



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 11:11 AM UTC

PDB ID : 8HLC / pdb_00008hlc
EMDB ID : EMD-34872
Title : S protein of SARS-CoV-2 in complex with 3711
Authors : Zhang, Y.Y.; Guo, Y.Y.; Zhou, Q.
Deposited on : 2022-11-29
Resolution : 2.80 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:

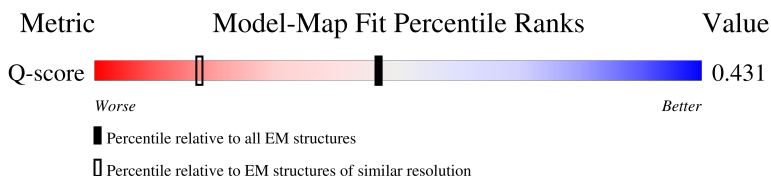
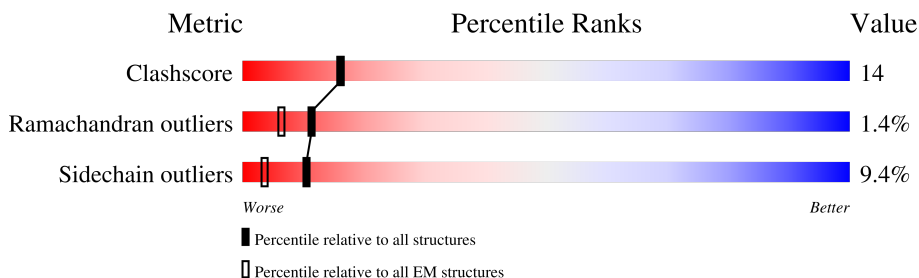
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 2.80 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	11806 (2.30 - 3.30)

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	
1	B	1283	
1	C	1283	
2	H	267	

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Mol	Chain	Length	Quality of chain
2	I	267	73% 60% 22% 15%
2	J	267	81% 60% 22% 15%
3	L	257	57% 65% 16% 17%
3	M	257	64% 65% 16% 17%
3	N	257	76% 64% 17% 17%
4	D	2	50% 100%
4	F	2	50% 50%
4	G	2	50% 100%
4	K	2	50% 50%
4	O	2	50% 100%
4	P	2	50% 50%
4	Q	2	100%
4	R	2	50% 50%
4	S	2	50% 50%
4	T	2	50% 100%
4	V	2	50% 50%
4	W	2	50% 50%
4	X	2	50% 50%
4	Y	2	50% 100%
4	Z	2	100%
4	a	2	50% 50%
4	b	2	50% 100%
4	d	2	100% 50%
4	e	2	50% 50%
4	f	2	50% 50%

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Mol	Chain	Length	Quality of chain
4	g	2	
4	h	2	
4	i	2	
5	E	3	
5	U	3	
5	c	3	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	NAG	A	1303	-	-	X	-
6	NAG	A	1304	-	-	X	-
6	NAG	B	1305	-	-	X	-
6	NAG	B	1306	-	-	X	-
6	NAG	C	1305	-	-	X	-
6	NAG	C	1306	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 36780 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	1081	Total	C	N	O	S	0	0
			8451	5395	1409	1607	40		
1	B	1081	Total	C	N	O	S	0	0
			8451	5395	1409	1607	40		
1	C	1081	Total	C	N	O	S	0	0
			8451	5395	1409	1607	40		

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 heavy chain of 3711.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	228	Total	C	N	O	S	0	0
			1708	1077	288	336	7		
2	I	228	Total	C	N	O	S	0	0
			1708	1077	288	336	7		
2	J	228	Total	C	N	O	S	0	0
			1708	1077	288	336	7		

- Molecule 3 is a protein called light chain of 3711.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	L	214	Total	C	N	O	S	0	0
			1647	1034	277	329	7		
3	M	214	Total	C	N	O	S	0	0
			1647	1034	277	329	7		
3	N	214	Total	C	N	O	S	0	0
			1647	1034	277	329	7		

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



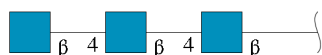
Mol	Chain	Residues	Atoms				AltConf	Trace
4	D	2	Total	C	N	O	0	0
			28	16	2	10		
4	F	2	Total	C	N	O	0	0
			28	16	2	10		
4	G	2	Total	C	N	O	0	0
			28	16	2	10		
4	K	2	Total	C	N	O	0	0
			28	16	2	10		
4	O	2	Total	C	N	O	0	0
			28	16	2	10		
4	P	2	Total	C	N	O	0	0
			28	16	2	10		
4	Q	2	Total	C	N	O	0	0
			28	16	2	10		
4	R	2	Total	C	N	O	0	0
			28	16	2	10		
4	S	2	Total	C	N	O	0	0
			28	16	2	10		
4	T	2	Total	C	N	O	0	0
			28	16	2	10		
4	V	2	Total	C	N	O	0	0
			28	16	2	10		
4	W	2	Total	C	N	O	0	0
			28	16	2	10		
4	X	2	Total	C	N	O	0	0
			28	16	2	10		
4	Y	2	Total	C	N	O	0	0
			28	16	2	10		
4	Z	2	Total	C	N	O	0	0
			28	16	2	10		
4	a	2	Total	C	N	O	0	0
			28	16	2	10		
4	b	2	Total	C	N	O	0	0
			28	16	2	10		
4	d	2	Total	C	N	O	0	0
			28	16	2	10		
4	e	2	Total	C	N	O	0	0
			28	16	2	10		
4	f	2	Total	C	N	O	0	0
			28	16	2	10		
4	g	2	Total	C	N	O	0	0
			28	16	2	10		
4	h	2	Total	C	N	O	0	0
			28	16	2	10		

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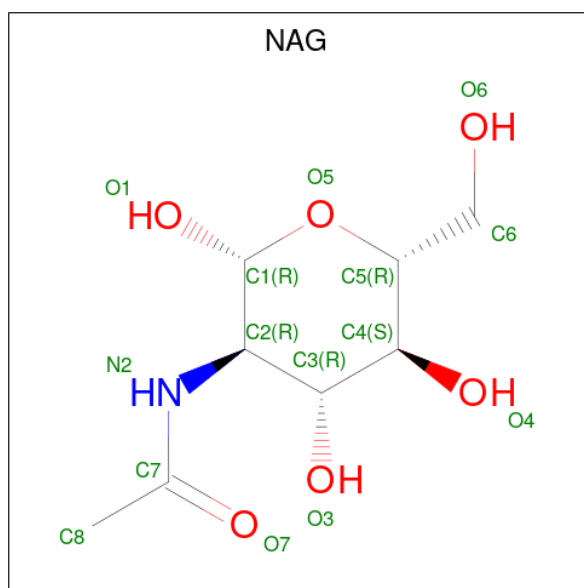
Mol	Chain	Residues	Atoms				AltConf	Trace
4	i	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
5	E	3	Total	C	N	O	0	0
			42	24	3	15		
5	U	3	Total	C	N	O	0	0
			42	24	3	15		
5	c	3	Total	C	N	O	0	0
			42	24	3	15		

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆) (labeled as "Ligand of Interest" by depositor).



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

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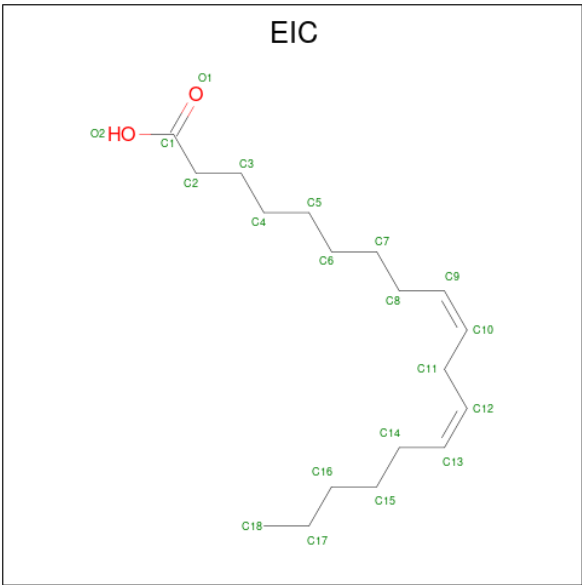
Mol	Chain	Residues	Atoms				AltConf
6	A	1	Total 14	C 8	N 1	O 5	0
6	A	1	Total 14	C 8	N 1	O 5	0
6	A	1	Total 14	C 8	N 1	O 5	0
6	A	1	Total 14	C 8	N 1	O 5	0
6	A	1	Total 14	C 8	N 1	O 5	0
6	A	1	Total 14	C 8	N 1	O 5	0
6	A	1	Total 14	C 8	N 1	O 5	0
6	A	1	Total 14	C 8	N 1	O 5	0
6	B	1	Total 14	C 8	N 1	O 5	0
6	B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

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

- Molecule 7 is LINOLEIC ACID (CCD ID: EIC) (formula: C₁₈H₃₂O₂) (labeled as "Ligand of Interest" by depositor).

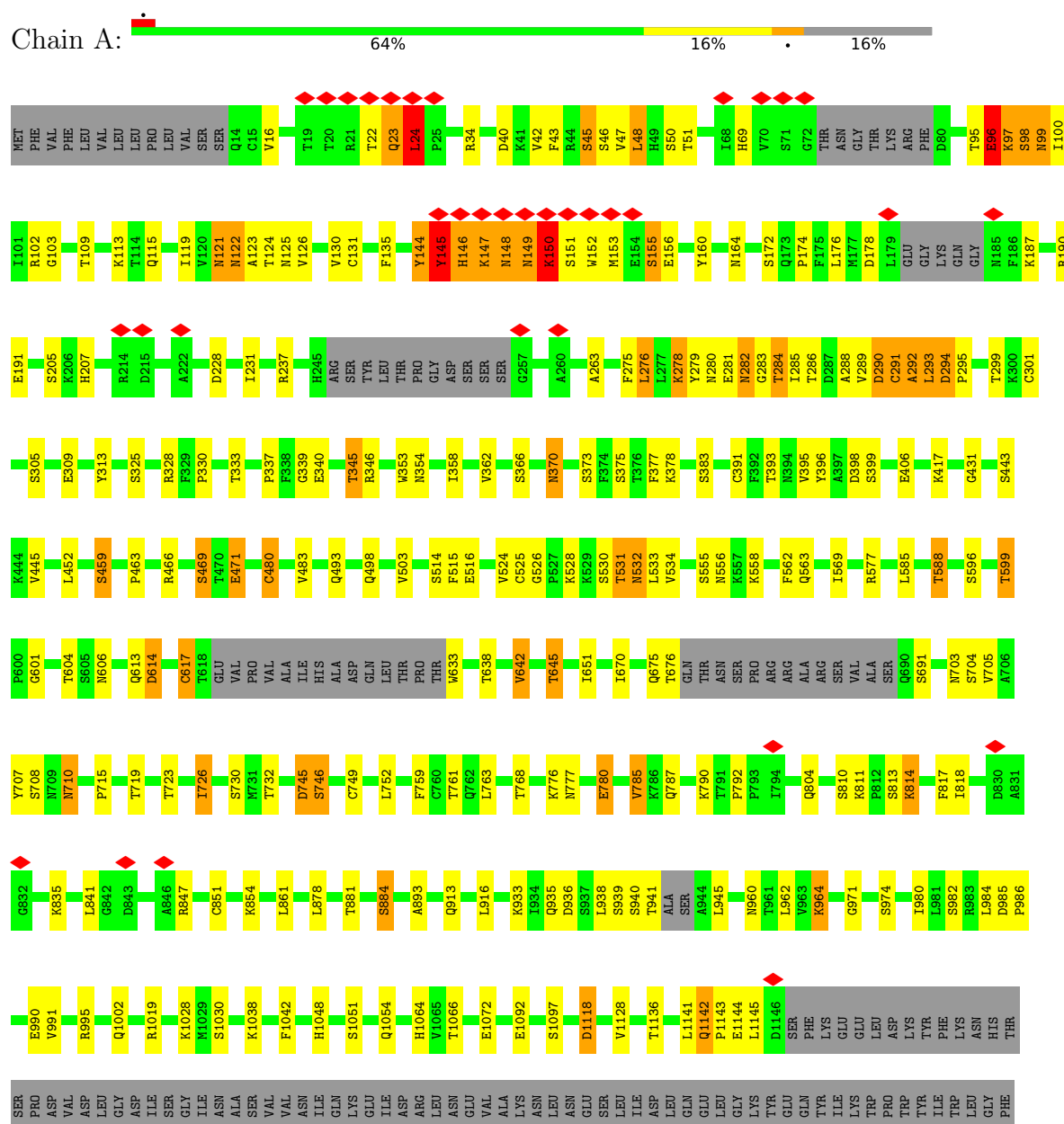


Mol	Chain	Residues	Atoms			AltConf
7	A	1	Total	C	O	0
			20	18	2	
7	B	1	Total	C	O	0
			20	18	2	
7	C	1	Total	C	O	0
			20	18	2	

