



Full wwPDB EM Validation Report ⓘ

Mar 19, 2026 – 10:26 PM UTC

PDB ID : 7DWX / pdb_00007dwx
EMDB ID : EMD-30888
Title : Conformation 1 of S-ACE2-B0AT1 ternary complex
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 : 8.30 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:

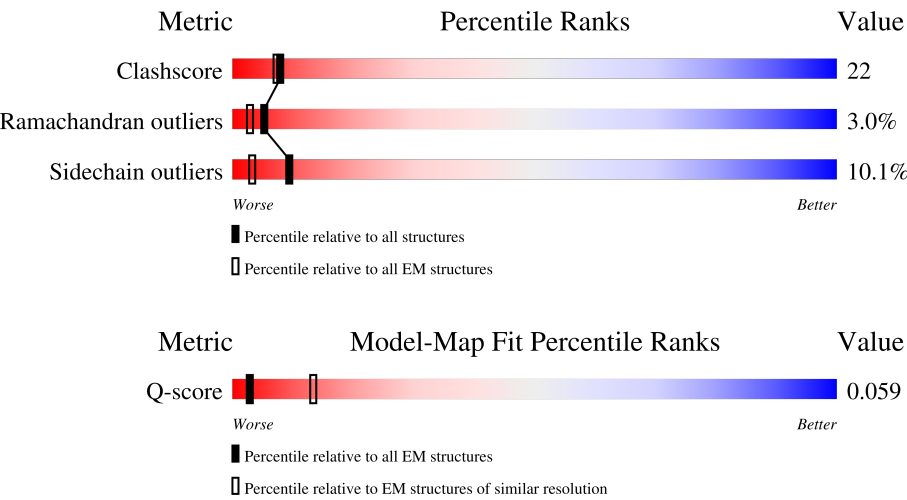
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 8.30 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.



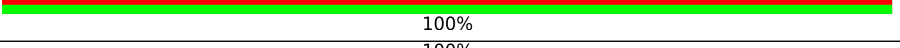
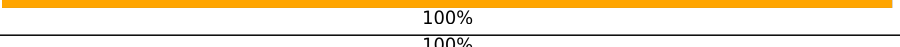
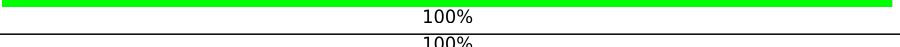
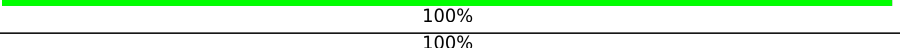
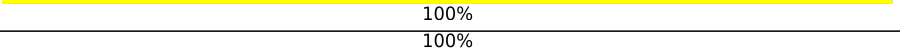
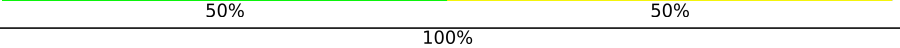
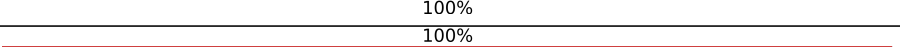
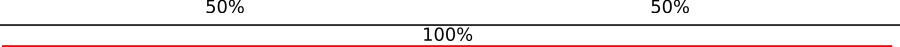
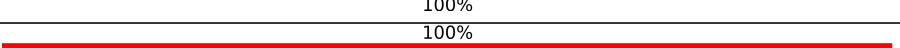
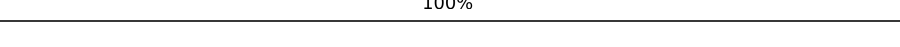
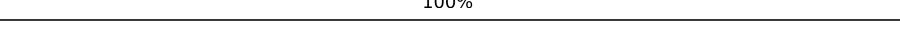
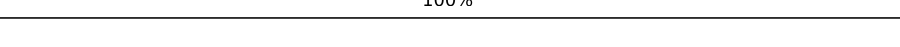
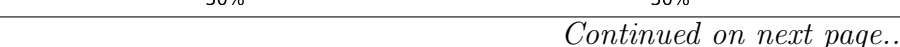
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	280 (7.82 - 8.80)

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	654	 5% 71% 18% • 7%
1	C	654	 6% 72% 17% • 7%
2	B	817	 • 76% 12% • 8%
2	D	817	 5% 76% 12% • 8%

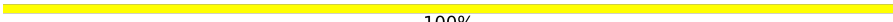
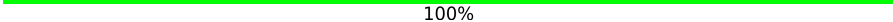
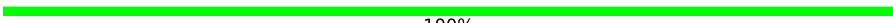
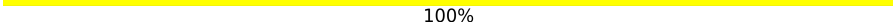
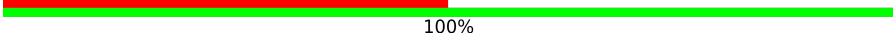
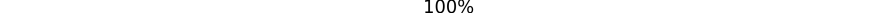
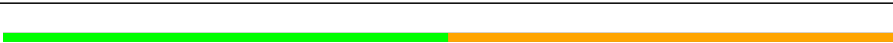
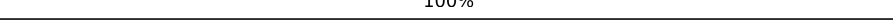
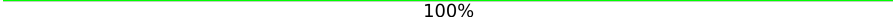
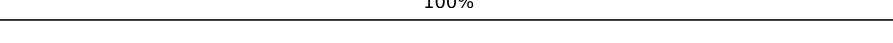
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Mol	Chain	Length	Quality of chain
3	E	1283	
3	F	1283	
3	G	1283	
3	H	1283	
3	I	1283	
3	J	1283	
4	0	2	
4	1	2	
4	2	2	
4	3	2	
4	4	2	
4	5	2	
4	6	2	
4	7	2	
4	8	2	
4	9	2	
4	AA	2	
4	BA	2	
4	CA	2	
4	DA	2	
4	EA	2	
4	FA	2	
4	K	2	
4	L	2	
4	M	2	

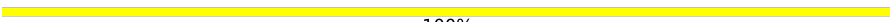
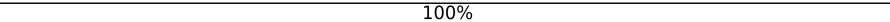
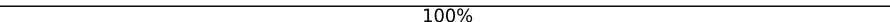
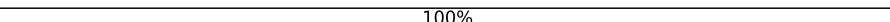
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Mol	Chain	Length	Quality of chain
4	N	2	 100%
4	O	2	 50% 100%
4	P	2	 50% 50%
4	Q	2	 100%
4	R	2	 100%
4	S	2	 50% 100%
4	T	2	 50% 50%
4	U	2	 100%
4	V	2	 50% 100%
4	W	2	 50% 50%
4	X	2	 100%
4	Y	2	 100%
4	Z	2	 100%
4	a	2	 100%
4	b	2	 50% 50%
4	c	2	 50% 50%
4	d	2	 50% 50%
4	e	2	 50% 50%
4	f	2	 50% 50%
4	g	2	 100%
4	h	2	 100%
4	i	2	 50% 50%
4	j	2	 50% 50%
4	k	2	 50% 100%
4	l	2	 100%

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Mol	Chain	Length	Quality of chain
4	m	2	 100%
4	n	2	 100%
4	o	2	 50% 50%
4	p	2	 50% 50%
4	q	2	 100%
4	r	2	 50% 50%
4	s	2	 100%
4	t	2	 100%
4	u	2	 100%
4	v	2	 100%
4	w	2	 50% 50%
4	x	2	 100%
4	y	2	 50% 50%
4	z	2	 100%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 71532 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 Sodium-dependent neutral amino acid transporter B(0)AT1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	605	Total	C	N	O	S	0	0
			4799	3171	744	854	30		
1	C	605	Total	C	N	O	S	0	0
			4799	3171	744	854	30		

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP Q695T7
A	-18	ALA	-	expression tag	UNP Q695T7
A	-17	ASP	-	expression tag	UNP Q695T7
A	-16	TYR	-	expression tag	UNP Q695T7
A	-15	LYS	-	expression tag	UNP Q695T7
A	-14	ASP	-	expression tag	UNP Q695T7
A	-13	ASP	-	expression tag	UNP Q695T7
A	-12	ASP	-	expression tag	UNP Q695T7
A	-11	ASP	-	expression tag	UNP Q695T7
A	-10	LYS	-	expression tag	UNP Q695T7
A	-9	SER	-	expression tag	UNP Q695T7
A	-8	GLY	-	expression tag	UNP Q695T7
A	-7	PRO	-	expression tag	UNP Q695T7
A	-6	ASP	-	expression tag	UNP Q695T7
A	-5	GLU	-	expression tag	UNP Q695T7
A	-4	VAL	-	expression tag	UNP Q695T7
A	-3	ASP	-	expression tag	UNP Q695T7
A	-2	ALA	-	expression tag	UNP Q695T7
A	-1	SER	-	expression tag	UNP Q695T7
A	0	GLY	-	expression tag	UNP Q695T7
A	1	ARG	-	expression tag	UNP Q695T7
C	-19	MET	-	initiating methionine	UNP Q695T7
C	-18	ALA	-	expression tag	UNP Q695T7
C	-17	ASP	-	expression tag	UNP Q695T7
C	-16	TYR	-	expression tag	UNP Q695T7
C	-15	LYS	-	expression tag	UNP Q695T7

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-14	ASP	-	expression tag	UNP Q695T7
C	-13	ASP	-	expression tag	UNP Q695T7
C	-12	ASP	-	expression tag	UNP Q695T7
C	-11	ASP	-	expression tag	UNP Q695T7
C	-10	LYS	-	expression tag	UNP Q695T7
C	-9	SER	-	expression tag	UNP Q695T7
C	-8	GLY	-	expression tag	UNP Q695T7
C	-7	PRO	-	expression tag	UNP Q695T7
C	-6	ASP	-	expression tag	UNP Q695T7
C	-5	GLU	-	expression tag	UNP Q695T7
C	-4	VAL	-	expression tag	UNP Q695T7
C	-3	ASP	-	expression tag	UNP Q695T7
C	-2	ALA	-	expression tag	UNP Q695T7
C	-1	SER	-	expression tag	UNP Q695T7
C	0	GLY	-	expression tag	UNP Q695T7
C	1	ARG	-	expression tag	UNP Q695T7

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	748	Total	C	N	O	S	0	0
			6089	3906	1018	1131	34		
2	D	748	Total	C	N	O	S	0	0
			6089	3906	1018	1131	34		

There are 26 discrepancies between the modelled and reference sequences:

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

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Chain	Residue	Modelled	Actual	Comment	Reference
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

- Molecule 3 is a protein called Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	1007	Total	C	N	O	S	0	0
			7872	5025	1310	1501	36		
3	F	1006	Total	C	N	O	S	0	0
			7866	5022	1309	1499	36		
3	G	1006	Total	C	N	O	S	0	0
			7866	5022	1309	1499	36		
3	H	1007	Total	C	N	O	S	0	0
			7872	5025	1310	1501	36		
3	I	1006	Total	C	N	O	S	0	0
			7866	5022	1309	1499	36		
3	J	1006	Total	C	N	O	S	0	0
			7866	5022	1309	1499	36		

There are 72 discrepancies between the modelled and reference sequences:

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

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

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

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



Mol	Chain	Residues	Atoms				AltConf	Trace
4	K	2	Total	C	N	O	0	0
			28	16	2	10		
4	L	2	Total	C	N	O	0	0
			28	16	2	10		
4	M	2	Total	C	N	O	0	0
			28	16	2	10		
4	N	2	Total	C	N	O	0	0
			28	16	2	10		
4	O	2	Total	C	N	O	0	0
			28	16	2	10		
4	P	2	Total	C	N	O	0	0
			28	16	2	10		

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

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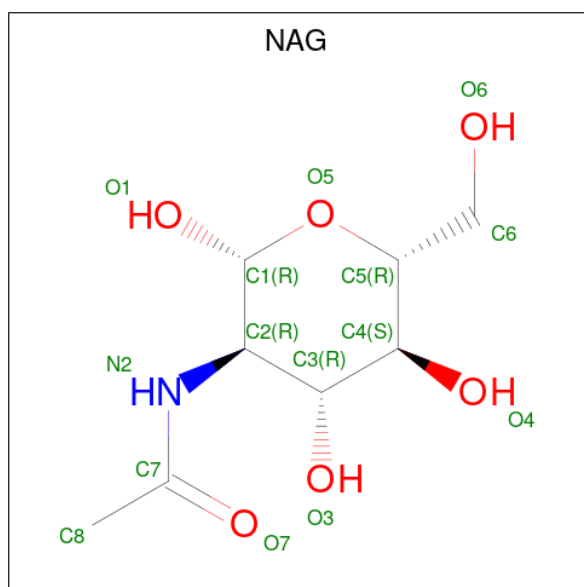
Mol	Chain	Residues	Atoms				AltConf	Trace
4	l	2	Total	C	N	O	0	0
			28	16	2	10		
4	m	2	Total	C	N	O	0	0
			28	16	2	10		
4	n	2	Total	C	N	O	0	0
			28	16	2	10		
4	o	2	Total	C	N	O	0	0
			28	16	2	10		
4	p	2	Total	C	N	O	0	0
			28	16	2	10		
4	q	2	Total	C	N	O	0	0
			28	16	2	10		
4	r	2	Total	C	N	O	0	0
			28	16	2	10		
4	s	2	Total	C	N	O	0	0
			28	16	2	10		
4	t	2	Total	C	N	O	0	0
			28	16	2	10		
4	u	2	Total	C	N	O	0	0
			28	16	2	10		
4	v	2	Total	C	N	O	0	0
			28	16	2	10		
4	w	2	Total	C	N	O	0	0
			28	16	2	10		
4	x	2	Total	C	N	O	0	0
			28	16	2	10		
4	y	2	Total	C	N	O	0	0
			28	16	2	10		
4	z	2	Total	C	N	O	0	0
			28	16	2	10		
4	0	2	Total	C	N	O	0	0
			28	16	2	10		
4	1	2	Total	C	N	O	0	0
			28	16	2	10		
4	2	2	Total	C	N	O	0	0
			28	16	2	10		
4	3	2	Total	C	N	O	0	0
			28	16	2	10		
4	4	2	Total	C	N	O	0	0
			28	16	2	10		
4	5	2	Total	C	N	O	0	0
			28	16	2	10		

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Mol	Chain	Residues	Atoms				AltConf	Trace
4	6	2	Total	C	N	O	0	0
			28	16	2	10		
4	7	2	Total	C	N	O	0	0
			28	16	2	10		
4	8	2	Total	C	N	O	0	0
			28	16	2	10		
4	9	2	Total	C	N	O	0	0
			28	16	2	10		
4	AA	2	Total	C	N	O	0	0
			28	16	2	10		
4	BA	2	Total	C	N	O	0	0
			28	16	2	10		
4	CA	2	Total	C	N	O	0	0
			28	16	2	10		
4	DA	2	Total	C	N	O	0	0
			28	16	2	10		
4	EA	2	Total	C	N	O	0	0
			28	16	2	10		
4	FA	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$) (labeled as "Ligand of Interest" by depositor).



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

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

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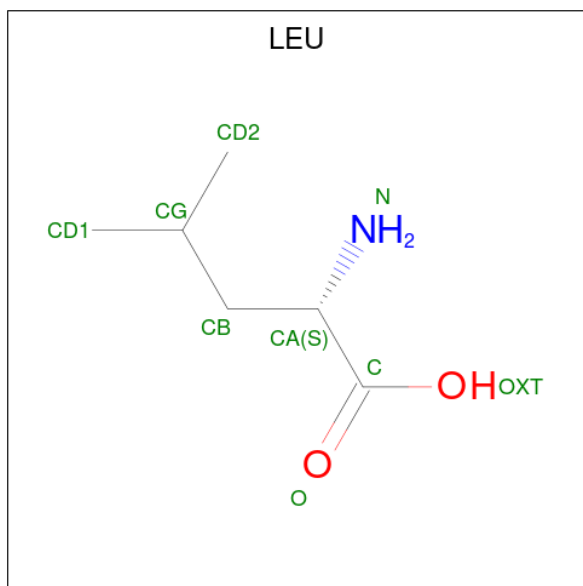
Mol	Chain	Residues	Atoms				AltConf
5	F	1	Total	C	N	O	0
			14	8	1	5	
5	F	1	Total	C	N	O	0
			14	8	1	5	
5	F	1	Total	C	N	O	0
			14	8	1	5	
5	F	1	Total	C	N	O	0
			14	8	1	5	
5	F	1	Total	C	N	O	0
			14	8	1	5	
5	F	1	Total	C	N	O	0
			14	8	1	5	
5	G	1	Total	C	N	O	0
			14	8	1	5	
5	G	1	Total	C	N	O	0
			14	8	1	5	
5	G	1	Total	C	N	O	0
			14	8	1	5	
5	G	1	Total	C	N	O	0
			14	8	1	5	
5	G	1	Total	C	N	O	0
			14	8	1	5	
5	G	1	Total	C	N	O	0
			14	8	1	5	
5	G	1	Total	C	N	O	0
			14	8	1	5	
5	H	1	Total	C	N	O	0
			14	8	1	5	
5	H	1	Total	C	N	O	0
			14	8	1	5	
5	H	1	Total	C	N	O	0
			14	8	1	5	
5	H	1	Total	C	N	O	0
			14	8	1	5	
5	H	1	Total	C	N	O	0
			14	8	1	5	

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Mol	Chain	Residues	Atoms				AltConf
5	H	1	Total	C	N	O	0
			14	8	1	5	
5	H	1	Total	C	N	O	0
			14	8	1	5	
5	H	1	Total	C	N	O	0
			14	8	1	5	
5	I	1	Total	C	N	O	0
			14	8	1	5	
5	I	1	Total	C	N	O	0
			14	8	1	5	
5	I	1	Total	C	N	O	0
			14	8	1	5	
5	I	1	Total	C	N	O	0
			14	8	1	5	
5	I	1	Total	C	N	O	0
			14	8	1	5	
5	I	1	Total	C	N	O	0
			14	8	1	5	
5	I	1	Total	C	N	O	0
			14	8	1	5	
5	I	1	Total	C	N	O	0
			14	8	1	5	
5	J	1	Total	C	N	O	0
			14	8	1	5	
5	J	1	Total	C	N	O	0
			14	8	1	5	
5	J	1	Total	C	N	O	0
			14	8	1	5	
5	J	1	Total	C	N	O	0
			14	8	1	5	
5	J	1	Total	C	N	O	0
			14	8	1	5	
5	J	1	Total	C	N	O	0
			14	8	1	5	

- Molecule 6 is LEUCINE (CCD ID: LEU) (formula: $C_6H_{13}NO_2$).



Mol	Chain	Residues	Atoms				AltConf
6	A	1	Total	C	N	O	0
			9	6	1	2	
6	C	1	Total	C	N	O	0
			9	6	1	2	

- Molecule 7 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
7	B	1	Total	Zn	0
			1	1	
7	D	1	Total	Zn	0
			1	1	

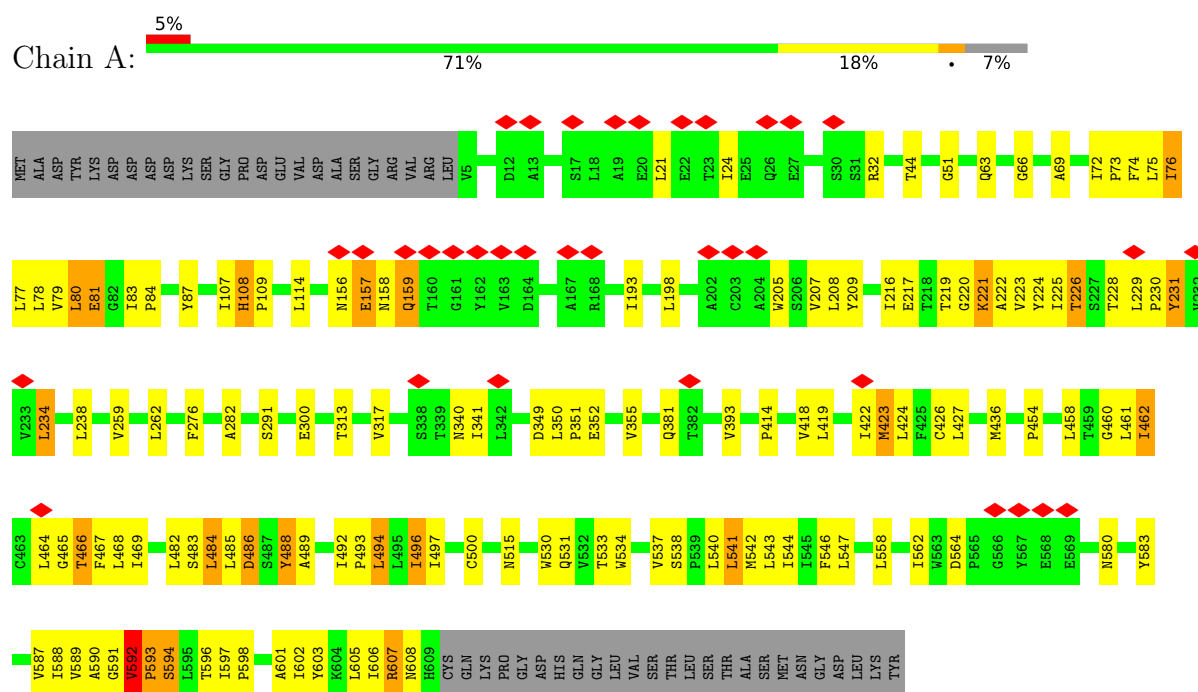
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		AltConf
8	B	4	Total	O	0
			4	4	
8	D	4	Total	O	0
			4	4	

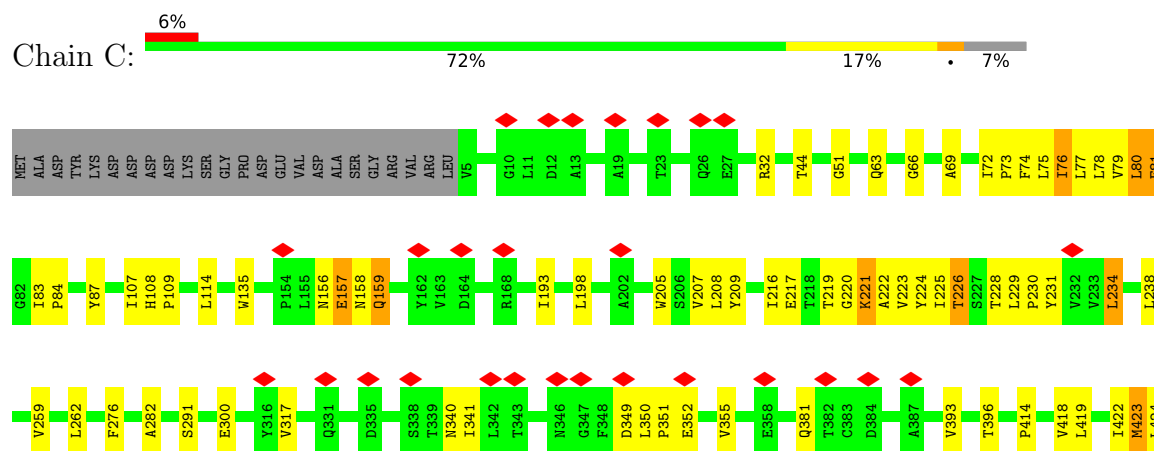
3 Residue-property plots

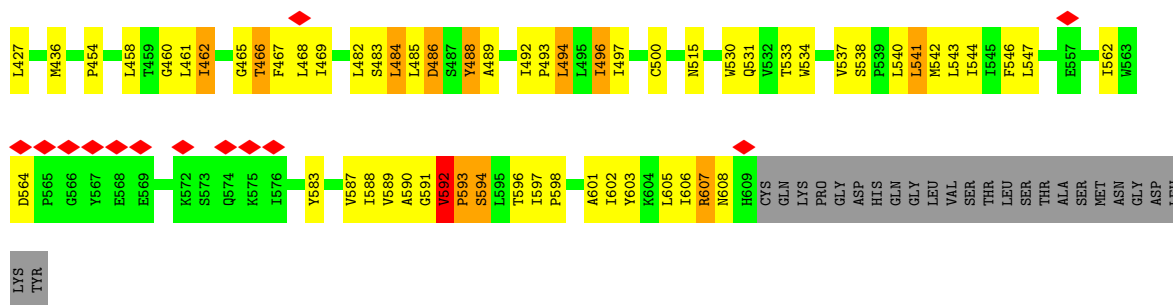
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Sodium-dependent neutral amino acid transporter B(0)AT1



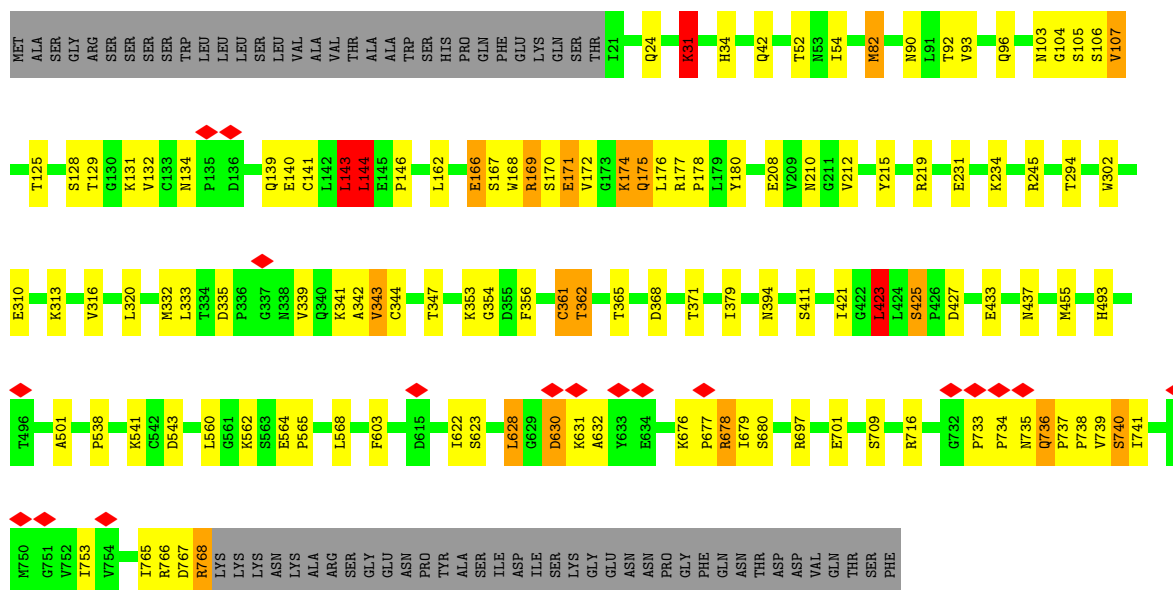
- Molecule 1: Sodium-dependent neutral amino acid transporter B(0)AT1





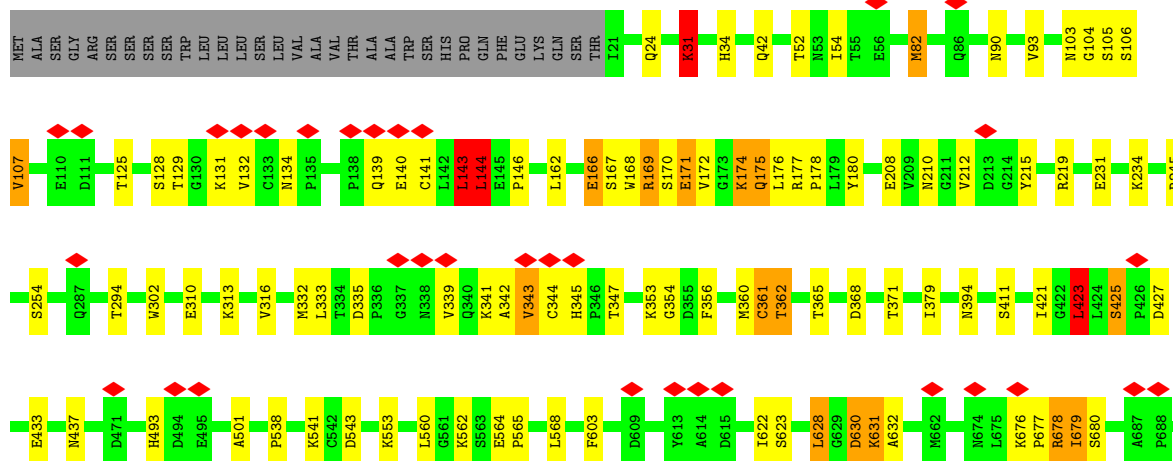
• Molecule 2: Angiotensin-converting enzyme 2

Chain B: 76% 12% 8%



• Molecule 2: Angiotensin-converting enzyme 2

Chain D: 5% 76% 12% 8%



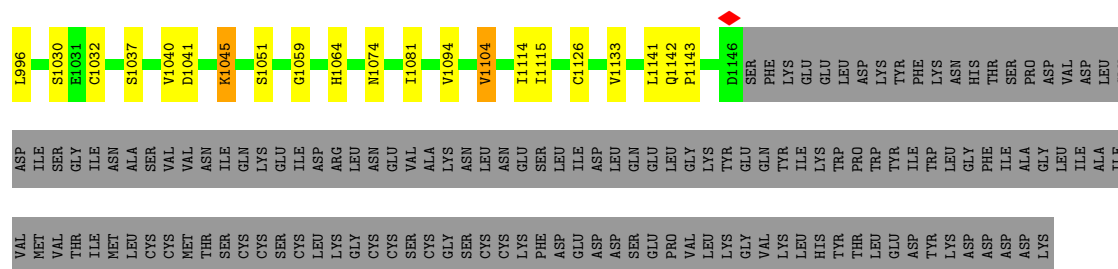


PHE	LYS	GLU	GLY	LEU	TRP	PRO	THR	ASP	LYS	TYR	PHE	LYS	ASN	HIS	THR	SER	PRO	ASP	LYS
GLN	TYR	ILE	GLY	TRP	LEU	TRP	THR	ASP	LYS	TYR	ILE	TRP	LEU	GLY	PHE	ILE	ALA	GLY	ASP
VAL	LYS	HIS	THR	LEU	GLU	LEU	ASP	ASP	ASP	LYS	VAL	THR	ASP	ASP	ASP	LYS	LYS	LYS	LYS

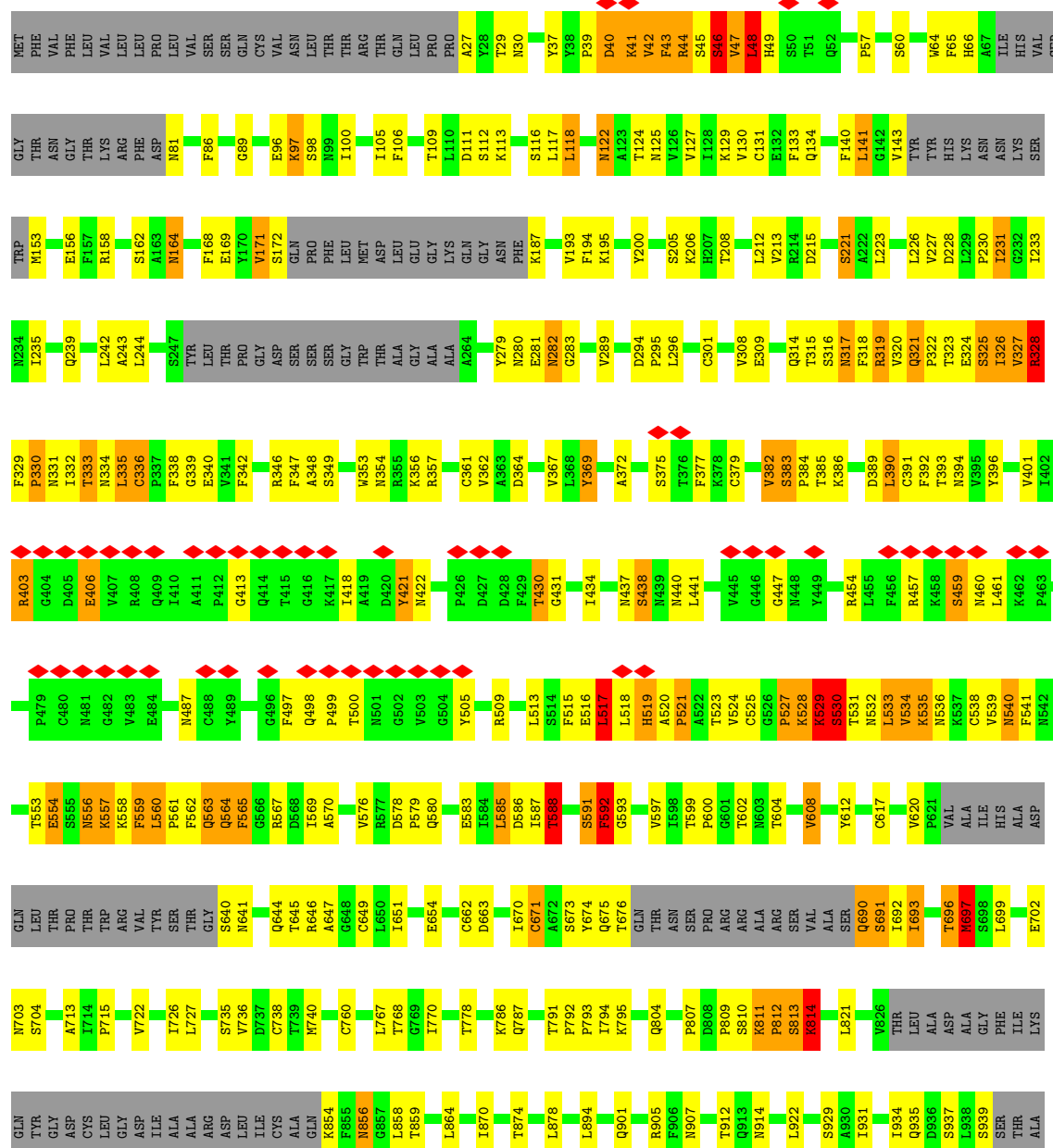
• Molecule 3: Spike glycoprotein

Chain F:  51% 20% 6% 22%

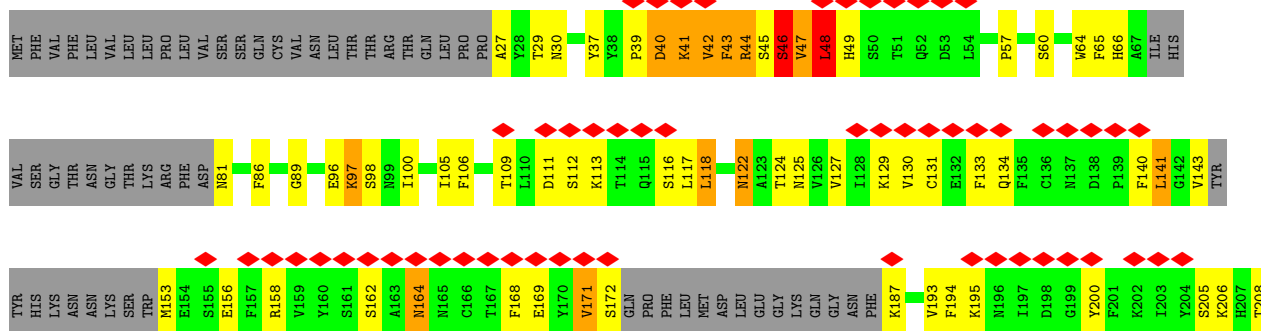
MET	PHE	VAL	PHE	LEU	VAL	VAL	LEU	LEU	PRO	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP
THR	ASN	GLY	THR	LYS	ARG	PHE	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP
M153	E156	E157	E158	S162	A163	M164	N165	C166	T167	F168	E169	E170	V171	S172	G173	P174	T175	D176	N177
P230	I231	I232	I233	N234	I235	Q239	L242	A243	N244	S247	TYR	THR	THR	PRO	GLY	ASP	SER	SER	SER
Q321	P322	T323	E324	S325	V327	R328	F329	P330	N331	I332	L335	C336	P337	F338	G339	E340	F341	F342	R346
F392	T393	N394	V395	V401	I402	R403	E406	V407	R408	A411	P412	T415	G416	K417	T418	A419	D420	Y421	N422
M481	G482	V483	M487	F497	Q498	D571	V576	B577	D578	P579	Q580	T581	L582	E583	I584	L585	D586	I587	T588
L560	P561	F562	Q563	Q564	F565	I569	A570	D571	V576	B577	D578	P579	Q580	T581	L582	E583	I584	L585	D586
TYR	SER	THR	GLY	S640	N641	Q644	T645	R646	A647	G648	C649	E654	H655	E661	C662	D663	G669	S673	Y674
C738	I742	C743	S746	T747	E748	C749	S758	Q762	V772	K776	Q779	Q787	I788	Y789	K790	T791	I794	P809	S810
G154	F855	N856	L864	E868	Y872	Q873	L878	T883	Q895	Q901	R905	G908	T912	L916	Q926	Q935	S939	S943	A944



• Molecule 3: Spike glycoprotein









- Molecule 3: Spike glycoprotein

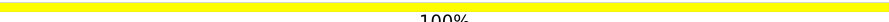
Frequency	Percentage
Daily	65%
Weekly	22%
Monthly	6%
Never	22%



Chain M:  50% 50%



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

Chain N:  100%



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

Chain O:  50% 100%



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

Chain P:  50% 50%

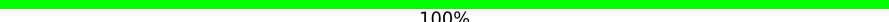


- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Q:  100%



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

Chain R:  100%



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

Chain S:  50% 100%

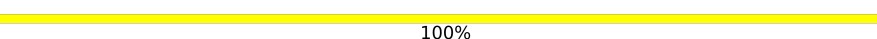


- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain T: 

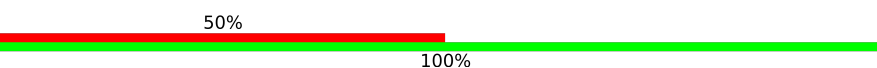


- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain U: 



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

Chain V: 

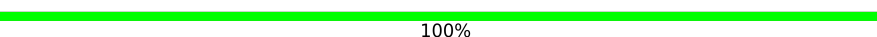


- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain W: 

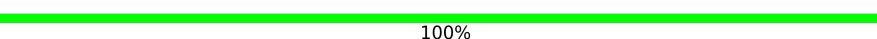


- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain X: 



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

Chain Y: 



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

Chain Z:  100%



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

Chain a:  100%



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

Chain b:  50% 50%



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

Chain c:  50% 50%



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

Chain d:  50% 50%



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

Chain e:  50% 50%



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



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



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



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



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



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



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

Chain l:  100%

NAG1
NAG2

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

Chain m:  100%

NAG1
NAG2

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

Chain n:  100%

NAG1
NAG2

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

Chain o:  50% 50% 50%

NAG1
NAG2

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

Chain p:  50% 50% 50%

NAG1
NAG2

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

Chain q:  100%

NAG1
NAG2

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

Chain r:  50% 50% 50%



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

Chain s:  100%



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

Chain t:  100%



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

Chain u:  100%
 100%

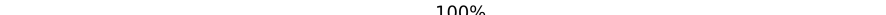


- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain v:  100%



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

Chain w:  100%
 50%  50%



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

Chain x:  100%
 50%  50%



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



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



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



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



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



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



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



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



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



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



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



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



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



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



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



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



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



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

Chain FA:  100%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	53141	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	1.786	Depositor
Minimum map value	-0.869	Depositor
Average map value	0.009	Depositor
Map value standard deviation	0.074	Depositor
Recommended contour level	0.3	Depositor
Map size ($\text{\AA}$)	521.76, 521.76, 521.76	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	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: ZN, 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	0.35	0/4940	0.70	9/6748 (0.1%)
1	C	0.34	0/4940	0.70	9/6748 (0.1%)
2	B	0.33	0/6252	0.61	4/8488 (0.0%)
2	D	0.33	0/6252	0.61	4/8488 (0.0%)
3	E	0.53	1/8048 (0.0%)	0.64	5/10947 (0.0%)
3	F	0.51	0/8042	0.63	2/10939 (0.0%)
3	G	0.51	0/8042	0.61	3/10939 (0.0%)
3	H	0.53	1/8048 (0.0%)	0.64	5/10947 (0.0%)
3	I	0.51	0/8042	0.63	2/10939 (0.0%)
3	J	0.51	0/8042	0.61	3/10939 (0.0%)
All	All	0.47	2/70648 (0.0%)	0.63	46/96122 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	698	SER	CA-C	-6.59	1.44	1.52
3	E	698	SER	CA-C	-6.51	1.44	1.52

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	157	GLU	N-CA-C	-10.67	99.18	111.03
1	A	157	GLU	N-CA-C	-10.63	99.23	111.03
2	D	143	LEU	N-CA-C	6.41	120.24	107.62
2	B	143	LEU	N-CA-C	6.40	120.23	107.62
3	H	538	CYS	N-CA-C	-6.40	100.83	110.24
3	E	538	CYS	N-CA-C	-6.33	100.93	110.24
2	D	144	LEU	N-CA-C	6.29	124.20	110.80
2	B	144	LEU	N-CA-C	6.28	124.17	110.80
2	B	31	LYS	N-CA-C	-6.24	104.56	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	31	LYS	N-CA-C	-6.20	104.60	111.36
2	D	362	THR	N-CA-C	6.02	119.34	109.76
2	B	362	THR	N-CA-C	6.00	119.31	109.76
3	J	86	PHE	CA-C-N	5.91	132.83	121.54
3	J	86	PHE	C-N-CA	5.91	132.83	121.54
3	H	86	PHE	CA-C-N	5.90	132.81	121.54
3	H	86	PHE	C-N-CA	5.90	132.81	121.54
3	G	86	PHE	CA-C-N	5.89	132.80	121.54
3	G	86	PHE	C-N-CA	5.89	132.80	121.54
3	E	86	PHE	CA-C-N	5.88	132.77	121.54
3	E	86	PHE	C-N-CA	5.88	132.77	121.54
3	F	86	PHE	CA-C-N	5.88	132.77	121.54
3	F	86	PHE	C-N-CA	5.88	132.77	121.54
3	I	86	PHE	CA-C-N	5.86	132.73	121.54
3	I	86	PHE	C-N-CA	5.86	132.73	121.54
3	E	588	THR	CA-C-N	-5.65	114.13	119.90
3	E	588	THR	C-N-CA	-5.65	114.13	119.90
3	H	588	THR	CA-C-N	-5.65	114.14	119.90
3	H	588	THR	C-N-CA	-5.65	114.14	119.90
1	A	494	LEU	CA-C-N	5.60	128.57	120.79
1	A	494	LEU	C-N-CA	5.60	128.57	120.79
1	A	216	ILE	CA-C-N	5.58	132.19	121.54
1	A	216	ILE	C-N-CA	5.58	132.19	121.54
1	C	216	ILE	CA-C-N	5.58	132.19	121.54
1	C	216	ILE	C-N-CA	5.58	132.19	121.54
1	C	494	LEU	CA-C-N	5.56	128.52	120.79
1	C	494	LEU	C-N-CA	5.56	128.52	120.79
1	A	231	TYR	N-CA-C	5.56	117.34	111.28
1	C	231	TYR	N-CA-C	5.55	117.33	111.28
3	J	369	TYR	N-CA-C	5.52	118.81	111.75
3	G	369	TYR	N-CA-C	5.50	118.79	111.75
1	C	488	TYR	N-CA-C	5.20	116.64	111.07
1	A	488	TYR	N-CA-C	5.17	116.60	111.07
1	C	496	ILE	N-CA-C	5.16	115.78	110.36
1	A	496	ILE	N-CA-C	5.15	115.76	110.36
1	C	349	ASP	N-CA-C	5.02	118.06	111.28
1	A	349	ASP	N-CA-C	5.01	118.05	111.28

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	4799	0	4762	156	0
1	C	4799	0	4762	153	0
2	B	6089	0	5901	157	0
2	D	6089	0	5901	152	0
3	E	7872	0	7674	441	0
3	F	7866	0	7663	458	0
3	G	7866	0	7663	504	0
3	H	7872	0	7670	453	0
3	I	7866	0	7663	458	0
3	J	7866	0	7663	503	0
4	0	28	0	25	0	0
4	1	28	0	25	1	0
4	2	28	0	25	3	0
4	3	28	0	25	0	0
4	4	28	0	25	0	0
4	5	28	0	25	0	0
4	6	28	0	25	1	0
4	7	28	0	25	0	0
4	8	28	0	25	0	0
4	9	28	0	25	3	0
4	AA	28	0	25	1	0
4	BA	28	0	25	0	0
4	CA	28	0	25	0	0
4	DA	28	0	25	1	0
4	EA	28	0	25	2	0
4	FA	28	0	25	0	0
4	K	28	0	25	0	0
4	L	28	0	25	0	0
4	M	28	0	25	0	0
4	N	28	0	25	6	0
4	O	28	0	25	0	0
4	P	28	0	25	0	0
4	Q	28	0	25	0	0
4	R	28	0	25	0	0
4	S	28	0	25	0	0
4	T	28	0	25	0	0
4	U	28	0	25	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	V	28	0	25	0	0
4	W	28	0	25	0	0
4	X	28	0	25	0	0
4	Y	28	0	25	0	0
4	Z	28	0	25	0	0
4	a	28	0	25	0	0
4	b	28	0	25	1	0
4	c	28	0	25	1	0
4	d	28	0	25	0	0
4	e	28	0	25	0	0
4	f	28	0	25	1	0
4	g	28	0	25	3	0
4	h	28	0	25	0	0
4	i	28	0	25	0	0
4	j	28	0	25	0	0
4	k	28	0	25	1	0
4	l	28	0	25	0	0
4	m	28	0	25	0	0
4	n	28	0	25	3	0
4	o	28	0	25	1	0
4	p	28	0	25	0	0
4	q	28	0	25	0	0
4	r	28	0	25	1	0
4	s	28	0	25	2	0
4	t	28	0	25	0	0
4	u	28	0	25	0	0
4	v	28	0	25	0	0
4	w	28	0	25	0	0
4	x	28	0	25	1	0
4	y	28	0	25	1	0
4	z	28	0	25	0	0
5	A	56	0	52	0	0
5	B	14	0	13	0	0
5	C	56	0	52	0	0
5	D	14	0	13	0	0
5	E	126	0	117	5	0
5	F	140	0	129	8	0
5	G	112	0	104	8	0
5	H	126	0	117	5	0
5	I	140	0	129	8	0
5	J	112	0	104	8	0
6	A	9	0	10	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	C	9	0	10	0	0
7	B	1	0	0	0	0
7	D	1	0	0	0	0
8	B	4	0	0	0	0
8	D	4	0	0	0	0
All	All	71532	0	69622	3146	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 22.

All (3146) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:431:GLY:HA2	3:F:515:PHE:CE1	1.25	1.71
3:I:431:GLY:HA2	3:I:515:PHE:CE1	1.25	1.62
3:H:740:MET:HE1	3:J:592:PHE:CD2	1.44	1.53
3:E:740:MET:HE1	3:G:592:PHE:CD2	1.44	1.52
3:G:431:GLY:HA2	3:G:515:PHE:CD1	1.51	1.45
5:I:1409:NAG:O4	5:I:1410:NAG:C1	1.63	1.45
3:J:431:GLY:HA2	3:J:515:PHE:CD1	1.51	1.45
5:F:1409:NAG:O4	5:F:1410:NAG:C1	1.63	1.44
3:G:654:GLU:HG3	3:G:693:ILE:CG2	1.48	1.42
3:J:654:GLU:HG3	3:J:693:ILE:CG2	1.48	1.39
3:J:528:LYS:HE2	3:J:530:SER:N	1.39	1.37
3:E:740:MET:HE1	3:G:592:PHE:CE2	1.62	1.34
3:G:528:LYS:HE2	3:G:530:SER:N	1.39	1.33
3:H:740:MET:HE1	3:J:592:PHE:CE2	1.62	1.33
3:E:550:GLY:HA2	3:E:590:CYS:SG	1.70	1.32
3:H:550:GLY:HA2	3:H:590:CYS:SG	1.70	1.32
3:H:225:PRO:HG2	3:J:562:PHE:CE2	1.64	1.31
3:E:225:PRO:HG2	3:G:562:PHE:CE2	1.64	1.31
3:H:703:ASN:HB2	3:I:787:GLN:OE1	1.28	1.30
3:F:324:GLU:OE2	3:F:539:VAL:HG23	1.34	1.25
3:I:324:GLU:OE2	3:I:539:VAL:HG23	1.34	1.25
1:A:205:TRP:CH2	1:A:466:THR:HG21	1.72	1.25
1:C:205:TRP:CH2	1:C:466:THR:HG21	1.72	1.25
3:E:740:MET:CE	3:G:592:PHE:CE2	2.20	1.24
3:H:740:MET:CE	3:J:592:PHE:CE2	2.20	1.24
3:H:745:ASP:HB2	3:J:319:ARG:NH1	1.52	1.24
3:E:703:ASN:HB2	3:F:787:GLN:OE1	1.28	1.23
3:G:393:THR:O	3:G:523:THR:HG21	1.34	1.23

