M557	SER	VAL	THR
C498	L558	ILE	THR	PHE
D499	R559	LYS	GLY	GLY
P500	L560	VAL	VAL	VAL
A501	G561	ARG	LYS	MET
S502	K562	ILE	ASP	GLY
L503	S563	LEU	VAL	ILE
F504	E564	SER	ASP	ILE
H505	P565	ALA	ILE	VAL
V506	W566	LEU	PRO	GLY
S507	T567	GLY	ARG	ILE
N508	L568	ASP	THR	ILE
D509	A569	LYS	GLU	LEU
Y510	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	MET	MET	ARG
Y516	A576	TYR	THR	ASP
T517	K577	LEU	PHE	THR
R518	N578	ARG	ARG	ARG
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	N280	D350	L410
GLY	M51	D111	E171	E231	I291	L351	S411
ARG	T52	K112	V172	E232	D292	G352	A412
ASP	M53	S113	K173	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	Z237	M297	R357	H417
ASN	N58	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
THR	M63	M123	Y183	Y243	D303	K363	L423
ILE	M64	S124	V184	V244	A304	V364	L424
GLN	A65	T125	V185	R245	Q305	T365	S425
PRO	G66	I126	L186	A246	R306	M366	P426
GLY	D67	Y127	K187	K247	I307	D367	D427
ASN	K68	S128	M188	L248	F308	D368	F428
PRO	M69	T129	E189	M249	K309	F369	Q429
ASN	S70	G130	M190	N250	E310	L370	E430
THR	A71	K131	A191	A251	A311	T371	D431
ASP	F72	V132	R192	Y252	E312	A372	N432
VAL	L73	C133	A193	P253	K313	H373	E433
SER	K74	M134	H194	S254	F314	H374	T434
LEU	E75	P135	H195	Y255	F315	E375	E435
THR	Q76	D136	V196	I256	V316	M376	I436
PHE	S77	M137	E197	S257	S317	G377	M437
ILE	T78	P138	D198	P258	V318	H378	F438
VAL	L79	Q139	Y199	I259	G319	I379	L439
ASP	A80	E140	Q200	G260	L320	Q380	L440
GLY	Q81	C141	D201	C261	P321	Y381	K441
VAL	M82	L142	Y202	L262	N322	Q382	Q442
ILE	R83	L143	W203	P263	M323	M383	A443
PRO	P84	L144	R204	A264	T324	A384	L444
ARG	L85	E145	G205	H265	Q325	Y385	T445
GLY	Q86	P146	D206	L266	G326	A386	I446
THR	E87	G147	Y207	L267	F327	A387	V447
LEU	I88	L148	E208	G268	W328	Q388	G448
ALA	Q89	M149	V209	D269	E329	P389	T449
ILE	N90	E150	M210	M270	N330	F390	L450
THR	L91	I151	G211	W271	S331	L391	P451
ASP	T92	M152	V212	G272	M332	L392	F452
ARG	V93	A153	D213	R273	L333	R393	T453
VAL	K94	M154	G214	F274	T334	N394	Y454
GLY	L95	S155	Y215	W275	D335	G395	M455
ILE	Q96	L156	D216	T276	P336	A396	L456
THR	L97	D157	Y217	N277	G337	N397	E457
ASP	Q98	Y158	S218	L278	N338	E398	K458
SER	A99	M159	R219	Y279	V339	G399	W459
VAL	L100	E160	Q220	S280	F400	H401	R460
ALA	Q101	R161	Q221	L281	K341	H402	W461
GLY	Q102	L162	L222	T282	A342	E403	M462
ILE	M103	W163	I223	V283	V343	A403	V463
ASP	G104	A164	E224	P284	C344	F464	F464
ARG	S105	W165	D225	F285	H345	G465	K465
THR	S106	E166	V226	G286	P346	E466	E466
GLY	V107	S167	E227	Q287	T347	I467	E467
ASP	L108	W168	H228	K288	A348	M468	I468

- 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%

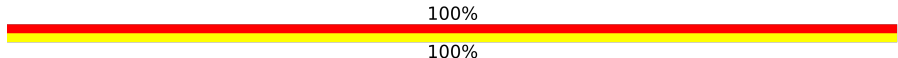


- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

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%

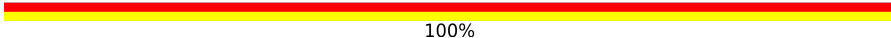


- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

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

5.1 Standard geometry

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

All (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
1	B	86	PHE	C-N-CA	5.88	132.77	121.54
1	C	86	PHE	CA-C-N	5.87	132.75	121.54
1	C	86	PHE	C-N-CA	5.87	132.75	121.54
1	A	86	PHE	CA-C-N	5.86	132.73	121.54
1	A	86	PHE	C-N-CA	5.86	132.73	121.54
1	B	530	SER	CB-CA-C	-5.66	110.07	116.63

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	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.