3 Residue-property plots [i](#)

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



ILE	ALA	GLY	LEU	ILE	ALA	ILE	VAL	MET	THR	ILE	MET	LEU	CYS	CYS	MET	THR	SER	CYS	CYS	SER	CYS	LEU	LYS	GLY	CYS	CYS	SER	CYS	GLY	SER	CYS	ASP	GLU	ASP	ASP	GLU	PRO	VAL	LEU	LYS	VAL	LYS	LEU	HIS	TYR	THR	LEU	GLY	GLU	ASP	TYR	LYS	ASP	ASP
ASP	ASP	LYS																																																				

- Molecule 1: Spike glycoprotein

Chain B:



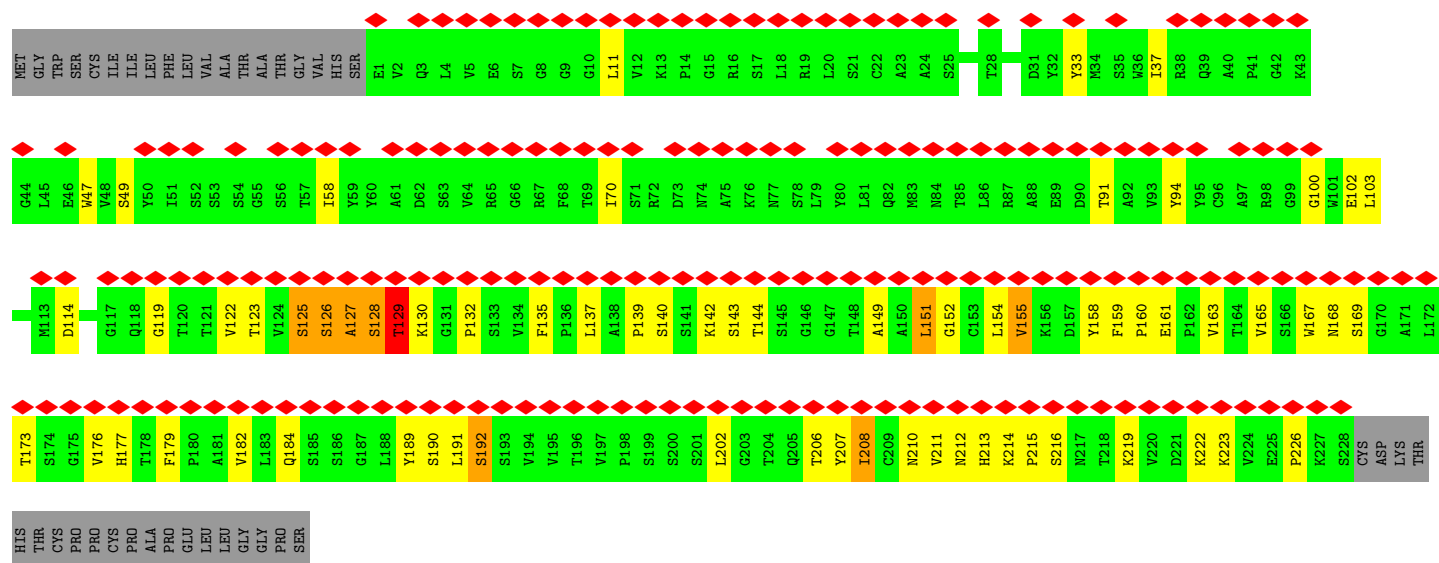
ASP LYS	ALA GLY	PRO ASP	P986	A829 D830	Q690 S691	L585	K417	A292 L293	K187	S98 N99
ALA LEU	ILE ASP	VAL ASP	E990 V991	K835	N703 S704	T588	L425	D294 E191	R190 E191	I100 PHE
ALA LEU	ALA LEU	ASP LEU	R995	L841	V705	S596	G431	T299 K300	D198 G103	R102 VAL
VAL ASP	ILE ASP	GLY ASP	R986	L841	V705	S596	G431	T299 K300	D198 G103	R102 VAL
MET VAL	MET VAL	ILE SER	Q1002	A845 A846	S708 N709	T599 P600	S443 K444	C301 F306	S205 H207	T109 LEU
VAL SER	VAL SER	GLY SER	R1019	A846	N710	G601	V445	F306	K113 LEU	VAL SER
ILE ASN	ILE ASN	ILE ASN	R847	R847	T719	T604	S459	E309	T114 Q115	SER
MET ASN	MET ASN	ASN ASN	K1028	C851	T719	S605	K462	Y313	L212 V213	Q14 C15
LEU SER	LEU SER	ALA SER	H1029	S1030	T723	N606	P463	E214	R214 V16	
CYS VAL	CYS VAL	VAL VAL	F1042	K854	I726	Q613	R466	S325	E224 G228	T19 T20
MET ASN	MET ASN	ASN ASN	H1048	L861	I726	D614	R466	S325	E224 G228	T19 T20
CYS GLN	CYS GLN	GLN LYS	S1051	L878	S730	T618	S469	T333	A123 T124	
CYS LYS	CYS LYS	LYS LYS	S1051	L878	M731	GLU	T470	T333	D228 L229	
SER GLY	SER GLY	GLY LYS	T881	T732	T732	VAL	E471	P337	P230 I231	T22
CYS ILE	CYS ILE	ILE ASP	Q1054	D745 S746	D745 S746	PRO VAL	C480 H481	F338 G339	R237 C131	Q23
LEU ASP	LEU ASP	ARG ASP	P1057	S884	S746	ALA	G482	E340	V130 C131	Q23
GLY ASN	GLY ASN	LEU ASN	H1064	A893	C749	ILE	V483	E340	V130 C131	L24
CYS GLY	CYS GLY	ASN GLY	H1064	A893	C749	ILE	V483	E340	V130 C131	L24
CYS GLY	CYS GLY	GLY GLY	V1065	Q913	L752	ALA	Q493	H245 R346	F135 ARG	R34
VAL GLY	VAL GLY	GLY GLY	T1066	L916	T761	ASP	V503	Y351 A352	Y144 Y145	Y37
ILE ASN	ILE ASN	ASN ASN	E1092	L916	T761	GLN	V503	Y351 A352	Y144 Y145	Y37
CYS LEU	CYS LEU	LEU ASN	S1097	K333	T768	THR	S514	N354	H146 K147	P39
CYS ASN	CYS ASN	ASN ASN	S1097	K333	T768	THR	S514	N354	H146 K147	P39
LYS GLY	LYS GLY	GLY GLY	D1118	I834	K776	THR	E516	I358	N148 N149	V42
PHE SER	PHE SER	SER SER	V1128	Q935	N777	W633	V524	V362	ASP SER	F43
ASP GLY	ASP GLY	ILE ASP	T1136	S937	E780	T638	C525	V362	SER SER	S45
ASP LEU	ASP LEU	ASP LEU	T1136	S939	E780	T638	G526	S366	SER SER	S46
GLN GLY	GLN GLY	GLN GLY	L1141	S940	V785	V642	P527	N370	G257 W258	L48
GLY GLY	GLY GLY	GLY GLY	Q1142	ALA	K786	T645	K528	N370	G257 W258	H49
PRO VAL	PRO VAL	LEU GLY	P1143	A944	K790	I651	K529	S373	T259 A260	S50
LEU LYS	LEU LYS	LYS TYR	E1144	L945	T791	T531	N532	S375	G261 A262	S50
LYS GLY	LYS GLY	TYR GLY	L1145	P792	P793	I670	L533	F375	A262 A263	T51
GLY GLY	GLY GLY	GLY GLY	D1146	L959	P793	T675	V534	K378	A263 A263	L54
VAL GLY	VAL GLY	GLY GLY	SER	N960	I794	T676	K378	K378	L276 L277	H69
LYS LEU	LYS LEU	TYR ILE	PHE	T961	Q804	GLN	K337	S383	L276 L277	V70
HIS TYR	HIS TYR	ILE TRP	GLU	L962	Q804	THR	S555	C391	K278 Y279	S71
TRP PRO	TRP PRO	TRP PRO	GLY	V963	S810	ASN	N556	F392	N280 G173	G72
TRP TRP	TRP TRP	TRP TRP	LEU	K964	K811	SER	K557	N393	N280 G173	
LYS TYR	LYS TYR	TRP TRP	ASP	G971	P812	PRO	K558	N394	N282 G173	
ASP PHE	ASP PHE	TRP TRP	LYS	S974	S813	ARG	F562	V395	L176 G283	ASN
ASP LYS	ASP LYS	TRP TRP	TYR	S974	K814	ALA	Q563	Y396	T284 D178	THR
ASN GLY	ASN GLY	TRP TRP	PHE	S974	K814	ALA	Q563	Y396	T284 D178	GLY
LYS PHE	LYS PHE	TRP TRP	LYS	I980	F817	ARG	I569	A397	L179 G179	ARG
ASP PHE	ASP PHE	TRP TRP	HIS	L861	I818	SER	I569	S399	D287 A288	PHE
ASP ASP	ASP ASP	GLY PHE	THR	S982	V826	ALA	R577	E406	GLY GLY	D80
ASP ASP	ASP ASP	GLY PHE	SER	S983	V826	ALA	R577	E406	GLY GLY	D80
		ILE		L984	D985	SER			LYS GLN	T95
				D985	D985				C291 F186	K97

- Molecule 1: Spike glycoprotein

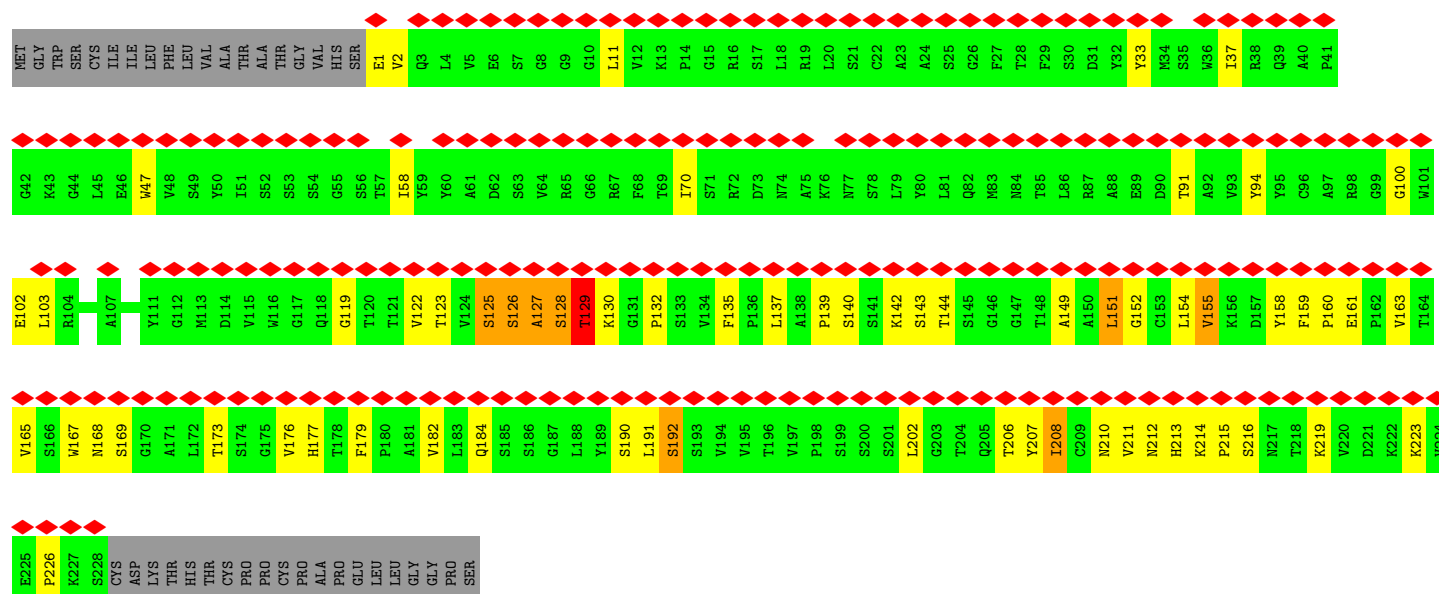
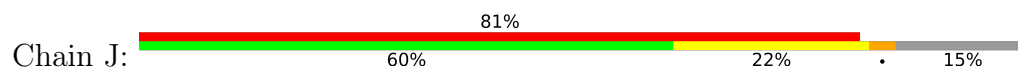
Chain C:



