



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 04:30 AM UTC

PDB ID : 7DX9 / pdb_00007dx9
EMDB ID : EMD-30900
Title : Trypsin-digested S protein of SARS-CoV-2 bound with PD of ACE2 in the conformation 3 (3 up RBD and 2 PD bound)
Authors : Yan, R.H.; Zhang, Y.Y.; Li, Y.N.; Ye, F.F.; Guo, Y.Y.; Xia, L.; Zhong, X.Y.; Chi, X.M.; Zhou, Q.
Deposited on : 2021-01-18
Resolution : 3.60 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:

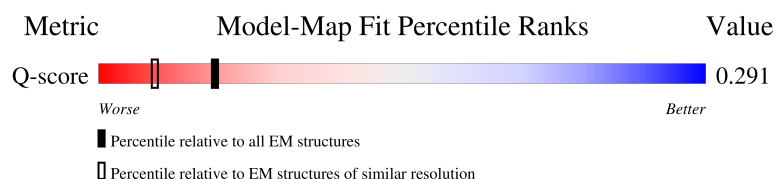
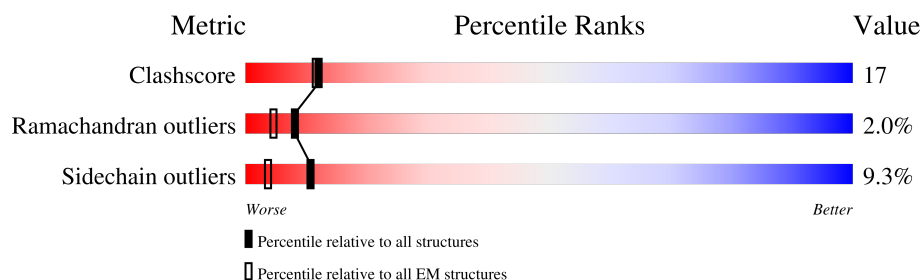
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

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

The reported resolution of this entry is 3.60 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	12797 (3.10 - 4.10)

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

Mol	Chain	Length	Quality of chain
1	A	1283	 15% 53% 21% 5% 22%
1	B	1283	 14% 50% 23% 5% 22%
1	C	1283	 39% 51% 23% 5% 22%
2	D	817	 65% 7% 27%

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Mol	Chain	Length	Quality of chain
2	E	817	
3	F	2	
3	G	2	
3	H	2	
3	I	2	
3	J	2	
3	K	2	
3	L	2	
3	M	2	
3	N	2	
3	O	2	
3	P	2	
3	Q	2	
3	R	2	
3	S	2	
3	T	2	
3	U	2	
3	V	2	
3	W	2	
3	X	2	
3	Y	2	
3	Z	2	
3	a	2	
3	b	2	
3	c	2	

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

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 34620 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Spike glycoprotein.

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

There are 36 discrepancies between the modelled and reference sequences:

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

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

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

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

There are 26 discrepancies between the modelled and reference sequences:

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

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

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



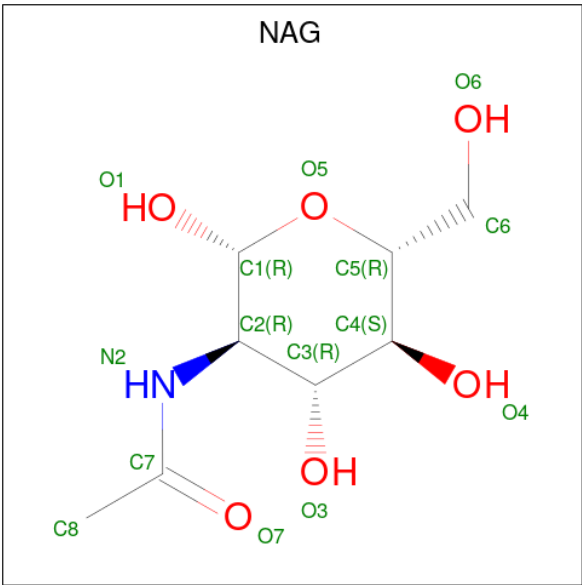
Mol	Chain	Residues	Atoms				AltConf	Trace
3	F	2	Total	C	N	O	0	0
			28	16	2	10		
3	G	2	Total	C	N	O	0	0
			28	16	2	10		
3	H	2	Total	C	N	O	0	0
			28	16	2	10		
3	I	2	Total	C	N	O	0	0
			28	16	2	10		
3	J	2	Total	C	N	O	0	0
			28	16	2	10		
3	K	2	Total	C	N	O	0	0
			28	16	2	10		
3	L	2	Total	C	N	O	0	0
			28	16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

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

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



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

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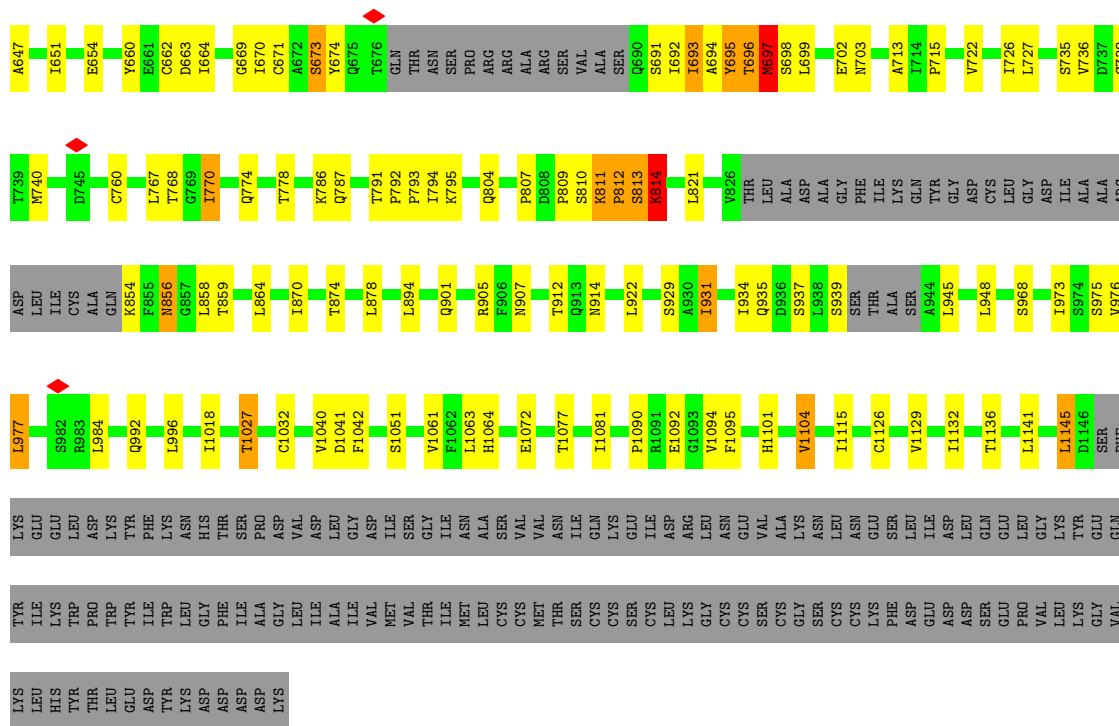
Mol	Chain	Residues	Atoms				AltConf
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4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

3 Residue-property plots

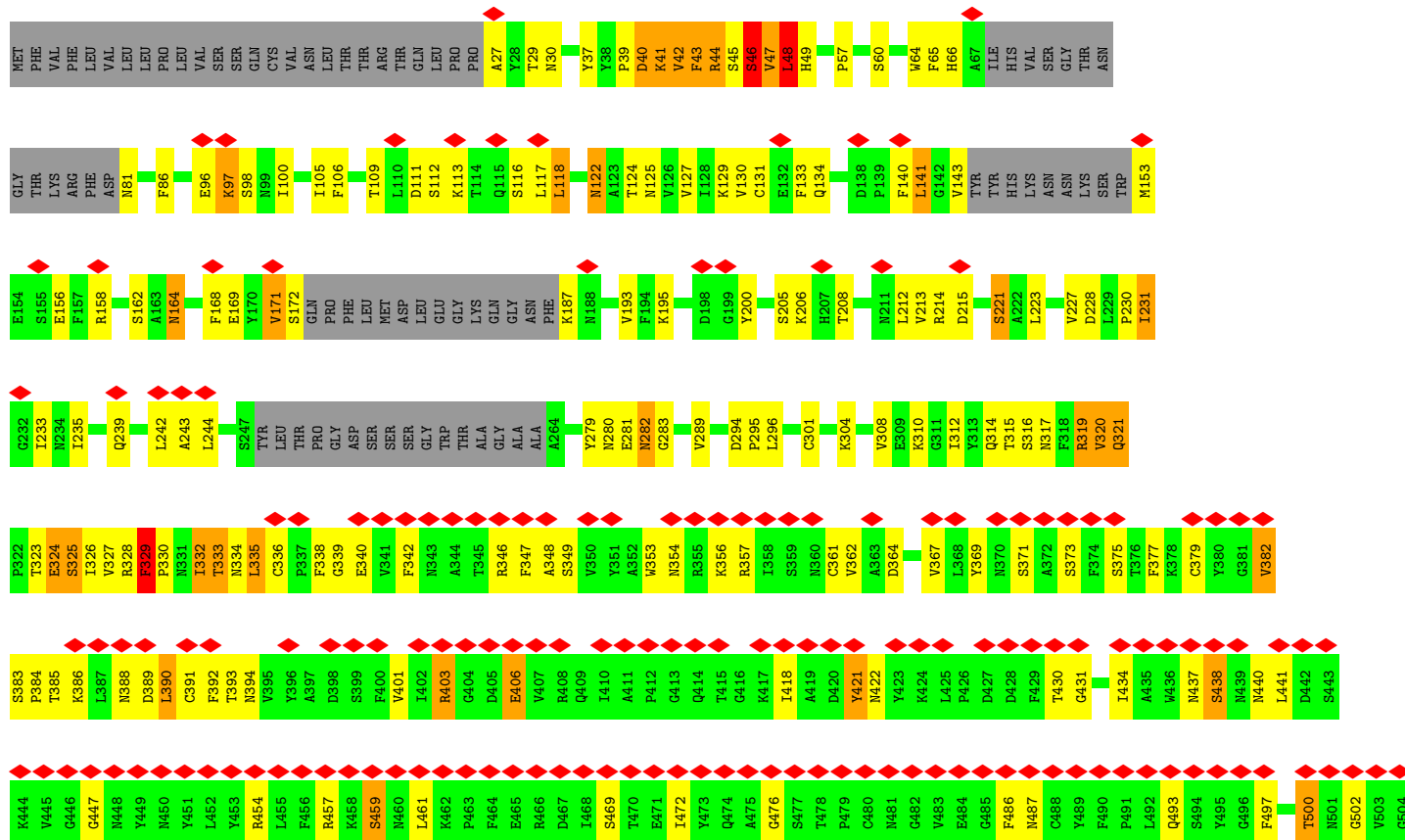
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

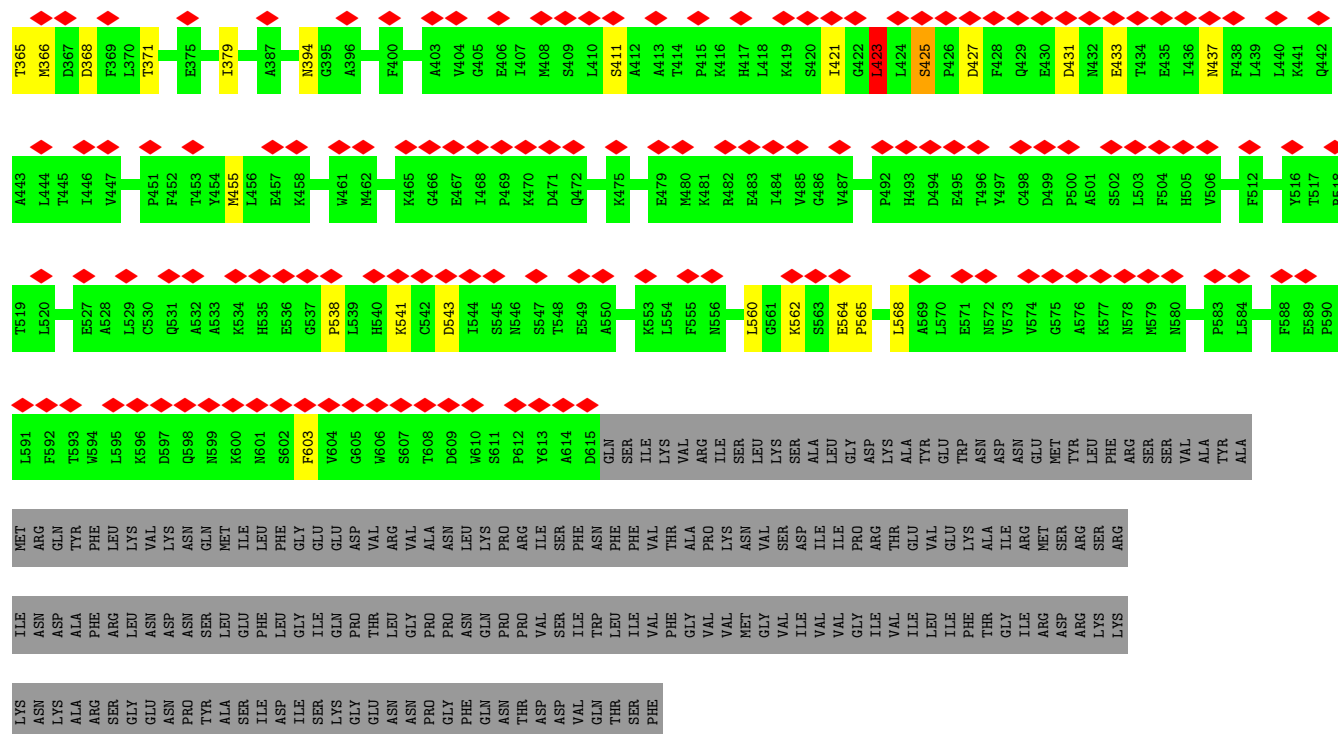
• Molecule 1: Spike glycoprotein



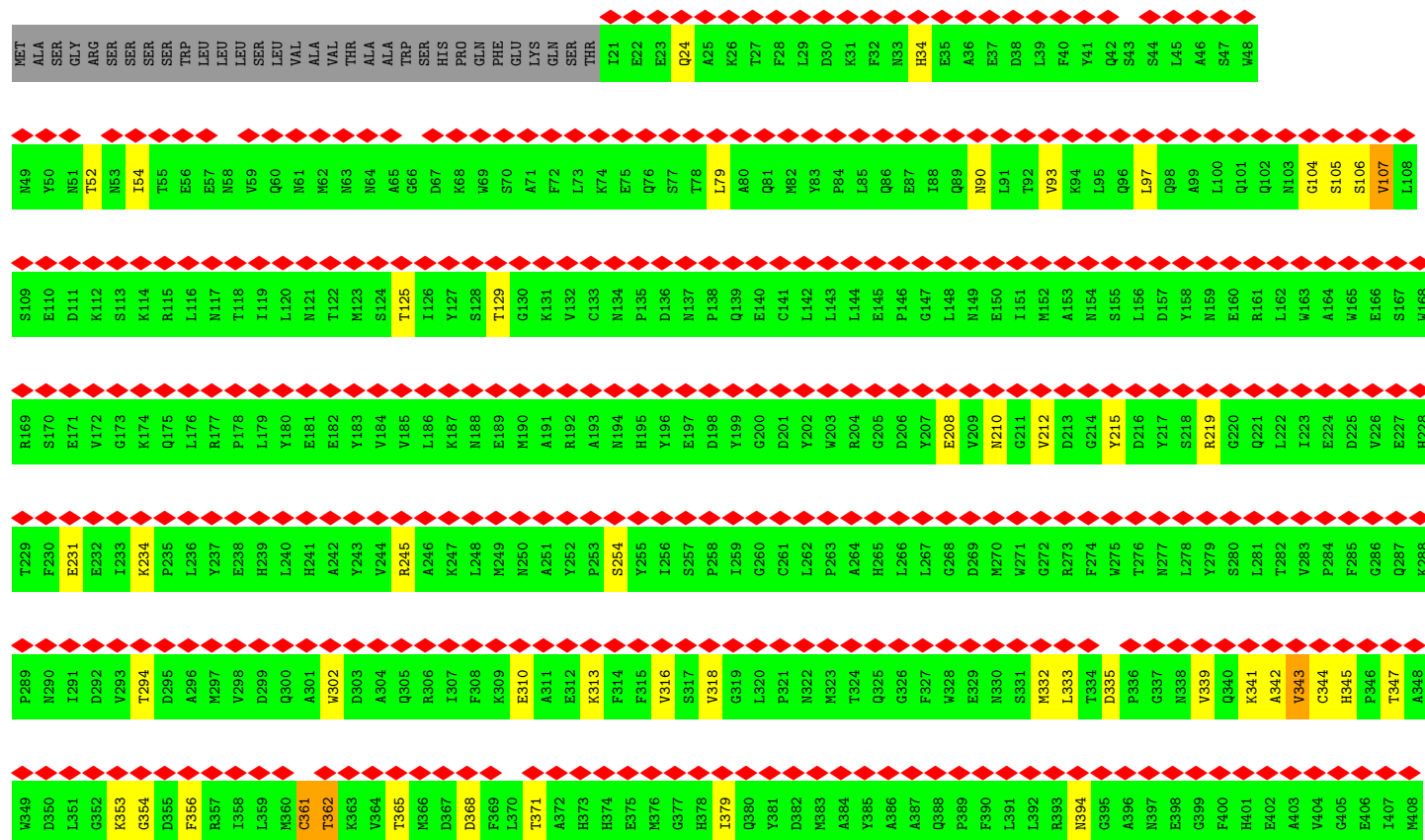


• Molecule 1: Spike glycoprotein



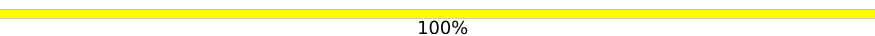


• Molecule 2: Angiotensin-converting enzyme 2



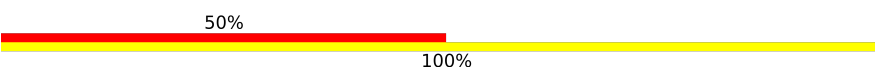
S409	L410	S411	A412	A413	T414	P415	K416	H417	L418	K419	S420	I421	G422	L423	L424	S425	P426	D427	F428	Q429	E430	D431	N432	E433	T434	E435	I436	N437	F438	L439	L440	K441	Q442	A443	L444	T445	I446	V447	G448	T449	L450	P451	F452	T453	Y454	M455	L456	E457	K458	W459	R460	W461	M462	V463	F464	K465	G466	E467	I468		
P469	K470	D471	Q472	W473	M474	K475	K476	W477	W478	E479	M480	K481	R482	E483	I484	V485	G486	V487	V488	E489	P490	V491	P492	H493	D494	E495	T496	Y497	C498	D499	P500	A501	S502	L503	F504	H505	V506	S507	N508	D509	Y510	S511	F512	I513	R514	Y515	Y516	T517	R518	T519	L520	Y521	Q522	F523	Q524	F525	Q526	E527	A528		
L529	C530	Q531	A532	A533	K534	H535	E536	G537	P538	L539	H540	K541	C542	D543	I544	S545	N546	S547	T548	E549	A550	G551	Q552	K553	L554	F555	N556	M557	L558	R559	L560	G561	K562	S563	E564	P565	W566	T567	L568	A569	L570	E571	N572	V573	V574	G575	A576	K577	N578	M579	N580	V581	R582	P583	L584	L585	N586	F587	F588		
E589	P590	L591	F592	T593	W594	L595	K596	D597	Q598	N599	K600	N601	S602	F603	V604	G605	W606	S607	T608	D609	W610	S611	P612	Y613	A614	D615	GLN	SER	ILE	LYS	VAL	THR	ALA	VAL	PRO	VAL	ILE	ARG	LYS	ASN	ILE	SER	LEU	LYS	ALA	TTR	D509	GLY	THR	ASN	ASP	ASN	GLU	MET	SER	ARG	ALA				
TYR	ALA	MET	ARG	GLN	TYR	PHE	LEU	VAL	ASN	ASN	GLN	MET	ILE	PHE	GLY	GLU	GLN	ASP	VAL	ARG	VAL	ALA	ASN	LEU	LYS	PRO	ARG	ILE	SER	PHE	ASN	PHE	ILE	VAL	THR	ILE	LYS	ALA	PRO	VAL	ILE	ARG	LYS	ASN	ILE	SER	LEU	LYS	ALA	TTR	D509	GLY	THR	ASN	ASP	ASN	GLU	MET	SER	ARG	ALA
SER	ARG	ILE	ASN	ASP	ALA	ARG	LEU	VAL	ASN	ASN	SER	LEU	GLU	PHE	ILE	GLY	GLN	PRO	THR	LEU	ARG	VAL	PRO	PRO	ASN	GLN	LYS	PRO	THR	ILE	LEU	TRP	ASN	PHE	ILE	VAL	THR	ILE	VAL	VAL	GLY	ILE	VAL	VAL	GLU	GLU	VAL	VAL	LYS	THR	ALA	ILE	GLY	ILE	ARG	ARG	ASP	ARG	ARG		
LYS	LYS	ASN	LYS	ALA	ARG	SER	GLY	GLU	PRO	TYR	ALA	SER	ILE	ASP	ILE	SER	LYS	GLY	GLU	ASN	ASN	PRO	GLY	PHE	GLN	ASN	THR	ASP	VAL	GLN	THR	SER	ILE	VAL	PHE	GLY	VAL	ILE	VAL	VAL	GLY	ILE	LEU	ILE	ILE	PHE	THR	GLY	ILE	ARG	ASP	ARG	ALA								

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

Chain F:  100%

MAG1
MAG2

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

Chain G:  50%
100%

MAG1
MAG2

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

Chain H:  50%
100%

MAG1
MAG2

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

Chain I:  50% 50%



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

Chain J:  50% 50%



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

Chain K:  100%



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

Chain L:  50% 100%

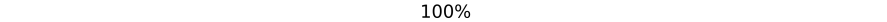


- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:  50% 100%



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

Chain N:  100% 100%



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

Chain O:  50% 50% 50%

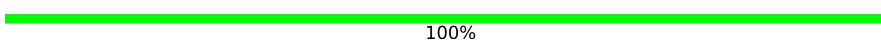


- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain P:  50% 50%



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

Chain Q:  100%

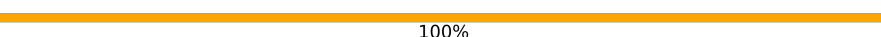


- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain R:  50% 50%

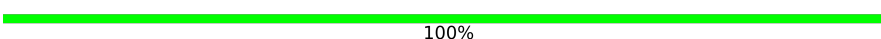


- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain S:  100%



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

Chain T:  100%



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

Chain U:  100%



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



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



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



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



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



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



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



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



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



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



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



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



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



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



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



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



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	14918	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.136	Depositor
Minimum map value	-0.070	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	313.056, 313.056, 313.056	wwPDB
Map dimensions	288, 288, 288	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.087, 1.087, 1.087	Depositor

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.51	0/8042	0.62	2/10939 (0.0%)
1	B	0.52	0/8042	0.60	2/10939 (0.0%)
1	C	0.52	1/8048 (0.0%)	0.62	2/10947 (0.0%)
2	D	0.30	0/4994	0.54	1/6785 (0.0%)
2	E	0.30	0/4994	0.54	1/6785 (0.0%)
All	All	0.46	1/34120 (0.0%)	0.59	8/46395 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	698	SER	CA-C	-6.60	1.44	1.52

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	362	THR	N-CA-C	6.03	119.35	109.76
2	D	362	THR	N-CA-C	6.03	119.34	109.76
1	B	86	PHE	CA-C-N	5.91	132.83	121.54
1	B	86	PHE	C-N-CA	5.91	132.83	121.54
1	C	86	PHE	CA-C-N	5.89	132.78	121.54
1	C	86	PHE	C-N-CA	5.89	132.78	121.54
1	A	86	PHE	CA-C-N	5.86	132.74	121.54
1	A	86	PHE	C-N-CA	5.86	132.74	121.54

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	7866	0	7666	343	0
1	B	7866	0	7664	371	0
1	C	7872	0	7669	384	0
2	D	4857	0	4624	68	0
2	E	4857	0	4624	67	0
3	F	28	0	25	1	0
3	G	28	0	25	3	0
3	H	28	0	25	0	0
3	I	28	0	25	0	0
3	J	28	0	25	0	0
3	K	28	0	25	1	0
3	L	28	0	25	0	0
3	M	28	0	25	0	0
3	N	28	0	25	4	0
3	O	28	0	25	1	0
3	P	28	0	25	0	0
3	Q	28	0	25	0	0
3	R	28	0	25	1	0
3	S	28	0	25	2	0
3	T	28	0	25	0	0
3	U	28	0	25	0	0
3	V	28	0	25	3	0
3	W	28	0	25	0	0
3	X	28	0	25	1	0
3	Y	28	0	25	1	0
3	Z	28	0	25	0	0
3	a	28	0	25	0	0
3	b	28	0	25	0	0
3	c	28	0	25	0	0
3	d	28	0	25	6	0
3	e	28	0	25	0	0
3	f	28	0	25	0	0
3	g	28	0	25	0	0
3	h	28	0	25	0	0
3	i	28	0	25	5	0
3	j	28	0	25	0	0
3	k	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	140	0	129	8	0
4	B	112	0	104	4	0
4	C	126	0	117	4	0
4	D	14	0	13	0	0
4	E	14	0	13	0	0
All	All	34620	0	33423	1175	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 17.