All (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
1:C:486:PHE:CE1	2:E:79:LEU:HD22	1.75	1.20
1:B:320:VAL:HG23	1:B:591:SER:O	1.45	1.15
1:A:340:GLU:OE2	1:A:356:LYS:HE2	1.47	1.14
1:B:519:HIS:ND1	1:C:41:LYS:HD2	1.63	1.13
1:B:340:GLU:OE2	1:B:356:LYS:HE2	1.47	1.13
1:C:523:THR:HG22	1:C:524:VAL:H	0.98	1.12
1:C:654:GLU:HG3	1:C:693:ILE:HG22	1.15	1.12
1:C:340:GLU:OE2	1:C:356:LYS:HE2	1.47	1.11
1:C:654:GLU:CG	1:C:693:ILE:CG2	2.28	1.11
1:A:230:PRO:CA	1:C:521:PRO:CG	2.29	1.11
1:A:523:THR:HG22	1:A:524:VAL:H	0.98	1.10
1:B:748:GLU:HG3	1:B:981:LEU:HD21	1.32	1.10
1:B:392:PHE:HB3	1:B:517:LEU:HD21	1.35	1.09
1:C:392:PHE:HB3	1:C:517:LEU:HD21	1.35	1.09
1:B:523:THR:HG22	1:B:524:VAL:H	0.98	1.08
1:A:392:PHE:HB3	1:A:517:LEU:HD21	1.35	1.08
1:B:560:LEU:HD23	1:B:563:GLN:OE1	1.52	1.08
1:A:230:PRO:CA	1:C:521:PRO:HG3	1.84	1.08
1:A:520:ALA:HB1	1:A:521:PRO:HD2	1.35	1.07
1:B:520:ALA:HB1	1:B:521:PRO:HD2	1.35	1.07
1:A:230:PRO:HA	1:C:521:PRO:HG3	1.30	1.07
1:C:662:CYS:HB2	1:C:697:MET:HE3	1.39	1.05
1:B:519:HIS:O	1:C:41:LYS:HD3	1.55	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:520:ALA:HB1	1:C:521:PRO:HD2	1.35	1.04
1:B:392:PHE:HB3	1:B:517:LEU:CD2	1.88	1.04
1:A:230:PRO:CB	1:C:521:PRO:CG	2.34	1.04
1:A:392:PHE:HB3	1:A:517:LEU:CD2	1.88	1.03
1:B:529:LYS:HA	1:B:529:LYS:HE3	1.40	1.03
1:C:674:TYR:HD1	1:C:691:SER:O	1.41	1.03
1:C:392:PHE:HB3	1:C:517:LEU:CD2	1.88	1.02
1:B:403:ARG:NH1	1:B:505:TYR:HE1	1.58	1.01
4:B:1409:NAG:C4	4:B:1410:NAG:C1	2.38	1.01
1:B:44:ARG:O	1:B:283:GLY:HA2	1.61	1.01
1:A:392:PHE:CB	1:A:517:LEU:HD21	1.91	1.00
1:A:523:THR:HG22	1:A:524:VAL:N	1.73	1.00
1:C:44:ARG:O	1:C:283:GLY:HA2	1.61	1.00
1:C:392:PHE:CB	1:C:517:LEU:HD21	1.91	0.99
1:A:44:ARG:O	1:A:283:GLY:HA2	1.61	0.99
1:B:523:THR:HG22	1:B:524:VAL:N	1.73	0.99
1:B:392:PHE:CB	1:B:517:LEU:HD21	1.91	0.99
1:C:654:GLU:O	1:C:693:ILE:HG22	1.62	0.99
1:B:748:GLU:CG	1:B:981:LEU:HD21	1.91	0.99
1:C:654:GLU:HG3	1:C:693:ILE:HG21	1.45	0.99
1:C:811:LYS:HB2	1:C:812:PRO:CD	1.91	0.98
1:A:230:PRO:HB2	1:C:521:PRO:HG2	1.03	0.98
1:C:486:PHE:CE1	2:E:79:LEU:CD2	2.47	0.98
1:A:486:PHE:CE1	2:D:79:LEU:CD2	2.47	0.98
2:D:302:TRP:CH2	2:D:423:LEU:HD11	1.99	0.98
1:A:230:PRO:CA	1:C:521:PRO:HG2	1.92	0.97
1:C:523:THR:HG22	1:C:524:VAL:N	1.73	0.97
2:E:302:TRP:CH2	2:E:423:LEU:HD11	1.99	0.97
1:A:346:ARG:NH2	1:A:347:PHE:O	1.98	0.97
1:C:328:ARG:NE	1:C:533:LEU:HD23	1.80	0.96
1:B:523:THR:CG2	1:B:524:VAL:H	1.77	0.96
1:B:403:ARG:NH1	1:B:505:TYR:CE1	2.33	0.96
1:A:523:THR:CG2	1:A:524:VAL:H	1.77	0.96
1:B:357:ARG:CZ	1:C:230:PRO:HB2	1.95	0.96
1:C:523:THR:CG2	1:C:524:VAL:H	1.77	0.96
1:B:328:ARG:NH1	1:B:533:LEU:HD23	1.81	0.95
1:B:346:ARG:NH2	1:B:347:PHE:O	1.98	0.95
1:C:346:ARG:NH2	1:C:347:PHE:O	1.98	0.94
1:A:42:VAL:HG22	1:C:565:PHE:CZ	2.02	0.94
1:A:703:ASN:OD1	1:B:789:TYR:HE1	1.50	0.94
1:B:332:ILE:HD12	1:B:332:ILE:H	1.32	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:302:TRP:HH2	2:D:423:LEU:HD11	1.34	0.93
1:C:328:ARG:HE	1:C:533:LEU:HD23	1.34	0.92
1:A:505:TYR:CD2	2:D:353:LYS:O	2.23	0.92
2:E:302:TRP:HH2	2:E:423:LEU:HD11	1.34	0.92
1:C:505:TYR:CD2	2:E:353:LYS:O	2.23	0.91
1:C:811:LYS:HB2	1:C:812:PRO:HD2	1.50	0.91
1:B:529:LYS:HA	1:B:529:LYS:CE	1.99	0.91
1:C:486:PHE:HE1	2:E:79:LEU:CD2	1.84	0.90
1:C:319:ARG:HH21	1:C:319:ARG:HG3	1.35	0.89
1:A:486:PHE:HE1	2:D:79:LEU:CD2	1.84	0.89
1:A:476:GLY:CA	2:D:24:GLN:HE21	1.85	0.89
1:C:476:GLY:CA	2:E:24:GLN:HE21	1.85	0.88
1:B:519:HIS:CE1	1:C:40:ASP:HB2	2.08	0.88
1:C:674:TYR:CD1	1:C:691:SER:O	2.26	0.87
1:A:42:VAL:HA	1:C:565:PHE:O	1.75	0.87
1:A:45:SER:O	1:A:47:VAL:HG22	1.75	0.87
1:A:319:ARG:NH2	1:B:740:MET:SD	2.47	0.87
1:C:45:SER:O	1:C:47:VAL:HG22	1.75	0.87
1:A:334:ASN:O	1:A:362:VAL:HB	1.74	0.87
1:B:45:SER:O	1:B:47:VAL:HG22	1.75	0.86
1:C:654:GLU:CG	1:C:693:ILE:HG22	1.98	0.86
2:E:105:SER:O	2:E:106:SER:OG	1.93	0.86
1:A:329:PHE:HB3	1:A:330:PRO:HD2	1.57	0.86
1:A:565:PHE:O	1:B:42:VAL:HA	1.75	0.86
1:A:46:SER:HA	1:A:279:TYR:O	1.76	0.86
1:C:392:PHE:CD2	1:C:517:LEU:HD21	2.11	0.86
1:C:674:TYR:CZ	1:C:690:GLN:N	2.44	0.86
2:D:335:ASP:HB3	2:D:361:CYS:SG	2.16	0.86
1:B:46:SER:HA	1:B:279:TYR:O	1.76	0.86
1:C:393:THR:O	1:C:523:THR:HG21	1.76	0.86
1:C:388:ASN:OD1	1:C:527:PRO:HD2	1.74	0.86
2:D:105:SER:O	2:D:106:SER:OG	1.93	0.86
1:B:392:PHE:CD2	1:B:517:LEU:HD21	2.11	0.85
1:A:319:ARG:HH22	1:B:740:MET:CG	1.89	0.85
1:A:393:THR:O	1:A:523:THR:HG21	1.75	0.85
2:E:335:ASP:HB3	2:E:361:CYS:SG	2.16	0.85
1:C:295:PRO:HB2	1:C:608:VAL:HG11	1.59	0.85
1:A:392:PHE:CD2	1:A:517:LEU:HD21	2.11	0.85
1:B:559:PHE:O	1:B:560:LEU:O	1.95	0.85
1:A:520:ALA:HB1	1:A:521:PRO:CD	2.06	0.85
1:A:729:VAL:HG13	1:A:1059:GLY:HA2	1.57	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:560:LEU:HB3	1:B:562:PHE:CE2	2.12	0.85
1:C:46:SER:HA	1:C:279:TYR:O	1.76	0.85
1:B:393:THR:O	1:B:523:THR:HG21	1.75	0.84
1:C:520:ALA:HB1	1:C:521:PRO:CD	2.06	0.84
1:B:520:ALA:HB1	1:B:521:PRO:CD	2.06	0.84
1:B:519:HIS:O	1:C:41:LYS:CD	2.26	0.84
1:C:516:GLU:O	1:C:517:LEU:HD22	1.78	0.84
1:B:516:GLU:O	1:B:517:LEU:HD22	1.78	0.83
1:A:230:PRO:C	1:C:521:PRO:CG	2.51	0.83
1:A:516:GLU:O	1:A:517:LEU:HD22	1.78	0.83
1:C:328:ARG:CZ	1:C:533:LEU:HD23	2.07	0.83
1:A:486:PHE:CZ	2:D:79:LEU:HD22	2.13	0.83
1:C:486:PHE:CZ	2:E:79:LEU:HD22	2.13	0.83
1:A:703:ASN:OD1	1:B:789:TYR:CE1	2.32	0.83
1:A:230:PRO:HB2	1:C:521:PRO:CG	2.00	0.82
1:A:230:PRO:HA	1:C:521:PRO:CG	2.01	0.82
1:B:901:GLN:HE21	1:B:905:ARG:HE	1.26	0.82
1:B:519:HIS:CE1	1:C:41:LYS:HD2	2.15	0.81
1:C:901:GLN:HE21	1:C:905:ARG:HE	1.27	0.81
1:B:519:HIS:ND1	1:C:41:LYS:CD	2.42	0.81
1:B:560:LEU:H	1:B:560:LEU:HD22	1.46	0.81
1:A:43:PHE:HD1	1:C:563:GLN:OE1	1.63	0.80
1:C:328:ARG:NH2	1:C:533:LEU:HD23	1.97	0.80
1:B:748:GLU:N	1:B:748:GLU:OE2	2.14	0.80
1:A:388:ASN:OD1	1:A:527:PRO:HD2	1.81	0.79
3:d:1:NAG:C3	3:d:2:NAG:HN2	1.95	0.79
3:i:1:NAG:C3	3:i:2:NAG:HN2	1.95	0.79
1:A:707:TYR:HB2	1:B:883:THR:HG23	1.65	0.79
1:B:743:CYS:SG	1:B:749:CYS:C	2.67	0.79
1:C:422:ASN:HD21	1:C:454:ARG:H	1.32	0.78
1:A:392:PHE:O	1:A:523:THR:HB	1.83	0.78
1:C:392:PHE:O	1:C:523:THR:HB	1.83	0.78
1:A:230:PRO:C	1:C:521:PRO:HG3	2.08	0.77
1:A:42:VAL:HG22	1:C:565:PHE:CE2	2.18	0.77
1:C:390:LEU:HD23	1:C:391:CYS:H	1.49	0.77
1:A:200:TYR:CE1	1:C:521:PRO:HB2	2.19	0.77
1:C:406:GLU:CD	1:C:418:ILE:HG13	2.10	0.77
1:C:654:GLU:HG3	1:C:693:ILE:HG23	1.58	0.77
1:B:392:PHE:O	1:B:523:THR:HB	1.83	0.77
1:A:319:ARG:HH22	1:B:740:MET:HG3	1.47	0.77
1:C:335:LEU:HA	1:C:362:VAL:HB	1.67	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:476:GLY:HA3	2:E:24:GLN:HE21	1.50	0.76
1:A:563:GLN:OE1	1:B:43:PHE:HD1	1.66	0.76
2:E:302:TRP:HH2	2:E:423:LEU:CD1	1.98	0.76
1:A:361:CYS:SG	1:A:524:VAL:HG21	2.25	0.76
1:A:406:GLU:CD	1:A:418:ILE:HG13	2.10	0.76
1:C:476:GLY:HA2	2:E:24:GLN:HE21	1.50	0.76
1:A:1125:ASN:H	1:A:1125:ASN:HD22	1.33	0.76
1:B:335:LEU:HA	1:B:362:VAL:HB	1.67	0.76
2:D:302:TRP:HH2	2:D:423:LEU:CD1	1.98	0.76
1:A:476:GLY:HA2	2:D:24:GLN:HE21	1.50	0.76
1:B:675:GLN:O	1:B:690:GLN:HG3	1.86	0.76
1:A:476:GLY:HA3	2:D:24:GLN:HE21	1.50	0.75
1:B:361:CYS:SG	1:B:524:VAL:HG21	2.25	0.75
1:B:406:GLU:CD	1:B:418:ILE:HG13	2.10	0.75
1:B:558:LYS:H	1:B:558:LYS:HD2	1.49	0.75
1:C:735:SER:OG	1:C:859:THR:CG2	2.34	0.75
1:A:390:LEU:HD23	1:A:391:CYS:H	1.49	0.75
1:B:357:ARG:HH12	1:B:394:ASN:ND2	1.84	0.75
1:B:390:LEU:HD23	1:B:391:CYS:H	1.49	0.75
1:B:559:PHE:HZ	1:B:566:GLY:N	1.84	0.75
1:A:422:ASN:HD21	1:A:454:ARG:H	1.32	0.75
1:A:826:VAL:HG13	1:A:1057:PRO:HG2	1.68	0.75
1:C:361:CYS:SG	1:C:524:VAL:HG21	2.25	0.75
1:B:403:ARG:HH11	1:B:505:TYR:HE1	1.33	0.75
2:E:335:ASP:CB	2:E:361:CYS:SG	2.75	0.75
1:A:703:ASN:CB	1:B:787:GLN:OE1	2.23	0.74
1:A:47:VAL:O	1:A:49:HIS:N	2.20	0.74
1:C:332:ILE:HD12	1:C:332:ILE:N	2.02	0.74
1:C:320:VAL:HG23	1:C:591:SER:O	1.87	0.74
1:B:47:VAL:O	1:B:49:HIS:N	2.20	0.74
1:B:321:GLN:CD	1:B:322:PRO:HD2	2.13	0.74
1:C:47:VAL:O	1:C:49:HIS:N	2.20	0.74
1:B:357:ARG:HH12	1:B:394:ASN:HD21	1.34	0.74
1:A:43:PHE:N	1:C:565:PHE:O	2.21	0.74
1:B:382:VAL:HA	1:C:983:ARG:O	1.88	0.74
1:C:654:GLU:O	1:C:693:ILE:CG2	2.35	0.74
2:D:335:ASP:CB	2:D:361:CYS:SG	2.75	0.74
1:B:422:ASN:HD21	1:B:454:ARG:H	1.32	0.73
1:C:654:GLU:C	1:C:693:ILE:HG22	2.14	0.73
1:C:811:LYS:CB	1:C:812:PRO:CD	2.66	0.73
1:B:560:LEU:CD2	1:B:563:GLN:OE1	2.34	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:319:ARG:HG3	1:C:319:ARG:NH2	2.03	0.72
1:B:392:PHE:HD2	1:B:517:LEU:HD21	1.53	0.72
1:A:392:PHE:HD2	1:A:517:LEU:HD21	1.54	0.72
1:C:391:CYS:HA	1:C:525:CYS:HB3	1.71	0.72
1:A:391:CYS:HA	1:A:525:CYS:HB3	1.71	0.72
1:B:533:LEU:HD11	1:B:535:LYS:CE	2.19	0.72
1:B:1142:GLN:HG3	1:B:1143:PRO:HD3	1.71	0.72
1:A:533:LEU:HD12	1:A:533:LEU:C	2.15	0.72
1:C:674:TYR:CE1	1:C:691:SER:N	2.57	0.72
1:B:973:ILE:HG12	1:B:992:GLN:HE21	1.53	0.71
1:A:790:LYS:NZ	1:C:702:GLU:OE2	2.20	0.71
1:C:326:ILE:HD12	1:C:326:ILE:O	1.90	0.71
1:A:565:PHE:CZ	1:B:42:VAL:HG22	2.25	0.71
1:C:124:THR:HG21	4:C:1402:NAG:HN2	1.56	0.71
4:B:1409:NAG:H4	4:B:1410:NAG:C1	2.21	0.71
1:C:392:PHE:HD2	1:C:517:LEU:HD21	1.53	0.71
1:C:363:ALA:O	1:C:527:PRO:HD3	1.91	0.70
1:B:124:THR:HG21	4:B:1402:NAG:HN2	1.56	0.70
1:A:329:PHE:O	1:A:580:GLN:HG2	1.91	0.70
1:A:340:GLU:OE2	1:A:356:LYS:CE	2.35	0.70
1:B:530:SER:O	1:B:531:THR:HB	1.91	0.70
1:B:559:PHE:O	1:B:560:LEU:C	2.35	0.70
1:A:124:THR:HG21	4:A:1402:NAG:HN2	1.56	0.70
1:A:187:LYS:N	1:A:212:LEU:O	2.25	0.70
1:A:200:TYR:CZ	1:C:521:PRO:HB2	2.26	0.70
1:C:945:LEU:HD12	1:C:948:LEU:HD12	1.74	0.70
1:C:41:LYS:HD2	1:C:41:LYS:H	1.57	0.69
1:C:340:GLU:OE2	1:C:356:LYS:CE	2.35	0.69
1:C:187:LYS:N	1:C:212:LEU:O	2.25	0.69
1:A:295:PRO:HB2	1:A:608:VAL:HG11	1.75	0.69
1:B:986:PRO:HB2	1:B:987:PRO:HD3	1.74	0.69
1:A:42:VAL:CG2	1:C:565:PHE:CZ	2.74	0.69
1:C:44:ARG:O	1:C:283:GLY:CA	2.40	0.69
1:B:187:LYS:N	1:B:212:LEU:O	2.25	0.69
1:A:45:SER:OG	1:A:46:SER:N	2.25	0.69
1:B:44:ARG:O	1:B:283:GLY:CA	2.40	0.68
1:B:392:PHE:CG	1:B:517:LEU:HD21	2.29	0.68
1:B:560:LEU:HB2	1:B:563:GLN:OE1	1.93	0.68
1:C:654:GLU:CG	1:C:693:ILE:HG23	2.19	0.68
1:A:391:CYS:CA	1:A:525:CYS:HB3	2.24	0.68
1:C:392:PHE:CG	1:C:517:LEU:HD21	2.29	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:43:PHE:CE1	1:B:283:GLY:HA3	2.29	0.67
1:B:326:ILE:HD11	1:B:543:PHE:CE1	2.29	0.67
1:B:519:HIS:CE1	1:C:41:LYS:H	2.12	0.67
1:C:96:GLU:OE1	1:C:98:SER:N	2.28	0.67
1:B:533:LEU:HD11	1:B:535:LYS:NZ	2.08	0.67
1:A:96:GLU:OE1	1:A:98:SER:N	2.28	0.67
1:C:43:PHE:CE1	1:C:283:GLY:HA3	2.29	0.67
1:C:45:SER:OG	1:C:46:SER:N	2.25	0.67
1:A:392:PHE:CG	1:A:517:LEU:HD21	2.29	0.67
1:C:328:ARG:HH21	1:C:533:LEU:HD23	1.58	0.67
1:A:43:PHE:CE1	1:A:283:GLY:HA3	2.29	0.67
1:A:329:PHE:CE1	1:A:544:ASN:HA	2.30	0.67
1:B:320:VAL:HG21	1:B:591:SER:HB2	1.77	0.67
1:B:320:VAL:CG2	1:B:591:SER:O	2.34	0.67
1:C:37:TYR:O	1:C:39:PRO:HD3	1.95	0.66
1:B:388:ASN:OD1	1:B:527:PRO:HD3	1.94	0.66
1:B:569:ILE:HD12	1:B:569:ILE:H	1.60	0.66
1:B:691:SER:O	1:B:692:ILE:HG13	1.96	0.66
1:A:187:LYS:HG2	1:A:213:VAL:HA	1.78	0.66
1:A:388:ASN:OD1	1:A:527:PRO:CD	2.43	0.66
1:B:535:LYS:O	1:B:536:ASN:HB2	1.95	0.66
1:B:1045:LYS:NZ	1:C:786:LYS:HE3	2.09	0.66
1:A:334:ASN:O	1:A:362:VAL:CB	2.42	0.66
1:C:187:LYS:HG2	1:C:213:VAL:HA	1.78	0.66
1:C:392:PHE:HD2	1:C:517:LEU:CD2	2.09	0.66
1:B:37:TYR:O	1:B:39:PRO:HD3	1.95	0.66
1:B:719:THR:HA	1:B:926:GLN:HE22	1.60	0.66
1:A:37:TYR:O	1:A:39:PRO:HD3	1.95	0.66
1:B:187:LYS:HG2	1:B:213:VAL:HA	1.78	0.66
1:B:96:GLU:OE1	1:B:98:SER:N	2.28	0.65
1:B:340:GLU:OE2	1:B:356:LYS:CE	2.35	0.65
1:B:323:THR:O	1:B:539:VAL:HG23	1.97	0.65
1:B:357:ARG:NH2	1:C:230:PRO:HB2	2.11	0.65
1:B:560:LEU:HB3	1:B:562:PHE:CD2	2.32	0.65
1:C:391:CYS:CA	1:C:525:CYS:HB3	2.24	0.65
1:C:493:GLN:OE1	2:E:34:HIS:CB	2.45	0.65
1:B:45:SER:OG	1:B:46:SER:N	2.25	0.65
1:C:569:ILE:H	1:C:569:ILE:HD12	1.61	0.65
1:B:392:PHE:HD2	1:B:517:LEU:CD2	2.09	0.65
1:A:493:GLN:OE1	2:D:34:HIS:CB	2.45	0.65
1:A:569:ILE:HD12	1:A:569:ILE:H	1.60	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:332:ILE:HG12	1:B:362:VAL:HG22	1.79	0.65
2:D:310:GLU:OE1	2:D:421:ILE:HD11	1.97	0.65
2:E:310:GLU:OE1	2:E:421:ILE:HD11	1.97	0.65
1:A:392:PHE:HD2	1:A:517:LEU:CD2	2.09	0.64
1:A:44:ARG:O	1:A:283:GLY:CA	2.40	0.64
1:A:533:LEU:HD11	1:A:535:LYS:HE3	1.78	0.64
1:B:535:LYS:HE2	1:B:585:LEU:CD2	2.27	0.64
1:B:569:ILE:CG1	1:C:47:VAL:HG11	2.27	0.64
1:B:326:ILE:HG22	1:B:534:VAL:HG22	1.79	0.64
1:C:321:GLN:HA	1:C:321:GLN:OE1	1.97	0.64
1:B:319:ARG:HB2	1:B:319:ARG:CZ	2.28	0.64
1:B:357:ARG:NH1	1:B:394:ASN:HD21	1.96	0.64
1:C:690:GLN:O	1:C:691:SER:HB3	1.98	0.64
1:A:854:LYS:HD2	1:A:854:LYS:N	2.13	0.64
1:C:406:GLU:CD	1:C:418:ILE:CG1	2.71	0.64
3:d:1:NAG:H3	3:d:2:NAG:HN2	1.63	0.63
1:A:43:PHE:CE1	1:A:282:ASN:O	2.52	0.63
1:B:406:GLU:CD	1:B:418:ILE:CG1	2.71	0.63
1:B:592:PHE:CZ	1:C:854:LYS:HE3	2.33	0.63
2:D:302:TRP:CZ3	2:D:423:LEU:HD11	2.34	0.63
1:C:522:ALA:O	1:C:523:THR:OG1	2.14	0.63
2:E:302:TRP:CZ3	2:E:423:LEU:HD11	2.34	0.63
1:A:700:GLY:O	1:A:701:ALA:O	2.17	0.63
1:A:117:LEU:HD12	1:A:118:LEU:H	1.64	0.63
1:C:388:ASN:OD1	1:C:527:PRO:CD	2.45	0.63
2:E:335:ASP:N	2:E:361:CYS:SG	2.72	0.63
1:B:326:ILE:HG21	1:B:534:VAL:HG23	1.79	0.63
1:B:326:ILE:HG22	1:B:534:VAL:CG2	2.28	0.63
1:B:527:PRO:O	1:B:528:LYS:HB3	1.98	0.63
1:C:96:GLU:OE1	1:C:97:LYS:N	2.32	0.63
1:C:124:THR:OG1	1:C:125:ASN:N	2.32	0.63
2:D:335:ASP:N	2:D:361:CYS:SG	2.72	0.63
3:i:1:NAG:H3	3:i:2:NAG:HN2	1.63	0.63
1:A:522:ALA:O	1:A:523:THR:OG1	2.14	0.62
1:A:43:PHE:HE1	1:A:282:ASN:O	1.83	0.62
1:A:124:THR:OG1	1:A:125:ASN:N	2.32	0.62
1:A:326:ILE:O	1:A:326:ILE:HG13	2.00	0.62
1:A:808:ASP:HB3	1:A:811:LYS:HD2	1.82	0.62
1:B:43:PHE:CE1	1:B:282:ASN:O	2.51	0.62
1:A:406:GLU:CD	1:A:418:ILE:CG1	2.71	0.62
1:B:117:LEU:HD12	1:B:118:LEU:H	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:326:ILE:CG2	1:B:534:VAL:CG2	2.77	0.62
1:A:96:GLU:OE1	1:A:97:LYS:N	2.32	0.62
1:A:457:ARG:NH1	1:A:459:SER:O	2.33	0.62
1:A:516:GLU:O	1:A:517:LEU:CD2	2.48	0.62
1:B:382:VAL:HB	1:C:983:ARG:HB2	1.81	0.62
1:C:43:PHE:CE1	1:C:282:ASN:O	2.52	0.62
1:C:813:SER:O	1:C:814:LYS:HE2	2.00	0.62
1:B:43:PHE:HE1	1:B:282:ASN:O	1.82	0.62
1:B:592:PHE:CE1	1:C:854:LYS:HE3	2.35	0.62
1:C:811:LYS:HB2	1:C:812:PRO:HD3	1.80	0.62
1:A:327:VAL:O	1:A:328:ARG:HD3	1.99	0.62
1:B:96:GLU:OE1	1:B:97:LYS:N	2.32	0.62
1:B:325:SER:HA	1:B:540:ASN:O	1.99	0.62
1:B:522:ALA:O	1:B:523:THR:OG1	2.14	0.62
1:A:530:SER:CB	1:A:580:GLN:NE2	2.63	0.61
1:B:326:ILE:HD12	1:B:326:ILE:O	2.00	0.61
1:B:124:THR:OG1	1:B:125:ASN:N	2.32	0.61
1:C:457:ARG:NH1	1:C:459:SER:O	2.33	0.61
1:A:1077:THR:HG22	1:A:1095:PHE:O	2.01	0.61
1:C:117:LEU:HD12	1:C:118:LEU:H	1.64	0.61
1:A:357:ARG:HH12	1:A:394:ASN:HD21	1.49	0.61
1:A:521:PRO:O	1:A:522:ALA:HB2	2.01	0.61
1:A:617:CYS:H	1:A:644:GLN:HE22	1.49	0.61
1:B:521:PRO:O	1:B:522:ALA:HB2	2.01	0.61
1:B:617:CYS:H	1:B:644:GLN:HE22	1.49	0.60
1:C:43:PHE:HE1	1:C:282:ASN:O	1.82	0.60
1:A:523:THR:HG22	1:A:524:VAL:HG12	1.83	0.60
1:B:523:THR:HG22	1:B:524:VAL:HG12	1.83	0.60
1:C:392:PHE:HB3	1:C:517:LEU:HD22	1.82	0.60
1:C:406:GLU:OE1	1:C:418:ILE:HG12	2.02	0.60
1:B:645:THR:HG22	1:B:647:ALA:H	1.66	0.60
1:A:406:GLU:OE1	1:A:418:ILE:HG12	2.02	0.60
1:B:406:GLU:OE1	1:B:418:ILE:HG12	2.02	0.60
1:C:327:VAL:HG12	1:C:328:ARG:N	2.16	0.60
1:A:164:ASN:OD1	1:A:164:ASN:N	2.35	0.60
1:A:392:PHE:HB3	1:A:517:LEU:HD22	1.82	0.60
1:C:523:THR:HG22	1:C:524:VAL:HG12	1.83	0.60
1:A:556:ASN:HD22	1:A:556:ASN:H	1.49	0.60
1:B:332:ILE:HG12	1:B:362:VAL:CG2	2.32	0.60
1:C:645:THR:HG22	1:C:647:ALA:H	1.66	0.60
1:C:521:PRO:O	1:C:522:ALA:HB2	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:328:ARG:HH21	1:C:533:LEU:CD2	2.15	0.59
2:D:212:VAL:HG21	2:D:565:PRO:HG3	1.84	0.59
1:C:533:LEU:O	1:C:533:LEU:HD12	2.02	0.59
1:A:141:LEU:HB2	1:A:156:GLU:HB2	1.85	0.59
1:B:565:PHE:O	1:C:42:VAL:HA	2.02	0.59
1:B:592:PHE:CE1	1:C:854:LYS:CE	2.85	0.59
1:C:164:ASN:OD1	1:C:164:ASN:N	2.35	0.59
1:C:333:THR:OG1	1:C:334:ASN:N	2.32	0.59
1:A:563:GLN:CD	1:B:43:PHE:HA	2.27	0.59
1:B:328:ARG:NH2	1:B:578:ASP:OD2	2.35	0.59
1:B:516:GLU:O	1:B:517:LEU:CD2	2.48	0.59
1:C:674:TYR:CE1	1:C:690:GLN:N	2.71	0.59
1:A:645:THR:HG22	1:A:647:ALA:H	1.66	0.59
1:C:556:ASN:HD22	1:C:556:ASN:H	1.50	0.59
1:C:357:ARG:HH12	1:C:394:ASN:HD21	1.49	0.59
1:B:164:ASN:OD1	1:B:164:ASN:N	2.35	0.59
1:B:738:CYS:O	1:B:742:ILE:HG13	2.03	0.59
1:C:328:ARG:NH1	1:C:580:GLN:HB3	2.17	0.59
1:A:722:VAL:HA	1:A:1064:HIS:O	2.03	0.58
1:B:392:PHE:CD2	1:B:517:LEU:CD2	2.85	0.58
1:C:617:CYS:H	1:C:644:GLN:HE22	1.49	0.58
1:B:560:LEU:C	1:B:562:PHE:H	2.11	0.58
4:B:1405:NAG:H83	4:B:1405:NAG:H3	1.86	0.58
1:C:391:CYS:SG	1:C:523:THR:O	2.61	0.58
1:B:206:LYS:NZ	1:B:221:SER:OG	2.35	0.58
1:B:334:ASN:N	1:B:334:ASN:OD1	2.36	0.58
1:C:516:GLU:O	1:C:517:LEU:CD2	2.48	0.58
1:A:476:GLY:HA3	2:D:24:GLN:NE2	2.17	0.58
1:A:532:ASN:N	1:A:532:ASN:OD1	2.35	0.58
1:A:813:SER:O	1:A:813:SER:OG	2.18	0.58
1:B:338:PHE:O	1:B:340:GLU:N	2.37	0.58
1:B:565:PHE:O	1:B:565:PHE:HD1	1.86	0.58
1:C:206:LYS:NZ	1:C:221:SER:OG	2.35	0.58
1:C:476:GLY:HA3	2:E:24:GLN:NE2	2.18	0.58
2:E:212:VAL:HG21	2:E:565:PRO:HG3	1.84	0.58
1:A:48:LEU:HD13	1:A:48:LEU:H	1.69	0.58
1:A:206:LYS:NZ	1:A:221:SER:OG	2.35	0.58
1:A:318:PHE:CE2	1:A:320:VAL:CG2	2.86	0.58
1:A:438:SER:O	1:A:438:SER:OG	2.21	0.58
2:D:368:ASP:HA	2:D:371:THR:HG22	1.85	0.58
3:Y:2:NAG:H3	3:Y:2:NAG:H83	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:328:ARG:NH2	1:C:533:LEU:CD2	2.65	0.58
1:C:361:CYS:SG	1:C:524:VAL:CG2	2.92	0.58
1:A:523:THR:CG2	1:A:524:VAL:N	2.46	0.58
1:B:391:CYS:SG	1:B:523:THR:O	2.61	0.58
2:D:302:TRP:CH2	2:D:423:LEU:CD1	2.78	0.58
1:B:361:CYS:SG	1:B:524:VAL:CG2	2.92	0.58
1:B:392:PHE:HB3	1:B:517:LEU:HD22	1.82	0.58
1:B:519:HIS:CE1	1:C:41:LYS:N	2.72	0.58
1:B:560:LEU:HD22	1:B:560:LEU:N	2.16	0.58
1:C:338:PHE:O	1:C:340:GLU:N	2.37	0.58
1:C:811:LYS:CB	1:C:812:PRO:HD2	2.28	0.58
1:A:332:ILE:HG22	1:A:333:THR:N	2.19	0.58
2:E:368:ASP:HA	2:E:371:THR:HG22	1.85	0.58
1:A:334:ASN:C	1:A:362:VAL:HB	2.28	0.57
1:A:361:CYS:SG	1:A:524:VAL:CG2	2.92	0.57
1:A:901:GLN:HE21	1:A:905:ARG:HE	1.50	0.57
1:B:141:LEU:HB2	1:B:156:GLU:HB2	1.85	0.57
1:B:390:LEU:HD23	1:B:391:CYS:N	2.19	0.57
1:C:141:LEU:HB2	1:C:156:GLU:HB2	1.85	0.57
4:A:1405:NAG:H3	4:A:1405:NAG:H83	1.86	0.57
1:B:41:LYS:O	1:B:42:VAL:HB	2.04	0.57
1:B:332:ILE:HD12	1:B:332:ILE:N	2.03	0.57
1:C:105:ILE:HG12	1:C:239:GLN:HB2	1.87	0.57
1:A:338:PHE:O	1:A:340:GLU:N	2.37	0.57
1:B:47:VAL:O	1:B:47:VAL:HG23	2.04	0.57
1:B:357:ARG:CZ	1:C:230:PRO:CB	2.77	0.57
1:A:391:CYS:SG	1:A:523:THR:O	2.61	0.57
1:B:901:GLN:NE2	1:B:905:ARG:HE	1.99	0.57
1:A:318:PHE:CE2	1:A:320:VAL:HG23	2.39	0.57
1:A:338:PHE:C	1:A:340:GLU:H	2.13	0.57
1:A:335:LEU:HA	1:A:362:VAL:HB	1.86	0.57
1:A:530:SER:HB3	1:A:580:GLN:HE22	1.69	0.57
1:B:48:LEU:HD13	1:B:48:LEU:H	1.69	0.57
1:C:227:VAL:HG12	1:C:228:ASP:N	2.20	0.57
1:A:335:LEU:HD12	1:A:335:LEU:H	1.69	0.57
1:C:47:VAL:O	1:C:47:VAL:HG23	2.04	0.57
1:C:332:ILE:HD12	1:C:332:ILE:H	1.68	0.57
1:B:227:VAL:HG12	1:B:228:ASP:N	2.20	0.57
1:B:357:ARG:NH1	1:C:230:PRO:CB	2.68	0.57
1:B:663:ASP:OD2	1:B:673:SER:OG	2.22	0.57
1:C:804:GLN:HE21	1:C:935:GLN:HE22	1.52	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:533:LEU:O	1:B:533:LEU:HG	2.05	0.56
1:C:519:HIS:O	1:C:519:HIS:ND1	2.38	0.56
2:D:54:ILE:HD12	2:D:341:LYS:HG3	1.87	0.56
1:B:45:SER:O	1:B:279:TYR:HB2	2.05	0.56
1:B:559:PHE:HE2	1:B:564:GLN:O	1.88	0.56
3:Z:2:NAG:H3	3:Z:2:NAG:H83	1.87	0.56
1:A:47:VAL:O	1:A:47:VAL:HG23	2.04	0.56
1:B:353:TRP:H	1:B:353:TRP:CD1	2.24	0.56
1:B:533:LEU:CD1	1:B:535:LYS:CE	2.83	0.56
1:C:563:GLN:O	1:C:577:ARG:NH1	2.38	0.56
1:C:654:GLU:O	1:C:693:ILE:CB	2.53	0.56
1:C:735:SER:OG	1:C:859:THR:HG23	2.04	0.56
2:D:425:SER:HB3	2:D:427:ASP:OD1	2.06	0.56
1:B:560:LEU:O	1:B:562:PHE:N	2.36	0.56
1:C:338:PHE:C	1:C:340:GLU:H	2.13	0.56
1:A:329:PHE:HB3	1:A:330:PRO:CD	2.32	0.56
1:B:29:THR:HG22	1:B:30:ASN:H	1.70	0.56
1:B:105:ILE:HG12	1:B:239:GLN:HB2	1.87	0.56
1:C:550:GLY:HA2	1:C:590:CYS:SG	2.45	0.56
1:A:29:THR:HG22	1:A:30:ASN:H	1.70	0.56
1:A:41:LYS:O	1:A:42:VAL:HB	2.05	0.56
1:A:486:PHE:CZ	2:D:79:LEU:CD2	2.84	0.56
1:A:563:GLN:O	1:A:577:ARG:NH1	2.38	0.56
1:B:295:PRO:HB2	1:B:608:VAL:HG11	1.88	0.56
1:C:29:THR:HG22	1:C:30:ASN:H	1.70	0.56
1:C:48:LEU:HD13	1:C:48:LEU:H	1.69	0.56
4:C:1405:NAG:H3	4:C:1405:NAG:H83	1.86	0.56
1:A:105:ILE:HG12	1:A:239:GLN:HB2	1.87	0.56
1:A:406:GLU:OE1	1:A:418:ILE:CG1	2.54	0.56
1:A:699:LEU:HD22	1:B:873:TYR:CZ	2.40	0.56
1:C:663:ASP:OD2	1:C:673:SER:OG	2.22	0.56
2:D:335:ASP:N	2:D:335:ASP:OD1	2.39	0.56
2:E:54:ILE:HD12	2:E:341:LYS:HG3	1.87	0.56
2:E:425:SER:HB3	2:E:427:ASP:OD1	2.06	0.56
1:A:42:VAL:CA	1:C:565:PHE:O	2.50	0.56
1:C:45:SER:O	1:C:279:TYR:HB2	2.05	0.56
1:C:551:VAL:HB	1:C:588:THR:HG23	1.88	0.56
2:E:317:SER:HG	2:E:546:ASN:H	1.51	0.56
1:A:227:VAL:HG12	1:A:228:ASP:N	2.20	0.56
1:C:57:PRO:O	1:C:60:SER:OG	2.24	0.56
1:C:332:ILE:HG21	1:C:362:VAL:HG11	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:653:ALA:HB2	1:C:692:ILE:HG22	1.87	0.56
1:B:43:PHE:CG	1:B:44:ARG:N	2.74	0.55
1:B:559:PHE:HZ	1:B:566:GLY:CA	2.19	0.55
1:C:342:PHE:HB3	3:U:1:NAG:H82	1.87	0.55
1:C:406:GLU:OE1	1:C:418:ILE:CG1	2.54	0.55
3:J:2:NAG:H83	3:J:2:NAG:H3	1.87	0.55
1:A:45:SER:O	1:A:279:TYR:HB2	2.05	0.55
1:A:342:PHE:HB3	3:G:1:NAG:H82	1.87	0.55
1:B:57:PRO:O	1:B:60:SER:OG	2.24	0.55
1:B:329:PHE:HB3	1:B:330:PRO:HD2	1.88	0.55
1:B:535:LYS:HE2	1:B:585:LEU:HD22	1.89	0.55
1:A:519:HIS:O	1:A:519:HIS:ND1	2.38	0.55
1:B:357:ARG:NH1	1:B:394:ASN:ND2	2.54	0.55
1:C:353:TRP:CD1	1:C:353:TRP:H	2.23	0.55
1:A:45:SER:HA	1:A:280:ASN:O	2.06	0.55
1:A:392:PHE:HA	1:A:517:LEU:HD11	1.89	0.55
1:B:338:PHE:C	1:B:340:GLU:H	2.13	0.55
1:C:556:ASN:HD22	1:C:556:ASN:N	2.05	0.55
2:D:342:ALA:O	2:D:343:VAL:C	2.50	0.55
1:A:347:PHE:CE1	1:A:509:ARG:HD3	2.42	0.55
1:A:476:GLY:CA	2:D:24:GLN:NE2	2.65	0.55
1:B:328:ARG:HH22	1:B:580:GLN:HB2	1.70	0.55
1:B:342:PHE:HB3	3:N:1:NAG:H82	1.87	0.55
1:B:558:LYS:O	1:C:43:PHE:CE1	2.59	0.55
1:C:43:PHE:CG	1:C:44:ARG:N	2.74	0.55
1:B:559:PHE:CE1	1:C:43:PHE:CB	2.89	0.55
1:C:45:SER:HA	1:C:280:ASN:O	2.06	0.55
1:C:326:ILE:HD12	1:C:541:PHE:HA	1.88	0.55
2:D:231:GLU:HA	2:D:234:LYS:HD3	1.88	0.55
2:E:538:PRO:HD2	2:E:541:LYS:HD2	1.88	0.55
1:A:967:SER:O	1:A:967:SER:OG	2.24	0.55
1:B:406:GLU:OE1	1:B:418:ILE:CG1	2.54	0.55
1:A:43:PHE:CG	1:A:44:ARG:N	2.74	0.55
1:B:546:LEU:HD11	1:B:565:PHE:CD2	2.42	0.55
1:B:565:PHE:HD1	1:B:565:PHE:C	2.15	0.55
1:C:392:PHE:HA	1:C:517:LEU:HD11	1.89	0.55
1:C:438:SER:O	1:C:438:SER:OG	2.21	0.55
2:E:335:ASP:N	2:E:335:ASP:OD1	2.39	0.55
1:A:329:PHE:O	1:A:580:GLN:CG	2.55	0.55
1:A:353:TRP:CD1	1:A:353:TRP:H	2.24	0.55
1:B:45:SER:HA	1:B:280:ASN:O	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:347:PHE:CE1	1:C:509:ARG:HD3	2.42	0.55
3:N:1:NAG:H61	3:N:2:NAG:HN2	1.71	0.55
1:B:551:VAL:HB	1:B:588:THR:CG2	2.37	0.54
1:A:663:ASP:OD2	1:A:673:SER:OG	2.22	0.54
1:A:886:TRP:HH2	1:A:904:TYR:HD2	1.56	0.54
1:B:43:PHE:O	1:B:44:ARG:HG3	2.08	0.54
1:B:392:PHE:HA	1:B:517:LEU:HD11	1.89	0.54
1:A:556:ASN:HD22	1:A:556:ASN:N	2.05	0.54
1:A:43:PHE:O	1:A:44:ARG:HG3	2.08	0.54
1:A:530:SER:HB3	1:A:580:GLN:NE2	2.21	0.54
1:C:43:PHE:O	1:C:44:ARG:HG3	2.08	0.54
1:C:486:PHE:CZ	2:E:79:LEU:CD2	2.84	0.54
2:E:342:ALA:O	2:E:343:VAL:C	2.50	0.54
3:G:1:NAG:H61	3:G:2:NAG:HN2	1.71	0.54
1:A:699:LEU:HD22	1:B:873:TYR:CE2	2.42	0.54
1:B:347:PHE:CE1	1:B:509:ARG:HD3	2.42	0.54
1:B:438:SER:O	1:B:438:SER:OG	2.21	0.54
1:C:653:ALA:HA	1:C:692:ILE:O	2.08	0.54
1:A:111:ASP:OD1	1:A:134:GLN:NE2	2.41	0.54
1:C:421:TYR:HA	1:C:461:LEU:HG	1.89	0.54
1:A:43:PHE:CD1	1:C:563:GLN:OE1	2.52	0.54
1:A:100:ILE:O	1:A:242:LEU:HA	2.08	0.54
1:A:392:PHE:CD2	1:A:517:LEU:CD2	2.86	0.54
1:B:557:LYS:HE3	1:B:575:ALA:HB2	1.90	0.54
1:B:565:PHE:C	1:B:565:PHE:CD1	2.85	0.54
1:C:111:ASP:OD1	1:C:134:GLN:NE2	2.41	0.54
2:D:538:PRO:HD2	2:D:541:LYS:HD2	1.88	0.54
2:E:231:GLU:HA	2:E:234:LYS:HD3	1.88	0.54
1:B:551:VAL:HB	1:B:588:THR:HG22	1.89	0.54
3:U:1:NAG:H61	3:U:2:NAG:HN2	1.71	0.54
1:B:100:ILE:O	1:B:242:LEU:HA	2.08	0.54
1:B:391:CYS:HA	1:B:525:CYS:HB3	1.90	0.54
1:B:559:PHE:CZ	1:B:566:GLY:N	2.73	0.54
2:D:52:THR:OG1	2:D:332:MET:SD	2.66	0.53
1:A:327:VAL:O	1:A:328:ARG:CD	2.56	0.53
1:A:1141:LEU:HD12	1:C:1141:LEU:HD11	1.90	0.53
1:B:111:ASP:OD1	1:B:134:GLN:NE2	2.41	0.53
1:B:530:SER:O	1:B:531:THR:CB	2.56	0.53
1:B:570:ALA:HB1	1:C:963:VAL:CG1	2.39	0.53
2:D:105:SER:C	2:D:106:SER:HG	2.09	0.53
2:E:52:THR:OG1	2:E:332:MET:SD	2.66	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:57:PRO:O	1:A:60:SER:OG	2.24	0.53
1:B:748:GLU:HG3	1:B:981:LEU:CD2	2.23	0.53
1:C:41:LYS:O	1:C:42:VAL:HB	2.08	0.53
1:C:100:ILE:O	1:C:242:LEU:HA	2.08	0.53
1:A:505:TYR:CG	2:D:353:LYS:O	2.62	0.53
1:C:476:GLY:H	1:C:487:ASN:HB3	1.74	0.53
1:C:532:ASN:N	1:C:532:ASN:OD1	2.40	0.53
1:A:690:GLN:O	1:A:691:SER:HB3	2.09	0.53
1:B:544:ASN:O	1:B:544:ASN:ND2	2.41	0.53
1:B:560:LEU:HD23	1:B:563:GLN:CD	2.29	0.53
1:B:1142:GLN:HG3	1:B:1143:PRO:CD	2.37	0.53
1:C:64:TRP:HD1	1:C:65:PHE:N	2.07	0.53
3:I:2:NAG:H3	3:I:2:NAG:H83	1.90	0.53
1:A:325:SER:HA	1:A:540:ASN:O	2.09	0.53
1:A:363:ALA:O	1:A:527:PRO:HD3	2.08	0.53
1:A:565:PHE:CE2	1:B:42:VAL:HG22	2.44	0.53
1:B:328:ARG:HH11	1:B:533:LEU:HD23	1.66	0.53
1:C:505:TYR:CE2	2:E:353:LYS:C	2.87	0.53
1:A:894:LEU:HB3	1:C:713:ALA:HB3	1.90	0.53
1:B:328:ARG:HH21	1:B:580:GLN:HG3	1.73	0.53
1:B:516:GLU:C	1:B:517:LEU:CD2	2.82	0.53
1:C:325:SER:HB3	1:C:540:ASN:HB3	1.90	0.53
1:A:310:LYS:HB3	1:A:310:LYS:HZ2	1.74	0.53
1:A:516:GLU:C	1:A:517:LEU:CD2	2.82	0.53
1:C:516:GLU:C	1:C:517:LEU:CD2	2.82	0.53
2:D:90:ASN:HB3	2:D:93:VAL:HG12	1.91	0.53
1:A:421:TYR:HA	1:A:461:LEU:HG	1.90	0.52
1:B:1104:VAL:HG22	1:B:1115:ILE:HG12	1.91	0.52
3:d:1:NAG:H3	3:d:2:NAG:N2	2.24	0.52
2:E:245:ARG:NH1	2:E:603:PHE:O	2.42	0.52
1:A:505:TYR:CE2	2:D:353:LYS:C	2.87	0.52
1:A:544:ASN:O	1:A:544:ASN:ND2	2.41	0.52
1:C:544:ASN:ND2	1:C:544:ASN:O	2.41	0.52
1:B:1045:LYS:HZ2	1:C:786:LYS:HE3	1.72	0.52
3:i:1:NAG:H3	3:i:2:NAG:N2	2.24	0.52
1:A:476:GLY:H	1:A:487:ASN:HB3	1.74	0.52
1:C:324:GLU:CG	1:C:325:SER:N	2.73	0.52
1:C:505:TYR:CG	2:E:353:LYS:O	2.62	0.52
1:A:334:ASN:O	1:A:362:VAL:CG2	2.58	0.52
1:A:524:VAL:C	1:A:525:CYS:SG	2.93	0.52
1:C:48:LEU:CD1	1:C:48:LEU:N	2.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:326:ILE:HD12	1:C:326:ILE:C	2.34	0.52
1:C:326:ILE:HD11	1:C:541:PHE:CB	2.40	0.52
1:C:1101:HIS:CD2	3:Z:1:NAG:H5	2.45	0.52
2:D:394:ASN:HB2	2:D:562:LYS:HD2	1.92	0.52
2:E:90:ASN:HB3	2:E:93:VAL:HG12	1.91	0.52
1:B:64:TRP:HD1	1:B:65:PHE:N	2.07	0.52
1:B:391:CYS:CA	1:B:525:CYS:HB3	2.39	0.52
2:E:394:ASN:HB2	2:E:562:LYS:HD2	1.92	0.52
1:A:530:SER:OG	1:A:580:GLN:NE2	2.42	0.52
1:A:563:GLN:OE1	1:B:43:PHE:CD1	2.56	0.52
1:B:48:LEU:N	1:B:48:LEU:CD1	2.73	0.52
1:B:748:GLU:HG2	1:B:981:LEU:HD21	1.83	0.52
1:C:327:VAL:CG1	1:C:328:ARG:N	2.73	0.52
1:C:662:CYS:HB2	1:C:697:MET:CE	2.26	0.52
1:B:559:PHE:CE1	1:C:43:PHE:HB2	2.45	0.52
1:C:524:VAL:C	1:C:525:CYS:SG	2.93	0.52
1:A:64:TRP:HD1	1:A:65:PHE:N	2.07	0.51
1:A:318:PHE:CZ	1:A:320:VAL:HG22	2.46	0.51
1:A:493:GLN:OE1	2:D:34:HIS:HB3	2.10	0.51
1:A:565:PHE:CZ	1:B:42:VAL:CG2	2.93	0.51
1:A:854:LYS:N	1:A:854:LYS:CD	2.73	0.51
1:B:580:GLN:HB3	3:M:1:NAG:H5	1.91	0.51
1:C:493:GLN:OE1	2:E:34:HIS:HB3	2.10	0.51
2:D:425:SER:C	2:D:427:ASP:H	2.19	0.51
1:A:390:LEU:HD23	1:A:391:CYS:N	2.19	0.51
1:A:505:TYR:CE2	2:D:354:GLY:HA3	2.45	0.51
1:C:529:LYS:HE2	1:C:530:SER:H	1.75	0.51
1:C:715:PRO:HA	1:C:1072:GLU:HA	1.92	0.51
1:A:379:CYS:HB3	1:A:382:VAL:O	2.10	0.51
2:D:245:ARG:NH1	2:D:603:PHE:O	2.42	0.51
1:A:48:LEU:N	1:A:48:LEU:CD1	2.73	0.51
1:A:565:PHE:O	1:B:42:VAL:CA	2.55	0.51
2:D:104:GLY:O	2:D:107:VAL:HG22	2.10	0.51
1:A:901:GLN:NE2	1:A:905:ARG:HH21	2.08	0.51
1:B:569:ILE:HG12	1:C:47:VAL:CG1	2.41	0.51
1:C:348:ALA:HB2	1:C:354:ASN:ND2	2.26	0.51
1:C:379:CYS:HB3	1:C:382:VAL:O	2.10	0.51
1:A:310:LYS:HB3	1:A:310:LYS:NZ	2.25	0.51
1:B:320:VAL:CG2	1:B:591:SER:HB2	2.39	0.51
1:B:379:CYS:HB3	1:B:382:VAL:O	2.10	0.51
1:C:130:VAL:HB	1:C:168:PHE:HB3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:390:LEU:HD23	1:C:391:CYS:N	2.19	0.51
2:E:425:SER:C	2:E:427:ASP:H	2.19	0.51
1:A:319:ARG:NH2	1:B:740:MET:HG3	2.23	0.51
1:B:516:GLU:OE2	1:C:200:TYR:HE2	1.94	0.51
2:E:104:GLY:O	2:E:107:VAL:HG22	2.10	0.51
1:A:130:VAL:HB	1:A:168:PHE:HB3	1.93	0.51
1:A:329:PHE:CB	1:A:330:PRO:HD2	2.37	0.51
1:B:324:GLU:HG2	1:B:325:SER:N	2.24	0.51
1:C:131:CYS:H	1:C:133:PHE:HE1	1.59	0.51
2:E:433:GLU:O	2:E:437:ASN:ND2	2.44	0.51
1:C:392:PHE:CD2	1:C:517:LEU:CD2	2.85	0.50
1:C:505:TYR:CE2	2:E:354:GLY:HA3	2.45	0.50
1:A:41:LYS:N	1:A:41:LYS:CD	2.73	0.50
1:B:131:CYS:H	1:B:133:PHE:HE1	1.59	0.50
1:C:401:VAL:HG22	1:C:509:ARG:HG2	1.94	0.50
1:A:705:VAL:HB	1:B:883:THR:HG21	1.93	0.50
1:C:129:LYS:HG2	1:C:133:PHE:HZ	1.77	0.50
1:C:327:VAL:O	1:C:328:ARG:HG2	2.11	0.50
1:A:129:LYS:HG2	1:A:133:PHE:HZ	1.77	0.50
1:A:348:ALA:HB2	1:A:354:ASN:ND2	2.26	0.50
1:B:662:CYS:HB2	1:B:697:MET:HE3	1.93	0.50
2:D:433:GLU:O	2:D:437:ASN:ND2	2.44	0.50
1:A:388:ASN:CG	1:A:527:PRO:HD2	2.36	0.50
1:B:106:PHE:HB3	1:B:235:ILE:HD13	1.93	0.50
1:C:326:ILE:HD11	1:C:541:PHE:HB3	1.94	0.50
1:C:804:GLN:HE21	1:C:935:GLN:NE2	2.08	0.50
1:C:1032:CYS:O	1:C:1051:SER:HB2	2.11	0.50
1:C:329:PHE:HB3	1:C:330:PRO:HD2	1.93	0.50
1:B:348:ALA:HB2	1:B:354:ASN:ND2	2.26	0.50
1:B:560:LEU:CB	1:B:562:PHE:CE2	2.92	0.50
1:C:1090:PRO:HD3	1:C:1095:PHE:CE2	2.47	0.50
2:E:208:GLU:OE2	2:E:219:ARG:NH1	2.44	0.50
1:A:131:CYS:H	1:A:133:PHE:HE1	1.59	0.50
1:A:310:LYS:HE2	1:A:663:ASP:OD1	2.12	0.50
1:A:502:GLY:O	1:A:505:TYR:HB2	2.12	0.50
1:C:431:GLY:HA3	1:C:513:LEU:O	2.12	0.50
2:D:335:ASP:CA	2:D:361:CYS:SG	3.00	0.50
1:C:388:ASN:CG	1:C:527:PRO:HD2	2.37	0.49
1:A:106:PHE:HB3	1:A:235:ILE:HD13	1.93	0.49
1:A:328:ARG:HB3	1:A:328:ARG:HH21	1.77	0.49
1:A:335:LEU:HD12	1:A:335:LEU:N	2.26	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:735:SER:HB3	1:A:859:THR:HG22	1.94	0.49
1:C:807:PRO:O	1:C:809:PRO:HD3	2.12	0.49
2:E:302:TRP:CH2	2:E:423:LEU:CD1	2.78	0.49
2:D:208:GLU:OE2	2:D:219:ARG:NH1	2.44	0.49
1:A:401:VAL:HG22	1:A:509:ARG:HG2	1.94	0.49
3:R:1:NAG:H62	3:R:2:NAG:H2	1.93	0.49
1:B:130:VAL:HB	1:B:168:PHE:HB3	1.93	0.49
1:C:331:ASN:OD1	1:C:331:ASN:N	2.40	0.49
1:C:437:ASN:OD1	1:C:438:SER:N	2.46	0.49
1:C:502:GLY:O	1:C:505:TYR:HB2	2.12	0.49
1:B:335:LEU:C	1:B:362:VAL:O	2.56	0.49
1:B:401:VAL:HG22	1:B:509:ARG:HG2	1.94	0.49
1:C:122:ASN:OD1	1:C:122:ASN:N	2.46	0.49
1:B:41:LYS:CD	1:B:41:LYS:N	2.73	0.49
1:B:212:LEU:HD23	1:B:215:ASP:HB2	1.95	0.49
1:B:521:PRO:HA	1:B:564:GLN:HG3	1.94	0.49
1:B:524:VAL:C	1:B:525:CYS:SG	2.95	0.49
2:E:335:ASP:CA	2:E:361:CYS:SG	3.00	0.49
1:C:106:PHE:HB3	1:C:235:ILE:HD13	1.93	0.49
1:C:654:GLU:CA	1:C:693:ILE:HG22	2.43	0.49
1:A:171:VAL:HG12	1:A:172:SER:H	1.78	0.48
1:A:437:ASN:OD1	1:A:438:SER:N	2.46	0.48
1:A:896:ILE:HG13	1:A:897:PRO:HD2	1.95	0.48
1:B:308:VAL:O	1:B:601:GLY:HA2	2.13	0.48
1:B:431:GLY:HA3	1:B:513:LEU:O	2.12	0.48
1:B:437:ASN:OD1	1:B:438:SER:N	2.46	0.48
1:C:361:CYS:O	1:C:524:VAL:HG23	2.13	0.48
2:E:564:GLU:HB3	2:E:568:LEU:HD23	1.94	0.48
1:A:122:ASN:OD1	1:A:122:ASN:N	2.46	0.48
1:B:171:VAL:HG12	1:B:172:SER:H	1.78	0.48
1:A:361:CYS:O	1:A:524:VAL:HG23	2.13	0.48
1:A:520:ALA:CB	1:A:521:PRO:CD	2.79	0.48
1:B:122:ASN:OD1	1:B:122:ASN:N	2.46	0.48
1:A:524:VAL:HG22	1:A:525:CYS:N	2.27	0.48
1:B:328:ARG:NH2	1:B:580:GLN:HB2	2.28	0.48
1:B:357:ARG:NH1	1:C:230:PRO:HB2	2.27	0.48
1:B:533:LEU:CD1	1:B:535:LYS:NZ	2.77	0.48
1:C:335:LEU:C	1:C:362:VAL:O	2.56	0.48
1:C:524:VAL:HG22	1:C:525:CYS:N	2.27	0.48
1:A:227:VAL:HG12	1:A:228:ASP:H	1.79	0.48
1:A:231:ILE:HB	1:A:233:ILE:HG22	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:129:LYS:HG2	1:B:133:PHE:HZ	1.77	0.48
1:B:231:ILE:HB	1:B:233:ILE:HG22	1.95	0.48
1:C:332:ILE:HG23	1:C:362:VAL:HG21	1.94	0.48
1:C:533:LEU:HD12	1:C:533:LEU:C	2.38	0.48
1:C:1104:VAL:HG22	1:C:1115:ILE:HG12	1.95	0.48
2:D:564:GLU:HB3	2:D:568:LEU:HD23	1.94	0.48
1:A:935:GLN:O	1:A:939:SER:HB3	2.14	0.48
1:B:361:CYS:O	1:B:524:VAL:HG23	2.13	0.48
1:C:319:ARG:NH2	1:C:319:ARG:CG	2.73	0.48
1:A:42:VAL:HG22	1:C:565:PHE:CE1	2.47	0.48
1:A:328:ARG:HH21	1:A:328:ARG:CG	2.27	0.48
1:A:335:LEU:C	1:A:362:VAL:O	2.57	0.48
1:B:46:SER:O	1:B:47:VAL:HG13	2.14	0.48
1:C:171:VAL:HG12	1:C:172:SER:H	1.78	0.48
1:A:672:ALA:HA	1:A:693:ILE:O	2.14	0.48
1:B:535:LYS:HE2	1:B:585:LEU:HD21	1.96	0.48
1:C:212:LEU:HD23	1:C:215:ASP:HB2	1.95	0.48
1:C:653:ALA:CB	1:C:692:ILE:HG22	2.44	0.48
1:B:524:VAL:HG22	1:B:525:CYS:N	2.28	0.48
1:C:227:VAL:HG12	1:C:228:ASP:H	1.79	0.48
1:A:431:GLY:HA3	1:A:513:LEU:O	2.12	0.47
1:C:476:GLY:HA2	2:E:24:GLN:NE2	2.26	0.47
1:B:227:VAL:HG12	1:B:228:ASP:H	1.79	0.47
1:B:533:LEU:HD11	1:B:535:LYS:HE2	1.95	0.47
1:B:1045:LYS:HZ1	1:C:786:LYS:HE3	1.76	0.47
1:B:569:ILE:CG1	1:C:47:VAL:CG1	2.92	0.47
1:C:46:SER:O	1:C:47:VAL:HG13	2.14	0.47
1:C:516:GLU:C	1:C:517:LEU:HD23	2.39	0.47
2:D:421:ILE:HG13	2:D:421:ILE:O	2.14	0.47
1:A:516:GLU:C	1:A:517:LEU:HD23	2.39	0.47
1:B:310:LYS:HG2	1:B:664:ILE:HD11	1.95	0.47
1:C:231:ILE:HB	1:C:233:ILE:HG22	1.95	0.47
1:C:326:ILE:C	1:C:326:ILE:CD1	2.87	0.47
1:C:500:THR:O	1:C:500:THR:OG1	2.31	0.47
1:B:403:ARG:NH1	1:B:505:TYR:CD1	2.78	0.47
2:E:254:SER:O	2:E:254:SER:OG	2.31	0.47
3:i:2:NAG:H83	3:i:2:NAG:C3	2.45	0.47
1:A:669:GLY:N	1:B:864:LEU:O	2.46	0.47
1:A:886:TRP:CH2	1:A:904:TYR:HD2	2.31	0.47
1:B:516:GLU:C	1:B:517:LEU:HD23	2.39	0.47
1:B:710:ASN:N	1:B:710:ASN:HD22	2.11	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:486:PHE:HE1	2:E:79:LEU:CD1	2.27	0.47
1:A:486:PHE:HE1	2:D:79:LEU:CD1	2.27	0.47
1:A:316:SER:C	1:A:317:ASN:ND2	2.73	0.47
1:B:570:ALA:HB1	1:C:963:VAL:HG12	1.96	0.47
1:B:640:SER:OG	1:B:641:ASN:N	2.48	0.47
1:C:640:SER:OG	1:C:641:ASN:N	2.48	0.47
1:C:696:THR:O	1:C:697:MET:C	2.56	0.47
3:d:2:NAG:C3	3:d:2:NAG:H83	2.45	0.47
1:A:212:LEU:HD23	1:A:215:ASP:HB2	1.95	0.47
1:C:316:SER:C	1:C:317:ASN:ND2	2.73	0.47
1:C:973:ILE:HG12	1:C:992:GLN:HE21	1.79	0.47
1:A:117:LEU:HD12	1:A:118:LEU:N	2.30	0.46
1:B:729:VAL:HG13	1:B:1059:GLY:HA2	1.98	0.46
1:C:476:GLY:CA	2:E:24:GLN:NE2	2.65	0.46
1:C:560:LEU:O	1:C:562:PHE:N	2.47	0.46
1:C:726:ILE:HG12	1:C:1061:VAL:HG22	1.97	0.46
2:D:425:SER:C	2:D:427:ASP:N	2.73	0.46
1:A:46:SER:O	1:A:47:VAL:HG13	2.14	0.46
1:A:369:TYR:CE2	1:A:384:PRO:HB2	2.50	0.46
1:B:316:SER:C	1:B:317:ASN:ND2	2.73	0.46
1:B:364:ASP:O	1:B:367:VAL:HG12	2.15	0.46
1:C:393:THR:HA	1:C:523:THR:HB	1.98	0.46
1:C:804:GLN:HG3	1:C:935:GLN:HE22	1.80	0.46
2:D:333:LEU:O	2:D:362:THR:HG22	2.15	0.46
1:A:393:THR:HA	1:A:523:THR:HB	1.98	0.46
2:E:333:LEU:O	2:E:362:THR:HG22	2.15	0.46
1:B:537:LYS:O	1:B:538:CYS:C	2.58	0.46
2:E:560:LEU:HD22	2:E:564:GLU:HG3	1.98	0.46
1:A:640:SER:OG	1:A:641:ASN:N	2.48	0.46
1:A:1105:THR:HG22	1:A:1111:GLU:H	1.80	0.46
1:B:722:VAL:HA	1:B:1064:HIS:O	2.16	0.46
1:C:117:LEU:HD12	1:C:118:LEU:N	2.30	0.46
1:B:528:LYS:O	1:B:529:LYS:HG2	2.15	0.46
1:B:556:ASN:C	1:B:556:ASN:ND2	2.73	0.46
1:C:977:LEU:HD12	1:C:996:LEU:HD12	1.98	0.46
1:A:912:THR:OG1	1:A:914:ASN:ND2	2.48	0.46
1:B:369:TYR:CE2	1:B:384:PRO:HB2	2.50	0.46
1:B:500:THR:O	1:B:500:THR:OG1	2.31	0.46
1:B:578:ASP:OD2	1:B:581:THR:HG22	2.16	0.46
1:B:710:ASN:HD22	1:B:710:ASN:H	1.62	0.46
1:A:41:LYS:N	1:A:41:LYS:HD3	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:364:ASP:O	1:A:367:VAL:HG12	2.15	0.46
1:A:565:PHE:O	1:B:43:PHE:N	2.49	0.46
1:B:393:THR:HA	1:B:523:THR:HB	1.97	0.46
1:B:1032:CYS:O	1:B:1051:SER:HB2	2.16	0.46
1:C:592:PHE:CD1	1:C:592:PHE:C	2.92	0.46
1:A:447:GLY:HA2	1:A:497:PHE:O	2.16	0.46
1:A:985:ASP:OD1	1:A:985:ASP:N	2.45	0.46
1:B:713:ALA:HB3	1:C:894:LEU:HB3	1.97	0.46
1:C:578:ASP:OD2	1:C:581:THR:HG22	2.16	0.46
2:D:52:THR:HA	2:D:342:ALA:HB1	1.98	0.46
2:E:421:ILE:O	2:E:421:ILE:HG13	2.14	0.46
1:A:505:TYR:CD2	2:D:353:LYS:C	2.93	0.46
1:B:316:SER:OG	1:B:317:ASN:N	2.48	0.46
1:B:758:SER:O	1:B:762:GLN:HG3	2.16	0.46
1:C:45:SER:O	1:C:279:TYR:CB	2.64	0.46
1:C:369:TYR:CE2	1:C:384:PRO:HB2	2.50	0.46
1:A:127:VAL:HG11	4:A:1402:NAG:H61	1.98	0.45
1:A:328:ARG:NH2	1:A:578:ASP:OD1	2.50	0.45
1:C:377:PHE:CD2	1:C:434:ILE:HG12	2.51	0.45
2:D:560:LEU:HD22	2:D:564:GLU:HG3	1.98	0.45
2:E:105:SER:C	2:E:106:SER:HG	2.07	0.45
1:B:570:ALA:CB	1:C:963:VAL:CG1	2.94	0.45
2:E:52:THR:HA	2:E:342:ALA:HB1	1.98	0.45
2:E:425:SER:C	2:E:427:ASP:N	2.73	0.45
1:A:48:LEU:HD13	1:A:48:LEU:N	2.32	0.45
1:C:48:LEU:HD13	1:C:48:LEU:N	2.32	0.45
1:C:153:MET:N	1:C:153:MET:SD	2.90	0.45
1:C:364:ASP:O	1:C:367:VAL:HG12	2.15	0.45
1:A:654:GLU:HG3	1:A:693:ILE:HG22	1.99	0.45
1:A:903:ALA:HB1	1:A:913:GLN:HG2	1.98	0.45
1:B:45:SER:O	1:B:279:TYR:CB	2.64	0.45
2:D:431:ASP:OD1	2:D:431:ASP:N	2.44	0.45
1:A:1094:VAL:HG22	1:A:1107:ARG:HG2	1.98	0.45
1:B:646:ARG:O	1:B:646:ARG:HG3	2.17	0.45
1:C:29:THR:HG22	1:C:30:ASN:N	2.31	0.45
1:C:338:PHE:C	1:C:340:GLU:N	2.75	0.45
1:A:316:SER:OG	1:A:317:ASN:N	2.48	0.45
1:A:318:PHE:CE2	1:A:320:VAL:HG22	2.52	0.45
1:A:560:LEU:O	1:A:562:PHE:N	2.47	0.45
1:B:338:PHE:C	1:B:340:GLU:N	2.75	0.45
1:C:523:THR:CG2	1:C:524:VAL:N	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:703:ASN:C	1:C:703:ASN:HD22	2.24	0.45
1:A:29:THR:HG22	1:A:30:ASN:N	2.31	0.45
1:A:153:MET:SD	1:A:153:MET:N	2.90	0.45
1:A:338:PHE:C	1:A:340:GLU:N	2.75	0.45
1:A:1090:PRO:HD3	1:A:1095:PHE:CE2	2.51	0.45
1:B:41:LYS:N	1:B:41:LYS:HD3	2.31	0.45
1:B:153:MET:SD	1:B:153:MET:N	2.90	0.45
1:C:447:GLY:HA2	1:C:497:PHE:O	2.16	0.45
2:D:208:GLU:OE1	2:D:210:ASN:ND2	2.50	0.45
1:B:447:GLY:HA2	1:B:497:PHE:O	2.16	0.45
1:B:565:PHE:HE1	1:C:42:VAL:HG22	1.81	0.45
1:B:655:HIS:HD2	1:B:694:ALA:O	2.00	0.45
1:A:45:SER:O	1:A:279:TYR:CB	2.64	0.45
1:A:187:LYS:HE3	1:A:213:VAL:HG12	1.99	0.45
1:A:578:ASP:OD2	1:A:581:THR:HG22	2.16	0.45
1:B:127:VAL:HG11	4:B:1402:NAG:H61	1.98	0.45
1:B:324:GLU:CG	1:B:325:SER:N	2.79	0.45
1:C:493:GLN:OE1	2:E:34:HIS:CG	2.70	0.45
1:C:1141:LEU:O	1:C:1145:LEU:HD12	2.16	0.45
1:A:377:PHE:CD2	1:A:434:ILE:HG12	2.51	0.45
1:B:29:THR:HG22	1:B:30:ASN:N	2.31	0.45
1:C:127:VAL:HG11	4:C:1402:NAG:H61	1.98	0.45
1:C:187:LYS:HE3	1:C:213:VAL:HG12	1.99	0.45
1:A:486:PHE:CE1	2:D:79:LEU:HD21	2.48	0.44
1:B:533:LEU:CD1	1:B:535:LYS:HZ1	2.30	0.44
2:E:356:PHE:HB3	2:E:379:ILE:HD12	1.98	0.44
1:A:134:GLN:HB3	1:A:162:SER:HB2	2.00	0.44
1:A:440:ASN:ND2	1:A:441:LEU:HG	2.32	0.44
1:A:617:CYS:HB2	1:A:649:CYS:HB2	1.87	0.44
1:B:825:LYS:HB3	1:B:825:LYS:HE2	1.79	0.44
1:C:520:ALA:CB	1:C:521:PRO:CD	2.79	0.44
1:C:995:ARG:HE	1:C:995:ARG:HB3	1.66	0.44
1:A:551:VAL:HB	1:A:588:THR:HG23	2.00	0.44
1:C:691:SER:OG	1:C:692:ILE:N	2.50	0.44
1:C:1040:VAL:O	1:C:1041:ASP:HB2	2.16	0.44
1:B:328:ARG:HD3	1:B:531:THR:O	2.17	0.44
1:B:519:HIS:O	1:C:41:LYS:CE	2.65	0.44
1:B:521:PRO:O	1:B:522:ALA:CB	2.66	0.44
1:C:646:ARG:HG3	1:C:646:ARG:O	2.17	0.44
1:B:377:PHE:CD2	1:B:434:ILE:HG12	2.51	0.44
1:B:569:ILE:HG13	1:C:47:VAL:HG11	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:748:GLU:N	1:B:748:GLU:CD	2.73	0.44
1:C:140:PHE:CG	1:C:244:LEU:HD11	2.53	0.44
2:D:356:PHE:HB3	2:D:379:ILE:HD12	1.98	0.44
1:B:48:LEU:HD13	1:B:48:LEU:N	2.32	0.44
1:B:187:LYS:HE3	1:B:213:VAL:HG12	1.99	0.44
1:B:393:THR:O	1:B:523:THR:CG2	2.58	0.44
1:B:134:GLN:HB3	1:B:162:SER:HB2	2.00	0.44
1:B:294:ASP:N	1:B:294:ASP:OD1	2.50	0.44
1:B:321:GLN:NE2	1:B:322:PRO:HD2	2.32	0.44
1:B:560:LEU:HD23	1:C:43:PHE:HD1	1.82	0.44
1:C:134:GLN:HB3	1:C:162:SER:HB2	2.00	0.44
1:A:130:VAL:HG21	1:A:231:ILE:HD12	2.00	0.44
1:A:476:GLY:HA2	2:D:24:GLN:NE2	2.26	0.44
1:B:1045:LYS:NZ	1:C:786:LYS:CE	2.79	0.44
2:E:208:GLU:OE1	2:E:210:ASN:ND2	2.50	0.44
1:A:140:PHE:CG	1:A:244:LEU:HD11	2.53	0.43
1:A:493:GLN:OE1	2:D:34:HIS:CG	2.70	0.43
1:A:546:LEU:HD11	1:A:565:PHE:CG	2.53	0.43
1:A:646:ARG:O	1:A:646:ARG:HG3	2.17	0.43
1:A:660:TYR:O	1:A:698:SER:HB2	2.17	0.43
1:C:1081:ILE:HG12	1:C:1095:PHE:CE2	2.53	0.43
1:A:1104:VAL:HG22	1:A:1115:ILE:HG12	2.01	0.43
1:B:140:PHE:CG	1:B:244:LEU:HD11	2.53	0.43
1:B:141:LEU:O	1:B:243:ALA:HA	2.18	0.43
1:C:130:VAL:HG21	1:C:231:ILE:HD12	2.00	0.43
1:B:319:ARG:HG3	1:B:319:ARG:HH21	1.84	0.43
1:B:332:ILE:HB	1:B:333:THR:H	1.55	0.43
1:B:519:HIS:HE1	1:C:41:LYS:N	2.14	0.43
1:B:559:PHE:CE2	1:B:564:GLN:O	2.70	0.43
1:B:669:GLY:N	1:C:864:LEU:O	2.49	0.43
1:C:127:VAL:HG21	4:C:1402:NAG:H5	2.01	0.43
1:C:316:SER:OG	1:C:317:ASN:N	2.48	0.43
2:D:313:LYS:HA	2:D:316:VAL:HG12	2.00	0.43
1:A:230:PRO:C	1:C:521:PRO:HG2	2.34	0.43
1:A:1097:SER:HA	1:A:1101:HIS:O	2.19	0.43
1:B:327:VAL:O	1:B:530:SER:O	2.36	0.43
1:B:440:ASN:ND2	1:B:441:LEU:HG	2.32	0.43
1:A:312:ILE:HG13	1:A:598:ILE:HG13	2.00	0.43
1:A:390:LEU:O	1:A:525:CYS:HB3	2.18	0.43
1:A:959:LEU:HD23	1:A:959:LEU:HA	1.78	0.43
1:B:117:LEU:HD12	1:B:118:LEU:N	2.30	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:127:VAL:HG21	4:B:1402:NAG:H5	2.00	0.43
1:C:390:LEU:O	1:C:525:CYS:HB3	2.18	0.43
1:C:486:PHE:CE1	2:E:79:LEU:HD21	2.47	0.43
3:i:1:NAG:C3	3:i:2:NAG:N2	2.74	0.43
1:A:113:LYS:O	1:A:113:LYS:NZ	2.31	0.43
1:A:795:LYS:HB3	1:A:797:PHE:CE2	2.54	0.43
1:A:1032:CYS:O	1:A:1051:SER:HB2	2.18	0.43
1:B:520:ALA:CB	1:B:521:PRO:CD	2.79	0.43
1:C:546:LEU:HD11	1:C:565:PHE:CG	2.53	0.43
1:A:612:TYR:HE1	1:A:651:ILE:HD12	1.84	0.43
3:G:1:NAG:H61	3:G:2:NAG:N2	2.33	0.43
1:A:328:ARG:HD2	1:A:328:ARG:HA	1.71	0.43
1:B:332:ILE:HD13	1:B:362:VAL:HG21	2.00	0.43
1:B:558:LYS:HD2	1:B:558:LYS:N	2.27	0.43
1:C:793:PRO:HG2	1:C:794:ILE:HD12	2.00	0.43
1:A:569:ILE:O	1:A:570:ALA:HB3	2.19	0.43
1:C:440:ASN:ND2	1:C:441:LEU:HG	2.32	0.43
1:C:486:PHE:HE1	2:E:79:LEU:HD21	1.77	0.43
1:C:569:ILE:O	1:C:570:ALA:HB3	2.19	0.43
1:C:1027:THR:HG22	1:C:1042:PHE:HZ	1.83	0.43
3:N:1:NAG:H61	3:N:2:NAG:N2	2.33	0.43
1:A:131:CYS:HB3	1:A:164:ASN:O	2.19	0.43
1:A:294:ASP:OD1	1:A:294:ASP:N	2.50	0.43
1:B:569:ILE:O	1:B:570:ALA:HB3	2.19	0.43
1:C:931:ILE:HD13	1:C:931:ILE:HA	1.86	0.43
3:U:1:NAG:H61	3:U:2:NAG:N2	2.33	0.43
1:B:130:VAL:HG21	1:B:231:ILE:HD12	2.00	0.42
1:C:294:ASP:OD1	1:C:294:ASP:N	2.50	0.42
1:C:296:LEU:HD11	1:C:602:THR:HG22	2.01	0.42
1:C:612:TYR:HE1	1:C:651:ILE:HD12	1.84	0.42
1:A:48:LEU:H	1:A:48:LEU:CD1	2.32	0.42
1:A:141:LEU:O	1:A:243:ALA:HA	2.18	0.42
1:B:986:PRO:CB	1:B:987:PRO:HD3	2.45	0.42
1:C:27:ALA:HB3	1:C:64:TRP:HB3	2.01	0.42
1:C:141:LEU:O	1:C:243:ALA:HA	2.18	0.42
1:C:304:LYS:HE3	1:C:304:LYS:HB3	1.78	0.42
1:C:722:VAL:HA	1:C:1064:HIS:O	2.19	0.42
1:A:533:LEU:C	1:A:533:LEU:CD1	2.86	0.42
1:B:27:ALA:HB3	1:B:64:TRP:HB3	2.01	0.42
1:A:27:ALA:HB3	1:A:64:TRP:HB3	2.01	0.42
1:B:560:LEU:HB2	1:B:563:GLN:CD	2.45	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:580:GLN:O	3:M:1:NAG:O4	2.38	0.42
1:B:612:TYR:HE1	1:B:651:ILE:HD12	1.84	0.42
1:C:735:SER:OG	1:C:859:THR:HG22	2.17	0.42
1:A:112:SER:O	1:A:113:LYS:HB3	2.20	0.42
1:A:521:PRO:O	1:A:522:ALA:CB	2.66	0.42
1:A:565:PHE:CE1	1:B:42:VAL:HG22	2.54	0.42
1:A:703:ASN:HB2	1:B:787:GLN:CD	2.26	0.42
1:B:131:CYS:HB3	1:B:164:ASN:O	2.19	0.42
1:B:327:VAL:O	1:B:531:THR:HB	2.19	0.42
1:B:776:LYS:HE3	1:B:776:LYS:HB3	1.65	0.42
1:C:112:SER:O	1:C:113:LYS:HB3	2.20	0.42
1:C:674:TYR:HE1	1:C:691:SER:N	2.12	0.42
1:C:784:GLN:HE21	1:C:784:GLN:HB3	1.63	0.42
1:C:792:PRO:O	1:C:795:LYS:NZ	2.52	0.42
1:C:912:THR:OG1	1:C:914:ASN:ND2	2.52	0.42
2:E:212:VAL:HG23	2:E:215:TYR:HB2	2.02	0.42
2:E:313:LYS:HA	2:E:316:VAL:HG12	2.00	0.42
1:A:127:VAL:HG21	4:A:1402:NAG:H5	2.01	0.42
1:A:670:ILE:HA	1:A:695:TYR:O	2.20	0.42
1:A:758:SER:O	1:A:762:GLN:HG3	2.19	0.42
1:A:325:SER:HB3	1:A:540:ASN:O	2.19	0.42
1:A:325:SER:C	1:A:326:ILE:HG23	2.44	0.42
1:A:524:VAL:CG2	1:A:525:CYS:N	2.83	0.42
1:B:112:SER:O	1:B:113:LYS:HB3	2.20	0.42
1:C:332:ILE:N	1:C:332:ILE:CD1	2.73	0.42
1:A:502:GLY:HA3	2:D:354:GLY:O	2.20	0.42
1:B:748:GLU:CG	1:B:981:LEU:CD2	2.81	0.42
1:C:131:CYS:HB3	1:C:164:ASN:O	2.19	0.42
1:C:280:ASN:OD1	1:C:281:GLU:N	2.50	0.42
3:V:1:NAG:H3	3:V:1:NAG:H83	2.02	0.42
1:A:406:GLU:CG	1:A:418:ILE:HG13	2.50	0.42
1:A:933:LYS:HB2	1:A:933:LYS:HE3	1.86	0.42
1:A:973:ILE:HG23	1:A:992:GLN:NE2	2.35	0.42
1:B:653:ALA:CB	1:B:692:ILE:HG22	2.50	0.42
1:B:794:ILE:H	1:B:794:ILE:HG13	1.69	0.42
1:C:505:TYR:CD2	2:E:353:LYS:C	2.93	0.42
1:A:99:ASN:O	1:A:102:ARG:NE	2.35	0.41
1:A:328:ARG:CG	1:A:328:ARG:NH2	2.83	0.41
1:A:886:TRP:HH2	1:A:904:TYR:CD2	2.35	0.41
1:B:99:ASN:O	1:B:102:ARG:NE	2.35	0.41
1:B:322:PRO:HA	1:B:538:CYS:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:560:LEU:CD2	1:B:560:LEU:N	2.83	0.41
1:C:48:LEU:H	1:C:48:LEU:CD1	2.32	0.41
1:C:393:THR:H	1:C:517:LEU:HD22	1.85	0.41
1:C:524:VAL:CG2	1:C:525:CYS:N	2.83	0.41
1:B:310:LYS:CG	1:B:664:ILE:HD11	2.50	0.41
1:C:973:ILE:HG23	1:C:992:GLN:NE2	2.35	0.41
2:E:39:LEU:HD23	2:E:39:LEU:HA	1.93	0.41
3:d:2:NAG:H83	3:d:2:NAG:H3	2.02	0.41
1:A:964:LYS:HE3	1:C:570:ALA:HA	2.01	0.41
1:B:569:ILE:HG12	1:C:47:VAL:HG12	2.02	0.41
4:B:1409:NAG:O4	4:B:1410:NAG:O5	2.28	0.41
1:C:502:GLY:HA3	2:E:354:GLY:O	2.20	0.41
1:C:736:VAL:HG23	1:C:858:LEU:HD23	2.02	0.41
1:C:985:ASP:OD1	1:C:985:ASP:N	2.46	0.41
1:A:43:PHE:HA	1:C:563:GLN:CD	2.45	0.41
1:A:309:GLU:H	1:A:309:GLU:HG2	1.71	0.41
1:A:699:LEU:HD12	1:B:872:GLN:CD	2.45	0.41
1:C:193:VAL:HG23	1:C:223:LEU:CD2	2.51	0.41
1:C:959:LEU:HD23	1:C:959:LEU:HA	1.93	0.41
2:D:212:VAL:HG23	2:D:215:TYR:HB2	2.02	0.41
1:A:393:THR:H	1:A:517:LEU:HD22	1.85	0.41
1:A:770:ILE:HG21	1:A:770:ILE:HD13	1.76	0.41
1:B:390:LEU:O	1:B:525:CYS:HB3	2.19	0.41
1:B:523:THR:O	1:B:525:CYS:SG	2.79	0.41
1:C:617:CYS:HB2	1:C:649:CYS:HB2	1.87	0.41
2:D:411:SER:OG	2:D:543:ASP:OD1	2.38	0.41
1:B:388:ASN:CG	1:B:527:PRO:HD3	2.45	0.41
1:B:406:GLU:CG	1:B:418:ILE:HG13	2.50	0.41
1:B:516:GLU:OE2	1:C:200:TYR:CE2	2.73	0.41
1:B:557:LYS:HE3	1:B:575:ALA:CB	2.50	0.41
1:C:393:THR:O	1:C:523:THR:CG2	2.58	0.41
2:D:21:ILE:HD12	2:D:21:ILE:HA	1.97	0.41
1:A:193:VAL:HG23	1:A:223:LEU:CD2	2.51	0.41
1:A:226:LEU:HB3	1:A:227:VAL:HG23	2.03	0.41
1:A:280:ASN:OD1	1:A:281:GLU:N	2.51	0.41
1:B:45:SER:OG	1:B:281:GLU:HA	2.21	0.41
1:A:1051:SER:OG	1:A:1064:HIS:ND1	2.46	0.41
1:B:193:VAL:HG23	1:B:223:LEU:CD2	2.51	0.41
1:B:654:GLU:HG3	1:B:693:ILE:HG22	2.03	0.41
1:C:347:PHE:CD1	1:C:509:ARG:HD3	2.56	0.41
1:C:854:LYS:HE2	1:C:854:LYS:HB3	1.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:870:ILE:O	1:C:874:THR:HG23	2.21	0.41
2:E:21:ILE:HD12	2:E:21:ILE:HA	1.97	0.41
1:A:486:PHE:CE1	2:D:79:LEU:HD13	2.56	0.41
1:A:1123:SER:O	1:A:1123:SER:OG	2.39	0.41
1:B:532:ASN:OD1	1:B:532:ASN:N	2.53	0.41
1:B:959:LEU:HD12	1:B:959:LEU:HA	1.90	0.41
1:C:200:TYR:CE1	1:C:230:PRO:HB3	2.56	0.41
1:C:856:ASN:O	1:C:856:ASN:ND2	2.48	0.41
3:d:1:NAG:C3	3:d:2:NAG:N2	2.74	0.41
1:A:166:CYS:HB3	1:A:169:GLU:OE1	2.21	0.40
1:A:371:SER:C	1:A:373:SER:H	2.29	0.40
1:A:694:ALA:O	1:A:695:TYR:HB3	2.22	0.40
1:B:127:VAL:HG22	1:B:171:VAL:HG13	2.04	0.40
1:B:212:LEU:HD12	1:B:212:LEU:HA	1.78	0.40
1:B:226:LEU:HB3	1:B:227:VAL:HG23	2.03	0.40
1:B:310:LYS:CD	1:B:664:ILE:HD11	2.51	0.40
1:B:542:ASN:HA	1:B:546:LEU:O	2.21	0.40
1:C:542:ASN:HA	1:C:546:LEU:O	2.21	0.40
2:D:455:MET:HE3	2:D:455:MET:HB3	1.80	0.40
1:A:45:SER:O	1:A:47:VAL:N	2.54	0.40
1:A:45:SER:OG	1:A:281:GLU:HA	2.21	0.40
1:A:318:PHE:HE2	1:A:320:VAL:CG2	2.32	0.40
1:B:89:GLY:HA2	1:B:194:PHE:O	2.22	0.40
1:B:166:CYS:HB3	1:B:169:GLU:OE1	2.21	0.40
1:C:166:CYS:HB3	1:C:169:GLU:OE1	2.21	0.40
1:C:213:VAL:HG23	1:C:214:ARG:N	2.36	0.40
1:C:486:PHE:CE1	2:E:79:LEU:HD13	2.56	0.40
1:C:654:GLU:HG2	1:C:693:ILE:HG23	2.02	0.40
1:C:821:LEU:HD22	1:C:939:SER:HB3	2.03	0.40
2:D:366:MET:HE3	2:D:366:MET:HB2	2.01	0.40
1:A:200:TYR:CE1	1:A:230:PRO:HB3	2.56	0.40
1:A:347:PHE:CD1	1:A:509:ARG:HD3	2.56	0.40
1:A:708:SER:OG	1:A:711:SER:HB2	2.22	0.40
1:A:1105:THR:HG21	1:A:1110:TYR:CD1	2.57	0.40
1:B:213:VAL:HG23	1:B:214:ARG:N	2.36	0.40
1:B:227:VAL:CG1	1:B:228:ASP:N	2.84	0.40
1:B:309:GLU:H	1:B:309:GLU:HG2	1.71	0.40
1:B:1040:VAL:O	1:B:1041:ASP:HB2	2.21	0.40
1:C:46:SER:C	1:C:47:VAL:HG13	2.47	0.40
1:C:127:VAL:HG22	1:C:171:VAL:HG13	2.04	0.40
2:D:294:THR:HG23	2:D:365:THR:HA	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:200:TYR:CE1	1:B:230:PRO:HB3	2.56	0.40
1:B:600:PRO:HB3	1:B:674:TYR:HB2	2.04	0.40
1:B:692:ILE:HD13	1:B:692:ILE:HG21	1.93	0.40
1:C:45:SER:O	1:C:47:VAL:N	2.54	0.40
1:C:100:ILE:HG22	1:C:242:LEU:HD23	2.04	0.40
1:C:342:PHE:CB	3:U:1:NAG:H82	2.52	0.40
2:E:476:LYS:HB3	2:E:476:LYS:HE3	1.92	0.40
1:A:39:PRO:C	1:A:40:ASP:CG	2.90	0.40
1:A:227:VAL:CG1	1:A:228:ASP:N	2.84	0.40
1:A:334:ASN:O	1:A:362:VAL:HG21	2.21	0.40
1:A:486:PHE:HE1	2:D:79:LEU:HD21	1.77	0.40
1:A:879:ALA:O	1:A:883:THR:HB	2.22	0.40
1:B:329:PHE:HB3	1:B:330:PRO:CD	2.51	0.40
1:B:347:PHE:CD1	1:B:509:ARG:HD3	2.56	0.40
1:B:369:TYR:CZ	1:B:384:PRO:HB2	2.57	0.40
1:B:524:VAL:CG2	1:B:525:CYS:N	2.83	0.40
2:E:411:SER:OG	2:E:543:ASP:OD1	2.38	0.40
2:E:424:LEU:HD23	2:E:424:LEU:HA	1.87	0.40