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:745:ASP:HB2	3:G:319:ARG:NH1	1.52	1.23
3:J:393:THR:O	3:J:523:THR:HG21	1.34	1.22
3:F:431:GLY:CA	3:F:515:PHE:CE1	2.21	1.22
3:H:225:PRO:CG	3:J:562:PHE:CE2	2.23	1.22
3:I:431:GLY:CA	3:I:515:PHE:CE1	2.21	1.21
3:F:326:ILE:HD12	3:F:534:VAL:CG2	1.71	1.20
3:I:326:ILE:HD12	3:I:534:VAL:CG2	1.71	1.20
3:E:225:PRO:CG	3:G:562:PHE:CE2	2.23	1.20
3:G:431:GLY:CA	3:G:515:PHE:CD1	2.26	1.18
3:J:431:GLY:CA	3:J:515:PHE:CD1	2.26	1.18
3:J:528:LYS:CE	3:J:530:SER:HB2	1.74	1.18
3:F:320:VAL:HG23	3:F:591:SER:O	1.40	1.18
3:J:322:PRO:HG3	3:J:538:CYS:SG	1.84	1.17
3:J:431:GLY:CA	3:J:515:PHE:HD1	1.57	1.17
3:F:519:HIS:CD2	3:F:565:PHE:HZ	1.62	1.16
3:G:322:PRO:HG3	3:G:538:CYS:SG	1.84	1.16
3:G:528:LYS:CE	3:G:530:SER:HB2	1.74	1.16
3:I:320:VAL:HG23	3:I:591:SER:O	1.40	1.16
3:I:326:ILE:CD1	3:I:534:VAL:HG23	1.75	1.16
3:G:528:LYS:NZ	3:G:530:SER:HB2	1.61	1.15
3:I:519:HIS:CD2	3:I:565:PHE:HZ	1.62	1.15
3:J:546:LEU:HD11	3:J:565:PHE:HD2	1.10	1.15
3:J:528:LYS:NZ	3:J:530:SER:HB2	1.61	1.14
3:E:654:GLU:HG3	3:E:693:ILE:HG22	1.18	1.14
3:G:431:GLY:CA	3:G:515:PHE:HD1	1.57	1.14
3:F:326:ILE:CD1	3:F:534:VAL:HG23	1.75	1.14
3:I:329:PHE:HB3	3:I:330:PRO:HD2	1.19	1.14
3:I:340:GLU:OE2	3:I:356:LYS:HE2	1.47	1.14
3:I:329:PHE:HD2	3:I:528:LYS:HG2	1.13	1.13
3:F:329:PHE:HD2	3:F:528:LYS:HG2	1.13	1.13
3:G:340:GLU:OE2	3:G:356:LYS:HE2	1.47	1.13
3:E:565:PHE:O	3:F:42:VAL:HA	1.48	1.13
3:F:329:PHE:CD2	3:F:528:LYS:HG2	1.84	1.12
3:I:329:PHE:CD2	3:I:528:LYS:HG2	1.85	1.12
3:F:340:GLU:OE2	3:F:356:LYS:HE2	1.47	1.12
3:G:546:LEU:HD11	3:G:565:PHE:HD2	1.10	1.12
3:F:326:ILE:HD11	3:F:539:VAL:HG21	1.27	1.12
3:I:326:ILE:HD11	3:I:539:VAL:HG21	1.27	1.12
3:H:520:ALA:HB1	3:H:521:PRO:HD2	1.27	1.11
3:H:565:PHE:O	3:I:42:VAL:HA	1.48	1.11
3:J:340:GLU:OE2	3:J:356:LYS:HE2	1.47	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:329:PHE:HB3	3:F:330:PRO:HD2	1.19	1.11
3:H:654:GLU:HG3	3:H:693:ILE:HG22	1.18	1.11
3:I:328:ARG:HD2	3:I:578:ASP:OD1	1.51	1.10
3:F:328:ARG:HD2	3:F:578:ASP:OD1	1.51	1.10
3:F:388:ASN:OD1	3:F:527:PRO:HD3	1.52	1.10
3:H:329:PHE:HB3	3:H:330:PRO:HD2	1.25	1.10
3:H:341:VAL:CG2	3:H:356:LYS:HD3	1.83	1.09
1:C:81:GLU:OE2	1:C:541:LEU:HB3	1.51	1.09
3:J:560:LEU:HB3	3:J:561:PRO:HD2	1.30	1.09
2:D:34:HIS:CE1	3:H:493:GLN:HG3	1.88	1.08
2:B:82:MET:HG3	3:E:486:PHE:CE2	1.89	1.08
2:D:82:MET:HG3	3:H:486:PHE:CE2	1.89	1.08
3:G:316:SER:C	3:G:317:ASN:HD22	1.61	1.08
3:H:393:THR:O	3:H:523:THR:HG21	1.51	1.08
3:I:388:ASN:OD1	3:I:527:PRO:HD3	1.52	1.08
4:N:1:NAG:H62	4:N:2:NAG:HN2	1.17	1.08
3:F:326:ILE:HG23	3:F:533:LEU:HA	1.35	1.08
1:A:81:GLU:OE2	1:A:541:LEU:HB3	1.51	1.07
2:B:34:HIS:CE1	3:E:493:GLN:HG3	1.88	1.07
3:J:316:SER:C	3:J:317:ASN:HD22	1.61	1.07
3:E:329:PHE:HB3	3:E:330:PRO:HD2	1.25	1.07
3:J:654:GLU:CG	3:J:693:ILE:HG22	1.83	1.07
3:F:519:HIS:CD2	3:F:565:PHE:CZ	2.42	1.07
3:G:654:GLU:CG	3:G:693:ILE:HG22	1.83	1.07
3:H:475:ALA:HB1	3:H:487:ASN:HB3	1.35	1.07
3:E:475:ALA:HB1	3:E:487:ASN:HB3	1.35	1.07
3:F:562:PHE:CE2	3:G:41:LYS:HD2	1.89	1.07
3:F:748:GLU:HG3	3:F:981:LEU:HD21	1.32	1.07
3:E:341:VAL:CG2	3:E:356:LYS:HD3	1.83	1.06
3:E:523:THR:CG2	3:E:524:VAL:H	1.69	1.06
3:E:523:THR:HG22	3:E:524:VAL:N	1.66	1.06
3:I:562:PHE:CE2	3:J:41:LYS:HD2	1.89	1.06
3:I:748:GLU:HG3	3:I:981:LEU:HD21	1.32	1.06
3:G:560:LEU:HB3	3:G:561:PRO:HD2	1.30	1.06
3:I:326:ILE:HG23	3:I:533:LEU:HA	1.35	1.06
3:I:519:HIS:CD2	3:I:565:PHE:CZ	2.42	1.06
3:J:528:LYS:HZ1	3:J:530:SER:HB2	1.13	1.06
1:A:592:VAL:HG23	1:A:593:PRO:CD	1.87	1.05
3:H:740:MET:CE	3:J:592:PHE:CD2	2.39	1.05
3:I:675:GLN:O	3:I:690:GLN:HG3	1.56	1.05
3:F:521:PRO:HA	3:F:564:GLN:NE2	1.72	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:U:1:NAG:H62	4:U:2:NAG:HN2	1.18	1.05
3:H:745:ASP:CB	3:J:319:ARG:HH11	1.70	1.04
3:I:521:PRO:HA	3:I:564:GLN:NE2	1.72	1.04
1:C:592:VAL:HG23	1:C:593:PRO:CD	1.87	1.04
1:C:221:LYS:H	1:C:221:LYS:HD2	1.19	1.04
3:G:333:THR:O	3:G:362:VAL:HG23	1.56	1.04
3:F:675:GLN:O	3:F:690:GLN:HG3	1.56	1.04
3:E:740:MET:CE	3:G:592:PHE:CD2	2.39	1.04
3:E:745:ASP:CB	3:G:319:ARG:HH11	1.70	1.04
1:A:492:ILE:CG2	1:A:493:PRO:HD3	1.88	1.03
1:C:205:TRP:CZ2	1:C:466:THR:CG2	2.42	1.03
3:J:333:THR:O	3:J:362:VAL:HG23	1.56	1.03
1:C:492:ILE:CG2	1:C:493:PRO:HD3	1.88	1.03
3:G:528:LYS:HZ1	3:G:530:SER:HB2	1.11	1.02
3:J:654:GLU:CG	3:J:693:ILE:CG2	2.36	1.02
1:A:205:TRP:CZ2	1:A:466:THR:CG2	2.42	1.02
3:E:475:ALA:CB	3:E:487:ASN:HB3	1.88	1.02
3:H:475:ALA:CB	3:H:487:ASN:HB3	1.88	1.02
3:I:403:ARG:NH1	3:I:505:TYR:HE1	1.58	1.02
1:A:221:LYS:H	1:A:221:LYS:HD2	1.19	1.02
3:I:326:ILE:CD1	3:I:534:VAL:CG2	2.33	1.02
3:I:558:LYS:NZ	5:J:1405:NAG:HN2	1.57	1.02
2:B:177:ARG:HB3	2:B:178:PRO:HD3	1.42	1.01
2:D:177:ARG:HB3	2:D:178:PRO:HD3	1.42	1.01
3:F:558:LYS:NZ	5:G:1405:NAG:HN2	1.57	1.01
3:G:654:GLU:CG	3:G:693:ILE:CG2	2.36	1.01
1:A:492:ILE:HG23	1:A:493:PRO:CD	1.90	1.01
3:G:403:ARG:NH1	3:G:505:TYR:HE1	1.58	1.01
3:F:403:ARG:NH1	3:F:505:TYR:HE1	1.58	1.01
3:H:392:PHE:HB3	3:H:517:LEU:HD21	1.41	1.01
5:I:1409:NAG:C4	5:I:1410:NAG:C1	2.38	1.01
1:C:492:ILE:HG23	1:C:493:PRO:CD	1.90	1.01
3:I:44:ARG:O	3:I:283:GLY:HA2	1.61	1.01
5:F:1409:NAG:C4	5:F:1410:NAG:C1	2.38	1.01
3:J:403:ARG:NH1	3:J:505:TYR:HE1	1.58	1.01
3:G:326:ILE:CG2	3:G:541:PHE:HA	1.92	1.00
1:C:592:VAL:CG2	1:C:593:PRO:HD3	1.91	1.00
3:E:225:PRO:HD2	3:G:562:PHE:CZ	1.96	1.00
3:F:326:ILE:CD1	3:F:534:VAL:CG2	2.33	1.00
3:H:225:PRO:HD2	3:J:562:PHE:CZ	1.96	1.00
1:A:583:TYR:O	1:A:587:VAL:HG23	1.62	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:736:GLN:H	2:D:737:PRO:HD2	1.25	1.00
1:A:592:VAL:CG2	1:A:593:PRO:HD3	1.91	1.00
1:C:583:TYR:O	1:C:587:VAL:HG23	1.62	1.00
3:H:44:ARG:O	3:H:283:GLY:HA2	1.61	1.00
3:E:44:ARG:O	3:E:283:GLY:HA2	1.61	0.99
3:H:524:VAL:HG22	3:H:525:CYS:H	1.27	0.99
3:E:341:VAL:HG22	3:E:356:LYS:HD3	1.44	0.99
3:I:748:GLU:CG	3:I:981:LEU:HD21	1.91	0.99
3:J:44:ARG:O	3:J:283:GLY:HA2	1.61	0.99
1:A:454:PRO:HG3	2:B:768:ARG:NH2	1.77	0.99
3:F:748:GLU:CG	3:F:981:LEU:HD21	1.91	0.99
3:G:811:LYS:HB2	3:G:812:PRO:CD	1.91	0.99
1:A:229:LEU:HB3	1:A:230:PRO:HD3	1.44	0.99
3:G:44:ARG:O	3:G:283:GLY:HA2	1.61	0.99
3:J:326:ILE:CG2	3:J:541:PHE:HA	1.91	0.99
3:F:325:SER:HA	3:F:540:ASN:O	1.63	0.99
3:J:811:LYS:HB2	3:J:812:PRO:CD	1.91	0.99
3:I:325:SER:HA	3:I:540:ASN:O	1.63	0.99
3:H:392:PHE:HB3	3:H:517:LEU:CD2	1.93	0.98
1:C:454:PRO:HG3	2:D:768:ARG:NH2	1.77	0.98
3:G:523:THR:HG22	3:G:524:VAL:H	1.29	0.98
2:B:302:TRP:CH2	2:B:423:LEU:HD11	1.99	0.98
3:E:523:THR:HG22	3:E:524:VAL:H	0.84	0.98
3:F:44:ARG:O	3:F:283:GLY:HA2	1.61	0.98
3:J:523:THR:HG22	3:J:524:VAL:H	1.29	0.98
2:D:34:HIS:CE1	3:H:493:GLN:CG	2.47	0.98
3:F:329:PHE:CD2	3:F:528:LYS:HB3	1.99	0.98
3:I:329:PHE:CD2	3:I:528:LYS:HB3	1.99	0.97
2:B:34:HIS:ND1	3:E:493:GLN:HG3	1.78	0.97
3:H:329:PHE:HB3	3:H:330:PRO:CD	1.94	0.97
3:J:392:PHE:O	3:J:523:THR:HB	1.64	0.97
1:C:229:LEU:HB3	1:C:230:PRO:HD3	1.44	0.97
2:B:736:GLN:H	2:B:737:PRO:HD2	1.25	0.97
1:C:592:VAL:HG23	1:C:593:PRO:HD3	0.97	0.97
3:H:346:ARG:NH2	3:H:347:PHE:O	1.98	0.97
1:A:492:ILE:HG23	1:A:493:PRO:HD3	0.97	0.97
1:C:159:GLN:HE21	2:D:733:PRO:HB3	1.30	0.97
3:E:346:ARG:NH2	3:E:347:PHE:O	1.98	0.97
3:G:403:ARG:NH1	3:G:505:TYR:CE1	2.33	0.97
2:D:34:HIS:ND1	3:H:493:GLN:HG3	1.78	0.96
3:E:326:ILE:HD13	3:E:533:LEU:HA	1.45	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:327:VAL:HA	3:F:542:ASN:O	1.63	0.96
1:C:205:TRP:CZ2	1:C:466:THR:HG23	1.99	0.96
3:F:346:ARG:NH2	3:F:347:PHE:O	1.98	0.96
3:G:392:PHE:O	3:G:523:THR:HB	1.65	0.96
3:I:346:ARG:NH2	3:I:347:PHE:O	1.98	0.96
3:G:346:ARG:NH2	3:G:347:PHE:O	1.98	0.96
2:B:34:HIS:CE1	3:E:493:GLN:CG	2.47	0.96
3:F:403:ARG:NH1	3:F:505:TYR:CE1	2.33	0.96
3:E:529:LYS:HG2	3:E:530:SER:N	1.80	0.96
3:I:327:VAL:HA	3:I:542:ASN:O	1.63	0.96
3:F:357:ARG:NH2	3:G:230:PRO:CG	2.29	0.96
3:F:411:ALA:HB1	3:F:412:PRO:HD2	1.47	0.96
3:I:360:ASN:HA	3:I:523:THR:CG2	1.96	0.96
3:I:403:ARG:NH1	3:I:505:TYR:CE1	2.33	0.96
3:F:360:ASN:HA	3:F:523:THR:CG2	1.96	0.96
3:H:529:LYS:HG2	3:H:530:SER:N	1.80	0.96
3:I:357:ARG:NH2	3:J:230:PRO:CG	2.29	0.95
3:H:341:VAL:HG22	3:H:356:LYS:HD3	1.44	0.95
1:A:592:VAL:HG23	1:A:593:PRO:HD3	0.97	0.95
2:D:82:MET:HG3	3:H:486:PHE:CZ	2.01	0.95
2:D:678:ARG:HH21	2:D:678:ARG:HG3	1.32	0.95
3:H:520:ALA:HB1	3:H:521:PRO:CD	1.96	0.95
3:J:403:ARG:NH1	3:J:505:TYR:CE1	2.33	0.95
2:D:302:TRP:CH2	2:D:423:LEU:HD11	1.99	0.95
3:H:326:ILE:HD13	3:H:533:LEU:HA	1.46	0.95
3:J:346:ARG:NH2	3:J:347:PHE:O	1.98	0.95
1:C:492:ILE:HG23	1:C:493:PRO:HD3	0.97	0.95
3:E:329:PHE:HB3	3:E:330:PRO:CD	1.94	0.95
3:G:560:LEU:HB3	3:G:561:PRO:CD	1.97	0.95
3:I:411:ALA:HB1	3:I:412:PRO:HD2	1.47	0.95
3:J:528:LYS:CE	3:J:530:SER:N	2.30	0.95
1:A:205:TRP:CZ2	1:A:466:THR:HG23	1.99	0.95
1:A:159:GLN:HE21	2:B:733:PRO:HB3	1.30	0.94
3:H:703:ASN:OD1	3:I:789:TYR:HE1	1.50	0.94
2:B:82:MET:HG3	3:E:486:PHE:CZ	2.01	0.94
3:G:528:LYS:CE	3:G:530:SER:N	2.30	0.94
3:G:811:LYS:HB2	3:G:812:PRO:HD2	1.50	0.94
3:J:528:LYS:CD	3:J:529:LYS:H	1.81	0.94
3:J:546:LEU:HD11	3:J:565:PHE:CD2	2.03	0.94
3:J:811:LYS:HB2	3:J:812:PRO:HD2	1.50	0.94
3:E:703:ASN:OD1	3:F:789:TYR:HE1	1.50	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:528:LYS:CD	3:G:529:LYS:H	1.81	0.94
3:H:392:PHE:CB	3:H:517:LEU:HD21	1.97	0.94
2:B:302:TRP:HH2	2:B:423:LEU:HD11	1.34	0.93
3:G:546:LEU:HD11	3:G:565:PHE:CD2	2.03	0.93
2:B:678:ARG:HH21	2:B:678:ARG:HG3	1.32	0.93
2:B:34:HIS:ND1	3:E:493:GLN:CG	2.32	0.93
3:G:318:PHE:CZ	3:G:620:VAL:O	2.21	0.93
3:G:431:GLY:HA2	3:G:515:PHE:CE1	2.02	0.93
3:J:318:PHE:CZ	3:J:620:VAL:O	2.21	0.93
3:E:319:ARG:HH21	3:E:319:ARG:HG3	1.35	0.92
3:J:431:GLY:HA2	3:J:515:PHE:CE1	2.03	0.92
3:E:42:VAL:HA	3:G:565:PHE:O	1.70	0.92
3:J:369:TYR:CZ	3:J:384:PRO:HB2	2.03	0.92
3:G:369:TYR:CZ	3:G:384:PRO:HB2	2.04	0.92
3:J:560:LEU:HB3	3:J:561:PRO:CD	1.97	0.92
2:D:34:HIS:ND1	3:H:493:GLN:CG	2.32	0.92
1:A:205:TRP:CZ2	1:A:466:THR:HG21	2.05	0.92
3:F:520:ALA:HB1	3:F:521:PRO:HD2	1.51	0.92
3:F:319:ARG:HH22	3:G:740:MET:HE2	1.34	0.92
3:I:562:PHE:HE2	3:J:41:LYS:HD2	1.34	0.91
3:J:528:LYS:HE2	3:J:529:LYS:C	1.95	0.91
3:H:42:VAL:HA	3:J:565:PHE:O	1.70	0.91
3:I:319:ARG:HH22	3:J:740:MET:HE2	1.34	0.91
3:E:983:ARG:O	3:G:382:VAL:HA	1.71	0.91
3:I:329:PHE:HB3	3:I:330:PRO:CD	2.00	0.91
3:H:654:GLU:HG3	3:H:693:ILE:CG2	2.01	0.91
1:A:205:TRP:CH2	1:A:466:THR:CG2	2.54	0.91
2:D:302:TRP:HH2	2:D:423:LEU:HD11	1.33	0.91
1:C:492:ILE:HG21	1:C:590:ALA:HB1	1.53	0.91
3:I:320:VAL:HG12	3:I:321:GLN:H	1.35	0.91
3:H:740:MET:HE2	3:J:592:PHE:CE2	2.06	0.90
3:H:340:GLU:OE1	3:H:340:GLU:N	2.03	0.90
3:I:360:ASN:CA	3:I:523:THR:HG23	2.01	0.90
3:H:319:ARG:HG3	3:H:319:ARG:HH21	1.35	0.90
3:F:562:PHE:HE2	3:G:41:LYS:HD2	1.34	0.90
3:F:320:VAL:HG12	3:F:321:GLN:H	1.35	0.90
3:I:520:ALA:HB1	3:I:521:PRO:HD2	1.51	0.90
1:C:205:TRP:CZ2	1:C:466:THR:HG21	2.05	0.90
3:G:528:LYS:CE	3:G:530:SER:CB	2.48	0.90
3:G:535:LYS:HD3	3:G:554:GLU:OE2	1.70	0.90
3:F:360:ASN:CA	3:F:523:THR:HG23	2.01	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:528:LYS:CE	3:J:530:SER:CB	2.48	0.90
3:F:558:LYS:HZ2	5:G:1405:NAG:HN2	1.10	0.90
3:E:340:GLU:OE1	3:E:340:GLU:N	2.03	0.89
3:G:528:LYS:HE2	3:G:529:LYS:C	1.95	0.89
3:G:322:PRO:CG	3:G:538:CYS:SG	2.61	0.89
1:A:588:ILE:O	1:A:592:VAL:HG22	1.71	0.89
3:J:322:PRO:CG	3:J:538:CYS:SG	2.61	0.89
1:A:489:ALA:HB2	1:A:589:VAL:CG1	2.03	0.89
3:E:740:MET:HE2	3:G:592:PHE:CE2	2.06	0.89
3:I:308:VAL:O	3:I:601:GLY:HA2	1.73	0.89
3:E:225:PRO:CG	3:G:562:PHE:HE2	1.86	0.89
3:E:654:GLU:HG3	3:E:693:ILE:CG2	2.01	0.89
3:F:329:PHE:HB3	3:F:330:PRO:CD	2.00	0.89
3:H:295:PRO:HB2	3:H:608:VAL:HG11	1.54	0.89
3:H:983:ARG:O	3:J:382:VAL:HA	1.71	0.89
3:I:558:LYS:HZ2	5:J:1405:NAG:HN2	1.07	0.89
3:J:535:LYS:HD3	3:J:554:GLU:OE2	1.70	0.89
3:I:324:GLU:CD	3:I:539:VAL:HG23	1.98	0.89
1:A:591:GLY:O	1:A:592:VAL:C	2.15	0.89
1:C:588:ILE:O	1:C:592:VAL:HG22	1.71	0.89
3:H:392:PHE:CD2	3:H:517:LEU:HD21	2.08	0.89
3:F:308:VAL:O	3:F:601:GLY:HA2	1.72	0.88
3:F:388:ASN:OD1	3:F:527:PRO:CD	2.21	0.88
3:G:332:ILE:O	3:G:333:THR:OG1	1.91	0.88
1:A:492:ILE:HG21	1:A:590:ALA:HB1	1.53	0.88
3:F:324:GLU:OE2	3:F:539:VAL:CG2	2.22	0.88
3:G:662:CYS:HB2	3:G:697:MET:HE3	1.54	0.88
3:H:327:VAL:HB	3:H:530:SER:HA	1.54	0.88
3:I:326:ILE:CD1	3:I:539:VAL:HG21	2.03	0.88
3:E:295:PRO:HB2	3:E:608:VAL:HG11	1.54	0.88
3:I:388:ASN:OD1	3:I:527:PRO:CD	2.21	0.88
3:E:327:VAL:HB	3:E:530:SER:HA	1.54	0.88
3:E:550:GLY:CA	3:E:590:CYS:SG	2.61	0.88
3:G:543:PHE:HE2	3:G:578:ASP:OD1	1.56	0.88
3:H:550:GLY:CA	3:H:590:CYS:SG	2.61	0.88
3:F:326:ILE:CD1	3:F:539:VAL:HG21	2.03	0.88
3:G:392:PHE:HE2	3:G:517:LEU:CD2	1.87	0.88
3:F:530:SER:O	3:F:531:THR:OG1	1.91	0.88
3:F:324:GLU:CD	3:F:539:VAL:HG23	1.98	0.87
1:C:489:ALA:HB2	1:C:589:VAL:CG1	2.03	0.87
3:G:392:PHE:CE2	3:G:517:LEU:HD22	2.09	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:362:VAL:HG13	3:H:527:PRO:HB3	1.55	0.87
3:F:360:ASN:HA	3:F:523:THR:HG23	1.54	0.87
3:E:740:MET:CE	3:G:592:PHE:HE2	1.85	0.87
3:H:225:PRO:CG	3:J:562:PHE:HE2	1.86	0.87
3:I:530:SER:O	3:I:531:THR:OG1	1.91	0.87
3:I:571:ASP:HB2	3:J:967:SER:CB	2.04	0.87
3:I:570:ALA:HB2	3:J:963:VAL:HG12	1.54	0.87
3:J:662:CYS:HB2	3:J:697:MET:HE3	1.54	0.87
3:F:431:GLY:HA2	3:F:515:PHE:CZ	2.09	0.87
3:E:478:THR:HG23	3:E:479:PRO:HD2	1.55	0.87
3:F:571:ASP:HB2	3:G:967:SER:CB	2.04	0.87
3:J:332:ILE:O	3:J:333:THR:OG1	1.91	0.87
3:J:543:PHE:HE2	3:J:578:ASP:OD1	1.56	0.87
1:C:205:TRP:CH2	1:C:466:THR:CG2	2.54	0.87
3:I:360:ASN:HA	3:I:523:THR:HG23	1.54	0.87
3:F:570:ALA:HB2	3:G:963:VAL:HG12	1.54	0.87
3:H:538:CYS:HG	3:H:590:CYS:HG	0.91	0.87
3:J:392:PHE:HE2	3:J:517:LEU:CD2	1.87	0.87
3:J:392:PHE:CE2	3:J:517:LEU:HD22	2.09	0.87
3:E:45:SER:O	3:E:47:VAL:HG22	1.75	0.86
3:E:475:ALA:CB	3:E:487:ASN:CB	2.52	0.86
3:I:45:SER:O	3:I:47:VAL:HG22	1.75	0.86
1:C:220:GLY:O	1:C:223:VAL:HG12	1.75	0.86
1:A:220:GLY:O	1:A:223:VAL:HG12	1.75	0.86
2:D:105:SER:O	2:D:106:SER:OG	1.93	0.86
2:B:335:ASP:HB3	2:B:361:CYS:SG	2.16	0.86
3:F:523:THR:HG22	3:F:524:VAL:H	1.40	0.86
3:H:45:SER:O	3:H:47:VAL:HG22	1.75	0.86
3:H:478:THR:HG23	3:H:479:PRO:HD2	1.55	0.86
3:E:46:SER:HA	3:E:279:TYR:O	1.76	0.86
3:F:388:ASN:C	3:F:527:PRO:HD2	2.01	0.86
3:G:45:SER:O	3:G:47:VAL:HG22	1.75	0.86
3:H:475:ALA:CB	3:H:487:ASN:CB	2.52	0.86
3:F:46:SER:HA	3:F:279:TYR:O	1.76	0.86
3:F:329:PHE:CD2	3:F:528:LYS:CG	2.57	0.86
3:G:46:SER:HA	3:G:279:TYR:O	1.76	0.86
3:I:46:SER:HA	3:I:279:TYR:O	1.76	0.86
3:J:45:SER:O	3:J:47:VAL:HG22	1.75	0.86
3:H:46:SER:HA	3:H:279:TYR:O	1.76	0.86
3:H:490:PHE:CD1	3:H:491:PRO:HD2	2.11	0.86
3:I:326:ILE:HD12	3:I:534:VAL:HG23	0.88	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:490:PHE:CD1	3:E:491:PRO:HD2	2.11	0.86
3:I:388:ASN:C	3:I:527:PRO:HD2	2.01	0.86
2:D:335:ASP:HB3	2:D:361:CYS:SG	2.16	0.86
3:I:329:PHE:CD2	3:I:528:LYS:CG	2.57	0.86
3:I:523:THR:HG22	3:I:524:VAL:H	1.40	0.86
3:J:46:SER:HA	3:J:279:TYR:O	1.76	0.85
3:G:316:SER:C	3:G:317:ASN:ND2	2.33	0.85
3:H:729:VAL:HG13	3:H:1059:GLY:HA2	1.57	0.85
3:G:654:GLU:HG3	3:G:693:ILE:HG22	0.86	0.85
1:C:83:ILE:HB	1:C:84:PRO:HD3	1.59	0.85
3:F:326:ILE:HD12	3:F:534:VAL:HG23	0.88	0.85
3:J:316:SER:C	3:J:317:ASN:ND2	2.33	0.85
2:B:34:HIS:CE1	3:E:493:GLN:HB3	2.11	0.85
3:F:431:GLY:HA2	3:F:515:PHE:HE1	1.02	0.85
3:F:617:CYS:H	3:F:644:GLN:HE22	1.21	0.85
3:J:528:LYS:HE2	3:J:530:SER:H	1.41	0.85
1:C:591:GLY:O	1:C:592:VAL:C	2.15	0.85
3:F:45:SER:O	3:F:47:VAL:HG22	1.75	0.85
3:J:369:TYR:CE2	3:J:384:PRO:HB2	2.12	0.85
3:I:431:GLY:HA2	3:I:515:PHE:CZ	2.09	0.85
3:J:320:VAL:O	3:J:322:PRO:HD3	1.75	0.85
2:D:34:HIS:CE1	3:H:493:GLN:HB3	2.11	0.85
3:G:320:VAL:O	3:G:322:PRO:HD3	1.75	0.85
3:I:431:GLY:HA2	3:I:515:PHE:HE1	1.02	0.85
3:J:654:GLU:HG3	3:J:693:ILE:HG22	0.87	0.85
2:B:105:SER:O	2:B:106:SER:OG	1.93	0.84
3:E:729:VAL:HG13	3:E:1059:GLY:HA2	1.57	0.84
3:J:329:PHE:HB3	3:J:330:PRO:HD2	1.59	0.84
3:E:320:VAL:CG2	3:E:591:SER:HB2	2.07	0.84
3:E:472:ILE:HD12	3:E:482:GLY:HA2	1.59	0.84
3:I:324:GLU:OE2	3:I:539:VAL:CG2	2.22	0.84
3:F:431:GLY:CA	3:F:515:PHE:HE1	1.75	0.84
3:G:329:PHE:HB3	3:G:330:PRO:HD2	1.59	0.84
3:E:336:CYS:HB2	3:E:362:VAL:O	1.77	0.84
3:F:562:PHE:CD2	3:G:41:LYS:HD2	2.12	0.84
3:E:475:ALA:HB3	3:E:487:ASN:O	1.78	0.84
3:H:740:MET:CE	3:J:592:PHE:HE2	1.85	0.84
3:J:318:PHE:HZ	3:J:620:VAL:O	1.60	0.84
1:A:83:ILE:HB	1:A:84:PRO:HD3	1.59	0.84
3:H:320:VAL:CG2	3:H:591:SER:HB2	2.07	0.84
3:I:901:GLN:HE21	3:I:905:ARG:HE	1.26	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:393:THR:C	3:G:523:THR:HG21	2.03	0.84
3:H:472:ILE:HD12	3:H:482:GLY:HA2	1.59	0.84
3:H:536:ASN:O	3:H:537:LYS:HG2	1.78	0.84
3:J:393:THR:C	3:J:523:THR:HG21	2.03	0.84
3:J:528:LYS:HE3	3:J:530:SER:HB2	1.60	0.84
3:E:536:ASN:O	3:E:537:LYS:HG2	1.78	0.84
3:G:528:LYS:HE2	3:G:530:SER:H	1.41	0.83
3:H:516:GLU:O	3:H:517:LEU:HD22	1.78	0.83
3:H:225:PRO:HD2	3:J:562:PHE:HZ	1.42	0.83
3:I:617:CYS:H	3:I:644:GLN:HE22	1.21	0.83
1:A:221:LYS:HD2	1:A:221:LYS:N	1.93	0.83
3:F:901:GLN:HE21	3:F:905:ARG:HE	1.26	0.83
3:J:528:LYS:CG	3:J:529:LYS:H	1.91	0.83
3:G:335:LEU:O	3:G:336:CYS:O	1.97	0.83
3:J:335:LEU:O	3:J:336:CYS:O	1.97	0.83
1:C:221:LYS:HD2	1:C:221:LYS:N	1.93	0.83
2:D:170:SER:O	2:D:174:LYS:HG2	1.79	0.83
3:G:369:TYR:CE2	3:G:384:PRO:HB2	2.12	0.83
3:G:393:THR:O	3:G:523:THR:CG2	2.24	0.83
3:H:335:LEU:H	3:H:335:LEU:HD12	1.44	0.83
3:J:328:ARG:NE	3:J:533:LEU:HD22	1.93	0.83
3:F:520:ALA:HB1	3:F:521:PRO:CD	2.09	0.83
3:G:528:LYS:CG	3:G:529:LYS:H	1.91	0.83
3:H:329:PHE:O	3:H:579:PRO:HB2	1.79	0.83
3:H:703:ASN:OD1	3:I:789:TYR:CE1	2.32	0.83
3:E:740:MET:HE1	3:G:592:PHE:HD2	1.38	0.82
3:I:532:ASN:OD1	3:I:533:LEU:HD12	1.77	0.82
3:F:532:ASN:OD1	3:F:533:LEU:HD12	1.77	0.82
3:I:520:ALA:HB1	3:I:521:PRO:CD	2.09	0.82
3:E:329:PHE:O	3:E:579:PRO:HB2	1.79	0.82
3:E:703:ASN:OD1	3:F:789:TYR:CE1	2.32	0.82
5:E:1405:NAG:O7	3:G:558:LYS:HE2	1.80	0.82
3:G:328:ARG:NE	3:G:533:LEU:HD22	1.93	0.82
3:H:475:ALA:HB3	3:H:487:ASN:O	1.78	0.82
3:I:525:CYS:HB3	3:I:528:LYS:HD2	1.61	0.82
1:A:72:ILE:O	1:A:76:ILE:HG23	1.80	0.82
3:F:319:ARG:HH22	3:G:740:MET:CE	1.93	0.82
3:G:528:LYS:HE3	3:G:530:SER:HB2	1.60	0.82
3:I:562:PHE:CD2	3:J:41:LYS:HD2	2.12	0.82
2:B:170:SER:O	2:B:174:LYS:HG2	1.78	0.82
3:H:529:LYS:HG2	3:H:530:SER:H	1.44	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:H:1405:NAG:O7	3:J:558:LYS:HE2	1.80	0.82
3:J:901:GLN:HE21	3:J:905:ARG:HE	1.27	0.82
3:J:528:LYS:HE3	3:J:530:SER:CB	2.10	0.82
3:E:320:VAL:HG23	3:E:591:SER:HB2	1.61	0.81
3:G:901:GLN:HE21	3:G:905:ARG:HE	1.27	0.81
1:C:229:LEU:HD23	1:C:426:CYS:SG	2.20	0.81
2:D:144:LEU:HD22	2:D:168:TRP:CH2	2.15	0.81
3:G:528:LYS:HE3	3:G:530:SER:CB	2.10	0.81
3:I:319:ARG:HH22	3:J:740:MET:CE	1.93	0.81
3:E:703:ASN:CB	3:F:787:GLN:OE1	2.23	0.81
3:F:525:CYS:HB3	3:F:528:LYS:HD2	1.61	0.81
3:G:318:PHE:HZ	3:G:620:VAL:O	1.60	0.81
3:H:486:PHE:CD1	3:H:487:ASN:ND2	2.49	0.81
1:A:229:LEU:HD23	1:A:426:CYS:SG	2.20	0.81
1:C:72:ILE:O	1:C:76:ILE:HG23	1.80	0.81
3:I:357:ARG:NH2	3:J:230:PRO:HG3	1.95	0.81
2:B:628:LEU:HD12	2:B:632:ALA:CB	2.10	0.81
3:E:486:PHE:CD1	3:E:487:ASN:ND2	2.49	0.81
3:F:326:ILE:HG21	3:F:328:ARG:HH21	1.46	0.81
2:B:144:LEU:HD22	2:B:168:TRP:CH2	2.15	0.81
3:H:320:VAL:HG23	3:H:591:SER:HB2	1.61	0.81
2:B:736:GLN:N	2:B:737:PRO:HD2	1.95	0.81
3:I:748:GLU:OE2	3:I:748:GLU:N	2.14	0.81
2:D:628:LEU:HD12	2:D:632:ALA:CB	2.10	0.80
1:A:454:PRO:HG3	2:B:768:ARG:HH21	1.46	0.80
3:G:392:PHE:CE2	3:G:517:LEU:CD2	2.65	0.80
3:I:533:LEU:HD22	3:I:534:VAL:N	1.97	0.80
3:J:392:PHE:CE2	3:J:517:LEU:CD2	2.65	0.80
2:D:736:GLN:N	2:D:737:PRO:HD2	1.95	0.80
1:C:597:ILE:HB	1:C:598:PRO:HD3	1.64	0.80
1:A:597:ILE:HB	1:A:598:PRO:HD3	1.64	0.80
3:E:617:CYS:H	3:E:644:GLN:HE22	1.29	0.80
3:F:535:LYS:HB2	3:F:535:LYS:NZ	1.97	0.80
3:I:329:PHE:CD2	3:I:528:LYS:CB	2.65	0.80
1:A:538:SER:O	1:A:542:MET:HE2	1.82	0.80
3:I:431:GLY:CA	3:I:515:PHE:HE1	1.75	0.80
3:G:392:PHE:HE2	3:G:517:LEU:HD21	1.47	0.79
3:H:498:GLN:HB2	3:H:501:ASN:HD21	1.48	0.79
3:E:538:CYS:HG	3:E:590:CYS:HG	0.81	0.79
3:F:357:ARG:NH2	3:G:230:PRO:HG3	1.95	0.79
3:F:748:GLU:N	3:F:748:GLU:OE2	2.14	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:81:GLU:OE2	1:C:541:LEU:CB	2.30	0.79
3:H:740:MET:HE1	3:J:592:PHE:HD2	1.37	0.79
3:H:519:HIS:ND1	3:H:519:HIS:O	2.15	0.79
3:E:498:GLN:HB2	3:E:501:ASN:HD21	1.48	0.79
3:I:295:PRO:HB2	3:I:608:VAL:HG11	1.64	0.79
1:A:81:GLU:OE2	1:A:541:LEU:CB	2.30	0.79
3:F:529:LYS:O	3:F:530:SER:O	2.01	0.79
3:J:326:ILE:HG13	3:J:327:VAL:N	1.97	0.79
3:J:528:LYS:HG3	3:J:529:LYS:N	1.97	0.79
3:H:390:LEU:HD23	3:H:391:CYS:H	1.48	0.79
3:I:326:ILE:HG21	3:I:328:ARG:HH21	1.46	0.79
3:I:529:LYS:O	3:I:530:SER:O	2.01	0.79
3:J:393:THR:O	3:J:523:THR:CG2	2.24	0.79
3:E:529:LYS:HG2	3:E:530:SER:H	1.44	0.79
3:H:543:PHE:HE2	3:H:578:ASP:OD1	1.66	0.79
3:I:535:LYS:HB2	3:I:535:LYS:NZ	1.97	0.79
3:J:326:ILE:HG23	3:J:541:PHE:HA	1.65	0.79
3:F:329:PHE:CD2	3:F:528:LYS:CB	2.65	0.78
3:J:560:LEU:CB	3:J:561:PRO:HD2	2.12	0.78
1:C:538:SER:O	1:C:542:MET:HE2	1.82	0.78
3:E:498:GLN:HB2	3:E:501:ASN:ND2	1.98	0.78
3:F:533:LEU:HD22	3:F:534:VAL:N	1.97	0.78
3:G:326:ILE:HG13	3:G:327:VAL:N	1.97	0.78
3:G:390:LEU:HD23	3:G:391:CYS:H	1.48	0.78
3:H:617:CYS:H	3:H:644:GLN:HE22	1.28	0.78
3:J:535:LYS:CD	3:J:554:GLU:OE2	2.32	0.78
3:F:295:PRO:HB2	3:F:608:VAL:HG11	1.64	0.78
3:G:326:ILE:HG23	3:G:541:PHE:HA	1.65	0.78
3:H:392:PHE:HD2	3:H:517:LEU:HD21	1.48	0.78
3:F:571:ASP:HB2	3:G:967:SER:HB3	1.65	0.78
3:H:422:ASN:HD21	3:H:454:ARG:H	1.32	0.78
3:I:535:LYS:HE2	3:I:554:GLU:CD	2.08	0.78
3:J:390:LEU:HD23	3:J:391:CYS:H	1.48	0.78
3:J:392:PHE:HE2	3:J:517:LEU:HD21	1.47	0.78
3:F:535:LYS:HE2	3:F:554:GLU:CD	2.08	0.78
3:F:676:THR:C	3:F:691:SER:H	1.92	0.78
3:G:587:ILE:HG22	3:G:588:THR:H	1.49	0.78
1:C:454:PRO:HG3	2:D:768:ARG:HH21	1.46	0.78
3:F:743:CYS:SG	3:F:749:CYS:C	2.67	0.78
3:G:535:LYS:CD	3:G:554:GLU:OE2	2.32	0.78
3:I:571:ASP:HB2	3:J:967:SER:HB3	1.65	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:390:LEU:HD23	3:E:391:CYS:H	1.49	0.77
3:G:403:ARG:HH11	3:G:505:TYR:HE1	1.32	0.77
3:I:323:THR:HB	3:I:324:GLU:OE1	1.85	0.77
3:I:360:ASN:CA	3:I:523:THR:CG2	2.60	0.77
3:I:743:CYS:SG	3:I:749:CYS:C	2.67	0.77
3:J:324:GLU:O	3:J:325:SER:OG	2.01	0.77
3:J:557:LYS:HB3	3:J:559:PHE:CE1	2.20	0.77
3:G:528:LYS:HG3	3:G:529:LYS:N	1.98	0.77
3:E:543:PHE:HE2	3:E:578:ASP:OD1	1.66	0.77
3:I:676:THR:C	3:I:691:SER:H	1.92	0.77
3:G:391:CYS:SG	3:G:524:VAL:O	2.43	0.77
3:E:328:ARG:CZ	3:E:533:LEU:HG	2.15	0.77
3:H:335:LEU:HA	3:H:362:VAL:HB	1.65	0.77
3:H:406:GLU:CD	3:H:418:ILE:HG13	2.10	0.77
3:I:535:LYS:HE2	3:I:554:GLU:OE2	1.85	0.77
3:J:391:CYS:SG	3:J:524:VAL:O	2.43	0.77
3:E:533:LEU:HD21	3:E:578:ASP:OD2	1.85	0.77
3:F:525:CYS:HB3	3:F:528:LYS:CG	2.15	0.77
3:H:498:GLN:HB2	3:H:501:ASN:ND2	1.98	0.77
3:E:406:GLU:CD	3:E:418:ILE:HG13	2.10	0.77
3:E:481:ASN:O	3:E:483:VAL:HG22	1.85	0.77
3:I:525:CYS:HB3	3:I:528:LYS:CG	2.15	0.77
3:J:323:THR:O	3:J:324:GLU:HG2	1.85	0.77
3:E:470:THR:CG2	3:E:490:PHE:CE1	2.68	0.77
3:E:477:SER:O	3:E:478:THR:OG1	2.03	0.77
3:G:324:GLU:O	3:G:325:SER:OG	2.01	0.77
3:G:535:LYS:HG2	3:G:536:ASN:OD1	1.85	0.77
3:H:707:TYR:HB2	3:I:883:THR:HG23	1.65	0.77
2:B:302:TRP:HH2	2:B:423:LEU:CD1	1.98	0.76
3:F:323:THR:HB	3:F:324:GLU:OE1	1.85	0.76
3:G:323:THR:O	3:G:324:GLU:HG2	1.85	0.76
3:H:328:ARG:CZ	3:H:533:LEU:HG	2.14	0.76
3:I:422:ASN:HD21	3:I:454:ARG:H	1.32	0.76
3:E:707:TYR:HB2	3:F:883:THR:HG23	1.65	0.76
3:F:617:CYS:HB2	3:F:644:GLN:NE2	1.99	0.76
3:J:406:GLU:CD	3:J:418:ILE:HG13	2.10	0.76
3:J:587:ILE:HG22	3:J:588:THR:H	1.49	0.76
3:E:327:VAL:HG11	3:E:529:LYS:O	1.86	0.76
3:G:431:GLY:HA3	3:G:515:PHE:HD1	1.49	0.76
3:G:528:LYS:CG	3:G:529:LYS:N	2.47	0.76
3:H:470:THR:CG2	3:H:490:PHE:CE1	2.68	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:475:ALA:HB3	3:H:487:ASN:CB	2.16	0.76
3:J:430:THR:HG21	3:J:517:LEU:HD23	1.66	0.76
3:J:431:GLY:HA3	3:J:515:PHE:HD1	1.49	0.76
3:F:422:ASN:HD21	3:F:454:ARG:H	1.32	0.76
3:H:328:ARG:NH1	3:H:533:LEU:HG	2.01	0.76
3:H:703:ASN:CB	3:I:787:GLN:OE1	2.23	0.76
3:I:617:CYS:HB2	3:I:644:GLN:NE2	1.99	0.76
1:A:492:ILE:HG21	1:A:590:ALA:CB	2.15	0.76
3:E:328:ARG:NH1	3:E:533:LEU:HG	2.00	0.76
3:E:475:ALA:HB3	3:E:487:ASN:CB	2.16	0.76
3:F:406:GLU:CD	3:F:418:ILE:HG13	2.10	0.76
3:G:430:THR:HG21	3:G:517:LEU:HD23	1.66	0.76
3:G:557:LYS:HB3	3:G:559:PHE:CE1	2.20	0.76
2:B:34:HIS:CE1	3:E:493:GLN:CB	2.69	0.76
2:D:302:TRP:HH2	2:D:423:LEU:CD1	1.98	0.76
3:E:225:PRO:HD2	3:G:562:PHE:HZ	1.42	0.76
3:I:403:ARG:HH11	3:I:505:TYR:HE1	1.32	0.76
3:I:406:GLU:CD	3:I:418:ILE:HG13	2.10	0.76
3:J:403:ARG:HH11	3:J:505:TYR:HE1	1.32	0.76
3:J:735:SER:OG	3:J:859:THR:CG2	2.34	0.76
1:C:492:ILE:HG21	1:C:590:ALA:CB	2.15	0.76
3:H:826:VAL:HG13	3:H:1057:PRO:HG2	1.68	0.76
2:B:768:ARG:HG2	2:B:768:ARG:HH11	1.49	0.76
1:C:159:GLN:HE21	2:D:733:PRO:CB	1.98	0.76
3:E:422:ASN:HD21	3:E:454:ARG:H	1.32	0.76
3:F:326:ILE:CD1	3:F:534:VAL:HG21	2.16	0.76
3:F:326:ILE:CG2	3:F:533:LEU:HA	2.16	0.76
3:J:535:LYS:HG2	3:J:536:ASN:OD1	1.85	0.76
1:A:222:ALA:O	1:A:226:THR:HG23	1.86	0.76
3:G:560:LEU:CB	3:G:561:PRO:HD2	2.12	0.76
3:H:481:ASN:O	3:H:483:VAL:HG22	1.85	0.76
1:C:222:ALA:O	1:C:226:THR:HG23	1.86	0.75
2:D:768:ARG:HG2	2:D:768:ARG:HH11	1.49	0.75
3:G:735:SER:OG	3:G:859:THR:CG2	2.34	0.75
2:B:736:GLN:H	2:B:737:PRO:CD	1.99	0.75
3:E:225:PRO:HG2	3:G:562:PHE:CD2	2.21	0.75
3:F:307:THR:HA	3:F:602:THR:OG1	1.87	0.75
3:F:360:ASN:CA	3:F:523:THR:CG2	2.60	0.75
3:F:535:LYS:HE2	3:F:554:GLU:OE2	1.85	0.75
3:J:422:ASN:HD21	3:J:454:ARG:H	1.32	0.75
3:E:534:VAL:C	3:E:535:LYS:HG2	2.10	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:360:ASN:HA	3:F:523:THR:HG22	1.68	0.75
2:D:736:GLN:H	2:D:737:PRO:CD	1.99	0.75
3:H:534:VAL:C	3:H:535:LYS:HG2	2.10	0.75
3:H:470:THR:HG22	3:H:490:PHE:HE1	1.51	0.75
3:H:477:SER:O	3:H:478:THR:OG1	2.03	0.75
3:I:612:TYR:O	3:I:648:GLY:HA3	1.87	0.75
3:G:422:ASN:HD21	3:G:454:ARG:H	1.32	0.75
3:H:225:PRO:HG2	3:J:562:PHE:CD2	2.21	0.75
2:D:678:ARG:HG3	2:D:678:ARG:NH2	1.99	0.75
3:E:47:VAL:O	3:E:49:HIS:N	2.20	0.75
3:E:826:VAL:HG13	3:E:1057:PRO:HG2	1.68	0.75
3:H:533:LEU:HD21	3:H:578:ASP:OD2	1.85	0.75
2:B:678:ARG:HG3	2:B:678:ARG:NH2	1.99	0.75
1:C:78:LEU:HD23	1:C:79:VAL:N	2.02	0.75
3:E:520:ALA:HB1	3:E:521:PRO:HD2	1.69	0.75
3:F:47:VAL:O	3:F:49:HIS:N	2.20	0.75
1:A:159:GLN:HE21	2:B:733:PRO:CB	1.98	0.75
1:C:418:VAL:O	1:C:422:ILE:HG23	1.86	0.75
2:D:34:HIS:CE1	3:H:493:GLN:CB	2.69	0.75
2:D:82:MET:CG	3:H:486:PHE:CZ	2.70	0.75
3:G:406:GLU:CD	3:G:418:ILE:HG13	2.10	0.75
3:I:47:VAL:O	3:I:49:HIS:N	2.20	0.75
3:I:320:VAL:HG12	3:I:321:GLN:N	2.02	0.75
2:B:82:MET:CG	3:E:486:PHE:CZ	2.70	0.74
3:E:336:CYS:HB2	3:E:363:ALA:HA	1.69	0.74
3:J:528:LYS:CE	3:J:529:LYS:H	1.99	0.74
3:E:470:THR:HG22	3:E:490:PHE:HE1	1.51	0.74
3:E:1125:ASN:H	3:E:1125:ASN:HD22	1.33	0.74
3:H:1125:ASN:H	3:H:1125:ASN:HD22	1.33	0.74
3:G:327:VAL:HB	3:G:529:LYS:HB3	1.68	0.74
3:G:528:LYS:CE	3:G:529:LYS:H	2.00	0.74
3:F:612:TYR:O	3:F:648:GLY:HA3	1.87	0.74
3:J:327:VAL:HB	3:J:529:LYS:HB3	1.68	0.74
3:H:327:VAL:HG11	3:H:529:LYS:O	1.86	0.74
1:A:78:LEU:HD23	1:A:79:VAL:N	2.02	0.74
1:A:418:VAL:O	1:A:422:ILE:HG23	1.86	0.74
2:B:335:ASP:CB	2:B:361:CYS:SG	2.75	0.74
3:F:320:VAL:HG12	3:F:321:GLN:N	2.02	0.74
3:I:571:ASP:HB2	3:J:967:SER:HB2	1.68	0.74
3:H:326:ILE:CD1	3:H:533:LEU:HA	2.17	0.74
1:C:229:LEU:HB3	1:C:230:PRO:CD	2.17	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:571:ASP:HB2	3:G:967:SER:HB2	1.68	0.73
3:H:47:VAL:O	3:H:49:HIS:N	2.20	0.73
3:I:326:ILE:CD1	3:I:534:VAL:HG21	2.16	0.73
3:I:411:ALA:HB1	3:I:412:PRO:CD	2.18	0.73
3:E:326:ILE:CD1	3:E:533:LEU:HA	2.17	0.73
3:E:478:THR:CG2	3:E:479:PRO:HD2	2.18	0.73
3:E:983:ARG:HB2	3:G:382:VAL:HB	1.68	0.73
3:F:519:HIS:CG	3:F:565:PHE:CZ	2.76	0.73
2:D:335:ASP:CB	2:D:361:CYS:SG	2.75	0.73
3:F:326:ILE:O	3:F:327:VAL:HG22	1.87	0.73
3:H:565:PHE:O	3:I:42:VAL:CA	2.34	0.73
3:I:326:ILE:O	3:I:327:VAL:HG22	1.87	0.73
3:I:519:HIS:CG	3:I:565:PHE:CZ	2.76	0.73
3:E:361:CYS:O	3:E:524:VAL:HB	1.88	0.73
3:G:47:VAL:O	3:G:49:HIS:N	2.20	0.73
3:G:675:GLN:HG2	3:G:676:THR:N	2.02	0.73
3:I:307:THR:HA	3:I:602:THR:OG1	1.87	0.73
2:B:172:VAL:HG13	2:B:176:LEU:HD11	1.71	0.73
3:H:225:PRO:CD	3:J:562:PHE:CE2	2.71	0.73
3:H:790:LYS:NZ	3:J:702:GLU:OE2	2.21	0.73
3:H:983:ARG:HB2	3:J:382:VAL:HB	1.68	0.73
2:D:172:VAL:CG1	2:D:176:LEU:HD11	2.18	0.73
3:F:411:ALA:HB1	3:F:412:PRO:CD	2.18	0.73
3:I:360:ASN:HA	3:I:523:THR:HG22	1.68	0.73
3:I:525:CYS:O	3:I:526:GLY:O	2.06	0.73
2:B:172:VAL:CG1	2:B:176:LEU:HD11	2.18	0.73
3:H:524:VAL:HG22	3:H:525:CYS:N	2.02	0.73
1:C:205:TRP:CE2	1:C:466:THR:HG23	2.24	0.73
2:D:82:MET:CG	3:H:486:PHE:CE2	2.71	0.73
3:F:431:GLY:HA2	3:F:515:PHE:CD1	2.15	0.73
3:H:478:THR:CG2	3:H:479:PRO:HD2	2.18	0.73
3:H:536:ASN:C	3:H:537:LYS:HG2	2.13	0.73
3:I:326:ILE:CG2	3:I:533:LEU:HA	2.16	0.73
3:F:525:CYS:O	3:F:526:GLY:O	2.06	0.73
3:J:47:VAL:O	3:J:49:HIS:N	2.20	0.73
3:E:486:PHE:CG	3:E:487:ASN:ND2	2.57	0.73
3:E:492:LEU:C	3:E:493:GLN:NE2	2.47	0.73
3:G:587:ILE:HG22	3:G:588:THR:N	2.04	0.73
3:H:486:PHE:CG	3:H:487:ASN:ND2	2.57	0.73
3:I:535:LYS:HG2	3:I:536:ASN:OD1	1.88	0.73
3:J:587:ILE:HG22	3:J:588:THR:N	2.04	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:229:LEU:HB3	1:A:230:PRO:CD	2.17	0.72
3:F:535:LYS:HG2	3:F:536:ASN:OD1	1.88	0.72
3:G:431:GLY:CA	3:G:515:PHE:CE1	2.67	0.72
3:I:533:LEU:HD13	3:I:533:LEU:C	2.14	0.72
3:I:523:THR:HG22	3:I:524:VAL:N	2.03	0.72
3:E:225:PRO:CD	3:G:562:PHE:CE2	2.72	0.72
3:E:327:VAL:O	3:E:328:ARG:HD3	1.89	0.72
3:E:790:LYS:NZ	3:G:702:GLU:OE2	2.21	0.72
3:F:403:ARG:HH11	3:F:505:TYR:HE1	1.32	0.72
3:I:973:ILE:HG12	3:I:992:GLN:HE21	1.53	0.72
3:I:1142:GLN:HG3	3:I:1143:PRO:HD3	1.71	0.72
3:E:536:ASN:C	3:E:537:LYS:HG2	2.13	0.72
3:F:1142:GLN:HG3	3:F:1143:PRO:HD3	1.71	0.72
3:H:335:LEU:HD12	3:H:335:LEU:N	2.03	0.72
3:H:492:LEU:C	3:H:493:GLN:NE2	2.47	0.72
3:E:225:PRO:CD	3:G:562:PHE:CZ	2.71	0.72
3:F:533:LEU:C	3:F:533:LEU:HD13	2.14	0.72
3:H:987:PRO:HG3	3:I:427:ASP:OD2	1.88	0.72
1:A:209:TYR:HE2	1:A:460:GLY:CA	2.03	0.72
3:E:987:PRO:HG3	3:F:427:ASP:OD2	1.88	0.72
3:J:675:GLN:HG2	3:J:676:THR:N	2.03	0.72
2:B:736:GLN:N	2:B:737:PRO:CD	2.53	0.72
3:H:225:PRO:CD	3:J:562:PHE:CZ	2.71	0.72
3:J:431:GLY:CA	3:J:515:PHE:CE1	2.67	0.72
1:A:205:TRP:CE2	1:A:466:THR:HG23	2.23	0.72
3:J:534:VAL:O	3:J:535:LYS:HB2	1.90	0.72
3:G:534:VAL:O	3:G:535:LYS:HB2	1.90	0.71
3:I:431:GLY:HA2	3:I:515:PHE:CD1	2.15	0.71
3:E:319:ARG:HG3	3:E:319:ARG:NH2	2.03	0.71
3:G:393:THR:OG1	3:G:518:LEU:HB3	1.90	0.71
2:D:172:VAL:HG13	2:D:176:LEU:HD11	1.71	0.71
1:C:209:TYR:HE2	1:C:460:GLY:CA	2.03	0.71
3:F:357:ARG:NH2	3:G:230:PRO:CB	2.53	0.71
5:F:1409:NAG:H4	5:F:1410:NAG:C1	2.21	0.71
3:H:327:VAL:O	3:H:328:ARG:HD3	1.89	0.71
2:B:172:VAL:CG1	2:B:176:LEU:CD1	2.68	0.71
1:C:78:LEU:HD23	1:C:78:LEU:C	2.16	0.71
3:G:670:ILE:HG22	3:G:671:CYS:N	2.06	0.71
3:I:357:ARG:NH2	3:J:230:PRO:CB	2.53	0.71
3:J:393:THR:OG1	3:J:518:LEU:HB3	1.90	0.71
2:D:172:VAL:CG1	2:D:176:LEU:CD1	2.68	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:357:ARG:CZ	3:G:230:PRO:HG3	2.21	0.71
3:F:973:ILE:HG12	3:F:992:GLN:HE21	1.53	0.71
3:I:357:ARG:CZ	3:J:230:PRO:HG3	2.21	0.71
3:G:124:THR:HG21	5:G:1402:NAG:HN2	1.56	0.71
3:H:654:GLU:O	3:H:693:ILE:HA	1.91	0.71
1:C:465:GLY:O	1:C:469:ILE:HG12	1.91	0.70
3:E:654:GLU:O	3:E:693:ILE:HA	1.91	0.70
3:H:41:LYS:CD	3:H:41:LYS:H	2.04	0.70
3:I:525:CYS:HB3	3:I:528:LYS:CD	2.20	0.70
3:J:316:SER:O	3:J:317:ASN:ND2	2.24	0.70
3:J:431:GLY:HA3	3:J:515:PHE:CD1	2.24	0.70
3:J:670:ILE:HG22	3:J:671:CYS:N	2.06	0.70
3:E:740:MET:HE2	3:G:592:PHE:HE2	1.48	0.70
3:G:528:LYS:HZ1	3:G:530:SER:CB	1.98	0.70
3:J:528:LYS:CG	3:J:529:LYS:N	2.47	0.70
3:F:525:CYS:HB3	3:F:528:LYS:CD	2.20	0.70
5:I:1409:NAG:H4	5:I:1410:NAG:C1	2.21	0.70
1:A:465:GLY:O	1:A:469:ILE:HG12	1.91	0.70
3:H:393:THR:O	3:H:523:THR:CG2	2.34	0.70
3:I:320:VAL:CG2	3:I:591:SER:HB3	2.22	0.70
1:A:78:LEU:HD23	1:A:78:LEU:C	2.16	0.70
2:B:172:VAL:HG12	2:B:176:LEU:HD12	1.73	0.70
3:E:41:LYS:H	3:E:41:LYS:CD	2.04	0.70
3:F:320:VAL:CG2	3:F:591:SER:HB3	2.22	0.70
3:F:523:THR:HG22	3:F:524:VAL:N	2.03	0.70
3:H:482:GLY:C	3:H:483:VAL:HG22	2.17	0.70
3:E:745:ASP:HB2	3:G:319:ARG:HH11	0.74	0.70
1:A:209:TYR:CE2	1:A:460:GLY:CA	2.75	0.70
2:D:736:GLN:N	2:D:737:PRO:CD	2.53	0.70
3:F:525:CYS:CB	3:F:528:LYS:HD2	2.22	0.70
3:F:571:ASP:CB	3:G:967:SER:HB2	2.22	0.70
3:H:745:ASP:HB2	3:J:319:ARG:HH11	0.74	0.70
3:I:592:PHE:CD2	3:J:740:MET:SD	2.85	0.70
3:J:124:THR:HG21	5:J:1402:NAG:HN2	1.56	0.70
2:B:82:MET:CG	3:E:486:PHE:CE2	2.71	0.70
3:E:534:VAL:O	3:E:535:LYS:HG2	1.91	0.70
3:I:525:CYS:CB	3:I:528:LYS:HD2	2.22	0.70
3:J:187:LYS:N	3:J:212:LEU:O	2.25	0.70
1:C:72:ILE:HD12	1:C:72:ILE:H	1.57	0.70
3:E:594:GLY:O	3:E:613:GLN:HG2	1.92	0.70
3:H:594:GLY:O	3:H:613:GLN:HG2	1.92	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:187:LYS:N	3:I:212:LEU:O	2.25	0.70
3:J:523:THR:HG22	3:J:524:VAL:N	2.06	0.70
3:E:187:LYS:N	3:E:212:LEU:O	2.25	0.69
3:G:316:SER:O	3:G:317:ASN:ND2	2.24	0.69
1:A:209:TYR:CE2	1:A:460:GLY:HA2	2.27	0.69
3:G:326:ILE:HG22	3:G:541:PHE:HA	1.74	0.69
3:G:431:GLY:HA3	3:G:515:PHE:CD1	2.24	0.69
3:J:528:LYS:HG3	3:J:529:LYS:H	1.57	0.69
1:A:72:ILE:H	1:A:72:ILE:HD12	1.57	0.69
3:F:45:SER:OG	3:F:46:SER:N	2.25	0.69
3:F:388:ASN:O	3:F:526:GLY:HA3	1.92	0.69
3:G:187:LYS:N	3:G:212:LEU:O	2.25	0.69
3:J:326:ILE:HG22	3:J:541:PHE:HA	1.74	0.69
3:H:187:LYS:N	3:H:212:LEU:O	2.25	0.69
3:I:124:THR:HG21	5:I:1402:NAG:HN2	1.56	0.69
3:E:124:THR:HG21	5:E:1402:NAG:HN2	1.56	0.69
3:F:430:THR:O	3:F:515:PHE:HE1	1.75	0.69
3:G:328:ARG:NE	3:G:533:LEU:CD2	2.54	0.69
3:G:523:THR:HG22	3:G:524:VAL:N	2.06	0.69
3:H:124:THR:HG21	5:H:1402:NAG:HN2	1.56	0.69
3:H:392:PHE:HD2	3:H:517:LEU:CD2	2.05	0.69
3:I:986:PRO:HB2	3:I:987:PRO:HD3	1.74	0.69
1:C:209:TYR:CE2	1:C:460:GLY:CA	2.75	0.69
3:F:124:THR:HG21	5:F:1402:NAG:HN2	1.56	0.69
3:F:592:PHE:CD2	3:G:740:MET:SD	2.85	0.69
3:G:340:GLU:OE2	3:G:356:LYS:CE	2.35	0.69
3:I:388:ASN:OD1	3:I:527:PRO:HG3	1.93	0.69
3:J:45:SER:OG	3:J:46:SER:N	2.25	0.69
2:D:172:VAL:HG12	2:D:176:LEU:HD12	1.73	0.69
3:E:45:SER:OG	3:E:46:SER:N	2.25	0.69
3:H:326:ILE:O	3:H:326:ILE:HG13	1.92	0.69
3:I:430:THR:O	3:I:515:PHE:HE1	1.75	0.69
3:E:482:GLY:C	3:E:483:VAL:HG22	2.17	0.69
3:G:322:PRO:CB	3:G:538:CYS:O	2.41	0.69
3:G:528:LYS:HG3	3:G:529:LYS:H	1.57	0.69
3:H:362:VAL:CG1	3:H:527:PRO:HB3	2.23	0.69
3:H:487:ASN:O	3:H:488:CYS:HB2	1.91	0.69
3:H:740:MET:HE2	3:J:592:PHE:HE2	1.48	0.69
3:I:45:SER:OG	3:I:46:SER:N	2.25	0.69
3:I:388:ASN:OD1	3:I:527:PRO:CG	2.41	0.69
3:J:328:ARG:NE	3:J:533:LEU:CD2	2.54	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:587:ILE:C	3:J:588:THR:HG22	2.18	0.69
3:G:322:PRO:HB2	3:G:538:CYS:O	1.93	0.69
3:G:587:ILE:C	3:G:588:THR:HG22	2.18	0.69
3:H:470:THR:HG22	3:H:490:PHE:CE1	2.28	0.69
1:C:209:TYR:CE2	1:C:460:GLY:HA2	2.27	0.69
3:I:388:ASN:O	3:I:526:GLY:HA3	1.92	0.69
3:J:326:ILE:CG1	3:J:327:VAL:N	2.56	0.69
3:E:985:ASP:CG	3:G:383:SER:HB2	2.18	0.68
3:G:45:SER:OG	3:G:46:SER:N	2.25	0.68
3:H:985:ASP:CG	3:J:383:SER:HB2	2.18	0.68
3:J:322:PRO:HB2	3:J:538:CYS:O	1.93	0.68
1:A:454:PRO:CG	2:B:768:ARG:HH21	2.07	0.68
3:E:403:ARG:HG3	3:E:495:TYR:CE1	2.29	0.68
3:F:986:PRO:HB2	3:F:987:PRO:HD3	1.74	0.68
3:F:320:VAL:HG21	3:F:591:SER:HB3	1.75	0.68
2:D:34:HIS:ND1	3:H:493:GLN:HG2	2.09	0.68
3:F:388:ASN:OD1	3:F:527:PRO:HG3	1.93	0.68
3:J:945:LEU:HD12	3:J:948:LEU:HD12	1.75	0.68
2:B:739:VAL:O	2:B:740:SER:HB2	1.94	0.68
1:C:454:PRO:CG	2:D:768:ARG:HH21	2.07	0.68
3:F:187:LYS:N	3:F:212:LEU:O	2.25	0.68
3:G:326:ILE:CD1	3:G:327:VAL:H	2.07	0.68
3:H:45:SER:OG	3:H:46:SER:N	2.25	0.68
3:J:317:ASN:HD22	3:J:317:ASN:N	1.92	0.68
3:J:340:GLU:OE2	3:J:356:LYS:CE	2.35	0.68
3:E:487:ASN:O	3:E:488:CYS:HB2	1.91	0.68
3:G:317:ASN:HD22	3:G:317:ASN:N	1.92	0.68
3:G:326:ILE:HD12	3:G:531:THR:HB	1.76	0.68
3:G:518:LEU:HG	3:G:519:HIS:H	1.58	0.68
3:I:571:ASP:CB	3:J:967:SER:HB2	2.22	0.68
3:E:326:ILE:O	3:E:326:ILE:HG13	1.92	0.68
3:G:945:LEU:HD12	3:G:948:LEU:HD12	1.74	0.68
3:H:403:ARG:HG3	3:H:495:TYR:CE1	2.29	0.68
3:H:475:ALA:CB	3:H:487:ASN:C	2.67	0.68
3:H:534:VAL:O	3:H:535:LYS:HG2	1.91	0.68
3:J:322:PRO:CB	3:J:538:CYS:O	2.41	0.68
3:E:44:ARG:O	3:E:283:GLY:CA	2.40	0.68
3:I:535:LYS:HB2	3:I:535:LYS:HZ2	1.57	0.68
3:F:44:ARG:O	3:F:283:GLY:CA	2.40	0.68
3:I:320:VAL:HG21	3:I:591:SER:HB3	1.75	0.68
3:I:1045:LYS:NZ	3:J:786:LYS:HE3	2.09	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:326:ILE:HD12	3:J:531:THR:HB	1.76	0.68
3:G:369:TYR:CZ	3:G:384:PRO:CB	2.77	0.67
3:I:558:LYS:NZ	5:J:1405:NAG:N2	2.38	0.67
3:G:43:PHE:CE1	3:G:283:GLY:HA3	2.29	0.67
3:G:557:LYS:CB	3:G:559:PHE:HE1	2.06	0.67
3:I:43:PHE:CE1	3:I:283:GLY:HA3	2.29	0.67
3:J:557:LYS:CB	3:J:559:PHE:HE1	2.06	0.67
3:E:475:ALA:CB	3:E:487:ASN:C	2.67	0.67
3:F:43:PHE:CE1	3:F:283:GLY:HA3	2.29	0.67
3:G:44:ARG:O	3:G:283:GLY:CA	2.40	0.67
3:G:811:LYS:CB	3:G:812:PRO:CD	2.66	0.67
3:J:43:PHE:CE1	3:J:283:GLY:HA3	2.29	0.67
3:J:518:LEU:HG	3:J:519:HIS:H	1.58	0.67
3:H:96:GLU:OE1	3:H:98:SER:N	2.28	0.67
3:J:326:ILE:CD1	3:J:327:VAL:H	2.07	0.67
3:J:369:TYR:CZ	3:J:384:PRO:CB	2.77	0.67
3:J:578:ASP:OD2	3:J:585:LEU:HD11	1.95	0.67
3:J:96:GLU:OE1	3:J:98:SER:N	2.28	0.67
3:E:482:GLY:O	3:E:483:VAL:HG13	1.95	0.67
3:F:388:ASN:OD1	3:F:527:PRO:CG	2.41	0.67
3:H:482:GLY:O	3:H:483:VAL:HG13	1.95	0.67
3:I:44:ARG:O	3:I:283:GLY:CA	2.40	0.67
2:B:34:HIS:ND1	3:E:493:GLN:HG2	2.09	0.67
1:C:583:TYR:O	1:C:587:VAL:CG2	2.42	0.67
3:E:340:GLU:O	3:E:342:PHE:N	2.28	0.67
3:E:538:CYS:SG	3:E:590:CYS:CB	2.83	0.67
3:H:37:TYR:O	3:H:39:PRO:HD3	1.95	0.67
3:H:392:PHE:CG	3:H:517:LEU:HD21	2.30	0.67
3:J:44:ARG:O	3:J:283:GLY:CA	2.40	0.67
2:D:739:VAL:O	2:D:740:SER:HB2	1.94	0.67
3:E:43:PHE:CE1	3:E:283:GLY:HA3	2.29	0.67
3:E:552:LEU:HD23	3:E:587:ILE:HG12	1.75	0.67
3:F:558:LYS:NZ	5:G:1405:NAG:N2	2.38	0.67
3:F:1045:LYS:NZ	3:G:786:LYS:HE3	2.09	0.67
3:G:578:ASP:OD2	3:G:585:LEU:HD11	1.95	0.67
3:H:44:ARG:O	3:H:283:GLY:CA	2.40	0.67
3:G:326:ILE:CG1	3:G:327:VAL:N	2.56	0.67
3:H:538:CYS:SG	3:H:590:CYS:CB	2.83	0.67
3:H:552:LEU:HD23	3:H:587:ILE:HG12	1.75	0.67
3:I:96:GLU:OE1	3:I:98:SER:N	2.28	0.67
3:J:326:ILE:CG1	3:J:327:VAL:H	2.08	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:454:PRO:CG	2:D:768:ARG:NH2	2.58	0.67
3:I:719:THR:HA	3:I:926:GLN:HE22	1.60	0.67
3:J:528:LYS:HZ1	3:J:530:SER:CB	2.00	0.67
3:E:187:LYS:HG2	3:E:213:VAL:HA	1.77	0.66
3:F:96:GLU:OE1	3:F:98:SER:N	2.28	0.66
3:G:326:ILE:CG1	3:G:327:VAL:H	2.08	0.66
1:A:350:LEU:O	2:B:678:ARG:HB2	1.96	0.66
3:E:96:GLU:OE1	3:E:98:SER:N	2.28	0.66
3:F:312:ILE:HG13	3:F:598:ILE:HG13	1.76	0.66
3:G:96:GLU:OE1	3:G:98:SER:N	2.28	0.66
3:E:37:TYR:O	3:E:39:PRO:HD3	1.95	0.66
3:F:719:THR:HA	3:F:926:GLN:HE22	1.60	0.66
3:J:569:ILE:H	3:J:569:ILE:HD12	1.60	0.66
3:F:519:HIS:CG	3:F:565:PHE:CE1	2.84	0.66
3:G:569:ILE:H	3:G:569:ILE:HD12	1.60	0.66
3:I:382:VAL:O	3:I:383:SER:O	2.14	0.66
3:I:691:SER:O	3:I:692:ILE:HG13	1.96	0.66
3:F:382:VAL:O	3:F:383:SER:O	2.14	0.66
3:I:569:ILE:HG22	3:J:964:LYS:HE2	1.76	0.66
3:J:332:ILE:C	3:J:333:THR:HG1	1.99	0.66
2:B:630:ASP:O	2:B:631:LYS:HB2	1.96	0.66
2:D:177:ARG:HB3	2:D:178:PRO:CD	2.22	0.66
3:E:470:THR:HG22	3:E:490:PHE:CE1	2.28	0.66
3:G:37:TYR:O	3:G:39:PRO:HD3	1.95	0.66
3:H:187:LYS:HG2	3:H:213:VAL:HA	1.78	0.66
2:D:630:ASP:O	2:D:631:LYS:HB2	1.96	0.66
3:E:336:CYS:SG	3:E:337:PRO:HD2	2.35	0.66
3:G:543:PHE:CE2	3:G:578:ASP:OD1	2.44	0.66
3:H:43:PHE:CE1	3:H:283:GLY:HA3	2.29	0.66
3:H:340:GLU:O	3:H:342:PHE:N	2.28	0.66
3:J:37:TYR:O	3:J:39:PRO:HD3	1.95	0.66
1:C:350:LEU:O	2:D:678:ARG:HB2	1.95	0.66
3:G:326:ILE:HG13	3:G:328:ARG:H	1.61	0.66
3:G:670:ILE:HG22	3:G:671:CYS:H	1.60	0.66
3:J:654:GLU:HG3	3:J:693:ILE:HG23	1.68	0.66
1:A:454:PRO:CG	2:B:768:ARG:NH2	2.58	0.66
3:F:691:SER:O	3:F:692:ILE:HG13	1.96	0.66
3:I:521:PRO:CA	3:I:564:GLN:NE2	2.56	0.66
3:F:326:ILE:HG21	3:F:328:ARG:NH2	2.11	0.66
3:I:312:ILE:HG13	3:I:598:ILE:HG13	1.76	0.66
3:J:326:ILE:HG13	3:J:328:ARG:H	1.61	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:328:ARG:NH1	3:E:533:LEU:CG	2.59	0.65
3:F:37:TYR:O	3:F:39:PRO:HD3	1.95	0.65
3:F:388:ASN:CG	3:F:527:PRO:HG3	2.21	0.65
3:F:569:ILE:HG22	3:G:964:LYS:HE2	1.76	0.65
3:J:187:LYS:HG2	3:J:213:VAL:HA	1.77	0.65
2:B:177:ARG:HB3	2:B:178:PRO:CD	2.22	0.65
2:D:734:PRO:O	2:D:735:ASN:HB2	1.96	0.65
3:F:332:ILE:HG23	3:F:528:LYS:HZ1	1.60	0.65
3:H:328:ARG:NH1	3:H:533:LEU:CG	2.59	0.65
3:I:519:HIS:CG	3:I:565:PHE:CE1	2.84	0.65
3:I:569:ILE:H	3:I:569:ILE:HD12	1.60	0.65
3:J:670:ILE:HG22	3:J:671:CYS:H	1.60	0.65
3:I:326:ILE:HG21	3:I:328:ARG:NH2	2.11	0.65
3:E:594:GLY:O	3:E:613:GLN:CG	2.44	0.65
3:I:388:ASN:CG	3:I:527:PRO:HG3	2.21	0.65
3:J:543:PHE:CE2	3:J:578:ASP:OD1	2.44	0.65
2:B:734:PRO:O	2:B:735:ASN:HB2	1.96	0.65
3:F:569:ILE:H	3:F:569:ILE:HD12	1.60	0.65
1:A:594:SER:O	1:A:598:PRO:HD2	1.97	0.65
3:H:319:ARG:HG3	3:H:319:ARG:NH2	2.03	0.65
3:H:569:ILE:HD12	3:H:569:ILE:H	1.61	0.65
3:H:594:GLY:O	3:H:613:GLN:CG	2.45	0.65
3:I:187:LYS:HG2	3:I:213:VAL:HA	1.77	0.65
3:J:811:LYS:CB	3:J:812:PRO:CD	2.66	0.65
1:C:594:SER:O	1:C:598:PRO:HD2	1.97	0.65
3:J:396:TYR:HE2	3:J:516:GLU:OE2	1.80	0.65
3:E:565:PHE:O	3:F:42:VAL:CA	2.34	0.65
3:E:591:SER:O	3:E:592:PHE:HB3	1.95	0.65
3:F:308:VAL:O	3:F:601:GLY:CA	2.44	0.65
3:G:396:TYR:HE2	3:G:516:GLU:OE2	1.80	0.65
3:H:613:GLN:O	3:H:615:VAL:HG23	1.97	0.65
3:J:393:THR:OG1	3:J:518:LEU:CB	2.45	0.65
3:F:187:LYS:HG2	3:F:213:VAL:HA	1.78	0.65
3:I:37:TYR:O	3:I:39:PRO:HD3	1.95	0.65
3:G:187:LYS:HG2	3:G:213:VAL:HA	1.77	0.65
3:H:522:ALA:CB	3:I:200:TYR:OH	2.45	0.65
1:A:583:TYR:O	1:A:587:VAL:CG2	2.42	0.64
1:C:72:ILE:HB	1:C:73:PRO:HD3	1.79	0.64
3:G:327:VAL:HG21	3:G:529:LYS:HG2	1.79	0.64
3:H:591:SER:O	3:H:592:PHE:HB3	1.95	0.64
3:E:225:PRO:HG3	3:G:562:PHE:CE2	2.28	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:516:GLU:HG3	3:E:516:GLU:O	1.97	0.64
3:E:569:ILE:HD12	3:E:569:ILE:H	1.61	0.64
3:H:335:LEU:C	3:H:362:VAL:O	2.40	0.64
3:F:531:THR:HG22	3:F:532:ASN:N	2.12	0.64
1:A:543:LEU:HD12	1:A:543:LEU:O	1.97	0.64
3:G:811:LYS:HB2	3:G:812:PRO:HD3	1.80	0.64
3:I:406:GLU:CD	3:I:418:ILE:CG1	2.71	0.64
1:A:454:PRO:HG3	2:B:768:ARG:HH22	1.62	0.64
1:C:72:ILE:HD12	1:C:72:ILE:N	2.13	0.64
3:J:528:LYS:O	3:J:529:LYS:HB2	1.98	0.64
1:A:72:ILE:HB	1:A:73:PRO:HD3	1.79	0.64
3:G:528:LYS:O	3:G:529:LYS:HB2	1.98	0.64
3:G:690:GLN:O	3:G:691:SER:HB3	1.98	0.64
3:I:675:GLN:O	3:I:690:GLN:CG	2.42	0.64
3:J:327:VAL:HG21	3:J:529:LYS:HG2	1.78	0.64
2:B:310:GLU:OE1	2:B:421:ILE:HD11	1.97	0.64
2:D:310:GLU:OE1	2:D:421:ILE:HD11	1.97	0.64
3:G:393:THR:OG1	3:G:518:LEU:CB	2.45	0.64
3:E:613:GLN:O	3:E:615:VAL:HG23	1.97	0.64
2:B:177:ARG:CB	2:B:178:PRO:HD3	2.25	0.63
2:B:766:ARG:O	2:B:766:ARG:HG2	1.98	0.63
1:C:543:LEU:HD12	1:C:543:LEU:O	1.97	0.63
3:I:308:VAL:O	3:I:601:GLY:CA	2.44	0.63
3:J:533:LEU:N	3:J:533:LEU:HD23	2.13	0.63
3:F:43:PHE:CE1	3:F:282:ASN:O	2.52	0.63
3:F:406:GLU:CD	3:F:418:ILE:CG1	2.71	0.63
3:I:386:LYS:CE	3:J:985:ASP:HB3	2.29	0.63
3:I:531:THR:HG22	3:I:532:ASN:N	2.12	0.63
2:B:335:ASP:N	2:B:361:CYS:SG	2.72	0.63
2:D:335:ASP:N	2:D:361:CYS:SG	2.72	0.63
3:E:385:THR:HG1	3:E:386:LYS:HZ3	1.45	0.63
3:H:43:PHE:CE1	3:H:282:ASN:O	2.51	0.63
3:I:522:ALA:O	3:I:523:THR:OG1	2.16	0.63
3:J:560:LEU:CB	3:J:561:PRO:CD	2.68	0.63
3:J:811:LYS:HB2	3:J:812:PRO:HD3	1.80	0.63
2:D:353:LYS:HD2	3:H:505:TYR:HD2	1.63	0.63
3:G:406:GLU:CD	3:G:418:ILE:CG1	2.71	0.63
3:J:690:GLN:O	3:J:691:SER:HB3	1.98	0.63
1:A:72:ILE:HD12	1:A:72:ILE:N	2.13	0.63
3:F:340:GLU:OE2	3:F:356:LYS:CE	2.35	0.63
3:G:533:LEU:N	3:G:533:LEU:HD23	2.13	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:225:PRO:HG3	3:J:562:PHE:HE2	1.60	0.63
3:J:43:PHE:CE1	3:J:282:ASN:O	2.51	0.63
1:A:276:PHE:O	1:A:494:LEU:HD13	1.99	0.63
2:B:302:TRP:CZ3	2:B:423:LEU:HD11	2.34	0.63
1:C:276:PHE:O	1:C:494:LEU:HD13	1.98	0.63
3:E:225:PRO:HG3	3:G:562:PHE:HE2	1.60	0.63
3:E:406:GLU:CD	3:E:418:ILE:CG1	2.71	0.63
3:E:983:ARG:HA	3:G:382:VAL:HG23	1.81	0.63
3:F:534:VAL:HG12	3:F:535:LYS:H	1.64	0.63
3:G:43:PHE:CE1	3:G:282:ASN:O	2.52	0.63
3:J:406:GLU:CD	3:J:418:ILE:CG1	2.71	0.63
3:F:308:VAL:N	3:F:602:THR:OG1	2.32	0.63
3:F:324:GLU:HG2	3:F:539:VAL:CG2	2.29	0.63
3:F:386:LYS:CE	3:G:985:ASP:HB3	2.29	0.63
3:G:531:THR:HG22	3:G:532:ASN:H	1.64	0.63
3:I:324:GLU:HG2	3:I:539:VAL:CG2	2.29	0.63
3:I:569:ILE:HG13	3:J:47:VAL:HG11	1.80	0.63
3:J:529:LYS:O	3:J:531:THR:N	2.32	0.63
3:E:43:PHE:CE1	3:E:282:ASN:O	2.51	0.63
3:E:492:LEU:O	3:E:493:GLN:NE2	2.32	0.63
3:F:96:GLU:OE1	3:F:97:LYS:N	2.32	0.63
3:F:117:LEU:HD12	3:F:118:LEU:H	1.64	0.63
2:D:302:TRP:CZ3	2:D:423:LEU:HD11	2.34	0.63
3:F:535:LYS:HB2	3:F:535:LYS:HZ2	1.63	0.63
3:H:41:LYS:CE	3:J:564:GLN:OE1	2.47	0.63
3:H:406:GLU:CD	3:H:418:ILE:CG1	2.71	0.63
3:H:492:LEU:O	3:H:493:GLN:NE2	2.32	0.63
3:I:308:VAL:N	3:I:602:THR:OG1	2.32	0.63
3:I:534:VAL:HG12	3:I:535:LYS:H	1.64	0.63
3:E:41:LYS:CE	3:G:564:GLN:OE1	2.47	0.62
3:H:983:ARG:HA	3:J:382:VAL:HG23	1.81	0.62
3:H:43:PHE:HE1	3:H:282:ASN:O	1.82	0.62
3:H:475:ALA:HB2	3:H:487:ASN:C	2.25	0.62
2:B:353:LYS:HD2	3:E:505:TYR:HD2	1.63	0.62
3:E:96:GLU:OE1	3:E:97:LYS:N	2.32	0.62
3:F:613:GLN:O	3:F:615:VAL:HG23	1.99	0.62
3:G:43:PHE:HE1	3:G:282:ASN:O	1.82	0.62
3:G:528:LYS:HE2	3:G:530:SER:CA	2.28	0.62
1:C:76:ILE:HG13	1:C:77:LEU:N	2.13	0.62
3:F:308:VAL:O	3:F:602:THR:N	2.31	0.62
3:F:569:ILE:HG13	3:G:47:VAL:HG11	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:329:PHE:CB	3:H:330:PRO:CD	2.72	0.62
3:I:43:PHE:CE1	3:I:282:ASN:O	2.51	0.62
3:J:43:PHE:HE1	3:J:282:ASN:O	1.83	0.62
3:J:117:LEU:HD12	3:J:118:LEU:H	1.64	0.62
1:A:76:ILE:HG13	1:A:77:LEU:N	2.13	0.62
3:E:124:THR:OG1	3:E:125:ASN:N	2.32	0.62
3:F:43:PHE:HE1	3:F:282:ASN:O	1.83	0.62
3:G:560:LEU:CB	3:G:561:PRO:CD	2.68	0.62
3:G:654:GLU:HG3	3:G:693:ILE:HG23	1.68	0.62
3:H:225:PRO:HD2	3:J:562:PHE:CE2	2.34	0.62
3:J:457:ARG:NH1	3:J:459:SER:O	2.33	0.62
3:F:308:VAL:CG1	3:F:602:THR:HG23	2.30	0.62
3:F:363:ALA:HB2	3:F:524:VAL:HG23	1.82	0.62
3:G:117:LEU:HD12	3:G:118:LEU:H	1.64	0.62
3:I:117:LEU:HD12	3:I:118:LEU:H	1.64	0.62
2:B:143:LEU:O	2:B:146:PRO:HD2	2.00	0.62
3:H:96:GLU:OE1	3:H:97:LYS:N	2.32	0.62
3:H:335:LEU:CA	3:H:362:VAL:O	2.47	0.62
3:I:340:GLU:OE2	3:I:356:LYS:CE	2.35	0.62
3:I:613:GLN:O	3:I:615:VAL:HG23	1.99	0.62
2:B:768:ARG:HH11	2:B:768:ARG:CG	2.13	0.62
2:D:766:ARG:O	2:D:766:ARG:HG2	1.98	0.62
3:F:457:ARG:NH1	3:F:459:SER:O	2.33	0.62
3:H:117:LEU:HD12	3:H:118:LEU:H	1.64	0.62
3:I:43:PHE:HE1	3:I:282:ASN:O	1.82	0.62
3:I:96:GLU:OE1	3:I:97:LYS:N	2.32	0.62
3:I:308:VAL:O	3:I:602:THR:N	2.31	0.62
3:J:813:SER:O	3:J:814:LYS:HE2	2.00	0.62
3:E:457:ARG:NH1	3:E:459:SER:O	2.33	0.62
3:E:470:THR:HG22	3:E:470:THR:O	2.00	0.62
3:H:124:THR:OG1	3:H:125:ASN:N	2.32	0.62
1:A:607:ARG:NH2	1:A:607:ARG:HG3	2.15	0.62
2:D:143:LEU:O	2:D:146:PRO:HD2	2.00	0.62
3:E:808:ASP:HB3	3:E:811:LYS:HD2	1.82	0.62
3:G:529:LYS:O	3:G:531:THR:N	2.32	0.62
3:G:654:GLU:CG	3:G:693:ILE:HG23	2.28	0.62
3:G:813:SER:O	3:G:814:LYS:HE2	2.00	0.62
3:I:363:ALA:HB2	3:I:524:VAL:HG23	1.82	0.62
3:J:531:THR:HG22	3:J:532:ASN:H	1.64	0.62
1:A:159:GLN:NE2	2:B:733:PRO:HB3	2.10	0.61
3:E:475:ALA:HB2	3:E:487:ASN:C	2.25	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:700:GLY:O	3:E:701:ALA:O	2.17	0.61
3:I:326:ILE:HD13	3:I:326:ILE:N	2.15	0.61
3:E:41:LYS:HE2	3:G:564:GLN:OE1	2.00	0.61
3:J:96:GLU:OE1	3:J:97:LYS:N	2.32	0.61
3:E:117:LEU:HD12	3:E:118:LEU:H	1.64	0.61
3:E:518:LEU:O	3:E:519:HIS:HB2	2.00	0.61
3:H:457:ARG:NH1	3:H:459:SER:O	2.33	0.61
3:I:308:VAL:CG1	3:I:602:THR:HG23	2.30	0.61
2:B:735:ASN:ND2	2:B:737:PRO:HD2	2.16	0.61
3:E:357:ARG:HH12	3:E:394:ASN:HD21	1.49	0.61
3:F:519:HIS:NE2	3:F:565:PHE:CZ	2.68	0.61
3:F:521:PRO:CA	3:F:564:GLN:NE2	2.57	0.61
3:G:124:THR:OG1	3:G:125:ASN:N	2.32	0.61
3:G:369:TYR:OH	3:G:384:PRO:HG2	2.00	0.61
3:J:662:CYS:HB2	3:J:697:MET:CE	2.28	0.61
3:E:391:CYS:SG	3:E:523:THR:HB	2.41	0.61
3:E:813:SER:O	3:E:813:SER:OG	2.18	0.61
3:G:557:LYS:CB	3:G:559:PHE:CE1	2.83	0.61
3:H:41:LYS:HE2	3:J:564:GLN:OE1	2.00	0.61
3:H:475:ALA:CB	3:H:487:ASN:O	2.48	0.61
3:H:808:ASP:HB3	3:H:811:LYS:HD2	1.82	0.61
3:J:369:TYR:OH	3:J:384:PRO:HG2	2.00	0.61
2:B:353:LYS:HD2	3:E:505:TYR:CD2	2.36	0.61
3:H:470:THR:HG22	3:H:470:THR:O	2.00	0.61
1:A:234:LEU:HD21	1:A:317:VAL:HG22	1.83	0.61
1:C:454:PRO:HG3	2:D:768:ARG:HH22	1.62	0.61
2:D:628:LEU:HD12	2:D:632:ALA:HB2	1.83	0.61
2:D:768:ARG:HH11	2:D:768:ARG:CG	2.13	0.61
3:E:1077:THR:HG22	3:E:1095:PHE:O	2.01	0.61
3:F:357:ARG:HH12	3:F:394:ASN:HD21	1.49	0.61
3:F:535:LYS:CE	3:F:554:GLU:OE2	2.49	0.61
3:G:96:GLU:OE1	3:G:97:LYS:N	2.32	0.61
3:I:360:ASN:N	3:I:523:THR:CG2	2.64	0.61
3:J:557:LYS:CB	3:J:559:PHE:CE1	2.83	0.61
4:U:1:NAG:H62	4:U:2:NAG:N2	2.03	0.61
2:D:353:LYS:HD2	3:H:505:TYR:CD2	2.36	0.61
2:D:735:ASN:ND2	2:D:737:PRO:HD2	2.16	0.61
3:F:326:ILE:HD13	3:F:326:ILE:N	2.15	0.61
3:G:457:ARG:NH1	3:G:459:SER:O	2.33	0.61
3:H:700:GLY:O	3:H:701:ALA:O	2.17	0.61
3:E:320:VAL:HG21	3:E:591:SER:HB2	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:360:ASN:N	3:F:523:THR:CG2	2.64	0.61
3:I:326:ILE:HD11	3:I:534:VAL:CG2	2.30	0.61
3:I:519:HIS:NE2	3:I:565:PHE:CZ	2.68	0.61
3:E:225:PRO:HG2	3:G:562:PHE:CZ	2.31	0.61
3:E:645:THR:HG22	3:E:647:ALA:H	1.66	0.61
3:G:662:CYS:HB2	3:G:697:MET:CE	2.28	0.61
3:I:124:THR:OG1	3:I:125:ASN:N	2.32	0.61
3:I:357:ARG:HH12	3:I:394:ASN:HD21	1.49	0.61
3:J:357:ARG:HH12	3:J:394:ASN:HD21	1.49	0.61
2:B:628:LEU:HD12	2:B:632:ALA:HB2	1.83	0.60
3:E:43:PHE:HE1	3:E:282:ASN:O	1.82	0.60
3:F:124:THR:OG1	3:F:125:ASN:N	2.32	0.60
3:G:319:ARG:HH21	3:G:319:ARG:HG2	1.66	0.60
3:G:357:ARG:HH12	3:G:394:ASN:HD21	1.49	0.60
3:I:569:ILE:CG2	3:J:964:LYS:HE2	2.31	0.60
3:J:124:THR:OG1	3:J:125:ASN:N	2.33	0.60
3:J:528:LYS:HE2	3:J:530:SER:CA	2.27	0.60
3:J:556:ASN:H	3:J:556:ASN:HD22	1.50	0.60
3:J:645:THR:HG22	3:J:647:ALA:H	1.66	0.60
1:A:44:THR:HA	1:A:223:VAL:HG21	1.84	0.60
3:H:320:VAL:HG21	3:H:591:SER:HB2	1.81	0.60
3:I:570:ALA:HB2	3:J:963:VAL:CG1	2.31	0.60
3:I:617:CYS:N	3:I:644:GLN:HE22	1.96	0.60
3:J:295:PRO:HB2	3:J:608:VAL:HG11	1.84	0.60
2:B:628:LEU:HD12	2:B:632:ALA:HB1	1.82	0.60
3:F:532:ASN:CG	3:F:533:LEU:H	2.09	0.60
3:G:295:PRO:HB2	3:G:608:VAL:HG11	1.84	0.60
3:G:406:GLU:OE1	3:G:418:ILE:HG12	2.02	0.60
3:H:225:PRO:HG2	3:J:562:PHE:CZ	2.31	0.60
3:H:1077:THR:HG22	3:H:1095:PHE:O	2.01	0.60
3:I:457:ARG:NH1	3:I:459:SER:O	2.33	0.60
3:J:393:THR:HG21	3:J:518:LEU:HD22	1.83	0.60
3:J:557:LYS:CG	3:J:559:PHE:HE1	2.14	0.60
3:G:556:ASN:HD22	3:G:556:ASN:H	1.49	0.60
3:H:357:ARG:HH12	3:H:394:ASN:HD21	1.49	0.60
3:J:326:ILE:HG13	3:J:327:VAL:H	1.62	0.60
1:A:607:ARG:HH21	1:A:607:ARG:CG	2.15	0.60
3:E:406:GLU:OE1	3:E:418:ILE:HG12	2.02	0.60
3:F:406:GLU:OE1	3:F:418:ILE:HG12	2.02	0.60
3:G:326:ILE:HD12	3:G:327:VAL:H	1.65	0.60
3:G:393:THR:HG21	3:G:518:LEU:HD22	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:302:TRP:CH2	2:B:423:LEU:CD1	2.78	0.60
3:E:472:ILE:HG22	3:E:473:TYR:N	2.16	0.60
3:F:530:SER:C	3:F:531:THR:HG1	2.00	0.60
3:H:335:LEU:O	3:H:336:CYS:HB2	2.02	0.60
3:I:535:LYS:CE	3:I:554:GLU:OE2	2.49	0.60
3:F:329:PHE:HD2	3:F:528:LYS:CG	1.99	0.60
3:G:557:LYS:CG	3:G:559:PHE:HE1	2.15	0.60
3:G:645:THR:HG22	3:G:647:ALA:H	1.66	0.60
3:H:745:ASP:CB	3:J:319:ARG:NH1	2.46	0.60
3:I:570:ALA:CB	3:J:963:VAL:HG12	2.30	0.60
3:J:319:ARG:HH21	3:J:319:ARG:HG2	1.66	0.60
3:J:326:ILE:HD12	3:J:327:VAL:H	1.65	0.60
2:D:628:LEU:HD12	2:D:632:ALA:HB1	1.82	0.60
3:F:569:ILE:CG2	3:G:964:LYS:HE2	2.31	0.60
3:H:492:LEU:C	3:H:493:GLN:HE21	2.10	0.60
3:J:206:LYS:NZ	3:J:221:SER:OG	2.35	0.60
3:F:164:ASN:N	3:F:164:ASN:OD1	2.35	0.60
3:F:308:VAL:HG21	3:F:599:THR:HG21	1.84	0.60
3:G:164:ASN:OD1	3:G:164:ASN:N	2.35	0.60
3:I:395:VAL:HG23	3:I:524:VAL:HG11	1.84	0.60
1:A:51:GLY:HA2	1:A:427:LEU:HD13	1.84	0.59
1:C:607:ARG:HH21	1:C:607:ARG:CG	2.14	0.59
3:E:328:ARG:HG3	3:E:328:ARG:NH2	2.17	0.59
3:F:326:ILE:HD11	3:F:534:VAL:CG2	2.30	0.59
3:F:395:VAL:HG23	3:F:524:VAL:HG11	1.84	0.59
3:G:332:ILE:C	3:G:333:THR:HG1	2.00	0.59
1:C:234:LEU:HD21	1:C:317:VAL:HG22	1.83	0.59
1:C:607:ARG:NH2	1:C:607:ARG:HG3	2.15	0.59
3:F:206:LYS:NZ	3:F:221:SER:OG	2.35	0.59
3:G:326:ILE:HG13	3:G:327:VAL:H	1.62	0.59
3:H:206:LYS:NZ	3:H:221:SER:OG	2.35	0.59
3:I:532:ASN:CG	3:I:533:LEU:H	2.10	0.59
3:I:645:THR:HG22	3:I:647:ALA:H	1.66	0.59
2:B:172:VAL:HG13	2:B:176:LEU:CD1	2.32	0.59
2:B:212:VAL:HG21	2:B:565:PRO:HG3	1.84	0.59
3:E:556:ASN:H	3:E:556:ASN:HD22	1.50	0.59
3:G:206:LYS:NZ	3:G:221:SER:OG	2.35	0.59
3:G:335:LEU:O	3:G:335:LEU:HD12	2.02	0.59
3:G:546:LEU:CD1	3:G:565:PHE:HD2	2.01	0.59
3:I:406:GLU:OE1	3:I:418:ILE:HG12	2.02	0.59
3:I:556:ASN:HD22	3:I:556:ASN:H	1.49	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:736:GLN:O	2:D:736:GLN:NE2	2.35	0.59
3:F:617:CYS:N	3:F:644:GLN:HE22	1.96	0.59
3:G:327:VAL:O	3:G:329:PHE:CD1	2.55	0.59
3:H:552:LEU:CD2	3:H:587:ILE:HG12	2.32	0.59
2:B:736:GLN:O	2:B:736:GLN:NE2	2.35	0.59
1:C:205:TRP:CZ3	1:C:466:THR:HG21	2.36	0.59
3:E:329:PHE:O	3:E:579:PRO:CB	2.49	0.59
3:F:556:ASN:HD22	3:F:556:ASN:H	1.50	0.59
3:F:570:ALA:CB	3:G:963:VAL:HG12	2.30	0.59
3:I:206:LYS:NZ	3:I:221:SER:OG	2.35	0.59
3:I:308:VAL:HG21	3:I:599:THR:HG21	1.84	0.59
3:J:617:CYS:H	3:J:644:GLN:HE22	1.49	0.59
3:E:901:GLN:HE21	3:E:905:ARG:HE	1.50	0.59
3:F:557:LYS:HD2	3:G:43:PHE:HE2	1.66	0.59
3:H:141:LEU:HB2	3:H:156:GLU:HB2	1.85	0.59
3:H:406:GLU:OE1	3:H:418:ILE:HG12	2.02	0.59
3:H:486:PHE:CE1	3:H:487:ASN:ND2	2.69	0.59
3:H:533:LEU:HD12	3:H:533:LEU:N	2.16	0.59
3:I:164:ASN:OD1	3:I:164:ASN:N	2.35	0.59
3:I:357:ARG:HH22	3:J:230:PRO:CB	2.14	0.59
3:I:535:LYS:HD3	3:I:554:GLU:OE2	2.03	0.59
3:J:335:LEU:O	3:J:335:LEU:HD12	2.02	0.59
2:D:167:SER:O	2:D:171:GLU:HG2	2.03	0.59
3:E:475:ALA:CB	3:E:487:ASN:O	2.48	0.59
3:E:533:LEU:HD12	3:E:533:LEU:N	2.16	0.59
3:F:360:ASN:CB	3:F:523:THR:HG23	2.33	0.59
3:H:645:THR:HG22	3:H:647:ALA:H	1.66	0.59
3:I:521:PRO:HA	3:I:564:GLN:CD	2.27	0.59
3:E:141:LEU:HB2	3:E:156:GLU:HB2	1.85	0.59
3:E:225:PRO:HD2	3:G:562:PHE:CE2	2.34	0.59
3:F:675:GLN:O	3:F:690:GLN:CG	2.42	0.59
3:H:327:VAL:HG12	3:H:328:ARG:N	2.17	0.59
3:H:328:ARG:NH2	3:H:328:ARG:HG3	2.17	0.59
3:H:329:PHE:O	3:H:579:PRO:CB	2.49	0.59
3:H:472:ILE:HG22	3:H:473:TYR:N	2.16	0.59
3:H:543:PHE:CE2	3:H:578:ASP:OD1	2.54	0.59
3:I:141:LEU:HB2	3:I:156:GLU:HB2	1.85	0.59
3:J:528:LYS:CD	3:J:529:LYS:N	2.61	0.59
3:J:663:ASP:OD2	3:J:673:SER:HB2	2.03	0.59
2:D:172:VAL:HG13	2:D:176:LEU:CD1	2.32	0.59
3:F:521:PRO:O	3:F:564:GLN:NE2	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:663:ASP:OD2	3:G:673:SER:HB2	2.03	0.59
3:H:164:ASN:N	3:H:164:ASN:OD1	2.35	0.59
3:H:556:ASN:H	3:H:556:ASN:HD22	1.49	0.59
3:J:406:GLU:OE1	3:J:418:ILE:HG12	2.02	0.59
2:B:139:GLN:HG3	2:D:129:THR:O	2.02	0.59
2:B:167:SER:O	2:B:171:GLU:HG2	2.03	0.59
1:C:44:THR:HA	1:C:223:VAL:HG21	1.84	0.59
3:E:327:VAL:HG12	3:E:328:ARG:N	2.17	0.59
3:F:141:LEU:HB2	3:F:156:GLU:HB2	1.85	0.59
3:F:535:LYS:HD3	3:F:554:GLU:OE2	2.03	0.59
3:F:557:LYS:HD2	3:G:43:PHE:CE2	2.38	0.59
3:J:141:LEU:HB2	3:J:156:GLU:HB2	1.85	0.59
3:J:164:ASN:OD1	3:J:164:ASN:N	2.35	0.59
3:E:164:ASN:N	3:E:164:ASN:OD1	2.35	0.58
3:E:552:LEU:CD2	3:E:587:ILE:HG12	2.32	0.58
3:F:357:ARG:HH22	3:G:230:PRO:CB	2.14	0.58
3:F:645:THR:HG22	3:F:647:ALA:H	1.67	0.58
3:H:901:GLN:HE21	3:H:905:ARG:HE	1.50	0.58
3:I:521:PRO:O	3:I:564:GLN:NE2	2.36	0.58
3:J:327:VAL:O	3:J:329:PHE:CD1	2.55	0.58
1:C:51:GLY:HA2	1:C:427:LEU:HD13	1.84	0.58
3:I:329:PHE:HD2	3:I:528:LYS:CG	1.99	0.58
3:I:535:LYS:O	3:I:536:ASN:HB2	2.03	0.58
3:E:492:LEU:C	3:E:493:GLN:HE21	2.10	0.58
3:F:438:SER:O	3:F:438:SER:OG	2.21	0.58
3:F:558:LYS:HZ3	5:G:1405:NAG:HN2	1.47	0.58
3:G:328:ARG:HG3	3:G:533:LEU:HD22	1.85	0.58
3:H:520:ALA:CB	3:H:521:PRO:HD2	2.17	0.58
3:F:363:ALA:HB2	3:F:524:VAL:CG2	2.33	0.58
2:B:131:LYS:HB3	2:B:141:CYS:HB3	1.86	0.58
3:E:42:VAL:HG22	3:G:565:PHE:CE1	2.39	0.58
3:F:390:LEU:HD11	3:G:983:ARG:HB3	1.85	0.58
3:G:617:CYS:H	3:G:644:GLN:HE22	1.49	0.58
3:I:523:THR:O	3:I:525:CYS:N	2.36	0.58
3:I:557:LYS:HD2	3:J:43:PHE:HE2	1.66	0.58
3:I:738:CYS:O	3:I:742:ILE:HG13	2.03	0.58
2:B:129:THR:O	2:D:139:GLN:HG3	2.02	0.58
2:B:140:GLU:HG3	2:B:140:GLU:O	2.03	0.58
1:C:605:LEU:O	1:C:608:ASN:HB3	2.03	0.58
3:E:48:LEU:H	3:E:48:LEU:HD13	1.69	0.58
3:E:206:LYS:NZ	3:E:221:SER:OG	2.35	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:486:PHE:CE1	3:E:487:ASN:ND2	2.69	0.58
3:F:48:LEU:HD13	3:F:48:LEU:H	1.69	0.58
3:F:521:PRO:HA	3:F:564:GLN:CD	2.27	0.58
3:F:522:ALA:O	3:F:523:THR:OG1	2.16	0.58
3:G:141:LEU:HB2	3:G:156:GLU:HB2	1.84	0.58
3:G:528:LYS:HE2	3:G:529:LYS:H	1.69	0.58
3:G:811:LYS:CB	3:G:812:PRO:HD2	2.27	0.58
3:I:518:LEU:HD22	3:I:519:HIS:N	2.18	0.58
3:J:47:VAL:O	3:J:47:VAL:HG23	2.04	0.58
1:A:87:TYR:HD2	1:A:534:TRP:HZ2	1.52	0.58
2:B:368:ASP:HA	2:B:371:THR:HG22	1.85	0.58
3:F:738:CYS:O	3:F:742:ILE:HG13	2.03	0.58
3:I:320:VAL:CG1	3:I:321:GLN:H	2.13	0.58
1:C:87:TYR:HD2	1:C:534:TRP:HZ2	1.52	0.58
2:D:140:GLU:HG3	2:D:140:GLU:O	2.03	0.58
3:E:473:TYR:CG	3:E:474:GLN:N	2.72	0.58
3:G:392:PHE:CD2	3:G:517:LEU:HD22	2.38	0.58
5:H:1405:NAG:H83	5:H:1405:NAG:H3	1.86	0.58
3:I:390:LEU:HD11	3:J:983:ARG:HB3	1.85	0.58
3:I:533:LEU:HD22	3:I:534:VAL:O	2.03	0.58
1:A:205:TRP:CZ3	1:A:208:LEU:HD23	2.39	0.58
3:E:43:PHE:CE2	3:G:557:LYS:HG2	2.39	0.58
5:E:1405:NAG:H83	5:E:1405:NAG:H3	1.86	0.58
3:F:338:PHE:O	3:F:340:GLU:N	2.37	0.58
3:F:533:LEU:HD22	3:F:534:VAL:O	2.03	0.58
3:F:535:LYS:O	3:F:536:ASN:HB2	2.02	0.58
3:G:557:LYS:HB3	3:G:559:PHE:CD1	2.39	0.58
3:H:225:PRO:HG3	3:J:562:PHE:CE2	2.28	0.58
3:I:557:LYS:HD2	3:J:43:PHE:CE2	2.38	0.58
3:J:328:ARG:HG3	3:J:533:LEU:HD22	1.86	0.58
3:J:338:PHE:O	3:J:340:GLU:N	2.37	0.58
3:J:557:LYS:HB3	3:J:559:PHE:CD1	2.39	0.58
1:C:205:TRP:CZ3	1:C:208:LEU:HD23	2.39	0.58
3:E:576:VAL:HG22	3:E:587:ILE:HD11	1.86	0.58
3:E:722:VAL:HA	3:E:1064:HIS:O	2.03	0.58
3:G:48:LEU:H	3:G:48:LEU:HD13	1.69	0.58
3:H:47:VAL:O	3:H:47:VAL:HG23	2.04	0.58
3:H:576:VAL:HG22	3:H:587:ILE:HD11	1.86	0.58
3:H:963:VAL:HG12	3:J:570:ALA:HB1	1.85	0.58
3:F:321:GLN:NE2	3:F:322:PRO:HD2	2.19	0.57
3:F:518:LEU:HD22	3:F:519:HIS:N	2.18	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:523:THR:O	3:F:525:CYS:N	2.36	0.57
3:I:338:PHE:O	3:I:340:GLU:N	2.37	0.57
3:J:392:PHE:CD2	3:J:517:LEU:HD22	2.38	0.57
3:E:614:ASP:O	3:E:615:VAL:HG23	2.04	0.57
3:F:901:GLN:NE2	3:F:905:ARG:HE	1.99	0.57
3:I:47:VAL:O	3:I:47:VAL:HG23	2.04	0.57
3:I:332:ILE:HG23	3:I:528:LYS:HZ1	1.68	0.57
3:I:363:ALA:HB2	3:I:524:VAL:CG2	2.33	0.57
3:F:324:GLU:CG	3:F:539:VAL:HG23	2.34	0.57
3:G:528:LYS:CE	3:G:530:SER:CA	2.82	0.57
3:H:42:VAL:HG22	3:J:565:PHE:CE1	2.39	0.57
3:H:48:LEU:HD13	3:H:48:LEU:H	1.69	0.57
3:H:614:ASP:O	3:H:615:VAL:HG23	2.04	0.57
3:I:105:ILE:HG12	3:I:239:GLN:HB2	1.87	0.57
1:A:605:LEU:O	1:A:608:ASN:HB3	2.04	0.57
2:D:177:ARG:CB	2:D:178:PRO:HD3	2.25	0.57
3:E:329:PHE:CB	3:E:330:PRO:CD	2.73	0.57
3:E:963:VAL:HG12	3:G:570:ALA:HB1	1.85	0.57
3:I:360:ASN:CB	3:I:523:THR:HG23	2.33	0.57
3:I:382:VAL:C	3:I:383:SER:O	2.47	0.57
3:J:48:LEU:H	3:J:48:LEU:HD13	1.69	0.57
2:D:368:ASP:HA	2:D:371:THR:HG22	1.85	0.57
3:F:105:ILE:HG12	3:F:239:GLN:HB2	1.87	0.57
3:F:532:ASN:OD1	3:F:533:LEU:N	2.38	0.57
3:H:43:PHE:CE2	3:J:557:LYS:HG2	2.39	0.57
3:H:524:VAL:CG2	3:H:525:CYS:H	2.09	0.57
3:H:722:VAL:HA	3:H:1064:HIS:O	2.03	0.57
3:I:324:GLU:CG	3:I:539:VAL:HG23	2.34	0.57
3:J:328:ARG:CG	3:J:533:LEU:HD22	2.34	0.57
1:A:602:ILE:O	1:A:606:ILE:HG12	2.03	0.57
1:C:602:ILE:O	1:C:606:ILE:HG12	2.03	0.57
2:D:212:VAL:HG21	2:D:565:PRO:HG3	1.84	0.57
3:G:328:ARG:CG	3:G:533:LEU:HD22	2.34	0.57
3:G:338:PHE:O	3:G:340:GLU:N	2.37	0.57
3:H:105:ILE:HG12	3:H:239:GLN:HB2	1.87	0.57
3:H:392:PHE:HB3	3:H:517:LEU:HD22	1.82	0.57
3:I:48:LEU:HD13	3:I:48:LEU:H	1.69	0.57
3:I:321:GLN:NE2	3:I:322:PRO:HD2	2.19	0.57
3:I:411:ALA:CA	3:I:425:LEU:HD12	2.35	0.57
3:I:521:PRO:O	3:I:522:ALA:HB2	2.05	0.57
3:J:390:LEU:HD23	3:J:391:CYS:N	2.19	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:528:LYS:CE	3:J:530:SER:CA	2.82	0.57
3:J:578:ASP:CG	3:J:585:LEU:HD11	2.30	0.57
3:E:578:ASP:OD2	3:E:585:LEU:HD11	2.05	0.57
3:F:47:VAL:O	3:F:47:VAL:HG23	2.04	0.57
3:F:227:VAL:HG12	3:F:228:ASP:N	2.20	0.57
3:F:521:PRO:O	3:F:522:ALA:HB2	2.05	0.57
3:G:47:VAL:O	3:G:47:VAL:HG23	2.04	0.57
3:G:578:ASP:CG	3:G:585:LEU:HD11	2.30	0.57
3:G:592:PHE:N	3:G:592:PHE:CD1	2.73	0.57
3:J:528:LYS:HE2	3:J:529:LYS:H	1.69	0.57
1:A:87:TYR:CD2	1:A:534:TRP:HZ2	2.23	0.57
1:C:597:ILE:HB	1:C:598:PRO:CD	2.33	0.57
3:E:47:VAL:O	3:E:47:VAL:HG23	2.04	0.57
3:G:227:VAL:HG12	3:G:228:ASP:N	2.20	0.57
3:F:563:GLN:O	3:F:577:ARG:NH1	2.38	0.57
3:G:41:LYS:O	3:G:42:VAL:HB	2.05	0.57
3:I:901:GLN:NE2	3:I:905:ARG:HE	1.99	0.57
3:J:227:VAL:HG12	3:J:228:ASP:N	2.20	0.57
3:J:531:THR:HG22	3:J:532:ASN:N	2.20	0.57
3:J:565:PHE:O	3:J:565:PHE:HD1	1.87	0.57
4:s:2:NAG:H3	4:s:2:NAG:H83	1.87	0.57
4:y:2:NAG:H83	4:y:2:NAG:H3	1.87	0.57
4:EA:2:NAG:H3	4:EA:2:NAG:H83	1.87	0.57
3:E:45:SER:O	3:E:279:TYR:HB2	2.05	0.57
3:E:105:ILE:HG12	3:E:239:GLN:HB2	1.87	0.57
3:E:341:VAL:HG21	3:E:356:LYS:HD3	1.84	0.57
3:F:669:GLY:N	3:G:864:LEU:O	2.38	0.57
3:G:390:LEU:HD23	3:G:391:CYS:N	2.19	0.57
3:H:390:LEU:HD23	3:H:391:CYS:N	2.19	0.57
3:I:563:GLN:O	3:I:577:ARG:NH1	2.38	0.57
3:J:45:SER:O	3:J:279:TYR:HB2	2.05	0.57
4:r:2:NAG:H3	4:r:2:NAG:H83	1.86	0.57
4:DA:2:NAG:H83	4:DA:2:NAG:H3	1.86	0.57
3:G:342:PHE:HB3	4:n:1:NAG:H82	1.87	0.56
3:G:565:PHE:O	3:G:565:PHE:HD1	1.87	0.56
3:H:699:LEU:HD22	3:I:873:TYR:CZ	2.40	0.56
3:J:342:PHE:HB3	4:9:1:NAG:H82	1.87	0.56
3:J:735:SER:OG	3:J:859:THR:HG23	2.04	0.56
3:E:327:VAL:CG1	3:E:529:LYS:O	2.53	0.56
3:E:493:GLN:HE21	3:E:493:GLN:N	2.03	0.56
3:E:699:LEU:HD22	3:F:873:TYR:CZ	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:531:THR:HG22	3:G:532:ASN:N	2.20	0.56
3:H:563:GLN:O	3:H:577:ARG:NH1	2.38	0.56
3:I:438:SER:O	3:I:438:SER:OG	2.21	0.56
5:J:1405:NAG:H83	5:J:1405:NAG:H3	1.86	0.56
2:B:54:ILE:HD12	2:B:341:LYS:HG3	1.87	0.56
1:C:87:TYR:CD2	1:C:534:TRP:HZ2	2.23	0.56
2:D:167:SER:OG	2:D:168:TRP:N	2.39	0.56
3:F:41:LYS:O	3:F:42:VAL:HB	2.05	0.56
3:F:45:SER:O	3:F:279:TYR:HB2	2.05	0.56
3:F:411:ALA:CA	3:F:425:LEU:HD12	2.35	0.56
3:G:45:SER:O	3:G:279:TYR:HB2	2.05	0.56
3:G:338:PHE:C	3:G:340:GLU:H	2.13	0.56
3:H:227:VAL:HG12	3:H:228:ASP:N	2.20	0.56
3:I:41:LYS:O	3:I:42:VAL:HB	2.05	0.56
3:I:227:VAL:HG12	3:I:228:ASP:N	2.20	0.56
3:I:327:VAL:C	3:I:328:ARG:HG2	2.30	0.56
3:I:338:PHE:C	3:I:340:GLU:H	2.13	0.56
3:I:357:ARG:NH2	3:J:230:PRO:HB2	2.20	0.56
3:I:655:HIS:HD2	3:I:694:ALA:O	1.88	0.56
5:I:1405:NAG:H3	5:I:1405:NAG:H83	1.86	0.56
3:J:29:THR:HG22	3:J:30:ASN:H	1.70	0.56
4:c:2:NAG:H3	4:c:2:NAG:H83	1.87	0.56
2:B:425:SER:HB3	2:B:427:ASP:OD1	2.06	0.56
3:E:353:TRP:CD1	3:E:353:TRP:H	2.24	0.56
3:G:326:ILE:O	3:G:327:VAL:HG22	2.06	0.56
3:G:804:GLN:HE21	3:G:935:GLN:HE22	1.52	0.56
3:H:29:THR:HG22	3:H:30:ASN:H	1.70	0.56
3:H:327:VAL:CG1	3:H:529:LYS:O	2.53	0.56
3:J:338:PHE:C	3:J:340:GLU:H	2.13	0.56
3:J:811:LYS:CB	3:J:812:PRO:HD2	2.28	0.56
1:C:483:SER:O	1:C:486:ASP:HB3	2.06	0.56
2:D:425:SER:HB3	2:D:427:ASP:OD1	2.06	0.56
3:E:393:THR:OG1	3:E:518:LEU:N	2.39	0.56
3:F:655:HIS:HD2	3:F:694:ALA:O	1.88	0.56
3:H:45:SER:O	3:H:279:TYR:HB2	2.05	0.56
3:H:327:VAL:CB	3:H:530:SER:HA	2.31	0.56
3:H:578:ASP:OD2	3:H:585:LEU:HD11	2.05	0.56
3:I:530:SER:C	3:I:531:THR:HG1	2.02	0.56
3:I:576:VAL:HG22	3:I:587:ILE:HD11	1.88	0.56
3:J:326:ILE:O	3:J:327:VAL:HG22	2.06	0.56
2:B:335:ASP:N	2:B:335:ASP:OD1	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:735:ASN:O	2:D:736:GLN:HB3	2.05	0.56
3:E:475:ALA:HB3	3:E:487:ASN:C	2.29	0.56
3:F:357:ARG:NH2	3:G:230:PRO:HB2	2.20	0.56
3:G:438:SER:O	3:G:438:SER:OG	2.21	0.56
5:G:1405:NAG:H3	5:G:1405:NAG:H83	1.86	0.56
3:I:45:SER:O	3:I:279:TYR:HB2	2.05	0.56
3:J:546:LEU:CD1	3:J:565:PHE:HD2	2.01	0.56
2:D:765:ILE:C	2:D:767:ASP:H	2.14	0.56
3:E:29:THR:HG22	3:E:30:ASN:H	1.70	0.56
3:E:978:ASN:HD22	3:G:547:THR:HG22	1.71	0.56
3:F:43:PHE:CG	3:F:44:ARG:N	2.74	0.56
3:F:357:ARG:CZ	3:G:230:PRO:CG	2.81	0.56
3:F:570:ALA:HB2	3:G:963:VAL:CG1	2.31	0.56
5:F:1405:NAG:H3	5:F:1405:NAG:H83	1.86	0.56
3:H:406:GLU:OE1	3:H:418:ILE:CG1	2.54	0.56
3:H:493:GLN:HE21	3:H:493:GLN:N	2.03	0.56
3:H:978:ASN:ND2	3:J:547:THR:HG22	2.20	0.56
3:I:357:ARG:CZ	3:J:230:PRO:CG	2.81	0.56
2:D:54:ILE:HD12	2:D:341:LYS:HG3	1.87	0.56
3:E:563:GLN:O	3:E:577:ARG:NH1	2.38	0.56
3:F:29:THR:HG22	3:F:30:ASN:H	1.71	0.56
3:F:576:VAL:HG22	3:F:587:ILE:HD11	1.88	0.56
3:H:522:ALA:HB2	3:I:200:TYR:OH	2.05	0.56
3:I:515:PHE:CD1	3:I:515:PHE:N	2.73	0.56
3:J:41:LYS:O	3:J:42:VAL:HB	2.05	0.56
3:J:328:ARG:CZ	3:J:533:LEU:HD21	2.36	0.56
3:J:438:SER:O	3:J:438:SER:OG	2.21	0.56
3:J:557:LYS:HB3	3:J:559:PHE:HE1	1.64	0.56
2:B:167:SER:OG	2:B:168:TRP:N	2.39	0.56
1:C:205:TRP:CE2	1:C:466:THR:CG2	2.87	0.56
3:E:334:ASN:C	3:E:335:LEU:HG	2.30	0.56
3:E:406:GLU:OE1	3:E:418:ILE:CG1	2.54	0.56
3:F:360:ASN:HB3	3:F:523:THR:HG23	1.87	0.56
3:F:406:GLU:OE1	3:F:418:ILE:CG1	2.54	0.56
3:G:45:SER:HA	3:G:280:ASN:O	2.06	0.56
3:G:353:TRP:H	3:G:353:TRP:CD1	2.24	0.56
3:G:406:GLU:OE1	3:G:418:ILE:CG1	2.54	0.56
3:H:328:ARG:HG3	3:H:328:ARG:HH21	1.70	0.56
3:J:322:PRO:HB3	3:J:538:CYS:O	2.06	0.56
3:J:353:TRP:CD1	3:J:353:TRP:H	2.24	0.56
1:A:483:SER:O	1:A:486:ASP:HB3	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:597:ILE:HB	1:A:598:PRO:CD	2.33	0.56
1:C:489:ALA:HB2	1:C:589:VAL:HG12	1.88	0.56
3:E:45:SER:HA	3:E:280:ASN:O	2.06	0.56
3:E:489:TYR:CD1	3:E:489:TYR:N	2.73	0.56
3:E:543:PHE:CE2	3:E:578:ASP:OD1	2.54	0.56
3:F:327:VAL:C	3:F:328:ARG:HG2	2.30	0.56
3:G:328:ARG:CZ	3:G:533:LEU:HD21	2.36	0.56
3:H:45:SER:HA	3:H:280:ASN:O	2.06	0.56
3:H:538:CYS:SG	3:H:590:CYS:HB3	2.46	0.56
3:H:978:ASN:HD22	3:J:547:THR:HG22	1.71	0.56
3:I:406:GLU:OE1	3:I:418:ILE:CG1	2.54	0.56
3:I:532:ASN:OD1	3:I:533:LEU:N	2.37	0.56
3:J:105:ILE:HG12	3:J:239:GLN:HB2	1.87	0.56
3:J:406:GLU:OE1	3:J:418:ILE:CG1	2.54	0.56
3:J:587:ILE:CG2	3:J:588:THR:H	2.19	0.56
3:J:654:GLU:CG	3:J:693:ILE:HG23	2.27	0.56
3:J:674:TYR:HD1	3:J:691:SER:O	1.89	0.56
2:D:538:PRO:HD2	2:D:541:LYS:HD2	1.88	0.55
3:E:227:VAL:HG12	3:E:228:ASP:N	2.20	0.55
3:F:45:SER:HA	3:F:280:ASN:O	2.06	0.55
3:F:663:ASP:OD2	3:F:673:SER:OG	2.22	0.55
3:G:393:THR:HA	3:G:523:THR:OG1	2.06	0.55
3:G:533:LEU:HD23	3:G:533:LEU:H	1.69	0.55
3:G:675:GLN:O	3:G:690:GLN:HG3	2.06	0.55
3:H:614:ASP:O	3:H:615:VAL:CG2	2.54	0.55
3:I:43:PHE:CG	3:I:44:ARG:N	2.74	0.55
3:J:533:LEU:HD23	3:J:533:LEU:H	1.69	0.55
3:J:804:GLN:HE21	3:J:935:GLN:HE22	1.52	0.55
1:A:108:HIS:ND1	1:A:109:PRO:HD2	2.21	0.55
3:E:43:PHE:CG	3:E:44:ARG:N	2.74	0.55
3:E:663:ASP:OD2	3:E:673:SER:OG	2.22	0.55
3:E:978:ASN:ND2	3:G:547:THR:HG22	2.20	0.55
3:F:329:PHE:CG	3:F:528:LYS:HB3	2.41	0.55
3:G:105:ILE:HG12	3:G:239:GLN:HB2	1.87	0.55
3:H:57:PRO:O	3:H:60:SER:OG	2.24	0.55
3:I:29:THR:HG22	3:I:30:ASN:H	1.70	0.55
3:J:328:ARG:CZ	3:J:533:LEU:CD2	2.84	0.55
3:J:592:PHE:N	3:J:592:PHE:CD1	2.73	0.55
1:A:229:LEU:CB	1:A:230:PRO:HD3	2.29	0.55
2:B:735:ASN:O	2:B:736:GLN:HB3	2.05	0.55
2:B:765:ILE:C	2:B:767:ASP:H	2.14	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:131:LYS:HB3	2:D:141:CYS:HB3	1.86	0.55
3:F:342:PHE:HB3	4:g:1:NAG:H82	1.87	0.55
3:G:329:PHE:CB	3:G:330:PRO:HD2	2.36	0.55
3:H:985:ASP:N	3:J:383:SER:HB3	2.21	0.55
3:I:342:PHE:HB3	4:2:1:NAG:H82	1.87	0.55
3:I:669:GLY:N	3:J:864:LEU:O	2.38	0.55
3:I:1045:LYS:HZ2	3:J:786:LYS:HE3	1.71	0.55
3:J:530:SER:OG	3:J:580:GLN:NE2	2.39	0.55
4:n:1:NAG:H61	4:n:2:NAG:HN2	1.72	0.55
1:A:205:TRP:CZ3	1:A:466:THR:HG21	2.36	0.55
2:B:231:GLU:HA	2:B:234:LYS:HD3	1.88	0.55
3:E:328:ARG:HG3	3:E:328:ARG:HH21	1.69	0.55
3:E:538:CYS:SG	3:E:590:CYS:HB3	2.46	0.55
3:F:338:PHE:C	3:F:340:GLU:H	2.13	0.55
3:G:559:PHE:HB3	3:G:563:GLN:HB3	1.87	0.55
3:H:522:ALA:HB3	3:I:200:TYR:OH	2.06	0.55
3:J:591:SER:O	3:J:592:PHE:HB3	2.06	0.55
3:E:699:LEU:HD22	3:F:873:TYR:CE2	2.42	0.55
3:F:613:GLN:O	3:F:615:VAL:N	2.40	0.55
3:G:327:VAL:CB	3:G:529:LYS:HB3	2.35	0.55
3:H:347:PHE:CE1	3:H:509:ARG:HD3	2.42	0.55
3:E:347:PHE:CE1	3:E:509:ARG:HD3	2.42	0.55
3:I:386:LYS:HE2	3:J:985:ASP:HB3	1.88	0.55
3:I:430:THR:O	3:I:515:PHE:CE1	2.60	0.55
3:J:347:PHE:CE1	3:J:509:ARG:HD3	2.42	0.55
1:C:159:GLN:NE2	2:D:733:PRO:HB3	2.11	0.55
2:D:335:ASP:N	2:D:335:ASP:OD1	2.39	0.55
3:E:522:ALA:O	3:E:523:THR:OG1	2.23	0.55
3:E:675:GLN:O	3:E:690:GLN:NE2	2.36	0.55
3:G:43:PHE:CG	3:G:44:ARG:N	2.74	0.55
3:H:699:LEU:HD22	3:I:873:TYR:CE2	2.42	0.55
1:A:467:PHE:HD1	1:A:468:LEU:HD23	1.72	0.55
1:C:492:ILE:CG2	1:C:590:ALA:HB1	2.34	0.55
2:D:231:GLU:HA	2:D:234:LYS:HD3	1.88	0.55
3:E:521:PRO:O	3:E:522:ALA:HB2	2.06	0.55
3:H:43:PHE:CG	3:H:44:ARG:N	2.74	0.55
3:J:559:PHE:HB3	3:J:563:GLN:HB3	1.87	0.55
4:9:1:NAG:H61	4:9:2:NAG:HN2	1.72	0.55
3:E:985:ASP:N	3:G:383:SER:HB3	2.21	0.55
3:F:382:VAL:C	3:F:383:SER:O	2.47	0.55
3:F:515:PHE:CD1	3:F:515:PHE:N	2.73	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:328:ARG:CZ	3:G:533:LEU:CD2	2.84	0.55
3:G:530:SER:OG	3:G:580:GLN:NE2	2.39	0.55
3:G:674:TYR:HD1	3:G:691:SER:O	1.89	0.55