All (1175) 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)
4:A:1409:NAG:O4	4:A:1410:NAG:C1	1.63	1.45
1:C:329:PHE:CE1	1:C:544:ASN:HA	1.53	1.41
1:B:329:PHE:CE1	1:B:544:ASN:HA	1.60	1.35
1:A:787:GLN:OE1	1:C:703:ASN:HB2	1.28	1.25
1:C:326:ILE:HD12	1:C:532:ASN:O	1.27	1.23
1:A:486:PHE:CE1	2:D:79:LEU:HD22	1.75	1.21
1:C:486:PHE:CE1	2:E:79:LEU:HD22	1.75	1.19
1:C:329:PHE:CE2	1:C:528:LYS:HD3	1.80	1.16
1:C:329:PHE:CE1	1:C:544:ASN:CA	2.29	1.15
1:B:523:THR:HG22	1:B:524:VAL:H	0.98	1.15
1:C:523:THR:HG22	1:C:524:VAL:H	0.98	1.15
1:B:328:ARG:HH21	1:B:533:LEU:HD21	1.01	1.14
1:C:340:GLU:OE2	1:C:356:LYS:HE2	1.47	1.14
1:A:340:GLU:OE2	1:A:356:LYS:HE2	1.47	1.14
1:B:340:GLU:OE2	1:B:356:LYS:HE2	1.47	1.12
1:B:328:ARG:HH21	1:B:533:LEU:CD2	1.61	1.12
1:B:529:LYS:HE2	1:B:529:LYS:HA	1.18	1.11
1:C:329:PHE:CE2	1:C:528:LYS:CD	2.33	1.11
1:A:748:GLU:HG3	1:A:981:LEU:HD21	1.32	1.10
1:B:328:ARG:HD2	1:B:533:LEU:HD23	1.33	1.10
1:A:576:VAL:HG22	1:A:587:ILE:HD11	1.16	1.10
1:C:520:ALA:HB1	1:C:521:PRO:HD2	1.34	1.09
1:A:392:PHE:HB3	1:A:517:LEU:HD21	1.35	1.09
1:B:328:ARG:NH2	1:B:533:LEU:HD21	1.65	1.08
1:A:523:THR:HG22	1:A:524:VAL:H	0.98	1.08
1:B:329:PHE:HB3	1:B:330:PRO:HD2	1.34	1.08
1:A:520:ALA:HB1	1:A:521:PRO:HD2	1.35	1.08
1:B:520:ALA:HB1	1:B:521:PRO:HD2	1.35	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:329:PHE:CE1	1:B:544:ASN:CA	2.38	1.06
1:C:326:ILE:HG13	1:C:533:LEU:HA	1.33	1.05
1:C:392:PHE:HB3	1:C:517:LEU:HD21	1.35	1.05
1:A:392:PHE:HB3	1:A:517:LEU:CD2	1.88	1.04
1:B:392:PHE:HB3	1:B:517:LEU:HD21	1.34	1.04
1:C:392:PHE:HB3	1:C:517:LEU:CD2	1.88	1.04
1:B:662:CYS:CB	1:B:697:MET:HE3	1.88	1.03
1:B:654:GLU:HG3	1:B:693:ILE:HG22	1.41	1.02
1:B:392:PHE:HB3	1:B:517:LEU:CD2	1.88	1.01
1:B:662:CYS:HB2	1:B:697:MET:HE3	1.05	1.01
1:B:403:ARG:NH1	1:B:505:TYR:HE1	1.58	1.01
1:B:44:ARG:O	1:B:283:GLY:HA2	1.61	1.01
1:B:811:LYS:HB2	1:B:812:PRO:CD	1.91	1.00
1:A:44:ARG:O	1:A:283:GLY:HA2	1.61	1.00
1:A:392:PHE:CB	1:A:517:LEU:HD21	1.91	1.00
1:A:748:GLU:CG	1:A:981:LEU:HD21	1.91	1.00
4:A:1409:NAG:C4	4:A:1410:NAG:C1	2.38	0.99
1:B:392:PHE:CB	1:B:517:LEU:HD21	1.91	0.99
1:C:329:PHE:HE1	1:C:544:ASN:CB	1.74	0.99
1:C:392:PHE:CB	1:C:517:LEU:HD21	1.91	0.99
1:C:523:THR:HG22	1:C:524:VAL:N	1.73	0.99
1:A:523:THR:HG22	1:A:524:VAL:N	1.73	0.99
1:C:44:ARG:O	1:C:283:GLY:HA2	1.61	0.99
1:C:674:TYR:HH	1:C:690:GLN:N	1.59	0.98
1:C:329:PHE:HE1	1:C:544:ASN:CA	1.69	0.98
1:A:486:PHE:CE1	2:D:79:LEU:CD2	2.47	0.98
2:D:302:TRP:CH2	2:D:423:LEU:HD11	1.99	0.97
1:B:523:THR:CG2	1:B:524:VAL:H	1.77	0.97
1:C:523:THR:CG2	1:C:524:VAL:H	1.77	0.97
1:B:523:THR:HG22	1:B:524:VAL:N	1.73	0.97
1:C:486:PHE:CE1	2:E:79:LEU:CD2	2.47	0.97
1:A:523:THR:CG2	1:A:524:VAL:H	1.77	0.96
1:A:346:ARG:NH2	1:A:347:PHE:O	1.98	0.96
1:C:329:PHE:HE2	1:C:528:LYS:HD3	1.14	0.96
1:B:403:ARG:NH1	1:B:505:TYR:CE1	2.33	0.96
1:B:346:ARG:NH2	1:B:347:PHE:O	1.98	0.96
2:E:302:TRP:CH2	2:E:423:LEU:HD11	1.99	0.95
1:A:789:TYR:HE1	1:C:703:ASN:OD1	1.50	0.95
1:B:551:VAL:HB	1:B:588:THR:CG2	1.95	0.95
1:C:329:PHE:CE1	1:C:544:ASN:CB	2.49	0.95
1:C:346:ARG:NH2	1:C:347:PHE:O	1.98	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:551:VAL:HB	1:B:588:THR:HG23	1.48	0.95
1:B:530:SER:CB	1:B:580:GLN:NE2	2.30	0.95
1:A:576:VAL:CG2	1:A:587:ILE:HD11	1.97	0.94
1:C:674:TYR:CZ	1:C:690:GLN:N	2.35	0.94
1:C:505:TYR:CD2	2:E:353:LYS:O	2.21	0.94
1:C:674:TYR:HD1	1:C:691:SER:O	1.51	0.93
2:D:302:TRP:HH2	2:D:423:LEU:HD11	1.34	0.93
2:E:302:TRP:HH2	2:E:423:LEU:HD11	1.34	0.92
1:B:328:ARG:NH2	1:B:533:LEU:CD2	2.27	0.92
1:A:505:TYR:CD2	2:D:353:LYS:O	2.23	0.91
1:C:329:PHE:CD1	1:C:330:PRO:CD	2.53	0.91
1:A:200:TYR:CZ	1:C:521:PRO:HB2	2.05	0.91
1:B:811:LYS:HB2	1:B:812:PRO:HD2	1.50	0.91
1:C:530:SER:HB2	1:C:580:GLN:NE2	1.87	0.90
1:C:319:ARG:HH21	1:C:319:ARG:HG3	1.35	0.90
1:C:476:GLY:CA	2:E:24:GLN:HE21	1.85	0.89
1:A:476:GLY:CA	2:D:24:GLN:HE21	1.85	0.89
1:A:486:PHE:HE1	2:D:79:LEU:CD2	1.84	0.89
1:C:295:PRO:HB2	1:C:608:VAL:HG11	1.53	0.89
1:A:576:VAL:HG22	1:A:587:ILE:CD1	2.02	0.89
1:C:332:ILE:O	1:C:333:THR:OG1	1.91	0.89
1:B:329:PHE:HB3	1:B:330:PRO:CD	2.00	0.88
1:C:326:ILE:CG1	1:C:533:LEU:HA	2.04	0.88
1:C:329:PHE:CD1	1:C:330:PRO:HD2	2.10	0.87
1:C:486:PHE:HE1	2:E:79:LEU:CD2	1.84	0.87
1:A:45:SER:O	1:A:47:VAL:HG22	1.75	0.87
1:C:45:SER:O	1:C:47:VAL:HG22	1.75	0.87
1:B:329:PHE:CE1	1:B:544:ASN:CB	2.58	0.87
1:C:329:PHE:CG	1:C:330:PRO:HD2	2.10	0.87
1:B:45:SER:O	1:B:47:VAL:HG22	1.75	0.87
2:E:105:SER:O	2:E:106:SER:OG	1.93	0.87
1:C:729:VAL:HG13	1:C:1059:GLY:HA2	1.57	0.86
1:B:388:ASN:OD1	1:B:527:PRO:HD2	1.75	0.86
1:C:393:THR:O	1:C:523:THR:HG21	1.75	0.86
2:D:335:ASP:HB3	2:D:361:CYS:SG	2.16	0.86
1:B:392:PHE:CD2	1:B:517:LEU:HD21	2.11	0.86
1:B:46:SER:HA	1:B:279:TYR:O	1.76	0.86
1:B:393:THR:O	1:B:523:THR:HG21	1.76	0.86
1:C:392:PHE:CD2	1:C:517:LEU:HD21	2.11	0.86
1:B:530:SER:HB2	1:B:580:GLN:NE2	1.91	0.86
2:D:105:SER:O	2:D:106:SER:OG	1.93	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:565:PHE:O	1:B:42:VAL:HA	1.76	0.86
1:A:675:GLN:O	1:A:690:GLN:HG3	1.76	0.85
2:E:335:ASP:HB3	2:E:361:CYS:SG	2.16	0.85
1:B:520:ALA:HB1	1:B:521:PRO:CD	2.06	0.85
1:A:46:SER:HA	1:A:279:TYR:O	1.76	0.85
1:A:520:ALA:HB1	1:A:521:PRO:CD	2.06	0.85
1:C:334:ASN:O	1:C:362:VAL:HB	1.76	0.85
1:B:654:GLU:HG3	1:B:693:ILE:CG2	2.06	0.85
1:A:393:THR:O	1:A:523:THR:HG21	1.76	0.85
1:C:329:PHE:CD1	1:C:330:PRO:HD3	2.11	0.85
1:A:392:PHE:CD2	1:A:517:LEU:HD21	2.11	0.85
1:C:46:SER:HA	1:C:279:TYR:O	1.76	0.85
1:C:520:ALA:HB1	1:C:521:PRO:CD	2.06	0.84
1:A:42:VAL:HA	1:C:565:PHE:O	1.76	0.84
1:B:329:PHE:CZ	1:B:544:ASN:HA	2.13	0.83
1:C:516:GLU:O	1:C:517:LEU:HD22	1.78	0.83
1:C:530:SER:HB2	1:C:580:GLN:HE22	1.40	0.83
1:A:321:GLN:OE1	1:A:322:PRO:HD2	1.78	0.83
1:C:329:PHE:HE1	1:C:544:ASN:HA	1.22	0.83
1:C:856:ASN:HD22	1:C:856:ASN:H	1.26	0.83
1:A:486:PHE:CZ	2:D:79:LEU:HD22	2.13	0.83
1:C:486:PHE:CZ	2:E:79:LEU:HD22	2.13	0.83
1:A:516:GLU:O	1:A:517:LEU:HD22	1.78	0.83
1:A:789:TYR:CE1	1:C:703:ASN:OD1	2.32	0.82
1:B:516:GLU:O	1:B:517:LEU:HD22	1.78	0.82
1:B:565:PHE:O	1:C:42:VAL:HA	1.79	0.82
1:B:388:ASN:OD1	1:B:527:PRO:CD	2.26	0.82
1:C:674:TYR:CD1	1:C:691:SER:O	2.32	0.82
1:B:570:ALA:HA	1:C:964:LYS:HE3	1.62	0.82
1:A:901:GLN:HE21	1:A:905:ARG:HE	1.26	0.82
1:B:310:LYS:CG	1:B:664:ILE:HD11	2.10	0.82
1:B:901:GLN:HE21	1:B:905:ARG:HE	1.27	0.81
1:B:671:CYS:SG	1:B:697:MET:HB3	2.21	0.81
1:B:329:PHE:CD1	1:B:544:ASN:HB3	2.16	0.80
1:A:748:GLU:OE2	1:A:748:GLU:N	2.14	0.80
1:C:530:SER:CB	1:C:580:GLN:NE2	2.43	0.80
1:A:388:ASN:OD1	1:A:527:PRO:HD2	1.81	0.80
3:d:1:NAG:C3	3:d:2:NAG:HN2	1.95	0.80
3:i:1:NAG:C3	3:i:2:NAG:HN2	1.95	0.80
1:B:693:ILE:H	1:B:693:ILE:HD12	1.47	0.80
1:B:529:LYS:HE2	1:B:529:LYS:CA	2.08	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:329:PHE:HE1	1:B:544:ASN:HA	1.44	0.79
1:C:329:PHE:CE2	1:C:528:LYS:HD2	2.14	0.79
1:C:326:ILE:CD1	1:C:532:ASN:O	2.22	0.79
1:A:883:THR:HG23	1:C:707:TYR:HB2	1.65	0.79
1:B:534:VAL:HG23	1:B:535:LYS:N	1.98	0.78
1:A:743:CYS:SG	1:A:749:CYS:C	2.67	0.78
1:C:552:LEU:HD23	1:C:587:ILE:HG12	1.64	0.78
1:B:674:TYR:CD1	1:B:691:SER:O	2.37	0.78
1:A:392:PHE:O	1:A:523:THR:HB	1.83	0.78
1:B:392:PHE:O	1:B:523:THR:HB	1.83	0.78
1:A:335:LEU:HA	1:A:362:VAL:HB	1.67	0.78
1:C:390:LEU:HD23	1:C:391:CYS:H	1.49	0.77
1:C:335:LEU:HA	1:C:362:VAL:HB	1.67	0.77
1:C:422:ASN:HD21	1:C:454:ARG:H	1.32	0.77
1:C:476:GLY:HA3	2:E:24:GLN:HE21	1.50	0.77
1:B:406:GLU:CD	1:B:418:ILE:HG13	2.10	0.77
1:A:329:PHE:CE1	1:A:544:ASN:HA	2.20	0.77
1:A:332:ILE:O	1:A:333:THR:OG1	2.01	0.77
1:C:406:GLU:CD	1:C:418:ILE:HG13	2.10	0.77
1:A:787:GLN:OE1	1:C:703:ASN:CB	2.23	0.77
1:C:361:CYS:SG	1:C:524:VAL:HG21	2.25	0.77
1:C:392:PHE:O	1:C:523:THR:HB	1.83	0.77
1:A:529:LYS:HE2	1:A:530:SER:H	1.49	0.77
2:E:302:TRP:HH2	2:E:423:LEU:CD1	1.98	0.77
1:B:361:CYS:SG	1:B:524:VAL:HG21	2.25	0.76
1:B:403:ARG:HH11	1:B:505:TYR:HE1	1.32	0.76
1:C:326:ILE:HG13	1:C:533:LEU:CA	2.12	0.76
1:A:476:GLY:HA2	2:D:24:GLN:HE21	1.50	0.76
1:A:361:CYS:SG	1:A:524:VAL:HG21	2.25	0.76
1:A:406:GLU:CD	1:A:418:ILE:HG13	2.10	0.76
1:B:390:LEU:HD23	1:B:391:CYS:H	1.49	0.76
1:C:321:GLN:HA	1:C:321:GLN:OE1	1.85	0.76
1:C:326:ILE:HG23	1:C:532:ASN:O	1.85	0.76
1:C:826:VAL:HG13	1:C:1057:PRO:HG2	1.68	0.76
2:D:302:TRP:HH2	2:D:423:LEU:CD1	1.98	0.76
1:B:334:ASN:O	1:B:362:VAL:HB	1.85	0.76
1:B:329:PHE:HE1	1:B:544:ASN:CA	1.98	0.75
1:B:335:LEU:HA	1:B:362:VAL:HB	1.67	0.75
1:B:696:THR:O	1:B:697:MET:O	2.04	0.75
1:B:422:ASN:HD21	1:B:454:ARG:H	1.32	0.75
1:A:422:ASN:HD21	1:A:454:ARG:H	1.32	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:476:GLY:HA2	2:E:24:GLN:HE21	1.50	0.75
1:A:476:GLY:HA3	2:D:24:GLN:HE21	1.50	0.75
1:C:1125:ASN:H	1:C:1125:ASN:HD22	1.33	0.75
1:B:735:SER:OG	1:B:859:THR:CG2	2.34	0.75
1:A:47:VAL:O	1:A:49:HIS:N	2.20	0.75
1:A:390:LEU:HD23	1:A:391:CYS:H	1.49	0.75
1:B:328:ARG:HD2	1:B:533:LEU:CD2	2.14	0.74
2:E:335:ASP:CB	2:E:361:CYS:SG	2.75	0.74
1:B:47:VAL:O	1:B:49:HIS:N	2.20	0.74
1:C:329:PHE:HD1	1:C:330:PRO:HD3	1.49	0.74
1:B:329:PHE:CB	1:B:330:PRO:HD2	2.16	0.74
2:D:335:ASP:CB	2:D:361:CYS:SG	2.75	0.74
1:B:565:PHE:CZ	1:C:42:VAL:HG22	2.23	0.74
1:C:47:VAL:O	1:C:49:HIS:N	2.20	0.74
1:A:310:LYS:HB3	1:A:600:PRO:O	1.88	0.73
1:A:312:ILE:HG13	1:A:598:ILE:HG13	1.70	0.73
1:B:530:SER:HB2	1:B:580:GLN:HE21	1.50	0.73
1:B:392:PHE:HD2	1:B:517:LEU:HD21	1.53	0.73
1:A:392:PHE:HD2	1:A:517:LEU:HD21	1.53	0.73
1:A:533:LEU:HG	1:A:534:VAL:N	2.03	0.73
1:B:530:SER:HB3	1:B:580:GLN:NE2	2.03	0.72
1:C:392:PHE:HD2	1:C:517:LEU:HD21	1.53	0.72
1:A:1142:GLN:HG3	1:A:1143:PRO:HD3	1.71	0.72
1:A:973:ILE:HG12	1:A:992:GLN:HE21	1.53	0.72
1:B:340:GLU:OE2	1:B:356:LYS:CE	2.35	0.72
1:C:695:TYR:HD1	1:C:696:THR:N	1.87	0.72
1:B:811:LYS:CB	1:B:812:PRO:CD	2.66	0.72
1:C:340:GLU:OE2	1:C:356:LYS:CE	2.35	0.72
1:A:42:VAL:HG22	1:C:565:PHE:CZ	2.25	0.72
1:A:391:CYS:HA	1:A:525:CYS:HB3	1.71	0.72
1:A:340:GLU:OE2	1:A:356:LYS:CE	2.35	0.71
1:C:674:TYR:OH	1:C:690:GLN:N	2.23	0.71
1:C:329:PHE:CD1	1:C:544:ASN:HB3	2.25	0.71
1:B:702:GLU:OE2	1:C:790:LYS:NZ	2.20	0.71
1:C:391:CYS:HA	1:C:525:CYS:HB3	1.71	0.71
1:C:534:VAL:O	1:C:535:LYS:HG3	1.91	0.71
1:C:535:LYS:HD3	1:C:554:GLU:OE2	1.90	0.71
1:B:328:ARG:HD3	1:B:578:ASP:OD1	1.91	0.71
1:B:329:PHE:O	1:B:580:GLN:HG2	1.89	0.71
1:B:535:LYS:O	1:B:537:LYS:N	2.23	0.70
1:B:565:PHE:O	1:C:43:PHE:N	2.24	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:589:PRO:CD	1:C:854:LYS:HG2	2.20	0.70
4:A:1409:NAG:H4	4:A:1410:NAG:C1	2.21	0.70
1:B:529:LYS:HA	1:B:529:LYS:CE	2.04	0.70
1:C:124:THR:HG21	4:C:1402:NAG:HN2	1.56	0.70
1:C:551:VAL:HB	1:C:588:THR:HG23	1.73	0.70
1:A:124:THR:HG21	4:A:1402:NAG:HN2	1.56	0.70
1:A:187:LYS:N	1:A:212:LEU:O	2.25	0.70
1:B:124:THR:HG21	4:B:1402:NAG:HN2	1.56	0.70
1:A:325:SER:C	1:A:326:ILE:HD12	2.17	0.70
1:A:986:PRO:HB2	1:A:987:PRO:HD3	1.74	0.69
1:C:187:LYS:N	1:C:212:LEU:O	2.25	0.69
1:B:328:ARG:NH2	1:B:533:LEU:CG	2.55	0.69
1:B:45:SER:OG	1:B:46:SER:N	2.25	0.69
1:B:945:LEU:HD12	1:B:948:LEU:HD12	1.74	0.69
1:B:391:CYS:HA	1:B:525:CYS:HB3	1.74	0.69
1:A:563:GLN:OE1	1:B:43:PHE:HD1	1.76	0.69
1:B:329:PHE:CD1	1:B:544:ASN:CB	2.76	0.69
1:C:319:ARG:HG3	1:C:319:ARG:NH2	2.03	0.69
1:C:662:CYS:HB2	1:C:697:MET:HB3	1.74	0.69
1:B:187:LYS:N	1:B:212:LEU:O	2.25	0.68
1:C:44:ARG:O	1:C:283:GLY:CA	2.40	0.68
1:A:385:THR:HG1	1:A:386:LYS:HZ3	1.41	0.68
1:B:535:LYS:HB3	1:B:536:ASN:OD1	1.93	0.68
1:C:693:ILE:H	1:C:693:ILE:CD1	2.06	0.68
1:B:691:SER:OG	1:B:692:ILE:N	2.20	0.68
1:C:326:ILE:CG2	1:C:533:LEU:HA	2.23	0.68
1:A:45:SER:OG	1:A:46:SER:N	2.25	0.68
1:B:392:PHE:CG	1:B:517:LEU:HD21	2.29	0.68
1:B:44:ARG:O	1:B:283:GLY:CA	2.40	0.68
1:C:392:PHE:CG	1:C:517:LEU:HD21	2.29	0.68
1:B:329:PHE:O	1:B:579:PRO:HB2	1.94	0.68
1:B:589:PRO:CG	1:C:854:LYS:HG2	2.23	0.68
1:C:693:ILE:H	1:C:693:ILE:HD13	1.59	0.68
1:B:43:PHE:CE1	1:B:283:GLY:HA3	2.29	0.67
1:A:96:GLU:OE1	1:A:98:SER:N	2.28	0.67
1:B:308:VAL:O	1:B:601:GLY:HA2	1.94	0.67
1:B:329:PHE:HE1	1:B:544:ASN:CB	2.06	0.67
1:A:392:PHE:CG	1:A:517:LEU:HD21	2.29	0.67
1:C:391:CYS:CA	1:C:525:CYS:HB3	2.24	0.67
1:C:43:PHE:CE1	1:C:283:GLY:HA3	2.29	0.67
1:C:96:GLU:OE1	1:C:98:SER:N	2.28	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:37:TYR:O	1:C:39:PRO:HD3	1.95	0.67
1:A:719:THR:HA	1:A:926:GLN:HE22	1.60	0.67
1:A:1045:LYS:NZ	1:B:786:LYS:HE3	2.09	0.67
1:A:43:PHE:CE1	1:A:283:GLY:HA3	2.29	0.67
1:C:388:ASN:OD1	1:C:527:PRO:CD	2.42	0.67
1:B:96:GLU:OE1	1:B:98:SER:N	2.28	0.66
1:C:329:PHE:HE1	1:C:544:ASN:HB2	1.58	0.66
1:A:187:LYS:HG2	1:A:213:VAL:HA	1.77	0.66
1:B:187:LYS:HG2	1:B:213:VAL:HA	1.78	0.66
1:B:569:ILE:HD12	1:B:569:ILE:H	1.60	0.66
1:B:696:THR:O	1:B:697:MET:C	2.38	0.66
1:B:522:ALA:O	1:B:523:THR:OG1	2.14	0.66
1:A:388:ASN:OD1	1:A:527:PRO:CD	2.43	0.66
1:C:323:THR:C	1:C:324:GLU:HG2	2.21	0.66
1:C:392:PHE:HD2	1:C:517:LEU:CD2	2.09	0.66
1:C:326:ILE:HG21	1:C:533:LEU:HA	1.78	0.66
1:C:187:LYS:HG2	1:C:213:VAL:HA	1.78	0.66
1:B:37:TYR:O	1:B:39:PRO:HD3	1.95	0.65
1:A:37:TYR:O	1:A:39:PRO:HD3	1.95	0.65
1:B:391:CYS:CA	1:B:525:CYS:HB3	2.25	0.65
1:B:321:GLN:OE1	1:B:321:GLN:HA	1.97	0.65
1:A:563:GLN:CD	1:B:43:PHE:HA	2.22	0.65
1:B:662:CYS:HB2	1:B:697:MET:CE	2.01	0.65
1:B:392:PHE:HD2	1:B:517:LEU:CD2	2.09	0.65
1:C:569:ILE:H	1:C:569:ILE:HD12	1.60	0.65
1:C:856:ASN:OD1	1:C:966:LEU:CD1	2.44	0.65
1:A:522:ALA:O	1:A:523:THR:OG1	2.14	0.65
1:A:691:SER:O	1:A:692:ILE:HG13	1.96	0.65
1:A:493:GLN:OE1	2:D:34:HIS:CB	2.45	0.65
1:C:329:PHE:CZ	1:C:544:ASN:HA	2.28	0.65
2:E:310:GLU:OE1	2:E:421:ILE:HD11	1.97	0.65
1:A:44:ARG:O	1:A:283:GLY:CA	2.40	0.65
1:A:310:LYS:NZ	1:A:663:ASP:OD1	2.29	0.65
1:A:332:ILE:C	1:A:333:THR:HG1	2.01	0.65
1:A:392:PHE:HD2	1:A:517:LEU:CD2	2.09	0.65
1:B:693:ILE:HD12	1:B:693:ILE:N	2.12	0.65
1:B:534:VAL:HG23	1:B:535:LYS:H	1.62	0.64
1:A:308:VAL:O	1:A:601:GLY:HA2	1.97	0.64
2:D:310:GLU:OE1	2:D:421:ILE:HD11	1.97	0.64
1:A:200:TYR:CE2	1:C:521:PRO:HB2	2.32	0.64
1:C:493:GLN:OE1	2:E:34:HIS:CB	2.45	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:325:SER:HA	1:A:540:ASN:O	1.98	0.64
1:A:569:ILE:HD12	1:A:569:ILE:H	1.60	0.64
1:B:388:ASN:CG	1:B:527:PRO:HD2	2.23	0.64
1:C:329:PHE:O	1:C:579:PRO:HG2	1.97	0.64
1:B:670:ILE:HA	1:B:695:TYR:O	1.98	0.64
1:C:522:ALA:O	1:C:523:THR:OG1	2.14	0.64
1:A:534:VAL:C	1:A:535:LYS:HG2	2.23	0.64
1:C:674:TYR:CE1	1:C:690:GLN:N	2.65	0.64
3:d:1:NAG:H3	3:d:2:NAG:HN2	1.63	0.63
1:A:43:PHE:CE1	1:A:282:ASN:O	2.51	0.63
2:D:302:TRP:CZ3	2:D:423:LEU:HD11	2.34	0.63
1:C:45:SER:OG	1:C:46:SER:N	2.25	0.63
1:B:406:GLU:CD	1:B:418:ILE:CG1	2.71	0.63
1:C:700:GLY:O	1:C:701:ALA:O	2.17	0.63
1:C:406:GLU:CD	1:C:418:ILE:CG1	2.71	0.63
1:A:321:GLN:OE1	1:A:321:GLN:HA	1.96	0.63
2:D:335:ASP:N	2:D:361:CYS:SG	2.72	0.63
2:E:335:ASP:N	2:E:361:CYS:SG	2.72	0.63
1:A:117:LEU:HD12	1:A:118:LEU:H	1.64	0.63
1:A:42:VAL:HG22	1:C:565:PHE:CE2	2.34	0.63
1:B:43:PHE:CE1	1:B:282:ASN:O	2.51	0.63
1:C:536:ASN:O	1:C:537:LYS:HG2	1.99	0.63
1:C:695:TYR:CD1	1:C:696:THR:N	2.65	0.63
1:A:43:PHE:HE1	1:A:282:ASN:O	1.82	0.62
1:C:43:PHE:CE1	1:C:282:ASN:O	2.52	0.62
1:C:96:GLU:OE1	1:C:97:LYS:N	2.32	0.62
1:C:124:THR:OG1	1:C:125:ASN:N	2.32	0.62
1:A:124:THR:OG1	1:A:125:ASN:N	2.32	0.62
1:A:328:ARG:NH2	1:A:578:ASP:OD2	2.32	0.62
1:C:388:ASN:OD1	1:C:527:PRO:HD2	1.99	0.62
1:A:328:ARG:HG3	1:A:578:ASP:OD1	1.99	0.62
1:A:391:CYS:CA	1:A:525:CYS:HB3	2.24	0.62
1:B:565:PHE:CE2	1:C:42:VAL:HG22	2.35	0.62
1:A:457:ARG:NH1	1:A:459:SER:O	2.33	0.62
1:A:535:LYS:O	1:A:537:LYS:N	2.32	0.62
1:B:43:PHE:HE1	1:B:282:ASN:O	1.82	0.62
1:A:406:GLU:CD	1:A:418:ILE:CG1	2.71	0.62
1:B:117:LEU:HD12	1:B:118:LEU:H	1.64	0.62
1:B:457:ARG:NH1	1:B:459:SER:O	2.33	0.62
1:B:319:ARG:HG3	1:B:319:ARG:HH21	1.64	0.62
2:E:302:TRP:CZ3	2:E:423:LEU:HD11	2.34	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:457:ARG:NH1	1:C:459:SER:O	2.33	0.62
3:i:1:NAG:H3	3:i:2:NAG:HN2	1.63	0.62
1:C:808:ASP:HB3	1:C:811:LYS:HD2	1.82	0.62
1:A:516:GLU:O	1:A:517:LEU:CD2	2.48	0.62
1:C:117:LEU:HD12	1:C:118:LEU:H	1.64	0.62
1:A:96:GLU:OE1	1:A:97:LYS:N	2.32	0.61
1:B:96:GLU:OE1	1:B:97:LYS:N	2.32	0.61
1:B:530:SER:HB3	1:B:580:GLN:HE22	1.64	0.61
1:B:310:LYS:HG2	1:B:664:ILE:HD11	1.81	0.61
1:B:811:LYS:CB	1:B:812:PRO:HD2	2.28	0.61
1:B:813:SER:O	1:B:814:LYS:HE2	2.00	0.61
1:C:43:PHE:HE1	1:C:282:ASN:O	1.83	0.61
1:C:312:ILE:HG13	1:C:598:ILE:HG13	1.82	0.61
1:C:1077:THR:HG22	1:C:1095:PHE:O	2.01	0.61
1:C:541:PHE:CZ	1:C:587:ILE:HD13	2.35	0.61
1:A:521:PRO:O	1:A:522:ALA:HB2	2.01	0.61
1:C:532:ASN:OD1	1:C:533:LEU:N	2.33	0.61
1:B:124:THR:OG1	1:B:125:ASN:N	2.32	0.61
1:A:523:THR:HG22	1:A:524:VAL:HG12	1.83	0.61
1:A:617:CYS:H	1:A:644:GLN:HE22	1.49	0.61
1:B:357:ARG:HH12	1:B:394:ASN:HD21	1.49	0.61
1:B:388:ASN:OD1	1:B:527:PRO:HD3	2.01	0.61
1:A:357:ARG:HH12	1:A:394:ASN:HD21	1.49	0.61
1:A:392:PHE:HB3	1:A:517:LEU:HD22	1.82	0.61
1:B:617:CYS:H	1:B:644:GLN:HE22	1.49	0.61
1:C:523:THR:HG22	1:C:524:VAL:HG12	1.83	0.60
1:C:533:LEU:C	1:C:533:LEU:HD23	2.26	0.60
1:A:329:PHE:CD1	1:A:330:PRO:HD2	2.36	0.60
1:C:901:GLN:HE21	1:C:905:ARG:HE	1.50	0.60
1:A:406:GLU:OE1	1:A:418:ILE:HG12	2.02	0.60
1:B:328:ARG:NH2	1:B:533:LEU:HG	2.16	0.60
1:C:329:PHE:CD2	1:C:528:LYS:HD2	2.35	0.60
1:A:43:PHE:HD1	1:C:563:GLN:OE1	1.85	0.60
1:B:556:ASN:H	1:B:556:ASN:HD22	1.50	0.60
1:A:748:GLU:HG2	1:A:981:LEU:HD21	1.83	0.60
1:C:392:PHE:HB3	1:C:517:LEU:HD22	1.82	0.60
1:C:406:GLU:OE1	1:C:418:ILE:HG12	2.02	0.60
1:C:645:THR:HG22	1:C:647:ALA:H	1.66	0.60
1:C:662:CYS:HB2	1:C:697:MET:CB	2.31	0.60
1:A:164:ASN:OD1	1:A:164:ASN:N	2.35	0.60
1:B:319:ARG:HH21	1:B:319:ARG:CG	2.14	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:552:LEU:CD2	1:C:587:ILE:HG12	2.31	0.60
1:B:516:GLU:O	1:B:517:LEU:CD2	2.48	0.60
1:C:516:GLU:O	1:C:517:LEU:CD2	2.48	0.60
1:B:523:THR:HG22	1:B:524:VAL:HG12	1.83	0.60
1:B:645:THR:HG22	1:B:647:ALA:H	1.66	0.60
1:C:164:ASN:OD1	1:C:164:ASN:N	2.35	0.60
1:B:329:PHE:CB	1:B:330:PRO:CD	2.70	0.59
1:C:327:VAL:HG12	1:C:327:VAL:O	2.02	0.59
1:C:476:GLY:HA3	2:E:24:GLN:NE2	2.17	0.59
1:C:556:ASN:HD22	1:C:556:ASN:H	1.50	0.59
1:C:856:ASN:H	1:C:856:ASN:ND2	1.97	0.59
2:D:212:VAL:HG21	2:D:565:PRO:HG3	1.84	0.59
1:A:141:LEU:HB2	1:A:156:GLU:HB2	1.85	0.59
1:A:529:LYS:HE2	1:A:529:LYS:CA	2.31	0.59
1:B:406:GLU:OE1	1:B:418:ILE:HG12	2.02	0.59
1:B:521:PRO:O	1:B:522:ALA:HB2	2.01	0.59
1:C:521:PRO:O	1:C:522:ALA:HB2	2.01	0.59
1:A:556:ASN:HD22	1:A:556:ASN:H	1.49	0.59
1:C:505:TYR:CE2	2:E:353:LYS:C	2.80	0.59
1:C:617:CYS:H	1:C:644:GLN:HE22	1.49	0.59
1:B:164:ASN:OD1	1:B:164:ASN:N	2.35	0.59
1:A:322:PRO:HB3	1:A:538:CYS:SG	2.43	0.59
1:C:357:ARG:HH12	1:C:394:ASN:HD21	1.49	0.59
1:A:327:VAL:O	1:A:327:VAL:HG12	2.02	0.59
1:C:329:PHE:CE1	1:C:544:ASN:HB3	2.34	0.59
1:C:329:PHE:CB	1:C:330:PRO:HD2	2.33	0.59
1:C:813:SER:O	1:C:813:SER:OG	2.18	0.59
1:A:645:THR:HG22	1:A:647:ALA:H	1.66	0.59
1:A:901:GLN:NE2	1:A:905:ARG:HE	1.99	0.59
1:C:722:VAL:HA	1:C:1064:HIS:O	2.03	0.59
1:B:535:LYS:C	1:B:537:LYS:H	2.11	0.59
2:D:368:ASP:HA	2:D:371:THR:HG22	1.85	0.58
1:A:535:LYS:C	1:A:537:LYS:H	2.11	0.58
1:A:738:CYS:O	1:A:742:ILE:HG13	2.03	0.58
1:B:206:LYS:NZ	1:B:221:SER:OG	2.35	0.58
2:E:368:ASP:HA	2:E:371:THR:HG22	1.85	0.58
1:A:1045:LYS:HZ2	1:B:786:LYS:HE3	1.68	0.58
1:C:388:ASN:OD1	1:C:527:PRO:HD3	2.03	0.58
1:C:391:CYS:SG	1:C:523:THR:O	2.61	0.58
1:A:476:GLY:HA3	2:D:24:GLN:NE2	2.17	0.58
1:B:391:CYS:SG	1:B:523:THR:O	2.62	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:1405:NAG:H83	4:B:1405:NAG:H3	1.86	0.58
1:C:206:LYS:NZ	1:C:221:SER:OG	2.35	0.58
1:A:48:LEU:HD13	1:A:48:LEU:H	1.69	0.58
1:A:206:LYS:NZ	1:A:221:SER:OG	2.35	0.58
1:B:338:PHE:O	1:B:340:GLU:N	2.37	0.58
1:C:141:LEU:HB2	1:C:156:GLU:HB2	1.85	0.58
1:B:141:LEU:HB2	1:B:156:GLU:HB2	1.85	0.58
1:B:328:ARG:CD	1:B:578:ASP:OD1	2.52	0.58
1:C:530:SER:CB	1:C:580:GLN:HE21	2.17	0.58
2:E:212:VAL:HG21	2:E:565:PRO:HG3	1.84	0.58
2:D:302:TRP:CH2	2:D:423:LEU:CD1	2.78	0.58
3:R:2:NAG:H3	3:R:2:NAG:H83	1.86	0.58
1:B:323:THR:HG21	1:B:537:LYS:CE	2.34	0.57
1:B:361:CYS:SG	1:B:524:VAL:CG2	2.92	0.57
1:B:334:ASN:N	1:B:334:ASN:OD1	2.37	0.57
1:C:105:ILE:HG12	1:C:239:GLN:HB2	1.87	0.57
1:B:520:ALA:CB	1:B:521:PRO:CD	2.79	0.57
1:C:329:PHE:HD1	1:C:544:ASN:HB3	1.70	0.57
1:C:361:CYS:SG	1:C:524:VAL:CG2	2.92	0.57
1:A:361:CYS:SG	1:A:524:VAL:CG2	2.92	0.57
1:A:391:CYS:SG	1:A:523:THR:O	2.61	0.57
1:B:41:LYS:O	1:B:42:VAL:HB	2.05	0.57
1:B:48:LEU:HD13	1:B:48:LEU:H	1.69	0.57
1:B:319:ARG:HB2	1:B:319:ARG:NH2	2.19	0.57
1:C:41:LYS:O	1:C:42:VAL:HB	2.04	0.57
4:A:1405:NAG:H3	4:A:1405:NAG:H83	1.86	0.57
1:B:735:SER:OG	1:B:859:THR:HG23	2.04	0.57
1:C:48:LEU:HD13	1:C:48:LEU:H	1.69	0.57
1:C:227:VAL:HG12	1:C:228:ASP:N	2.20	0.57
1:B:47:VAL:O	1:B:47:VAL:HG23	2.04	0.57
1:A:47:VAL:O	1:A:47:VAL:HG23	2.04	0.57
1:C:47:VAL:O	1:C:47:VAL:HG23	2.04	0.57
1:C:670:ILE:HD13	1:C:695:TYR:O	2.04	0.57
1:B:45:SER:O	1:B:279:TYR:HB2	2.05	0.57
1:B:392:PHE:HB3	1:B:517:LEU:HD22	1.82	0.57
1:C:529:LYS:HG2	1:C:530:SER:N	2.20	0.57
1:A:338:PHE:C	1:A:340:GLU:H	2.13	0.57
1:A:338:PHE:O	1:A:340:GLU:N	2.37	0.57
1:B:592:PHE:CD1	1:B:593:GLY:N	2.73	0.57
1:B:669:GLY:O	1:B:696:THR:HA	2.04	0.57
1:C:320:VAL:HG23	1:C:591:SER:O	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:338:PHE:O	1:C:340:GLU:N	2.37	0.57
3:Y:2:NAG:H3	3:Y:2:NAG:H83	1.87	0.57
1:A:873:TYR:CZ	1:C:699:LEU:HD22	2.40	0.56
1:C:45:SER:O	1:C:279:TYR:HB2	2.05	0.56
1:C:338:PHE:C	1:C:340:GLU:H	2.13	0.56
2:D:54:ILE:HD12	2:D:341:LYS:HG3	1.87	0.56
1:A:105:ILE:HG12	1:A:239:GLN:HB2	1.87	0.56
1:C:519:HIS:O	1:C:519:HIS:ND1	2.38	0.56
1:C:535:LYS:HE2	1:C:554:GLU:OE1	2.04	0.56
1:B:29:THR:HG22	1:B:30:ASN:H	1.70	0.56
1:B:227:VAL:HG12	1:B:228:ASP:N	2.20	0.56
1:B:811:LYS:HB2	1:B:812:PRO:HD3	1.80	0.56
1:C:563:GLN:O	1:C:577:ARG:NH1	2.38	0.56
4:C:1405:NAG:H3	4:C:1405:NAG:H83	1.86	0.56
1:B:563:GLN:O	1:B:577:ARG:NH1	2.38	0.56
1:C:535:LYS:O	1:C:536:ASN:HB2	2.05	0.56
1:A:29:THR:HG22	1:A:30:ASN:H	1.70	0.56
1:B:804:GLN:HE21	1:B:935:GLN:HE22	1.52	0.56
2:D:425:SER:HB3	2:D:427:ASP:OD1	2.06	0.56
3:S:2:NAG:H83	3:S:2:NAG:H3	1.87	0.56
1:A:41:LYS:O	1:A:42:VAL:HB	2.05	0.56
1:A:227:VAL:HG12	1:A:228:ASP:N	2.20	0.56
1:A:406:GLU:OE1	1:A:418:ILE:CG1	2.54	0.56
1:C:310:LYS:NZ	1:C:663:ASP:OD1	2.37	0.56
1:C:332:ILE:C	1:C:333:THR:HG1	2.03	0.56
1:A:392:PHE:CD2	1:A:517:LEU:CD2	2.85	0.56
1:A:563:GLN:O	1:A:577:ARG:NH1	2.38	0.56
1:B:663:ASP:OD2	1:B:673:SER:OG	2.22	0.56
1:C:29:THR:HG22	1:C:30:ASN:H	1.70	0.56
1:A:329:PHE:HD1	1:A:330:PRO:HD2	1.70	0.56
1:B:570:ALA:HA	1:C:964:LYS:CE	2.35	0.56
1:C:353:TRP:CD1	1:C:353:TRP:H	2.24	0.56
1:C:663:ASP:OD2	1:C:673:SER:OG	2.22	0.56
1:B:338:PHE:C	1:B:340:GLU:H	2.13	0.56
2:D:335:ASP:N	2:D:335:ASP:OD1	2.39	0.56
1:A:45:SER:HA	1:A:280:ASN:O	2.06	0.56
1:B:105:ILE:HG12	1:B:239:GLN:HB2	1.87	0.56
1:C:486:PHE:CZ	2:E:79:LEU:CD2	2.84	0.56
2:D:231:GLU:HA	2:D:234:LYS:HD3	1.88	0.56
2:E:425:SER:HB3	2:E:427:ASP:OD1	2.06	0.56
1:A:519:HIS:O	1:A:519:HIS:ND1	2.38	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:406:GLU:OE1	1:B:418:ILE:CG1	2.54	0.55
1:C:57:PRO:O	1:C:60:SER:OG	2.24	0.55
1:C:390:LEU:HD23	1:C:391:CYS:N	2.19	0.55
2:E:54:ILE:HD12	2:E:341:LYS:HG3	1.87	0.55
1:B:353:TRP:H	1:B:353:TRP:CD1	2.24	0.55
1:C:406:GLU:OE1	1:C:418:ILE:CG1	2.54	0.55
1:C:660:TYR:O	1:C:698:SER:HB2	2.06	0.55
2:D:342:ALA:O	2:D:343:VAL:C	2.50	0.55
1:A:873:TYR:CE2	1:C:699:LEU:HD22	2.42	0.55
1:B:45:SER:HA	1:B:280:ASN:O	2.06	0.55
1:B:329:PHE:HD1	1:B:544:ASN:HB3	1.67	0.55
1:C:556:ASN:HD22	1:C:556:ASN:N	2.05	0.55
2:E:231:GLU:HA	2:E:234:LYS:HD3	1.88	0.55
3:N:1:NAG:H61	3:N:2:NAG:HN2	1.71	0.55
1:A:45:SER:O	1:A:279:TYR:HB2	2.05	0.55
1:A:347:PHE:CE1	1:A:509:ARG:HD3	2.42	0.55
1:A:392:PHE:HA	1:A:517:LEU:HD11	1.89	0.55
1:B:519:HIS:ND1	1:B:519:HIS:O	2.38	0.55
1:B:536:ASN:HA	1:B:551:VAL:HG13	1.88	0.55
1:B:556:ASN:HD22	1:B:556:ASN:N	2.05	0.55
1:A:295:PRO:HB2	1:A:608:VAL:HG11	1.89	0.55
1:C:45:SER:HA	1:C:280:ASN:O	2.06	0.55
1:B:342:PHE:HB3	3:N:1:NAG:H82	1.87	0.55
1:C:334:ASN:O	1:C:362:VAL:CB	2.52	0.55
1:A:342:PHE:HB3	3:G:1:NAG:H82	1.87	0.55
1:C:342:PHE:HB3	3:V:1:NAG:H82	1.87	0.55
1:C:347:PHE:CE1	1:C:509:ARG:HD3	2.42	0.55
1:C:392:PHE:HA	1:C:517:LEU:HD11	1.89	0.55
2:E:538:PRO:HD2	2:E:541:LYS:HD2	1.88	0.55
1:A:353:TRP:CD1	1:A:353:TRP:H	2.24	0.55
1:A:663:ASP:OD2	1:A:673:SER:OG	2.22	0.55
1:A:476:GLY:CA	2:D:24:GLN:NE2	2.65	0.55
2:D:105:SER:C	2:D:106:SER:HG	2.04	0.55
3:V:1:NAG:H61	3:V:2:NAG:HN2	1.71	0.55
1:A:556:ASN:HD22	1:A:556:ASN:N	2.05	0.54
1:C:43:PHE:CG	1:C:44:ARG:N	2.74	0.54
3:G:1:NAG:H61	3:G:2:NAG:HN2	1.72	0.54
1:B:392:PHE:HA	1:B:517:LEU:HD11	1.89	0.54
1:C:326:ILE:HG21	1:C:533:LEU:CA	2.38	0.54
1:C:421:TYR:HA	1:C:461:LEU:HG	1.90	0.54
1:A:43:PHE:O	1:A:44:ARG:HG3	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:43:PHE:CG	1:A:44:ARG:N	2.74	0.54
1:A:535:LYS:C	1:A:537:LYS:N	2.65	0.54
1:B:390:LEU:HD23	1:B:391:CYS:N	2.19	0.54
2:E:335:ASP:N	2:E:335:ASP:OD1	2.39	0.54
1:C:520:ALA:CB	1:C:521:PRO:CD	2.79	0.54
1:A:43:PHE:N	1:C:565:PHE:O	2.40	0.54
1:A:529:LYS:HE2	1:A:530:SER:N	2.17	0.54
1:B:43:PHE:O	1:B:44:ARG:HG3	2.08	0.54
1:C:43:PHE:O	1:C:44:ARG:HG3	2.08	0.54
1:B:43:PHE:CG	1:B:44:ARG:N	2.74	0.54
1:C:111:ASP:OD1	1:C:134:GLN:NE2	2.41	0.54
1:C:329:PHE:CB	1:C:530:SER:OG	2.56	0.54
1:A:100:ILE:O	1:A:242:LEU:HA	2.08	0.54
1:A:111:ASP:OD1	1:A:134:GLN:NE2	2.41	0.54
1:A:486:PHE:CZ	2:D:79:LEU:CD2	2.84	0.54
1:C:329:PHE:CB	1:C:330:PRO:CD	2.85	0.54
2:D:538:PRO:HD2	2:D:541:LYS:HD2	1.88	0.54
1:A:329:PHE:O	1:A:580:GLN:NE2	2.41	0.54
1:A:1142:GLN:HG3	1:A:1143:PRO:CD	2.37	0.54
1:B:347:PHE:CE1	1:B:509:ARG:HD3	2.42	0.54
1:C:329:PHE:CD2	1:C:528:LYS:CD	2.88	0.54
1:B:111:ASP:OD1	1:B:134:GLN:NE2	2.41	0.54
1:B:421:TYR:HA	1:B:461:LEU:HG	1.90	0.54
1:C:100:ILE:O	1:C:242:LEU:HA	2.08	0.54
2:E:342:ALA:O	2:E:343:VAL:C	2.50	0.54
1:B:438:SER:O	1:B:438:SER:OG	2.21	0.54
1:C:333:THR:O	1:C:334:ASN:C	2.51	0.54
2:D:52:THR:OG1	2:D:332:MET:SD	2.66	0.53
1:A:310:LYS:HA	1:A:599:THR:O	2.07	0.53
2:E:52:THR:OG1	2:E:332:MET:SD	2.66	0.53
1:A:326:ILE:HG22	1:A:327:VAL:N	2.22	0.53
3:X:2:NAG:H83	3:X:2:NAG:H3	1.90	0.53
1:A:57:PRO:O	1:A:60:SER:OG	2.24	0.53
1:A:363:ALA:O	1:A:527:PRO:HD3	2.08	0.53
1:B:100:ILE:O	1:B:242:LEU:HA	2.08	0.53
1:A:318:PHE:CD1	1:A:318:PHE:C	2.85	0.53
1:C:886:TRP:HH2	1:C:904:TYR:HD2	1.56	0.53
1:B:310:LYS:HA	1:B:599:THR:O	2.09	0.53
1:B:533:LEU:HD12	1:B:533:LEU:H	1.73	0.53
1:B:544:ASN:O	1:B:544:ASN:ND2	2.41	0.53
2:D:90:ASN:HB3	2:D:93:VAL:HG12	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:308:VAL:HG21	1:A:599:THR:HG21	1.91	0.53
1:A:320:VAL:HG12	1:A:321:GLN:N	2.23	0.53
1:A:565:PHE:CZ	1:B:42:VAL:HG22	2.44	0.53
1:B:307:THR:HA	1:B:602:THR:OG1	2.09	0.53
1:B:476:GLY:H	1:B:487:ASN:HB3	1.74	0.53
1:B:535:LYS:C	1:B:537:LYS:N	2.67	0.53
1:A:421:TYR:HA	1:A:461:LEU:HG	1.90	0.53
1:A:476:GLY:H	1:A:487:ASN:HB3	1.74	0.53
1:C:64:TRP:HD1	1:C:65:PHE:N	2.07	0.53
1:A:329:PHE:HD1	1:A:330:PRO:CD	2.22	0.53
1:B:516:GLU:C	1:B:517:LEU:CD2	2.82	0.53
1:C:516:GLU:C	1:C:517:LEU:CD2	2.82	0.53
1:A:505:TYR:CE2	2:D:353:LYS:C	2.87	0.52
1:A:516:GLU:C	1:A:517:LEU:CD2	2.82	0.52
1:A:329:PHE:O	1:A:580:GLN:HG2	2.08	0.52
1:B:57:PRO:O	1:B:60:SER:OG	2.24	0.52
1:C:505:TYR:CD2	2:E:353:LYS:C	2.86	0.52
1:B:713:ALA:HB3	1:C:894:LEU:HB3	1.90	0.52
1:B:1141:LEU:HD11	1:C:1141:LEU:HD12	1.90	0.52
1:C:901:GLN:NE2	1:C:905:ARG:HH21	2.08	0.52
2:E:90:ASN:HB3	2:E:93:VAL:HG12	1.91	0.52
1:B:329:PHE:HE1	1:B:544:ASN:HB2	1.73	0.52
1:B:589:PRO:HG3	1:C:854:LYS:HG2	1.90	0.52
1:C:326:ILE:HG21	1:C:533:LEU:CB	2.40	0.52
3:d:1:NAG:H3	3:d:2:NAG:N2	2.24	0.52
1:A:544:ASN:O	1:A:544:ASN:ND2	2.41	0.52
1:C:48:LEU:CD1	1:C:48:LEU:N	2.73	0.52
1:C:476:GLY:H	1:C:487:ASN:HB3	1.74	0.52
2:D:394:ASN:HB2	2:D:562:LYS:HD2	1.92	0.52
1:A:327:VAL:N	1:A:531:THR:OG1	2.43	0.52
1:B:324:GLU:O	1:B:539:VAL:CG2	2.58	0.52
1:B:549:THR:HG22	1:B:590:CYS:SG	2.49	0.52
1:C:544:ASN:ND2	1:C:544:ASN:O	2.41	0.52
1:A:325:SER:O	1:A:326:ILE:HD12	2.09	0.52
1:C:327:VAL:HG13	1:C:542:ASN:HB3	1.92	0.52
1:C:588:THR:OG1	1:C:589:PRO:HD2	2.10	0.52
1:A:64:TRP:HD1	1:A:65:PHE:N	2.07	0.52
1:B:1101:HIS:CD2	3:S:1:NAG:H5	2.45	0.52
2:E:302:TRP:CH2	2:E:423:LEU:CD1	2.78	0.52
1:A:524:VAL:C	1:A:525:CYS:SG	2.93	0.52
1:B:48:LEU:N	1:B:48:LEU:CD1	2.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:1:NAG:H62	3:F:2:NAG:H82	1.92	0.52
1:A:390:LEU:HD23	1:A:391:CYS:N	2.19	0.52
2:D:104:GLY:O	2:D:107:VAL:HG22	2.10	0.52
2:D:425:SER:C	2:D:427:ASP:H	2.18	0.52
3:i:1:NAG:H3	3:i:2:NAG:N2	2.24	0.52
1:A:326:ILE:CG2	1:A:327:VAL:N	2.73	0.51
1:A:493:GLN:OE1	2:D:34:HIS:HB3	2.10	0.51
1:B:319:ARG:CB	1:B:319:ARG:CZ	2.87	0.51
1:B:324:GLU:O	1:B:539:VAL:HG23	2.10	0.51
1:B:804:GLN:HE21	1:B:935:GLN:NE2	2.08	0.51
1:C:493:GLN:OE1	2:E:34:HIS:HB3	2.10	0.51
1:C:524:VAL:C	1:C:525:CYS:SG	2.93	0.51
1:B:715:PRO:HA	1:B:1072:GLU:HA	1.92	0.51
2:E:245:ARG:NH1	2:E:603:PHE:O	2.42	0.51
1:B:64:TRP:HD1	1:B:65:PHE:N	2.07	0.51
1:B:348:ALA:HB2	1:B:354:ASN:ND2	2.26	0.51
1:C:967:SER:O	1:C:967:SER:OG	2.24	0.51
2:D:245:ARG:NH1	2:D:603:PHE:O	2.42	0.51
1:A:505:TYR:CE2	2:D:354:GLY:HA3	2.45	0.51
1:A:505:TYR:CG	2:D:353:LYS:O	2.62	0.51
1:B:403:ARG:NH1	1:B:505:TYR:CD1	2.78	0.51
1:C:131:CYS:H	1:C:133:PHE:HE1	1.59	0.51
1:C:502:GLY:O	1:C:505:TYR:HB2	2.10	0.51
1:C:693:ILE:HD13	1:C:693:ILE:O	2.11	0.51
2:E:425:SER:C	2:E:427:ASP:H	2.18	0.51
1:A:1104:VAL:HG22	1:A:1115:ILE:HG12	1.91	0.51
1:C:130:VAL:HB	1:C:168:PHE:HB3	1.93	0.51
1:A:48:LEU:N	1:A:48:LEU:CD1	2.73	0.51
1:A:130:VAL:HB	1:A:168:PHE:HB3	1.93	0.51
1:A:379:CYS:HB3	1:A:382:VAL:O	2.10	0.51
1:C:329:PHE:CG	1:C:330:PRO:CD	2.85	0.51
2:E:394:ASN:HB2	2:E:562:LYS:HD2	1.92	0.51
1:A:591:SER:O	1:A:592:PHE:HB3	2.11	0.51
1:B:551:VAL:HB	1:B:588:THR:HG21	1.90	0.51
1:C:41:LYS:N	1:C:41:LYS:CD	2.73	0.51
2:D:433:GLU:O	2:D:437:ASN:ND2	2.44	0.51
1:C:129:LYS:HG2	1:C:133:PHE:HZ	1.77	0.51
1:C:661:GLU:HA	1:C:698:SER:HB3	1.93	0.51
1:A:326:ILE:N	1:A:326:ILE:CD1	2.74	0.50
1:A:438:SER:O	1:A:438:SER:OG	2.21	0.50
2:E:208:GLU:OE2	2:E:219:ARG:NH1	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1032:CYS:O	1:B:1051:SER:HB2	2.12	0.50
1:C:348:ALA:HB2	1:C:354:ASN:ND2	2.26	0.50
1:C:379:CYS:HB3	1:C:382:VAL:O	2.10	0.50
1:A:388:ASN:CG	1:A:527:PRO:HD2	2.36	0.50
1:A:748:GLU:HG3	1:A:981:LEU:CD2	2.23	0.50
1:B:327:VAL:O	1:B:531:THR:N	2.44	0.50
1:B:379:CYS:HB3	1:B:382:VAL:O	2.10	0.50
1:A:41:LYS:N	1:A:41:LYS:CD	2.73	0.50
1:B:106:PHE:HB3	1:B:235:ILE:HD13	1.93	0.50
1:B:131:CYS:H	1:B:133:PHE:HE1	1.59	0.50
1:B:401:VAL:HG22	1:B:509:ARG:HG2	1.94	0.50
1:C:392:PHE:CD2	1:C:517:LEU:CD2	2.85	0.50
2:D:208:GLU:OE2	2:D:219:ARG:NH1	2.44	0.50
1:A:533:LEU:CG	1:A:534:VAL:N	2.73	0.50
1:A:129:LYS:HG2	1:A:133:PHE:HZ	1.77	0.50
1:B:310:LYS:HG2	1:B:664:ILE:CD1	2.42	0.50
1:A:316:SER:OG	1:A:317:ASN:N	2.45	0.50
1:A:325:SER:HB3	1:A:540:ASN:HB3	1.94	0.50
1:A:502:GLY:O	1:A:505:TYR:HB2	2.12	0.50
1:A:591:SER:HB3	1:A:619:GLU:OE2	2.11	0.50
1:B:660:TYR:O	1:B:698:SER:N	2.44	0.50
2:D:335:ASP:CA	2:D:361:CYS:SG	3.00	0.50
2:E:104:GLY:O	2:E:107:VAL:HG22	2.10	0.50
1:A:520:ALA:CB	1:A:521:PRO:CD	2.79	0.50
1:A:655:HIS:HD2	1:A:694:ALA:O	1.95	0.50
1:B:319:ARG:NH2	1:B:319:ARG:CB	2.75	0.50
1:C:401:VAL:HG22	1:C:509:ARG:HG2	1.94	0.50
1:C:476:GLY:CA	2:E:24:GLN:NE2	2.65	0.50
1:C:735:SER:HB3	1:C:859:THR:HG22	1.94	0.50
1:B:333:THR:HG22	1:B:334:ASN:OD1	2.12	0.49
1:A:325:SER:CA	1:A:540:ASN:O	2.59	0.49
1:A:348:ALA:HB2	1:A:354:ASN:ND2	2.26	0.49
1:A:401:VAL:HG22	1:A:509:ARG:HG2	1.94	0.49
1:B:1090:PRO:HD3	1:B:1095:PHE:CE2	2.47	0.49
2:E:335:ASP:CA	2:E:361:CYS:SG	3.00	0.49
1:A:106:PHE:HB3	1:A:235:ILE:HD13	1.93	0.49
1:A:131:CYS:H	1:A:133:PHE:HE1	1.59	0.49
1:A:308:VAL:O	1:A:602:THR:N	2.39	0.49
1:A:324:GLU:CG	1:A:325:SER:N	2.73	0.49
1:B:524:VAL:C	1:B:525:CYS:SG	2.94	0.49
1:B:535:LYS:O	1:B:537:LYS:HG3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:363:ALA:O	1:B:527:PRO:HD3	2.12	0.49
1:A:662:CYS:HB2	1:A:697:MET:HE3	1.94	0.49
1:A:883:THR:HG21	1:C:705:VAL:HB	1.93	0.49
1:B:319:ARG:CG	1:B:319:ARG:NH2	2.73	0.49
1:B:41:LYS:CD	1:B:41:LYS:N	2.73	0.49
1:B:129:LYS:HG2	1:B:133:PHE:HZ	1.77	0.49
1:B:130:VAL:HB	1:B:168:PHE:HB3	1.93	0.49
1:C:335:LEU:C	1:C:362:VAL:O	2.56	0.49
1:C:438:SER:O	1:C:438:SER:OG	2.21	0.49
1:C:856:ASN:HD22	1:C:856:ASN:N	1.92	0.49
2:E:433:GLU:O	2:E:437:ASN:ND2	2.44	0.49
1:B:335:LEU:C	1:B:362:VAL:O	2.56	0.49
1:B:437:ASN:OD1	1:B:438:SER:N	2.46	0.49
1:C:431:GLY:HA3	1:C:513:LEU:O	2.12	0.49
1:C:437:ASN:OD1	1:C:438:SER:N	2.46	0.49
1:C:693:ILE:HD13	1:C:693:ILE:N	2.25	0.49
1:A:122:ASN:OD1	1:A:122:ASN:N	2.46	0.49
1:A:171:VAL:HG12	1:A:172:SER:H	1.78	0.49
1:A:308:VAL:CG1	1:A:602:THR:HG23	2.43	0.49
1:B:334:ASN:O	1:B:362:VAL:CB	2.60	0.49
1:B:807:PRO:O	1:B:809:PRO:HD3	2.12	0.49
1:C:106:PHE:HB3	1:C:235:ILE:HD13	1.93	0.49
2:E:564:GLU:HB3	2:E:568:LEU:HD23	1.95	0.49
3:K:1:NAG:H62	3:K:2:NAG:H2	1.93	0.49
1:B:329:PHE:CE1	1:B:544:ASN:HB2	2.44	0.49
1:B:392:PHE:CD2	1:B:517:LEU:CD2	2.85	0.49
1:B:431:GLY:HA3	1:B:513:LEU:O	2.12	0.49
1:A:321:GLN:OE1	1:A:322:PRO:CD	2.58	0.48
1:A:335:LEU:C	1:A:362:VAL:O	2.56	0.48
1:B:231:ILE:HB	1:B:233:ILE:HG22	1.95	0.48
1:B:361:CYS:O	1:B:524:VAL:HG23	2.13	0.48
1:A:431:GLY:HA3	1:A:513:LEU:O	2.12	0.48
1:B:212:LEU:HD23	1:B:215:ASP:HB2	1.95	0.48
1:C:325:SER:HA	1:C:540:ASN:O	2.13	0.48
1:C:361:CYS:O	1:C:524:VAL:HG23	2.13	0.48
1:A:437:ASN:OD1	1:A:438:SER:N	2.46	0.48
1:B:335:LEU:H	1:B:335:LEU:HD12	1.78	0.48
1:C:524:VAL:HG22	1:C:525:CYS:N	2.27	0.48
2:D:564:GLU:HB3	2:D:568:LEU:HD23	1.94	0.48
1:A:329:PHE:CB	1:A:330:PRO:HD2	2.43	0.48
1:A:710:ASN:N	1:A:710:ASN:HD22	2.11	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:171:VAL:HG12	1:B:172:SER:H	1.78	0.48
1:B:329:PHE:C	1:B:579:PRO:HB2	2.37	0.48
1:C:122:ASN:N	1:C:122:ASN:OD1	2.46	0.48
1:C:935:GLN:O	1:C:939:SER:HB3	2.14	0.48
1:C:985:ASP:OD1	1:C:985:ASP:N	2.45	0.48
1:A:310:LYS:HB3	1:A:600:PRO:C	2.37	0.48
1:A:361:CYS:O	1:A:524:VAL:HG23	2.13	0.48
1:B:122:ASN:OD1	1:B:122:ASN:N	2.46	0.48
1:C:886:TRP:CH2	1:C:904:TYR:HD2	2.31	0.48
1:C:212:LEU:HD23	1:C:215:ASP:HB2	1.95	0.48
1:C:319:ARG:NH2	1:C:319:ARG:CG	2.73	0.48
1:C:323:THR:O	1:C:324:GLU:HG2	2.13	0.48
1:A:227:VAL:HG12	1:A:228:ASP:H	1.79	0.48
1:B:328:ARG:CZ	1:B:533:LEU:HG	2.44	0.48
1:A:231:ILE:HB	1:A:233:ILE:HG22	1.95	0.48
1:B:323:THR:HG21	1:B:537:LYS:HE2	1.94	0.48
1:B:516:GLU:C	1:B:517:LEU:HD23	2.39	0.48
1:A:325:SER:C	1:A:326:ILE:CD1	2.85	0.48
1:A:524:VAL:HG22	1:A:525:CYS:N	2.27	0.48
1:B:46:SER:O	1:B:47:VAL:HG13	2.14	0.48
1:A:654:GLU:HG3	1:A:693:ILE:HG22	1.96	0.47
1:C:171:VAL:HG12	1:C:172:SER:H	1.78	0.47
1:A:776:LYS:HE3	1:A:776:LYS:HB3	1.65	0.47
1:A:486:PHE:HE1	2:D:79:LEU:CD1	2.27	0.47
1:B:524:VAL:HG22	1:B:525:CYS:N	2.28	0.47
1:B:528:LYS:O	1:B:529:LYS:HE2	2.14	0.47
1:B:670:ILE:HD13	1:B:695:TYR:O	2.14	0.47
1:C:46:SER:O	1:C:47:VAL:HG13	2.14	0.47
1:C:516:GLU:C	1:C:517:LEU:HD23	2.39	0.47
1:C:896:ILE:HG13	1:C:897:PRO:HD2	1.95	0.47
3:i:2:NAG:H83	3:i:2:NAG:C3	2.45	0.47
1:A:516:GLU:C	1:A:517:LEU:HD23	2.39	0.47
1:B:227:VAL:HG12	1:B:228:ASP:H	1.79	0.47
1:A:212:LEU:HD23	1:A:215:ASP:HB2	1.95	0.47
1:A:710:ASN:HD22	1:A:710:ASN:H	1.62	0.47
1:B:328:ARG:O	1:B:329:PHE:CG	2.68	0.47
1:C:500:THR:O	1:C:500:THR:OG1	2.31	0.47
1:B:308:VAL:HG21	1:B:599:THR:HG21	1.97	0.47
1:B:369:TYR:CE2	1:B:384:PRO:HB2	2.50	0.47
1:B:1104:VAL:HG22	1:B:1115:ILE:HG12	1.95	0.47
1:C:227:VAL:HG12	1:C:228:ASP:H	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:46:SER:O	1:A:47:VAL:HG13	2.14	0.47
1:A:529:LYS:HE2	1:A:529:LYS:HA	1.94	0.47
1:A:713:ALA:HB3	1:B:894:LEU:HB3	1.97	0.47
1:B:534:VAL:O	1:B:535:LYS:HG3	2.14	0.47
1:B:565:PHE:O	1:C:42:VAL:CA	2.58	0.47
1:C:385:THR:HG1	1:C:386:LYS:HZ3	1.59	0.47
1:C:551:VAL:HB	1:C:588:THR:CG2	2.44	0.47
1:C:640:SER:OG	1:C:641:ASN:N	2.48	0.47
1:C:690:GLN:N	1:C:690:GLN:CD	2.73	0.47
1:A:312:ILE:CG1	1:A:598:ILE:HG13	2.42	0.47
1:C:617:CYS:HB2	1:C:649:CYS:HB2	1.87	0.47
1:A:329:PHE:HB3	1:A:330:PRO:HD2	1.96	0.47
1:B:534:VAL:O	1:B:535:LYS:CG	2.63	0.47
1:B:640:SER:OG	1:B:641:ASN:N	2.48	0.47
1:B:973:ILE:HG12	1:B:992:GLN:HE21	1.79	0.47
1:C:231:ILE:HB	1:C:233:ILE:HG22	1.95	0.47
1:C:316:SER:C	1:C:317:ASN:ND2	2.73	0.47
1:C:912:THR:OG1	1:C:914:ASN:ND2	2.48	0.47
2:D:421:ILE:HG13	2:D:421:ILE:O	2.14	0.47
1:A:729:VAL:HG13	1:A:1059:GLY:HA2	1.97	0.47
2:D:333:LEU:O	2:D:362:THR:HG22	2.15	0.47
3:d:2:NAG:C3	3:d:2:NAG:H83	2.45	0.47
1:A:117:LEU:HD12	1:A:118:LEU:N	2.30	0.46
1:A:530:SER:CB	1:A:580:GLN:HE22	2.28	0.46
1:C:364:ASP:O	1:C:367:VAL:HG12	2.15	0.46
1:B:804:GLN:HG3	1:B:935:GLN:HE22	1.80	0.46
1:A:326:ILE:C	1:A:327:VAL:HG23	2.40	0.46
1:B:310:LYS:CD	1:B:664:ILE:HD11	2.45	0.46
1:B:703:ASN:HD22	1:B:703:ASN:C	2.24	0.46
1:C:403:ARG:NH1	1:C:505:TYR:CE1	2.84	0.46
1:C:505:TYR:CG	2:E:353:LYS:O	2.65	0.46
1:C:533:LEU:C	1:C:534:VAL:HG13	2.41	0.46
1:C:560:LEU:O	1:C:562:PHE:N	2.47	0.46
1:C:671:CYS:SG	1:C:697:MET:HB3	2.56	0.46
2:E:52:THR:HA	2:E:342:ALA:HB1	1.98	0.46
1:A:393:THR:HA	1:A:523:THR:HB	1.98	0.46
1:B:313:TYR:O	1:B:596:SER:HA	2.16	0.46
1:C:41:LYS:N	1:C:41:LYS:HD3	2.31	0.46
1:C:660:TYR:C	1:C:698:SER:HB2	2.39	0.46
1:A:722:VAL:HA	1:A:1064:HIS:O	2.16	0.46
1:C:1105:THR:HG22	1:C:1111:GLU:H	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:421:ILE:O	2:E:421:ILE:HG13	2.14	0.46
1:A:334:ASN:O	1:A:362:VAL:HB	2.15	0.46
1:A:369:TYR:CE2	1:A:384:PRO:HB2	2.50	0.46
1:B:560:LEU:O	1:B:562:PHE:N	2.47	0.46
2:D:425:SER:C	2:D:427:ASP:N	2.73	0.46
1:A:41:LYS:N	1:A:41:LYS:HD3	2.31	0.46
1:A:447:GLY:HA2	1:A:497:PHE:O	2.16	0.46
1:A:640:SER:OG	1:A:641:ASN:N	2.48	0.46
1:B:726:ILE:HG12	1:B:1061:VAL:HG22	1.97	0.46
1:C:45:SER:O	1:C:279:TYR:CB	2.64	0.46
1:C:369:TYR:CE2	1:C:384:PRO:HB2	2.50	0.46
1:A:42:VAL:CG2	1:C:565:PHE:CZ	2.98	0.46
1:B:325:SER:C	1:B:326:ILE:HG23	2.41	0.46
1:C:29:THR:HG22	1:C:30:ASN:N	2.31	0.46
1:C:447:GLY:HA2	1:C:497:PHE:O	2.16	0.46
1:C:673:SER:O	1:C:693:ILE:HD13	2.16	0.46
2:E:333:LEU:O	2:E:362:THR:HG22	2.15	0.46
1:A:536:ASN:N	1:A:536:ASN:OD1	2.47	0.46
1:C:316:SER:OG	1:C:317:ASN:N	2.48	0.46
1:B:45:SER:O	1:B:279:TYR:CB	2.64	0.46
1:C:335:LEU:HD12	1:C:335:LEU:H	1.80	0.46
1:C:486:PHE:HE1	2:E:79:LEU:CD1	2.27	0.46
1:A:758:SER:O	1:A:762:GLN:HG3	2.16	0.45
1:A:1032:CYS:O	1:A:1051:SER:HB2	2.16	0.45
1:B:310:LYS:HG3	1:B:664:ILE:HD11	1.95	0.45
1:B:322:PRO:HA	1:B:538:CYS:O	2.16	0.45
1:B:977:LEU:HD12	1:B:996:LEU:HD12	1.98	0.45
1:A:127:VAL:HG11	4:A:1402:NAG:H61	1.98	0.45
1:A:364:ASP:O	1:A:367:VAL:HG12	2.15	0.45
1:B:364:ASP:O	1:B:367:VAL:HG12	2.15	0.45
1:C:1094:VAL:HG22	1:C:1107:ARG:HG2	1.98	0.45
2:E:425:SER:C	2:E:427:ASP:N	2.73	0.45
1:A:308:VAL:HG13	1:A:602:THR:HG23	1.98	0.45
1:A:530:SER:CB	1:A:580:GLN:NE2	2.80	0.45
1:A:560:LEU:O	1:A:562:PHE:N	2.47	0.45
1:B:329:PHE:O	1:B:579:PRO:HG2	2.17	0.45
1:B:578:ASP:OD2	1:B:581:THR:HG22	2.16	0.45
1:B:1141:LEU:O	1:B:1145:LEU:HD12	2.16	0.45
1:C:117:LEU:HD12	1:C:118:LEU:N	2.30	0.45
1:C:388:ASN:CG	1:C:527:PRO:HD2	2.42	0.45
1:C:578:ASP:OD2	1:C:581:THR:HG22	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:153:MET:SD	1:A:153:MET:N	2.90	0.45
1:B:536:ASN:OD1	1:B:536:ASN:N	2.49	0.45
1:C:377:PHE:CD2	1:C:434:ILE:HG12	2.51	0.45
1:C:693:ILE:CD1	1:C:693:ILE:N	2.73	0.45
2:D:560:LEU:HD22	2:D:564:GLU:HG3	1.98	0.45
1:A:48:LEU:HD13	1:A:48:LEU:N	2.32	0.45
1:A:505:TYR:CD2	2:D:353:LYS:C	2.93	0.45
1:A:1045:LYS:HZ1	1:B:786:LYS:HE3	1.81	0.45
4:A:1409:NAG:O4	4:A:1410:NAG:O5	2.28	0.45
1:B:377:PHE:CD2	1:B:434:ILE:HG12	2.51	0.45
1:C:48:LEU:HD13	1:C:48:LEU:N	2.32	0.45
2:D:52:THR:HA	2:D:342:ALA:HB1	1.98	0.45
2:D:208:GLU:OE1	2:D:210:ASN:ND2	2.50	0.45
2:E:560:LEU:HD22	2:E:564:GLU:HG3	1.97	0.45
1:A:29:THR:HG22	1:A:30:ASN:N	2.31	0.45
1:B:738:CYS:HB3	1:B:760:CYS:HB3	1.92	0.45
1:C:153:MET:N	1:C:153:MET:SD	2.90	0.45
1:A:377:PHE:CD2	1:A:434:ILE:HG12	2.51	0.45
1:B:589:PRO:HD2	1:C:854:LYS:HG2	1.98	0.45
1:C:329:PHE:CD1	1:C:544:ASN:CB	2.88	0.45
1:C:329:PHE:C	1:C:579:PRO:HG2	2.42	0.45
1:C:654:GLU:HG3	1:C:693:ILE:HG22	1.98	0.45
1:A:338:PHE:C	1:A:340:GLU:N	2.75	0.45
1:B:393:THR:HA	1:B:523:THR:HB	1.98	0.45
1:B:646:ARG:O	1:B:646:ARG:HG3	2.17	0.45
1:C:187:LYS:HE3	1:C:213:VAL:HG12	1.99	0.45
2:E:208:GLU:OE1	2:E:210:ASN:ND2	2.50	0.45
1:A:578:ASP:OD2	1:A:581:THR:HG22	2.16	0.45
1:B:127:VAL:HG11	4:B:1402:NAG:H61	1.98	0.45
1:C:127:VAL:HG11	4:C:1402:NAG:H61	1.98	0.45
1:C:393:THR:HA	1:C:523:THR:HB	1.98	0.45
1:C:493:GLN:OE1	2:E:34:HIS:CG	2.70	0.45
1:C:1090:PRO:HD3	1:C:1095:PHE:CE2	2.51	0.45
2:E:356:PHE:HB3	2:E:379:ILE:HD12	1.98	0.45
1:A:440:ASN:ND2	1:A:441:LEU:HG	2.32	0.45
1:A:617:CYS:HB2	1:A:649:CYS:HB2	1.87	0.45
1:B:447:GLY:HA2	1:B:497:PHE:O	2.16	0.45
1:B:1040:VAL:O	1:B:1041:ASP:HB2	2.16	0.45
1:A:187:LYS:HE3	1:A:213:VAL:HG12	1.99	0.44
1:B:29:THR:HG22	1:B:30:ASN:N	2.31	0.44
1:B:153:MET:SD	1:B:153:MET:N	2.90	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:523:THR:CG2	1:C:524:VAL:N	2.46	0.44
2:D:356:PHE:HB3	2:D:379:ILE:HD12	1.98	0.44
2:D:455:MET:HE3	2:D:455:MET:HB3	1.79	0.44
1:B:931:ILE:HD13	1:B:931:ILE:HA	1.86	0.44
1:A:986:PRO:CB	1:A:987:PRO:HD3	2.46	0.44
1:B:294:ASP:N	1:B:294:ASP:OD1	2.50	0.44
1:B:295:PRO:HB2	1:B:608:VAL:HG11	1.97	0.44
1:B:316:SER:OG	1:B:317:ASN:N	2.50	0.44
1:B:440:ASN:ND2	1:B:441:LEU:HG	2.32	0.44
1:C:140:PHE:CG	1:C:244:LEU:HD11	2.53	0.44
1:C:330:PRO:HA	1:C:579:PRO:HB2	2.00	0.44
1:C:653:ALA:HA	1:C:692:ILE:O	2.17	0.44
1:C:694:ALA:O	1:C:695:TYR:HB3	2.17	0.44
1:C:903:ALA:HB1	1:C:913:GLN:HG2	1.98	0.44
1:A:45:SER:O	1:A:279:TYR:CB	2.64	0.44
1:A:327:VAL:HB	1:A:531:THR:OG1	2.18	0.44
1:A:592:PHE:CD1	1:A:592:PHE:C	2.95	0.44
1:B:41:LYS:N	1:B:41:LYS:HD3	2.31	0.44
1:B:134:GLN:HB3	1:B:162:SER:HB2	2.00	0.44
1:C:294:ASP:OD1	1:C:294:ASP:N	2.50	0.44
1:C:334:ASN:O	1:C:362:VAL:CG2	2.65	0.44
1:C:393:THR:O	1:C:523:THR:CG2	2.58	0.44
1:A:134:GLN:HB3	1:A:162:SER:HB2	2.00	0.44
1:A:521:PRO:O	1:A:522:ALA:CB	2.66	0.44
1:C:646:ARG:O	1:C:646:ARG:HG3	2.17	0.44
1:A:486:PHE:CE1	2:D:79:LEU:HD21	2.48	0.44
1:B:338:PHE:C	1:B:340:GLU:N	2.75	0.44
1:B:1027:THR:HG22	1:B:1042:PHE:HZ	1.83	0.44
1:C:854:LYS:O	1:C:855:PHE:CD1	2.70	0.44
1:B:793:PRO:HG2	1:B:794:ILE:HD12	2.00	0.44
1:C:134:GLN:HB3	1:C:162:SER:HB2	2.00	0.44
1:C:653:ALA:HB1	1:C:692:ILE:O	2.18	0.44
1:A:130:VAL:HG21	1:A:231:ILE:HD12	2.00	0.44
1:B:140:PHE:CG	1:B:244:LEU:HD11	2.53	0.44
1:B:588:THR:OG1	1:B:589:PRO:HD2	2.18	0.44
1:B:740:MET:HE2	1:B:856:ASN:HA	1.99	0.44
1:C:440:ASN:ND2	1:C:441:LEU:HG	2.32	0.44
1:C:486:PHE:CE1	2:E:79:LEU:HD21	2.48	0.44
1:C:533:LEU:HG	1:C:534:VAL:N	2.33	0.44
2:E:313:LYS:HA	2:E:316:VAL:HG12	2.00	0.44
3:N:1:NAG:H61	3:N:2:NAG:N2	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:320:VAL:CG1	1:A:321:GLN:N	2.80	0.43
1:A:500:THR:O	1:A:500:THR:OG1	2.31	0.43
1:B:595:VAL:HG12	1:B:596:SER:N	2.33	0.43
1:C:1097:SER:HA	1:C:1101:HIS:O	2.18	0.43
2:D:313:LYS:HA	2:D:316:VAL:HG12	2.00	0.43
1:A:140:PHE:CG	1:A:244:LEU:HD11	2.53	0.43
1:A:546:LEU:HD11	1:A:565:PHE:CG	2.53	0.43
1:B:187:LYS:HE3	1:B:213:VAL:HG12	1.99	0.43
1:B:534:VAL:CG2	1:B:535:LYS:H	2.24	0.43
1:C:127:VAL:HG21	4:C:1402:NAG:H5	2.01	0.43
1:C:521:PRO:O	1:C:522:ALA:CB	2.66	0.43
1:C:1032:CYS:O	1:C:1051:SER:HB2	2.18	0.43
1:A:307:THR:HA	1:A:602:THR:OG1	2.18	0.43
1:A:748:GLU:N	1:A:748:GLU:CD	2.73	0.43
1:B:141:LEU:O	1:B:243:ALA:HA	2.18	0.43
1:B:1081:ILE:HG12	1:B:1095:PHE:CE2	2.53	0.43
1:C:390:LEU:O	1:C:525:CYS:HB3	2.18	0.43
1:A:493:GLN:OE1	2:D:34:HIS:CG	2.70	0.43
1:C:536:ASN:C	1:C:537:LYS:HG2	2.43	0.43
1:C:670:ILE:CD1	1:C:695:TYR:O	2.65	0.43
2:D:431:ASP:OD1	2:D:431:ASP:N	2.44	0.43
2:E:97:LEU:HD23	2:E:97:LEU:HA	1.88	0.43
1:A:328:ARG:HD3	1:A:328:ARG:HA	1.61	0.43
1:A:646:ARG:O	1:A:646:ARG:HG3	2.17	0.43
1:C:130:VAL:HG21	1:C:231:ILE:HD12	2.00	0.43
1:C:326:ILE:HG22	1:C:327:VAL:N	2.33	0.43
1:A:333:THR:OG1	1:A:334:ASN:N	2.50	0.43
1:A:669:GLY:N	1:B:864:LEU:O	2.51	0.43
1:B:48:LEU:HD13	1:B:48:LEU:N	2.32	0.43
1:B:326:ILE:HG13	1:B:541:PHE:HA	2.01	0.43
1:C:329:PHE:O	1:C:580:GLN:HG2	2.19	0.43
1:C:546:LEU:HD11	1:C:565:PHE:CG	2.53	0.43
1:C:795:LYS:HB3	1:C:797:PHE:CE2	2.54	0.43
1:A:390:LEU:O	1:A:525:CYS:HB3	2.18	0.43
1:A:569:ILE:O	1:A:570:ALA:HB3	2.19	0.43
1:A:1045:LYS:NZ	1:B:786:LYS:CE	2.79	0.43
1:B:127:VAL:HG21	4:B:1402:NAG:H5	2.01	0.43
1:C:1104:VAL:HG22	1:C:1115:ILE:HG12	2.01	0.43
3:G:1:NAG:H61	3:G:2:NAG:N2	2.33	0.43
1:A:612:TYR:HE1	1:A:651:ILE:HD12	1.84	0.43
1:B:674:TYR:HA	1:B:691:SER:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:V:1:NAG:H61	3:V:2:NAG:N2	2.33	0.43
1:A:476:GLY:HA2	2:D:24:GLN:NE2	2.26	0.43
1:A:592:PHE:CD1	1:A:593:GLY:N	2.87	0.43
1:B:130:VAL:HG21	1:B:231:ILE:HD12	2.00	0.43
1:C:141:LEU:O	1:C:243:ALA:HA	2.18	0.43
1:C:886:TRP:HH2	1:C:904:TYR:CD2	2.35	0.43
1:A:131:CYS:HB3	1:A:164:ASN:O	2.19	0.43
1:B:27:ALA:HB3	1:B:64:TRP:HB3	2.01	0.43
1:C:27:ALA:HB3	1:C:64:TRP:HB3	2.01	0.43
1:C:569:ILE:O	1:C:570:ALA:HB3	2.19	0.43
1:C:612:TYR:HE1	1:C:651:ILE:HD12	1.84	0.43
1:C:676:THR:HB	1:C:693:ILE:HG21	2.00	0.43
3:d:1:NAG:C3	3:d:2:NAG:N2	2.74	0.43
1:A:48:LEU:H	1:A:48:LEU:CD1	2.32	0.42
1:A:127:VAL:HG21	4:A:1402:NAG:H5	2.00	0.42
1:B:117:LEU:HD12	1:B:118:LEU:N	2.30	0.42
1:B:792:PRO:O	1:B:795:LYS:NZ	2.52	0.42
1:B:912:THR:OG1	1:B:914:ASN:ND2	2.51	0.42
1:C:535:LYS:HE2	1:C:554:GLU:CD	2.44	0.42
1:C:933:LYS:HB2	1:C:933:LYS:HE3	1.86	0.42
1:A:27:ALA:HB3	1:A:64:TRP:HB3	2.01	0.42
1:B:523:THR:CG2	1:B:524:VAL:N	2.46	0.42
1:B:546:LEU:HD11	1:B:565:PHE:CG	2.53	0.42
1:B:569:ILE:O	1:B:570:ALA:HB3	2.19	0.42
1:C:673:SER:O	1:C:693:ILE:CD1	2.67	0.42
1:C:856:ASN:OD1	1:C:966:LEU:HD11	2.17	0.42
2:E:455:MET:HE3	2:E:455:MET:HB3	1.80	0.42
2:E:513:ILE:HD12	2:E:513:ILE:HA	1.94	0.42
1:A:825:LYS:HB3	1:A:825:LYS:HE2	1.79	0.42
1:B:212:LEU:HD12	1:B:212:LEU:HA	1.78	0.42
1:B:536:ASN:HA	1:B:551:VAL:CG1	2.48	0.42
1:B:722:VAL:HA	1:B:1064:HIS:O	2.19	0.42
1:C:112:SER:O	1:C:113:LYS:HB3	2.20	0.42
1:C:476:GLY:HA2	2:E:24:GLN:NE2	2.26	0.42
1:C:758:SER:O	1:C:762:GLN:HG3	2.19	0.42
1:A:42:VAL:CA	1:C:565:PHE:O	2.58	0.42
1:A:141:LEU:O	1:A:243:ALA:HA	2.18	0.42
1:C:502:GLY:HA3	2:E:354:GLY:O	2.20	0.42
1:A:112:SER:O	1:A:113:LYS:HB3	2.20	0.42
1:A:502:GLY:HA3	2:D:354:GLY:O	2.20	0.42
1:B:856:ASN:O	1:B:856:ASN:ND2	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:973:ILE:HG23	1:B:992:GLN:NE2	2.35	0.42
1:C:131:CYS:HB3	1:C:164:ASN:O	2.19	0.42
1:B:326:ILE:C	1:B:327:VAL:HG23	2.44	0.42
1:B:535:LYS:O	1:B:537:LYS:CG	2.68	0.42
1:C:392:PHE:CA	1:C:517:LEU:HD21	2.49	0.42
1:A:406:GLU:CG	1:A:418:ILE:HG13	2.50	0.42
1:A:996:LEU:HD23	1:A:996:LEU:HA	1.92	0.42
1:B:131:CYS:HB3	1:B:164:ASN:O	2.19	0.42
1:B:612:TYR:HE1	1:B:651:ILE:HD12	1.84	0.42
1:B:736:VAL:HG23	1:B:858:LEU:HD23	2.02	0.42
1:C:48:LEU:H	1:C:48:LEU:CD1	2.32	0.42
1:C:524:VAL:CG2	1:C:525:CYS:N	2.83	0.42
1:C:754:LEU:HA	1:C:754:LEU:HD23	1.85	0.42
1:C:973:ILE:HG23	1:C:992:GLN:NE2	2.35	0.42
2:E:212:VAL:HG23	2:E:215:TYR:HB2	2.02	0.42
1:A:294:ASP:N	1:A:294:ASP:OD1	2.50	0.42
1:A:552:LEU:CD2	1:A:587:ILE:HG12	2.50	0.42
1:C:326:ILE:HG13	1:C:533:LEU:C	2.44	0.42
1:C:393:THR:H	1:C:517:LEU:HD22	1.85	0.42
3:i:2:NAG:H83	3:i:2:NAG:H3	2.02	0.42
1:A:591:SER:CB	1:A:619:GLU:OE2	2.67	0.42
1:B:393:THR:H	1:B:517:LEU:HD22	1.85	0.42
3:d:2:NAG:H83	3:d:2:NAG:H3	2.02	0.42
1:A:326:ILE:C	1:A:327:VAL:CG2	2.93	0.41
1:A:329:PHE:O	1:A:580:GLN:CG	2.68	0.41
1:B:48:LEU:H	1:B:48:LEU:CD1	2.32	0.41
1:B:523:THR:O	1:B:525:CYS:SG	2.78	0.41
1:B:112:SER:O	1:B:113:LYS:HB3	2.20	0.41
1:B:500:THR:O	1:B:500:THR:OG1	2.31	0.41
1:B:674:TYR:HD1	1:B:691:SER:O	1.96	0.41
1:A:524:VAL:CG2	1:A:525:CYS:N	2.83	0.41
2:E:411:SER:OG	2:E:543:ASP:OD1	2.38	0.41
2:E:125:THR:O	2:E:129:THR:OG1	2.32	0.41
1:A:393:THR:O	1:A:523:THR:CG2	2.58	0.41
1:B:821:LEU:HD22	1:B:939:SER:HB3	2.03	0.41
1:C:193:VAL:HG23	1:C:223:LEU:CD2	2.51	0.41
1:C:304:LYS:HE3	1:C:304:LYS:HB3	1.78	0.41
2:E:254:SER:O	2:E:254:SER:OG	2.31	0.41
1:A:99:ASN:O	1:A:102:ARG:NE	2.35	0.41
1:A:310:LYS:HZ3	1:A:663:ASP:CG	2.26	0.41
1:B:390:LEU:O	1:B:525:CYS:HB3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:406:GLU:CG	1:B:418:ILE:HG13	2.50	0.41
1:B:460:ASN:OD1	1:B:460:ASN:N	2.53	0.41
1:B:542:ASN:HA	1:B:546:LEU:O	2.21	0.41
1:A:226:LEU:HB3	1:A:227:VAL:HG23	2.03	0.41
1:A:393:THR:H	1:A:517:LEU:HD22	1.85	0.41
1:B:521:PRO:O	1:B:522:ALA:CB	2.66	0.41
1:C:691:SER:C	1:C:692:ILE:HG12	2.44	0.41
2:D:212:VAL:HG23	2:D:215:TYR:HB2	2.02	0.41
1:A:984:LEU:HD23	1:A:988:GLU:HB3	2.03	0.41
1:B:589:PRO:O	1:B:590:CYS:C	2.64	0.41
1:A:166:CYS:HB3	1:A:169:GLU:OE1	2.21	0.41
1:A:193:VAL:HG23	1:A:223:LEU:CD2	2.51	0.41
1:A:331:ASN:O	1:A:332:ILE:HG12	2.21	0.41
1:A:563:GLN:OE1	1:B:43:PHE:CD1	2.65	0.41
1:B:45:SER:OG	1:B:281:GLU:HA	2.21	0.41
1:B:329:PHE:O	1:B:579:PRO:CB	2.67	0.41
1:B:870:ILE:O	1:B:874:THR:HG23	2.21	0.41
1:B:984:LEU:HD23	1:B:984:LEU:HA	1.91	0.41
1:C:347:PHE:CD1	1:C:509:ARG:HD3	2.56	0.41
1:C:406:GLU:CG	1:C:418:ILE:HG13	2.50	0.41
1:C:542:ASN:HA	1:C:546:LEU:O	2.21	0.41
2:D:21:ILE:HD12	2:D:21:ILE:HA	1.97	0.41
2:D:366:MET:HE3	2:D:366:MET:HB2	2.01	0.41
2:D:411:SER:OG	2:D:543:ASP:OD1	2.38	0.41
3:O:1:NAG:H3	3:O:1:NAG:H83	2.02	0.41
1:A:535:LYS:HG3	1:A:536:ASN:OD1	2.21	0.41
1:A:735:SER:O	1:A:859:THR:HG22	2.21	0.41
1:B:524:VAL:CG2	1:B:525:CYS:N	2.83	0.41
1:C:371:SER:C	1:C:373:SER:H	2.30	0.41
1:A:45:SER:OG	1:A:281:GLU:HA	2.21	0.40
1:A:200:TYR:CE1	1:A:230:PRO:HB3	2.56	0.40
1:A:371:SER:C	1:A:373:SER:H	2.30	0.40
1:A:486:PHE:HE1	2:D:79:LEU:HD21	1.77	0.40
1:A:1040:VAL:O	1:A:1041:ASP:HB2	2.21	0.40
1:B:166:CYS:HB3	1:B:169:GLU:OE1	2.21	0.40
1:B:226:LEU:HB3	1:B:227:VAL:HG23	2.03	0.40
1:A:46:SER:C	1:A:47:VAL:HG13	2.46	0.40
1:A:308:VAL:N	1:A:602:THR:OG1	2.54	0.40
1:A:392:PHE:CA	1:A:517:LEU:HD21	2.49	0.40
1:B:200:TYR:CE1	1:B:230:PRO:HB3	2.56	0.40
1:B:213:VAL:HG23	1:B:214:ARG:N	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:309:GLU:H	1:B:309:GLU:HG2	1.71	0.40
1:B:325:SER:C	1:B:326:ILE:CG2	2.94	0.40
1:B:694:ALA:O	1:B:695:TYR:HB3	2.21	0.40
1:C:200:TYR:CE1	1:C:230:PRO:HB3	2.56	0.40
1:C:280:ASN:OD1	1:C:281:GLU:N	2.50	0.40
2:D:294:THR:HG23	2:D:365:THR:HA	2.03	0.40
2:E:318:VAL:HG21	2:E:544:ILE:HD12	2.03	0.40
1:A:39:PRO:C	1:A:40:ASP:CG	2.90	0.40
1:A:45:SER:O	1:A:47:VAL:N	2.54	0.40
1:A:227:VAL:CG1	1:A:228:ASP:N	2.84	0.40
1:B:99:ASN:O	1:B:102:ARG:NE	2.35	0.40
1:B:227:VAL:CG1	1:B:228:ASP:N	2.84	0.40
1:B:342:PHE:CB	3:N:1:NAG:H82	2.51	0.40
1:B:670:ILE:HG23	1:B:695:TYR:O	2.21	0.40
1:B:770:ILE:O	1:B:774:GLN:HG2	2.21	0.40
1:C:213:VAL:HG23	1:C:214:ARG:N	2.36	0.40
1:C:486:PHE:CE1	2:E:79:LEU:HD13	2.56	0.40
1:C:662:CYS:CB	1:C:697:MET:HB3	2.47	0.40
1:C:691:SER:OG	1:C:692:ILE:N	2.54	0.40
1:A:325:SER:HB3	1:A:540:ASN:O	2.20	0.40
1:A:534:VAL:C	1:A:535:LYS:CG	2.92	0.40
1:A:981:LEU:HD12	1:A:981:LEU:HA	1.89	0.40
1:B:89:GLY:HA2	1:B:194:PHE:O	2.22	0.40
1:B:127:VAL:HG22	1:B:171:VAL:HG13	2.04	0.40
1:B:193:VAL:HG23	1:B:223:LEU:CD2	2.51	0.40
1:B:347:PHE:CD1	1:B:509:ARG:HD3	2.56	0.40
1:B:854:LYS:HE2	1:B:854:LYS:HB3	1.88	0.40
1:C:100:ILE:HG22	1:C:242:LEU:HD23	2.04	0.40
1:A:309:GLU:H	1:A:309:GLU:HG2	1.71	0.40
1:A:340:GLU:HG3	1:A:341:VAL:N	2.37	0.40
1:A:505:TYR:CE2	2:D:353:LYS:O	2.73	0.40
1:A:872:GLN:CD	1:C:699:LEU:HD12	2.45	0.40
1:B:64:TRP:CD1	1:B:65:PHE:N	2.89	0.40
1:B:187:LYS:N	1:B:187:LYS:HE2	2.37	0.40
1:B:371:SER:C	1:B:373:SER:H	2.30	0.40
1:B:393:THR:O	1:B:523:THR:CG2	2.58	0.40
1:B:767:LEU:HD23	1:B:767:LEU:HA	1.85	0.40
1:C:187:LYS:N	1:C:187:LYS:HE2	2.37	0.40
1:C:369:TYR:CZ	1:C:384:PRO:HB2	2.57	0.40
2:E:294:THR:HG23	2:E:365:THR:HA	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	988/1283 (77%)	865 (88%)	95 (10%)	28 (3%)	4	26
1	B	988/1283 (77%)	862 (87%)	98 (10%)	28 (3%)	4	26
1	C	989/1283 (77%)	868 (88%)	98 (10%)	23 (2%)	5	30
2	D	593/817 (73%)	563 (95%)	28 (5%)	2 (0%)	36	65
2	E	593/817 (73%)	564 (95%)	27 (5%)	2 (0%)	36	65
All	All	4151/5483 (76%)	3722 (90%)	346 (8%)	83 (2%)	8	32