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

All (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
1	C	518	LEU
1	C	691	SER
1	C	814	LYS
1	A	41	LYS
1	A	46	SER
1	A	339	GLY
1	C	41	LYS
1	C	46	SER
1	C	324	GLU
1	C	339	GLY
1	C	528	LYS
1	C	529	LYS
1	C	697	MET
1	C	810	SER
2	D	343	VAL
2	E	343	VAL
1	A	43	PHE
1	A	336	CYS
1	C	43	PHE
1	C	331	ASN
1	C	336	CYS
1	C	522	ALA
1	C	527	PRO
2	D	423	LEU
2	E	423	LEU
1	A	44	ARG
1	A	349	SER
1	C	44	ARG
1	C	349	SER
1	C	520	ALA
1	C	813	SER
1	A	40	ASP
1	A	42	VAL
1	A	47	VAL
1	C	40	ASP
1	C	42	VAL
1	C	47	VAL

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Mol	Chain	Res	Type
1	C	812	PRO
1	C	811	LYS
1	A	326	ILE

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
3	NAG	J	2	3	14,14,15	0.42	0	17,19,21	1.49	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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
3	NAG	d	2	3	14,14,15	0.31	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	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
3	NAG	N	2	3	-	3/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
3	NAG	f	2	3	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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

All (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
3	P	1	NAG	C1-O5-C5	3.39	116.73	112.19
3	J	2	NAG	C1-C2-N2	2.64	114.59	110.43
3	I	2	NAG	C1-C2-N2	2.60	114.53	110.43
3	h	2	NAG	C1-O5-C5	2.53	115.58	112.19
3	c	2	NAG	C1-O5-C5	2.50	115.54	112.19
3	Z	2	NAG	C1-C2-N2	2.44	114.27	110.43
3	R	1	NAG	O4-C4-C3	-2.33	104.89	110.38
3	Q	1	NAG	C1-O5-C5	2.31	115.29	112.19
3	W	1	NAG	C1-O5-C5	2.29	115.26	112.19
3	V	1	NAG	C1-C2-N2	2.16	113.83	110.43
3	L	1	NAG	C1-O5-C5	2.12	115.03	112.19
3	J	2	NAG	C1-O5-C5	2.11	115.02	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	R	2	NAG	C1-O5-C5	2.08	114.97	112.19
3	f	2	NAG	C1-O5-C5	2.07	114.97	112.19
3	k	2	NAG	C1-O5-C5	2.07	114.95	112.19
3	Y	2	NAG	C1-C2-N2	2.05	113.66	110.43
3	H	1	NAG	C1-O5-C5	2.02	114.89	112.19

There are no chirality outliers.

All (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
3	i	1	NAG	C8-C7-N2-C2
3	i	1	NAG	O7-C7-N2-C2
3	i	2	NAG	C3-C2-N2-C7
3	i	2	NAG	C8-C7-N2-C2
3	i	2	NAG	O7-C7-N2-C2
3	V	2	NAG	O5-C5-C6-O6
3	X	1	NAG	O5-C5-C6-O6
3	W	2	NAG	O5-C5-C6-O6
3	F	2	NAG	O5-C5-C6-O6
3	K	1	NAG	O5-C5-C6-O6
3	M	2	NAG	O5-C5-C6-O6
3	R	1	NAG	O5-C5-C6-O6
3	T	2	NAG	O5-C5-C6-O6
3	f	2	NAG	O5-C5-C6-O6
3	k	2	NAG	O5-C5-C6-O6
3	b	1	NAG	O5-C5-C6-O6
3	g	1	NAG	O5-C5-C6-O6
3	h	2	NAG	O5-C5-C6-O6
3	c	2	NAG	O5-C5-C6-O6
3	F	2	NAG	C4-C5-C6-O6
3	M	2	NAG	C4-C5-C6-O6
3	R	1	NAG	C4-C5-C6-O6
3	T	2	NAG	C4-C5-C6-O6
3	W	1	NAG	O5-C5-C6-O6
3	R	2	NAG	O5-C5-C6-O6
3	c	1	NAG	O5-C5-C6-O6
3	h	1	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	K	1	NAG	C4-C5-C6-O6
3	W	1	NAG	C4-C5-C6-O6
3	X	1	NAG	C4-C5-C6-O6
3	c	2	NAG	C4-C5-C6-O6
3	h	2	NAG	C4-C5-C6-O6
3	S	1	NAG	C4-C5-C6-O6
3	W	2	NAG	C4-C5-C6-O6
3	Y	2	NAG	O5-C5-C6-O6
3	V	2	NAG	C4-C5-C6-O6
3	R	2	NAG	C4-C5-C6-O6
3	b	2	NAG	C4-C5-C6-O6
3	g	2	NAG	C4-C5-C6-O6
3	S	2	NAG	O5-C5-C6-O6
3	Y	2	NAG	C4-C5-C6-O6
3	f	2	NAG	C4-C5-C6-O6
3	k	2	NAG	C4-C5-C6-O6
3	b	1	NAG	C4-C5-C6-O6
3	g	1	NAG	C4-C5-C6-O6
3	V	1	NAG	O5-C5-C6-O6
3	b	2	NAG	O5-C5-C6-O6
3	g	2	NAG	O5-C5-C6-O6
3	V	1	NAG	C4-C5-C6-O6
3	I	2	NAG	C8-C7-N2-C2
3	I	2	NAG	O7-C7-N2-C2
3	J	2	NAG	C8-C7-N2-C2
3	J	2	NAG	O7-C7-N2-C2
3	Q	2	NAG	C8-C7-N2-C2
3	Q	2	NAG	O7-C7-N2-C2
3	V	1	NAG	C8-C7-N2-C2
3	V	1	NAG	O7-C7-N2-C2
3	Y	2	NAG	C8-C7-N2-C2
3	Y	2	NAG	O7-C7-N2-C2
3	Z	2	NAG	C8-C7-N2-C2
3	Z	2	NAG	O7-C7-N2-C2
3	c	1	NAG	C4-C5-C6-O6
3	h	1	NAG	C4-C5-C6-O6
3	I	1	NAG	C4-C5-C6-O6
3	S	2	NAG	C4-C5-C6-O6
3	J	1	NAG	C4-C5-C6-O6
3	S	1	NAG	O5-C5-C6-O6
3	I	1	NAG	O5-C5-C6-O6
3	J	1	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	K	2	NAG	C4-C5-C6-O6
3	K	2	NAG	O5-C5-C6-O6
3	Z	1	NAG	O5-C5-C6-O6
3	Z	1	NAG	C4-C5-C6-O6
3	L	1	NAG	C4-C5-C6-O6
3	L	1	NAG	O5-C5-C6-O6
3	Z	2	NAG	O5-C5-C6-O6
3	Q	2	NAG	O5-C5-C6-O6
3	V	1	NAG	C1-C2-N2-C7
3	T	1	NAG	O5-C5-C6-O6
3	F	1	NAG	O5-C5-C6-O6
3	M	1	NAG	O5-C5-C6-O6
3	Q	1	NAG	C4-C5-C6-O6
3	H	2	NAG	C4-C5-C6-O6
3	a	2	NAG	C4-C5-C6-O6
3	H	2	NAG	O5-C5-C6-O6
3	Y	1	NAG	C4-C5-C6-O6
3	K	2	NAG	C3-C2-N2-C7
3	P	1	NAG	C3-C2-N2-C7
3	R	2	NAG	C3-C2-N2-C7
3	X	2	NAG	C3-C2-N2-C7
3	Z	2	NAG	C3-C2-N2-C7
3	a	2	NAG	O5-C5-C6-O6
3	O	2	NAG	C4-C5-C6-O6
3	J	2	NAG	C4-C5-C6-O6
3	Y	1	NAG	O5-C5-C6-O6
3	J	2	NAG	O5-C5-C6-O6
3	I	2	NAG	C1-C2-N2-C7
3	J	2	NAG	C1-C2-N2-C7
3	K	2	NAG	C1-C2-N2-C7
3	X	2	NAG	C1-C2-N2-C7
3	Y	2	NAG	C1-C2-N2-C7
3	Z	2	NAG	C1-C2-N2-C7
3	N	2	NAG	C4-C5-C6-O6
3	G	2	NAG	C3-C2-N2-C7
3	I	2	NAG	C3-C2-N2-C7
3	J	2	NAG	C3-C2-N2-C7
3	N	2	NAG	C3-C2-N2-C7
3	U	2	NAG	C3-C2-N2-C7
3	V	1	NAG	C3-C2-N2-C7
3	Y	2	NAG	C3-C2-N2-C7
3	U	2	NAG	C4-C5-C6-O6

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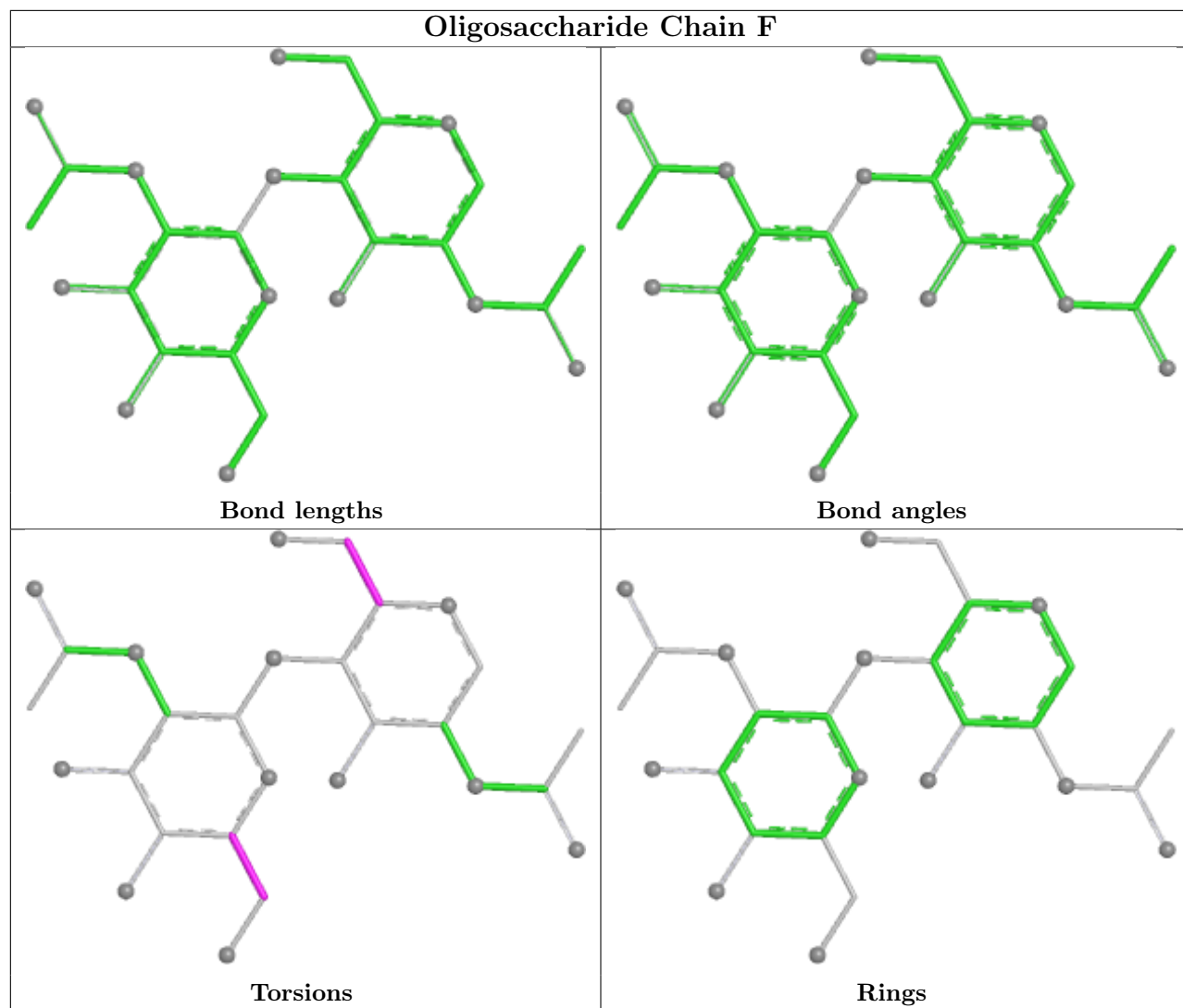
Mol	Chain	Res	Type	Atoms
3	Q	1	NAG	O5-C5-C6-O6
3	G	2	NAG	C4-C5-C6-O6
3	N	2	NAG	O5-C5-C6-O6
3	U	2	NAG	O5-C5-C6-O6
3	G	2	NAG	O5-C5-C6-O6

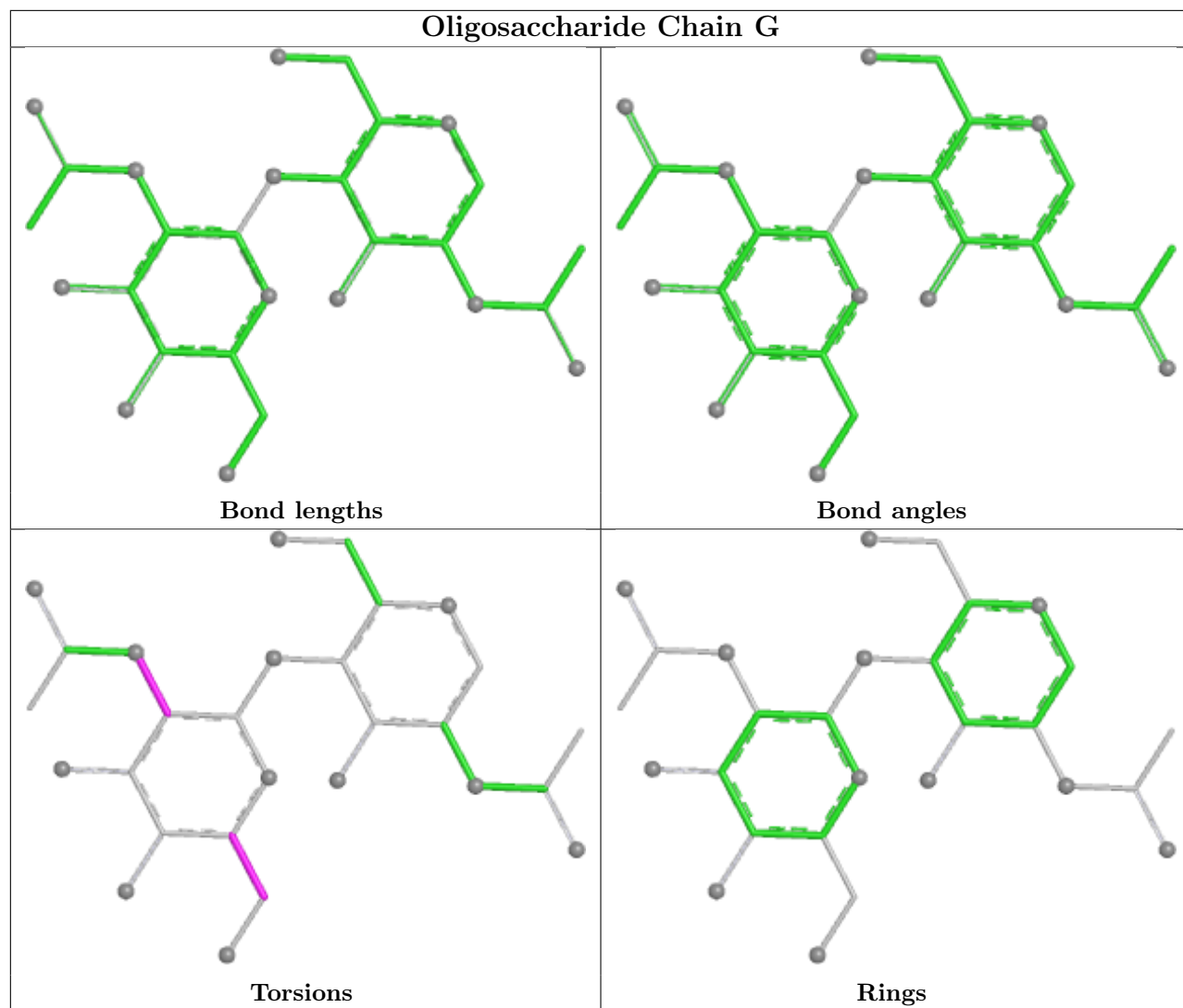
There are no ring outliers.

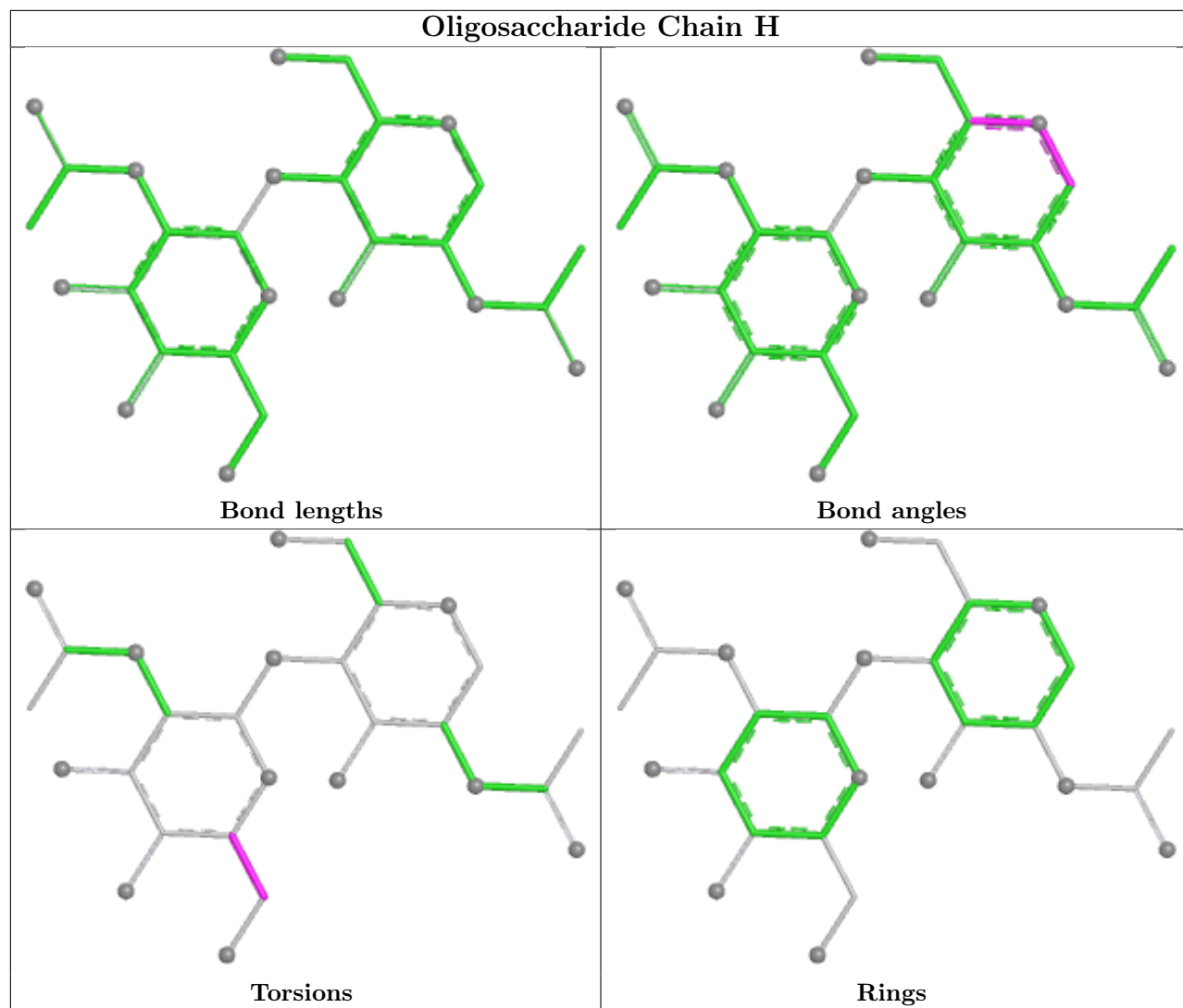
19 monomers are involved in 30 short contacts:

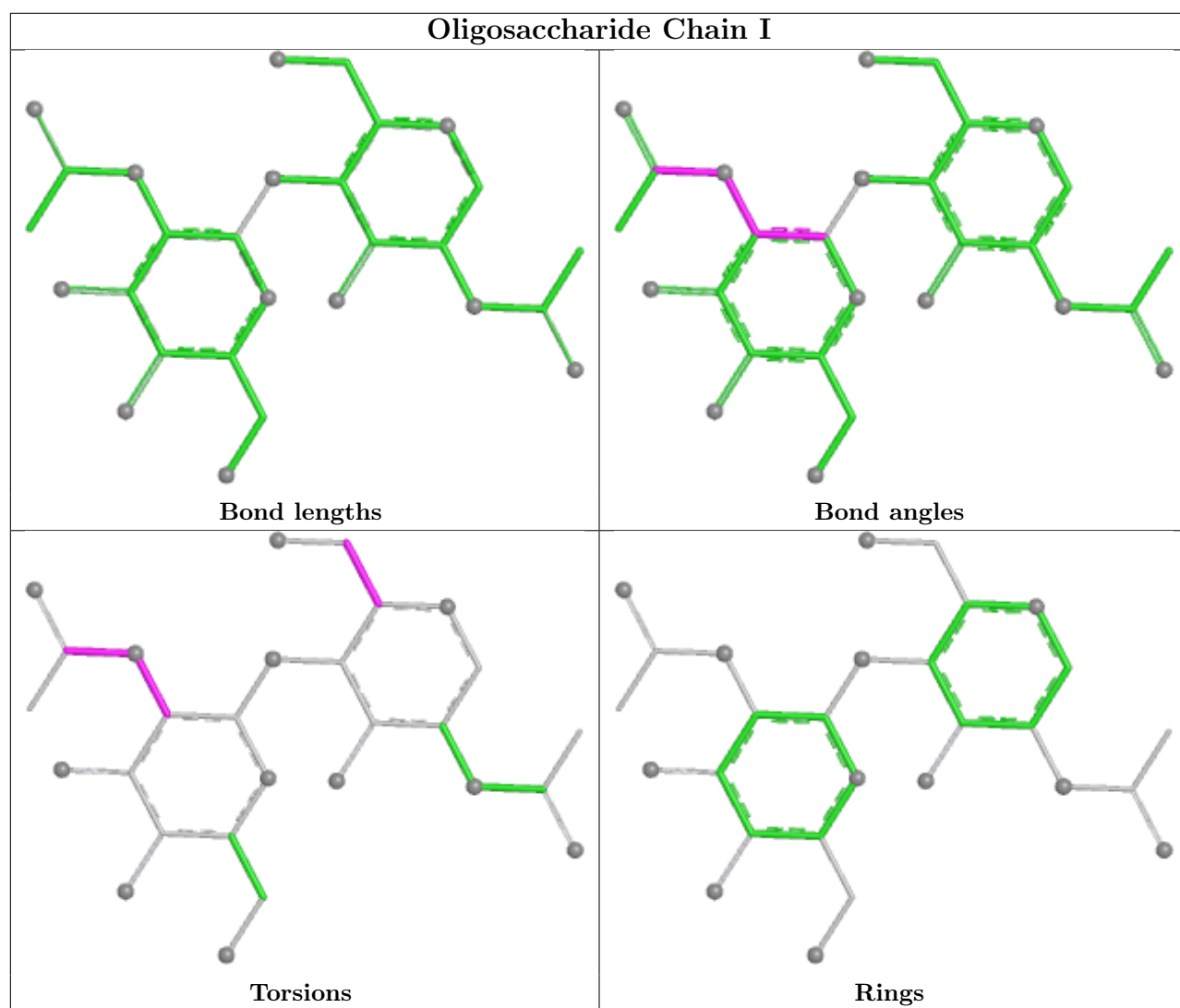
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	U	2	NAG	2	0
3	N	2	NAG	2	0
3	G	1	NAG	3	0
3	J	2	NAG	1	0
3	I	2	NAG	1	0
3	G	2	NAG	2	0
3	M	1	NAG	2	0
3	U	1	NAG	4	0
3	V	1	NAG	1	0
3	R	1	NAG	1	0
3	d	1	NAG	4	0
3	i	1	NAG	4	0
3	R	2	NAG	1	0
3	i	2	NAG	5	0
3	Z	1	NAG	1	0
3	Z	2	NAG	1	0
3	Y	2	NAG	1	0
3	d	2	NAG	6	0
3	N	1	NAG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

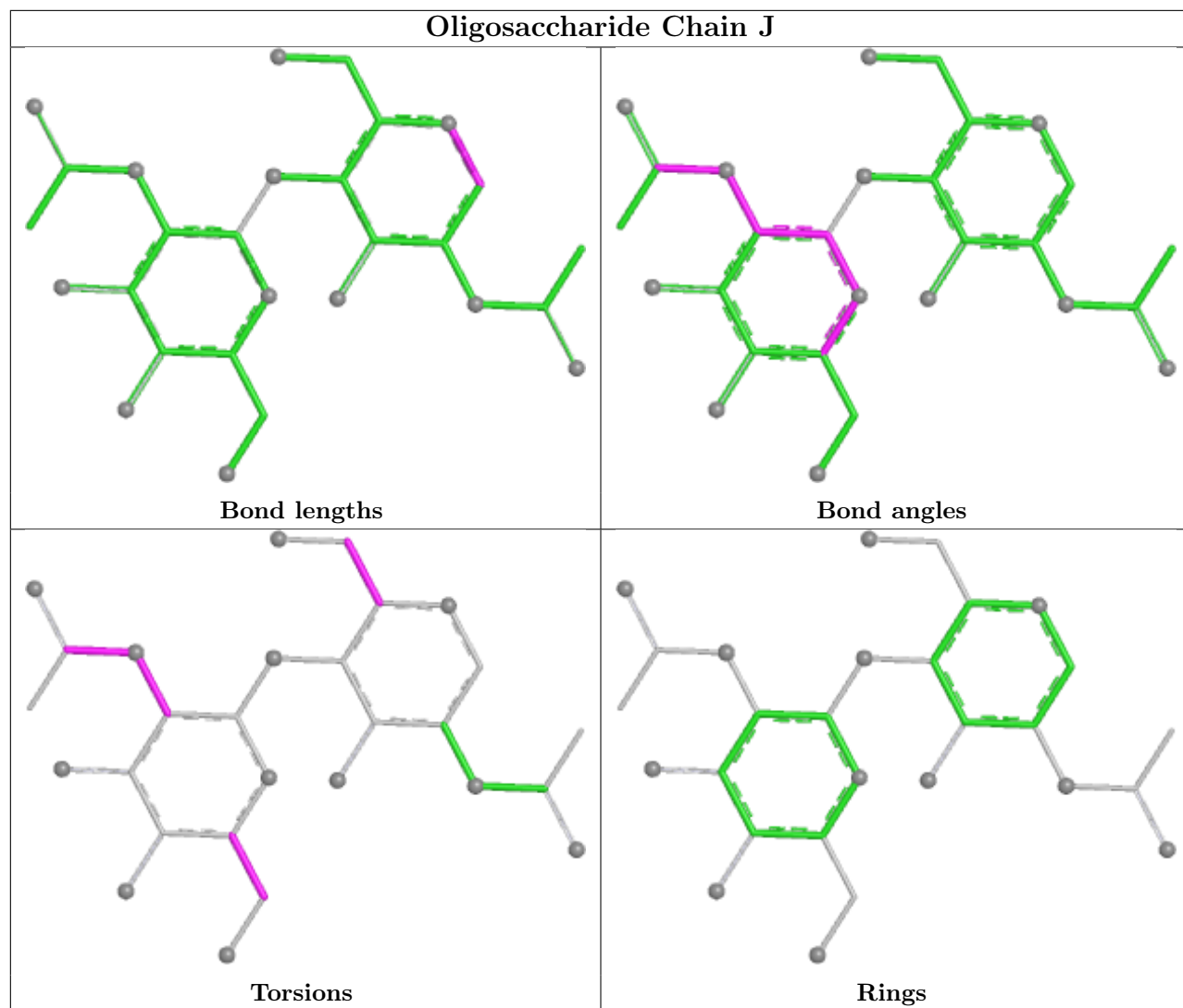
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