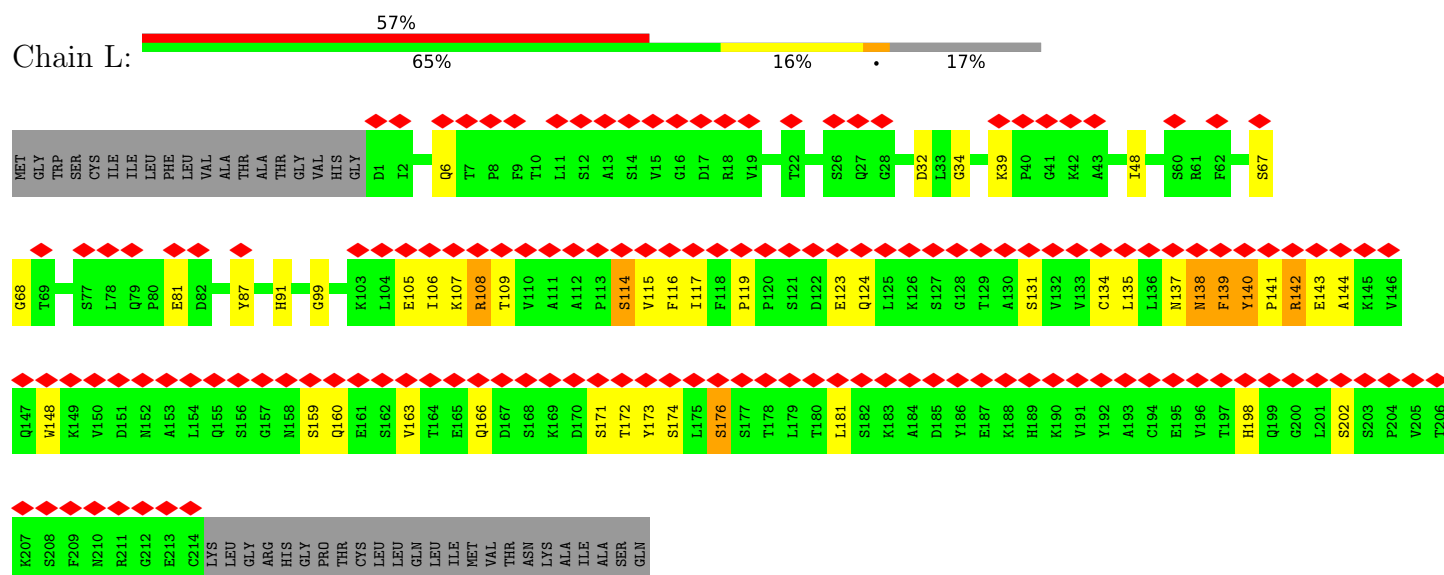
- Molecule 2: heavy chain of 3711



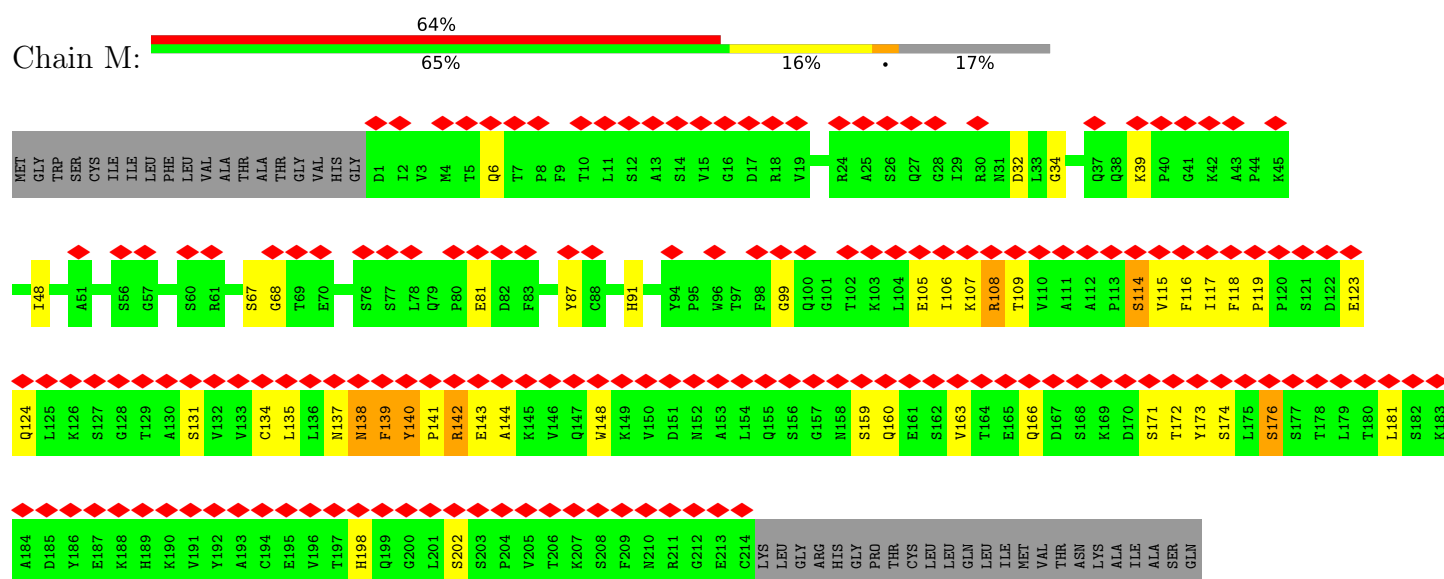
- Molecule 2: heavy chain of 3711



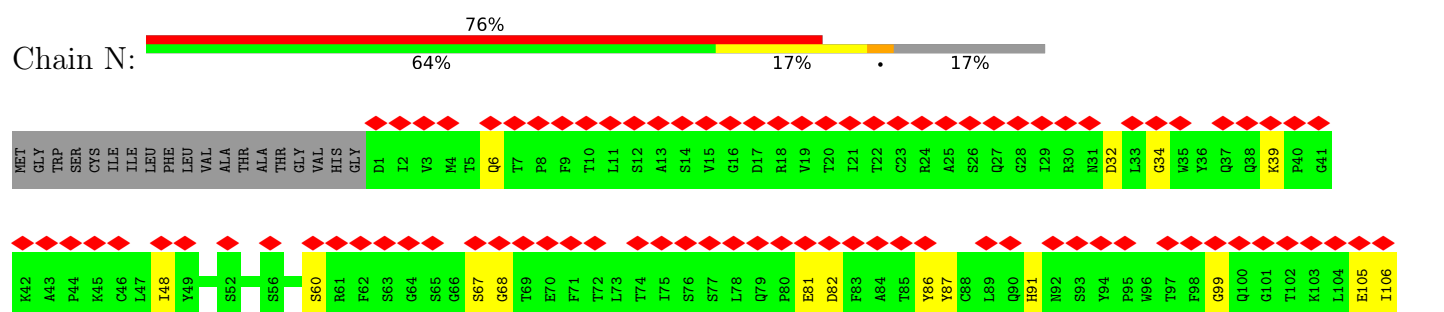
- Molecule 3: light chain of 3711

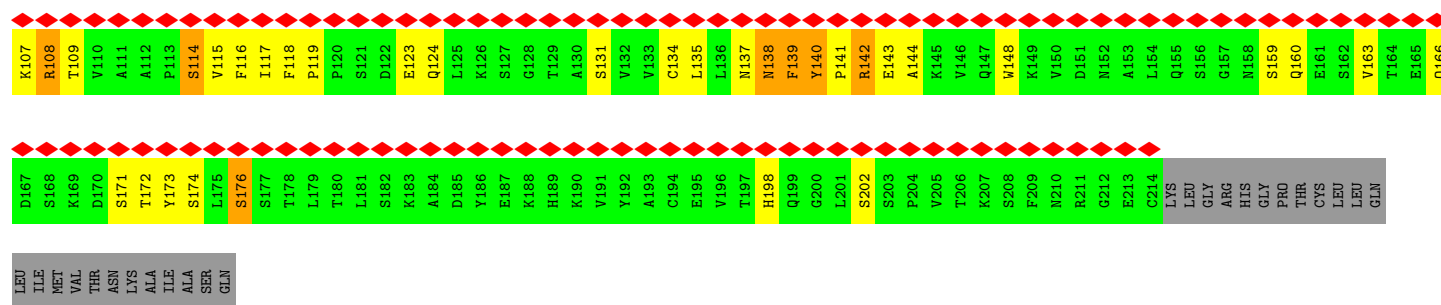


- Molecule 3: light chain of 3711



- Molecule 3: light chain of 3711





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



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



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



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



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





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



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



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



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



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



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





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



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



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



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



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



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





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



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



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



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



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



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





- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-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	175006	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)	1200	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.252	Depositor
Minimum map value	-0.129	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.007	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, EIC

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.35	0/8646	0.52	1/11767 (0.0%)
1	B	0.35	0/8646	0.52	1/11767 (0.0%)
1	C	0.35	0/8646	0.52	2/11767 (0.0%)
2	H	0.26	0/1749	0.59	0/2379
2	I	0.26	0/1749	0.59	0/2379
2	J	0.26	0/1749	0.59	0/2379
3	L	0.36	0/1684	0.60	0/2287
3	M	0.36	0/1684	0.60	0/2287
3	N	0.36	0/1684	0.60	0/2287
All	All	0.34	0/36237	0.54	4/49299 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	847	ARG	N-CA-C	-5.43	107.66	114.56
1	B	847	ARG	N-CA-C	-5.43	107.66	114.56
1	A	847	ARG	N-CA-C	-5.41	107.69	114.56
1	C	278	LYS	N-CA-C	-5.36	102.11	110.42

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	8451	0	8216	227	0
1	B	8451	0	8216	223	0
1	C	8451	0	8214	204	0
2	H	1708	0	1672	68	0
2	I	1708	0	1672	72	0
2	J	1708	0	1672	70	0
3	L	1647	0	1604	60	0
3	M	1647	0	1604	60	0
3	N	1647	0	1604	64	0
4	D	28	0	25	0	0
4	F	28	0	25	5	0
4	G	28	0	25	0	0
4	K	28	0	25	0	0
4	O	28	0	25	1	0
4	P	28	0	25	6	0
4	Q	28	0	25	0	0
4	R	28	0	25	1	0
4	S	28	0	25	0	0
4	T	28	0	25	0	0
4	V	28	0	25	6	0
4	W	28	0	25	2	0
4	X	28	0	25	0	0
4	Y	28	0	25	1	0
4	Z	28	0	25	0	0
4	a	28	0	25	0	0
4	b	28	0	25	0	0
4	d	28	0	25	3	0
4	e	28	0	25	1	0
4	f	28	0	25	0	0
4	g	28	0	25	1	0
4	h	28	0	25	0	0
4	i	28	0	25	0	0
5	E	42	0	37	2	0
5	U	42	0	37	2	0
5	c	42	0	37	2	0
6	A	140	0	129	15	0
6	B	196	0	179	22	0
6	C	196	0	179	22	0
7	A	20	0	31	4	0
7	B	20	0	31	4	0
7	C	20	0	31	2	0
All	All	36780	0	35740	1030	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 14.