All (83) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	48	LEU
1	A	331	ASN
1	A	518	LEU
1	A	536	ASN
1	B	48	LEU
1	B	329	PHE
1	B	331	ASN
1	B	518	LEU
1	B	536	ASN
1	B	697	MET
1	B	814	LYS
1	C	48	LEU
1	C	325	SER
1	C	518	LEU
1	C	695	TYR
1	C	701	ALA
1	A	41	LYS
1	A	46	SER
1	A	339	GLY
1	A	534	VAL
1	A	591	SER

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Mol	Chain	Res	Type
1	A	742	ILE
1	A	743	CYS
1	B	41	LYS
1	B	46	SER
1	B	332	ILE
1	B	339	GLY
1	B	534	VAL
1	B	695	TYR
1	B	810	SER
1	C	41	LYS
1	C	46	SER
1	C	339	GLY
1	C	531	THR
1	C	534	VAL
2	D	343	VAL
2	E	343	VAL
1	A	43	PHE
1	A	332	ILE
1	A	336	CYS
1	A	522	ALA
1	A	535	LYS
1	B	43	PHE
1	B	333	THR
1	B	336	CYS
1	B	522	ALA
1	C	43	PHE
1	C	324	GLU
1	C	333	THR
1	C	336	CYS
1	C	522	ALA
1	C	710	ASN
2	D	423	LEU
2	E	423	LEU
1	A	44	ARG
1	A	324	GLU
1	A	333	THR
1	A	349	SER
1	A	520	ALA
1	A	746	SER
1	B	44	ARG
1	B	349	SER
1	B	520	ALA

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Mol	Chain	Res	Type
1	B	813	SER
1	C	44	ARG
1	C	349	SER
1	C	520	ALA
1	A	40	ASP
1	A	42	VAL
1	A	47	VAL
1	A	327	VAL
1	A	328	ARG
1	B	40	ASP
1	B	42	VAL
1	B	47	VAL
1	B	812	PRO
1	C	40	ASP
1	C	42	VAL
1	C	47	VAL
1	B	811	LYS
1	C	329	PHE
1	B	594	GLY
1	A	526	GLY

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.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	881/1122 (78%)	780 (88%)	101 (12%)	5	25
1	B	881/1122 (78%)	773 (88%)	108 (12%)	4	23
1	C	882/1122 (79%)	762 (86%)	120 (14%)	3	20
2	D	525/721 (73%)	517 (98%)	8 (2%)	57	70
2	E	525/721 (73%)	517 (98%)	8 (2%)	57	70
All	All	3694/4808 (77%)	3349 (91%)	345 (9%)	11	32

All (345) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	ASP
1	A	46	SER
1	A	48	LEU
1	A	66	HIS
1	A	81	ASN
1	A	97	LYS
1	A	109	THR
1	A	116	SER
1	A	118	LEU
1	A	122	ASN
1	A	141	LEU
1	A	143	VAL
1	A	158	ARG
1	A	164	ASN
1	A	169	GLU
1	A	171	VAL
1	A	195	LYS
1	A	205	SER
1	A	208	THR
1	A	221	SER
1	A	231	ILE
1	A	282	ASN
1	A	289	VAL
1	A	296	LEU
1	A	301	CYS
1	A	308	VAL
1	A	314	GLN
1	A	315	THR
1	A	324	GLU
1	A	325	SER
1	A	326	ILE
1	A	335	LEU
1	A	375	SER
1	A	382	VAL
1	A	383	SER
1	A	389	ASP
1	A	390	LEU
1	A	403	ARG
1	A	406	GLU
1	A	421	TYR
1	A	430	THR
1	A	438	SER
1	A	459	SER

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Mol	Chain	Res	Type
1	A	469	SER
1	A	472	ILE
1	A	500	THR
1	A	514	SER
1	A	517	LEU
1	A	518	LEU
1	A	525	CYS
1	A	529	LYS
1	A	531	THR
1	A	536	ASN
1	A	537	LYS
1	A	540	ASN
1	A	546	LEU
1	A	553	THR
1	A	554	GLU
1	A	556	ASN
1	A	576	VAL
1	A	583	GLU
1	A	585	LEU
1	A	588	THR
1	A	592	PHE
1	A	599	THR
1	A	602	THR
1	A	608	VAL
1	A	673	SER
1	A	710	ASN
1	A	729	VAL
1	A	735	SER
1	A	747	THR
1	A	748	GLU
1	A	772	VAL
1	A	779	GLN
1	A	787	GLN
1	A	791	THR
1	A	811	LYS
1	A	855	PHE
1	A	856	ASN
1	A	868	GLU
1	A	878	LEU
1	A	912	THR
1	A	916	LEU
1	A	935	GLN

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Mol	Chain	Res	Type
1	A	968	SER
1	A	969	ASN
1	A	974	SER
1	A	976	VAL
1	A	991	VAL
1	A	1030	SER
1	A	1037	SER
1	A	1045	LYS
1	A	1074	ASN
1	A	1081	ILE
1	A	1094	VAL
1	A	1104	VAL
1	A	1114	ILE
1	A	1126	CYS
1	A	1133	VAL
1	A	1141	LEU
1	B	40	ASP
1	B	46	SER
1	B	48	LEU
1	B	66	HIS
1	B	81	ASN
1	B	97	LYS
1	B	109	THR
1	B	116	SER
1	B	118	LEU
1	B	122	ASN
1	B	141	LEU
1	B	143	VAL
1	B	158	ARG
1	B	164	ASN
1	B	169	GLU
1	B	171	VAL
1	B	195	LYS
1	B	205	SER
1	B	208	THR
1	B	221	SER
1	B	231	ILE
1	B	282	ASN
1	B	289	VAL
1	B	296	LEU
1	B	301	CYS
1	B	308	VAL

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Mol	Chain	Res	Type
1	B	310	LYS
1	B	314	GLN
1	B	315	THR
1	B	319	ARG
1	B	324	GLU
1	B	326	ILE
1	B	328	ARG
1	B	333	THR
1	B	334	ASN
1	B	335	LEU
1	B	375	SER
1	B	382	VAL
1	B	383	SER
1	B	389	ASP
1	B	390	LEU
1	B	403	ARG
1	B	406	GLU
1	B	421	TYR
1	B	430	THR
1	B	438	SER
1	B	459	SER
1	B	469	SER
1	B	472	ILE
1	B	500	THR
1	B	514	SER
1	B	517	LEU
1	B	518	LEU
1	B	525	CYS
1	B	529	LYS
1	B	531	THR
1	B	533	LEU
1	B	535	LYS
1	B	536	ASN
1	B	540	ASN
1	B	546	LEU
1	B	553	THR
1	B	554	GLU
1	B	556	ASN
1	B	576	VAL
1	B	583	GLU
1	B	585	LEU
1	B	588	THR

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Mol	Chain	Res	Type
1	B	591	SER
1	B	599	THR
1	B	602	THR
1	B	608	VAL
1	B	673	SER
1	B	693	ILE
1	B	696	THR
1	B	697	MET
1	B	699	LEU
1	B	727	LEU
1	B	768	THR
1	B	770	ILE
1	B	778	THR
1	B	787	GLN
1	B	791	THR
1	B	814	LYS
1	B	856	ASN
1	B	878	LEU
1	B	907	ASN
1	B	922	LEU
1	B	929	SER
1	B	931	ILE
1	B	934	ILE
1	B	937	SER
1	B	968	SER
1	B	975	SER
1	B	976	VAL
1	B	977	LEU
1	B	1018	ILE
1	B	1027	THR
1	B	1063	LEU
1	B	1077	THR
1	B	1092	GLU
1	B	1094	VAL
1	B	1104	VAL
1	B	1126	CYS
1	B	1129	VAL
1	B	1132	ILE
1	B	1136	THR
1	B	1145	LEU
1	C	40	ASP
1	C	46	SER

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Mol	Chain	Res	Type
1	C	48	LEU
1	C	66	HIS
1	C	81	ASN
1	C	97	LYS
1	C	109	THR
1	C	116	SER
1	C	118	LEU
1	C	122	ASN
1	C	141	LEU
1	C	143	VAL
1	C	158	ARG
1	C	164	ASN
1	C	169	GLU
1	C	171	VAL
1	C	195	LYS
1	C	205	SER
1	C	208	THR
1	C	221	SER
1	C	231	ILE
1	C	282	ASN
1	C	289	VAL
1	C	296	LEU
1	C	301	CYS
1	C	308	VAL
1	C	314	GLN
1	C	315	THR
1	C	319	ARG
1	C	320	VAL
1	C	321	GLN
1	C	328	ARG
1	C	329	PHE
1	C	332	ILE
1	C	335	LEU
1	C	375	SER
1	C	382	VAL
1	C	383	SER
1	C	389	ASP
1	C	390	LEU
1	C	403	ARG
1	C	406	GLU
1	C	421	TYR
1	C	430	THR

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Mol	Chain	Res	Type
1	C	438	SER
1	C	459	SER
1	C	469	SER
1	C	472	ILE
1	C	500	THR
1	C	514	SER
1	C	517	LEU
1	C	518	LEU
1	C	525	CYS
1	C	528	LYS
1	C	533	LEU
1	C	540	ASN
1	C	546	LEU
1	C	553	THR
1	C	554	GLU
1	C	556	ASN
1	C	576	VAL
1	C	583	GLU
1	C	585	LEU
1	C	588	THR
1	C	591	SER
1	C	599	THR
1	C	602	THR
1	C	608	VAL
1	C	673	SER
1	C	690	GLN
1	C	693	ILE
1	C	696	THR
1	C	702	GLU
1	C	704	SER
1	C	705	VAL
1	C	719	THR
1	C	722	VAL
1	C	729	VAL
1	C	730	SER
1	C	738	CYS
1	C	746	SER
1	C	772	VAL
1	C	773	GLU
1	C	785	VAL
1	C	787	GLN
1	C	791	THR

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Mol	Chain	Res	Type
1	C	826	VAL
1	C	854	LYS
1	C	856	ASN
1	C	868	GLU
1	C	878	LEU
1	C	883	THR
1	C	902	MET
1	C	916	LEU
1	C	929	SER
1	C	939	SER
1	C	951	VAL
1	C	960	ASN
1	C	967	SER
1	C	973	ILE
1	C	976	VAL
1	C	991	VAL
1	C	994	ASP
1	C	998	THR
1	C	1005	GLN
1	C	1018	ILE
1	C	1039	ARG
1	C	1074	ASN
1	C	1076	THR
1	C	1077	THR
1	C	1092	GLU
1	C	1094	VAL
1	C	1100	THR
1	C	1104	VAL
1	C	1114	ILE
1	C	1123	SER
1	C	1125	ASN
1	C	1132	ILE
1	C	1142	GLN
1	C	1144	GLU
2	D	107	VAL
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

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Mol	Chain	Res	Type
2	E	107	VAL
2	E	339	VAL
2	E	344	CYS
2	E	345	HIS
2	E	347	THR
2	E	361	CYS
2	E	423	LEU
2	E	425	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (122) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	134	GLN
1	A	137	ASN
1	A	188	ASN
1	A	317	ASN
1	A	394	ASN
1	A	422	ASN
1	A	440	ASN
1	A	450	ASN
1	A	498	GLN
1	A	556	ASN
1	A	580	GLN
1	A	644	GLN
1	A	655	HIS
1	A	658	ASN
1	A	675	GLN
1	A	690	GLN
1	A	703	ASN
1	A	710	ASN
1	A	804	GLN
1	A	901	GLN
1	A	914	ASN
1	A	920	GLN
1	A	926	GLN
1	A	949	GLN
1	A	957	GLN
1	A	960	ASN
1	A	992	GLN
1	A	1011	GLN
1	A	1083	HIS
1	A	1101	HIS

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Mol	Chain	Res	Type
1	B	134	GLN
1	B	137	ASN
1	B	188	ASN
1	B	317	ASN
1	B	394	ASN
1	B	422	ASN
1	B	440	ASN
1	B	450	ASN
1	B	498	GLN
1	B	556	ASN
1	B	580	GLN
1	B	644	GLN
1	B	658	ASN
1	B	675	GLN
1	B	703	ASN
1	B	764	ASN
1	B	779	GLN
1	B	784	GLN
1	B	804	GLN
1	B	901	GLN
1	B	907	ASN
1	B	914	ASN
1	B	926	GLN
1	B	935	GLN
1	B	949	GLN
1	B	992	GLN
1	B	1010	GLN
1	B	1011	GLN
1	B	1071	GLN
1	B	1101	HIS
1	B	1125	ASN
1	C	134	GLN
1	C	137	ASN
1	C	188	ASN
1	C	314	GLN
1	C	317	ASN
1	C	394	ASN
1	C	422	ASN
1	C	440	ASN
1	C	450	ASN
1	C	487	ASN
1	C	498	GLN

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Mol	Chain	Res	Type
1	C	536	ASN
1	C	556	ASN
1	C	580	GLN
1	C	644	GLN
1	C	658	ASN
1	C	675	GLN
1	C	690	GLN
1	C	703	ASN
1	C	755	GLN
1	C	762	GLN
1	C	764	ASN
1	C	787	GLN
1	C	824	ASN
1	C	856	ASN
1	C	901	GLN
1	C	914	ASN
1	C	926	GLN
1	C	949	GLN
1	C	969	ASN
1	C	992	GLN
1	C	1010	GLN
1	C	1054	GLN
1	C	1125	ASN
2	D	24	GLN
2	D	58	ASN
2	D	63	ASN
2	D	96	GLN
2	D	117	ASN
2	D	121	ASN
2	D	175	GLN
2	D	277	ASN
2	D	300	GLN
2	D	417	HIS
2	D	508	ASN
2	D	572	ASN
2	D	586	ASN
2	D	599	ASN
2	E	24	GLN
2	E	58	ASN
2	E	96	GLN
2	E	117	ASN
2	E	121	ASN

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Mol	Chain	Res	Type
2	E	175	GLN
2	E	277	ASN
2	E	300	GLN
2	E	417	HIS
2	E	508	ASN
2	E	572	ASN
2	E	586	ASN
2	E	599	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

64 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	NAG	F	1	1,3	14,14,15	0.51	0	17,19,21	0.51	0
3	NAG	F	2	3	14,14,15	0.25	0	17,19,21	0.61	0
3	NAG	G	1	1,3	14,14,15	0.55	0	17,19,21	0.58	0
3	NAG	G	2	3	14,14,15	0.30	0	17,19,21	0.47	0
3	NAG	H	1	1,3	14,14,15	0.30	0	17,19,21	0.42	0
3	NAG	H	2	3	14,14,15	0.40	0	17,19,21	0.38	0
3	NAG	I	1	1,3	14,14,15	0.36	0	17,19,21	1.17	1 (5%)
3	NAG	I	2	3	14,14,15	0.25	0	17,19,21	0.49	0
3	NAG	J	1	1,3	14,14,15	0.31	0	17,19,21	0.71	1 (5%)
3	NAG	J	2	3	14,14,15	0.21	0	17,19,21	0.41	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	K	1	1,3	14,14,15	0.70	1 (7%)	17,19,21	0.91	1 (5%)
3	NAG	K	2	3	14,14,15	0.35	0	17,19,21	0.72	1 (5%)
3	NAG	L	1	1,3	14,14,15	0.20	0	17,19,21	0.45	0
3	NAG	L	2	3	14,14,15	0.27	0	17,19,21	0.39	0
3	NAG	M	1	1,3	14,14,15	0.52	0	17,19,21	0.52	0
3	NAG	M	2	3	14,14,15	0.26	0	17,19,21	0.61	0
3	NAG	N	1	1,3	14,14,15	0.57	0	17,19,21	0.58	0
3	NAG	N	2	3	14,14,15	0.29	0	17,19,21	0.48	0
3	NAG	O	1	1,3	14,14,15	0.23	0	17,19,21	1.45	2 (11%)
3	NAG	O	2	3	14,14,15	0.19	0	17,19,21	0.53	0
3	NAG	P	1	1,3	14,14,15	0.52	0	17,19,21	0.73	1 (5%)
3	NAG	P	2	3	14,14,15	0.38	0	17,19,21	0.48	0
3	NAG	Q	1	1,3	14,14,15	0.40	0	17,19,21	0.40	0
3	NAG	Q	2	3	14,14,15	0.19	0	17,19,21	0.77	0
3	NAG	R	1	1,3	14,14,15	0.36	0	17,19,21	0.49	0
3	NAG	R	2	3	14,14,15	0.58	0	17,19,21	1.38	2 (11%)
3	NAG	S	1	1,3	14,14,15	0.63	1 (7%)	17,19,21	0.45	0
3	NAG	S	2	3	14,14,15	0.34	0	17,19,21	1.43	2 (11%)
3	NAG	T	1	1,3	14,14,15	0.38	0	17,19,21	0.46	0
3	NAG	T	2	3	14,14,15	0.24	0	17,19,21	0.50	0
3	NAG	U	1	1,3	14,14,15	0.52	0	17,19,21	0.51	0
3	NAG	U	2	3	14,14,15	0.24	0	17,19,21	0.61	0
3	NAG	V	1	1,3	14,14,15	0.57	1 (7%)	17,19,21	0.58	0
3	NAG	V	2	3	14,14,15	0.29	0	17,19,21	0.48	0
3	NAG	W	1	1,3	14,14,15	0.31	0	17,19,21	0.64	1 (5%)
3	NAG	W	2	3	14,14,15	0.51	0	17,19,21	0.48	0
3	NAG	X	1	1,3	14,14,15	0.37	0	17,19,21	0.74	0
3	NAG	X	2	3	14,14,15	0.29	0	17,19,21	1.40	2 (11%)
3	NAG	Y	1	1,3	14,14,15	0.67	1 (7%)	17,19,21	0.71	0
3	NAG	Y	2	3	14,14,15	0.42	0	17,19,21	1.48	3 (17%)
3	NAG	Z	1	1,3	14,14,15	0.66	1 (7%)	17,19,21	0.67	0
3	NAG	Z	2	3	14,14,15	0.28	0	17,19,21	0.67	0
3	NAG	a	1	1,3	14,14,15	0.24	0	17,19,21	0.70	1 (5%)
3	NAG	a	2	3	14,14,15	0.17	0	17,19,21	0.50	0
3	NAG	b	1	2,3	14,14,15	0.59	1 (7%)	17,19,21	0.74	0
3	NAG	b	2	3	14,14,15	0.55	0	17,19,21	0.38	0
3	NAG	c	1	2,3	14,14,15	0.41	0	17,19,21	0.67	0
3	NAG	c	2	3	14,14,15	0.28	0	17,19,21	0.71	1 (5%)
3	NAG	d	1	2,3	14,14,15	0.29	0	17,19,21	0.57	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	d	2	3	14,14,15	0.30	0	17,19,21	0.58	0
3	NAG	e	1	2,3	14,14,15	0.31	0	17,19,21	0.53	0
3	NAG	e	2	3	14,14,15	0.36	0	17,19,21	0.49	0
3	NAG	f	1	2,3	14,14,15	0.22	0	17,19,21	0.64	0
3	NAG	f	2	3	14,14,15	0.35	0	17,19,21	0.60	1 (5%)
3	NAG	g	1	2,3	14,14,15	0.59	1 (7%)	17,19,21	0.74	0
3	NAG	g	2	3	14,14,15	0.56	0	17,19,21	0.39	0
3	NAG	h	1	2,3	14,14,15	0.40	0	17,19,21	0.67	0
3	NAG	h	2	3	14,14,15	0.28	0	17,19,21	0.70	1 (5%)
3	NAG	i	1	2,3	14,14,15	0.29	0	17,19,21	0.57	0
3	NAG	i	2	3	14,14,15	0.29	0	17,19,21	0.57	0
3	NAG	j	1	2,3	14,14,15	0.32	0	17,19,21	0.54	0
3	NAG	j	2	3	14,14,15	0.37	0	17,19,21	0.49	0
3	NAG	k	1	2,3	14,14,15	0.23	0	17,19,21	0.62	0
3	NAG	k	2	3	14,14,15	0.34	0	17,19,21	0.61	1 (5%)

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

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	N	2	3	-	3/6/23/26	0/1/1/1
3	NAG	O	1	1,3	-	6/6/23/26	0/1/1/1
3	NAG	O	2	3	-	2/6/23/26	0/1/1/1
3	NAG	P	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	P	2	3	-	2/6/23/26	0/1/1/1
3	NAG	Q	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	Q	2	3	-	2/6/23/26	0/1/1/1
3	NAG	R	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	R	2	3	-	6/6/23/26	0/1/1/1
3	NAG	S	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	S	2	3	-	5/6/23/26	0/1/1/1
3	NAG	T	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	T	2	3	-	2/6/23/26	0/1/1/1
3	NAG	U	1	1,3	-	1/6/23/26	0/1/1/1
3	NAG	U	2	3	-	2/6/23/26	0/1/1/1
3	NAG	V	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	V	2	3	-	3/6/23/26	0/1/1/1
3	NAG	W	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	W	2	3	-	2/6/23/26	0/1/1/1
3	NAG	X	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	X	2	3	-	4/6/23/26	0/1/1/1
3	NAG	Y	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	Y	2	3	-	6/6/23/26	0/1/1/1
3	NAG	Z	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	Z	2	3	-	4/6/23/26	0/1/1/1
3	NAG	a	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	a	2	3	-	0/6/23/26	0/1/1/1
3	NAG	b	1	2,3	-	2/6/23/26	0/1/1/1
3	NAG	b	2	3	-	2/6/23/26	0/1/1/1
3	NAG	c	1	2,3	-	2/6/23/26	0/1/1/1
3	NAG	c	2	3	-	2/6/23/26	0/1/1/1
3	NAG	d	1	2,3	-	2/6/23/26	0/1/1/1
3	NAG	d	2	3	-	3/6/23/26	0/1/1/1
3	NAG	e	1	2,3	-	0/6/23/26	0/1/1/1
3	NAG	e	2	3	-	0/6/23/26	0/1/1/1
3	NAG	f	1	2,3	-	0/6/23/26	0/1/1/1

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

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	K	1	NAG	O5-C1	-2.53	1.39	1.43
3	Z	1	NAG	O5-C1	-2.41	1.39	1.43
3	Y	1	NAG	O5-C1	-2.19	1.40	1.43
3	g	1	NAG	O5-C1	-2.05	1.40	1.43
3	S	1	NAG	O5-C1	-2.05	1.40	1.43
3	b	1	NAG	O5-C1	-2.04	1.40	1.43
3	V	1	NAG	O5-C1	-2.01	1.40	1.43

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	O	1	NAG	C2-N2-C7	4.99	129.59	122.90
3	Y	2	NAG	C2-N2-C7	4.67	129.16	122.90
3	S	2	NAG	C2-N2-C7	4.61	129.08	122.90
3	R	2	NAG	C2-N2-C7	4.57	129.03	122.90
3	X	2	NAG	C2-N2-C7	4.53	128.97	122.90
3	I	1	NAG	C1-O5-C5	3.37	116.70	112.19
3	Y	2	NAG	C1-C2-N2	2.61	114.55	110.43
3	X	2	NAG	C1-C2-N2	2.59	114.52	110.43
3	c	2	NAG	C1-O5-C5	2.50	115.53	112.19
3	h	2	NAG	C1-O5-C5	2.46	115.49	112.19
3	S	2	NAG	C1-C2-N2	2.44	114.28	110.43
3	K	1	NAG	O4-C4-C3	-2.35	104.84	110.38
3	P	1	NAG	C1-O5-C5	2.33	115.31	112.19
3	J	1	NAG	C1-O5-C5	2.32	115.29	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	O	1	NAG	C1-C2-N2	2.14	113.80	110.43
3	Y	2	NAG	C1-O5-C5	2.11	115.01	112.19
3	a	1	NAG	C1-O5-C5	2.10	115.00	112.19
3	k	2	NAG	C1-O5-C5	2.09	114.98	112.19
3	K	2	NAG	C1-O5-C5	2.06	114.95	112.19
3	f	2	NAG	C1-O5-C5	2.06	114.94	112.19
3	R	2	NAG	C1-C2-N2	2.04	113.65	110.43
3	W	1	NAG	C1-O5-C5	2.01	114.89	112.19

There are no chirality outliers.