3:H:479:PRO:O	3:H:480:CYS:HB3	2.07	0.55
3:J:45:SER:HA	3:J:280:ASN:O	2.06	0.55
3:J:327:VAL:CB	3:J:529:LYS:HB3	2.35	0.55
3:J:541:PHE:CZ	3:J:587:ILE:HD13	2.42	0.55
3:J:556:ASN:HD22	3:J:556:ASN:N	2.05	0.55
1:A:484:LEU:HG	1:A:485:LEU:N	2.21	0.55
2:D:342:ALA:O	2:D:343:VAL:C	2.50	0.55
3:E:57:PRO:O	3:E:60:SER:OG	2.25	0.55
3:E:556:ASN:HD22	3:E:556:ASN:N	2.05	0.55
3:G:57:PRO:O	3:G:60:SER:OG	2.24	0.55
3:G:735:SER:OG	3:G:859:THR:HG23	2.04	0.55
3:H:353:TRP:CD1	3:H:353:TRP:H	2.24	0.55
3:H:565:PHE:CE2	3:I:42:VAL:HG22	2.42	0.55
3:I:421:TYR:HA	3:I:461:LEU:HG	1.89	0.55
3:J:523:THR:CG2	3:J:524:VAL:H	2.12	0.55
3:J:592:PHE:N	3:J:592:PHE:HD1	2.05	0.55
1:C:484:LEU:HG	1:C:485:LEU:N	2.21	0.54
2:D:172:VAL:CG1	2:D:176:LEU:HD12	2.36	0.54
3:F:332:ILE:HG23	3:F:528:LYS:NZ	2.22	0.54
3:F:353:TRP:CD1	3:F:353:TRP:H	2.23	0.54
3:F:748:GLU:HG2	3:F:981:LEU:HD21	1.83	0.54
3:G:322:PRO:HB3	3:G:538:CYS:O	2.06	0.54
3:G:591:SER:O	3:G:592:PHE:HB3	2.06	0.54
3:H:489:TYR:CD1	3:H:489:TYR:N	2.73	0.54
3:I:663:ASP:OD2	3:I:673:SER:OG	2.22	0.54
3:J:559:PHE:HD1	3:J:559:PHE:N	2.05	0.54
3:J:675:GLN:O	3:J:690:GLN:HG3	2.06	0.54
1:C:83:ILE:HB	1:C:84:PRO:CD	2.35	0.54
2:D:739:VAL:O	2:D:740:SER:CB	2.56	0.54
3:F:386:LYS:HE2	3:G:985:ASP:HB3	1.88	0.54
3:G:329:PHE:HB3	3:G:330:PRO:CD	2.36	0.54
3:I:45:SER:HA	3:I:280:ASN:O	2.06	0.54
3:I:57:PRO:O	3:I:60:SER:OG	2.25	0.54
3:I:613:GLN:O	3:I:615:VAL:N	2.40	0.54
3:E:614:ASP:O	3:E:615:VAL:CG2	2.54	0.54
3:F:111:ASP:OD1	3:F:134:GLN:NE2	2.41	0.54
3:G:328:ARG:NH1	3:G:533:LEU:HD21	2.22	0.54
3:H:392:PHE:HA	3:H:517:LEU:HD11	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:663:ASP:OD2	3:H:673:SER:OG	2.22	0.54
3:I:353:TRP:CD1	3:I:353:TRP:H	2.24	0.54
3:J:43:PHE:CG	3:J:44:ARG:N	2.74	0.54
3:J:57:PRO:O	3:J:60:SER:OG	2.24	0.54
3:J:393:THR:HA	3:J:523:THR:OG1	2.06	0.54
1:C:108:HIS:ND1	1:C:109:PRO:HD2	2.21	0.54
3:E:326:ILE:HD13	3:E:533:LEU:CA	2.30	0.54
3:G:329:PHE:H	3:G:530:SER:HA	1.72	0.54
3:G:528:LYS:CD	3:G:529:LYS:N	2.62	0.54
4:2:1:NAG:H61	4:2:2:NAG:HN2	1.72	0.54
3:E:544:ASN:O	3:E:544:ASN:ND2	2.41	0.54
3:G:556:ASN:HD22	3:G:556:ASN:N	2.05	0.54
3:G:559:PHE:N	3:G:559:PHE:HD1	2.05	0.54
3:H:111:ASP:OD1	3:H:134:GLN:NE2	2.41	0.54
3:I:43:PHE:O	3:I:44:ARG:HG3	2.08	0.54
3:I:111:ASP:OD1	3:I:134:GLN:NE2	2.41	0.54
3:I:748:GLU:HG2	3:I:981:LEU:HD21	1.83	0.54
3:J:111:ASP:OD1	3:J:134:GLN:NE2	2.41	0.54
3:J:559:PHE:CD1	3:J:559:PHE:N	2.76	0.54
4:N:1:NAG:H62	4:N:2:NAG:N2	2.02	0.54
1:A:414:PRO:O	1:A:418:VAL:HG23	2.07	0.54
3:F:57:PRO:O	3:F:60:SER:OG	2.25	0.54
3:F:347:PHE:CE1	3:F:509:ARG:HD3	2.42	0.54
3:F:421:TYR:HA	3:F:461:LEU:HG	1.90	0.54
3:F:535:LYS:CD	3:F:554:GLU:OE2	2.56	0.54
3:F:592:PHE:HD2	3:G:740:MET:HE1	1.72	0.54
3:G:43:PHE:O	3:G:44:ARG:HG3	2.08	0.54
3:G:111:ASP:OD1	3:G:134:GLN:NE2	2.41	0.54
3:G:347:PHE:CE1	3:G:509:ARG:HD3	2.42	0.54
3:H:341:VAL:HG21	3:H:356:LYS:HD3	1.84	0.54
3:I:332:ILE:HG23	3:I:528:LYS:NZ	2.22	0.54
3:I:347:PHE:CE1	3:I:509:ARG:HD3	2.42	0.54
3:I:556:ASN:HD22	3:I:556:ASN:N	2.05	0.54
3:E:111:ASP:OD1	3:E:134:GLN:NE2	2.41	0.54
3:E:327:VAL:CB	3:E:530:SER:HA	2.31	0.54
3:E:565:PHE:CE2	3:F:42:VAL:HG22	2.42	0.54
3:E:669:GLY:N	3:F:864:LEU:O	2.40	0.54
3:G:29:THR:HG22	3:G:30:ASN:H	1.71	0.54
3:G:559:PHE:CD1	3:G:559:PHE:N	2.76	0.54
3:H:556:ASN:HD22	3:H:556:ASN:N	2.05	0.54
3:H:614:ASP:C	3:H:615:VAL:HG23	2.33	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:654:GLU:O	3:H:693:ILE:CA	2.56	0.54
3:J:329:PHE:H	3:J:530:SER:HA	1.72	0.54
1:A:205:TRP:CE2	1:A:466:THR:CG2	2.87	0.54
2:B:144:LEU:HD22	2:B:168:TRP:CZ2	2.43	0.54
2:B:734:PRO:O	2:B:735:ASN:CB	2.56	0.54
2:D:52:THR:OG1	2:D:332:MET:SD	2.66	0.54
3:E:478:THR:CG2	3:E:479:PRO:CD	2.86	0.54
3:F:100:ILE:O	3:F:242:LEU:HA	2.08	0.54
3:G:541:PHE:CZ	3:G:587:ILE:HD13	2.42	0.54
3:H:438:SER:O	3:H:438:SER:OG	2.21	0.54
3:H:669:GLY:N	3:I:864:LEU:O	2.40	0.54
2:B:342:ALA:O	2:B:343:VAL:C	2.50	0.54
3:I:329:PHE:CG	3:I:528:LYS:HB3	2.41	0.54
4:g:1:NAG:H61	4:g:2:NAG:HN2	1.72	0.54
1:A:593:PRO:O	1:A:596:THR:HB	2.09	0.54
2:B:538:PRO:HD2	2:B:541:LYS:HD2	1.88	0.54
1:C:467:PHE:HD1	1:C:468:LEU:HD23	1.72	0.54
1:C:603:TYR:CD1	1:C:603:TYR:C	2.85	0.54
3:E:614:ASP:C	3:E:615:VAL:HG23	2.33	0.54
3:F:327:VAL:HG22	3:F:531:THR:HB	1.90	0.54
3:H:41:LYS:O	3:H:42:VAL:HB	2.08	0.54
3:H:43:PHE:O	3:H:44:ARG:HG3	2.08	0.54
3:H:100:ILE:O	3:H:242:LEU:HA	2.08	0.54
3:H:544:ASN:O	3:H:544:ASN:ND2	2.41	0.54
3:H:565:PHE:CZ	3:I:42:VAL:HG22	2.43	0.54
3:H:675:GLN:O	3:H:690:GLN:NE2	2.36	0.54
3:I:360:ASN:HB3	3:I:523:THR:HG23	1.87	0.54
3:I:535:LYS:CD	3:I:554:GLU:OE2	2.56	0.54
3:J:43:PHE:O	3:J:44:ARG:HG3	2.08	0.54
3:J:100:ILE:O	3:J:242:LEU:HA	2.08	0.54
3:J:328:ARG:NH1	3:J:533:LEU:HD21	2.22	0.54
3:J:333:THR:O	3:J:362:VAL:CG2	2.44	0.54
2:B:697:ARG:NH1	2:B:701:GLU:OE2	2.41	0.53
2:D:697:ARG:NH1	2:D:701:GLU:OE2	2.41	0.53
3:E:482:GLY:O	3:E:483:VAL:HG22	2.08	0.53
3:E:894:LEU:HB3	3:G:713:ALA:HB3	1.90	0.53
3:F:357:ARG:NH2	3:G:230:PRO:HG2	2.21	0.53
3:F:617:CYS:SG	3:F:649:CYS:CB	2.96	0.53
3:H:894:LEU:HB3	3:J:713:ALA:HB3	1.90	0.53
3:J:544:ASN:O	3:J:544:ASN:ND2	2.41	0.53
2:B:739:VAL:O	2:B:740:SER:CB	2.56	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:209:TYR:HE2	1:C:460:GLY:N	2.07	0.53
3:E:100:ILE:O	3:E:242:LEU:HA	2.08	0.53
3:F:43:PHE:O	3:F:44:ARG:HG3	2.08	0.53
3:H:516:GLU:O	3:H:517:LEU:CD2	2.53	0.53
3:I:357:ARG:HH22	3:J:230:PRO:CG	2.19	0.53
3:I:569:ILE:HG12	3:J:47:VAL:HG12	1.89	0.53
3:I:1142:GLN:HG3	3:I:1143:PRO:CD	2.37	0.53
3:J:385:THR:HG1	3:J:386:LYS:HZ3	1.54	0.53
1:C:414:PRO:O	1:C:418:VAL:HG23	2.07	0.53
2:D:105:SER:C	2:D:106:SER:HG	2.05	0.53
2:D:734:PRO:O	2:D:735:ASN:CB	2.56	0.53
3:E:41:LYS:O	3:E:42:VAL:HB	2.08	0.53
3:E:488:CYS:C	3:E:489:TYR:CG	2.86	0.53
3:F:320:VAL:CG1	3:F:321:GLN:H	2.13	0.53
3:I:100:ILE:O	3:I:242:LEU:HA	2.08	0.53
3:I:327:VAL:HG22	3:I:531:THR:HB	1.91	0.53
3:I:328:ARG:CZ	3:I:533:LEU:HB2	2.38	0.53
3:I:617:CYS:SG	3:I:649:CYS:CB	2.96	0.53
1:A:209:TYR:HE2	1:A:460:GLY:N	2.07	0.53
2:B:52:THR:OG1	2:B:332:MET:SD	2.66	0.53
2:D:31:LYS:NZ	3:H:493:GLN:OE1	2.42	0.53
3:F:569:ILE:HG12	3:G:47:VAL:HG12	1.89	0.53
3:G:421:TYR:HA	3:G:461:LEU:HG	1.89	0.53
3:I:580:GLN:O	4:I:1:NAG:H83	2.08	0.53
3:E:43:PHE:O	3:E:44:ARG:HG3	2.08	0.53
3:E:475:ALA:HB3	3:E:487:ASN:HB2	1.89	0.53
3:F:580:GLN:O	4:f:1:NAG:H83	2.08	0.53
3:J:674:TYR:CD1	3:J:691:SER:O	2.61	0.53
2:D:144:LEU:HD22	2:D:168:TRP:CZ2	2.43	0.53
3:E:421:TYR:HA	3:E:461:LEU:HG	1.90	0.53
3:E:479:PRO:O	3:E:480:CYS:HB3	2.07	0.53
3:F:544:ASN:ND2	3:F:544:ASN:O	2.41	0.53
3:F:556:ASN:HD22	3:F:556:ASN:N	2.05	0.53
3:G:592:PHE:N	3:G:592:PHE:HD1	2.05	0.53
3:G:674:TYR:CD1	3:G:691:SER:O	2.61	0.53
3:H:475:ALA:HB3	3:H:487:ASN:C	2.29	0.53
3:H:488:CYS:C	3:H:489:TYR:CG	2.86	0.53
3:J:369:TYR:CZ	3:J:384:PRO:HG2	2.43	0.53
1:C:607:ARG:HH21	1:C:607:ARG:HG3	1.72	0.53
2:D:622:ILE:HB	2:D:679:ILE:CG2	2.39	0.53
3:E:390:LEU:HD23	3:E:391:CYS:N	2.19	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:565:PHE:CZ	3:F:42:VAL:HG22	2.43	0.53
3:G:100:ILE:O	3:G:242:LEU:HA	2.08	0.53
3:G:544:ASN:O	3:G:544:ASN:ND2	2.41	0.53
3:H:64:TRP:HD1	3:H:65:PHE:N	2.07	0.53
3:H:421:TYR:HA	3:H:461:LEU:HG	1.90	0.53
3:H:886:TRP:HH2	3:H:904:TYR:HD2	1.56	0.53
3:I:393:THR:OG1	3:I:520:ALA:HB3	2.09	0.53
3:I:1104:VAL:HG22	3:I:1115:ILE:HG12	1.91	0.53
1:A:603:TYR:CD1	1:A:603:TYR:C	2.85	0.53
2:B:31:LYS:NZ	3:E:493:GLN:OE1	2.42	0.53
1:C:598:PRO:O	1:C:602:ILE:HG12	2.09	0.53
3:G:330:PRO:HA	3:G:579:PRO:HB2	1.91	0.53
3:G:600:PRO:HB3	3:G:674:TYR:CB	2.39	0.53
3:H:473:TYR:CG	3:H:474:GLN:N	2.72	0.53
3:I:544:ASN:ND2	3:I:544:ASN:O	2.41	0.53
3:J:64:TRP:HD1	3:J:65:PHE:N	2.07	0.53
1:A:230:PRO:HG3	1:A:426:CYS:HB3	1.91	0.53
2:B:622:ILE:HB	2:B:679:ILE:CG2	2.39	0.53
3:E:1141:LEU:HD12	3:G:1141:LEU:HD11	1.90	0.53
3:F:64:TRP:HD1	3:F:65:PHE:N	2.07	0.53
3:I:592:PHE:HD2	3:J:740:MET:HE1	1.72	0.53
2:B:631:LYS:HB2	2:B:631:LYS:HZ3	1.74	0.53
3:F:328:ARG:CZ	3:F:533:LEU:HB2	2.38	0.53
3:F:1045:LYS:HZ1	3:G:786:LYS:HE3	1.72	0.53
3:G:369:TYR:CZ	3:G:384:PRO:HG2	2.43	0.53
3:H:578:ASP:CG	3:H:585:LEU:HD11	2.34	0.53
3:I:562:PHE:CE2	3:J:41:LYS:CD	2.80	0.53
3:J:326:ILE:C	3:J:327:VAL:CG2	2.82	0.53
3:J:330:PRO:HA	3:J:579:PRO:HB2	1.91	0.53
3:J:421:TYR:HA	3:J:461:LEU:HG	1.90	0.53
3:J:600:PRO:HB3	3:J:674:TYR:CB	2.39	0.53
1:C:230:PRO:HG3	1:C:426:CYS:HB3	1.91	0.52
3:F:393:THR:OG1	3:F:520:ALA:HB3	2.09	0.52
3:F:518:LEU:CD2	3:F:519:HIS:N	2.72	0.52
3:G:587:ILE:CG2	3:G:588:THR:H	2.19	0.52
3:H:323:THR:O	3:H:324:GLU:HG2	2.09	0.52
3:H:478:THR:CG2	3:H:479:PRO:CD	2.86	0.52
3:J:295:PRO:HB3	3:J:597:VAL:HG22	1.90	0.52
3:J:476:GLY:H	3:J:487:ASN:HB3	1.74	0.52
3:E:694:ALA:O	3:E:695:TYR:HB3	2.10	0.52
3:F:476:GLY:H	3:F:487:ASN:HB3	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:1104:VAL:HG22	3:F:1115:ILE:HG12	1.91	0.52
3:H:338:PHE:O	3:H:339:GLY:C	2.51	0.52
3:H:392:PHE:CD2	3:H:517:LEU:CD2	2.83	0.52
3:I:517:LEU:HD22	3:I:517:LEU:H	1.74	0.52
3:I:518:LEU:CD2	3:I:519:HIS:N	2.72	0.52
2:B:105:SER:C	2:B:106:SER:HG	2.02	0.52
2:D:90:ASN:HB3	2:D:93:VAL:HG12	1.91	0.52
2:D:631:LYS:HB2	2:D:631:LYS:HZ3	1.74	0.52
3:G:476:GLY:H	3:G:487:ASN:HB3	1.74	0.52
3:I:335:LEU:HD23	3:I:336:CYS:O	2.09	0.52
3:I:476:GLY:H	3:I:487:ASN:HB3	1.74	0.52
3:I:748:GLU:HG3	3:I:981:LEU:CD2	2.23	0.52
3:J:328:ARG:NH2	3:J:580:GLN:HG3	2.24	0.52
1:A:489:ALA:HB2	1:A:589:VAL:HG12	1.88	0.52
2:B:90:ASN:HB3	2:B:93:VAL:HG12	1.91	0.52
2:D:741:ILE:O	2:D:741:ILE:HG22	2.09	0.52
3:E:578:ASP:CG	3:E:585:LEU:HD11	2.34	0.52
3:H:694:ALA:O	3:H:695:TYR:HB3	2.10	0.52
3:I:64:TRP:HD1	3:I:65:PHE:N	2.07	0.52
2:B:245:ARG:NH1	2:B:603:PHE:O	2.42	0.52
1:C:78:LEU:CD2	1:C:79:VAL:N	2.73	0.52
2:D:245:ARG:NH1	2:D:603:PHE:O	2.43	0.52
3:E:48:LEU:N	3:E:48:LEU:CD1	2.73	0.52
3:E:64:TRP:HD1	3:E:65:PHE:N	2.07	0.52
3:E:886:TRP:HH2	3:E:904:TYR:HD2	1.56	0.52
3:F:570:ALA:CB	3:G:963:VAL:CG1	2.88	0.52
3:F:1142:GLN:HG3	3:F:1143:PRO:CD	2.37	0.52
3:G:326:ILE:C	3:G:327:VAL:CG2	2.82	0.52
3:H:1141:LEU:HD12	3:J:1141:LEU:HD11	1.90	0.52
1:A:193:ILE:HG22	1:A:198:LEU:HD22	1.91	0.52
1:A:492:ILE:CG2	1:A:590:ALA:HB1	2.33	0.52
2:B:735:ASN:CG	2:B:736:GLN:N	2.68	0.52
1:C:193:ILE:HG22	1:C:198:LEU:HD22	1.91	0.52
3:E:336:CYS:CB	3:E:363:ALA:HA	2.39	0.52
3:E:472:ILE:CG2	3:E:473:TYR:N	2.73	0.52
3:G:64:TRP:HD1	3:G:65:PHE:N	2.07	0.52
3:G:328:ARG:NH2	3:G:580:GLN:HG3	2.24	0.52
3:H:41:LYS:HE3	3:J:564:GLN:OE1	2.09	0.52
3:H:475:ALA:HB3	3:H:487:ASN:HB2	1.89	0.52
3:I:328:ARG:NH2	3:I:533:LEU:HB2	2.25	0.52
3:I:570:ALA:CB	3:J:963:VAL:CG1	2.88	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:317:ASN:HA	3:J:593:GLY:O	2.10	0.52
1:C:593:PRO:O	1:C:596:THR:HB	2.09	0.52
3:E:319:ARG:NH2	3:E:319:ARG:CG	2.73	0.52
3:E:745:ASP:CB	3:G:319:ARG:NH1	2.46	0.52
3:E:901:GLN:NE2	3:E:905:ARG:HH21	2.08	0.52
3:G:295:PRO:HB3	3:G:597:VAL:HG22	1.90	0.52
3:H:482:GLY:O	3:H:483:VAL:HG22	2.08	0.52
3:H:538:CYS:HG	3:H:590:CYS:CB	2.12	0.52
3:J:330:PRO:HG2	3:J:331:ASN:H	1.75	0.52
1:A:231:TYR:HH	1:A:313:THR:HG1	1.58	0.52
1:A:607:ARG:HG3	1:A:607:ARG:HH21	1.72	0.52
3:G:330:PRO:HG2	3:G:331:ASN:H	1.75	0.52
3:G:591:SER:C	3:G:592:PHE:HD1	2.18	0.52
3:G:804:GLN:HE21	3:G:935:GLN:NE2	2.08	0.52
3:H:327:VAL:CG1	3:H:329:PHE:CE2	2.92	0.52
3:H:327:VAL:CG1	3:H:328:ARG:N	2.73	0.52
4:U:1:NAG:C6	4:U:2:NAG:HN2	2.06	0.52
2:D:162:LEU:HD12	2:D:162:LEU:O	2.10	0.52
3:E:520:ALA:HB1	3:E:521:PRO:CD	2.38	0.52
3:G:1101:HIS:CD2	4:s:1:NAG:H5	2.45	0.52
3:J:670:ILE:CG2	3:J:671:CYS:N	2.73	0.52
4:b:2:NAG:H3	4:b:2:NAG:H83	1.90	0.52
2:B:162:LEU:HD12	2:B:162:LEU:O	2.09	0.52
2:D:176:LEU:HD13	2:D:501:ALA:O	2.10	0.52
2:D:735:ASN:CG	2:D:736:GLN:N	2.68	0.52
3:E:323:THR:O	3:E:324:GLU:HG2	2.09	0.52
3:F:335:LEU:HD23	3:F:336:CYS:O	2.09	0.52
3:H:813:SER:O	3:H:813:SER:OG	2.18	0.52
3:J:591:SER:C	3:J:592:PHE:HD1	2.18	0.52
3:J:1101:HIS:CD2	4:EA:1:NAG:H5	2.45	0.52
4:x:2:NAG:H3	4:x:2:NAG:H83	1.90	0.52
1:C:238:LEU:HD12	1:C:238:LEU:O	2.10	0.51
2:D:425:SER:C	2:D:427:ASP:H	2.19	0.51
3:E:524:VAL:C	3:E:525:CYS:SG	2.93	0.51
3:F:328:ARG:NH2	3:F:533:LEU:HB2	2.25	0.51
3:F:430:THR:C	3:F:515:PHE:HE1	2.17	0.51
3:F:531:THR:CG2	3:F:532:ASN:N	2.72	0.51
3:F:562:PHE:CD2	3:G:41:LYS:CD	2.88	0.51
1:C:454:PRO:HB3	2:D:768:ARG:HH21	1.75	0.51
3:G:48:LEU:N	3:G:48:LEU:CD1	2.73	0.51
3:H:48:LEU:CD1	3:H:48:LEU:N	2.73	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:472:ILE:CG2	3:H:473:TYR:N	2.73	0.51
3:I:41:LYS:N	3:I:41:LYS:CD	2.73	0.51
3:I:48:LEU:N	3:I:48:LEU:CD1	2.73	0.51
3:I:379:CYS:HB3	3:I:382:VAL:O	2.10	0.51
3:J:332:ILE:HG12	3:J:333:THR:N	2.25	0.51
2:B:628:LEU:HB2	2:B:632:ALA:HB2	1.92	0.51
2:B:741:ILE:O	2:B:741:ILE:HG22	2.09	0.51
3:E:327:VAL:CG1	3:E:329:PHE:CE2	2.92	0.51
3:F:403:ARG:NH1	3:F:505:TYR:CD1	2.78	0.51
3:F:517:LEU:HD22	3:F:517:LEU:H	1.74	0.51
3:H:379:CYS:HB3	3:H:382:VAL:O	2.10	0.51
3:I:498:GLN:HB3	3:I:499:PRO:HD2	1.92	0.51
3:I:562:PHE:CD2	3:J:41:LYS:CD	2.88	0.51
1:A:225:ILE:O	1:A:225:ILE:HG22	2.09	0.51
1:A:598:PRO:O	1:A:602:ILE:HG12	2.09	0.51
1:C:79:VAL:O	1:C:79:VAL:HG12	2.10	0.51
1:C:225:ILE:O	1:C:225:ILE:HG22	2.09	0.51
3:E:327:VAL:CG1	3:E:328:ARG:N	2.73	0.51
3:E:379:CYS:HB3	3:E:382:VAL:O	2.10	0.51
3:F:498:GLN:HB3	3:F:499:PRO:HD2	1.92	0.51
3:I:308:VAL:HG12	3:I:602:THR:HG23	1.92	0.51
3:I:531:THR:CG2	3:I:532:ASN:N	2.73	0.51
3:J:41:LYS:CD	3:J:41:LYS:N	2.73	0.51
3:J:348:ALA:HB2	3:J:354:ASN:ND2	2.26	0.51
2:B:172:VAL:CG1	2:B:176:LEU:HD12	2.36	0.51
2:B:394:ASN:HB2	2:B:562:LYS:HD2	1.92	0.51
1:C:66:GLY:HA3	1:C:69:ALA:HB3	1.93	0.51
3:E:329:PHE:O	3:E:579:PRO:CG	2.59	0.51
3:G:333:THR:O	3:G:362:VAL:CG2	2.44	0.51
3:G:348:ALA:HB2	3:G:354:ASN:ND2	2.26	0.51
3:G:498:GLN:HB3	3:G:499:PRO:HD2	1.92	0.51
3:I:430:THR:C	3:I:515:PHE:HE1	2.17	0.51
3:J:48:LEU:N	3:J:48:LEU:CD1	2.73	0.51
2:D:104:GLY:O	2:D:107:VAL:HG22	2.10	0.51
3:F:335:LEU:HD23	3:F:336:CYS:N	2.26	0.51
3:G:41:LYS:CD	3:G:41:LYS:N	2.73	0.51
3:J:329:PHE:CB	3:J:330:PRO:HD2	2.36	0.51
3:J:670:ILE:CG2	3:J:671:CYS:H	2.23	0.51
2:B:104:GLY:O	2:B:107:VAL:HG22	2.10	0.51
3:E:654:GLU:O	3:E:693:ILE:CA	2.56	0.51
3:F:48:LEU:N	3:F:48:LEU:CD1	2.73	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:332:ILE:HD12	3:F:332:ILE:O	2.11	0.51
3:F:592:PHE:CE2	3:G:740:MET:SD	3.04	0.51
3:H:493:GLN:NE2	3:H:493:GLN:CA	2.73	0.51
3:J:587:ILE:O	3:J:588:THR:HG22	2.10	0.51
1:A:467:PHE:C	1:A:467:PHE:CD1	2.89	0.51
2:B:176:LEU:HD13	2:B:501:ALA:O	2.10	0.51
2:B:433:GLU:O	2:B:437:ASN:ND2	2.44	0.51
2:D:394:ASN:HB2	2:D:562:LYS:HD2	1.92	0.51
3:E:348:ALA:HB2	3:E:354:ASN:ND2	2.26	0.51
3:E:705:VAL:HB	3:F:883:THR:HG21	1.93	0.51
3:F:308:VAL:HG12	3:F:602:THR:HG23	1.92	0.51
3:F:379:CYS:HB3	3:F:382:VAL:O	2.10	0.51
3:F:551:VAL:HB	3:F:588:THR:HG23	1.92	0.51
3:G:326:ILE:CG2	3:G:541:PHE:CA	2.80	0.51
3:G:332:ILE:HG12	3:G:333:THR:N	2.25	0.51
3:H:329:PHE:O	3:H:579:PRO:CG	2.59	0.51
3:I:592:PHE:CE2	3:J:740:MET:SD	3.04	0.51
3:J:498:GLN:HB3	3:J:499:PRO:HD2	1.92	0.51
1:A:238:LEU:HD12	1:A:238:LEU:O	2.10	0.51
1:A:454:PRO:CB	2:B:768:ARG:HH21	2.24	0.51
1:A:454:PRO:HB3	2:B:768:ARG:HH21	1.76	0.51
3:F:130:VAL:HB	3:F:168:PHE:HB3	1.93	0.51
3:F:748:GLU:HG3	3:F:981:LEU:CD2	2.23	0.51
3:G:317:ASN:HA	3:G:593:GLY:O	2.10	0.51
3:G:379:CYS:HB3	3:G:382:VAL:O	2.10	0.51
3:G:654:GLU:O	3:G:693:ILE:HG22	2.11	0.51
3:I:551:VAL:HB	3:I:588:THR:HG23	1.92	0.51
3:J:131:CYS:H	3:J:133:PHE:HE1	1.59	0.51
3:J:518:LEU:CG	3:J:519:HIS:H	2.24	0.51
2:D:628:LEU:HB2	2:D:632:ALA:HB2	1.92	0.51
3:E:41:LYS:HE3	3:G:564:GLN:OE1	2.09	0.51
3:E:438:SER:O	3:E:438:SER:OG	2.21	0.51
3:G:670:ILE:CG2	3:G:671:CYS:H	2.23	0.51
3:H:500:THR:C	3:H:501:ASN:HD22	2.19	0.51
3:I:523:THR:CG2	3:I:524:VAL:H	2.12	0.51
3:J:361:CYS:SG	3:J:524:VAL:HG21	2.51	0.51
3:E:336:CYS:N	3:E:362:VAL:O	2.44	0.50
3:F:614:ASP:OD2	3:G:854:LYS:HD2	2.12	0.50
3:G:131:CYS:H	3:G:133:PHE:HE1	1.59	0.50
3:H:516:GLU:C	3:H:517:LEU:CD2	2.84	0.50
3:H:653:ALA:HA	3:H:692:ILE:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:901:GLN:NE2	3:H:905:ARG:HH21	2.08	0.50
3:H:983:ARG:CB	3:J:382:VAL:HB	2.40	0.50
3:I:130:VAL:HB	3:I:168:PHE:HB3	1.93	0.50
3:J:379:CYS:HB3	3:J:382:VAL:O	2.10	0.50
3:J:675:GLN:HG2	3:J:676:THR:H	1.72	0.50
2:B:425:SER:C	2:B:427:ASP:H	2.19	0.50
3:F:348:ALA:HB2	3:F:354:ASN:ND2	2.26	0.50
3:G:715:PRO:HA	3:G:1072:GLU:HA	1.92	0.50
3:H:490:PHE:CD1	3:H:491:PRO:CD	2.91	0.50
3:H:705:VAL:HB	3:I:883:THR:HG21	1.93	0.50
3:J:106:PHE:HB3	3:J:235:ILE:HD13	1.93	0.50
3:J:804:GLN:HE21	3:J:935:GLN:NE2	2.08	0.50
3:E:983:ARG:CB	3:G:382:VAL:HB	2.40	0.50
3:F:569:ILE:CG1	3:G:47:VAL:CG1	2.89	0.50
3:G:394:ASN:HB2	3:G:516:GLU:OE1	2.12	0.50
3:H:401:VAL:HG22	3:H:509:ARG:HG2	1.94	0.50
3:I:335:LEU:HD23	3:I:336:CYS:N	2.26	0.50
3:J:715:PRO:HA	3:J:1072:GLU:HA	1.92	0.50
3:J:1032:CYS:O	3:J:1051:SER:HB2	2.12	0.50
2:B:208:GLU:OE2	2:B:219:ARG:NH1	2.44	0.50
3:F:129:LYS:HG2	3:F:133:PHE:HZ	1.76	0.50
3:G:106:PHE:HB3	3:G:235:ILE:HD13	1.93	0.50
3:G:670:ILE:CG2	3:G:671:CYS:N	2.73	0.50
3:I:332:ILE:HD12	3:I:332:ILE:O	2.11	0.50
1:A:79:VAL:O	1:A:79:VAL:HG12	2.10	0.50
3:E:653:ALA:HA	3:E:692:ILE:O	2.11	0.50
3:F:401:VAL:HG22	3:F:509:ARG:HG2	1.94	0.50
3:F:524:VAL:O	3:F:524:VAL:HG22	2.12	0.50
3:G:130:VAL:HB	3:G:168:PHE:HB3	1.93	0.50
3:G:328:ARG:CD	3:G:533:LEU:HD22	2.42	0.50
3:H:348:ALA:HB2	3:H:354:ASN:ND2	2.26	0.50
3:I:324:GLU:CG	3:I:539:VAL:CG2	2.89	0.50
3:I:524:VAL:O	3:I:524:VAL:HG22	2.12	0.50
3:I:529:LYS:C	3:I:530:SER:O	2.55	0.50
3:E:106:PHE:HB3	3:E:235:ILE:HD13	1.93	0.50
3:G:361:CYS:SG	3:G:524:VAL:HG21	2.51	0.50
3:H:735:SER:HB3	3:H:859:THR:HG22	1.94	0.50
3:H:967:SER:O	3:H:967:SER:OG	2.24	0.50
1:C:467:PHE:CD1	1:C:467:PHE:C	2.89	0.50
3:E:479:PRO:HG2	3:E:480:CYS:H	1.77	0.50
3:E:735:SER:HB3	3:E:859:THR:HG22	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:324:GLU:CG	3:F:539:VAL:CG2	2.89	0.50
3:G:403:ARG:NH1	3:G:505:TYR:CD1	2.78	0.50
3:G:587:ILE:O	3:G:588:THR:HG22	2.10	0.50
3:J:328:ARG:CD	3:J:533:LEU:HD22	2.42	0.50
3:J:654:GLU:O	3:J:693:ILE:HG22	2.11	0.50
3:F:357:ARG:HH22	3:G:230:PRO:CG	2.19	0.50
3:G:604:THR:CG2	3:G:674:TYR:CE2	2.95	0.50
3:I:320:VAL:CG1	3:I:321:GLN:N	2.73	0.50
3:I:348:ALA:HB2	3:I:354:ASN:ND2	2.26	0.50
3:I:518:LEU:C	3:I:518:LEU:HD23	2.36	0.50
3:I:614:ASP:OD2	3:J:854:LYS:HD2	2.12	0.50
3:J:604:THR:CG2	3:J:674:TYR:CE2	2.95	0.50
1:A:66:GLY:HA3	1:A:69:ALA:HB3	1.93	0.50
1:A:78:LEU:CD2	1:A:79:VAL:N	2.73	0.50
2:B:143:LEU:CD2	2:B:143:LEU:C	2.85	0.50
3:F:518:LEU:HD23	3:F:518:LEU:C	2.36	0.50
3:F:529:LYS:C	3:F:530:SER:O	2.55	0.50
3:G:332:ILE:HD12	3:G:528:LYS:CB	2.42	0.50
1:A:80:LEU:HD13	1:A:537:VAL:HG11	1.94	0.49
1:C:80:LEU:HD13	1:C:537:VAL:HG11	1.94	0.49
2:D:208:GLU:OE2	2:D:219:ARG:NH1	2.44	0.49
3:E:325:SER:O	3:E:325:SER:OG	2.28	0.49
3:E:336:CYS:HB2	3:E:362:VAL:C	2.37	0.49
3:E:500:THR:C	3:E:501:ASN:HD22	2.19	0.49
3:F:319:ARG:NH2	3:G:740:MET:CE	2.71	0.49
3:F:320:VAL:HG21	3:F:591:SER:CB	2.42	0.49
3:F:529:LYS:NZ	3:F:529:LYS:CB	2.75	0.49
3:G:675:GLN:HG2	3:G:676:THR:H	1.72	0.49
3:H:106:PHE:HB3	3:H:235:ILE:HD13	1.93	0.49
3:H:129:LYS:HG2	3:H:133:PHE:HZ	1.76	0.49
3:I:106:PHE:HB3	3:I:235:ILE:HD13	1.93	0.49
3:I:319:ARG:NH2	3:J:740:MET:CE	2.71	0.49
3:I:401:VAL:HG22	3:I:509:ARG:HG2	1.94	0.49
3:J:361:CYS:O	3:J:524:VAL:HG23	2.12	0.49
1:C:207:VAL:HG22	2:D:753:ILE:HG13	1.94	0.49
3:E:129:LYS:HG2	3:E:133:PHE:HZ	1.77	0.49
3:E:523:THR:CG2	3:E:524:VAL:N	2.41	0.49
3:F:382:VAL:O	3:F:383:SER:C	2.55	0.49
3:F:578:ASP:OD2	3:F:581:THR:HG22	2.12	0.49
3:F:1045:LYS:HZ2	3:G:786:LYS:HE3	1.77	0.49
3:I:320:VAL:HG21	3:I:591:SER:CB	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:518:LEU:CD2	3:I:518:LEU:C	2.86	0.49
3:I:529:LYS:O	3:I:529:LYS:HG2	2.11	0.49
3:I:529:LYS:NZ	3:I:529:LYS:CB	2.75	0.49
3:I:533:LEU:O	3:I:534:VAL:HG22	2.12	0.49
3:I:569:ILE:CG1	3:J:47:VAL:CG1	2.89	0.49
3:I:612:TYR:O	3:I:648:GLY:CA	2.58	0.49
3:J:129:LYS:HG2	3:J:133:PHE:HZ	1.77	0.49
3:J:130:VAL:HB	3:J:168:PHE:HB3	1.93	0.49
3:J:394:ASN:HB2	3:J:516:GLU:OE1	2.12	0.49
2:D:564:GLU:HB3	2:D:568:LEU:HD23	1.95	0.49
3:E:130:VAL:HB	3:E:168:PHE:HB3	1.93	0.49
3:F:106:PHE:HB3	3:F:235:ILE:HD13	1.93	0.49
3:G:807:PRO:O	3:G:809:PRO:HD3	2.12	0.49
3:G:1090:PRO:HD3	3:G:1095:PHE:CE2	2.47	0.49
3:I:129:LYS:HG2	3:I:133:PHE:HZ	1.76	0.49
3:I:382:VAL:O	3:I:383:SER:C	2.55	0.49
1:C:454:PRO:CB	2:D:768:ARG:HH21	2.24	0.49
2:D:143:LEU:C	2:D:143:LEU:CD2	2.85	0.49
2:D:335:ASP:CA	2:D:361:CYS:SG	3.00	0.49
2:D:433:GLU:O	2:D:437:ASN:ND2	2.44	0.49
3:E:475:ALA:CB	3:E:487:ASN:CA	2.91	0.49
3:H:131:CYS:H	3:H:133:PHE:HE1	1.59	0.49
3:H:326:ILE:CD1	3:H:533:LEU:HB3	2.43	0.49
3:I:131:CYS:H	3:I:133:PHE:HE1	1.59	0.49
1:C:467:PHE:CD1	1:C:468:LEU:HD23	2.47	0.49
3:E:326:ILE:CD1	3:E:533:LEU:HB3	2.43	0.49
3:E:437:ASN:OD1	3:E:438:SER:N	2.46	0.49
3:F:41:LYS:CD	3:F:41:LYS:N	2.73	0.49
3:H:528:LYS:CD	3:H:528:LYS:N	2.73	0.49
3:J:122:ASN:OD1	3:J:122:ASN:N	2.46	0.49
3:J:807:PRO:O	3:J:809:PRO:HD3	2.12	0.49
4:k:1:NAG:H62	4:k:2:NAG:H2	1.93	0.49
2:B:335:ASP:CA	2:B:361:CYS:SG	3.00	0.49
3:F:326:ILE:HD11	3:F:534:VAL:HG21	1.93	0.49
3:F:533:LEU:C	3:F:534:VAL:CG2	2.85	0.49
3:F:533:LEU:O	3:F:534:VAL:HG22	2.12	0.49
3:G:122:ASN:OD1	3:G:122:ASN:N	2.46	0.49
3:G:129:LYS:HG2	3:G:133:PHE:HZ	1.77	0.49
3:G:316:SER:OG	3:G:317:ASN:N	2.45	0.49
3:H:475:ALA:CB	3:H:487:ASN:CA	2.91	0.49
3:I:403:ARG:NH1	3:I:505:TYR:CD1	2.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:437:ASN:OD1	3:I:438:SER:N	2.46	0.49
3:I:578:ASP:OD2	3:I:581:THR:HG22	2.12	0.49
3:J:329:PHE:HB3	3:J:330:PRO:CD	2.36	0.49
1:A:352:GLU:OE2	2:B:623:SER:CB	2.61	0.49
3:E:493:GLN:NE2	3:E:493:GLN:CA	2.73	0.49
3:F:437:ASN:OD1	3:F:438:SER:N	2.46	0.49
3:F:533:LEU:HD22	3:F:534:VAL:H	1.76	0.49
3:H:482:GLY:C	3:H:483:VAL:CG2	2.85	0.49
3:J:332:ILE:HD12	3:J:528:LYS:CB	2.42	0.49
3:J:401:VAL:HG22	3:J:509:ARG:HG2	1.94	0.49
2:B:768:ARG:CG	2:B:768:ARG:NH1	2.73	0.49
1:C:488:TYR:O	1:C:492:ILE:HG22	2.13	0.49
2:D:678:ARG:O	2:D:679:ILE:HB	2.13	0.49
3:E:517:LEU:HD22	3:E:518:LEU:H	1.77	0.49
3:F:131:CYS:H	3:F:133:PHE:HE1	1.59	0.49
3:F:518:LEU:CD2	3:F:518:LEU:C	2.86	0.49
3:F:529:LYS:O	3:F:529:LYS:HG2	2.11	0.49
3:G:171:VAL:HG12	3:G:172:SER:H	1.78	0.49
3:G:437:ASN:OD1	3:G:438:SER:N	2.46	0.49
3:G:1032:CYS:O	3:G:1051:SER:HB2	2.12	0.49
3:I:171:VAL:HG12	3:I:172:SER:H	1.78	0.49
3:I:533:LEU:C	3:I:534:VAL:CG2	2.85	0.49
3:J:171:VAL:HG12	3:J:172:SER:H	1.78	0.49
3:J:361:CYS:SG	3:J:524:VAL:CG2	3.00	0.49
3:J:437:ASN:OD1	3:J:438:SER:N	2.46	0.49
3:E:131:CYS:H	3:E:133:PHE:HE1	1.59	0.49
3:F:430:THR:O	3:F:515:PHE:CE1	2.60	0.49
3:G:212:LEU:HD23	3:G:215:ASP:HB2	1.95	0.49
3:H:130:VAL:HB	3:H:168:PHE:HB3	1.93	0.49
3:J:231:ILE:HB	3:J:233:ILE:HG22	1.95	0.49
3:J:326:ILE:CG2	3:J:541:PHE:CA	2.80	0.49
3:J:562:PHE:N	3:J:562:PHE:CD1	2.81	0.49
3:J:1090:PRO:HD3	3:J:1095:PHE:CE2	2.47	0.49
1:C:352:GLU:OE2	2:D:623:SER:CB	2.61	0.49
3:E:500:THR:O	3:E:500:THR:OG1	2.31	0.49
3:F:212:LEU:HD23	3:F:215:ASP:HB2	1.95	0.49
3:F:535:LYS:NZ	3:F:535:LYS:CB	2.73	0.49
3:F:612:TYR:O	3:F:648:GLY:CA	2.58	0.49
3:I:363:ALA:CB	3:I:524:VAL:CG2	2.90	0.49
1:A:83:ILE:HB	1:A:84:PRO:CD	2.35	0.48
2:D:676:LYS:HB3	2:D:677:PRO:HD2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:401:VAL:HG22	3:E:509:ARG:HG2	1.94	0.48
3:E:482:GLY:C	3:E:483:VAL:CG2	2.86	0.48
3:E:501:ASN:HD22	3:E:501:ASN:N	2.11	0.48
3:E:534:VAL:C	3:E:535:LYS:CG	2.86	0.48
3:E:896:ILE:HG13	3:E:897:PRO:HD2	1.96	0.48
3:F:363:ALA:CB	3:F:524:VAL:CG2	2.90	0.48
3:F:382:VAL:HG22	3:F:383:SER:O	2.13	0.48
3:F:533:LEU:C	3:F:533:LEU:CD1	2.85	0.48
3:G:557:LYS:HE3	3:G:586:ASP:OD1	2.13	0.48
3:G:562:PHE:N	3:G:562:PHE:CD1	2.81	0.48
3:H:896:ILE:HG13	3:H:897:PRO:HD2	1.96	0.48
3:I:122:ASN:N	3:I:122:ASN:OD1	2.46	0.48
3:I:329:PHE:CE2	3:I:528:LYS:HG2	2.44	0.48
3:I:529:LYS:O	3:I:530:SER:C	2.56	0.48
3:J:212:LEU:HD23	3:J:215:ASP:HB2	1.95	0.48
3:J:403:ARG:NH1	3:J:505:TYR:CD1	2.78	0.48
3:J:696:THR:O	3:J:697:MET:C	2.56	0.48
4:6:1:NAG:H62	4:6:2:NAG:H2	1.93	0.48
1:A:340:ASN:HD21	1:A:381:GLN:HB2	1.78	0.48
2:B:678:ARG:O	2:B:679:ILE:HB	2.13	0.48
3:E:171:VAL:HG12	3:E:172:SER:H	1.78	0.48
3:E:533:LEU:CD2	3:E:578:ASP:OD2	2.60	0.48
3:E:985:ASP:N	3:E:985:ASP:OD1	2.45	0.48
3:F:431:GLY:HA3	3:F:513:LEU:O	2.12	0.48
3:G:231:ILE:HB	3:G:233:ILE:HG22	1.95	0.48
3:G:361:CYS:SG	3:G:524:VAL:CG2	3.00	0.48
3:G:401:VAL:HG22	3:G:509:ARG:HG2	1.94	0.48
3:H:431:GLY:HA3	3:H:513:LEU:O	2.12	0.48
3:H:703:ASN:HB2	3:I:787:GLN:CD	2.26	0.48
3:J:316:SER:OG	3:J:317:ASN:N	2.45	0.48
3:E:383:SER:HG	3:E:386:LYS:HZ1	1.55	0.48
3:F:562:PHE:CE2	3:G:41:LYS:CD	2.80	0.48
3:G:326:ILE:CG1	3:G:328:ARG:H	2.26	0.48
3:H:200:TYR:OH	3:J:394:ASN:ND2	2.45	0.48
3:I:212:LEU:HD23	3:I:215:ASP:HB2	1.95	0.48
3:I:431:GLY:HA3	3:I:513:LEU:O	2.12	0.48
3:J:557:LYS:HE3	3:J:586:ASP:OD1	2.13	0.48
1:A:467:PHE:CD1	1:A:468:LEU:HD23	2.47	0.48
2:B:676:LYS:HB3	2:B:677:PRO:HD2	1.95	0.48
2:D:302:TRP:CH2	2:D:423:LEU:CD1	2.78	0.48
3:E:431:GLY:HA3	3:E:513:LEU:O	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:171:VAL:HG12	3:F:172:SER:H	1.78	0.48
3:G:361:CYS:O	3:G:524:VAL:HG23	2.12	0.48
3:H:122:ASN:OD1	3:H:122:ASN:N	2.46	0.48
3:H:437:ASN:OD1	3:H:438:SER:N	2.46	0.48
3:H:987:PRO:HG3	3:I:427:ASP:CG	2.38	0.48
3:I:1045:LYS:HZ1	3:J:786:LYS:HE3	1.78	0.48
1:A:538:SER:O	1:A:542:MET:CE	2.59	0.48
1:A:591:GLY:O	1:A:593:PRO:N	2.46	0.48
2:B:34:HIS:HE1	3:E:493:GLN:HG3	1.66	0.48
3:E:886:TRP:CH2	3:E:904:TYR:HD2	2.31	0.48
3:E:967:SER:O	3:E:967:SER:OG	2.24	0.48
3:E:987:PRO:HG3	3:F:427:ASP:CG	2.38	0.48
3:E:200:TYR:OH	3:G:394:ASN:ND2	2.45	0.48
3:E:524:VAL:HG22	3:E:525:CYS:N	2.27	0.48
3:E:935:GLN:O	3:E:939:SER:HB3	2.14	0.48
3:G:523:THR:CG2	3:G:524:VAL:H	2.12	0.48
3:H:171:VAL:HG12	3:H:172:SER:H	1.78	0.48
3:I:710:ASN:HD22	3:I:710:ASN:H	1.62	0.48
2:B:564:GLU:HB3	2:B:568:LEU:HD23	1.95	0.48
1:C:591:GLY:O	1:C:593:PRO:N	2.46	0.48
2:D:34:HIS:HE1	3:H:493:GLN:HG3	1.66	0.48
3:E:523:THR:HG22	3:E:524:VAL:HG12	1.96	0.48
3:E:524:VAL:C	3:E:525:CYS:HG	2.21	0.48
3:F:710:ASN:HD22	3:F:710:ASN:H	1.62	0.48
3:F:710:ASN:HD22	3:F:710:ASN:N	2.11	0.48
3:G:587:ILE:CG2	3:G:588:THR:N	2.73	0.48
3:H:479:PRO:HG2	3:H:480:CYS:H	1.77	0.48
3:I:231:ILE:HB	3:I:233:ILE:HG22	1.95	0.48
1:A:207:VAL:HG22	2:B:753:ILE:HG13	1.94	0.48
1:A:276:PHE:C	1:A:494:LEU:HD13	2.39	0.48
1:A:488:TYR:O	1:A:492:ILE:HG22	2.13	0.48
1:C:276:PHE:C	1:C:494:LEU:HD13	2.39	0.48
2:D:421:ILE:O	2:D:421:ILE:HG13	2.14	0.48
3:E:335:LEU:HB3	3:E:364:ASP:OD2	2.14	0.48
3:E:478:THR:HG22	3:E:479:PRO:N	2.28	0.48
3:E:985:ASP:CG	3:G:383:SER:CB	2.86	0.48
3:F:614:ASP:CG	3:G:854:LYS:HD2	2.39	0.48
3:F:776:LYS:HE3	3:F:776:LYS:HB3	1.65	0.48
3:H:328:ARG:HH21	3:H:328:ARG:CG	2.27	0.48
3:H:501:ASN:HD22	3:H:501:ASN:N	2.11	0.48
3:H:985:ASP:N	3:H:985:ASP:OD1	2.45	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:326:ILE:CG1	3:J:328:ARG:H	2.26	0.48
1:A:544:ILE:C	1:A:546:PHE:N	2.71	0.48
1:C:340:ASN:HD21	1:C:381:GLN:HB2	1.79	0.48
3:E:122:ASN:OD1	3:E:122:ASN:N	2.46	0.48
3:E:328:ARG:HH21	3:E:328:ARG:CG	2.27	0.48
3:F:122:ASN:N	3:F:122:ASN:OD1	2.46	0.48
3:F:329:PHE:CE2	3:F:528:LYS:HB3	2.48	0.48
3:J:46:SER:O	3:J:47:VAL:HG13	2.14	0.48
3:H:478:THR:HG22	3:H:479:PRO:N	2.28	0.48
3:H:486:PHE:CD2	3:H:487:ASN:ND2	2.82	0.48
3:H:935:GLN:O	3:H:939:SER:HB3	2.14	0.48
3:I:614:ASP:CG	3:J:854:LYS:HD2	2.39	0.48
3:J:1104:VAL:HG22	3:J:1115:ILE:HG12	1.95	0.48
2:B:175:GLN:O	2:B:178:PRO:HD2	2.14	0.47
3:E:46:SER:O	3:E:47:VAL:HG13	2.14	0.47
3:G:335:LEU:O	3:G:336:CYS:C	2.55	0.47
3:G:1104:VAL:HG22	3:G:1115:ILE:HG12	1.95	0.47
3:H:46:SER:O	3:H:47:VAL:HG13	2.14	0.47
3:H:231:ILE:HB	3:H:233:ILE:HG22	1.95	0.47
3:H:576:VAL:CG2	3:H:587:ILE:HD11	2.44	0.47
3:H:886:TRP:CH2	3:H:904:TYR:HD2	2.31	0.47
3:J:332:ILE:CG1	3:J:333:THR:N	2.77	0.47
3:E:225:PRO:CG	3:G:562:PHE:CZ	2.87	0.47
3:G:528:LYS:CE	3:G:529:LYS:C	2.79	0.47
3:H:325:SER:O	3:H:325:SER:OG	2.28	0.47
3:H:534:VAL:C	3:H:535:LYS:CG	2.86	0.47
3:H:985:ASP:CG	3:J:383:SER:CB	2.86	0.47
3:I:329:PHE:CB	3:I:330:PRO:HD2	2.11	0.47
3:I:382:VAL:HG22	3:I:383:SER:O	2.13	0.47
3:I:710:ASN:HD22	3:I:710:ASN:N	2.11	0.47
3:F:231:ILE:HB	3:F:233:ILE:HG22	1.95	0.47
3:F:357:ARG:HH22	3:G:230:PRO:HG3	1.77	0.47
3:H:340:GLU:H	3:H:340:GLU:CD	2.09	0.47
3:I:558:LYS:HZ3	5:J:1405:NAG:HN2	1.51	0.47
1:A:221:LYS:O	1:A:224:TYR:HB2	2.15	0.47
1:C:341:ILE:HD12	1:C:355:VAL:HG12	1.97	0.47
1:C:489:ALA:HB2	1:C:589:VAL:HG11	1.91	0.47
1:C:540:LEU:O	1:C:544:ILE:HG12	2.15	0.47
3:E:227:VAL:HG12	3:E:228:ASP:H	1.79	0.47
3:E:231:ILE:HB	3:E:233:ILE:HG22	1.95	0.47
3:E:565:PHE:O	3:F:43:PHE:N	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:333:THR:O	3:H:335:LEU:N	2.48	0.47
3:I:535:LYS:NZ	3:I:535:LYS:CB	2.73	0.47
2:B:139:GLN:CG	2:D:129:THR:O	2.63	0.47
3:E:490:PHE:CD1	3:E:491:PRO:CD	2.91	0.47
3:E:576:VAL:CG2	3:E:587:ILE:HD11	2.44	0.47
3:G:600:PRO:HB3	3:G:674:TYR:HB3	1.96	0.47
3:G:804:GLN:HG3	3:G:935:GLN:HE22	1.80	0.47
3:H:369:TYR:CE2	3:H:384:PRO:HB2	2.50	0.47
3:I:987:PRO:HG2	3:J:413:GLY:HA3	1.97	0.47
3:J:327:VAL:O	3:J:328:ARG:C	2.58	0.47
1:C:544:ILE:C	1:C:546:PHE:N	2.71	0.47
3:E:316:SER:C	3:E:317:ASN:ND2	2.73	0.47
3:F:560:LEU:O	3:F:562:PHE:N	2.47	0.47
3:G:535:LYS:O	3:G:536:ASN:HB2	2.15	0.47
3:G:557:LYS:CD	3:G:559:PHE:HE1	2.27	0.47
3:I:562:PHE:CD2	3:J:41:LYS:CE	2.98	0.47
1:A:489:ALA:HB2	1:A:589:VAL:HG11	1.91	0.47
2:B:129:THR:O	2:D:139:GLN:CG	2.63	0.47
2:B:421:ILE:HG13	2:B:421:ILE:O	2.14	0.47
2:B:425:SER:C	2:B:427:ASP:N	2.73	0.47
2:B:736:GLN:NE2	2:B:736:GLN:C	2.73	0.47
1:C:114:LEU:HD21	1:C:500:CYS:HB3	1.97	0.47
1:C:156:ASN:HB2	1:C:158:ASN:O	2.15	0.47
1:C:229:LEU:CB	1:C:230:PRO:HD3	2.29	0.47
1:C:538:SER:O	1:C:542:MET:CE	2.59	0.47
2:D:736:GLN:NE2	2:D:736:GLN:C	2.73	0.47
3:E:617:CYS:H	3:E:644:GLN:NE2	2.06	0.47
3:E:983:ARG:CA	3:G:382:VAL:HG23	2.42	0.47
3:F:329:PHE:CE2	3:F:528:LYS:HG2	2.44	0.47
3:G:46:SER:O	3:G:47:VAL:HG13	2.14	0.47
3:G:227:VAL:HG12	3:G:228:ASP:H	1.79	0.47
3:G:696:THR:O	3:G:697:MET:C	2.56	0.47
3:H:327:VAL:HG11	3:H:329:PHE:HE2	1.80	0.47
3:H:335:LEU:H	3:H:335:LEU:CD1	2.11	0.47
3:I:326:ILE:HD13	3:I:326:ILE:H	1.78	0.47
3:I:560:LEU:O	3:I:562:PHE:N	2.47	0.47
3:J:335:LEU:O	3:J:336:CYS:C	2.55	0.47
1:A:352:GLU:OE2	2:B:623:SER:HB3	2.14	0.47
2:B:333:LEU:O	2:B:362:THR:HG22	2.15	0.47
3:E:369:TYR:CE2	3:E:384:PRO:HB2	2.50	0.47
3:F:46:SER:O	3:F:47:VAL:HG13	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:987:PRO:HG2	3:G:413:GLY:HA3	1.97	0.47
3:G:369:TYR:HE2	3:G:385:THR:HG23	1.80	0.47
3:H:212:LEU:HD23	3:H:215:ASP:HB2	1.95	0.47
3:H:983:ARG:CA	3:J:382:VAL:HG23	2.42	0.47
3:J:535:LYS:O	3:J:536:ASN:HB2	2.15	0.47
1:A:540:LEU:O	1:A:544:ILE:HG12	2.14	0.47
2:D:333:LEU:O	2:D:362:THR:HG22	2.15	0.47
3:E:486:PHE:CD2	3:E:487:ASN:ND2	2.82	0.47
3:E:528:LYS:CD	3:E:528:LYS:N	2.73	0.47
3:F:307:THR:CA	3:F:602:THR:OG1	2.60	0.47
3:H:41:LYS:H	3:H:41:LYS:HD2	1.77	0.47
3:H:316:SER:C	3:H:317:ASN:ND2	2.73	0.47
3:H:912:THR:OG1	3:H:914:ASN:ND2	2.48	0.47
3:I:46:SER:O	3:I:47:VAL:HG13	2.14	0.47
3:J:227:VAL:HG12	3:J:228:ASP:H	1.79	0.47
3:J:557:LYS:CD	3:J:559:PHE:HE1	2.27	0.47
2:D:425:SER:C	2:D:427:ASP:N	2.73	0.47
2:D:768:ARG:CG	2:D:768:ARG:NH1	2.73	0.47
3:E:212:LEU:HD23	3:E:215:ASP:HB2	1.95	0.47
3:E:393:THR:HG21	3:E:518:LEU:HB3	1.95	0.47
3:F:748:GLU:N	3:F:748:GLU:CD	2.73	0.47
3:G:117:LEU:HD12	3:G:118:LEU:N	2.30	0.47
1:A:114:LEU:HD21	1:A:500:CYS:HB3	1.97	0.46
2:B:34:HIS:HE1	3:E:493:GLN:HB3	1.76	0.46
3:E:912:THR:OG1	3:E:914:ASN:ND2	2.48	0.46
3:E:1105:THR:HG22	3:E:1111:GLU:H	1.80	0.46
3:F:640:SER:OG	3:F:641:ASN:N	2.48	0.46
3:G:332:ILE:CG1	3:G:333:THR:N	2.77	0.46
3:G:973:ILE:HG12	3:G:992:GLN:HE21	1.79	0.46
3:H:29:THR:HG22	3:H:30:ASN:N	2.31	0.46
1:A:156:ASN:HB2	1:A:158:ASN:O	2.15	0.46
2:B:177:ARG:CB	2:B:178:PRO:CD	2.89	0.46
3:E:393:THR:OG1	3:E:517:LEU:HD23	2.15	0.46
3:F:227:VAL:HG12	3:F:228:ASP:H	1.79	0.46
3:F:411:ALA:O	3:F:425:LEU:HB2	2.16	0.46
3:H:560:LEU:O	3:H:562:PHE:N	2.47	0.46
3:H:565:PHE:O	3:I:43:PHE:N	2.47	0.46
3:I:364:ASP:O	3:I:367:VAL:HG12	2.15	0.46
3:J:973:ILE:HG12	3:J:992:GLN:HE21	1.79	0.46
3:F:562:PHE:CD2	3:G:41:LYS:CE	2.98	0.46
3:G:327:VAL:O	3:G:328:ARG:C	2.58	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:364:ASP:O	3:G:367:VAL:HG12	2.15	0.46
3:G:640:SER:OG	3:G:641:ASN:N	2.48	0.46
3:I:227:VAL:HG12	3:I:228:ASP:H	1.79	0.46
3:I:516:GLU:OE1	3:I:517:LEU:N	2.48	0.46
3:J:127:VAL:HG11	5:J:1402:NAG:H61	1.98	0.46
3:J:640:SER:OG	3:J:641:ASN:N	2.48	0.46
3:J:804:GLN:HG3	3:J:935:GLN:HE22	1.80	0.46
4:N:2:NAG:C3	4:N:2:NAG:H83	2.45	0.46
1:A:341:ILE:HD12	1:A:355:VAL:HG12	1.96	0.46
2:B:24:GLN:NE2	3:E:487:ASN:OD1	2.48	0.46
2:B:560:LEU:HD22	2:B:564:GLU:HG3	1.98	0.46
1:C:74:PHE:CD2	1:C:75:LEU:HD23	2.51	0.46
1:C:221:LYS:O	1:C:224:TYR:HB2	2.15	0.46
1:C:352:GLU:OE2	2:D:623:SER:HB3	2.14	0.46
3:F:516:GLU:OE1	3:F:517:LEU:N	2.48	0.46
3:H:364:ASP:O	3:H:367:VAL:HG12	2.15	0.46
3:H:477:SER:C	3:H:478:THR:HG1	2.15	0.46
3:I:29:THR:HG22	3:I:30:ASN:N	2.31	0.46
3:I:326:ILE:HD11	3:I:539:VAL:CG2	2.20	0.46
3:J:561:PRO:HG2	3:J:562:PHE:HD1	1.80	0.46
2:B:174:LYS:HG2	2:B:174:LYS:H	1.54	0.46
1:C:159:GLN:HG2	2:D:733:PRO:HB3	1.98	0.46
3:E:327:VAL:HG11	3:E:329:PHE:HE2	1.80	0.46
3:E:1090:PRO:HD3	3:E:1095:PHE:CE2	2.51	0.46
3:G:326:ILE:CD1	3:G:531:THR:HB	2.44	0.46
3:G:528:LYS:HD2	3:G:529:LYS:H	1.76	0.46
3:G:561:PRO:HG2	3:G:562:PHE:HD1	1.80	0.46
3:G:703:ASN:C	3:G:703:ASN:HD22	2.24	0.46
3:H:227:VAL:HG12	3:H:228:ASP:H	1.79	0.46
3:H:326:ILE:HD12	3:H:533:LEU:HB3	1.97	0.46
3:H:532:ASN:HD22	3:H:532:ASN:HA	1.59	0.46
3:H:536:ASN:C	3:H:537:LYS:CG	2.87	0.46
3:H:594:GLY:H	3:H:613:GLN:HB2	1.81	0.46
3:H:617:CYS:H	3:H:644:GLN:NE2	2.05	0.46
3:I:41:LYS:N	3:I:41:LYS:HD3	2.31	0.46
3:I:729:VAL:HG13	3:I:1059:GLY:HA2	1.97	0.46
3:J:703:ASN:C	3:J:703:ASN:HD22	2.24	0.46
1:C:592:VAL:CG2	1:C:593:PRO:CD	2.72	0.46
3:F:29:THR:HG22	3:F:30:ASN:N	2.31	0.46
3:F:364:ASP:O	3:F:367:VAL:HG12	2.15	0.46
3:F:369:TYR:CE2	3:F:384:PRO:HB2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:729:VAL:HG13	3:F:1059:GLY:HA2	1.97	0.46
3:I:411:ALA:O	3:I:425:LEU:HB2	2.16	0.46
3:J:977:LEU:HD12	3:J:996:LEU:HD12	1.98	0.46
2:D:175:GLN:O	2:D:178:PRO:HD2	2.14	0.46
3:E:537:LYS:O	3:E:538:CYS:C	2.59	0.46
3:G:127:VAL:HG11	5:G:1402:NAG:H61	1.98	0.46
3:G:326:ILE:O	3:G:327:VAL:CG2	2.64	0.46
3:H:117:LEU:HD12	3:H:118:LEU:N	2.30	0.46
3:H:525:CYS:SG	3:H:526:GLY:N	2.89	0.46
3:I:127:VAL:HG11	5:I:1402:NAG:H61	1.98	0.46
3:I:357:ARG:NH2	3:J:230:PRO:HG2	2.21	0.46
3:J:324:GLU:CG	3:J:539:VAL:HG23	2.45	0.46
3:J:369:TYR:HE2	3:J:385:THR:HG23	1.80	0.46
3:J:600:PRO:HB3	3:J:674:TYR:HB3	1.96	0.46
2:B:716:ARG:NH1	2:D:709:SER:OG	2.49	0.46
3:E:560:LEU:O	3:E:562:PHE:N	2.47	0.46
3:F:377:PHE:CD2	3:F:434:ILE:HG12	2.51	0.46
3:F:447:GLY:HA2	3:F:497:PHE:O	2.16	0.46
3:F:1032:CYS:O	3:F:1051:SER:HB2	2.16	0.46
3:H:1090:PRO:HD3	3:H:1095:PHE:CE2	2.51	0.46
3:I:117:LEU:HD12	3:I:118:LEU:N	2.30	0.46
3:I:369:TYR:CE2	3:I:384:PRO:HB2	2.50	0.46
3:I:613:GLN:C	3:I:615:VAL:N	2.73	0.46
3:J:364:ASP:O	3:J:367:VAL:HG12	2.16	0.46
4:U:2:NAG:C3	4:U:2:NAG:H83	2.45	0.46
1:C:340:ASN:HD21	1:C:381:GLN:H	1.64	0.46
3:E:41:LYS:H	3:E:41:LYS:HD2	1.77	0.46
3:E:328:ARG:NE	3:E:533:LEU:HG	2.30	0.46
3:E:470:THR:CG2	3:E:490:PHE:CZ	2.98	0.46
3:E:594:GLY:H	3:E:613:GLN:HB2	1.81	0.46
3:F:127:VAL:HG11	5:F:1402:NAG:H61	1.98	0.46
3:G:41:LYS:N	3:G:41:LYS:HD3	2.31	0.46
3:G:324:GLU:CG	3:G:539:VAL:HG23	2.46	0.46
3:G:393:THR:HA	3:G:523:THR:HG1	1.81	0.46
3:G:528:LYS:HE2	3:G:529:LYS:N	2.31	0.46
3:H:361:CYS:O	3:H:524:VAL:HG23	2.15	0.46
3:J:326:ILE:O	3:J:327:VAL:CG2	2.64	0.46
3:J:377:PHE:CD2	3:J:434:ILE:HG12	2.51	0.46
3:J:447:GLY:HA2	3:J:497:PHE:O	2.16	0.46
3:J:726:ILE:HG12	3:J:1061:VAL:HG22	1.97	0.46
3:F:45:SER:O	3:F:279:TYR:CB	2.64	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:310:LYS:HB2	3:F:310:LYS:HE3	1.75	0.46
3:F:529:LYS:O	3:F:530:SER:C	2.56	0.46
3:G:535:LYS:HB2	3:G:535:LYS:HE3	1.77	0.46
3:G:977:LEU:HD12	3:G:996:LEU:HD12	1.98	0.46
3:H:328:ARG:NE	3:H:533:LEU:HG	2.30	0.46
3:I:316:SER:OG	3:I:317:ASN:N	2.49	0.46
3:J:41:LYS:N	3:J:41:LYS:HD3	2.31	0.46
1:A:458:LEU:O	1:A:462:ILE:HD13	2.16	0.45
2:D:356:PHE:HB3	2:D:379:ILE:HD12	1.98	0.45
2:D:560:LEU:HD22	2:D:564:GLU:HG3	1.98	0.45
3:E:326:ILE:HD12	3:E:533:LEU:HB3	1.97	0.45
3:E:364:ASP:O	3:E:367:VAL:HG12	2.15	0.45
3:F:326:ILE:HD13	3:F:326:ILE:H	1.79	0.45
3:F:392:PHE:N	3:F:392:PHE:CD1	2.84	0.45
3:G:45:SER:O	3:G:279:TYR:CB	2.64	0.45
3:G:377:PHE:CD2	3:G:434:ILE:HG12	2.51	0.45
3:G:561:PRO:HG2	3:G:562:PHE:CD1	2.51	0.45
3:I:713:ALA:HB3	3:J:894:LEU:HB3	1.97	0.45
3:J:326:ILE:CD1	3:J:531:THR:HB	2.44	0.45
3:J:326:ILE:C	3:J:327:VAL:HG23	2.40	0.45
3:E:29:THR:HG22	3:E:30:ASN:N	2.31	0.45
3:E:903:ALA:HB1	3:E:913:GLN:HG2	1.98	0.45
3:F:613:GLN:C	3:F:615:VAL:N	2.73	0.45
3:F:758:SER:O	3:F:762:GLN:HG3	2.16	0.45
3:G:29:THR:HG22	3:G:30:ASN:N	2.31	0.45
3:H:470:THR:CG2	3:H:490:PHE:CZ	2.98	0.45
3:H:1105:THR:HG22	3:H:1111:GLU:H	1.80	0.45
3:I:500:THR:HG23	3:I:500:THR:O	2.16	0.45
1:A:32:ARG:NH2	1:A:291:SER:OG	2.46	0.45
2:B:52:THR:HA	2:B:342:ALA:HB1	1.98	0.45
2:B:709:SER:OG	2:D:716:ARG:NH1	2.49	0.45
1:C:496:ILE:HD11	1:C:546:PHE:CE1	2.52	0.45
3:E:403:ARG:NH1	3:E:405:ASP:OD1	2.43	0.45
3:F:153:MET:N	3:F:153:MET:SD	2.90	0.45
3:F:500:THR:HG23	3:F:500:THR:O	2.16	0.45
3:F:713:ALA:HB3	3:G:894:LEU:HB3	1.97	0.45
3:G:326:ILE:C	3:G:327:VAL:HG23	2.40	0.45
3:G:646:ARG:O	3:G:646:ARG:HG3	2.17	0.45
3:H:377:PHE:CD2	3:H:434:ILE:HG12	2.52	0.45
3:H:520:ALA:CB	3:H:521:PRO:CD	2.71	0.45
3:H:903:ALA:HB1	3:H:913:GLN:HG2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:153:MET:N	3:J:153:MET:SD	2.90	0.45
3:J:500:THR:HG23	3:J:500:THR:O	2.17	0.45
1:A:601:ALA:O	1:A:605:LEU:HG	2.17	0.45
2:B:735:ASN:CG	2:B:736:GLN:H	2.24	0.45
1:C:32:ARG:NH2	1:C:291:SER:OG	2.46	0.45
2:D:52:THR:HA	2:D:342:ALA:HB1	1.98	0.45
3:E:153:MET:N	3:E:153:MET:SD	2.90	0.45
3:E:477:SER:C	3:E:478:THR:HG1	2.11	0.45
3:F:48:LEU:HD13	3:F:48:LEU:N	2.32	0.45
3:F:536:ASN:HA	3:F:551:VAL:HG13	1.99	0.45
3:G:295:PRO:HB3	3:G:597:VAL:CG2	2.46	0.45
3:G:527:PRO:O	3:G:528:LYS:HB2	2.17	0.45
3:G:726:ILE:HG12	3:G:1061:VAL:HG22	1.97	0.45
3:H:45:SER:O	3:H:279:TYR:CB	2.64	0.45
3:H:1094:VAL:HG22	3:H:1107:ARG:HG2	1.98	0.45
3:I:45:SER:O	3:I:279:TYR:CB	2.64	0.45
3:I:307:THR:CA	3:I:602:THR:OG1	2.60	0.45
3:I:325:SER:CA	3:I:540:ASN:O	2.50	0.45
3:J:527:PRO:O	3:J:528:LYS:HB2	2.17	0.45
3:F:41:LYS:N	3:F:41:LYS:HD3	2.31	0.45
3:F:520:ALA:CB	3:F:521:PRO:CD	2.82	0.45
3:G:153:MET:SD	3:G:153:MET:N	2.90	0.45
3:H:447:GLY:HA2	3:H:497:PHE:O	2.16	0.45
3:H:533:LEU:HD21	3:H:578:ASP:CG	2.40	0.45
3:I:48:LEU:HD13	3:I:48:LEU:N	2.32	0.45
3:I:529:LYS:NZ	3:I:529:LYS:HB3	2.32	0.45
3:I:758:SER:O	3:I:762:GLN:HG3	2.16	0.45
3:J:646:ARG:O	3:J:646:ARG:HG3	2.17	0.45
2:B:677:PRO:C	2:B:679:ILE:N	2.75	0.45
2:D:677:PRO:C	2:D:679:ILE:N	2.75	0.45
2:D:735:ASN:CG	2:D:736:GLN:H	2.24	0.45
3:E:493:GLN:NE2	3:E:493:GLN:N	2.65	0.45
3:G:48:LEU:HD13	3:G:48:LEU:N	2.32	0.45
3:G:1040:VAL:O	3:G:1041:ASP:HB2	2.17	0.45
3:G:1141:LEU:O	3:G:1145:LEU:HD12	2.16	0.45
3:H:153:MET:N	3:H:153:MET:SD	2.90	0.45
3:H:537:LYS:O	3:H:538:CYS:C	2.58	0.45
3:I:363:ALA:CB	3:I:524:VAL:HG23	2.47	0.45
3:I:447:GLY:HA2	3:I:497:PHE:O	2.16	0.45
3:I:528:LYS:HB2	3:I:528:LYS:HZ3	1.82	0.45
3:I:536:ASN:HA	3:I:551:VAL:HG13	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:722:VAL:HA	3:I:1064:HIS:O	2.16	0.45
3:I:1032:CYS:O	3:I:1051:SER:HB2	2.16	0.45
3:J:295:PRO:HB3	3:J:597:VAL:CG2	2.46	0.45
3:J:319:ARG:HD3	3:J:319:ARG:HA	1.90	0.45
3:J:528:LYS:CE	3:J:529:LYS:C	2.79	0.45
3:J:561:PRO:HG2	3:J:562:PHE:CD1	2.51	0.45
1:A:496:ILE:HD11	1:A:546:PHE:CE1	2.52	0.45
2:B:208:GLU:OE1	2:B:210:ASN:ND2	2.50	0.45
1:C:462:ILE:N	1:C:462:ILE:CD1	2.80	0.45
3:F:326:ILE:C	3:F:327:VAL:HG13	2.41	0.45
3:F:329:PHE:N	3:F:329:PHE:HD1	2.14	0.45
3:F:722:VAL:HA	3:F:1064:HIS:O	2.16	0.45
3:H:385:THR:HG1	3:H:386:LYS:HZ3	1.59	0.45
3:H:403:ARG:NH1	3:H:405:ASP:OD1	2.43	0.45
3:I:153:MET:N	3:I:153:MET:SD	2.90	0.45
3:I:329:PHE:N	3:I:329:PHE:HD1	2.14	0.45
3:I:377:PHE:CD2	3:I:434:ILE:HG12	2.51	0.45
3:I:417:LYS:NZ	3:J:372:ALA:HB3	2.32	0.45
3:I:640:SER:OG	3:I:641:ASN:N	2.48	0.45
3:J:45:SER:O	3:J:279:TYR:CB	2.64	0.45
1:A:74:PHE:CD2	1:A:75:LEU:HD23	2.51	0.45
1:A:74:PHE:HD2	1:A:75:LEU:HD23	1.82	0.45
1:A:159:GLN:HG2	2:B:733:PRO:HB3	1.98	0.45
1:A:340:ASN:HD21	1:A:381:GLN:H	1.64	0.45
1:C:458:LEU:O	1:C:462:ILE:HD13	2.16	0.45
3:E:45:SER:O	3:E:279:TYR:CB	2.64	0.45
3:E:377:PHE:CD2	3:E:434:ILE:HG12	2.51	0.45
3:E:447:GLY:HA2	3:E:497:PHE:O	2.16	0.45
3:E:533:LEU:HD21	3:E:578:ASP:CG	2.40	0.45
3:G:500:THR:O	3:G:500:THR:HG23	2.17	0.45
3:H:516:GLU:C	3:H:517:LEU:HD22	2.39	0.45
3:H:676:THR:C	3:H:690:GLN:HB3	2.42	0.45
3:I:326:ILE:HG23	3:I:533:LEU:CA	2.25	0.45
3:I:748:GLU:CG	3:I:981:LEU:CD2	2.81	0.45
3:J:617:CYS:HB2	3:J:649:CYS:HB2	1.87	0.45
3:J:1141:LEU:O	3:J:1145:LEU:HD12	2.16	0.45
1:A:544:ILE:O	1:A:547:LEU:N	2.47	0.45
2:B:132:VAL:O	2:B:141:CYS:HA	2.17	0.45
1:C:562:ILE:HG22	1:C:564:ASP:HB2	1.99	0.45
3:E:127:VAL:HG11	5:E:1402:NAG:H61	1.98	0.45
3:E:329:PHE:O	3:E:579:PRO:HG2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:363:ALA:CB	3:F:524:VAL:HG23	2.47	0.45
3:H:329:PHE:O	3:H:579:PRO:HG2	2.17	0.45
3:I:326:ILE:HD11	3:I:534:VAL:HG21	1.93	0.45
3:I:1045:LYS:NZ	3:J:786:LYS:CE	2.79	0.45
3:J:29:THR:HG22	3:J:30:ASN:N	2.31	0.45
3:J:332:ILE:HD12	3:J:528:LYS:HB2	1.98	0.45
3:J:528:LYS:HE2	3:J:529:LYS:N	2.31	0.45
1:A:462:ILE:CD1	1:A:462:ILE:N	2.80	0.45
2:D:208:GLU:OE1	2:D:210:ASN:ND2	2.50	0.45
3:E:331:ASN:O	3:E:333:THR:N	2.50	0.45
3:E:676:THR:C	3:E:690:GLN:HB3	2.42	0.45
3:F:417:LYS:NZ	3:G:372:ALA:HB3	2.32	0.45
3:G:319:ARG:HD3	3:G:319:ARG:HA	1.90	0.45
3:I:187:LYS:HE3	3:I:213:VAL:HG12	1.99	0.45
3:I:329:PHE:N	3:I:329:PHE:CD1	2.84	0.45
3:J:48:LEU:HD13	3:J:48:LEU:N	2.32	0.45
3:J:430:THR:CG2	3:J:517:LEU:HD23	2.41	0.45
1:C:544:ILE:O	1:C:547:LEU:N	2.47	0.44
1:C:601:ALA:O	1:C:605:LEU:HG	2.17	0.44
3:E:117:LEU:HD12	3:E:118:LEU:N	2.30	0.44
3:F:294:ASP:N	3:F:294:ASP:OD1	2.50	0.44
3:F:519:HIS:ND1	3:F:565:PHE:CE1	2.85	0.44
3:F:529:LYS:NZ	3:F:529:LYS:HB3	2.32	0.44
5:F:1409:NAG:O4	5:F:1410:NAG:O5	2.28	0.44
3:G:559:PHE:HD1	3:G:559:PHE:H	1.65	0.44
3:H:127:VAL:HG11	5:H:1402:NAG:H61	1.98	0.44
3:H:316:SER:OG	3:H:317:ASN:N	2.48	0.44
3:H:340:GLU:C	3:H:342:PHE:N	2.75	0.44
3:J:1040:VAL:O	3:J:1041:ASP:HB2	2.17	0.44
1:A:351:PRO:HD3	2:B:677:PRO:HG2	1.99	0.44
1:C:74:PHE:HD2	1:C:75:LEU:HD23	1.82	0.44
2:D:176:LEU:O	2:D:180:TYR:HB2	2.17	0.44
3:E:316:SER:OG	3:E:317:ASN:N	2.48	0.44
3:E:1094:VAL:HG22	3:E:1107:ARG:HG2	1.98	0.44
3:F:329:PHE:N	3:F:329:PHE:CD1	2.84	0.44
3:F:390:LEU:HD11	3:G:983:ARG:CB	2.46	0.44
3:G:447:GLY:HA2	3:G:497:PHE:O	2.16	0.44
3:H:646:ARG:O	3:H:646:ARG:HG3	2.17	0.44
3:I:134:GLN:HB3	3:I:162:SER:HB2	2.00	0.44
3:J:440:ASN:ND2	3:J:441:LEU:HG	2.32	0.44
1:C:221:LYS:H	1:C:221:LYS:CD	2.08	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:340:GLU:H	3:E:340:GLU:CD	2.09	0.44
3:E:440:ASN:ND2	3:E:441:LEU:HG	2.32	0.44
3:E:529:LYS:CG	3:E:530:SER:N	2.65	0.44
3:G:674:TYR:CD2	3:G:674:TYR:O	2.70	0.44
3:G:1081:ILE:HG12	3:G:1095:PHE:CE2	2.53	0.44
3:H:331:ASN:O	3:H:333:THR:N	2.50	0.44
3:I:655:HIS:CD2	3:I:694:ALA:O	2.70	0.44
3:J:559:PHE:HD1	3:J:559:PHE:H	1.65	0.44
3:J:591:SER:C	3:J:592:PHE:CD1	2.95	0.44
3:J:674:TYR:CD2	3:J:674:TYR:O	2.70	0.44
3:F:134:GLN:HB3	3:F:162:SER:HB2	2.00	0.44
3:F:187:LYS:HE3	3:F:213:VAL:HG12	1.99	0.44
3:F:212:LEU:HD12	3:F:212:LEU:HA	1.78	0.44
3:H:47:VAL:HG11	3:J:569:ILE:HG13	2.00	0.44
3:I:326:ILE:C	3:I:327:VAL:HG13	2.41	0.44
3:J:117:LEU:HD12	3:J:118:LEU:N	2.30	0.44
3:J:187:LYS:HE3	3:J:213:VAL:HG12	1.99	0.44
3:J:565:PHE:O	3:J:565:PHE:CD1	2.70	0.44
3:J:740:MET:HE2	3:J:740:MET:HB2	1.92	0.44
3:J:1081:ILE:HG12	3:J:1095:PHE:CE2	2.53	0.44
2:B:24:GLN:HE21	3:E:487:ASN:CG	2.26	0.44
1:C:351:PRO:HD3	2:D:677:PRO:HG2	1.99	0.44
3:E:334:ASN:OD1	3:E:334:ASN:N	2.51	0.44
3:E:707:TYR:HB2	3:F:883:THR:CG2	2.43	0.44
3:G:134:GLN:HB3	3:G:162:SER:HB2	2.00	0.44
3:G:187:LYS:HE3	3:G:213:VAL:HG12	1.99	0.44
3:G:338:PHE:C	3:G:340:GLU:N	2.75	0.44
3:H:294:ASP:N	3:H:294:ASP:OD1	2.50	0.44
3:H:440:ASN:ND2	3:H:441:LEU:HG	2.32	0.44
3:I:519:HIS:ND1	3:I:565:PHE:CE1	2.85	0.44
3:I:533:LEU:HD22	3:I:534:VAL:H	1.76	0.44
3:I:676:THR:C	3:I:691:SER:N	2.70	0.44
2:B:176:LEU:O	2:B:180:TYR:HB2	2.17	0.44
3:E:47:VAL:HG11	3:G:569:ILE:HG13	2.00	0.44
3:E:187:LYS:HE3	3:E:213:VAL:HG12	1.99	0.44
3:E:328:ARG:O	3:E:329:PHE:CG	2.71	0.44
3:F:613:GLN:C	3:F:615:VAL:H	2.26	0.44
3:F:676:THR:C	3:F:691:SER:N	2.70	0.44
3:G:332:ILE:HD12	3:G:528:LYS:HB2	1.98	0.44
3:G:430:THR:CG2	3:G:517:LEU:HD23	2.41	0.44
3:G:440:ASN:ND2	3:G:441:LEU:HG	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:390:LEU:HD11	3:J:983:ARG:CB	2.46	0.44
3:I:392:PHE:CD1	3:I:392:PHE:N	2.84	0.44
3:J:134:GLN:HB3	3:J:162:SER:HB2	2.00	0.44
3:J:431:GLY:HA3	3:J:513:LEU:O	2.18	0.44
3:J:931:ILE:HD13	3:J:931:ILE:HA	1.86	0.44
1:A:229:LEU:HD23	1:A:426:CYS:HG	1.77	0.44
2:D:166:GLU:OE1	2:D:493:HIS:HE1	2.01	0.44
3:E:328:ARG:NH1	3:E:533:LEU:HD21	2.33	0.44
3:E:646:ARG:O	3:E:646:ARG:HG3	2.17	0.44
3:E:675:GLN:O	3:E:690:GLN:HG3	2.18	0.44
3:E:854:LYS:O	3:E:855:PHE:CD1	2.71	0.44
3:F:646:ARG:O	3:F:646:ARG:HG3	2.17	0.44
3:G:617:CYS:HB2	3:G:649:CYS:HB2	1.87	0.44
3:G:735:SER:OG	3:G:859:THR:HG22	2.17	0.44
3:G:856:ASN:O	3:G:856:ASN:ND2	2.48	0.44
3:H:493:GLN:NE2	3:H:493:GLN:N	2.65	0.44
1:A:606:ILE:C	1:A:608:ASN:N	2.74	0.44
3:F:325:SER:CA	3:F:540:ASN:O	2.50	0.44
3:F:440:ASN:ND2	3:F:441:LEU:HG	2.32	0.44
3:G:140:PHE:CG	3:G:244:LEU:HD11	2.53	0.44
3:G:767:LEU:HD23	3:G:767:LEU:HA	1.85	0.44
3:H:328:ARG:NH1	3:H:533:LEU:HD21	2.33	0.44
3:H:675:GLN:O	3:H:690:GLN:HG3	2.18	0.44
3:H:854:LYS:O	3:H:855:PHE:CD1	2.71	0.44
3:I:329:PHE:CE2	3:I:528:LYS:HB3	2.48	0.44
1:A:230:PRO:HB3	1:A:427:LEU:CD2	2.48	0.44
2:B:171:GLU:HG2	2:B:171:GLU:H	1.47	0.44
2:D:254:SER:O	2:D:254:SER:OG	2.31	0.44
3:H:141:LEU:O	3:H:243:ALA:HA	2.18	0.44
3:H:326:ILE:HD13	3:H:533:LEU:CA	2.30	0.44
3:H:328:ARG:O	3:H:329:PHE:CG	2.71	0.44
3:H:1032:CYS:O	3:H:1051:SER:HB2	2.18	0.44
3:I:294:ASP:OD1	3:I:294:ASP:N	2.50	0.44
5:I:1409:NAG:O4	5:I:1410:NAG:O5	2.28	0.44
1:A:219:THR:HG22	1:A:219:THR:O	2.18	0.43
1:A:562:ILE:HG22	1:A:564:ASP:HB2	1.99	0.43
1:C:606:ILE:C	1:C:608:ASN:N	2.74	0.43
2:D:353:LYS:HA	3:H:505:TYR:CE2	2.53	0.43
3:E:48:LEU:HD13	3:E:48:LEU:N	2.32	0.43
3:F:117:LEU:HD12	3:F:118:LEU:N	2.30	0.43
3:F:130:VAL:HG21	3:F:231:ILE:HD12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:391:CYS:C	3:F:392:PHE:CD1	2.96	0.43
3:F:525:CYS:HB3	3:F:528:LYS:HG2	1.95	0.43
3:F:528:LYS:NZ	3:F:528:LYS:HB2	2.33	0.43
3:G:328:ARG:NH2	3:G:580:GLN:CD	2.76	0.43
3:G:591:SER:C	3:G:592:PHE:CD1	2.95	0.43
3:G:691:SER:OG	3:G:692:ILE:N	2.50	0.43
3:G:912:THR:OG1	3:G:914:ASN:ND2	2.51	0.43
3:H:613:GLN:HG2	3:H:613:GLN:H	1.65	0.43
3:I:140:PHE:CG	3:I:244:LEU:HD11	2.53	0.43
3:I:141:LEU:O	3:I:243:ALA:HA	2.18	0.43
3:I:518:LEU:O	3:I:519:HIS:CB	2.66	0.43
1:A:87:TYR:CD2	1:A:534:TRP:CZ2	3.06	0.43
2:B:353:LYS:HA	3:E:505:TYR:CE2	2.53	0.43
2:B:356:PHE:HB3	2:B:379:ILE:HD12	1.98	0.43
2:D:132:VAL:O	2:D:141:CYS:HA	2.17	0.43
3:E:41:LYS:HB2	3:E:42:VAL:H	1.64	0.43
3:E:141:LEU:O	3:E:243:ALA:HA	2.18	0.43
3:F:323:THR:C	3:F:324:GLU:CD	2.86	0.43
3:G:431:GLY:HA3	3:G:513:LEU:O	2.18	0.43
3:H:140:PHE:CG	3:H:244:LEU:HD11	2.53	0.43
3:H:187:LYS:HE3	3:H:213:VAL:HG12	1.99	0.43
3:H:529:LYS:CG	3:H:530:SER:N	2.65	0.43
3:H:533:LEU:CD2	3:H:578:ASP:OD2	2.60	0.43
3:I:130:VAL:HG21	3:I:231:ILE:HD12	2.00	0.43
4:N:1:NAG:C6	4:N:2:NAG:HN2	2.06	0.43
2:D:24:GLN:NE2	3:H:487:ASN:CG	2.77	0.43
3:E:130:VAL:HG21	3:E:231:ILE:HD12	2.00	0.43
3:G:130:VAL:HG21	3:G:231:ILE:HD12	2.00	0.43
3:H:391:CYS:HB3	3:H:525:CYS:HB2	1.49	0.43
3:H:640:SER:OG	3:H:641:ASN:N	2.48	0.43
3:H:1104:VAL:HG22	3:H:1115:ILE:HG12	2.00	0.43
3:I:388:ASN:O	3:I:390:LEU:N	2.52	0.43
3:J:130:VAL:HG21	3:J:231:ILE:HD12	2.00	0.43
2:B:313:LYS:HA	2:B:316:VAL:HG12	2.00	0.43
1:C:591:GLY:C	1:C:593:PRO:HD2	2.43	0.43
2:D:24:GLN:NE2	3:H:487:ASN:OD1	2.48	0.43
2:D:313:LYS:HA	2:D:316:VAL:HG12	2.00	0.43
3:E:127:VAL:HG21	5:E:1402:NAG:H5	2.01	0.43
3:E:569:ILE:O	3:E:570:ALA:HB3	2.19	0.43
3:F:141:LEU:O	3:F:243:ALA:HA	2.18	0.43
3:F:388:ASN:O	3:F:390:LEU:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:654:GLU:O	3:F:693:ILE:HA	2.18	0.43
3:G:294:ASP:OD1	3:G:294:ASP:N	2.50	0.43
3:H:127:VAL:HG21	5:H:1402:NAG:H5	2.01	0.43
3:I:323:THR:C	3:I:324:GLU:CD	2.86	0.43
3:J:535:LYS:HB2	3:J:535:LYS:HE3	1.77	0.43
2:D:24:GLN:HE21	3:H:487:ASN:CG	2.26	0.43
3:F:592:PHE:HD2	3:G:740:MET:CE	2.31	0.43
3:H:335:LEU:CB	3:H:362:VAL:O	2.67	0.43
3:H:795:LYS:HB3	3:H:797:PHE:CE2	2.54	0.43
3:J:141:LEU:O	3:J:243:ALA:HA	2.18	0.43
3:J:1027:THR:HG22	3:J:1042:PHE:HZ	1.83	0.43
1:A:591:GLY:C	1:A:593:PRO:HD2	2.43	0.43
2:B:24:GLN:NE2	3:E:487:ASN:CG	2.77	0.43
3:E:1104:VAL:HG22	3:E:1115:ILE:HG12	2.00	0.43
3:H:130:VAL:HG21	3:H:231:ILE:HD12	2.00	0.43
3:H:134:GLN:HB3	3:H:162:SER:HB2	2.00	0.43
3:I:330:PRO:HB2	3:I:331:ASN:H	1.70	0.43
3:I:391:CYS:C	3:I:392:PHE:CD1	2.96	0.43
3:I:855:PHE:HB3	3:I:856:ASN:H	1.72	0.43
3:J:520:ALA:N	3:J:521:PRO:HD3	2.34	0.43
4:g:1:NAG:H61	4:g:2:NAG:N2	2.33	0.43
4:2:1:NAG:H61	4:2:2:NAG:N2	2.33	0.43
2:B:166:GLU:OE1	2:B:493:HIS:HE1	2.01	0.43
2:D:144:LEU:O	2:D:144:LEU:HD12	2.19	0.43
3:E:140:PHE:CG	3:E:244:LEU:HD11	2.53	0.43
3:E:546:LEU:HD11	3:E:565:PHE:CG	2.53	0.43
3:E:594:GLY:CA	3:E:613:GLN:HG3	2.48	0.43
3:E:1032:CYS:O	3:E:1051:SER:HB2	2.18	0.43
3:F:140:PHE:CG	3:F:244:LEU:HD11	2.53	0.43
3:F:546:LEU:HD11	3:F:565:PHE:CG	2.53	0.43
3:F:569:ILE:CG1	3:G:47:VAL:HG12	2.48	0.43
3:G:740:MET:HE2	3:G:740:MET:HB2	1.92	0.43
3:G:792:PRO:O	3:G:795:LYS:NZ	2.52	0.43
3:I:440:ASN:ND2	3:I:441:LEU:HG	2.32	0.43
3:I:519:HIS:CG	3:I:565:PHE:HE1	2.33	0.43
3:I:569:ILE:O	3:I:570:ALA:HB3	2.19	0.43
3:J:328:ARG:NH2	3:J:580:GLN:CD	2.76	0.43
3:E:336:CYS:CB	3:E:362:VAL:O	2.59	0.43
3:F:27:ALA:HB3	3:F:64:TRP:HB3	2.01	0.43
3:F:131:CYS:HB3	3:F:164:ASN:O	2.19	0.43
3:F:569:ILE:O	3:F:570:ALA:HB3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:48:LEU:H	3:G:48:LEU:CD1	2.32	0.43
3:H:206:LYS:HZ3	3:H:208:THR:HG23	1.84	0.43
3:H:328:ARG:NH1	3:H:533:LEU:CD2	2.82	0.43
3:H:472:ILE:HD12	3:H:483:VAL:H	1.84	0.43
3:H:569:ILE:O	3:H:570:ALA:HB3	2.19	0.43
3:H:1097:SER:HA	3:H:1101:HIS:O	2.18	0.43
3:I:529:LYS:HB3	3:I:529:LYS:HZ3	1.84	0.43
3:I:613:GLN:C	3:I:615:VAL:H	2.26	0.43
3:I:646:ARG:O	3:I:646:ARG:HG3	2.17	0.43
3:J:912:THR:OG1	3:J:914:ASN:ND2	2.51	0.43
4:9:1:NAG:H61	4:9:2:NAG:N2	2.33	0.43
1:A:205:TRP:CE3	1:A:208:LEU:HD23	2.54	0.43
1:A:492:ILE:CG2	1:A:590:ALA:CB	2.94	0.43
1:C:230:PRO:HB3	1:C:427:LEU:CD2	2.48	0.43
3:E:134:GLN:HB3	3:E:162:SER:HB2	1.99	0.43
3:E:340:GLU:C	3:E:342:PHE:N	2.75	0.43
3:G:309:GLU:H	3:G:309:GLU:HG2	1.71	0.43
3:G:326:ILE:HG22	3:G:540:ASN:O	2.19	0.43
3:G:520:ALA:N	3:G:521:PRO:HD3	2.34	0.43
3:G:793:PRO:HG2	3:G:794:ILE:HD12	2.00	0.43
3:G:1027:THR:HG22	3:G:1042:PHE:HZ	1.83	0.43
3:I:546:LEU:HD11	3:I:565:PHE:CG	2.53	0.43
3:I:592:PHE:HD2	3:J:740:MET:CE	2.31	0.43
3:I:654:GLU:O	3:I:693:ILE:HA	2.18	0.43
3:J:48:LEU:H	3:J:48:LEU:CD1	2.32	0.43
3:J:99:ASN:O	3:J:102:ARG:NE	2.35	0.43
3:J:140:PHE:CG	3:J:244:LEU:HD11	2.53	0.43
3:J:324:GLU:CG	3:J:325:SER:N	2.81	0.43
1:C:229:LEU:CB	1:C:230:PRO:CD	2.88	0.43
1:C:422:ILE:HG13	1:C:423:MET:N	2.33	0.43
3:E:328:ARG:NH1	3:E:533:LEU:CD2	2.82	0.43
3:E:795:LYS:HB3	3:E:797:PHE:CE2	2.54	0.43
3:F:329:PHE:CB	3:F:330:PRO:CD	2.77	0.43
3:F:518:LEU:O	3:F:519:HIS:CB	2.66	0.43
3:G:141:LEU:O	3:G:243:ALA:HA	2.18	0.43
3:H:594:GLY:CA	3:H:613:GLN:HG3	2.48	0.43
3:I:386:LYS:NZ	3:J:985:ASP:HB3	2.34	0.43
3:I:416:GLY:O	3:I:420:ASP:HB2	2.18	0.43
3:I:986:PRO:CB	3:I:987:PRO:HD3	2.46	0.43
3:J:369:TYR:CZ	3:J:384:PRO:CG	3.02	0.43
3:J:569:ILE:O	3:J:570:ALA:HB3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:722:VAL:HA	3:J:1064:HIS:O	2.19	0.43
3:E:131:CYS:HB3	3:E:164:ASN:O	2.19	0.42
3:E:933:LYS:HB2	3:E:933:LYS:HE3	1.86	0.42
3:E:940:SER:O	3:E:940:SER:OG	2.33	0.42
3:E:959:LEU:HA	3:E:959:LEU:HD23	1.78	0.42
3:G:524:VAL:C	3:G:525:CYS:SG	3.02	0.42
3:G:565:PHE:O	3:G:565:PHE:CD1	2.70	0.42
3:G:565:PHE:CD1	3:G:565:PHE:C	2.96	0.42
3:G:722:VAL:HA	3:G:1064:HIS:O	2.19	0.42
3:H:27:ALA:HB3	3:H:64:TRP:HB3	2.01	0.42
3:H:758:SER:O	3:H:762:GLN:HG3	2.19	0.42
3:J:131:CYS:HB3	3:J:164:ASN:O	2.19	0.42
3:J:324:GLU:C	3:J:325:SER:HG	2.18	0.42
3:J:854:LYS:HE2	3:J:854:LYS:HB3	1.88	0.42
4:n:1:NAG:H61	4:n:2:NAG:N2	2.33	0.42
3:E:27:ALA:HB3	3:E:64:TRP:HB3	2.01	0.42
3:E:640:SER:OG	3:E:641:ASN:N	2.48	0.42
3:E:1097:SER:HA	3:E:1101:HIS:O	2.18	0.42
3:G:324:GLU:CG	3:G:325:SER:N	2.81	0.42
3:G:385:THR:HG1	3:G:386:LYS:HZ3	1.59	0.42
3:G:518:LEU:HG	3:G:519:HIS:N	2.31	0.42
3:G:528:LYS:O	3:G:529:LYS:CB	2.66	0.42
3:G:569:ILE:O	3:G:570:ALA:HB3	2.19	0.42
3:H:335:LEU:HA	3:H:362:VAL:O	2.20	0.42
3:H:546:LEU:HD11	3:H:565:PHE:CG	2.53	0.42
3:I:131:CYS:HB3	3:I:164:ASN:O	2.19	0.42
3:I:528:LYS:NZ	3:I:528:LYS:HB2	2.33	0.42
3:J:294:ASP:OD1	3:J:294:ASP:N	2.50	0.42
3:J:691:SER:OG	3:J:692:ILE:N	2.50	0.42
2:B:738:PRO:HD2	2:B:739:VAL:HG12	2.01	0.42
1:C:83:ILE:HG22	1:C:530:TRP:CZ3	2.54	0.42
3:E:478:THR:HG22	3:E:479:PRO:CD	2.49	0.42
3:E:758:SER:O	3:E:762:GLN:HG3	2.19	0.42
3:F:562:PHE:HD2	3:G:41:LYS:CE	2.33	0.42
3:H:472:ILE:HD12	3:H:482:GLY:CA	2.41	0.42
3:H:472:ILE:CD1	3:H:482:GLY:HA2	2.40	0.42
3:I:320:VAL:HG23	3:I:591:SER:C	2.32	0.42
3:J:327:VAL:HG12	3:J:329:PHE:CE1	2.54	0.42
3:J:793:PRO:HG2	3:J:794:ILE:HD12	2.00	0.42
2:B:125:THR:O	2:B:129:THR:OG1	2.28	0.42
2:B:354:GLY:O	3:E:502:GLY:HA3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:327:VAL:HG12	3:G:329:PHE:CE1	2.54	0.42
3:I:319:ARG:NH2	3:J:740:MET:HE2	2.16	0.42
3:I:525:CYS:HB3	3:I:528:LYS:HG2	1.95	0.42
3:J:27:ALA:HB3	3:J:64:TRP:HB3	2.01	0.42
3:J:127:VAL:HG21	5:J:1402:NAG:H5	2.01	0.42
3:J:767:LEU:HD23	3:J:767:LEU:HA	1.85	0.42
1:A:259:VAL:HA	1:A:262:LEU:HD13	2.01	0.42
2:B:103:ASN:H	4:N:1:NAG:H82	1.85	0.42
1:C:219:THR:O	1:C:219:THR:HG22	2.18	0.42
1:C:282:ALA:HB1	1:C:497:ILE:HB	2.01	0.42
1:C:533:THR:HA	1:C:537:VAL:HB	2.02	0.42
2:D:738:PRO:HD2	2:D:739:VAL:HG12	2.01	0.42
3:E:112:SER:O	3:E:113:LYS:HB3	2.20	0.42
3:E:703:ASN:HB2	3:F:787:GLN:CD	2.26	0.42
3:F:328:ARG:CD	3:F:578:ASP:OD1	2.44	0.42
3:F:964:LYS:HB2	3:F:964:LYS:HE3	1.77	0.42
3:G:393:THR:HA	3:G:523:THR:CB	2.49	0.42
3:G:854:LYS:HE2	3:G:854:LYS:HB3	1.88	0.42
3:H:41:LYS:HD2	3:H:41:LYS:N	2.35	0.42
3:H:320:VAL:HG21	3:H:591:SER:CB	2.48	0.42
3:I:27:ALA:HB3	3:I:64:TRP:HB3	2.01	0.42
3:J:112:SER:O	3:J:113:LYS:HB3	2.20	0.42
3:J:328:ARG:HH22	3:J:580:GLN:CD	2.28	0.42
3:J:393:THR:HA	3:J:523:THR:CB	2.49	0.42
3:J:856:ASN:O	3:J:856:ASN:ND2	2.48	0.42
1:A:72:ILE:HB	1:A:73:PRO:CD	2.49	0.42
1:A:83:ILE:HG22	1:A:530:TRP:CZ3	2.54	0.42
1:A:515:ASN:HD21	1:A:531:GLN:HE22	1.67	0.42
1:C:63:GLN:HE22	1:C:393:VAL:HG21	1.84	0.42
1:C:544:ILE:C	1:C:546:PHE:H	2.28	0.42
3:F:127:VAL:HG21	5:F:1402:NAG:H5	2.01	0.42
3:F:310:LYS:HA	3:F:599:THR:O	2.19	0.42
3:F:386:LYS:NZ	3:G:985:ASP:HB3	2.34	0.42
3:F:1045:LYS:NZ	3:G:786:LYS:CE	2.79	0.42
3:G:27:ALA:HB3	3:G:64:TRP:HB3	2.01	0.42
3:G:321:GLN:H	3:G:321:GLN:HG2	1.52	0.42
3:H:212:LEU:HD12	3:H:212:LEU:HA	1.78	0.42
3:J:524:VAL:C	3:J:525:CYS:SG	3.02	0.42
4:U:2:NAG:H83	4:U:2:NAG:H3	2.02	0.42
1:A:422:ILE:HG13	1:A:423:MET:N	2.33	0.42
1:C:205:TRP:CE3	1:C:208:LEU:HD23	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:125:THR:O	2:D:129:THR:OG1	2.28	0.42
3:E:524:VAL:CG2	3:E:525:CYS:N	2.83	0.42
3:F:316:SER:OG	3:F:317:ASN:N	2.49	0.42
3:G:369:TYR:CZ	3:G:384:PRO:CG	3.02	0.42
3:H:99:ASN:O	3:H:102:ARG:NE	2.35	0.42
3:I:531:THR:CG2	3:I:532:ASN:H	2.33	0.42
3:J:326:ILE:HG22	3:J:540:ASN:O	2.19	0.42
3:J:565:PHE:CD1	3:J:565:PHE:C	2.96	0.42
3:J:973:ILE:HG23	3:J:992:GLN:NE2	2.34	0.42
1:A:282:ALA:HB1	1:A:497:ILE:HB	2.01	0.42
1:A:544:ILE:O	1:A:546:PHE:N	2.53	0.42
2:B:144:LEU:HD12	2:B:144:LEU:O	2.19	0.42
1:C:87:TYR:CD2	1:C:534:TRP:CZ2	3.06	0.42
2:D:212:VAL:HG23	2:D:215:TYR:HB2	2.02	0.42
2:D:354:GLY:O	3:H:502:GLY:HA3	2.20	0.42
3:E:294:ASP:N	3:E:294:ASP:OD1	2.50	0.42
3:G:328:ARG:HH22	3:G:580:GLN:CD	2.28	0.42
3:I:127:VAL:HG21	5:I:1402:NAG:H5	2.01	0.42
3:I:533:LEU:C	3:I:533:LEU:CD1	2.85	0.42
3:J:321:GLN:H	3:J:321:GLN:HG2	1.52	0.42
2:B:82:MET:HB3	3:E:486:PHE:CZ	2.55	0.42
2:B:379:ILE:HD13	2:B:379:ILE:HA	1.92	0.42
1:C:515:ASN:HD21	1:C:531:GLN:HE22	1.67	0.42
2:D:360:MET:HE3	2:D:360:MET:HB2	1.86	0.42
3:E:406:GLU:CG	3:E:418:ILE:HG13	2.50	0.42
3:E:886:TRP:HH2	3:E:904:TYR:CD2	2.35	0.42
3:F:328:ARG:O	3:F:579:PRO:HG2	2.20	0.42
3:F:416:GLY:O	3:F:420:ASP:HB2	2.19	0.42
3:H:41:LYS:HB2	3:H:42:VAL:H	1.64	0.42
3:H:326:ILE:CD1	3:H:533:LEU:CA	2.94	0.42
3:I:310:LYS:HA	3:I:599:THR:O	2.19	0.42
3:I:562:PHE:HD2	3:J:41:LYS:CE	2.33	0.42
3:I:569:ILE:CG1	3:J:47:VAL:HG11	2.45	0.42
1:A:63:GLN:HE22	1:A:393:VAL:HG21	1.83	0.42
1:C:436:MET:HE1	1:C:462:ILE:HG22	2.02	0.42
2:D:379:ILE:HD13	2:D:379:ILE:HA	1.92	0.42
3:E:41:LYS:HD2	3:E:41:LYS:N	2.35	0.42
3:E:973:ILE:HG23	3:E:992:GLN:NE2	2.35	0.42
3:F:531:THR:CG2	3:F:532:ASN:H	2.33	0.42
3:F:655:HIS:CD2	3:F:694:ALA:O	2.70	0.42
3:I:569:ILE:HG13	3:J:47:VAL:CG1	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:735:SER:OG	3:J:859:THR:HG22	2.17	0.42
1:A:229:LEU:HD12	1:A:229:LEU:HA	1.78	0.41
1:A:436:MET:HE1	1:A:462:ILE:HG22	2.02	0.41
1:C:87:TYR:HE1	1:C:300:GLU:HA	1.84	0.41
3:E:329:PHE:CB	3:E:330:PRO:HD2	2.18	0.41
3:G:127:VAL:HG21	5:G:1402:NAG:H5	2.01	0.41
3:G:560:LEU:HD23	3:G:560:LEU:HA	1.84	0.41
3:G:612:TYR:HE1	3:G:651:ILE:HD12	1.84	0.41
3:I:113:LYS:O	3:I:113:LYS:NZ	2.31	0.41
3:J:304:LYS:HE3	3:J:304:LYS:HB3	1.78	0.41
3:J:328:ARG:HG2	3:J:328:ARG:HH21	1.85	0.41
4:AA:1:NAG:H83	4:AA:1:NAG:H3	2.02	0.41
2:D:82:MET:HB3	3:H:486:PHE:CZ	2.55	0.41
2:D:174:LYS:HG2	2:D:174:LYS:H	1.54	0.41
3:F:996:LEU:HD23	3:F:996:LEU:HA	1.92	0.41
3:H:131:CYS:HB3	3:H:164:ASN:O	2.19	0.41
3:H:478:THR:HG22	3:H:479:PRO:CD	2.49	0.41
3:H:519:HIS:O	3:H:519:HIS:CG	2.70	0.41
3:H:973:ILE:HG23	3:H:992:GLN:NE2	2.35	0.41
3:J:322:PRO:CB	3:J:538:CYS:SG	3.07	0.41
3:J:792:PRO:O	3:J:795:LYS:NZ	2.52	0.41
3:J:995:ARG:HE	3:J:995:ARG:HB3	1.67	0.41
3:E:472:ILE:HD12	3:E:483:VAL:H	1.84	0.41
3:E:473:TYR:CD2	3:E:474:GLN:N	2.72	0.41
3:E:594:GLY:C	3:E:613:GLN:HG3	2.45	0.41
3:G:112:SER:O	3:G:113:LYS:HB3	2.20	0.41
3:G:131:CYS:HB3	3:G:164:ASN:O	2.19	0.41
3:H:112:SER:O	3:H:113:LYS:HB3	2.20	0.41
3:H:480:CYS:SG	3:H:480:CYS:O	2.79	0.41
3:I:112:SER:O	3:I:113:LYS:HB3	2.20	0.41
3:J:518:LEU:HG	3:J:519:HIS:N	2.30	0.41
3:J:612:TYR:HE1	3:J:651:ILE:HD12	1.84	0.41
3:J:870:ILE:O	3:J:874:THR:HG23	2.21	0.41
4:N:2:NAG:H83	4:N:2:NAG:H3	2.02	0.41
1:C:72:ILE:HB	1:C:73:PRO:CD	2.49	0.41
1:C:135:TRP:HZ3	1:C:396:THR:HG21	1.86	0.41
1:C:209:TYR:CD2	1:C:460:GLY:HA2	2.55	0.41
1:C:544:ILE:O	1:C:546:PHE:N	2.53	0.41
3:F:542:ASN:HA	3:F:546:LEU:O	2.21	0.41
3:I:390:LEU:HA	3:I:390:LEU:HD23	1.81	0.41
3:I:569:ILE:CG1	3:J:47:VAL:HG12	2.48	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:168:TRP:CH2	2:B:172:VAL:HG21	2.55	0.41
1:C:589:VAL:HG12	1:C:589:VAL:O	2.20	0.41
3:F:227:VAL:CG1	3:F:228:ASP:N	2.84	0.41
3:F:319:ARG:NH2	3:G:740:MET:HE2	2.16	0.41
3:F:326:ILE:HG23	3:F:533:LEU:CA	2.25	0.41
3:F:655:HIS:HA	3:F:694:ALA:O	2.20	0.41
3:F:855:PHE:HB3	3:F:856:ASN:H	1.72	0.41
3:G:280:ASN:OD1	3:G:281:GLU:N	2.51	0.41
3:G:736:VAL:HG23	3:G:858:LEU:HD23	2.02	0.41
3:H:406:GLU:CG	3:H:418:ILE:HG13	2.50	0.41
3:H:594:GLY:C	3:H:613:GLN:HG3	2.45	0.41
3:I:411:ALA:HA	3:I:425:LEU:HD12	2.02	0.41
3:I:528:LYS:H	3:I:528:LYS:HG3	1.61	0.41
3:I:562:PHE:CD2	3:J:41:LYS:HE3	2.56	0.41
2:D:103:ASN:H	4:U:1:NAG:H82	1.85	0.41
2:D:553:LYS:HE3	2:D:553:LYS:HB3	1.88	0.41
3:E:320:VAL:HG12	3:E:321:GLN:N	2.36	0.41
3:E:470:THR:HG21	3:E:490:PHE:CZ	2.56	0.41
3:E:523:THR:O	3:E:525:CYS:SG	2.77	0.41
3:F:308:VAL:HG13	3:F:602:THR:HG23	2.02	0.41
3:F:522:ALA:C	3:F:523:THR:HG1	2.19	0.41
3:G:226:LEU:HB3	3:G:227:VAL:HG23	2.03	0.41
3:G:406:GLU:CG	3:G:418:ILE:HG13	2.50	0.41
3:H:193:VAL:HG23	3:H:223:LEU:CD2	2.51	0.41
3:H:690:GLN:HB2	3:H:691:SER:H	1.69	0.41
3:I:655:HIS:HA	3:I:694:ALA:O	2.20	0.41
3:J:528:LYS:O	3:J:529:LYS:CB	2.66	0.41
1:A:427:LEU:HD23	1:A:427:LEU:HA	1.91	0.41
1:A:533:THR:HA	1:A:537:VAL:HB	2.02	0.41
2:B:736:GLN:C	2:B:736:GLN:CD	2.89	0.41
1:C:72:ILE:N	1:C:72:ILE:CD1	2.83	0.41
3:E:45:SER:OG	3:E:281:GLU:HA	2.21	0.41
3:E:362:VAL:HA	3:E:524:VAL:HG23	2.02	0.41
3:E:699:LEU:HD12	3:F:872:GLN:CD	2.45	0.41
3:F:528:LYS:H	3:F:528:LYS:HG3	1.61	0.41
3:G:193:VAL:HG23	3:G:223:LEU:CD2	2.51	0.41
3:H:309:GLU:H	3:H:309:GLU:HG2	1.71	0.41
3:H:470:THR:HG21	3:H:490:PHE:CZ	2.56	0.41
3:H:473:TYR:CD2	3:H:474:GLN:N	2.72	0.41
3:H:500:THR:O	3:H:500:THR:OG1	2.31	0.41
3:I:193:VAL:HG23	3:I:223:LEU:CD2	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:227:VAL:CG1	3:I:228:ASP:N	2.84	0.41
3:I:308:VAL:HG13	3:I:602:THR:HG23	2.02	0.41
3:I:328:ARG:O	3:I:579:PRO:HG2	2.20	0.41
3:I:542:ASN:HA	3:I:546:LEU:O	2.21	0.41
3:I:996:LEU:HD23	3:I:996:LEU:HA	1.92	0.41
3:J:45:SER:OG	3:J:281:GLU:HA	2.21	0.41
3:J:226:LEU:HB3	3:J:227:VAL:HG23	2.03	0.41
3:J:309:GLU:H	3:J:309:GLU:HG2	1.71	0.41
3:J:464:PHE:HZ	3:J:514:SER:HG	1.61	0.41
3:J:542:ASN:HA	3:J:546:LEU:O	2.21	0.41
3:J:907:ASN:HD22	3:J:907:ASN:HA	1.64	0.41
1:A:87:TYR:HE1	1:A:300:GLU:HA	1.84	0.41
1:A:592:VAL:CG2	1:A:593:PRO:CD	2.72	0.41
2:B:294:THR:HG23	2:B:365:THR:HA	2.03	0.41
2:B:411:SER:OG	2:B:543:ASP:OD1	2.38	0.41
1:C:221:LYS:N	1:C:221:LYS:CD	2.73	0.41
2:D:168:TRP:CH2	2:D:172:VAL:HG21	2.55	0.41
2:D:171:GLU:HG2	2:D:171:GLU:H	1.47	0.41
2:D:736:GLN:C	2:D:736:GLN:CD	2.89	0.41
3:E:326:ILE:CD1	3:E:533:LEU:CA	2.94	0.41
3:E:490:PHE:HD1	3:E:490:PHE:HA	1.75	0.41
3:F:112:SER:O	3:F:113:LYS:HB3	2.20	0.41
3:F:193:VAL:HG23	3:F:223:LEU:CD2	2.51	0.41
3:F:309:GLU:H	3:F:309:GLU:HG2	1.71	0.41
3:F:406:GLU:CG	3:F:418:ILE:HG13	2.50	0.41
3:F:562:PHE:CD2	3:G:41:LYS:HE3	2.56	0.41
3:F:794:ILE:H	3:F:794:ILE:HG13	1.69	0.41
3:G:45:SER:OG	3:G:281:GLU:HA	2.21	0.41
3:H:616:ASN:O	3:H:618:THR:N	2.47	0.41
3:H:886:TRP:HH2	3:H:904:TYR:CD2	2.35	0.41
3:I:45:SER:O	3:I:47:VAL:N	2.54	0.41
3:I:676:THR:HB	3:I:693:ILE:HG21	2.03	0.41
3:J:406:GLU:CG	3:J:418:ILE:HG13	2.50	0.41
3:J:517:LEU:HD13	3:J:517:LEU:HA	1.90	0.41
4:o:1:NAG:H3	4:o:1:NAG:H83	2.02	0.41
1:A:209:TYR:O	1:A:209:TYR:CD1	2.74	0.41
1:A:436:MET:HE1	1:A:462:ILE:CG2	2.51	0.41
1:A:558:LEU:HD23	1:A:558:LEU:HA	1.93	0.41
2:B:212:VAL:HG23	2:B:215:TYR:HB2	2.02	0.41
1:C:72:ILE:H	1:C:72:ILE:CD1	2.30	0.41
1:C:209:TYR:O	1:C:209:TYR:CD1	2.74	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:460:ASN:N	3:E:460:ASN:OD1	2.53	0.41
3:E:472:ILE:CD1	3:E:483:VAL:N	2.84	0.41
3:E:484:GLU:H	3:E:484:GLU:HG3	1.61	0.41
3:E:705:VAL:HG12	3:F:895:GLN:HB3	2.03	0.41
3:F:324:GLU:HG2	3:F:539:VAL:HG23	1.96	0.41
3:G:322:PRO:CB	3:G:538:CYS:SG	3.07	0.41
3:G:973:ILE:HG23	3:G:992:GLN:NE2	2.35	0.41
3:H:213:VAL:HG23	3:H:214:ARG:N	2.36	0.41
3:H:319:ARG:NH2	3:H:319:ARG:CG	2.73	0.41
3:H:472:ILE:CD1	3:H:483:VAL:N	2.84	0.41
3:H:542:ASN:HA	3:H:546:LEU:O	2.21	0.41
3:I:226:LEU:HB3	3:I:227:VAL:HG23	2.03	0.41
3:J:45:SER:O	3:J:47:VAL:N	2.54	0.41
3:J:193:VAL:HG23	3:J:223:LEU:CD2	2.51	0.41
3:J:369:TYR:CE1	3:J:384:PRO:CB	3.04	0.41
1:A:107:ILE:O	1:A:108:HIS:CB	2.69	0.41
1:A:482:LEU:O	1:A:486:ASP:CB	2.69	0.41
2:B:167:SER:O	2:B:168:TRP:C	2.64	0.41
3:E:363:ALA:H	3:E:524:VAL:HG21	1.86	0.41
3:F:460:ASN:OD1	3:F:460:ASN:N	2.53	0.41
3:F:676:THR:HB	3:F:693:ILE:HG21	2.03	0.41
3:G:200:TYR:CE1	3:G:230:PRO:HB3	2.56	0.41
3:G:319:ARG:HG2	3:G:319:ARG:NH2	2.35	0.41
3:H:64:TRP:CD1	3:H:65:PHE:N	2.89	0.41
3:H:705:VAL:HG12	3:I:895:GLN:HB3	2.03	0.41
3:I:460:ASN:OD1	3:I:460:ASN:N	2.53	0.41
3:J:736:VAL:HG23	3:J:858:LEU:HD23	2.02	0.41
3:J:821:LEU:HD22	3:J:939:SER:HB3	2.03	0.41
1:A:21:LEU:HA	1:A:24:ILE:HG22	2.03	0.40
1:A:351:PRO:HD3	2:B:677:PRO:CG	2.51	0.40
2:B:455:MET:HE3	2:B:455:MET:HB3	1.79	0.40
2:B:739:VAL:O	2:B:739:VAL:HG22	2.21	0.40
1:C:259:VAL:HA	1:C:262:LEU:HD13	2.01	0.40
1:C:436:MET:HE1	1:C:462:ILE:CG2	2.51	0.40
2:D:411:SER:OG	2:D:543:ASP:OD1	2.38	0.40
3:E:193:VAL:HG23	3:E:223:LEU:CD2	2.51	0.40
3:E:227:VAL:CG1	3:E:228:ASP:N	2.84	0.40
3:E:480:CYS:O	3:E:480:CYS:SG	2.79	0.40
3:E:542:ASN:HA	3:E:546:LEU:O	2.21	0.40
3:F:89:GLY:HA2	3:F:194:PHE:O	2.21	0.40
3:G:738:CYS:HB3	3:G:760:CYS:HB3	1.92	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:821:LEU:HD22	3:G:939:SER:HB3	2.03	0.40
3:H:393:THR:HG23	3:H:523:THR:OG1	2.21	0.40
3:H:699:LEU:HD12	3:I:872:GLN:CD	2.45	0.40
3:I:187:LYS:N	3:I:187:LYS:HE2	2.37	0.40
3:I:213:VAL:HG23	3:I:214:ARG:N	2.36	0.40
3:I:329:PHE:CB	3:I:330:PRO:CD	2.77	0.40
3:I:406:GLU:CG	3:I:418:ILE:HG13	2.50	0.40
3:I:855:PHE:HD1	3:I:855:PHE:HA	1.81	0.40
3:J:200:TYR:CE1	3:J:230:PRO:HB3	2.56	0.40
3:J:770:ILE:O	3:J:774:GLN:HG2	2.21	0.40
3:E:64:TRP:CD1	3:E:65:PHE:N	2.89	0.40
3:E:166:CYS:HB3	3:E:169:GLU:OE1	2.21	0.40
3:F:166:CYS:HB3	3:F:169:GLU:OE1	2.21	0.40
3:F:529:LYS:HB3	3:F:529:LYS:HZ3	1.86	0.40
3:G:328:ARG:HG2	3:G:328:ARG:HH21	1.85	0.40
3:G:369:TYR:CE1	3:G:384:PRO:CB	3.04	0.40
3:H:187:LYS:N	3:H:187:LYS:HE2	2.37	0.40
3:H:707:TYR:HB2	3:I:883:THR:CG2	2.43	0.40
3:H:959:LEU:HD23	3:H:959:LEU:HA	1.78	0.40
3:I:576:VAL:CG2	3:I:587:ILE:HD11	2.49	0.40
3:I:931:ILE:HD13	3:I:931:ILE:HA	1.88	0.40
1:A:544:ILE:C	1:A:546:PHE:H	2.28	0.40
1:A:589:VAL:HG12	1:A:589:VAL:O	2.20	0.40
2:B:320:LEU:HD23	2:B:320:LEU:HA	1.92	0.40
1:C:81:GLU:OE2	1:C:541:LEU:HD23	2.21	0.40
3:E:472:ILE:CD1	3:E:483:VAL:H	2.34	0.40
3:E:536:ASN:C	3:E:537:LYS:CG	2.87	0.40
3:F:46:SER:C	3:F:47:VAL:HG13	2.46	0.40
3:F:187:LYS:N	3:F:187:LYS:HE2	2.37	0.40
3:F:411:ALA:HA	3:F:425:LEU:HD12	2.02	0.40
3:F:518:LEU:O	3:F:519:HIS:HB2	2.22	0.40
3:F:1040:VAL:O	3:F:1041:ASP:HB2	2.21	0.40
3:G:460:ASN:OD1	3:G:460:ASN:N	2.53	0.40
3:G:524:VAL:HG22	3:G:525:CYS:N	2.37	0.40
3:G:703:ASN:HD22	3:G:704:SER:N	2.19	0.40
3:H:45:SER:O	3:H:47:VAL:N	2.54	0.40
3:H:113:LYS:O	3:H:113:LYS:NZ	2.31	0.40
3:H:227:VAL:CG1	3:H:228:ASP:N	2.84	0.40
3:H:369:TYR:CZ	3:H:384:PRO:HB2	2.57	0.40
3:I:310:LYS:HB2	3:I:310:LYS:HE3	1.75	0.40
3:I:735:SER:O	3:I:859:THR:HG22	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:825:LYS:HE2	3:I:825:LYS:HB3	1.79	0.40
1:A:209:TYR:CD2	1:A:460:GLY:HA2	2.55	0.40
1:A:580:ASN:HD22	1:A:580:ASN:HA	1.65	0.40
3:E:187:LYS:N	3:E:187:LYS:HE2	2.36	0.40
3:E:226:LEU:HB3	3:E:227:VAL:HG23	2.03	0.40
3:F:213:VAL:HG23	3:F:214:ARG:N	2.36	0.40
3:F:390:LEU:HD23	3:F:390:LEU:HA	1.81	0.40
3:F:395:VAL:CG2	3:F:524:VAL:HG11	2.50	0.40
3:F:533:LEU:HD22	3:F:534:VAL:C	2.47	0.40
3:F:984:LEU:HD23	3:F:988:GLU:HB3	2.03	0.40
3:G:45:SER:O	3:G:47:VAL:N	2.54	0.40
3:G:100:ILE:HG22	3:G:242:LEU:HD23	2.04	0.40
3:G:187:LYS:N	3:G:187:LYS:HE2	2.37	0.40
3:H:200:TYR:CE1	3:H:230:PRO:HB3	2.56	0.40
3:H:530:SER:C	3:H:531:THR:CG2	2.94	0.40
3:I:810:SER:O	3:I:810:SER:OG	2.35	0.40
3:J:347:PHE:CD1	3:J:509:ARG:HD3	2.56	0.40
1:A:464:LEU:HD12	1:A:464:LEU:HA	1.86	0.40
2:B:92:THR:HG22	2:B:96:GLN:HE21	1.87	0.40
1:C:107:ILE:O	1:C:108:HIS:CB	2.69	0.40
1:C:482:LEU:O	1:C:486:ASP:CB	2.69	0.40
2:D:294:THR:HG23	2:D:365:THR:HA	2.03	0.40
3:E:45:SER:O	3:E:47:VAL:N	2.54	0.40
3:E:200:TYR:CE1	3:E:230:PRO:HB3	2.56	0.40
3:E:322:PRO:HB3	3:E:538:CYS:C	2.47	0.40
3:E:340:GLU:C	3:E:342:PHE:H	2.30	0.40
3:E:369:TYR:CZ	3:E:384:PRO:HB2	2.57	0.40
3:F:200:TYR:CE1	3:F:230:PRO:HB3	2.56	0.40
3:F:226:LEU:HB3	3:F:227:VAL:HG23	2.03	0.40
3:F:329:PHE:CB	3:F:330:PRO:HD2	2.11	0.40
3:F:519:HIS:CG	3:F:565:PHE:HE1	2.33	0.40
3:F:523:THR:CG2	3:F:524:VAL:H	2.12	0.40
3:F:576:VAL:CG2	3:F:587:ILE:HD11	2.49	0.40
3:F:981:LEU:HD12	3:F:981:LEU:HA	1.89	0.40
3:G:89:GLY:HA2	3:G:194:PHE:O	2.22	0.40
3:G:518:LEU:CG	3:G:519:HIS:H	2.24	0.40
3:G:870:ILE:O	3:G:874:THR:HG23	2.21	0.40
3:H:127:VAL:HG22	3:H:171:VAL:HG13	2.04	0.40
3:H:371:SER:C	3:H:373:SER:H	2.30	0.40
3:H:472:ILE:CD1	3:H:483:VAL:H	2.34	0.40
3:I:89:GLY:HA2	3:I:194:PHE:O	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:1040:VAL:O	3:I:1041:ASP:HB2	2.21	0.40
3:J:213:VAL:HG23	3:J:214:ARG:N	2.36	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	603/654 (92%)	540 (90%)	59 (10%)	4 (1%)	18	56
1	C	531/654 (81%)	483 (91%)	45 (8%)	3 (1%)	21	59
2	B	394/817 (48%)	356 (90%)	34 (9%)	4 (1%)	12	49
2	D	731/817 (90%)	671 (92%)	50 (7%)	10 (1%)	9	40
3	E	989/1283 (77%)	841 (85%)	113 (11%)	35 (4%)	3	20
3	F	988/1283 (77%)	855 (86%)	96 (10%)	37 (4%)	2	20
3	G	988/1283 (77%)	842 (85%)	106 (11%)	40 (4%)	2	18
3	H	989/1283 (77%)	841 (85%)	112 (11%)	36 (4%)	2	20
3	I	988/1283 (77%)	855 (86%)	96 (10%)	37 (4%)	2	20
3	J	988/1283 (77%)	842 (85%)	106 (11%)	40 (4%)	2	18
All	All	8189/10640 (77%)	7126 (87%)	817 (10%)	246 (3%)	5	23