All (1030) 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)
6:C:1313:NAG:O4	6:C:1314:NAG:C1	1.69	1.38
6:A:1309:NAG:O4	6:A:1310:NAG:C1	1.69	1.37
6:B:1313:NAG:O4	6:B:1314:NAG:C1	1.69	1.36
6:B:1305:NAG:O4	6:B:1306:NAG:C1	1.86	1.24
6:A:1303:NAG:O4	6:A:1304:NAG:C1	1.86	1.23
1:A:463:PRO:HB2	1:B:198:ASP:OD1	1.36	1.23
6:C:1305:NAG:O4	6:C:1306:NAG:C1	1.86	1.22
1:C:24:LEU:HD11	1:C:69:HIS:CD2	1.83	1.13
1:B:24:LEU:HD11	1:B:69:HIS:CD2	1.82	1.13
2:I:11:LEU:HD12	2:I:159:PHE:CZ	1.83	1.13
1:A:24:LEU:HD11	1:A:69:HIS:CD2	1.82	1.13
2:J:11:LEU:HD12	2:J:159:PHE:CZ	1.83	1.12
2:H:11:LEU:HD12	2:H:159:PHE:CZ	1.83	1.12
1:A:339:GLY:HA3	4:P:1:NAG:H82	1.31	1.10
1:B:339:GLY:HA3	6:B:1302:NAG:H82	1.31	1.09
3:M:114:SER:HB2	3:M:116:PHE:CZ	1.89	1.08
3:N:114:SER:HB2	3:N:116:PHE:CZ	1.89	1.08
3:L:114:SER:HB2	3:L:116:PHE:CZ	1.89	1.07
1:C:339:GLY:HA3	6:C:1302:NAG:H82	1.31	1.07
1:B:358:ILE:CD1	7:B:1315:EIC:H182	1.84	1.07
1:B:124:THR:O	1:B:125:ASN:ND2	1.88	1.06
1:A:124:THR:O	1:A:125:ASN:ND2	1.88	1.06
1:C:124:THR:O	1:C:125:ASN:ND2	1.88	1.06
1:A:95:THR:HG22	1:A:187:LYS:HE2	1.37	1.05
1:A:339:GLY:CA	4:P:1:NAG:H82	1.87	1.05
1:C:339:GLY:CA	6:C:1302:NAG:H82	1.87	1.05
1:C:95:THR:HG22	1:C:187:LYS:HE2	1.37	1.04
1:B:339:GLY:CA	6:B:1302:NAG:H82	1.87	1.04
1:B:95:THR:HG22	1:B:187:LYS:HE2	1.37	1.03
1:A:339:GLY:HA3	4:P:1:NAG:C8	1.89	1.02
1:B:339:GLY:HA3	6:B:1302:NAG:C8	1.89	1.02
1:C:339:GLY:HA3	6:C:1302:NAG:C8	1.89	1.02
1:B:358:ILE:HD13	7:B:1315:EIC:H182	1.06	1.02
1:B:145:TYR:HB3	1:B:153:MET:HA	1.46	0.98
2:H:11:LEU:HD12	2:H:159:PHE:CE2	1.99	0.98
1:C:145:TYR:HB3	1:C:153:MET:HA	1.46	0.98
2:I:11:LEU:HD12	2:I:159:PHE:CE2	1.99	0.98
2:J:11:LEU:CD1	2:J:159:PHE:CZ	2.47	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:11:LEU:HD12	2:J:159:PHE:CE2	1.99	0.97
2:H:11:LEU:CD1	2:H:159:PHE:CZ	2.47	0.96
1:A:145:TYR:HB3	1:A:153:MET:HA	1.46	0.96
2:I:11:LEU:CD1	2:I:159:PHE:CZ	2.47	0.95
1:B:24:LEU:HD11	1:B:69:HIS:HD2	1.33	0.94
6:C:1305:NAG:H62	6:C:1306:NAG:C7	1.99	0.93
1:B:23:GLN:O	1:B:24:LEU:HB2	1.68	0.93
6:B:1305:NAG:HO4	6:B:1306:NAG:C1	1.71	0.93
2:J:11:LEU:CD1	2:J:159:PHE:CE2	2.52	0.92
6:A:1303:NAG:HO4	6:A:1304:NAG:C1	1.80	0.92
1:B:1144:GLU:C	1:B:1145:LEU:HD23	1.95	0.92
2:I:11:LEU:CD1	2:I:159:PHE:CE2	2.52	0.92
1:A:1144:GLU:C	1:A:1145:LEU:HD23	1.95	0.92
6:C:1313:NAG:HO4	6:C:1314:NAG:C1	1.79	0.92
6:B:1305:NAG:H62	6:B:1306:NAG:C7	1.99	0.91
3:N:142:ARG:HE	3:N:163:VAL:HG11	1.35	0.91
6:A:1303:NAG:H62	6:A:1304:NAG:C7	1.99	0.91
2:H:11:LEU:CD1	2:H:159:PHE:CE2	2.52	0.91
1:A:23:GLN:O	1:A:24:LEU:HB2	1.68	0.91
1:C:1144:GLU:C	1:C:1145:LEU:HD23	1.95	0.91
1:C:23:GLN:O	1:C:24:LEU:HB2	1.68	0.91
3:L:142:ARG:HE	3:L:163:VAL:HG11	1.35	0.91
3:M:142:ARG:HE	3:M:163:VAL:HG11	1.35	0.90
1:C:24:LEU:HD11	1:C:69:HIS:HD2	1.33	0.90
2:I:182:VAL:CG2	3:M:160:GLN:OE1	2.21	0.89
2:J:182:VAL:CG2	3:N:160:GLN:OE1	2.21	0.89
2:H:182:VAL:CG2	3:L:160:GLN:OE1	2.21	0.89
1:A:24:LEU:HD11	1:A:69:HIS:HD2	1.33	0.89
1:B:940:SER:O	1:B:941:THR:OG1	1.91	0.88
1:A:940:SER:O	1:A:941:THR:OG1	1.91	0.88
1:C:940:SER:O	1:C:941:THR:OG1	1.91	0.88
3:M:114:SER:HB2	3:M:116:PHE:HZ	1.38	0.88
1:B:362:VAL:HG13	1:B:526:GLY:O	1.74	0.88
1:B:358:ILE:HD13	7:B:1315:EIC:C18	2.01	0.88
1:B:276:LEU:HB3	1:B:289:VAL:HG12	1.57	0.87
1:A:122:ASN:OD1	1:A:123:ALA:N	2.08	0.87
2:H:11:LEU:HD12	2:H:159:PHE:HZ	1.39	0.86
1:B:122:ASN:OD1	1:B:123:ALA:N	2.08	0.86
1:A:283:GLY:O	1:A:284:THR:OG1	1.94	0.86
1:C:122:ASN:OD1	1:C:123:ALA:N	2.08	0.86
1:B:283:GLY:O	1:B:284:THR:OG1	1.94	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:362:VAL:HG13	1:A:526:GLY:O	1.74	0.85
1:C:362:VAL:HG13	1:C:526:GLY:O	1.74	0.85
6:B:1313:NAG:HO4	6:B:1314:NAG:C1	1.87	0.85
1:C:283:GLY:O	1:C:284:THR:OG1	1.94	0.85
2:J:143:SER:HA	3:N:116:PHE:HB3	1.59	0.85
1:B:396:TYR:OH	1:C:230:PRO:HG3	1.77	0.84
3:N:114:SER:HB2	3:N:116:PHE:HZ	1.38	0.84
1:A:45:SER:O	1:A:47:VAL:HG23	1.77	0.84
2:I:143:SER:HA	3:M:116:PHE:HB3	1.59	0.84
1:B:563:GLN:HG2	1:C:41:LYS:O	1.78	0.84
1:C:45:SER:O	1:C:47:VAL:HG23	1.77	0.84
3:M:106:ILE:HD12	3:M:166:GLN:OE1	1.78	0.84
1:B:45:SER:O	1:B:47:VAL:HG23	1.77	0.83
2:I:11:LEU:HD12	2:I:159:PHE:HZ	1.38	0.83
3:N:139:PHE:CD1	3:N:173:TYR:O	2.32	0.83
3:L:139:PHE:CD1	3:L:173:TYR:O	2.32	0.83
1:C:145:TYR:CB	1:C:153:MET:HA	2.08	0.83
2:H:143:SER:HA	3:L:116:PHE:HB3	1.59	0.83
3:L:106:ILE:HD12	3:L:166:GLN:OE1	1.78	0.83
1:B:145:TYR:CB	1:B:153:MET:HA	2.08	0.83
2:I:125:SER:OG	2:I:159:PHE:HE1	1.62	0.83
3:N:106:ILE:HD12	3:N:166:GLN:OE1	1.78	0.83
1:A:145:TYR:CB	1:A:153:MET:HA	2.08	0.83
2:H:125:SER:OG	2:H:159:PHE:HE1	1.62	0.83
1:A:123:ALA:HB3	5:E:1:NAG:H82	1.60	0.82
1:B:103:GLY:HA3	1:B:119:ILE:O	1.79	0.82
3:L:114:SER:HB2	3:L:116:PHE:HZ	1.38	0.82
2:J:125:SER:OG	2:J:159:PHE:HE1	1.62	0.82
1:C:148:ASN:C	1:C:149:ASN:HD22	1.88	0.82
1:C:123:ALA:HB3	5:c:1:NAG:H82	1.60	0.82
1:B:148:ASN:C	1:B:149:ASN:HD22	1.88	0.82
6:C:1305:NAG:HO4	6:C:1306:NAG:C1	1.90	0.82
3:M:139:PHE:CD1	3:M:173:TYR:O	2.32	0.82
1:C:103:GLY:HA3	1:C:119:ILE:O	1.79	0.82
2:J:11:LEU:HD12	2:J:159:PHE:HZ	1.39	0.82
2:J:125:SER:HG	2:J:159:PHE:HE1	0.83	0.81
1:A:103:GLY:HA3	1:A:119:ILE:O	1.79	0.81
1:B:123:ALA:HB3	5:U:1:NAG:H82	1.60	0.81
2:I:135:PHE:CE2	3:M:124:GLN:HG3	2.15	0.81
2:J:135:PHE:CE2	3:N:124:GLN:HG3	2.16	0.81
1:A:148:ASN:C	1:A:149:ASN:HD22	1.88	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:125:SER:HG	2:H:159:PHE:HE1	0.82	0.81
2:H:135:PHE:CE2	3:L:124:GLN:HG3	2.16	0.81
1:B:278:LYS:HD2	1:B:286:THR:OG1	1.80	0.80
1:B:817:PHE:CE2	1:B:935:GLN:NE2	2.50	0.80
1:C:817:PHE:CE2	1:C:935:GLN:NE2	2.50	0.80
3:N:139:PHE:HD1	3:N:173:TYR:O	1.65	0.80
1:A:817:PHE:CE2	1:A:935:GLN:NE2	2.50	0.80
2:I:125:SER:HG	2:I:159:PHE:HE1	0.81	0.79
3:M:139:PHE:HD1	3:M:173:TYR:O	1.65	0.79
6:A:1305:NAG:H3	6:A:1305:NAG:C8	2.13	0.79
6:C:1307:NAG:H3	6:C:1307:NAG:C8	2.13	0.78
3:M:139:PHE:CE2	3:M:142:ARG:HA	2.18	0.78
3:L:139:PHE:CE2	3:L:142:ARG:HA	2.18	0.78
3:L:139:PHE:HD1	3:L:173:TYR:O	1.65	0.78
1:A:275:PHE:CE1	1:A:290:ASP:HB2	2.18	0.78
1:A:293:LEU:HD22	1:A:294:ASP:N	1.98	0.78
6:B:1307:NAG:H3	6:B:1307:NAG:C8	2.13	0.78
1:B:351:TYR:OH	4:d:2:NAG:C8	2.32	0.78
3:N:139:PHE:CE2	3:N:142:ARG:HA	2.18	0.78
1:B:95:THR:CG2	1:B:187:LYS:HE2	2.13	0.77
1:B:599:THR:HG23	1:B:601:GLY:H	1.50	0.77
1:C:599:THR:HG23	1:C:601:GLY:H	1.50	0.77
1:A:396:TYR:OH	1:B:230:PRO:HG3	1.84	0.76
1:A:599:THR:HG23	1:A:601:GLY:H	1.49	0.76
3:M:137:ASN:O	3:M:138:ASN:O	2.04	0.76
3:N:140:TYR:HB3	3:N:141:PRO:HD3	1.68	0.75
1:C:95:THR:CG2	1:C:187:LYS:HE2	2.13	0.75
3:N:137:ASN:O	3:N:138:ASN:O	2.04	0.75