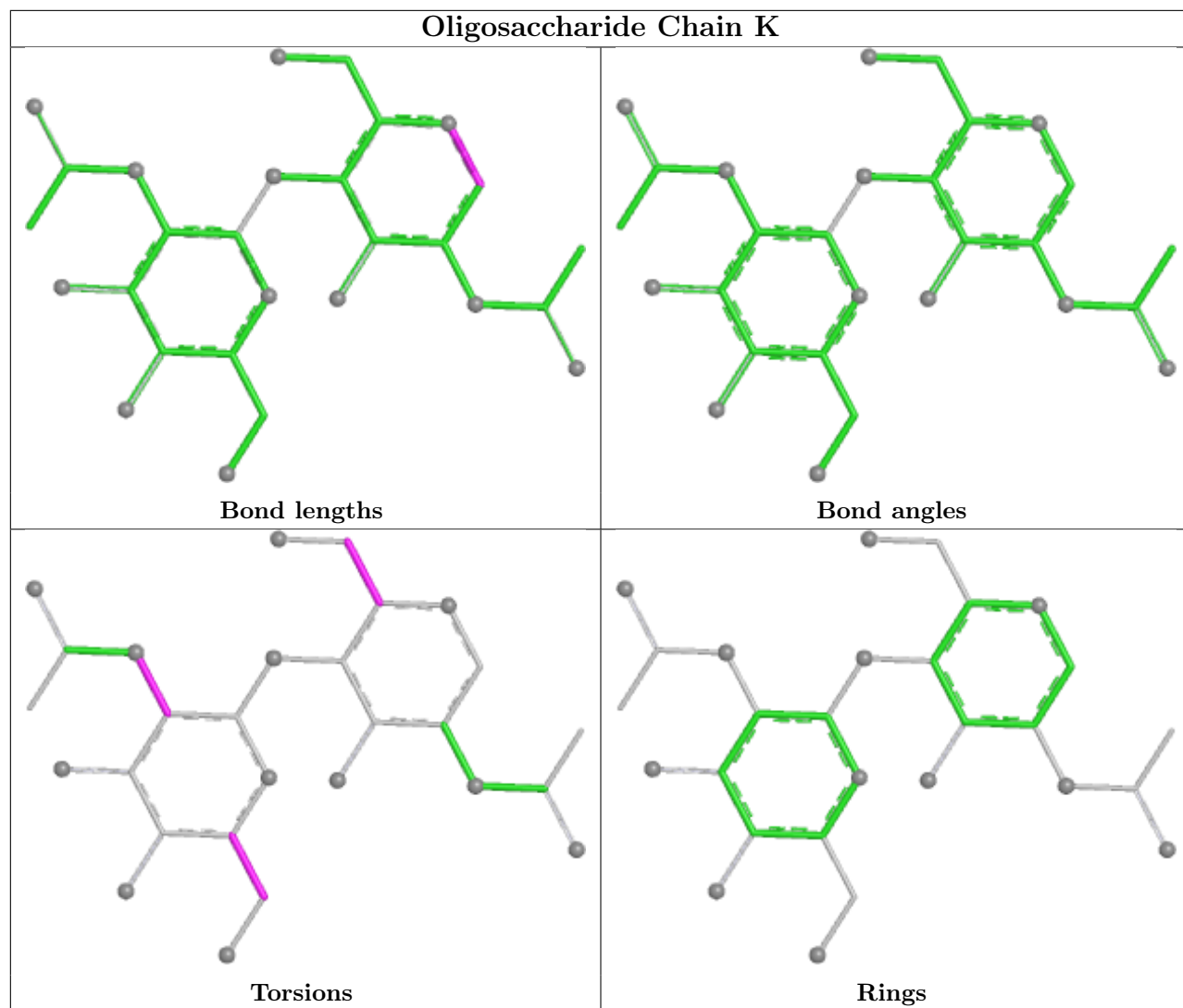


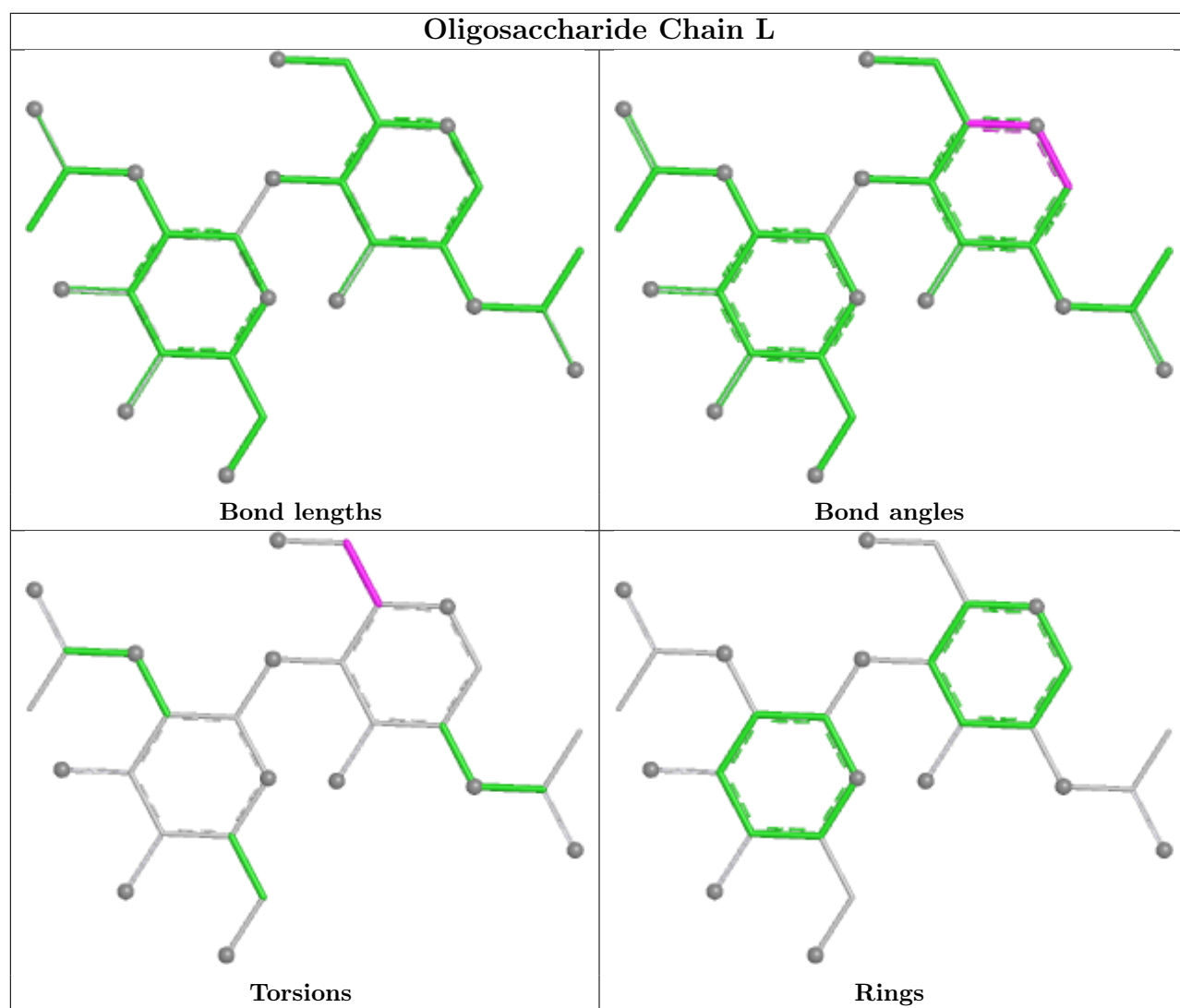


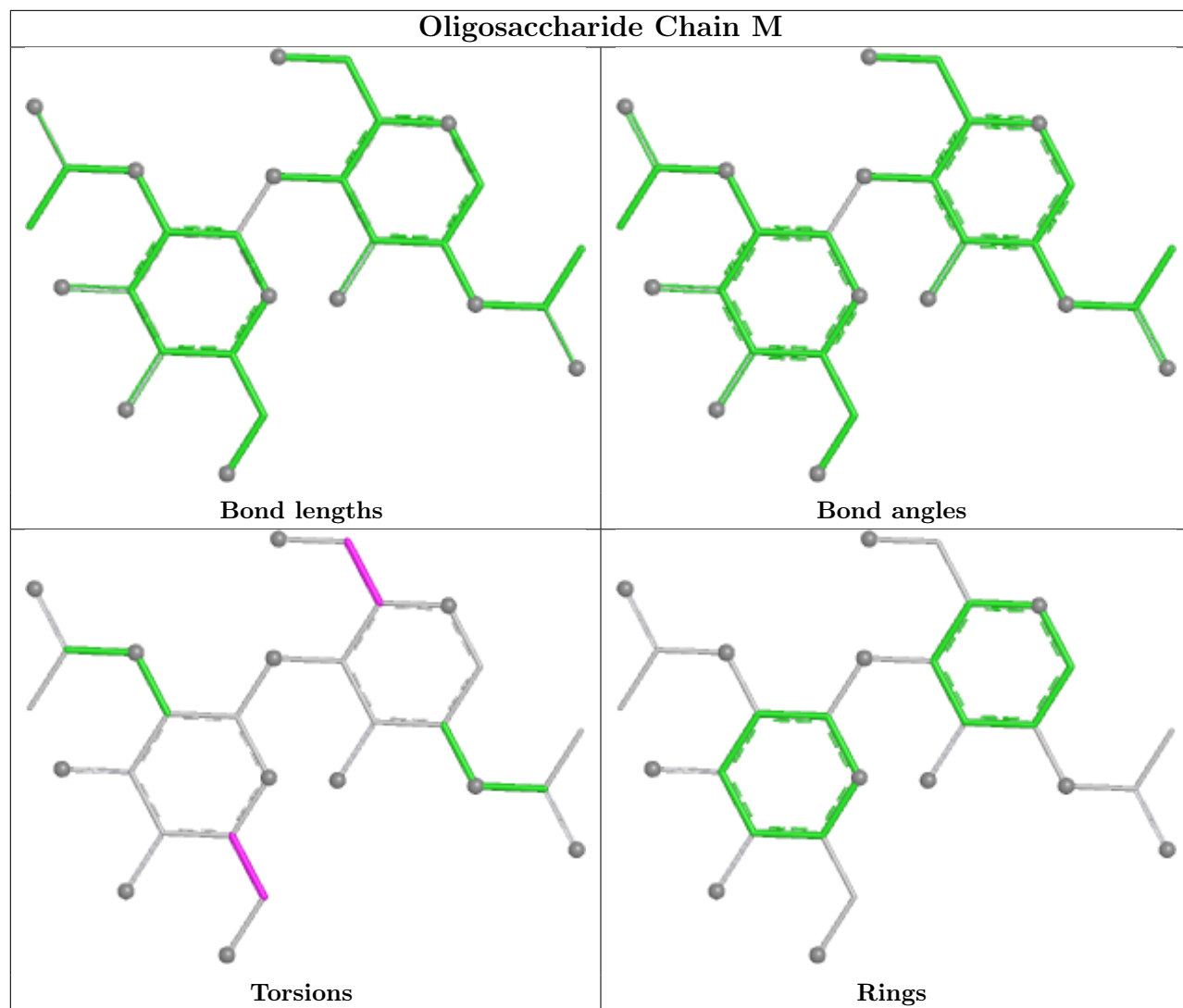


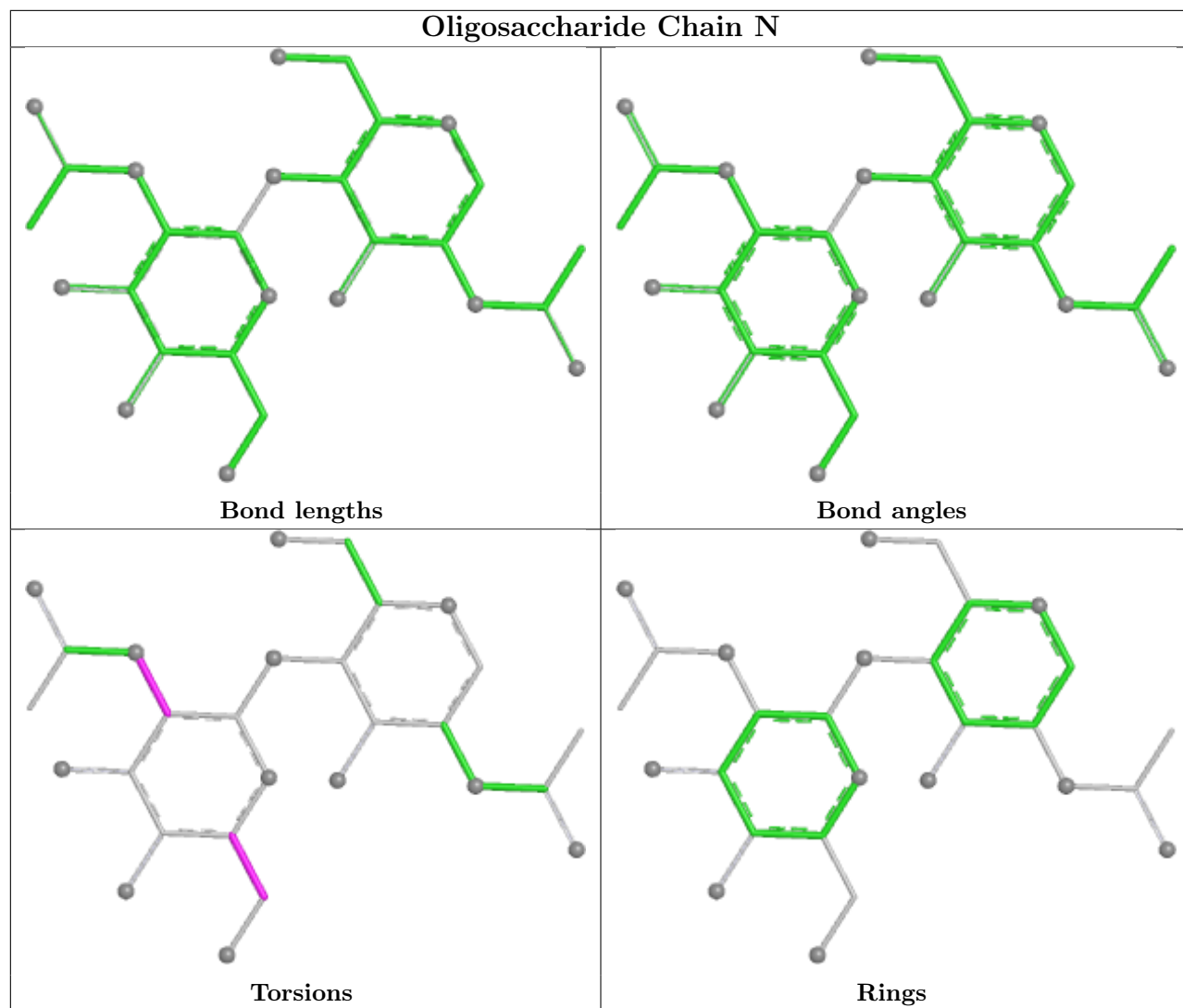


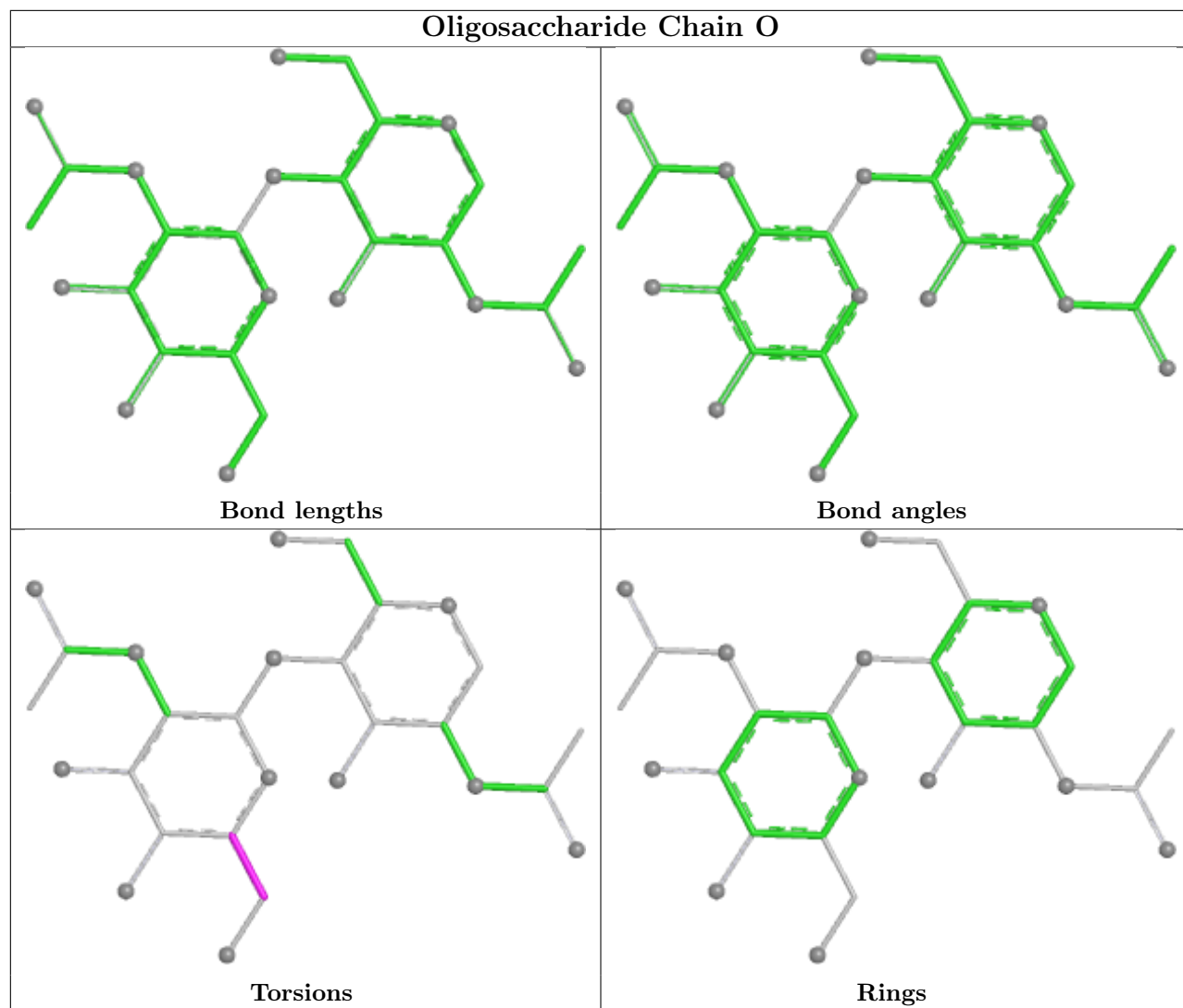


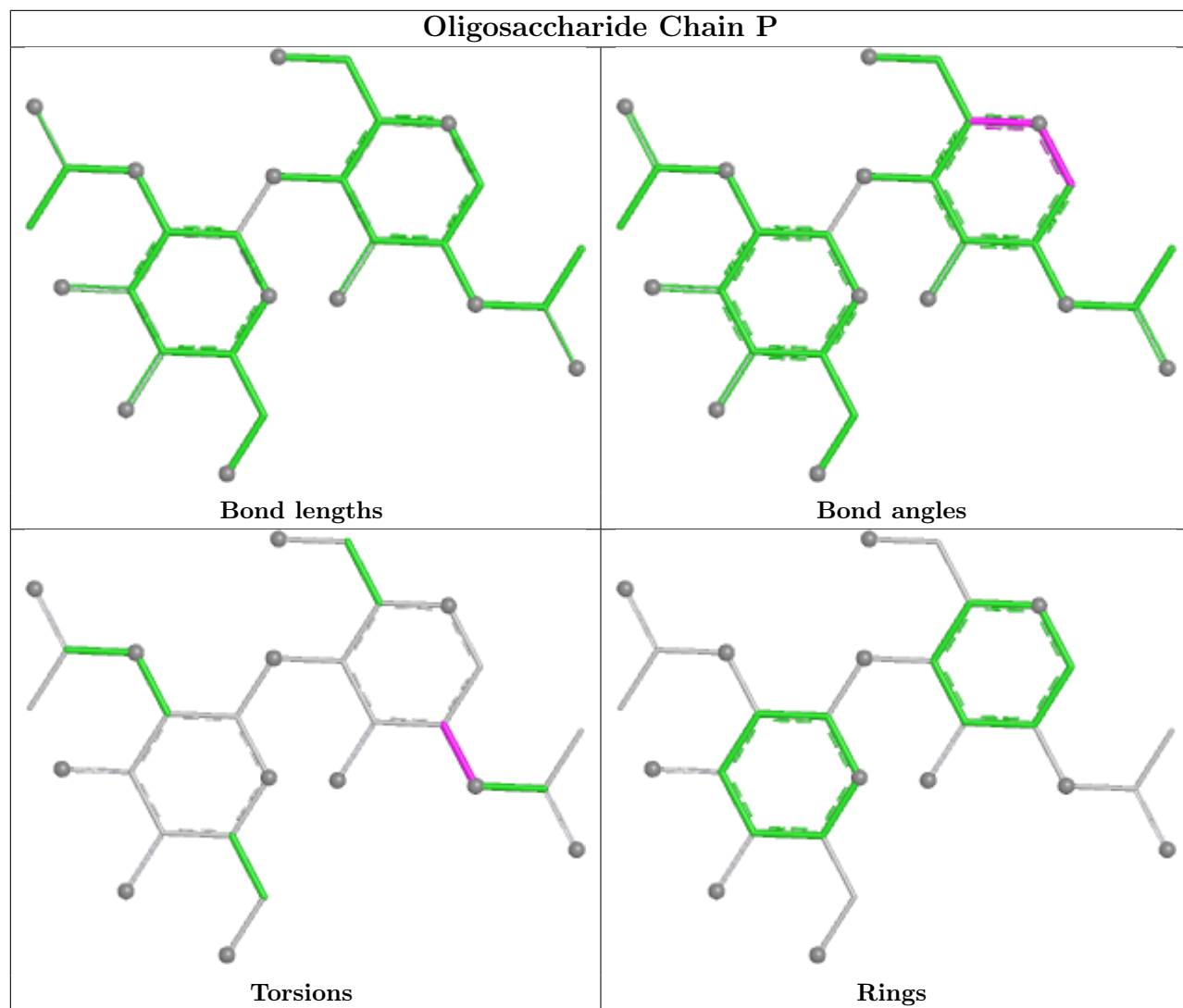


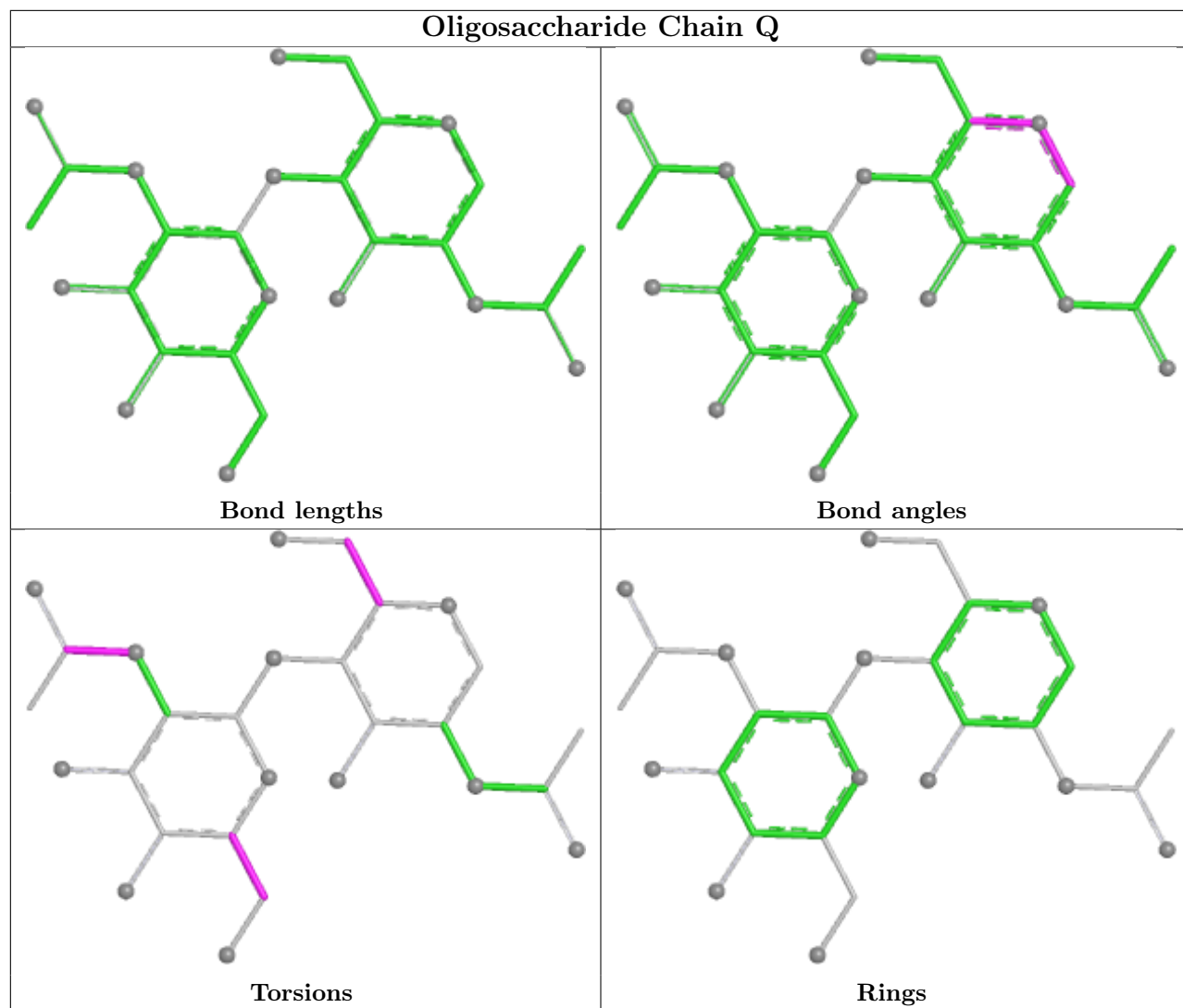


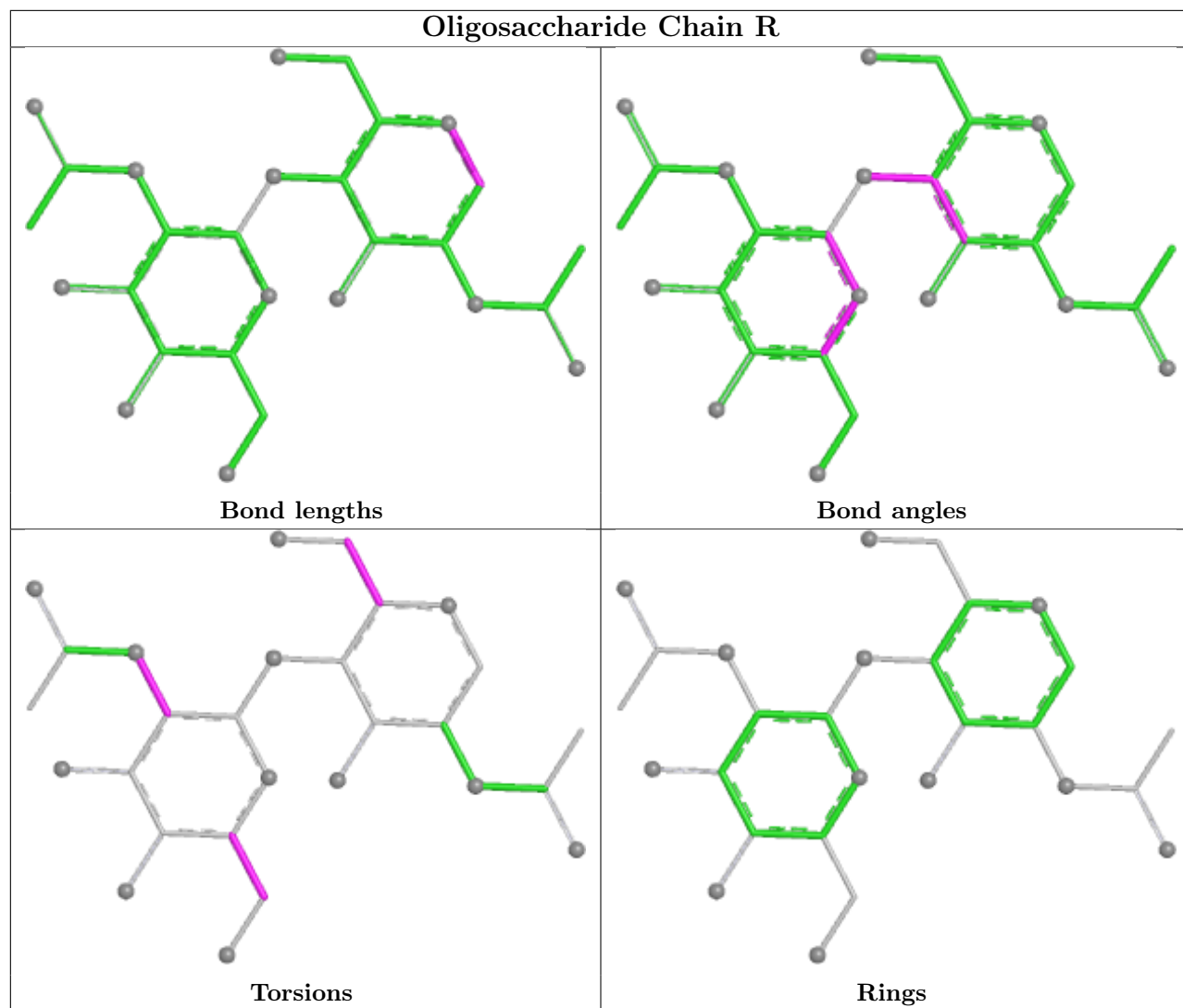


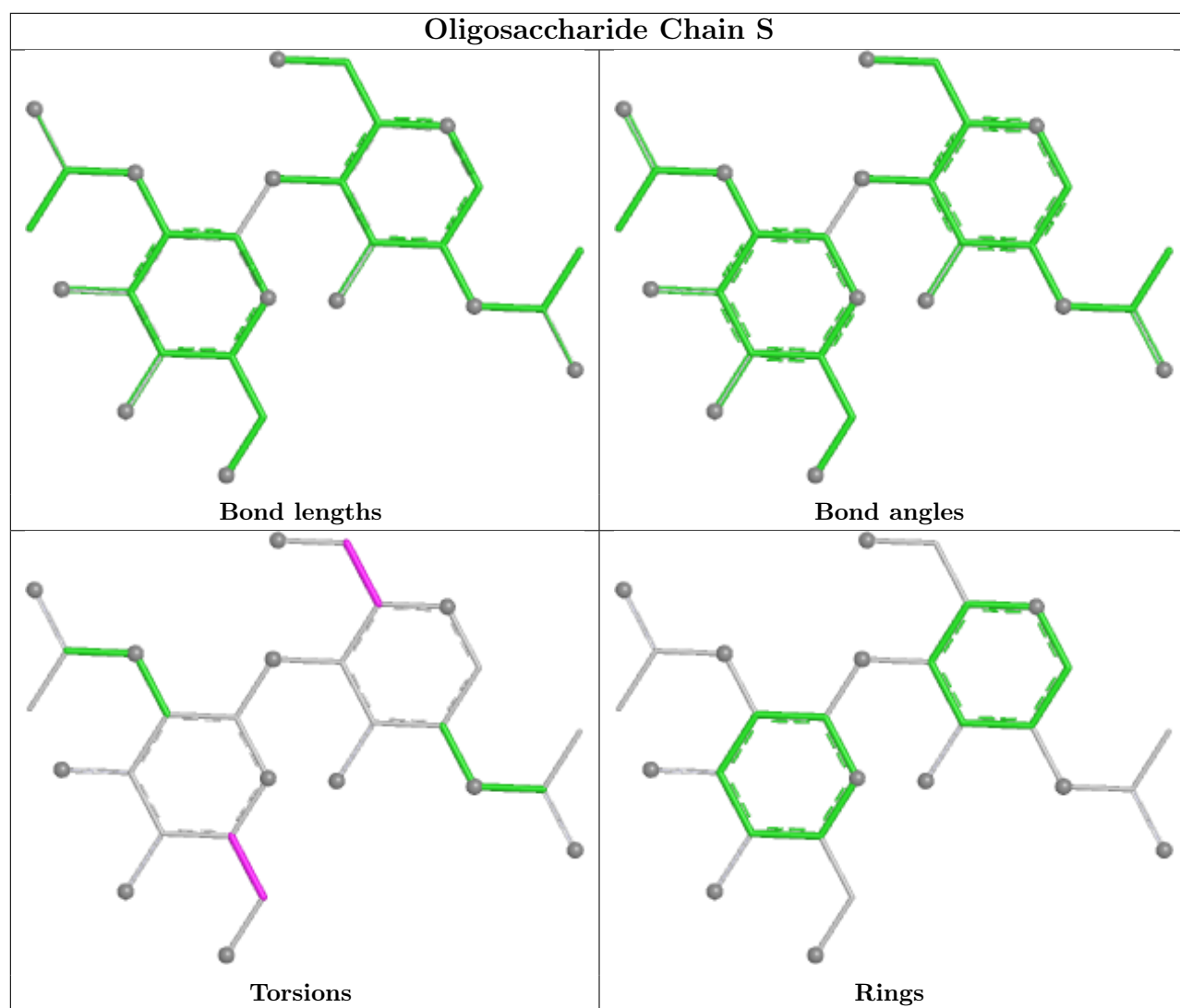


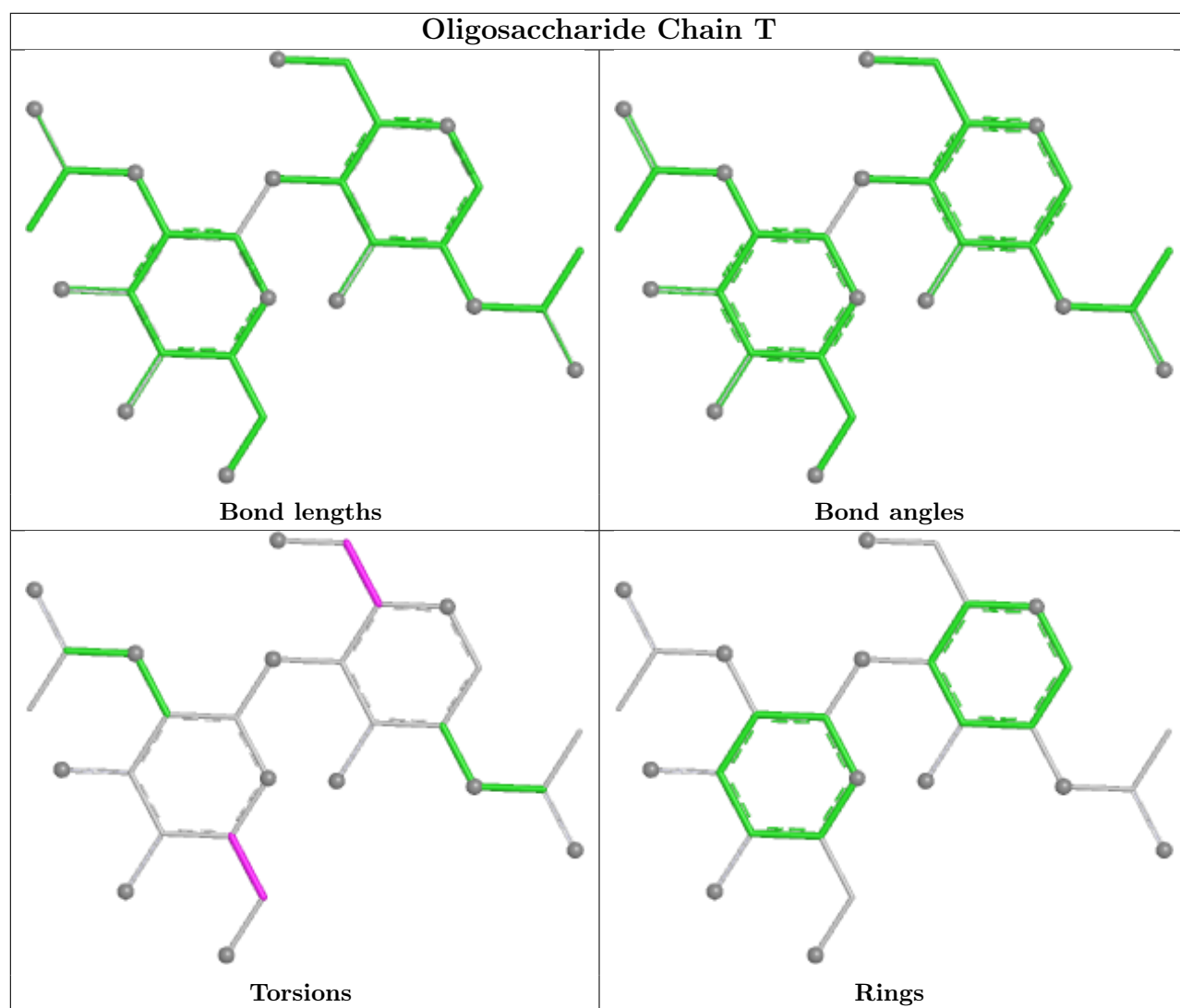


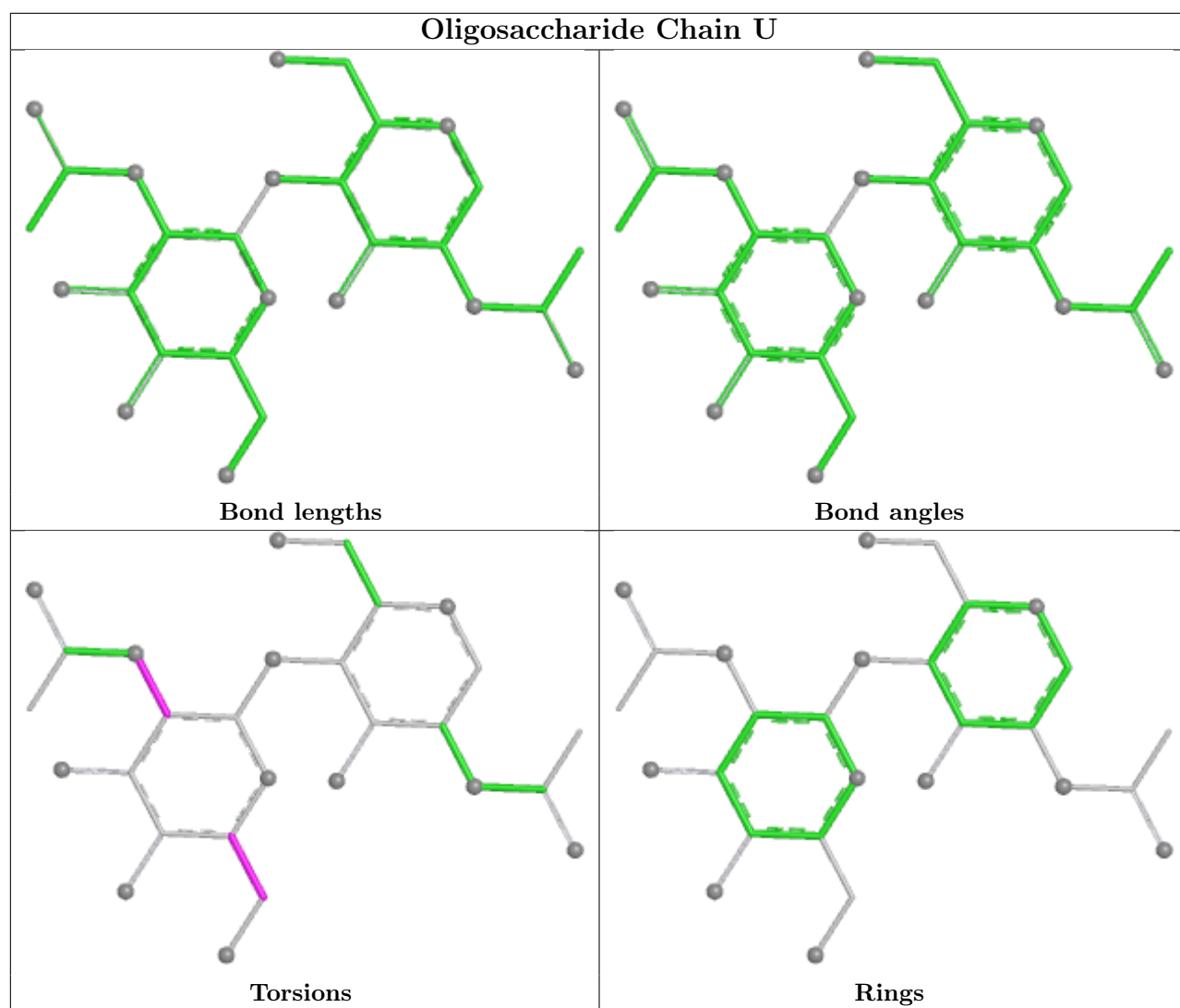


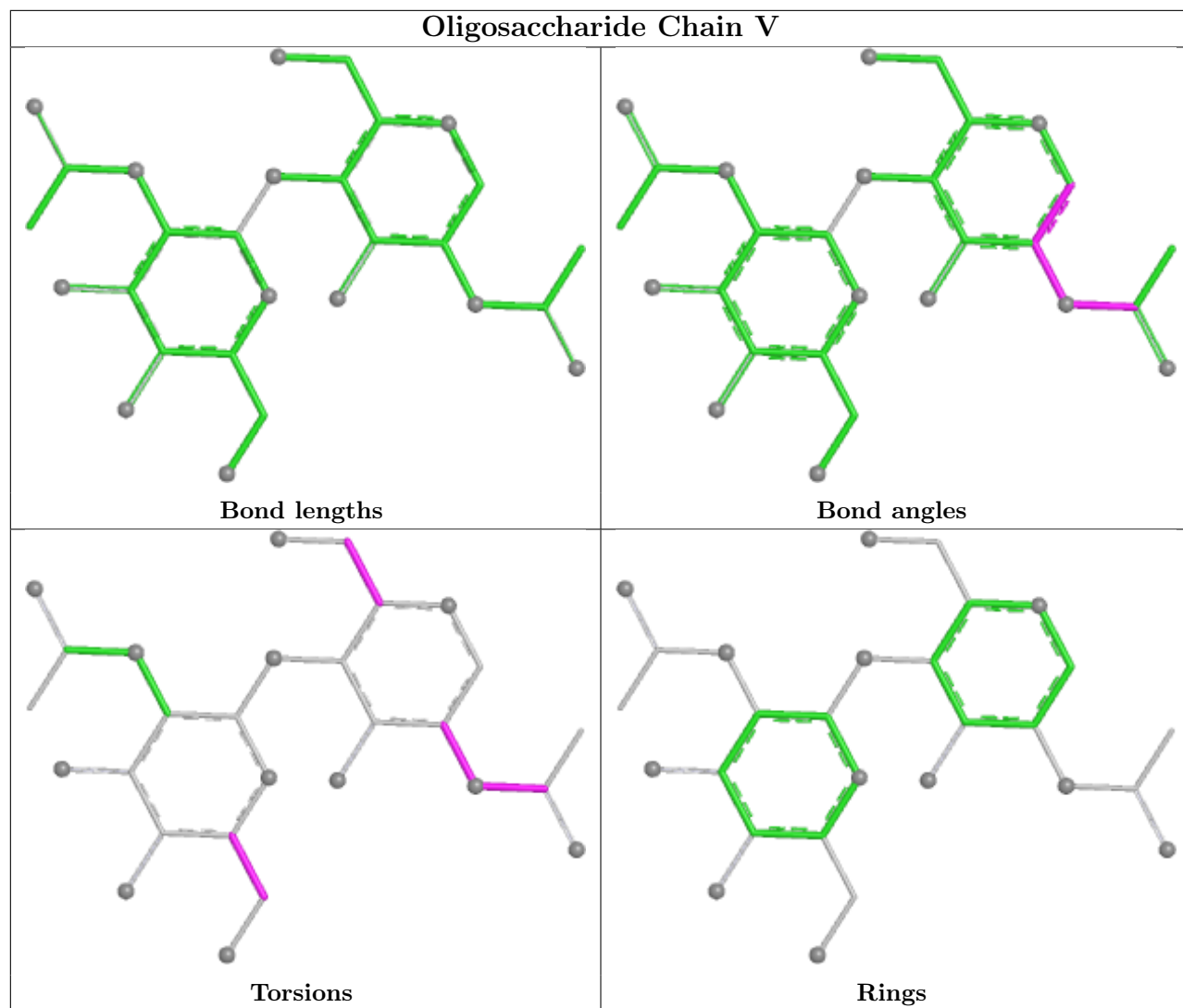


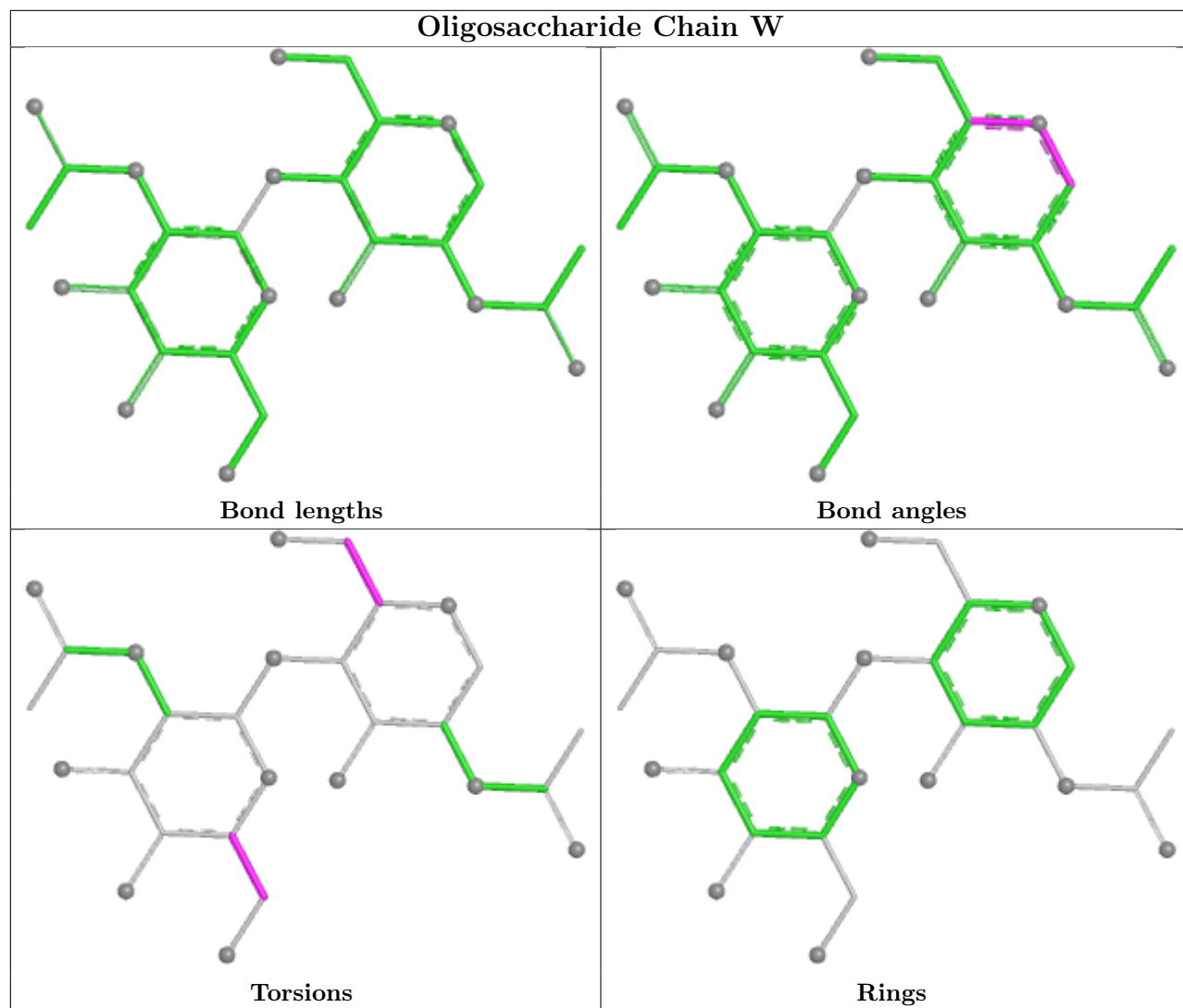


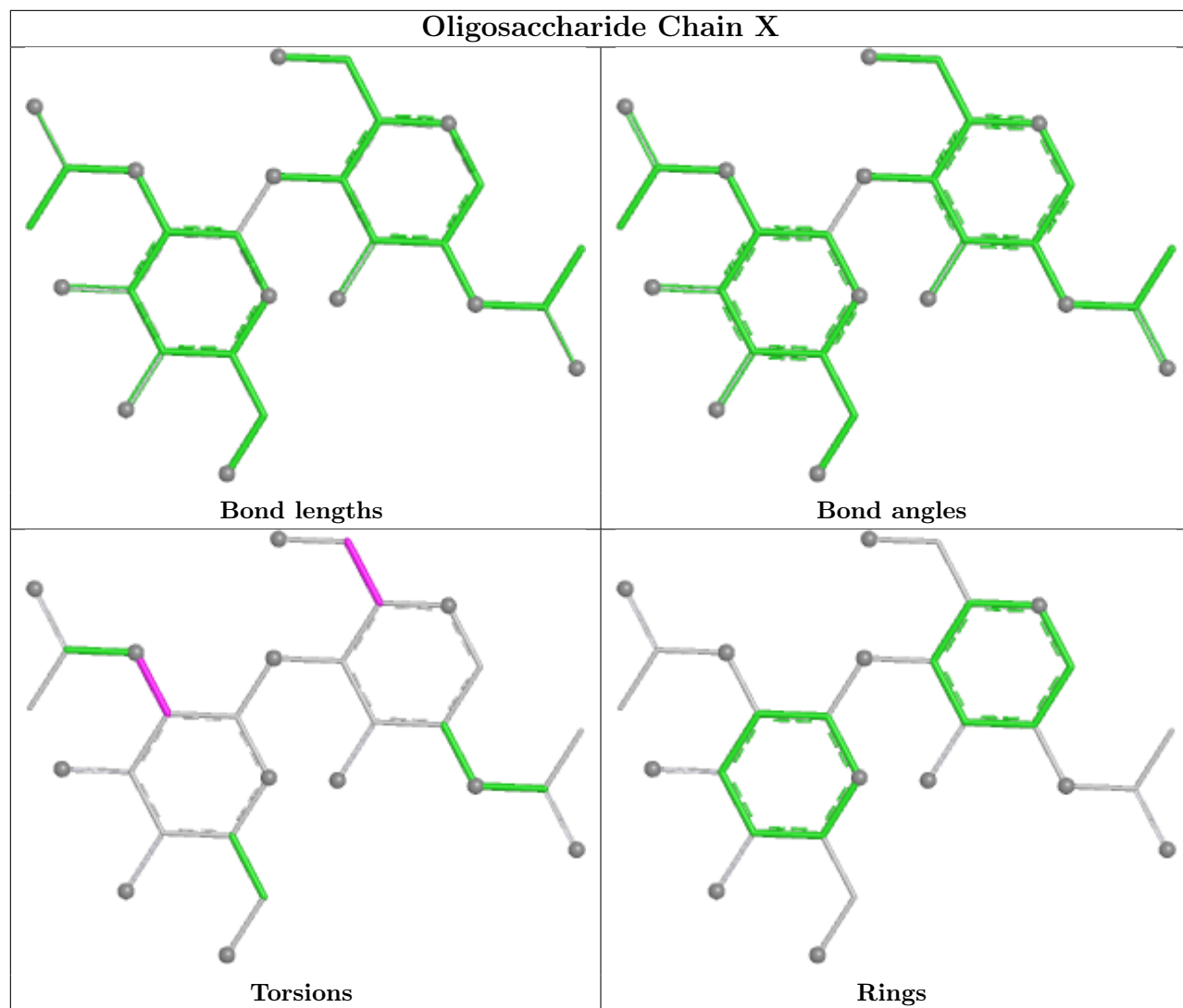


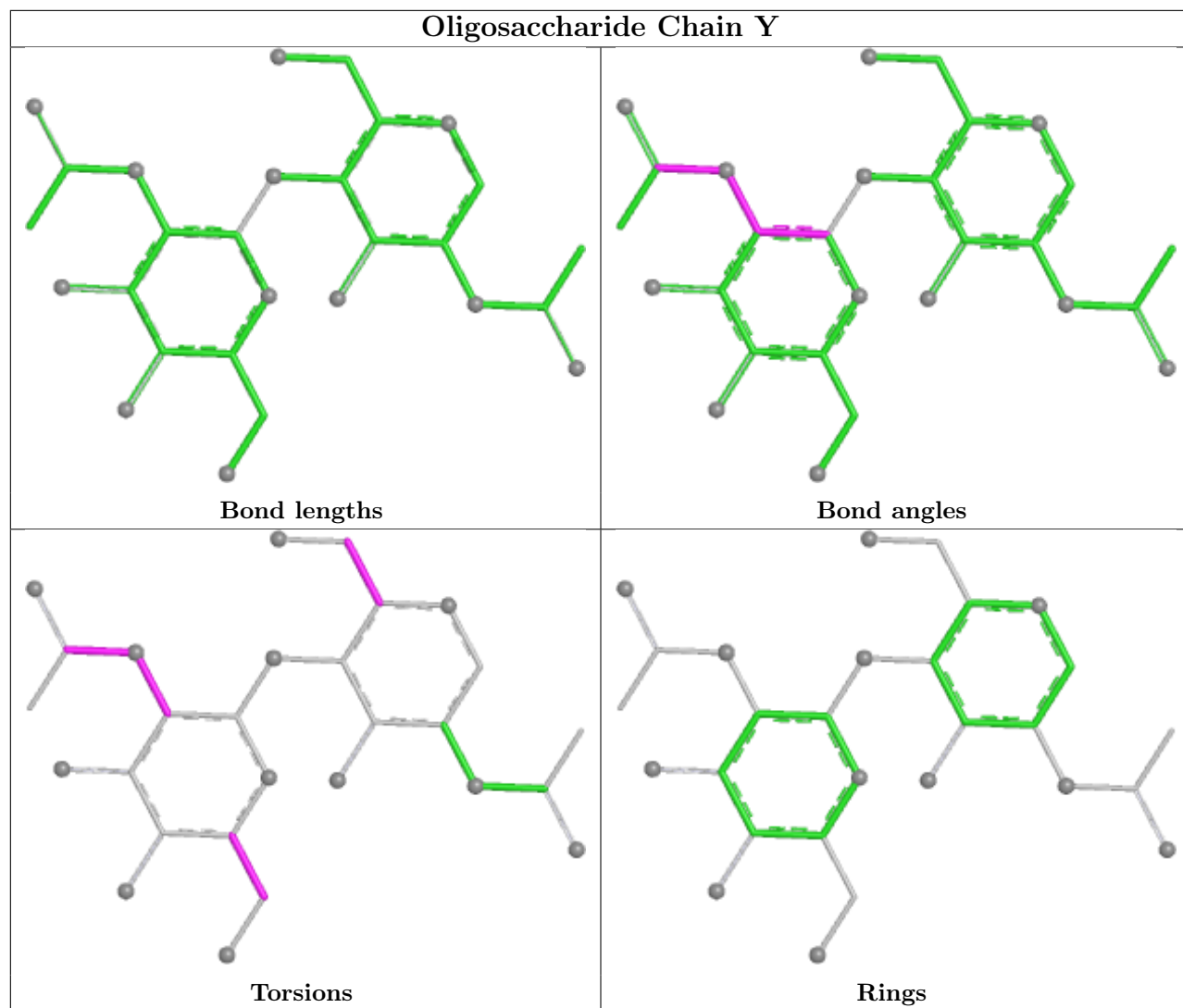


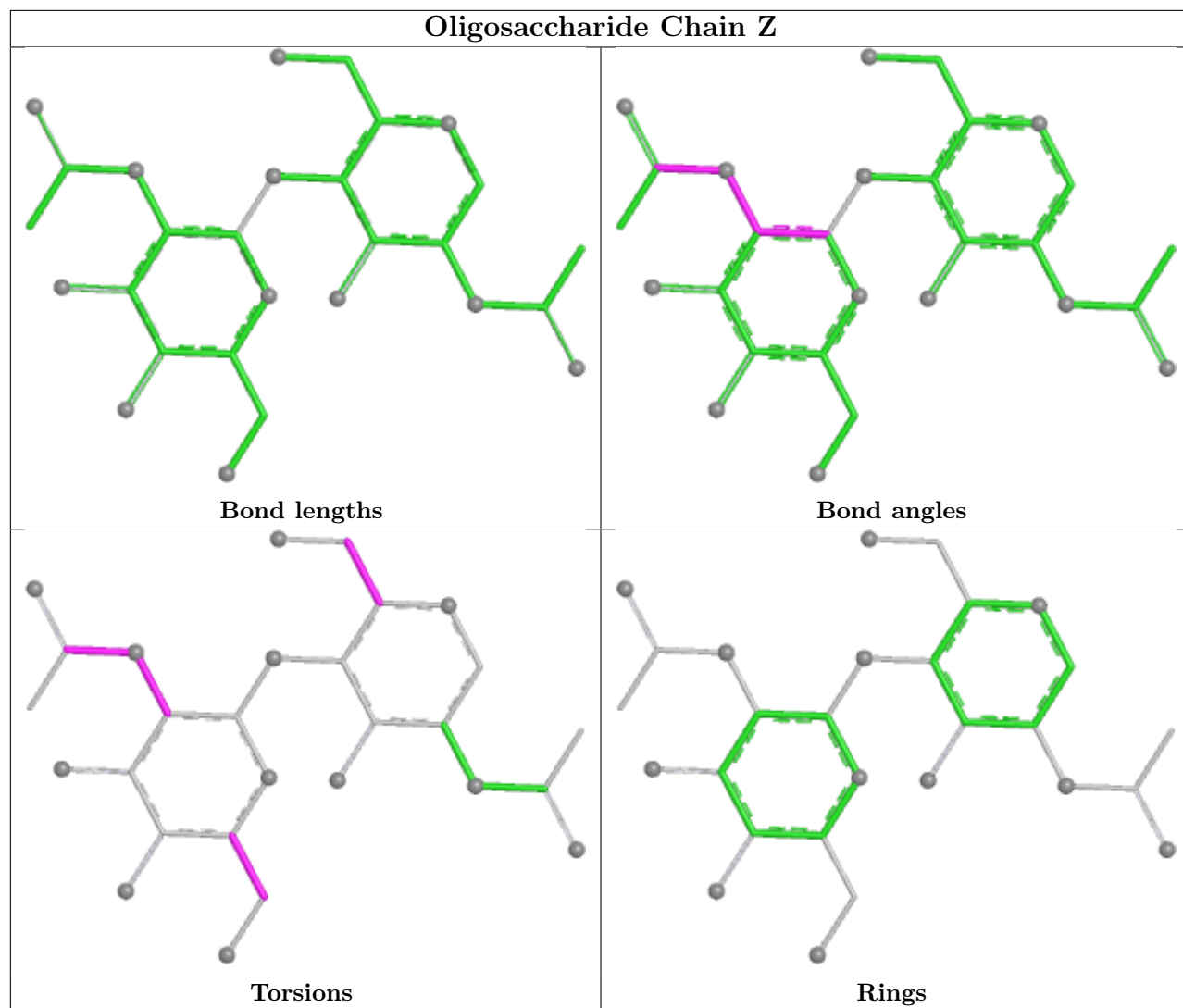