All (246) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	144	LEU
2	D	144	LEU
2	D	631	LYS
2	D	736	GLN
3	E	48	LEU

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Mol	Chain	Res	Type
3	E	332	ILE
3	E	341	VAL
3	E	479	PRO
3	E	483	VAL
3	E	691	SER
3	E	701	ALA
3	E	855	PHE
3	F	48	LEU
3	F	326	ILE
3	F	388	ASN
3	F	519	HIS
3	F	524	VAL
3	F	526	GLY
3	F	530	SER
3	F	614	ASP
3	G	48	LEU
3	G	336	CYS
3	G	529	LYS
3	G	530	SER
3	G	534	VAL
3	G	560	LEU
3	G	564	GLN
3	G	691	SER
3	G	814	LYS
3	H	48	LEU
3	H	332	ILE
3	H	334	ASN
3	H	341	VAL
3	H	479	PRO
3	H	483	VAL
3	H	521	PRO
3	H	691	SER
3	H	701	ALA
3	H	855	PHE
3	I	48	LEU
3	I	326	ILE
3	I	388	ASN
3	I	519	HIS
3	I	524	VAL
3	I	526	GLY
3	I	530	SER
3	I	614	ASP

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Mol	Chain	Res	Type
3	J	48	LEU
3	J	336	CYS
3	J	529	LYS
3	J	530	SER
3	J	534	VAL
3	J	560	LEU
3	J	564	GLN
3	J	691	SER
3	J	814	LYS
2	B	343	VAL
2	D	343	VAL
2	D	679	ILE
2	D	735	ASN
2	D	739	VAL
3	E	41	LYS
3	E	46	SER
3	E	334	ASN
3	E	339	GLY
3	E	481	ASN
3	E	482	GLY
3	E	484	GLU
3	E	488	CYS
3	F	41	LYS
3	F	46	SER
3	F	324	GLU
3	F	327	VAL
3	F	330	PRO
3	F	339	GLY
3	F	389	ASP
3	F	523	THR
3	F	532	ASN
3	F	742	ILE
3	F	743	CYS
3	G	41	LYS
3	G	46	SER
3	G	327	VAL
3	G	328	ARG
3	G	330	PRO
3	G	333	THR
3	G	335	LEU
3	G	339	GLY
3	G	535	LYS

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Mol	Chain	Res	Type
3	G	588	THR
3	G	697	MET
3	G	810	SER
3	H	41	LYS
3	H	46	SER
3	H	339	GLY
3	H	481	ASN
3	H	482	GLY
3	H	484	GLU
3	H	488	CYS
3	H	520	ALA
3	I	41	LYS
3	I	46	SER
3	I	324	GLU
3	I	327	VAL
3	I	330	PRO
3	I	339	GLY
3	I	389	ASP
3	I	523	THR
3	I	532	ASN
3	I	742	ILE
3	I	743	CYS
3	J	41	LYS
3	J	46	SER
3	J	327	VAL
3	J	328	ARG
3	J	330	PRO
3	J	333	THR
3	J	335	LEU
3	J	339	GLY
3	J	535	LYS
3	J	588	THR
3	J	697	MET
3	J	810	SER
1	A	486	ASP
2	B	169	ARG
2	B	423	LEU
1	C	486	ASP
2	D	169	ARG
2	D	423	LEU
3	E	43	PHE
3	E	324	GLU

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Mol	Chain	Res	Type
3	E	333	THR
3	E	519	HIS
3	E	614	ASP
3	E	695	TYR
3	E	710	ASN
3	F	43	PHE
3	F	320	VAL
3	F	383	SER
3	F	521	PRO
3	F	590	CYS
3	G	43	PHE
3	G	517	LEU
3	G	527	PRO
3	G	528	LYS
3	G	591	SER
3	H	43	PHE
3	H	324	GLU
3	H	614	ASP
3	H	695	TYR
3	H	710	ASN
3	I	43	PHE
3	I	320	VAL
3	I	383	SER
3	I	521	PRO
3	I	590	CYS
3	J	43	PHE
3	J	517	LEU
3	J	527	PRO
3	J	528	LYS
3	J	591	SER
1	A	108	HIS
1	A	592	VAL
1	C	592	VAL
3	E	44	ARG
3	E	329	PHE
3	E	349	SER
3	E	472	ILE
3	E	480	CYS
3	E	522	ALA
3	E	592	PHE
3	F	44	ARG
3	F	349	SER

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Mol	Chain	Res	Type
3	F	518	LEU
3	F	531	THR
3	F	746	SER
3	G	44	ARG
3	G	325	SER
3	G	349	SER
3	G	519	HIS
3	G	592	PHE
3	G	813	SER
3	H	44	ARG
3	H	329	PHE
3	H	349	SER
3	H	472	ILE
3	H	480	CYS
3	H	523	THR
3	H	592	PHE
3	I	44	ARG
3	I	349	SER
3	I	518	LEU
3	I	531	THR
3	I	746	SER
3	J	44	ARG
3	J	325	SER
3	J	349	SER
3	J	519	HIS
3	J	592	PHE
3	J	813	SER
3	E	40	ASP
3	E	42	VAL
3	E	47	VAL
3	E	617	CYS
3	F	40	ASP
3	F	42	VAL
3	F	47	VAL
3	F	520	ALA
3	F	522	ALA
3	F	616	ASN
3	G	40	ASP
3	G	42	VAL
3	G	47	VAL
3	G	812	PRO
3	H	40	ASP

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Mol	Chain	Res	Type
3	H	42	VAL
3	H	47	VAL
3	H	525	CYS
3	H	617	CYS
3	I	40	ASP
3	I	42	VAL
3	I	47	VAL
3	I	520	ALA
3	I	522	ALA
3	I	616	ASN
3	J	40	ASP
3	J	42	VAL
3	J	47	VAL
3	J	812	PRO
3	E	523	THR
3	G	334	ASN
3	G	811	LYS
3	H	336	CYS
3	J	334	ASN
3	J	811	LYS
3	G	521	PRO
3	J	521	PRO
1	A	593	PRO
1	C	593	PRO
3	F	384	PRO
3	I	384	PRO
3	F	534	VAL
3	I	534	VAL
2	D	738	PRO
3	G	326	ILE
3	J	326	ILE

5.3.2 Protein sidechains ⓘ

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

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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	531/572 (93%)	510 (96%)	21 (4%)	28	49
1	C	531/572 (93%)	510 (96%)	21 (4%)	28	49
2	B	662/721 (92%)	637 (96%)	25 (4%)	29	50
2	D	662/721 (92%)	636 (96%)	26 (4%)	28	49
3	E	882/1122 (79%)	756 (86%)	126 (14%)	3	13
3	F	881/1122 (78%)	771 (88%)	110 (12%)	4	16
3	G	881/1122 (78%)	776 (88%)	105 (12%)	5	18
3	H	882/1122 (79%)	757 (86%)	125 (14%)	3	13
3	I	881/1122 (78%)	771 (88%)	110 (12%)	4	16
3	J	881/1122 (78%)	776 (88%)	105 (12%)	5	18
All	All	7674/9318 (82%)	6900 (90%)	774 (10%)	9	23

All (774) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	76	ILE
1	A	80	LEU
1	A	81	GLU
1	A	157	GLU
1	A	159	GLN
1	A	217	GLU
1	A	221	LYS
1	A	226	THR
1	A	228	THR
1	A	234	LEU
1	A	419	LEU
1	A	423	MET
1	A	424	LEU
1	A	461	LEU
1	A	462	ILE
1	A	466	THR
1	A	484	LEU
1	A	541	LEU
1	A	592	VAL
1	A	594	SER
1	A	607	ARG
2	B	31	LYS

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Mol	Chain	Res	Type
2	B	42	GLN
2	B	82	MET
2	B	107	VAL
2	B	128	SER
2	B	134	ASN
2	B	143	LEU
2	B	166	GLU
2	B	169	ARG
2	B	171	GLU
2	B	174	LYS
2	B	175	GLN
2	B	339	VAL
2	B	344	CYS
2	B	347	THR
2	B	361	CYS
2	B	423	LEU
2	B	425	SER
2	B	628	LEU
2	B	630	ASP
2	B	678	ARG
2	B	680	SER
2	B	736	GLN
2	B	740	SER
2	B	768	ARG
1	C	76	ILE
1	C	80	LEU
1	C	81	GLU
1	C	157	GLU
1	C	159	GLN
1	C	217	GLU
1	C	221	LYS
1	C	226	THR
1	C	228	THR
1	C	234	LEU
1	C	419	LEU
1	C	423	MET
1	C	424	LEU
1	C	461	LEU
1	C	462	ILE
1	C	466	THR
1	C	484	LEU
1	C	541	LEU

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Mol	Chain	Res	Type
1	C	592	VAL
1	C	594	SER
1	C	607	ARG
2	D	31	LYS
2	D	42	GLN
2	D	82	MET
2	D	107	VAL
2	D	128	SER
2	D	134	ASN
2	D	143	LEU
2	D	166	GLU
2	D	169	ARG
2	D	171	GLU
2	D	174	LYS
2	D	175	GLN
2	D	339	VAL
2	D	344	CYS
2	D	345	HIS
2	D	347	THR
2	D	361	CYS
2	D	423	LEU
2	D	425	SER
2	D	628	LEU
2	D	630	ASP
2	D	678	ARG
2	D	680	SER
2	D	736	GLN
2	D	740	SER
2	D	768	ARG
3	E	40	ASP
3	E	41	LYS
3	E	46	SER
3	E	48	LEU
3	E	66	HIS
3	E	81	ASN
3	E	97	LYS
3	E	109	THR
3	E	116	SER
3	E	118	LEU
3	E	122	ASN
3	E	141	LEU
3	E	143	VAL

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Mol	Chain	Res	Type
3	E	158	ARG
3	E	164	ASN
3	E	169	GLU
3	E	171	VAL
3	E	195	LYS
3	E	205	SER
3	E	208	THR
3	E	221	SER
3	E	231	ILE
3	E	282	ASN
3	E	289	VAL
3	E	296	LEU
3	E	301	CYS
3	E	308	VAL
3	E	314	GLN
3	E	315	THR
3	E	319	ARG
3	E	324	GLU
3	E	328	ARG
3	E	333	THR
3	E	334	ASN
3	E	335	LEU
3	E	340	GLU
3	E	375	SER
3	E	382	VAL
3	E	383	SER
3	E	389	ASP
3	E	390	LEU
3	E	406	GLU
3	E	421	TYR
3	E	430	THR
3	E	438	SER
3	E	459	SER
3	E	469	SER
3	E	483	VAL
3	E	484	GLU
3	E	487	ASN
3	E	489	TYR
3	E	490	PHE
3	E	493	GLN
3	E	500	THR
3	E	501	ASN

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Mol	Chain	Res	Type
3	E	514	SER
3	E	516	GLU
3	E	517	LEU
3	E	518	LEU
3	E	525	CYS
3	E	528	LYS
3	E	529	LYS
3	E	532	ASN
3	E	533	LEU
3	E	540	ASN
3	E	546	LEU
3	E	553	THR
3	E	556	ASN
3	E	576	VAL
3	E	583	GLU
3	E	585	LEU
3	E	599	THR
3	E	602	THR
3	E	608	VAL
3	E	617	CYS
3	E	619	GLU
3	E	673	SER
3	E	692	ILE
3	E	696	THR
3	E	702	GLU
3	E	704	SER
3	E	705	VAL
3	E	719	THR
3	E	722	VAL
3	E	729	VAL
3	E	730	SER
3	E	738	CYS
3	E	746	SER
3	E	772	VAL
3	E	773	GLU
3	E	785	VAL
3	E	787	GLN
3	E	791	THR
3	E	826	VAL
3	E	855	PHE
3	E	868	GLU
3	E	878	LEU

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Mol	Chain	Res	Type
3	E	883	THR
3	E	902	MET
3	E	916	LEU
3	E	929	SER
3	E	939	SER
3	E	951	VAL
3	E	960	ASN
3	E	967	SER
3	E	973	ILE
3	E	976	VAL
3	E	991	VAL
3	E	994	ASP
3	E	998	THR
3	E	1005	GLN
3	E	1018	ILE
3	E	1039	ARG
3	E	1074	ASN
3	E	1076	THR
3	E	1077	THR
3	E	1092	GLU
3	E	1094	VAL
3	E	1100	THR
3	E	1104	VAL
3	E	1114	ILE
3	E	1123	SER
3	E	1125	ASN
3	E	1132	ILE
3	E	1142	GLN
3	E	1144	GLU
3	F	40	ASP
3	F	46	SER
3	F	48	LEU
3	F	66	HIS
3	F	81	ASN
3	F	97	LYS
3	F	109	THR
3	F	116	SER
3	F	118	LEU
3	F	122	ASN
3	F	141	LEU
3	F	143	VAL
3	F	158	ARG

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Mol	Chain	Res	Type
3	F	164	ASN
3	F	169	GLU
3	F	171	VAL
3	F	195	LYS
3	F	205	SER
3	F	208	THR
3	F	221	SER
3	F	231	ILE
3	F	282	ASN
3	F	289	VAL
3	F	296	LEU
3	F	301	CYS
3	F	308	VAL
3	F	314	GLN
3	F	315	THR
3	F	323	THR
3	F	326	ILE
3	F	327	VAL
3	F	332	ILE
3	F	336	CYS
3	F	375	SER
3	F	382	VAL
3	F	383	SER
3	F	386	LYS
3	F	389	ASP
3	F	403	ARG
3	F	406	GLU
3	F	408	ARG
3	F	415	THR
3	F	417	LYS
3	F	421	TYR
3	F	430	THR
3	F	438	SER
3	F	459	SER
3	F	469	SER
3	F	472	ILE
3	F	514	SER
3	F	515	PHE
3	F	517	LEU
3	F	518	LEU
3	F	519	HIS
3	F	525	CYS

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Mol	Chain	Res	Type
3	F	528	LYS
3	F	529	LYS
3	F	533	LEU
3	F	534	VAL
3	F	535	LYS
3	F	540	ASN
3	F	546	LEU
3	F	553	THR
3	F	554	GLU
3	F	556	ASN
3	F	576	VAL
3	F	583	GLU
3	F	585	LEU
3	F	588	THR
3	F	592	PHE
3	F	599	THR
3	F	602	THR
3	F	608	VAL
3	F	611	LEU
3	F	613	GLN
3	F	617	CYS
3	F	673	SER
3	F	710	ASN
3	F	729	VAL
3	F	735	SER
3	F	747	THR
3	F	748	GLU
3	F	772	VAL
3	F	779	GLN
3	F	787	GLN
3	F	791	THR
3	F	811	LYS
3	F	855	PHE
3	F	856	ASN
3	F	868	GLU
3	F	878	LEU
3	F	912	THR
3	F	916	LEU
3	F	935	GLN
3	F	968	SER
3	F	969	ASN
3	F	974	SER

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Mol	Chain	Res	Type
3	F	976	VAL
3	F	991	VAL
3	F	1030	SER
3	F	1037	SER
3	F	1045	LYS
3	F	1074	ASN
3	F	1081	ILE
3	F	1094	VAL
3	F	1104	VAL
3	F	1114	ILE
3	F	1126	CYS
3	F	1133	VAL
3	F	1141	LEU
3	G	40	ASP
3	G	46	SER
3	G	48	LEU
3	G	66	HIS
3	G	81	ASN
3	G	97	LYS
3	G	109	THR
3	G	116	SER
3	G	118	LEU
3	G	122	ASN
3	G	141	LEU
3	G	143	VAL
3	G	158	ARG
3	G	164	ASN
3	G	169	GLU
3	G	171	VAL
3	G	195	LYS
3	G	205	SER
3	G	208	THR
3	G	221	SER
3	G	231	ILE
3	G	282	ASN
3	G	289	VAL
3	G	296	LEU
3	G	301	CYS
3	G	308	VAL
3	G	314	GLN
3	G	315	THR
3	G	317	ASN