All (121) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	d	1	NAG	C8-C7-N2-C2
3	d	1	NAG	O7-C7-N2-C2
3	d	2	NAG	C3-C2-N2-C7
3	d	2	NAG	C8-C7-N2-C2
3	d	2	NAG	O7-C7-N2-C2
3	i	1	NAG	C8-C7-N2-C2
3	i	1	NAG	O7-C7-N2-C2
3	i	2	NAG	C3-C2-N2-C7
3	i	2	NAG	C8-C7-N2-C2
3	i	2	NAG	O7-C7-N2-C2
3	O	2	NAG	O5-C5-C6-O6
3	Q	1	NAG	O5-C5-C6-O6
3	P	2	NAG	O5-C5-C6-O6
3	F	2	NAG	O5-C5-C6-O6
3	K	1	NAG	O5-C5-C6-O6
3	M	2	NAG	O5-C5-C6-O6
3	U	2	NAG	O5-C5-C6-O6
3	Z	1	NAG	O5-C5-C6-O6
3	f	2	NAG	O5-C5-C6-O6
3	k	2	NAG	O5-C5-C6-O6
3	b	1	NAG	O5-C5-C6-O6
3	g	1	NAG	O5-C5-C6-O6
3	c	2	NAG	O5-C5-C6-O6
3	h	2	NAG	O5-C5-C6-O6
3	F	2	NAG	C4-C5-C6-O6
3	K	1	NAG	C4-C5-C6-O6
3	M	2	NAG	C4-C5-C6-O6
3	U	2	NAG	C4-C5-C6-O6
3	P	1	NAG	O5-C5-C6-O6

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

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

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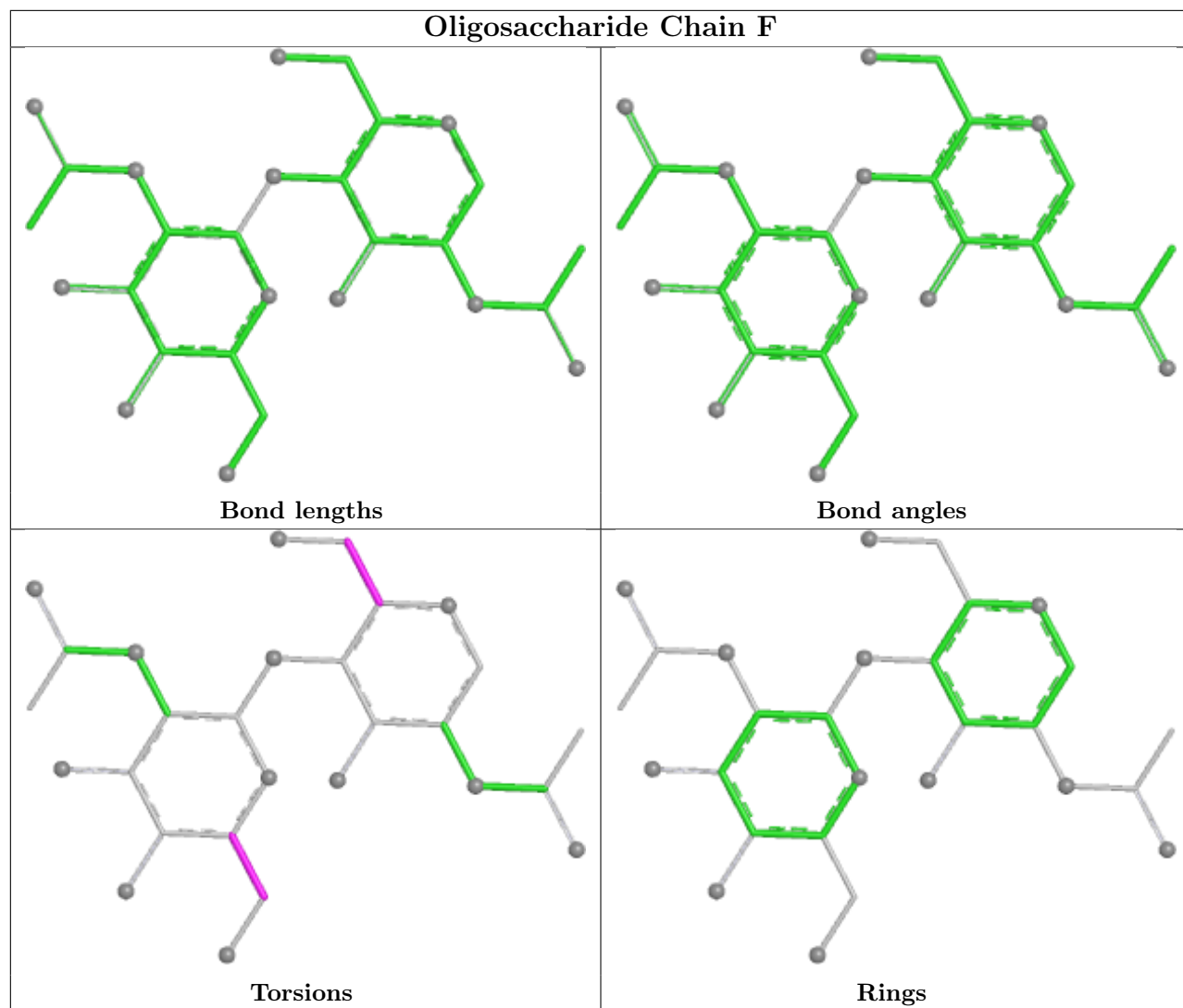
Mol	Chain	Res	Type	Atoms
3	Y	2	NAG	C3-C2-N2-C7
3	V	2	NAG	C4-C5-C6-O6
3	G	2	NAG	C4-C5-C6-O6
3	N	2	NAG	C4-C5-C6-O6
3	J	1	NAG	O5-C5-C6-O6
3	V	2	NAG	O5-C5-C6-O6
3	N	2	NAG	O5-C5-C6-O6
3	G	2	NAG	O5-C5-C6-O6

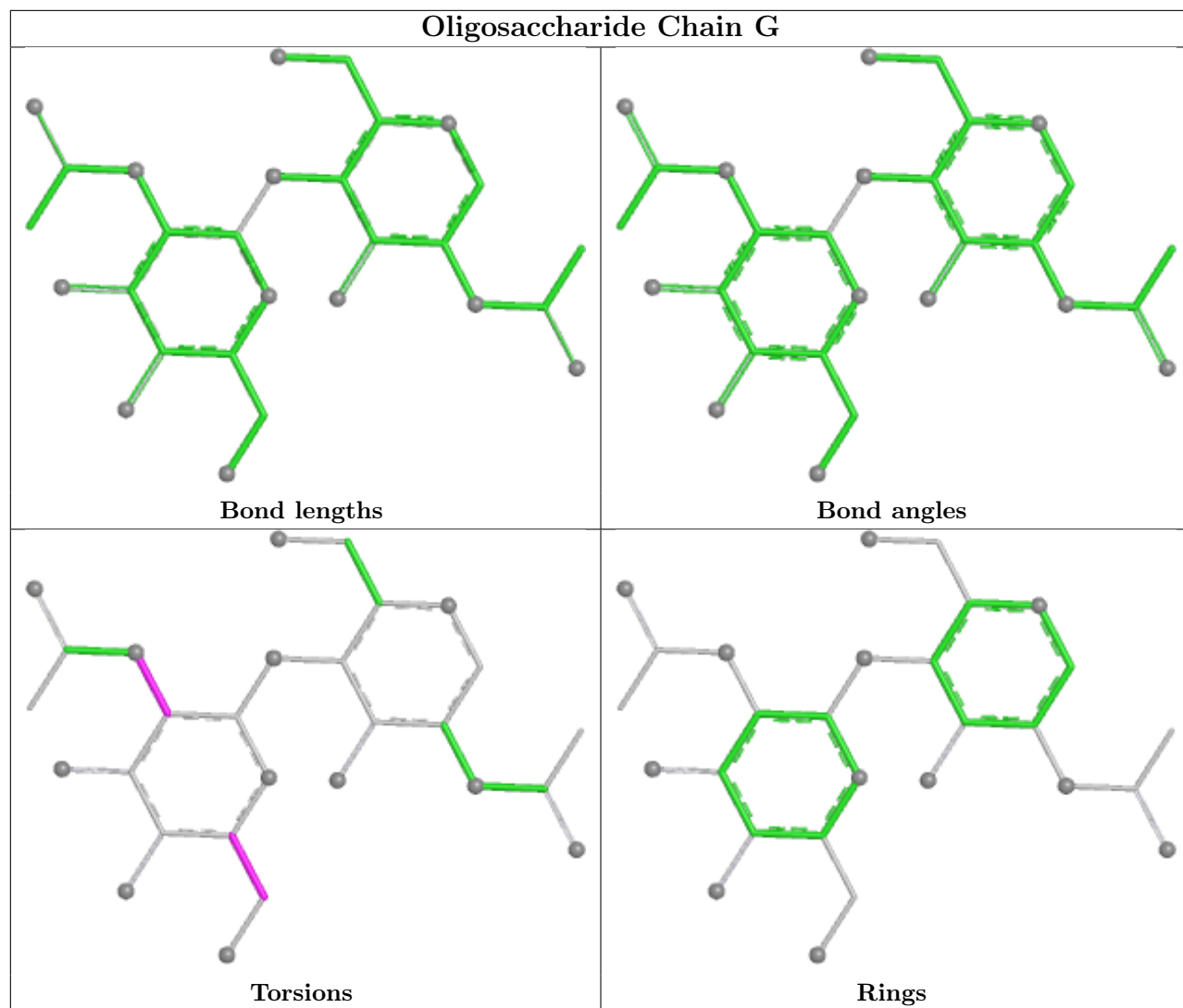
There are no ring outliers.

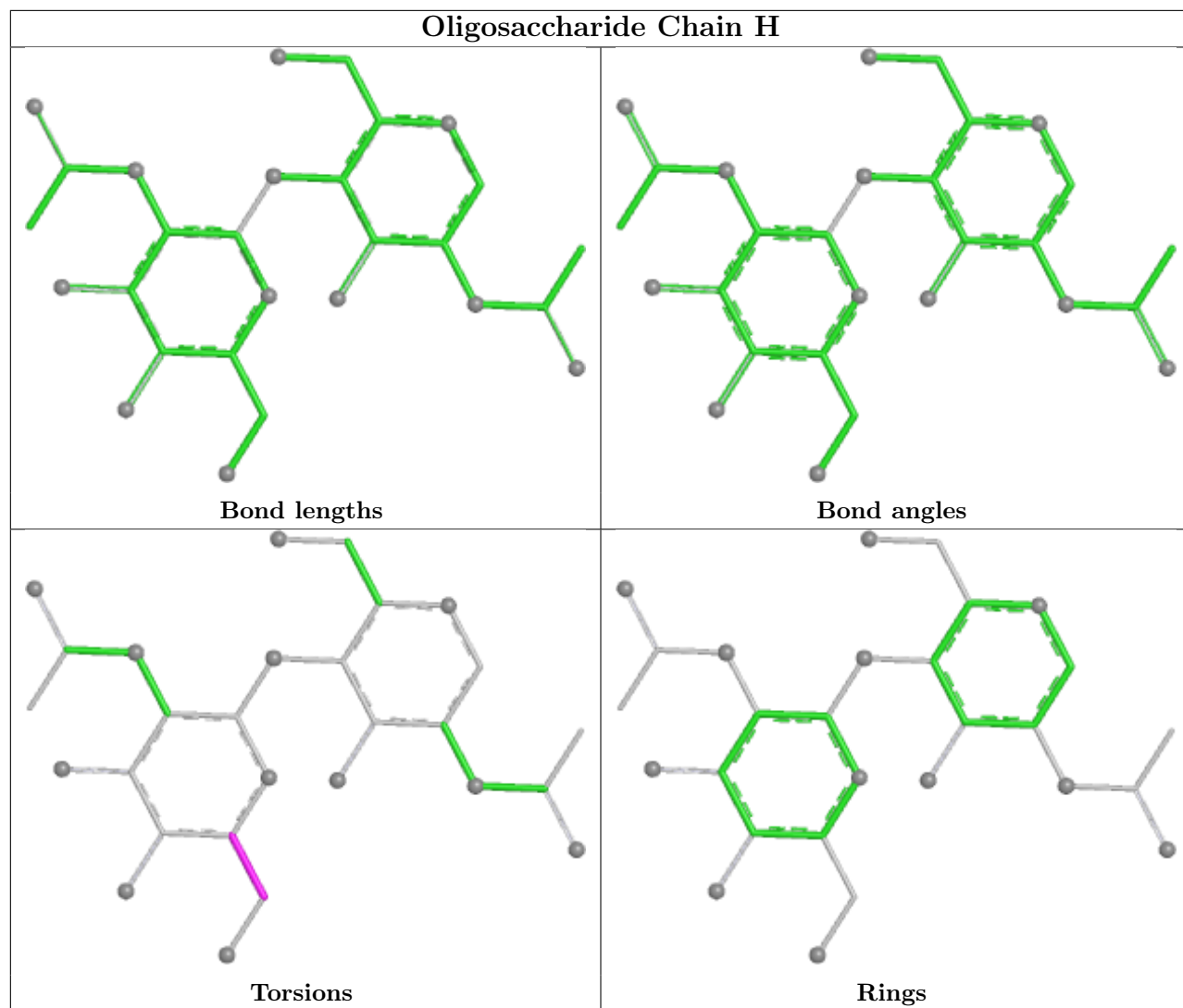
20 monomers are involved in 29 short contacts:

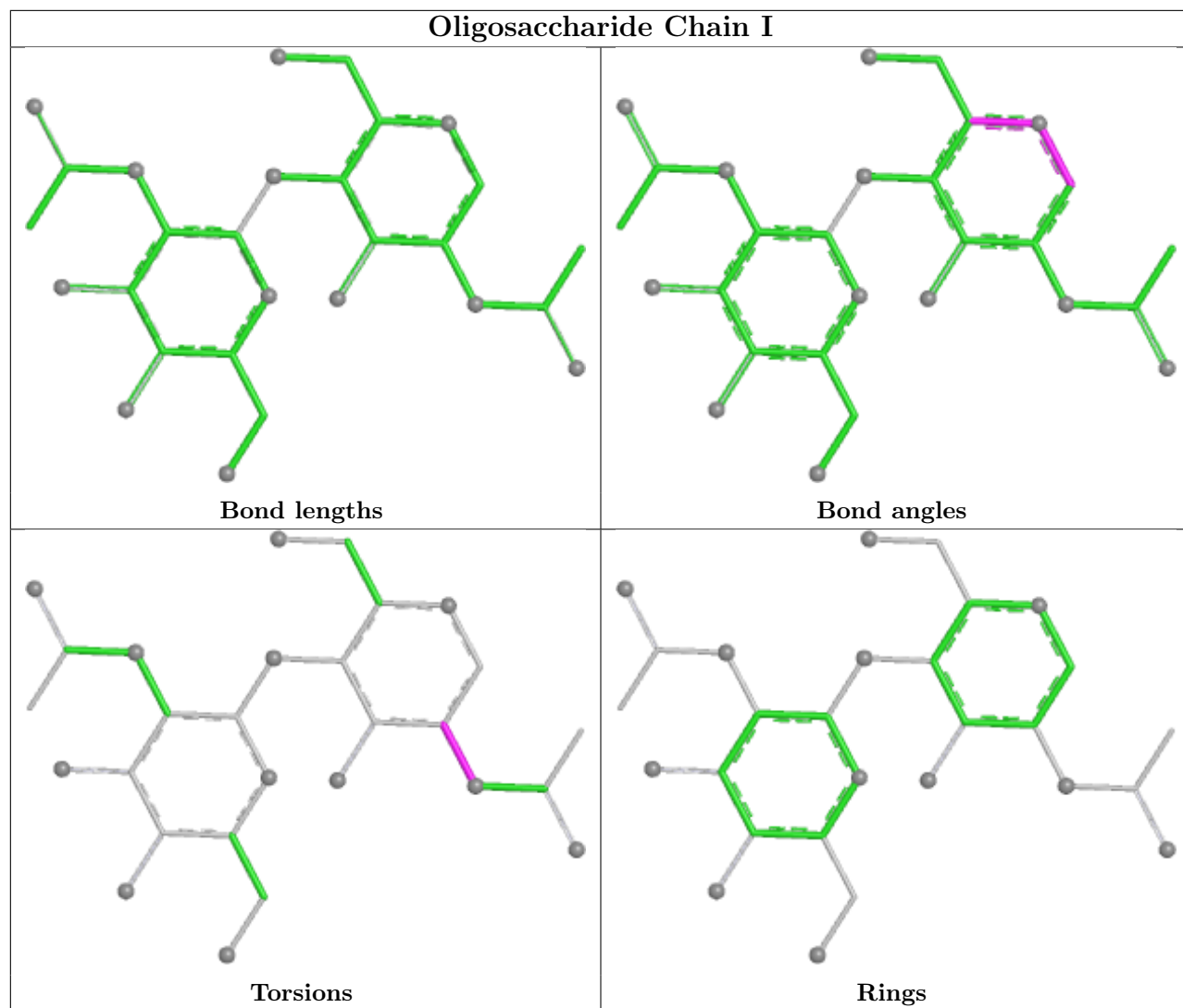
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	N	1	NAG	4	0
3	K	1	NAG	1	0
3	R	2	NAG	1	0
3	S	2	NAG	1	0
3	d	2	NAG	6	0
3	i	1	NAG	3	0
3	X	2	NAG	1	0
3	Y	2	NAG	1	0
3	V	1	NAG	3	0
3	V	2	NAG	2	0
3	i	2	NAG	5	0
3	O	1	NAG	1	0
3	F	2	NAG	1	0
3	G	2	NAG	2	0
3	G	1	NAG	3	0
3	F	1	NAG	1	0
3	S	1	NAG	1	0
3	N	2	NAG	2	0
3	d	1	NAG	4	0
3	K	2	NAG	1	0

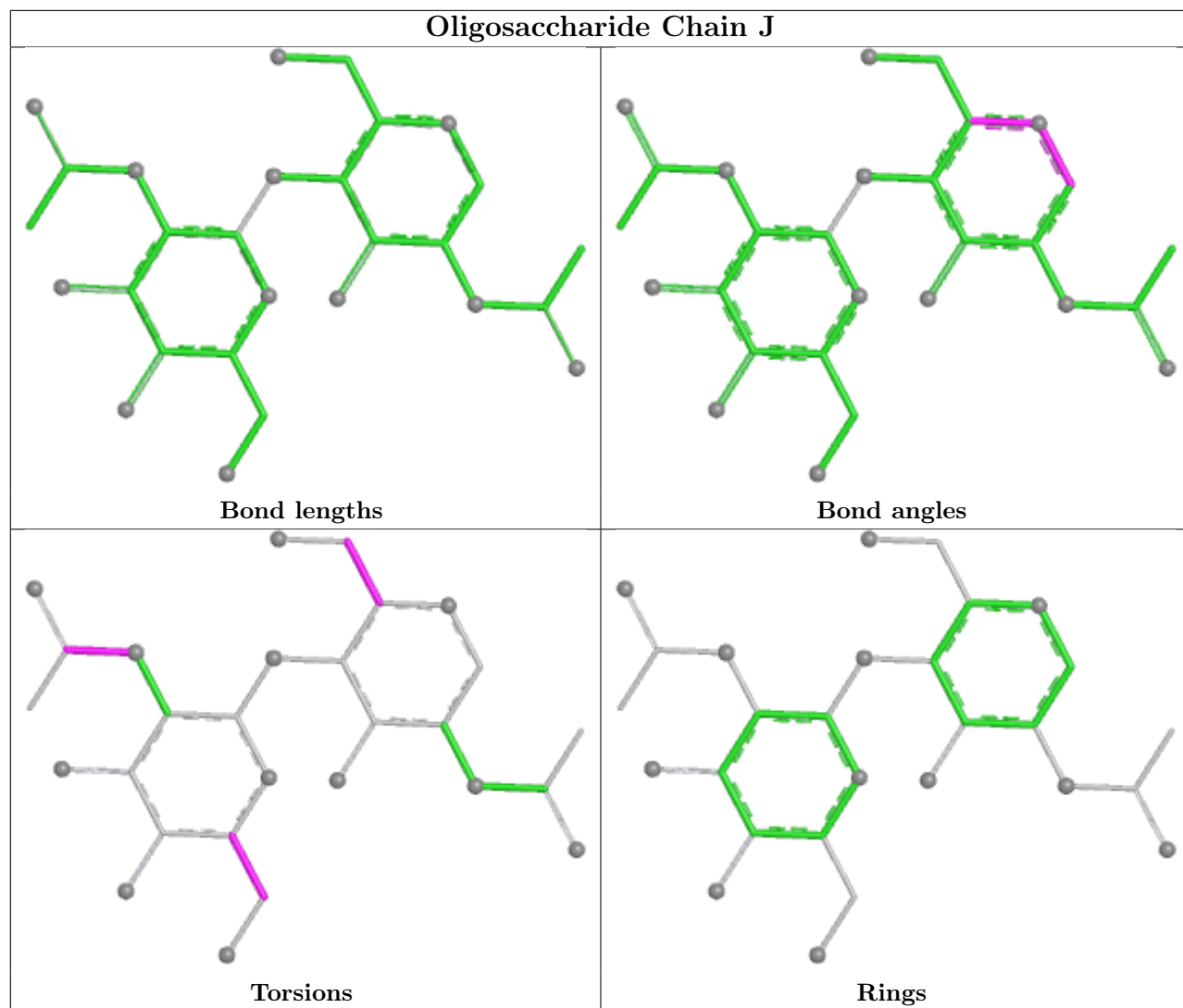
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