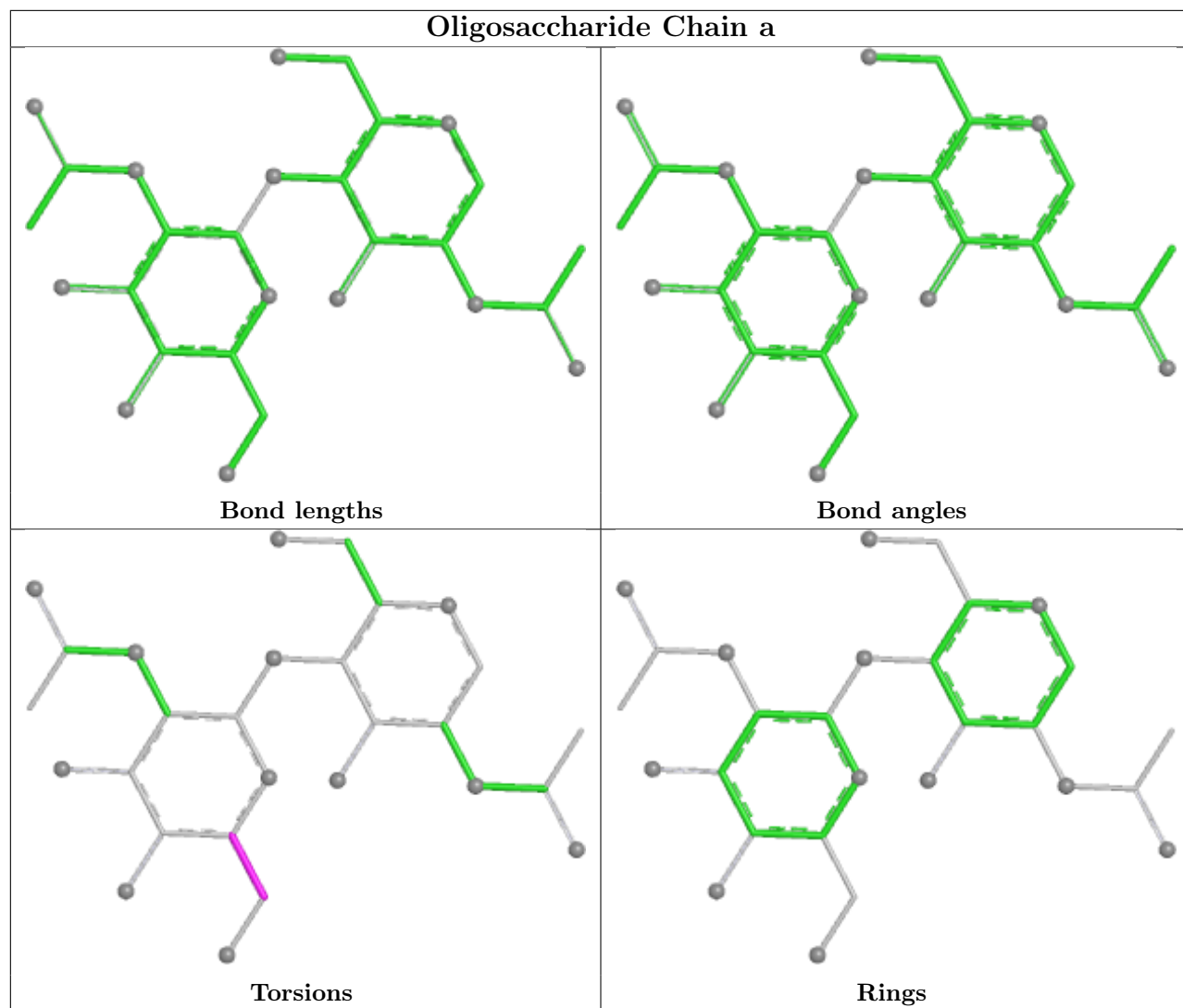


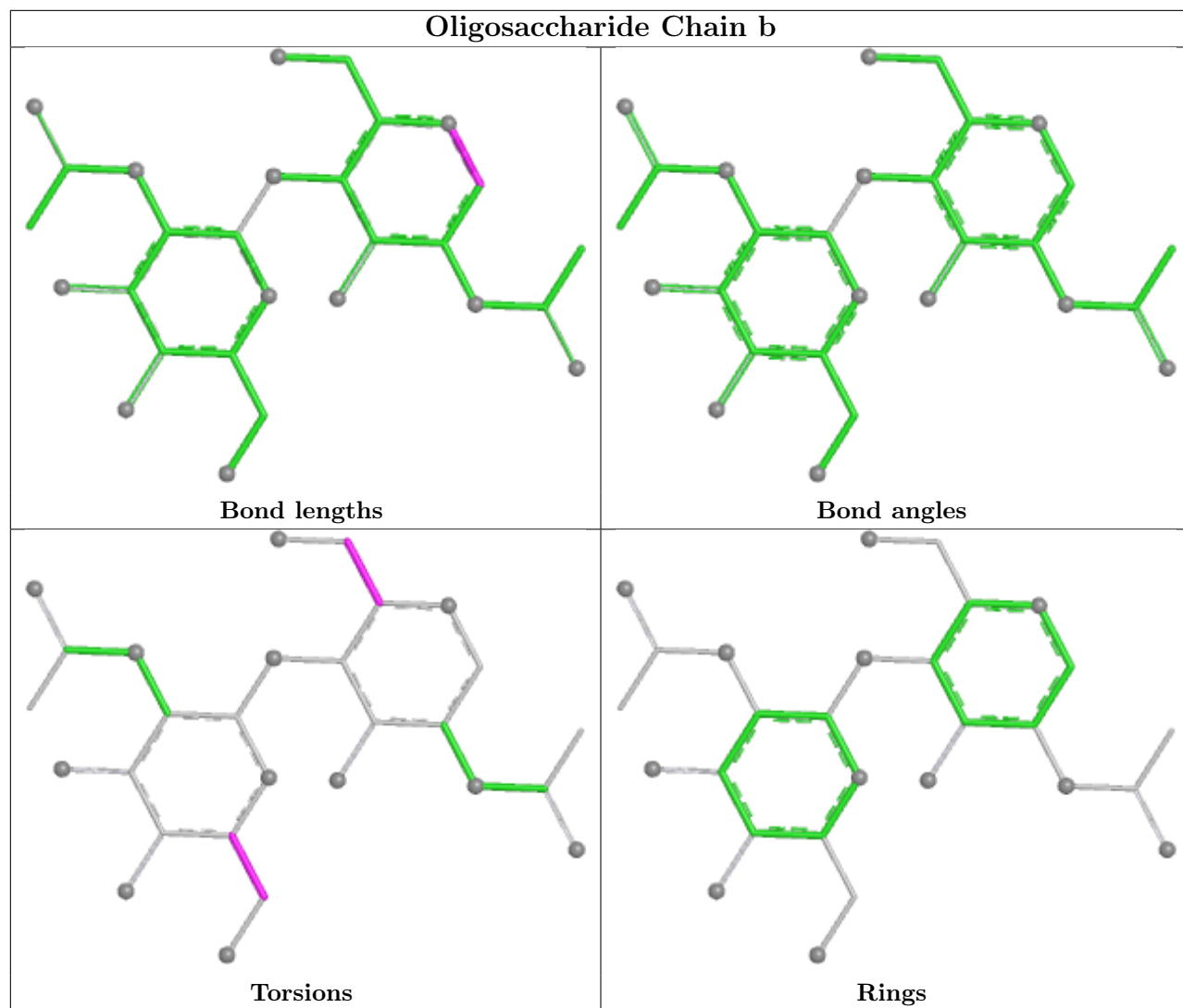


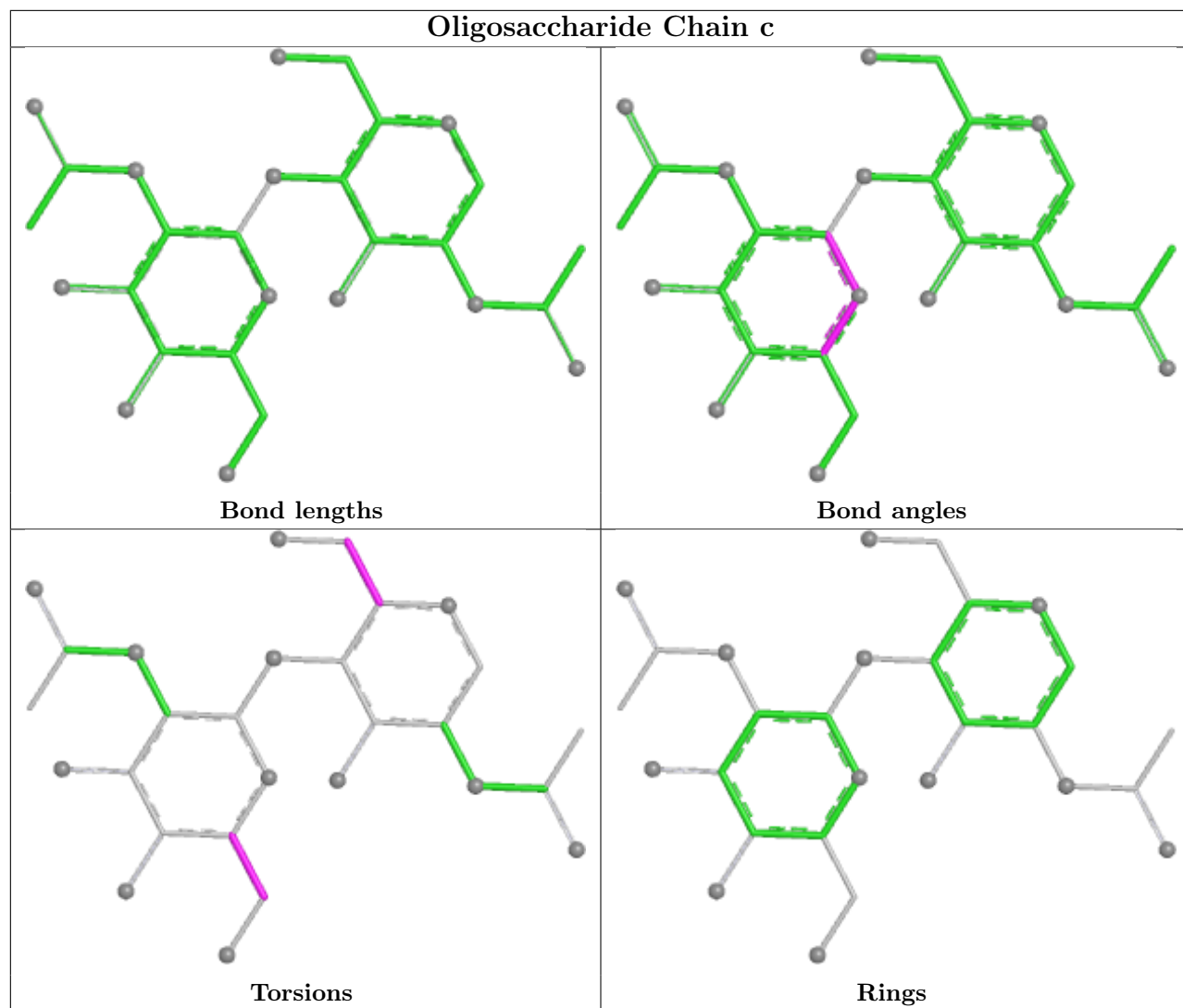


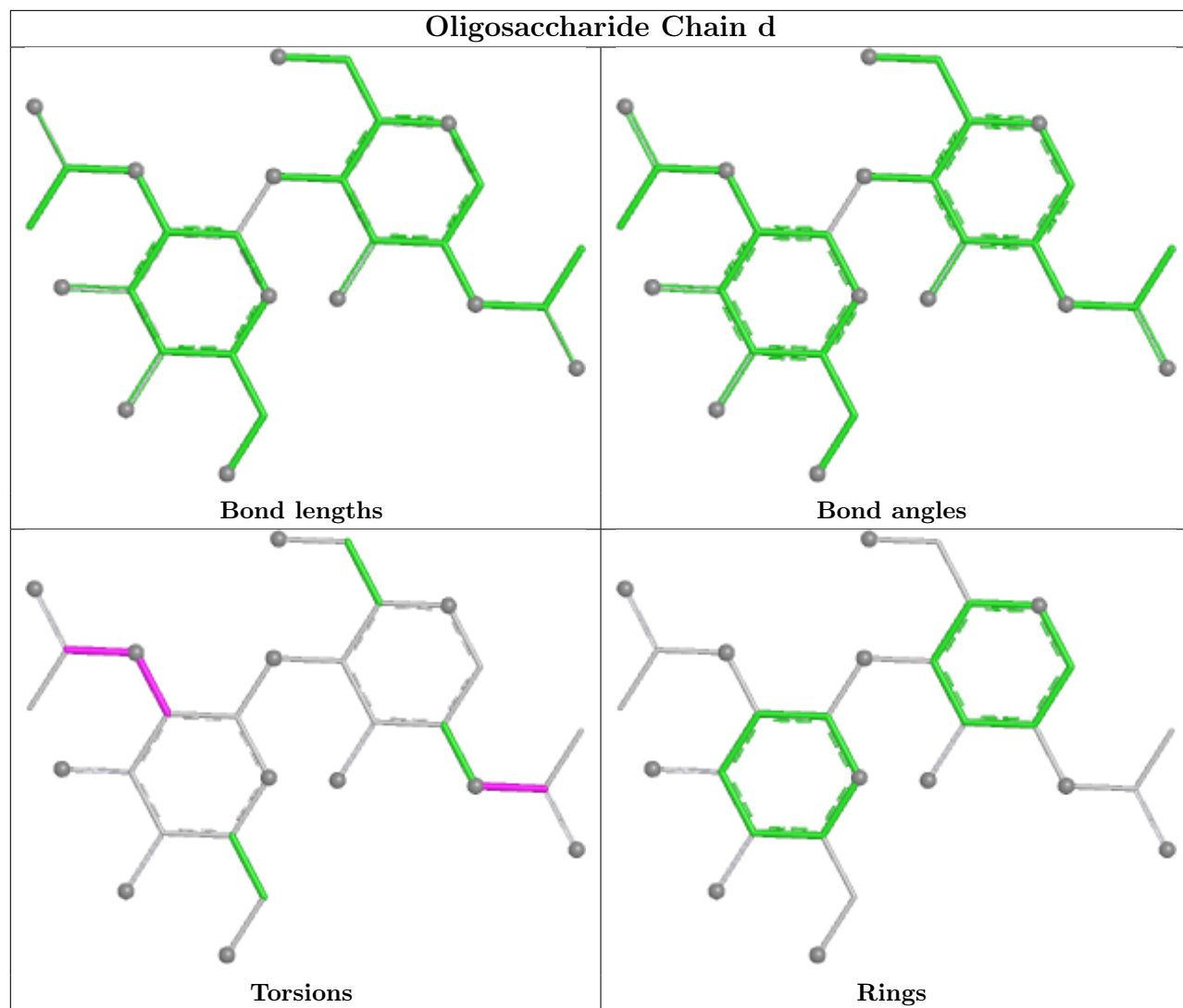


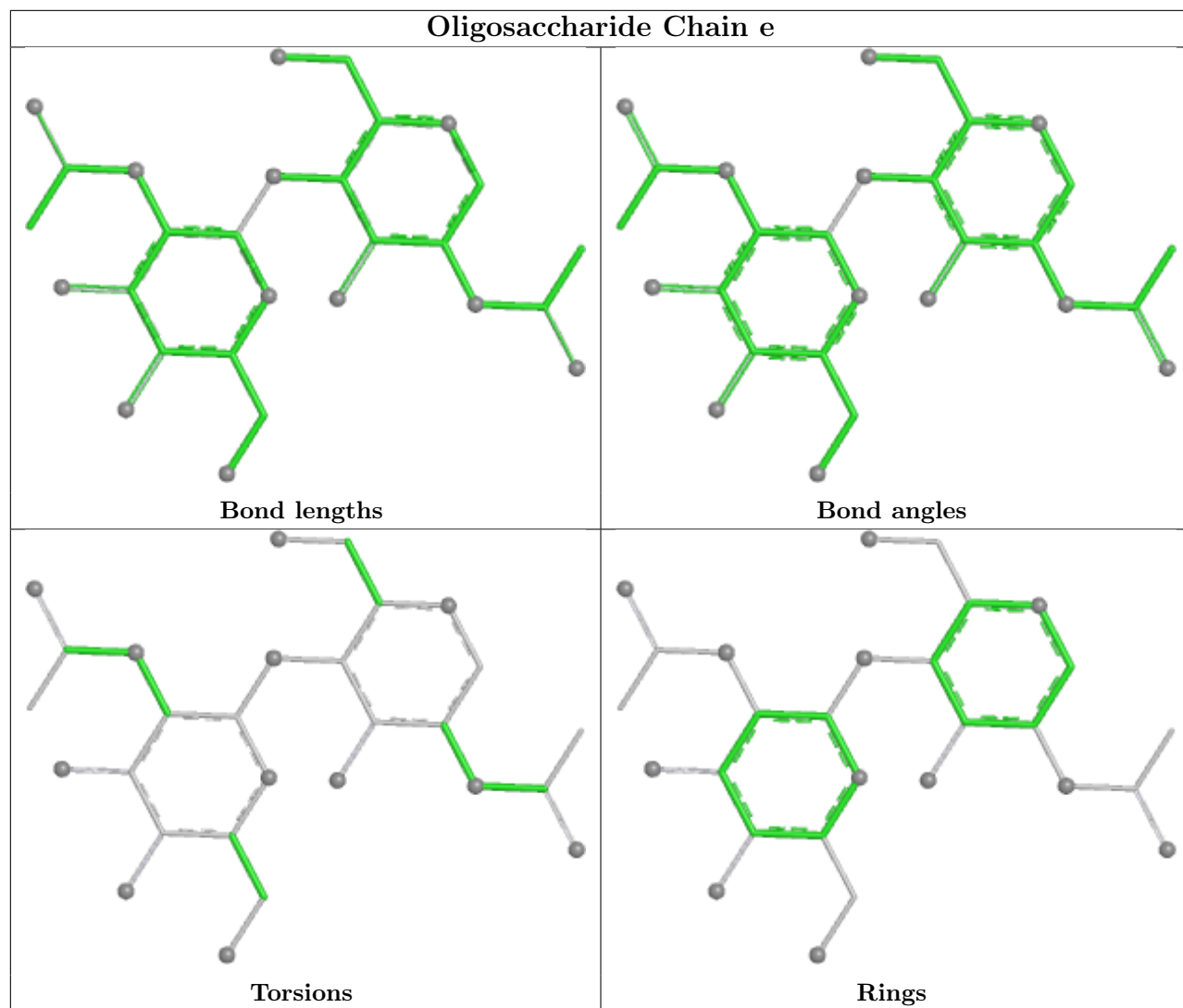


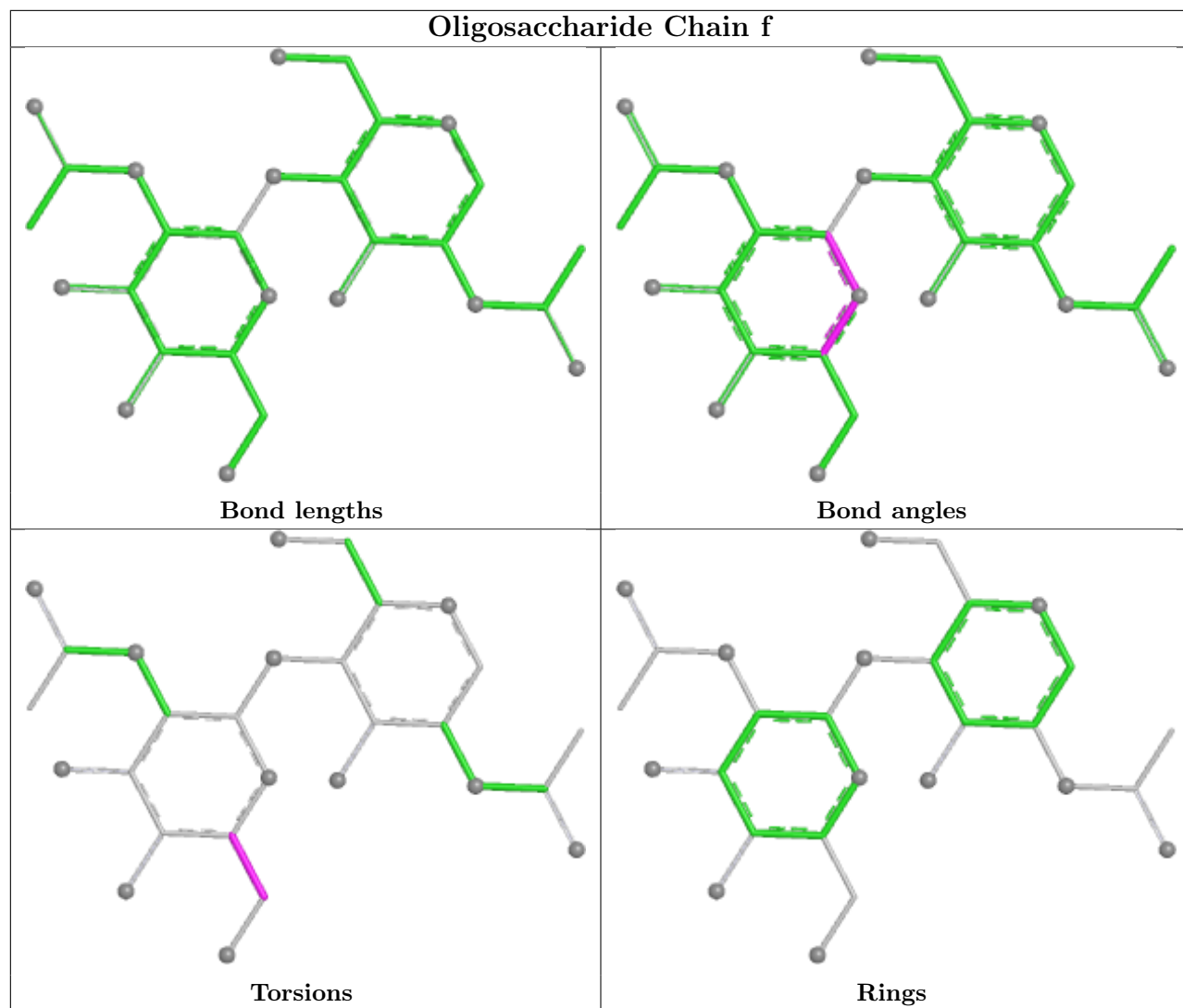


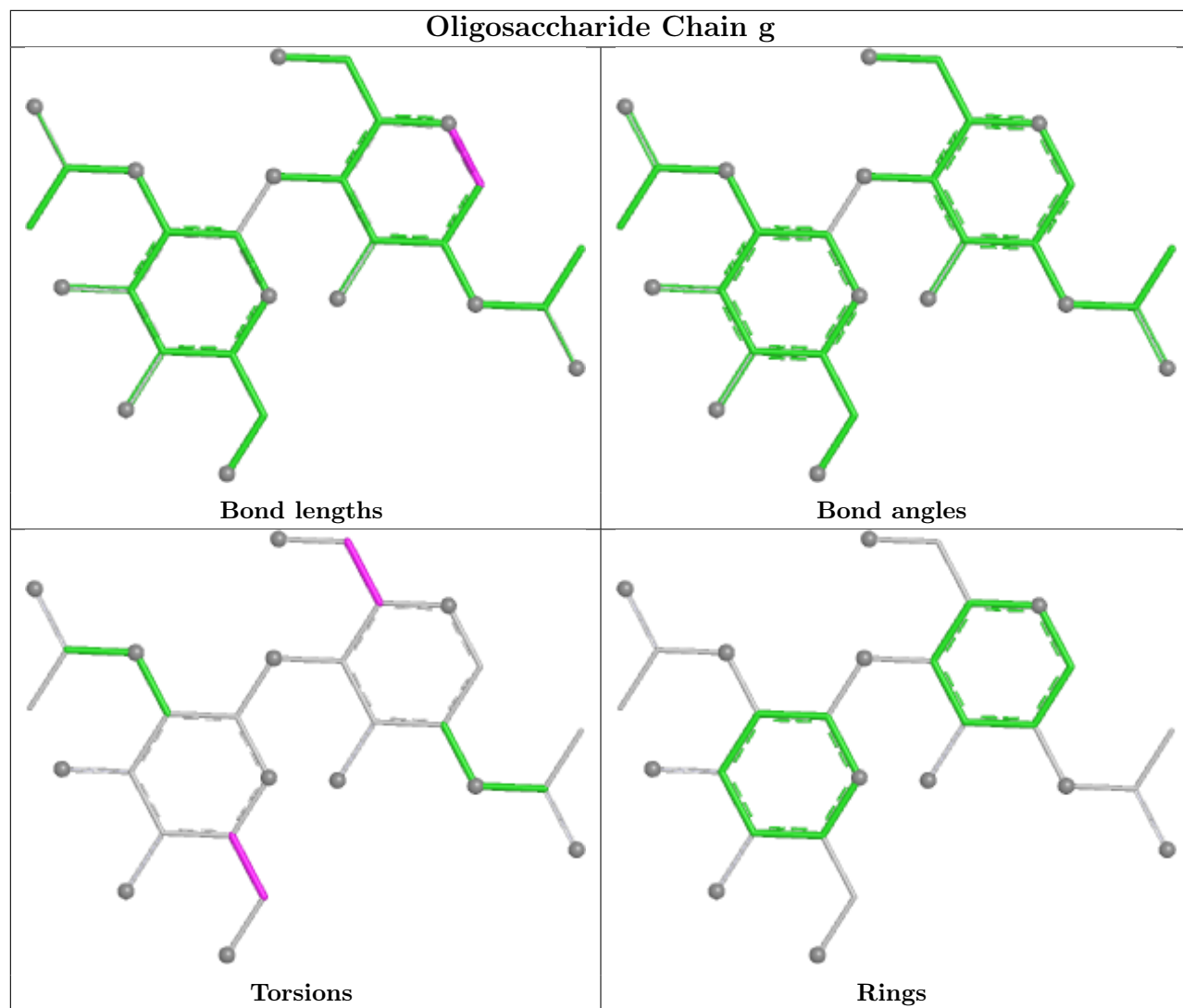


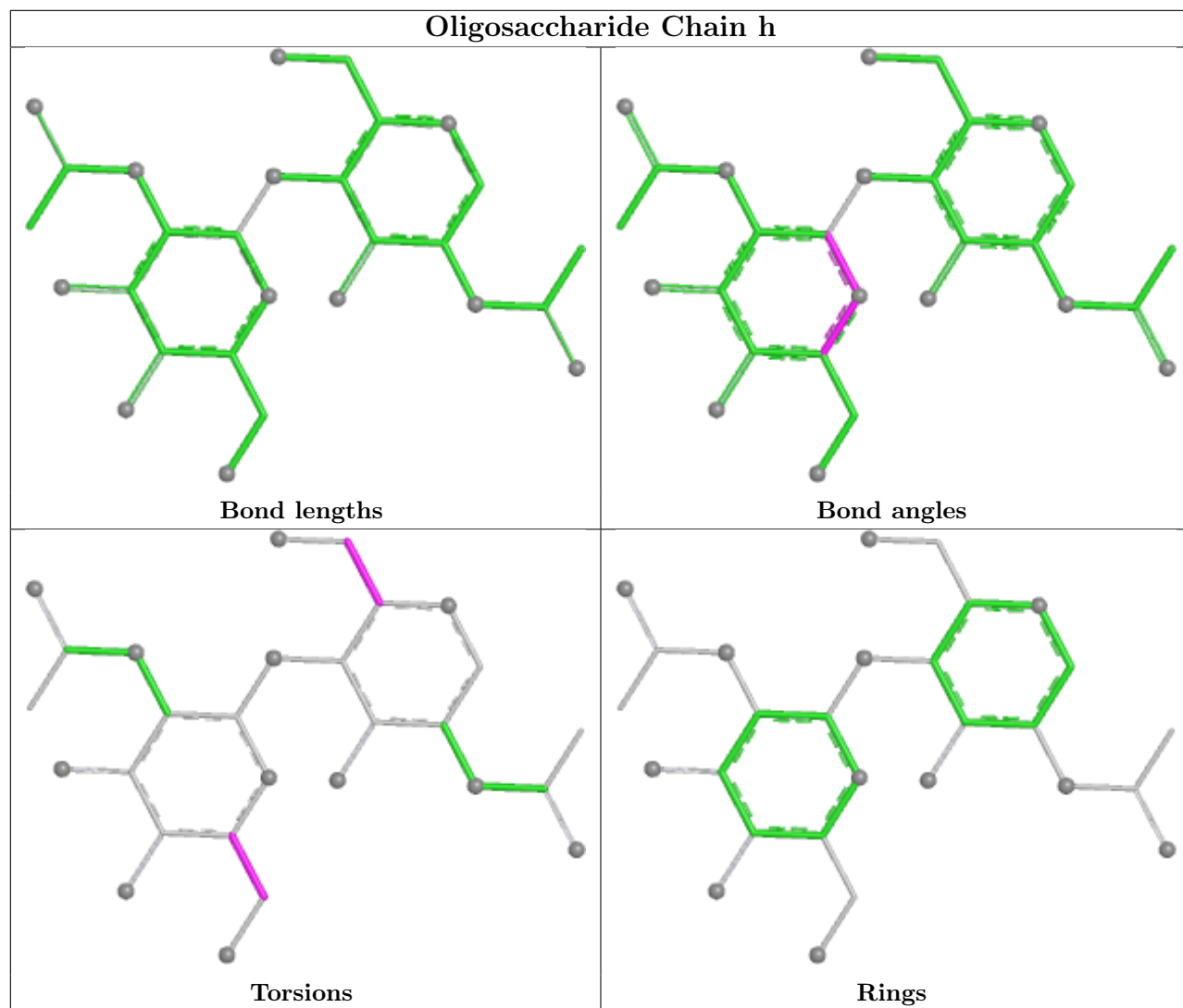


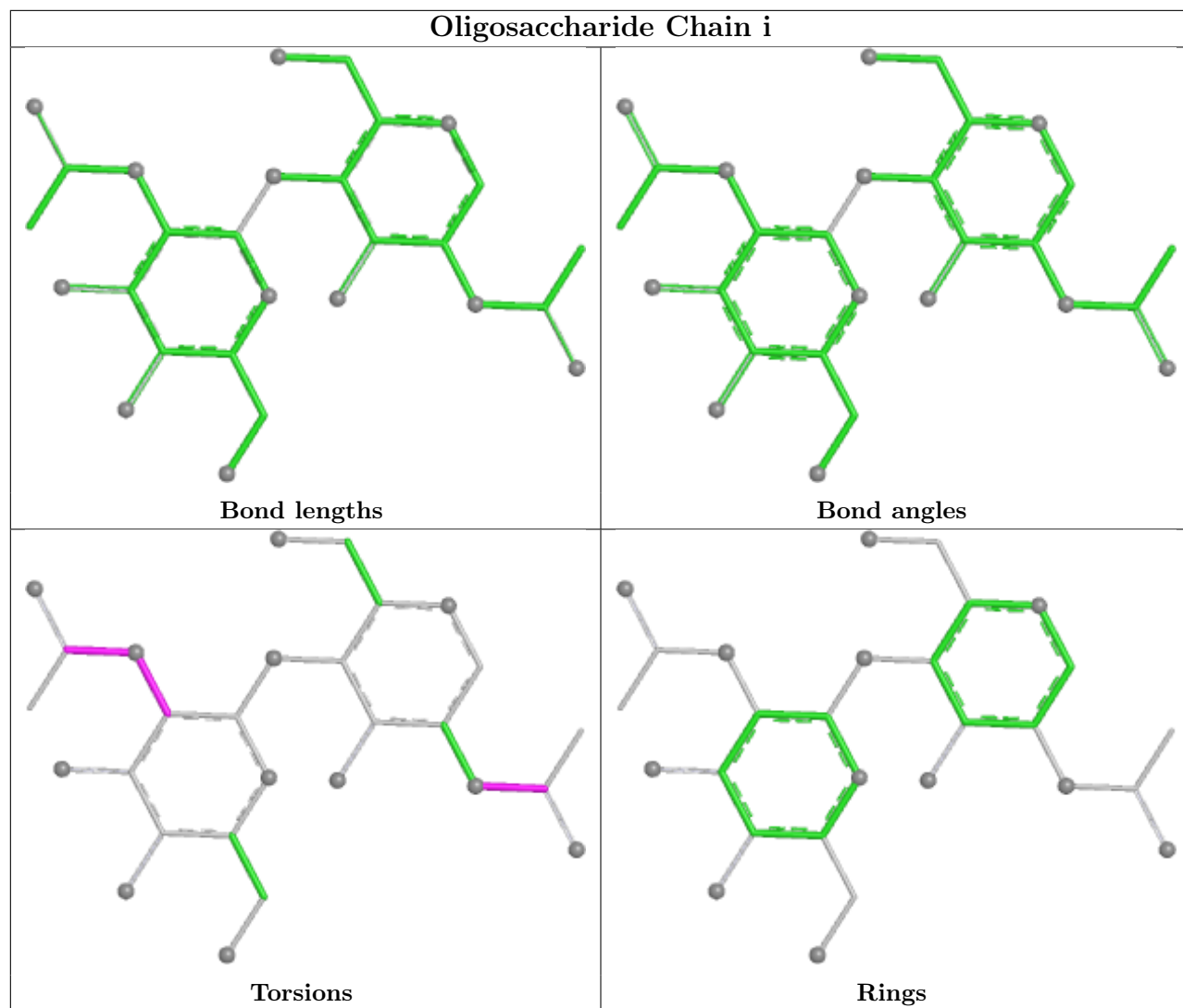


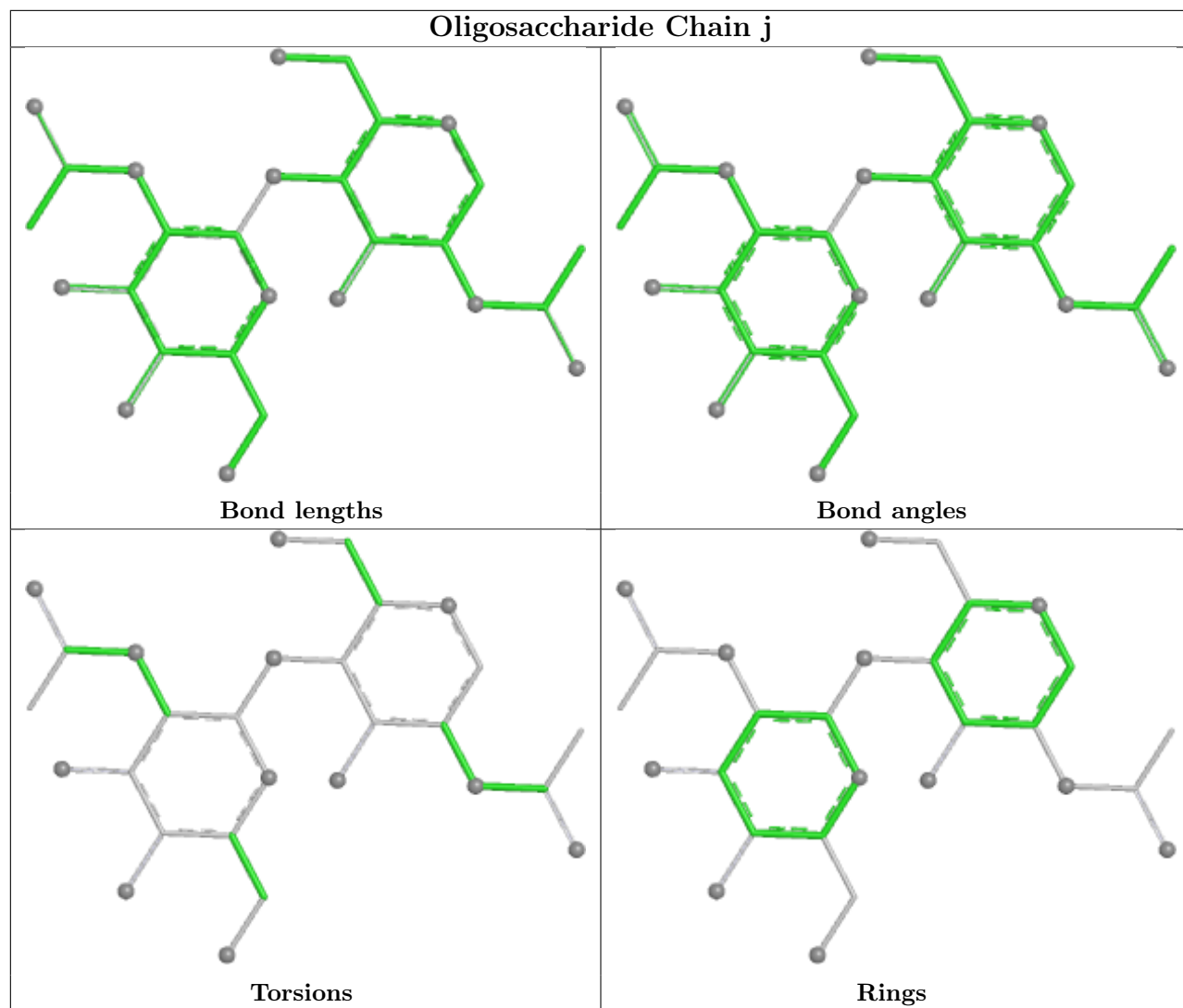


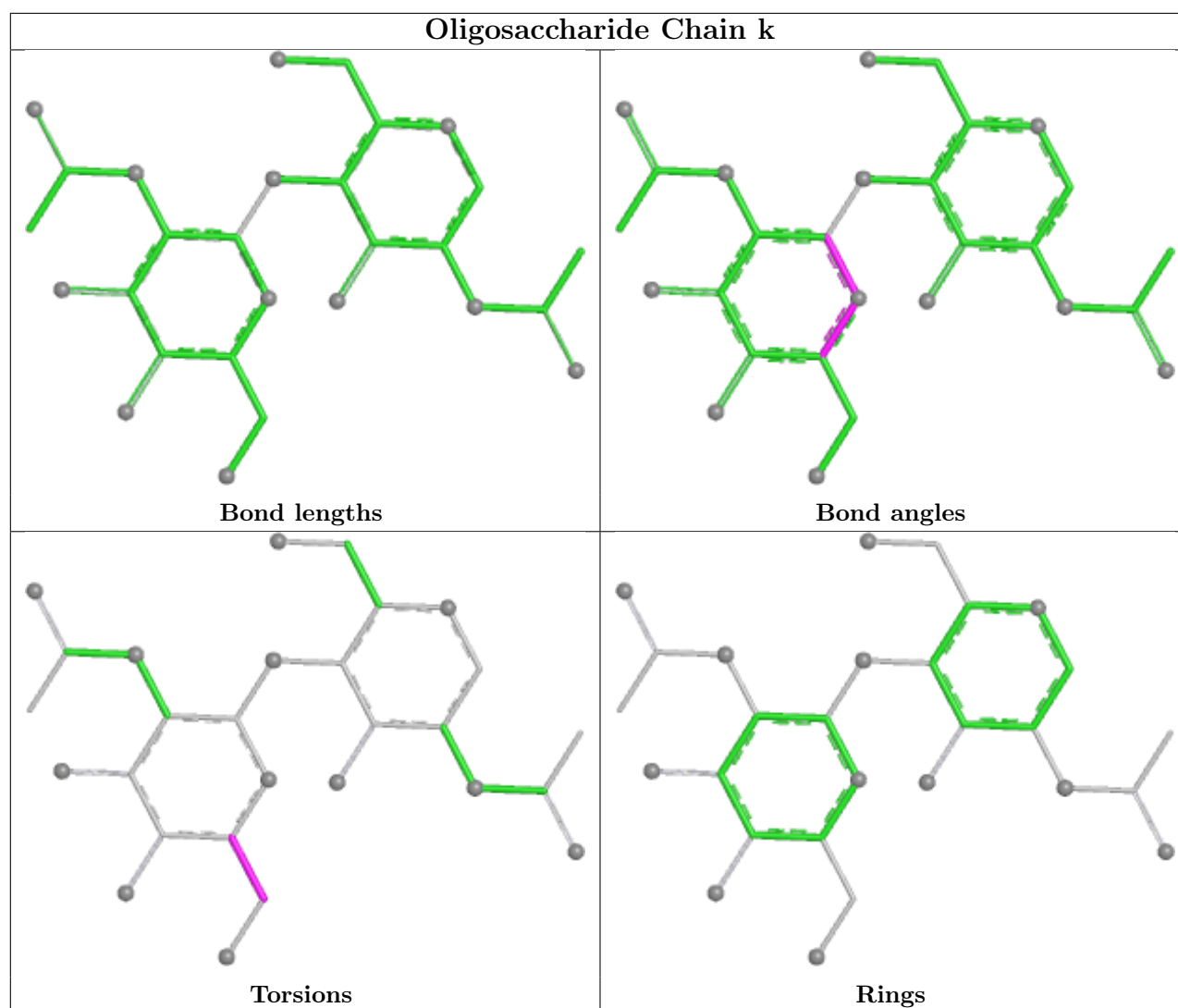












5.6 Ligand geometry [i](#)

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

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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.