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Mol	Chain	Res	Type
3	G	319	ARG
3	G	321	GLN
3	G	328	ARG
3	G	375	SER
3	G	382	VAL
3	G	383	SER
3	G	389	ASP
3	G	390	LEU
3	G	403	ARG
3	G	406	GLU
3	G	421	TYR
3	G	430	THR
3	G	438	SER
3	G	459	SER
3	G	469	SER
3	G	472	ILE
3	G	517	LEU
3	G	529	LYS
3	G	530	SER
3	G	533	LEU
3	G	540	ASN
3	G	546	LEU
3	G	553	THR
3	G	554	GLU
3	G	556	ASN
3	G	557	LYS
3	G	559	PHE
3	G	563	GLN
3	G	565	PHE
3	G	567	ARG
3	G	576	VAL
3	G	583	GLU
3	G	585	LEU
3	G	588	THR
3	G	592	PHE
3	G	599	THR
3	G	602	THR
3	G	608	VAL
3	G	671	CYS
3	G	690	GLN
3	G	693	ILE
3	G	696	THR

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Mol	Chain	Res	Type
3	G	697	MET
3	G	699	LEU
3	G	727	LEU
3	G	768	THR
3	G	770	ILE
3	G	778	THR
3	G	787	GLN
3	G	791	THR
3	G	814	LYS
3	G	856	ASN
3	G	878	LEU
3	G	907	ASN
3	G	922	LEU
3	G	929	SER
3	G	931	ILE
3	G	934	ILE
3	G	937	SER
3	G	968	SER
3	G	975	SER
3	G	976	VAL
3	G	977	LEU
3	G	988	GLU
3	G	1018	ILE
3	G	1027	THR
3	G	1063	LEU
3	G	1077	THR
3	G	1092	GLU
3	G	1094	VAL
3	G	1104	VAL
3	G	1126	CYS
3	G	1129	VAL
3	G	1132	ILE
3	G	1136	THR
3	G	1145	LEU
3	H	40	ASP
3	H	41	LYS
3	H	46	SER
3	H	48	LEU
3	H	66	HIS
3	H	81	ASN
3	H	97	LYS
3	H	109	THR

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Mol	Chain	Res	Type
3	H	116	SER
3	H	118	LEU
3	H	122	ASN
3	H	141	LEU
3	H	143	VAL
3	H	158	ARG
3	H	164	ASN
3	H	169	GLU
3	H	171	VAL
3	H	195	LYS
3	H	205	SER
3	H	208	THR
3	H	221	SER
3	H	231	ILE
3	H	282	ASN
3	H	289	VAL
3	H	296	LEU
3	H	301	CYS
3	H	308	VAL
3	H	314	GLN
3	H	315	THR
3	H	319	ARG
3	H	324	GLU
3	H	328	ARG
3	H	333	THR
3	H	335	LEU
3	H	336	CYS
3	H	340	GLU
3	H	375	SER
3	H	382	VAL
3	H	383	SER
3	H	389	ASP
3	H	390	LEU
3	H	406	GLU
3	H	421	TYR
3	H	430	THR
3	H	438	SER
3	H	459	SER
3	H	469	SER
3	H	483	VAL
3	H	484	GLU
3	H	487	ASN

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Mol	Chain	Res	Type
3	H	489	TYR
3	H	490	PHE
3	H	493	GLN
3	H	500	THR
3	H	501	ASN
3	H	514	SER
3	H	517	LEU
3	H	518	LEU
3	H	523	THR
3	H	528	LYS
3	H	529	LYS
3	H	532	ASN
3	H	533	LEU
3	H	540	ASN
3	H	546	LEU
3	H	553	THR
3	H	556	ASN
3	H	576	VAL
3	H	583	GLU
3	H	585	LEU
3	H	599	THR
3	H	602	THR
3	H	608	VAL
3	H	617	CYS
3	H	619	GLU
3	H	673	SER
3	H	692	ILE
3	H	696	THR
3	H	702	GLU
3	H	704	SER
3	H	705	VAL
3	H	719	THR
3	H	722	VAL
3	H	729	VAL
3	H	730	SER
3	H	738	CYS
3	H	746	SER
3	H	772	VAL
3	H	773	GLU
3	H	785	VAL
3	H	787	GLN
3	H	791	THR

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Mol	Chain	Res	Type
3	H	826	VAL
3	H	855	PHE
3	H	868	GLU
3	H	878	LEU
3	H	883	THR
3	H	902	MET
3	H	916	LEU
3	H	929	SER
3	H	939	SER
3	H	951	VAL
3	H	960	ASN
3	H	967	SER
3	H	973	ILE
3	H	976	VAL
3	H	991	VAL
3	H	994	ASP
3	H	998	THR
3	H	1005	GLN
3	H	1018	ILE
3	H	1039	ARG
3	H	1074	ASN
3	H	1076	THR
3	H	1077	THR
3	H	1092	GLU
3	H	1094	VAL
3	H	1100	THR
3	H	1104	VAL
3	H	1114	ILE
3	H	1123	SER
3	H	1125	ASN
3	H	1132	ILE
3	H	1142	GLN
3	H	1144	GLU
3	I	40	ASP
3	I	46	SER
3	I	48	LEU
3	I	66	HIS
3	I	81	ASN
3	I	97	LYS
3	I	109	THR
3	I	116	SER
3	I	118	LEU

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Mol	Chain	Res	Type
3	I	122	ASN
3	I	141	LEU
3	I	143	VAL
3	I	158	ARG
3	I	164	ASN
3	I	169	GLU
3	I	171	VAL
3	I	195	LYS
3	I	205	SER
3	I	208	THR
3	I	221	SER
3	I	231	ILE
3	I	282	ASN
3	I	289	VAL
3	I	296	LEU
3	I	301	CYS
3	I	308	VAL
3	I	314	GLN
3	I	315	THR
3	I	323	THR
3	I	326	ILE
3	I	327	VAL
3	I	332	ILE
3	I	336	CYS
3	I	375	SER
3	I	382	VAL
3	I	383	SER
3	I	386	LYS
3	I	389	ASP
3	I	403	ARG
3	I	406	GLU
3	I	408	ARG
3	I	415	THR
3	I	417	LYS
3	I	421	TYR
3	I	430	THR
3	I	438	SER
3	I	459	SER
3	I	469	SER
3	I	472	ILE
3	I	514	SER
3	I	515	PHE

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Mol	Chain	Res	Type
3	I	517	LEU
3	I	518	LEU
3	I	519	HIS
3	I	525	CYS
3	I	528	LYS
3	I	529	LYS
3	I	533	LEU
3	I	534	VAL
3	I	535	LYS
3	I	540	ASN
3	I	546	LEU
3	I	553	THR
3	I	554	GLU
3	I	556	ASN
3	I	576	VAL
3	I	583	GLU
3	I	585	LEU
3	I	588	THR
3	I	592	PHE
3	I	599	THR
3	I	602	THR
3	I	608	VAL
3	I	611	LEU
3	I	613	GLN
3	I	617	CYS
3	I	673	SER
3	I	710	ASN
3	I	729	VAL
3	I	735	SER
3	I	747	THR
3	I	748	GLU
3	I	772	VAL
3	I	779	GLN
3	I	787	GLN
3	I	791	THR
3	I	811	LYS
3	I	855	PHE
3	I	856	ASN
3	I	868	GLU
3	I	878	LEU
3	I	912	THR
3	I	916	LEU

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Mol	Chain	Res	Type
3	I	935	GLN
3	I	968	SER
3	I	969	ASN
3	I	974	SER
3	I	976	VAL
3	I	991	VAL
3	I	1030	SER
3	I	1037	SER
3	I	1045	LYS
3	I	1074	ASN
3	I	1081	ILE
3	I	1094	VAL
3	I	1104	VAL
3	I	1114	ILE
3	I	1126	CYS
3	I	1133	VAL
3	I	1141	LEU
3	J	40	ASP
3	J	46	SER
3	J	48	LEU
3	J	66	HIS
3	J	81	ASN
3	J	97	LYS
3	J	109	THR
3	J	116	SER
3	J	118	LEU
3	J	122	ASN
3	J	141	LEU
3	J	143	VAL
3	J	158	ARG
3	J	164	ASN
3	J	169	GLU
3	J	171	VAL
3	J	195	LYS
3	J	205	SER
3	J	208	THR
3	J	221	SER
3	J	231	ILE
3	J	282	ASN
3	J	289	VAL
3	J	296	LEU
3	J	301	CYS

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Mol	Chain	Res	Type
3	J	308	VAL
3	J	314	GLN
3	J	315	THR
3	J	317	ASN
3	J	319	ARG
3	J	321	GLN
3	J	328	ARG
3	J	375	SER
3	J	382	VAL
3	J	383	SER
3	J	389	ASP
3	J	390	LEU
3	J	403	ARG
3	J	406	GLU
3	J	421	TYR
3	J	430	THR
3	J	438	SER
3	J	459	SER
3	J	469	SER
3	J	472	ILE
3	J	517	LEU
3	J	529	LYS
3	J	530	SER
3	J	533	LEU
3	J	540	ASN
3	J	546	LEU
3	J	553	THR
3	J	554	GLU
3	J	556	ASN
3	J	557	LYS
3	J	559	PHE
3	J	563	GLN
3	J	565	PHE
3	J	567	ARG
3	J	576	VAL
3	J	583	GLU
3	J	585	LEU
3	J	588	THR
3	J	592	PHE
3	J	599	THR
3	J	602	THR
3	J	608	VAL

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Mol	Chain	Res	Type
3	J	671	CYS
3	J	690	GLN
3	J	693	ILE
3	J	696	THR
3	J	697	MET
3	J	699	LEU
3	J	727	LEU
3	J	768	THR
3	J	770	ILE
3	J	778	THR
3	J	787	GLN
3	J	791	THR
3	J	814	LYS
3	J	856	ASN
3	J	878	LEU
3	J	907	ASN
3	J	922	LEU
3	J	929	SER
3	J	931	ILE
3	J	934	ILE
3	J	937	SER
3	J	968	SER
3	J	975	SER
3	J	976	VAL
3	J	977	LEU
3	J	988	GLU
3	J	1018	ILE
3	J	1027	THR
3	J	1063	LEU
3	J	1077	THR
3	J	1092	GLU
3	J	1094	VAL
3	J	1104	VAL
3	J	1126	CYS
3	J	1129	VAL
3	J	1132	ILE
3	J	1136	THR
3	J	1145	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (252) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	GLN
1	A	63	GLN
1	A	94	GLN
1	A	142	ASN
1	A	159	GLN
1	A	298	ASN
1	A	310	ASN
1	A	340	ASN
1	A	515	ASN
1	A	580	ASN
1	A	609	HIS
2	B	58	ASN
2	B	63	ASN
2	B	89	GLN
2	B	96	GLN
2	B	117	ASN
2	B	139	GLN
2	B	159	ASN
2	B	175	GLN
2	B	277	ASN
2	B	300	GLN
2	B	417	HIS
2	B	493	HIS
2	B	508	ASN
2	B	572	ASN
2	B	586	ASN
2	B	599	ASN
2	B	735	ASN
2	B	736	GLN
1	C	26	GLN
1	C	63	GLN
1	C	94	GLN
1	C	142	ASN
1	C	159	GLN
1	C	310	ASN
1	C	340	ASN
1	C	386	ASN
1	C	515	ASN
1	C	580	ASN
1	C	609	HIS
2	D	58	ASN
2	D	63	ASN
2	D	89	GLN

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Mol	Chain	Res	Type
2	D	96	GLN
2	D	117	ASN
2	D	121	ASN
2	D	139	GLN
2	D	159	ASN
2	D	175	GLN
2	D	277	ASN
2	D	300	GLN
2	D	417	HIS
2	D	472	GLN
2	D	493	HIS
2	D	508	ASN
2	D	572	ASN
2	D	586	ASN
2	D	599	ASN
2	D	735	ASN
2	D	736	GLN
3	E	134	GLN
3	E	137	ASN
3	E	188	ASN
3	E	317	ASN
3	E	394	ASN
3	E	422	ASN
3	E	440	ASN
3	E	450	ASN
3	E	474	GLN
3	E	501	ASN
3	E	532	ASN
3	E	556	ASN
3	E	644	GLN
3	E	658	ASN
3	E	675	GLN
3	E	703	ASN
3	E	755	GLN
3	E	762	GLN
3	E	764	ASN
3	E	787	GLN
3	E	824	ASN
3	E	901	GLN
3	E	914	ASN
3	E	926	GLN
3	E	949	GLN

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Mol	Chain	Res	Type
3	E	969	ASN
3	E	992	GLN
3	E	1010	GLN
3	E	1054	GLN
3	E	1113	GLN
3	E	1125	ASN
3	F	134	GLN
3	F	137	ASN
3	F	188	ASN
3	F	317	ASN
3	F	334	ASN
3	F	394	ASN
3	F	422	ASN
3	F	440	ASN
3	F	450	ASN
3	F	498	GLN
3	F	542	ASN
3	F	556	ASN
3	F	564	GLN
3	F	613	GLN
3	F	644	GLN
3	F	655	HIS
3	F	658	ASN
3	F	675	GLN
3	F	690	GLN
3	F	703	ASN
3	F	710	ASN
3	F	804	GLN
3	F	901	GLN
3	F	914	ASN
3	F	920	GLN
3	F	926	GLN
3	F	949	GLN
3	F	957	GLN
3	F	960	ASN
3	F	992	GLN
3	F	1011	GLN
3	F	1083	HIS
3	F	1101	HIS
3	G	134	GLN
3	G	137	ASN
3	G	188	ASN

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Mol	Chain	Res	Type
3	G	314	GLN
3	G	317	ASN
3	G	321	GLN
3	G	394	ASN
3	G	422	ASN
3	G	440	ASN
3	G	450	ASN
3	G	498	GLN
3	G	556	ASN
3	G	644	GLN
3	G	658	ASN
3	G	690	GLN
3	G	703	ASN
3	G	764	ASN
3	G	779	GLN
3	G	784	GLN
3	G	804	GLN
3	G	901	GLN
3	G	907	ASN
3	G	914	ASN
3	G	926	GLN
3	G	935	GLN
3	G	992	GLN
3	G	1010	GLN
3	G	1011	GLN
3	G	1071	GLN
3	G	1101	HIS
3	G	1125	ASN
3	G	1135	ASN
3	H	134	GLN
3	H	137	ASN
3	H	188	ASN
3	H	317	ASN
3	H	394	ASN
3	H	422	ASN
3	H	440	ASN
3	H	450	ASN
3	H	474	GLN
3	H	501	ASN
3	H	532	ASN
3	H	556	ASN
3	H	644	GLN

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Mol	Chain	Res	Type
3	H	658	ASN
3	H	675	GLN
3	H	703	ASN
3	H	755	GLN
3	H	762	GLN
3	H	787	GLN
3	H	901	GLN
3	H	914	ASN
3	H	926	GLN
3	H	949	GLN
3	H	969	ASN
3	H	992	GLN
3	H	1010	GLN
3	H	1054	GLN
3	H	1125	ASN
3	I	134	GLN
3	I	137	ASN
3	I	188	ASN
3	I	317	ASN
3	I	334	ASN
3	I	394	ASN
3	I	422	ASN
3	I	440	ASN
3	I	450	ASN
3	I	498	GLN
3	I	542	ASN
3	I	556	ASN
3	I	564	GLN
3	I	644	GLN
3	I	655	HIS
3	I	658	ASN
3	I	675	GLN
3	I	690	GLN
3	I	703	ASN
3	I	710	ASN
3	I	804	GLN
3	I	901	GLN
3	I	914	ASN
3	I	920	GLN
3	I	926	GLN
3	I	949	GLN
3	I	957	GLN

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Mol	Chain	Res	Type
3	I	960	ASN
3	I	992	GLN
3	I	1011	GLN
3	I	1083	HIS
3	I	1101	HIS
3	J	134	GLN
3	J	137	ASN
3	J	188	ASN
3	J	239	GLN
3	J	314	GLN
3	J	317	ASN
3	J	321	GLN
3	J	394	ASN
3	J	422	ASN
3	J	440	ASN
3	J	450	ASN
3	J	498	GLN
3	J	542	ASN
3	J	556	ASN
3	J	644	GLN
3	J	658	ASN
3	J	703	ASN
3	J	764	ASN
3	J	779	GLN
3	J	784	GLN
3	J	804	GLN
3	J	901	GLN
3	J	907	ASN
3	J	914	ASN
3	J	926	GLN
3	J	935	GLN
3	J	949	GLN
3	J	992	GLN
3	J	1010	GLN
3	J	1011	GLN
3	J	1058	HIS
3	J	1071	GLN
3	J	1101	HIS
3	J	1106	GLN
3	J	1125	ASN
3	J	1135	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

116 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	$\# Z > 2$
4	NAG	0	1	3,4	14,14,15	0.25	0	17,19,21	0.70	1 (5%)
4	NAG	0	2	4	14,14,15	0.15	0	17,19,21	0.50	0
4	NAG	1	1	3,4	14,14,15	0.28	0	17,19,21	0.57	0
4	NAG	1	2	4	14,14,15	0.24	0	17,19,21	0.60	0
4	NAG	2	1	3,4	14,14,15	0.58	1 (7%)	17,19,21	0.58	0
4	NAG	2	2	4	14,14,15	0.31	0	17,19,21	0.48	0
4	NAG	3	1	3,4	14,14,15	0.29	0	17,19,21	0.42	0
4	NAG	3	2	4	14,14,15	0.43	0	17,19,21	0.38	0
4	NAG	4	1	3,4	14,14,15	0.37	0	17,19,21	1.16	1 (5%)
4	NAG	4	2	4	14,14,15	0.28	0	17,19,21	0.50	0
4	NAG	5	1	3,4	14,14,15	0.31	0	17,19,21	0.72	1 (5%)
4	NAG	5	2	4	14,14,15	0.20	0	17,19,21	0.42	0
4	NAG	6	1	3,4	14,14,15	0.73	1 (7%)	17,19,21	0.91	1 (5%)
4	NAG	6	2	4	14,14,15	0.33	0	17,19,21	0.73	1 (5%)
4	NAG	7	1	3,4	14,14,15	0.21	0	17,19,21	0.44	0
4	NAG	7	2	4	14,14,15	0.27	0	17,19,21	0.38	0
4	NAG	8	1	3,4	14,14,15	0.52	0	17,19,21	0.51	0
4	NAG	8	2	4	14,14,15	0.25	0	17,19,21	0.59	0
4	NAG	9	1	3,4	14,14,15	0.55	0	17,19,21	0.58	0
4	NAG	9	2	4	14,14,15	0.29	0	17,19,21	0.48	0
4	NAG	AA	1	3,4	14,14,15	0.23	0	17,19,21	1.45	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	AA	2	4	14,14,15	0.19	0	17,19,21	0.53	0
4	NAG	BA	1	3,4	14,14,15	0.52	0	17,19,21	0.73	1 (5%)
4	NAG	BA	2	4	14,14,15	0.41	0	17,19,21	0.48	0
4	NAG	CA	1	3,4	14,14,15	0.37	0	17,19,21	0.41	0
4	NAG	CA	2	4	14,14,15	0.19	0	17,19,21	0.77	0
4	NAG	DA	1	3,4	14,14,15	0.36	0	17,19,21	0.49	0
4	NAG	DA	2	4	14,14,15	0.60	0	17,19,21	1.39	2 (11%)
4	NAG	EA	1	3,4	14,14,15	0.63	1 (7%)	17,19,21	0.44	0
4	NAG	EA	2	4	14,14,15	0.33	0	17,19,21	1.44	2 (11%)
4	NAG	FA	1	3,4	14,14,15	0.39	0	17,19,21	0.46	0
4	NAG	FA	2	4	14,14,15	0.24	0	17,19,21	0.52	0
4	NAG	K	1	4,1	14,14,15	0.33	0	17,19,21	0.53	0
4	NAG	K	2	4	14,14,15	0.33	0	17,19,21	0.51	0
4	NAG	L	1	2,4	14,14,15	0.58	0	17,19,21	0.73	0
4	NAG	L	2	4	14,14,15	0.55	0	17,19,21	0.38	0
4	NAG	M	1	2,4	14,14,15	0.40	0	17,19,21	0.66	0
4	NAG	M	2	4	14,14,15	0.29	0	17,19,21	0.71	1 (5%)
4	NAG	N	1	2,4	14,14,15	0.28	0	17,19,21	0.57	0
4	NAG	N	2	4	14,14,15	0.30	0	17,19,21	0.56	0
4	NAG	O	1	2,4	14,14,15	0.31	0	17,19,21	0.53	0
4	NAG	O	2	4	14,14,15	0.37	0	17,19,21	0.48	0
4	NAG	P	1	2,4	14,14,15	0.24	0	17,19,21	0.63	0
4	NAG	P	2	4	14,14,15	0.33	0	17,19,21	0.61	1 (5%)
4	NAG	Q	1	2,4	14,14,15	0.24	0	17,19,21	0.58	0
4	NAG	Q	2	4	14,14,15	0.23	0	17,19,21	0.59	0
4	NAG	R	1	4,1	14,14,15	0.34	0	17,19,21	0.53	0
4	NAG	R	2	4	14,14,15	0.33	0	17,19,21	0.49	0
4	NAG	S	1	2,4	14,14,15	0.57	0	17,19,21	0.74	0
4	NAG	S	2	4	14,14,15	0.54	0	17,19,21	0.37	0
4	NAG	T	1	2,4	14,14,15	0.39	0	17,19,21	0.66	0
4	NAG	T	2	4	14,14,15	0.28	0	17,19,21	0.71	1 (5%)
4	NAG	U	1	2,4	14,14,15	0.28	0	17,19,21	0.57	0
4	NAG	U	2	4	14,14,15	0.30	0	17,19,21	0.56	0
4	NAG	V	1	2,4	14,14,15	0.33	0	17,19,21	0.53	0
4	NAG	V	2	4	14,14,15	0.35	0	17,19,21	0.48	0
4	NAG	W	1	2,4	14,14,15	0.23	0	17,19,21	0.63	0
4	NAG	W	2	4	14,14,15	0.34	0	17,19,21	0.61	1 (5%)
4	NAG	X	1	2,4	14,14,15	0.25	0	17,19,21	0.58	0
4	NAG	X	2	4	14,14,15	0.23	0	17,19,21	0.59	0
4	NAG	Y	1	3,4	14,14,15	0.51	0	17,19,21	0.52	0
4	NAG	Y	2	4	14,14,15	0.25	0	17,19,21	0.61	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	Z	1	3,4	14,14,15	0.28	0	17,19,21	0.57	0
4	NAG	Z	2	4	14,14,15	0.29	0	17,19,21	0.56	0
4	NAG	a	1	3,4	14,14,15	0.31	0	17,19,21	0.64	0
4	NAG	a	2	4	14,14,15	0.51	0	17,19,21	0.49	0
4	NAG	b	1	3,4	14,14,15	0.35	0	17,19,21	0.74	0
4	NAG	b	2	4	14,14,15	0.31	0	17,19,21	1.40	2 (11%)
4	NAG	c	1	3,4	14,14,15	0.68	1 (7%)	17,19,21	0.71	0
4	NAG	c	2	4	14,14,15	0.41	0	17,19,21	1.49	3 (17%)
4	NAG	d	1	3,4	14,14,15	0.66	1 (7%)	17,19,21	0.68	0
4	NAG	d	2	4	14,14,15	0.28	0	17,19,21	0.67	0
4	NAG	e	1	3,4	14,14,15	0.24	0	17,19,21	0.71	1 (5%)
4	NAG	e	2	4	14,14,15	0.18	0	17,19,21	0.50	0
4	NAG	f	1	3,4	14,14,15	0.29	0	17,19,21	0.56	0
4	NAG	f	2	4	14,14,15	0.24	0	17,19,21	0.60	0
4	NAG	g	1	3,4	14,14,15	0.56	0	17,19,21	0.58	0
4	NAG	g	2	4	14,14,15	0.31	0	17,19,21	0.48	0
4	NAG	h	1	3,4	14,14,15	0.31	0	17,19,21	0.41	0
4	NAG	h	2	4	14,14,15	0.42	0	17,19,21	0.38	0
4	NAG	i	1	3,4	14,14,15	0.37	0	17,19,21	1.17	1 (5%)
4	NAG	i	2	4	14,14,15	0.25	0	17,19,21	0.49	0
4	NAG	j	1	3,4	14,14,15	0.30	0	17,19,21	0.72	1 (5%)
4	NAG	j	2	4	14,14,15	0.21	0	17,19,21	0.42	0
4	NAG	k	1	3,4	14,14,15	0.73	1 (7%)	17,19,21	0.91	1 (5%)
4	NAG	k	2	4	14,14,15	0.33	0	17,19,21	0.73	1 (5%)
4	NAG	l	1	3,4	14,14,15	0.21	0	17,19,21	0.45	0
4	NAG	l	2	4	14,14,15	0.29	0	17,19,21	0.39	0
4	NAG	m	1	3,4	14,14,15	0.53	0	17,19,21	0.51	0
4	NAG	m	2	4	14,14,15	0.24	0	17,19,21	0.60	0
4	NAG	n	1	3,4	14,14,15	0.56	0	17,19,21	0.58	0
4	NAG	n	2	4	14,14,15	0.29	0	17,19,21	0.47	0
4	NAG	o	1	3,4	14,14,15	0.22	0	17,19,21	1.45	2 (11%)
4	NAG	o	2	4	14,14,15	0.20	0	17,19,21	0.53	0
4	NAG	p	1	3,4	14,14,15	0.53	0	17,19,21	0.74	1 (5%)
4	NAG	p	2	4	14,14,15	0.41	0	17,19,21	0.48	0
4	NAG	q	1	3,4	14,14,15	0.38	0	17,19,21	0.40	0
4	NAG	q	2	4	14,14,15	0.20	0	17,19,21	0.77	0
4	NAG	r	1	3,4	14,14,15	0.35	0	17,19,21	0.48	0
4	NAG	r	2	4	14,14,15	0.60	0	17,19,21	1.39	2 (11%)
4	NAG	s	1	3,4	14,14,15	0.63	1 (7%)	17,19,21	0.45	0
4	NAG	s	2	4	14,14,15	0.33	0	17,19,21	1.44	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	t	1	3,4	14,14,15	0.38	0	17,19,21	0.47	0
4	NAG	t	2	4	14,14,15	0.23	0	17,19,21	0.52	0
4	NAG	u	1	3,4	14,14,15	0.51	0	17,19,21	0.51	0
4	NAG	u	2	4	14,14,15	0.24	0	17,19,21	0.61	0
4	NAG	v	1	3,4	14,14,15	0.28	0	17,19,21	0.57	0
4	NAG	v	2	4	14,14,15	0.29	0	17,19,21	0.56	0
4	NAG	w	1	3,4	14,14,15	0.32	0	17,19,21	0.65	1 (5%)
4	NAG	w	2	4	14,14,15	0.51	0	17,19,21	0.49	0
4	NAG	x	1	3,4	14,14,15	0.36	0	17,19,21	0.74	0
4	NAG	x	2	4	14,14,15	0.33	0	17,19,21	1.40	2 (11%)
4	NAG	y	1	3,4	14,14,15	0.68	1 (7%)	17,19,21	0.71	0
4	NAG	y	2	4	14,14,15	0.40	0	17,19,21	1.48	3 (17%)
4	NAG	z	1	3,4	14,14,15	0.66	1 (7%)	17,19,21	0.68	0
4	NAG	z	2	4	14,14,15	0.27	0	17,19,21	0.66	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	0	1	3,4	-	2/6/23/26	0/1/1/1
4	NAG	0	2	4	-	0/6/23/26	0/1/1/1
4	NAG	1	1	3,4	-	2/6/23/26	0/1/1/1
4	NAG	1	2	4	-	2/6/23/26	0/1/1/1
4	NAG	2	1	3,4	-	0/6/23/26	0/1/1/1
4	NAG	2	2	4	-	3/6/23/26	0/1/1/1
4	NAG	3	1	3,4	-	0/6/23/26	0/1/1/1
4	NAG	3	2	4	-	1/6/23/26	0/1/1/1
4	NAG	4	1	3,4	-	1/6/23/26	0/1/1/1
4	NAG	4	2	4	-	0/6/23/26	0/1/1/1
4	NAG	5	1	3,4	-	2/6/23/26	0/1/1/1
4	NAG	5	2	4	-	3/6/23/26	0/1/1/1
4	NAG	6	1	3,4	-	2/6/23/26	0/1/1/1
4	NAG	6	2	4	-	3/6/23/26	0/1/1/1
4	NAG	7	1	3,4	-	2/6/23/26	0/1/1/1
4	NAG	7	2	4	-	2/6/23/26	0/1/1/1
4	NAG	8	1	3,4	-	1/6/23/26	0/1/1/1
4	NAG	8	2	4	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	9	1	3,4	-	0/6/23/26	0/1/1/1
4	NAG	9	2	4	-	3/6/23/26	0/1/1/1
4	NAG	AA	1	3,4	-	6/6/23/26	0/1/1/1
4	NAG	AA	2	4	-	2/6/23/26	0/1/1/1
4	NAG	BA	1	3,4	-	2/6/23/26	0/1/1/1
4	NAG	BA	2	4	-	2/6/23/26	0/1/1/1
4	NAG	CA	1	3,4	-	2/6/23/26	0/1/1/1
4	NAG	CA	2	4	-	2/6/23/26	0/1/1/1
4	NAG	DA	1	3,4	-	2/6/23/26	0/1/1/1
4	NAG	DA	2	4	-	6/6/23/26	0/1/1/1
4	NAG	EA	1	3,4	-	2/6/23/26	0/1/1/1
4	NAG	EA	2	4	-	5/6/23/26	0/1/1/1
4	NAG	FA	1	3,4	-	0/6/23/26	0/1/1/1
4	NAG	FA	2	4	-	2/6/23/26	0/1/1/1
4	NAG	K	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	K	2	4	-	2/6/23/26	0/1/1/1
4	NAG	L	1	2,4	-	2/6/23/26	0/1/1/1
4	NAG	L	2	4	-	2/6/23/26	0/1/1/1
4	NAG	M	1	2,4	-	2/6/23/26	0/1/1/1
4	NAG	M	2	4	-	2/6/23/26	0/1/1/1
4	NAG	N	1	2,4	-	2/6/23/26	0/1/1/1
4	NAG	N	2	4	-	3/6/23/26	0/1/1/1
4	NAG	O	1	2,4	-	0/6/23/26	0/1/1/1
4	NAG	O	2	4	-	0/6/23/26	0/1/1/1
4	NAG	P	1	2,4	-	0/6/23/26	0/1/1/1
4	NAG	P	2	4	-	2/6/23/26	0/1/1/1
4	NAG	Q	1	2,4	-	0/6/23/26	0/1/1/1
4	NAG	Q	2	4	-	2/6/23/26	0/1/1/1
4	NAG	R	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	R	2	4	-	2/6/23/26	0/1/1/1
4	NAG	S	1	2,4	-	2/6/23/26	0/1/1/1
4	NAG	S	2	4	-	2/6/23/26	0/1/1/1
4	NAG	T	1	2,4	-	2/6/23/26	0/1/1/1
4	NAG	T	2	4	-	2/6/23/26	0/1/1/1
4	NAG	U	1	2,4	-	2/6/23/26	0/1/1/1
4	NAG	U	2	4	-	3/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	V	1	2,4	-	0/6/23/26	0/1/1/1
4	NAG	V	2	4	-	0/6/23/26	0/1/1/1
4	NAG	W	1	2,4	-	0/6/23/26	0/1/1/1
4	NAG	W	2	4	-	2/6/23/26	0/1/1/1
4	NAG	X	1	2,4	-	0/6/23/26	0/1/1/1
4	NAG	X	2	4	-	2/6/23/26	0/1/1/1
4	NAG	Y	1	3,4	-	1/6/23/26	0/1/1/1
4	NAG	Y	2	4	-	2/6/23/26	0/1/1/1
4	NAG	Z	1	3,4	-	3/6/23/26	0/1/1/1
4	NAG	Z	2	4	-	4/6/23/26	0/1/1/1
4	NAG	a	1	3,4	-	0/6/23/26	0/1/1/1
4	NAG	a	2	4	-	2/6/23/26	0/1/1/1
4	NAG	b	1	3,4	-	2/6/23/26	0/1/1/1
4	NAG	b	2	4	-	4/6/23/26	0/1/1/1
4	NAG	c	1	3,4	-	2/6/23/26	0/1/1/1
4	NAG	c	2	4	-	6/6/23/26	0/1/1/1
4	NAG	d	1	3,4	-	2/6/23/26	0/1/1/1
4	NAG	d	2	4	-	4/6/23/26	0/1/1/1
4	NAG	e	1	3,4	-	2/6/23/26	0/1/1/1
4	NAG	e	2	4	-	0/6/23/26	0/1/1/1
4	NAG	f	1	3,4	-	2/6/23/26	0/1/1/1
4	NAG	f	2	4	-	2/6/23/26	0/1/1/1
4	NAG	g	1	3,4	-	0/6/23/26	0/1/1/1
4	NAG	g	2	4	-	3/6/23/26	0/1/1/1
4	NAG	h	1	3,4	-	0/6/23/26	0/1/1/1
4	NAG	h	2	4	-	1/6/23/26	0/1/1/1
4	NAG	i	1	3,4	-	1/6/23/26	0/1/1/1
4	NAG	i	2	4	-	0/6/23/26	0/1/1/1
4	NAG	j	1	3,4	-	2/6/23/26	0/1/1/1
4	NAG	j	2	4	-	3/6/23/26	0/1/1/1
4	NAG	k	1	3,4	-	2/6/23/26	0/1/1/1
4	NAG	k	2	4	-	3/6/23/26	0/1/1/1
4	NAG	l	1	3,4	-	2/6/23/26	0/1/1/1
4	NAG	l	2	4	-	2/6/23/26	0/1/1/1
4	NAG	m	1	3,4	-	1/6/23/26	0/1/1/1
4	NAG	m	2	4	-	2/6/23/26	0/1/1/1
4	NAG	n	1	3,4	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	n	2	4	-	3/6/23/26	0/1/1/1
4	NAG	o	1	3,4	-	6/6/23/26	0/1/1/1
4	NAG	o	2	4	-	2/6/23/26	0/1/1/1
4	NAG	p	1	3,4	-	2/6/23/26	0/1/1/1
4	NAG	p	2	4	-	2/6/23/26	0/1/1/1
4	NAG	q	1	3,4	-	2/6/23/26	0/1/1/1
4	NAG	q	2	4	-	2/6/23/26	0/1/1/1
4	NAG	r	1	3,4	-	2/6/23/26	0/1/1/1
4	NAG	r	2	4	-	6/6/23/26	0/1/1/1
4	NAG	s	1	3,4	-	2/6/23/26	0/1/1/1
4	NAG	s	2	4	-	5/6/23/26	0/1/1/1
4	NAG	t	1	3,4	-	0/6/23/26	0/1/1/1
4	NAG	t	2	4	-	2/6/23/26	0/1/1/1
4	NAG	u	1	3,4	-	1/6/23/26	0/1/1/1
4	NAG	u	2	4	-	2/6/23/26	0/1/1/1
4	NAG	v	1	3,4	-	3/6/23/26	0/1/1/1
4	NAG	v	2	4	-	4/6/23/26	0/1/1/1
4	NAG	w	1	3,4	-	0/6/23/26	0/1/1/1
4	NAG	w	2	4	-	2/6/23/26	0/1/1/1
4	NAG	x	1	3,4	-	2/6/23/26	0/1/1/1
4	NAG	x	2	4	-	4/6/23/26	0/1/1/1
4	NAG	y	1	3,4	-	2/6/23/26	0/1/1/1
4	NAG	y	2	4	-	6/6/23/26	0/1/1/1
4	NAG	z	1	3,4	-	2/6/23/26	0/1/1/1
4	NAG	z	2	4	-	4/6/23/26	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	6	1	NAG	O5-C1	-2.63	1.39	1.43
4	k	1	NAG	O5-C1	-2.62	1.39	1.43
4	d	1	NAG	O5-C1	-2.39	1.39	1.43
4	z	1	NAG	O5-C1	-2.39	1.39	1.43
4	c	1	NAG	O5-C1	-2.22	1.40	1.43
4	y	1	NAG	O5-C1	-2.21	1.40	1.43
4	s	1	NAG	O5-C1	-2.05	1.40	1.43
4	EA	1	NAG	O5-C1	-2.05	1.40	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	2	1	NAG	O5-C1	-2.03	1.40	1.43

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	AA	1	NAG	C2-N2-C7	4.99	129.59	122.90
4	o	1	NAG	C2-N2-C7	4.99	129.59	122.90
4	c	2	NAG	C2-N2-C7	4.72	129.22	122.90
4	y	2	NAG	C2-N2-C7	4.65	129.13	122.90
4	s	2	NAG	C2-N2-C7	4.64	129.12	122.90
4	DA	2	NAG	C2-N2-C7	4.61	129.08	122.90
4	EA	2	NAG	C2-N2-C7	4.60	129.07	122.90
4	r	2	NAG	C2-N2-C7	4.60	129.06	122.90
4	x	2	NAG	C2-N2-C7	4.58	129.04	122.90
4	b	2	NAG	C2-N2-C7	4.57	129.03	122.90
4	i	1	NAG	C1-O5-C5	3.37	116.70	112.19
4	4	1	NAG	C1-O5-C5	3.33	116.65	112.19
4	y	2	NAG	C1-C2-N2	2.63	114.57	110.43
4	c	2	NAG	C1-C2-N2	2.61	114.55	110.43
4	x	2	NAG	C1-C2-N2	2.53	114.42	110.43
4	b	2	NAG	C1-C2-N2	2.53	114.42	110.43
4	M	2	NAG	C1-O5-C5	2.50	115.54	112.19
4	s	2	NAG	C1-C2-N2	2.50	114.36	110.43
4	T	2	NAG	C1-O5-C5	2.50	115.53	112.19
4	EA	2	NAG	C1-C2-N2	2.47	114.33	110.43
4	6	1	NAG	O4-C4-C3	-2.35	104.85	110.38
4	5	1	NAG	C1-O5-C5	2.34	115.33	112.19
4	k	1	NAG	O4-C4-C3	-2.34	104.85	110.38
4	p	1	NAG	C1-O5-C5	2.34	115.32	112.19
4	j	1	NAG	C1-O5-C5	2.30	115.27	112.19
4	BA	1	NAG	C1-O5-C5	2.28	115.25	112.19
4	AA	1	NAG	C1-C2-N2	2.20	113.90	110.43
4	o	1	NAG	C1-C2-N2	2.18	113.87	110.43
4	y	2	NAG	C1-O5-C5	2.16	115.08	112.19
4	e	1	NAG	C1-O5-C5	2.15	115.07	112.19
4	c	2	NAG	C1-O5-C5	2.14	115.06	112.19
4	0	1	NAG	C1-O5-C5	2.13	115.04	112.19
4	P	2	NAG	C1-O5-C5	2.09	114.99	112.19
4	W	2	NAG	C1-O5-C5	2.09	114.98	112.19
4	6	2	NAG	C1-O5-C5	2.05	114.94	112.19
4	k	2	NAG	C1-O5-C5	2.05	114.94	112.19
4	w	1	NAG	C1-O5-C5	2.04	114.93	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	r	2	NAG	C1-C2-N2	2.04	113.65	110.43
4	DA	2	NAG	C1-C2-N2	2.03	113.64	110.43

There are no chirality outliers.

All (230) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	N	1	NAG	O7-C7-N2-C2
4	N	2	NAG	C3-C2-N2-C7
4	N	2	NAG	C8-C7-N2-C2
4	N	2	NAG	O7-C7-N2-C2
4	U	1	NAG	O7-C7-N2-C2
4	U	2	NAG	C3-C2-N2-C7
4	U	2	NAG	C8-C7-N2-C2
4	U	2	NAG	O7-C7-N2-C2
4	Z	1	NAG	C8-C7-N2-C2
4	Z	1	NAG	O7-C7-N2-C2
4	Z	2	NAG	C8-C7-N2-C2
4	Z	2	NAG	O7-C7-N2-C2
4	v	1	NAG	C8-C7-N2-C2
4	v	1	NAG	O7-C7-N2-C2
4	v	2	NAG	C8-C7-N2-C2
4	v	2	NAG	O7-C7-N2-C2
4	Q	2	NAG	O5-C5-C6-O6
4	X	2	NAG	O5-C5-C6-O6
4	N	1	NAG	C8-C7-N2-C2
4	U	1	NAG	C8-C7-N2-C2
4	o	2	NAG	O5-C5-C6-O6
4	p	2	NAG	O5-C5-C6-O6
4	q	1	NAG	O5-C5-C6-O6
4	AA	2	NAG	O5-C5-C6-O6
4	BA	2	NAG	O5-C5-C6-O6
4	CA	1	NAG	O5-C5-C6-O6
4	P	2	NAG	O5-C5-C6-O6
4	W	2	NAG	O5-C5-C6-O6
4	Y	2	NAG	O5-C5-C6-O6
4	d	1	NAG	O5-C5-C6-O6
4	f	2	NAG	O5-C5-C6-O6
4	k	1	NAG	O5-C5-C6-O6
4	m	2	NAG	O5-C5-C6-O6
4	u	2	NAG	O5-C5-C6-O6
4	z	1	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	1	2	NAG	O5-C5-C6-O6
4	6	1	NAG	O5-C5-C6-O6
4	8	2	NAG	O5-C5-C6-O6
4	L	1	NAG	O5-C5-C6-O6
4	S	1	NAG	O5-C5-C6-O6
4	M	2	NAG	O5-C5-C6-O6
4	T	2	NAG	O5-C5-C6-O6
4	Y	2	NAG	C4-C5-C6-O6
4	f	2	NAG	C4-C5-C6-O6
4	k	1	NAG	C4-C5-C6-O6
4	m	2	NAG	C4-C5-C6-O6
4	u	2	NAG	C4-C5-C6-O6
4	1	2	NAG	C4-C5-C6-O6
4	6	1	NAG	C4-C5-C6-O6
4	8	2	NAG	C4-C5-C6-O6
4	p	1	NAG	O5-C5-C6-O6
4	BA	1	NAG	O5-C5-C6-O6
4	M	1	NAG	O5-C5-C6-O6
4	T	1	NAG	O5-C5-C6-O6
4	k	2	NAG	O5-C5-C6-O6
4	6	2	NAG	O5-C5-C6-O6
4	Q	2	NAG	C4-C5-C6-O6
4	X	2	NAG	C4-C5-C6-O6
4	Z	2	NAG	C4-C5-C6-O6
4	d	1	NAG	C4-C5-C6-O6
4	v	2	NAG	C4-C5-C6-O6
4	z	1	NAG	C4-C5-C6-O6
4	M	2	NAG	C4-C5-C6-O6
4	T	2	NAG	C4-C5-C6-O6
4	p	1	NAG	C4-C5-C6-O6
4	q	1	NAG	C4-C5-C6-O6
4	BA	1	NAG	C4-C5-C6-O6
4	CA	1	NAG	C4-C5-C6-O6
4	l	1	NAG	C4-C5-C6-O6
4	p	2	NAG	C4-C5-C6-O6
4	7	1	NAG	C4-C5-C6-O6
4	BA	2	NAG	C4-C5-C6-O6
4	Z	2	NAG	O5-C5-C6-O6
4	v	2	NAG	O5-C5-C6-O6
4	r	2	NAG	O5-C5-C6-O6
4	DA	2	NAG	O5-C5-C6-O6
4	o	2	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	AA	2	NAG	C4-C5-C6-O6
4	L	2	NAG	C4-C5-C6-O6
4	S	2	NAG	C4-C5-C6-O6
4	k	2	NAG	C4-C5-C6-O6
4	6	2	NAG	C4-C5-C6-O6
4	l	2	NAG	O5-C5-C6-O6
4	7	2	NAG	O5-C5-C6-O6
4	P	2	NAG	C4-C5-C6-O6
4	W	2	NAG	C4-C5-C6-O6
4	r	2	NAG	C4-C5-C6-O6
4	DA	2	NAG	C4-C5-C6-O6
4	L	1	NAG	C4-C5-C6-O6
4	S	1	NAG	C4-C5-C6-O6
4	o	1	NAG	O5-C5-C6-O6
4	AA	1	NAG	O5-C5-C6-O6
4	L	2	NAG	O5-C5-C6-O6
4	S	2	NAG	O5-C5-C6-O6
4	o	1	NAG	C4-C5-C6-O6
4	b	2	NAG	C8-C7-N2-C2
4	b	2	NAG	O7-C7-N2-C2
4	c	2	NAG	C8-C7-N2-C2
4	c	2	NAG	O7-C7-N2-C2
4	j	2	NAG	C8-C7-N2-C2
4	j	2	NAG	O7-C7-N2-C2
4	o	1	NAG	C8-C7-N2-C2
4	o	1	NAG	O7-C7-N2-C2
4	r	2	NAG	C8-C7-N2-C2
4	r	2	NAG	O7-C7-N2-C2
4	s	2	NAG	C8-C7-N2-C2
4	s	2	NAG	O7-C7-N2-C2
4	x	2	NAG	C8-C7-N2-C2
4	x	2	NAG	O7-C7-N2-C2
4	y	2	NAG	C8-C7-N2-C2
4	y	2	NAG	O7-C7-N2-C2
4	5	2	NAG	C8-C7-N2-C2
4	5	2	NAG	O7-C7-N2-C2
4	AA	1	NAG	C8-C7-N2-C2
4	AA	1	NAG	O7-C7-N2-C2
4	DA	2	NAG	C8-C7-N2-C2
4	DA	2	NAG	O7-C7-N2-C2
4	EA	2	NAG	C8-C7-N2-C2
4	EA	2	NAG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
4	M	1	NAG	C4-C5-C6-O6
4	T	1	NAG	C4-C5-C6-O6
4	AA	1	NAG	C4-C5-C6-O6
4	b	1	NAG	C4-C5-C6-O6
4	c	1	NAG	C4-C5-C6-O6
4	x	1	NAG	C4-C5-C6-O6
4	l	2	NAG	C4-C5-C6-O6
4	y	1	NAG	C4-C5-C6-O6
4	7	2	NAG	C4-C5-C6-O6
4	f	1	NAG	O5-C5-C6-O6
4	l	1	NAG	O5-C5-C6-O6
4	1	1	NAG	O5-C5-C6-O6
4	7	1	NAG	O5-C5-C6-O6
4	f	1	NAG	C4-C5-C6-O6
4	1	1	NAG	C4-C5-C6-O6
4	b	1	NAG	O5-C5-C6-O6
4	x	1	NAG	O5-C5-C6-O6
4	c	1	NAG	O5-C5-C6-O6
4	y	1	NAG	O5-C5-C6-O6
4	d	2	NAG	C4-C5-C6-O6
4	z	2	NAG	C4-C5-C6-O6
4	d	2	NAG	O5-C5-C6-O6
4	z	2	NAG	O5-C5-C6-O6
4	EA	1	NAG	O5-C5-C6-O6
4	s	1	NAG	O5-C5-C6-O6
4	s	1	NAG	C4-C5-C6-O6
4	EA	1	NAG	C4-C5-C6-O6
4	e	1	NAG	C4-C5-C6-O6
4	0	1	NAG	C4-C5-C6-O6
4	e	1	NAG	O5-C5-C6-O6
4	0	1	NAG	O5-C5-C6-O6
4	s	2	NAG	O5-C5-C6-O6
4	EA	2	NAG	O5-C5-C6-O6
4	Z	1	NAG	C3-C2-N2-C7
4	v	1	NAG	C3-C2-N2-C7
4	K	2	NAG	C4-C5-C6-O6
4	R	2	NAG	C4-C5-C6-O6
4	K	2	NAG	O5-C5-C6-O6
4	R	2	NAG	O5-C5-C6-O6
4	j	2	NAG	O5-C5-C6-O6
4	5	2	NAG	O5-C5-C6-O6
4	o	1	NAG	C1-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
4	AA	1	NAG	C1-C2-N2-C7
4	8	1	NAG	O5-C5-C6-O6
4	m	1	NAG	O5-C5-C6-O6
4	u	1	NAG	O5-C5-C6-O6
4	Y	1	NAG	O5-C5-C6-O6
4	j	1	NAG	C4-C5-C6-O6
4	5	1	NAG	C4-C5-C6-O6
4	a	2	NAG	C4-C5-C6-O6
4	w	2	NAG	C4-C5-C6-O6
4	a	2	NAG	O5-C5-C6-O6
4	t	2	NAG	C4-C5-C6-O6
4	FA	2	NAG	C4-C5-C6-O6
4	w	2	NAG	O5-C5-C6-O6
4	r	1	NAG	C4-C5-C6-O6
4	DA	1	NAG	C4-C5-C6-O6
4	d	2	NAG	C3-C2-N2-C7
4	i	1	NAG	C3-C2-N2-C7
4	k	2	NAG	C3-C2-N2-C7
4	q	2	NAG	C3-C2-N2-C7
4	s	2	NAG	C3-C2-N2-C7
4	z	2	NAG	C3-C2-N2-C7
4	4	1	NAG	C3-C2-N2-C7
4	6	2	NAG	C3-C2-N2-C7
4	CA	2	NAG	C3-C2-N2-C7
4	t	2	NAG	O5-C5-C6-O6
4	FA	2	NAG	O5-C5-C6-O6
4	h	2	NAG	C4-C5-C6-O6
4	3	2	NAG	C4-C5-C6-O6
4	y	2	NAG	C4-C5-C6-O6
4	c	2	NAG	C4-C5-C6-O6
4	DA	1	NAG	O5-C5-C6-O6
4	r	1	NAG	O5-C5-C6-O6
4	b	2	NAG	C1-C2-N2-C7
4	c	2	NAG	C1-C2-N2-C7
4	d	2	NAG	C1-C2-N2-C7
4	q	2	NAG	C1-C2-N2-C7
4	r	2	NAG	C1-C2-N2-C7
4	s	2	NAG	C1-C2-N2-C7
4	x	2	NAG	C1-C2-N2-C7
4	y	2	NAG	C1-C2-N2-C7
4	z	2	NAG	C1-C2-N2-C7
4	CA	2	NAG	C1-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
4	DA	2	NAG	C1-C2-N2-C7
4	EA	2	NAG	C1-C2-N2-C7
4	c	2	NAG	O5-C5-C6-O6
4	y	2	NAG	O5-C5-C6-O6
4	2	2	NAG	C4-C5-C6-O6
4	b	2	NAG	C3-C2-N2-C7
4	c	2	NAG	C3-C2-N2-C7
4	g	2	NAG	C3-C2-N2-C7
4	n	2	NAG	C3-C2-N2-C7
4	o	1	NAG	C3-C2-N2-C7
4	r	2	NAG	C3-C2-N2-C7
4	x	2	NAG	C3-C2-N2-C7
4	y	2	NAG	C3-C2-N2-C7
4	2	2	NAG	C3-C2-N2-C7
4	9	2	NAG	C3-C2-N2-C7
4	AA	1	NAG	C3-C2-N2-C7
4	DA	2	NAG	C3-C2-N2-C7
4	EA	2	NAG	C3-C2-N2-C7
4	9	2	NAG	C4-C5-C6-O6
4	n	2	NAG	C4-C5-C6-O6
4	g	2	NAG	C4-C5-C6-O6
4	j	1	NAG	O5-C5-C6-O6
4	5	1	NAG	O5-C5-C6-O6
4	2	2	NAG	O5-C5-C6-O6
4	g	2	NAG	O5-C5-C6-O6
4	9	2	NAG	O5-C5-C6-O6
4	n	2	NAG	O5-C5-C6-O6

There are no ring outliers.

30 monomers are involved in 40 short contacts:

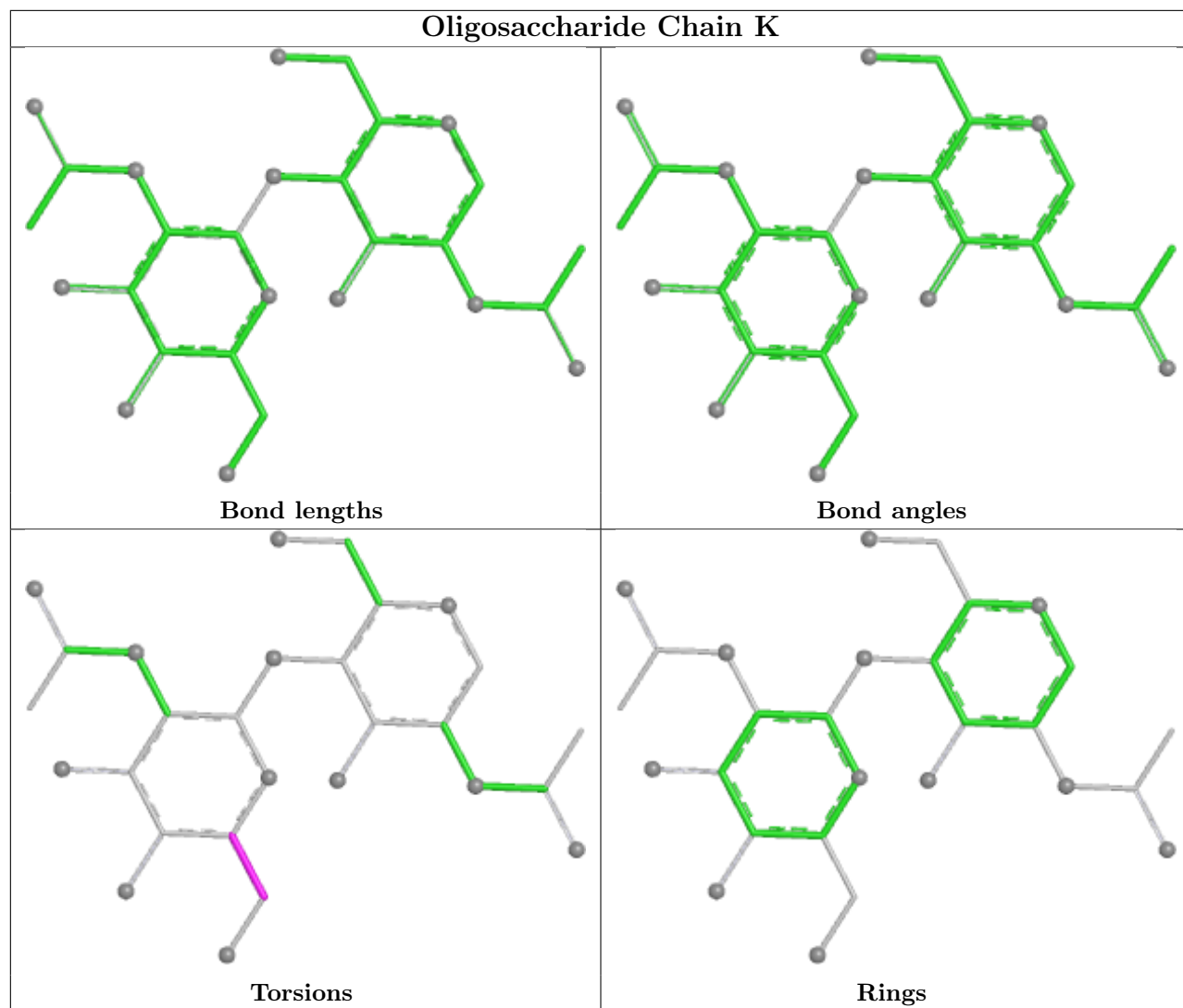
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	s	1	NAG	1	0
4	2	1	NAG	3	0
4	s	2	NAG	1	0
4	r	2	NAG	1	0
4	EA	1	NAG	1	0
4	9	1	NAG	3	0
4	b	2	NAG	1	0
4	k	2	NAG	1	0
4	N	2	NAG	5	0
4	EA	2	NAG	1	0

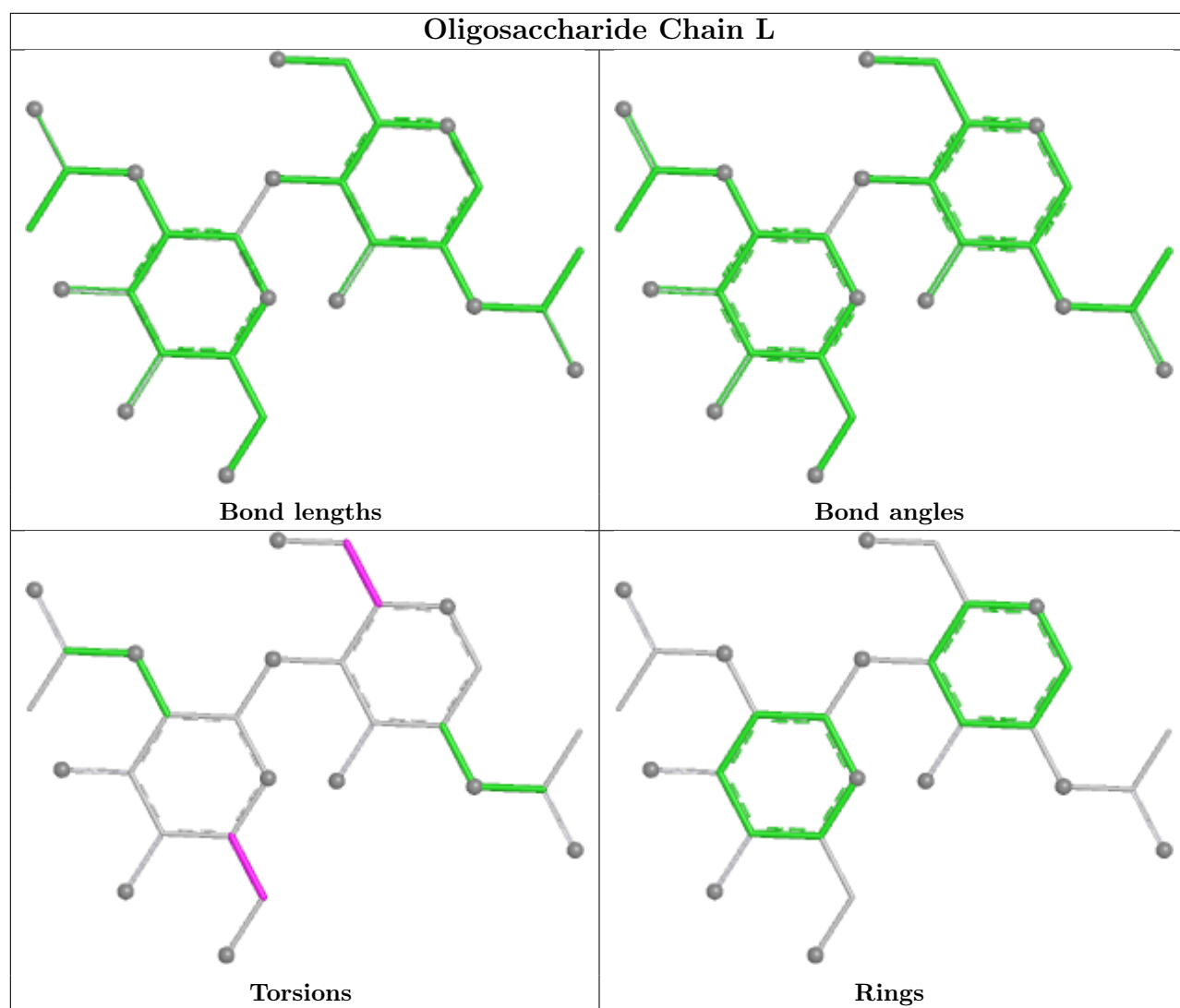
Continued on next page...

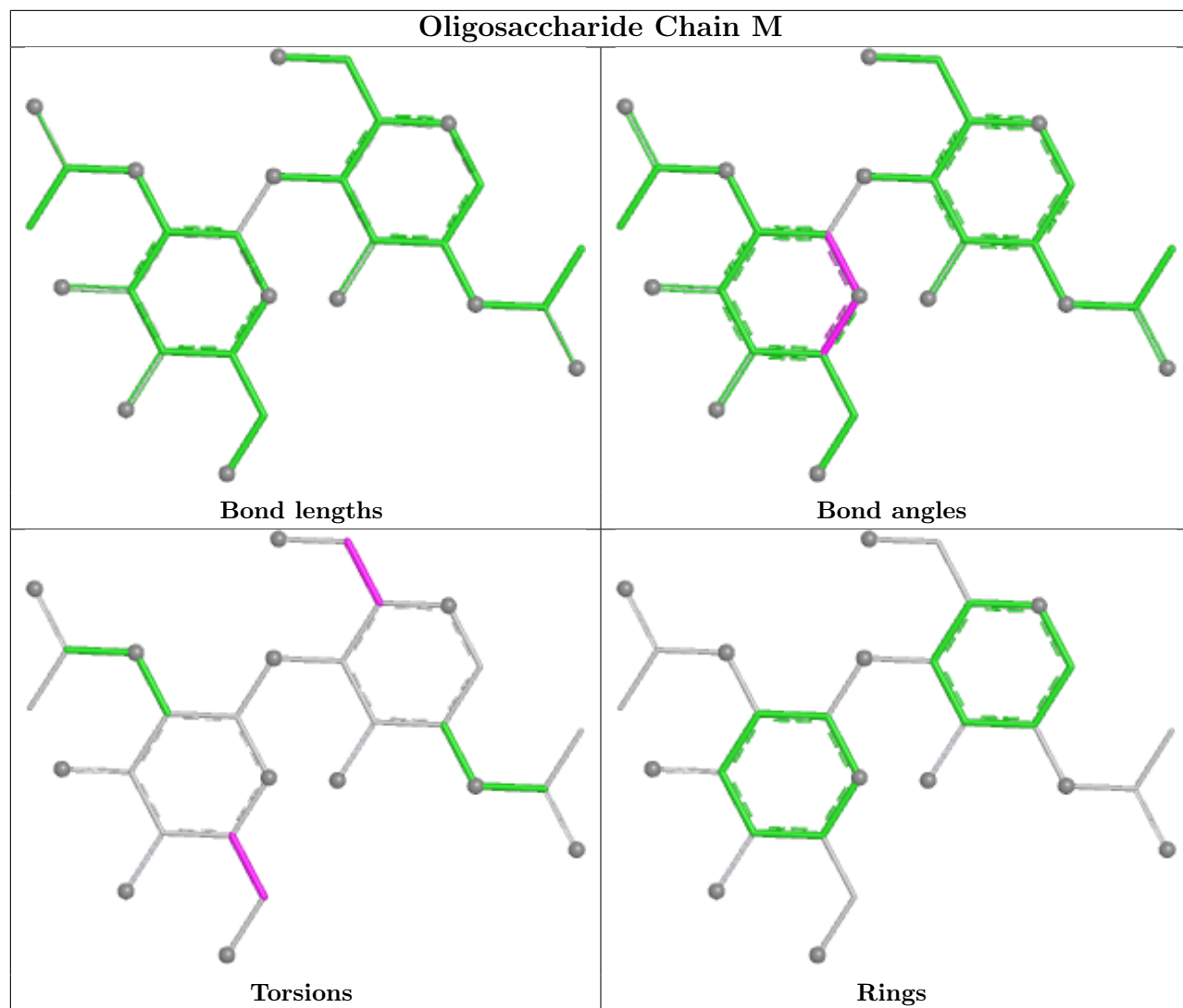
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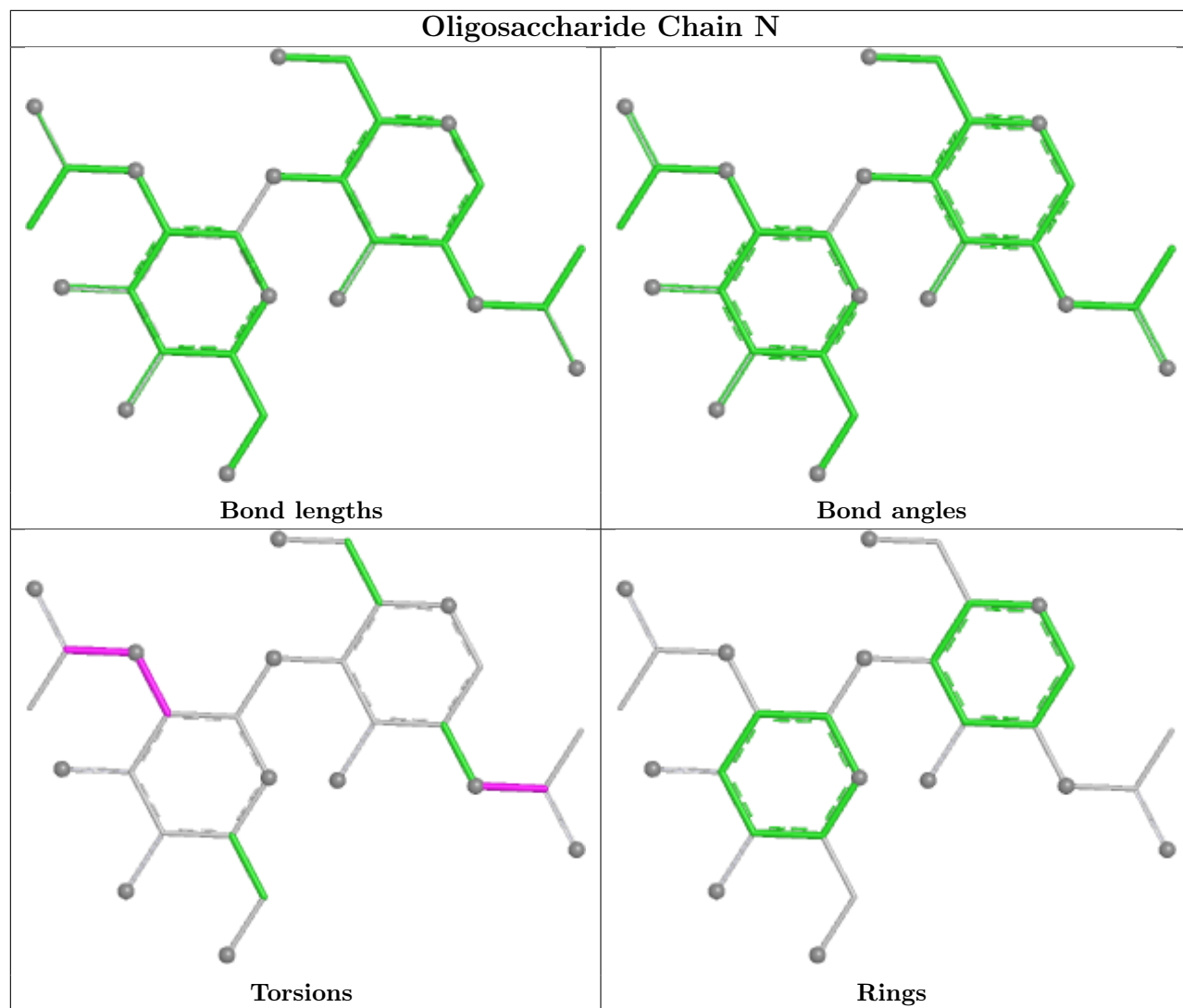
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	U	2	NAG	5	0
4	n	2	NAG	2	0
4	c	2	NAG	1	0
4	f	1	NAG	1	0
4	U	1	NAG	4	0
4	AA	1	NAG	1	0
4	DA	2	NAG	1	0
4	k	1	NAG	1	0
4	9	2	NAG	2	0
4	n	1	NAG	3	0
4	y	2	NAG	1	0
4	o	1	NAG	1	0
4	x	2	NAG	1	0
4	6	1	NAG	1	0
4	6	2	NAG	1	0
4	N	1	NAG	4	0
4	2	2	NAG	2	0
4	g	1	NAG	3	0
4	g	2	NAG	2	0
4	1	1	NAG	1	0

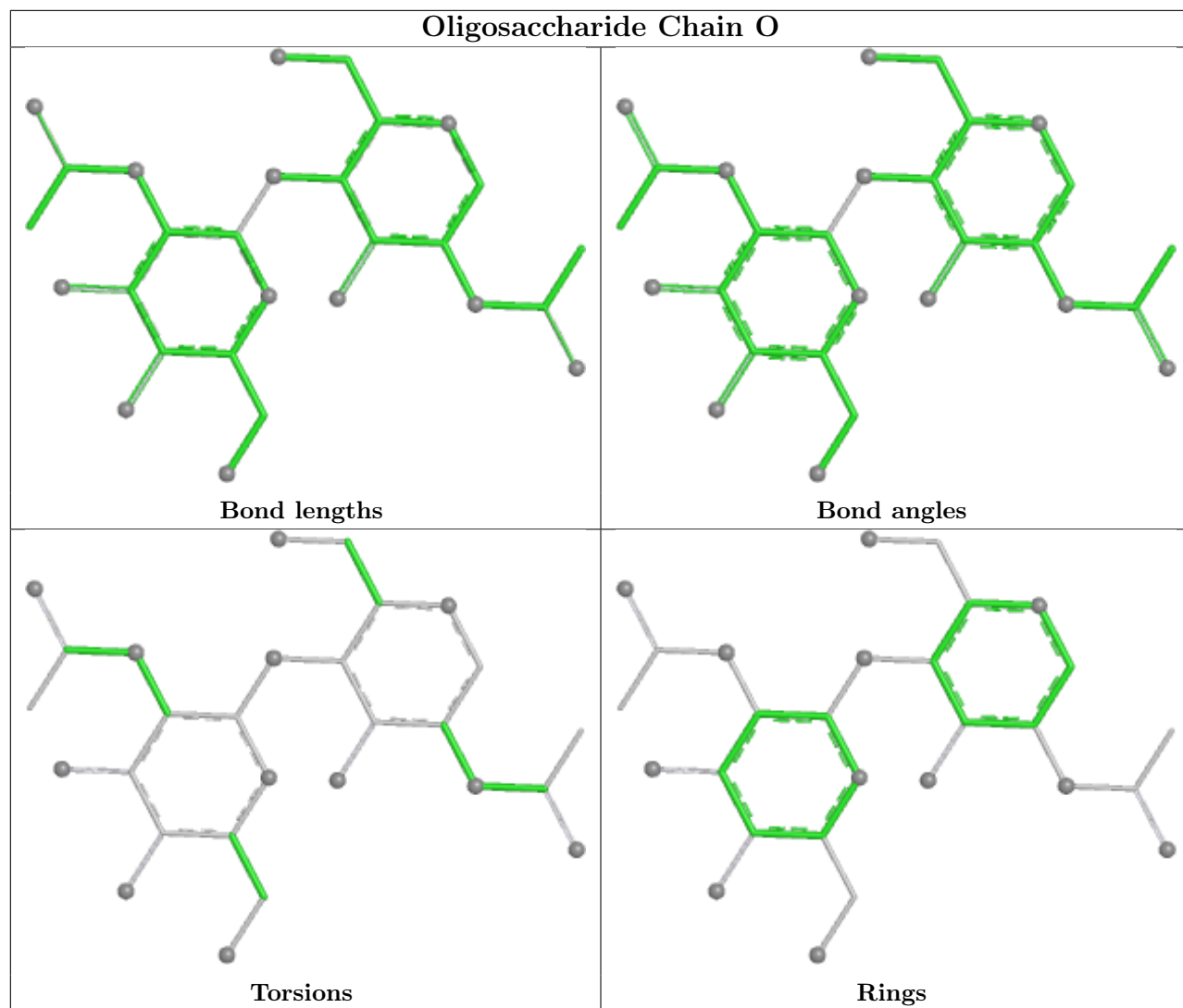
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