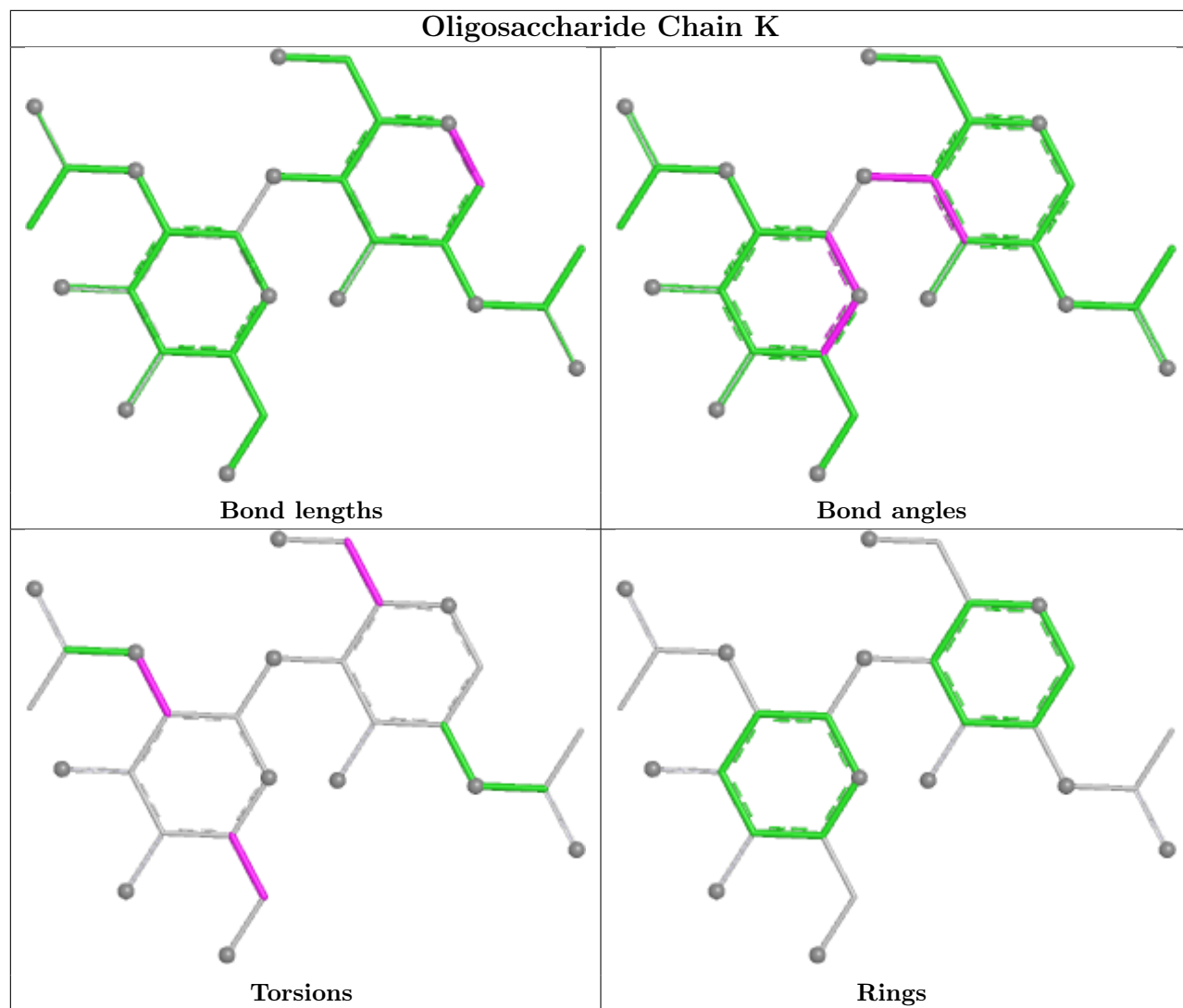


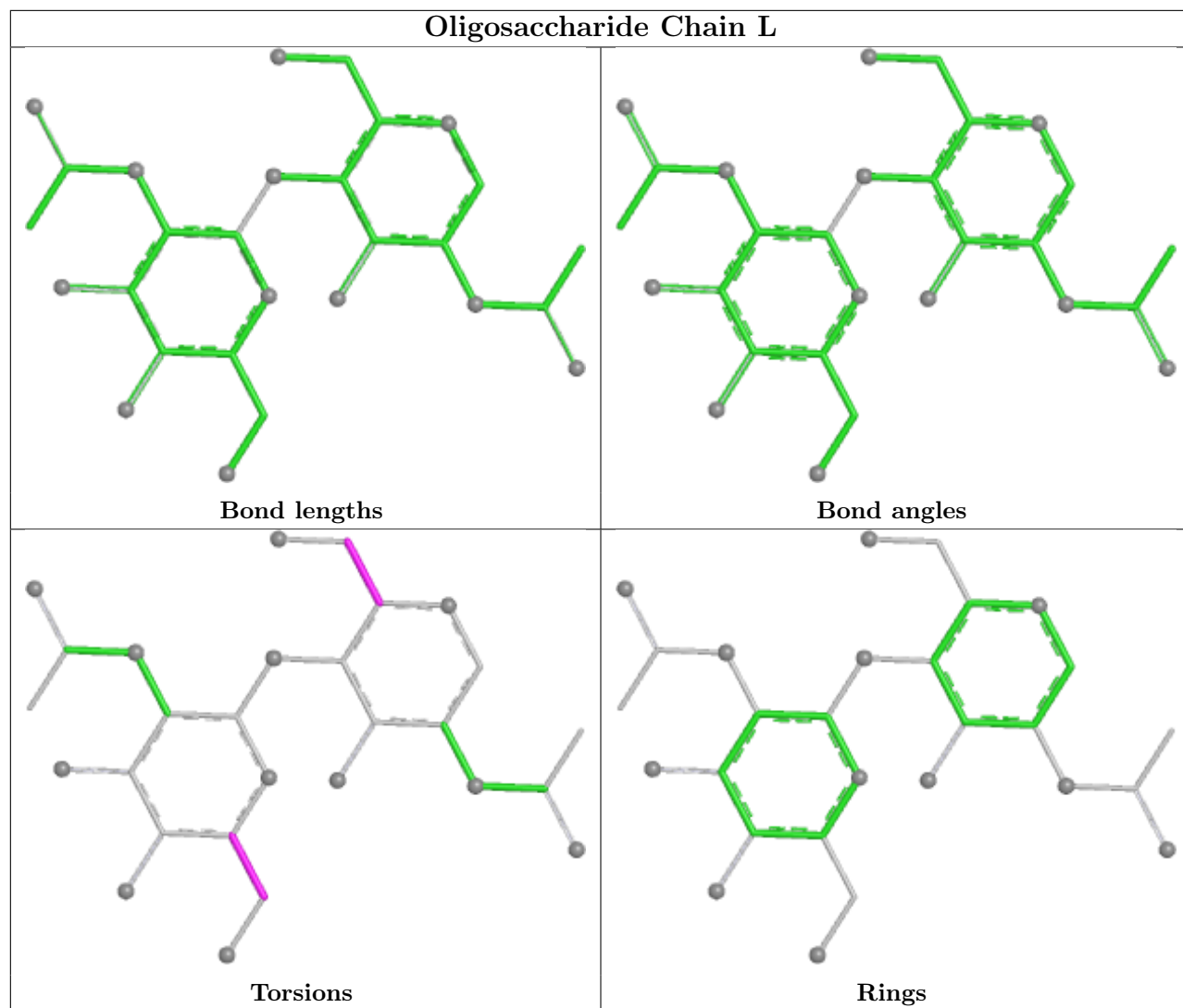


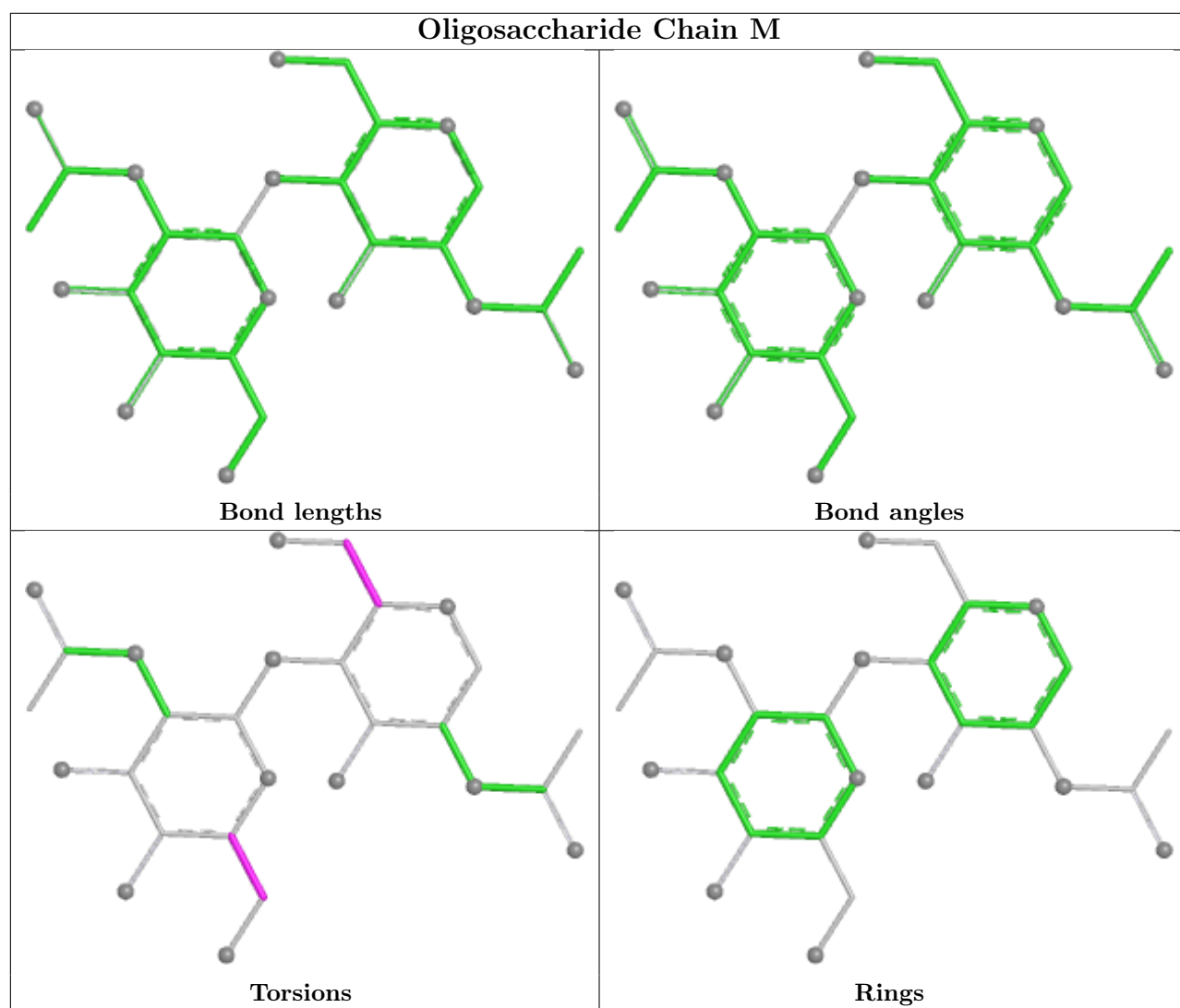


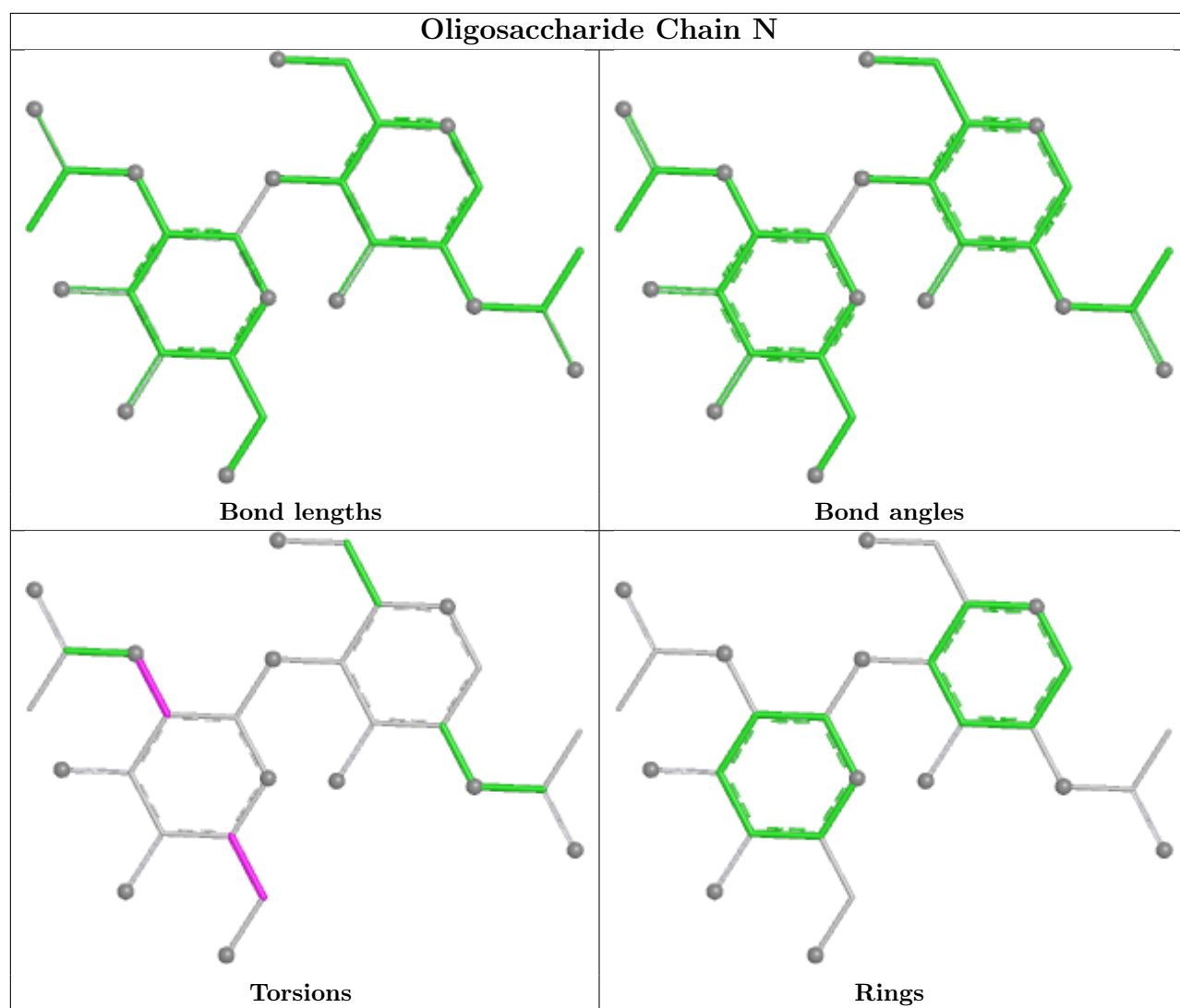


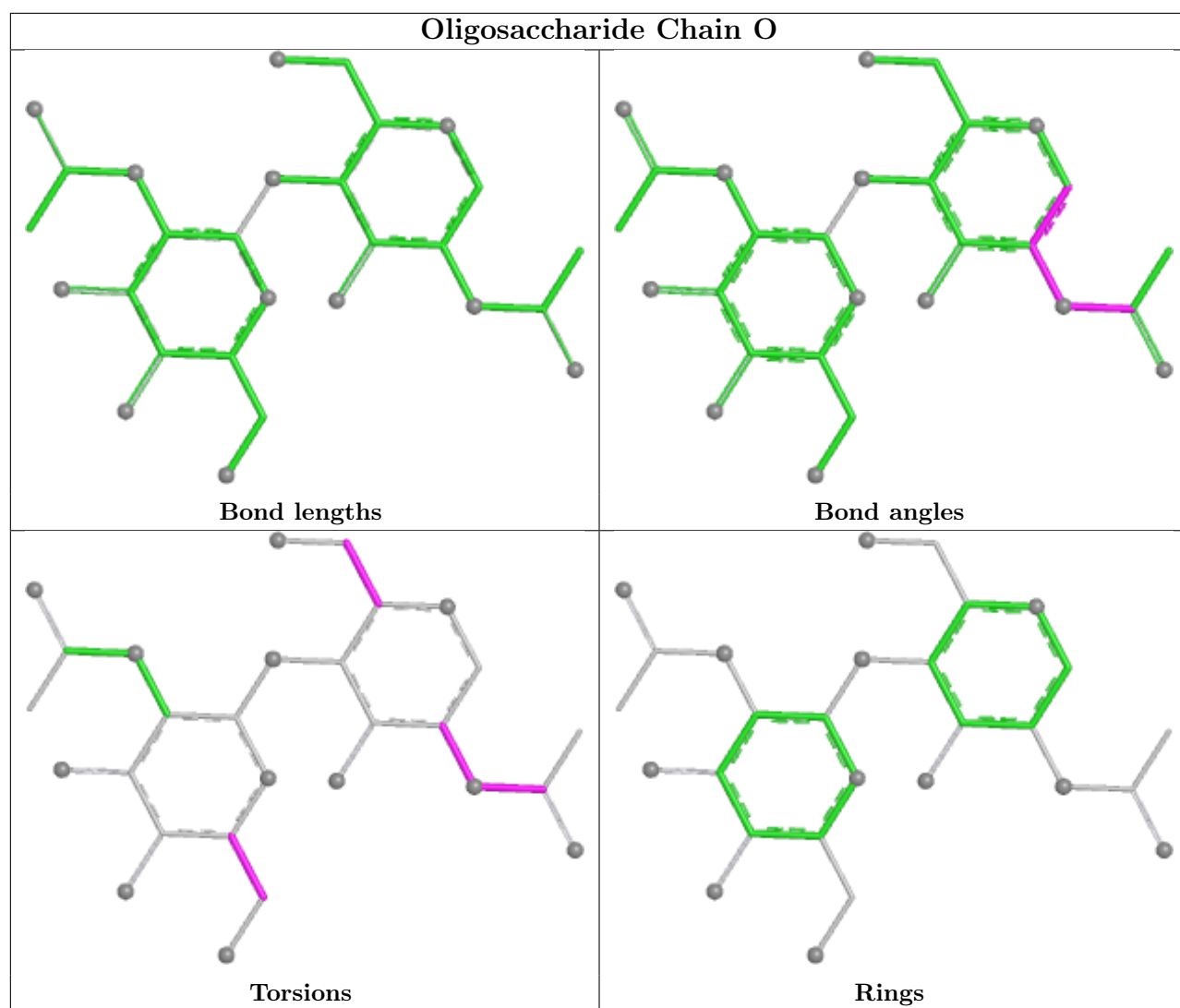


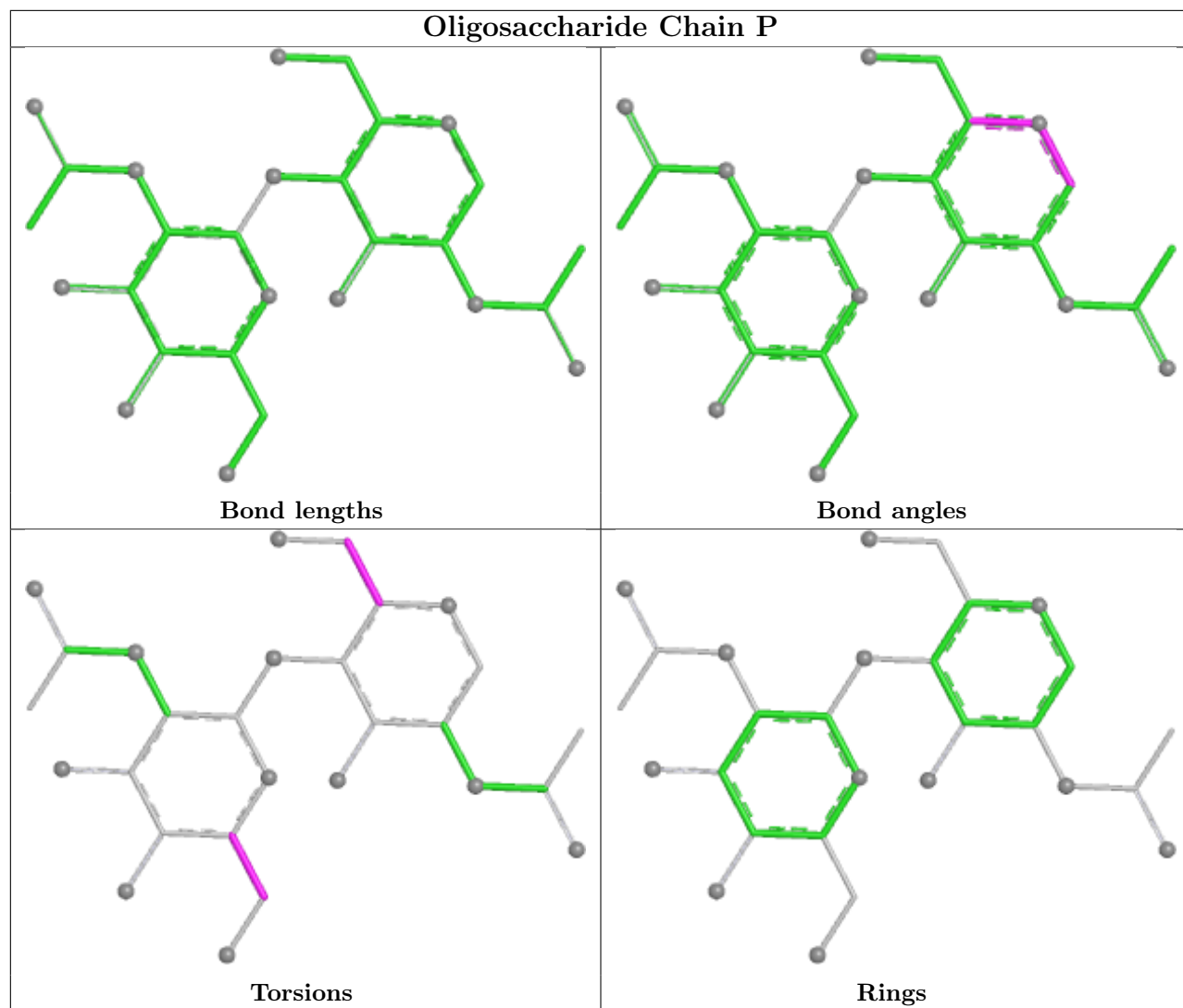


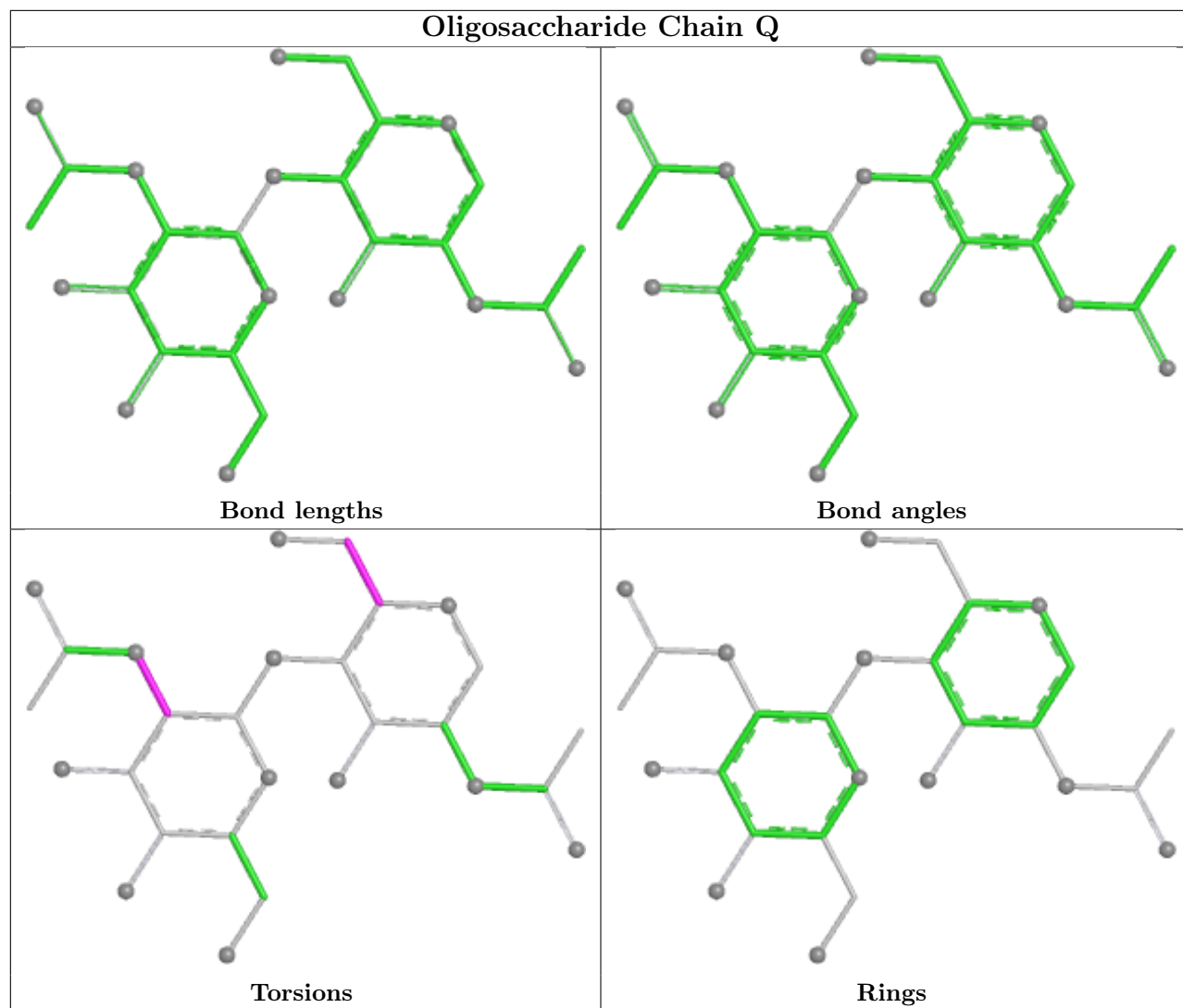


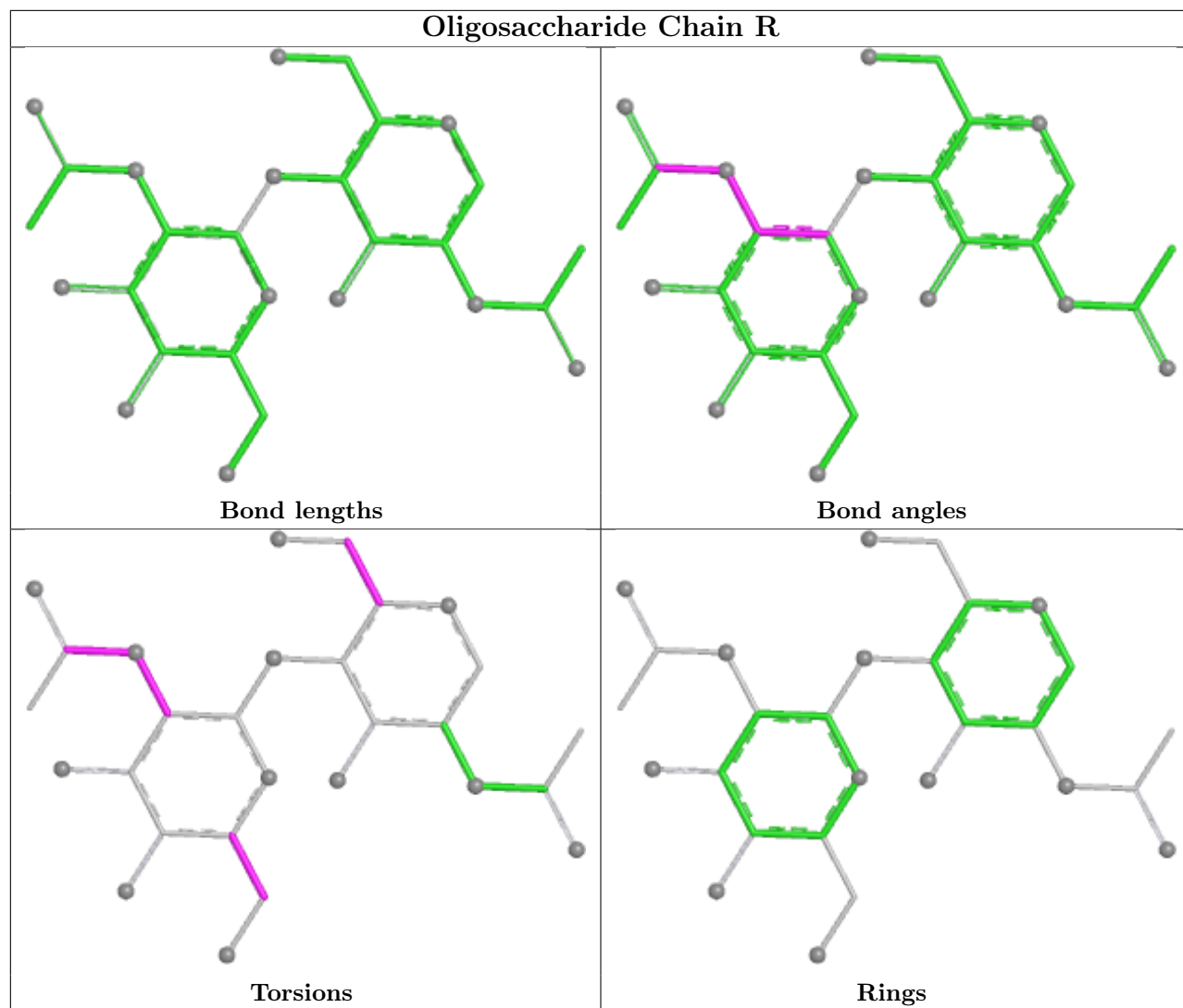


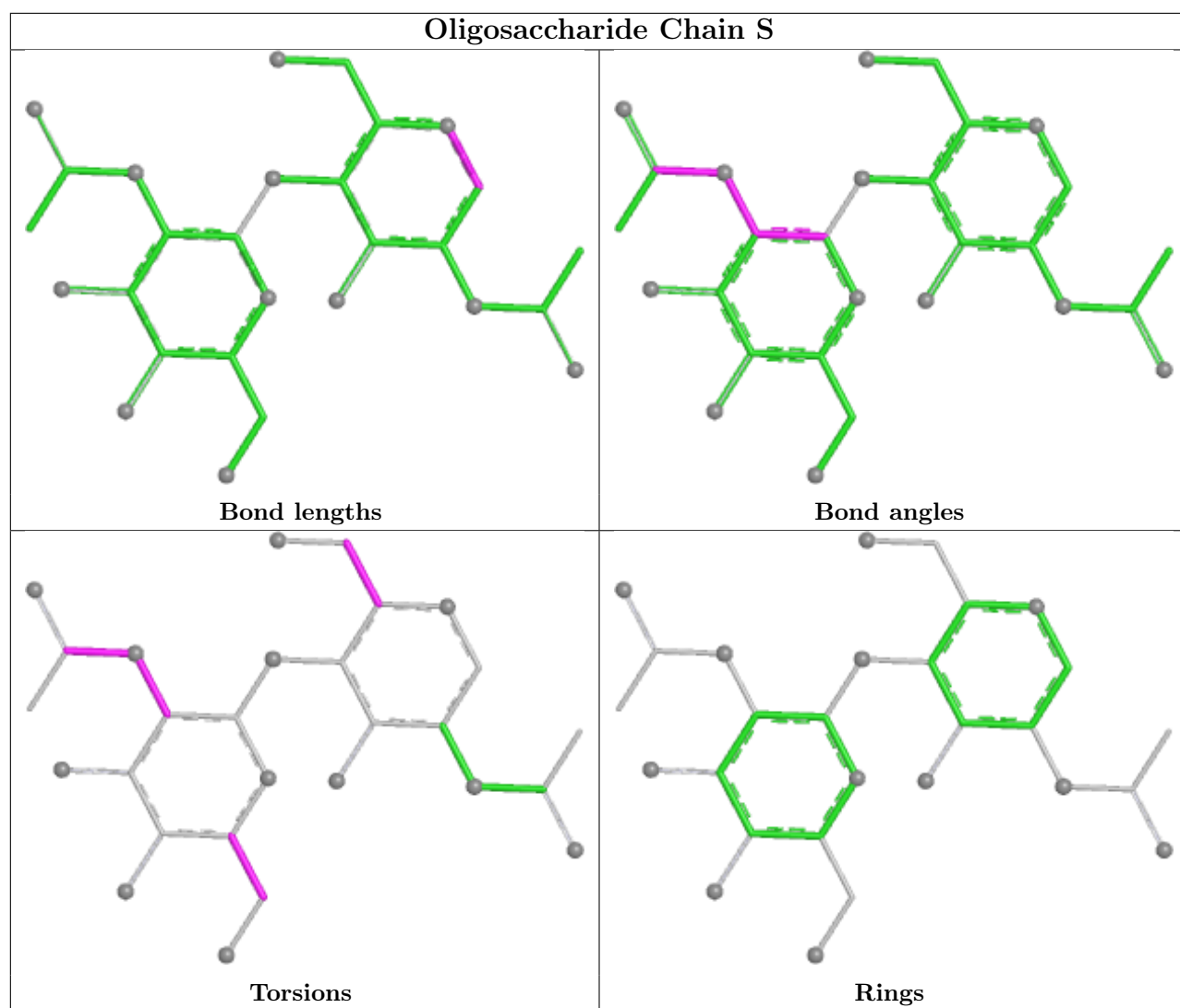


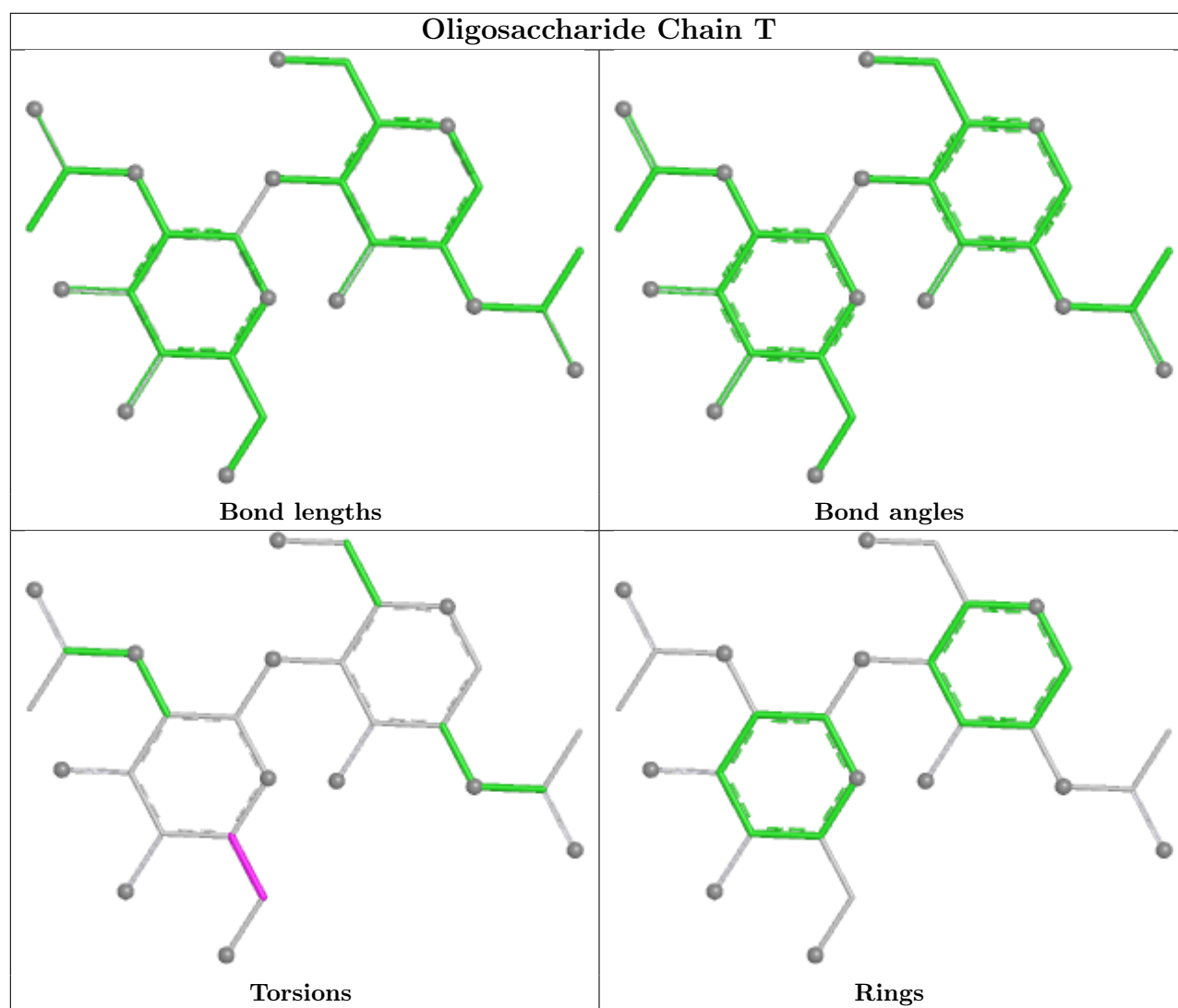


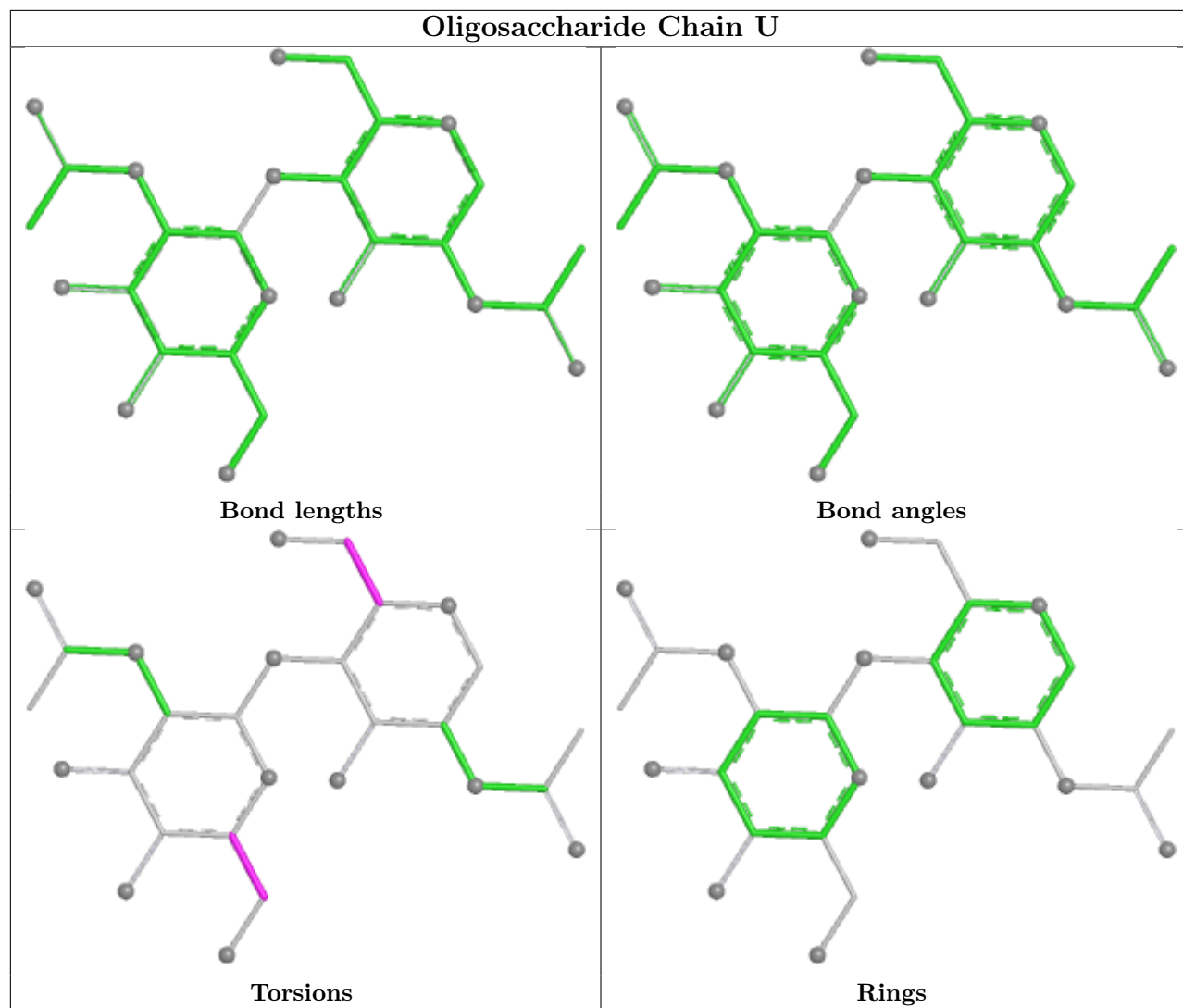


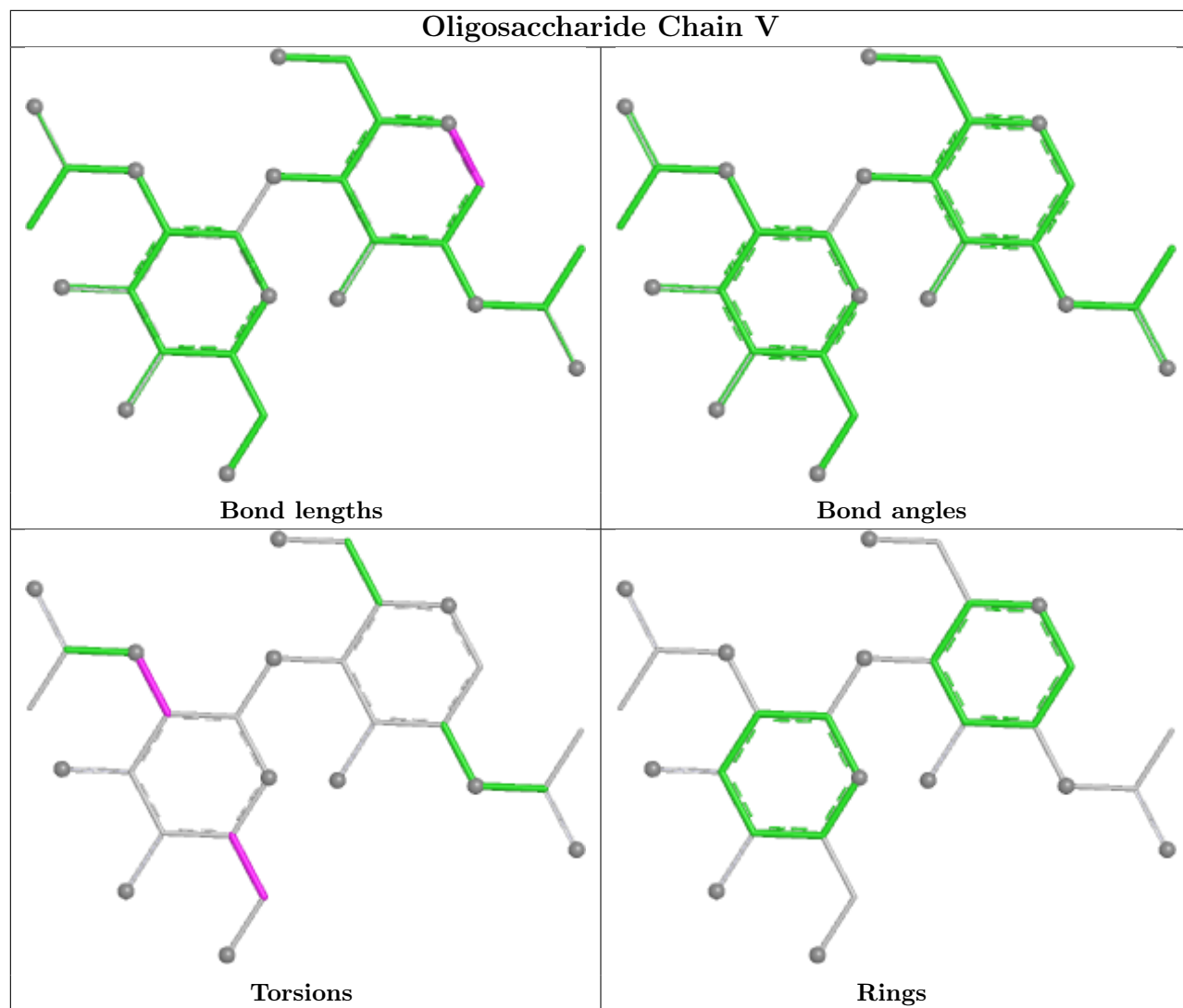


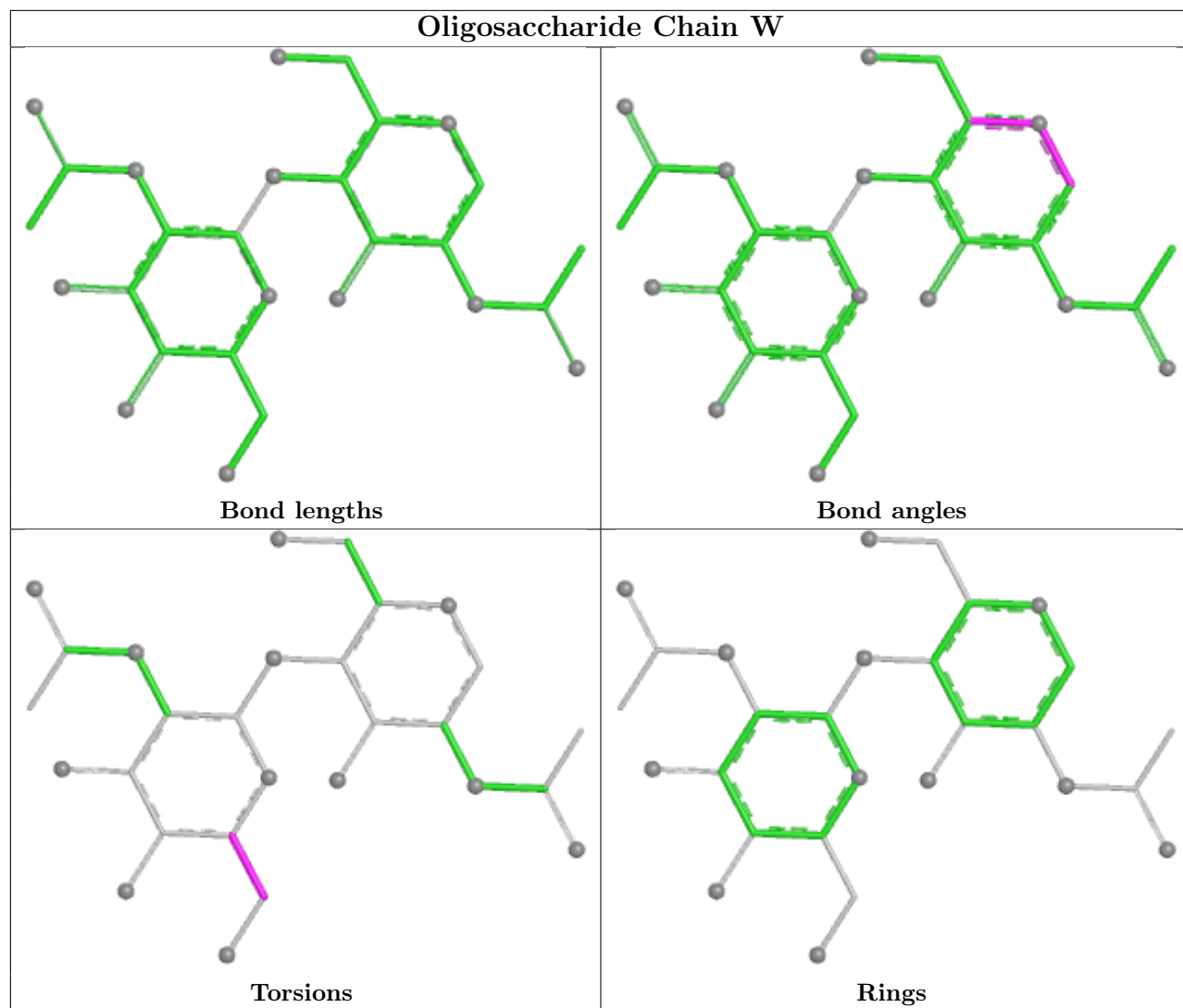


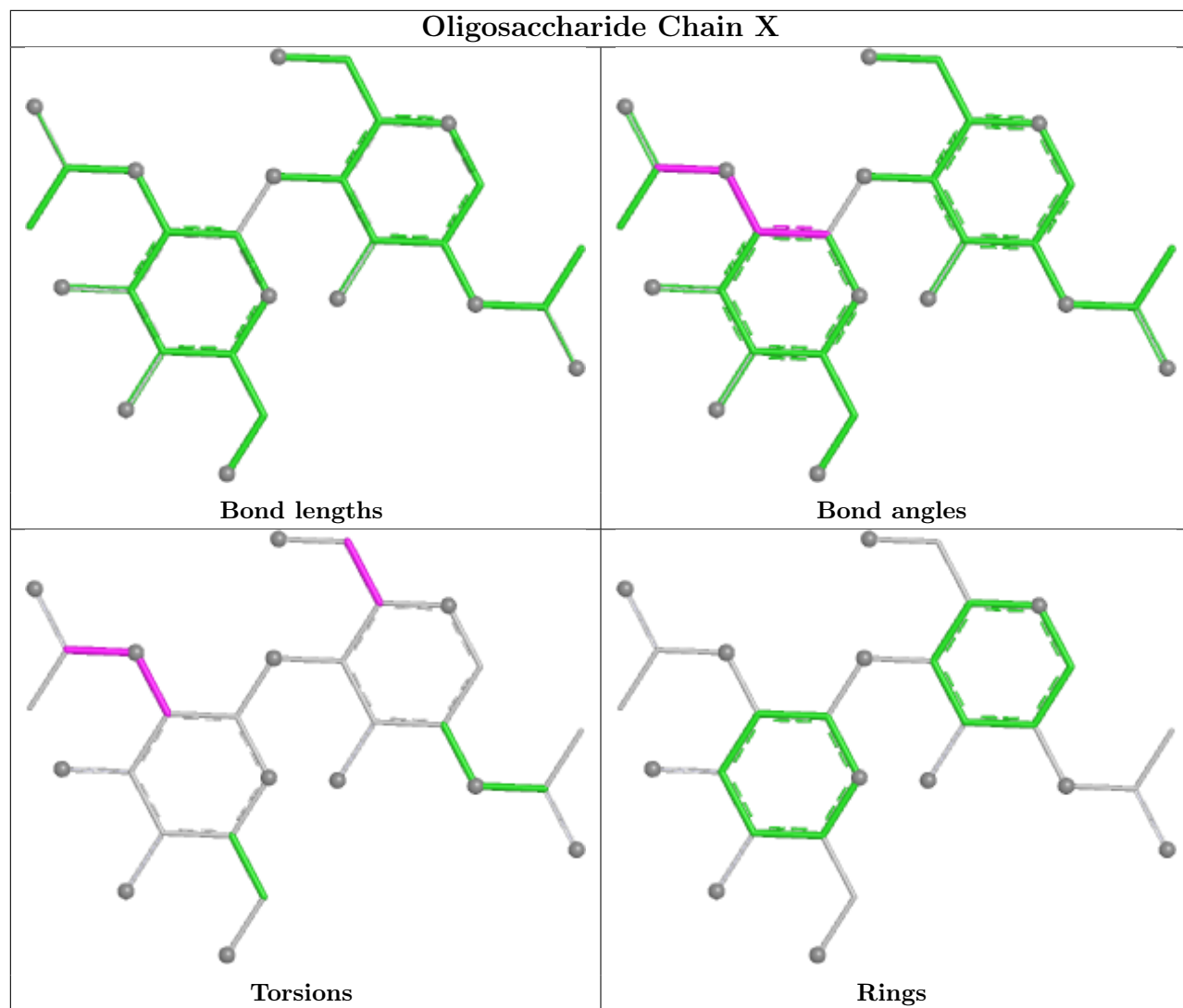


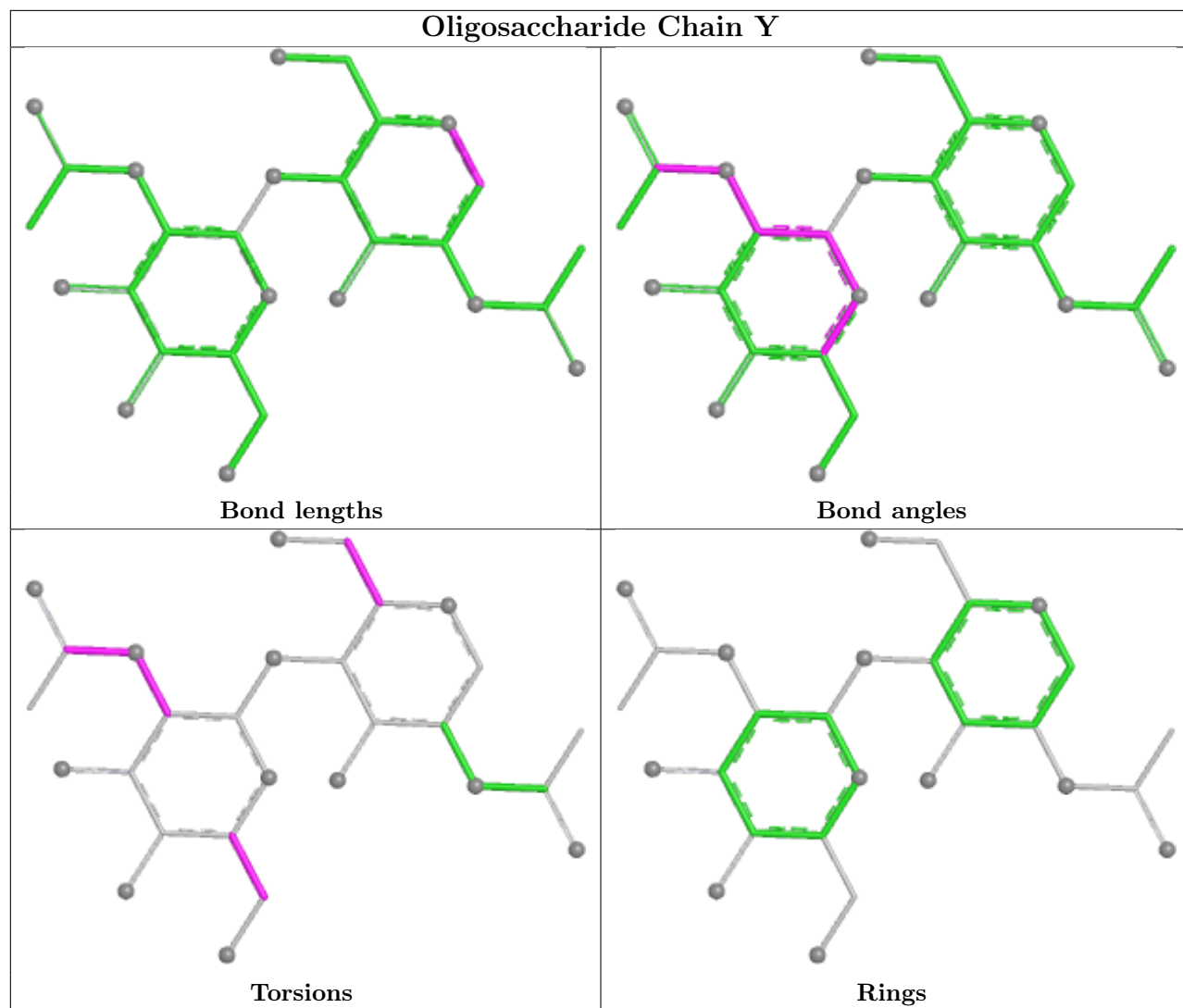


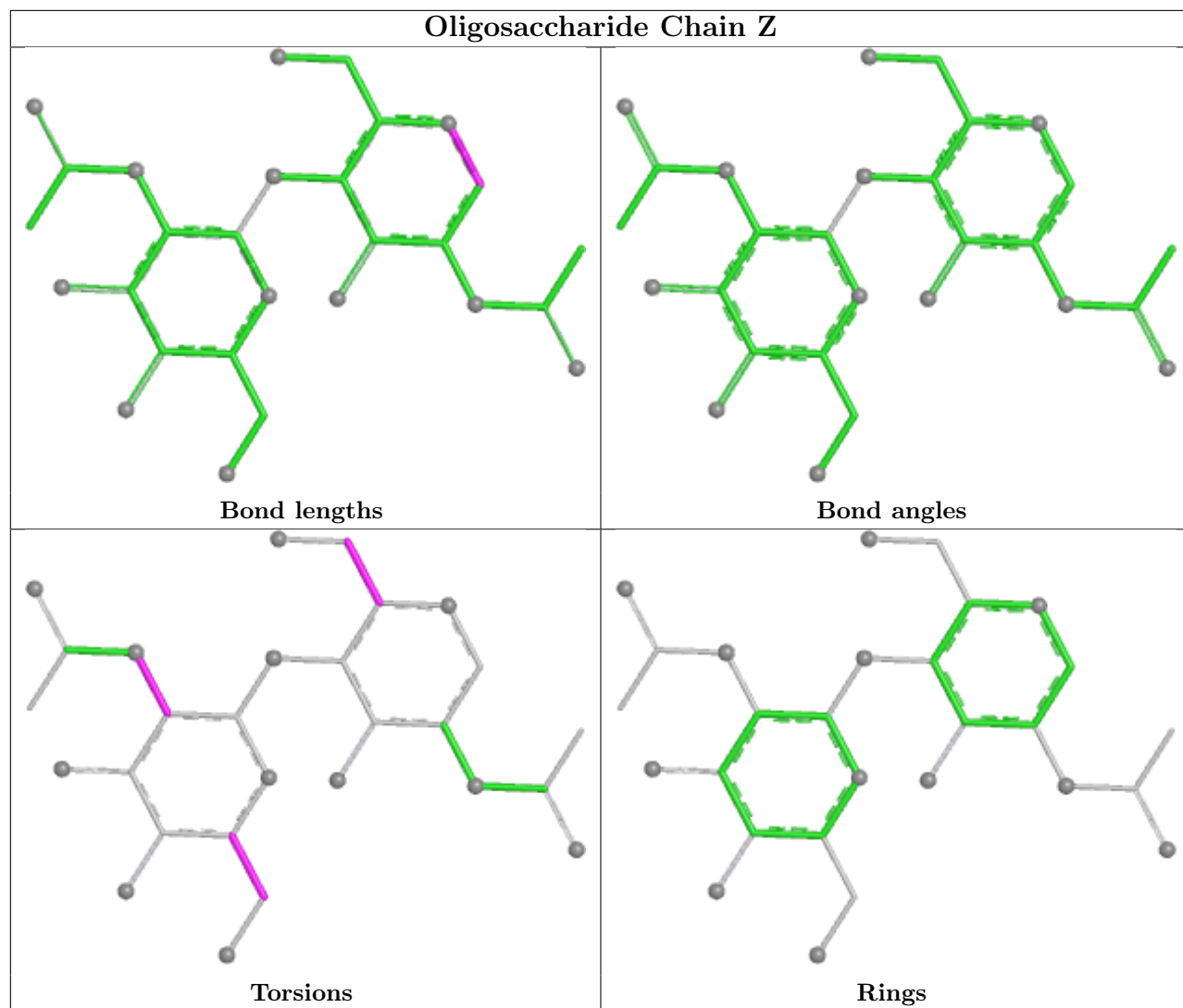


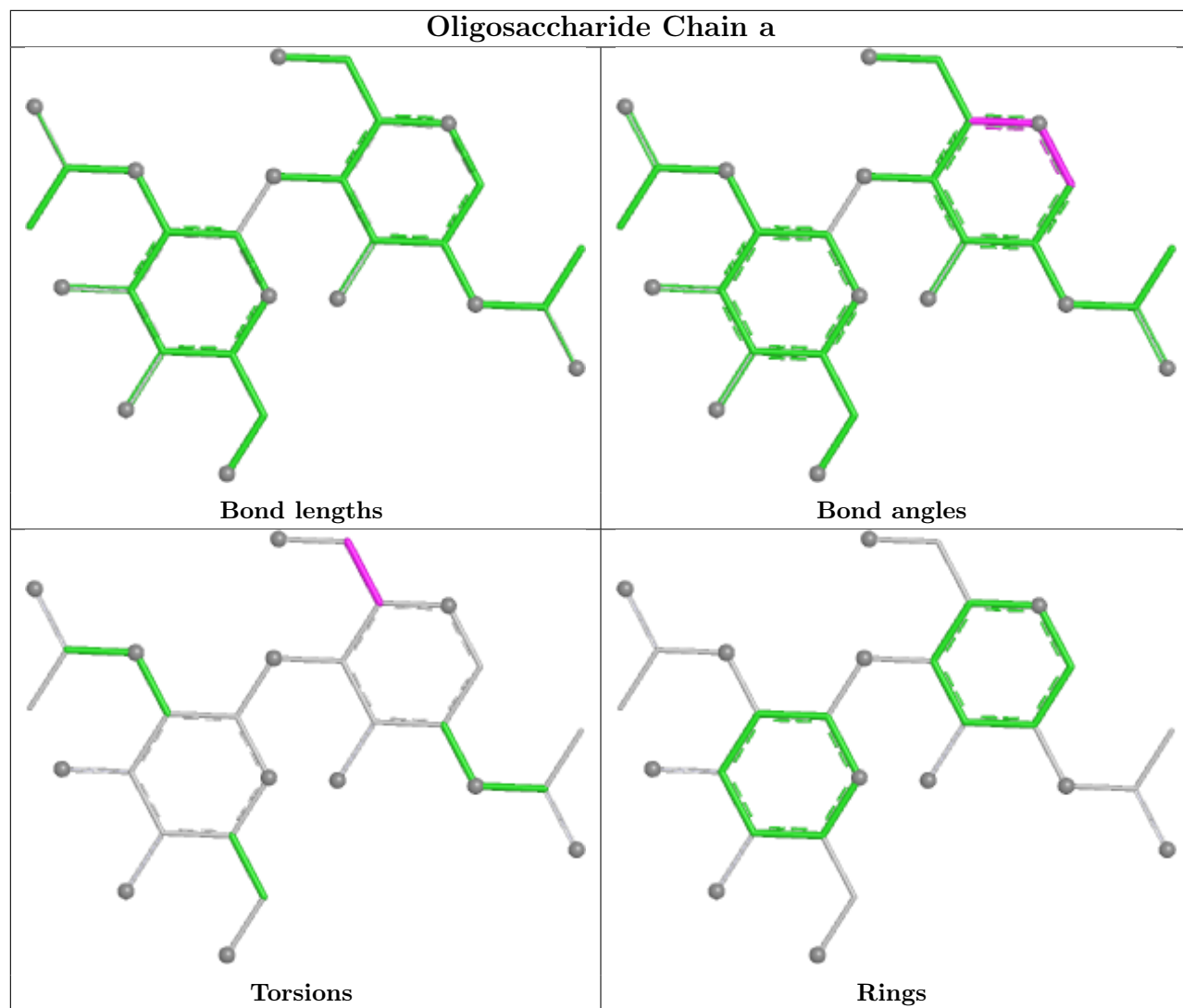


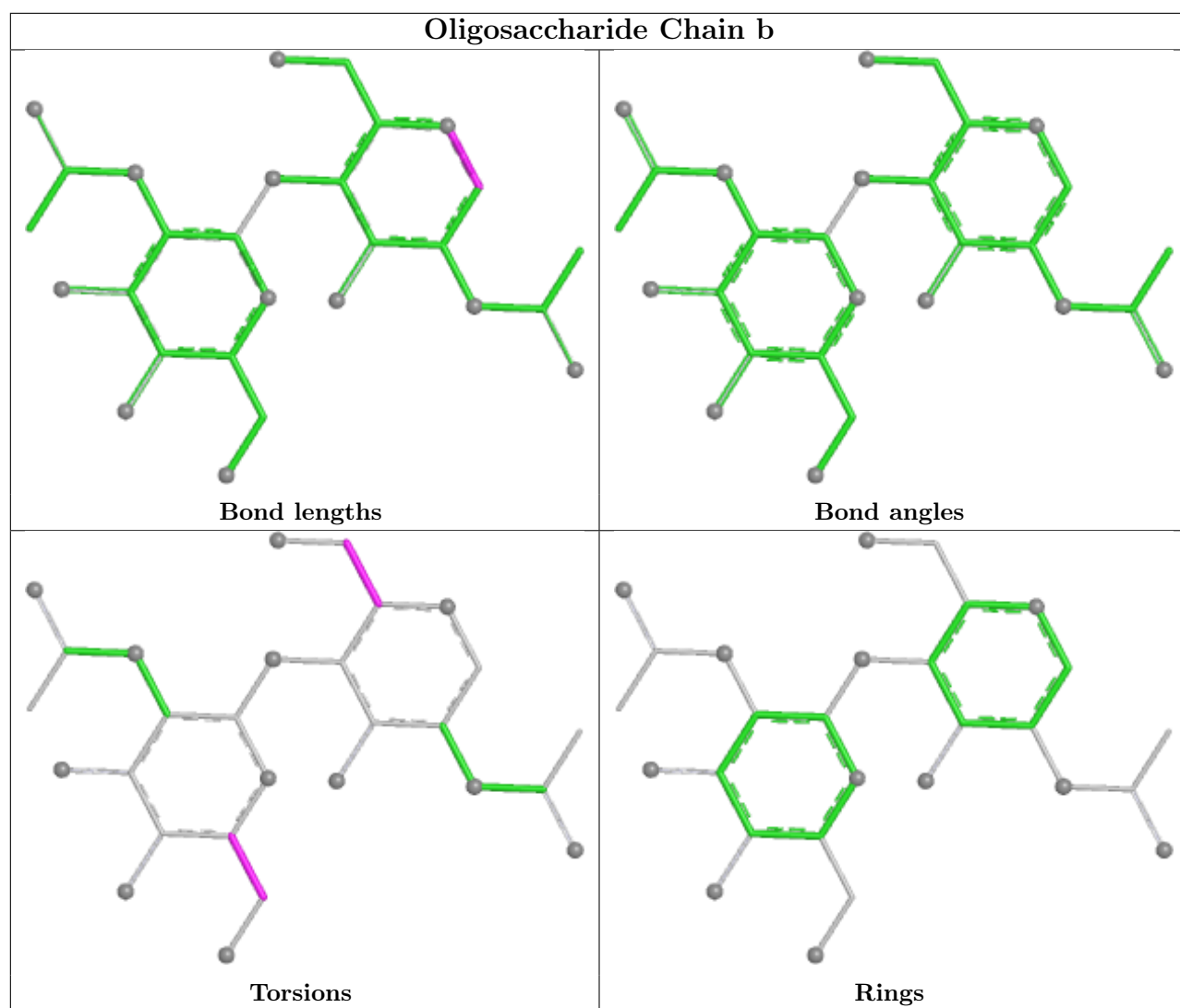


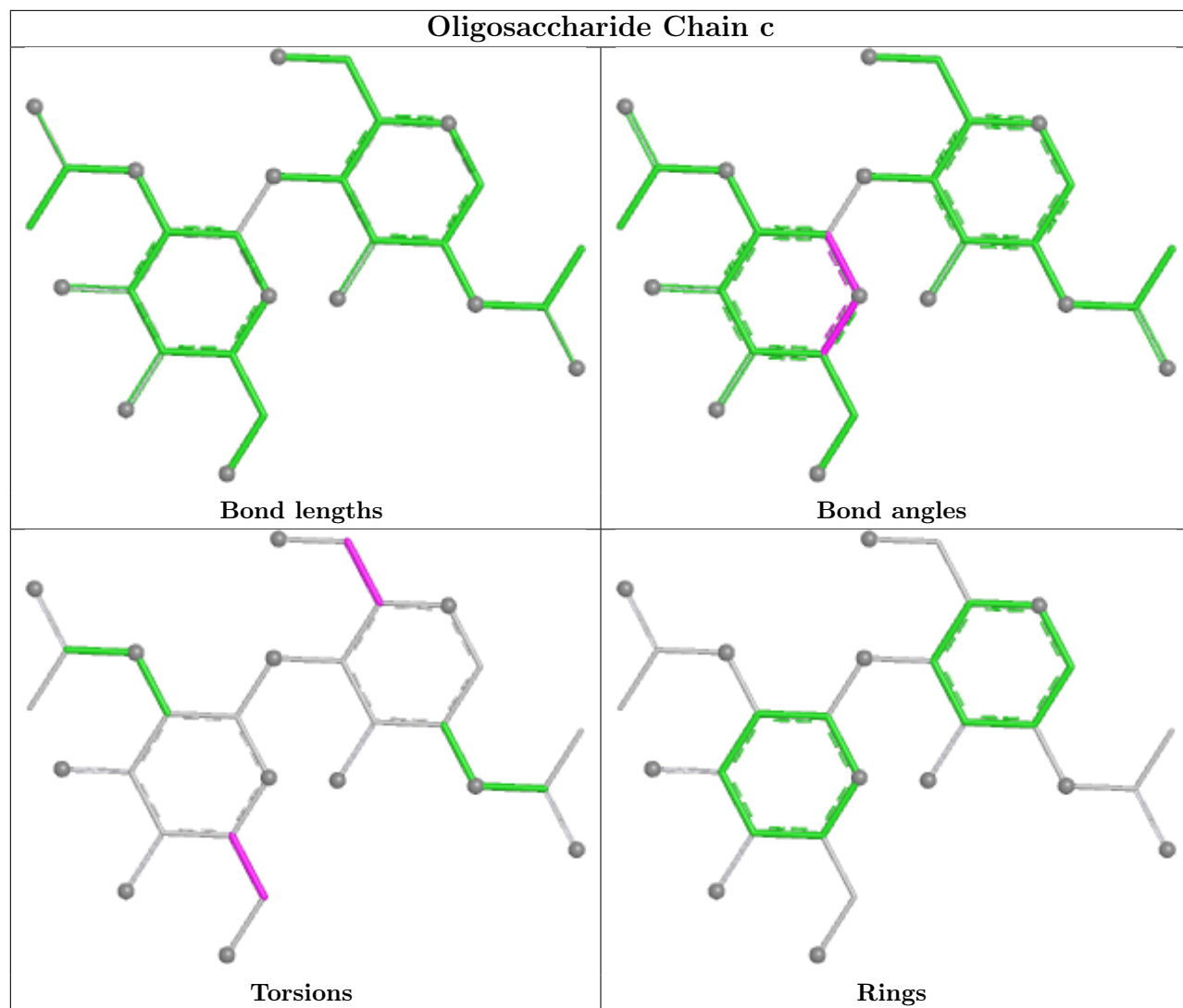


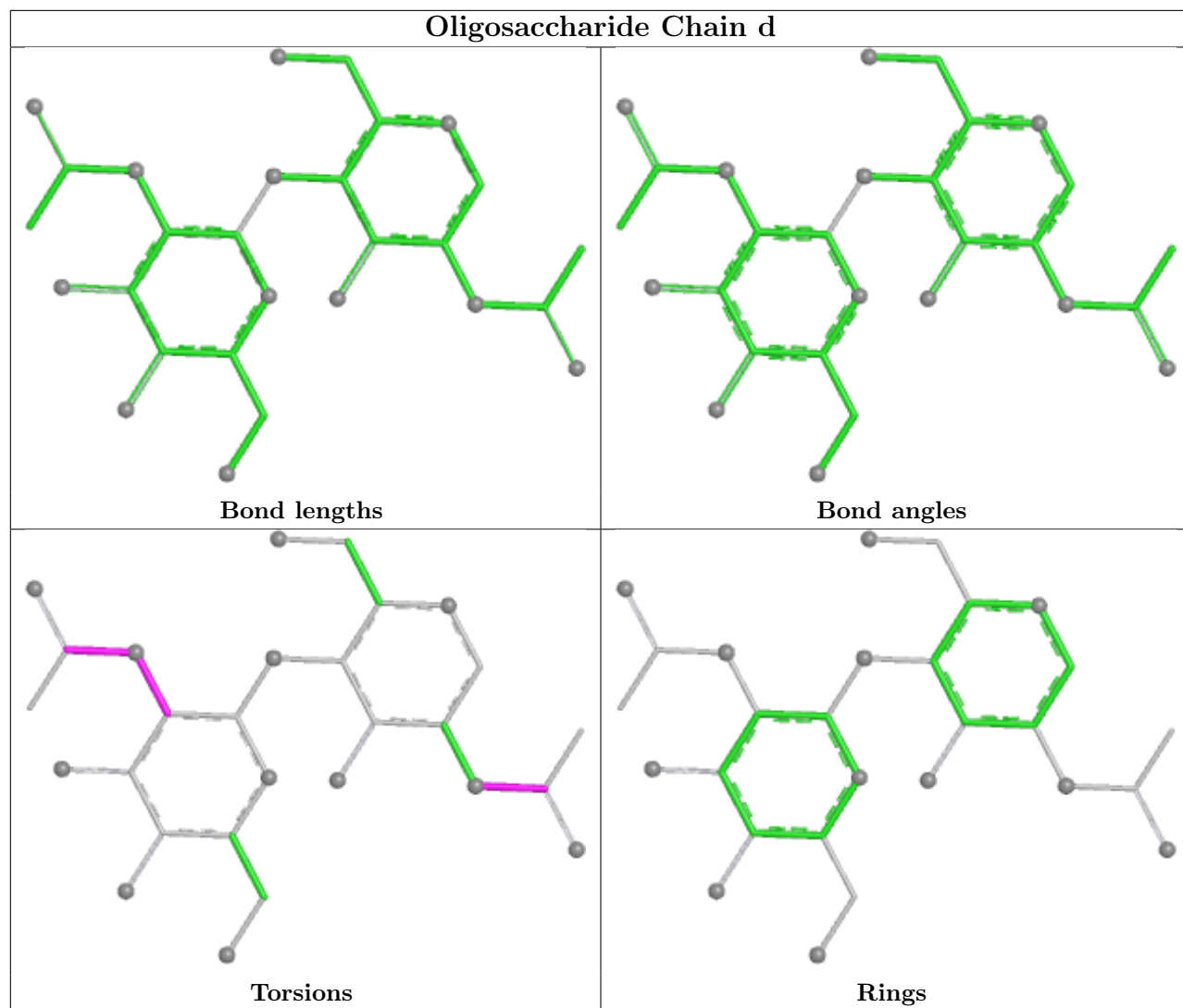


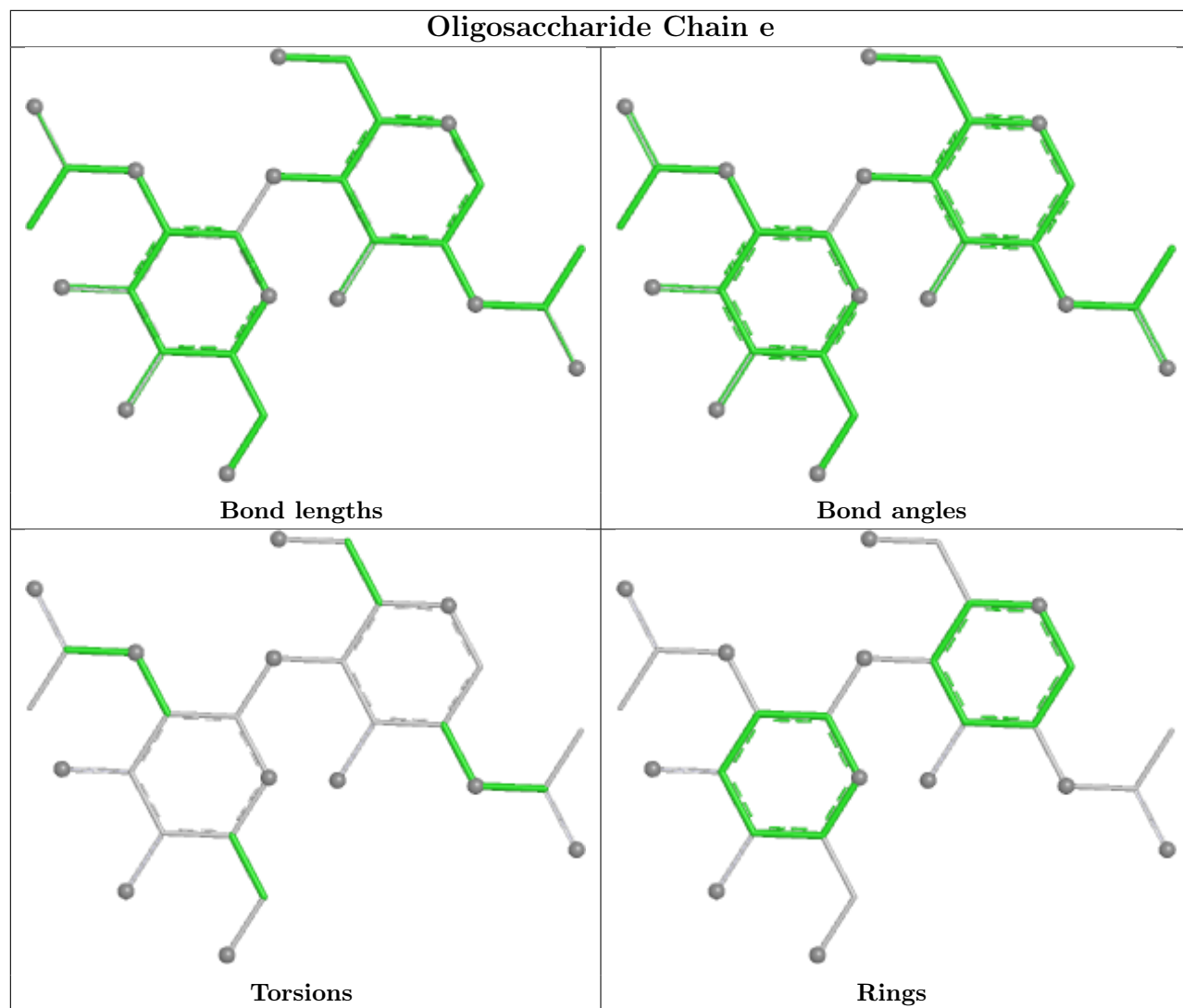


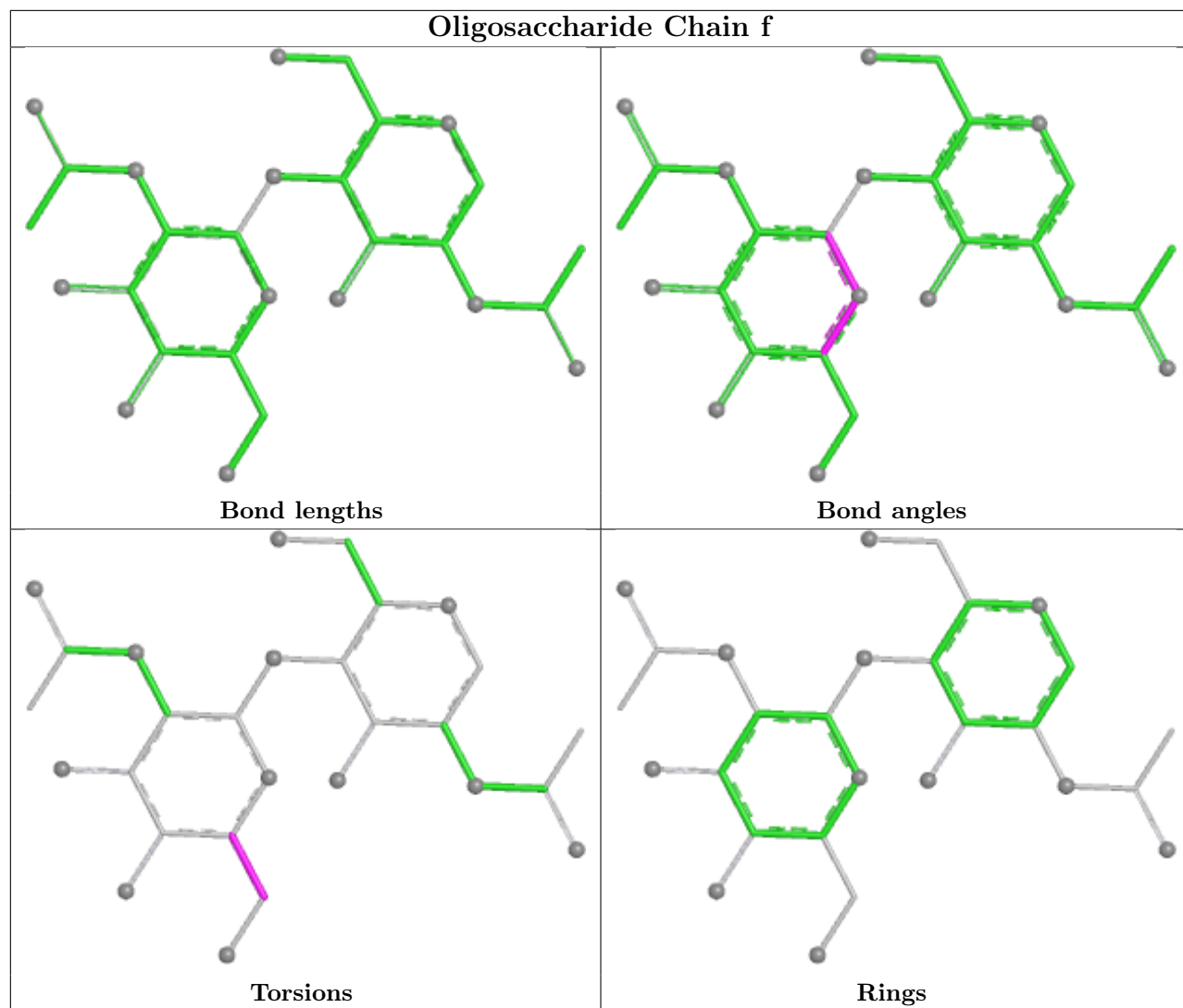


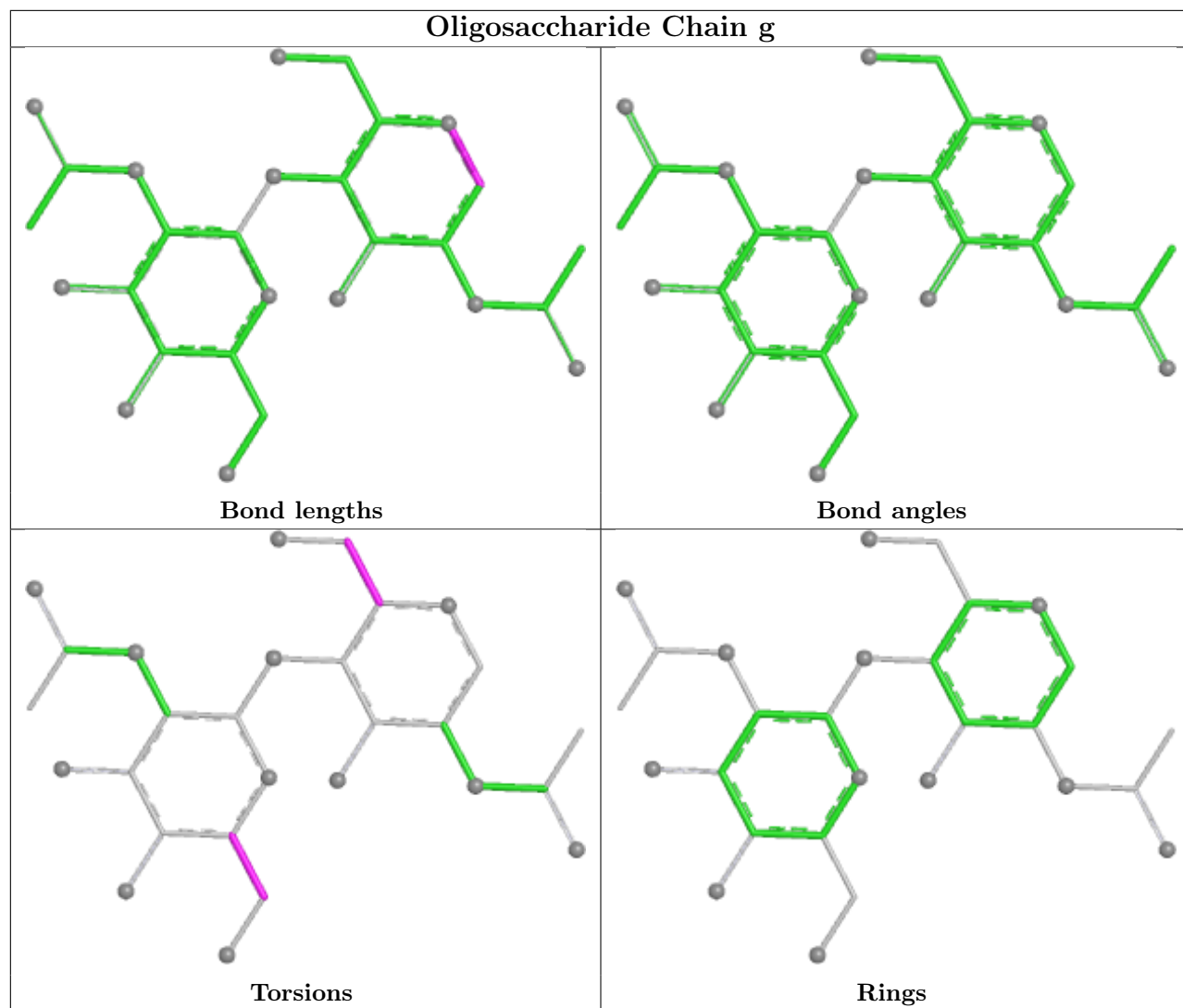


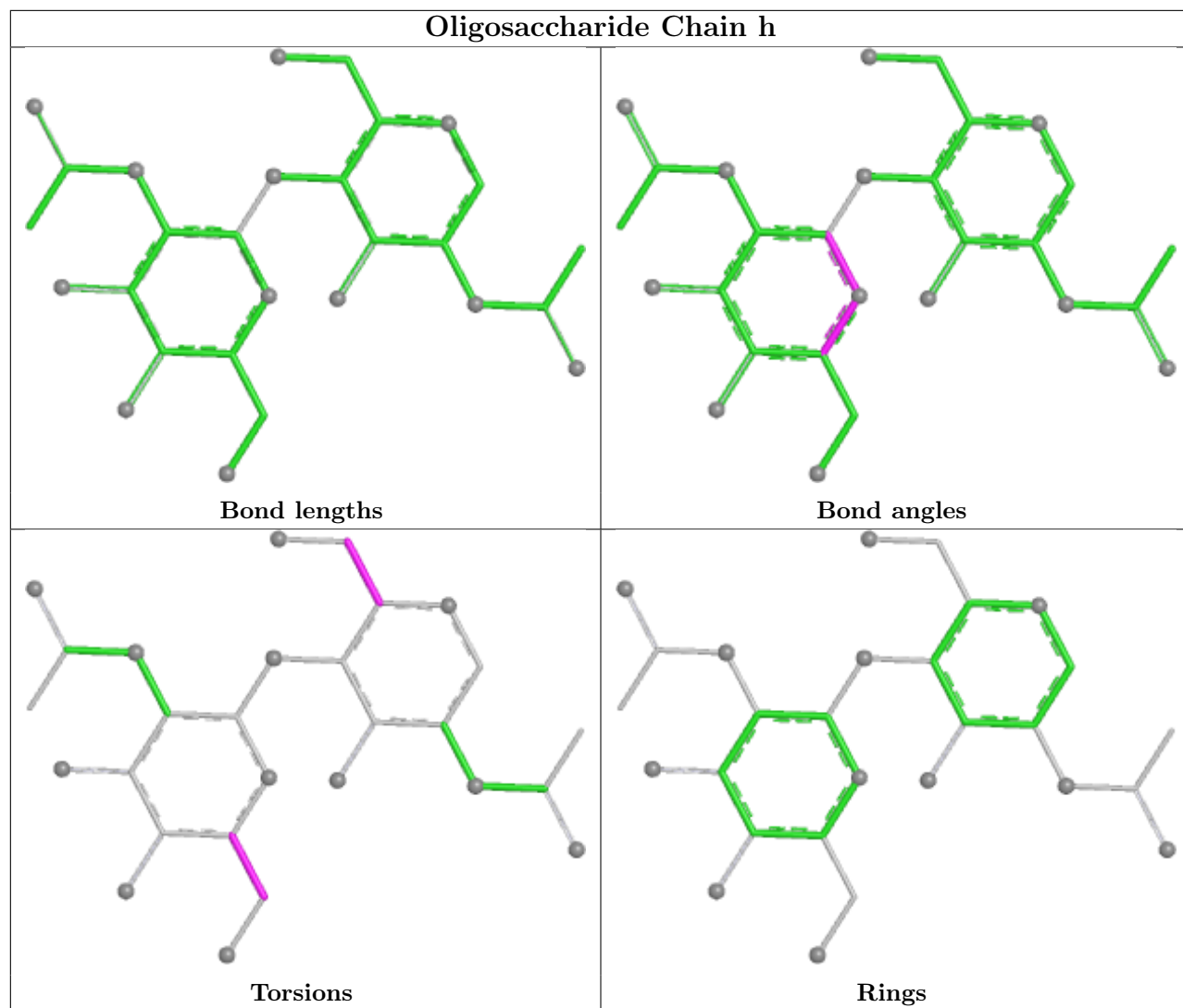


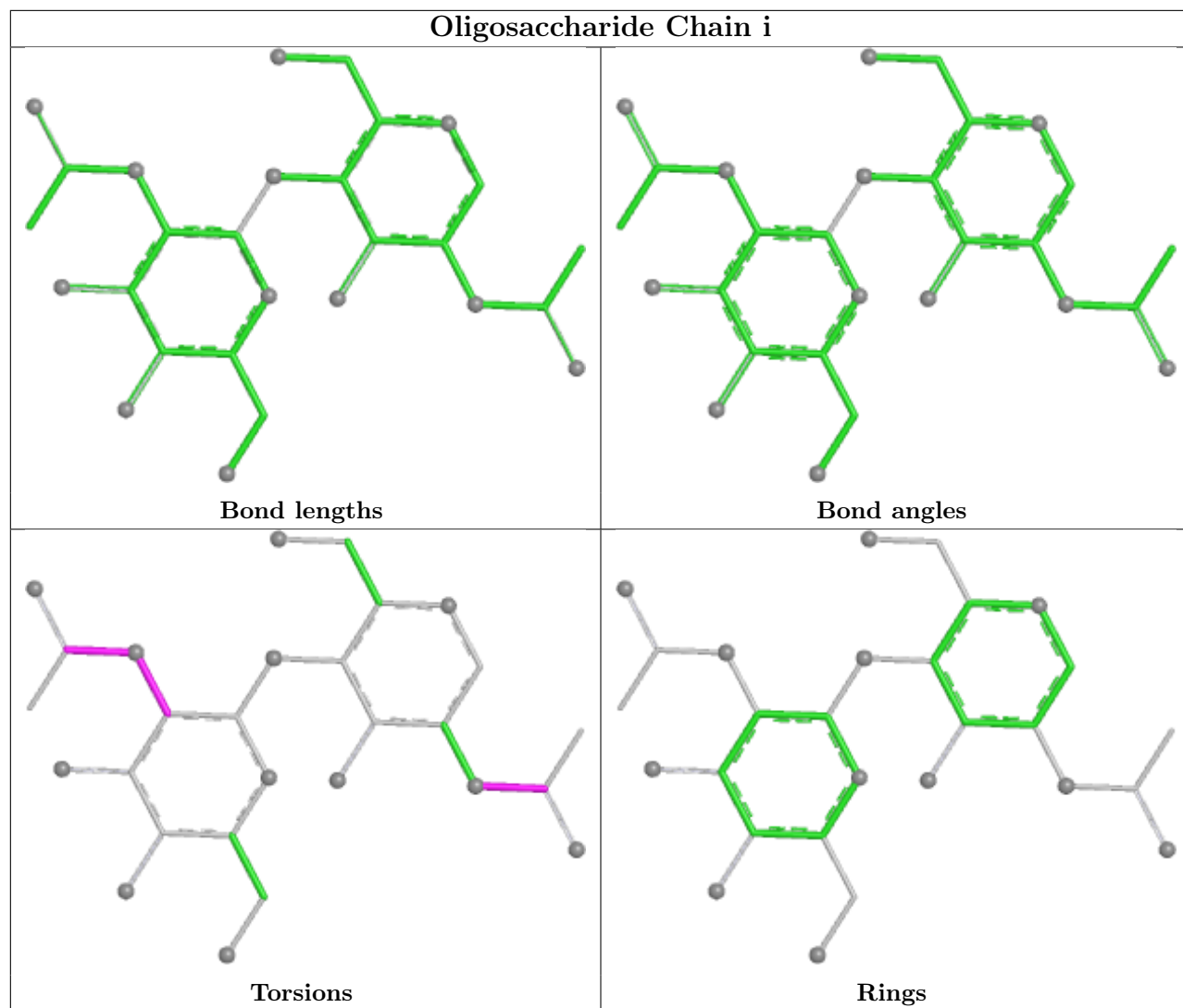


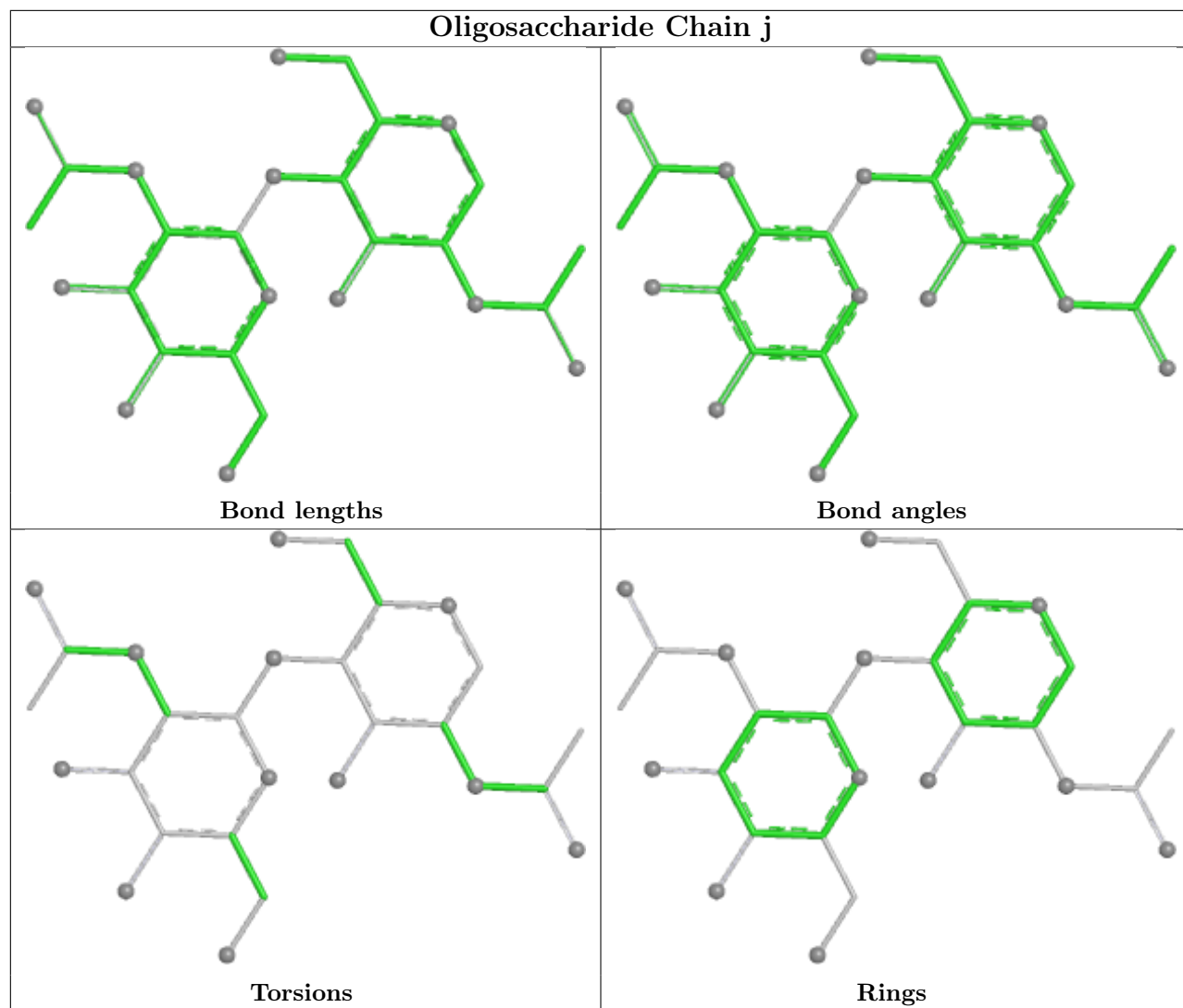


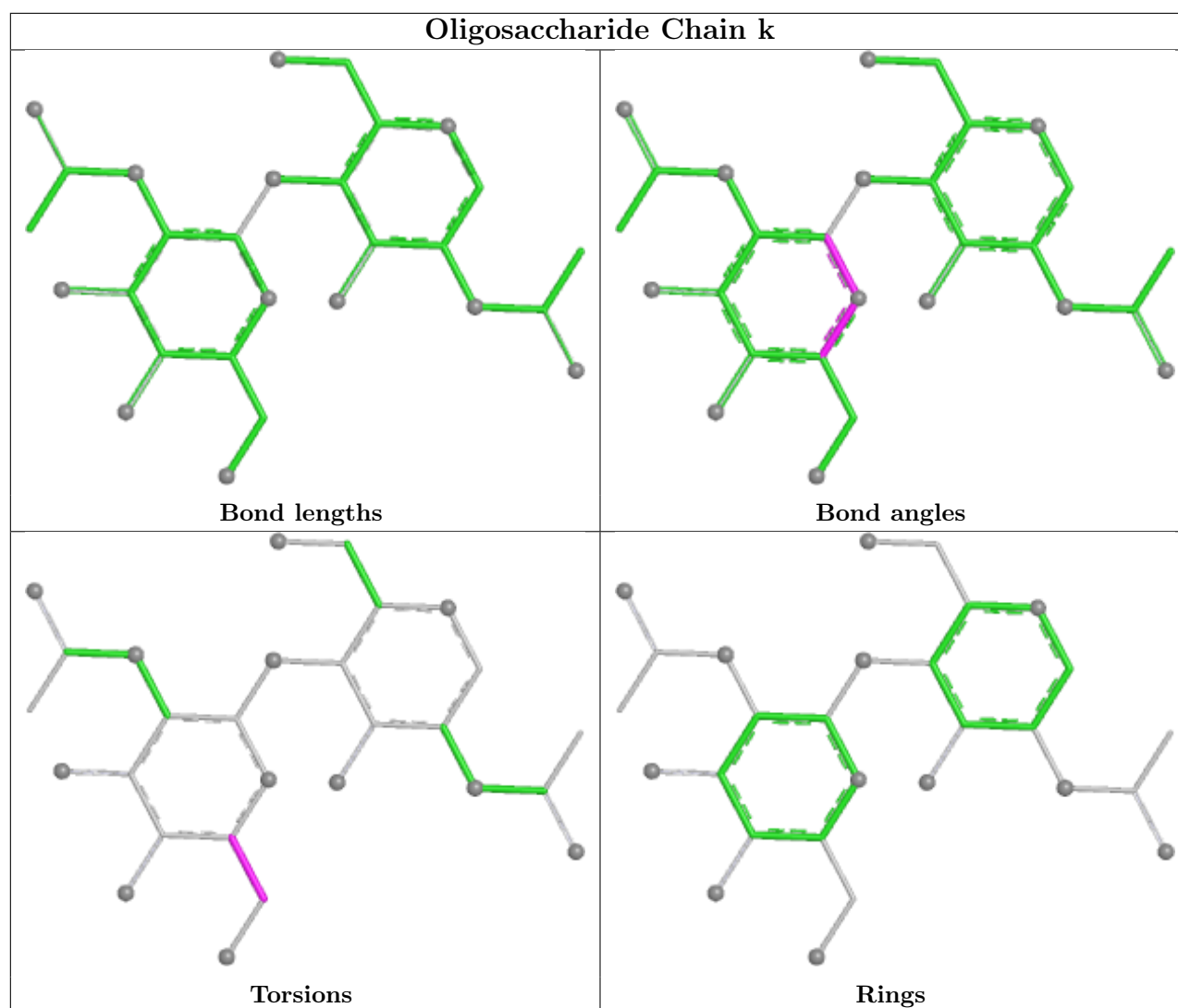












5.6 Ligand geometry [i](#)

29 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	NAG	A	1406	1	14,14,15	0.29	0	17,19,21	0.40	0
4	NAG	C	1407	1	14,14,15	0.24	0	17,19,21	0.51	0
4	NAG	C	1403	1	14,14,15	0.19	0	17,19,21	0.44	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	B	1404	1	14,14,15	0.49	0	17,19,21	0.55	0
4	NAG	A	1409	1	14,14,15	0.43	0	17,19,21	1.14	2 (11%)
4	NAG	A	1410	-	14,14,15	0.36	0	17,19,21	0.42	0
4	NAG	E	901	2	14,14,15	0.38	0	17,19,21	0.61	1 (5%)
4	NAG	B	1405	1	14,14,15	0.60	0	17,19,21	1.33	2 (11%)
4	NAG	A	1407	1	14,14,15	0.23	0	17,19,21	0.51	0
4	NAG	C	1406	1	14,14,15	0.28	0	17,19,21	0.40	0
4	NAG	C	1408	1	14,14,15	0.32	0	17,19,21	0.40	0
4	NAG	B	1403	1	14,14,15	0.19	0	17,19,21	0.44	0
4	NAG	C	1401	1	14,14,15	0.31	0	17,19,21	0.35	0
4	NAG	C	1405	1	14,14,15	0.60	0	17,19,21	1.34	2 (11%)
4	NAG	D	901	2	14,14,15	0.38	0	17,19,21	0.62	1 (5%)
4	NAG	C	1402	1	14,14,15	0.21	0	17,19,21	0.66	0
4	NAG	A	1408	1	14,14,15	0.34	0	17,19,21	0.39	0
4	NAG	C	1404	1	14,14,15	0.50	0	17,19,21	0.55	0
4	NAG	B	1402	1	14,14,15	0.23	0	17,19,21	0.66	0
4	NAG	A	1404	1	14,14,15	0.51	0	17,19,21	0.54	0
4	NAG	B	1408	1	14,14,15	0.34	0	17,19,21	0.40	0
4	NAG	A	1402	1	14,14,15	0.22	0	17,19,21	0.66	0
4	NAG	A	1405	1	14,14,15	0.59	0	17,19,21	1.34	2 (11%)