1:B:463:PRO:HB2	1:C:198:ASP:OD1	1.87	0.75
1:A:95:THR:CG2	1:A:187:LYS:HE2	2.13	0.74
3:L:137:ASN:O	3:L:138:ASN:O	2.04	0.74
1:C:155:SER:O	1:C:156:GLU:HG2	1.87	0.74
1:A:452:LEU:CD1	4:V:2:NAG:C8	2.66	0.74
3:L:140:TYR:HB3	3:L:141:PRO:HD3	1.68	0.74
2:I:182:VAL:HG22	3:M:160:GLN:OE1	1.87	0.74
1:C:1144:GLU:O	1:C:1145:LEU:HD23	1.88	0.74
1:A:155:SER:O	1:A:156:GLU:HG2	1.88	0.74
6:B:1307:NAG:H3	6:B:1307:NAG:H82	1.70	0.73
1:B:24:LEU:CD1	1:B:69:HIS:HD2	2.01	0.73
3:M:140:TYR:HB3	3:M:141:PRO:HD3	1.68	0.73
2:J:11:LEU:HD23	2:J:11:LEU:C	2.14	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:358:ILE:HD13	7:C:1315:EIC:H172	1.68	0.73
2:J:182:VAL:HG22	3:N:160:GLN:OE1	1.87	0.73
1:A:24:LEU:CD1	1:A:69:HIS:HD2	2.01	0.73
1:B:155:SER:O	1:B:156:GLU:HG2	1.87	0.73
6:B:1305:NAG:H62	6:B:1306:NAG:C8	2.19	0.73
1:C:339:GLY:HA2	6:C:1302:NAG:H82	1.70	0.73
2:I:11:LEU:C	2:I:11:LEU:HD23	2.14	0.73
6:A:1305:NAG:H3	6:A:1305:NAG:H82	1.70	0.73
6:A:1309:NAG:HO4	6:A:1310:NAG:C1	2.01	0.73
1:B:339:GLY:HA2	6:B:1302:NAG:H82	1.71	0.73
1:C:1142:GLN:OE1	1:C:1142:GLN:N	2.21	0.73
1:A:1142:GLN:N	1:A:1142:GLN:OE1	2.21	0.72
2:H:182:VAL:HG22	3:L:160:GLN:OE1	1.87	0.72
1:B:47:VAL:HG12	1:B:48:LEU:N	2.04	0.72
1:A:293:LEU:HD22	1:A:293:LEU:C	2.14	0.72
1:B:95:THR:HG22	1:B:187:LYS:CE	2.18	0.72
1:B:1142:GLN:N	1:B:1142:GLN:OE1	2.21	0.72
1:A:339:GLY:HA2	4:P:1:NAG:H82	1.70	0.72
1:A:452:LEU:CD1	4:V:2:NAG:H83	2.18	0.72
1:B:1144:GLU:O	1:B:1145:LEU:HD23	1.88	0.72
1:C:24:LEU:CD1	1:C:69:HIS:HD2	2.01	0.72
2:H:11:LEU:HD23	2:H:11:LEU:C	2.14	0.72
3:N:139:PHE:CE1	3:N:173:TYR:C	2.68	0.72
1:A:47:VAL:HG12	1:A:48:LEU:N	2.04	0.71
1:A:1144:GLU:O	1:A:1145:LEU:HD23	1.88	0.71
6:A:1303:NAG:H62	6:A:1304:NAG:C8	2.19	0.71
3:M:139:PHE:CE1	3:M:173:TYR:C	2.68	0.71
3:M:140:TYR:CD2	3:M:141:PRO:HD3	2.25	0.71
1:B:146:HIS:CG	1:B:147:LYS:HE3	2.26	0.71
1:B:293:LEU:HD13	1:B:293:LEU:O	1.91	0.71
1:B:351:TYR:OH	4:d:2:NAG:H81	1.90	0.71
1:B:370:ASN:OD1	1:B:370:ASN:N	2.22	0.71
6:C:1305:NAG:H62	6:C:1306:NAG:C8	2.19	0.71
6:C:1307:NAG:H3	6:C:1307:NAG:H82	1.71	0.71
3:L:140:TYR:CD2	3:L:141:PRO:HD3	2.25	0.71
1:A:370:ASN:N	1:A:370:ASN:OD1	2.22	0.71
1:C:146:HIS:CG	1:C:147:LYS:HE3	2.26	0.71
3:L:139:PHE:CE1	3:L:173:TYR:C	2.68	0.71
1:C:370:ASN:OD1	1:C:370:ASN:N	2.22	0.71
1:B:24:LEU:CD1	1:B:69:HIS:CD2	2.69	0.71
3:N:140:TYR:CD2	3:N:141:PRO:HD3	2.25	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:146:HIS:CG	1:A:147:LYS:HE3	2.26	0.71
1:B:47:VAL:HG12	1:B:48:LEU:H	1.56	0.71
1:B:345:THR:HG23	1:B:346:ARG:HG3	1.72	0.71
1:A:345:THR:HG23	1:A:346:ARG:HG3	1.72	0.70
1:C:345:THR:HG23	1:C:346:ARG:HG3	1.72	0.70
1:A:47:VAL:HG12	1:A:48:LEU:H	1.56	0.70
1:C:47:VAL:HG12	1:C:48:LEU:N	2.04	0.70
2:J:128:SER:C	2:J:129:THR:HG22	2.17	0.70
2:H:128:SER:C	2:H:129:THR:HG22	2.17	0.70
3:L:139:PHE:H	3:L:172:THR:HB	1.57	0.69
3:N:139:PHE:H	3:N:172:THR:HB	1.57	0.69
2:I:128:SER:C	2:I:129:THR:HG22	2.17	0.69
1:C:47:VAL:HG12	1:C:48:LEU:H	1.56	0.69
1:B:50:SER:O	1:B:51:THR:OG1	2.09	0.69
1:B:146:HIS:HA	1:B:153:MET:CG	2.23	0.69
1:C:50:SER:O	1:C:51:THR:OG1	2.09	0.68
1:A:24:LEU:CD1	1:A:69:HIS:CD2	2.69	0.68
1:A:146:HIS:HA	1:A:153:MET:CG	2.23	0.68
1:C:287:ASP:OD1	1:C:306:PHE:HE2	1.76	0.68
1:B:358:ILE:CD1	7:B:1315:EIC:C18	2.67	0.68
3:M:139:PHE:H	3:M:172:THR:HB	1.57	0.68
1:C:24:LEU:CD1	1:C:69:HIS:CD2	2.69	0.68
1:C:95:THR:CG2	1:C:187:LYS:CE	2.72	0.68
3:M:108:ARG:NH1	3:M:109:THR:O	2.27	0.68
1:C:146:HIS:HA	1:C:153:MET:CG	2.23	0.68
1:A:113:LYS:HB3	1:C:471:GLU:OE1	1.94	0.68
3:N:108:ARG:NH1	3:N:109:THR:O	2.27	0.68
1:A:95:THR:HG22	1:A:187:LYS:CE	2.18	0.67
1:A:95:THR:CG2	1:A:187:LYS:CE	2.72	0.67
1:A:97:LYS:HD3	1:A:97:LYS:C	2.19	0.67
1:A:452:LEU:HD12	4:V:2:NAG:H81	1.74	0.67
1:C:97:LYS:HD3	1:C:97:LYS:C	2.19	0.67
1:C:1144:GLU:HA	1:C:1144:GLU:OE2	1.94	0.67
1:A:97:LYS:NZ	1:A:97:LYS:O	2.28	0.67
1:A:1144:GLU:OE2	1:A:1144:GLU:HA	1.94	0.67
1:B:97:LYS:O	1:B:97:LYS:NZ	2.28	0.67
1:A:471:GLU:OE1	1:B:113:LYS:HB3	1.95	0.67
1:B:97:LYS:HD3	1:B:97:LYS:C	2.19	0.67
1:B:95:THR:CG2	1:B:187:LYS:CE	2.72	0.66
3:L:114:SER:CB	3:L:116:PHE:CZ	2.75	0.66
1:C:97:LYS:NZ	1:C:97:LYS:O	2.28	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:139:PHE:HE2	3:L:142:ARG:HA	1.61	0.66
1:C:406:GLU:OE2	1:C:417:LYS:NZ	2.27	0.66
1:C:940:SER:C	1:C:941:THR:HG1	2.00	0.66
1:B:283:GLY:C	1:B:284:THR:HG1	2.00	0.66
1:B:351:TYR:OH	4:d:2:NAG:H82	1.95	0.66
1:A:452:LEU:HD13	4:V:2:NAG:H83	1.76	0.65
3:L:108:ARG:NH1	3:L:109:THR:O	2.27	0.65
1:B:1144:GLU:OE2	1:B:1144:GLU:HA	1.95	0.65
3:M:114:SER:CB	3:M:116:PHE:CZ	2.75	0.65
1:B:562:PHE:CD2	1:C:41:LYS:HD3	2.32	0.65
2:I:182:VAL:HG21	3:M:160:GLN:OE1	1.97	0.65
1:B:146:HIS:HA	1:B:153:MET:HG3	1.79	0.65
1:A:50:SER:O	1:A:51:THR:OG1	2.09	0.64
1:A:776:LYS:O	1:A:780:GLU:HG2	1.97	0.64
1:B:96:GLU:OE2	1:B:99:ASN:HA	1.98	0.64
1:B:776:LYS:O	1:B:780:GLU:HG2	1.97	0.64
2:J:125:SER:C	2:J:127:ALA:H	2.05	0.64
1:B:940:SER:C	1:B:941:THR:HG1	1.99	0.64
3:N:116:PHE:CD2	3:N:135:LEU:HD23	2.33	0.64
1:A:96:GLU:OE2	1:A:99:ASN:HA	1.98	0.64
1:A:406:GLU:OE2	1:A:417:LYS:NZ	2.27	0.64
3:M:140:TYR:HD2	3:M:141:PRO:HD3	1.63	0.64
3:L:116:PHE:CD2	3:L:135:LEU:HD23	2.33	0.64
1:C:776:LYS:O	1:C:780:GLU:HG2	1.97	0.64
1:C:96:GLU:OE2	1:C:99:ASN:HA	1.98	0.64
1:A:293:LEU:O	1:A:294:ASP:HB2	1.95	0.64
1:C:24:LEU:HD21	1:C:69:HIS:NE2	2.13	0.64
1:C:146:HIS:HA	1:C:153:MET:HG3	1.80	0.63
2:H:182:VAL:HG21	3:L:160:GLN:OE1	1.97	0.63
1:A:24:LEU:HD21	1:A:69:HIS:NE2	2.13	0.63
1:A:469:SER:HB2	1:B:113:LYS:O	1.97	0.63
3:N:139:PHE:HE2	3:N:142:ARG:HA	1.61	0.63
2:H:125:SER:C	2:H:127:ALA:H	2.05	0.63
2:I:212:ASN:HB3	2:I:219:LYS:HE2	1.79	0.63
1:A:817:PHE:HE2	1:A:935:GLN:NE2	1.97	0.63
2:H:11:LEU:HD11	2:H:159:PHE:CZ	2.33	0.63
3:M:116:PHE:CD2	3:M:135:LEU:HD23	2.33	0.63
2:H:137:LEU:HD11	2:H:154:LEU:HB2	1.81	0.63
2:H:212:ASN:HB3	2:H:219:LYS:HE2	1.79	0.63
1:C:817:PHE:HE2	1:C:935:GLN:NE2	1.97	0.63
2:H:165:VAL:HG22	2:H:211:VAL:HG22	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:140:TYR:HD2	3:L:141:PRO:HD3	1.63	0.63
1:B:24:LEU:HD21	1:B:69:HIS:NE2	2.13	0.63
2:I:11:LEU:HD11	2:I:159:PHE:CZ	2.33	0.63
2:I:125:SER:C	2:I:127:ALA:H	2.05	0.63
2:J:182:VAL:HG21	3:N:160:GLN:OE1	1.97	0.63
2:J:212:ASN:HB3	2:J:219:LYS:HE2	1.79	0.63
1:B:406:GLU:OE2	1:B:417:LYS:NZ	2.27	0.63
1:C:96:GLU:HG2	1:C:97:LYS:N	2.14	0.63
2:I:137:LEU:HD11	2:I:154:LEU:HB2	1.80	0.63
2:J:11:LEU:HD11	2:J:159:PHE:CZ	2.33	0.62
3:N:140:TYR:HD2	3:N:141:PRO:HD3	1.63	0.62
1:C:48:LEU:HD12	1:C:278:LYS:HB3	1.81	0.62
1:A:145:TYR:C	1:A:153:MET:HG3	2.24	0.62
1:B:145:TYR:C	1:B:153:MET:HG3	2.25	0.62