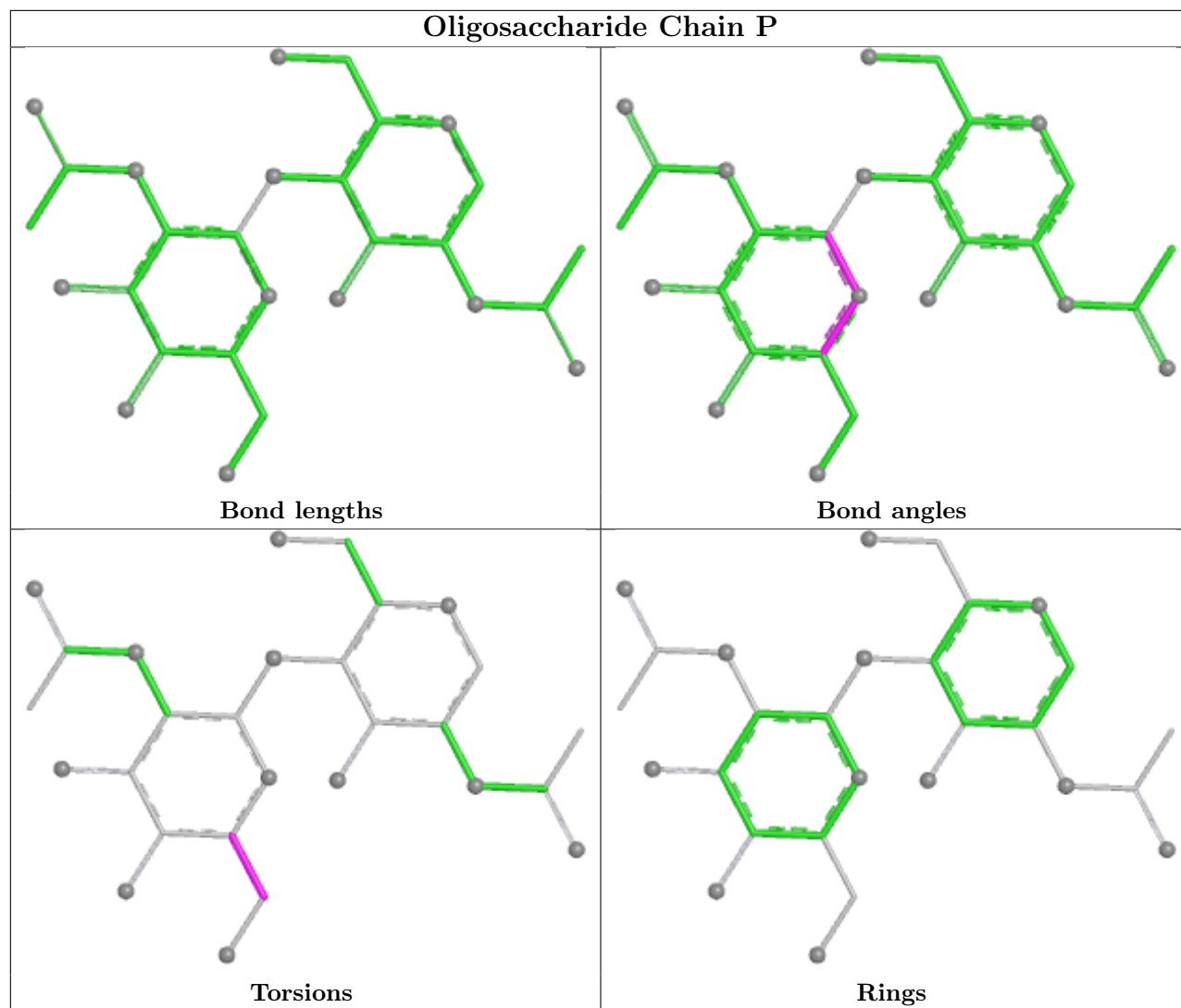


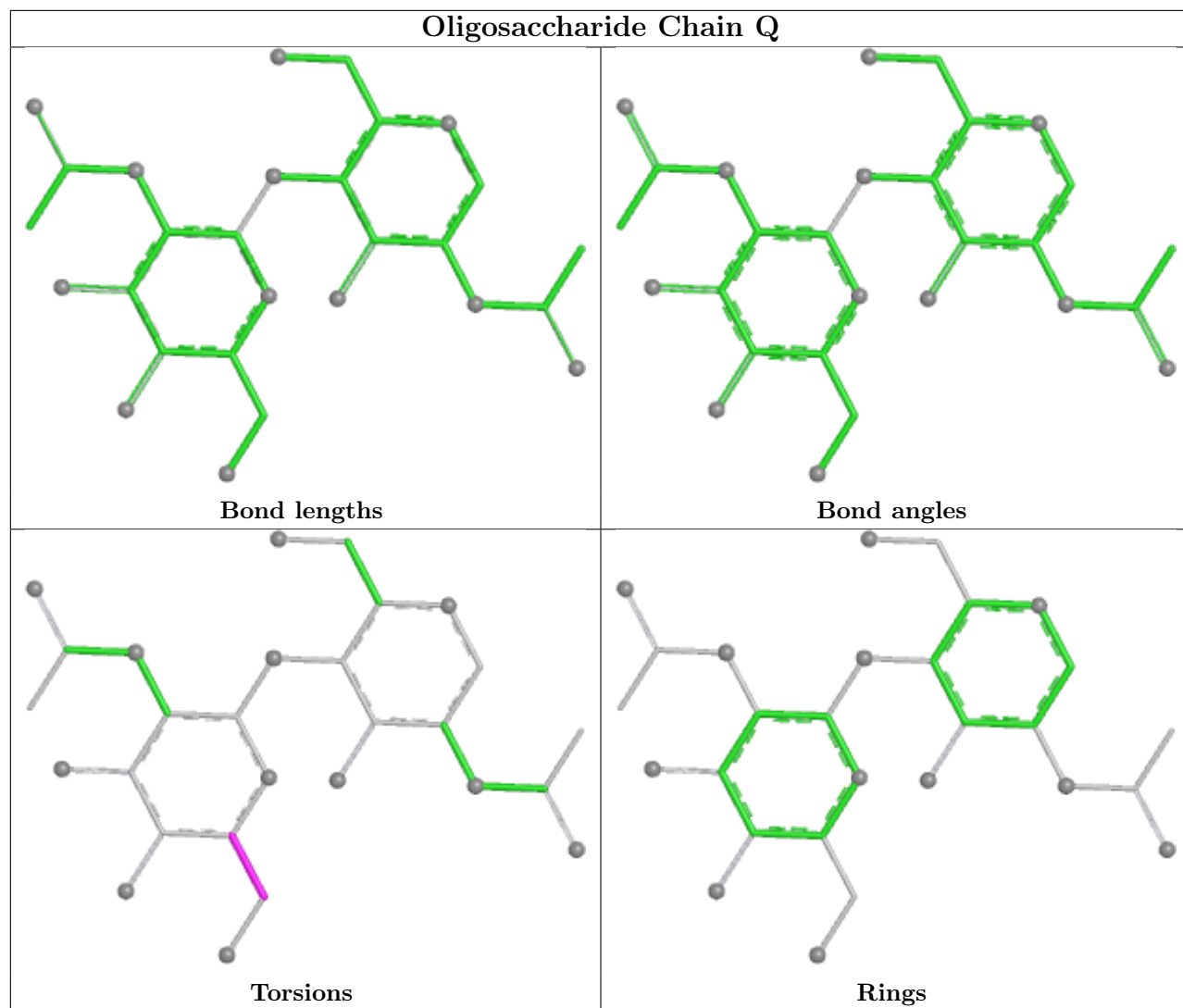


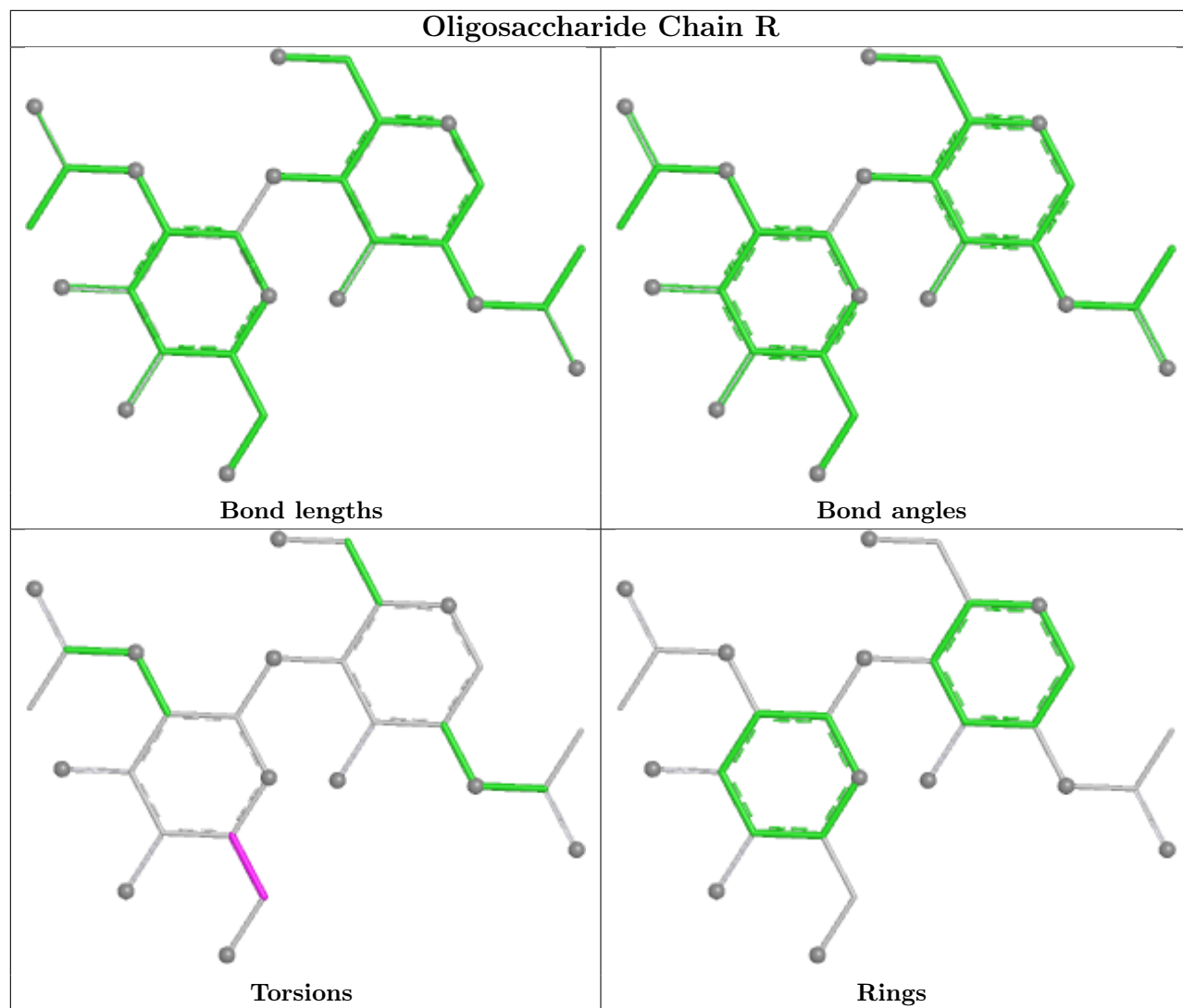


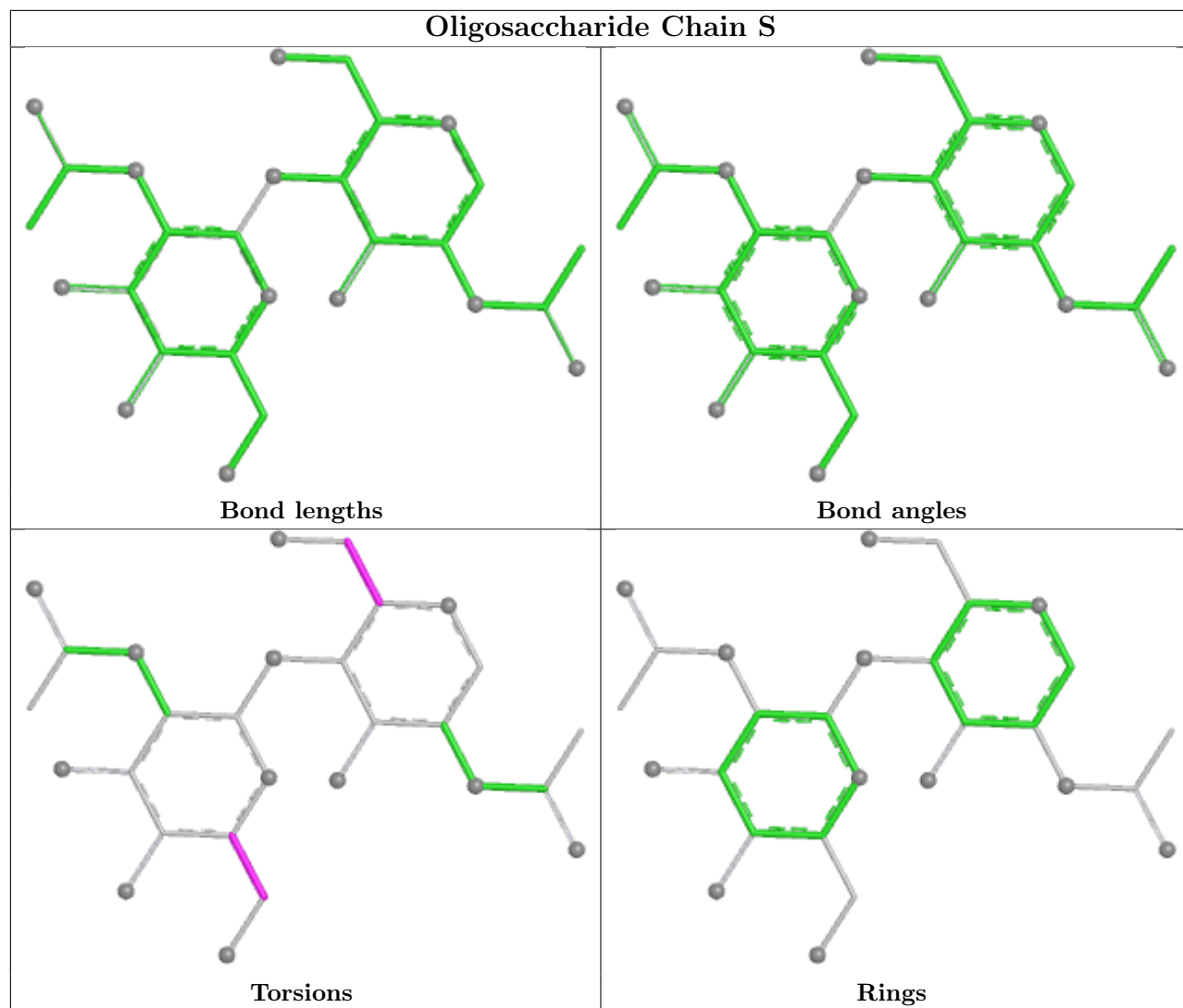


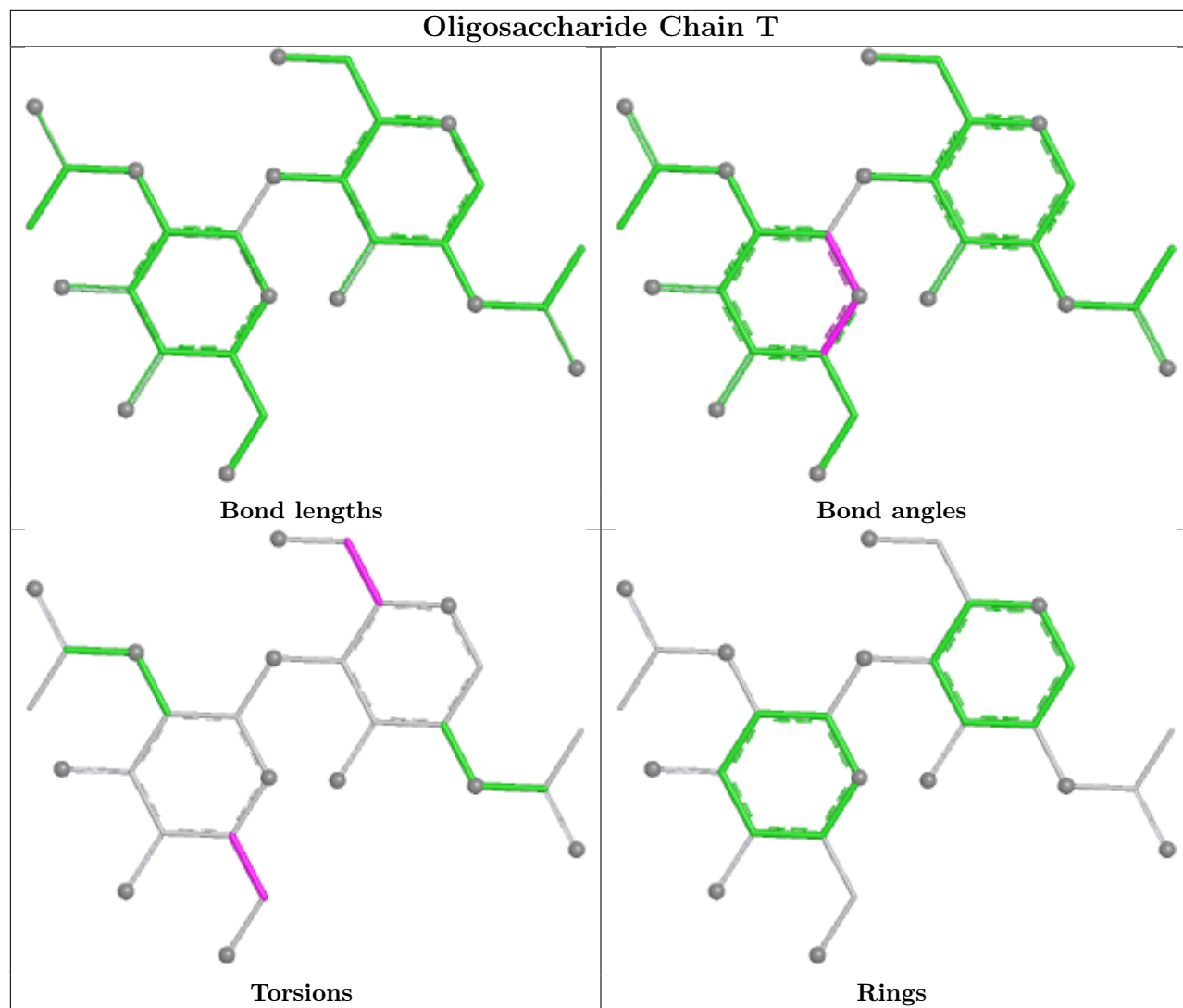


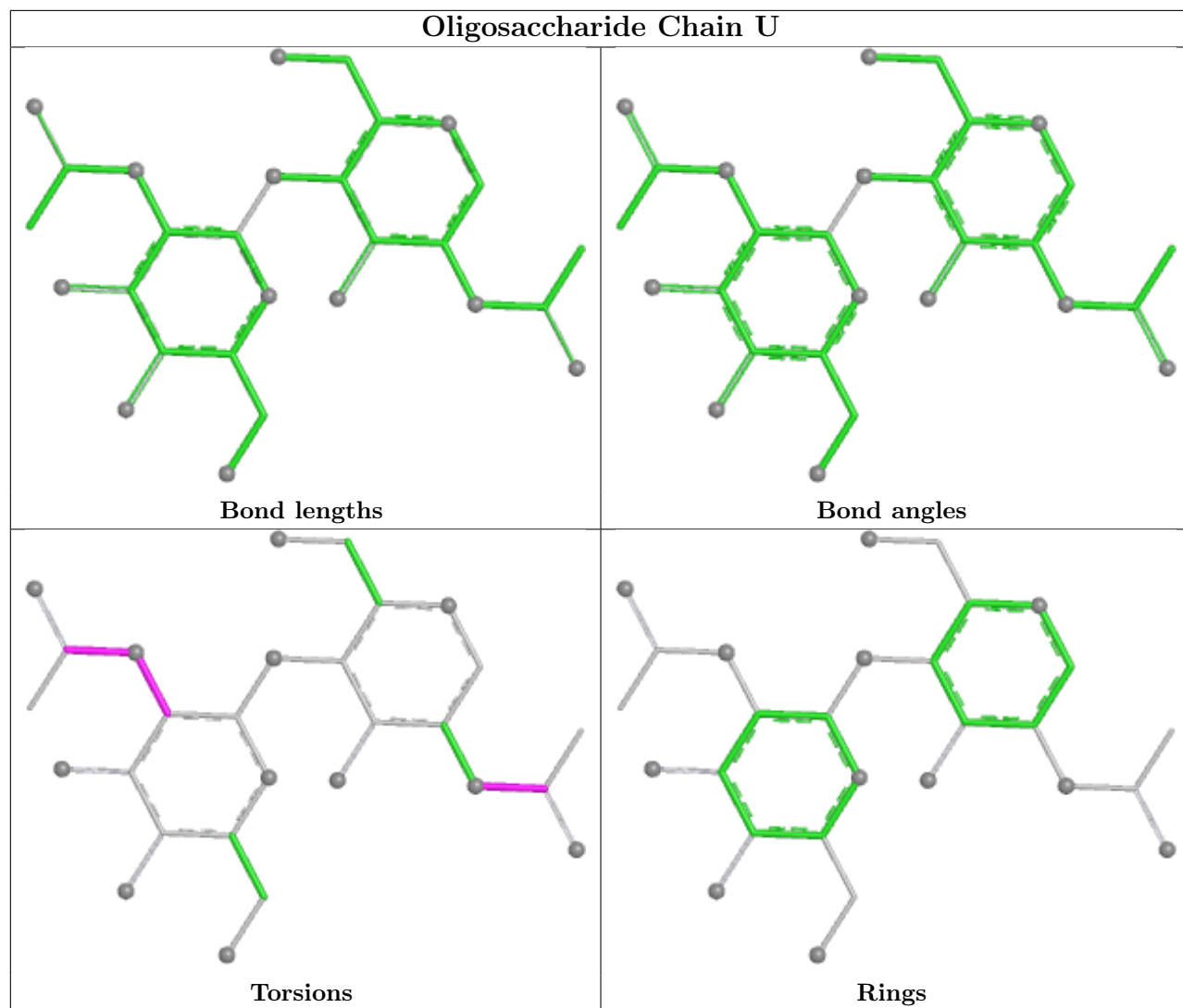


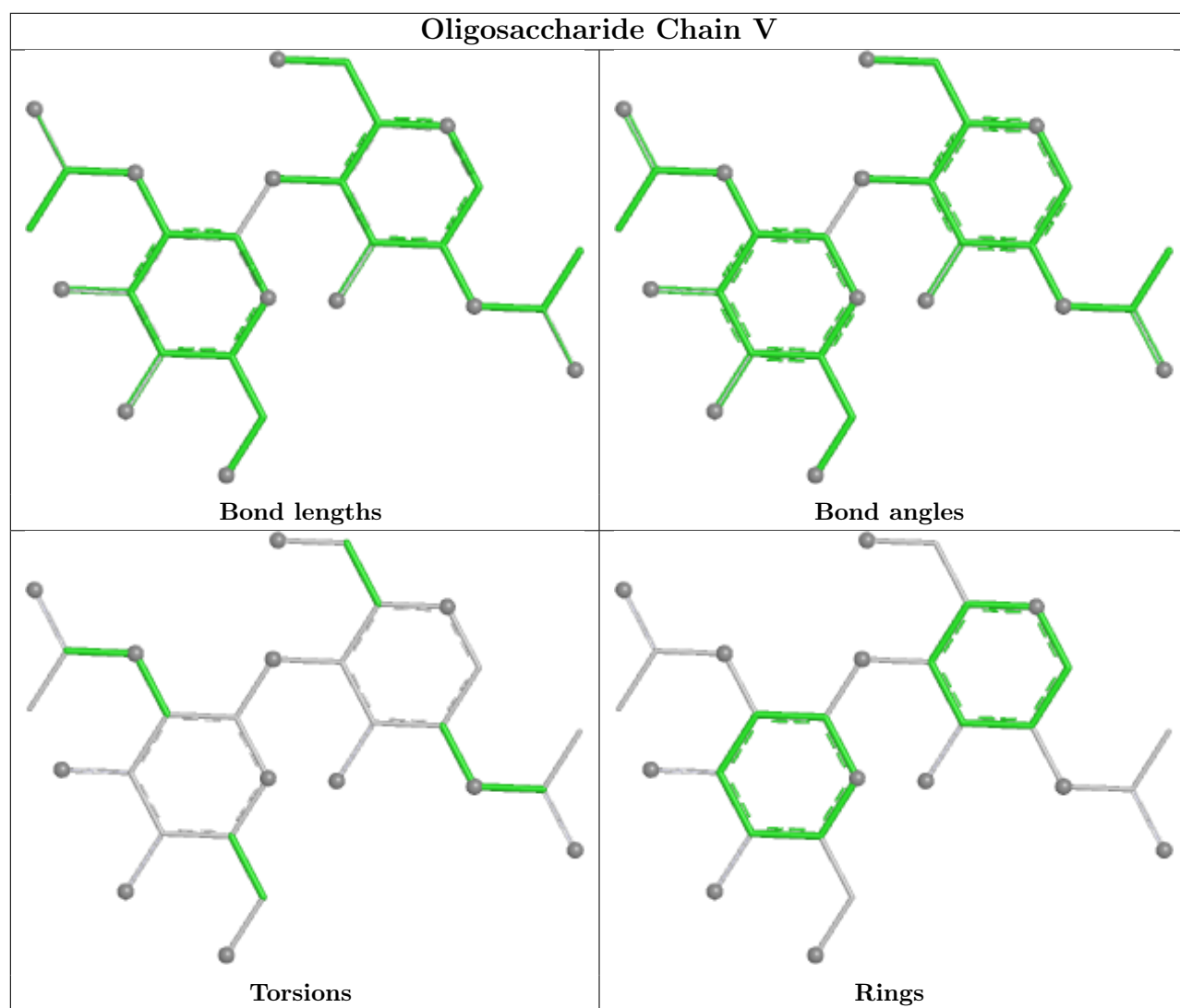


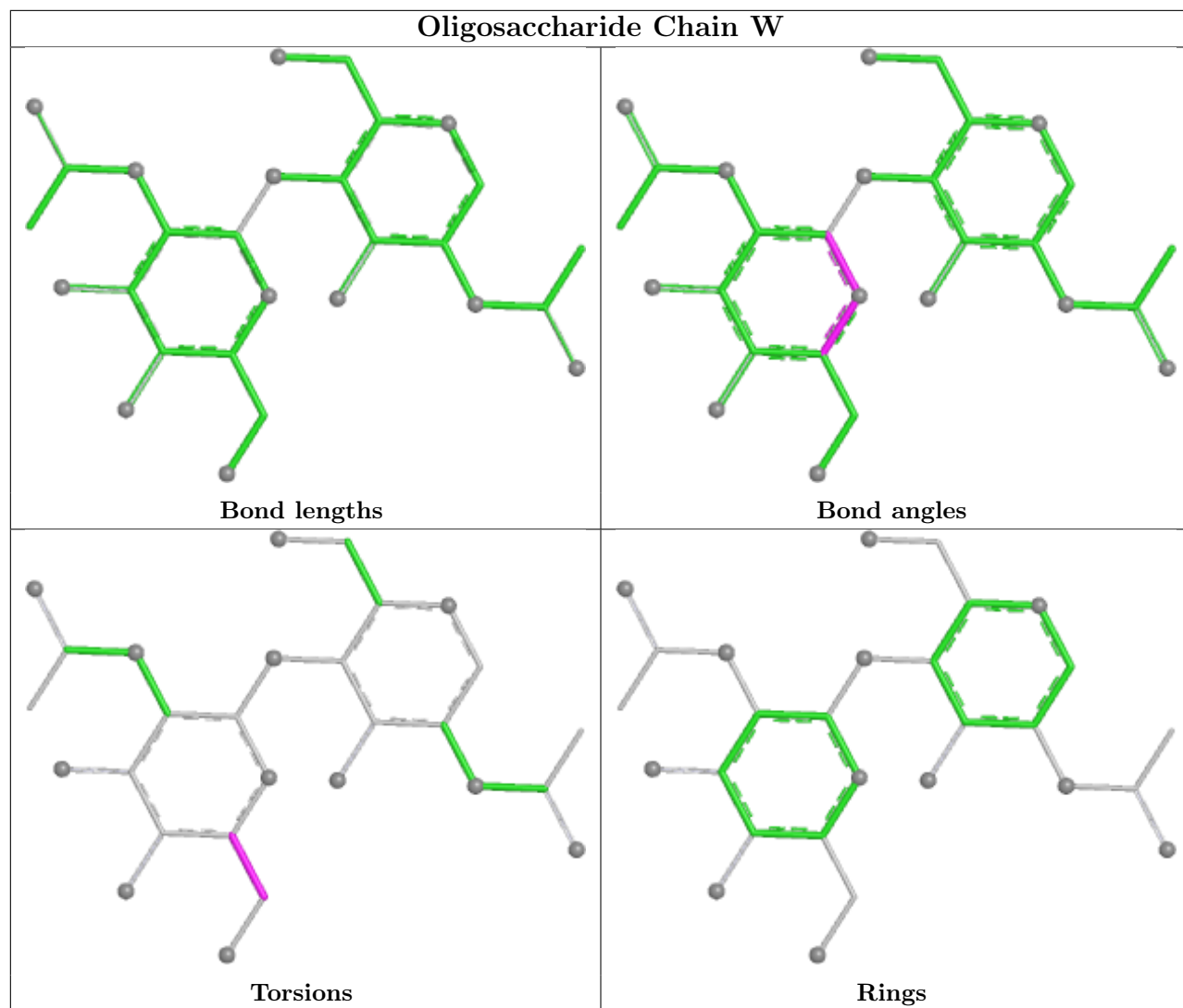


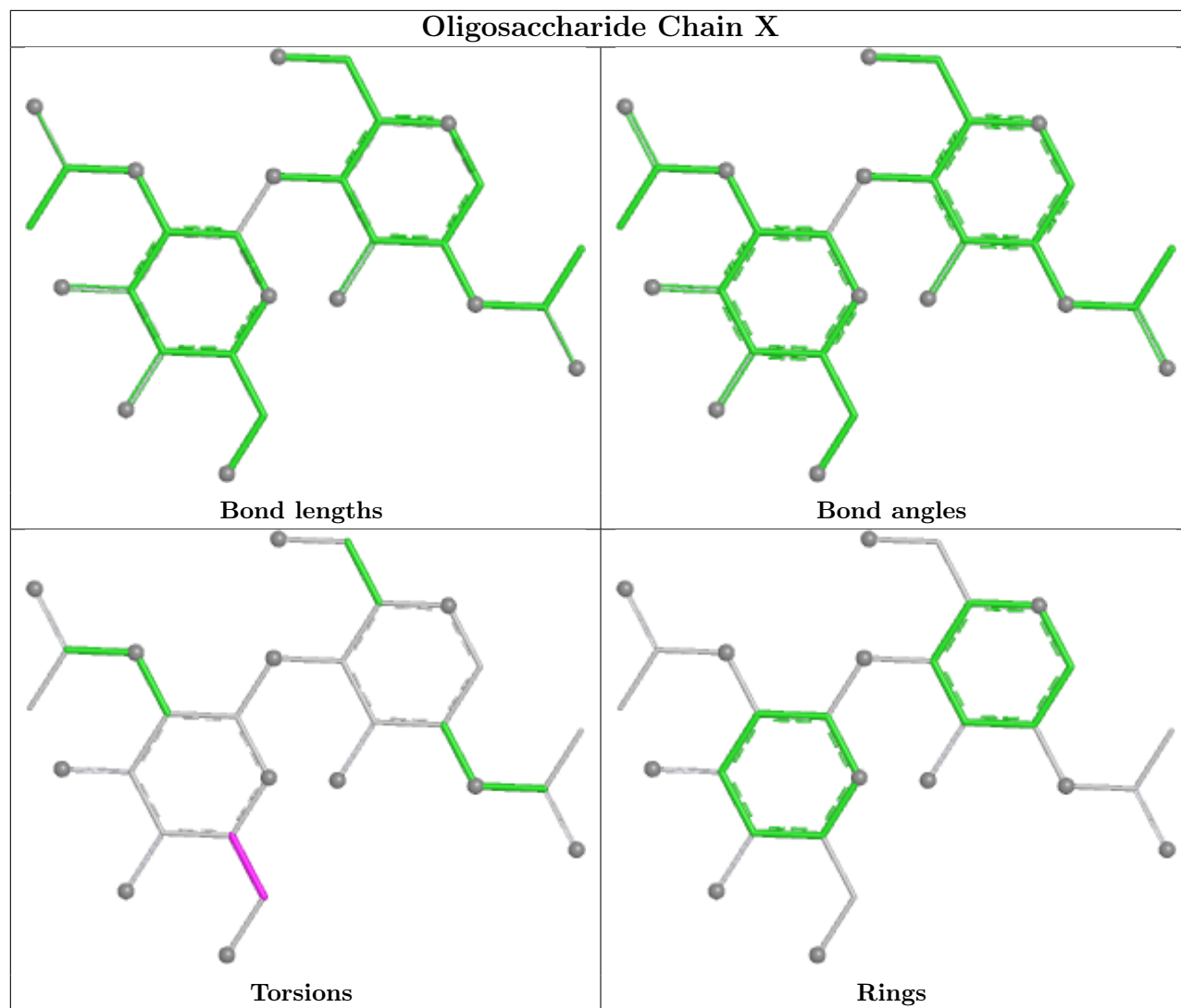


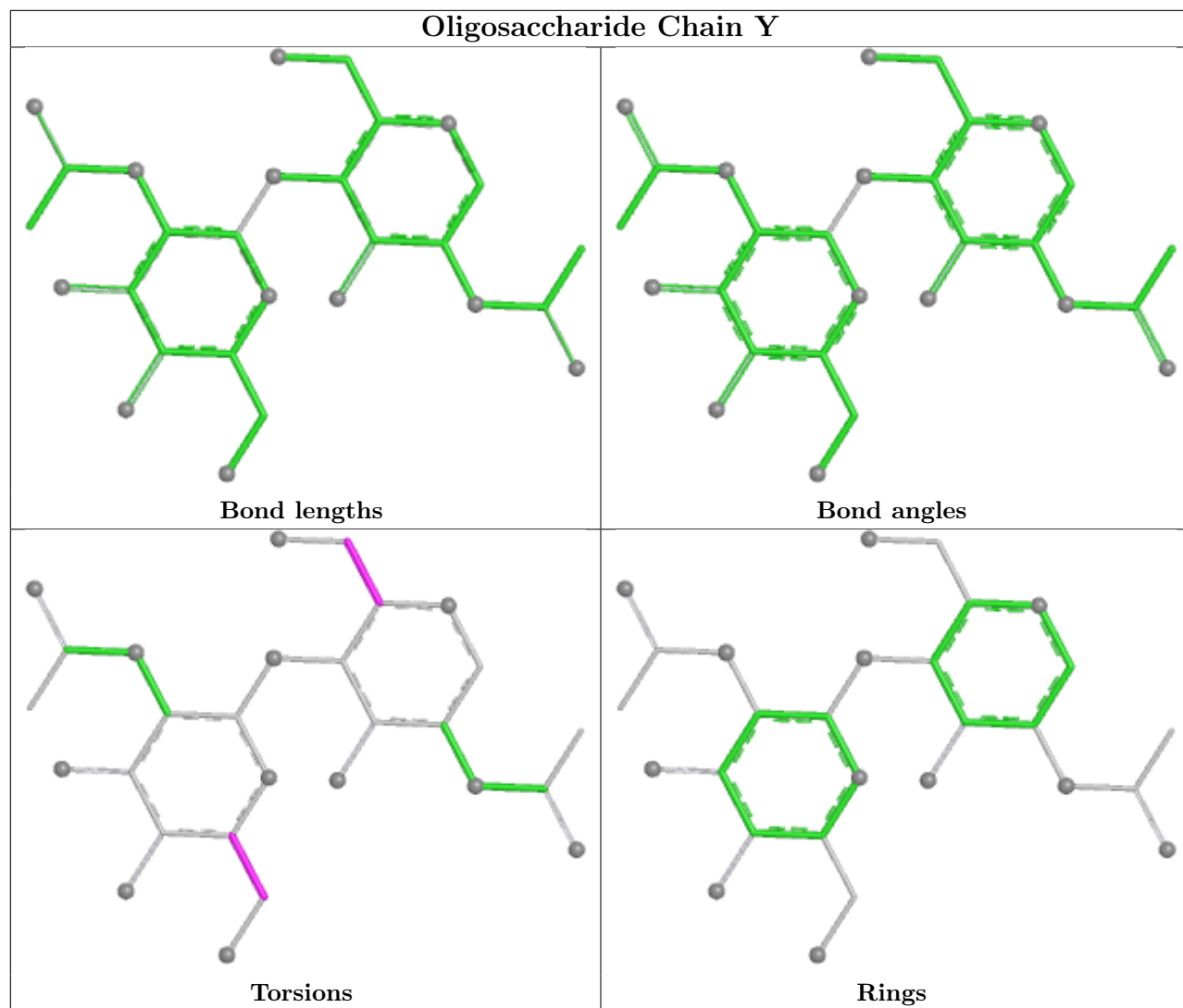


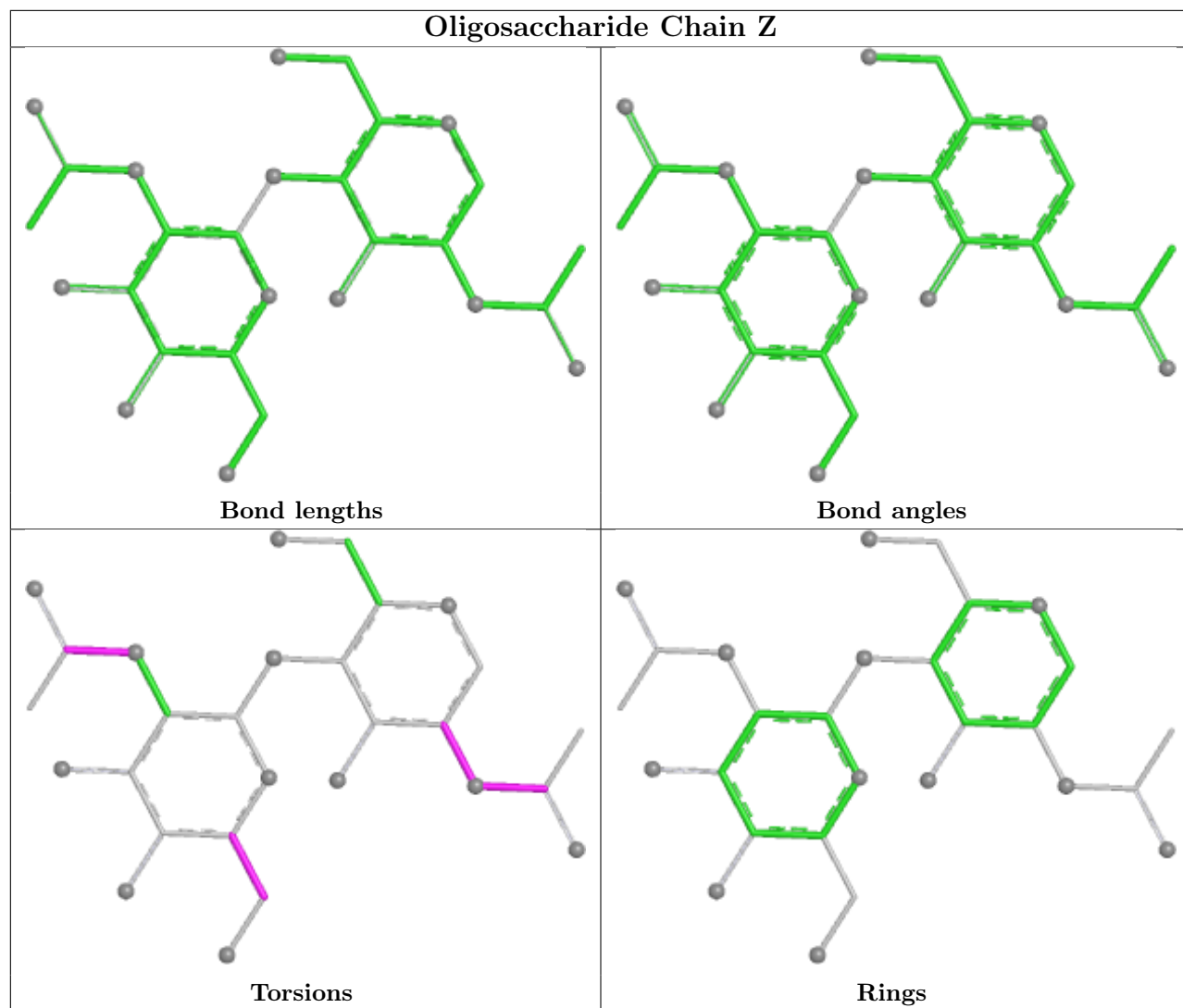


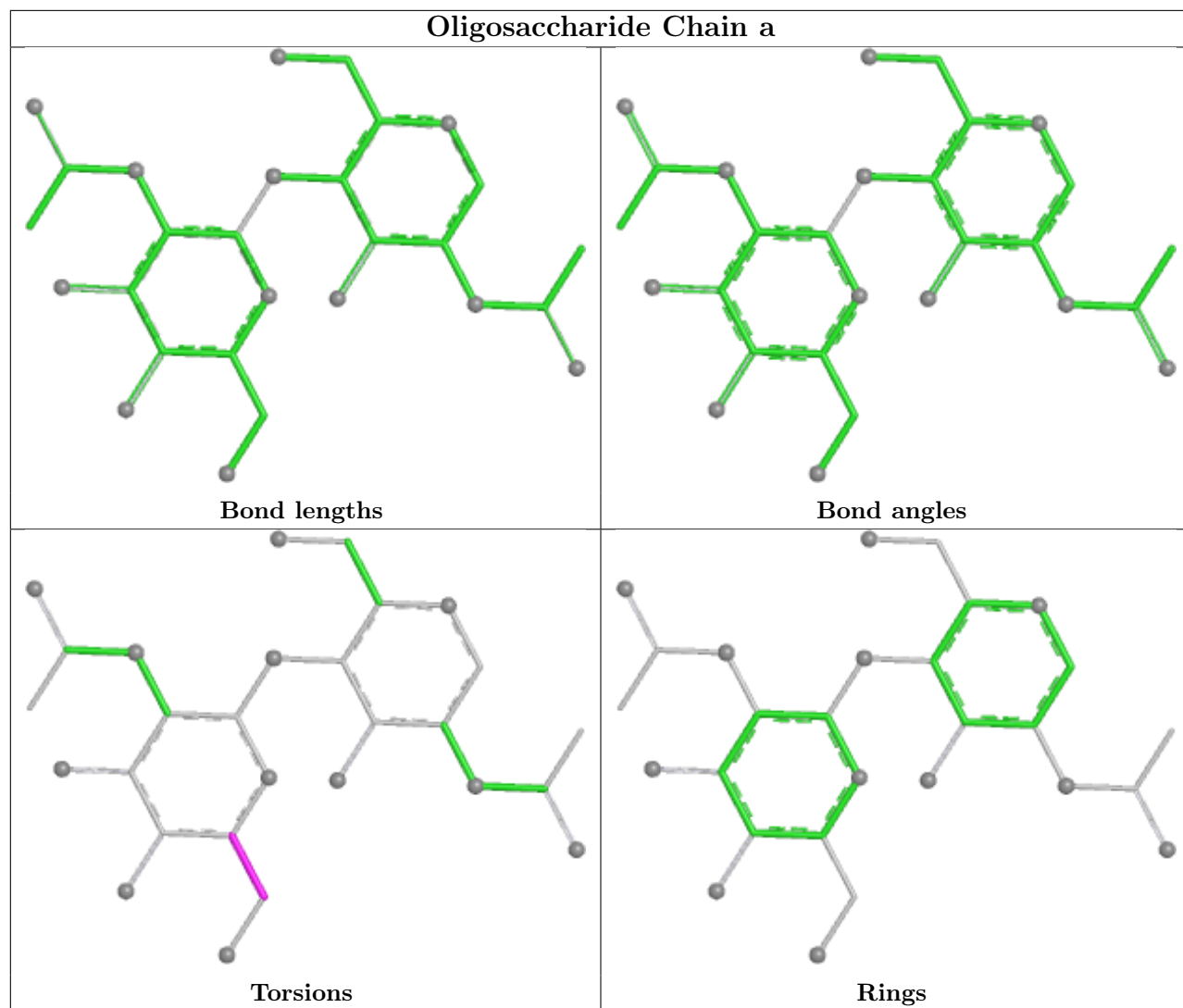


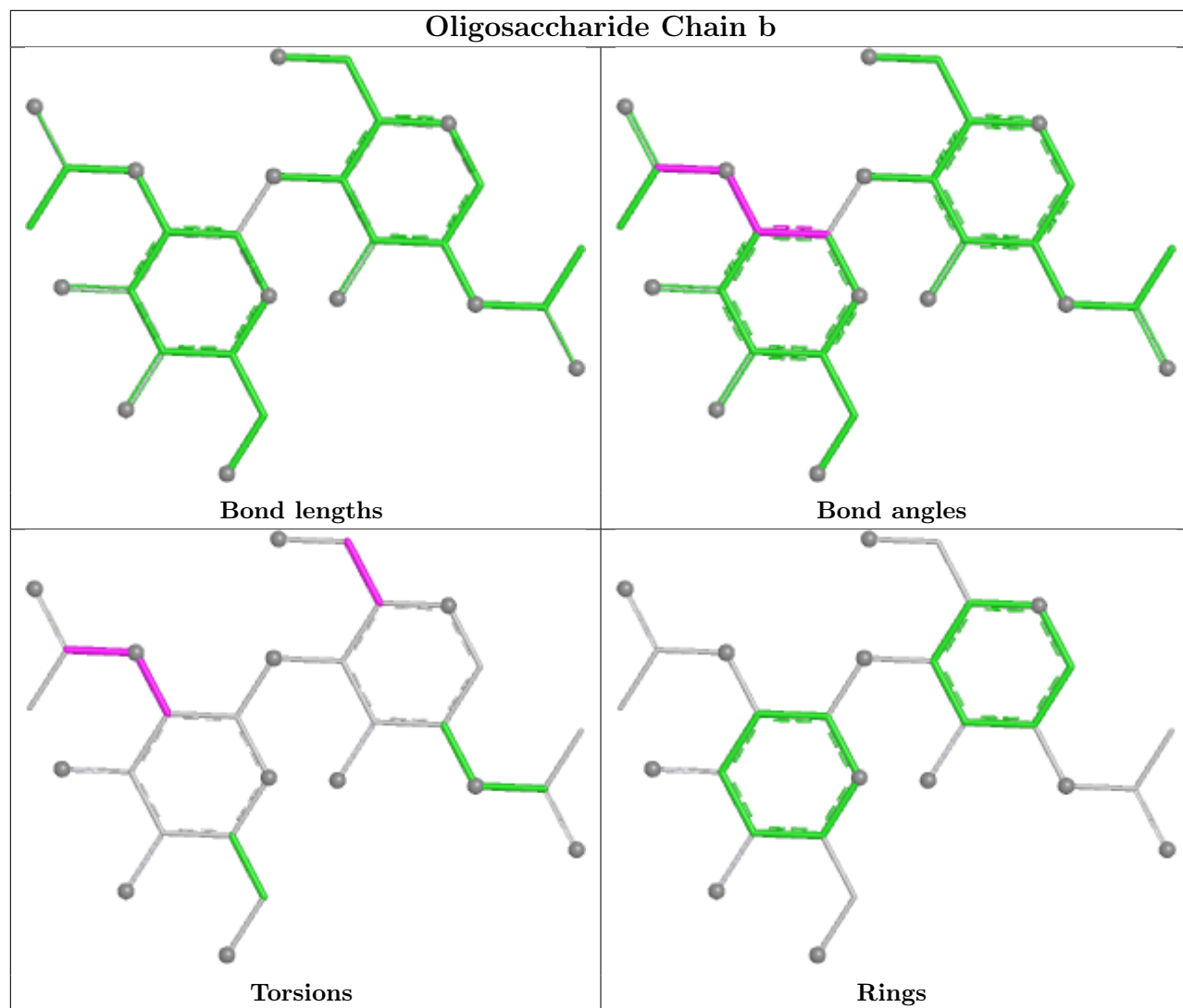


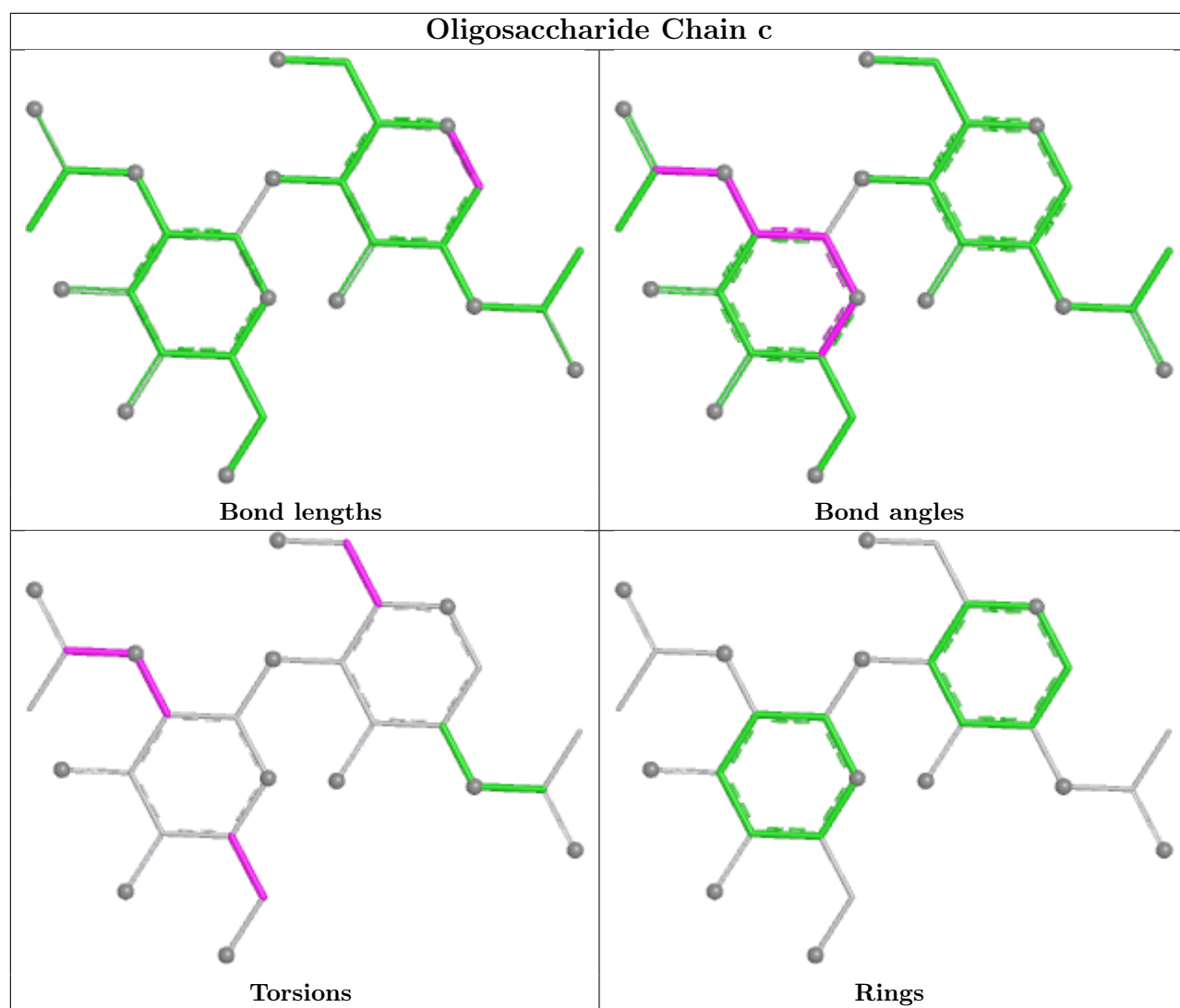


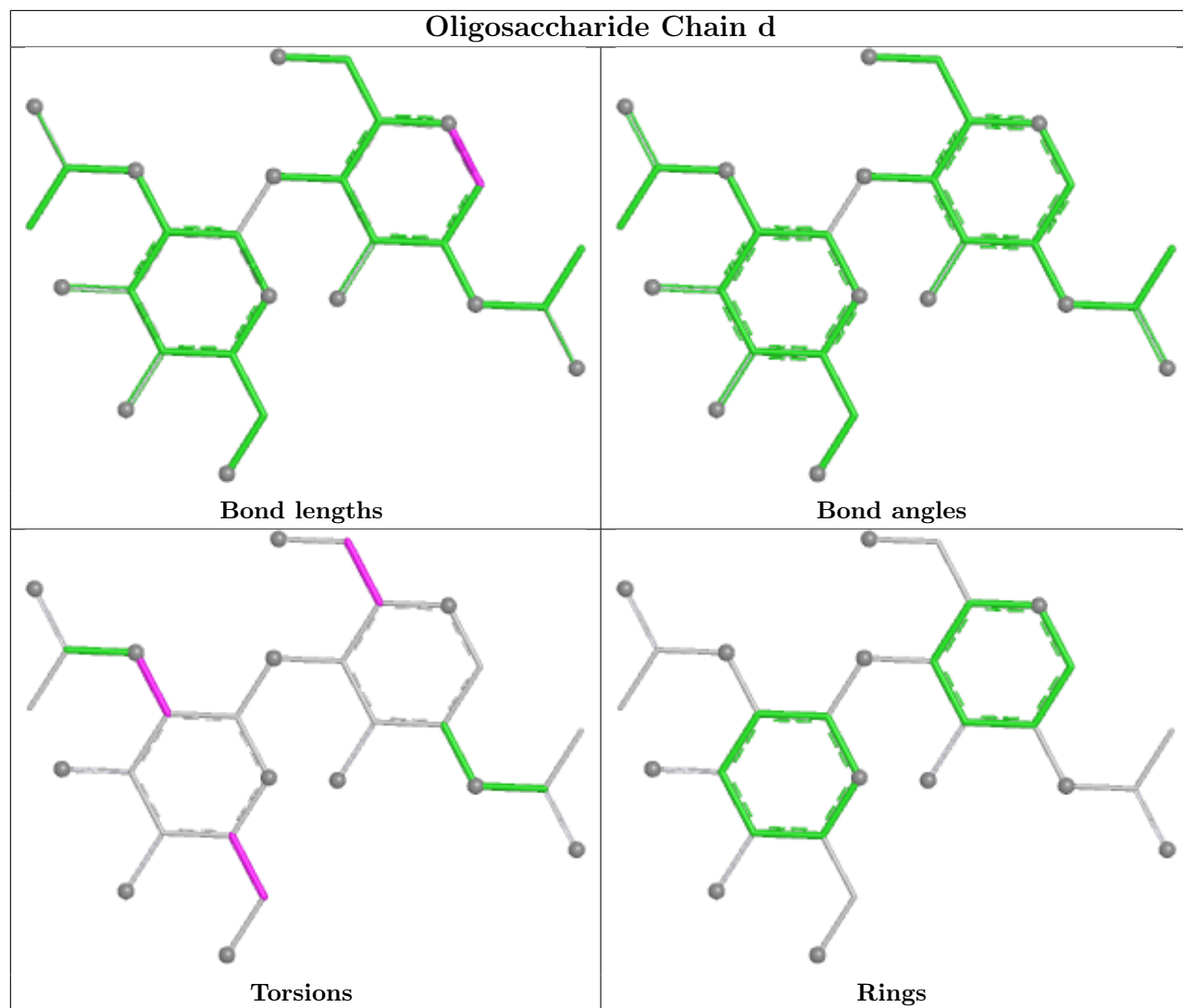


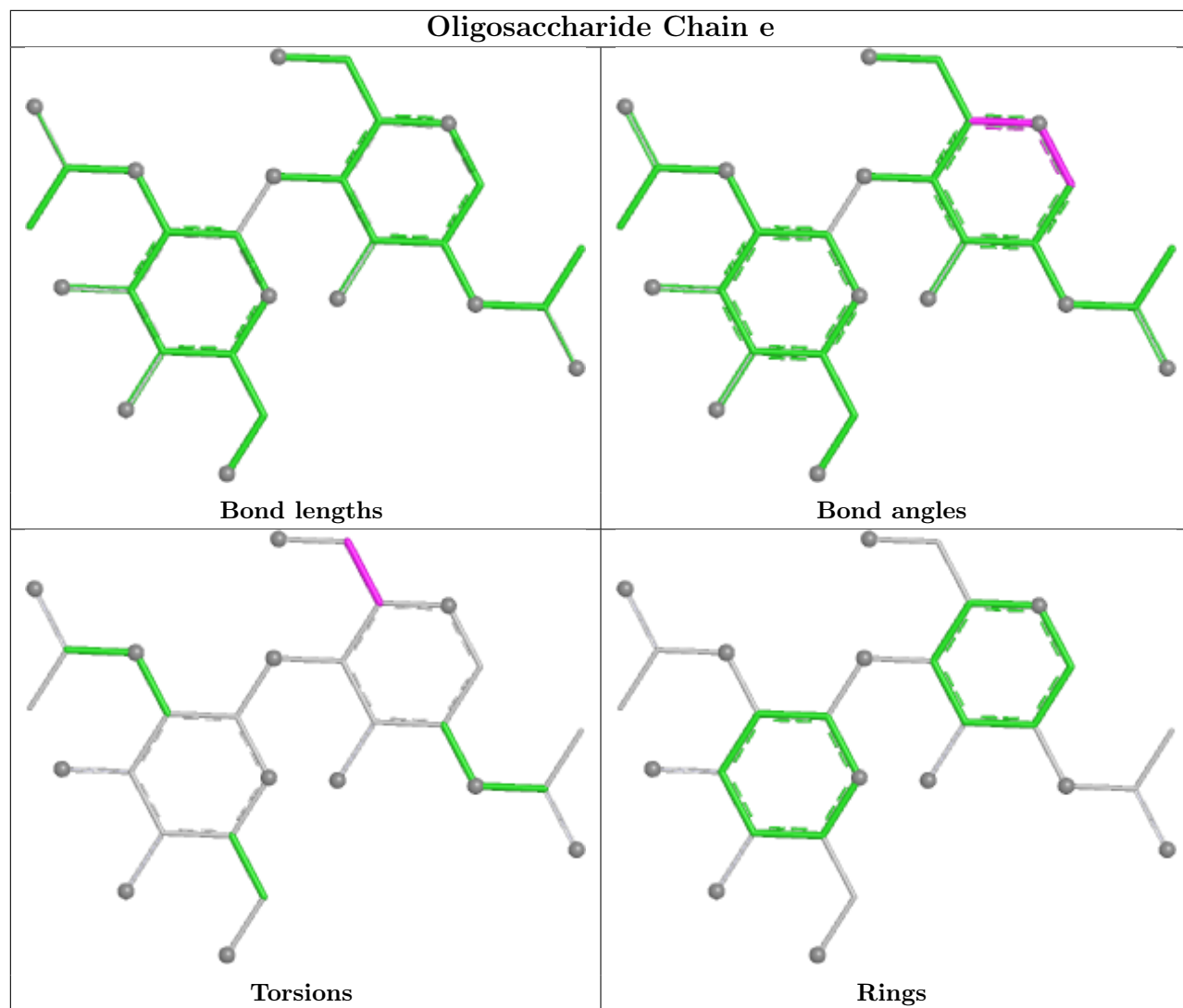


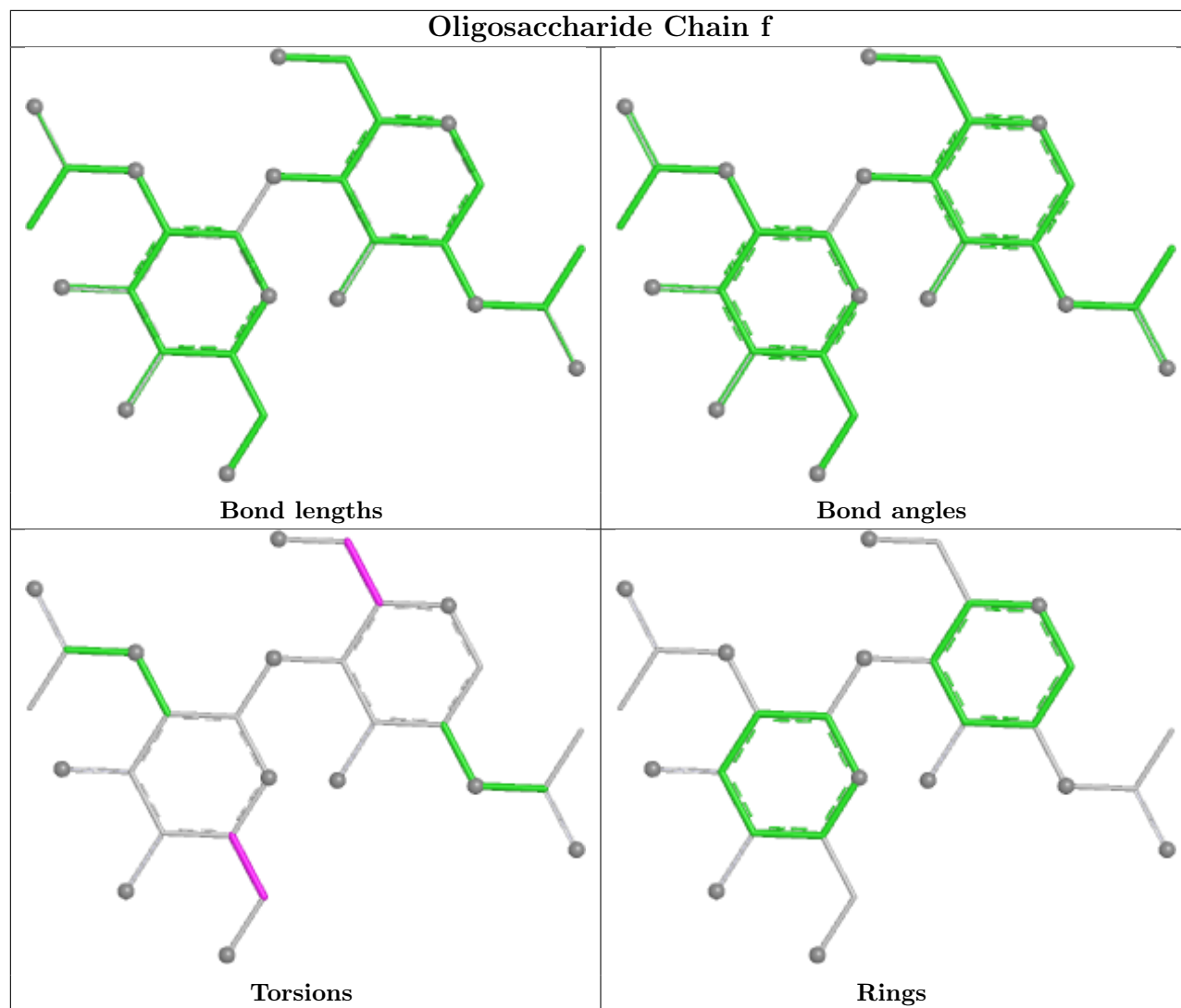


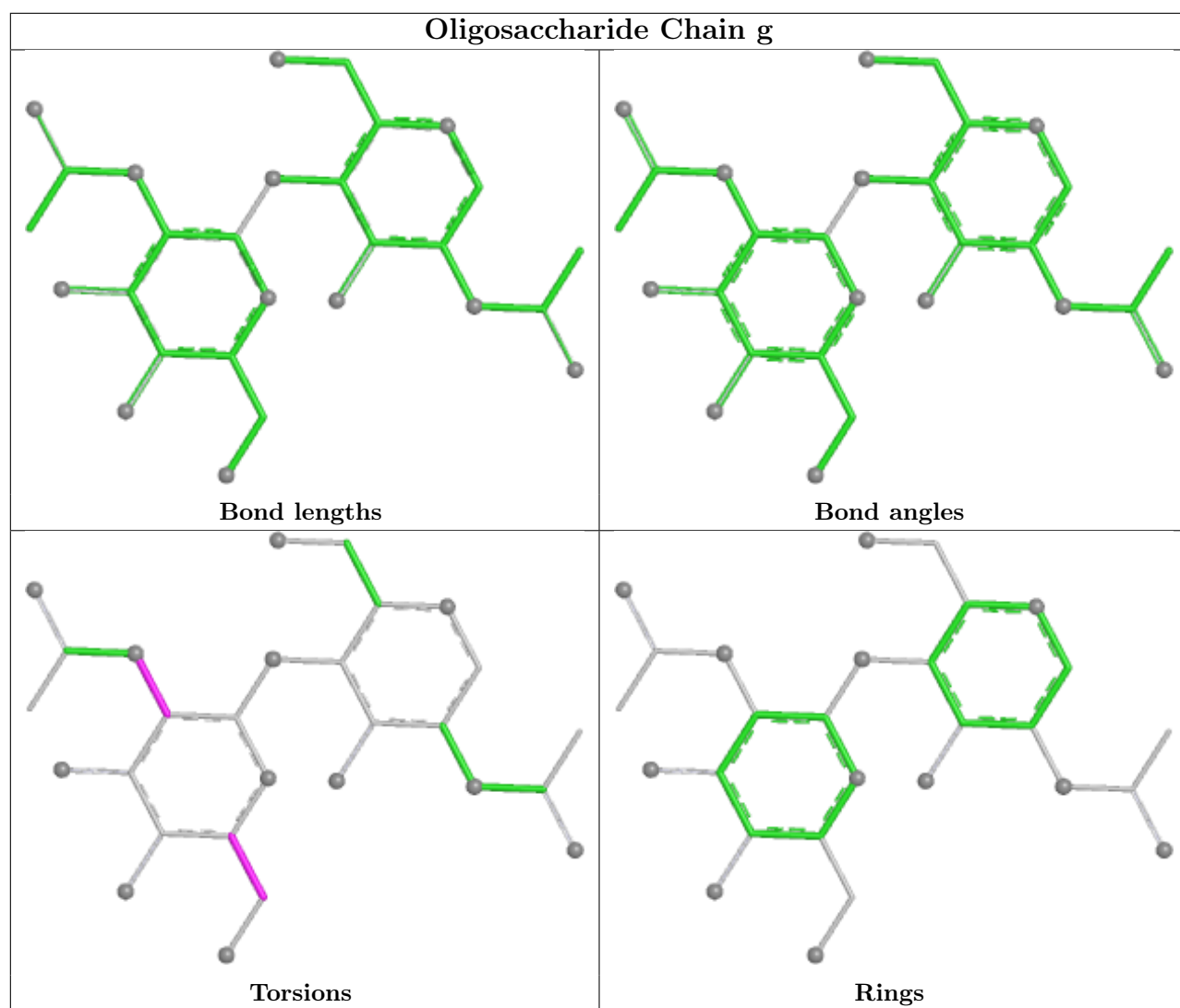


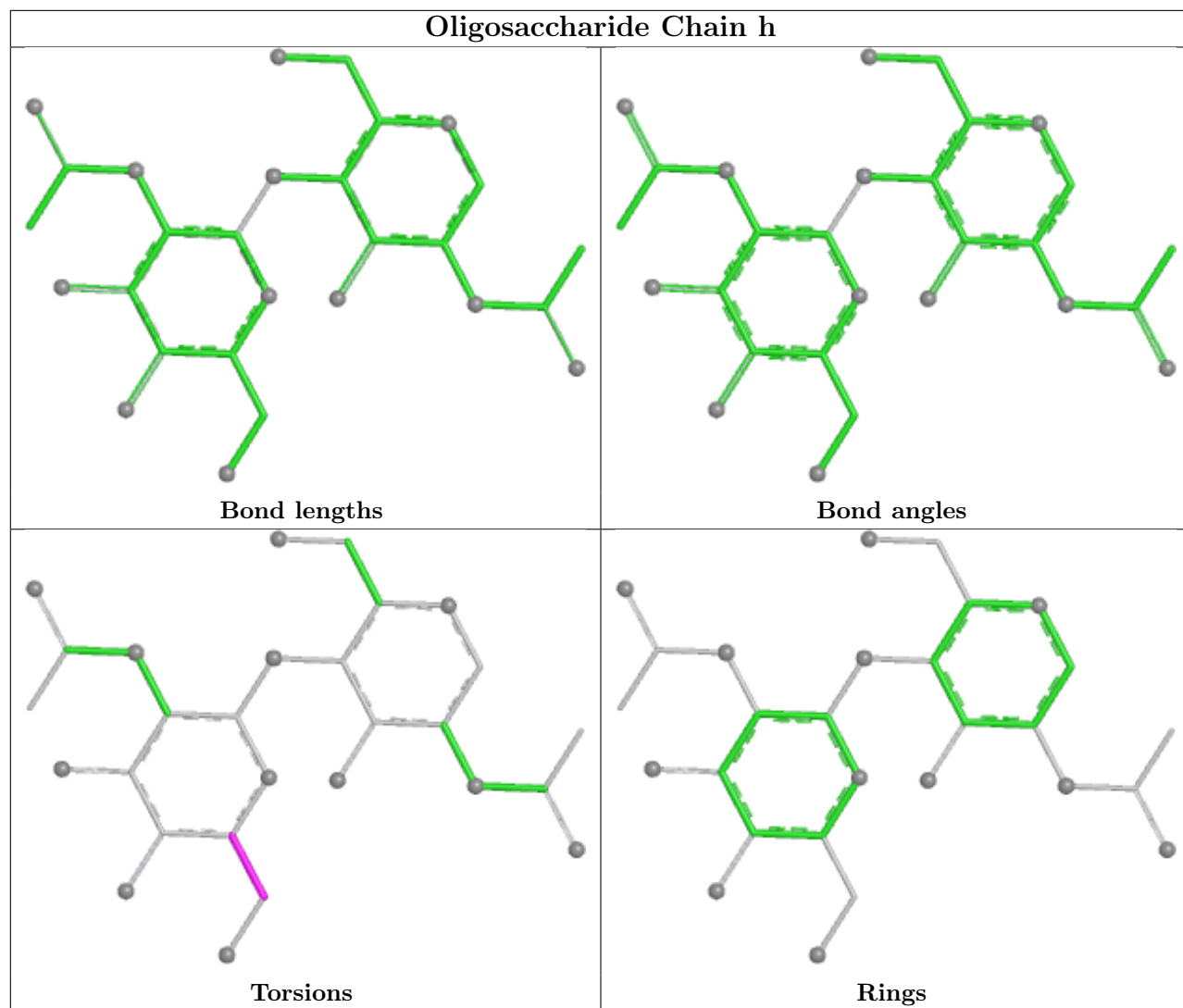


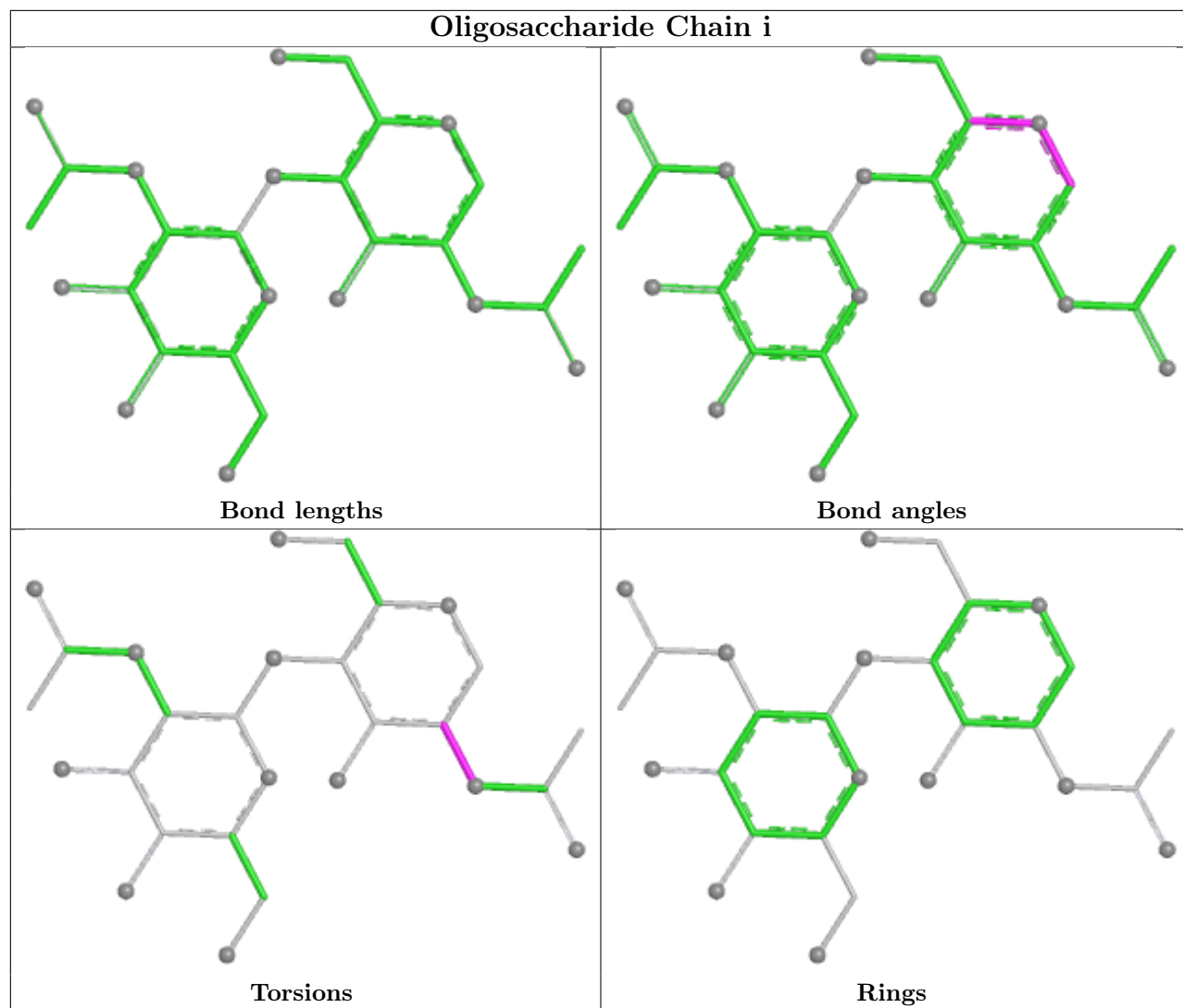


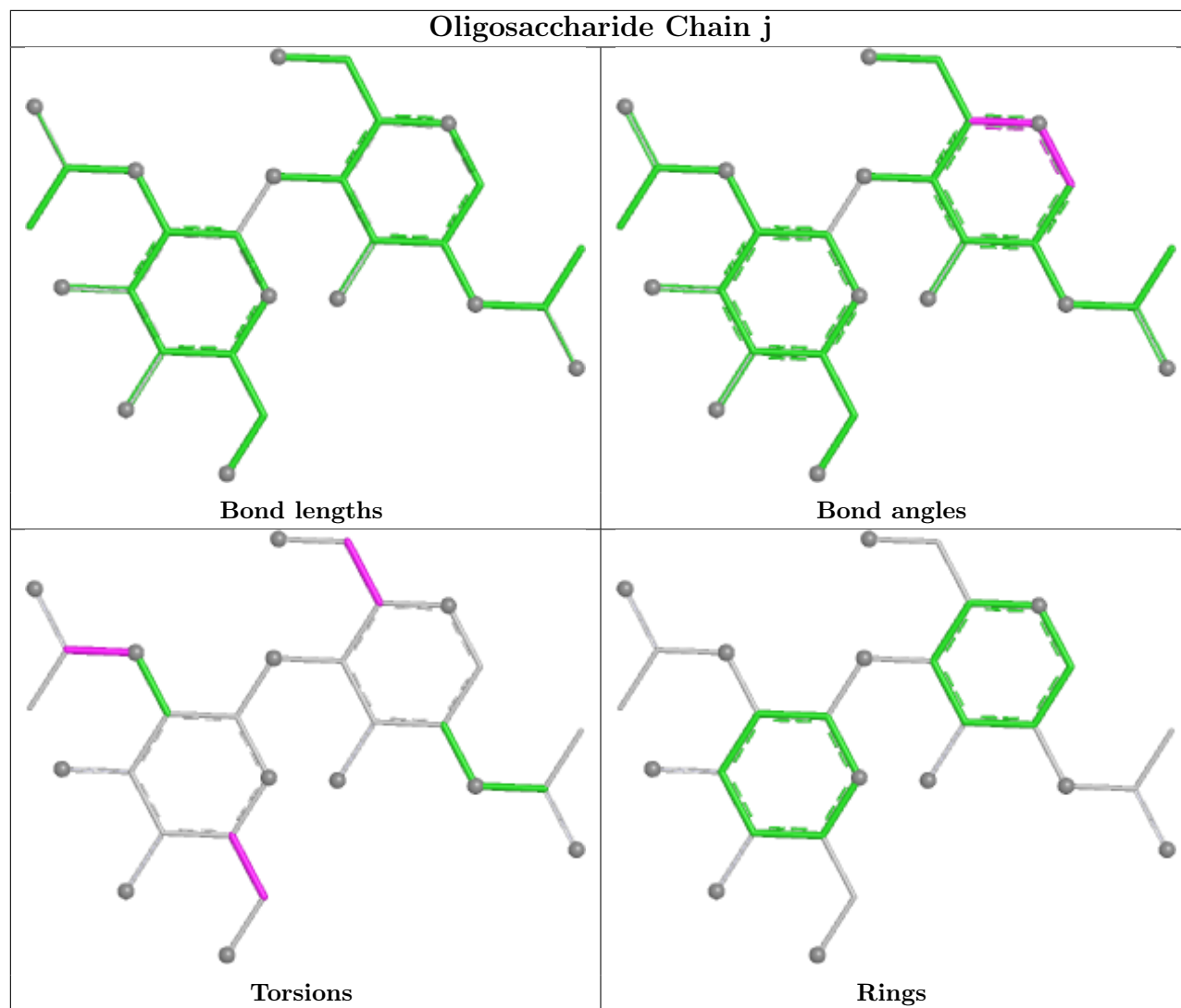


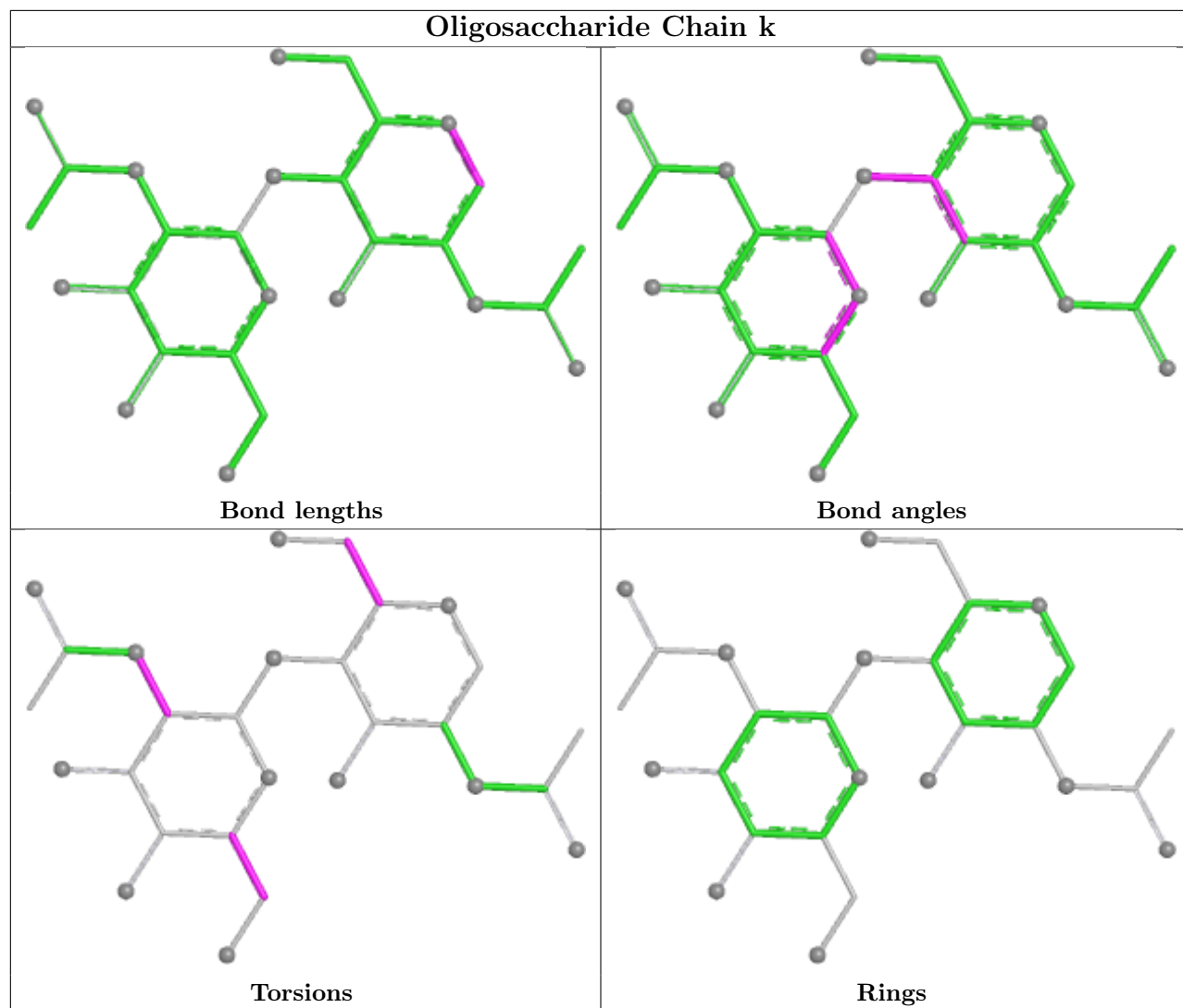


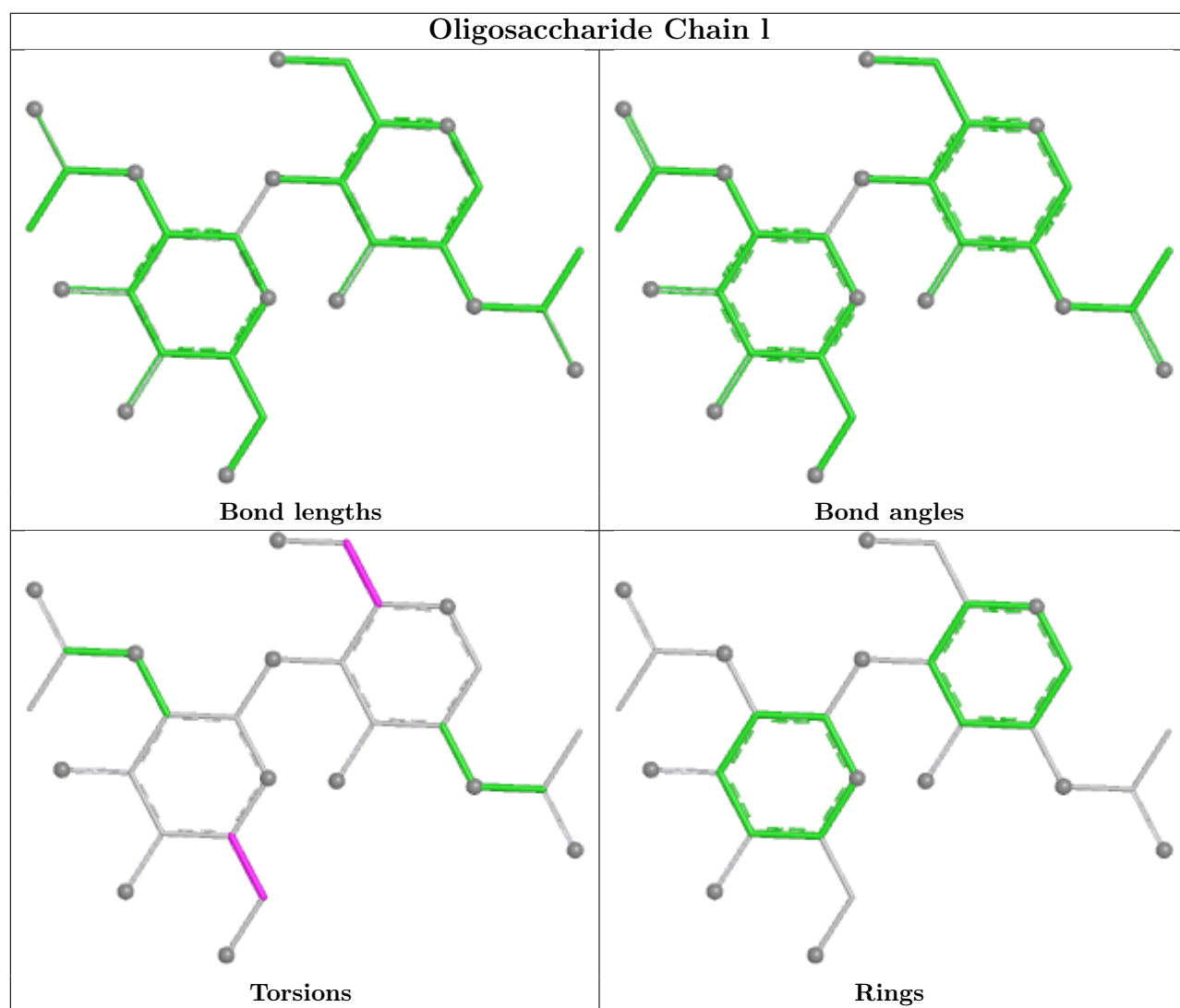


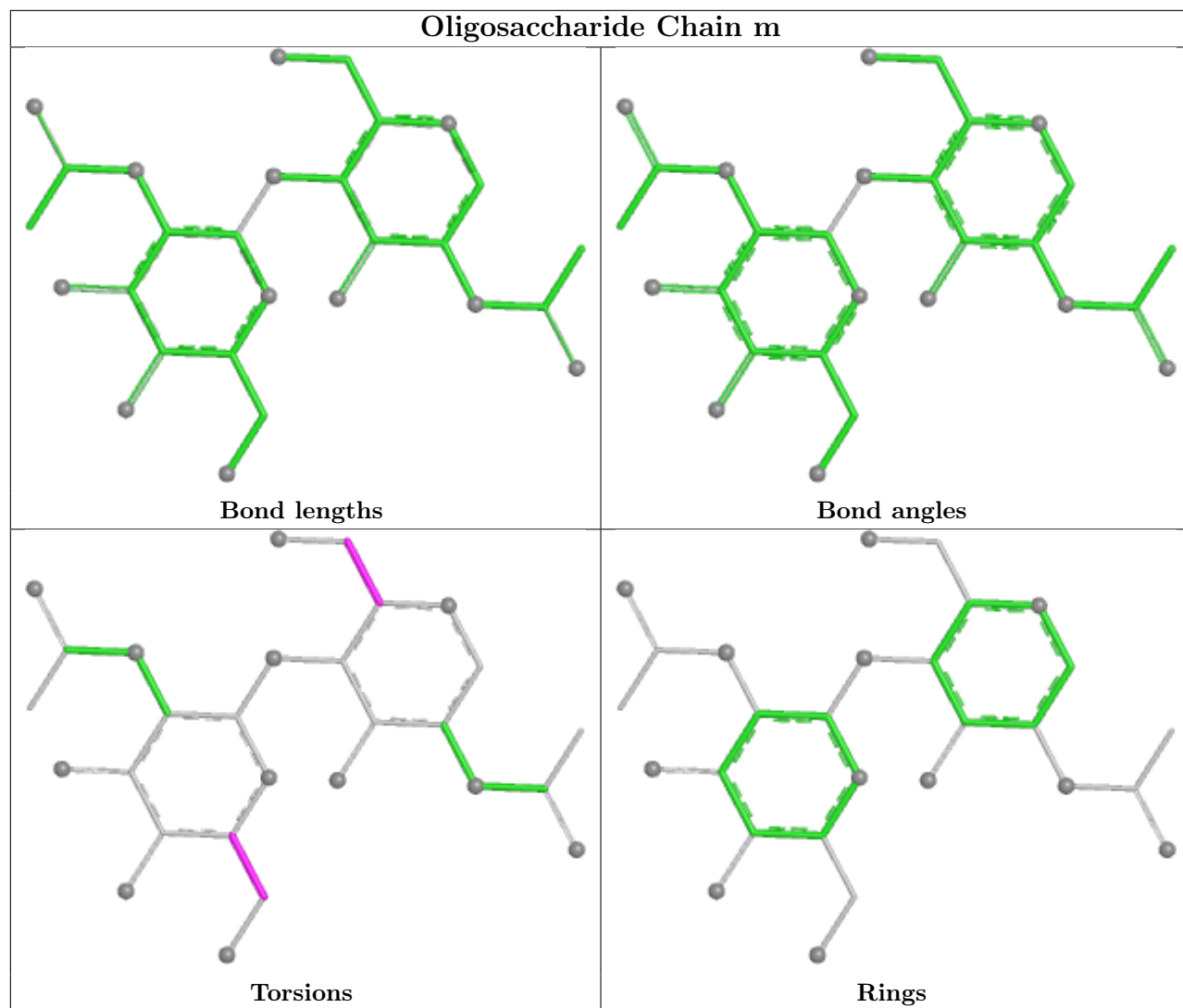


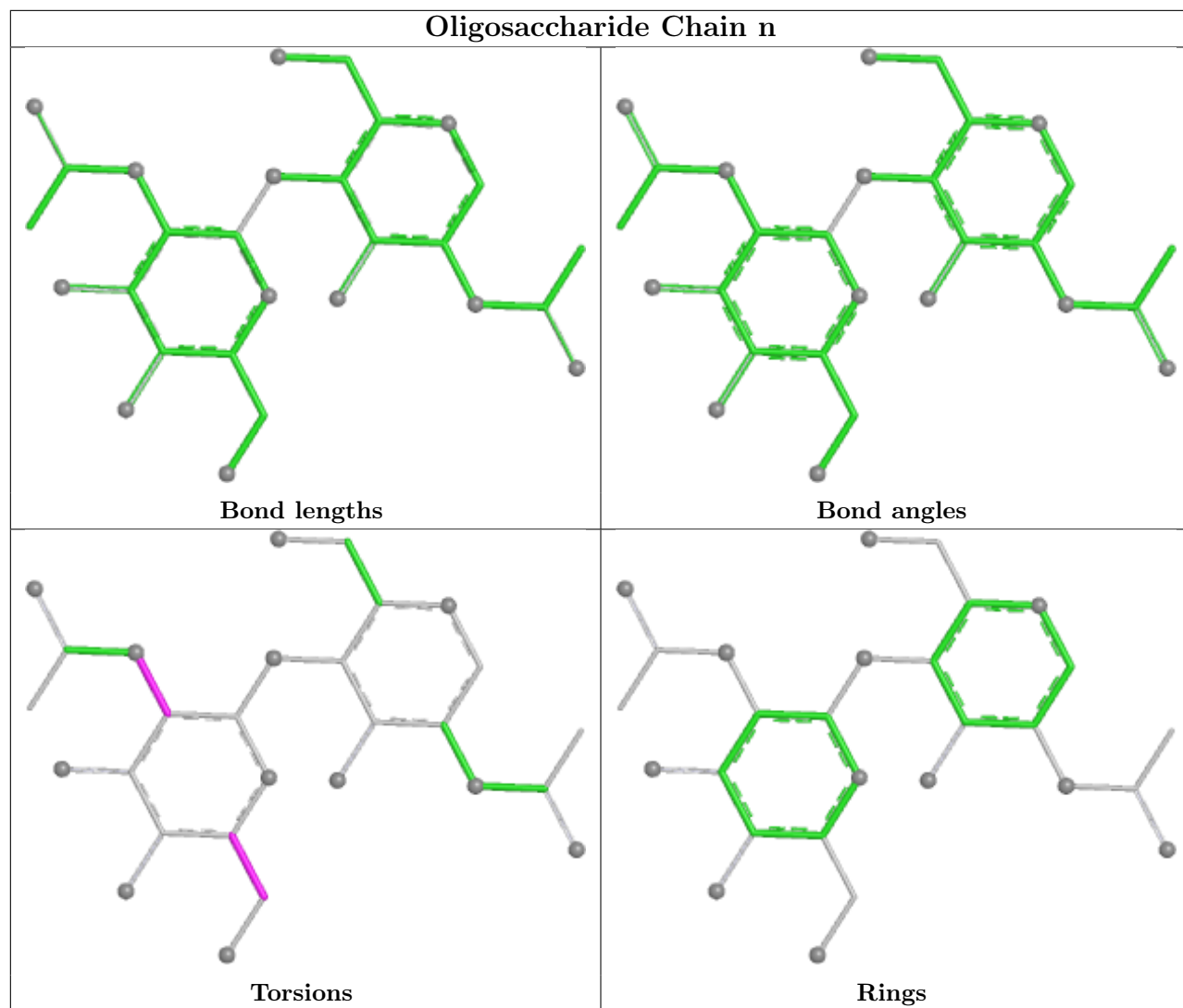


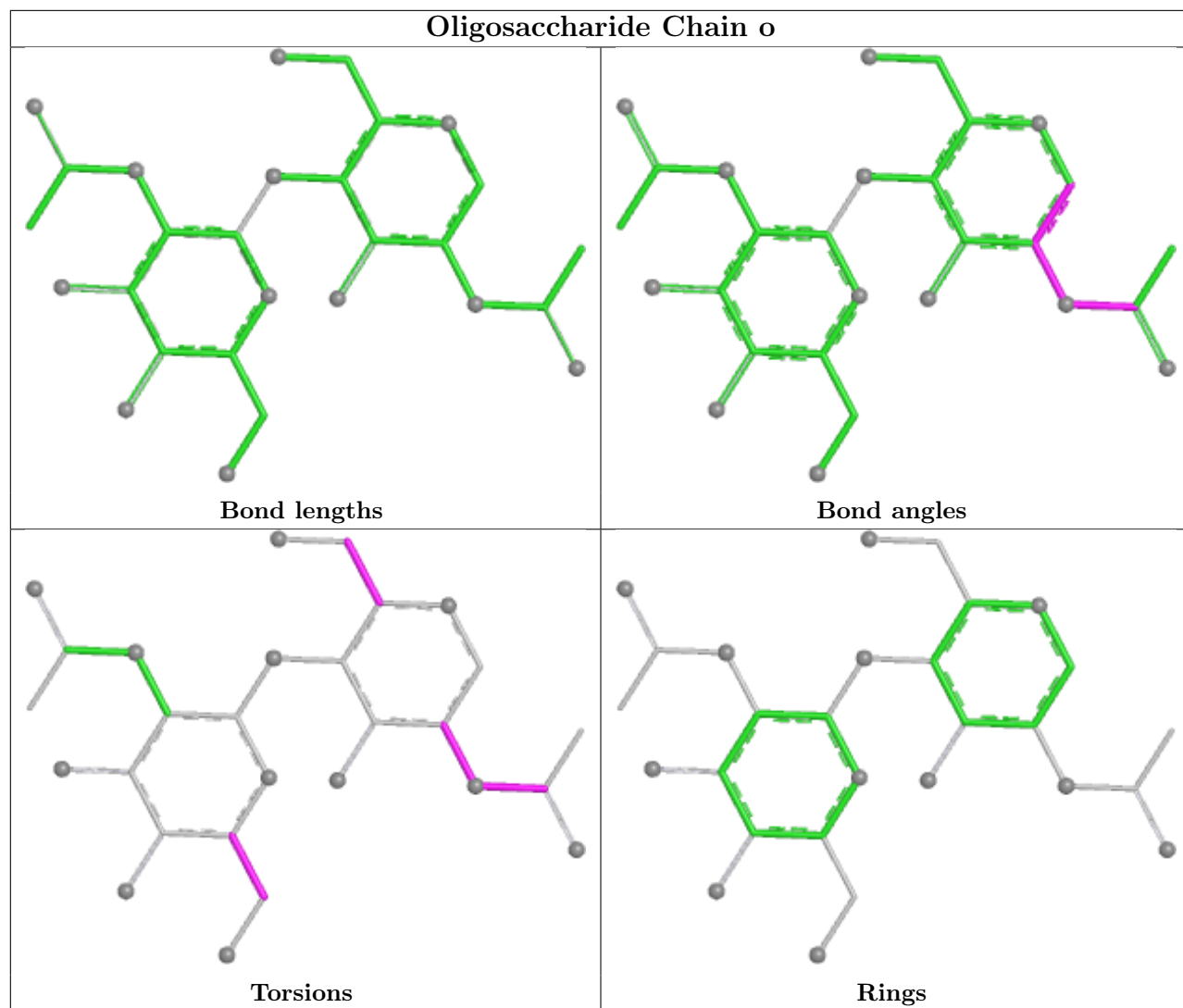


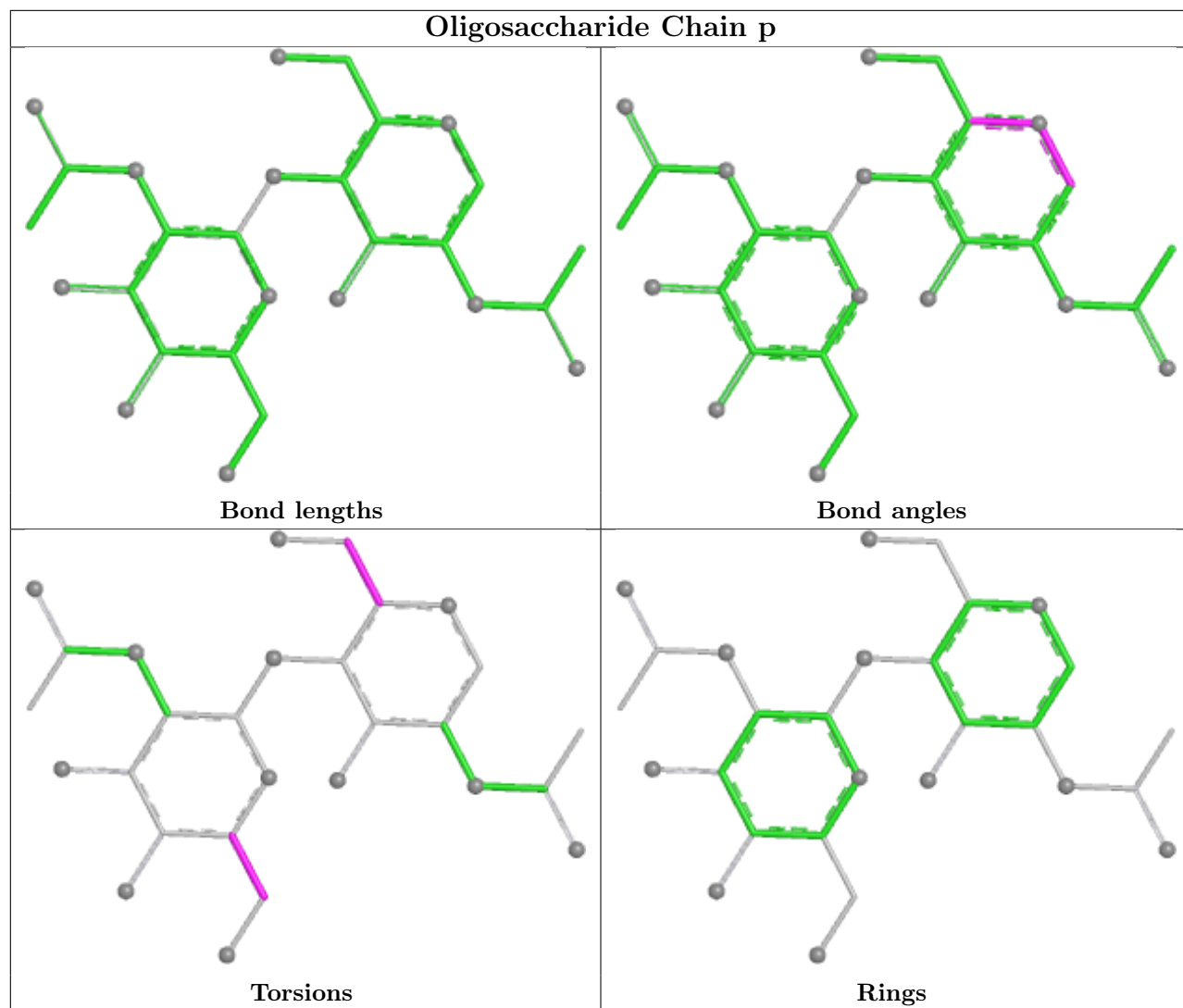


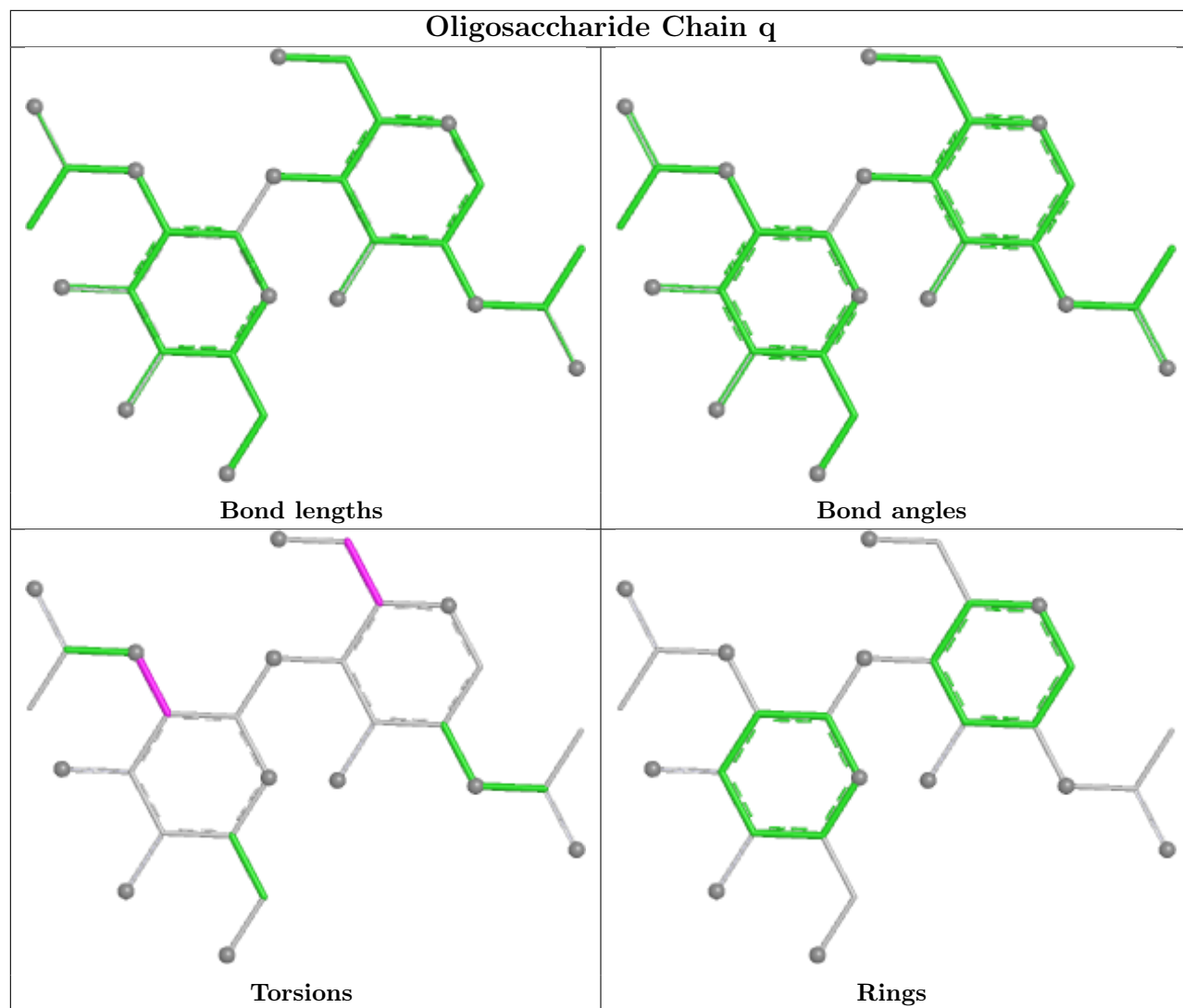


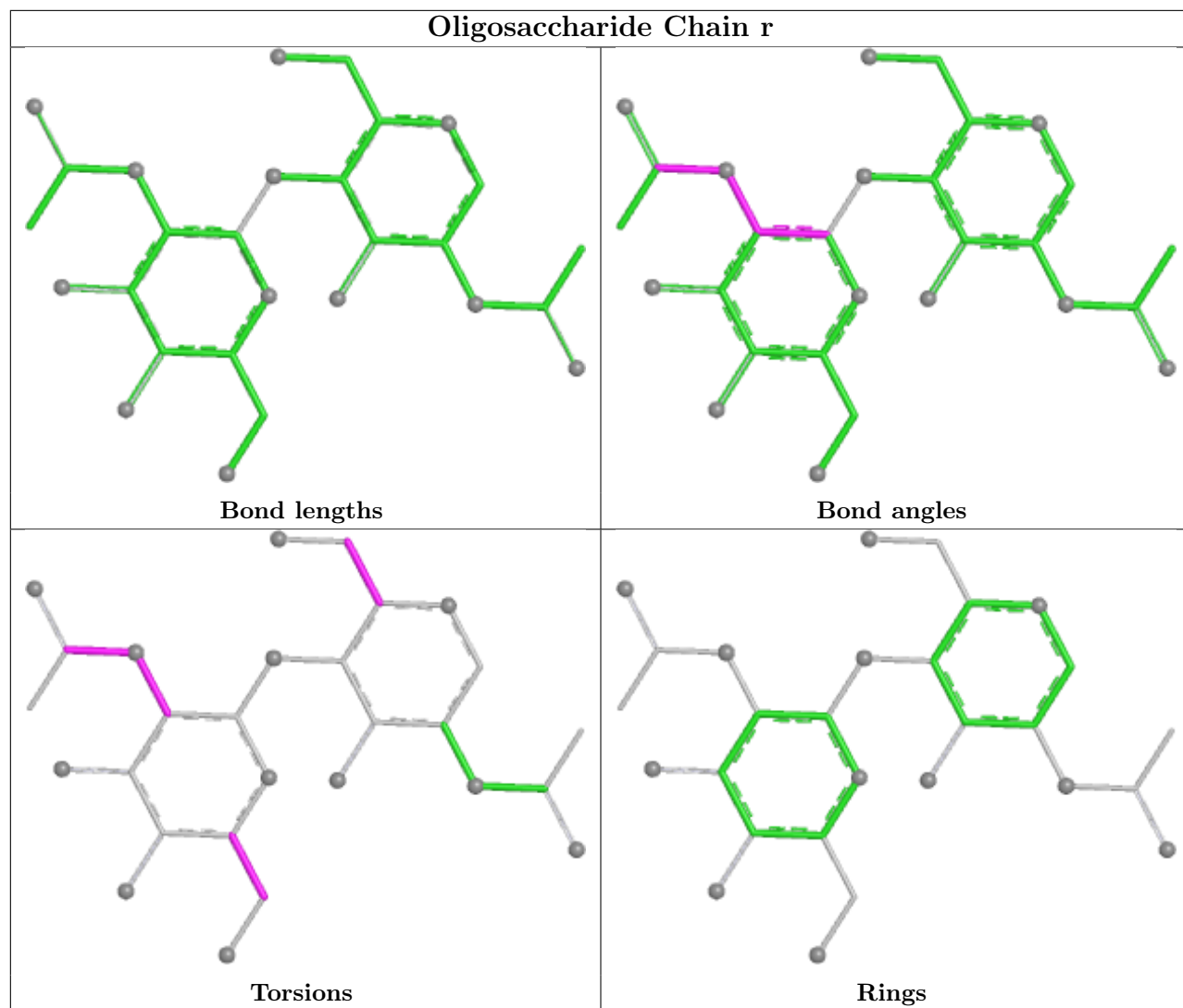


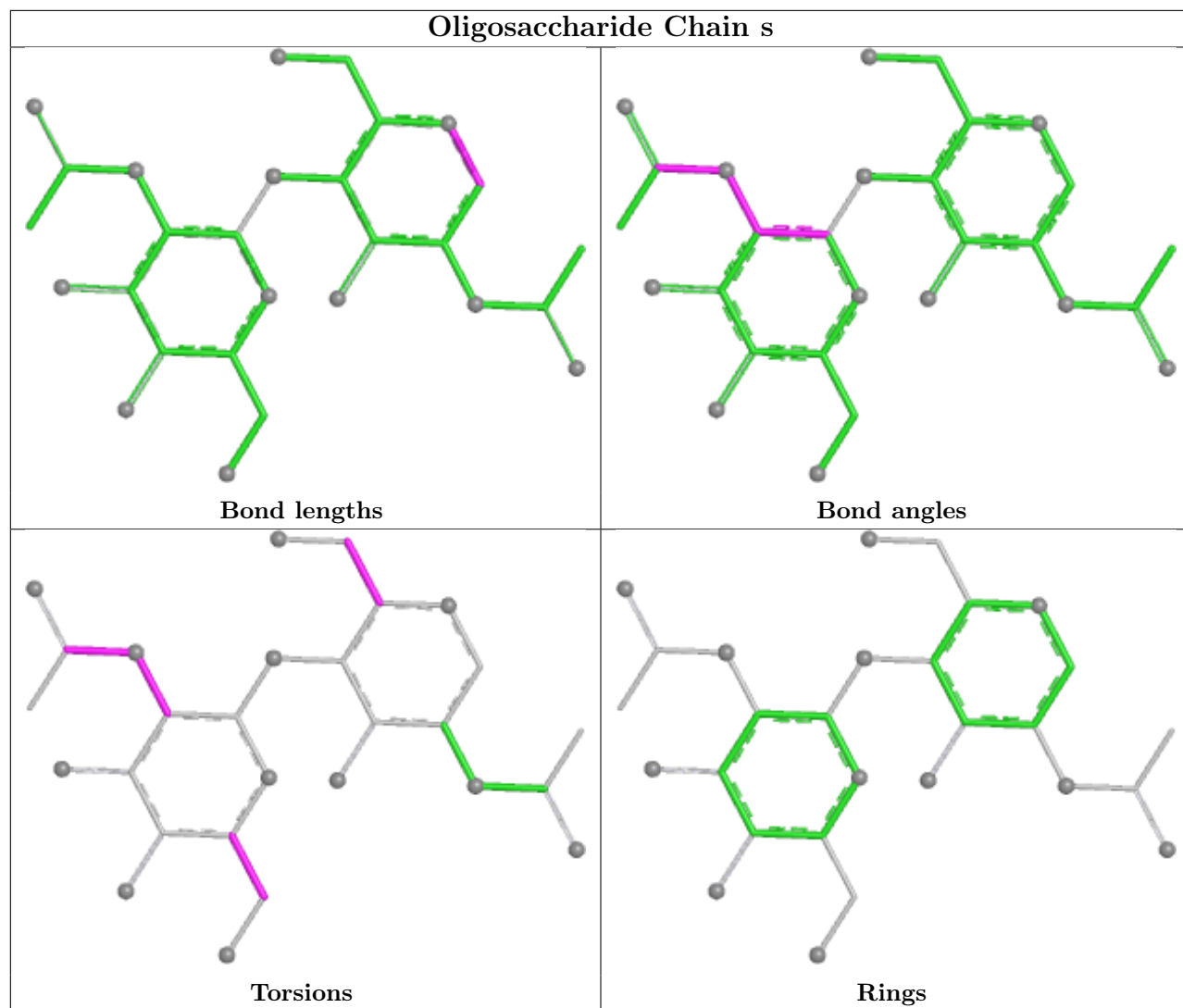


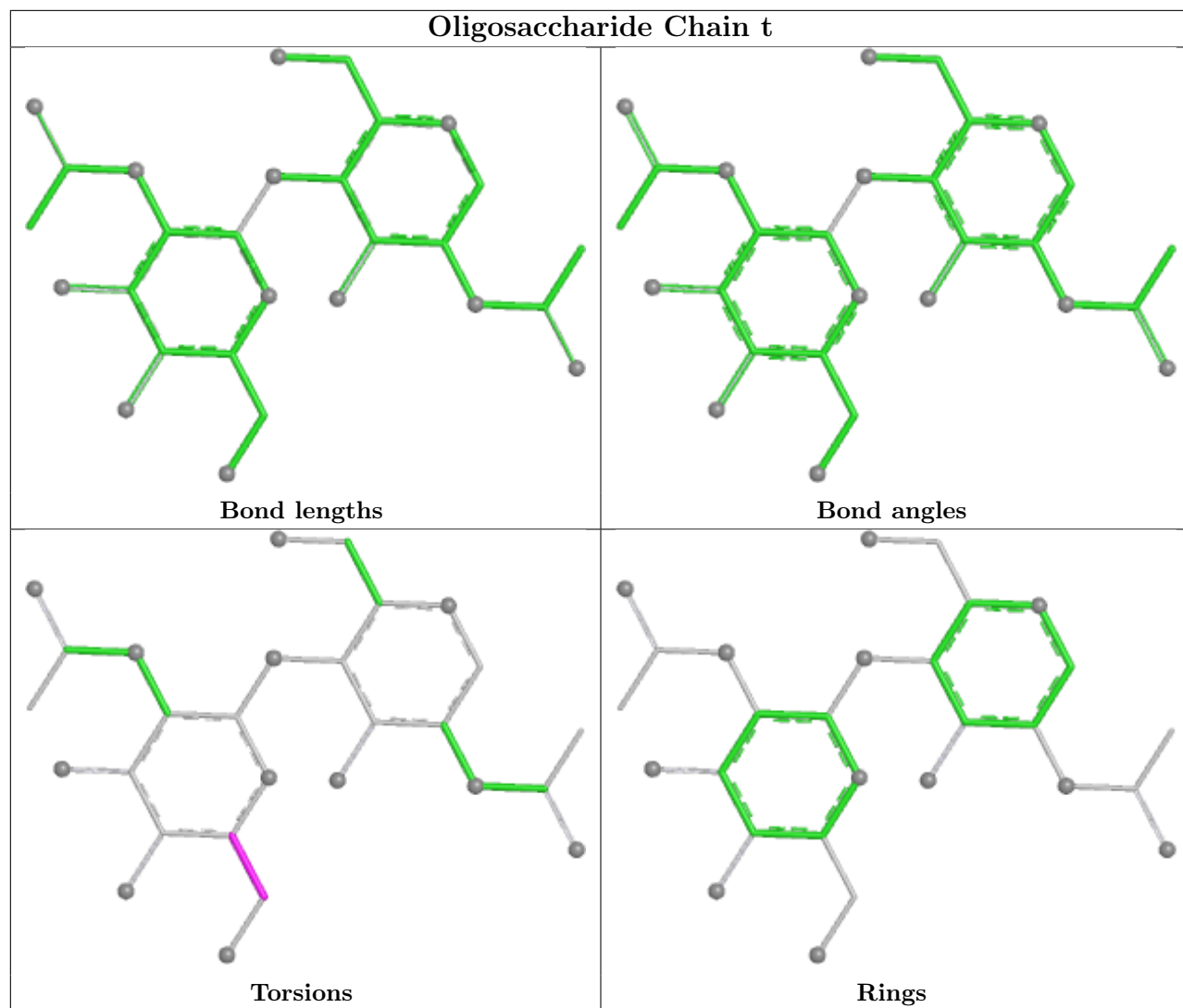


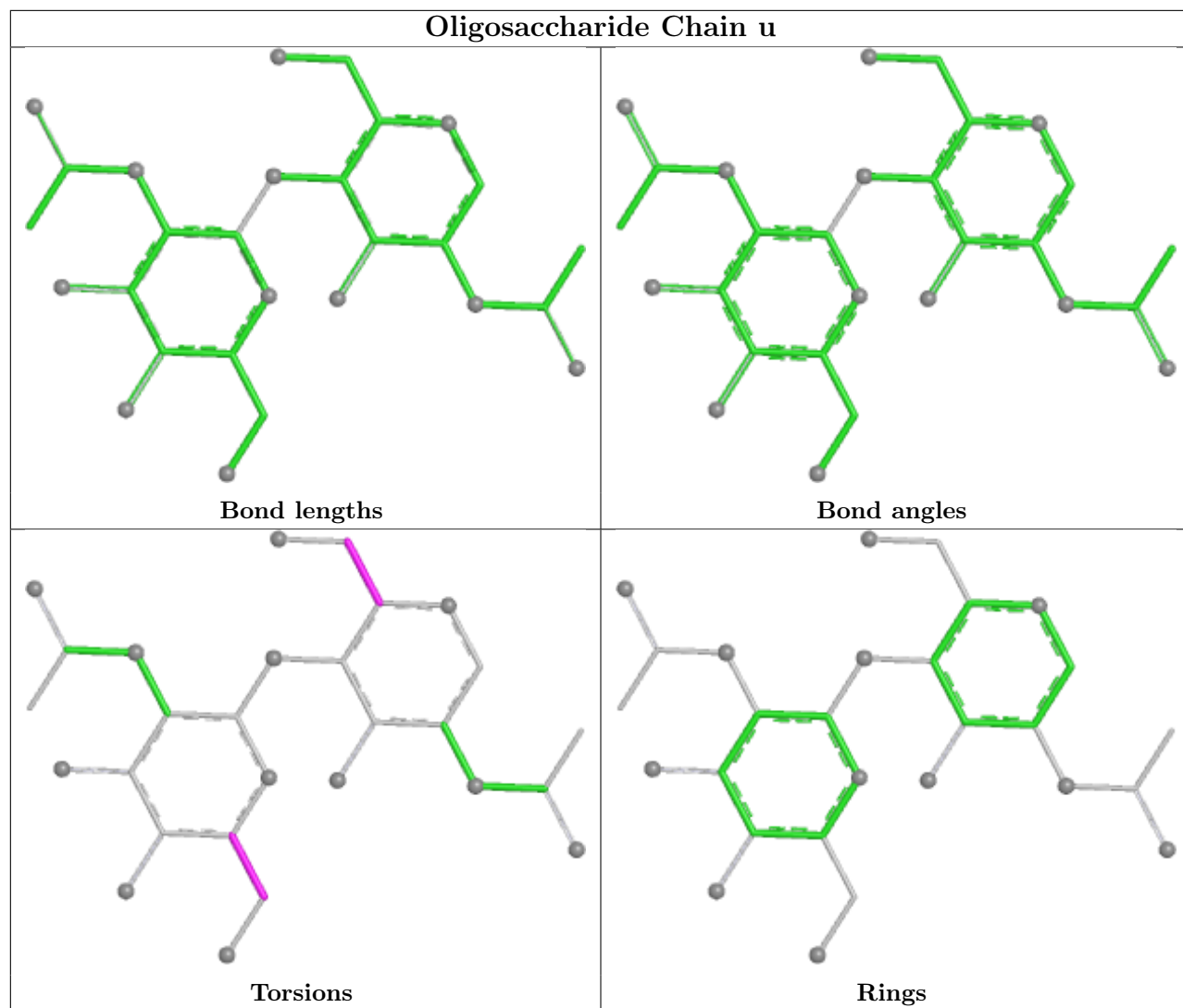


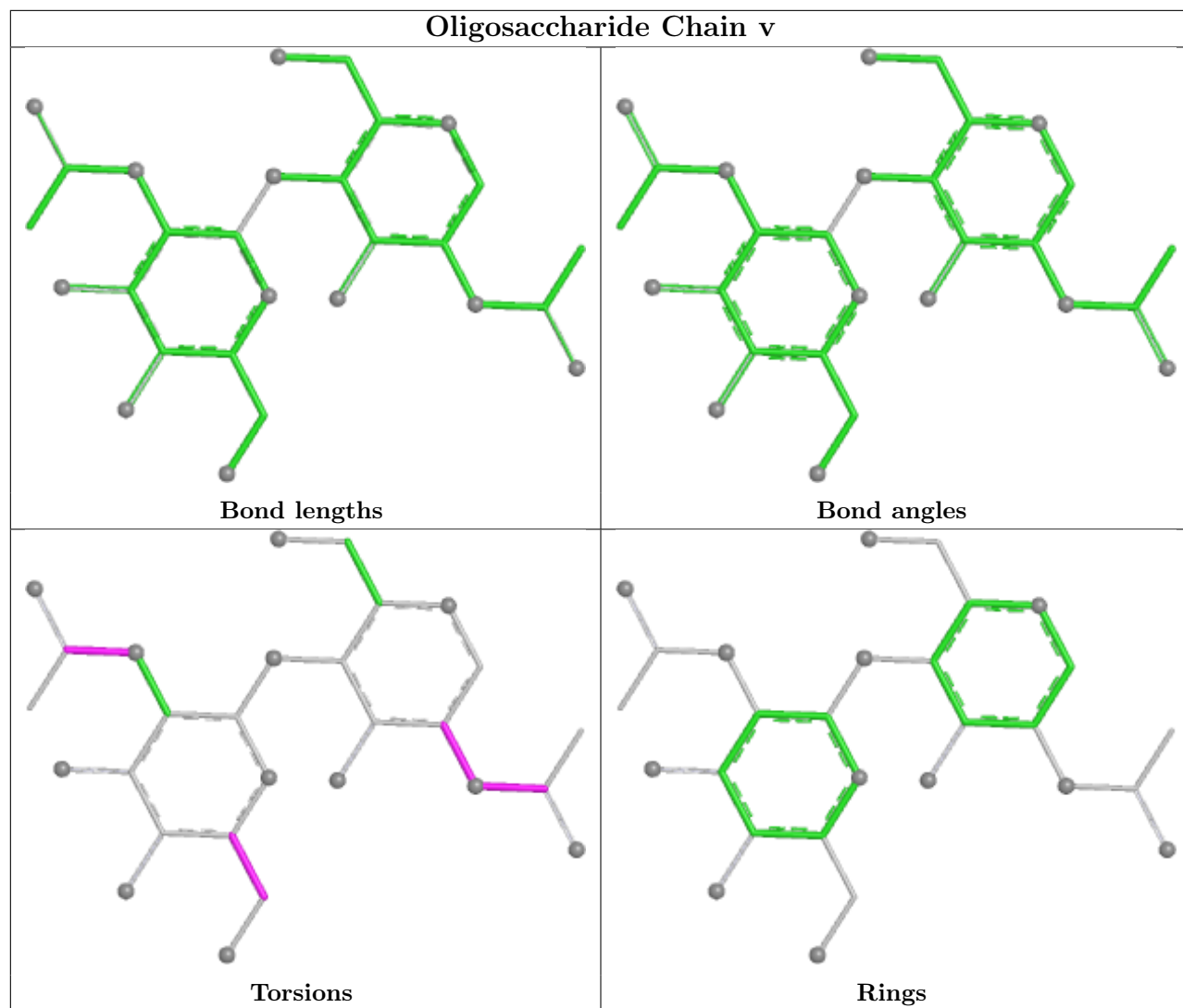


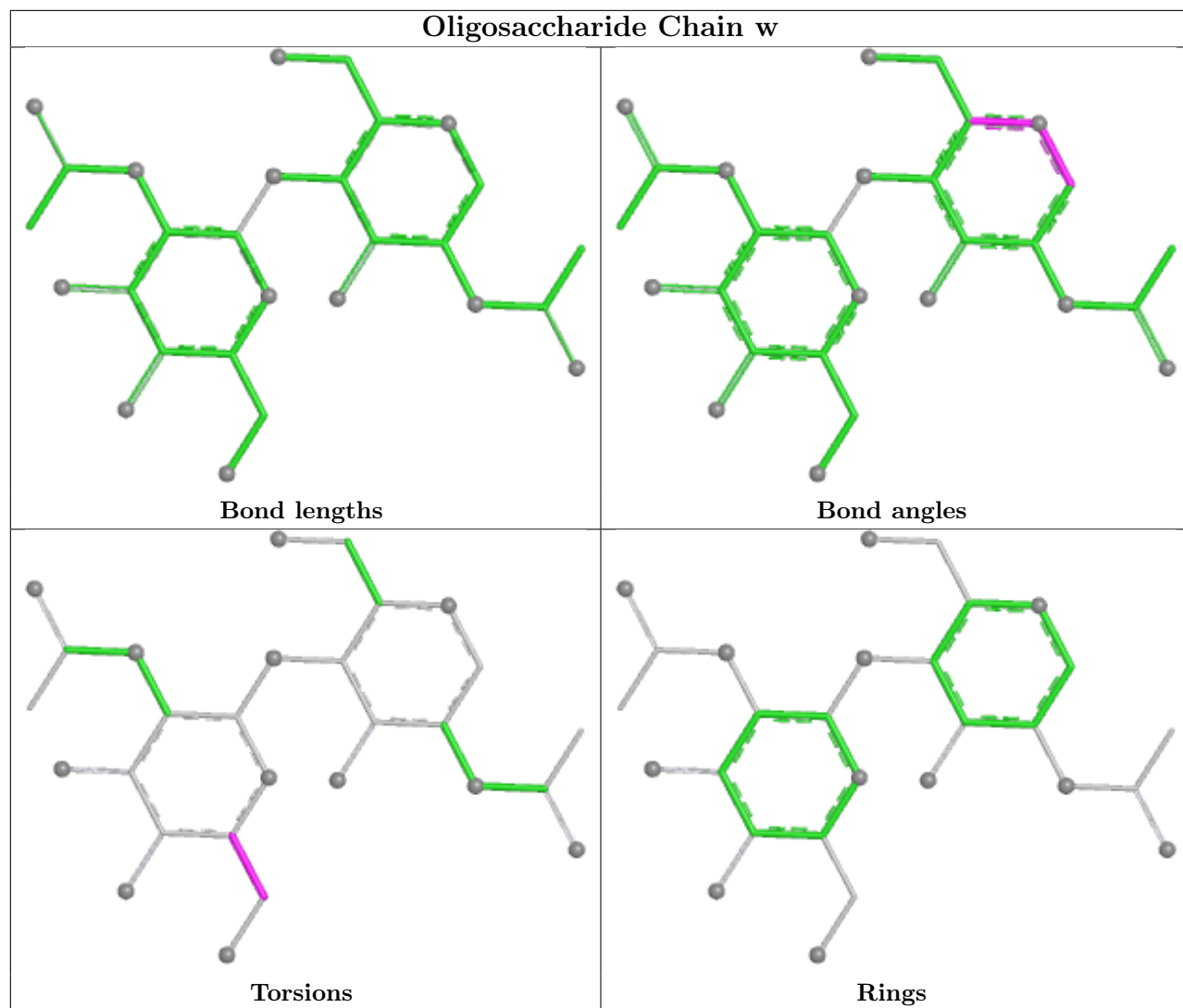


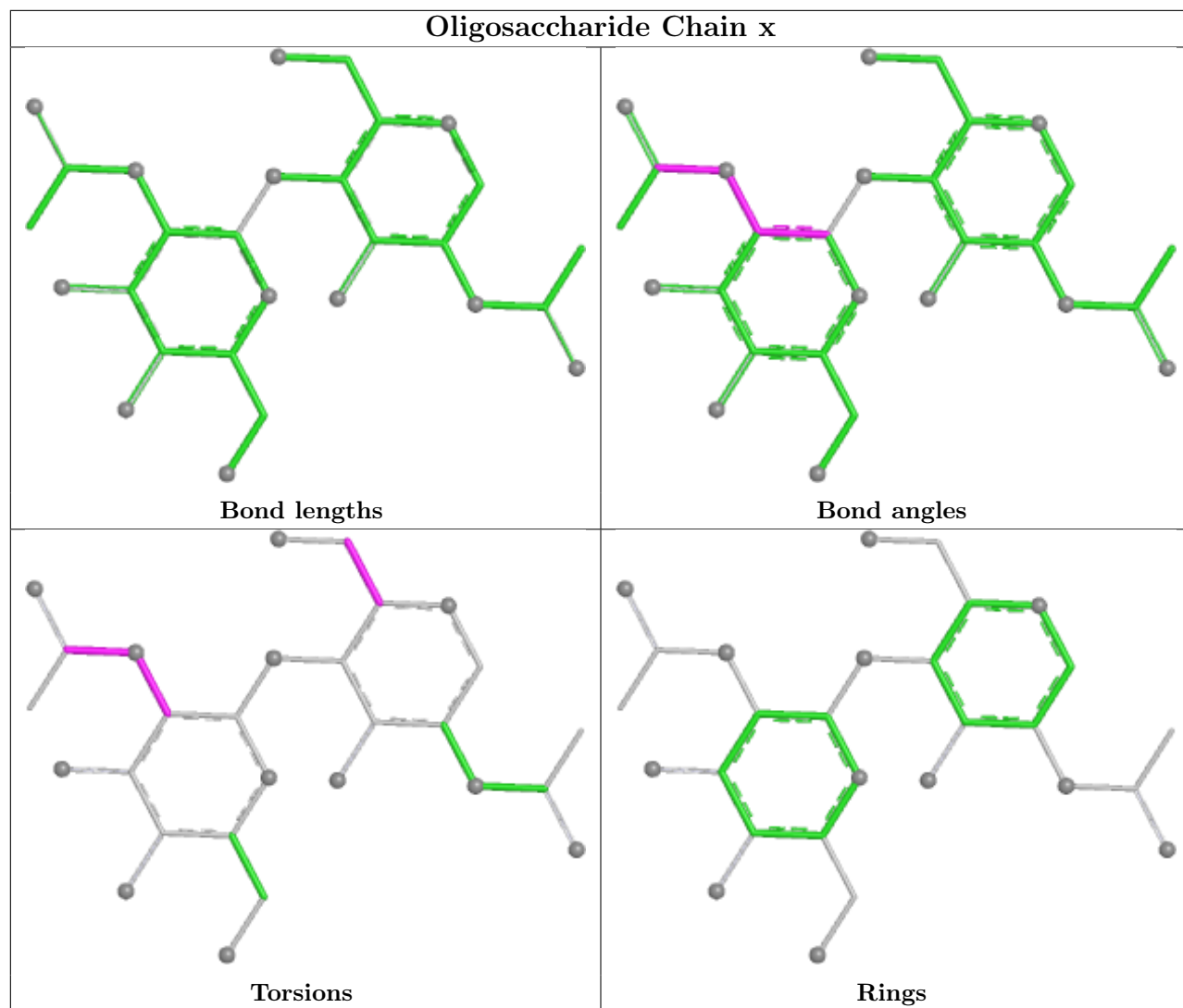


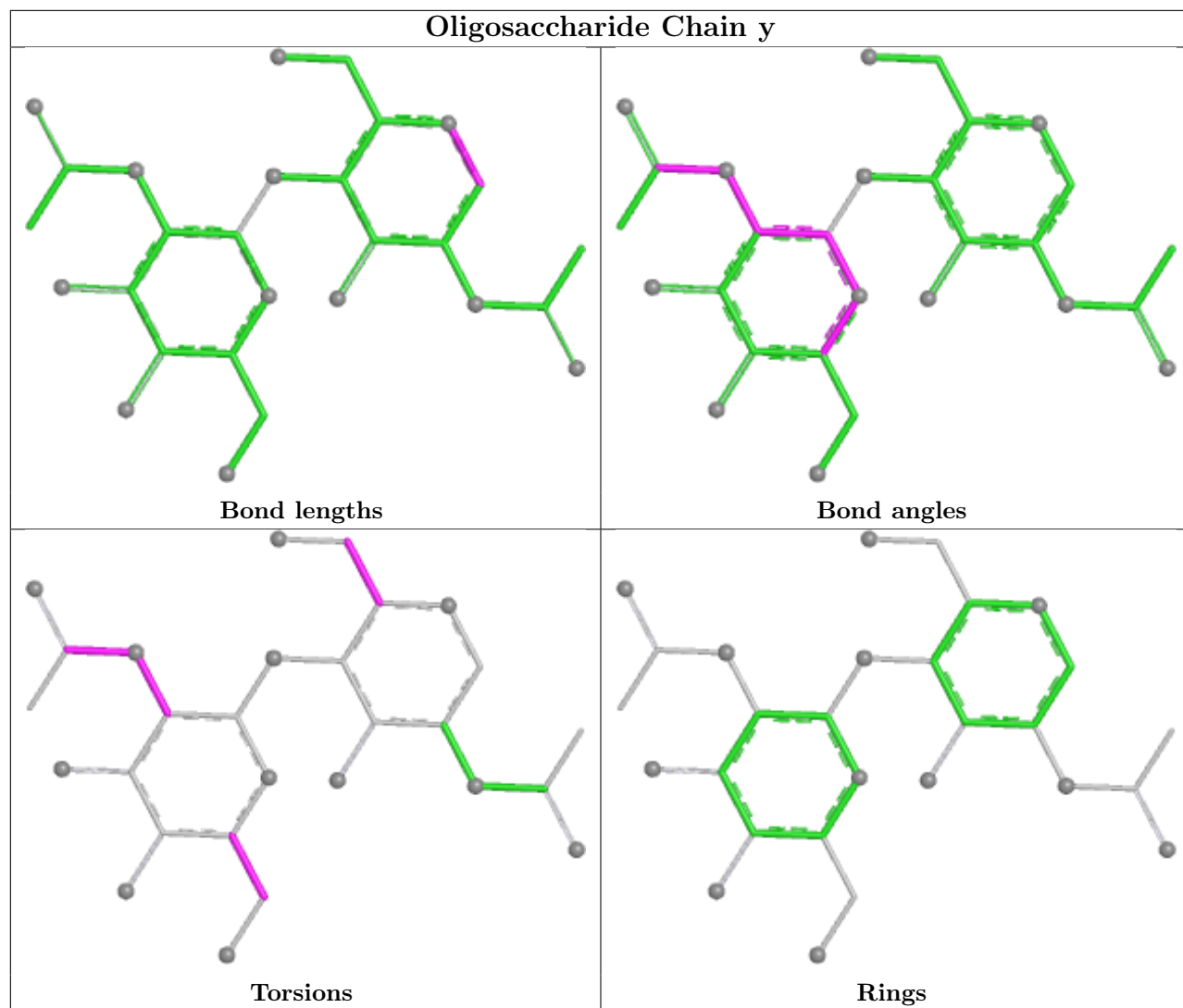


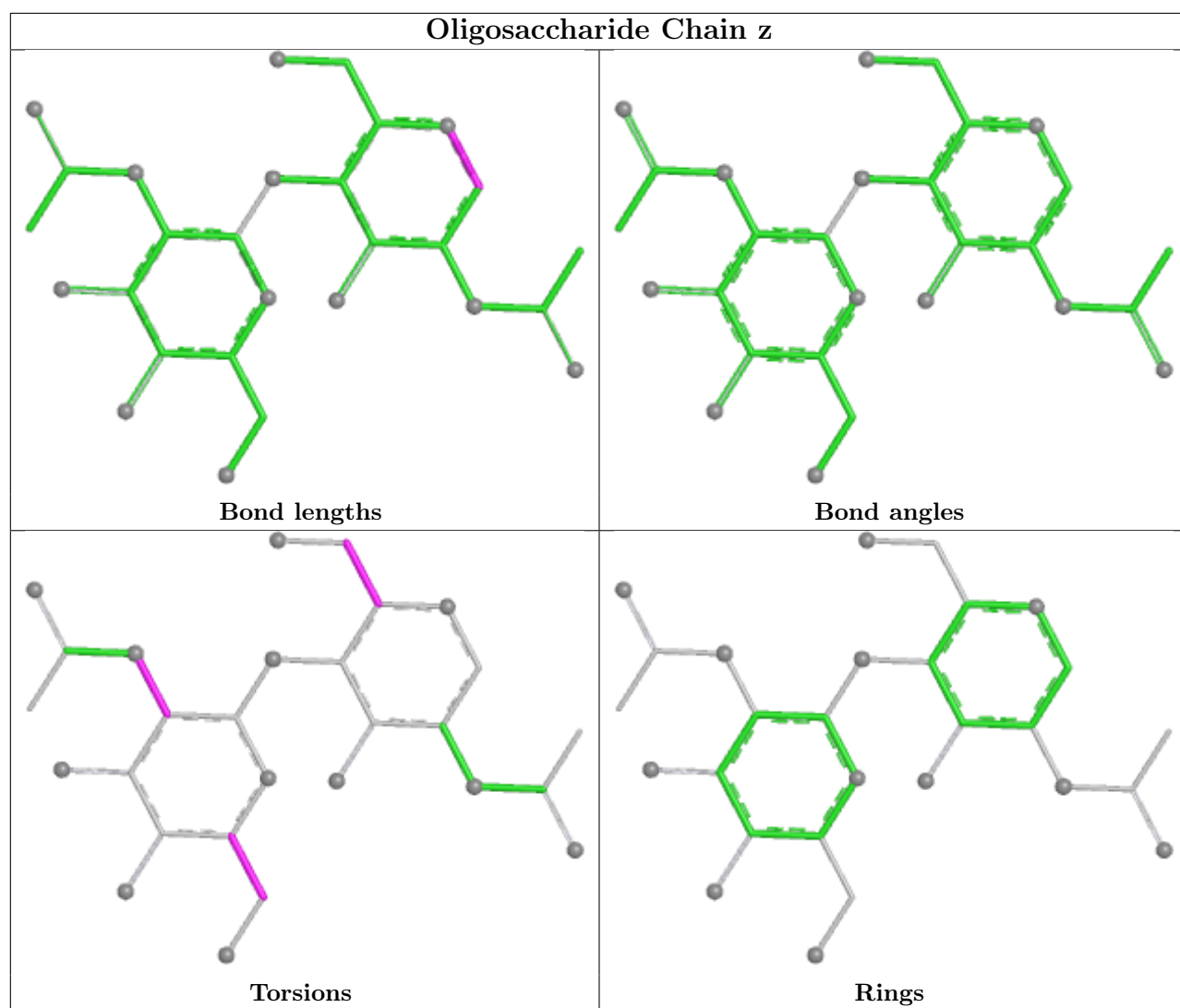


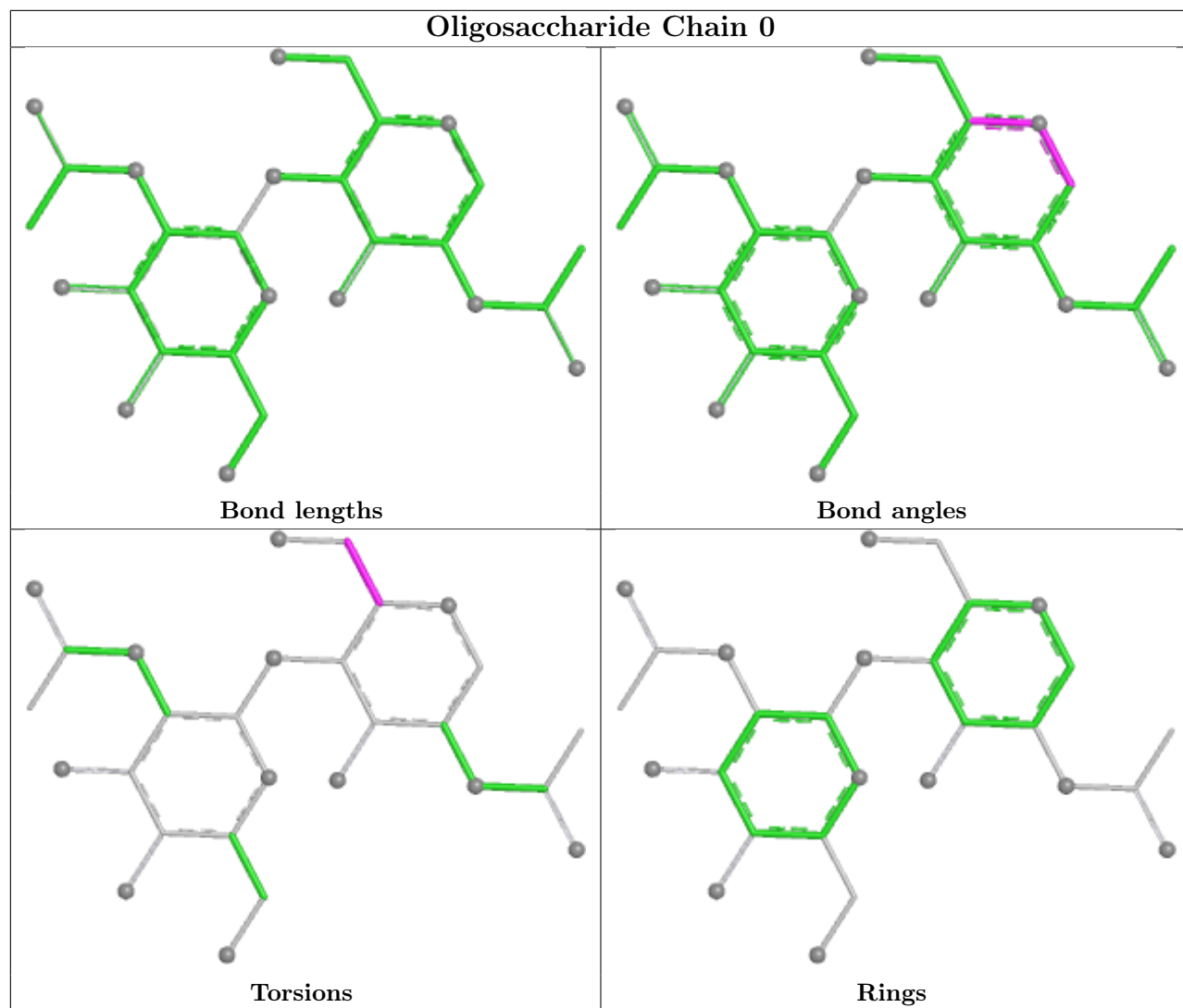


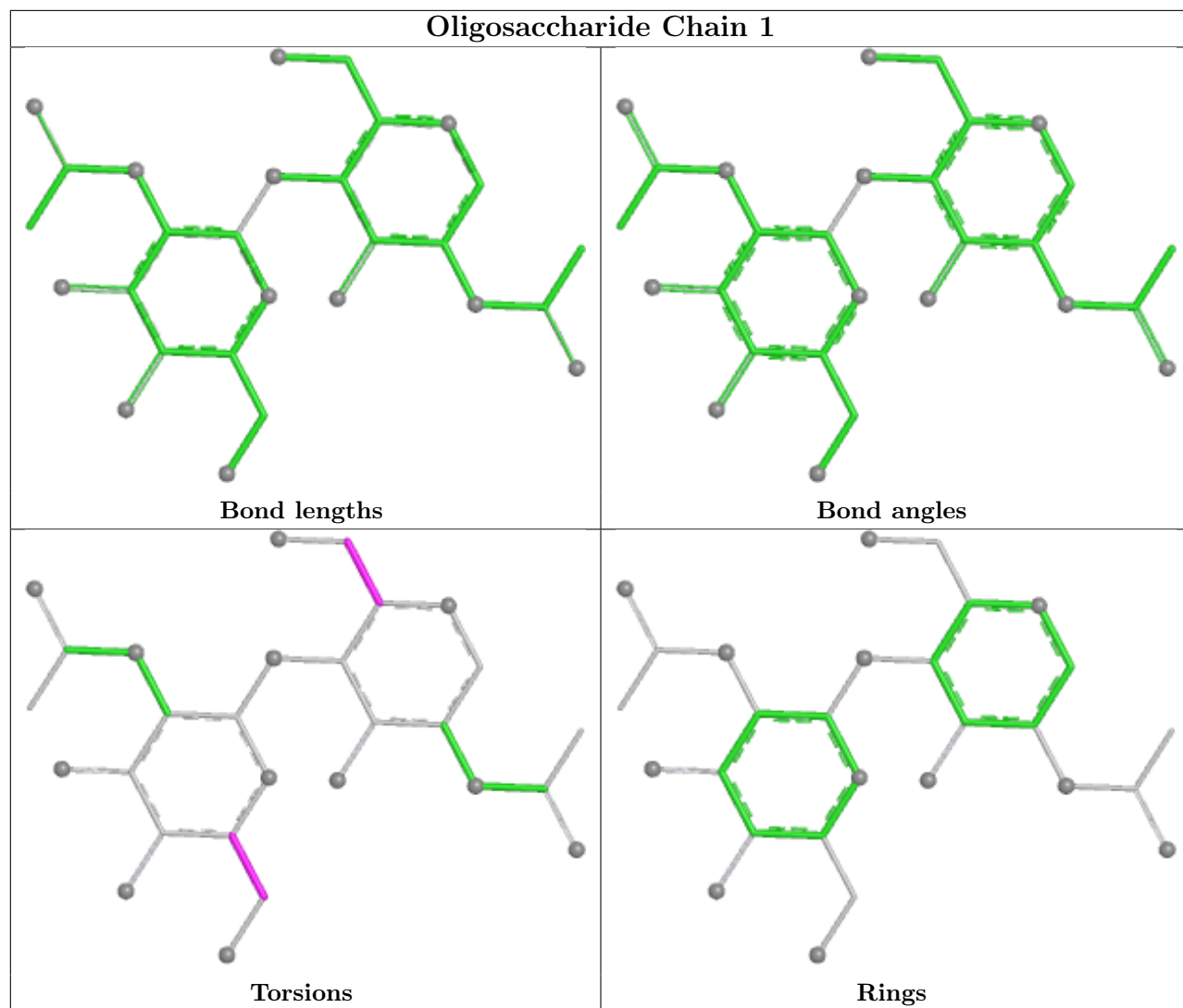


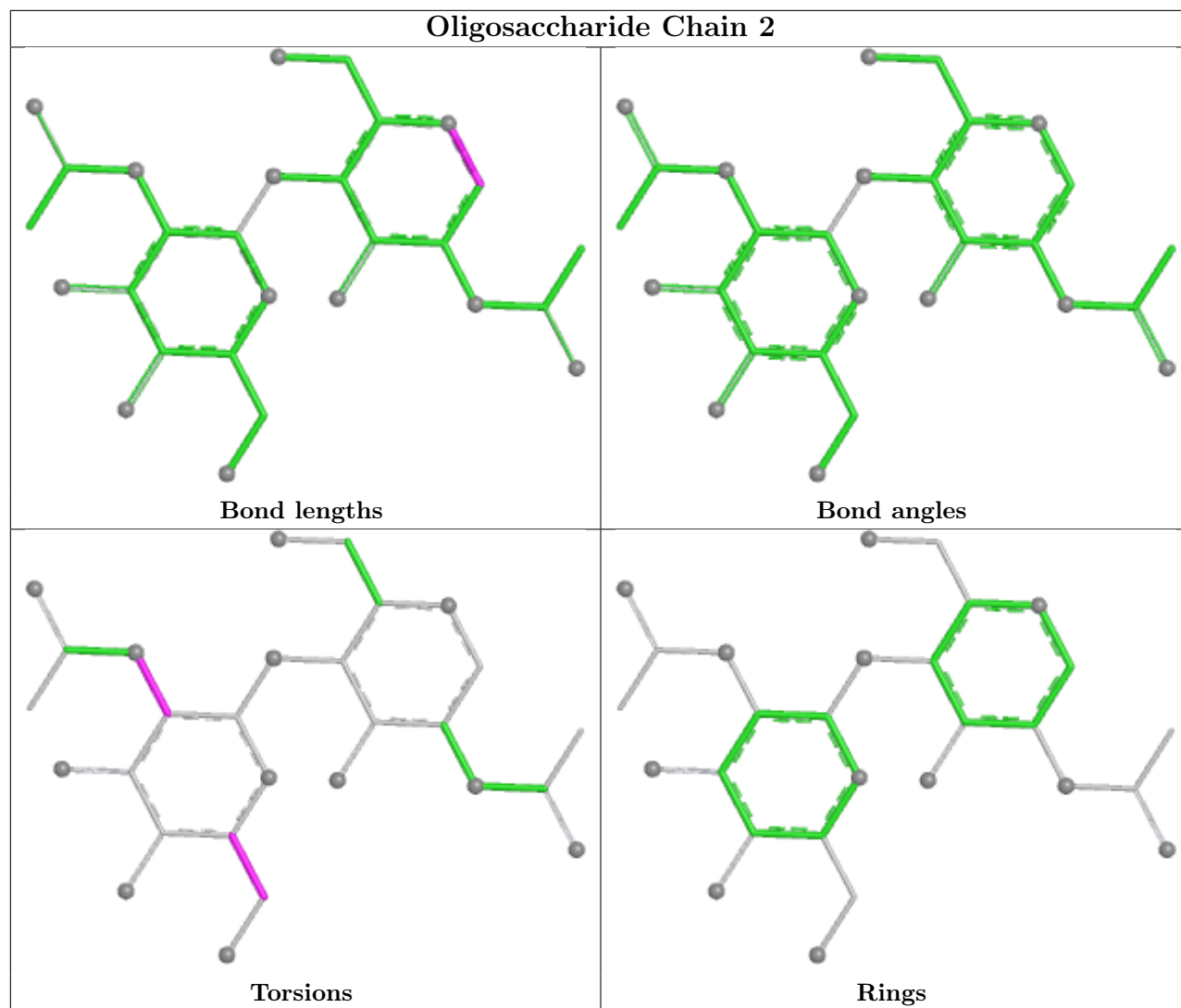


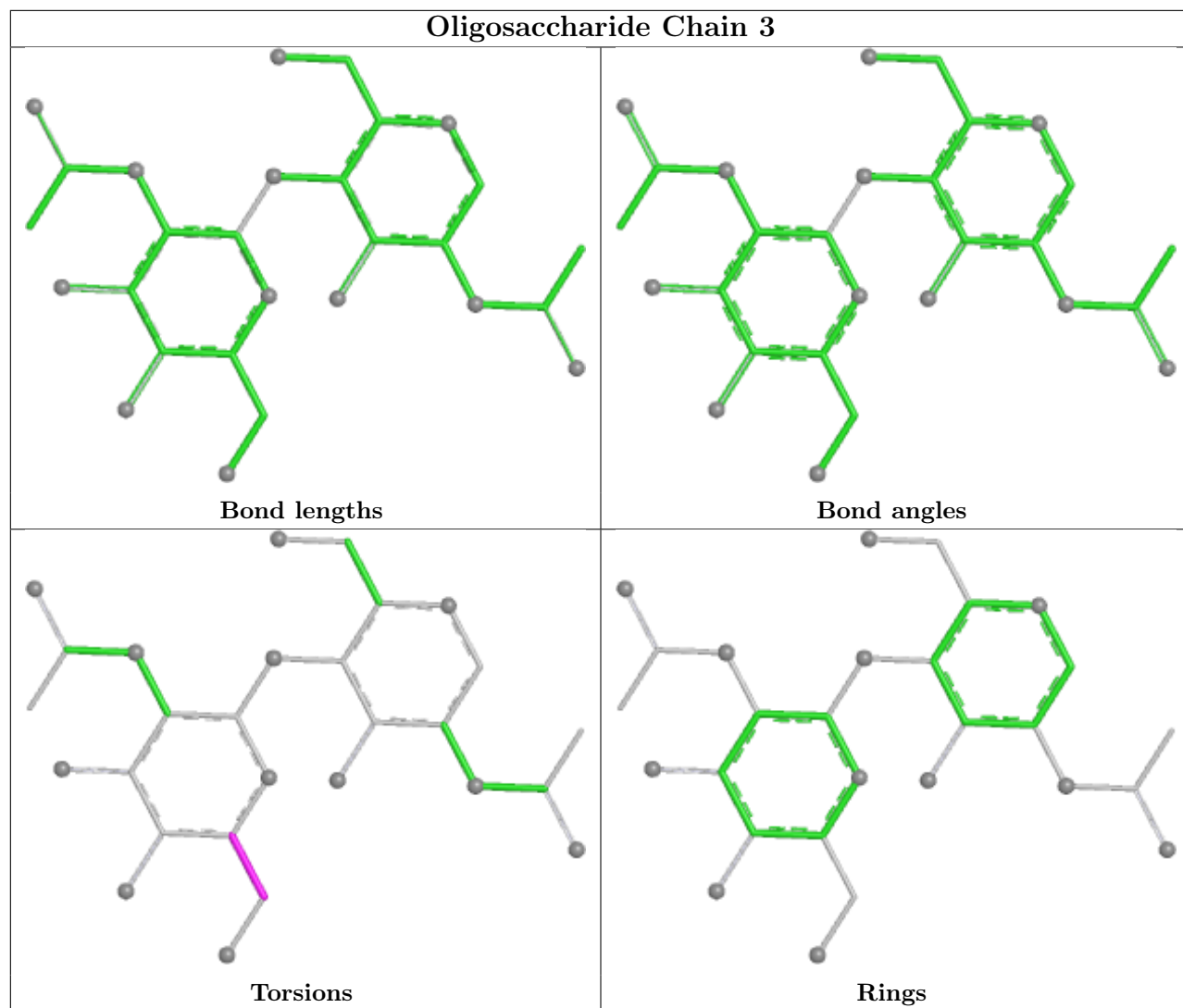


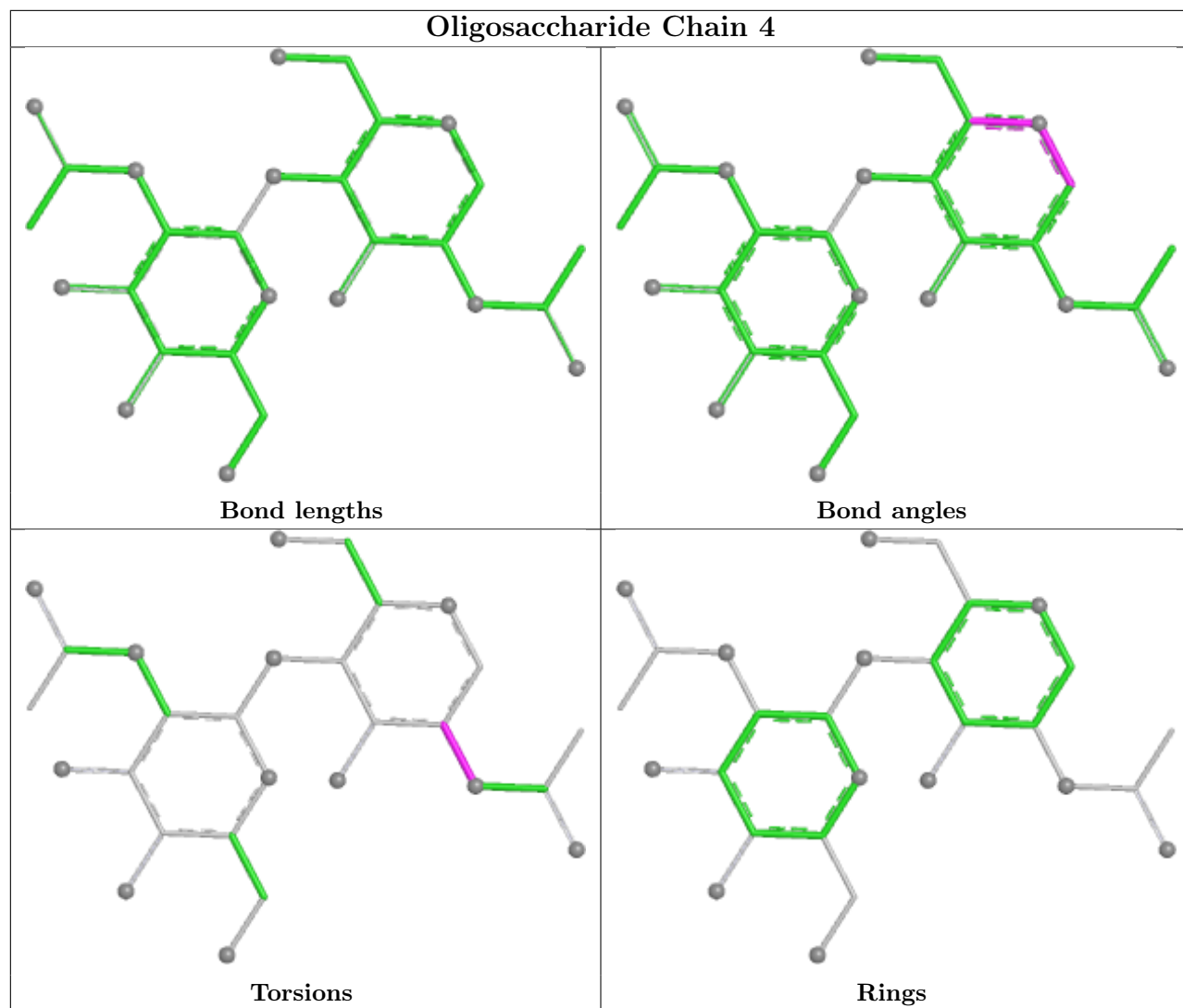


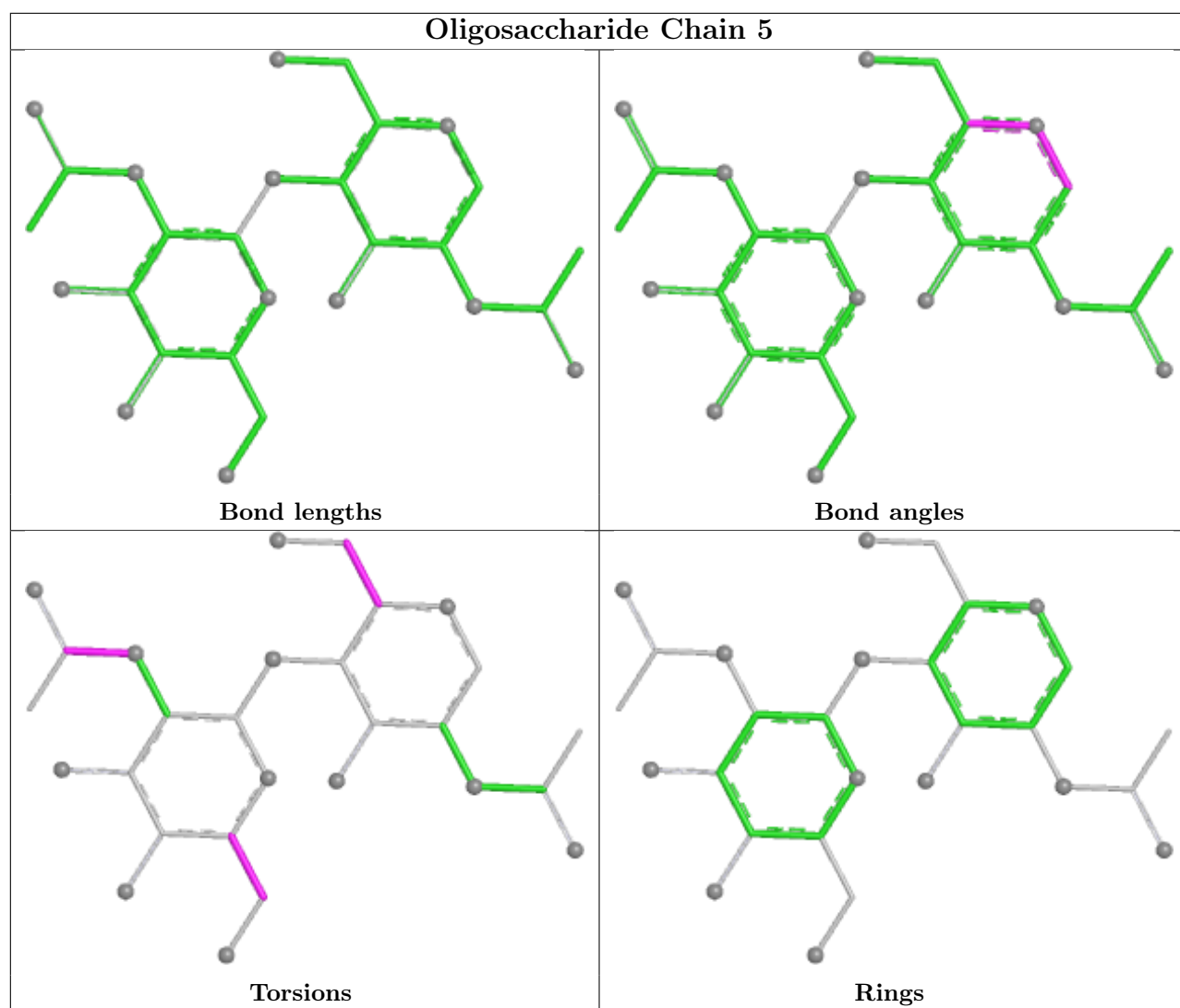


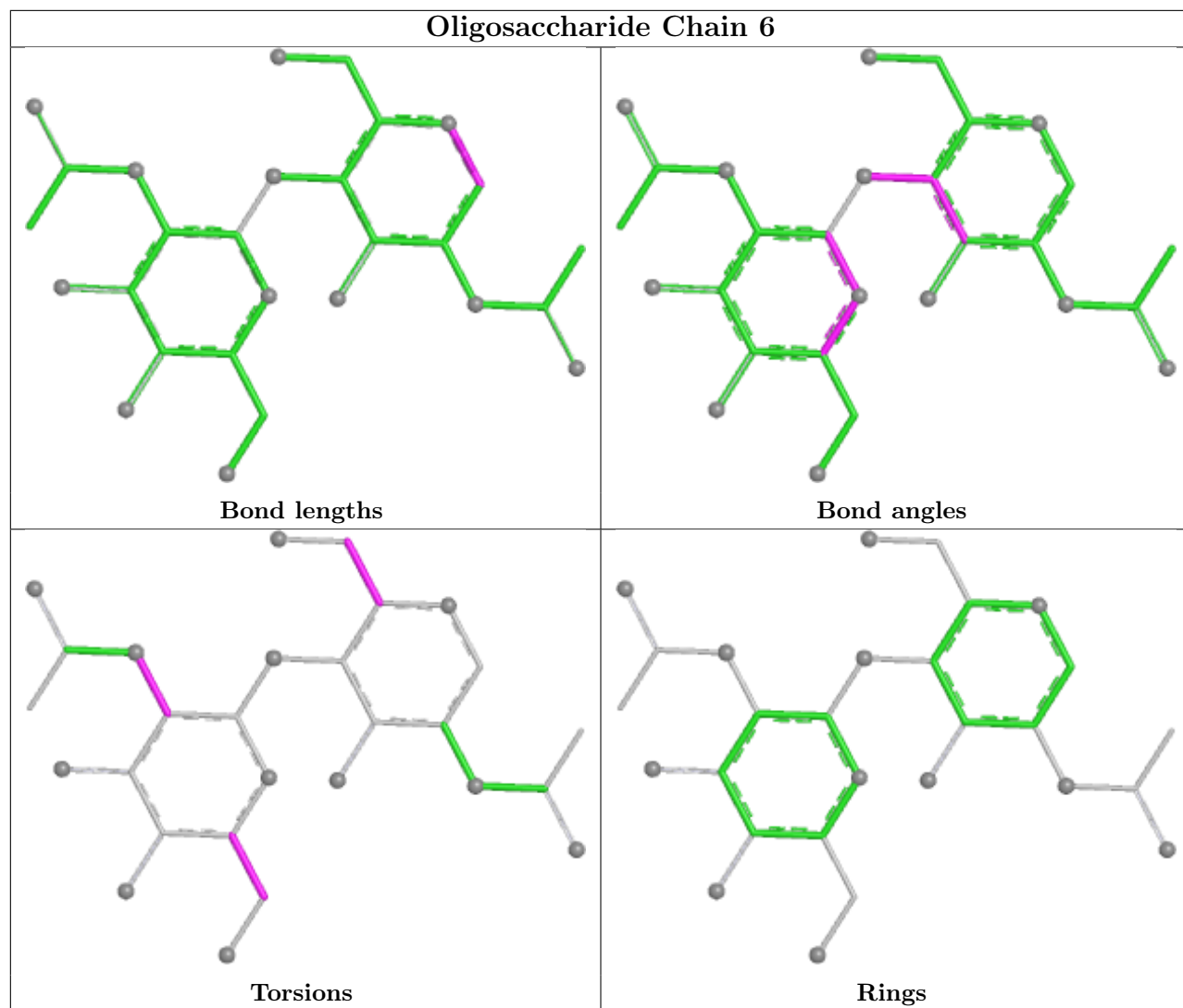


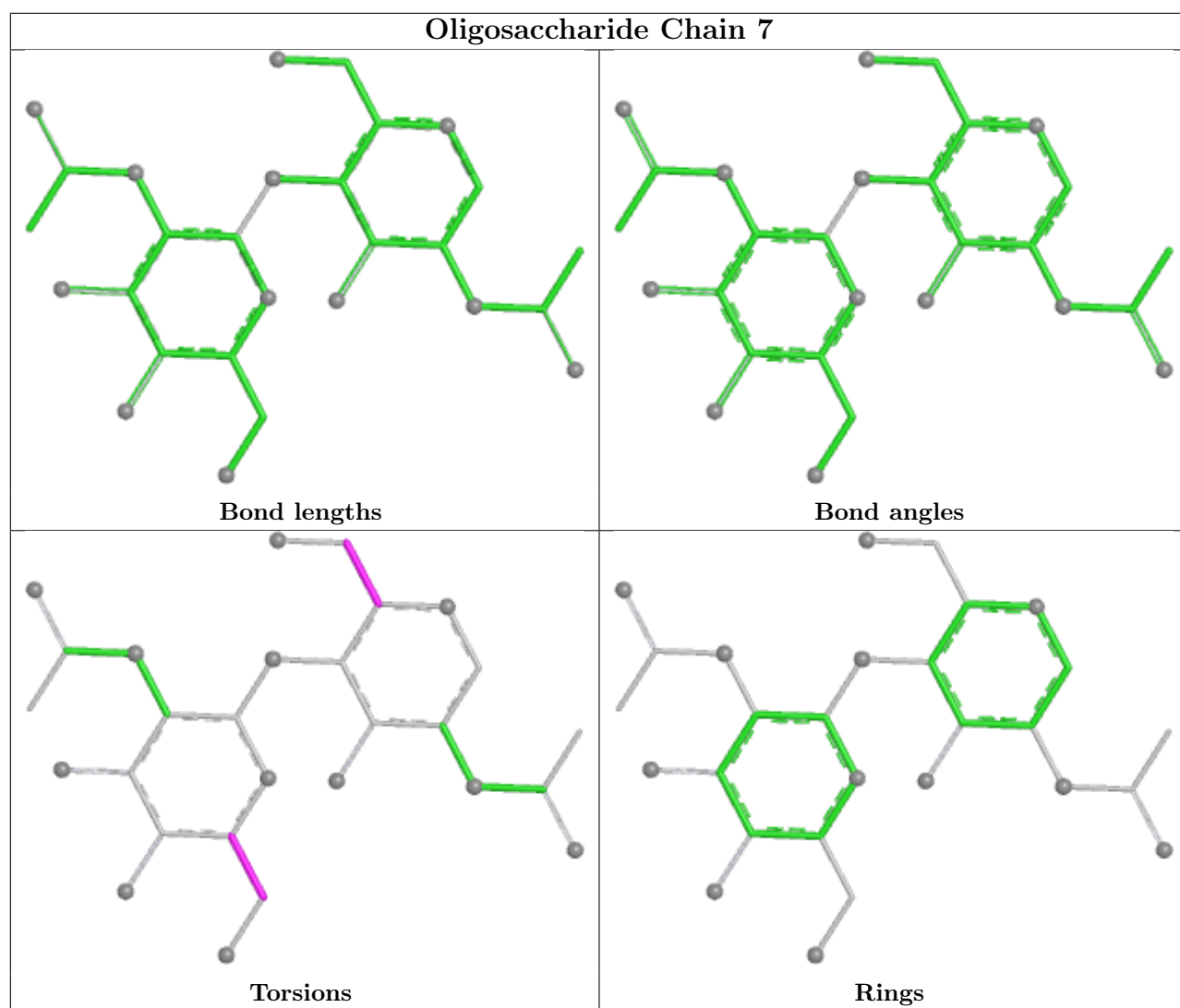


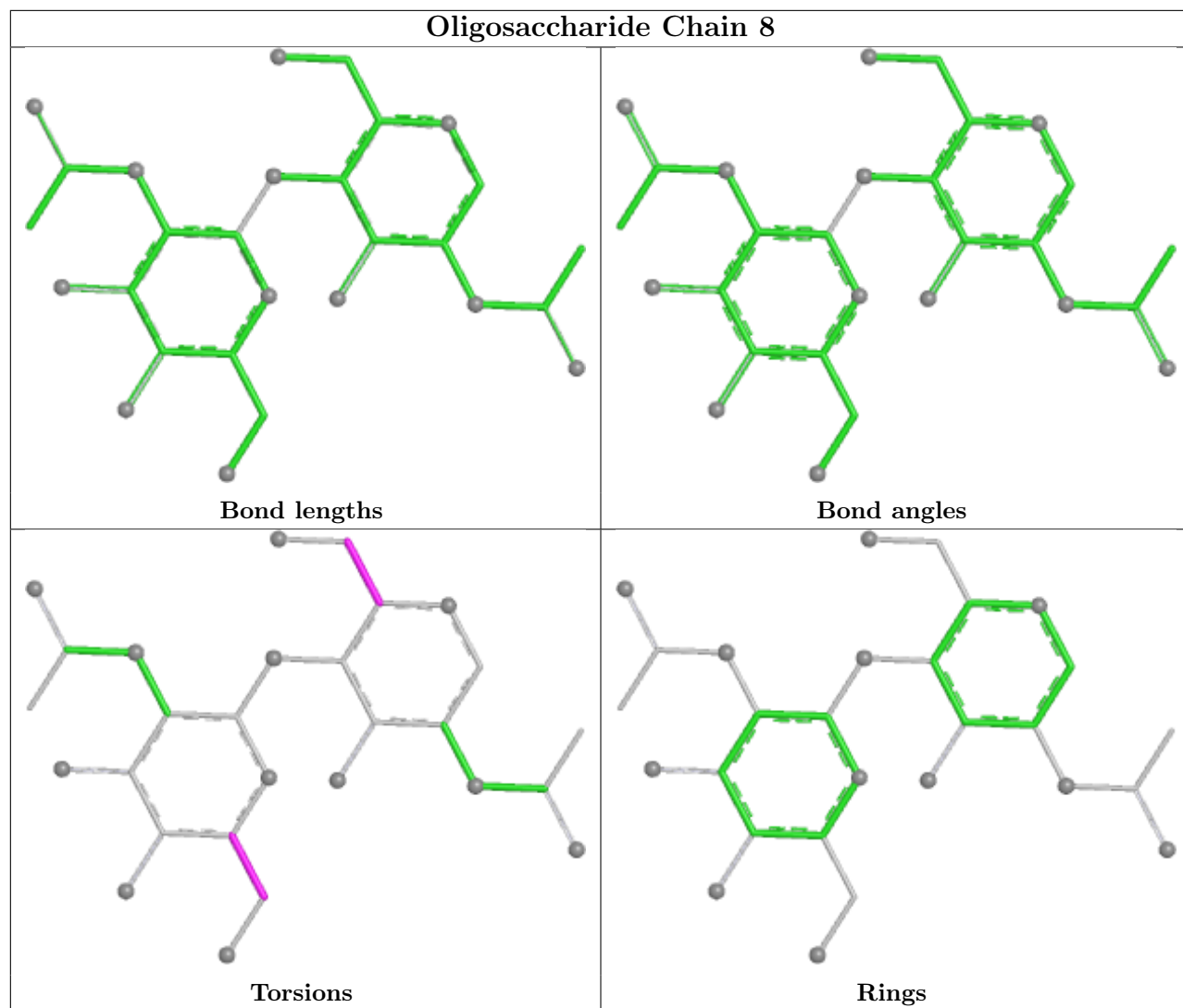


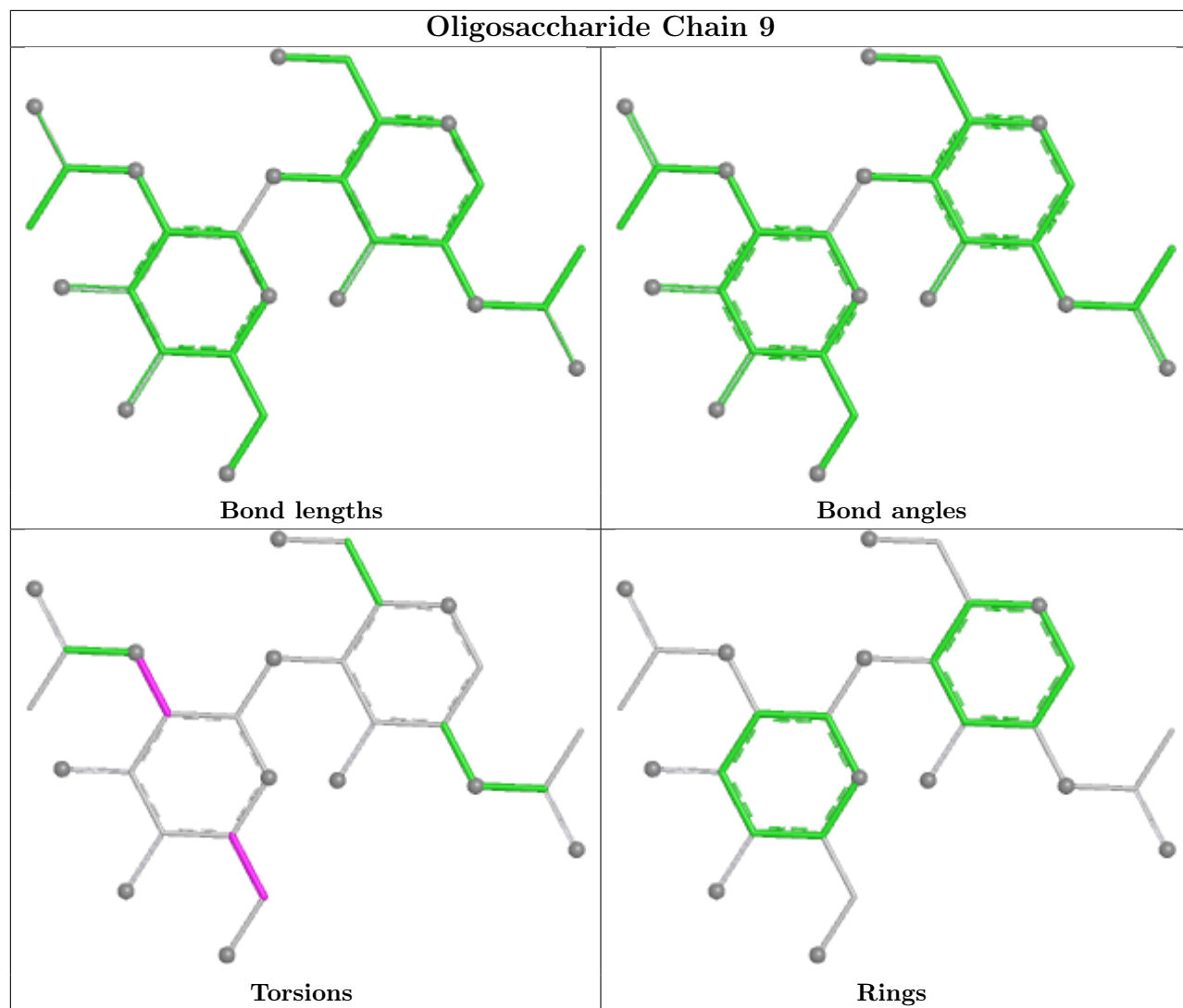


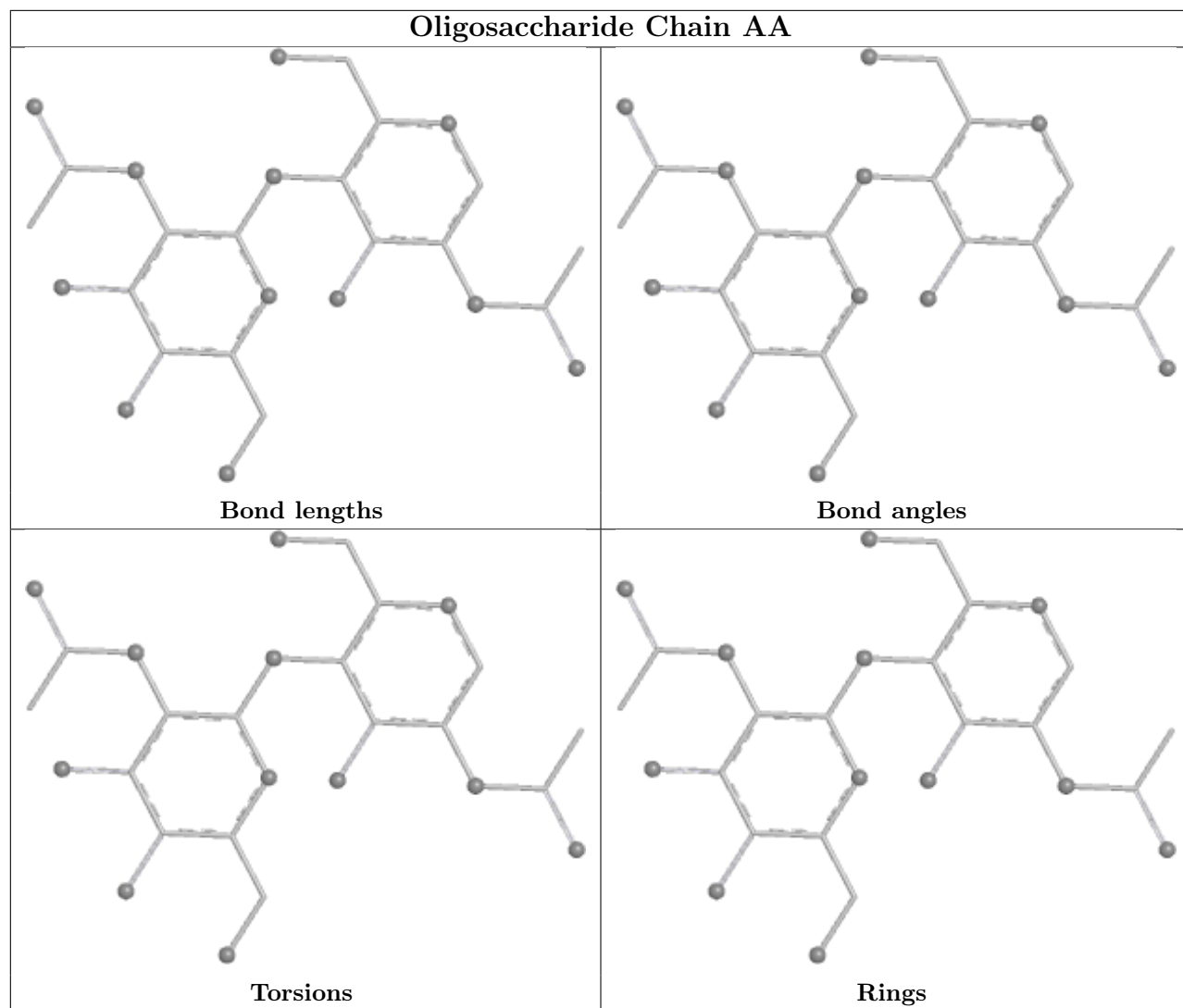


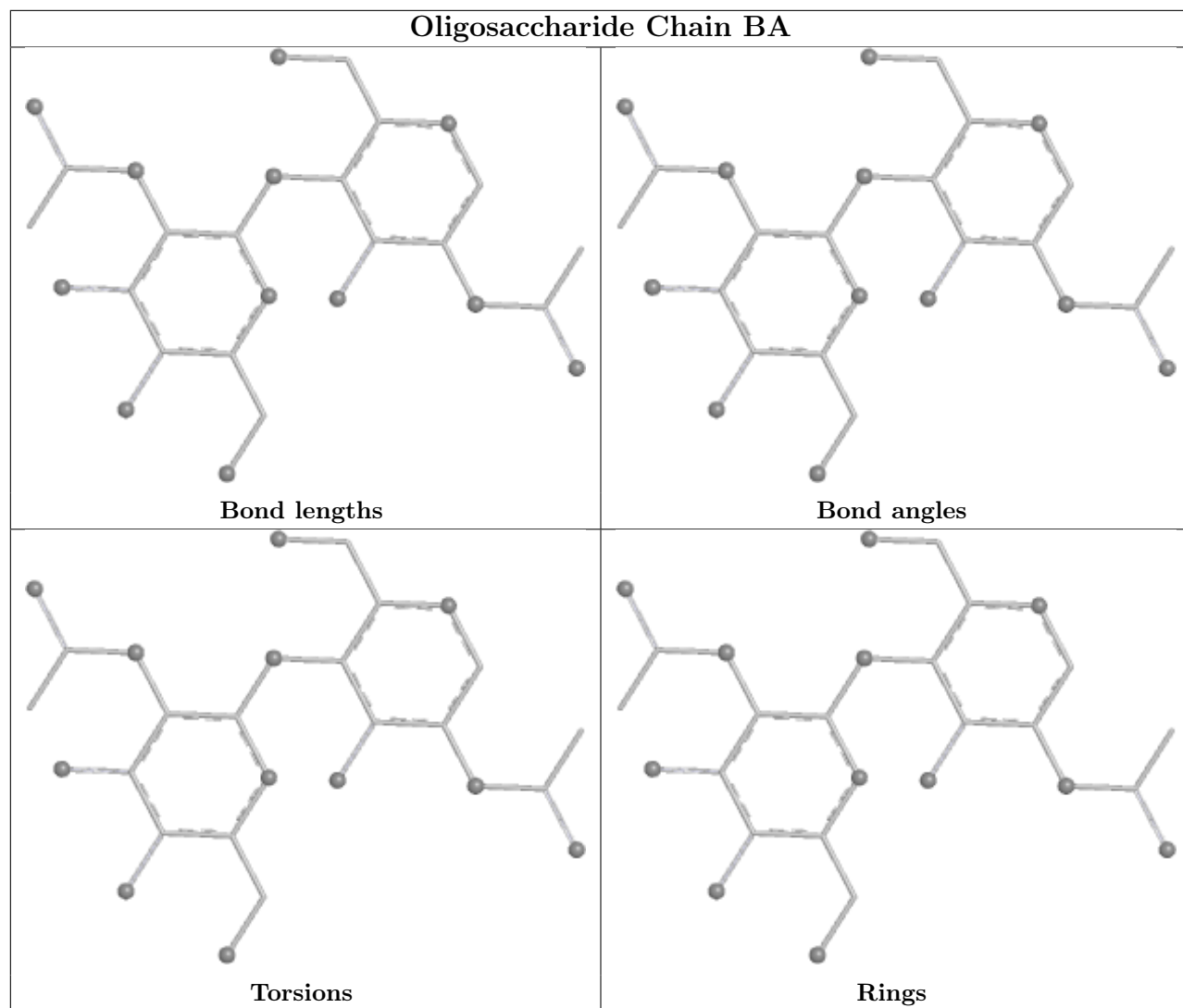


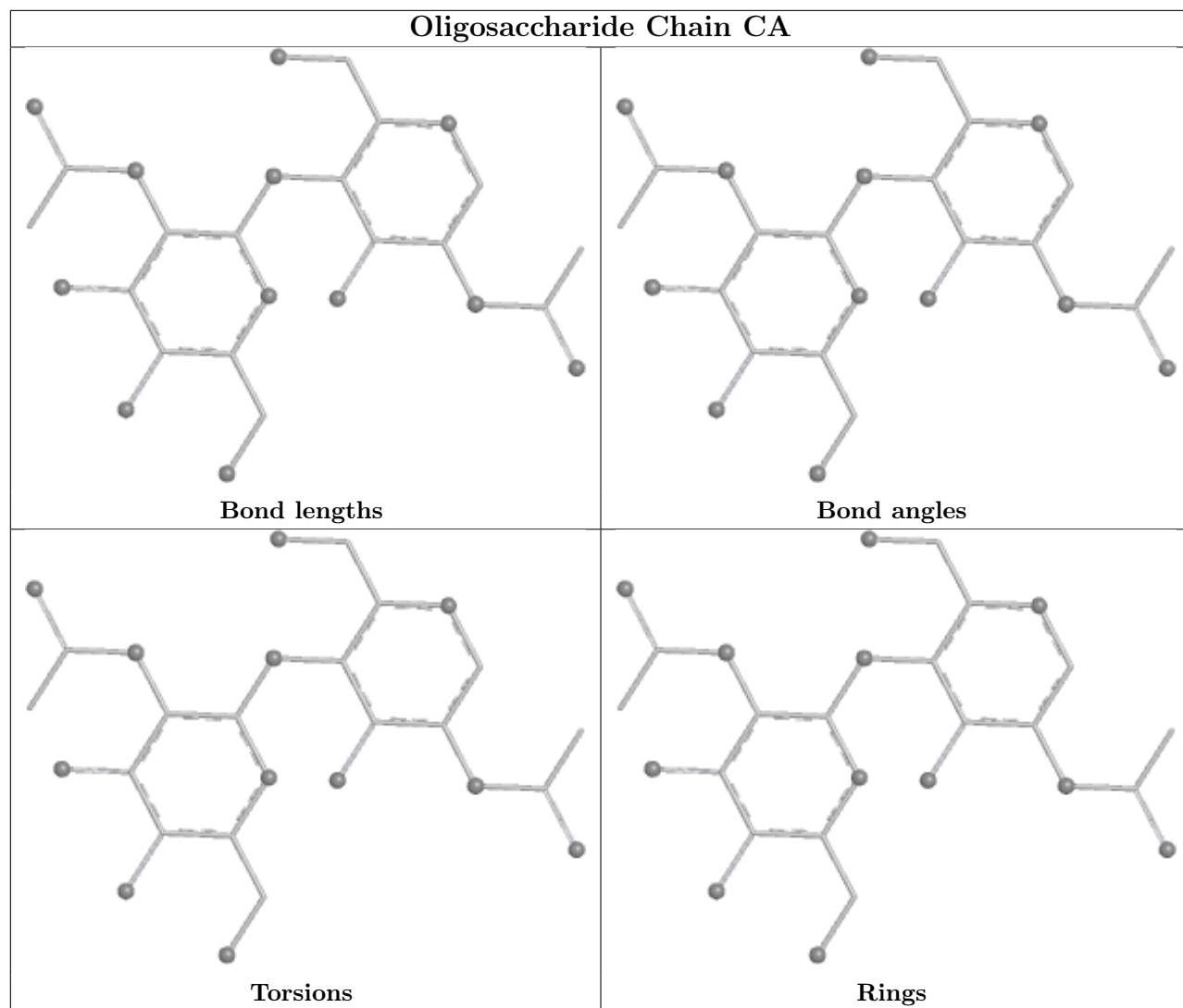


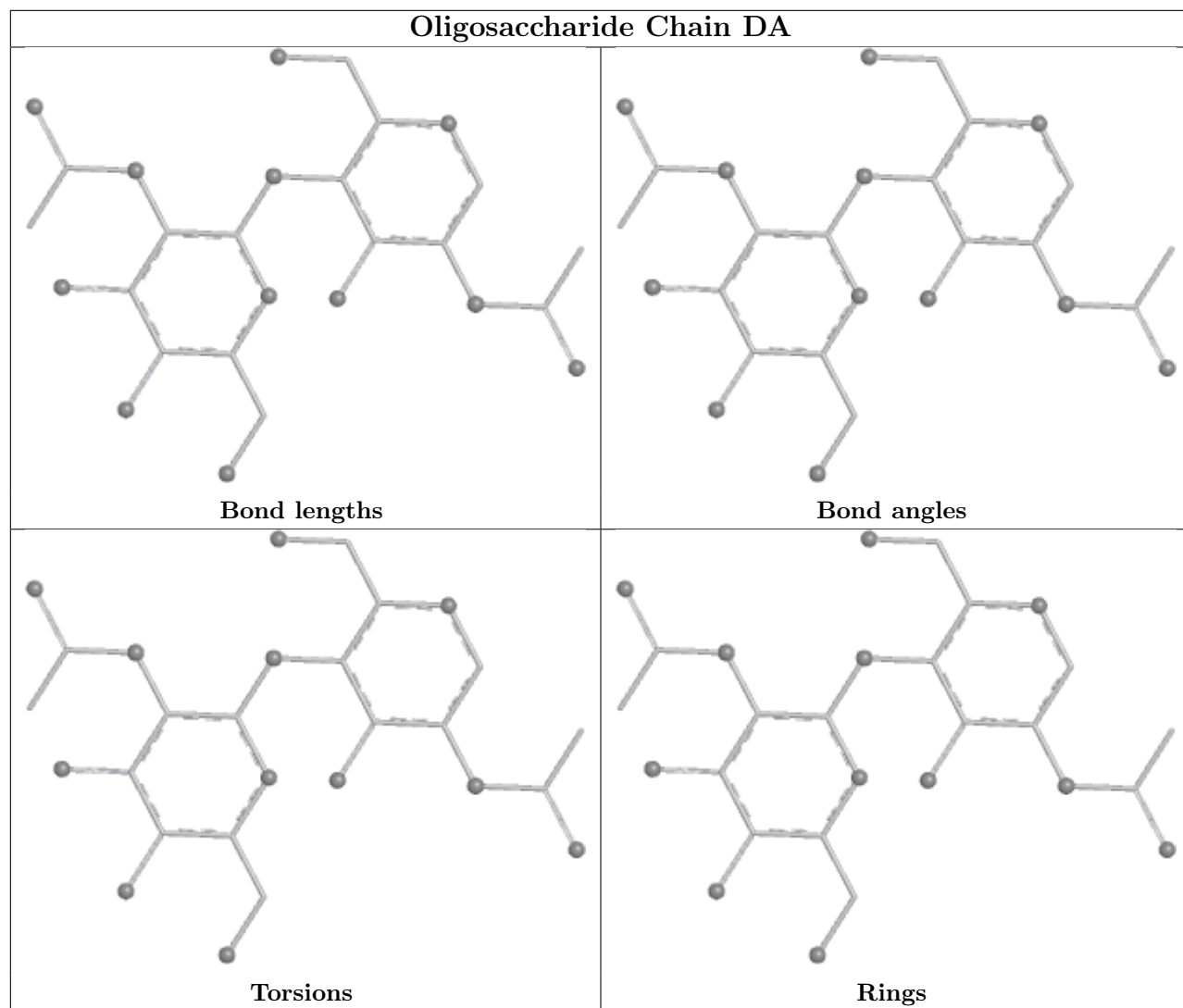


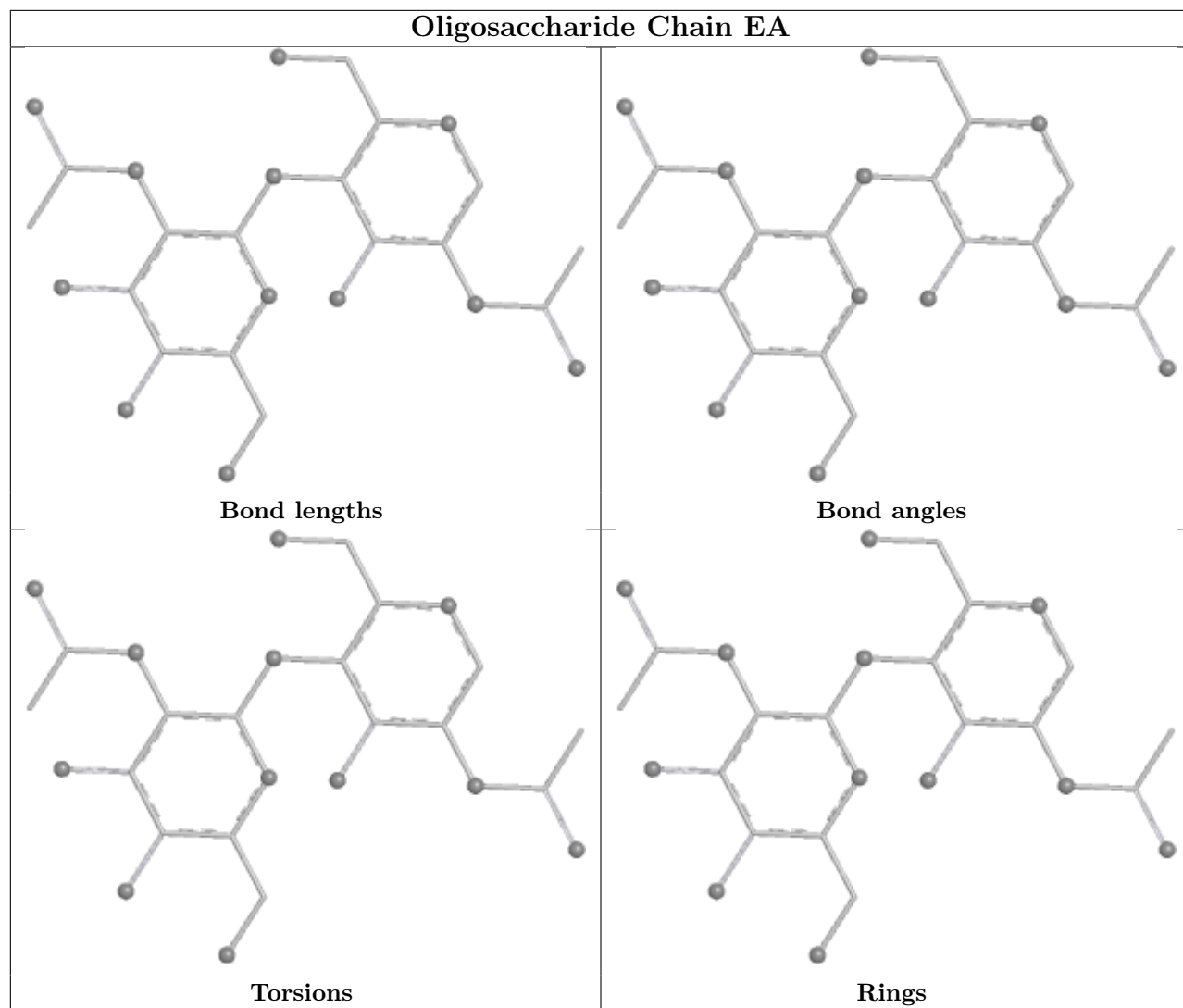


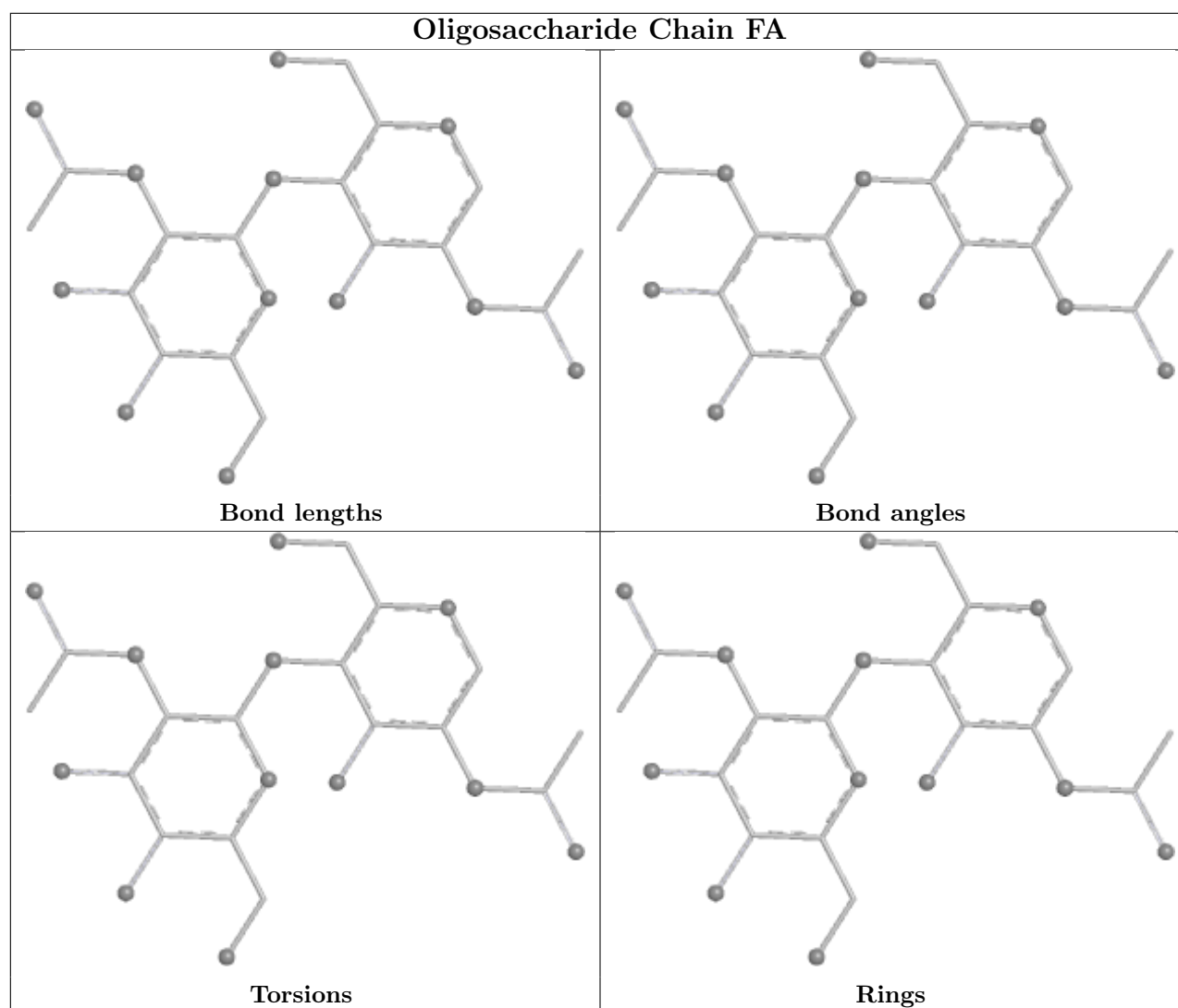












5.6 Ligand geometry [i](#)

Of 68 ligands modelled in this entry, 2 are monoatomic - leaving 66 for Mogul analysis.

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	$\# Z > 2$
5	NAG	E	1403	3	14,14,15	0.18	0	17,19,21	0.44	0
5	NAG	G	1402	3	14,14,15	0.21	0	17,19,21	0.67	0
5	NAG	B	901	2	14,14,15	0.39	0	17,19,21	0.61	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	NAG	F	1407	3	14,14,15	0.26	0	17,19,21	0.52	0
5	NAG	E	1409	3	14,14,15	0.48	0	17,19,21	0.38	0
5	NAG	F	1402	3	14,14,15	0.22	0	17,19,21	0.66	0
5	NAG	I	1410	-	14,14,15	0.37	0	17,19,21	0.43	0
5	NAG	F	1405	3	14,14,15	0.60	0	17,19,21	1.34	2 (11%)
5	NAG	I	1404	3	14,14,15	0.50	0	17,19,21	0.54	0
5	NAG	H	1405	3	14,14,15	0.60	0	17,19,21	1.34	2 (11%)
5	NAG	E	1404	3	14,14,15	0.51	0	17,19,21	0.55	0
5	NAG	J	1404	3	14,14,15	0.51	0	17,19,21	0.55	0
5	NAG	G	1405	3	14,14,15	0.60	0	17,19,21	1.34	2 (11%)
5	NAG	I	1406	3	14,14,15	0.29	0	17,19,21	0.41	0
5	NAG	C	701	1	14,14,15	0.37	0	17,19,21	0.45	0
6	LEU	C	705	-	6,8,8	1.02	1 (16%)	5,10,10	1.27	1 (20%)
5	NAG	J	1401	3	14,14,15	0.32	0	17,19,21	0.34	0
5	NAG	G	1407	3	14,14,15	0.24	0	17,19,21	0.51	0
5	NAG	J	1406	3	14,14,15	0.29	0	17,19,21	0.40	0
5	NAG	G	1403	3	14,14,15	0.20	0	17,19,21	0.44	0
5	NAG	F	1406	3	14,14,15	0.30	0	17,19,21	0.41	0
5	NAG	H	1407	3	14,14,15	0.25	0	17,19,21	0.51	0
5	NAG	H	1406	3	14,14,15	0.28	0	17,19,21	0.40	0
5	NAG	I	1401	3	14,14,15	0.31	0	17,19,21	0.36	0
5	NAG	H	1409	3	14,14,15	0.48	0	17,19,21	0.38	0
5	NAG	F	1409	3	14,14,15	0.42	0	17,19,21	1.15	2 (11%)
5	NAG	J	1403	3	14,14,15	0.20	0	17,19,21	0.44	0
5	NAG	J	1405	3	14,14,15	0.62	0	17,19,21	1.34	2 (11%)
5	NAG	C	702	1	14,14,15	0.36	0	17,19,21	0.42	0
5	NAG	I	1408	3	14,14,15	0.34	0	17,19,21	0.39	0
5	NAG	J	1408	3	14,14,15	0.33	0	17,19,21	0.40	0
5	NAG	E	1407	3	14,14,15	0.25	0	17,19,21	0.52	0
5	NAG	F	1403	3	14,14,15	0.20	0	17,19,21	0.44	0
5	NAG	H	1402	3	14,14,15	0.22	0	17,19,21	0.66	0
5	NAG	H	1401	3	14,14,15	0.32	0	17,19,21	0.35	0
5	NAG	A	701	1	14,14,15	0.36	0	17,19,21	0.45	0
5	NAG	E	1405	3	14,14,15	0.60	0	17,19,21	1.35	2 (11%)
5	NAG	G	1406	3	14,14,15	0.27	0	17,19,21	0.40	0
5	NAG	A	702	1	14,14,15	0.37	0	17,19,21	0.42	0
5	NAG	H	1403	3	14,14,15	0.17	0	17,19,21	0.44	0
5	NAG	F	1401	3	14,14,15	0.32	0	17,19,21	0.35	0
5	NAG	D	901	2	14,14,15	0.39	0	17,19,21	0.61	1 (5%)
5	NAG	G	1401	3	14,14,15	0.30	0	17,19,21	0.34	0
5	NAG	F	1408	3	14,14,15	0.32	0	17,19,21	0.40	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	G	1408	3	14,14,15	0.33	0	17,19,21	0.41	0
5	NAG	I	1409	3	14,14,15	0.43	0	17,19,21	1.15	2 (11%)
5	NAG	F	1404	3	14,14,15	0.51	0	17,19,21	0.55	0
5	NAG	H	1408	3	14,14,15	0.34	0	17,19,21	0.40	0
5	NAG	A	704	1	14,14,15	0.38	0	17,19,21	0.57	0
5	NAG	E	1408	3	14,14,15	0.34	0	17,19,21	0.40	0
5	NAG	A	703	1	14,14,15	0.41	0	17,19,21	0.67	1 (5%)
5	NAG	I	1403	3	14,14,15	0.20	0	17,19,21	0.45	0
5	NAG	F	1410	-	14,14,15	0.38	0	17,19,21	0.44	0
5	NAG	E	1401	3	14,14,15	0.31	0	17,19,21	0.36	0
5	NAG	E	1402	3	14,14,15	0.22	0	17,19,21	0.66	0
5	NAG	E	1406	3	14,14,15	0.28	0	17,19,21	0.40	0
5	NAG	G	1404	3	14,14,15	0.50	0	17,19,21	0.55	0
5	NAG	I	1402	3	14,14,15	0.21	0	17,19,21	0.66	0
5	NAG	I	1407	3	14,14,15	0.28	0	17,19,21	0.52	0
5	NAG	J	1402	3	14,14,15	0.20	0	17,19,21	0.66	0
5	NAG	H	1404	3	14,14,15	0.50	0	17,19,21	0.54	0
5	NAG	I	1405	3	14,14,15	0.60	0	17,19,21	1.35	2 (11%)
5	NAG	J	1407	3	14,14,15	0.24	0	17,19,21	0.52	0
6	LEU	A	705	-	6,8,8	1.03	1 (16%)	5,10,10	1.27	1 (20%)
5	NAG	C	704	1	14,14,15	0.38	0	17,19,21	0.57	0
5	NAG	C	703	1	14,14,15	0.40	0	17,19,21	0.66	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
5	NAG	E	1403	3	-	2/6/23/26	0/1/1/1
5	NAG	G	1402	3	-	2/6/23/26	0/1/1/1
5	NAG	B	901	2	-	2/6/23/26	0/1/1/1
5	NAG	F	1407	3	-	0/6/23/26	0/1/1/1
5	NAG	E	1409	3	-	2/6/23/26	0/1/1/1
5	NAG	F	1402	3	-	2/6/23/26	0/1/1/1
5	NAG	I	1410	-	-	0/6/23/26	0/1/1/1
5	NAG	F	1405	3	-	6/6/23/26	0/1/1/1
5	NAG	I	1404	3	-	2/6/23/26	0/1/1/1
5	NAG	H	1405	3	-	6/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	E	1404	3	-	2/6/23/26	0/1/1/1
5	NAG	J	1404	3	-	2/6/23/26	0/1/1/1
5	NAG	G	1405	3	-	6/6/23/26	0/1/1/1
5	NAG	I	1406	3	-	2/6/23/26	0/1/1/1
5	NAG	C	701	1	-	2/6/23/26	0/1/1/1
6	LEU	C	705	-	-	2/8/8/8	-
5	NAG	J	1401	3	-	2/6/23/26	0/1/1/1
5	NAG	G	1407	3	-	0/6/23/26	0/1/1/1
5	NAG	J	1406	3	-	2/6/23/26	0/1/1/1
5	NAG	G	1403	3	-	2/6/23/26	0/1/1/1
5	NAG	F	1406	3	-	2/6/23/26	0/1/1/1
5	NAG	H	1407	3	-	0/6/23/26	0/1/1/1
5	NAG	H	1406	3	-	2/6/23/26	0/1/1/1
5	NAG	I	1401	3	-	2/6/23/26	0/1/1/1
5	NAG	H	1409	3	-	2/6/23/26	0/1/1/1
5	NAG	F	1409	3	-	0/6/23/26	0/1/1/1
5	NAG	J	1403	3	-	2/6/23/26	0/1/1/1
5	NAG	J	1405	3	-	6/6/23/26	0/1/1/1
5	NAG	C	702	1	-	2/6/23/26	0/1/1/1
5	NAG	I	1408	3	-	2/6/23/26	0/1/1/1
5	NAG	J	1408	3	-	2/6/23/26	0/1/1/1
5	NAG	E	1407	3	-	0/6/23/26	0/1/1/1
5	NAG	F	1403	3	-	2/6/23/26	0/1/1/1
5	NAG	H	1402	3	-	2/6/23/26	0/1/1/1
5	NAG	H	1401	3	-	2/6/23/26	0/1/1/1
5	NAG	A	701	1	-	2/6/23/26	0/1/1/1
5	NAG	E	1405	3	-	6/6/23/26	0/1/1/1
5	NAG	G	1406	3	-	2/6/23/26	0/1/1/1
5	NAG	A	702	1	-	2/6/23/26	0/1/1/1
5	NAG	H	1403	3	-	2/6/23/26	0/1/1/1
5	NAG	F	1401	3	-	2/6/23/26	0/1/1/1
5	NAG	D	901	2	-	2/6/23/26	0/1/1/1
5	NAG	G	1401	3	-	2/6/23/26	0/1/1/1
5	NAG	F	1408	3	-	2/6/23/26	0/1/1/1
5	NAG	G	1408	3	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	I	1409	3	-	0/6/23/26	0/1/1/1
5	NAG	F	1404	3	-	2/6/23/26	0/1/1/1
5	NAG	H	1408	3	-	2/6/23/26	0/1/1/1
5	NAG	A	704	1	-	0/6/23/26	0/1/1/1
5	NAG	E	1408	3	-	2/6/23/26	0/1/1/1
5	NAG	A	703	1	-	2/6/23/26	0/1/1/1
5	NAG	I	1403	3	-	2/6/23/26	0/1/1/1
5	NAG	F	1410	-	-	0/6/23/26	0/1/1/1
5	NAG	E	1401	3	-	2/6/23/26	0/1/1/1
5	NAG	E	1402	3	-	2/6/23/26	0/1/1/1
5	NAG	E	1406	3	-	2/6/23/26	0/1/1/1
5	NAG	G	1404	3	-	2/6/23/26	0/1/1/1
5	NAG	I	1402	3	-	2/6/23/26	0/1/1/1
5	NAG	I	1407	3	-	0/6/23/26	0/1/1/1
5	NAG	J	1402	3	-	2/6/23/26	0/1/1/1
5	NAG	H	1404	3	-	2/6/23/26	0/1/1/1
5	NAG	I	1405	3	-	6/6/23/26	0/1/1/1
5	NAG	J	1407	3	-	0/6/23/26	0/1/1/1
6	LEU	A	705	-	-	2/8/8/8	-
5	NAG	C	704	1	-	0/6/23/26	0/1/1/1
5	NAG	C	703	1	-	2/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	705	LEU	OXT-C	-2.41	1.23	1.30
6	C	705	LEU	OXT-C	-2.38	1.23	1.30

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	1405	NAG	C2-N2-C7	4.62	129.09	122.90
5	I	1405	NAG	C2-N2-C7	4.61	129.08	122.90
5	H	1405	NAG	C2-N2-C7	4.61	129.07	122.90
5	G	1405	NAG	C2-N2-C7	4.59	129.05	122.90
5	F	1405	NAG	C2-N2-C7	4.59	129.04	122.90
5	J	1405	NAG	C2-N2-C7	4.58	129.03	122.90
6	C	705	LEU	OXT-C-O	-2.82	117.67	124.08
6	A	705	LEU	OXT-C-O	-2.81	117.71	124.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	1409	NAG	C8-C7-N2	2.29	119.92	116.12
5	I	1409	NAG	C8-C7-N2	2.29	119.91	116.12
5	F	1409	NAG	C2-N2-C7	-2.26	119.88	122.90
5	I	1409	NAG	C2-N2-C7	-2.21	119.94	122.90
5	H	1405	NAG	C1-C2-N2	2.13	113.79	110.43
5	I	1405	NAG	C1-C2-N2	2.13	113.79	110.43
5	F	1405	NAG	C1-C2-N2	2.11	113.76	110.43
5	B	901	NAG	C1-O5-C5	2.09	114.98	112.19
5	E	1405	NAG	C1-C2-N2	2.08	113.72	110.43
5	G	1405	NAG	C1-C2-N2	2.08	113.71	110.43
5	J	1405	NAG	C1-C2-N2	2.07	113.69	110.43
5	D	901	NAG	C1-O5-C5	2.05	114.94	112.19
5	A	703	NAG	C1-O5-C5	2.05	114.93	112.19
5	C	703	NAG	C1-O5-C5	2.02	114.90	112.19

There are no chirality outliers.

All (132) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	705	LEU	N-CA-CB-CG
6	C	705	LEU	N-CA-CB-CG
5	A	701	NAG	O5-C5-C6-O6
5	C	701	NAG	O5-C5-C6-O6
5	E	1406	NAG	O5-C5-C6-O6
5	F	1406	NAG	O5-C5-C6-O6
5	G	1406	NAG	O5-C5-C6-O6
5	H	1406	NAG	O5-C5-C6-O6
5	I	1406	NAG	O5-C5-C6-O6
5	J	1406	NAG	O5-C5-C6-O6
5	A	701	NAG	C4-C5-C6-O6
5	C	701	NAG	C4-C5-C6-O6
5	E	1404	NAG	O5-C5-C6-O6
5	F	1402	NAG	O5-C5-C6-O6
5	F	1404	NAG	O5-C5-C6-O6
5	G	1402	NAG	O5-C5-C6-O6
5	G	1404	NAG	O5-C5-C6-O6
5	H	1404	NAG	O5-C5-C6-O6
5	I	1402	NAG	O5-C5-C6-O6
5	I	1404	NAG	O5-C5-C6-O6
5	J	1402	NAG	O5-C5-C6-O6
5	J	1404	NAG	O5-C5-C6-O6
5	J	1405	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
5	E	1402	NAG	O5-C5-C6-O6
5	F	1401	NAG	O5-C5-C6-O6
5	G	1401	NAG	O5-C5-C6-O6
5	H	1402	NAG	O5-C5-C6-O6
5	I	1401	NAG	O5-C5-C6-O6
5	J	1401	NAG	O5-C5-C6-O6
5	E	1402	NAG	C4-C5-C6-O6
5	F	1402	NAG	C4-C5-C6-O6
5	G	1402	NAG	C4-C5-C6-O6
5	H	1402	NAG	C4-C5-C6-O6
5	I	1402	NAG	C4-C5-C6-O6
5	J	1402	NAG	C4-C5-C6-O6
5	E	1401	NAG	O5-C5-C6-O6
5	E	1405	NAG	O5-C5-C6-O6
5	F	1405	NAG	O5-C5-C6-O6
5	G	1405	NAG	O5-C5-C6-O6
5	H	1401	NAG	O5-C5-C6-O6
5	H	1405	NAG	O5-C5-C6-O6
5	I	1405	NAG	O5-C5-C6-O6
5	E	1409	NAG	C4-C5-C6-O6
5	H	1409	NAG	C4-C5-C6-O6
5	E	1405	NAG	C4-C5-C6-O6
5	F	1405	NAG	C4-C5-C6-O6
5	G	1405	NAG	C4-C5-C6-O6
5	H	1405	NAG	C4-C5-C6-O6
5	I	1405	NAG	C4-C5-C6-O6
5	J	1405	NAG	C4-C5-C6-O6
5	J	1408	NAG	O5-C5-C6-O6
5	E	1408	NAG	O5-C5-C6-O6
5	F	1408	NAG	O5-C5-C6-O6
5	G	1408	NAG	O5-C5-C6-O6
5	H	1408	NAG	O5-C5-C6-O6
5	I	1408	NAG	O5-C5-C6-O6
5	E	1409	NAG	O5-C5-C6-O6
5	H	1409	NAG	O5-C5-C6-O6
5	E	1406	NAG	C4-C5-C6-O6
5	F	1406	NAG	C4-C5-C6-O6
5	G	1406	NAG	C4-C5-C6-O6
5	H	1406	NAG	C4-C5-C6-O6
5	I	1406	NAG	C4-C5-C6-O6
5	J	1406	NAG	C4-C5-C6-O6
5	A	703	NAG	C8-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
5	A	703	NAG	O7-C7-N2-C2
5	C	703	NAG	C8-C7-N2-C2
5	C	703	NAG	O7-C7-N2-C2
5	E	1405	NAG	C8-C7-N2-C2
5	E	1405	NAG	O7-C7-N2-C2
5	F	1405	NAG	C8-C7-N2-C2
5	F	1405	NAG	O7-C7-N2-C2
5	G	1405	NAG	C8-C7-N2-C2
5	G	1405	NAG	O7-C7-N2-C2
5	H	1405	NAG	C8-C7-N2-C2
5	H	1405	NAG	O7-C7-N2-C2
5	I	1405	NAG	C8-C7-N2-C2
5	I	1405	NAG	O7-C7-N2-C2
5	J	1405	NAG	C8-C7-N2-C2
5	J	1405	NAG	O7-C7-N2-C2
5	A	702	NAG	O5-C5-C6-O6
5	C	702	NAG	O5-C5-C6-O6
5	E	1404	NAG	C4-C5-C6-O6
5	F	1404	NAG	C4-C5-C6-O6
5	G	1404	NAG	C4-C5-C6-O6
5	H	1404	NAG	C4-C5-C6-O6
5	I	1404	NAG	C4-C5-C6-O6
5	J	1404	NAG	C4-C5-C6-O6
5	B	901	NAG	O5-C5-C6-O6
5	D	901	NAG	O5-C5-C6-O6
5	G	1403	NAG	O5-C5-C6-O6
5	E	1403	NAG	C4-C5-C6-O6
5	F	1403	NAG	C4-C5-C6-O6
5	G	1403	NAG	C4-C5-C6-O6
5	H	1403	NAG	C4-C5-C6-O6
5	I	1403	NAG	C4-C5-C6-O6
5	J	1403	NAG	C4-C5-C6-O6
5	E	1403	NAG	O5-C5-C6-O6
5	F	1403	NAG	O5-C5-C6-O6
5	H	1403	NAG	O5-C5-C6-O6
5	I	1403	NAG	O5-C5-C6-O6
5	J	1403	NAG	O5-C5-C6-O6
5	F	1408	NAG	C4-C5-C6-O6
5	I	1408	NAG	C4-C5-C6-O6
5	J	1408	NAG	C4-C5-C6-O6
5	E	1408	NAG	C4-C5-C6-O6
5	G	1408	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
5	H	1408	NAG	C4-C5-C6-O6
5	C	702	NAG	C4-C5-C6-O6
5	A	702	NAG	C4-C5-C6-O6
5	E	1401	NAG	C4-C5-C6-O6
5	F	1401	NAG	C4-C5-C6-O6
5	H	1401	NAG	C4-C5-C6-O6
5	I	1401	NAG	C4-C5-C6-O6
5	J	1401	NAG	C4-C5-C6-O6
5	G	1401	NAG	C4-C5-C6-O6
5	B	901	NAG	C4-C5-C6-O6
5	D	901	NAG	C4-C5-C6-O6
5	E	1405	NAG	C1-C2-N2-C7
5	F	1405	NAG	C1-C2-N2-C7
5	G	1405	NAG	C1-C2-N2-C7
5	H	1405	NAG	C1-C2-N2-C7
5	I	1405	NAG	C1-C2-N2-C7
5	J	1405	NAG	C1-C2-N2-C7
5	E	1405	NAG	C3-C2-N2-C7
5	F	1405	NAG	C3-C2-N2-C7
5	G	1405	NAG	C3-C2-N2-C7
5	H	1405	NAG	C3-C2-N2-C7
5	I	1405	NAG	C3-C2-N2-C7
5	J	1405	NAG	C3-C2-N2-C7
6	A	705	LEU	OXT-C-CA-N
6	C	705	LEU	OXT-C-CA-N

There are no ring outliers.

16 monomers are involved in 42 short contacts:

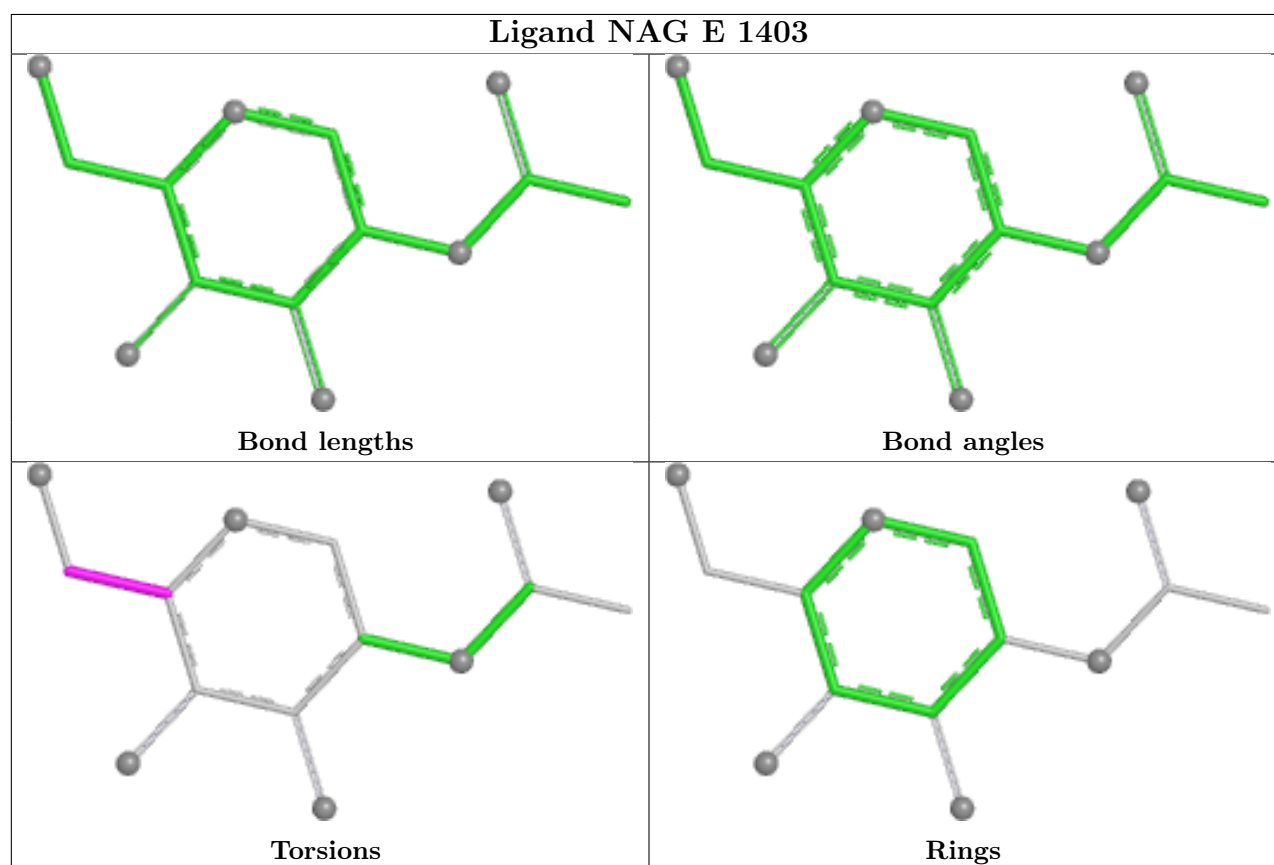
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	G	1402	NAG	3	0
5	F	1402	NAG	3	0
5	I	1410	NAG	4	0
5	F	1405	NAG	1	0
5	H	1405	NAG	2	0
5	G	1405	NAG	5	0
5	F	1409	NAG	4	0
5	J	1405	NAG	5	0
5	H	1402	NAG	3	0
5	E	1405	NAG	2	0
5	I	1409	NAG	4	0
5	F	1410	NAG	4	0

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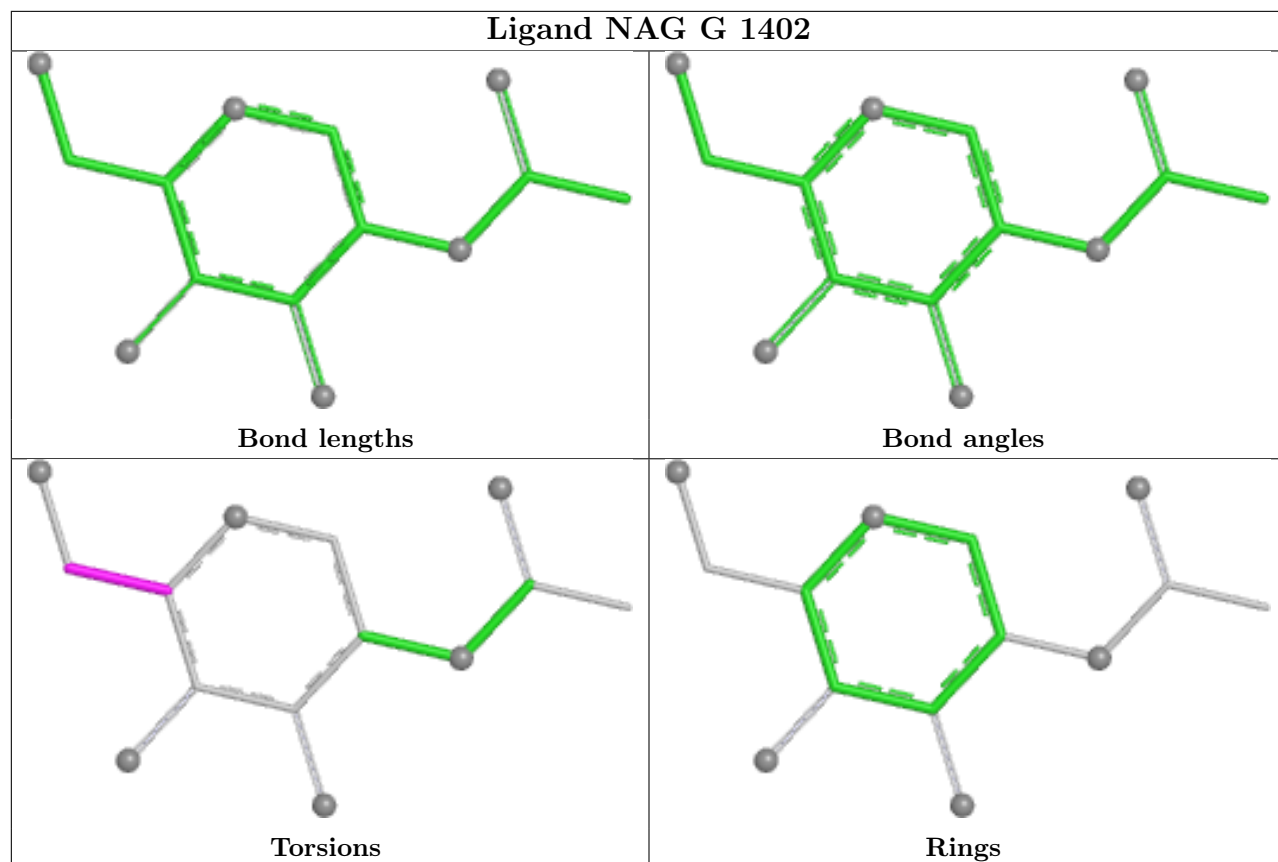
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	E	1402	NAG	3	0
5	I	1402	NAG	3	0
5	J	1402	NAG	3	0
5	I	1405	NAG	1	0

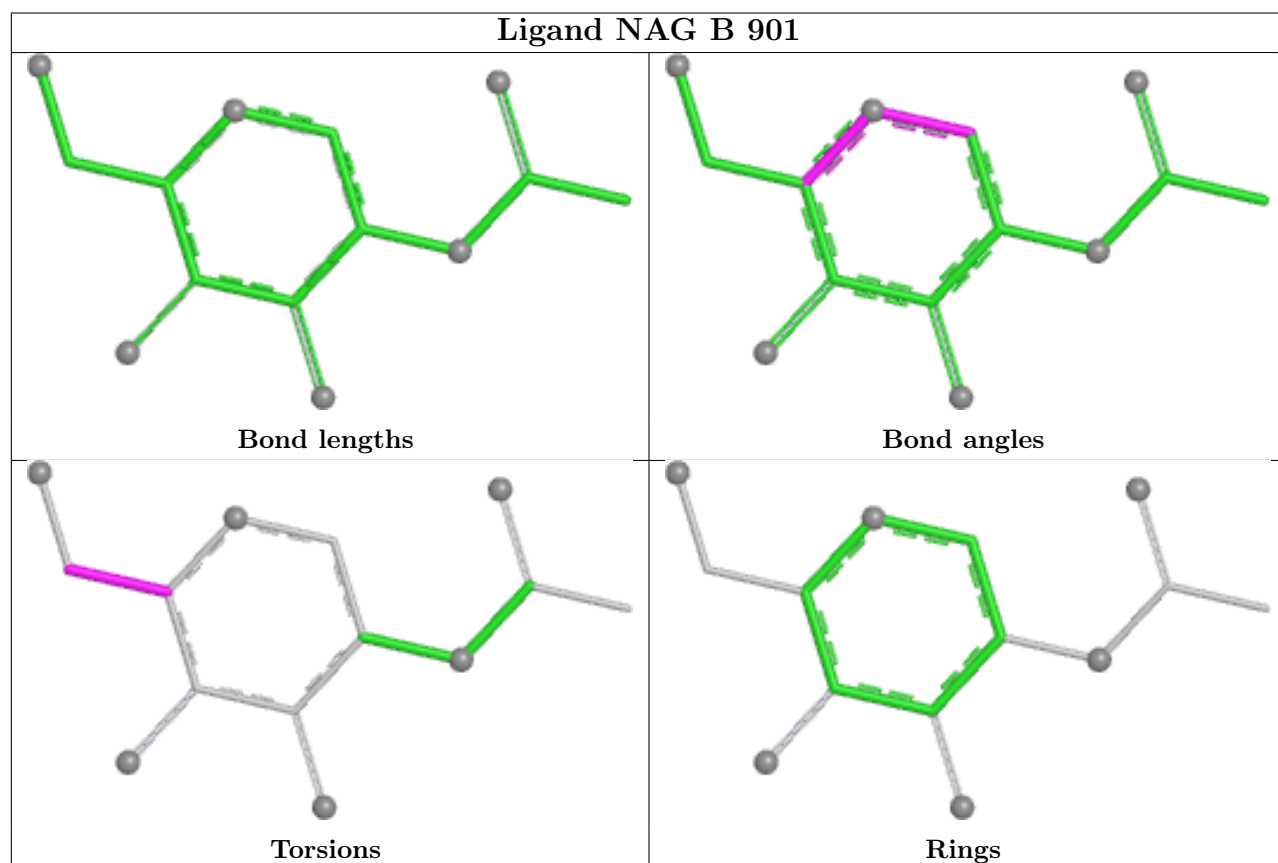
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

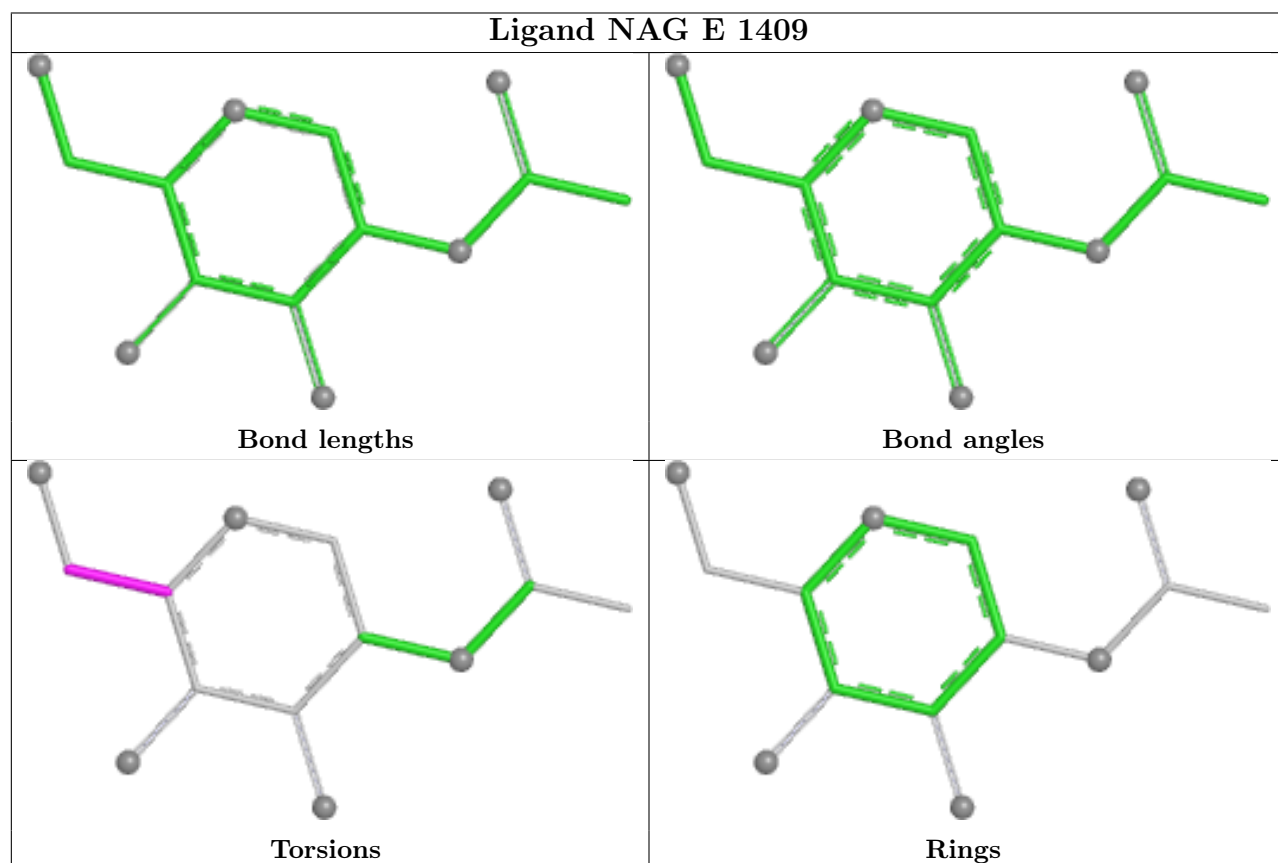
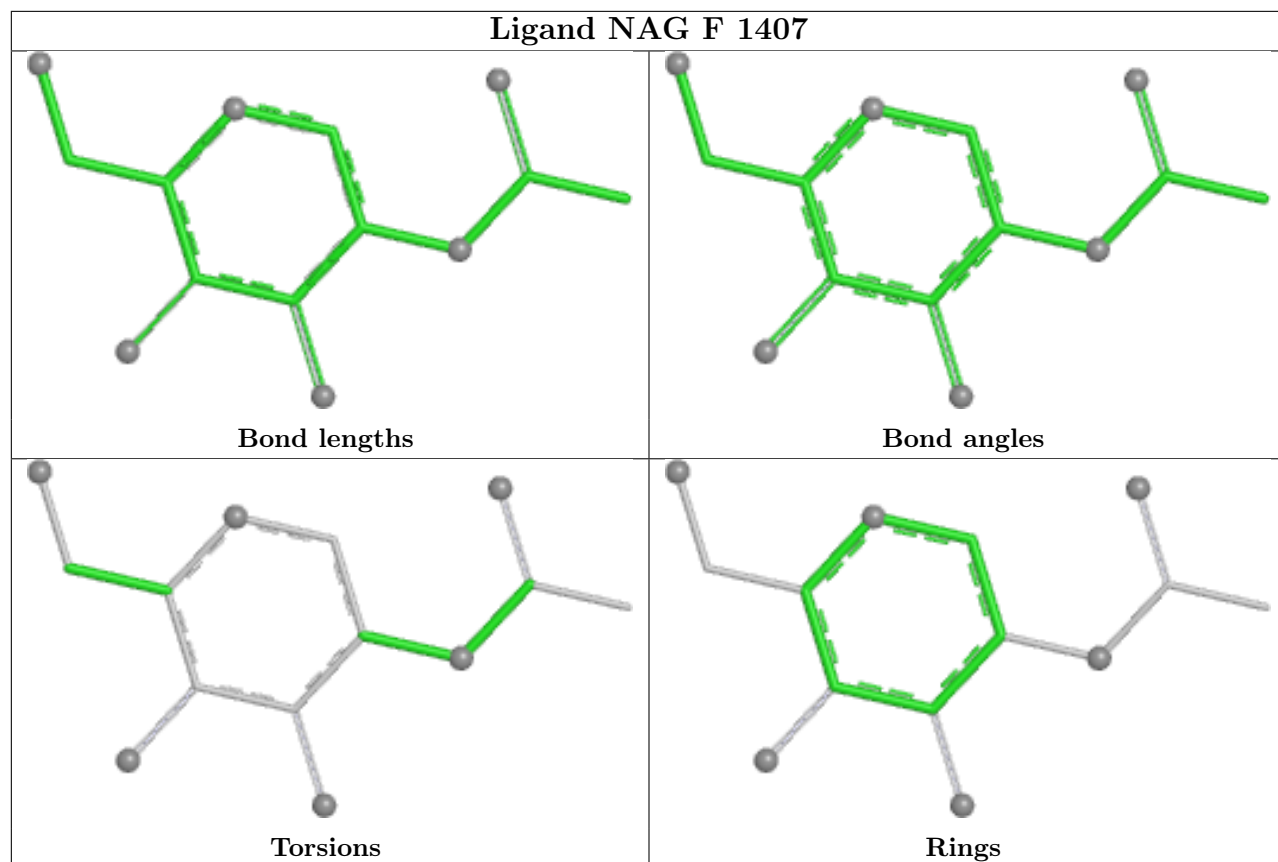


Ligand NAG G 1402

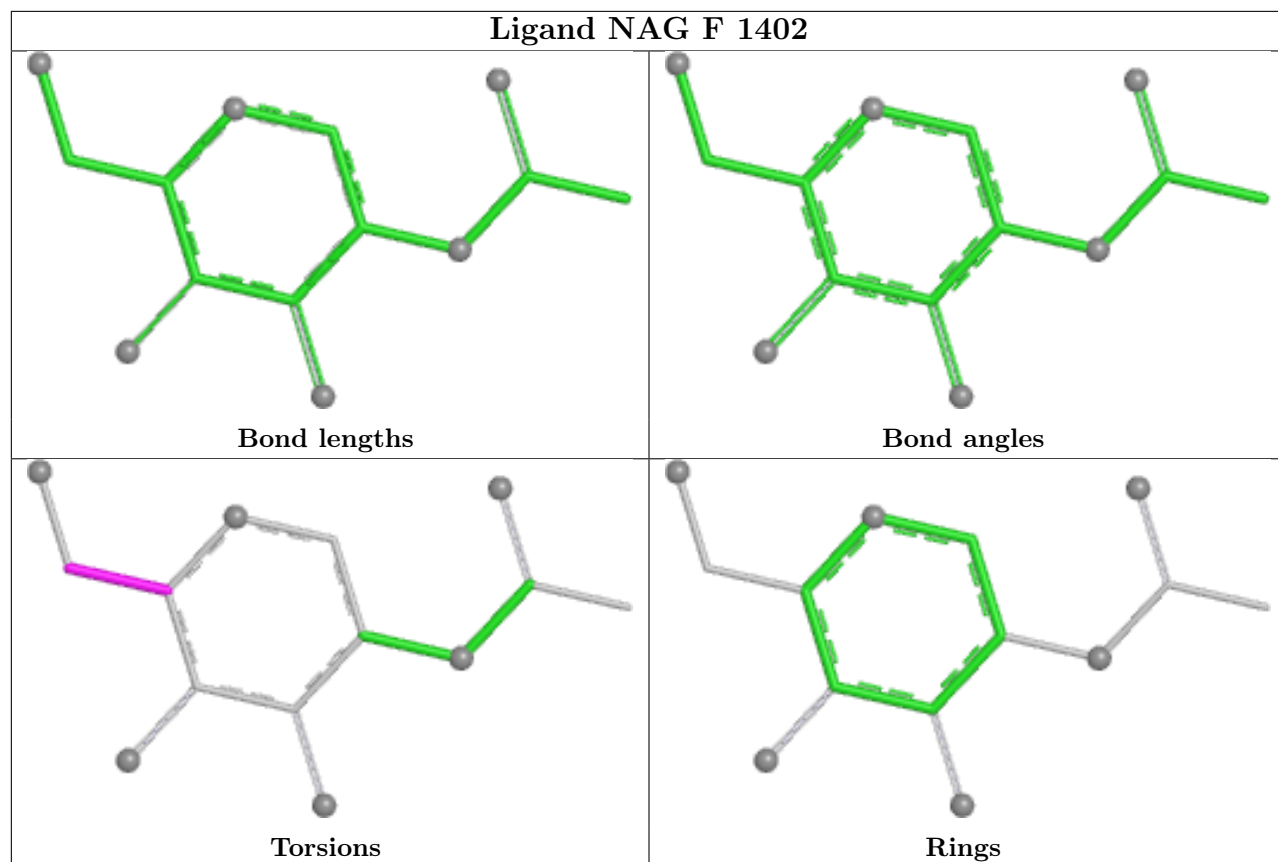


Ligand NAG B 901

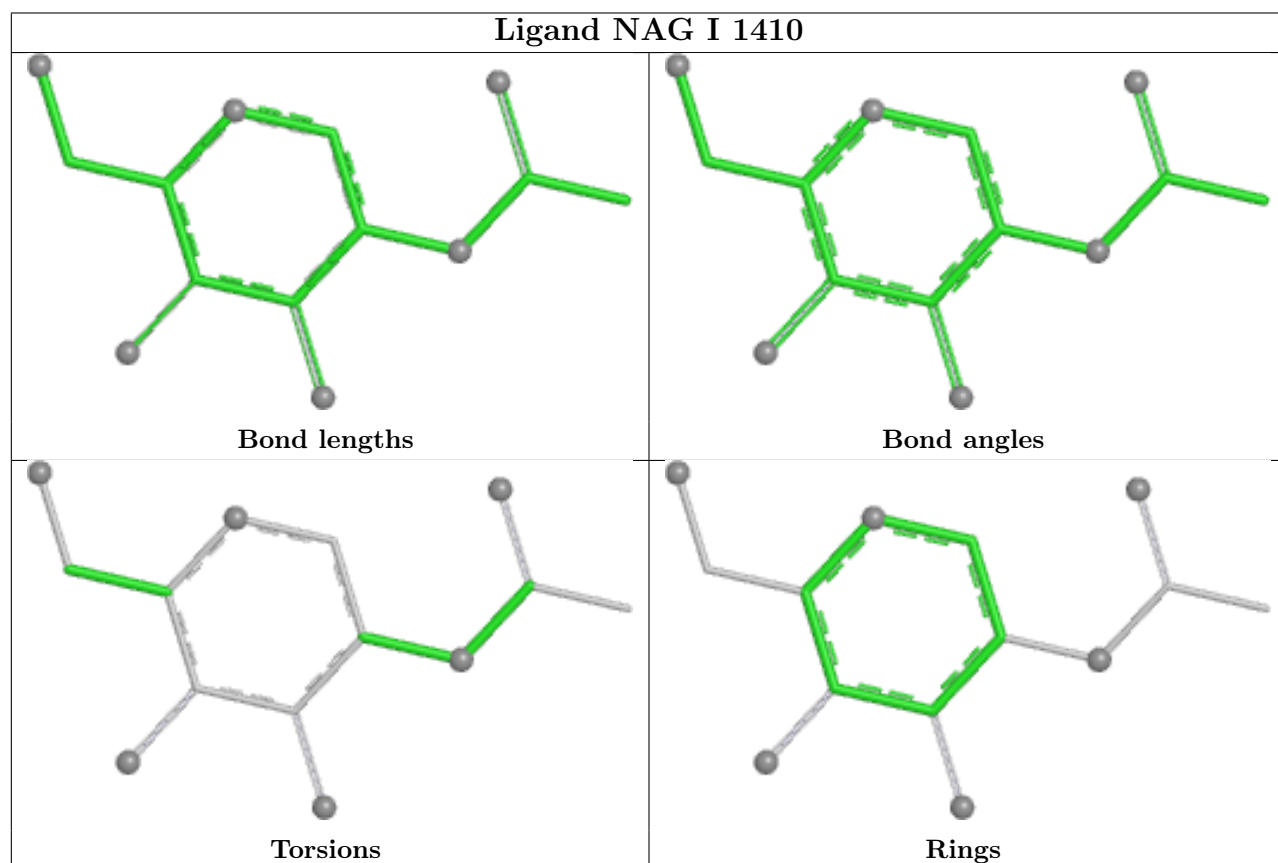


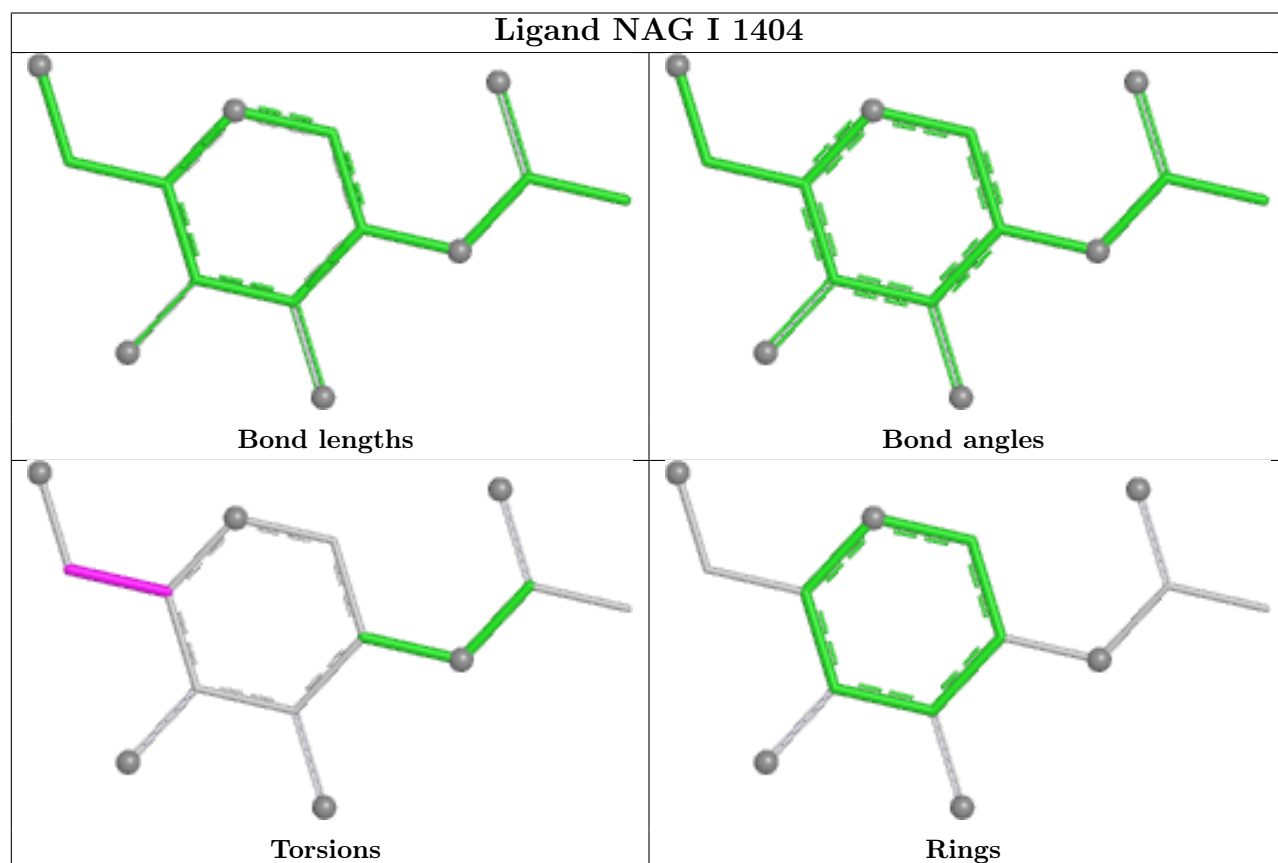
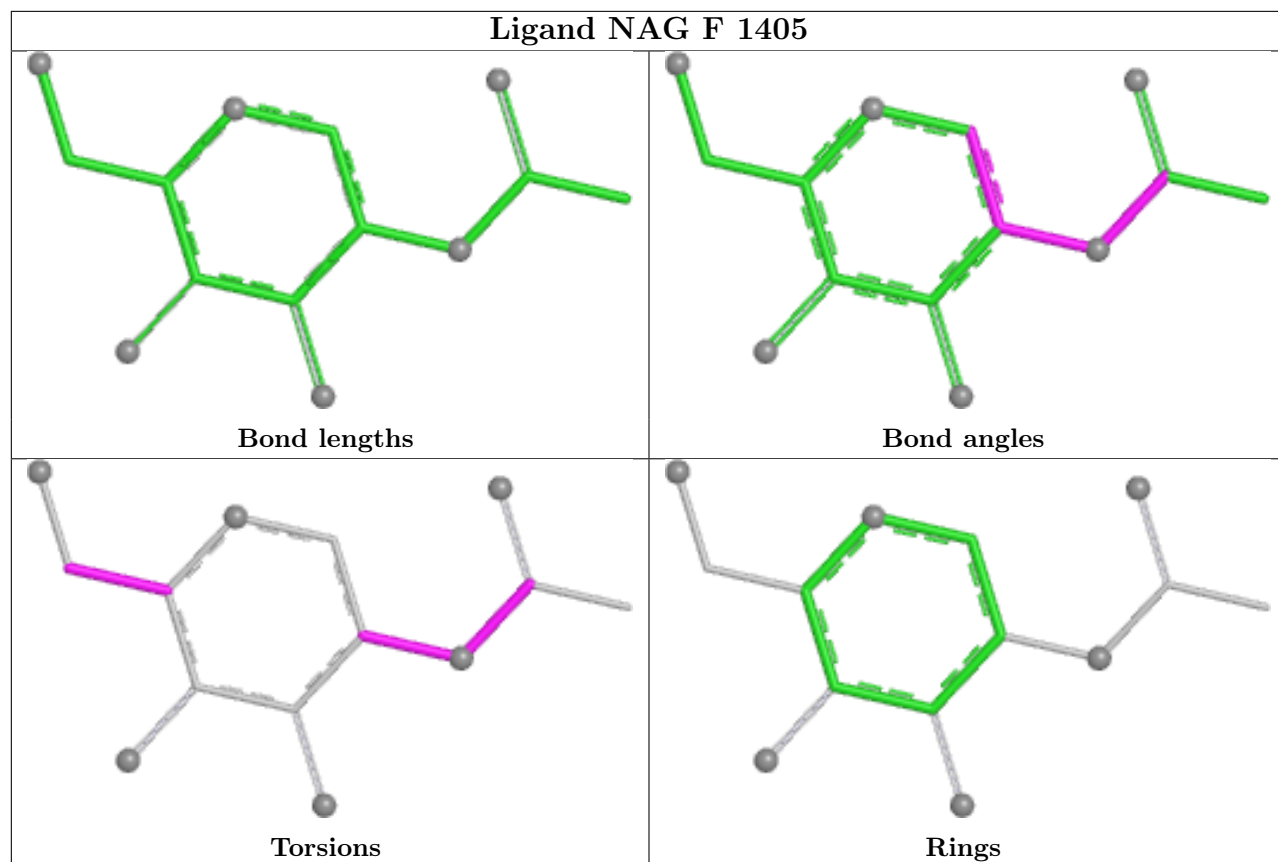