All (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
4	C	1405	NAG	C1-C2-N2	2.13	113.79	110.43
4	E	901	NAG	C1-O5-C5	2.11	115.02	112.19
4	A	1405	NAG	C1-C2-N2	2.11	113.76	110.43
4	B	1405	NAG	C1-C2-N2	2.11	113.76	110.43
4	D	901	NAG	C1-O5-C5	2.09	114.99	112.19

There are no chirality outliers.

All (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
4	B	1402	NAG	O5-C5-C6-O6
4	B	1404	NAG	O5-C5-C6-O6
4	C	1402	NAG	O5-C5-C6-O6
4	C	1404	NAG	O5-C5-C6-O6
4	C	1405	NAG	O5-C5-C6-O6
4	A	1401	NAG	O5-C5-C6-O6
4	B	1401	NAG	O5-C5-C6-O6
4	C	1401	NAG	O5-C5-C6-O6
4	A	1402	NAG	C4-C5-C6-O6
4	B	1402	NAG	C4-C5-C6-O6
4	C	1402	NAG	C4-C5-C6-O6
4	A	1405	NAG	O5-C5-C6-O6
4	B	1405	NAG	O5-C5-C6-O6
4	A	1409	NAG	C4-C5-C6-O6
4	A	1405	NAG	C4-C5-C6-O6
4	B	1405	NAG	C4-C5-C6-O6
4	C	1405	NAG	C4-C5-C6-O6
4	C	1408	NAG	O5-C5-C6-O6
4	A	1408	NAG	O5-C5-C6-O6
4	B	1408	NAG	O5-C5-C6-O6
4	A	1409	NAG	O5-C5-C6-O6
4	A	1406	NAG	C4-C5-C6-O6
4	B	1406	NAG	C4-C5-C6-O6
4	C	1406	NAG	C4-C5-C6-O6
4	A	1405	NAG	C8-C7-N2-C2
4	A	1405	NAG	O7-C7-N2-C2
4	B	1405	NAG	C8-C7-N2-C2
4	B	1405	NAG	O7-C7-N2-C2
4	C	1405	NAG	C8-C7-N2-C2
4	C	1405	NAG	O7-C7-N2-C2
4	A	1404	NAG	C4-C5-C6-O6
4	B	1404	NAG	C4-C5-C6-O6
4	C	1404	NAG	C4-C5-C6-O6
4	D	901	NAG	O5-C5-C6-O6
4	E	901	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	A	1403	NAG	C4-C5-C6-O6
4	B	1403	NAG	C4-C5-C6-O6
4	C	1403	NAG	C4-C5-C6-O6
4	A	1403	NAG	O5-C5-C6-O6
4	B	1403	NAG	O5-C5-C6-O6
4	C	1403	NAG	O5-C5-C6-O6
4	A	1408	NAG	C4-C5-C6-O6
4	B	1408	NAG	C4-C5-C6-O6
4	C	1408	NAG	C4-C5-C6-O6
4	A	1401	NAG	C4-C5-C6-O6
4	B	1401	NAG	C4-C5-C6-O6
4	C	1401	NAG	C4-C5-C6-O6
4	D	901	NAG	C4-C5-C6-O6
4	E	901	NAG	C4-C5-C6-O6
4	A	1405	NAG	C1-C2-N2-C7
4	B	1405	NAG	C1-C2-N2-C7
4	C	1405	NAG	C1-C2-N2-C7
4	A	1405	NAG	C3-C2-N2-C7
4	B	1405	NAG	C3-C2-N2-C7
4	C	1405	NAG	C3-C2-N2-C7

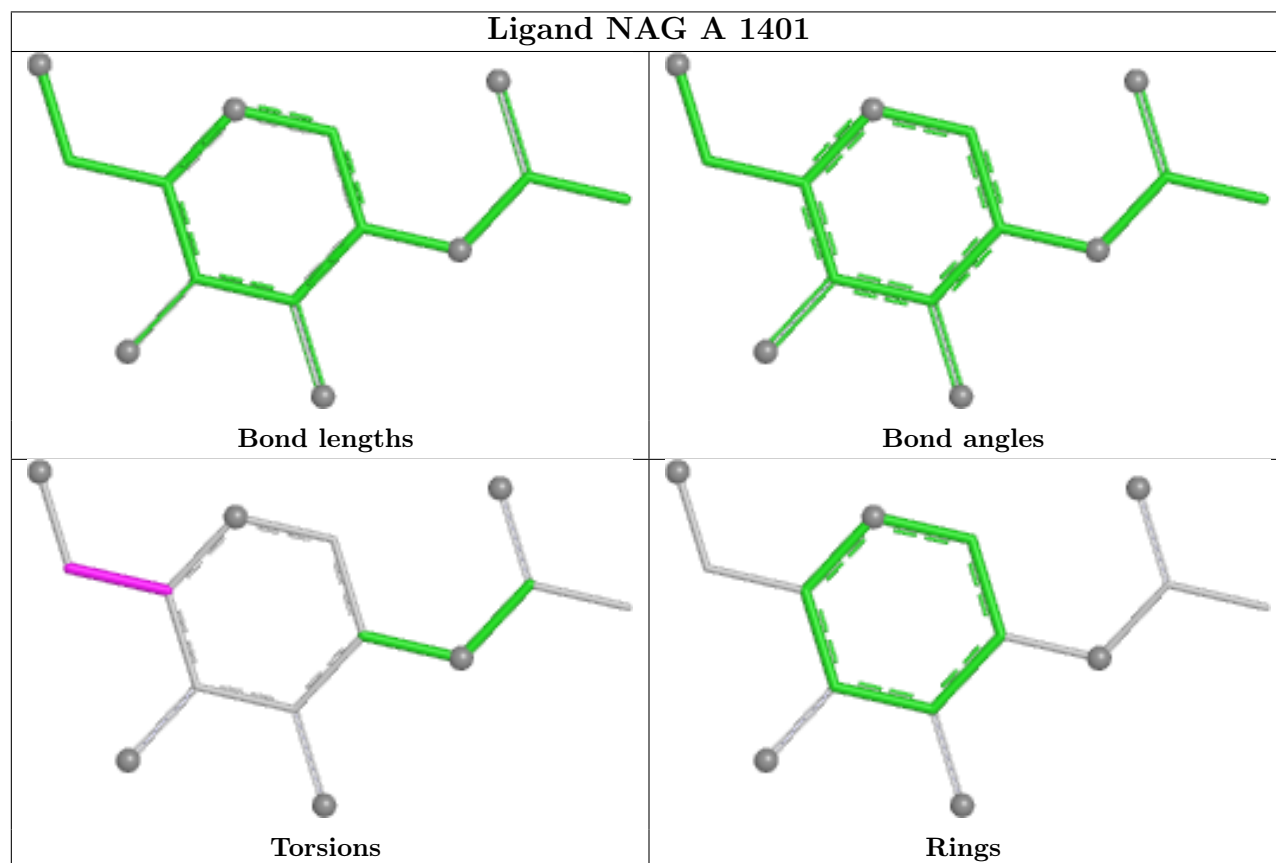
There are no ring outliers.

8 monomers are involved in 16 short contacts:

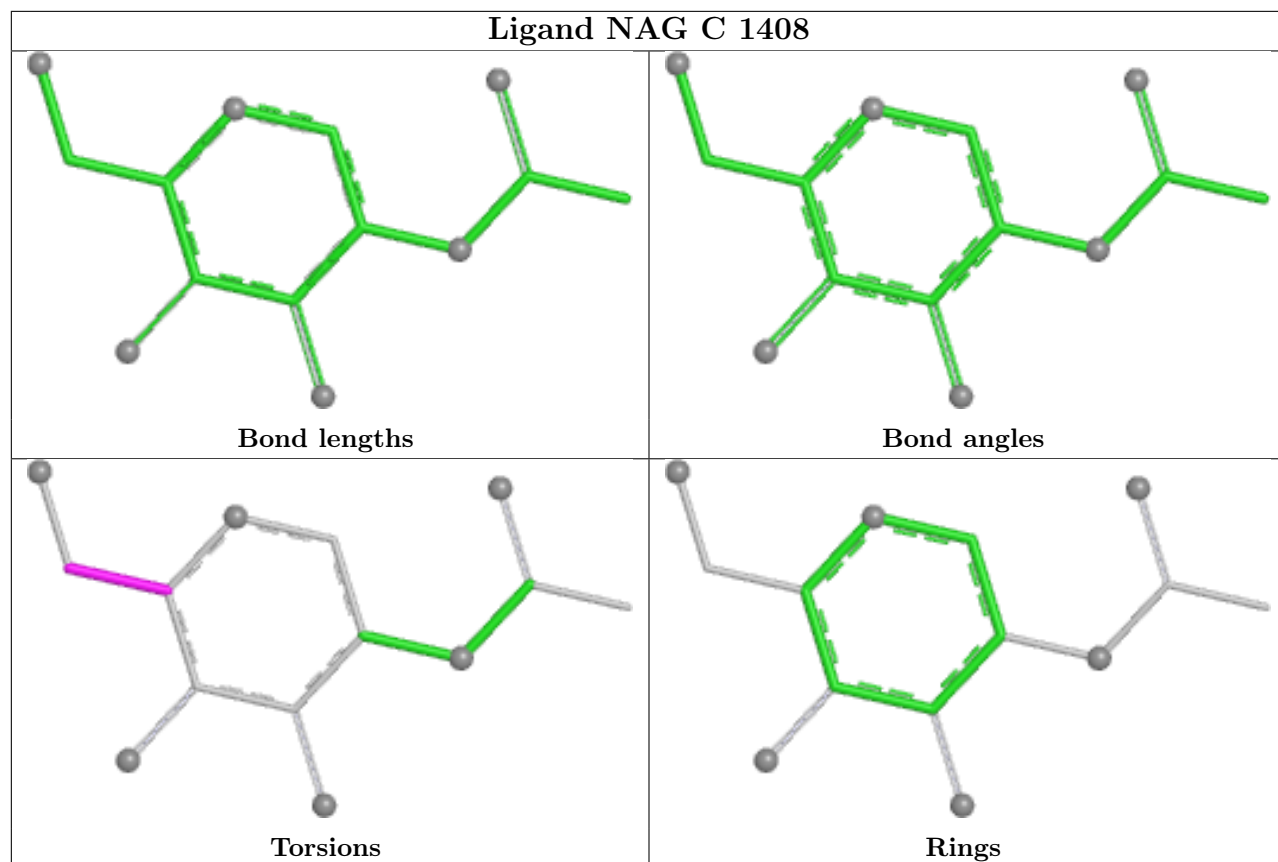
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1405	NAG	1	0
4	C	1405	NAG	1	0
4	B	1402	NAG	3	0
4	A	1405	NAG	1	0
4	C	1402	NAG	3	0
4	B	1409	NAG	4	0
4	B	1410	NAG	4	0
4	A	1402	NAG	3	0

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

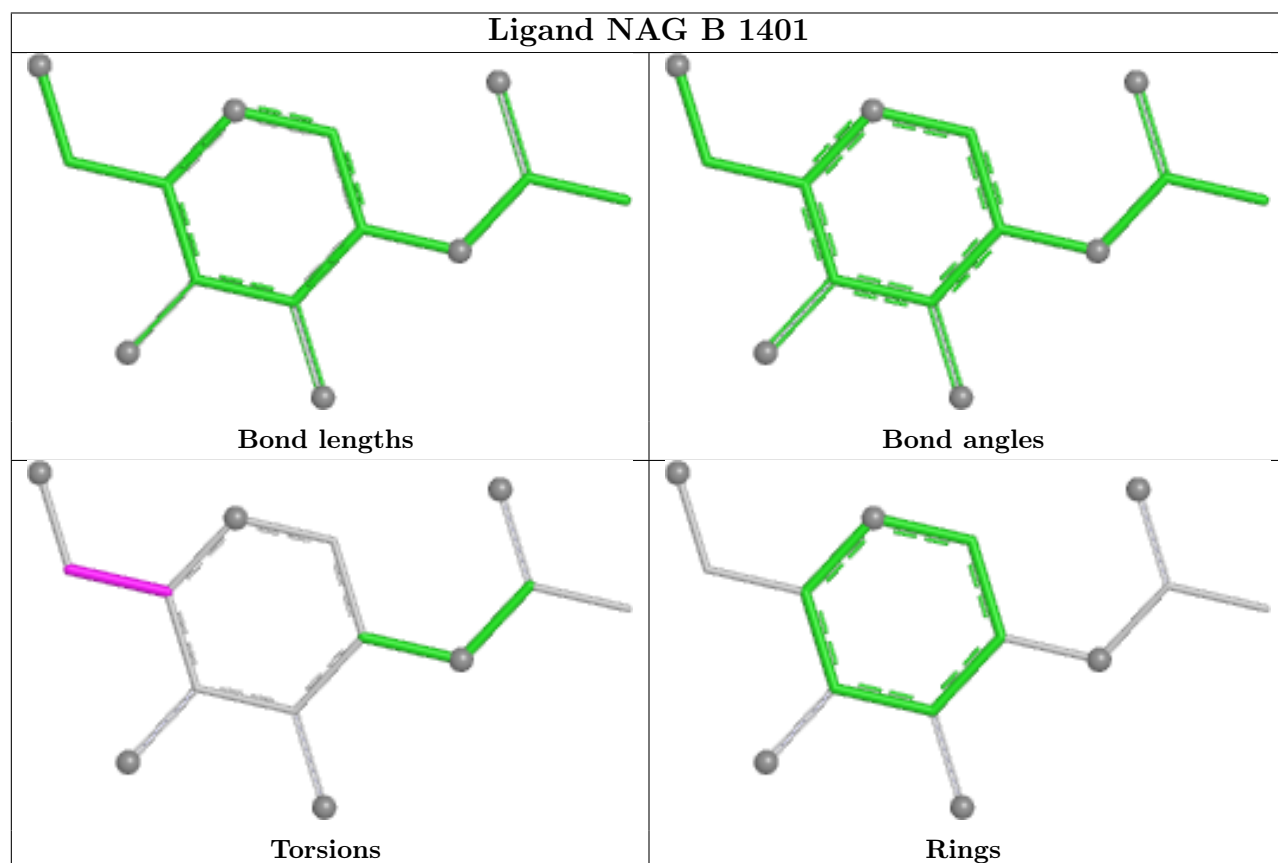
average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



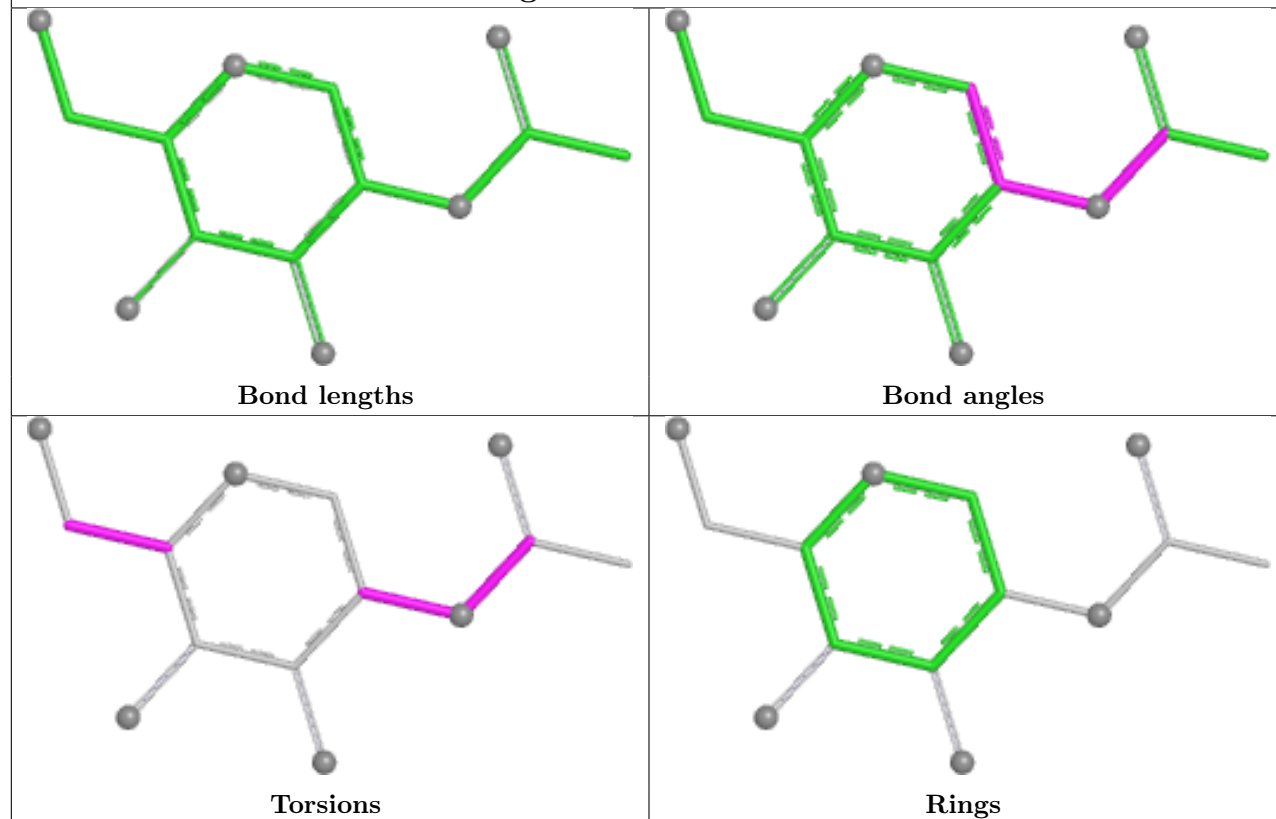
Ligand NAG C 1408



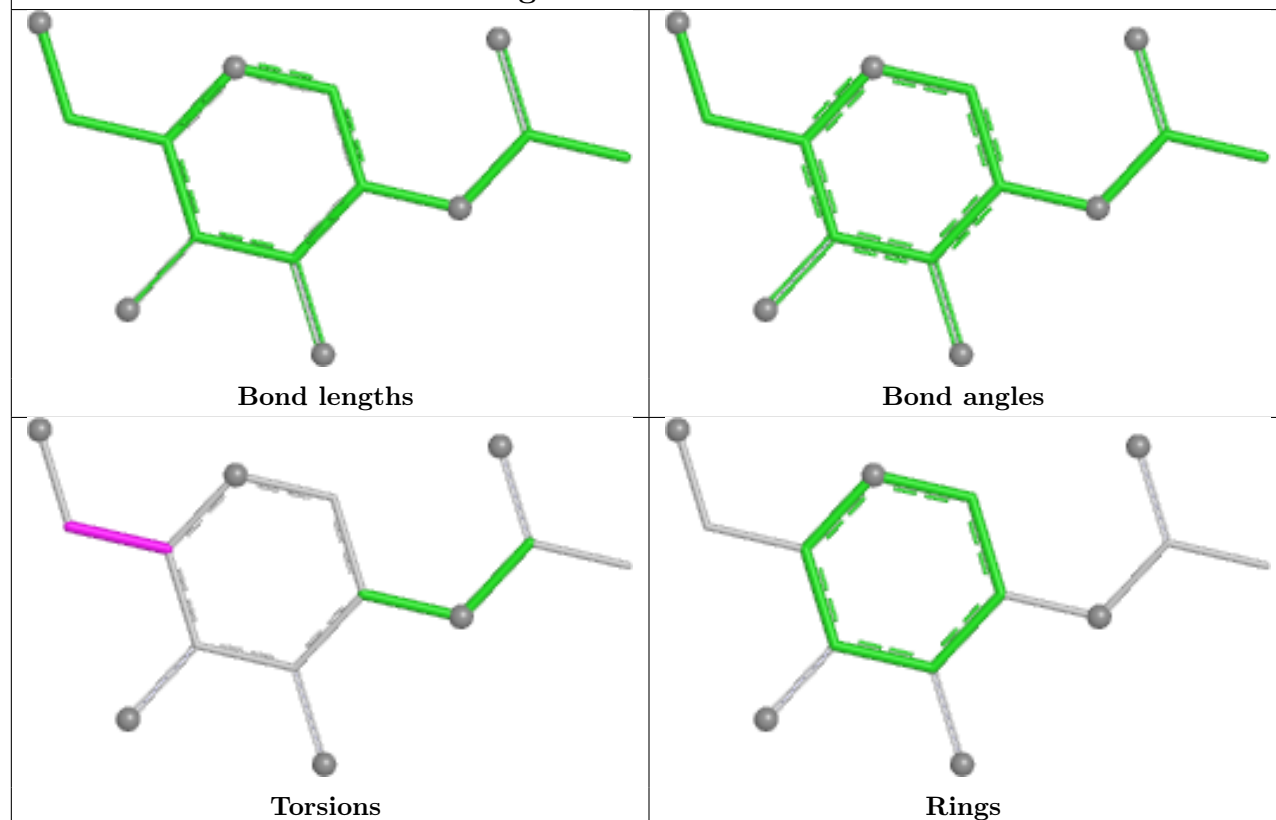
Ligand NAG B 1401



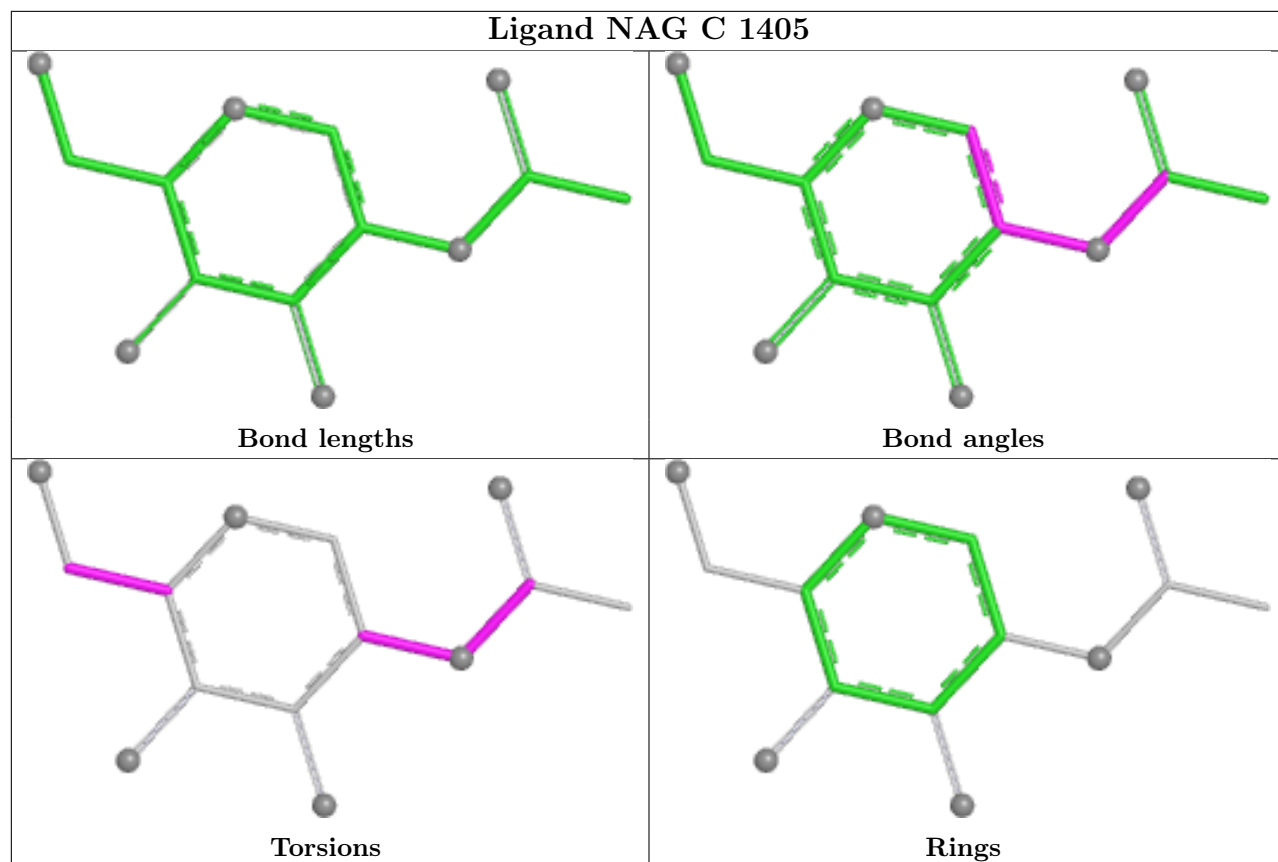
Ligand NAG B 1405



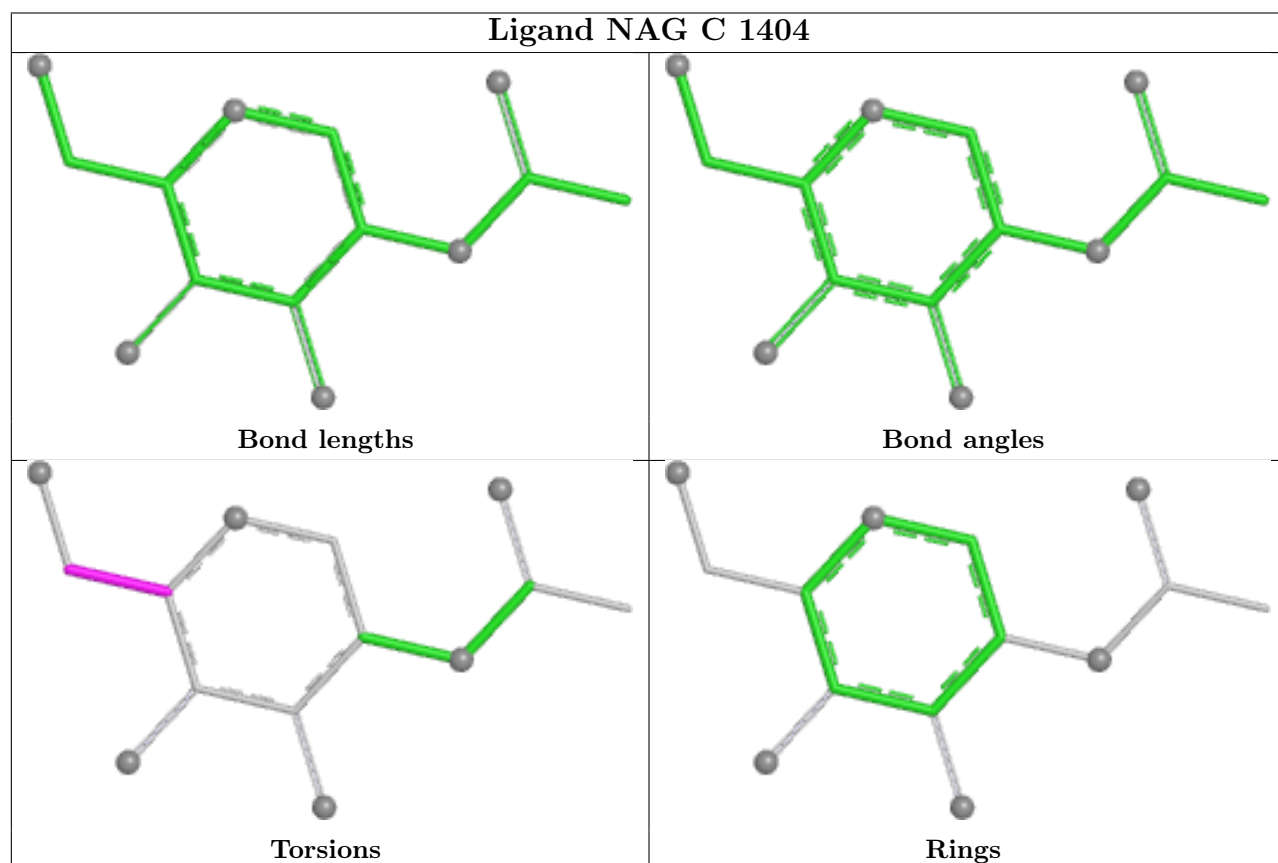
Ligand NAG A 1409



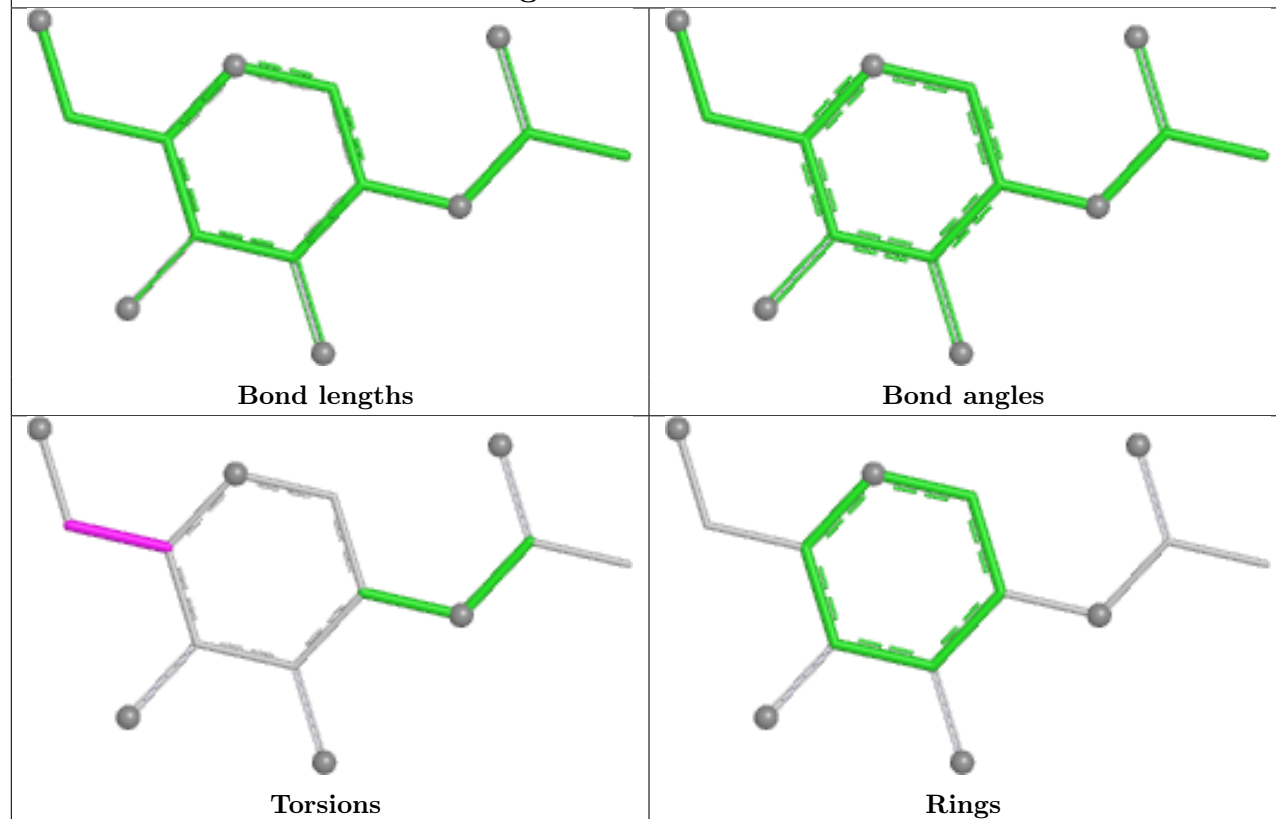
Ligand NAG C 1405



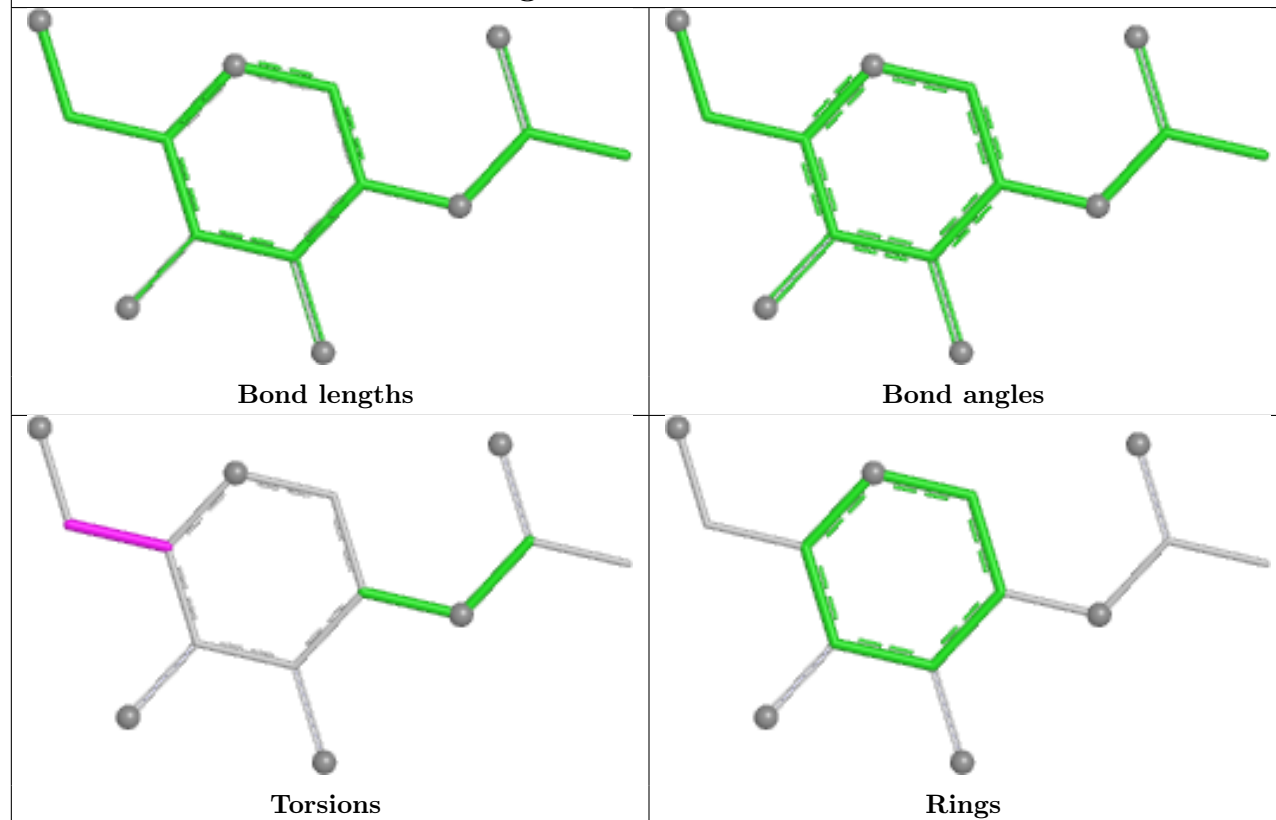
Ligand NAG C 1404

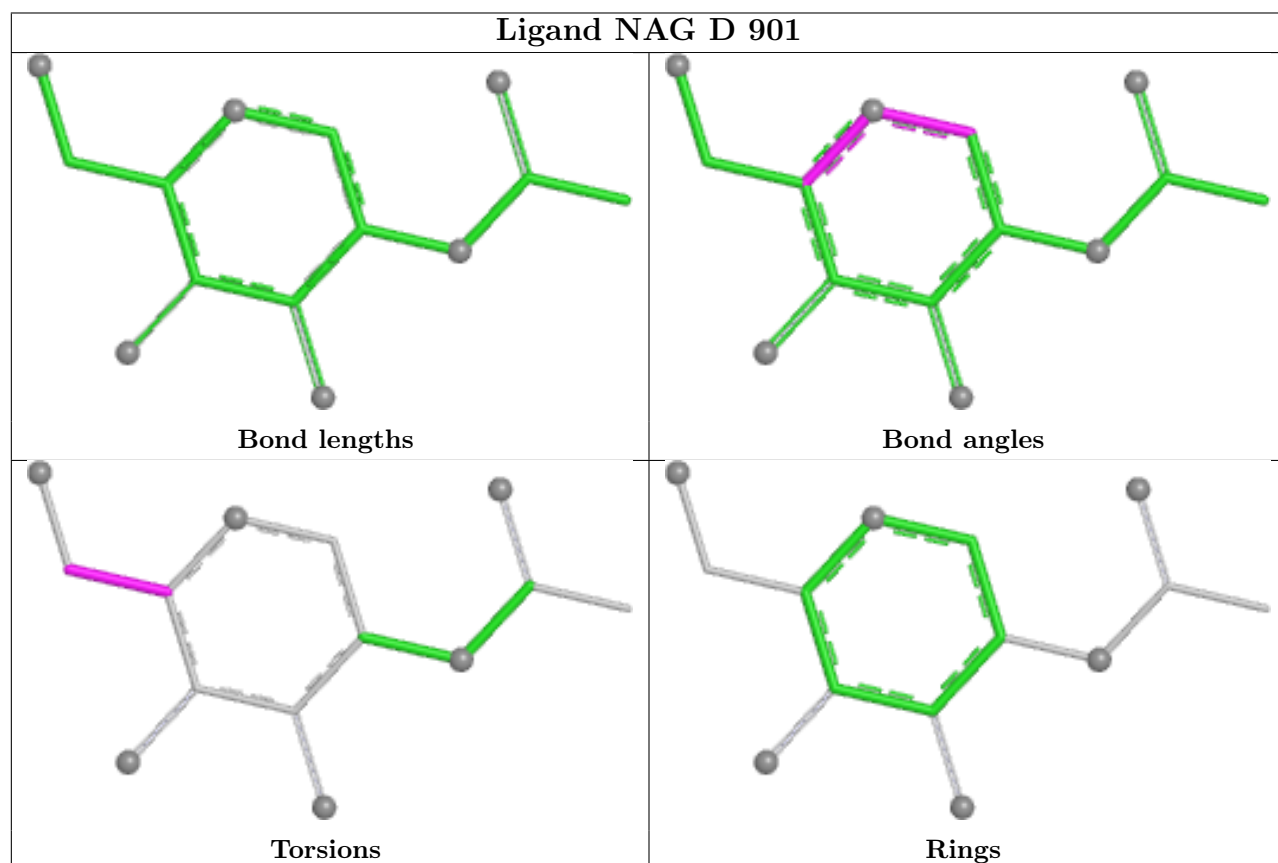
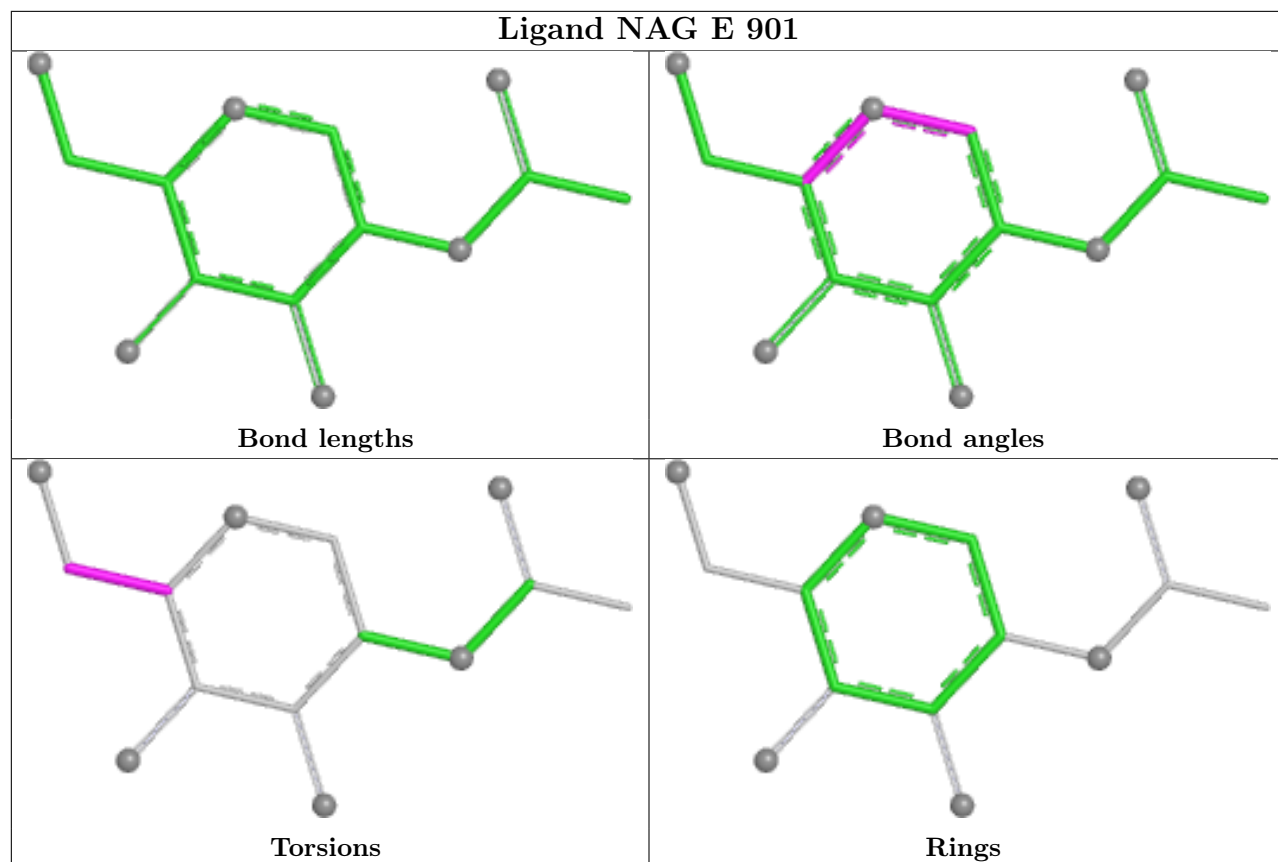