1:C:48:LEU:CD1	1:C:278:LYS:HB3	2.29	0.62
3:L:142:ARG:NE	3:L:163:VAL:HG11	2.13	0.62
1:B:562:PHE:HD2	1:C:41:LYS:HD3	1.63	0.62
1:A:146:HIS:HA	1:A:153:MET:HG3	1.79	0.62
1:A:745:ASP:N	1:A:745:ASP:OD1	2.32	0.62
6:A:1303:NAG:H62	6:A:1304:NAG:H82	1.82	0.62
1:A:48:LEU:HD12	1:A:278:LYS:CB	2.30	0.62
1:B:96:GLU:HG2	1:B:97:LYS:N	2.14	0.62
6:C:1305:NAG:H62	6:C:1306:NAG:H82	1.82	0.61
1:A:293:LEU:O	1:A:293:LEU:HD13	1.99	0.61
6:B:1305:NAG:H62	6:B:1306:NAG:H82	1.82	0.61
1:C:22:THR:O	1:C:23:GLN:C	2.43	0.61
2:I:165:VAL:HG22	2:I:211:VAL:HG22	1.81	0.61
2:J:137:LEU:HD11	2:J:154:LEU:HB2	1.80	0.61
1:A:96:GLU:HG2	1:A:97:LYS:N	2.14	0.61
2:H:94:TYR:O	2:H:119:GLY:HA2	2.01	0.61
2:J:94:TYR:O	2:J:119:GLY:HA2	2.01	0.61
1:A:940:SER:C	1:A:941:THR:HG1	2.03	0.61
1:C:745:ASP:OD1	1:C:745:ASP:N	2.32	0.61
1:C:95:THR:HG22	1:C:187:LYS:CE	2.18	0.61
3:M:116:PHE:HE2	3:M:137:ASN:HB2	1.65	0.61
1:B:813:SER:C	1:B:814:LYS:HD2	2.26	0.61
3:L:116:PHE:HE2	3:L:137:ASN:HB2	1.65	0.61
2:J:165:VAL:HG22	2:J:211:VAL:HG22	1.81	0.61
1:B:745:ASP:OD1	1:B:745:ASP:N	2.32	0.61
1:A:459:SER:HB3	4:W:2:NAG:H81	1.82	0.61
1:B:22:THR:O	1:B:23:GLN:C	2.43	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:813:SER:C	1:A:814:LYS:HD2	2.26	0.60
2:I:94:TYR:O	2:I:119:GLY:HA2	2.01	0.60
1:A:278:LYS:HD2	1:A:286:THR:OG1	1.99	0.60
1:A:283:GLY:C	1:A:284:THR:HG1	1.99	0.60
1:C:145:TYR:C	1:C:153:MET:HG3	2.25	0.60
1:C:813:SER:C	1:C:814:LYS:HD2	2.26	0.60
1:C:123:ALA:O	1:C:124:THR:OG1	2.17	0.60
1:A:148:ASN:C	1:A:150:LYS:H	2.10	0.60
1:A:291:CYS:SG	1:A:301:CYS:CB	2.90	0.60
3:N:116:PHE:HE2	3:N:137:ASN:HB2	1.65	0.60
1:A:452:LEU:CD1	4:V:2:NAG:H81	2.32	0.60
1:A:278:LYS:CD	1:A:286:THR:OG1	2.50	0.60
1:A:22:THR:O	1:A:23:GLN:C	2.43	0.59
1:A:814:LYS:HD2	1:A:814:LYS:N	2.17	0.59
1:B:48:LEU:HD12	1:B:278:LYS:CB	2.32	0.59
2:J:142:LYS:HE3	3:N:119:PRO:HD3	1.84	0.59
3:N:114:SER:CB	3:N:116:PHE:CZ	2.75	0.59
1:C:339:GLY:HA3	6:C:1302:NAG:H81	1.80	0.59
1:A:339:GLY:HA3	4:P:1:NAG:H81	1.80	0.59
1:B:814:LYS:HD2	1:B:814:LYS:N	2.17	0.59
1:C:148:ASN:C	1:C:150:LYS:H	2.10	0.59
1:C:283:GLY:C	1:C:284:THR:HG1	2.04	0.59
1:B:339:GLY:HA3	6:B:1302:NAG:H81	1.80	0.59
3:M:139:PHE:HE2	3:M:142:ARG:HA	1.61	0.59
1:C:293:LEU:O	1:C:294:ASP:HB2	2.03	0.59
1:C:814:LYS:HD2	1:C:814:LYS:N	2.18	0.59
2:I:142:LYS:HE3	3:M:119:PRO:HD3	1.84	0.59
3:N:142:ARG:NE	3:N:163:VAL:HG11	2.13	0.59
3:L:6:GLN:HE21	3:L:99:GLY:HA3	1.68	0.58
3:M:6:GLN:HE21	3:M:99:GLY:HA3	1.68	0.58
3:N:6:GLN:HE21	3:N:99:GLY:HA3	1.68	0.58
1:B:123:ALA:O	1:B:124:THR:OG1	2.17	0.58
1:B:817:PHE:HE2	1:B:935:GLN:NE2	1.97	0.58
2:I:161:GLU:H	2:I:161:GLU:CD	2.12	0.58
1:B:777:ASN:OD1	1:B:1019:ARG:NH1	2.32	0.58
2:H:142:LYS:HE3	3:L:119:PRO:HD3	1.84	0.58
4:Y:1:NAG:H62	4:Y:2:NAG:H82	1.84	0.58
1:B:148:ASN:C	1:B:150:LYS:H	2.10	0.58
3:L:140:TYR:HB3	3:L:141:PRO:CD	2.34	0.58
3:L:6:GLN:HE22	3:L:87:TYR:HA	1.69	0.58
6:C:1305:NAG:C6	6:C:1306:NAG:C7	2.80	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:48:LEU:CD1	1:A:278:LYS:HB3	2.34	0.58
2:H:161:GLU:CD	2:H:161:GLU:H	2.12	0.58
1:A:126:VAL:HG12	1:A:172:SER:O	2.05	0.57
1:B:123:ALA:C	1:B:124:THR:HG23	2.29	0.57
1:C:123:ALA:C	1:C:124:THR:HG23	2.29	0.57
1:B:126:VAL:HG12	1:B:172:SER:O	2.05	0.57
1:C:811:LYS:HB2	1:C:813:SER:O	2.04	0.57
2:J:161:GLU:CD	2:J:161:GLU:H	2.12	0.57
3:N:6:GLN:HE22	3:N:87:TYR:HA	1.69	0.57
1:A:811:LYS:HB2	1:A:813:SER:O	2.05	0.57
1:B:811:LYS:O	1:B:814:LYS:NZ	2.38	0.57
3:M:6:GLN:HE22	3:M:87:TYR:HA	1.69	0.57
1:C:811:LYS:O	1:C:814:LYS:NZ	2.38	0.57
3:M:115:VAL:O	3:M:116:PHE:CD1	2.58	0.56
1:A:777:ASN:OD1	1:A:1019:ARG:NH1	2.31	0.56
1:C:24:LEU:HD21	1:C:69:HIS:CD2	2.40	0.56
3:L:115:VAL:O	3:L:116:PHE:CD1	2.58	0.56
1:A:176:LEU:HD13	1:A:207:HIS:HB2	1.87	0.56
1:B:102:ARG:NH1	1:B:121:ASN:O	2.39	0.56
1:B:811:LYS:HB2	1:B:813:SER:O	2.04	0.56
6:C:1312:NAG:H83	6:C:1312:NAG:H3	1.87	0.56
3:N:108:ARG:HG3	3:N:171:SER:HB2	1.88	0.56
1:C:777:ASN:OD1	1:C:1019:ARG:NH1	2.31	0.56
3:L:108:ARG:HG3	3:L:171:SER:HB2	1.88	0.56
1:A:24:LEU:HD21	1:A:69:HIS:CD2	2.40	0.56
1:C:102:ARG:NH1	1:C:121:ASN:O	2.38	0.56
1:A:123:ALA:C	1:A:124:THR:HG23	2.29	0.56
1:B:176:LEU:HD13	1:B:207:HIS:HB2	1.87	0.56
1:B:276:LEU:CB	1:B:289:VAL:HG12	2.34	0.56
1:B:337:PRO:HB2	1:B:340:GLU:HG2	1.88	0.56
3:N:140:TYR:HB3	3:N:141:PRO:CD	2.34	0.56
4:R:2:NAG:H3	4:R:2:NAG:H83	1.87	0.56
1:A:811:LYS:O	1:A:814:LYS:NZ	2.38	0.56
2:H:132:PRO:HB2	2:H:155:VAL:HG23	1.88	0.56
1:B:24:LEU:HD21	1:B:69:HIS:CD2	2.41	0.56
1:B:148:ASN:C	1:B:149:ASN:ND2	2.62	0.56
1:C:126:VAL:HG12	1:C:172:SER:O	2.05	0.56
1:C:176:LEU:HD13	1:C:207:HIS:HB2	1.87	0.56
3:L:114:SER:CB	3:L:116:PHE:HZ	2.16	0.56
1:A:148:ASN:C	1:A:149:ASN:ND2	2.62	0.56
1:B:146:HIS:ND1	1:B:147:LYS:HG2	2.21	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:139:PHE:CD1	3:L:173:TYR:C	2.84	0.56
3:N:115:VAL:O	3:N:116:PHE:CD1	2.58	0.56
1:B:278:LYS:HD2	1:B:286:THR:HG1	1.72	0.55
1:C:148:ASN:C	1:C:149:ASN:ND2	2.62	0.55
1:A:123:ALA:O	1:A:124:THR:OG1	2.17	0.55
1:C:48:LEU:HD12	1:C:278:LYS:CB	2.36	0.55
3:M:140:TYR:HB3	3:M:141:PRO:CD	2.34	0.55
1:A:155:SER:O	1:A:156:GLU:CG	2.55	0.55
1:A:146:HIS:ND1	1:A:147:LYS:HG2	2.21	0.55
1:A:960:ASN:O	1:A:964:LYS:HG3	2.06	0.55
2:H:212:ASN:HD22	2:H:214:LYS:HE3	1.72	0.55
1:A:146:HIS:CD2	1:A:147:LYS:HE3	2.42	0.55
1:B:123:ALA:HB3	5:U:1:NAG:C8	2.35	0.55
1:B:941:THR:HG22	1:B:941:THR:O	2.06	0.55
1:C:146:HIS:CD2	1:C:147:LYS:HE3	2.42	0.55
1:C:278:LYS:HD2	1:C:286:THR:OG1	2.07	0.55
2:J:33:TYR:H	2:J:100:GLY:HA3	1.72	0.55
1:A:145:TYR:HB3	1:A:153:MET:CA	2.29	0.55
1:A:146:HIS:N	1:A:153:MET:HG3	2.22	0.55
1:C:280:ASN:HB2	1:C:284:THR:O	2.07	0.55
3:M:108:ARG:HG3	3:M:171:SER:HB2	1.88	0.55
3:M:142:ARG:NE	3:M:163:VAL:HG11	2.13	0.55
2:J:132:PRO:HB2	2:J:155:VAL:HG23	1.88	0.55
1:A:126:VAL:HG13	1:A:126:VAL:O	2.06	0.55
1:A:941:THR:O	1:A:941:THR:HG22	2.06	0.55
1:B:145:TYR:HB3	1:B:153:MET:CA	2.29	0.55
6:B:1312:NAG:H3	6:B:1312:NAG:H83	1.87	0.55
2:I:33:TYR:H	2:I:100:GLY:HA3	1.72	0.55
2:I:212:ASN:HD22	2:I:214:LYS:HE3	1.72	0.55
1:A:291:CYS:HG	1:A:301:CYS:CB	2.15	0.55
1:A:480:CYS:O	1:A:483:VAL:HG22	2.07	0.55
1:B:146:HIS:CD2	1:B:147:LYS:HE3	2.42	0.55
1:A:562:PHE:HZ	1:B:38:TYR:CD2	2.25	0.54
2:I:132:PRO:HB2	2:I:155:VAL:HG23	1.88	0.54
2:I:139:PRO:HG3	2:I:151:LEU:HD23	1.89	0.54
3:M:140:TYR:CB	3:M:141:PRO:HD3	2.37	0.54
1:A:337:PRO:HB2	1:A:340:GLU:HG2	1.88	0.54
1:C:337:PRO:HB2	1:C:340:GLU:HG2	1.88	0.54
2:H:139:PRO:HG3	2:H:151:LEU:HD23	1.89	0.54
3:L:140:TYR:CB	3:L:141:PRO:HD3	2.37	0.54
1:B:155:SER:O	1:B:156:GLU:CG	2.55	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:960:ASN:O	1:B:964:LYS:HG3	2.06	0.54