4	NAG	A	1403	1	14,14,15	0.20	0	17,19,21	0.43	0
4	NAG	B	1401	1	14,14,15	0.30	0	17,19,21	0.35	0
4	NAG	C	1409	1	14,14,15	0.49	0	17,19,21	0.36	0
4	NAG	A	1401	1	14,14,15	0.31	0	17,19,21	0.35	0
4	NAG	B	1407	1	14,14,15	0.24	0	17,19,21	0.52	0
4	NAG	B	1406	1	14,14,15	0.28	0	17,19,21	0.40	0

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

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

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

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	1405	NAG	C2-N2-C7	4.60	129.06	122.90
4	B	1405	NAG	C2-N2-C7	4.57	129.02	122.90
4	A	1405	NAG	C2-N2-C7	4.56	129.02	122.90
4	A	1409	NAG	C8-C7-N2	2.30	119.93	116.12
4	A	1409	NAG	C2-N2-C7	-2.21	119.94	122.90
4	A	1405	NAG	C1-C2-N2	2.11	113.76	110.43
4	B	1405	NAG	C1-C2-N2	2.11	113.75	110.43
4	C	1405	NAG	C1-C2-N2	2.10	113.75	110.43
4	D	901	NAG	C1-O5-C5	2.10	115.01	112.19
4	E	901	NAG	C1-O5-C5	2.04	114.92	112.19

There are no chirality outliers.

All (60) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1406	NAG	O5-C5-C6-O6
4	B	1406	NAG	O5-C5-C6-O6
4	C	1406	NAG	O5-C5-C6-O6
4	A	1402	NAG	O5-C5-C6-O6
4	A	1404	NAG	O5-C5-C6-O6
4	B	1402	NAG	O5-C5-C6-O6
4	B	1404	NAG	O5-C5-C6-O6
4	C	1402	NAG	O5-C5-C6-O6
4	C	1404	NAG	O5-C5-C6-O6
4	A	1401	NAG	O5-C5-C6-O6
4	B	1401	NAG	O5-C5-C6-O6
4	C	1401	NAG	O5-C5-C6-O6
4	A	1402	NAG	C4-C5-C6-O6
4	B	1402	NAG	C4-C5-C6-O6
4	C	1402	NAG	C4-C5-C6-O6
4	A	1405	NAG	O5-C5-C6-O6
4	B	1405	NAG	O5-C5-C6-O6
4	C	1405	NAG	O5-C5-C6-O6
4	C	1409	NAG	C4-C5-C6-O6
4	A	1405	NAG	C4-C5-C6-O6
4	B	1405	NAG	C4-C5-C6-O6
4	C	1405	NAG	C4-C5-C6-O6
4	A	1408	NAG	O5-C5-C6-O6
4	B	1408	NAG	O5-C5-C6-O6
4	C	1408	NAG	O5-C5-C6-O6
4	C	1409	NAG	O5-C5-C6-O6
4	A	1406	NAG	C4-C5-C6-O6
4	B	1406	NAG	C4-C5-C6-O6
4	C	1406	NAG	C4-C5-C6-O6
4	A	1405	NAG	C8-C7-N2-C2
4	A	1405	NAG	O7-C7-N2-C2
4	B	1405	NAG	C8-C7-N2-C2
4	B	1405	NAG	O7-C7-N2-C2
4	C	1405	NAG	C8-C7-N2-C2
4	C	1405	NAG	O7-C7-N2-C2
4	A	1404	NAG	C4-C5-C6-O6
4	B	1404	NAG	C4-C5-C6-O6
4	C	1404	NAG	C4-C5-C6-O6
4	D	901	NAG	O5-C5-C6-O6
4	E	901	NAG	O5-C5-C6-O6

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

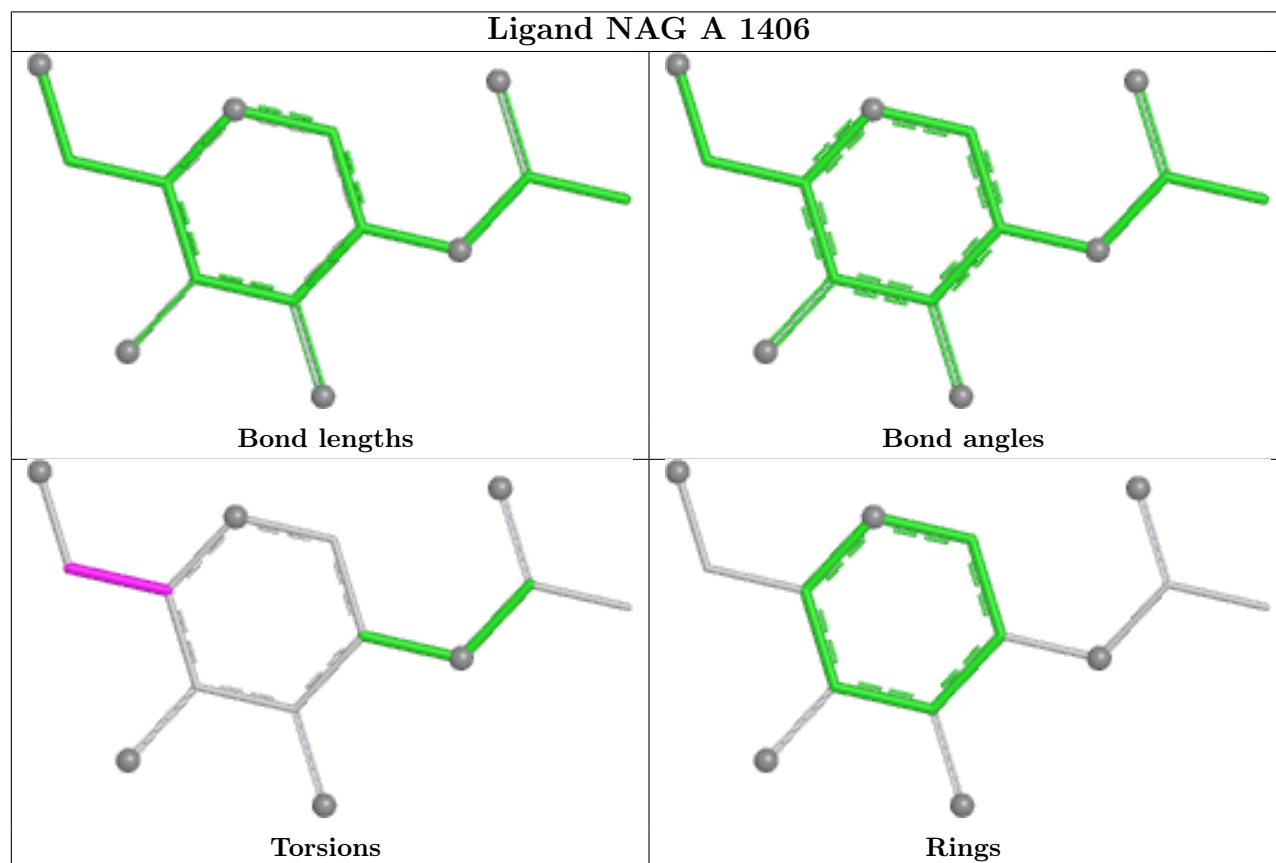
There are no ring outliers.

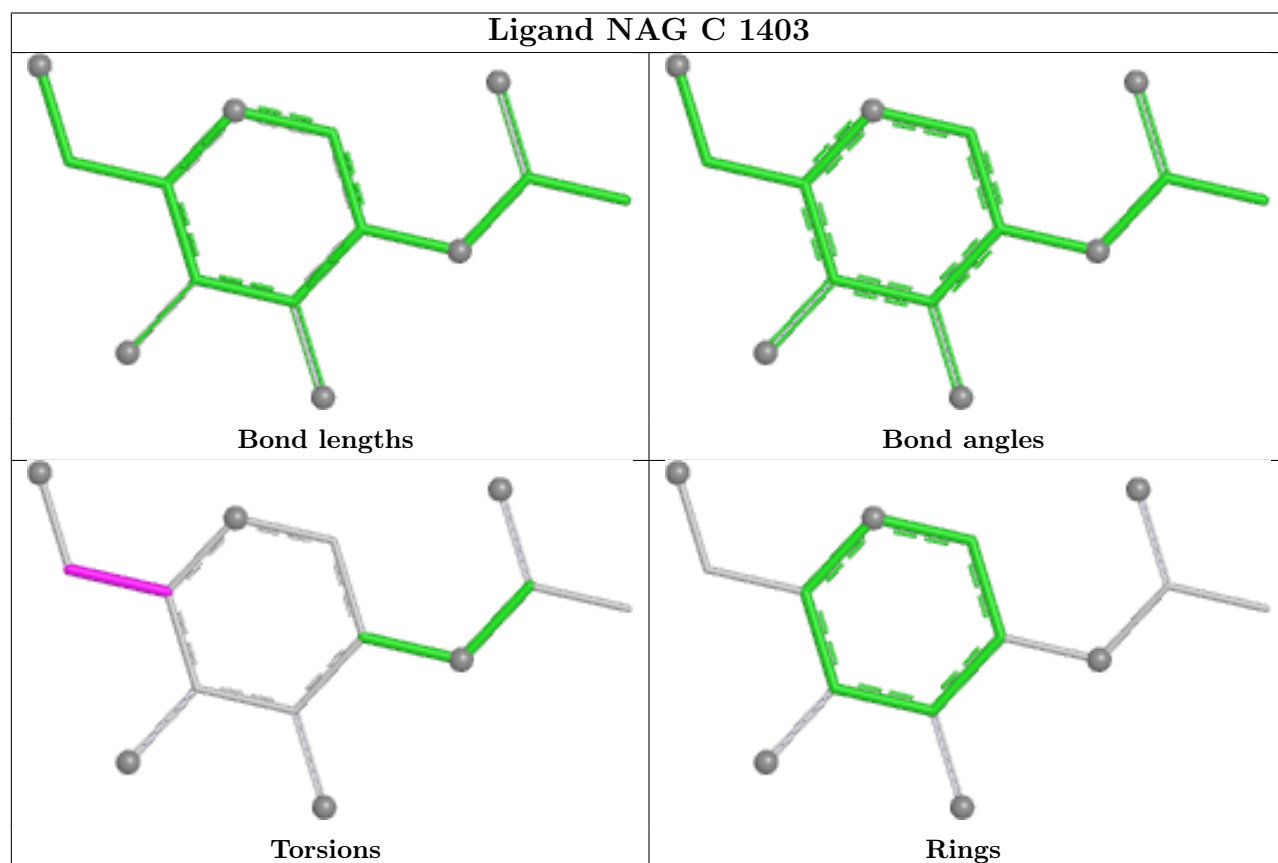
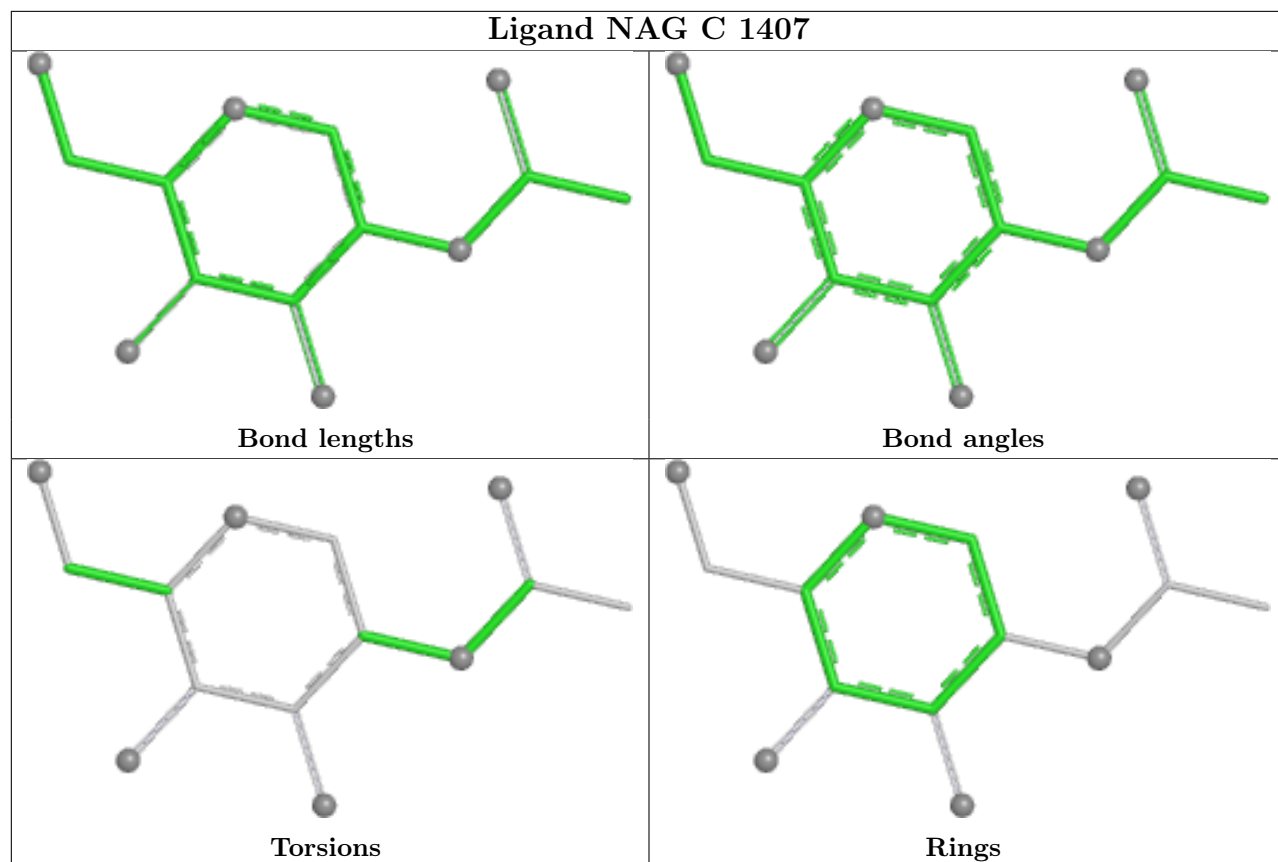
8 monomers are involved in 16 short contacts:

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

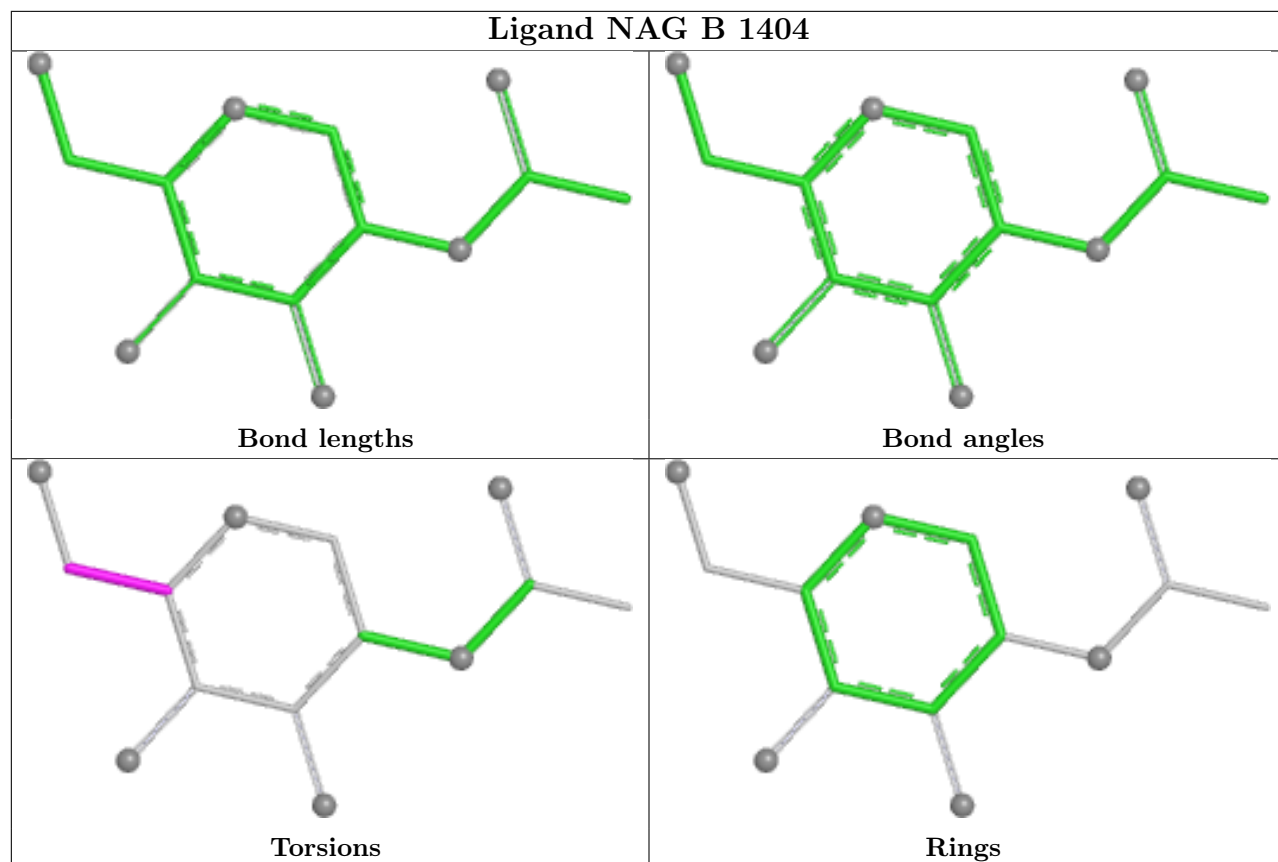
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