Ligand NAG F 1402

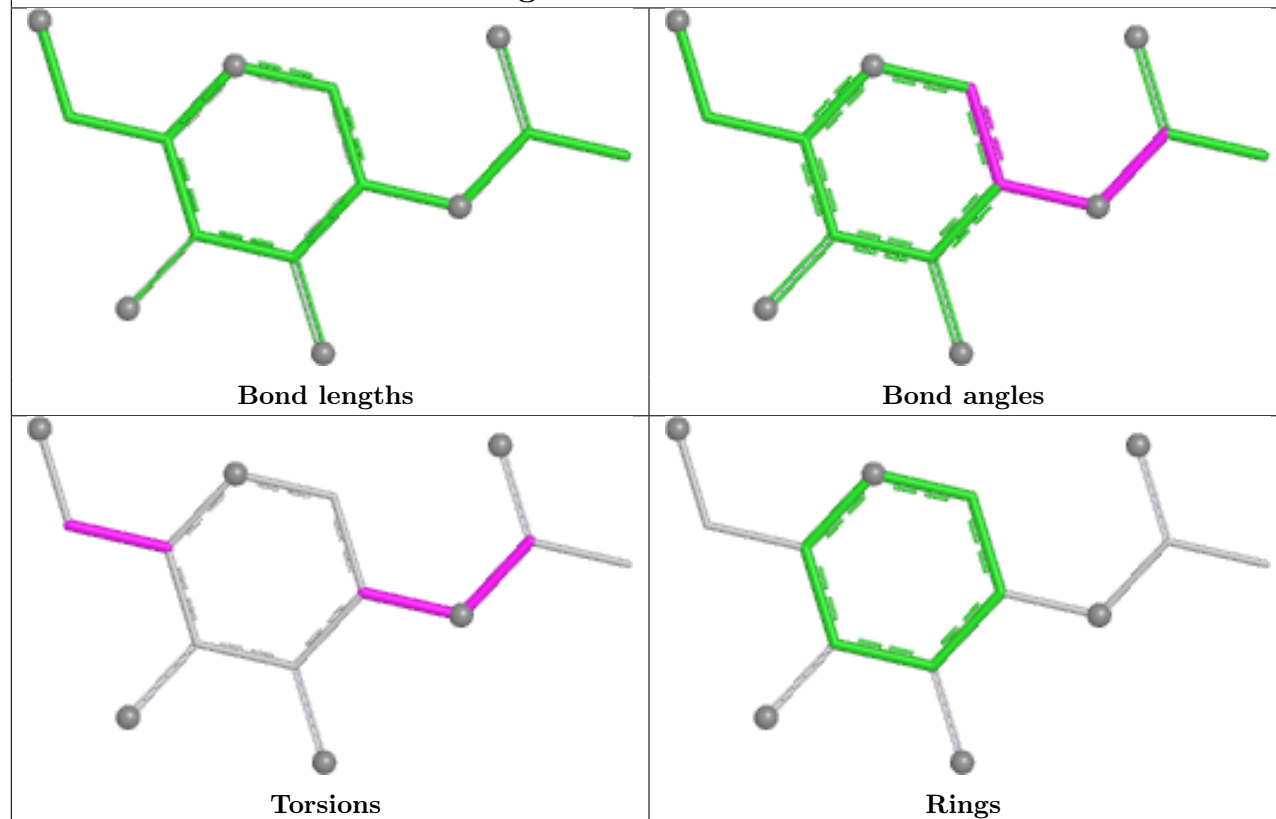


Ligand NAG I 1410

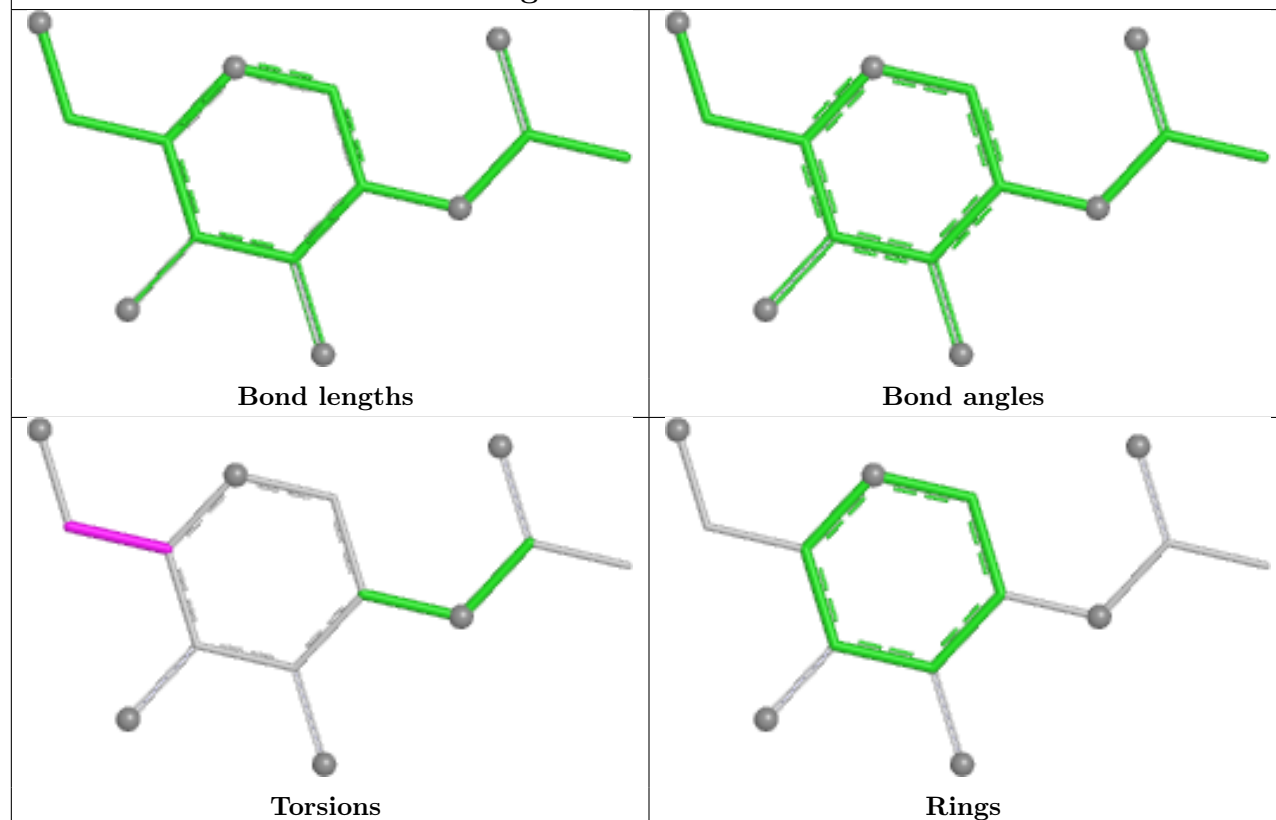


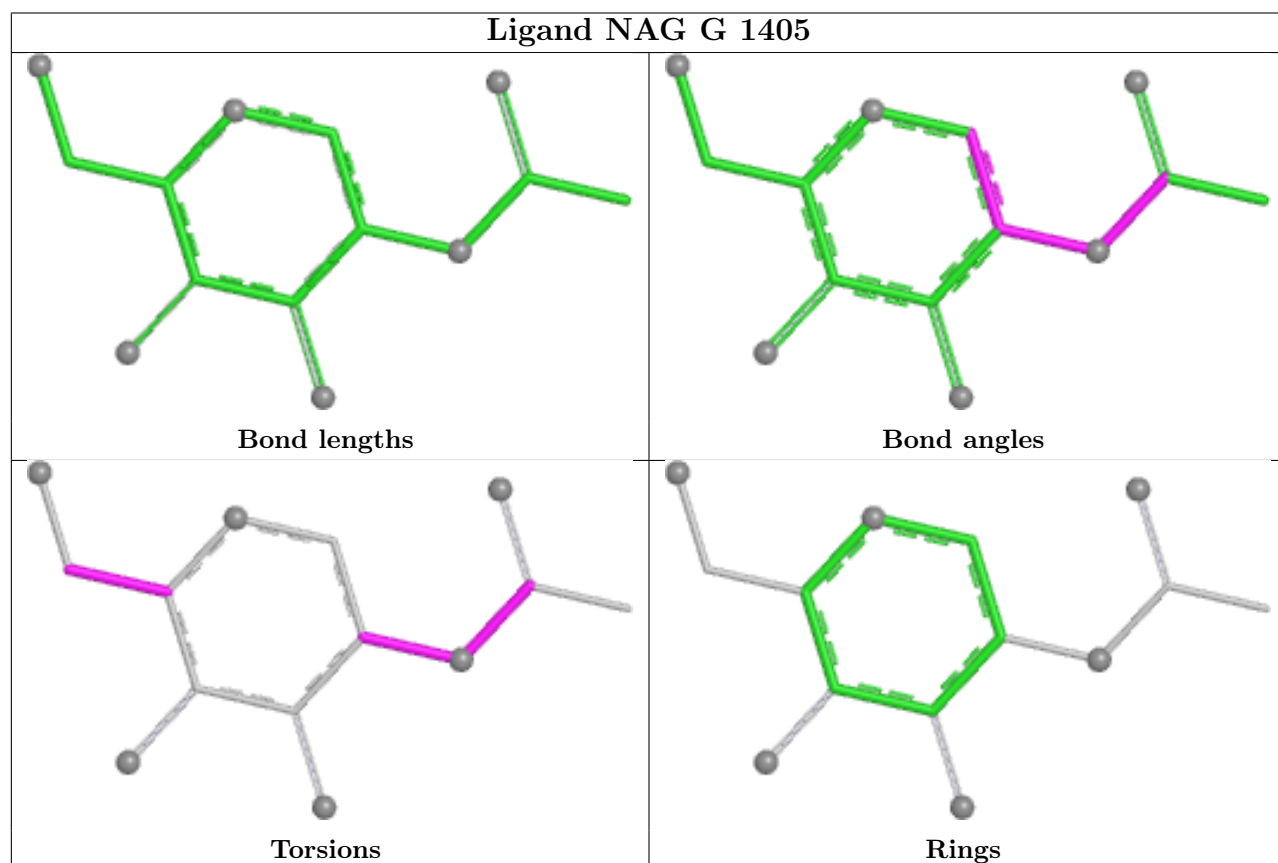
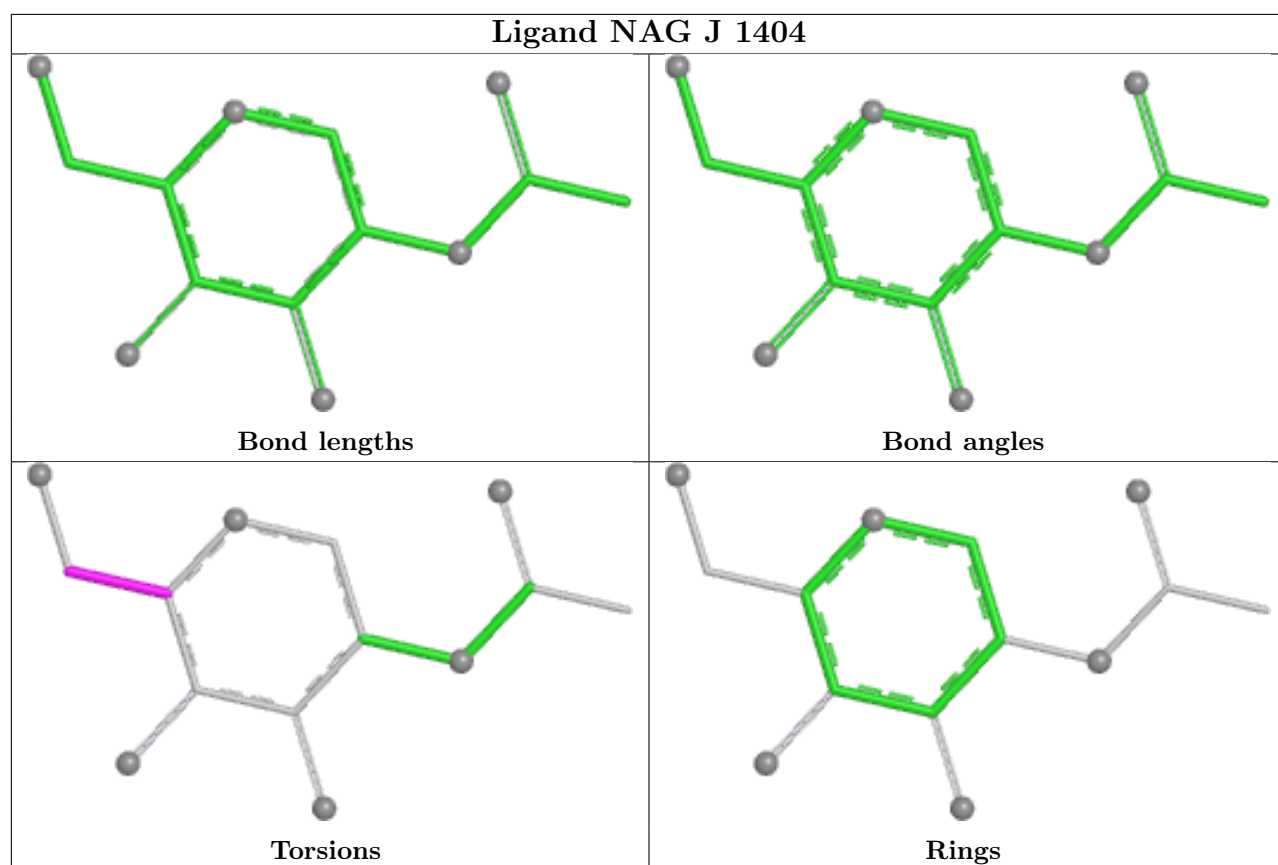


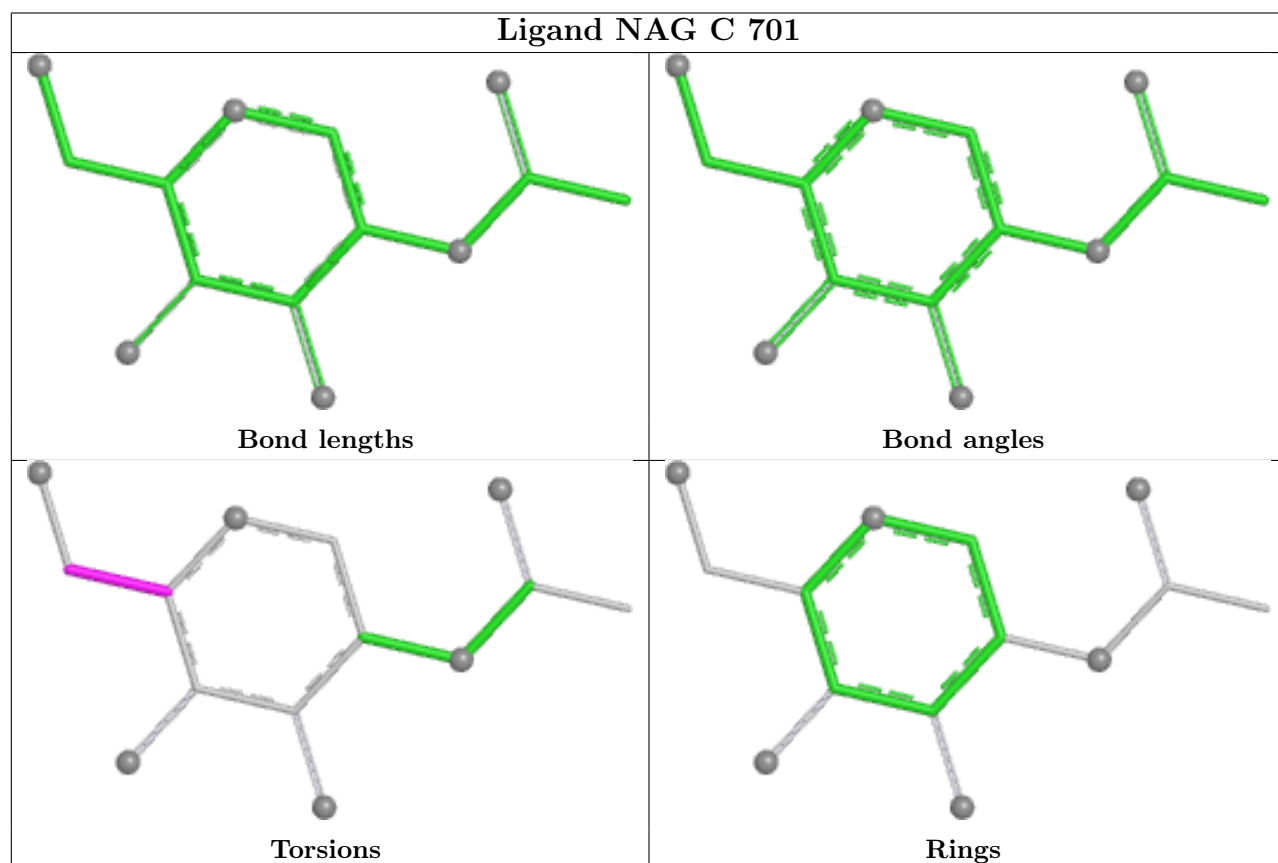
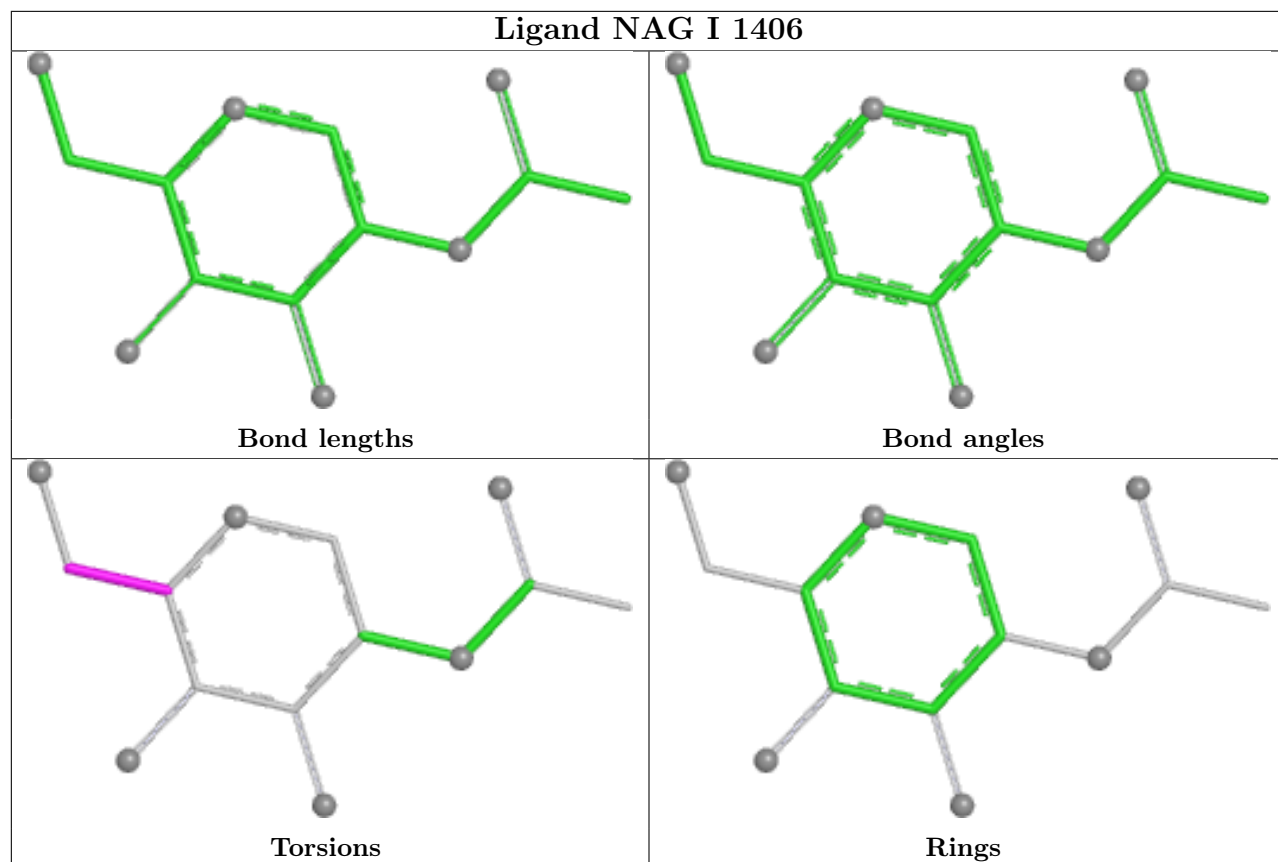
Ligand NAG H 1405



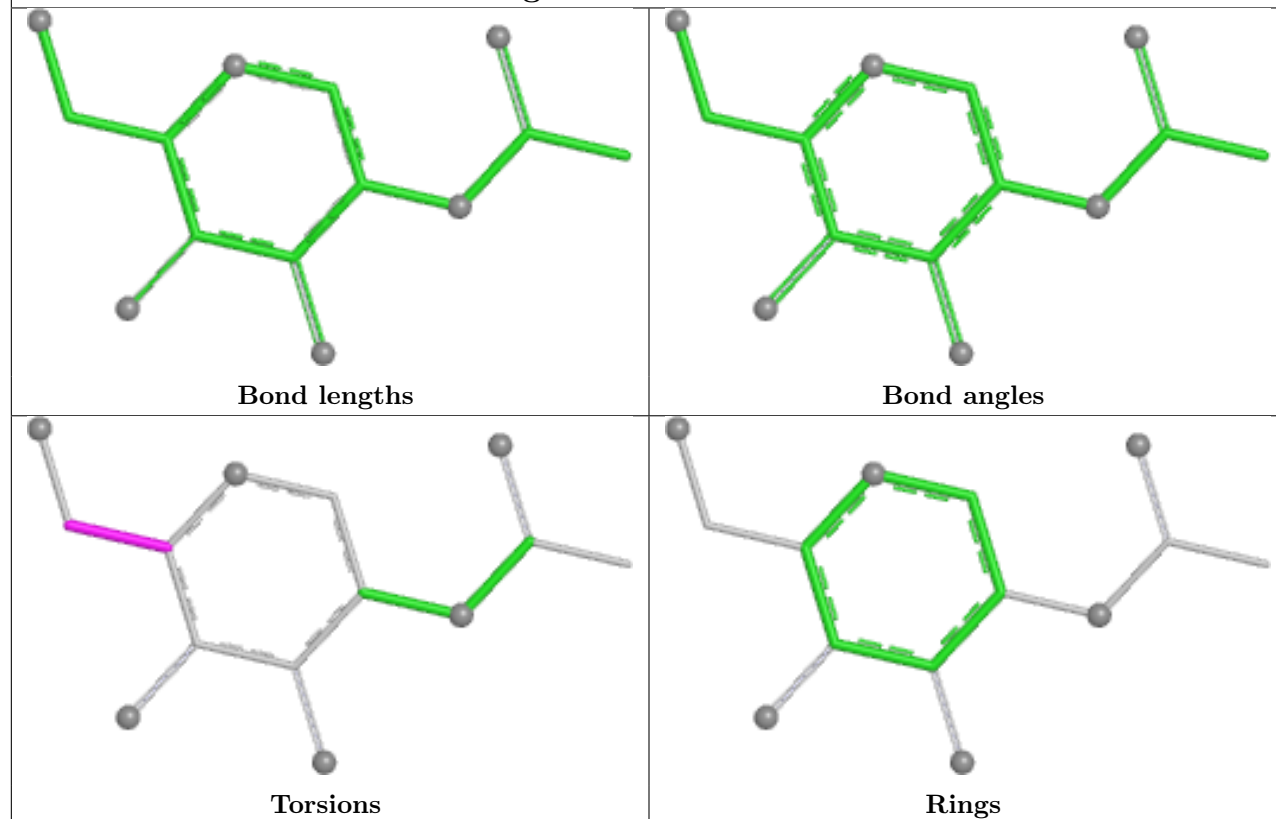
Ligand NAG E 1404



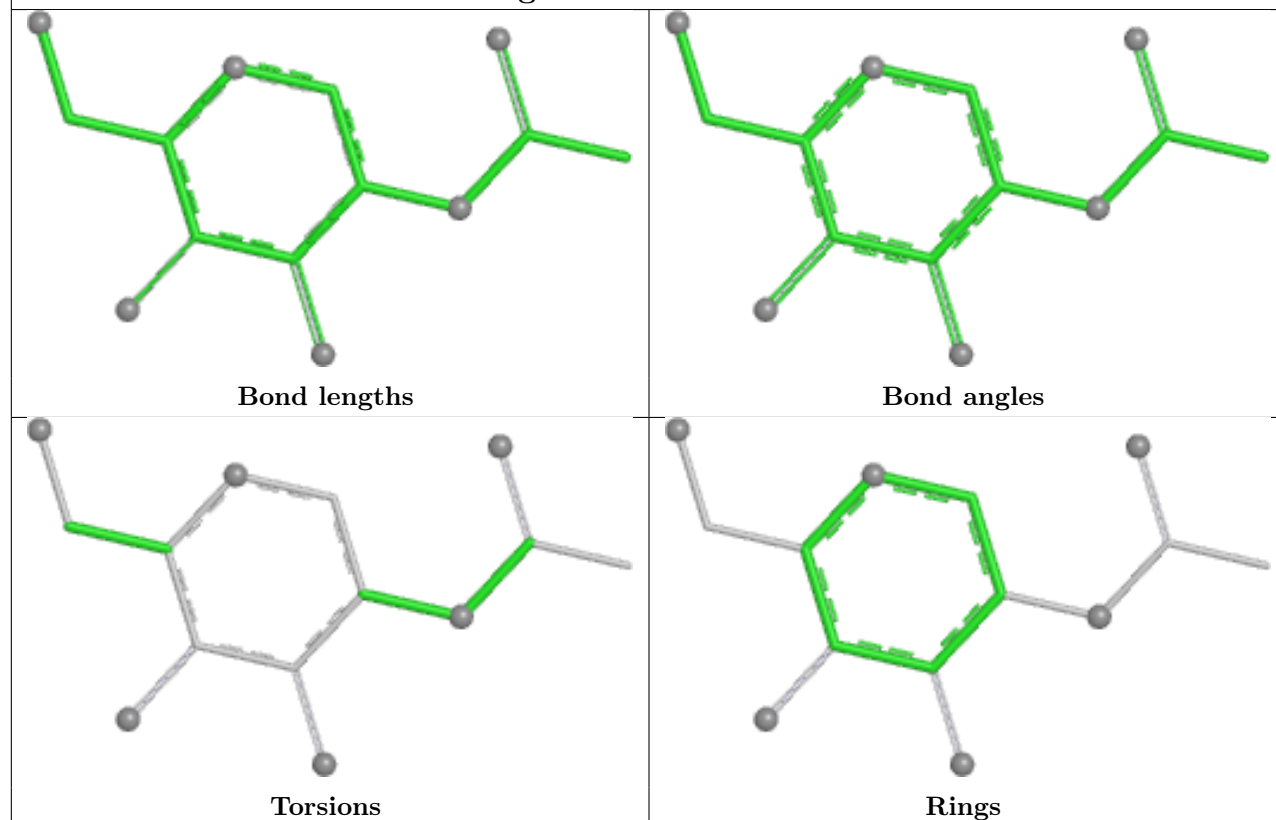




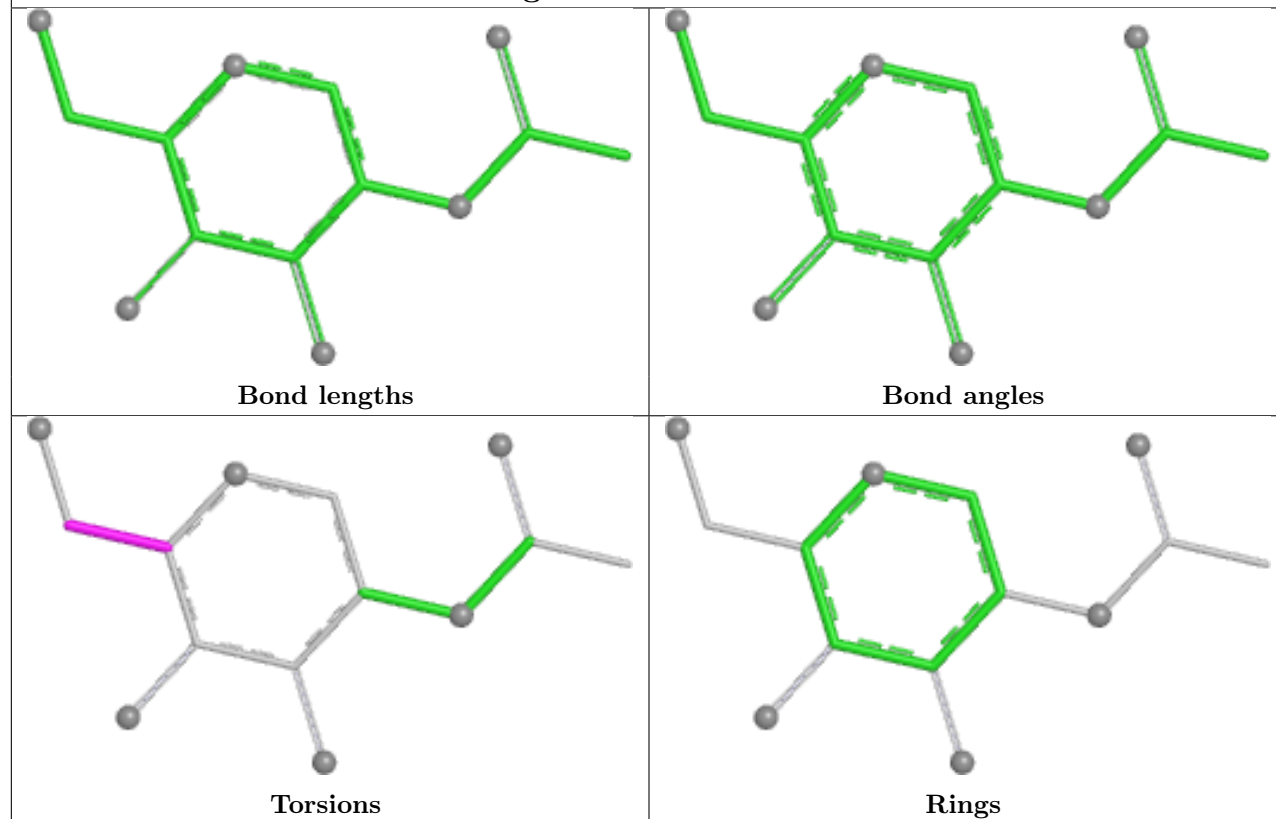
Ligand NAG J 1401



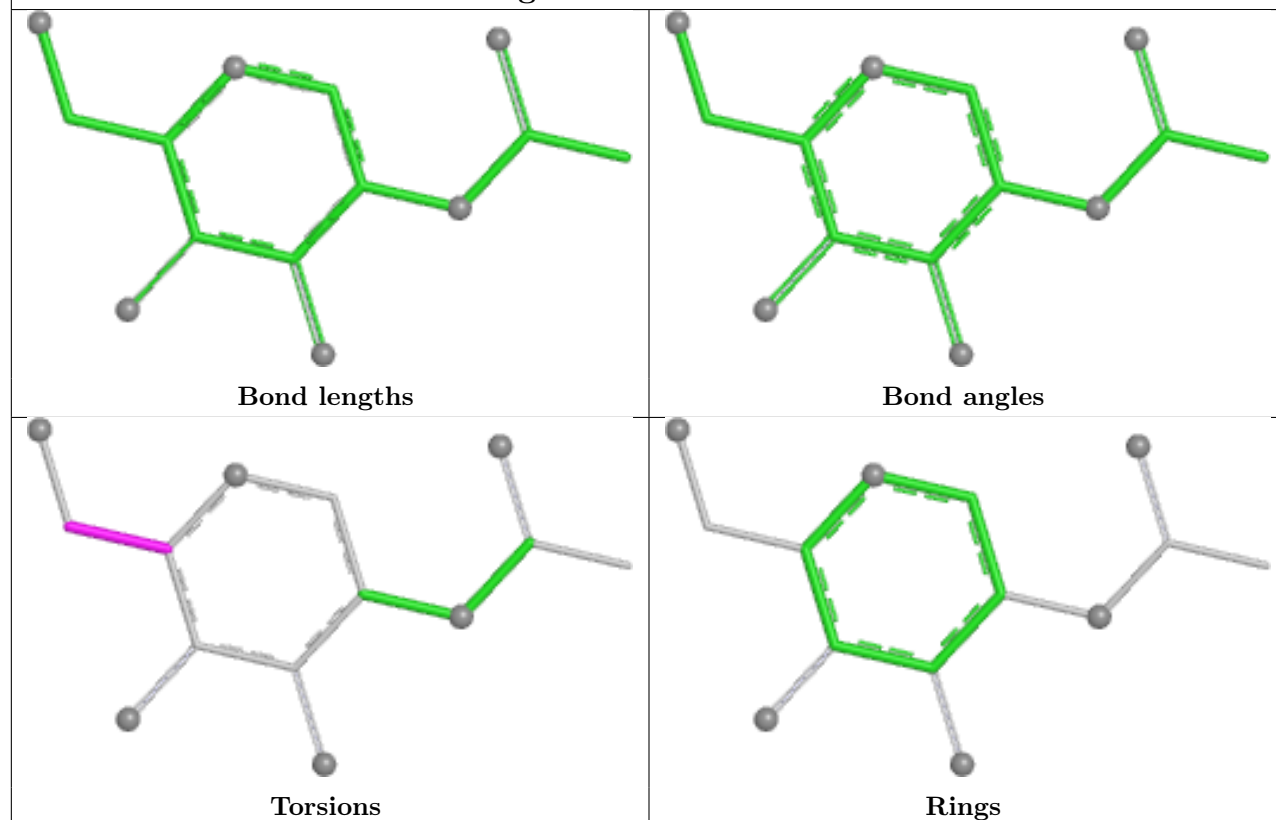
Ligand NAG G 1407



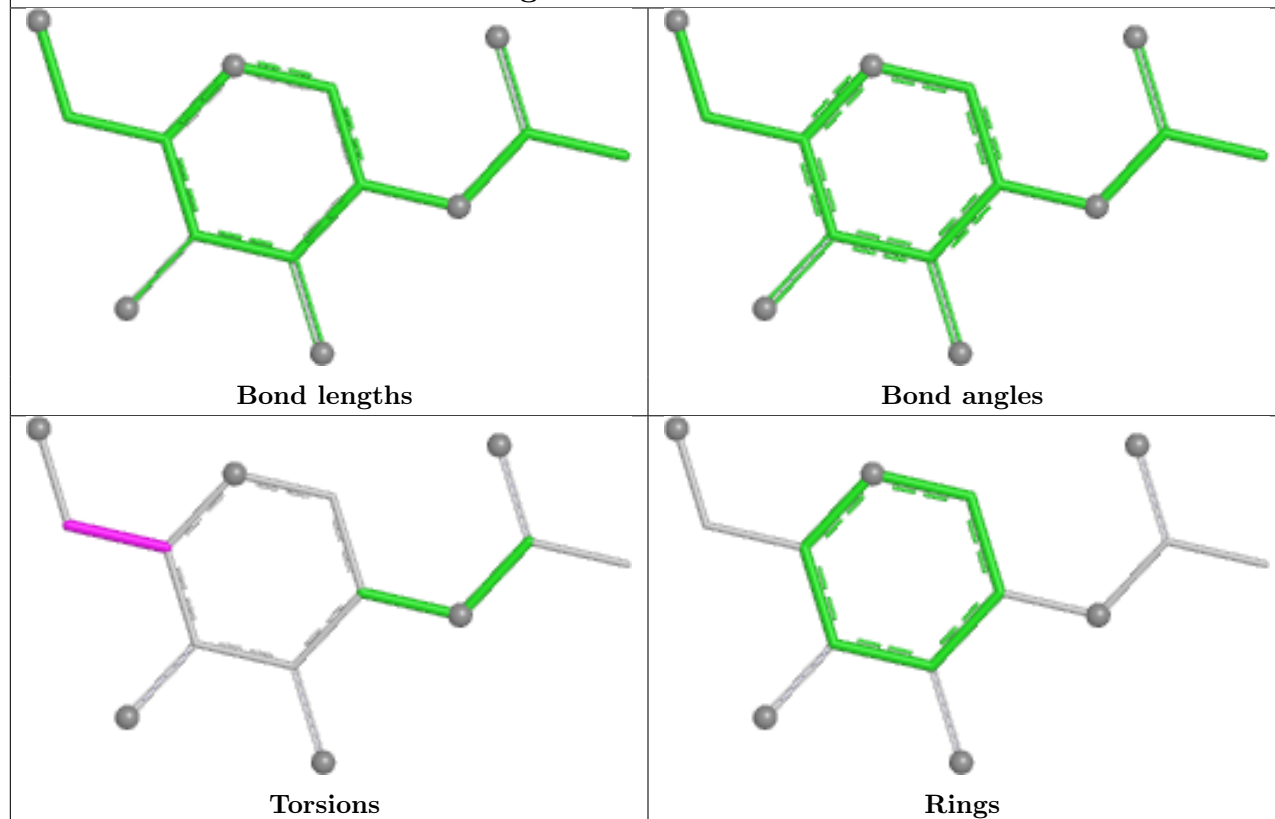
Ligand NAG J 1406



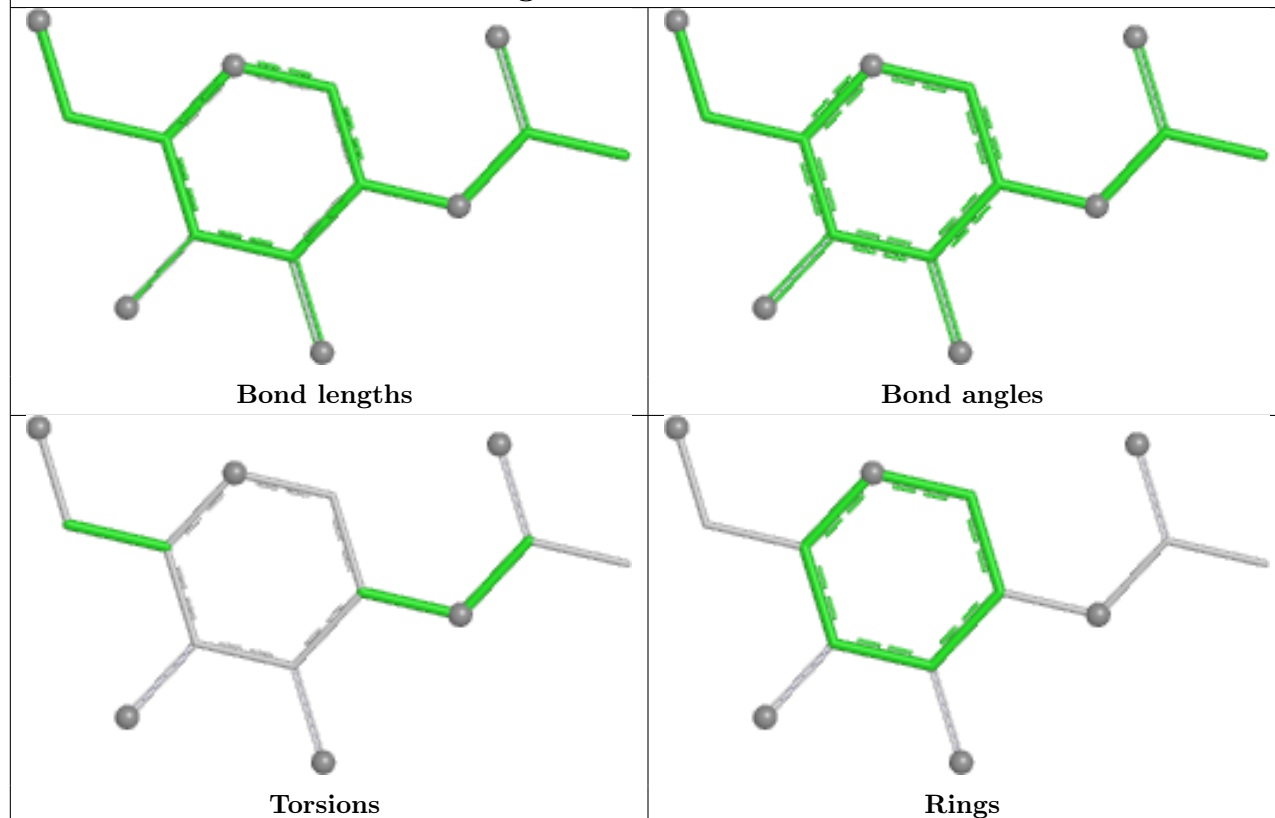
Ligand NAG G 1403



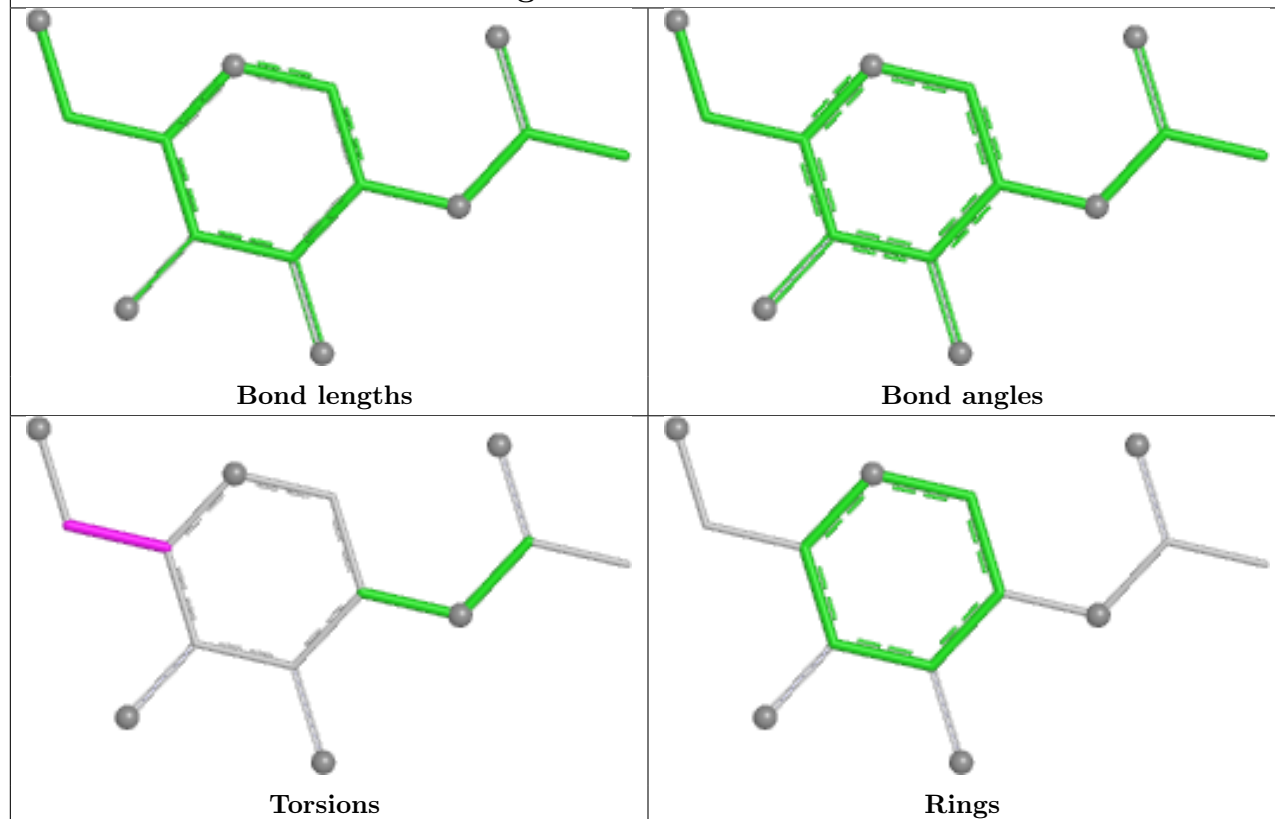
Ligand NAG F 1406



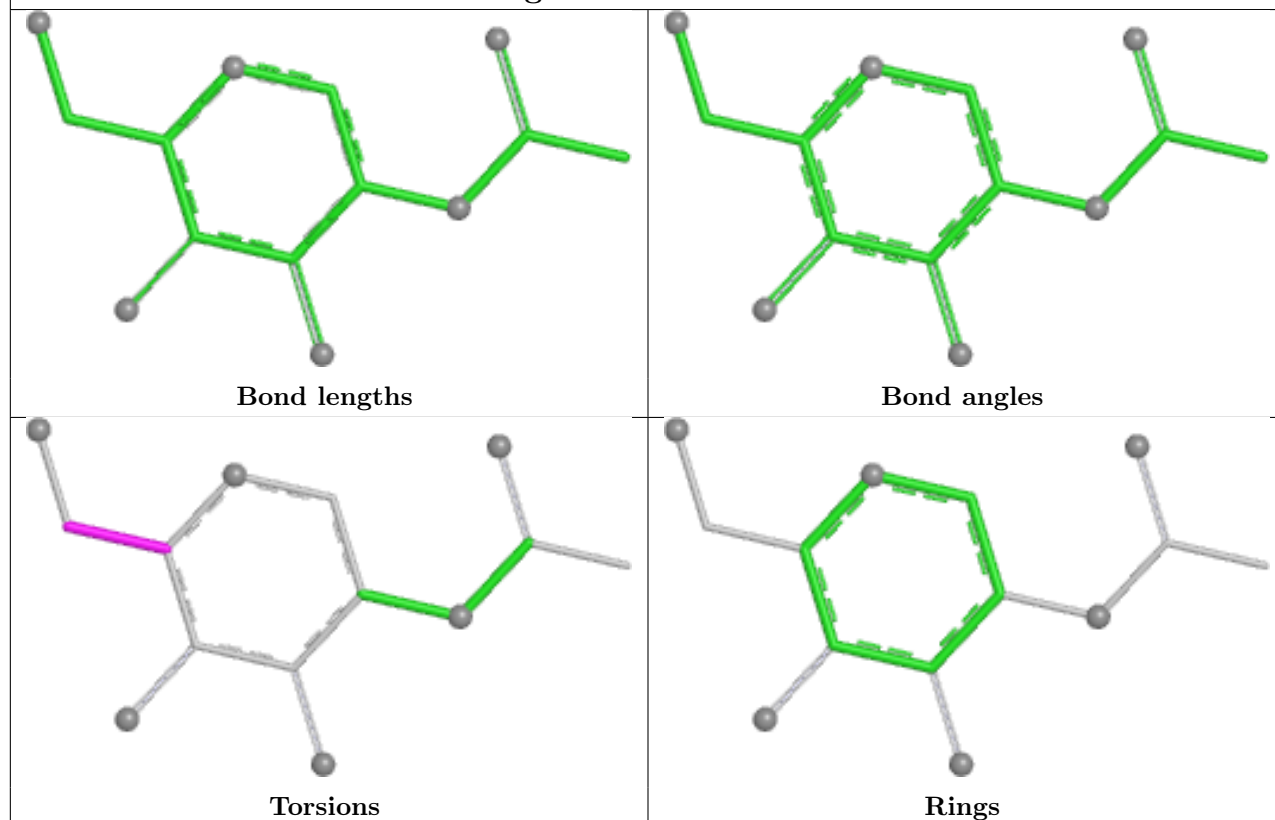
Ligand NAG H 1407



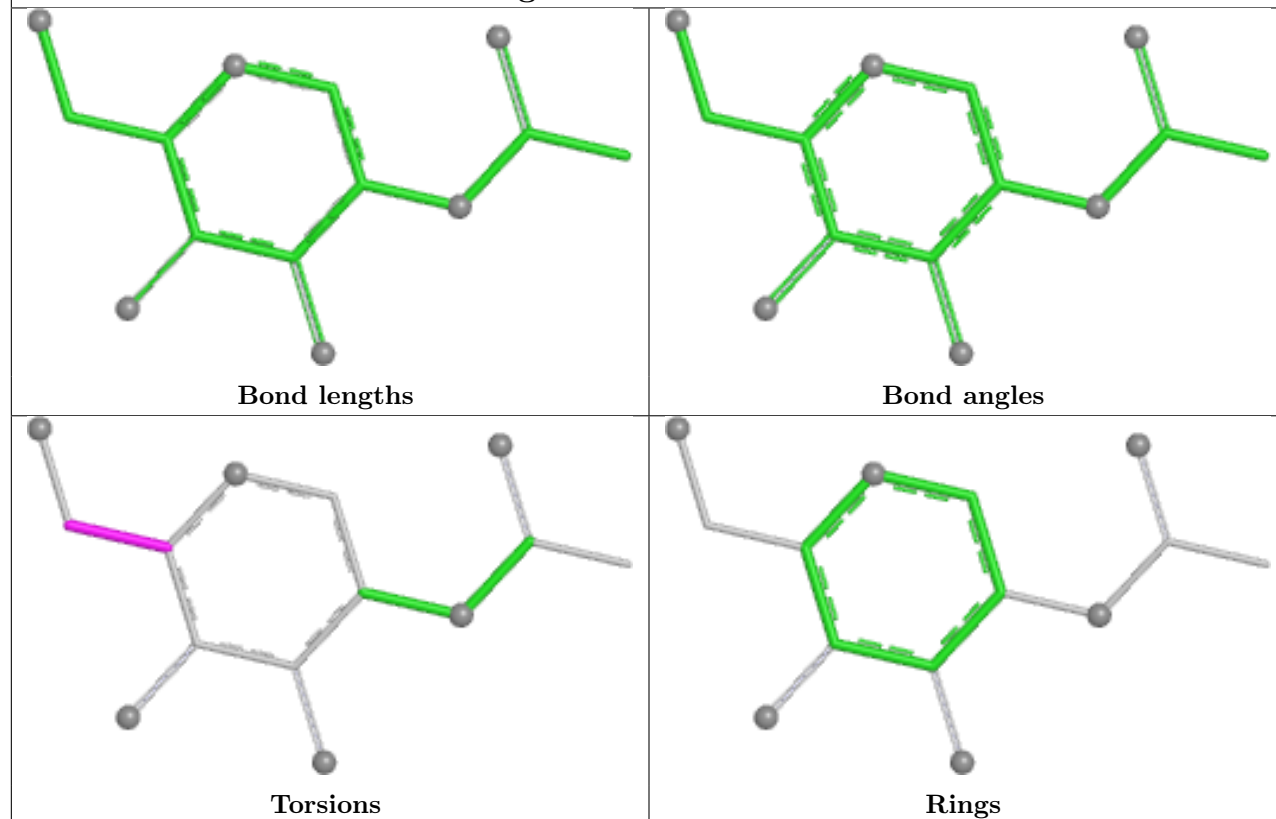
Ligand NAG H 1406



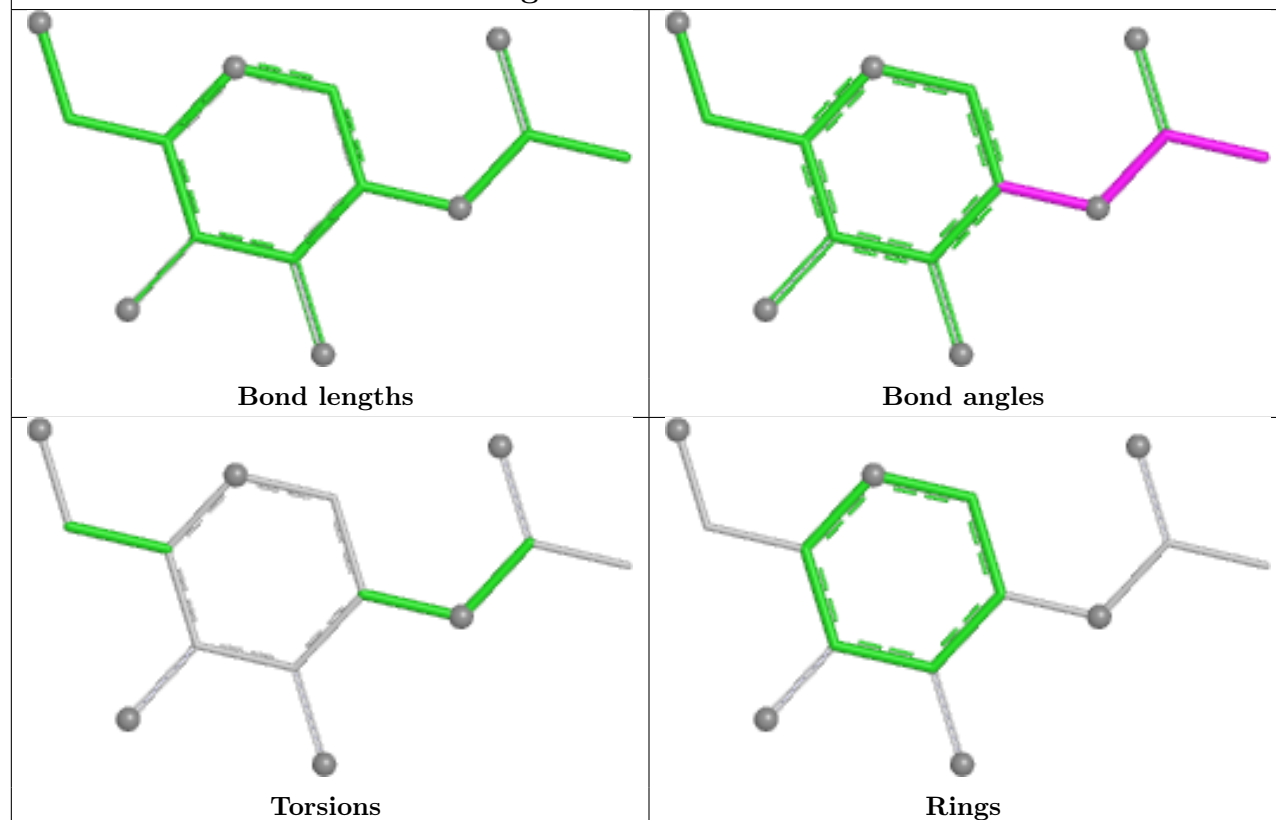
Ligand NAG I 1401

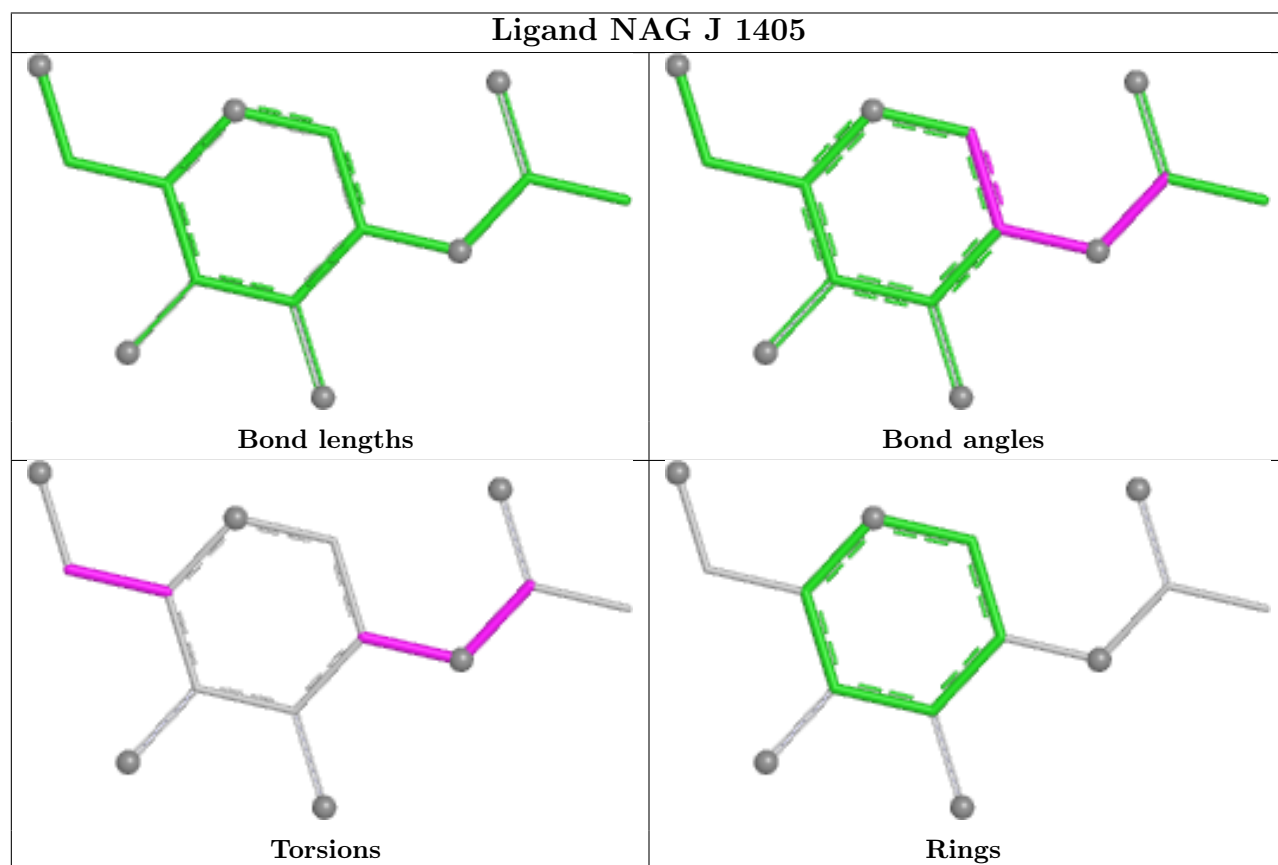
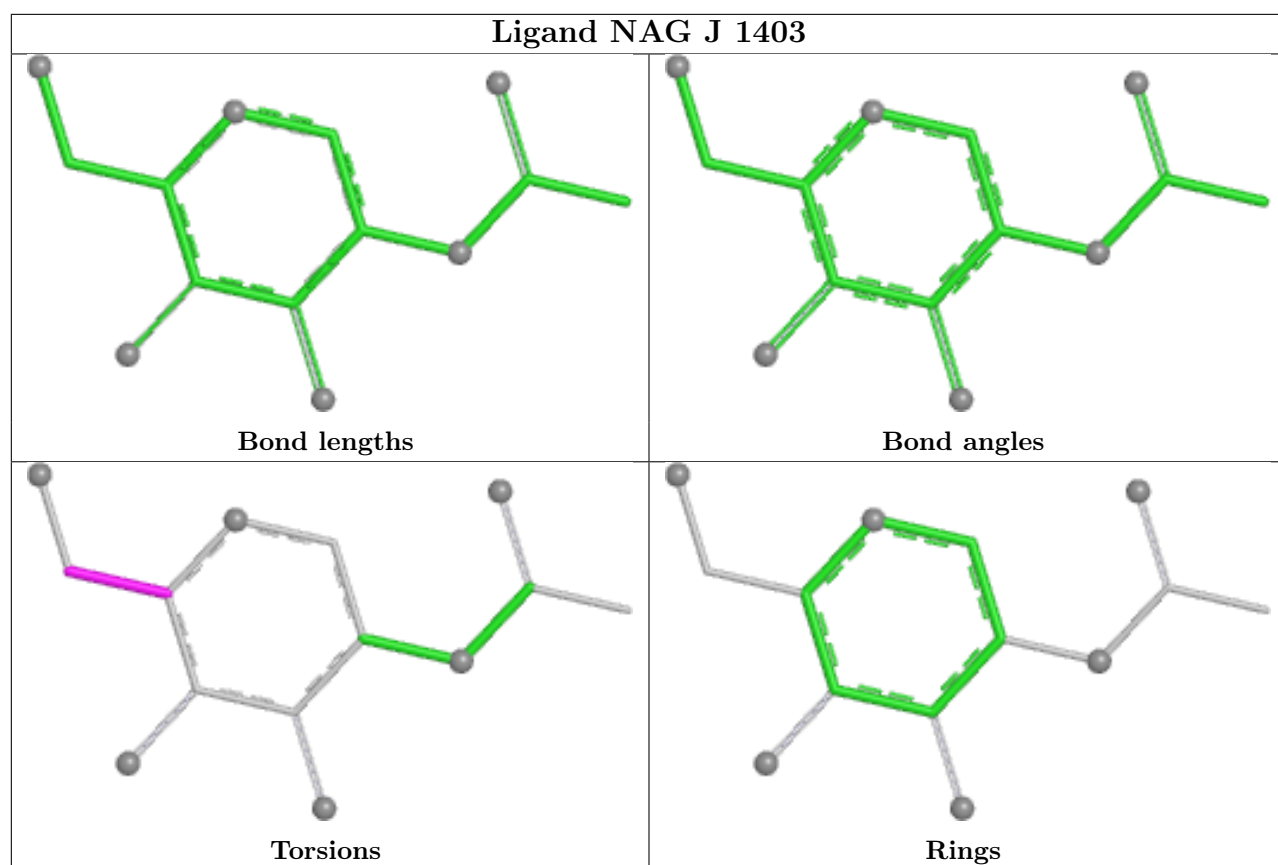


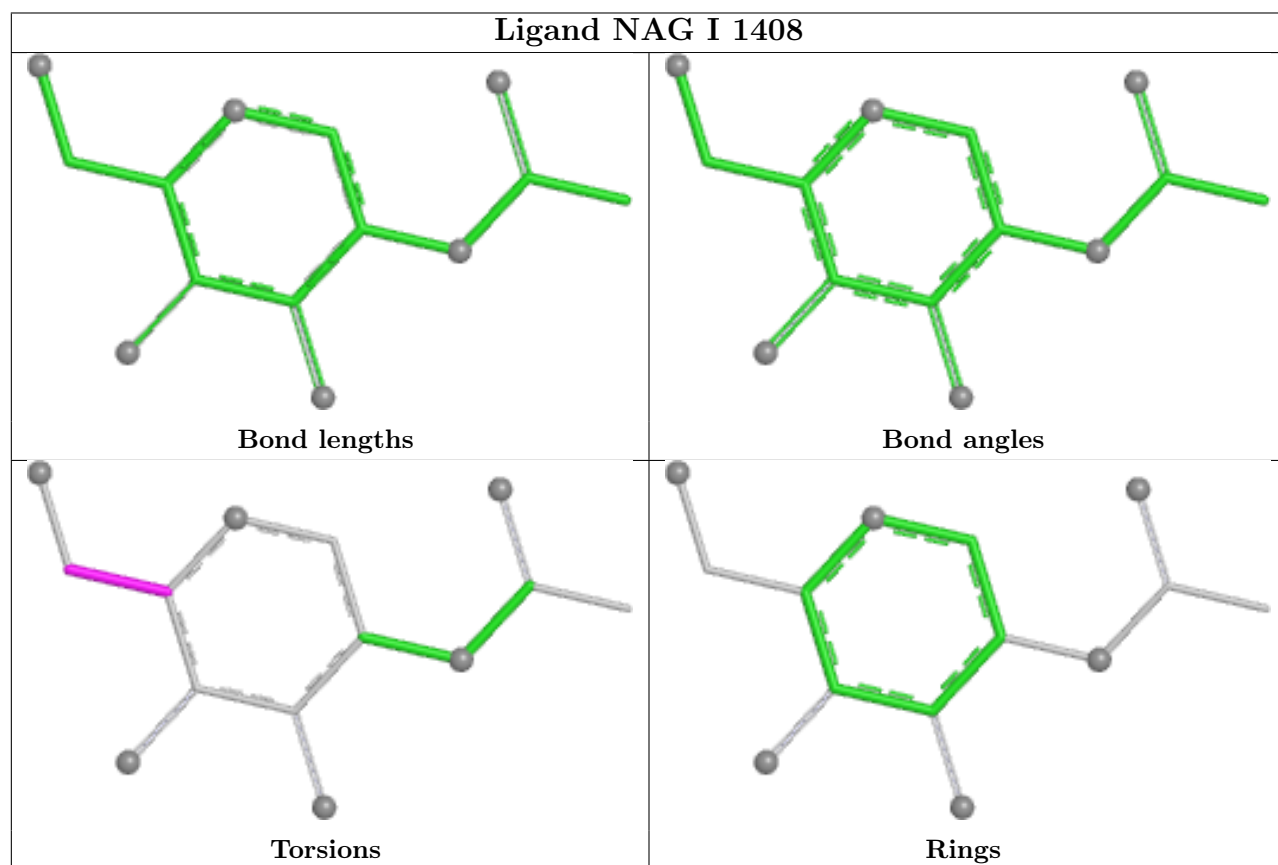
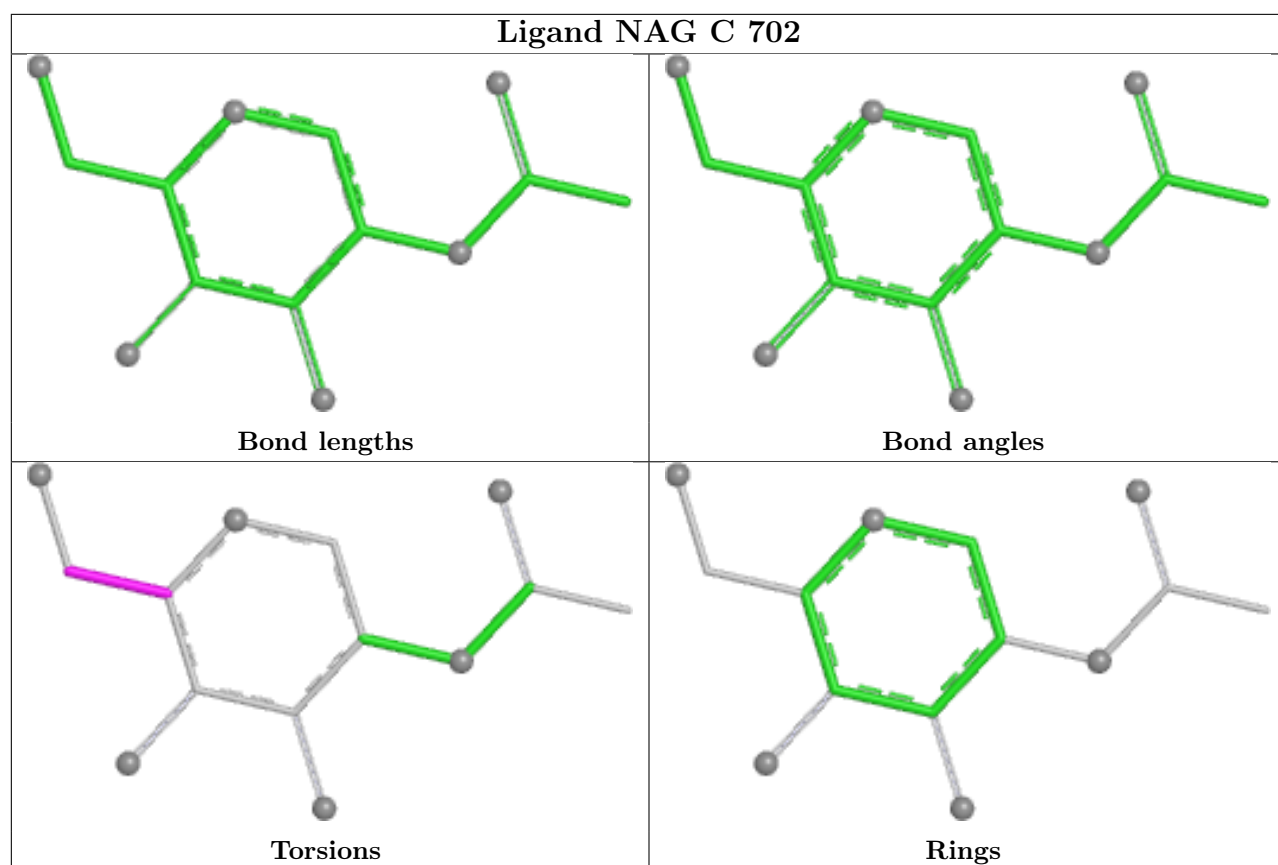
Ligand NAG H 1409

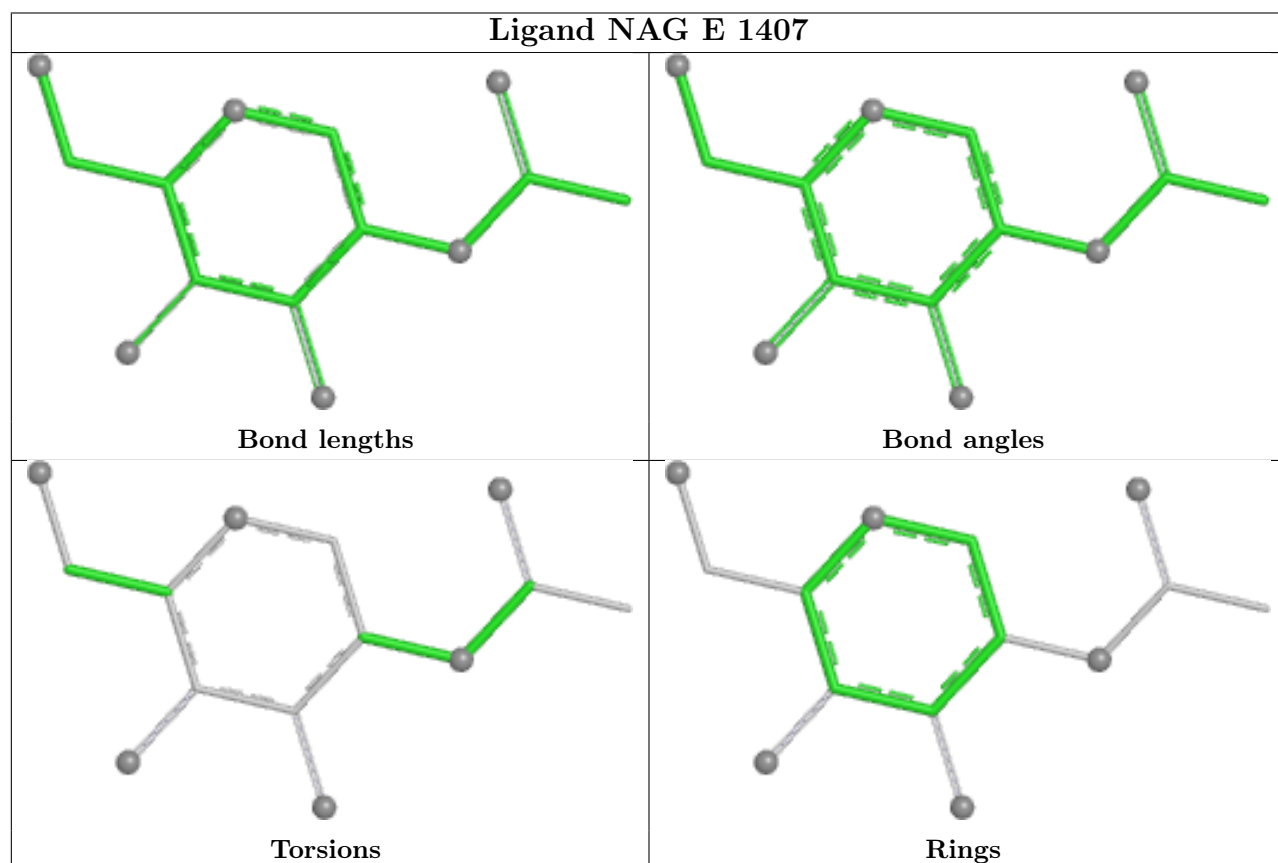
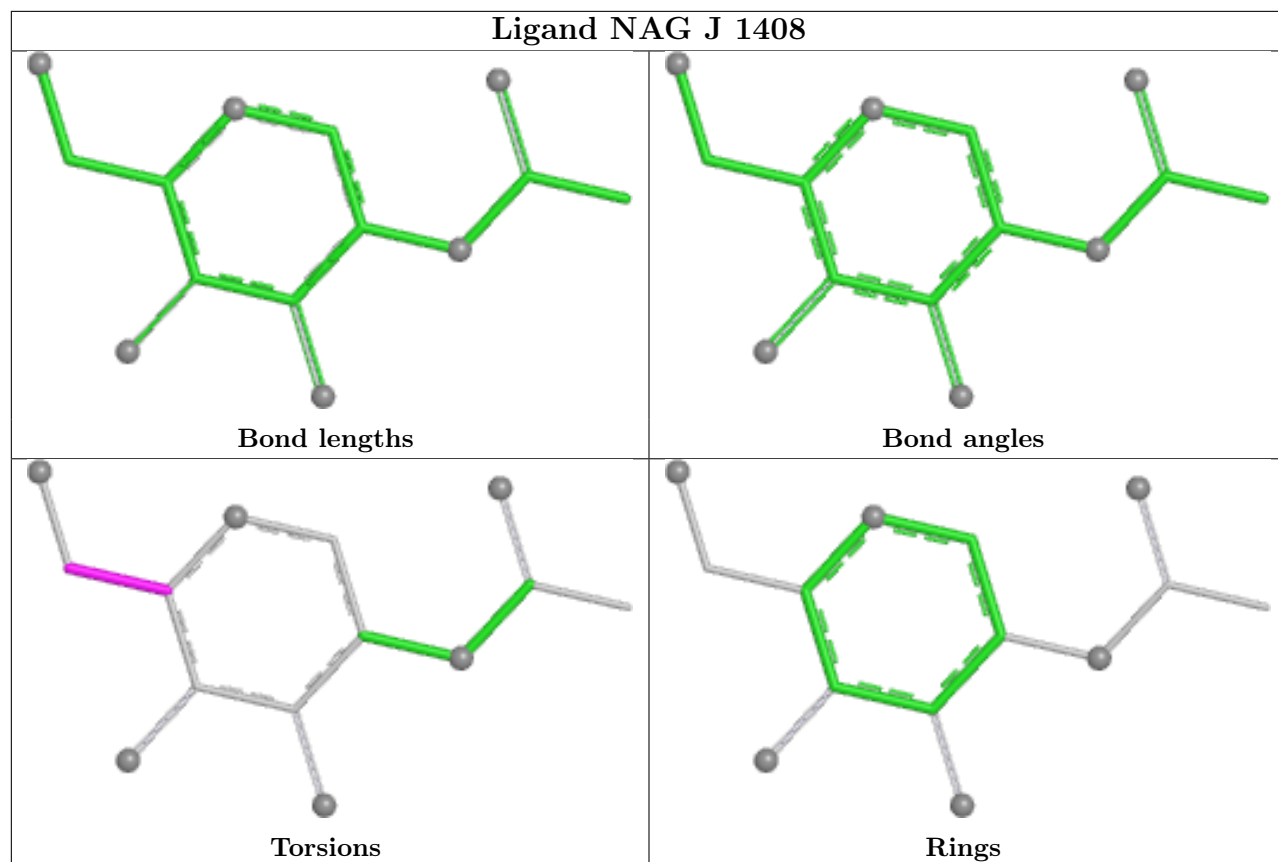


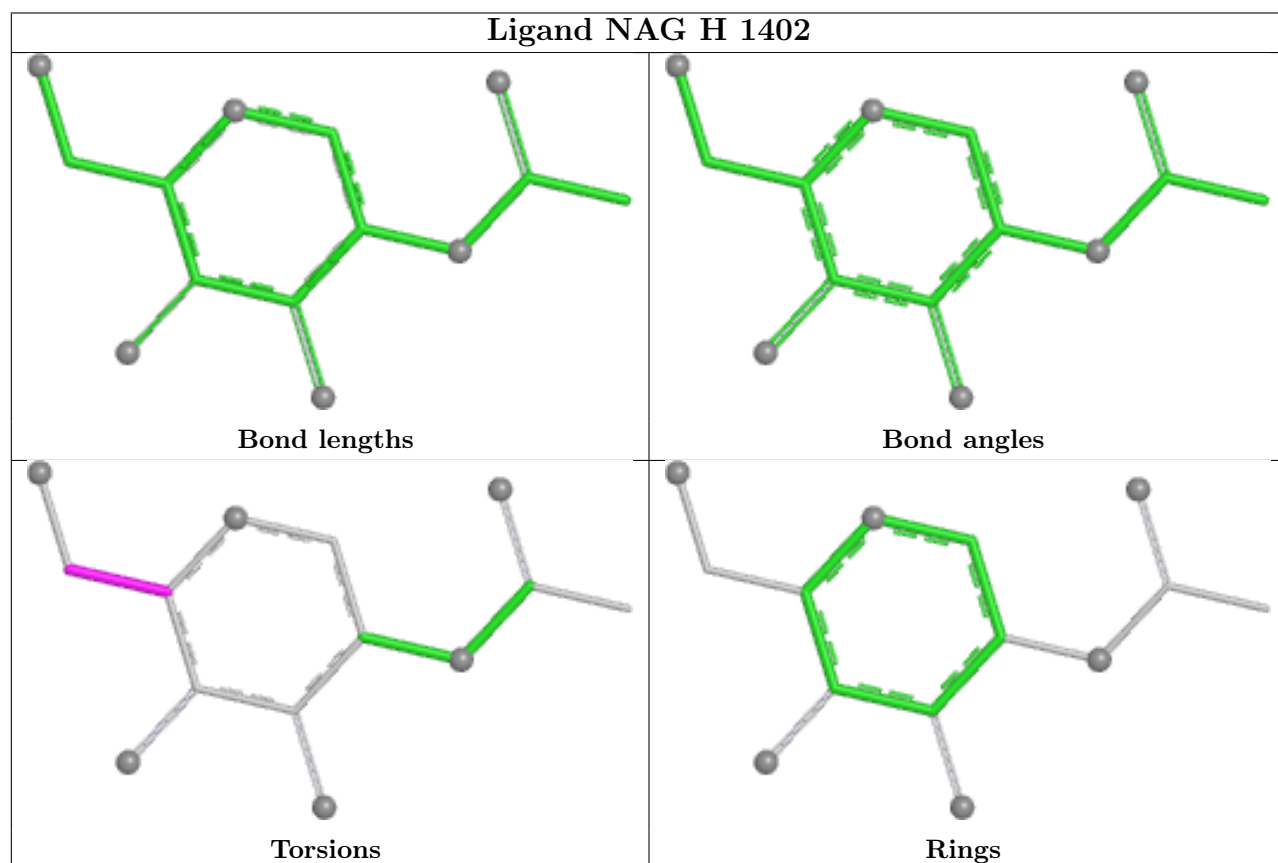
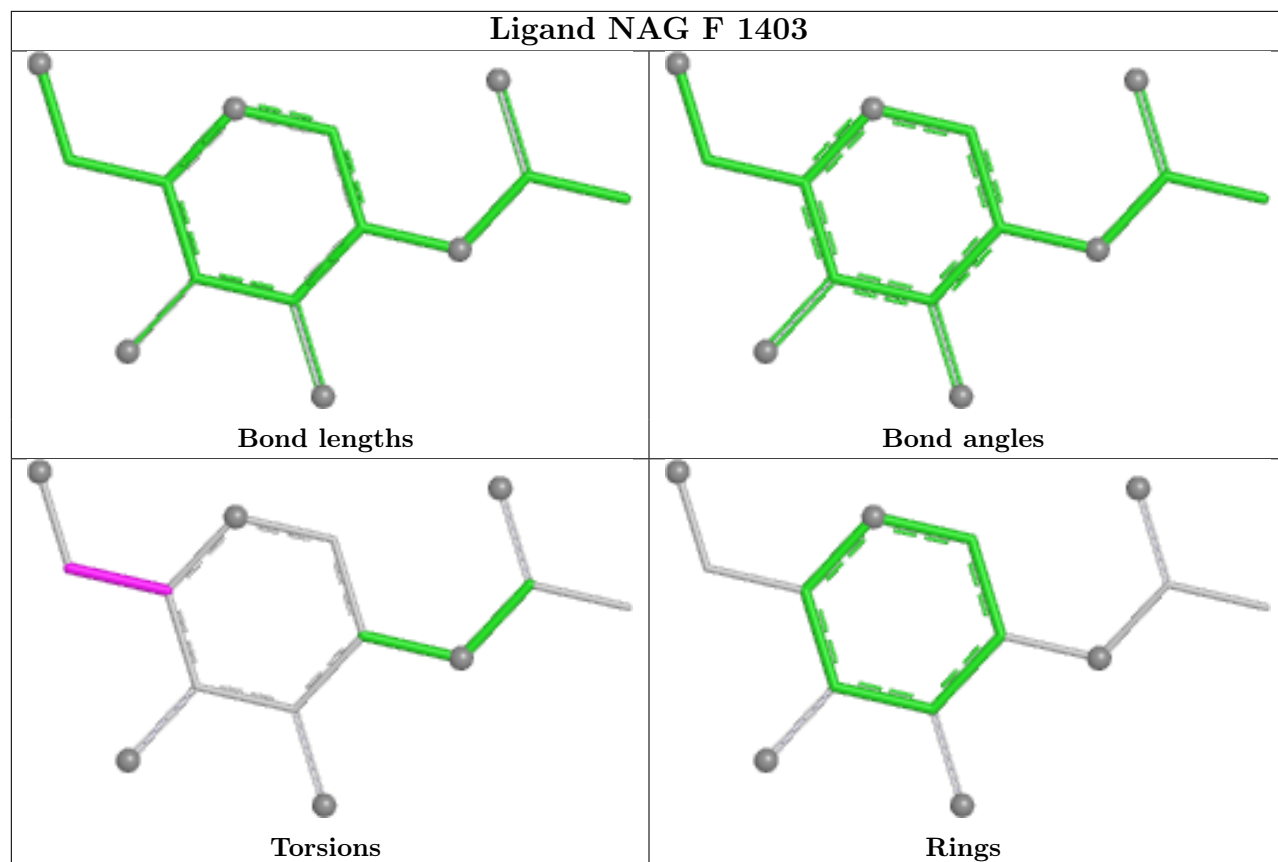
Ligand NAG F 1409



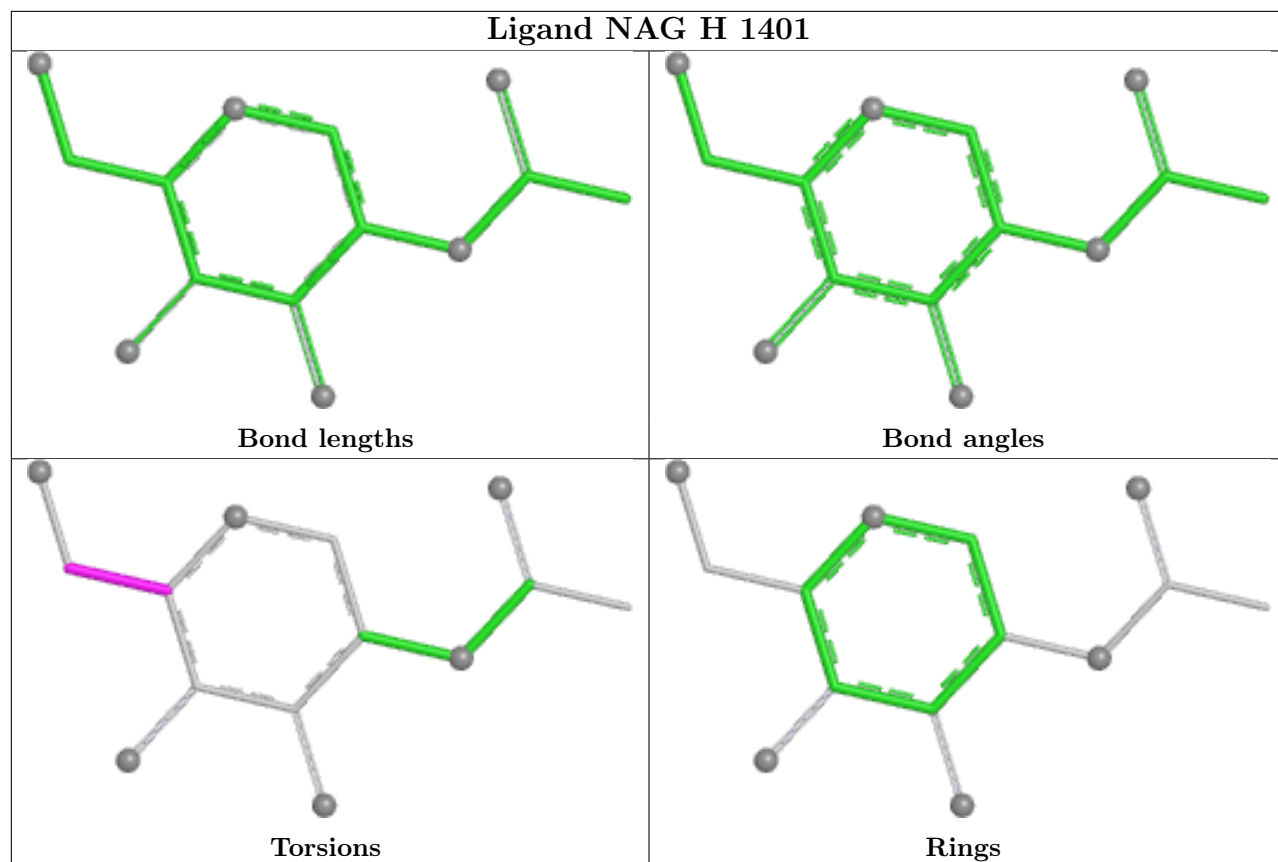




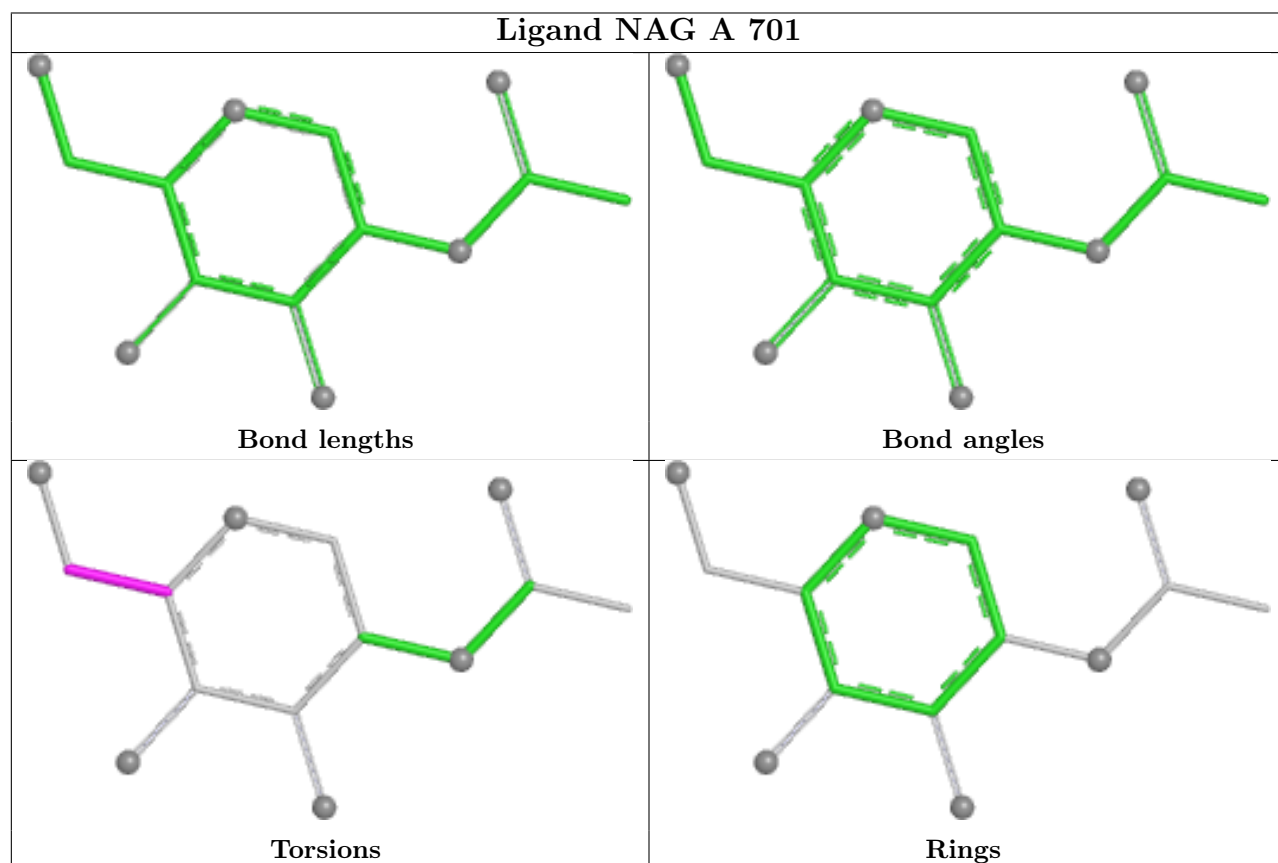


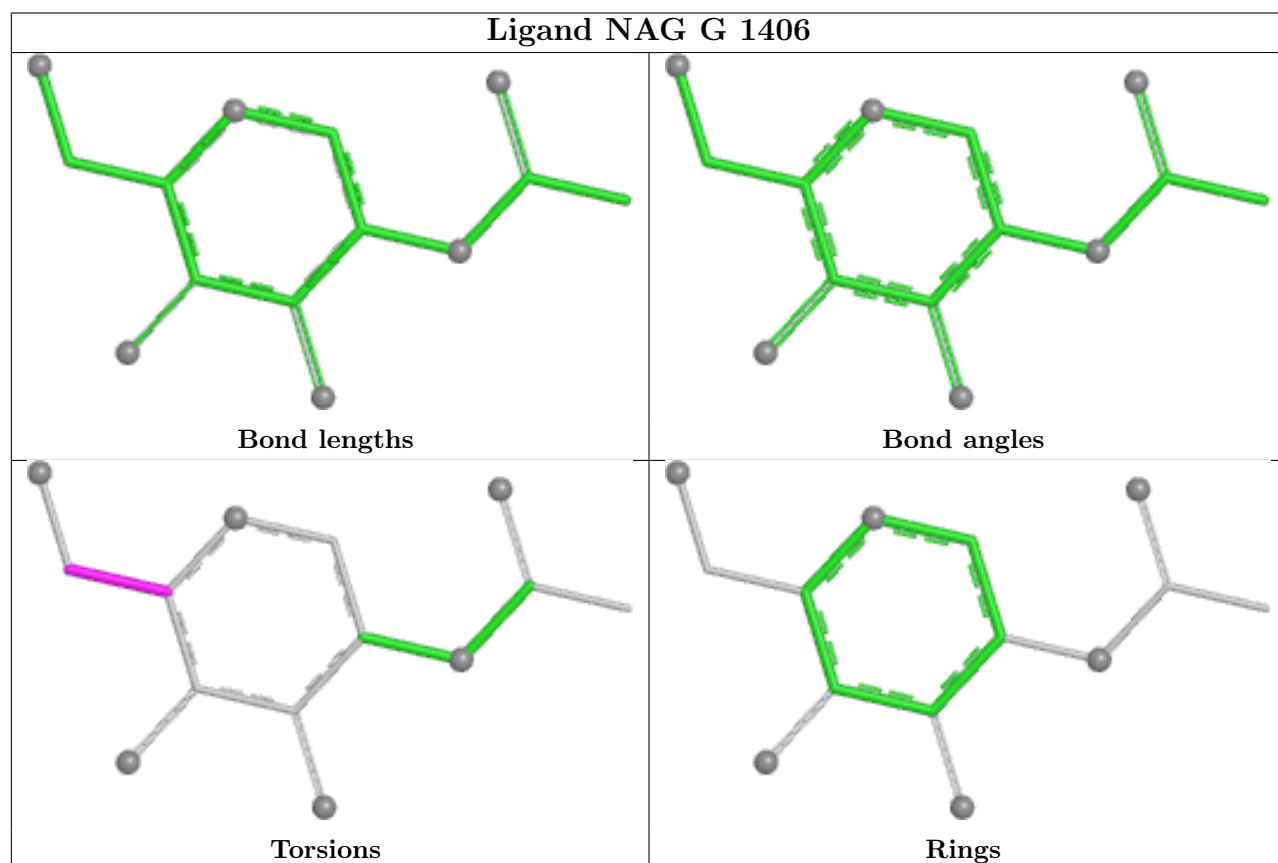
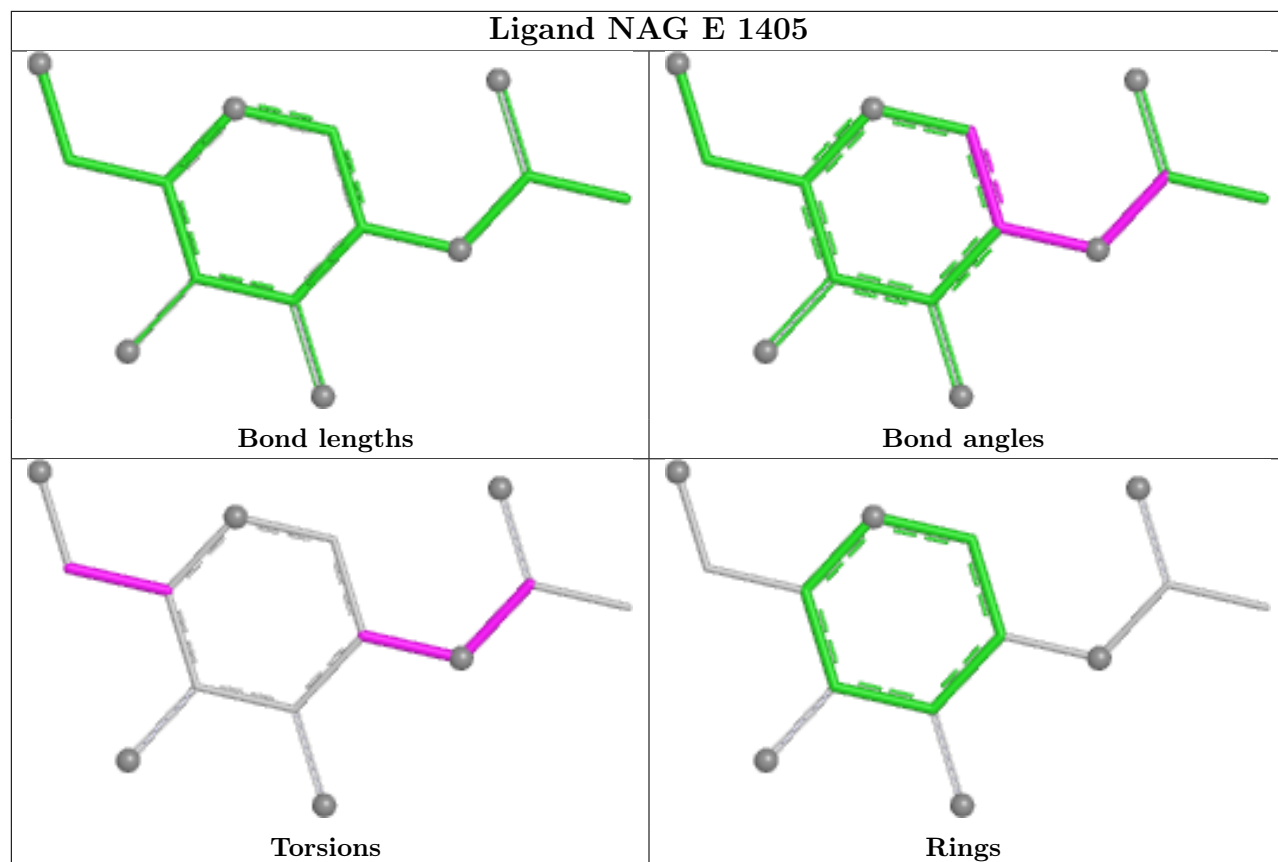


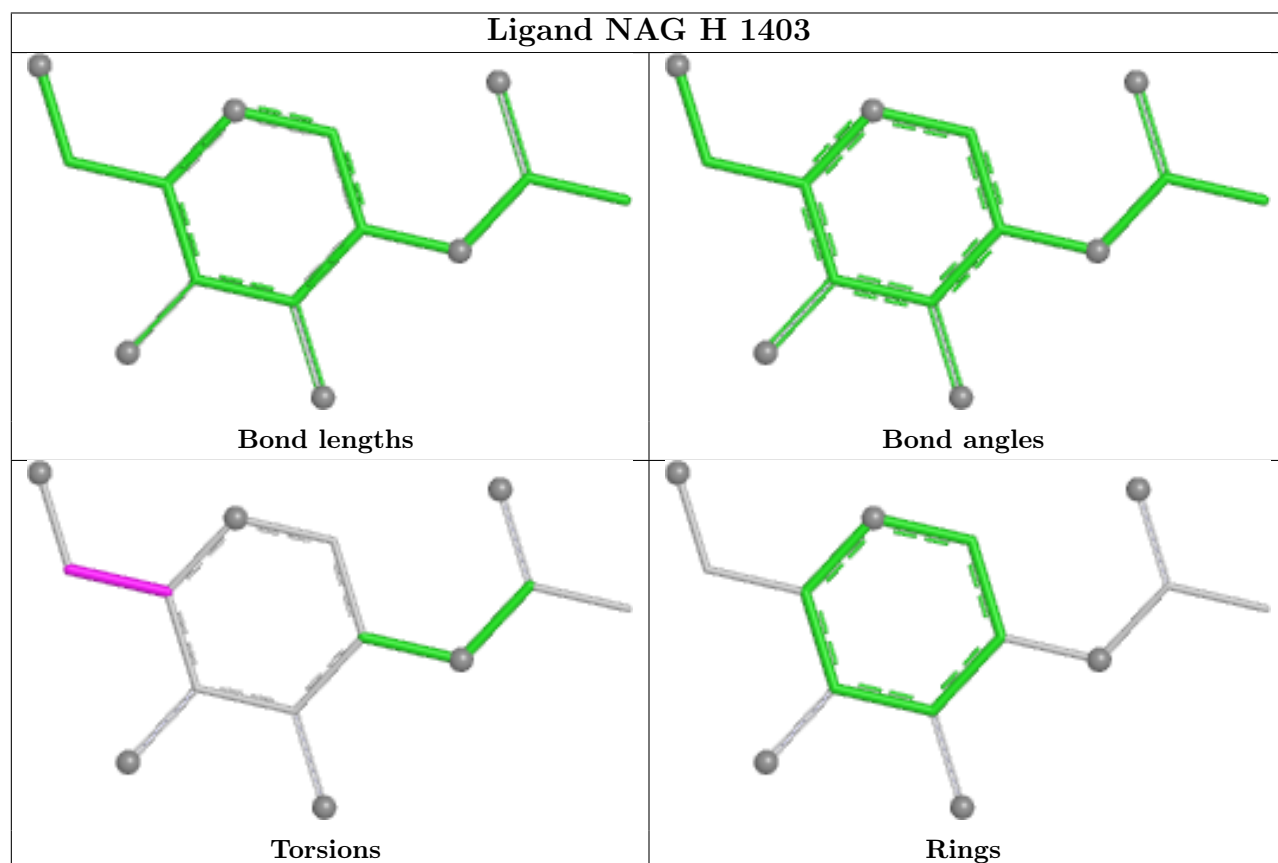
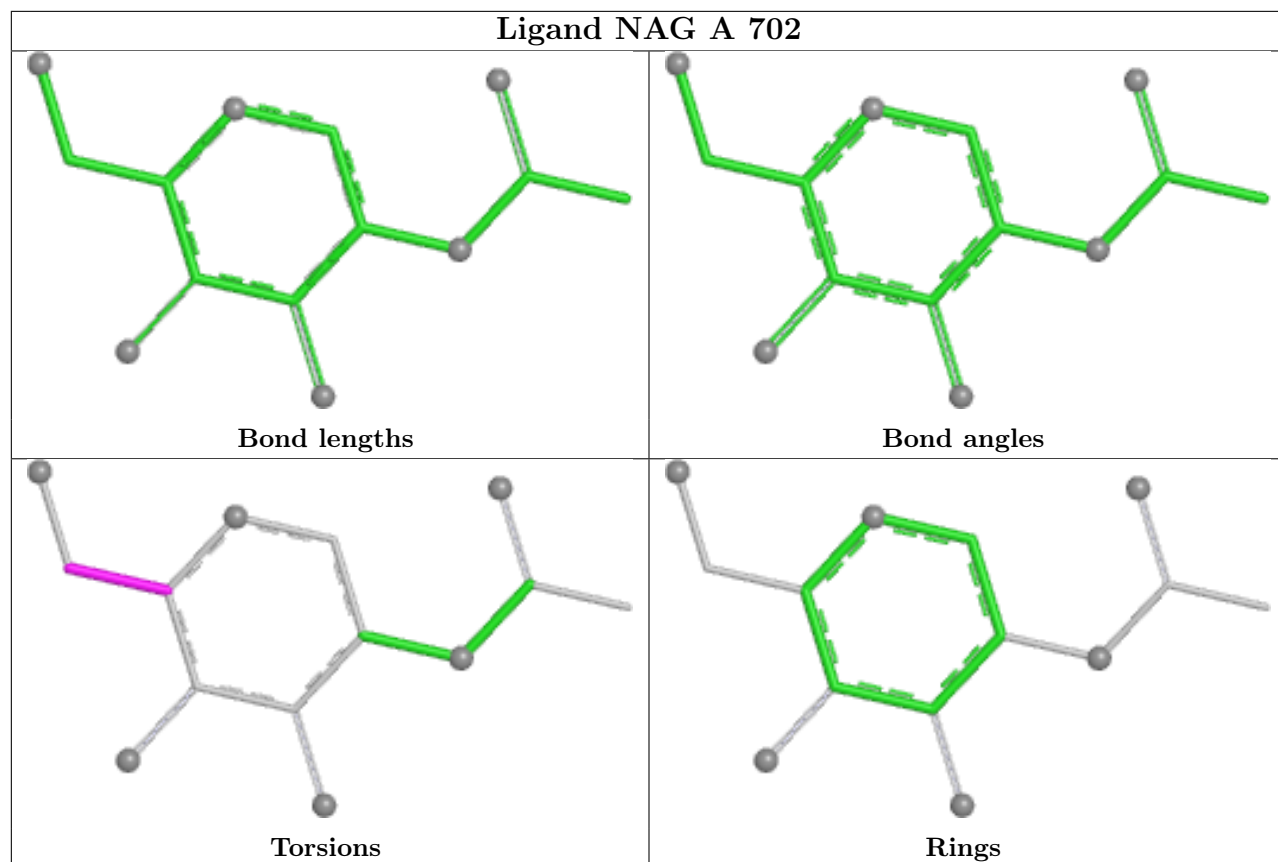
Ligand NAG H 1401