1:C:146:HIS:N	1:C:153:MET:HG3	2.22	0.54
2:I:152:GLY:HA2	2:I:167:TRP:HZ2	1.73	0.54
2:J:212:ASN:HD22	2:J:214:LYS:HE3	1.72	0.54
1:A:48:LEU:HD12	1:A:278:LYS:HB3	1.89	0.54
1:B:280:ASN:HB2	1:B:284:THR:O	2.07	0.54
1:C:145:TYR:HB3	1:C:153:MET:CA	2.29	0.54
1:C:941:THR:HG22	1:C:941:THR:O	2.06	0.54
1:C:960:ASN:O	1:C:964:LYS:HG3	2.06	0.54
3:N:32:ASP:HB3	3:N:91:HIS:HB2	1.90	0.54
1:B:276:LEU:O	1:B:288:ALA:HA	2.08	0.54
1:C:146:HIS:ND1	1:C:147:LYS:HG2	2.21	0.54
3:M:114:SER:CB	3:M:116:PHE:HZ	2.16	0.54
1:A:1142:GLN:HB2	1:A:1143:PRO:HD3	1.89	0.54
1:C:281:GLU:HG2	1:C:282:ASN:OD1	2.08	0.54
1:B:1142:GLN:HB2	1:B:1143:PRO:HD3	1.89	0.54
1:C:146:HIS:CA	1:C:153:MET:HG3	2.38	0.54
2:H:152:GLY:HA2	2:H:167:TRP:HZ2	1.73	0.54
2:J:139:PRO:HG3	2:J:151:LEU:HD23	1.89	0.54
1:A:280:ASN:HB2	1:A:284:THR:O	2.07	0.54
1:B:146:HIS:N	1:B:153:MET:HG3	2.22	0.54
1:B:480:CYS:O	1:B:483:VAL:HG22	2.07	0.54
1:C:1142:GLN:HB2	1:C:1143:PRO:HD3	1.89	0.54
2:H:33:TYR:H	2:H:100:GLY:HA3	1.72	0.54
3:M:139:PHE:CD1	3:M:173:TYR:C	2.84	0.54
1:A:276:LEU:O	1:A:288:ALA:HA	2.08	0.54
1:A:562:PHE:HZ	1:B:38:TYR:HD2	1.55	0.54
3:N:139:PHE:CD1	3:N:173:TYR:C	2.84	0.54
6:A:1308:NAG:H83	6:A:1308:NAG:H3	1.90	0.53
1:B:126:VAL:HG13	1:B:126:VAL:O	2.06	0.53
1:B:281:GLU:HG2	1:B:282:ASN:OD1	2.08	0.53
6:C:1310:NAG:H83	6:C:1310:NAG:H3	1.90	0.53
3:M:141:PRO:O	3:M:198:HIS:NE2	2.40	0.53
2:I:127:ALA:O	2:I:128:SER:HB3	2.08	0.53
3:M:67:SER:OG	3:M:68:GLY:N	2.42	0.53
2:J:152:GLY:HA2	2:J:167:TRP:HZ2	1.73	0.53
3:N:140:TYR:CB	3:N:141:PRO:HD3	2.37	0.53
1:B:146:HIS:HA	1:B:153:MET:HG2	1.91	0.53
6:B:1310:NAG:H83	6:B:1310:NAG:H3	1.90	0.53
3:L:32:ASP:HB3	3:L:91:HIS:HB2	1.90	0.53
3:M:32:ASP:HB3	3:M:91:HIS:HB2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:480:CYS:O	1:C:483:VAL:HG22	2.07	0.53
2:H:127:ALA:O	2:H:128:SER:HB3	2.08	0.53
1:C:126:VAL:O	1:C:126:VAL:HG13	2.06	0.53
1:C:155:SER:O	1:C:156:GLU:CG	2.55	0.53
1:A:146:HIS:CA	1:A:153:MET:HG3	2.38	0.53
1:A:841:LEU:HD12	1:C:588:THR:HG21	1.91	0.53
1:B:1118:ASP:N	1:B:1118:ASP:OD1	2.42	0.53
1:C:452:LEU:CD1	4:F:2:NAG:H81	2.39	0.53
1:A:123:ALA:HB3	5:E:1:NAG:C8	2.35	0.53
1:A:146:HIS:HA	1:A:153:MET:HG2	1.91	0.53
1:A:396:TYR:CZ	1:B:230:PRO:HG3	2.44	0.53
1:B:146:HIS:CA	1:B:153:MET:HG3	2.38	0.53
1:A:1118:ASP:OD1	1:A:1118:ASP:N	2.42	0.53
1:C:276:LEU:HB3	1:C:289:VAL:HG12	1.91	0.53
3:N:141:PRO:O	3:N:198:HIS:NE2	2.40	0.53
2:J:127:ALA:O	2:J:128:SER:HB3	2.08	0.53
1:C:146:HIS:HA	1:C:153:MET:HG2	1.91	0.52
3:N:116:PHE:HD2	3:N:135:LEU:HD23	1.72	0.52
1:A:281:GLU:HG2	1:A:282:ASN:OD1	2.08	0.52
6:B:1305:NAG:C6	6:B:1306:NAG:C7	2.80	0.52
3:N:67:SER:OG	3:N:68:GLY:N	2.42	0.52
1:A:102:ARG:NH1	1:A:121:ASN:O	2.39	0.52
1:C:452:LEU:CD1	4:F:2:NAG:C8	2.87	0.52
1:A:96:GLU:HB2	1:A:263:ALA:CB	2.40	0.52
1:A:228:ASP:N	1:A:228:ASP:OD1	2.42	0.52
1:A:452:LEU:HD12	4:V:2:NAG:C8	2.37	0.52
1:B:462:LYS:HG2	4:e:1:NAG:C8	2.39	0.52
1:C:123:ALA:HB3	5:c:1:NAG:C8	2.35	0.52
3:L:67:SER:OG	3:L:68:GLY:N	2.42	0.52
3:M:140:TYR:CD2	3:M:141:PRO:CD	2.93	0.52
1:A:792:PRO:HG3	1:C:707:TYR:HB3	1.92	0.52
1:C:96:GLU:HB2	1:C:263:ALA:CB	2.40	0.52
1:A:282:ASN:OD1	1:A:282:ASN:N	2.43	0.52
6:A:1303:NAG:C6	6:A:1304:NAG:C7	2.80	0.52
1:C:1142:GLN:N	1:C:1143:PRO:CD	2.73	0.52
1:B:228:ASP:OD1	1:B:228:ASP:N	2.42	0.52
1:C:276:LEU:O	1:C:288:ALA:HA	2.08	0.52
1:A:113:LYS:HB3	1:C:471:GLU:CD	2.35	0.52
1:C:47:VAL:CG1	1:C:48:LEU:H	2.22	0.52
1:C:282:ASN:OD1	1:C:282:ASN:N	2.43	0.52
2:I:128:SER:O	2:I:129:THR:HG22	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:134:CYS:HB2	3:M:148:TRP:CH2	2.45	0.52
1:B:96:GLU:HB2	1:B:263:ALA:CB	2.40	0.51
1:C:354:ASN:O	1:C:398:ASP:HA	2.10	0.51
2:H:128:SER:O	2:H:129:THR:HG22	2.09	0.51
2:J:128:SER:O	2:J:129:THR:HG22	2.09	0.51
1:A:1142:GLN:N	1:A:1143:PRO:CD	2.73	0.51
1:B:1142:GLN:N	1:B:1143:PRO:CD	2.73	0.51
1:A:178:ASP:OD1	1:A:178:ASP:N	2.44	0.51
1:C:228:ASP:OD1	1:C:228:ASP:N	2.42	0.51
1:C:178:ASP:N	1:C:178:ASP:OD1	2.44	0.51
3:L:116:PHE:HD2	3:L:135:LEU:HD23	1.72	0.51
2:J:143:SER:OG	3:N:118:PHE:CE1	2.60	0.51
3:N:140:TYR:CD2	3:N:141:PRO:CD	2.93	0.51
1:B:354:ASN:O	1:B:398:ASP:HA	2.10	0.51
3:L:139:PHE:CE1	3:L:173:TYR:HB2	2.46	0.51
3:N:134:CYS:HB2	3:N:148:TRP:CH2	2.46	0.51
1:A:642:VAL:HG13	1:A:651:ILE:HG12	1.93	0.51
1:B:47:VAL:CG1	1:B:48:LEU:H	2.22	0.51
3:M:116:PHE:HD2	3:M:135:LEU:HD23	1.72	0.51
1:A:113:LYS:O	1:C:469:SER:HB2	2.11	0.51
1:A:276:LEU:HB3	1:A:289:VAL:HG12	1.91	0.51
1:A:354:ASN:O	1:A:398:ASP:HA	2.10	0.51
2:J:135:PHE:HE2	3:N:124:GLN:HG3	1.72	0.51
1:A:835:LYS:HD3	1:A:851:CYS:SG	2.51	0.51
2:H:91:THR:HG23	2:H:123:THR:HA	1.92	0.51
3:N:139:PHE:CE1	3:N:173:TYR:HB2	2.46	0.51
1:C:278:LYS:CD	1:C:286:THR:OG1	2.59	0.51
1:C:804:GLN:NE2	6:C:1309:NAG:O6	2.44	0.51
1:C:1118:ASP:OD1	1:C:1118:ASP:N	2.42	0.51
2:I:91:THR:HG23	2:I:123:THR:HA	1.92	0.51
1:A:47:VAL:CG1	1:A:48:LEU:N	2.72	0.50
1:B:642:VAL:HG13	1:B:651:ILE:HG12	1.93	0.50
3:M:139:PHE:CE1	3:M:173:TYR:HB2	2.46	0.50
2:J:91:THR:HG23	2:J:123:THR:HA	1.92	0.50
1:A:804:GLN:NE2	6:A:1307:NAG:O6	2.45	0.50
1:C:40:ASP:HB3	1:C:42:VAL:HG23	1.93	0.50
3:L:134:CYS:HB2	3:L:148:TRP:CH2	2.45	0.50
1:A:40:ASP:HB3	1:A:42:VAL:HG23	1.93	0.50
1:B:835:LYS:HD3	1:B:851:CYS:SG	2.51	0.50
1:C:309:GLU:O	1:C:313:TYR:OH	2.27	0.50
3:L:140:TYR:CD2	3:L:141:PRO:CD	2.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:125:SER:C	2:I:127:ALA:N	2.69	0.50
1:C:835:LYS:HD3	1:C:851:CYS:SG	2.51	0.50
3:L:141:PRO:O	3:L:198:HIS:NE2	2.40	0.50
2:J:58:ILE:HG23	2:J:70:ILE:HD12	1.94	0.50
1:A:148:ASN:C	1:A:150:LYS:N	2.70	0.50
1:B:178:ASP:OD1	1:B:178:ASP:N	2.44	0.50
1:B:282:ASN:OD1	1:B:282:ASN:N	2.43	0.50
1:A:562:PHE:CZ	1:B:38:TYR:HD2	2.30	0.50
2:H:11:LEU:CD1	2:H:159:PHE:HE2	2.20	0.50
2:H:58:ILE:HG23	2:H:70:ILE:HD12	1.94	0.50
2:J:168:ASN:ND2	2:J:206:THR:O	2.45	0.50
1:A:645:THR:CG2	1:A:670:ILE:HG13	2.42	0.50
1:B:804:GLN:NE2	6:B:1309:NAG:O6	2.44	0.50
1:C:645:THR:CG2	1:C:670:ILE:HG13	2.42	0.50
2:H:168:ASN:ND2	2:H:206:THR:O	2.45	0.50
1:B:40:ASP:HB3	1:B:42:VAL:HG23	1.93	0.49
1:B:176:LEU:O	1:B:190:ARG:NH2	2.45	0.49
3:N:139:PHE:CE1	3:N:173:TYR:CB	2.95	0.49
1:B:149:ASN:ND2	1:B:149:ASN:N	2.60	0.49
1:C:148:ASN:C	1:C:150:LYS:N	2.70	0.49
2:H:132:PRO:HD3	2:H:213:HIS:HD1	1.78	0.49
3:M:139:PHE:CE1	3:M:173:TYR:CB	2.95	0.49
1:B:148:ASN:C	1:B:150:LYS:N	2.70	0.49
1:B:151:SER:O	1:B:152:TRP:HB2	2.13	0.49
1:B:710:ASN:C	1:B:710:ASN:HD22	2.20	0.49
3:L:138:ASN:O	3:L:139:PHE:HB3	2.13	0.49
1:A:377:PHE:CE2	7:A:1311:EIC:H21	2.48	0.49
1:C:176:LEU:O	1:C:190:ARG:NH2	2.45	0.49
1:A:47:VAL:CG1	1:A:48:LEU:H	2.22	0.49