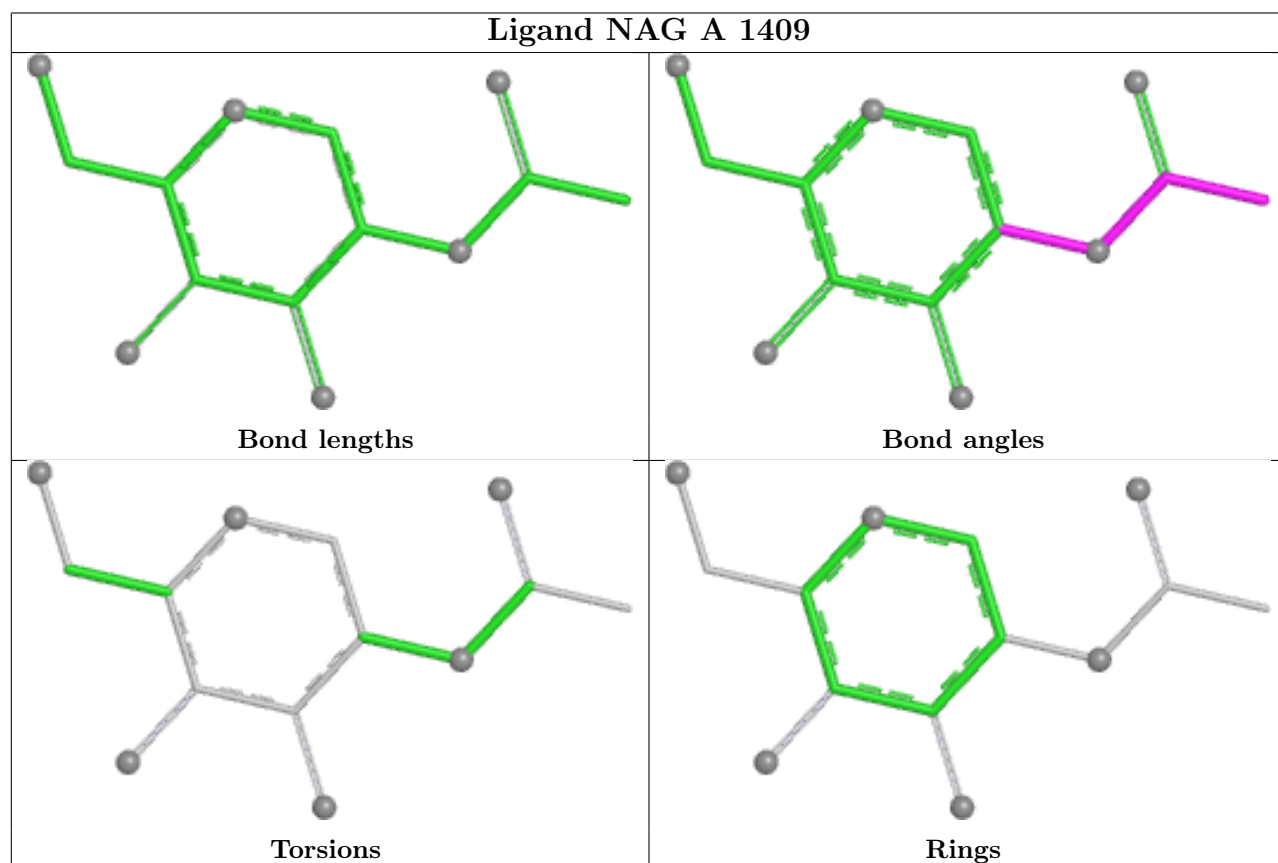




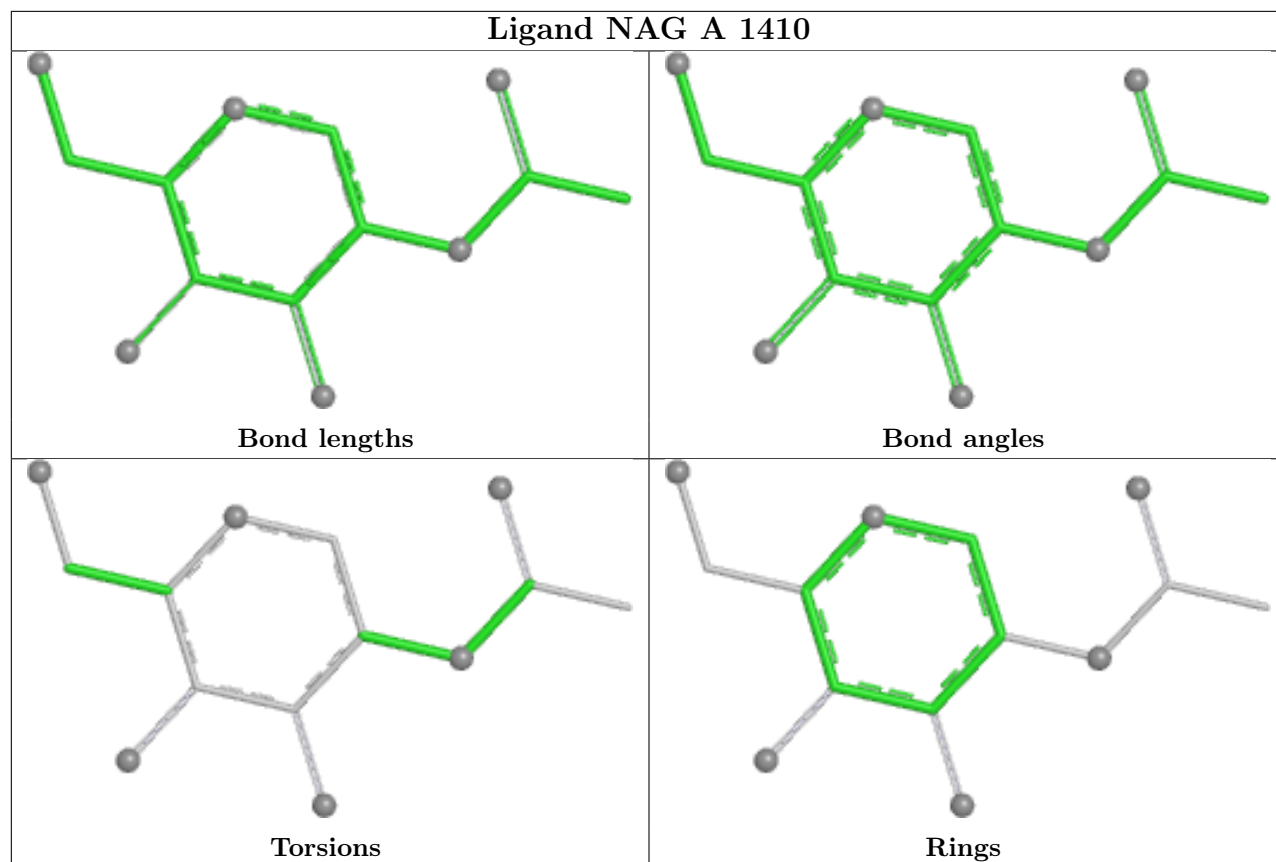
Ligand NAG B 1404



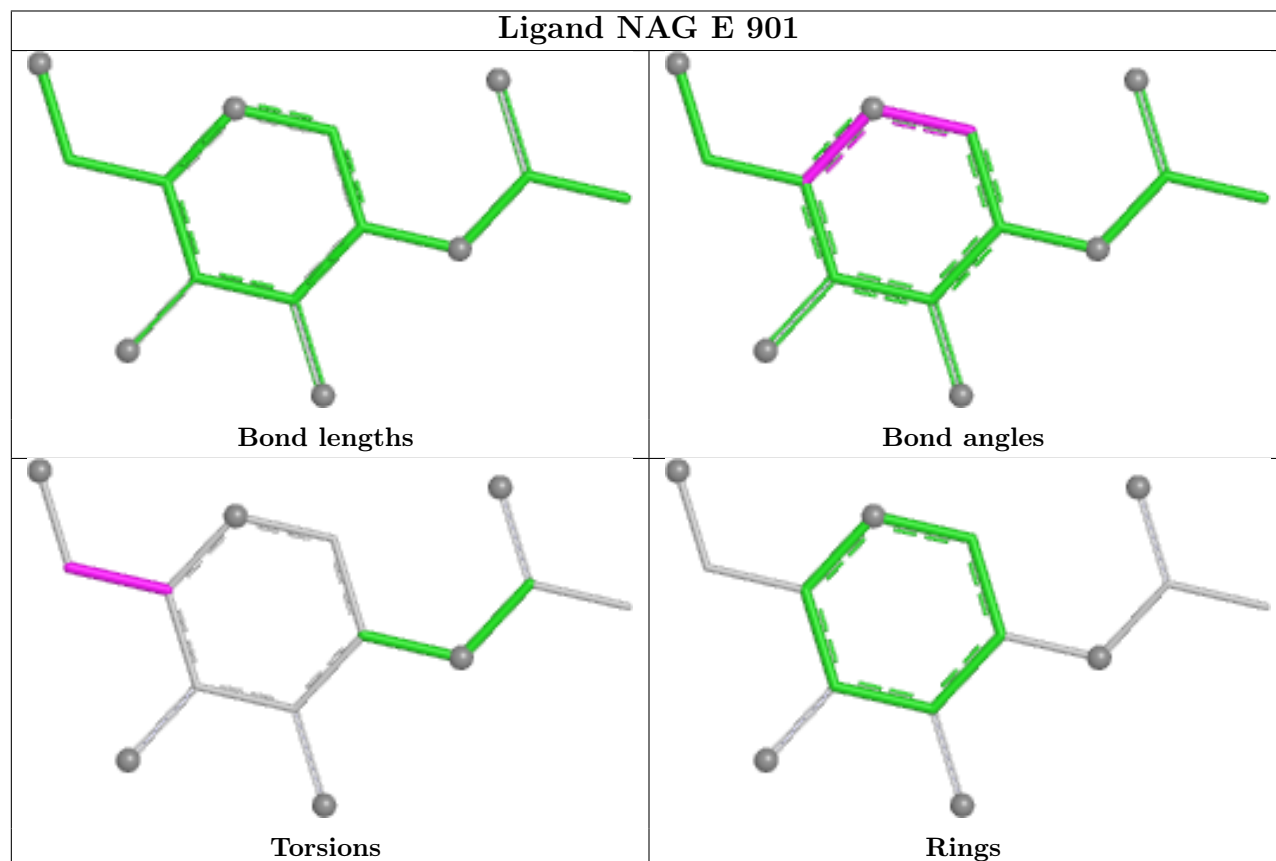
Ligand NAG A 1409



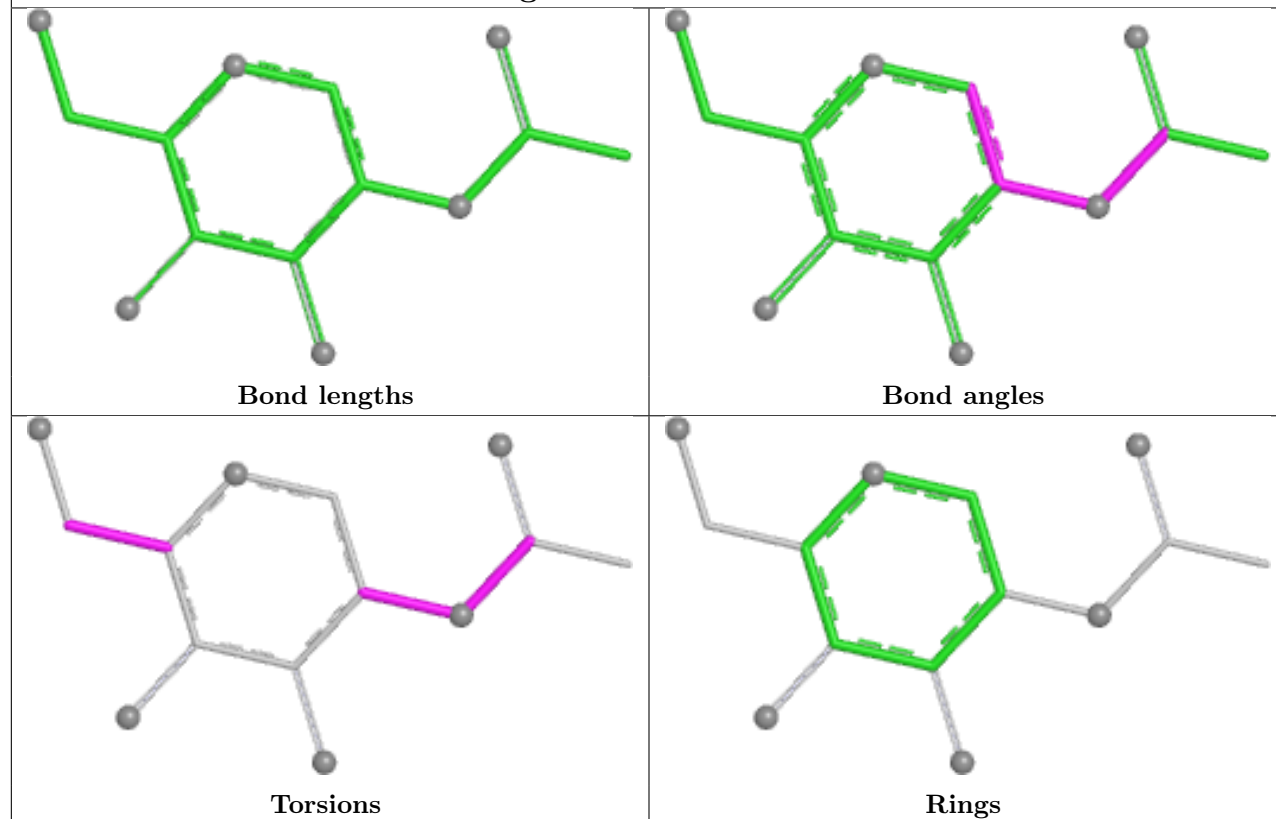
Ligand NAG A 1410



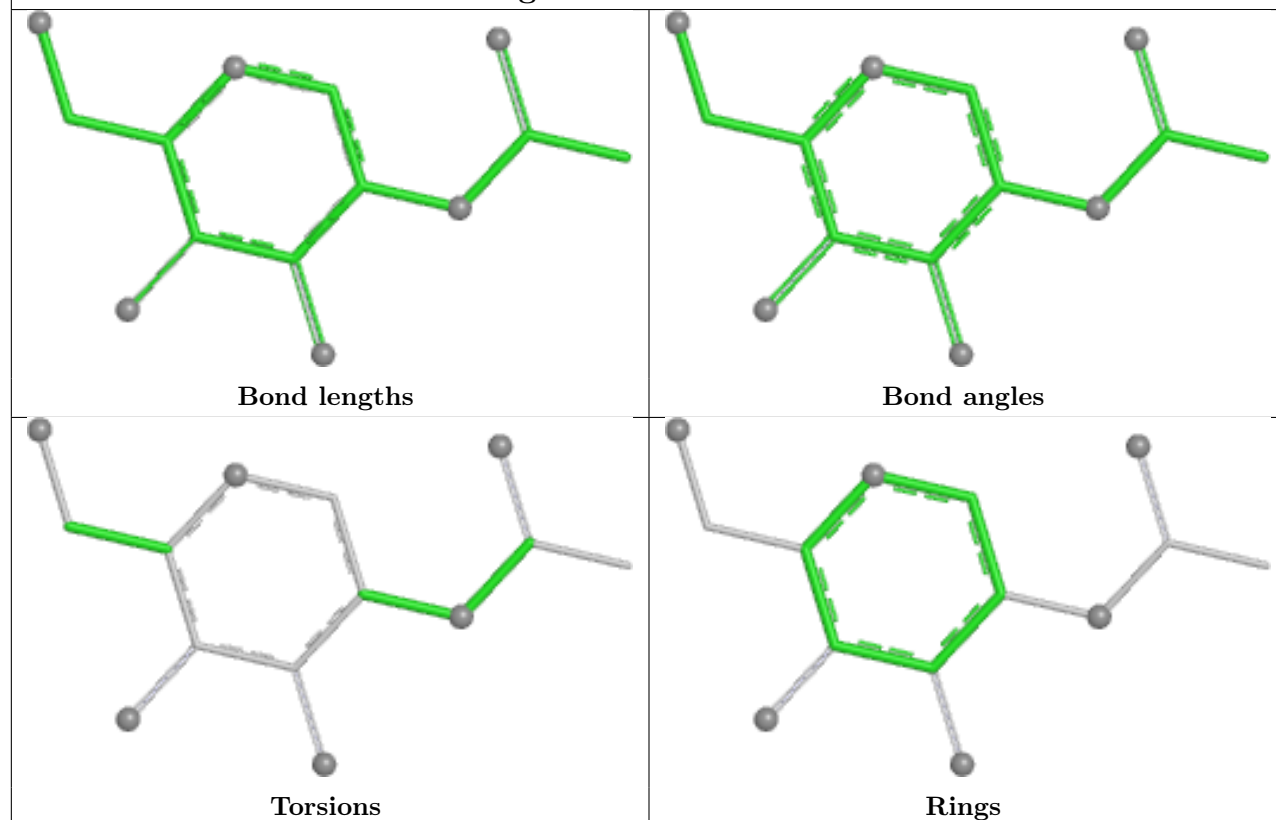
Ligand NAG E 901



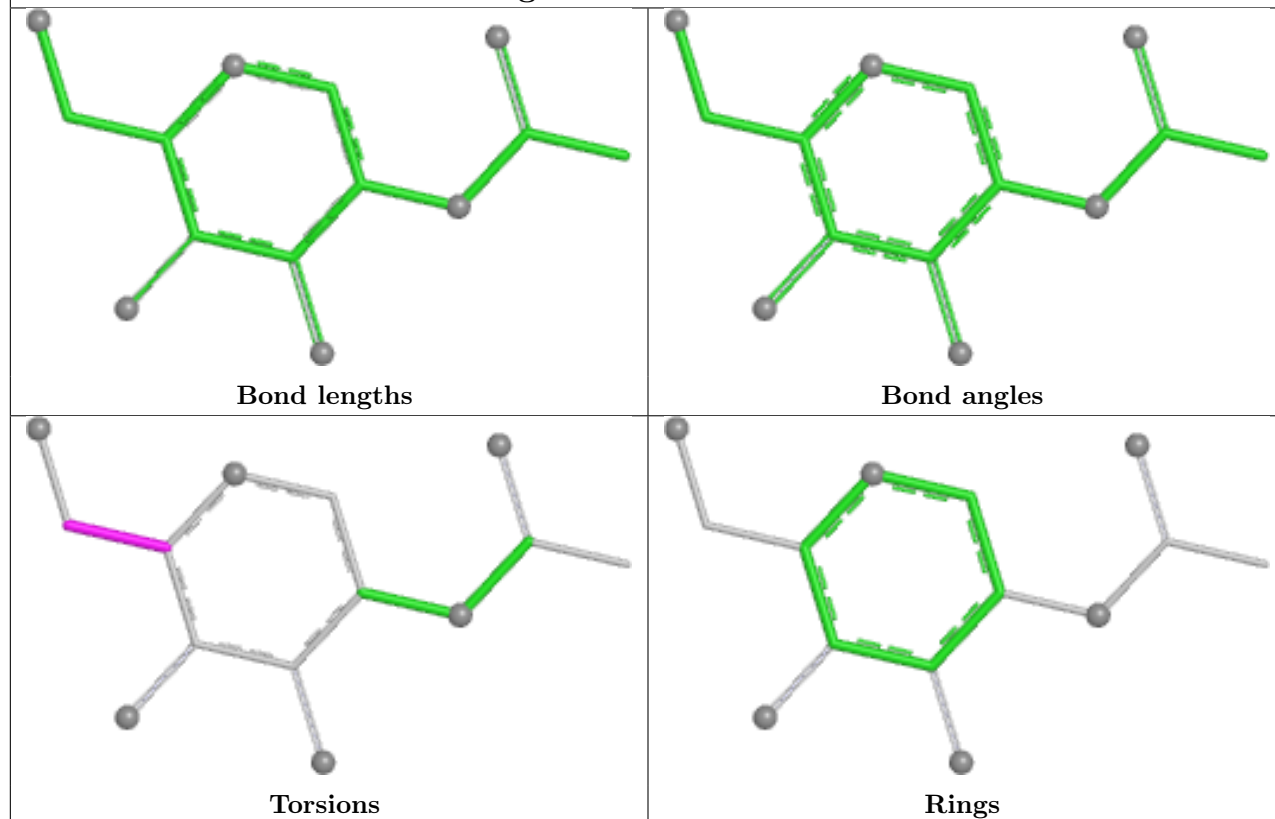
Ligand NAG B 1405



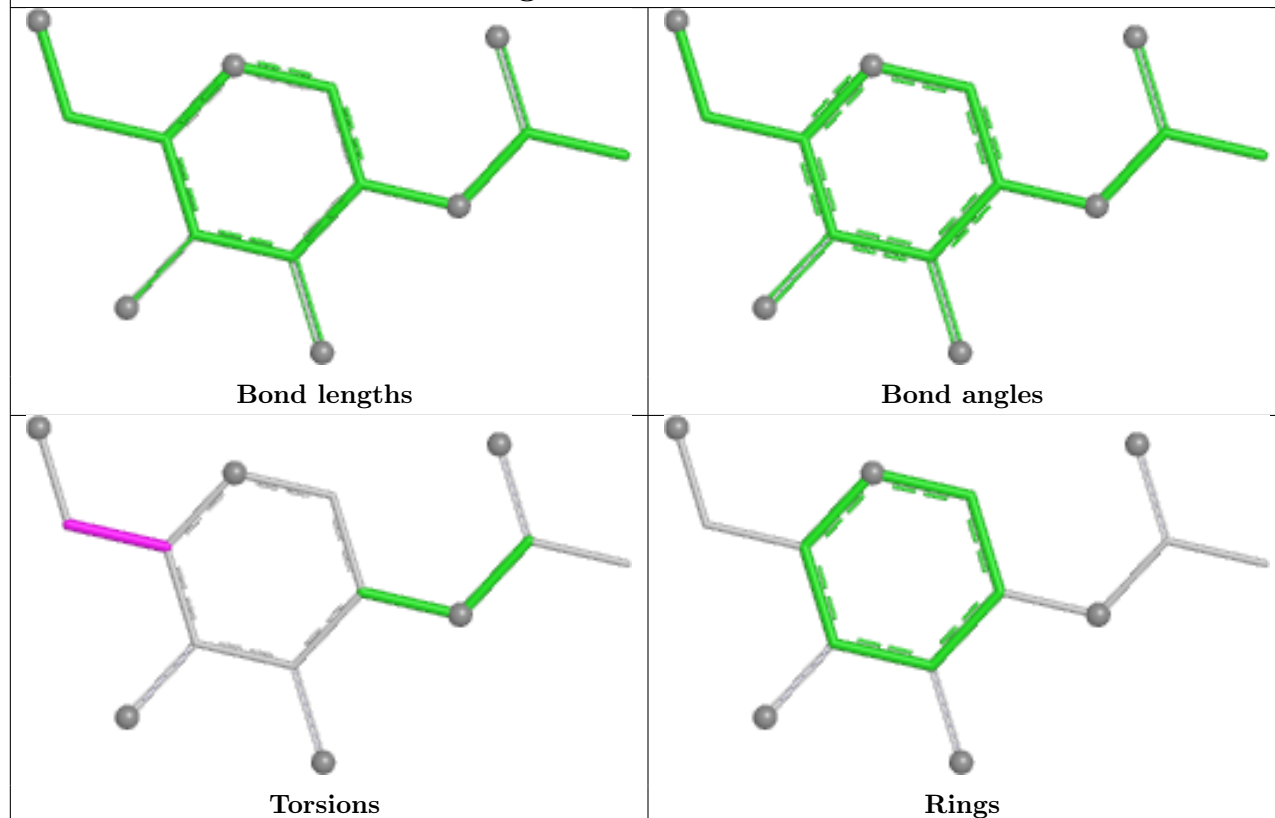
Ligand NAG A 1407



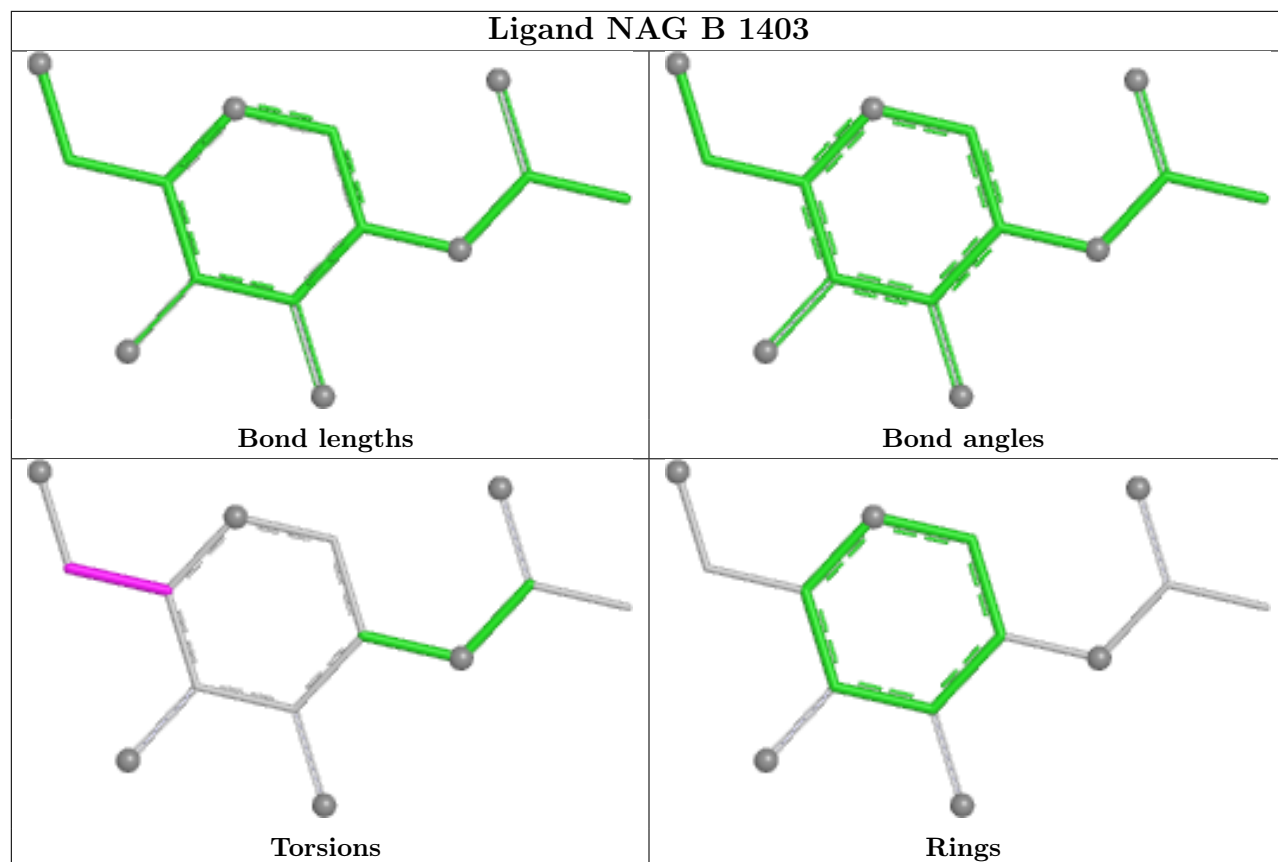
Ligand NAG C 1406



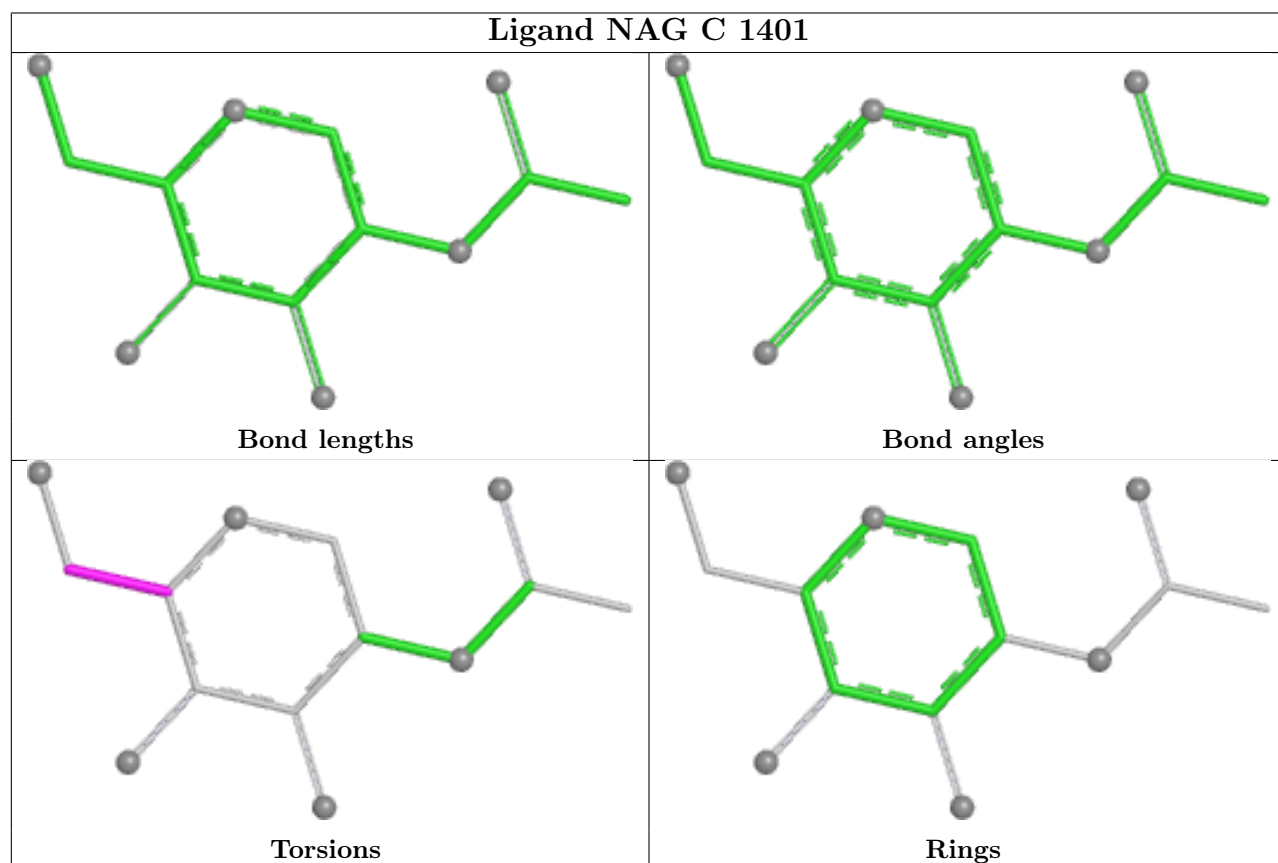
Ligand NAG C 1408



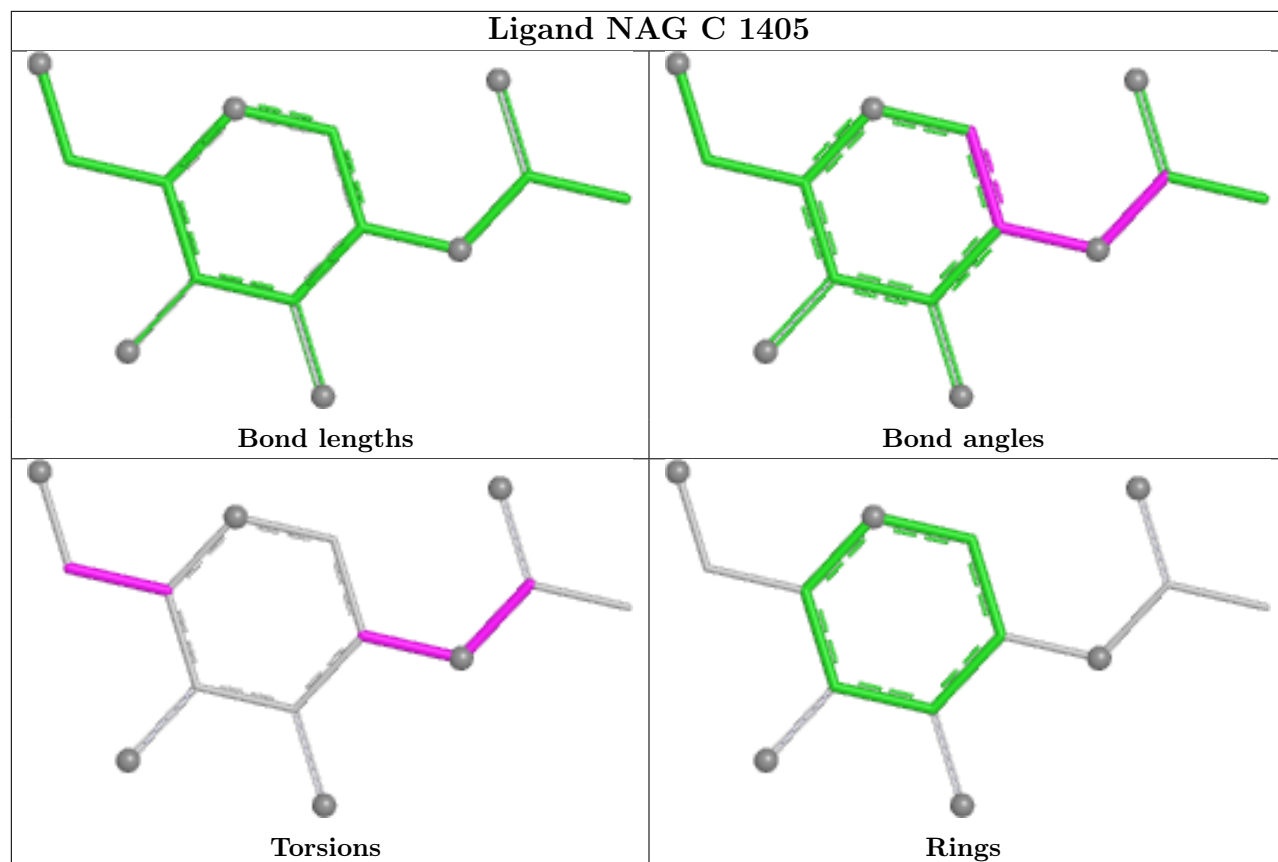
Ligand NAG B 1403



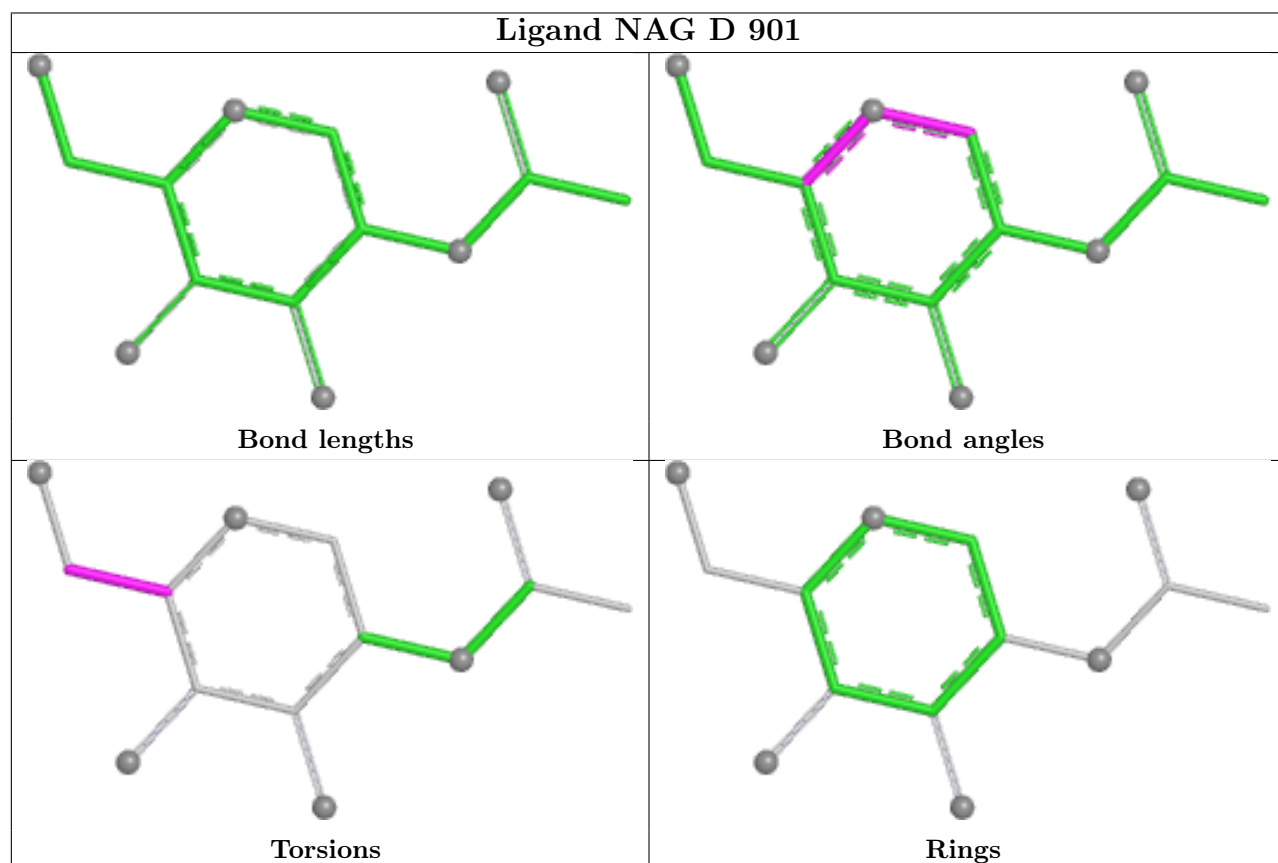
Ligand NAG C 1401



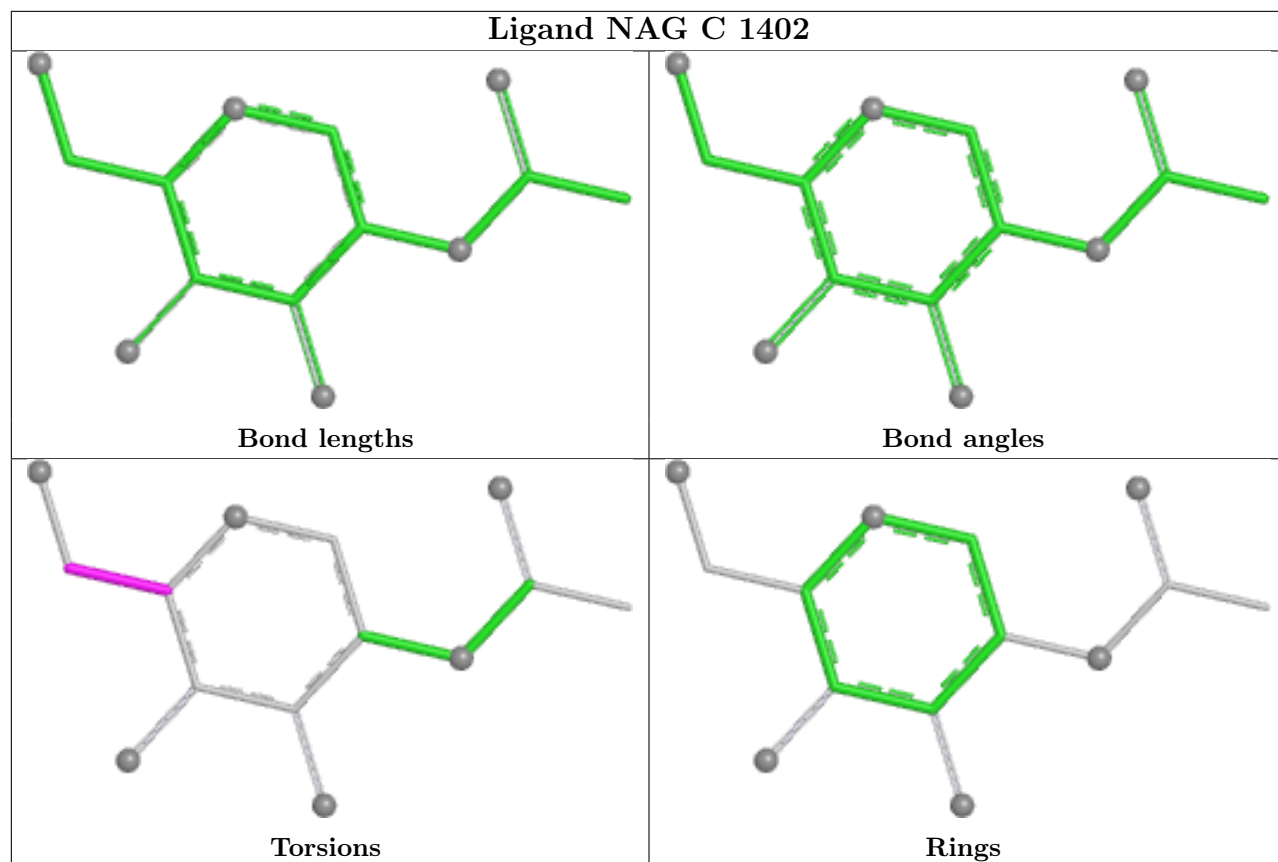
Ligand NAG C 1405



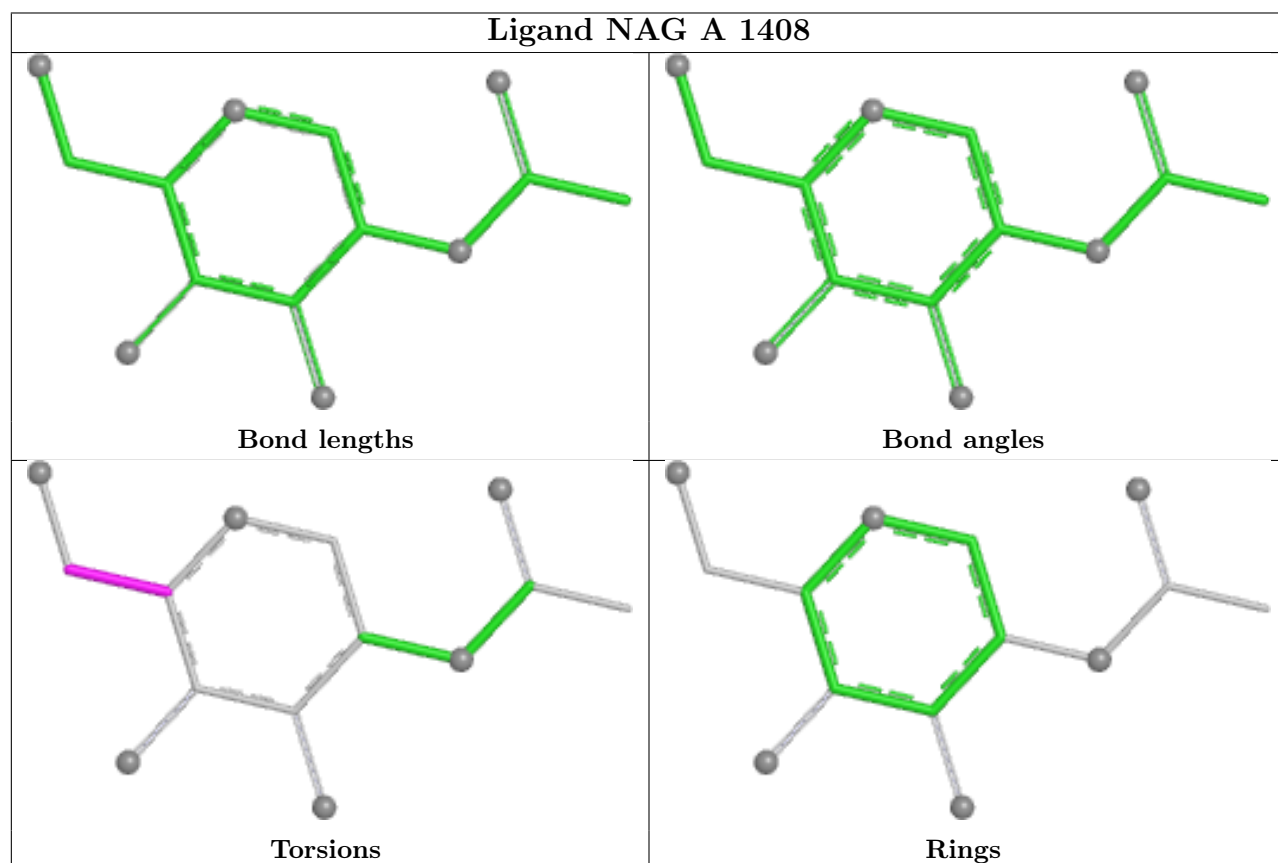
Ligand NAG D 901



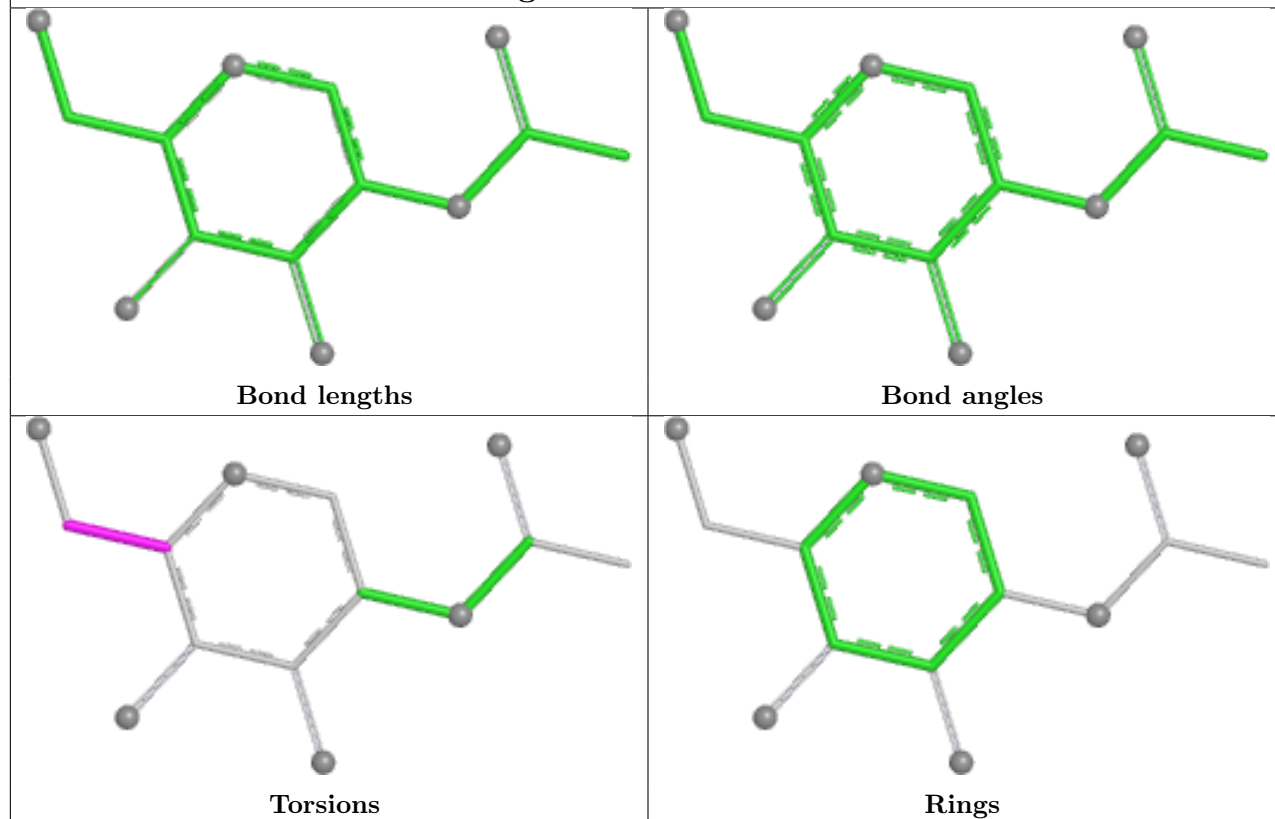
Ligand NAG C 1402



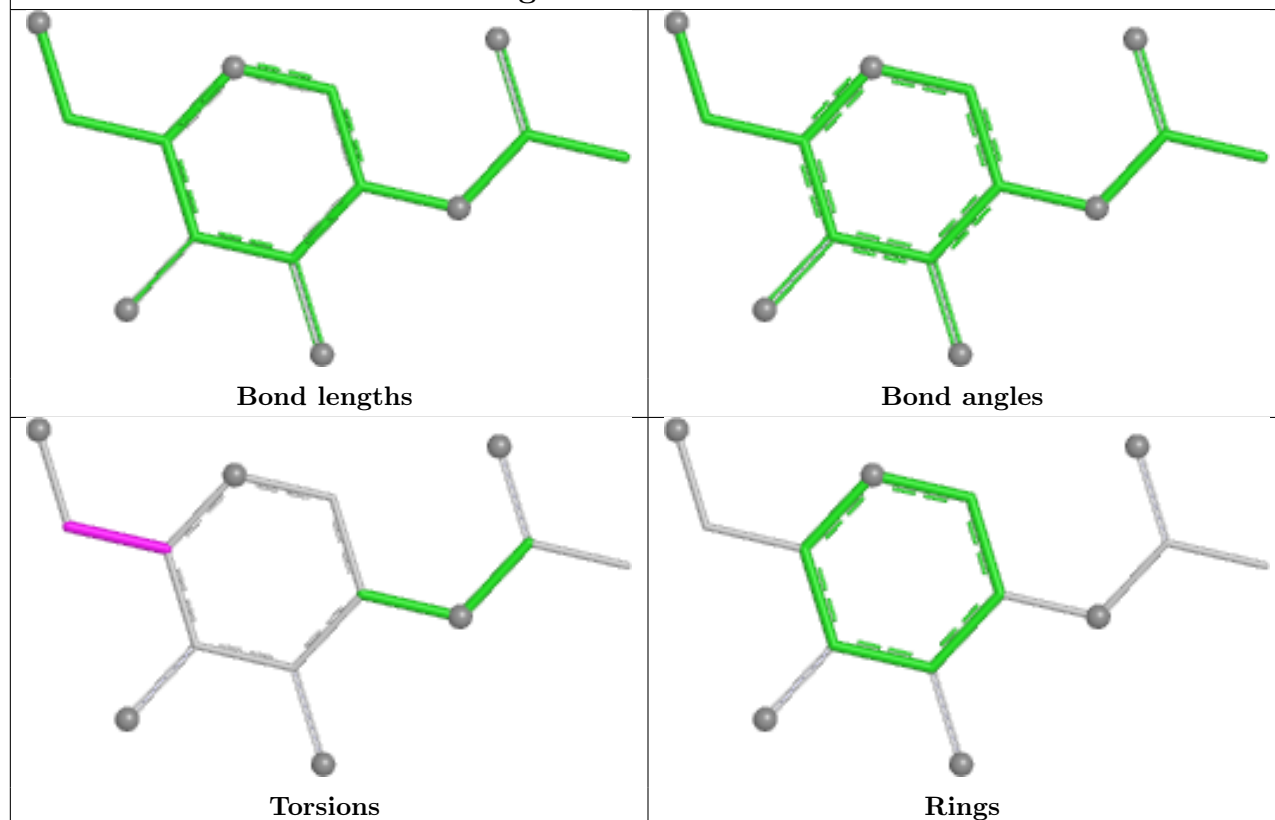
Ligand NAG A 1408



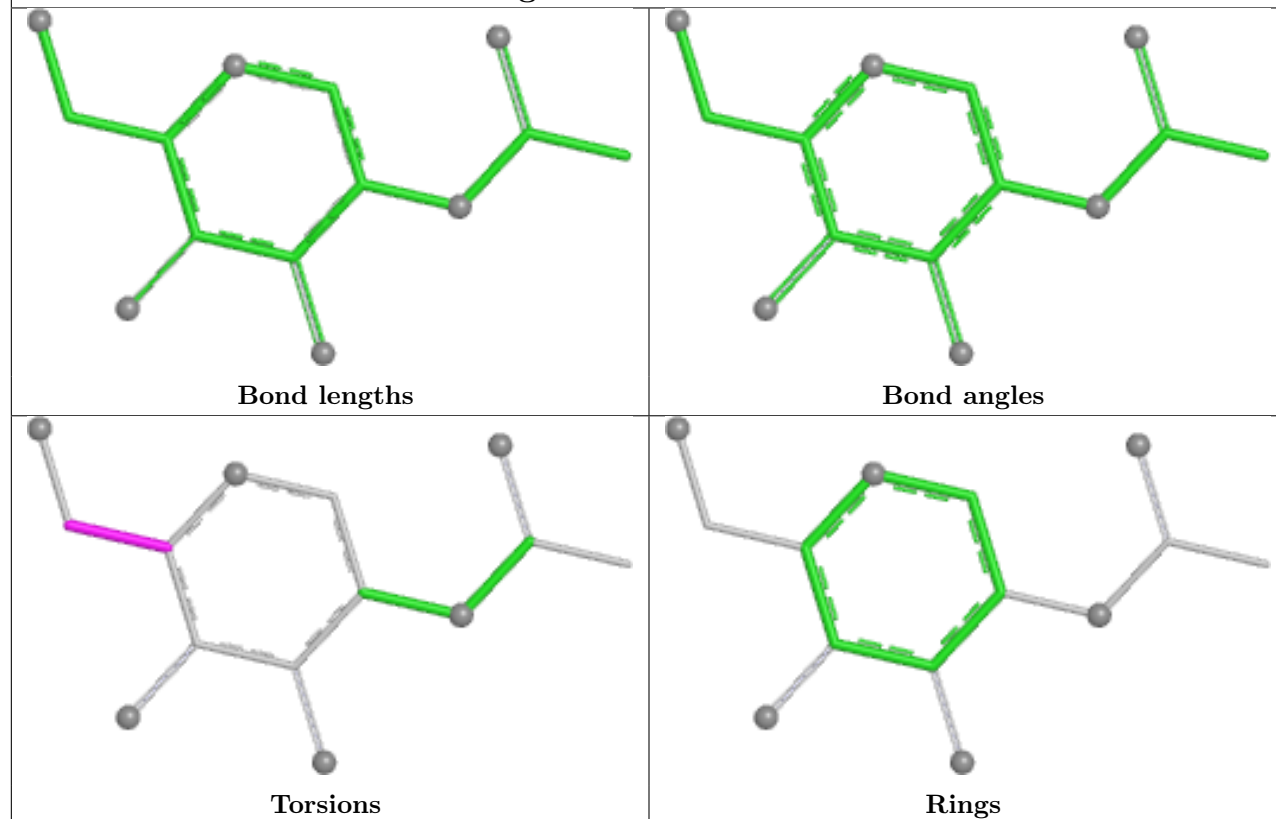
Ligand NAG C 1404



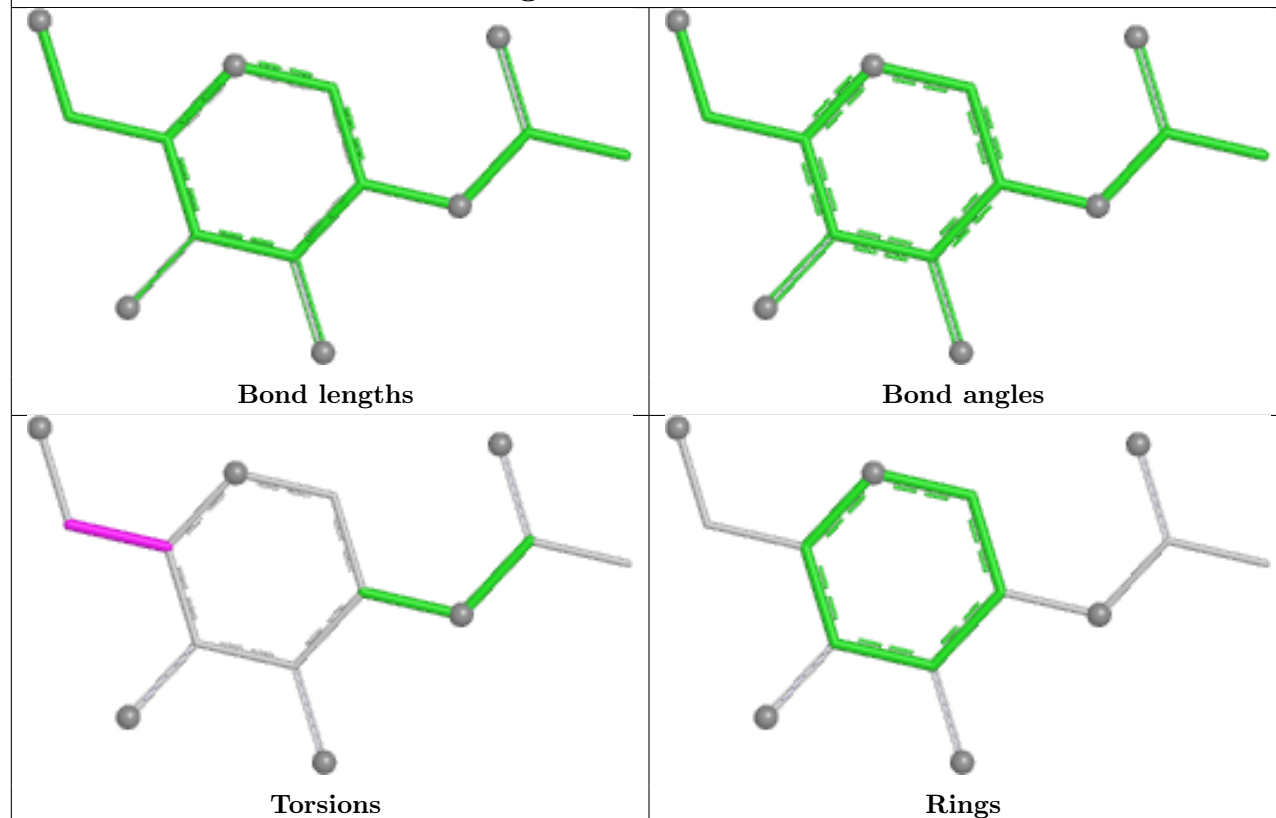
Ligand NAG B 1402



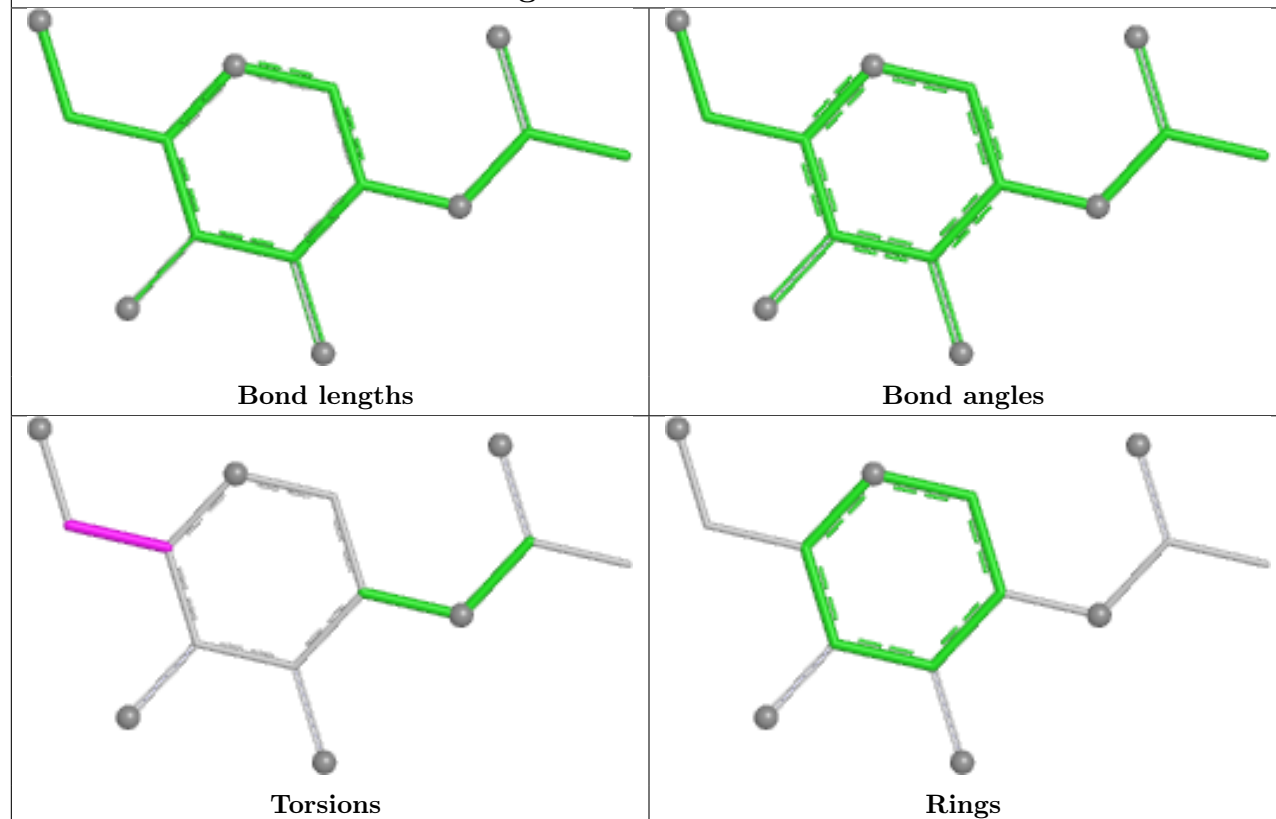
Ligand NAG A 1404



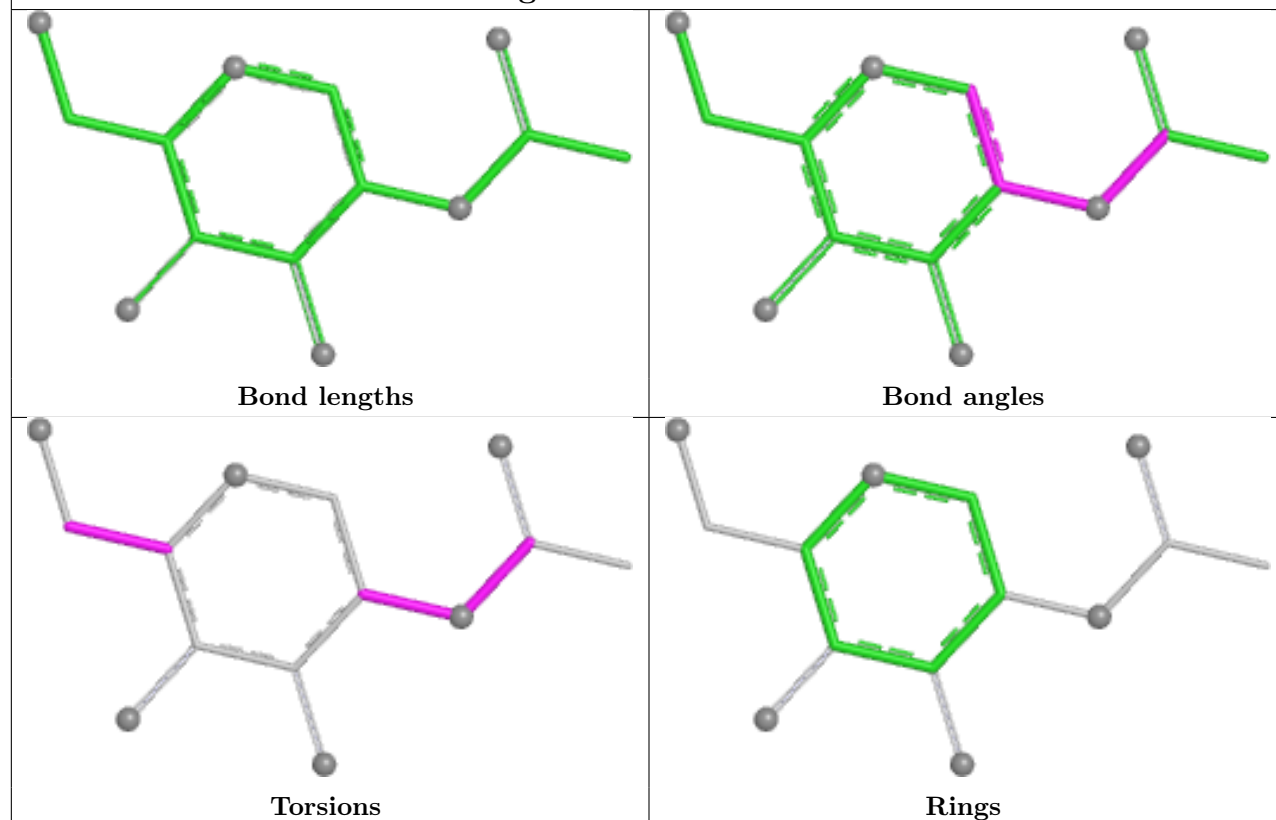
Ligand NAG B 1408



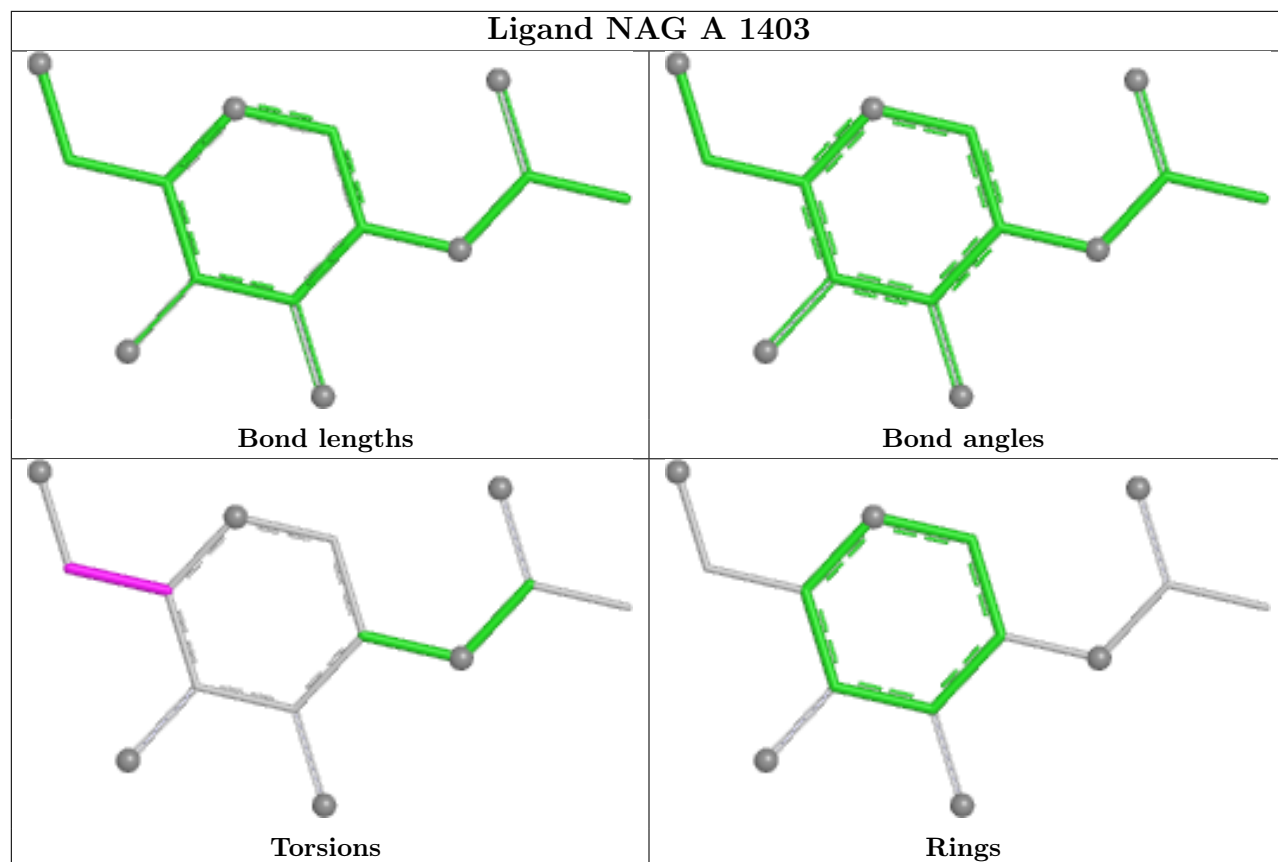
Ligand NAG A 1402



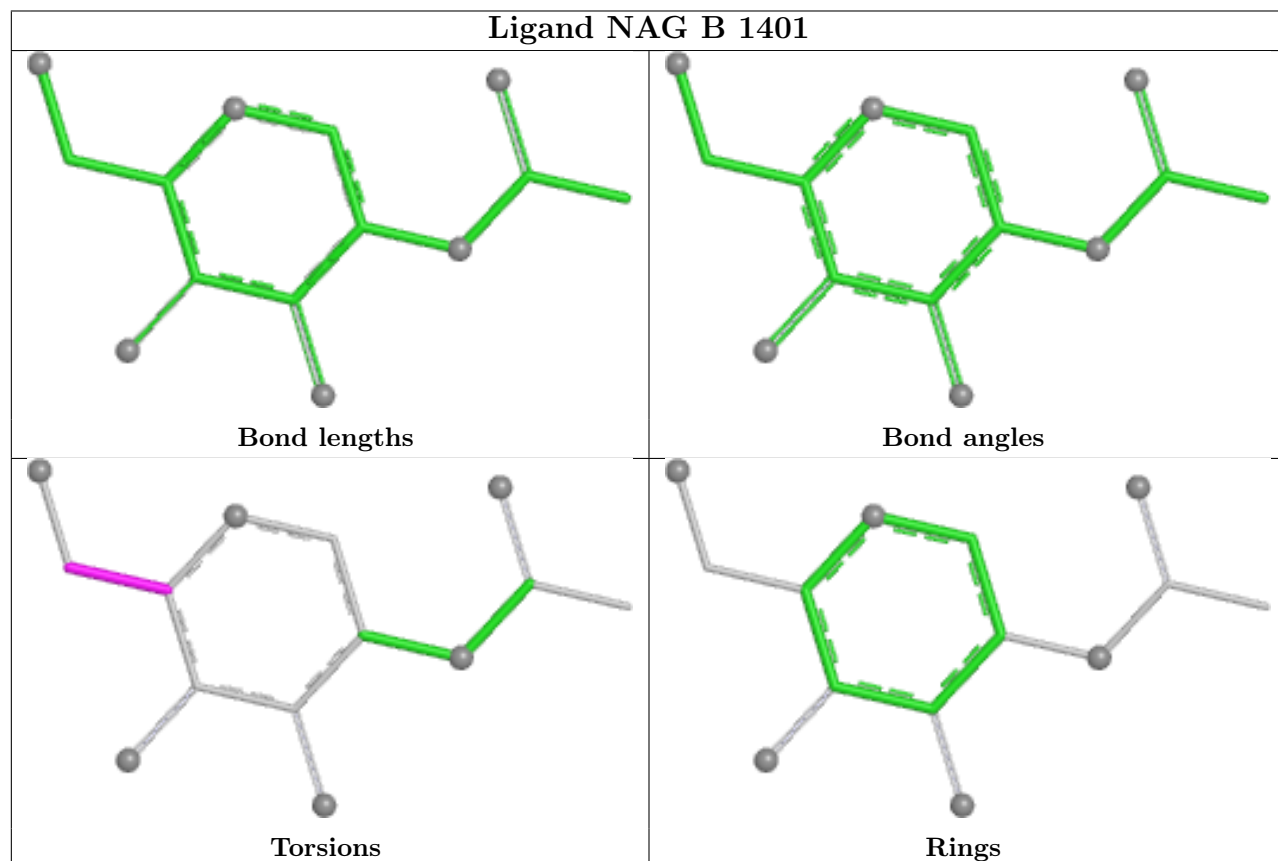
Ligand NAG A 1405

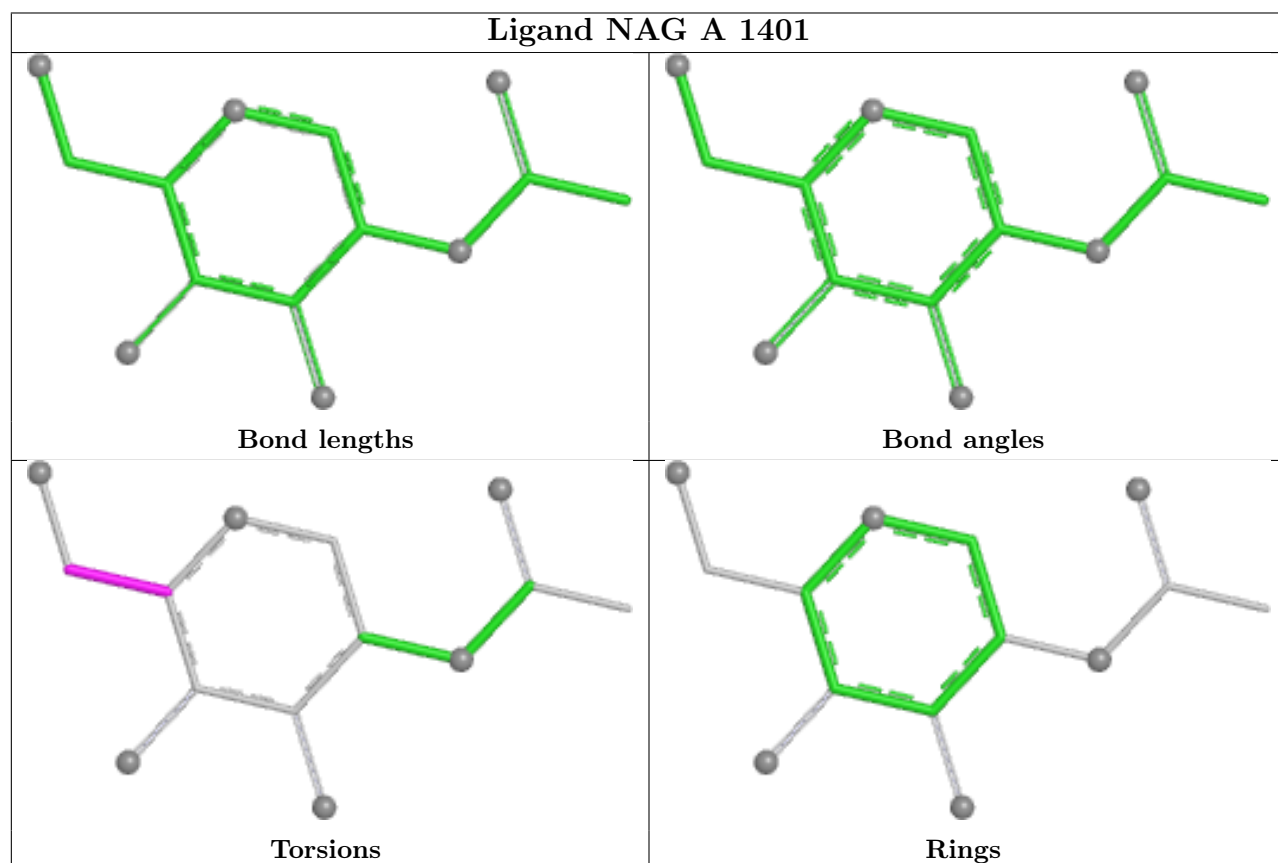
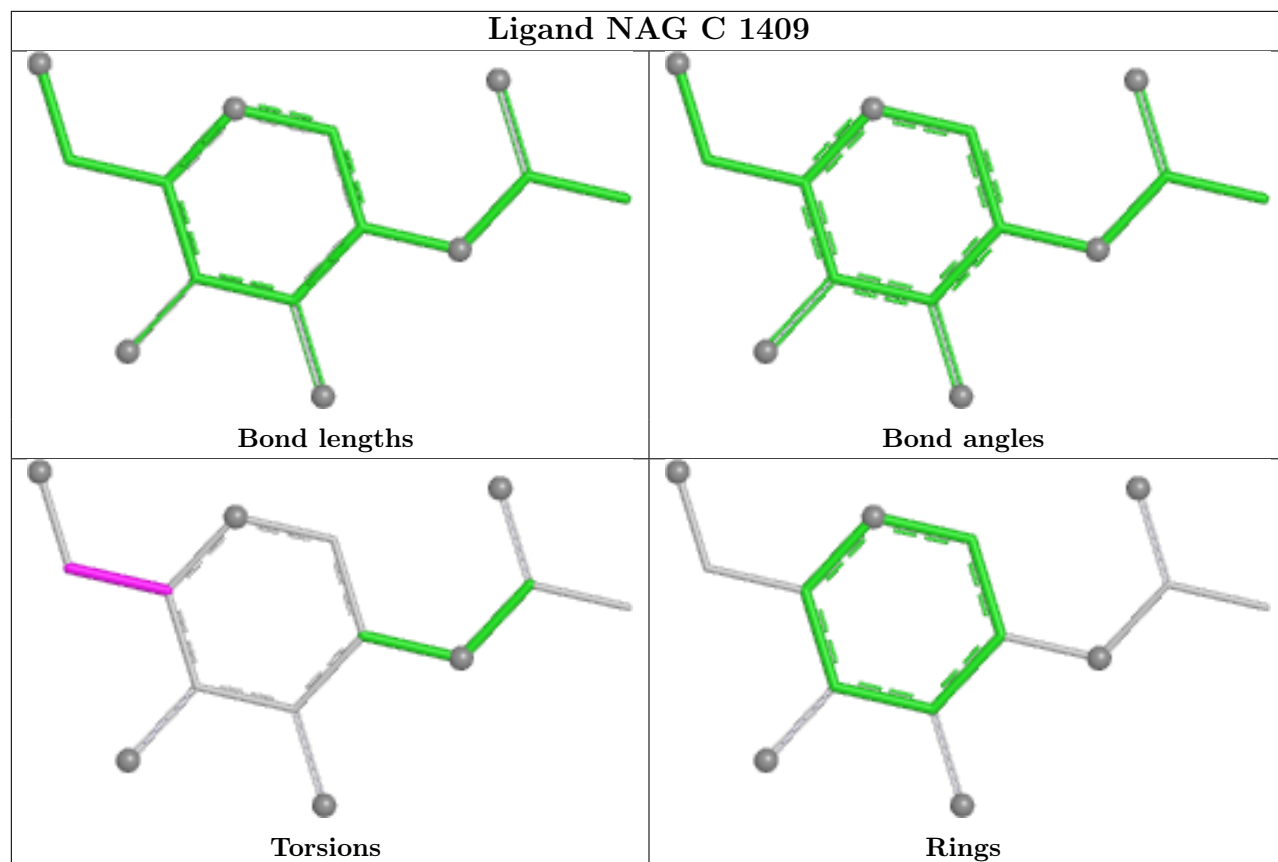


Ligand NAG A 1403

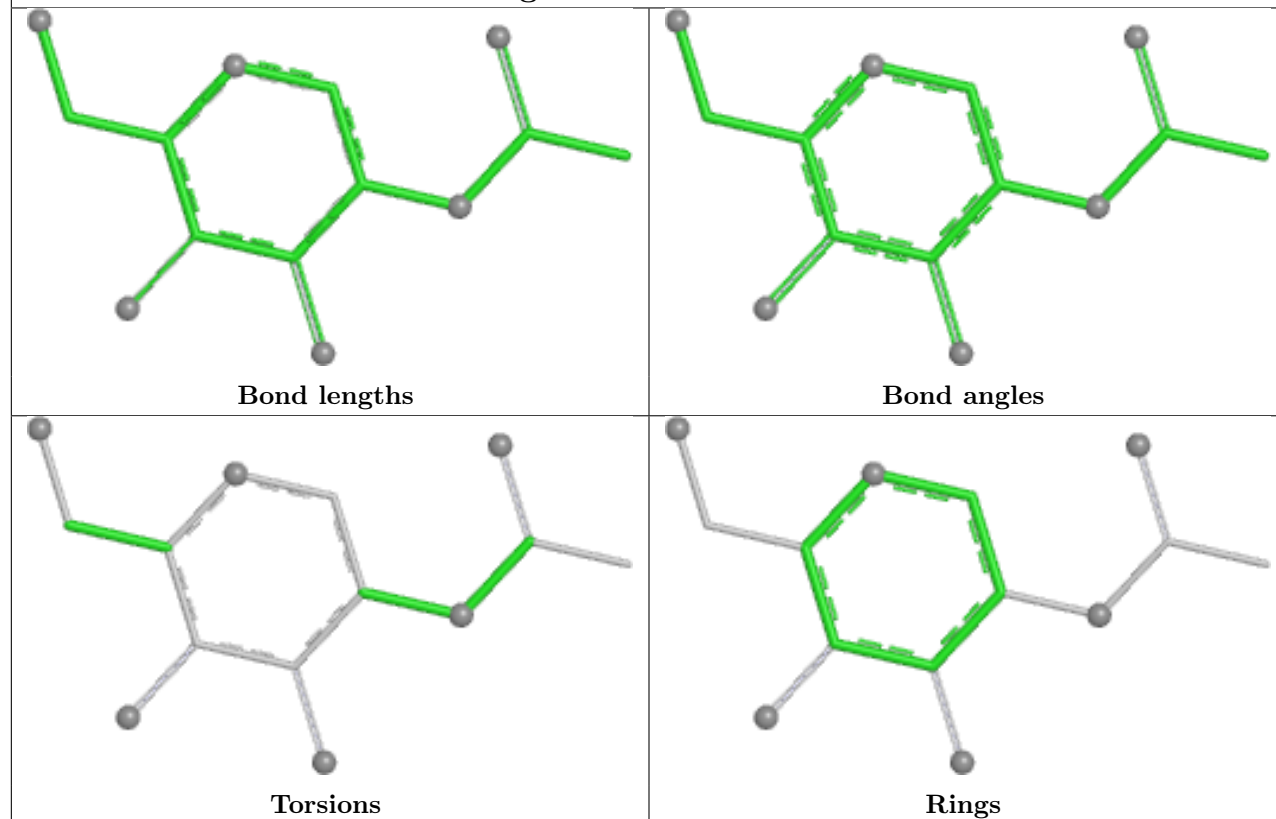


Ligand NAG B 1401

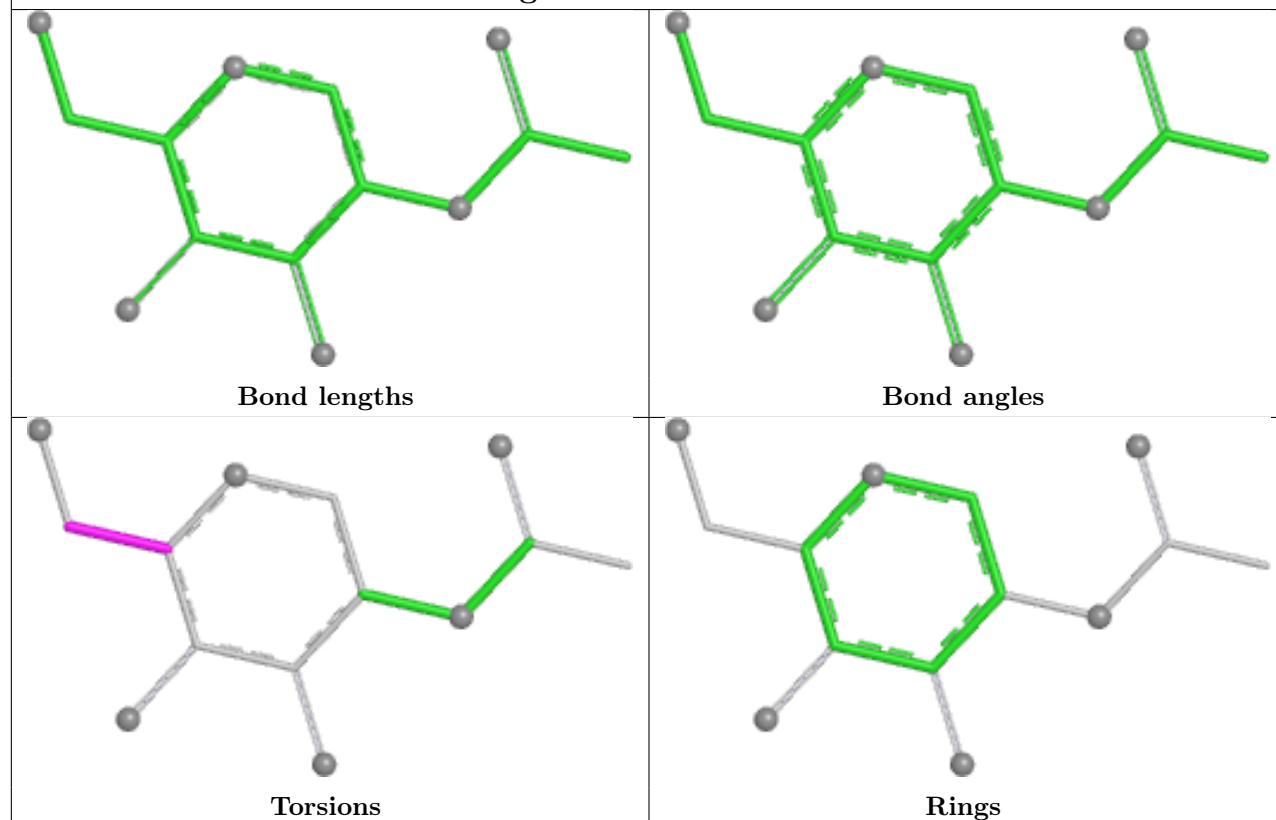




Ligand NAG B 1407



Ligand NAG B 1406



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.

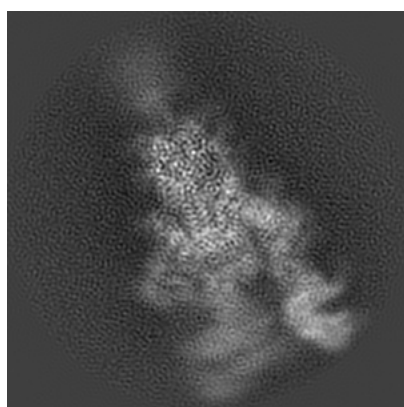
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-30900. These allow visual inspection of the internal detail of the map and identification of artifacts.

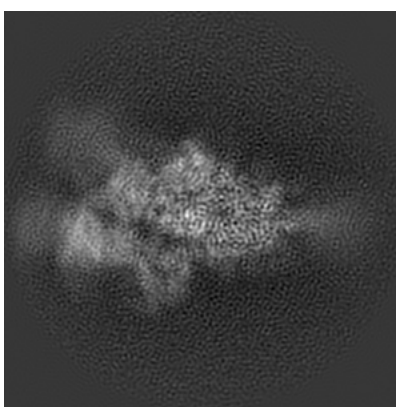
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

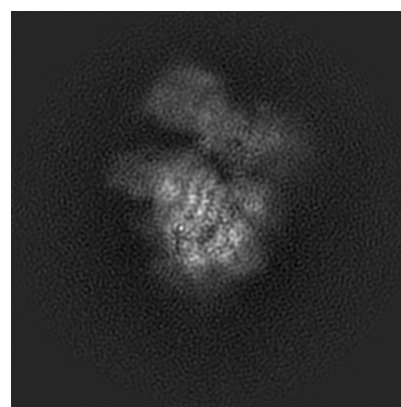
6.1.1 Primary map



X



Y

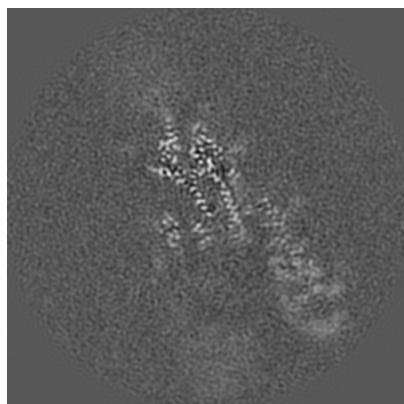


Z

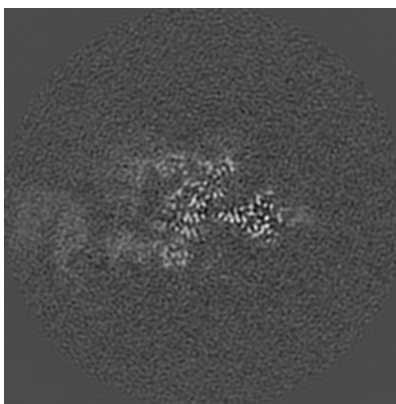
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

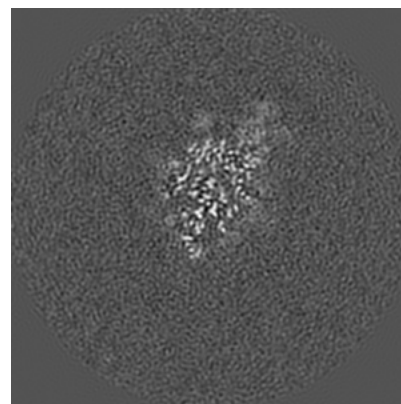
6.2.1 Primary map



X Index: 144



Y Index: 144

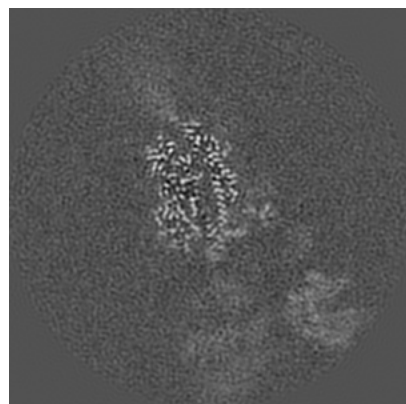


Z Index: 144

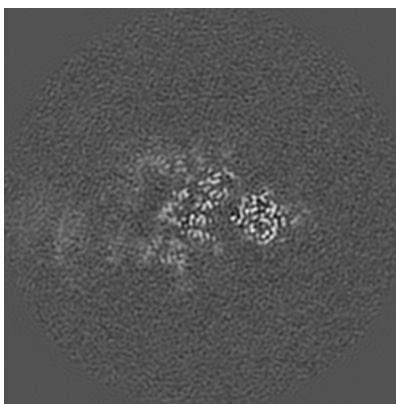
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

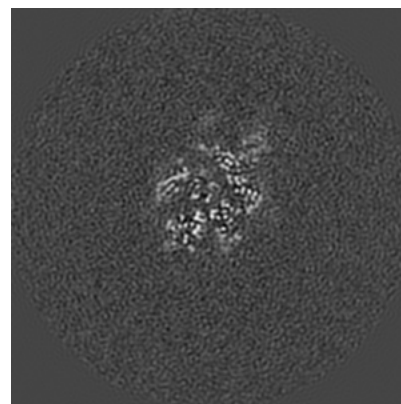