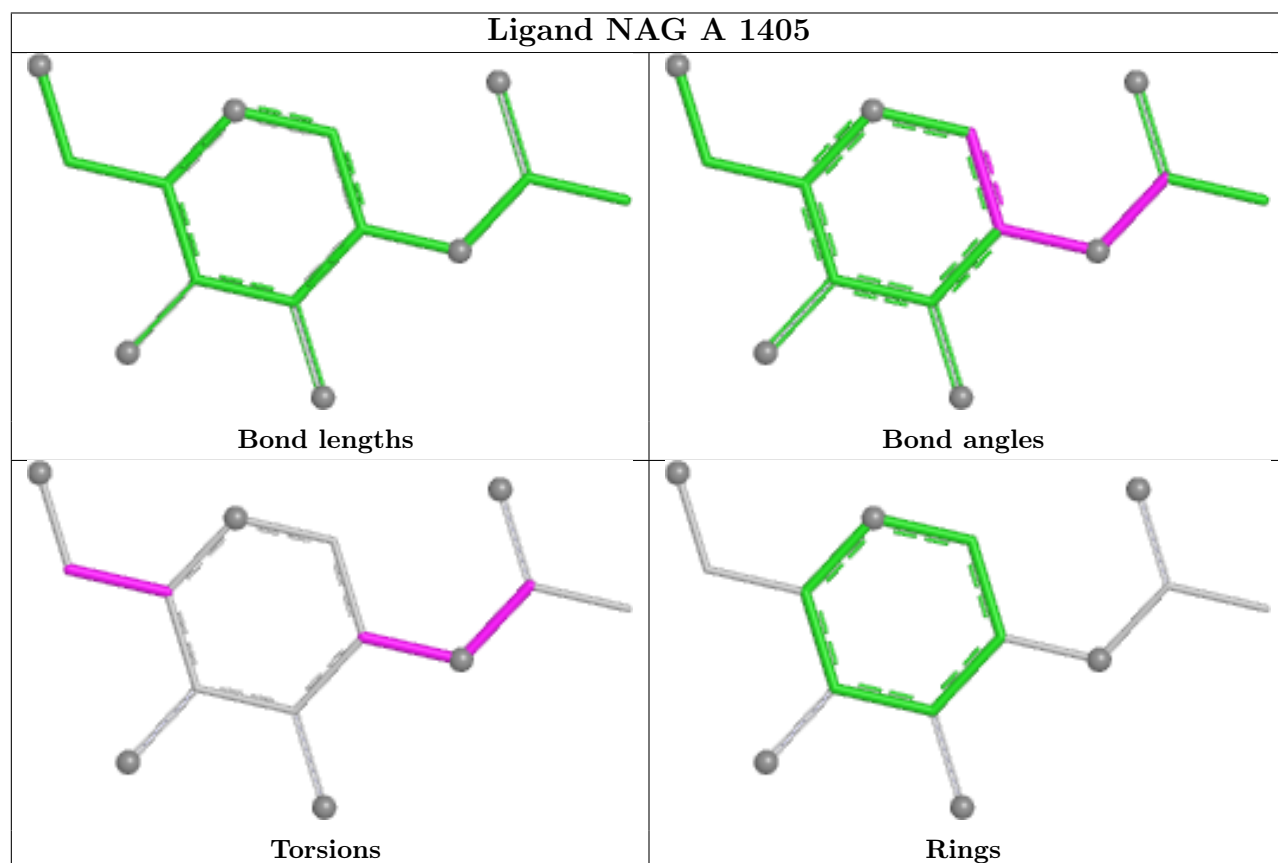
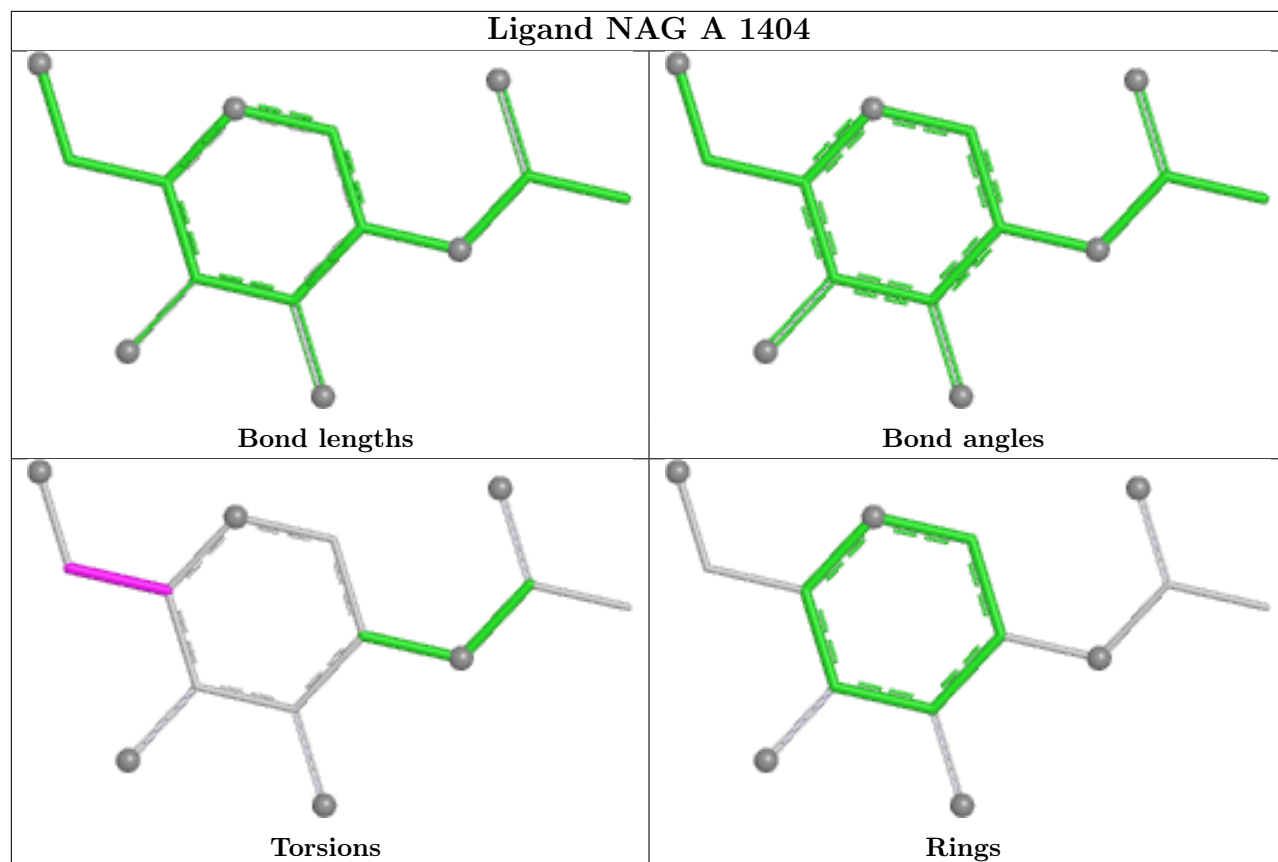
Ligand NAG B 1402

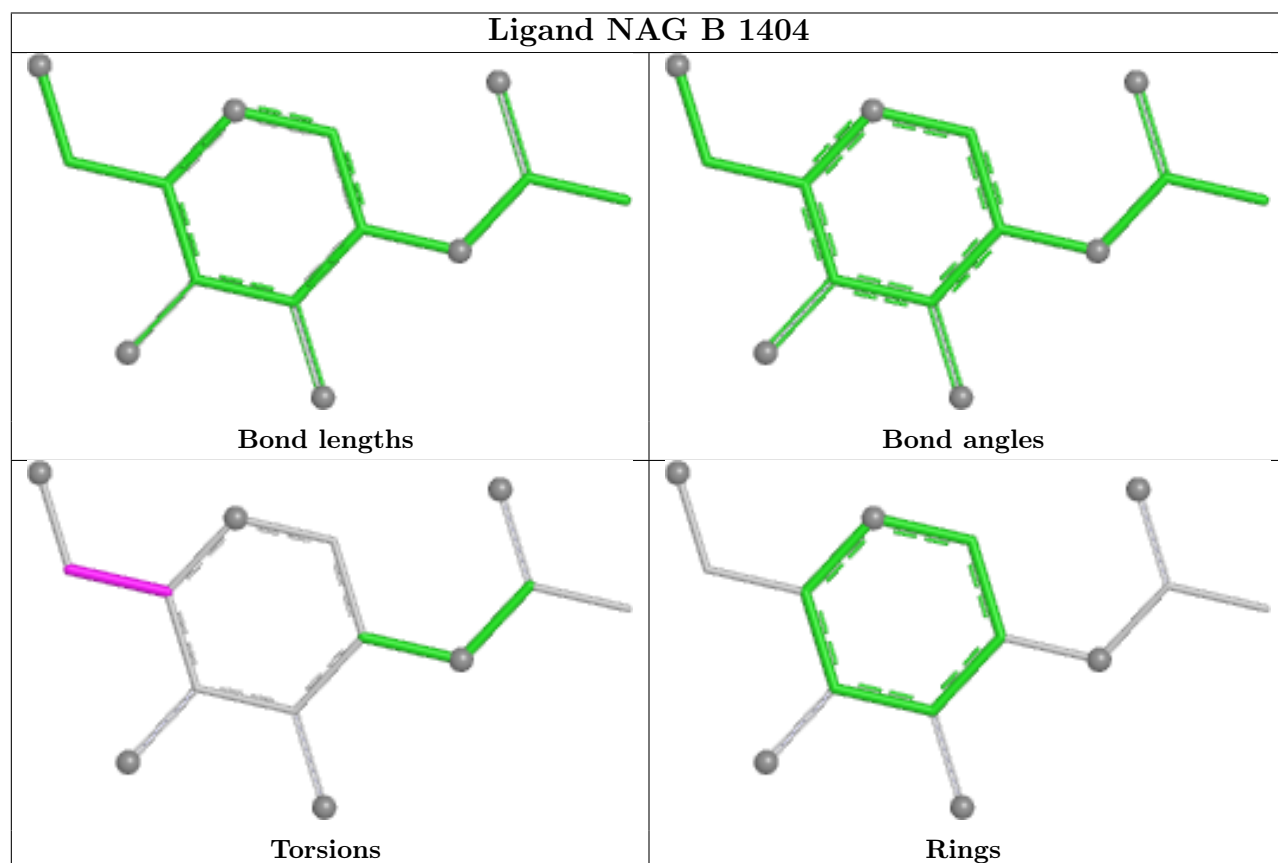
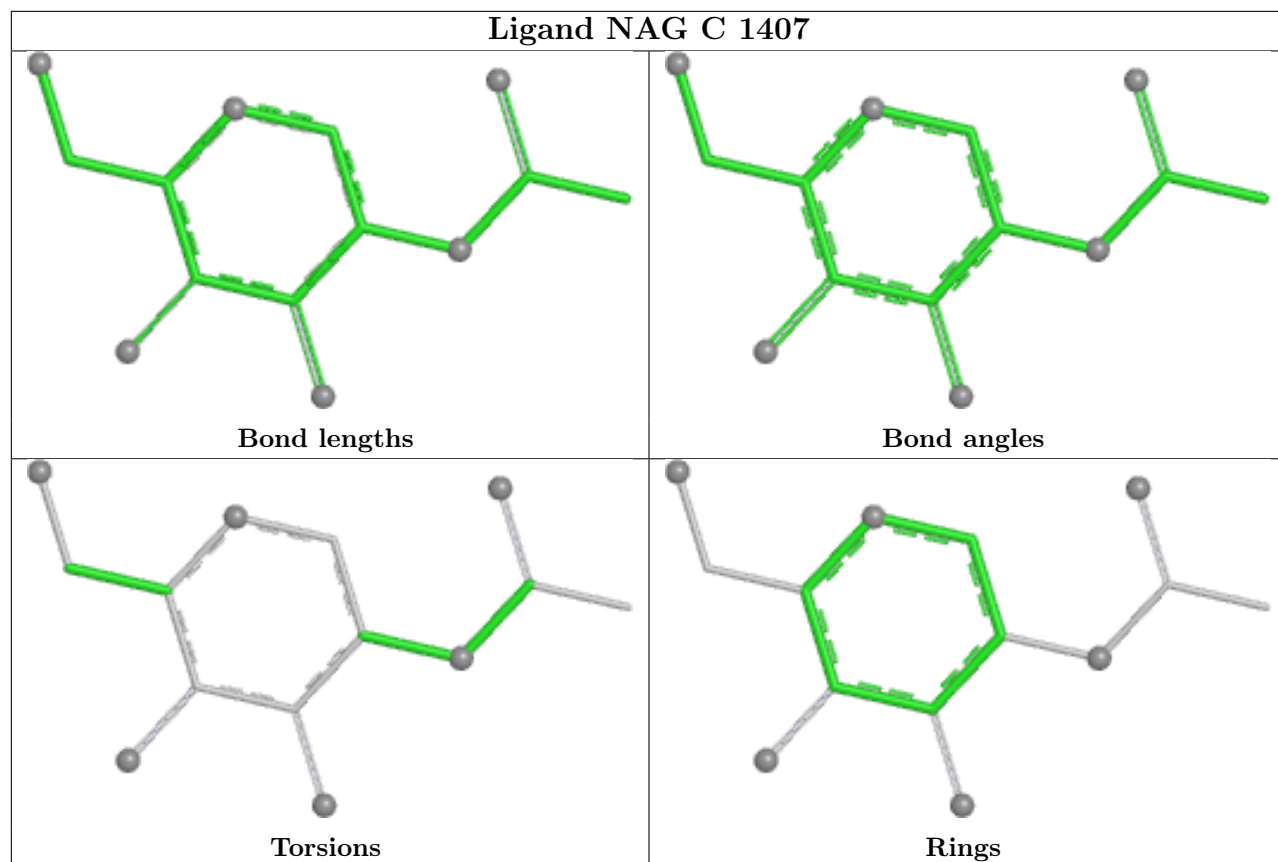


Ligand NAG A 1403

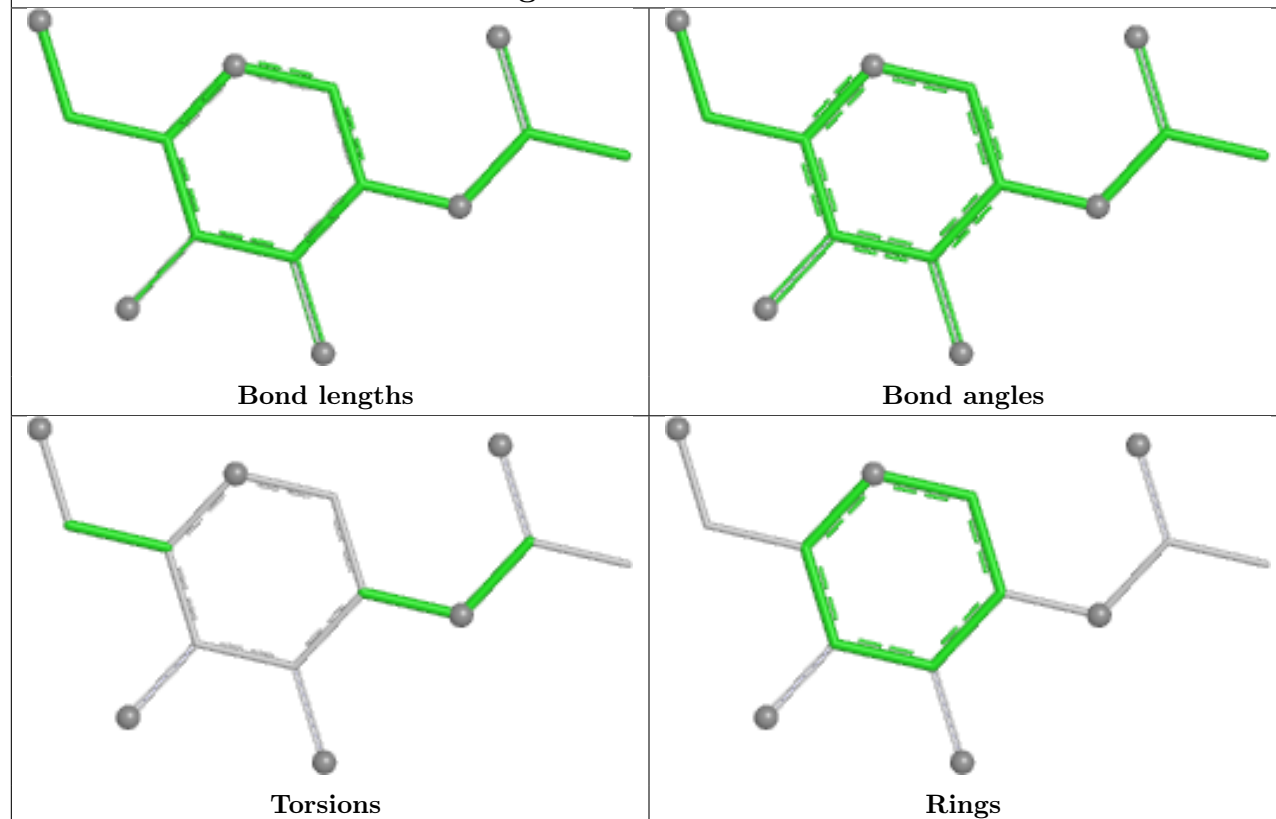




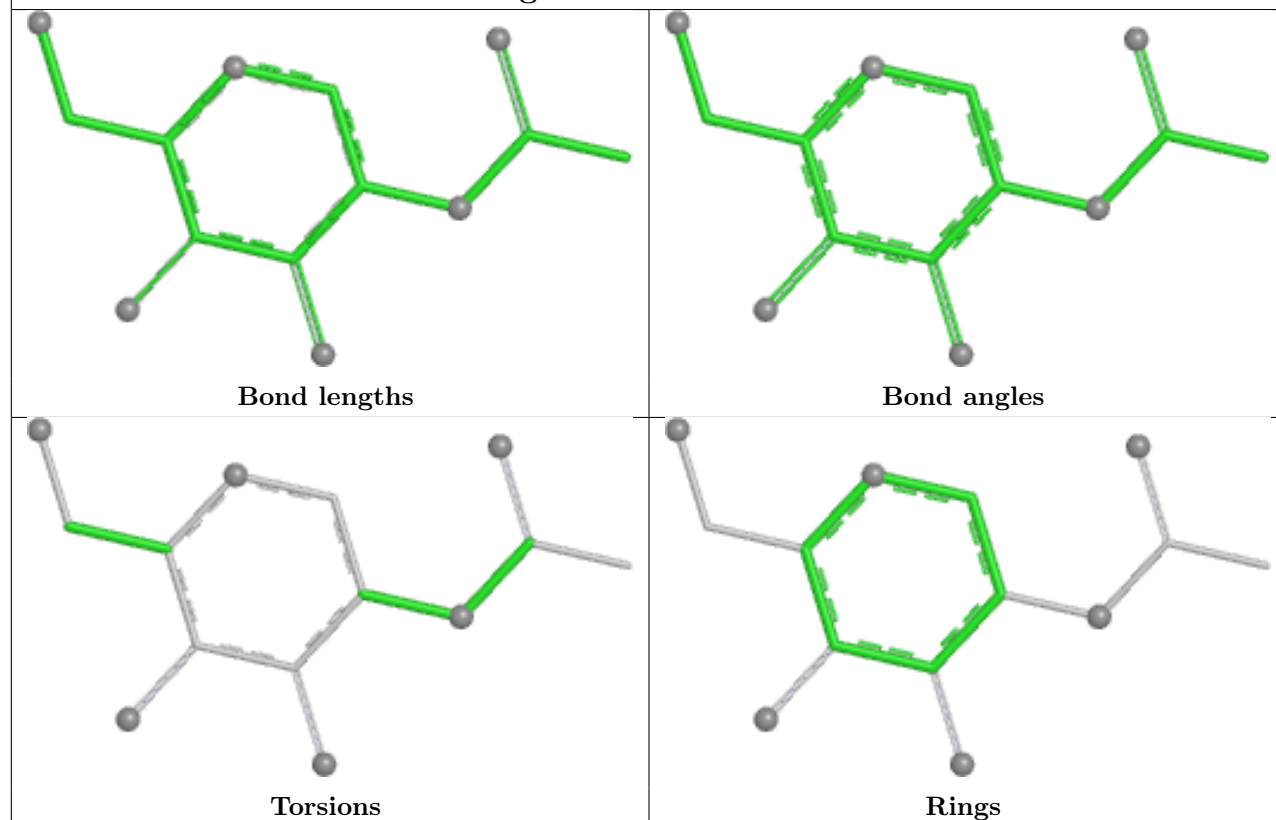




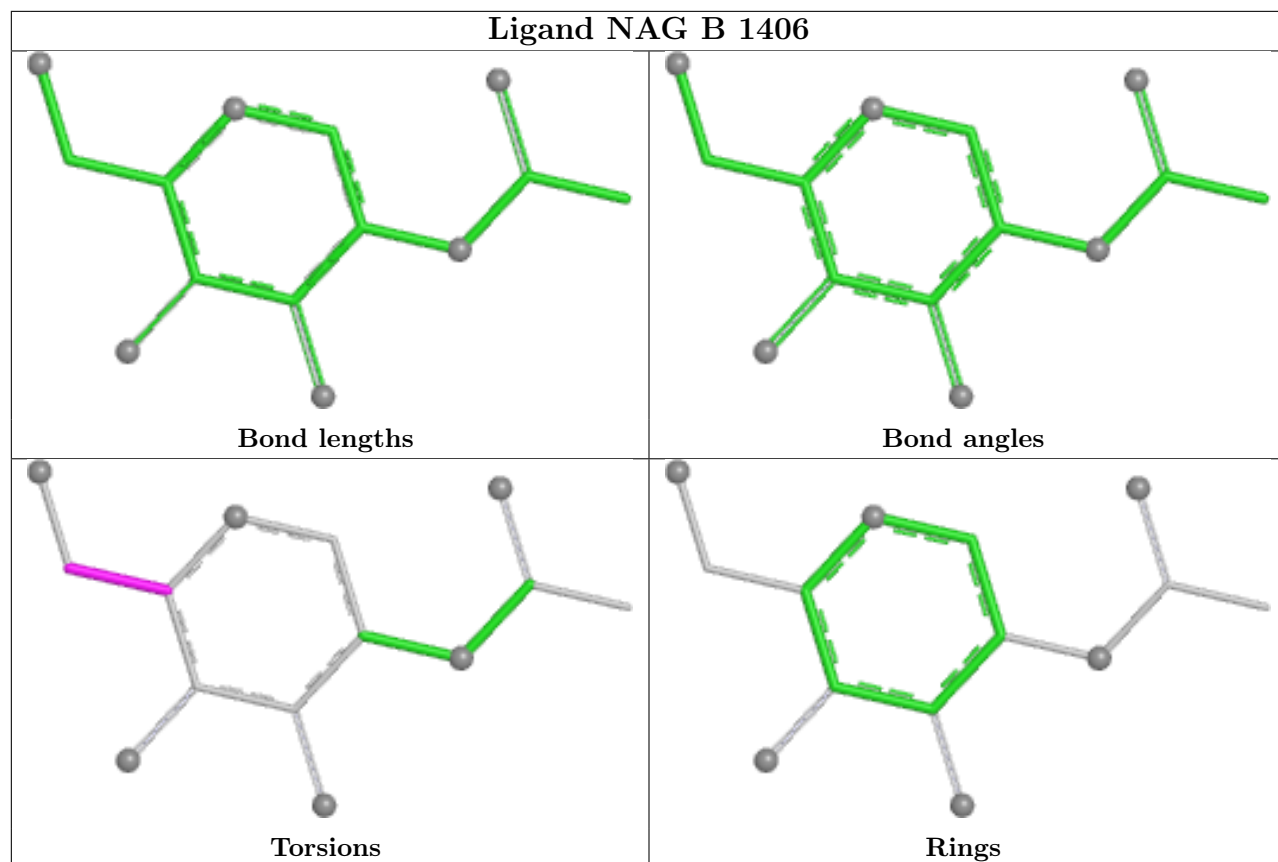
Ligand NAG A 1407



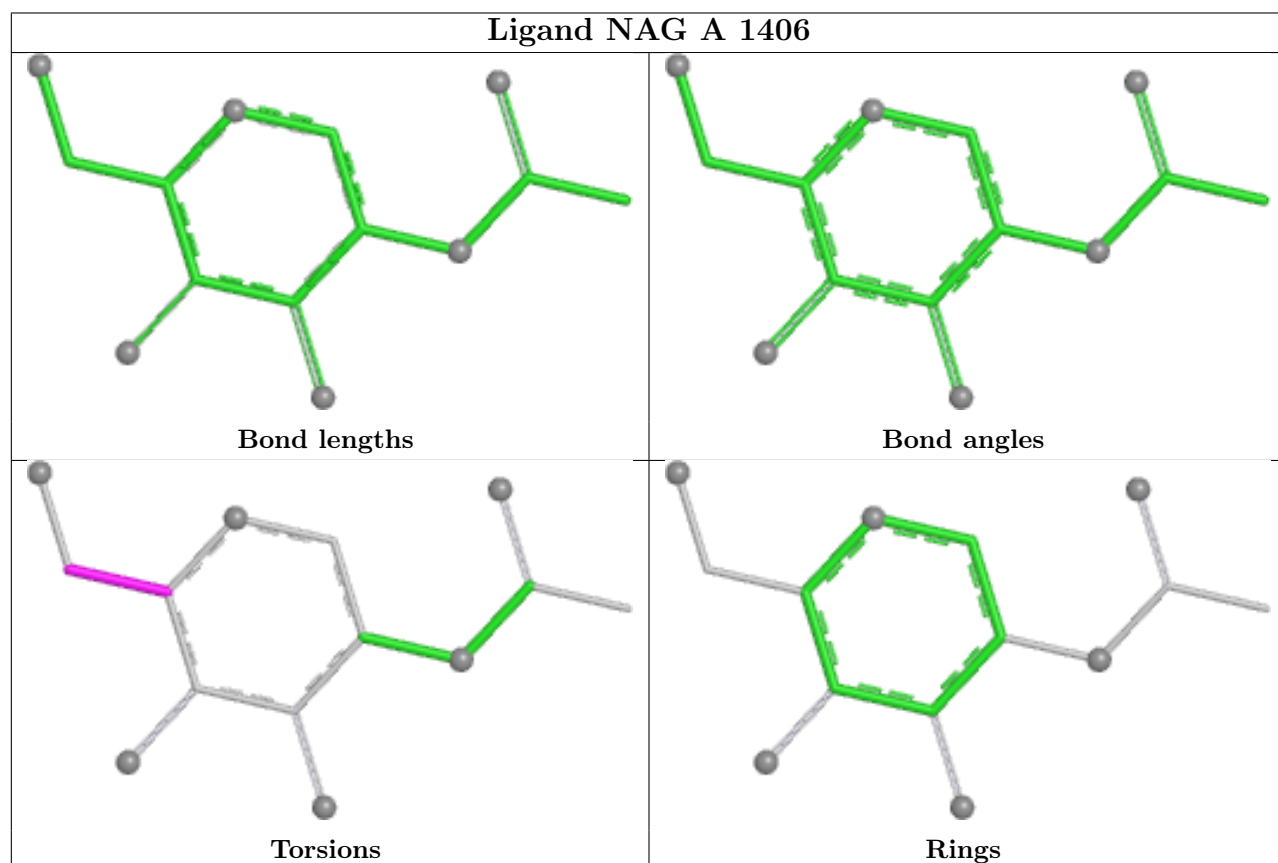
Ligand NAG B 1407

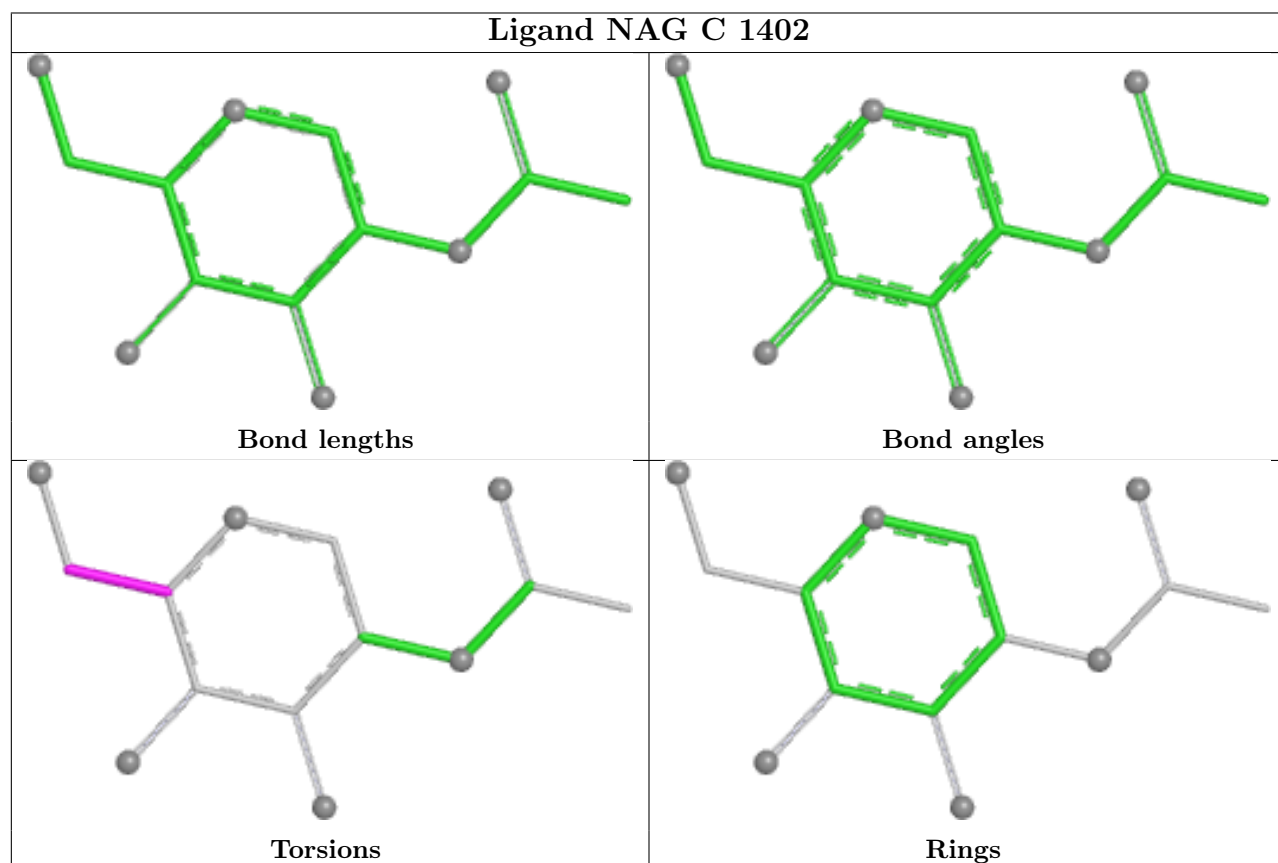
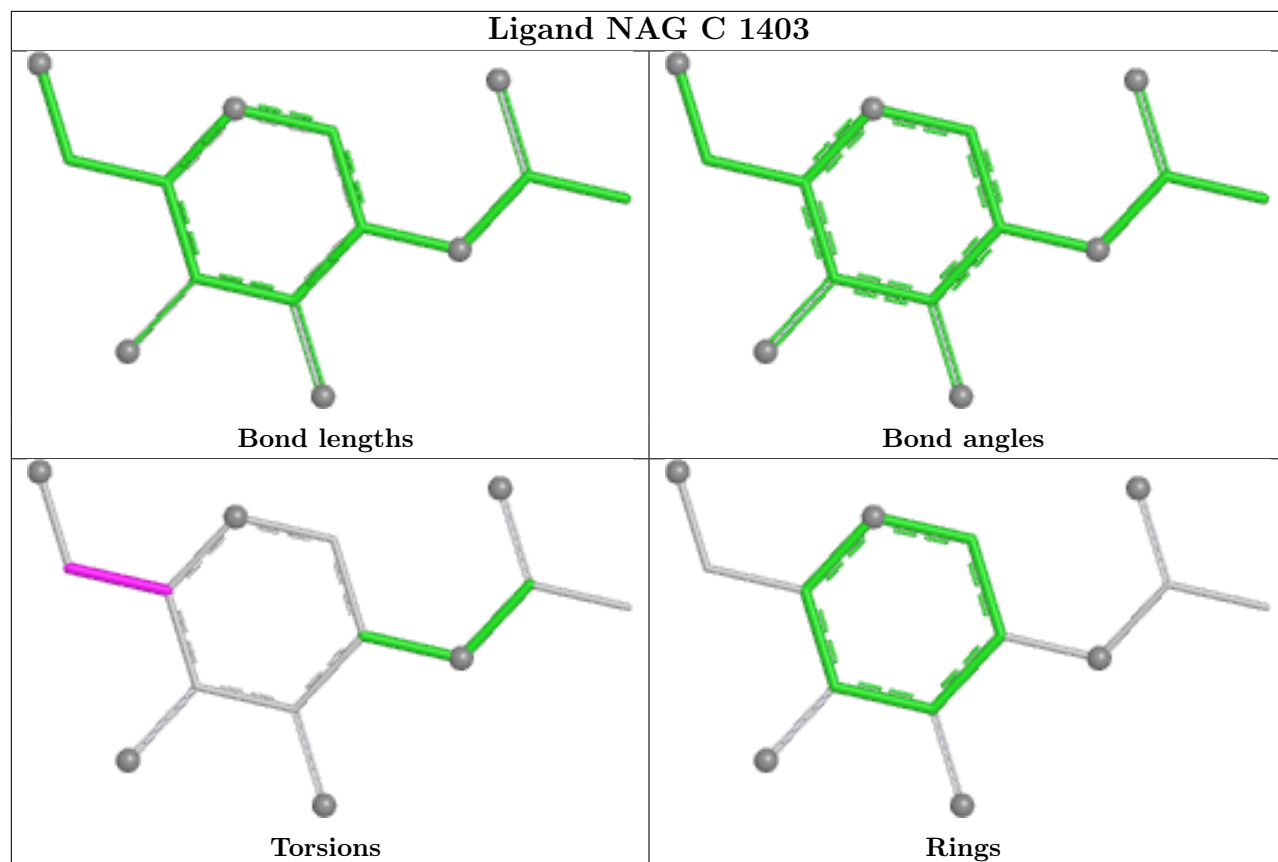