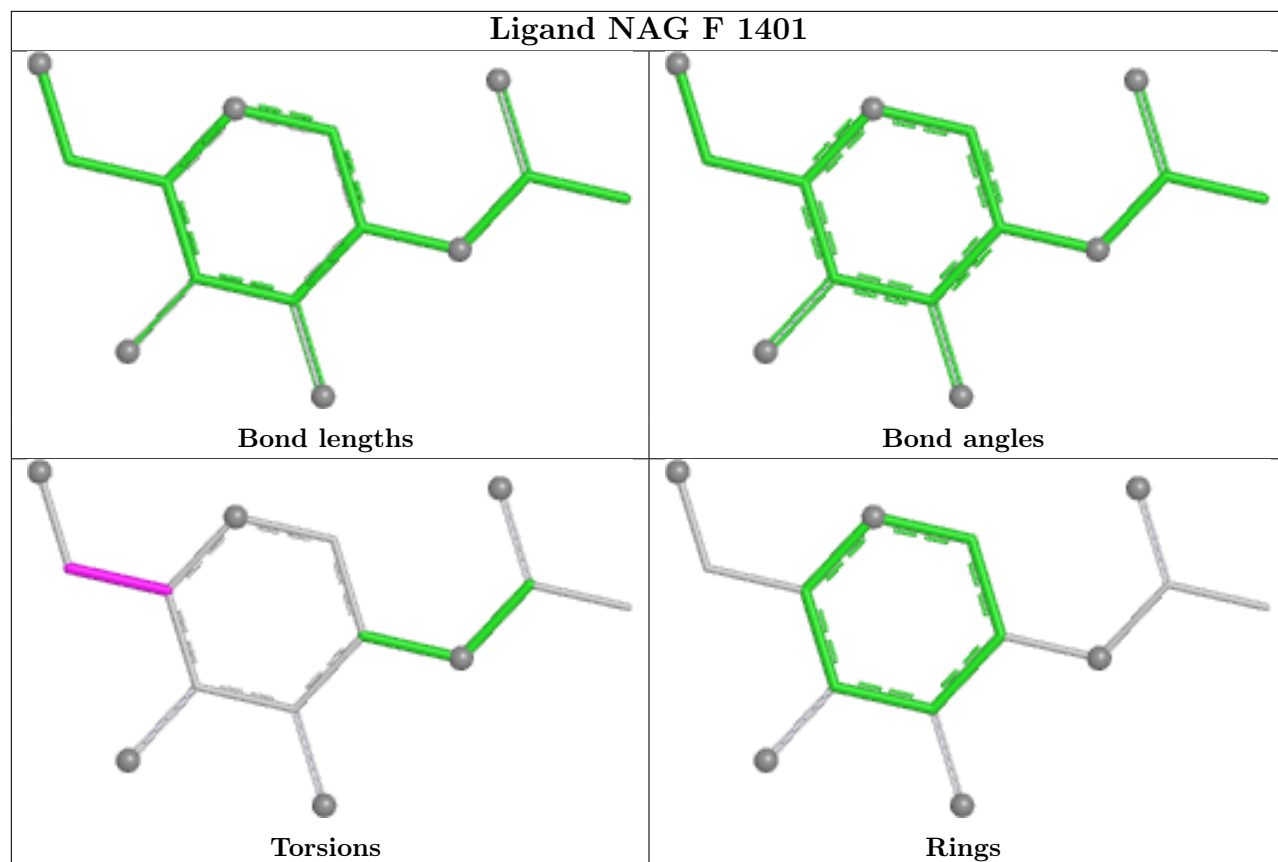
Ligand NAG A 701



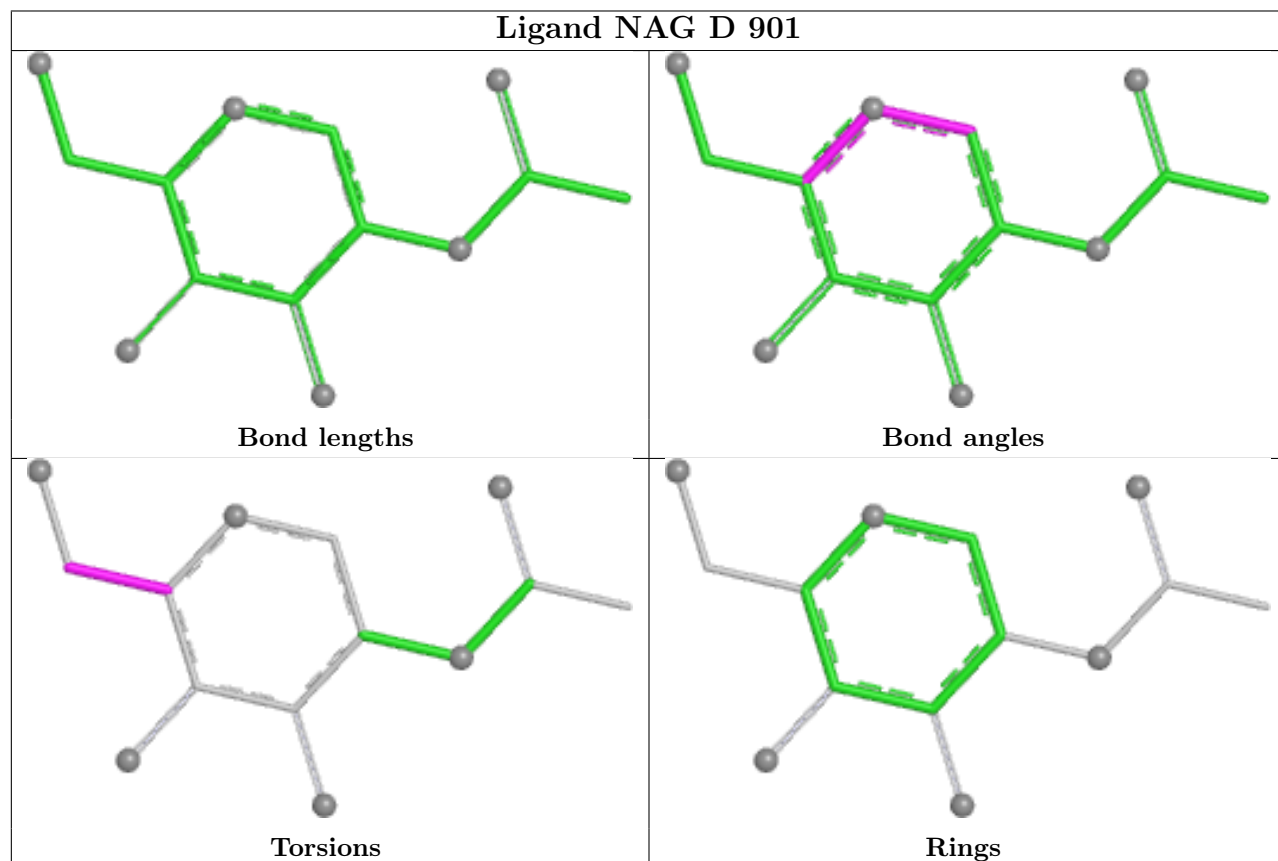




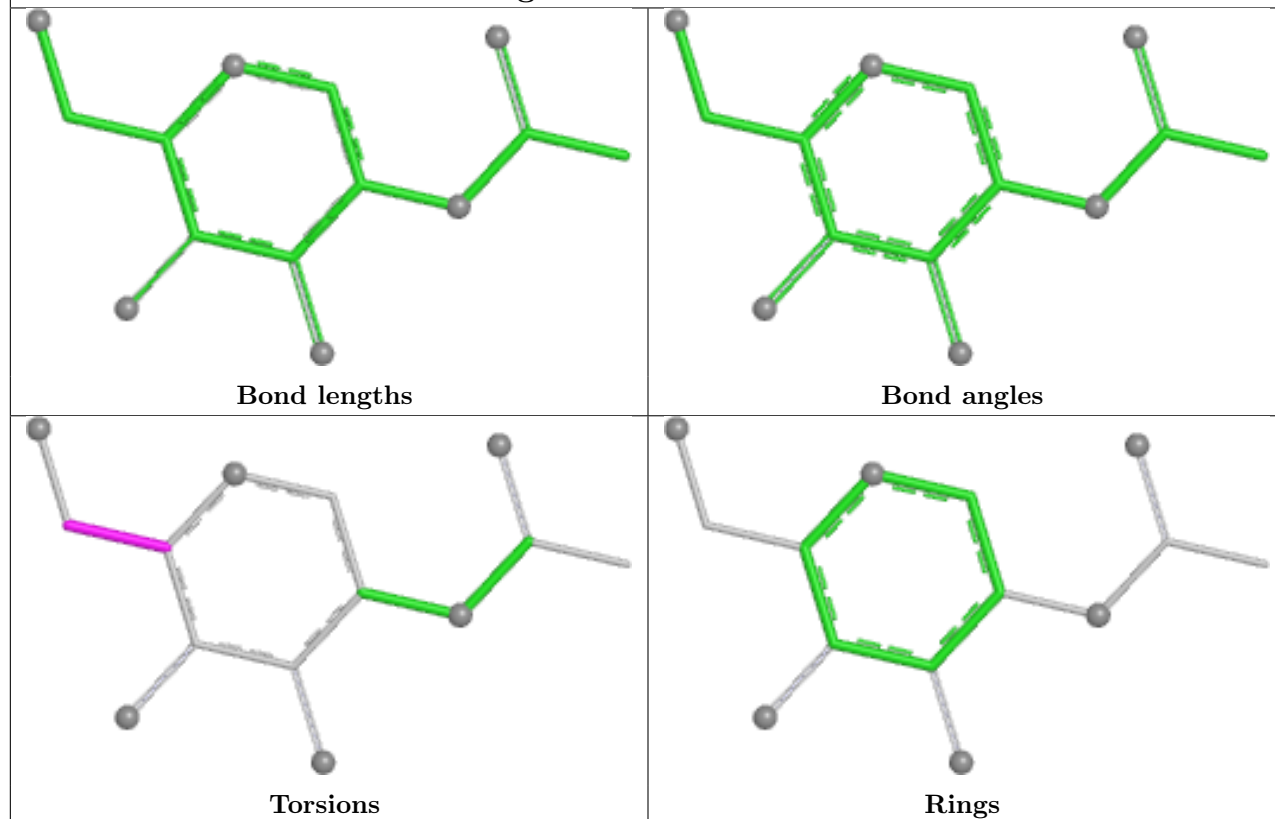
Ligand NAG F 1401



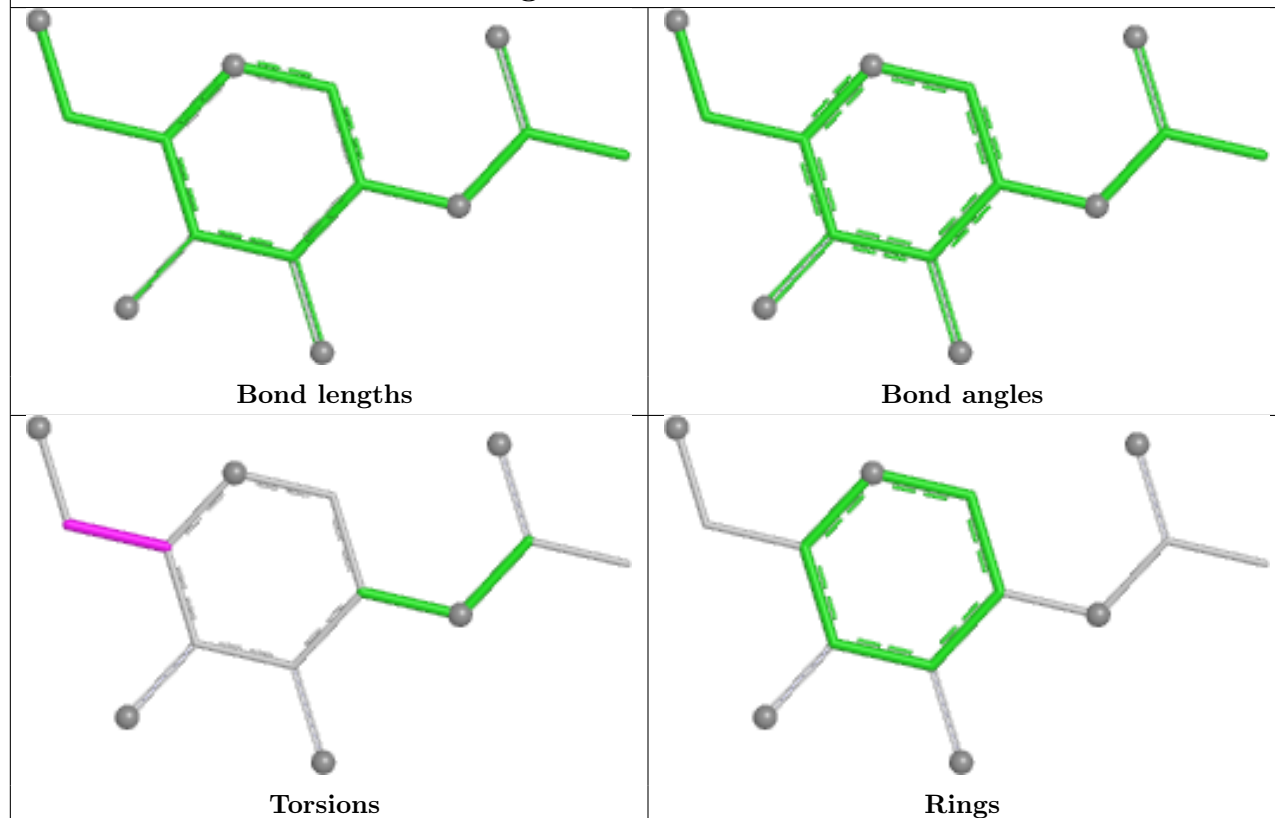
Ligand NAG D 901



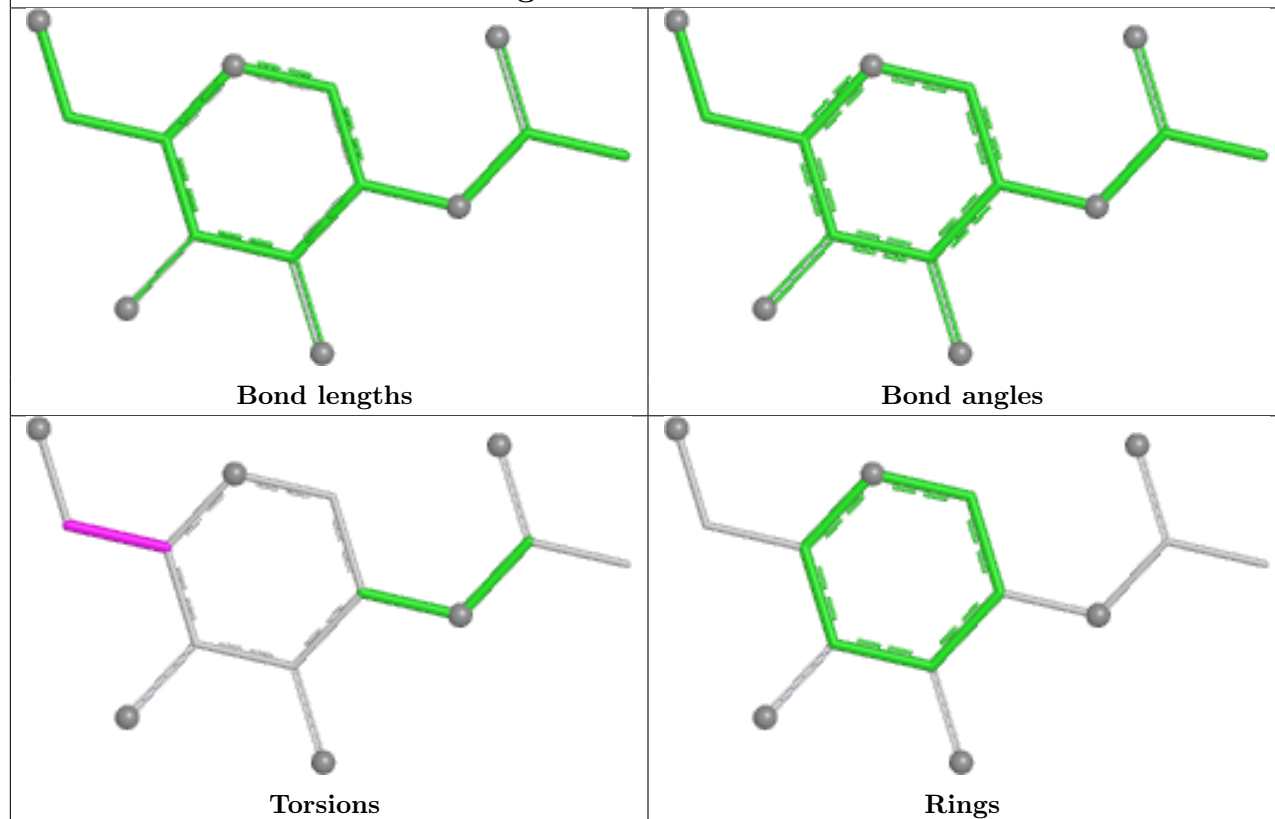
Ligand NAG G 1401



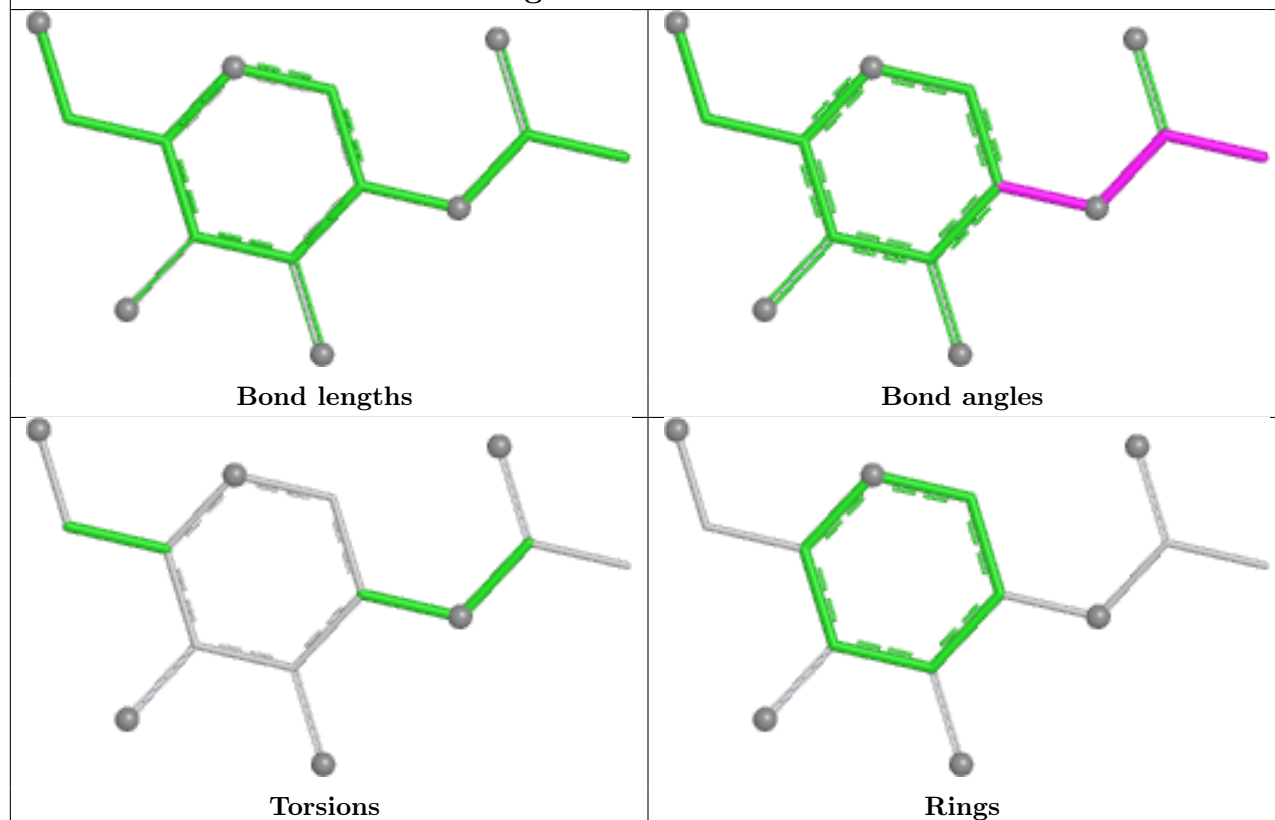
Ligand NAG F 1408

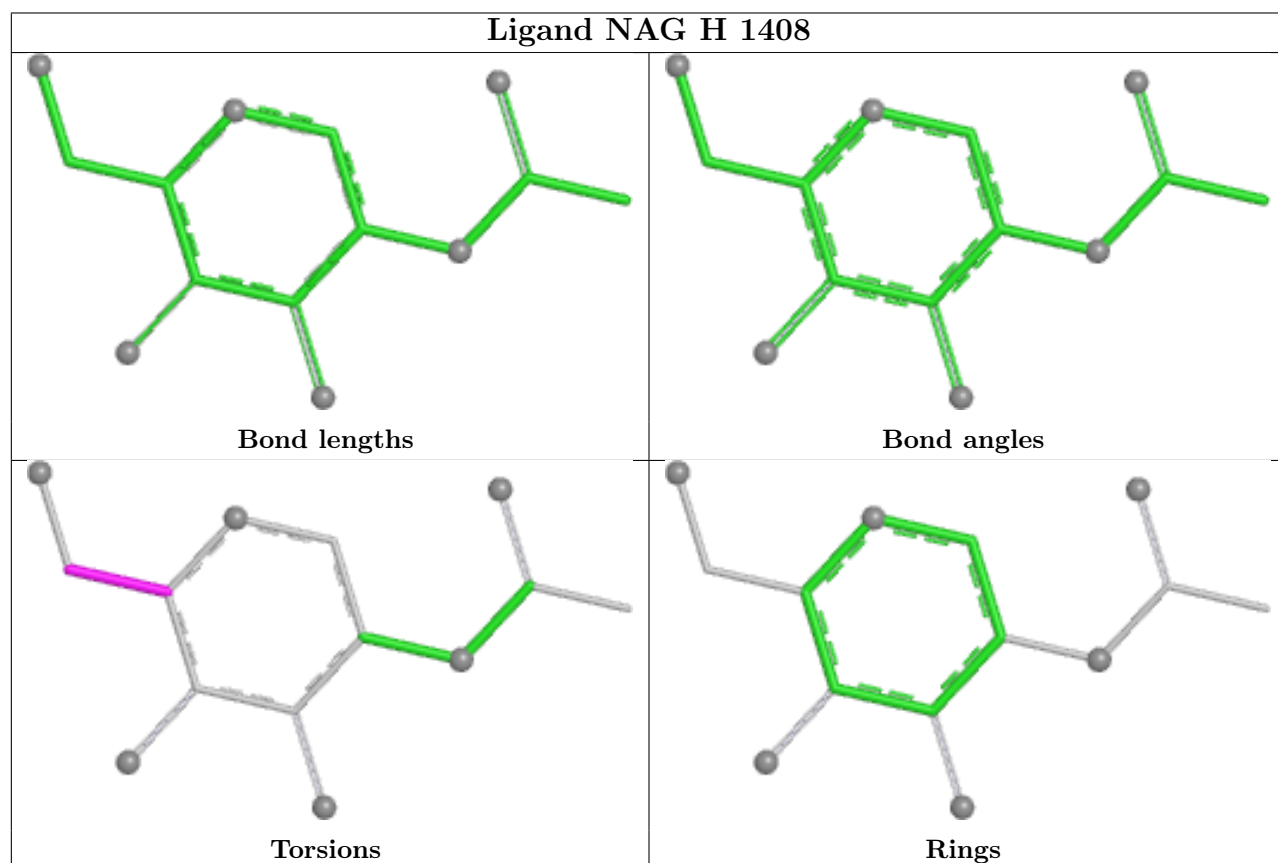
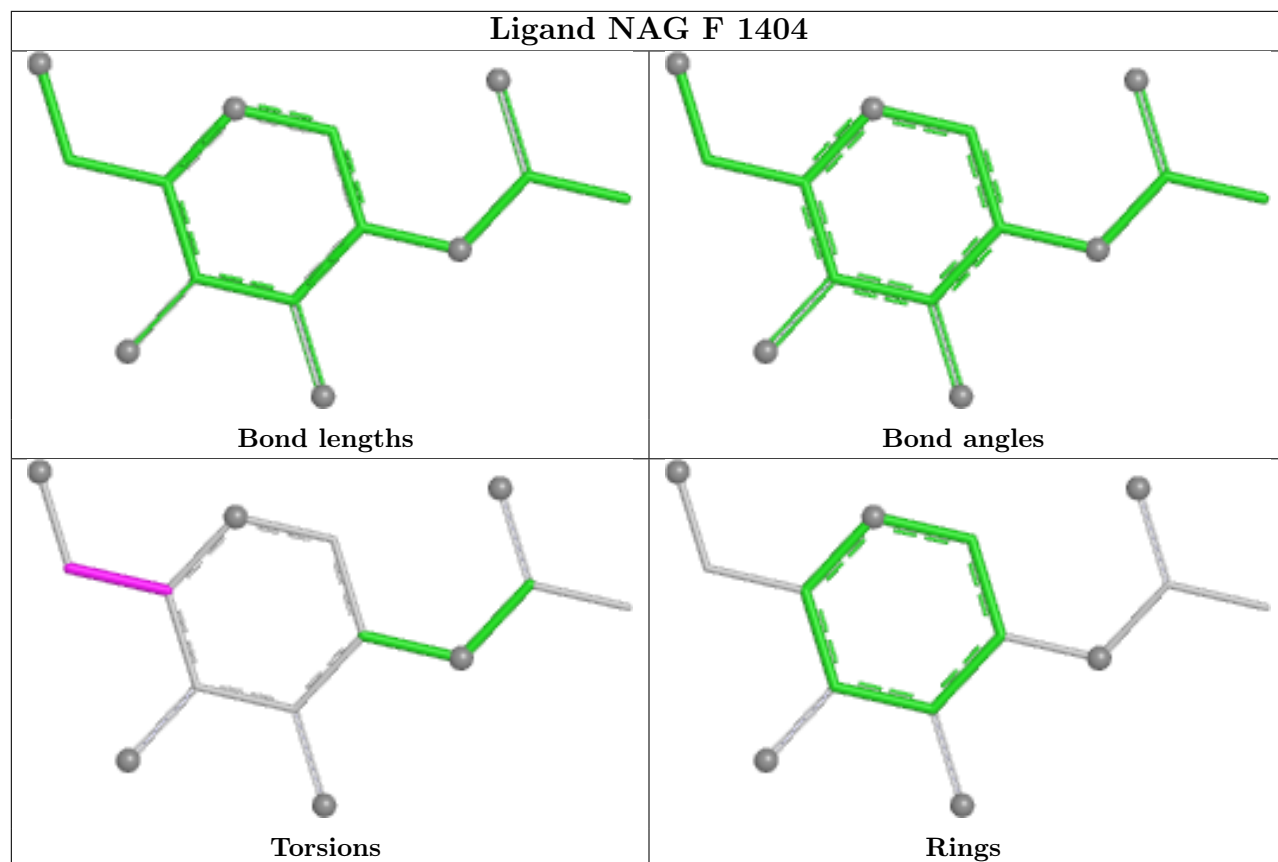


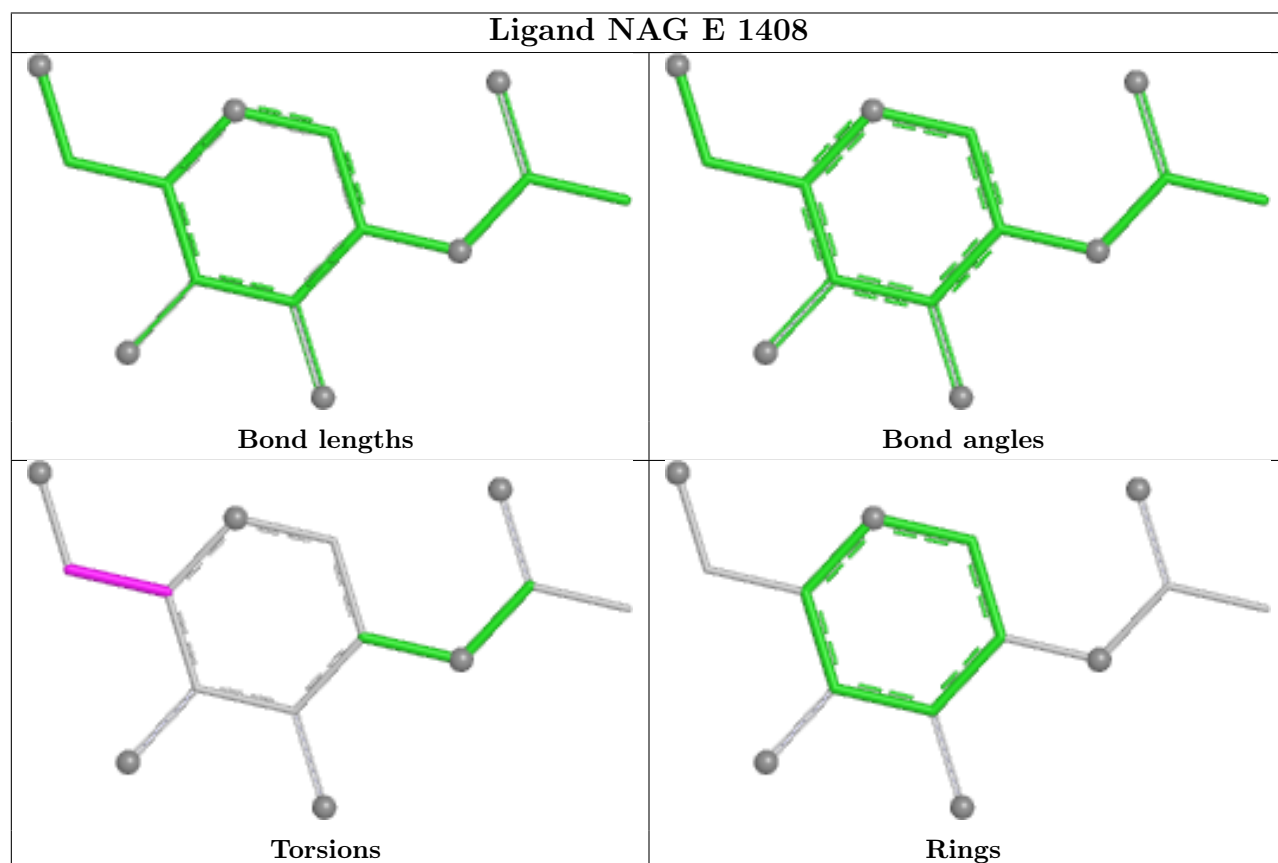
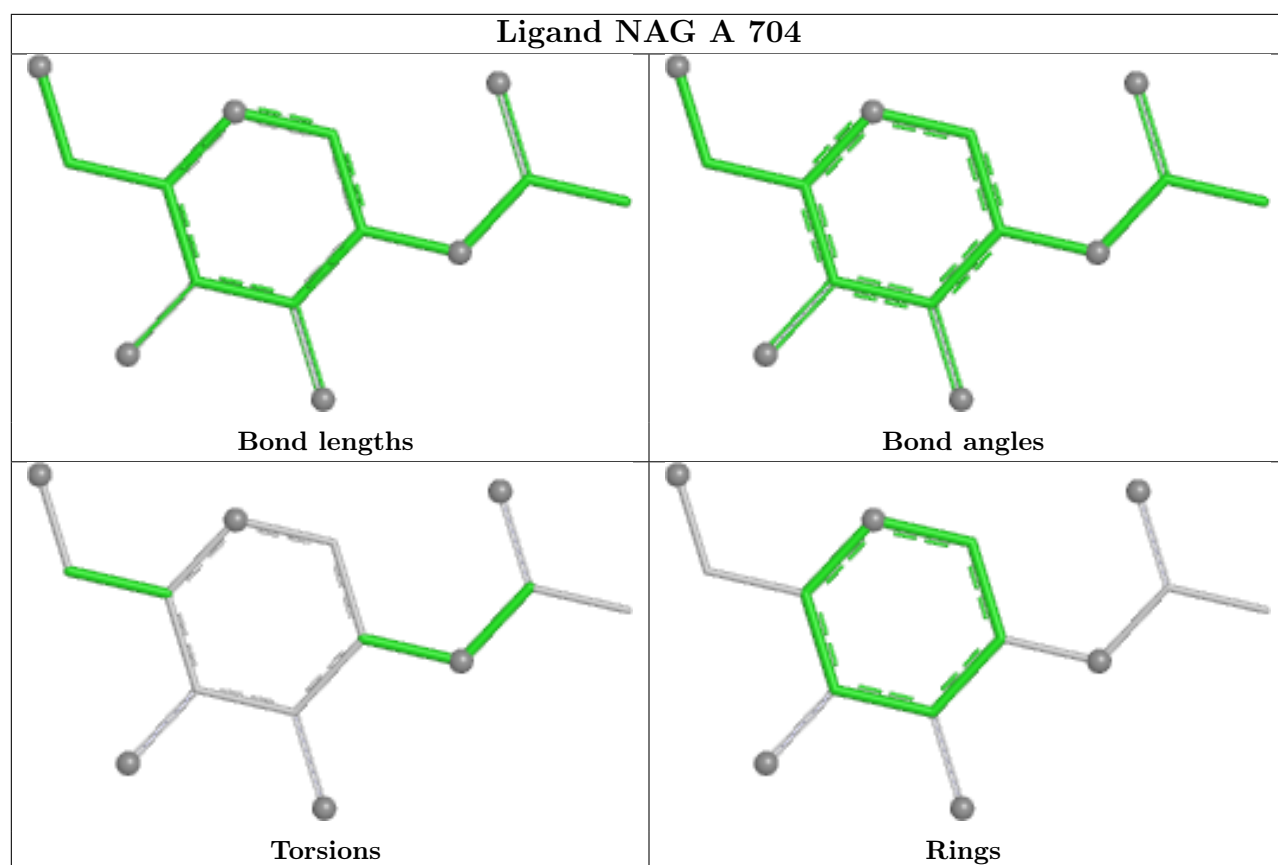
Ligand NAG G 1408

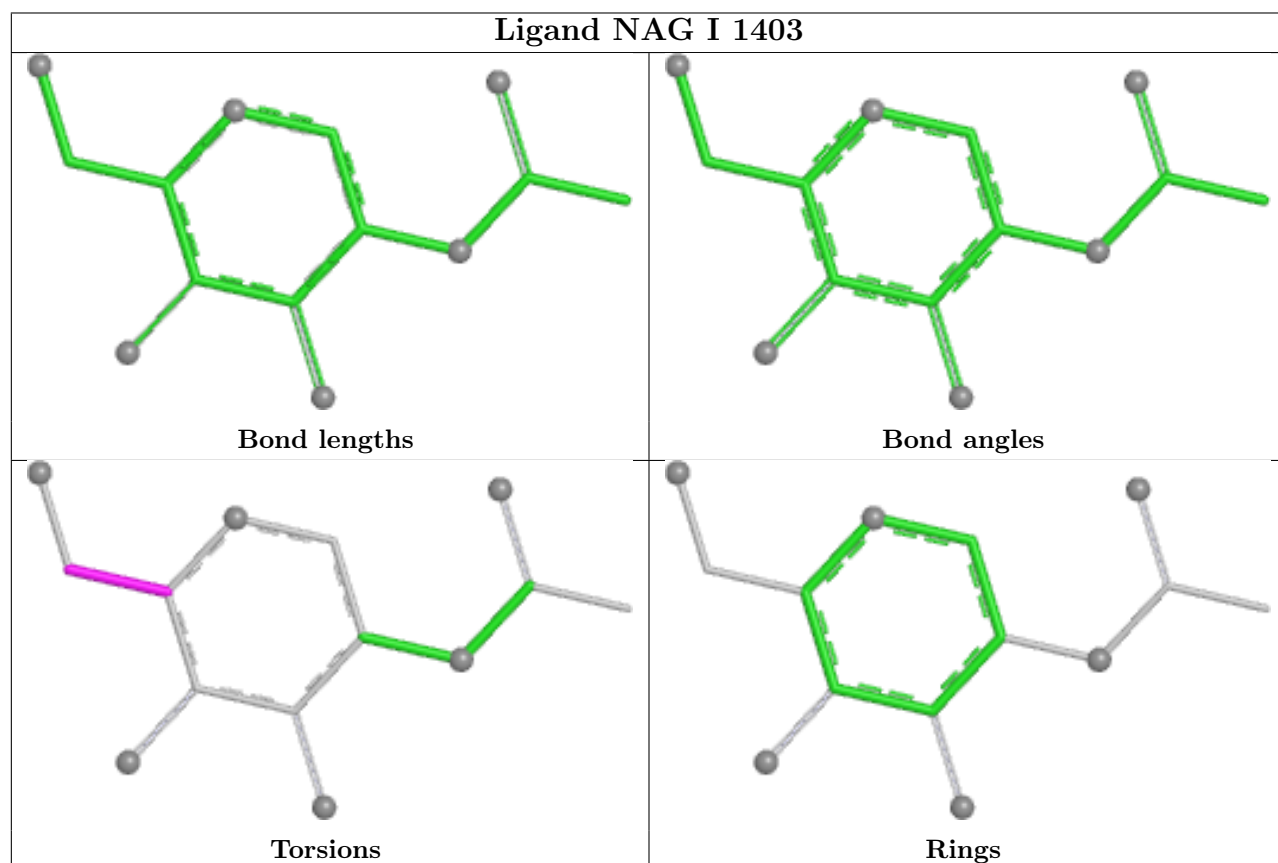
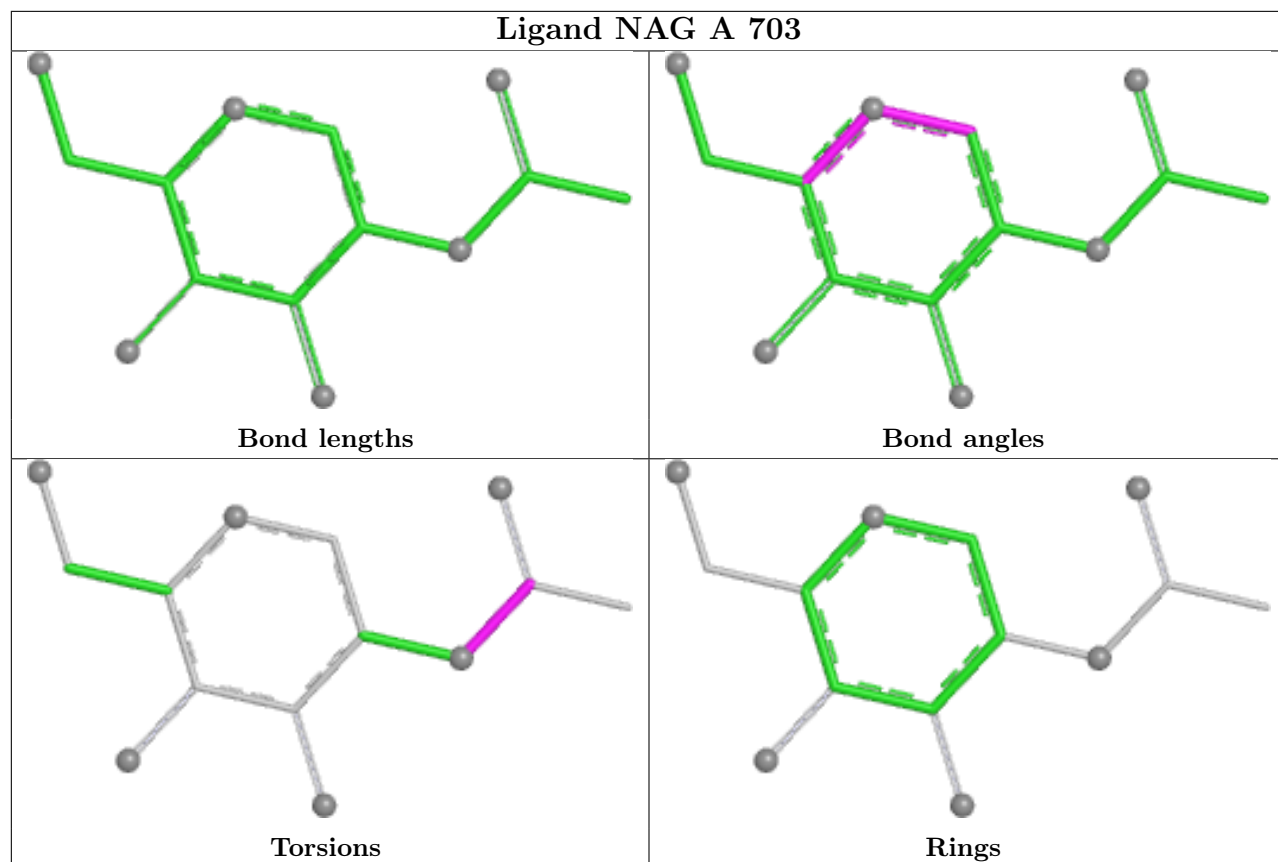


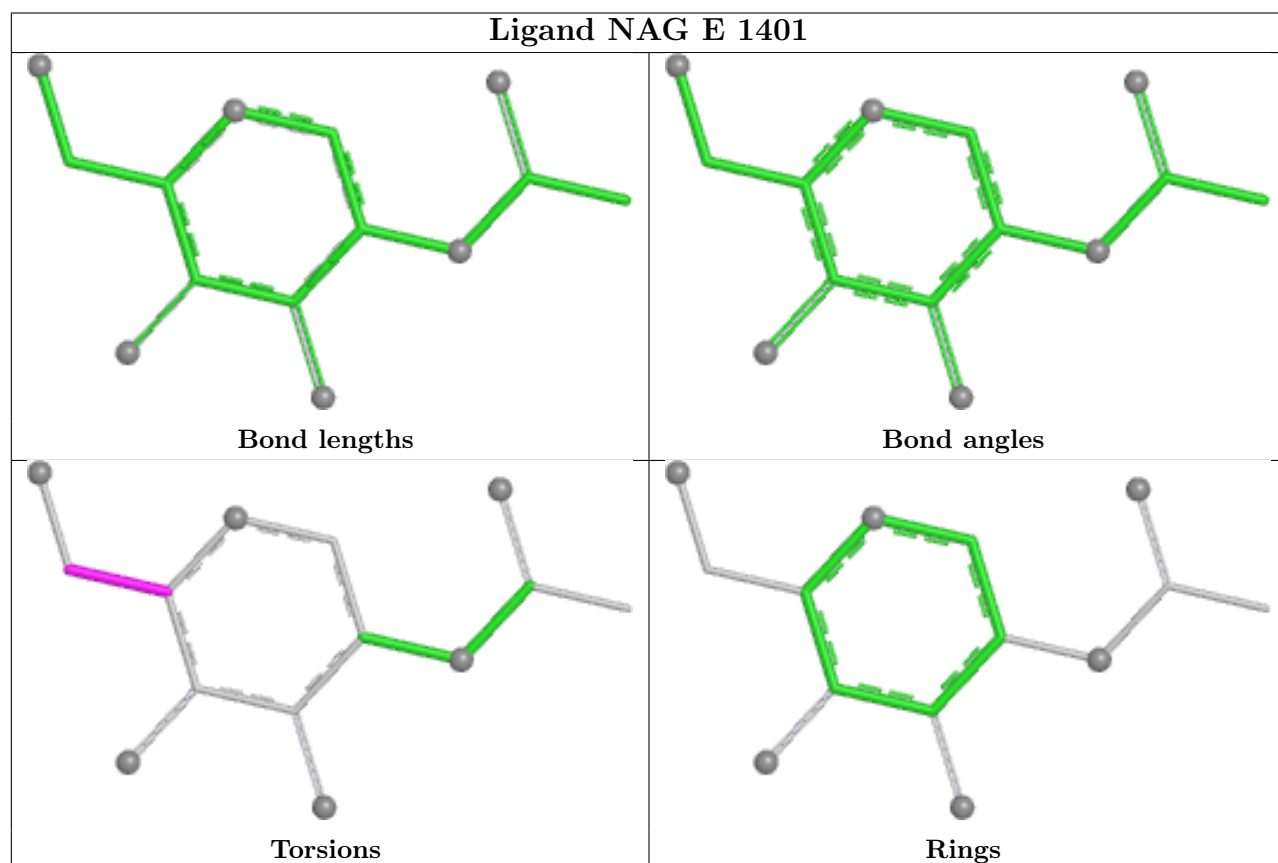
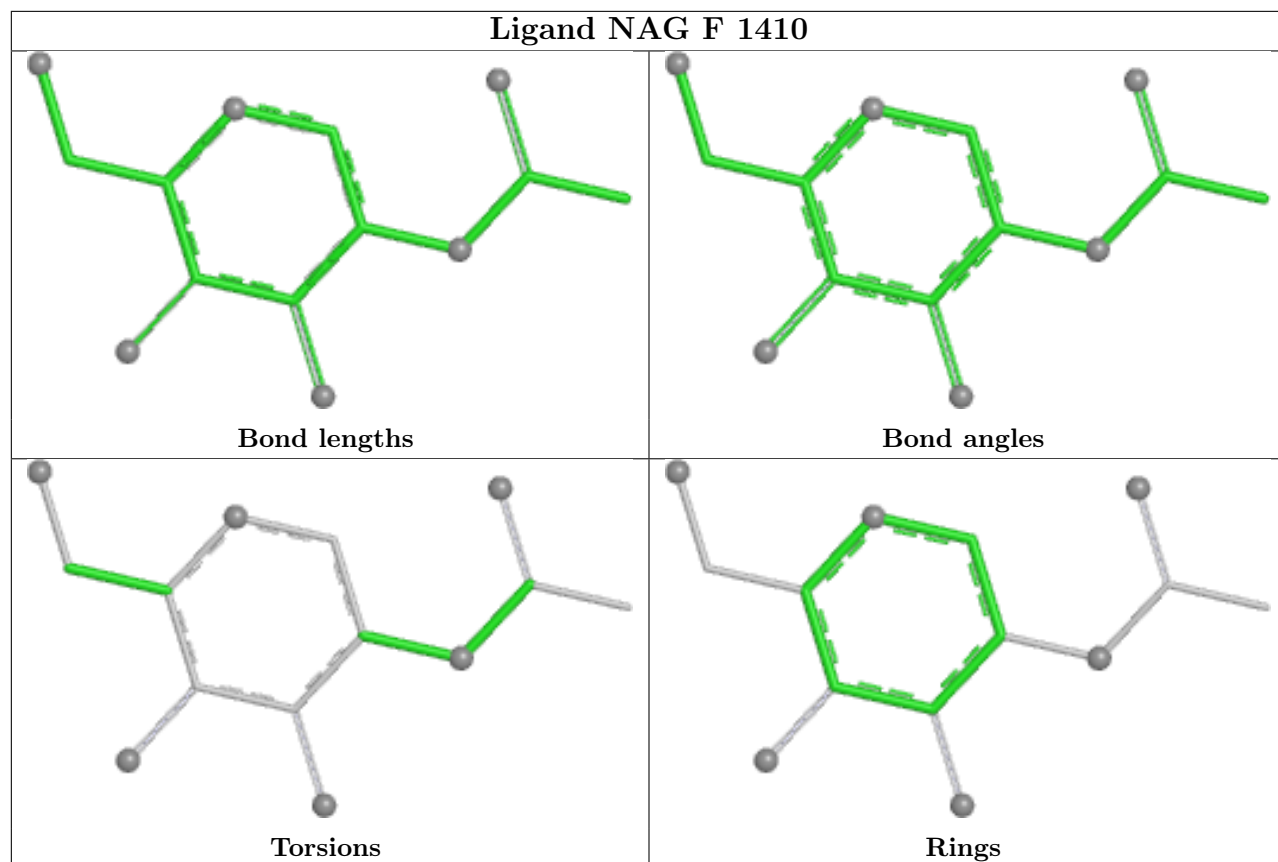
Ligand NAG I 1409



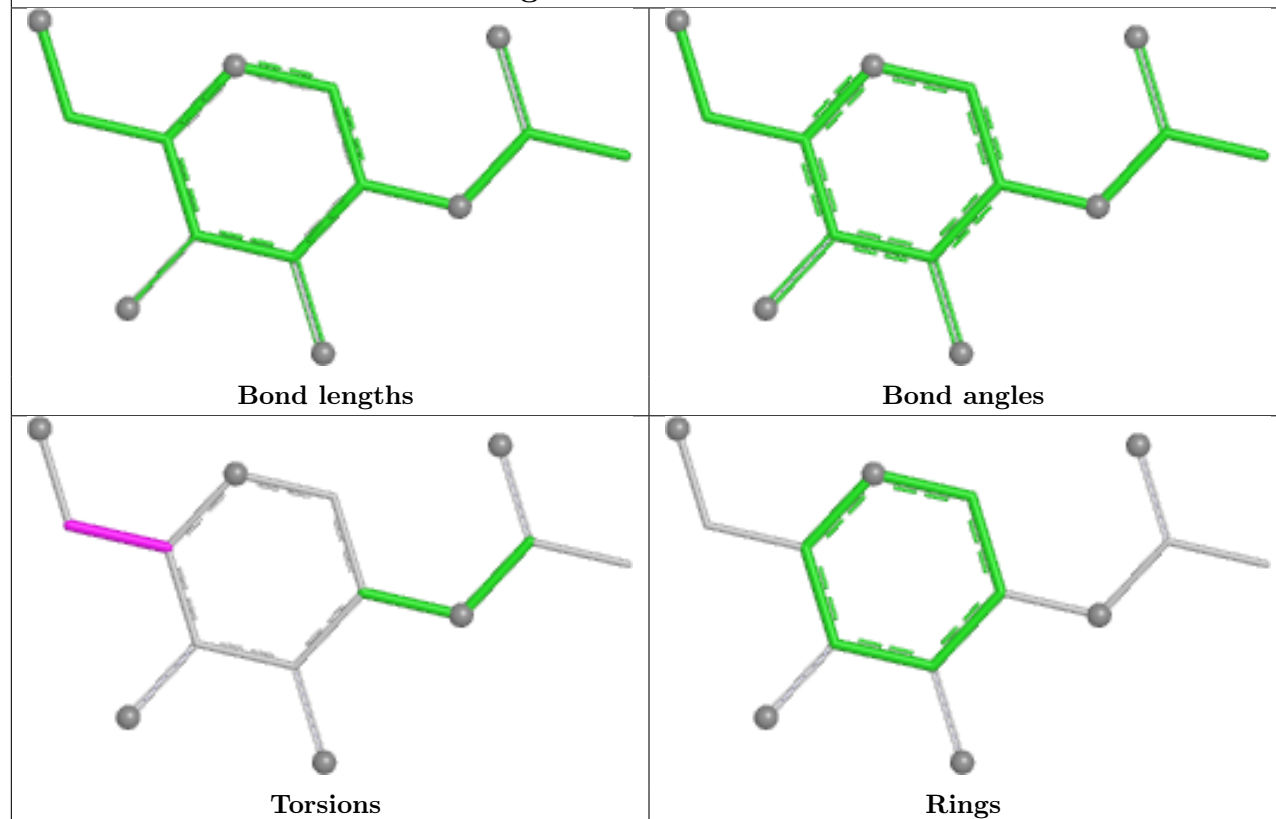




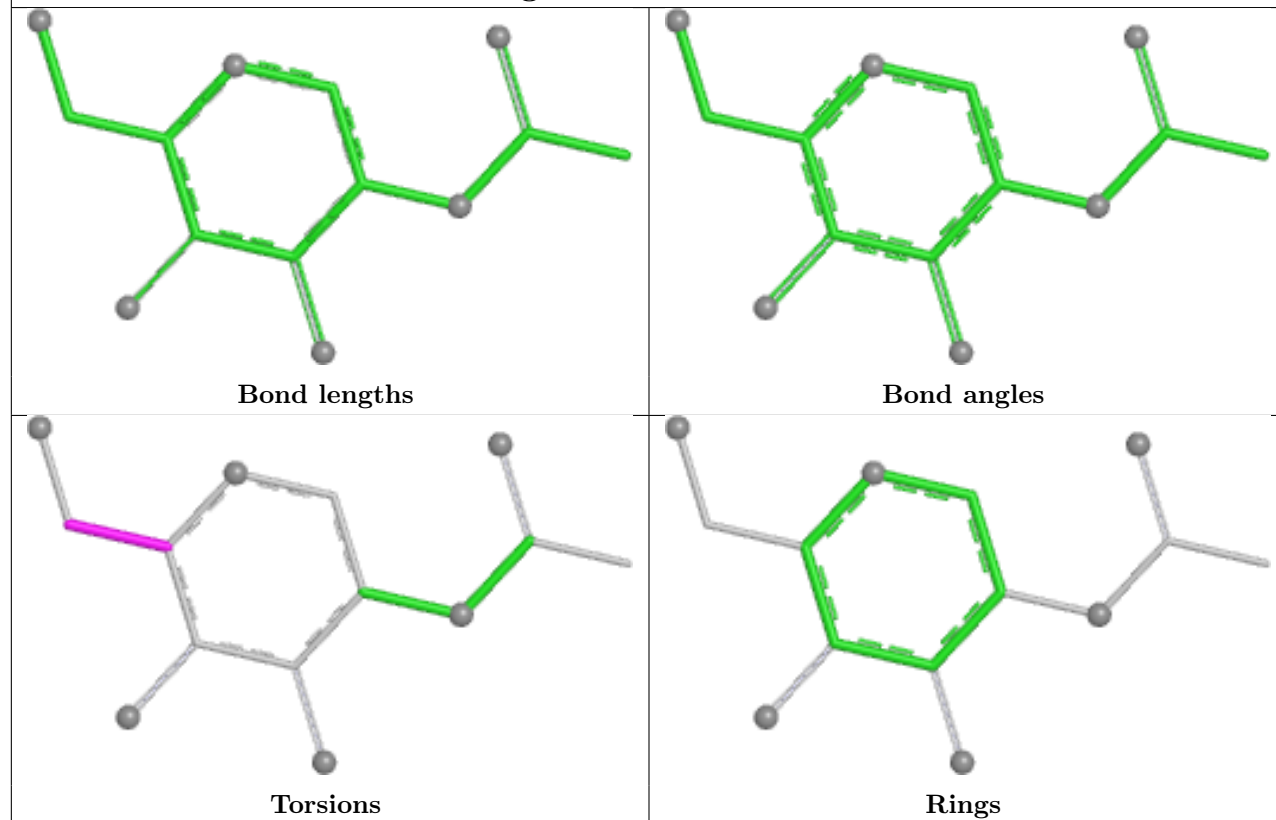




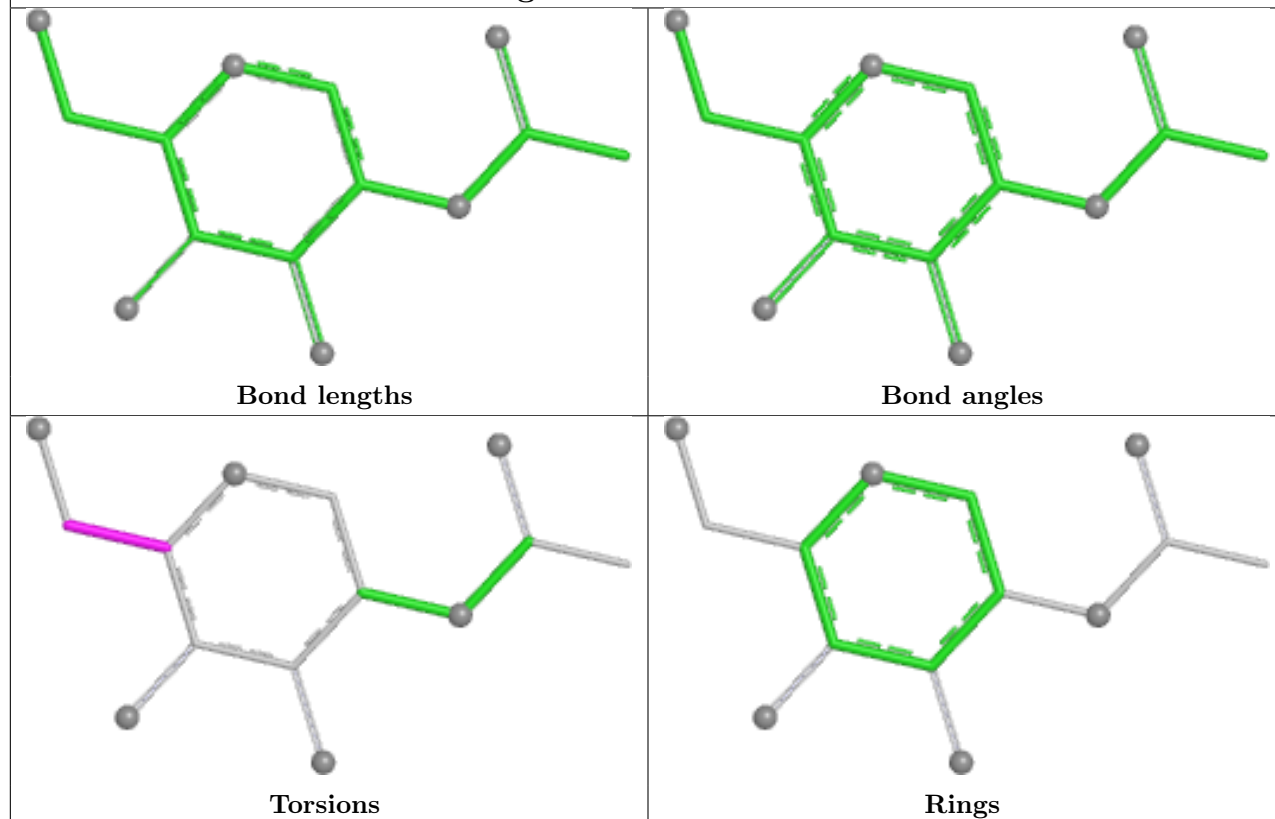
Ligand NAG E 1402



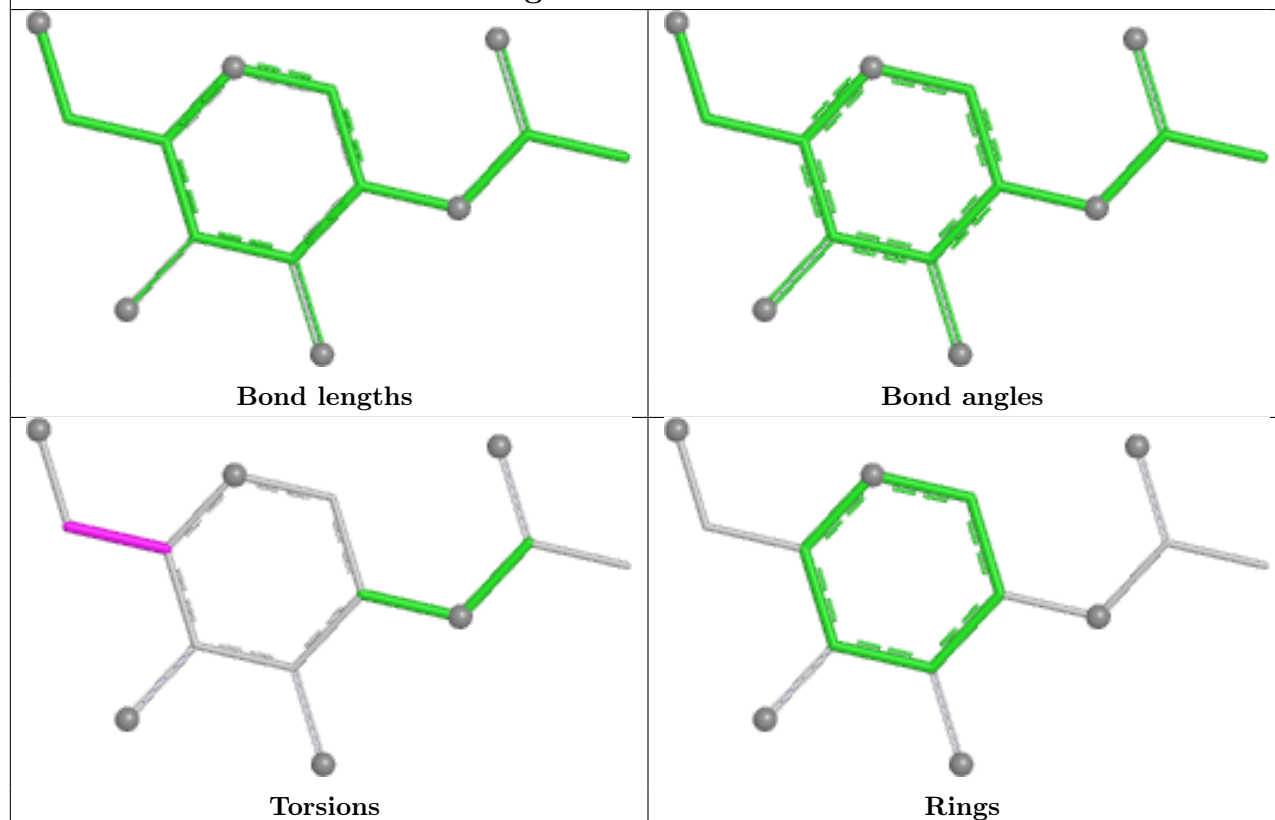
Ligand NAG E 1406

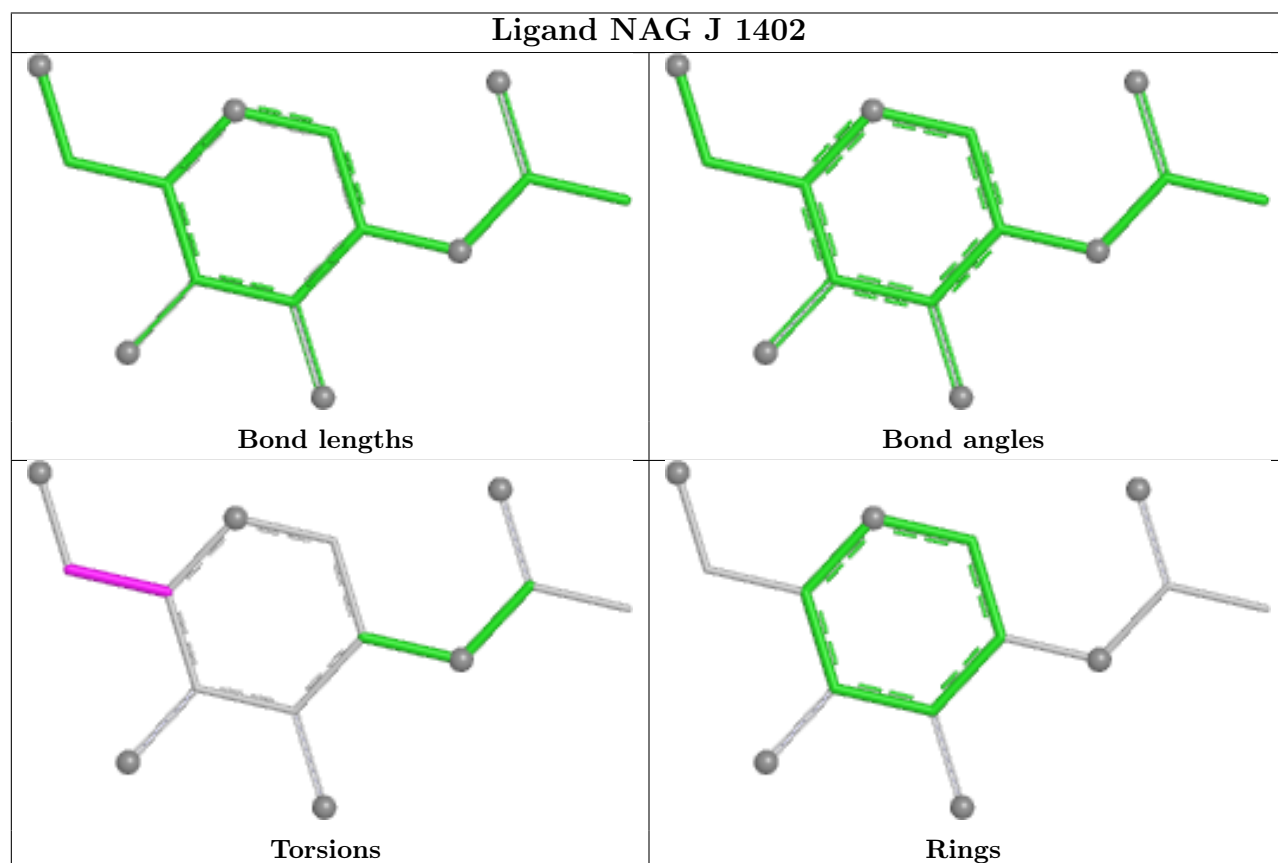
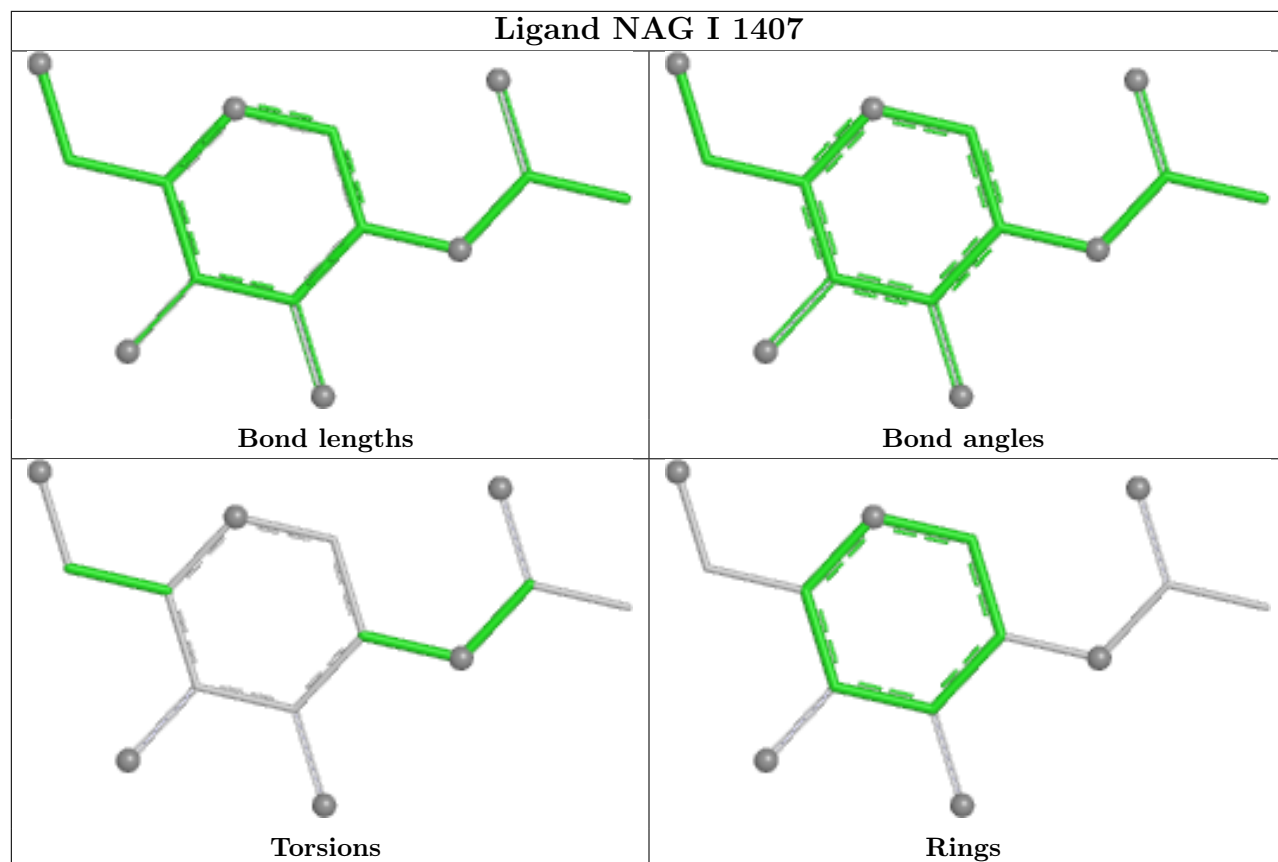


Ligand NAG G 1404

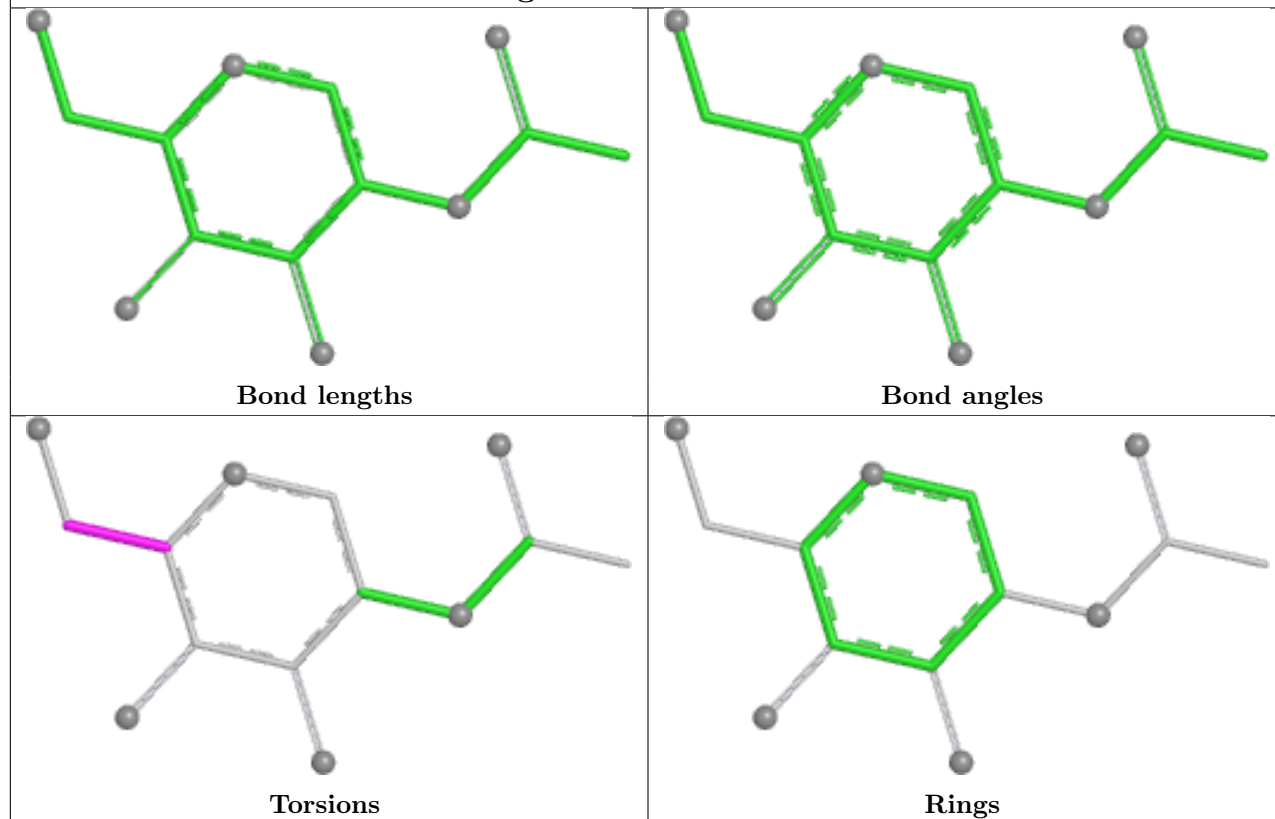


Ligand NAG I 1402

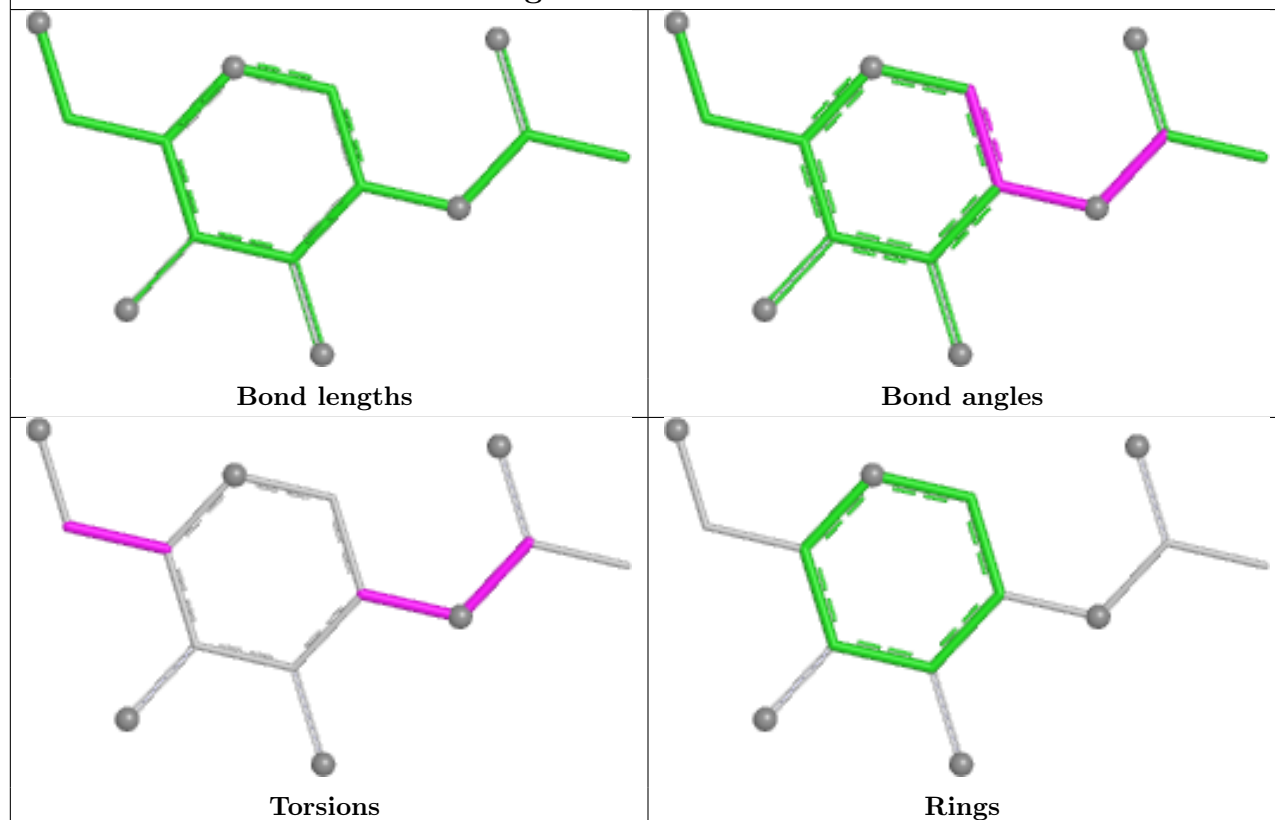




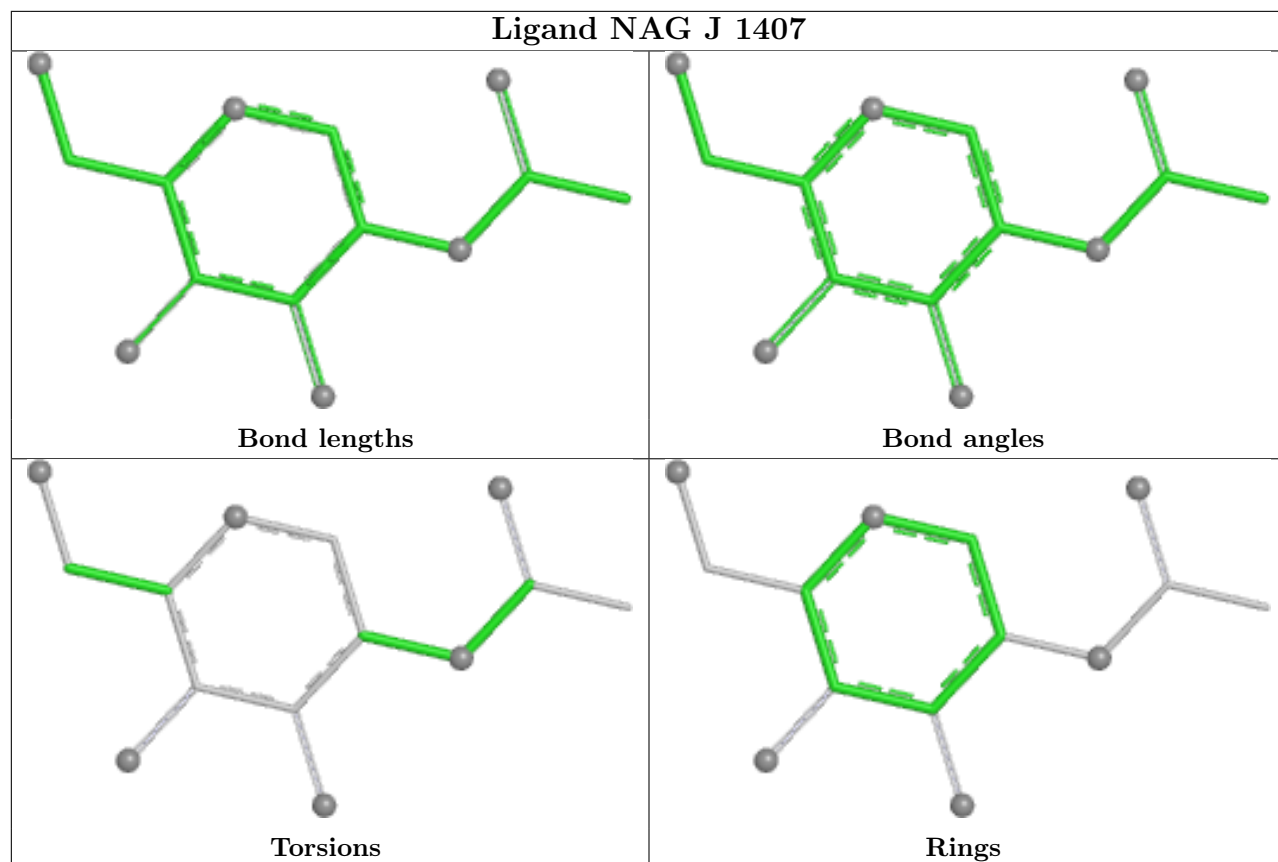
Ligand NAG H 1404



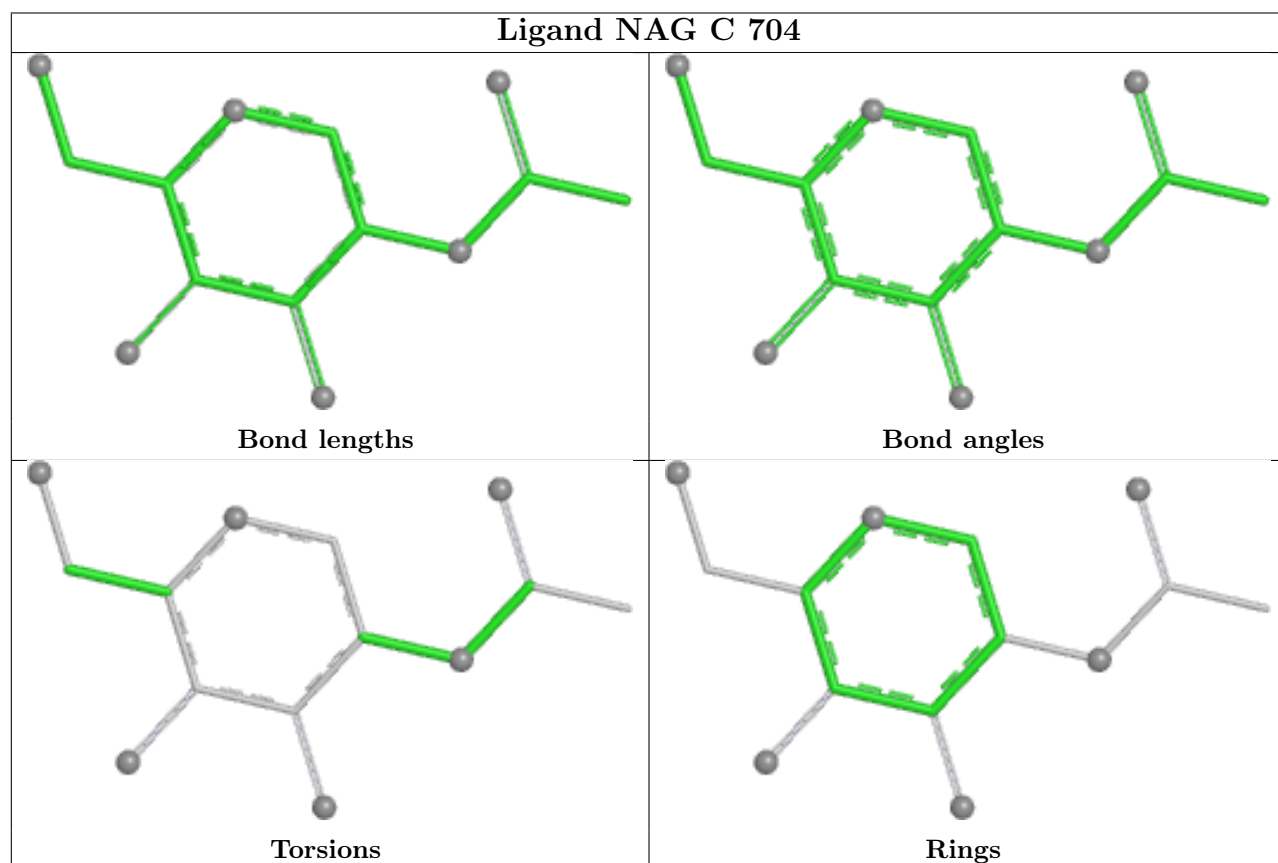
Ligand NAG I 1405

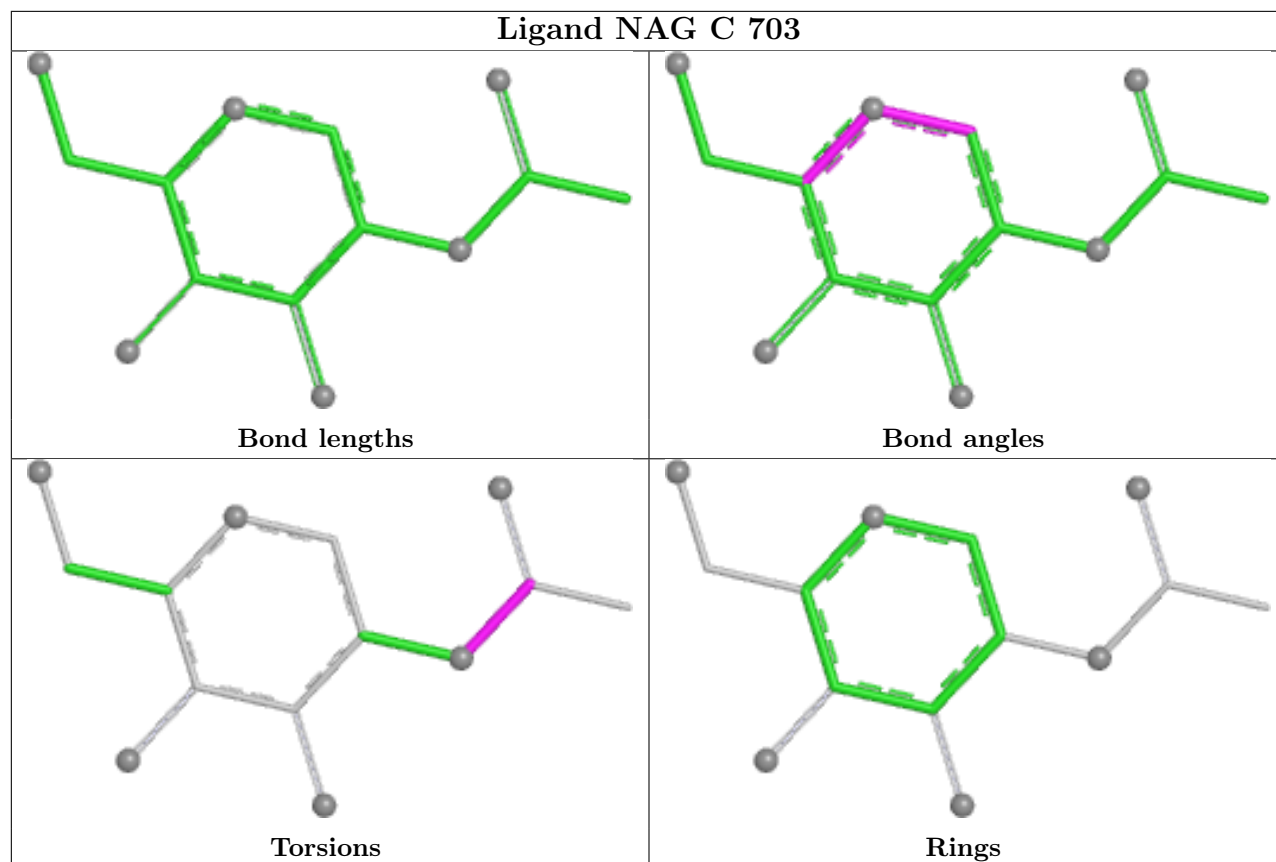


Ligand NAG J 1407



Ligand NAG C 704





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.

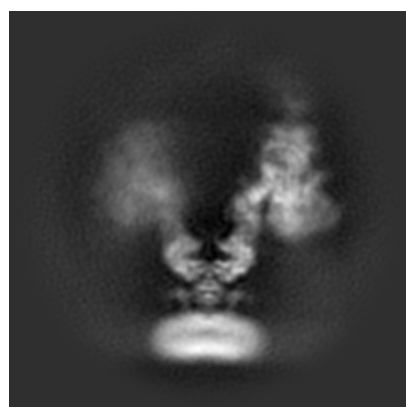
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-30888. These allow visual inspection of the internal detail of the map and identification of artifacts.

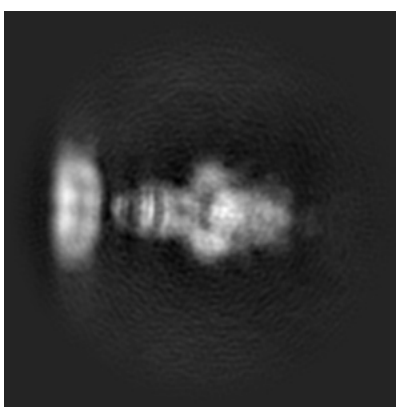
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

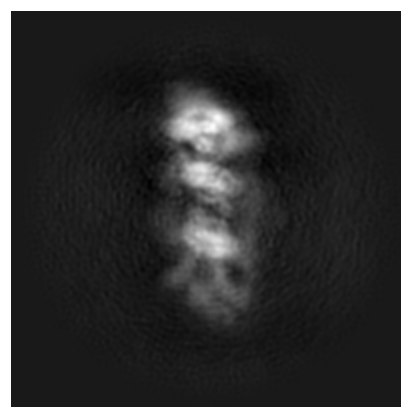
6.1.1 Primary map



X



Y

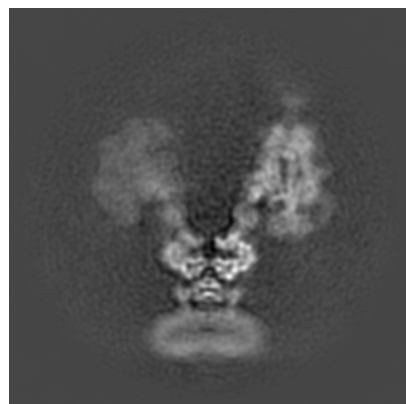


Z

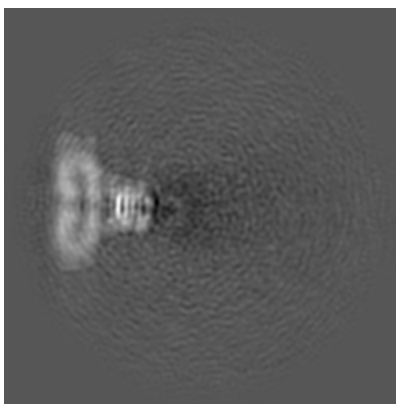
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

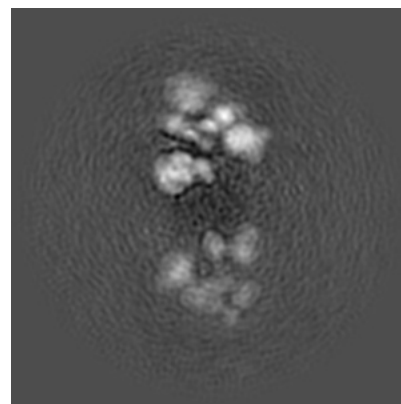
6.2.1 Primary map



X Index: 240



Y Index: 240

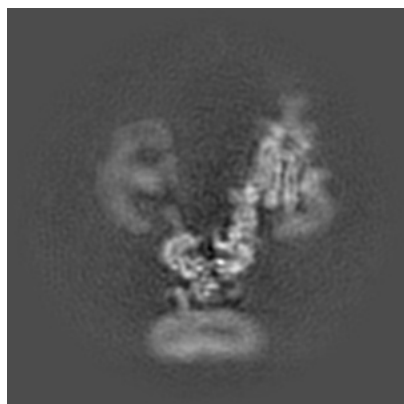


Z Index: 240

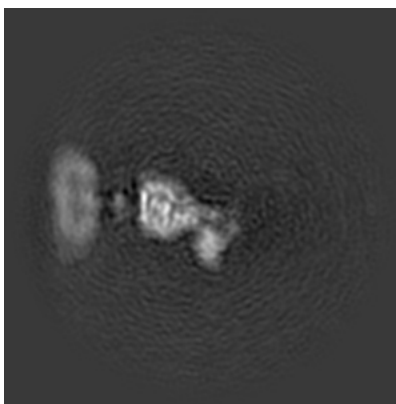
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

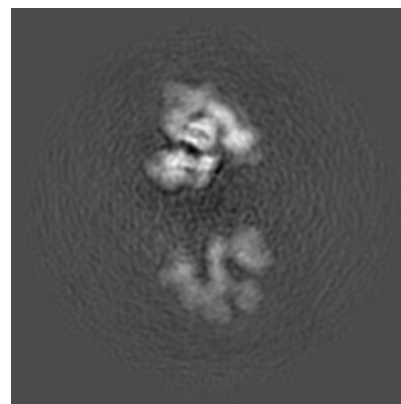
6.3.1 Primary map



X Index: 231



Y Index: 279

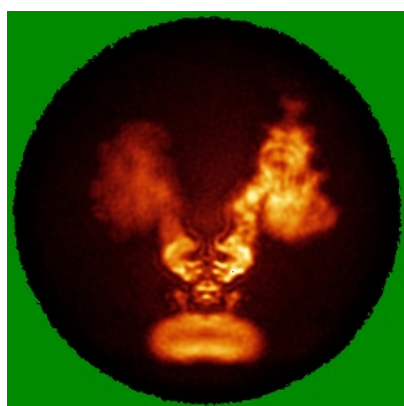


Z Index: 253

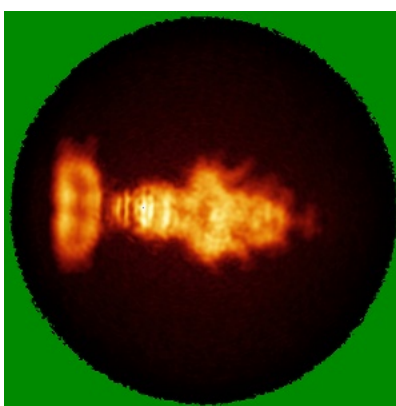
The images above show the largest variance slices of the map in three orthogonal directions.

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

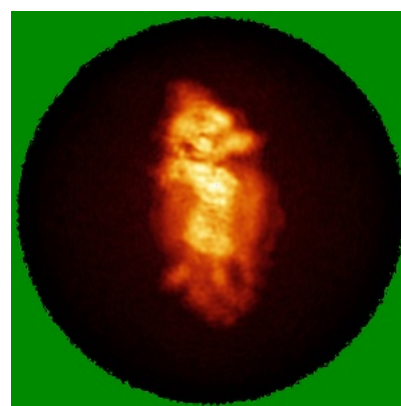
6.4.1 Primary map



X



Y

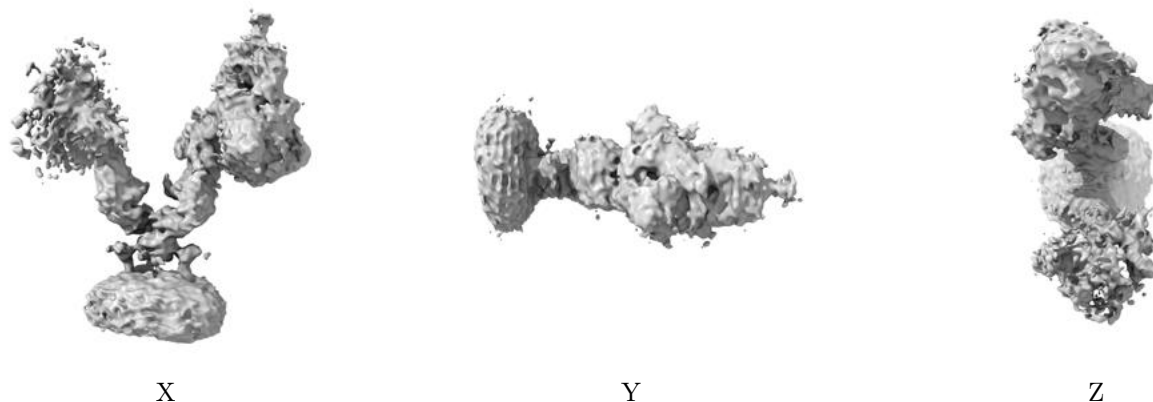


Z

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 0.3. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

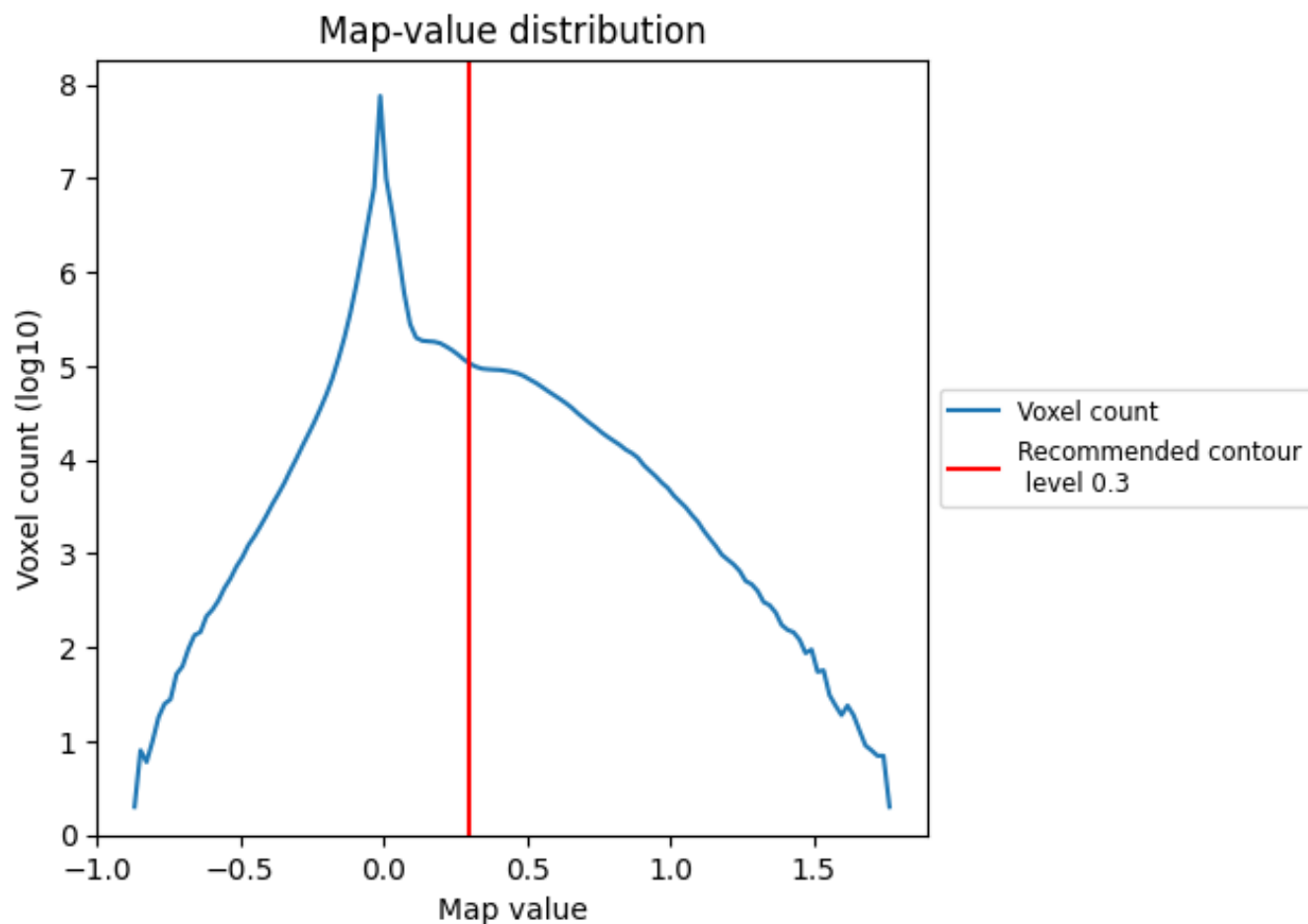
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

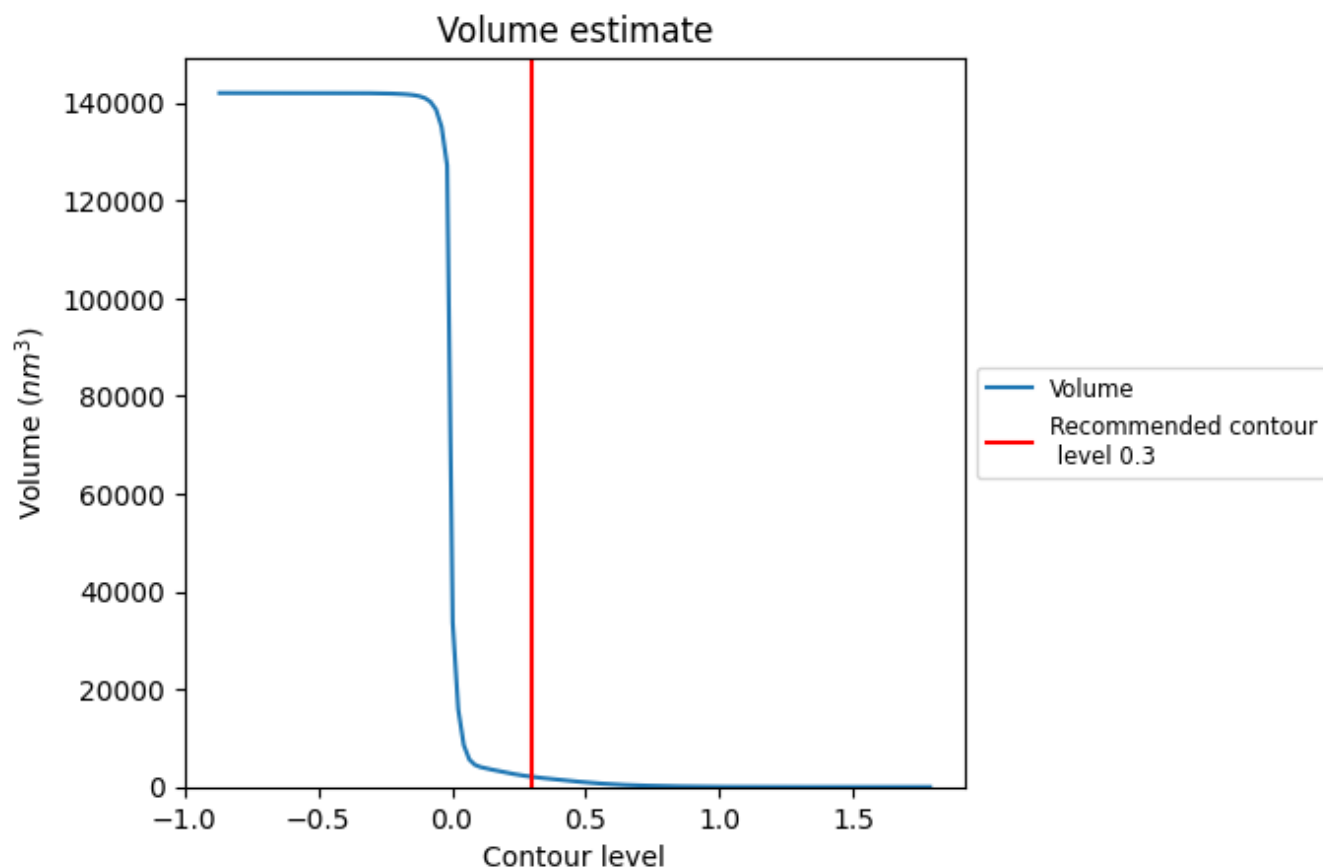
This section contains the results of statistical analysis of the map.

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.

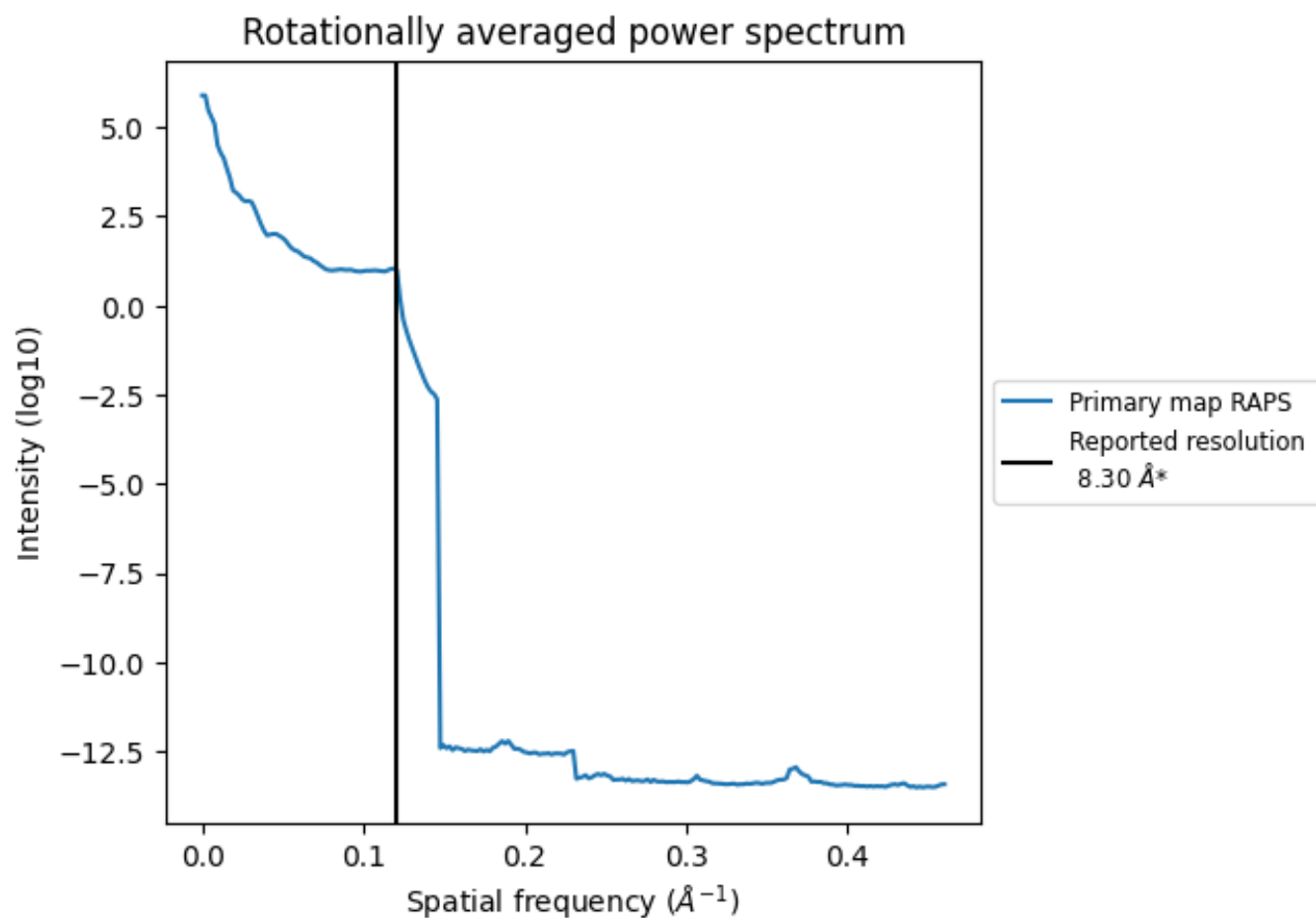
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2071 nm³; this corresponds to an approximate mass of 1871 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 0.120 Å⁻¹

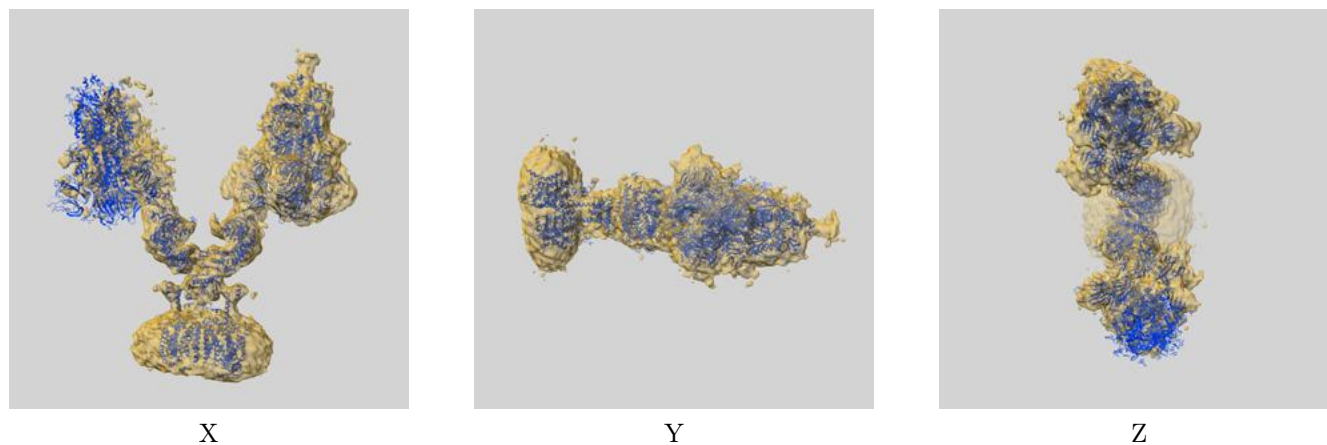
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit [i](#)

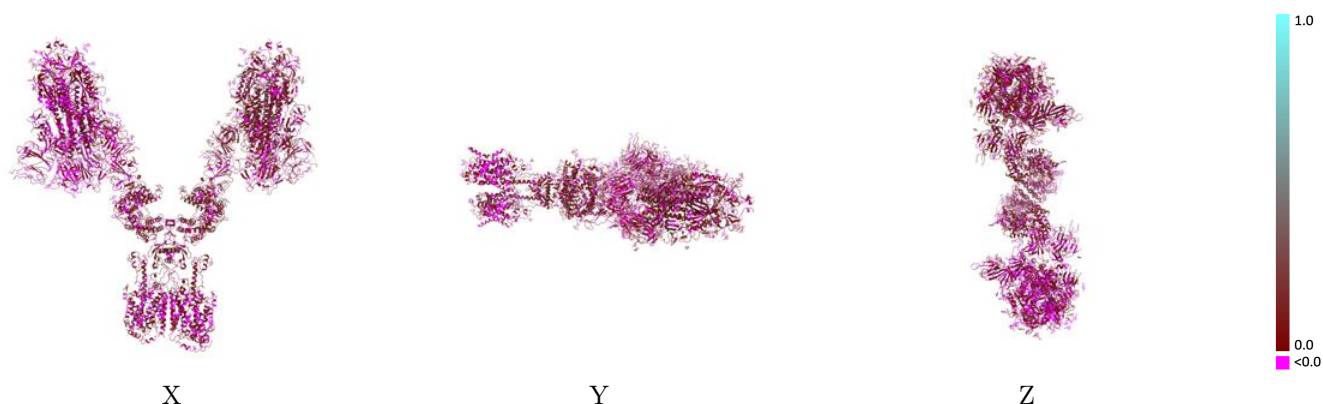
This section contains information regarding the fit between EMDB map EMD-30888 and PDB model 7DWX. Per-residue inclusion information can be found in [section 3](#) on [page 18](#).

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.3 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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

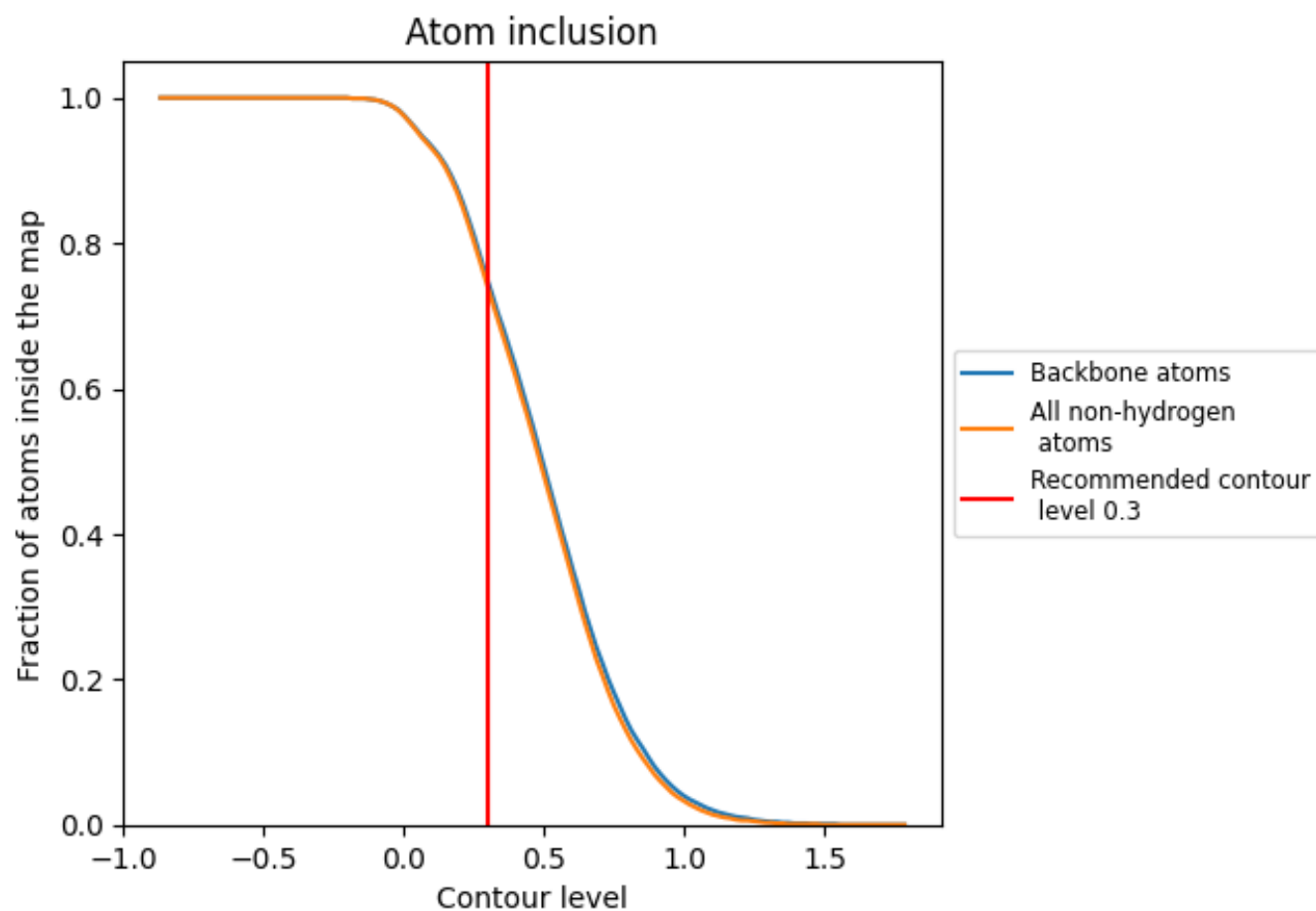


The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 75% of all backbone atoms, 74% 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 (0.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7380	 0.0590
0	 0.0000	 -0.1670
1	 0.0000	 0.2380
2	 0.0000	 -0.0390
3	 0.0000	 0.0190
4	 0.0360	 0.2120
5	 0.6070	 0.0500
6	 0.0000	 0.0020
7	 0.0000	 -0.2070
8	 0.1070	 -0.0560
9	 0.0360	 -0.0570
A	 0.9270	 0.0490
AA	 0.0000	 -0.0820
B	 0.9440	 0.1070
BA	 0.0000	 -0.0660
C	 0.9090	 0.0470
CA	 0.0000	 0.1500
D	 0.9070	 0.0910
DA	 0.0000	 -0.0150
E	 0.9640	 0.0800
EA	 0.0000	 -0.0910
F	 0.9470	 0.0870
FA	 0.0000	 -0.0470
G	 0.9250	 0.0690
H	 0.5640	 0.0340
I	 0.4230	 0.0240
J	 0.1580	 0.0150
K	 0.5360	 0.0770
L	 0.7140	 0.0810
M	 0.8210	 0.0720
N	 1.0000	 0.0400
O	 0.2140	 -0.0370
P	 0.8210	 0.0760
Q	 0.8210	 0.0990
R	 0.5360	 0.0400



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
S	 0.2860	 0.1170
T	 0.7860	 0.0600
U	 0.7860	 0.0600
V	 0.2500	 0.0480
W	 0.9290	 0.0700
X	 1.0000	 0.2210
Y	 1.0000	 0.2510
Z	 1.0000	 0.1410
a	 0.8930	 0.0060
b	 0.8210	 0.0300
c	 0.5710	 0.0880
d	 0.4640	 -0.0740
e	 0.5710	 0.1110
f	 0.3930	 0.0910
g	 0.8210	 -0.0920
h	 0.9290	 0.0370
i	 0.8210	 0.1070
j	 0.5710	 0.0380
k	 0.4290	 -0.0010
l	 0.7860	 0.0880
m	 0.9640	 0.1240
n	 1.0000	 0.1630
o	 0.5000	 -0.0350
p	 1.0000	 0.1070
q	 1.0000	 0.1420
r	 0.7500	 0.0740
s	 0.6790	 0.0080
t	 0.7500	 0.0860
u	 0.2500	 0.0420
v	 0.6430	 0.0270
w	 0.1430	 -0.0040
x	 0.0000	 0.1240
y	 0.0000	 -0.1520
z	 0.0000	 -0.1580