6.3.1 Primary map



X Index: 129



Y Index: 141

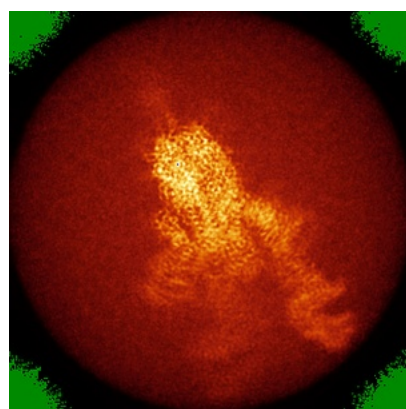


Z Index: 148

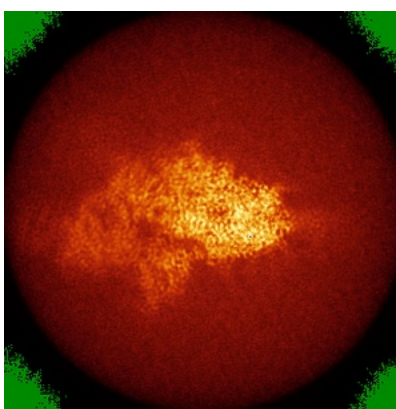
The images above show the largest variance slices of the map in three orthogonal directions.

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

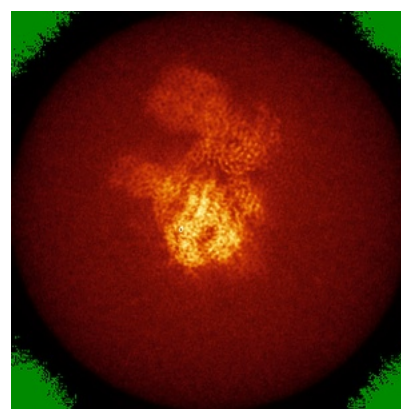
6.4.1 Primary map



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

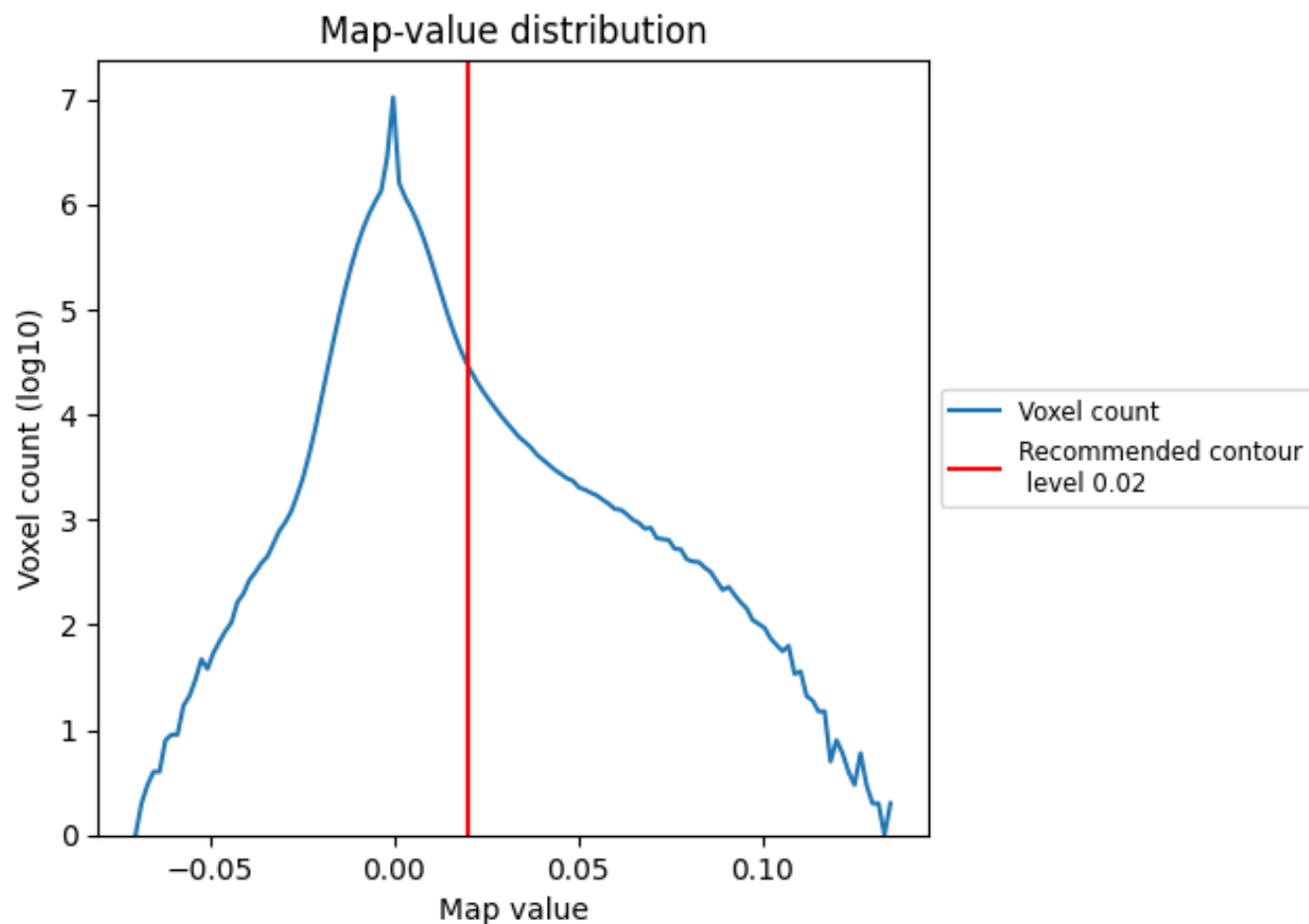
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

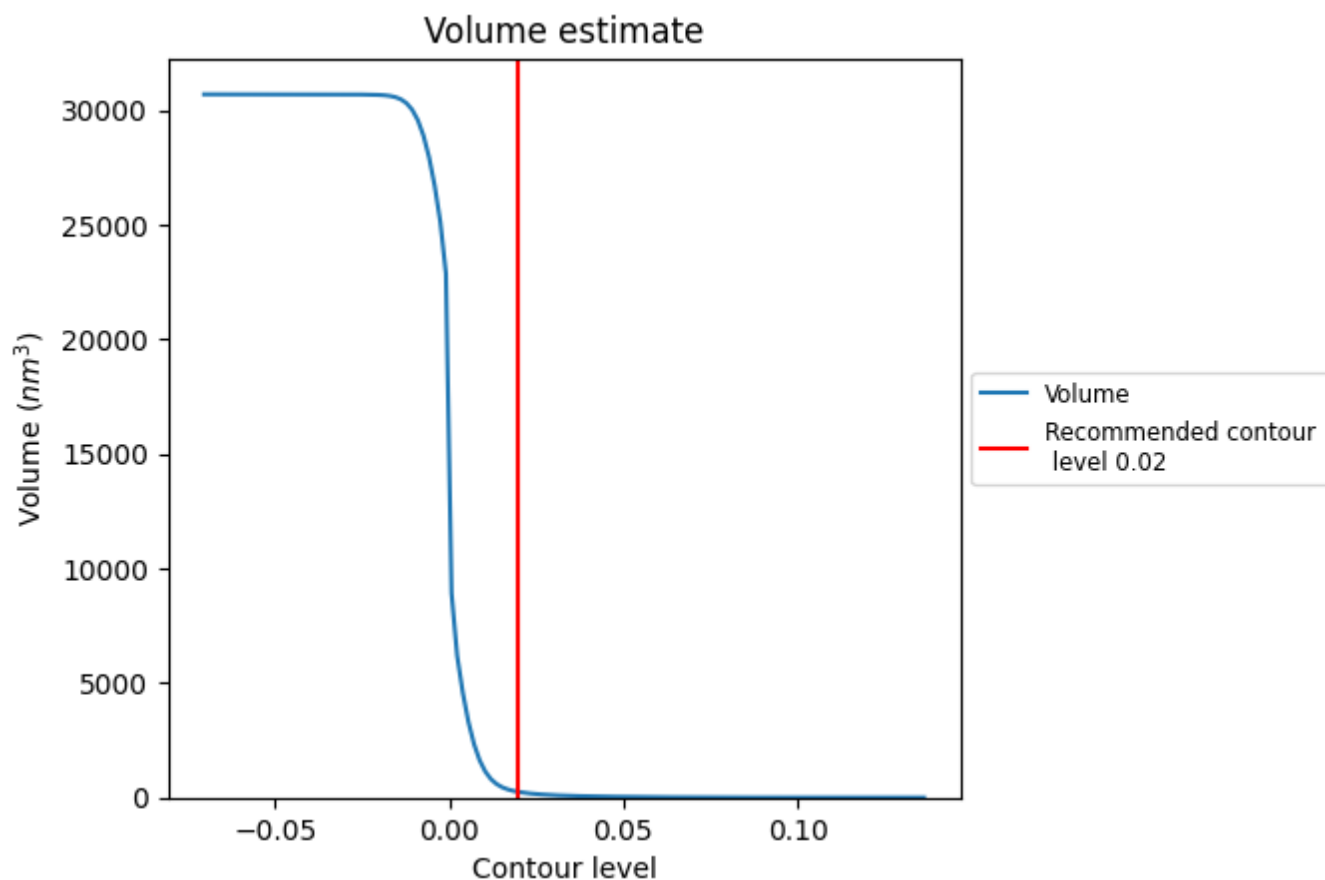
This section contains the results of statistical analysis of the map.

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.

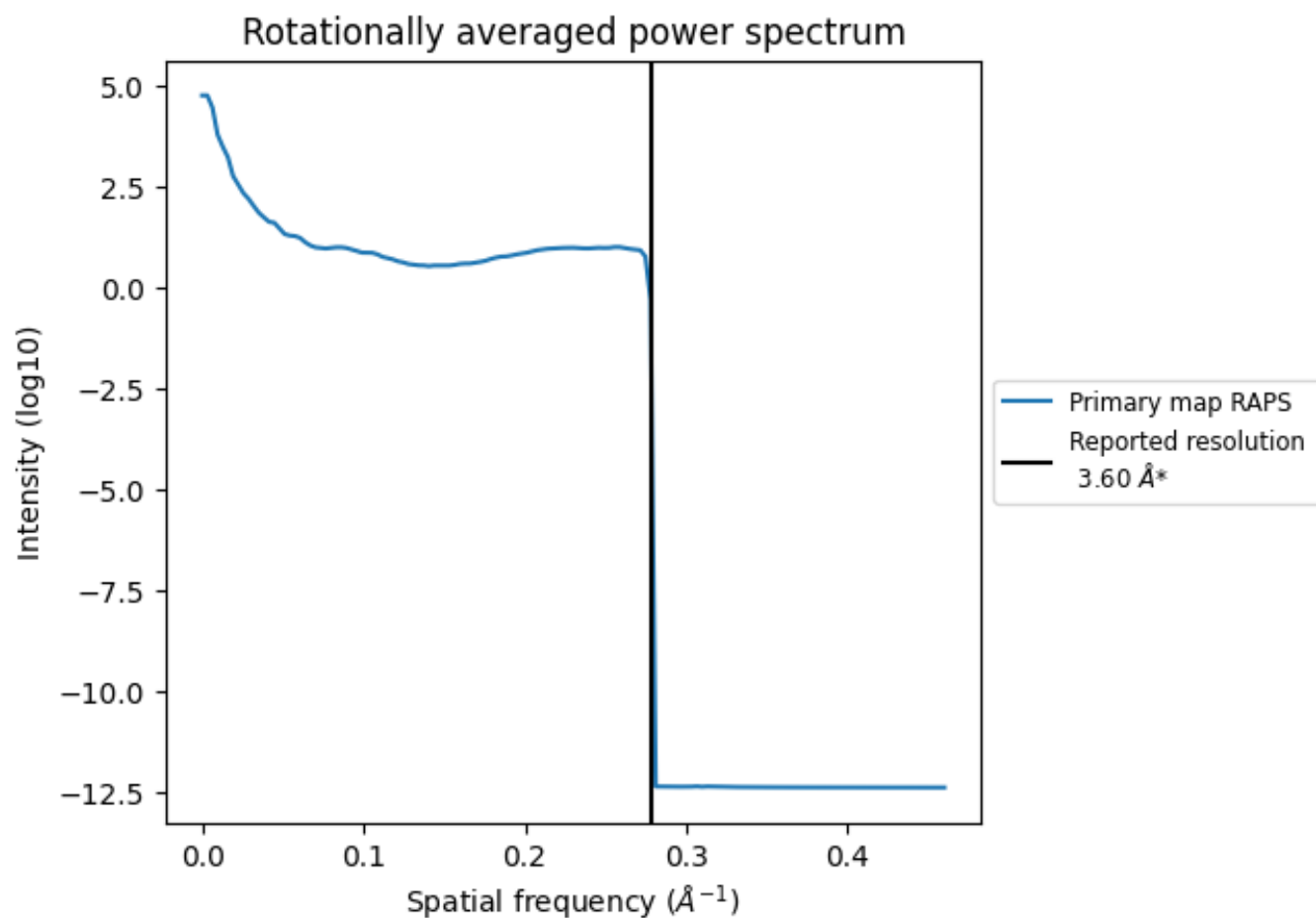
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 245 nm³; this corresponds to an approximate mass of 221 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 0.278 Å⁻¹

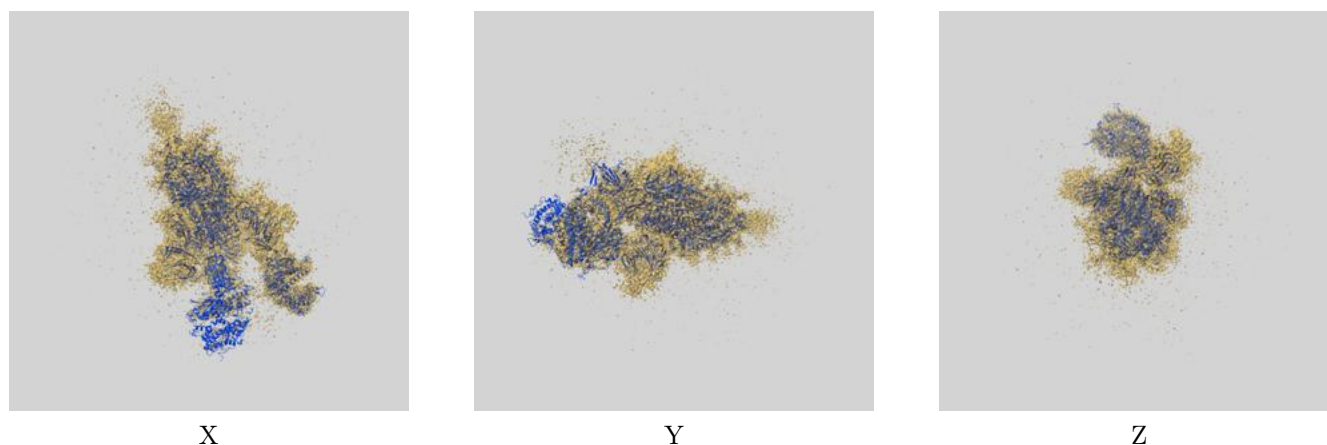
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit [i](#)

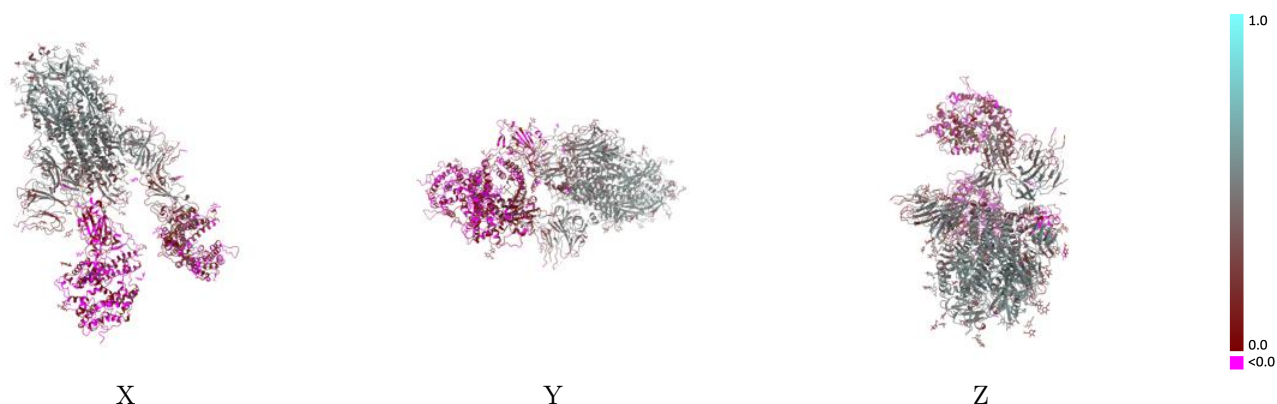
This section contains information regarding the fit between EMDB map EMD-30900 and PDB model 7DX9. Per-residue inclusion information can be found in section [3](#) on page [11](#).

9.1 Map-model overlay [i](#)



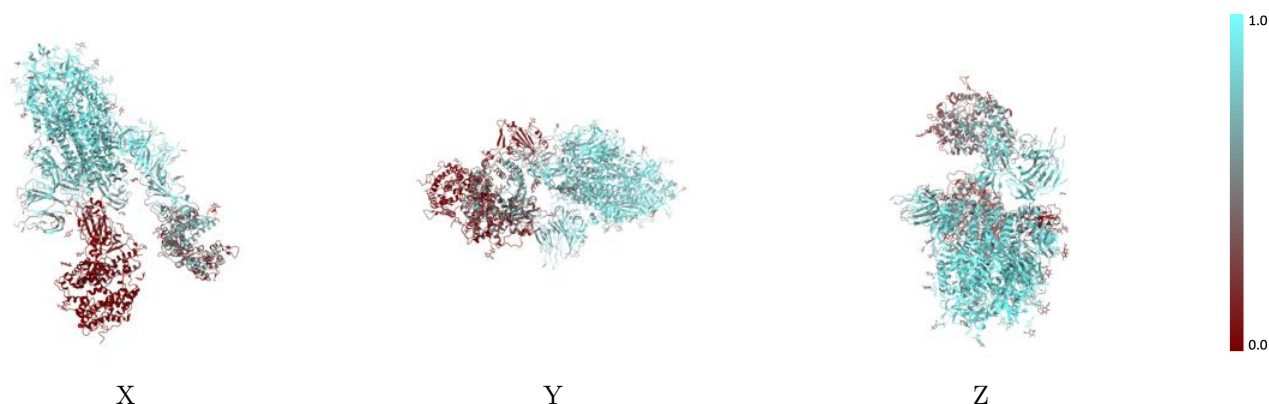
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



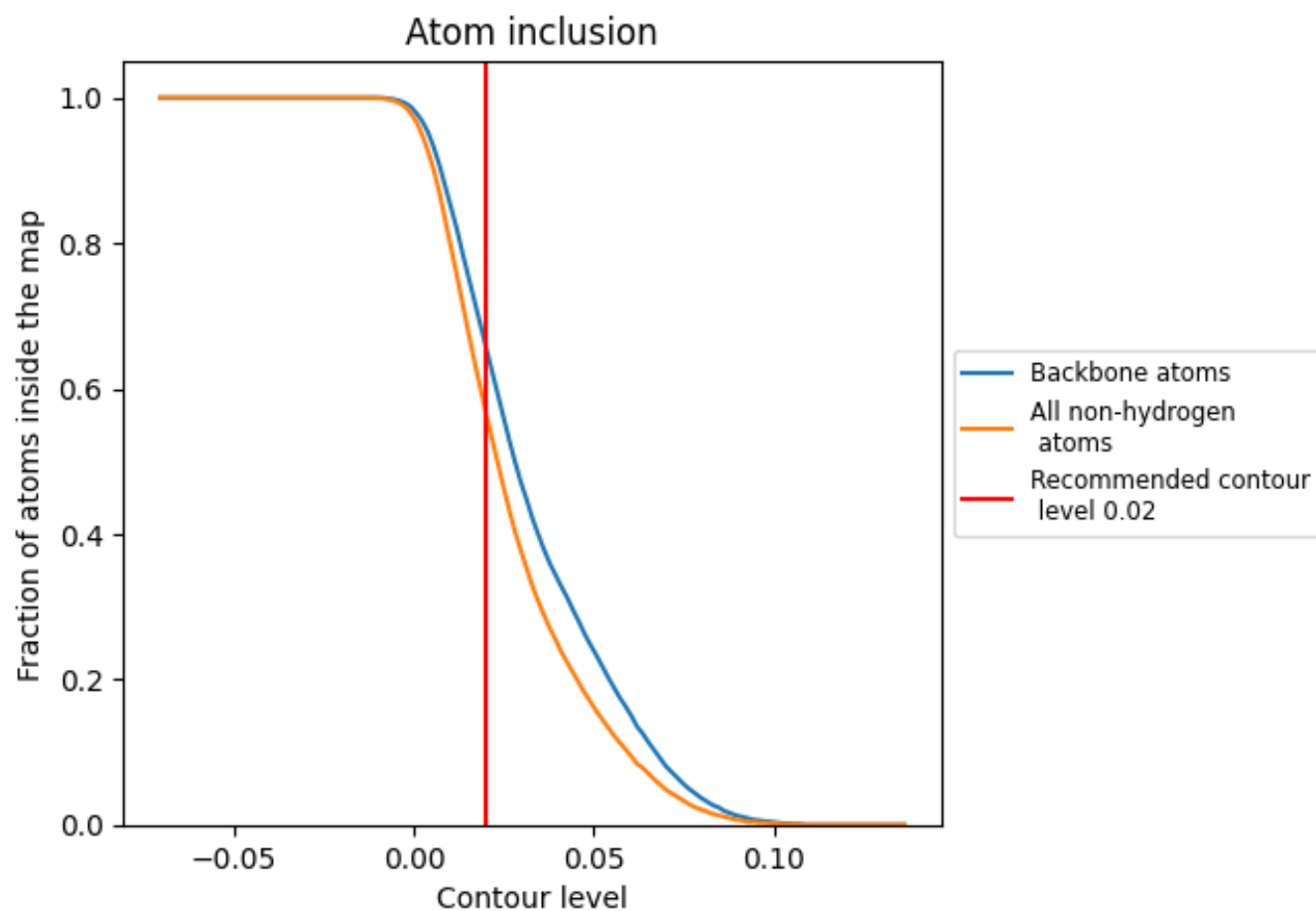
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.02).

9.4 Atom inclusion [i](#)



At the recommended contour level, 66% of all backbone atoms, 57% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5670	 0.2910
A	 0.7760	 0.4190
B	 0.6780	 0.3710
C	 0.6850	 0.3680
D	 0.3980	 0.1150
E	 0.0420	 0.0130
F	 0.7860	 0.3890
G	 0.5000	 0.0770
H	 0.5000	 0.2640
I	 0.7500	 0.4150
J	 0.6790	 0.3990
K	 0.7860	 0.4050
L	 0.6430	 0.3280
M	 0.3930	 0.1670
N	 0.0360	 0.0740
O	 0.4640	 0.2730
P	 0.7140	 0.4250
Q	 0.7140	 0.3730
R	 0.4640	 0.2930
S	 0.8210	 0.4580
T	 0.6430	 0.2690
U	 0.5710	 0.2850
V	 0.4290	 0.2150
W	 0.7860	 0.4330
X	 0.7140	 0.3360
Y	 0.4640	 0.3400
Z	 0.6790	 0.3080
a	 0.6070	 0.2590
b	 0.0360	 -0.0100
c	 0.1430	 -0.0460
d	 0.2860	 0.1590
e	 0.0360	 0.1650
f	 0.0710	 0.1640
g	 0.0000	 0.0170
h	 0.0000	 -0.0710



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Chain	Atom inclusion	Q-score
i	 0.0000	 -0.0430
j	 0.0000	 0.0690
k	 0.0000	 0.0340