Ligand NAG B 1406

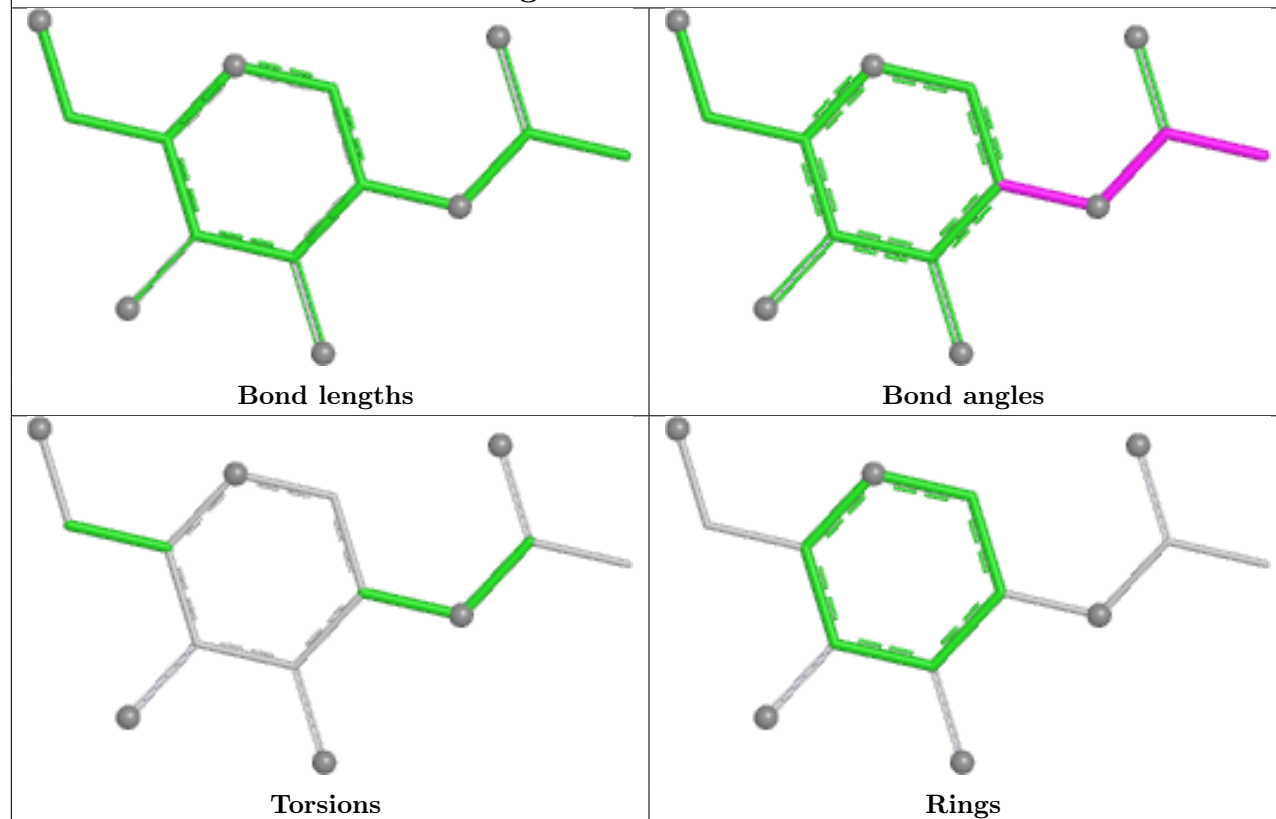


Ligand NAG A 1406

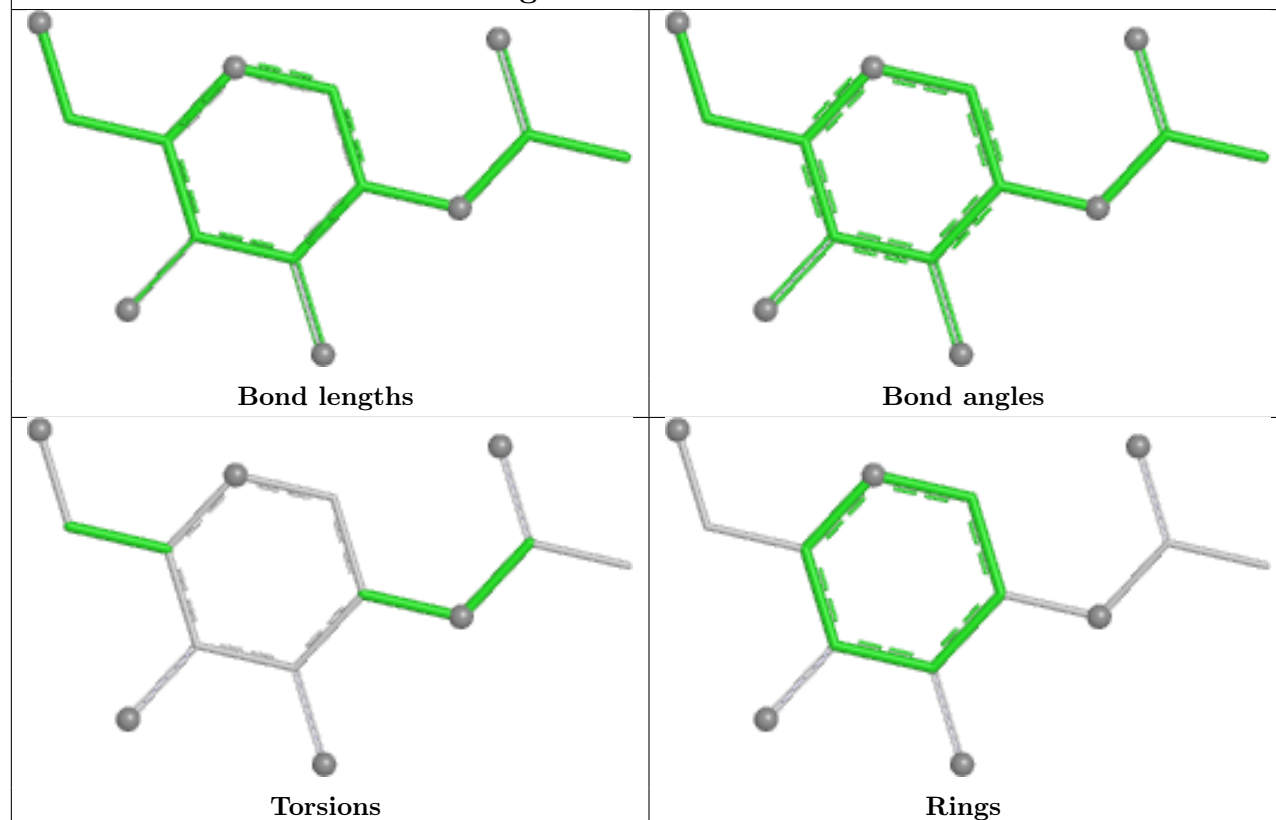




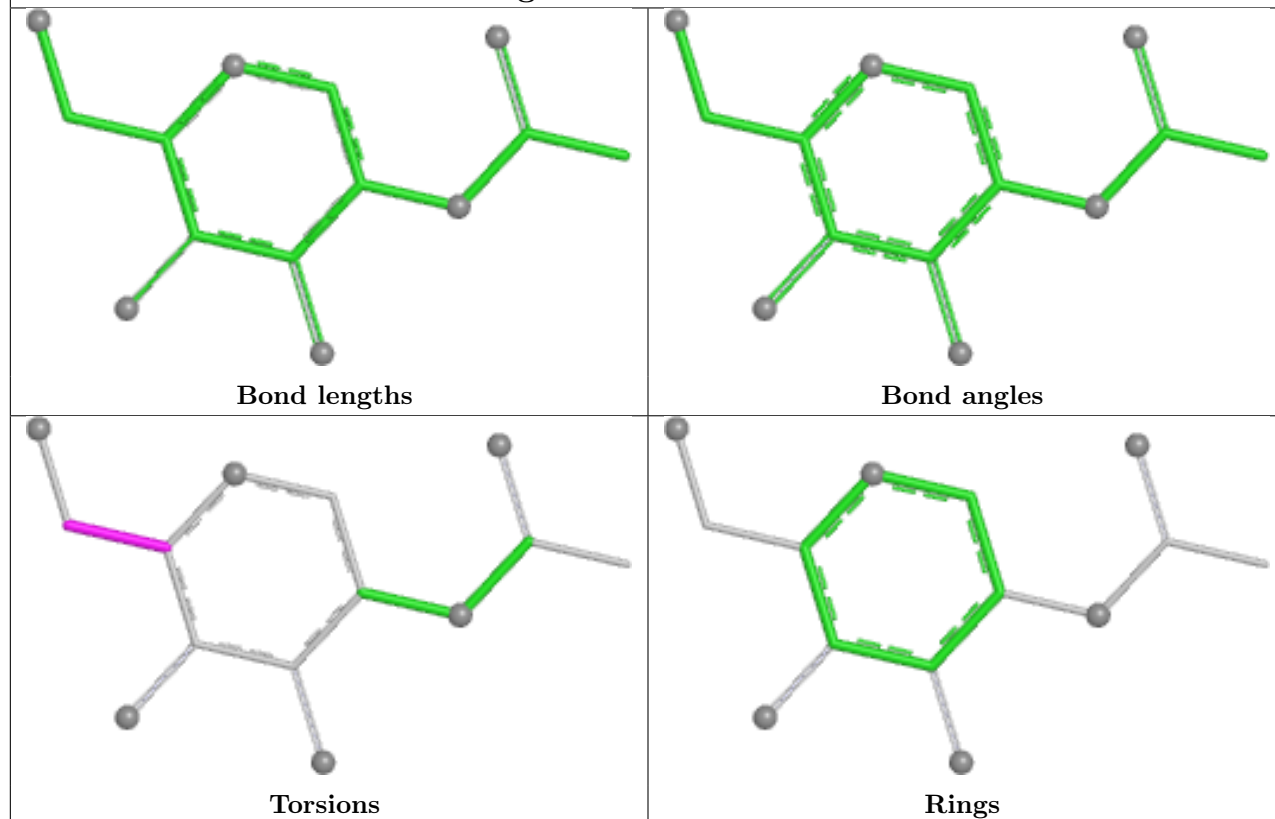
Ligand NAG B 1409



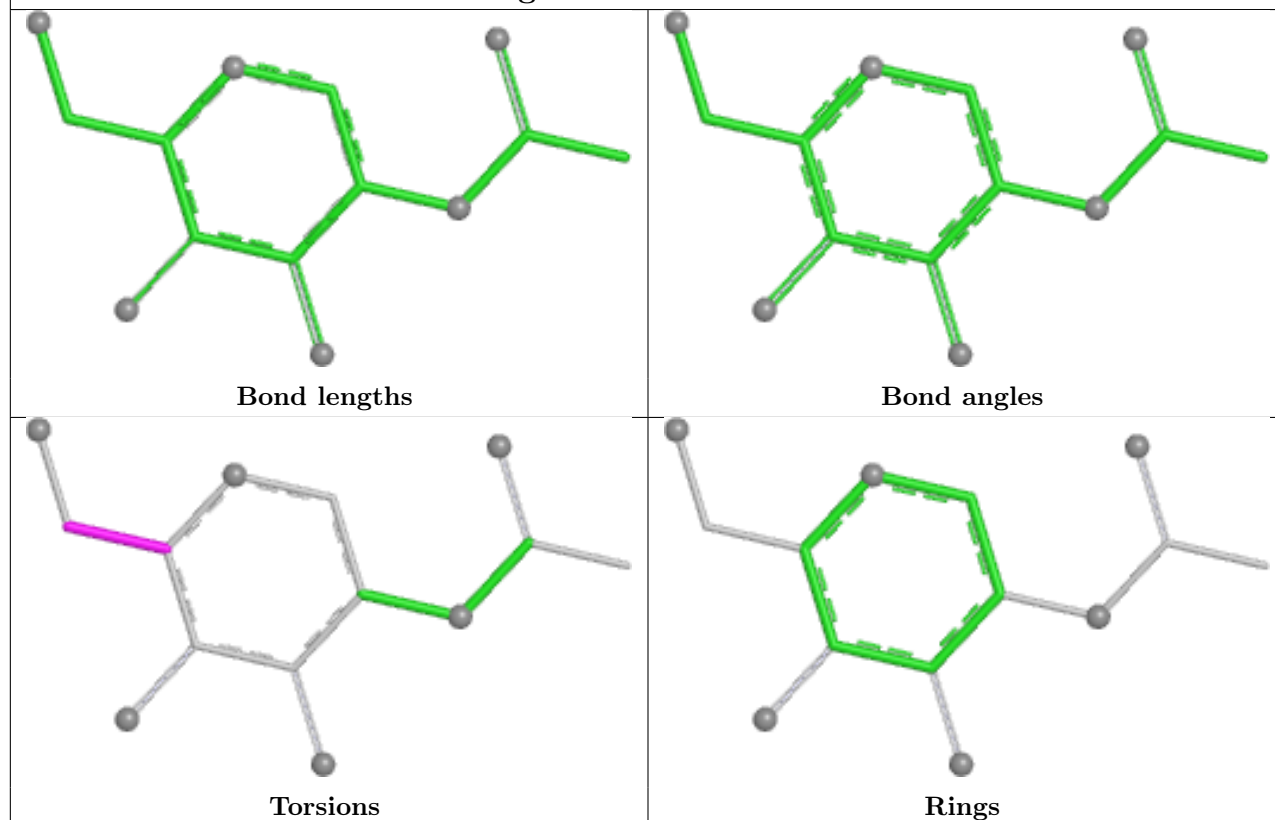
Ligand NAG B 1410



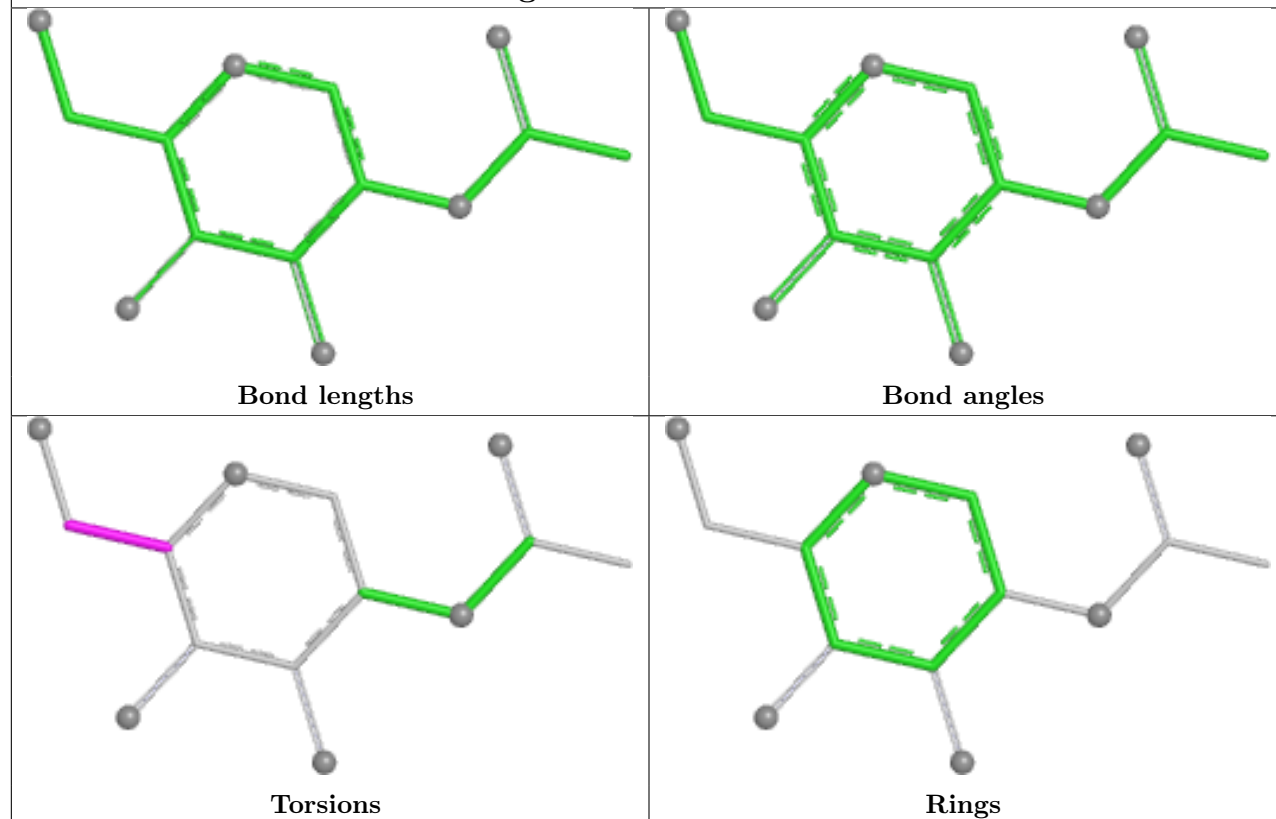
Ligand NAG A 1402



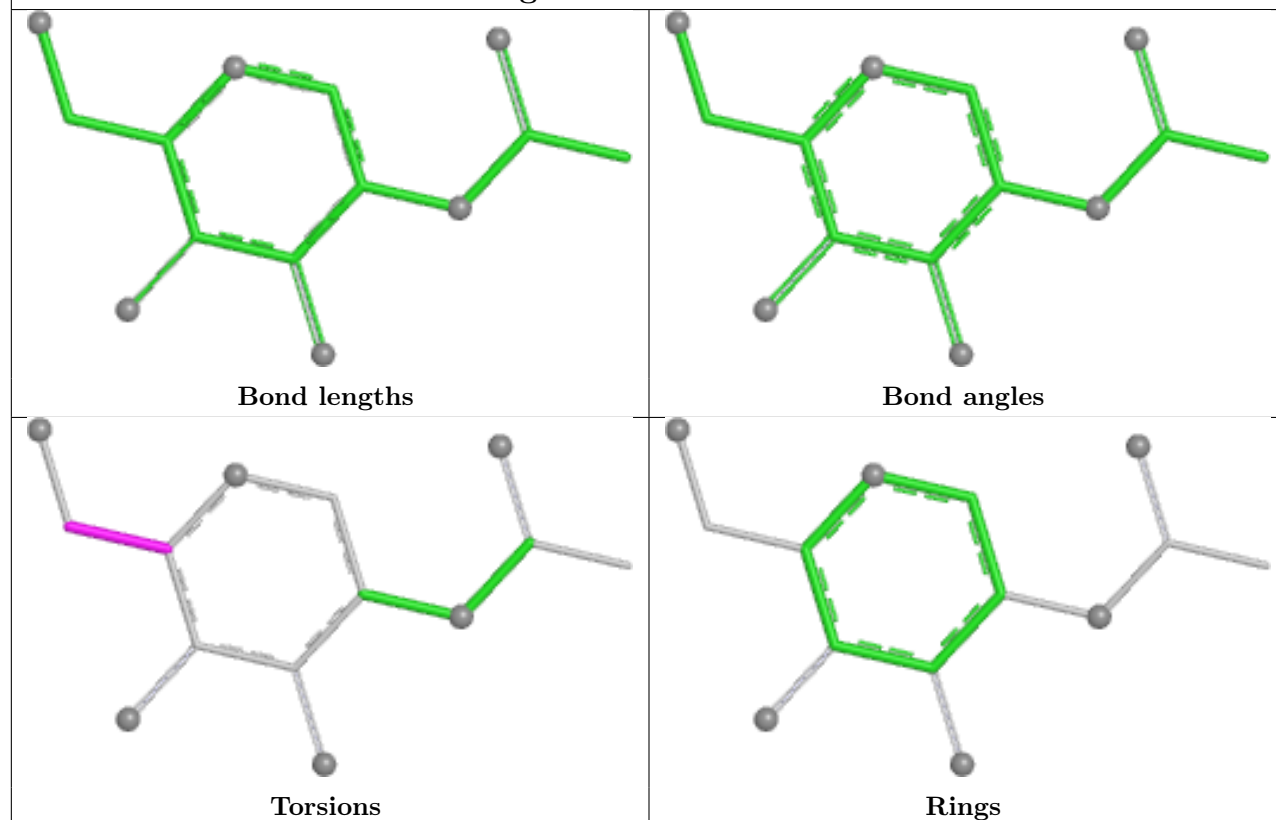
Ligand NAG C 1406



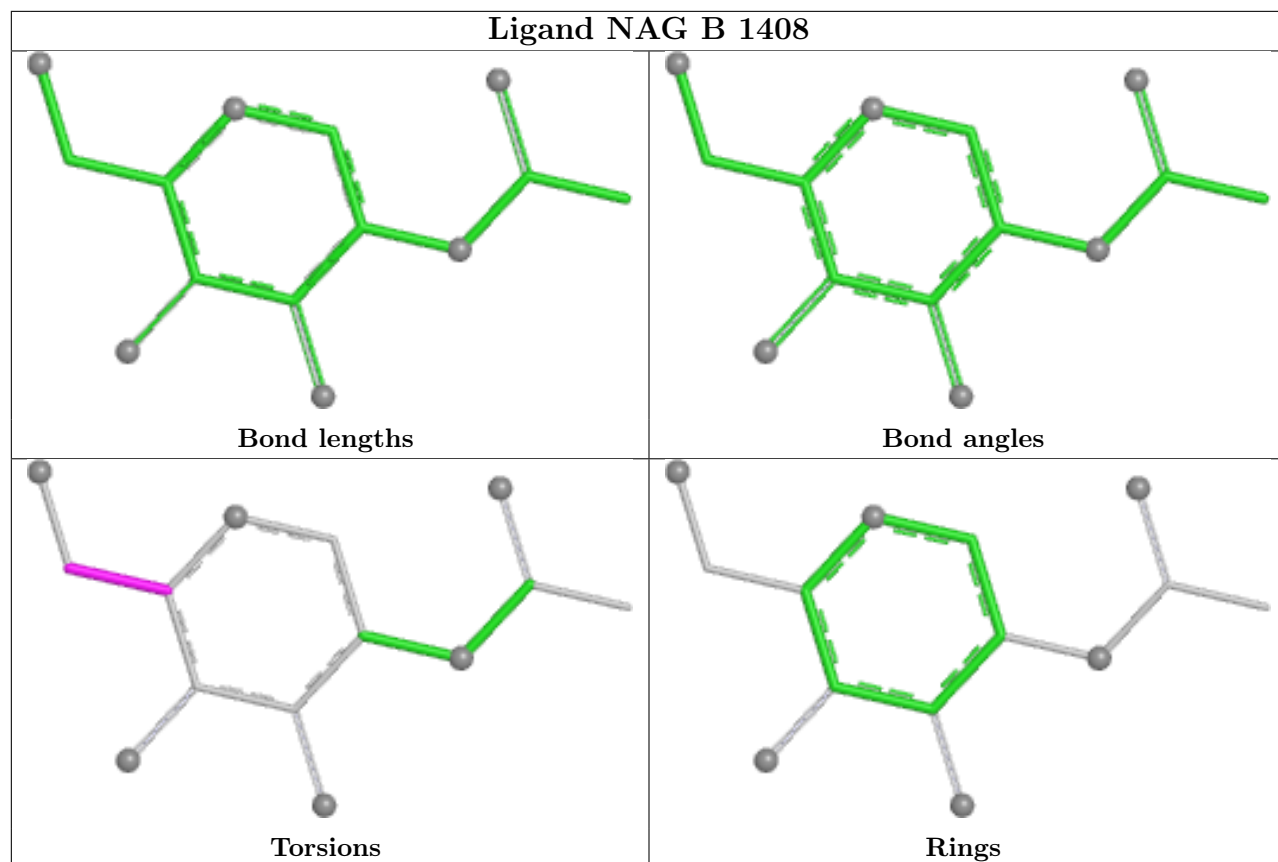
Ligand NAG A 1408



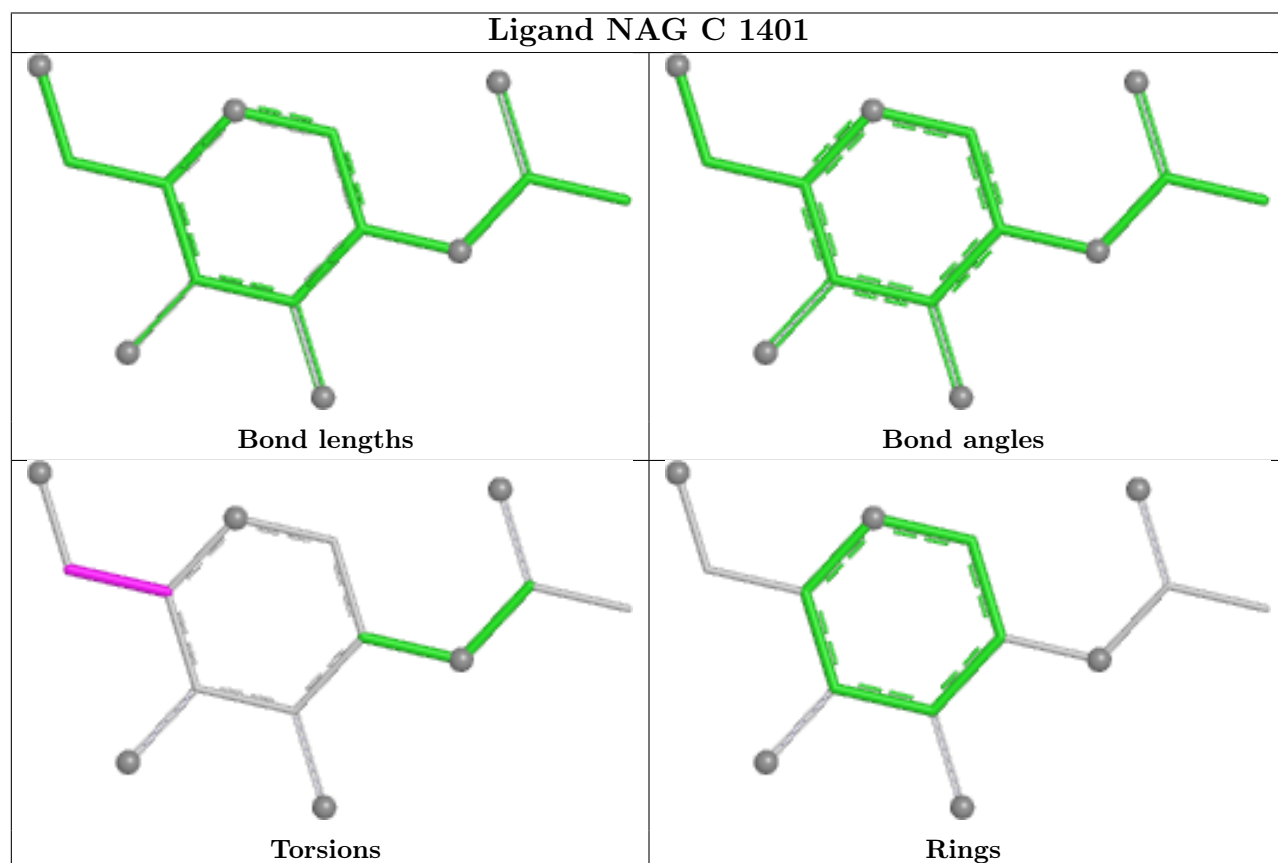
Ligand NAG B 1403



Ligand NAG B 1408



Ligand NAG C 1401



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.

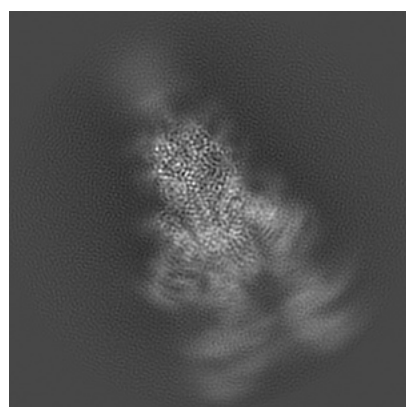
6 Map visualisation [i](#)

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.

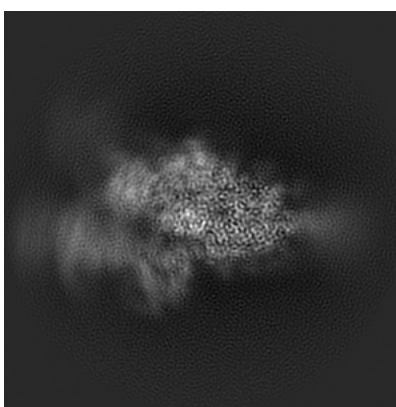
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

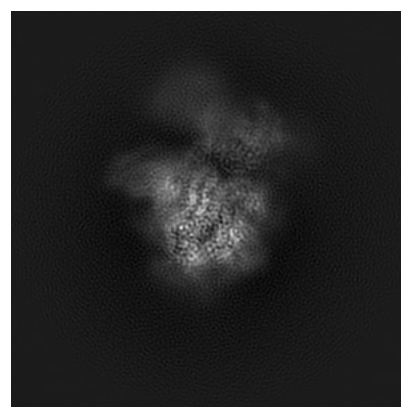
6.1.1 Primary map



X



Y

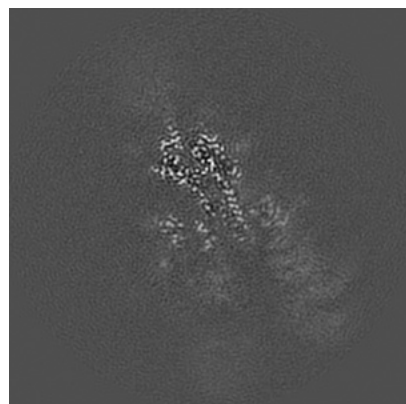


Z

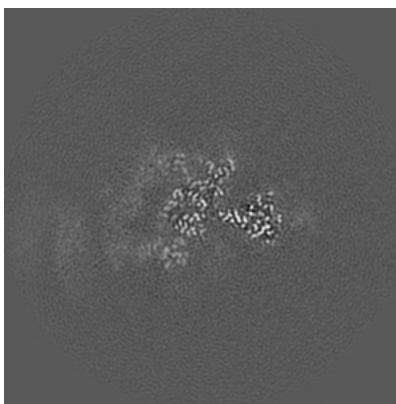
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

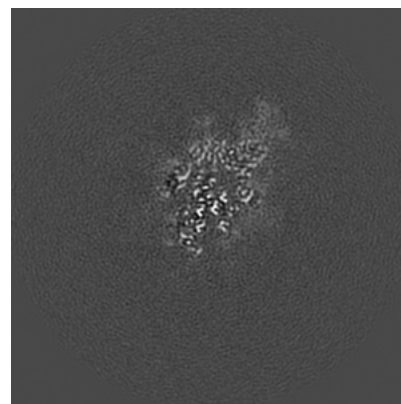
6.2.1 Primary map



X Index: 144



Y Index: 144

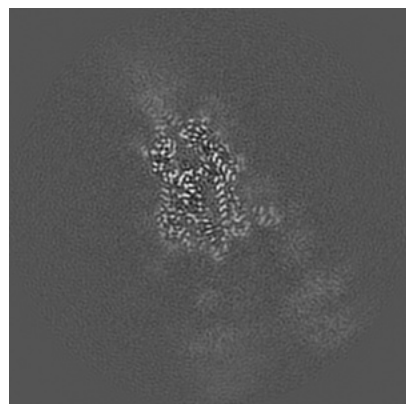


Z Index: 144

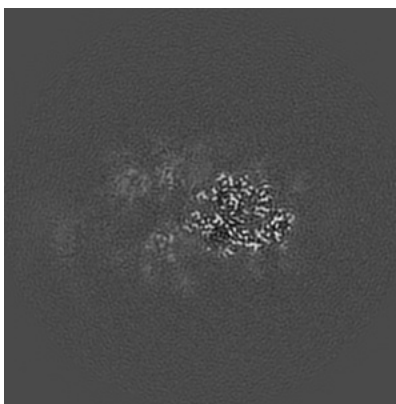
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

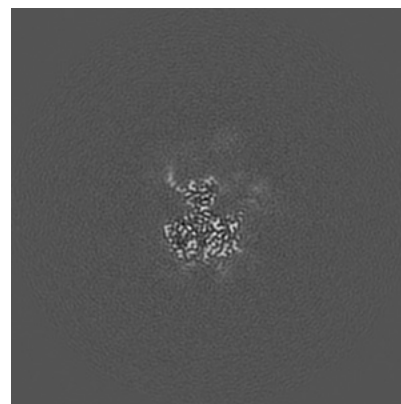
6.3.1 Primary map



X Index: 132



Y Index: 133

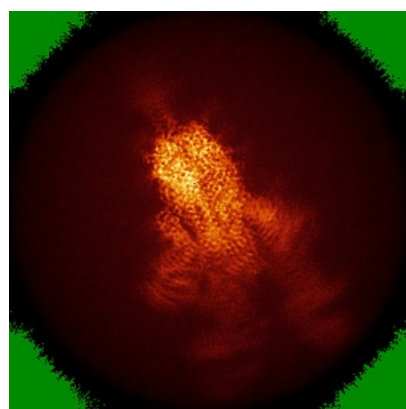


Z Index: 167

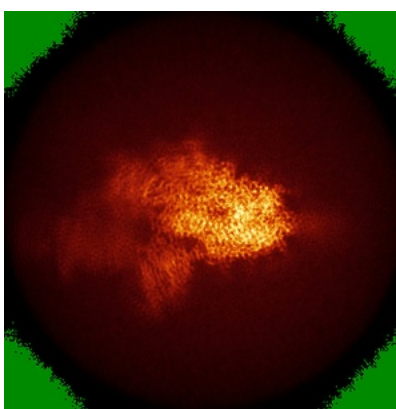
The images above show the largest variance slices of the map in three orthogonal directions.

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

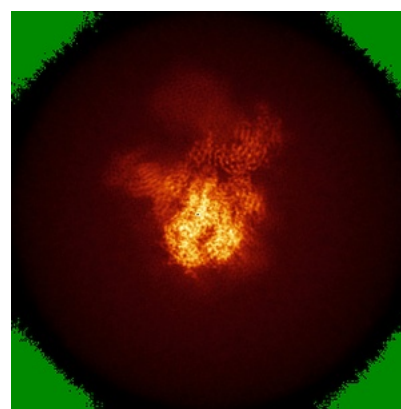
6.4.1 Primary map



X



Y

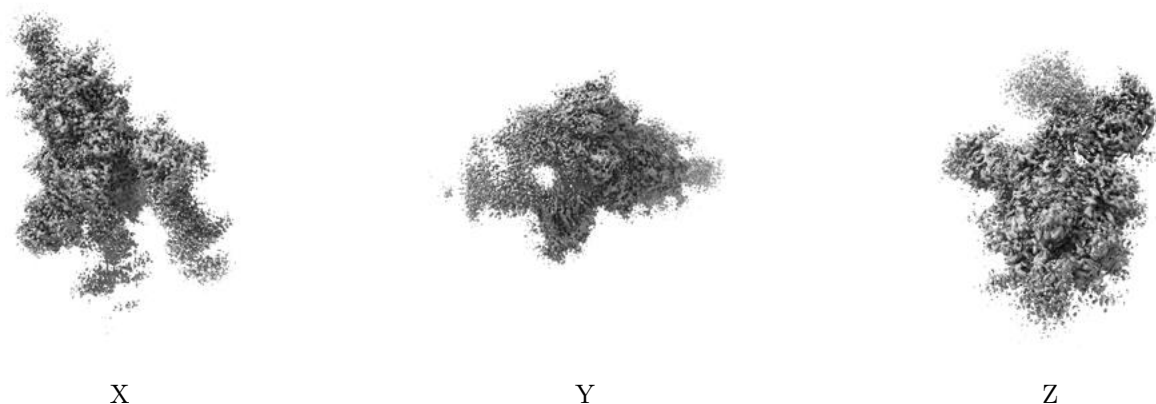


Z

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.

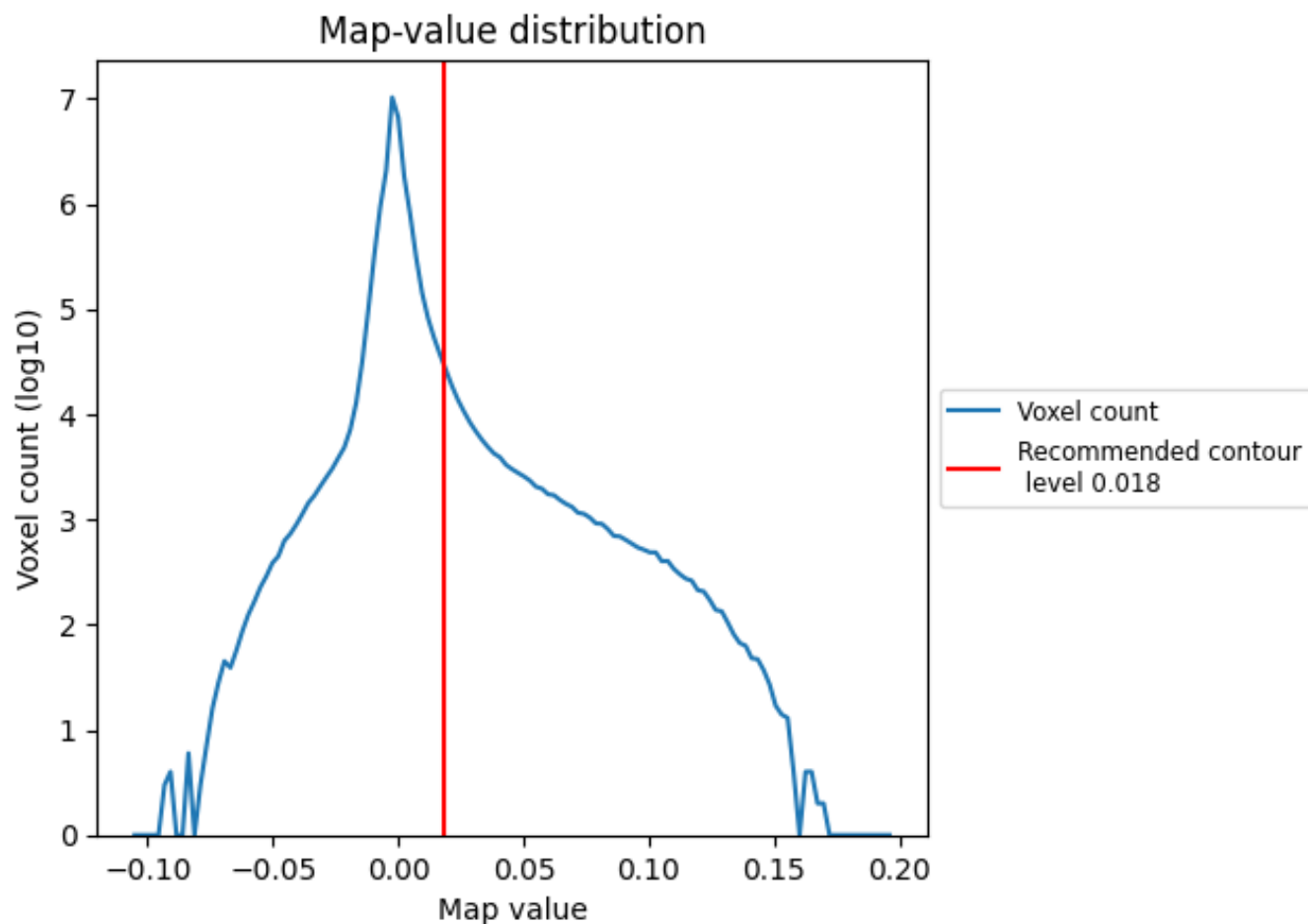
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

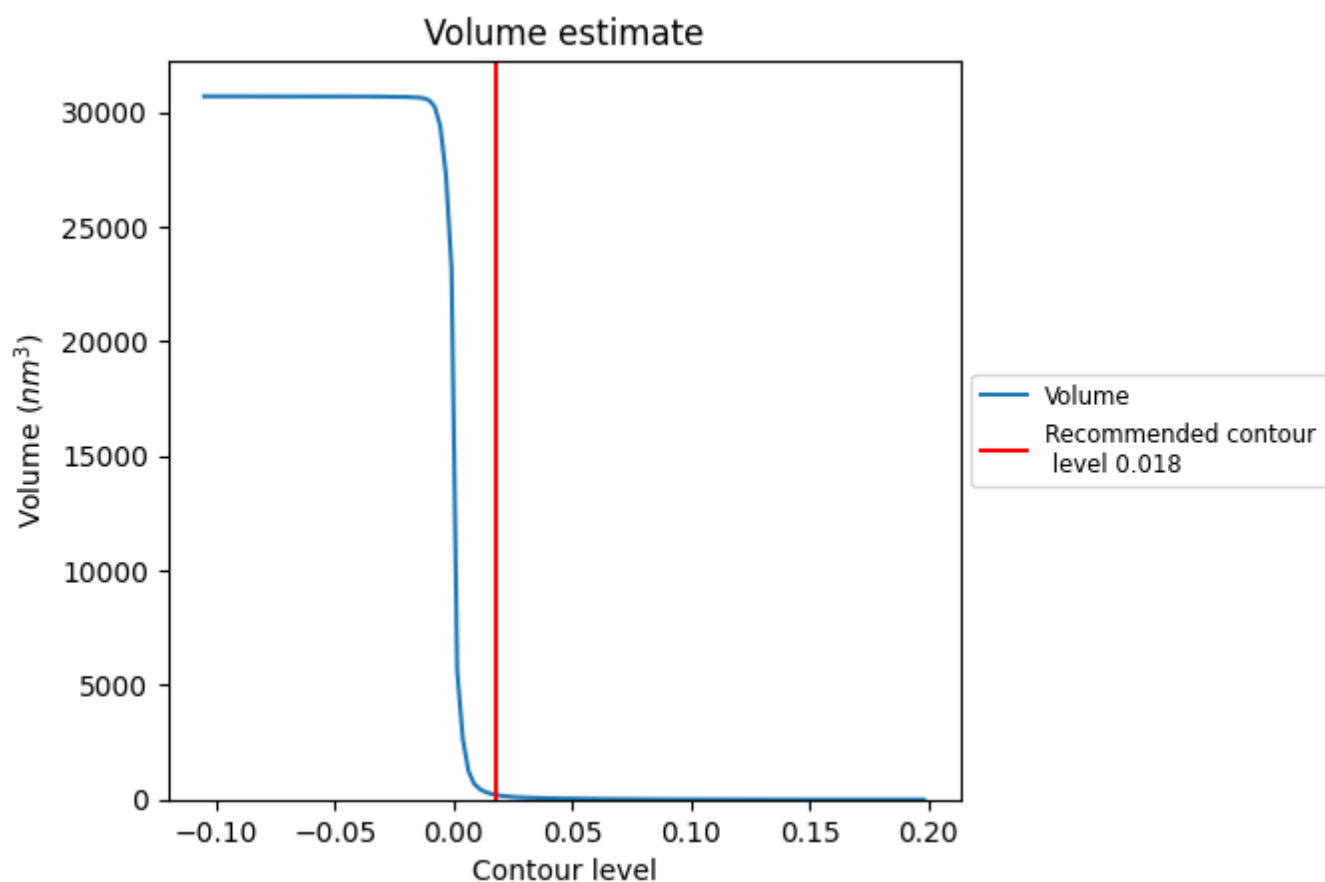
This section contains the results of statistical analysis of the map.

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.

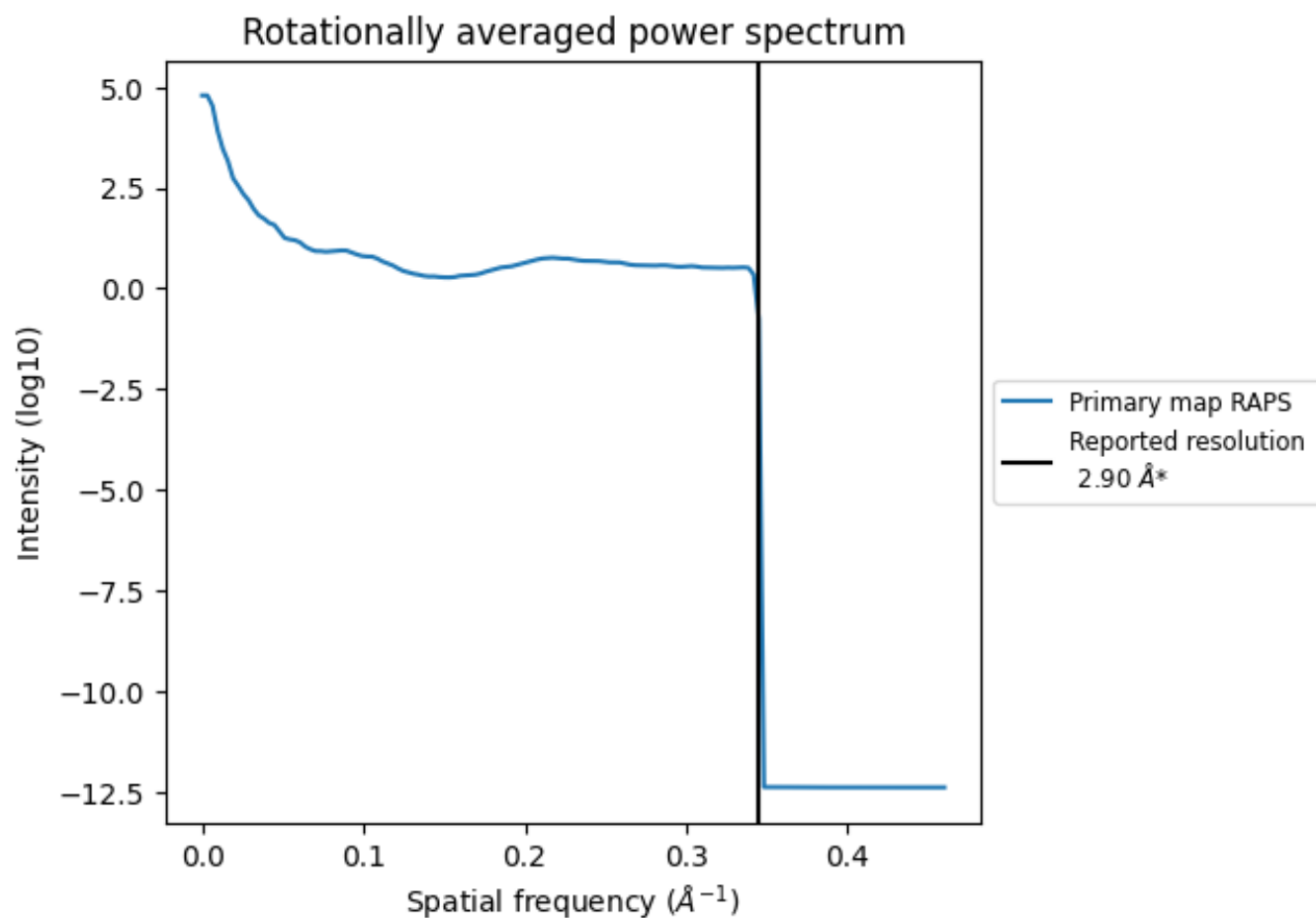
7.2 Volume estimate [i](#)



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

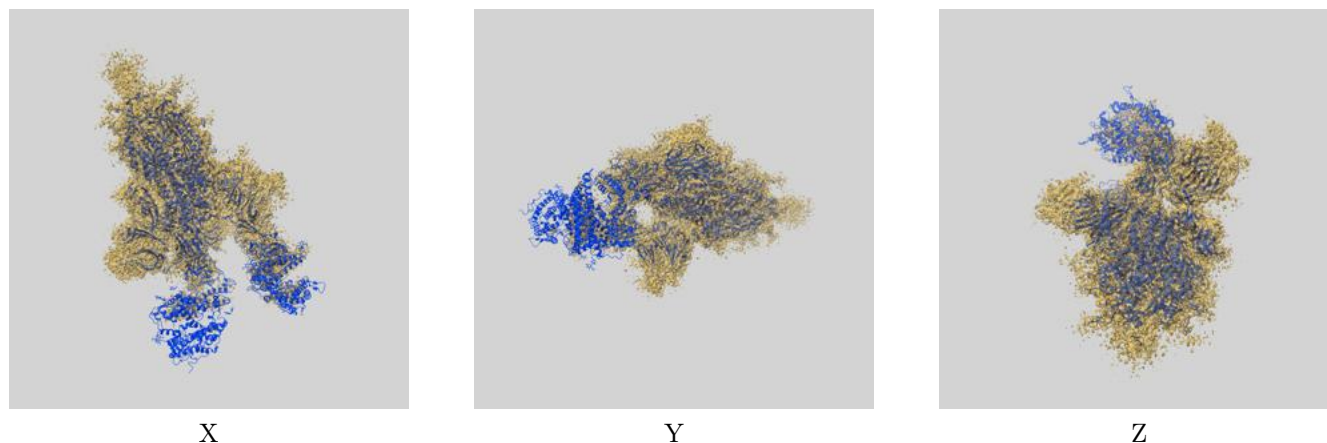
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

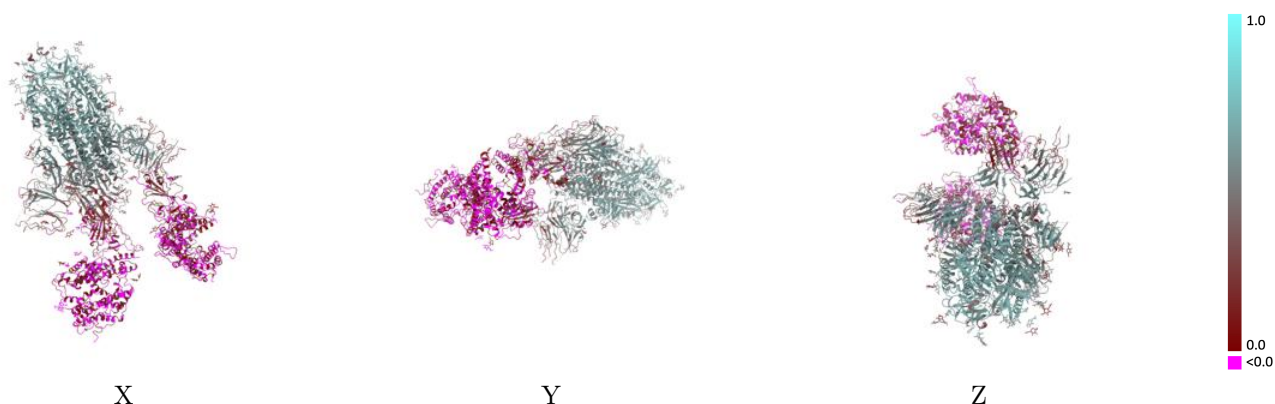
This section contains information regarding the fit between EMDB map EMD-30899 and PDB model 7DX8. Per-residue inclusion information can be found in section [3](#) on page [11](#).

9.1 Map-model overlay [i](#)



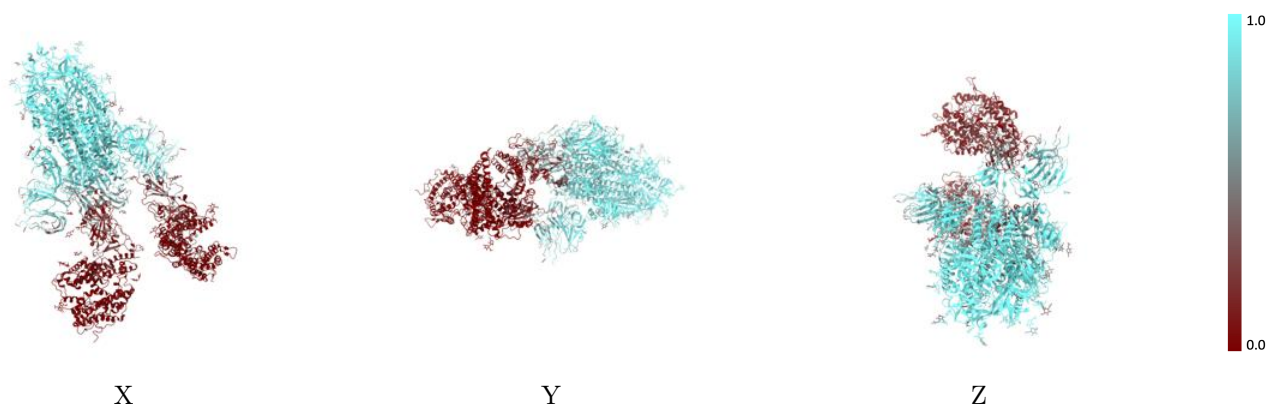
The images above show the 3D surface view of the map at the recommended contour level 0.018 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



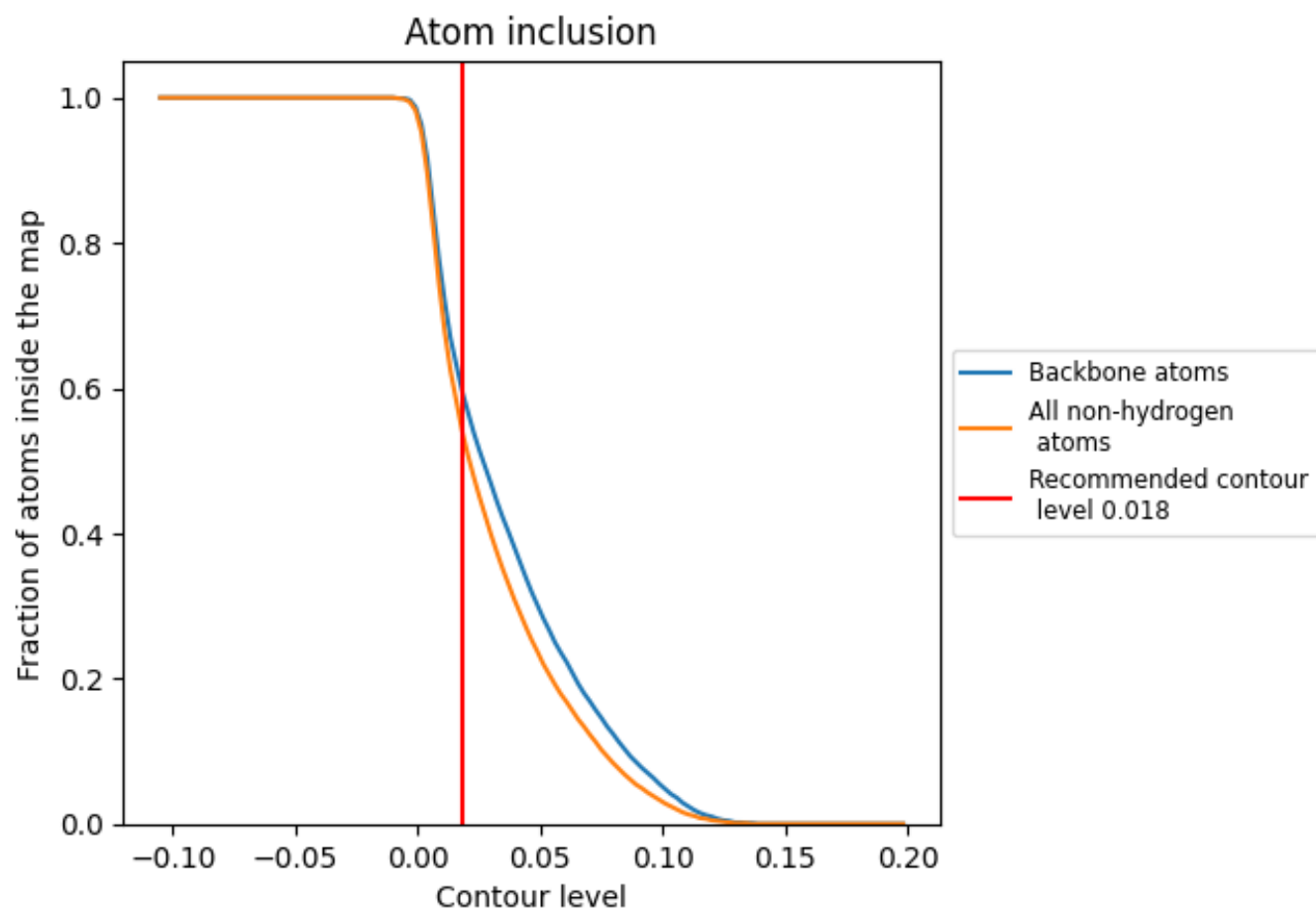
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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



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