1:B:146:HIS:ND1	1:B:146:HIS:N	2.60	0.49
1:C:1145:LEU:HD23	1:C:1145:LEU:N	2.26	0.49
1:A:985:ASP:OD1	1:C:383:SER:OG	2.23	0.49
1:B:23:GLN:O	1:B:24:LEU:CB	2.51	0.49
1:B:280:ASN:HB3	1:B:283:GLY:O	2.13	0.49
1:C:95:THR:HG21	1:C:187:LYS:CE	2.43	0.49
1:C:710:ASN:C	1:C:710:ASN:HD22	2.20	0.49
2:I:58:ILE:HG23	2:I:70:ILE:HD12	1.94	0.49
2:I:132:PRO:HD3	2:I:213:HIS:HD1	1.77	0.49
1:A:23:GLN:O	1:A:24:LEU:CB	2.51	0.49
1:A:176:LEU:O	1:A:190:ARG:NH2	2.45	0.49
1:B:1145:LEU:HD23	1:B:1145:LEU:N	2.26	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1145:LEU:HD23	1:A:1145:LEU:N	2.26	0.49
1:C:97:LYS:C	1:C:97:LYS:CD	2.86	0.49
1:C:149:ASN:ND2	1:C:149:ASN:N	2.60	0.49
2:I:127:ALA:HB3	2:I:159:PHE:CD1	2.48	0.49
2:H:127:ALA:HB3	2:H:159:PHE:CD1	2.48	0.49
3:N:138:ASN:O	3:N:139:PHE:HB3	2.13	0.49
1:C:115:GLN:HA	1:C:131:CYS:O	2.13	0.49
3:L:139:PHE:CE1	3:L:173:TYR:CB	2.95	0.49
1:C:151:SER:O	1:C:152:TRP:HB2	2.13	0.48
3:L:139:PHE:HE1	3:L:173:TYR:C	2.20	0.48
1:A:95:THR:HG21	1:A:187:LYS:CE	2.43	0.48
1:A:149:ASN:ND2	1:A:149:ASN:N	2.60	0.48
1:B:645:THR:CG2	1:B:670:ILE:HG13	2.42	0.48
2:I:168:ASN:ND2	2:I:206:THR:O	2.45	0.48
1:A:280:ASN:HB3	1:A:283:GLY:O	2.13	0.48
1:B:48:LEU:HD12	1:B:278:LYS:HB2	1.96	0.48
1:B:95:THR:HG21	1:B:187:LYS:CE	2.43	0.48
1:C:642:VAL:HG13	1:C:651:ILE:HG12	1.93	0.48
2:H:1:GLU:HB3	2:H:2:VAL:H	1.51	0.48
3:M:138:ASN:O	3:M:139:PHE:HB3	2.13	0.48
2:J:11:LEU:C	2:J:11:LEU:CD2	2.86	0.48
1:B:144:TYR:O	1:B:145:TYR:HB2	2.13	0.48
1:C:146:HIS:N	1:C:146:HIS:ND1	2.60	0.48
2:J:132:PRO:HD3	2:J:213:HIS:HD1	1.78	0.48
1:A:144:TYR:N	1:A:144:TYR:CD1	2.81	0.48
1:A:309:GLU:O	1:A:313:TYR:OH	2.27	0.48
2:J:127:ALA:HB3	2:J:159:PHE:CD1	2.48	0.48
1:A:144:TYR:HD1	1:A:144:TYR:H	1.61	0.48
1:A:50:SER:C	1:A:51:THR:HG1	2.11	0.48
1:A:144:TYR:O	1:A:145:TYR:HB2	2.13	0.48
1:A:710:ASN:HD22	1:A:710:ASN:C	2.20	0.48
1:B:144:TYR:N	1:B:144:TYR:CD1	2.81	0.48
1:C:533:LEU:HD21	1:C:585:LEU:HD11	1.96	0.48
1:B:533:LEU:HD21	1:B:585:LEU:HD11	1.96	0.48
1:C:47:VAL:CG1	1:C:48:LEU:N	2.72	0.48
2:J:163:VAL:HG22	2:J:213:HIS:CD2	2.49	0.48
1:A:291:CYS:O	1:A:293:LEU:N	2.47	0.48
1:C:144:TYR:O	1:C:145:TYR:HB2	2.13	0.48
1:A:275:PHE:HE1	1:A:290:ASP:HB2	1.76	0.47
1:A:533:LEU:HD21	1:A:585:LEU:HD11	1.96	0.47
2:H:160:PRO:HB2	2:H:213:HIS:NE2	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:151:SER:O	1:A:152:TRP:HB2	2.13	0.47
1:B:34:ARG:NH2	1:B:191:GLU:OE2	2.35	0.47
1:B:115:GLN:HA	1:B:131:CYS:O	2.13	0.47
1:B:144:TYR:HD1	1:B:144:TYR:H	1.61	0.47
1:C:144:TYR:HD1	1:C:144:TYR:H	1.61	0.47
1:B:146:HIS:CG	1:B:147:LYS:CE	2.97	0.47
1:B:309:GLU:O	1:B:313:TYR:OH	2.27	0.47
2:I:160:PRO:HB2	2:I:213:HIS:NE2	2.29	0.47
4:g:1:NAG:H62	4:g:2:NAG:H82	1.97	0.47
1:A:146:HIS:CG	1:A:147:LYS:CE	2.97	0.47
6:B:1307:NAG:H3	6:B:1307:NAG:H83	1.96	0.47
1:C:280:ASN:HB3	1:C:283:GLY:O	2.13	0.47
1:C:291:CYS:C	1:C:293:LEU:N	2.72	0.47
1:A:146:HIS:ND1	1:A:146:HIS:N	2.60	0.47
1:B:98:SER:C	1:B:99:ASN:ND2	2.73	0.47
1:B:291:CYS:C	1:B:293:LEU:N	2.73	0.47
1:C:1051:SER:OG	1:C:1064:HIS:HD2	1.97	0.47
2:H:163:VAL:HG22	2:H:213:HIS:CD2	2.49	0.47
1:A:34:ARG:NH2	1:A:191:GLU:OE2	2.35	0.47
1:A:97:LYS:C	1:A:97:LYS:CD	2.86	0.47
1:A:115:GLN:HA	1:A:131:CYS:O	2.13	0.47
1:A:126:VAL:HB	1:A:174:PRO:HA	1.97	0.47
1:B:1051:SER:OG	1:B:1064:HIS:HD2	1.97	0.47
1:A:986:PRO:O	1:A:990:GLU:HG3	2.15	0.47
1:B:986:PRO:O	1:B:990:GLU:HG3	2.15	0.47
2:I:163:VAL:HG22	2:I:213:HIS:CD2	2.49	0.47
1:A:1051:SER:OG	1:A:1064:HIS:HD2	1.97	0.47
2:H:144:THR:HG23	2:H:149:ALA:HB2	1.97	0.47
2:J:160:PRO:HB2	2:J:213:HIS:NE2	2.29	0.47
3:N:139:PHE:HE1	3:N:173:TYR:C	2.21	0.47
1:B:126:VAL:HB	1:B:174:PRO:HA	1.97	0.47
1:B:562:PHE:HZ	1:C:38:TYR:HD2	1.63	0.47
2:I:144:THR:HG23	2:I:149:ALA:HB2	1.97	0.47
1:B:817:PHE:CE2	1:B:935:GLN:CD	2.93	0.46
1:C:146:HIS:CG	1:C:147:LYS:CE	2.97	0.46
1:A:617:CYS:HB3	1:A:633:TRP:CE2	2.50	0.46
2:I:11:LEU:CD1	2:I:159:PHE:HE2	2.20	0.46
2:H:143:SER:CA	3:L:116:PHE:HB3	2.40	0.46
3:L:142:ARG:HH21	3:L:163:VAL:HB	1.80	0.46
1:A:98:SER:C	1:A:99:ASN:ND2	2.73	0.46
1:A:395:VAL:HG11	7:A:1311:EIC:H131	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:47:VAL:CG1	1:B:48:LEU:N	2.73	0.46
1:C:144:TYR:N	1:C:144:TYR:CD1	2.81	0.46
2:J:125:SER:C	2:J:127:ALA:N	2.69	0.46
3:N:142:ARG:HH21	3:N:163:VAL:HB	1.81	0.46
1:A:149:ASN:C	1:A:151:SER:N	2.73	0.46
1:B:617:CYS:HB3	1:B:633:TRP:CE2	2.50	0.46
3:M:142:ARG:HH21	3:M:163:VAL:HB	1.81	0.46
1:A:938:LEU:C	1:A:940:SER:N	2.73	0.46
1:B:48:LEU:CD1	1:B:278:LYS:HB3	2.46	0.46
1:C:126:VAL:HB	1:C:174:PRO:HA	1.97	0.46
1:C:817:PHE:CE2	1:C:935:GLN:CD	2.93	0.46
3:M:115:VAL:C	3:M:116:PHE:CG	2.93	0.46
1:B:144:TYR:N	1:B:144:TYR:HD1	2.14	0.46
3:L:115:VAL:C	3:L:116:PHE:CG	2.93	0.46
2:I:140:SER:HB3	2:I:142:LYS:HG2	1.98	0.46
2:I:213:HIS:CD2	2:I:215:PRO:HD2	2.51	0.46
3:M:139:PHE:HE1	3:M:173:TYR:C	2.21	0.46
2:J:144:THR:HG23	2:J:149:ALA:HB2	1.97	0.46
1:C:98:SER:C	1:C:99:ASN:ND2	2.73	0.46
1:A:47:VAL:O	1:A:278:LYS:HA	2.15	0.46
1:C:986:PRO:O	1:C:990:GLU:HG3	2.15	0.46
3:M:34:GLY:HA2	3:M:48:ILE:O	2.16	0.46
2:J:11:LEU:CD1	2:J:159:PHE:HE2	2.20	0.46
2:J:128:SER:C	2:J:129:THR:CG2	2.87	0.46
3:N:115:VAL:C	3:N:116:PHE:CG	2.93	0.46
1:A:145:TYR:C	1:A:147:LYS:N	2.73	0.46
1:A:707:TYR:HB3	1:B:792:PRO:HG3	1.98	0.46
1:B:1141:LEU:O	1:B:1144:GLU:HB2	2.16	0.46
6:B:1307:NAG:C8	6:B:1307:NAG:C3	2.87	0.46
1:C:144:TYR:HD1	1:C:144:TYR:N	2.14	0.45
1:C:145:TYR:C	1:C:147:LYS:N	2.73	0.45
1:C:339:GLY:CA	6:C:1302:NAG:C8	2.66	0.45
1:C:596:SER:OG	1:C:613:GLN:OE1	2.34	0.45
1:C:938:LEU:O	1:C:940:SER:N	2.49	0.45
1:A:144:TYR:N	1:A:144:TYR:HD1	2.14	0.45
1:B:1048:HIS:HA	1:B:1066:THR:HG22	1.98	0.45
3:M:140:TYR:CB	3:M:141:PRO:CD	2.94	0.45
2:J:213:HIS:CD2	2:J:215:PRO:HD2	2.51	0.45
3:N:114:SER:CB	3:N:116:PHE:HZ	2.16	0.45
1:A:817:PHE:CE2	1:A:935:GLN:CD	2.93	0.45
1:B:395:VAL:HG21	1:B:524:VAL:HG21	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:971:GLY:O	1:C:995:ARG:NH1	2.47	0.45
1:C:1048:HIS:HA	1:C:1066:THR:HG22	1.98	0.45
2:H:140:SER:HB3	2:H:142:LYS:HG2	1.98	0.45
3:L:34:GLY:HA2	3:L:48:ILE:O	2.16	0.45
1:A:938:LEU:O	1:A:940:SER:N	2.50	0.45
1:B:938:LEU:C	1:B:940:SER:N	2.73	0.45
1:C:391:CYS:HA	1:C:525:CYS:HA	1.99	0.45
2:J:140:SER:HB3	2:J:142:LYS:HG2	1.98	0.45
6:A:1303:NAG:H5	6:A:1304:NAG:O7	2.16	0.45
1:B:97:LYS:C	1:B:97:LYS:CD	2.86	0.45
1:B:99:ASN:ND2	1:B:99:ASN:N	2.64	0.45
1:C:452:LEU:HD12	4:F:2:NAG:H81	1.97	0.45
6:C:1305:NAG:H5	6:C:1306:NAG:O7	2.16	0.45
2:H:135:PHE:HE2	3:L:124:GLN:HG3	1.72	0.45
1:B:596:SER:OG	1:B:613:GLN:OE1	2.34	0.45
1:C:938:LEU:C	1:C:940:SER:N	2.73	0.45
2:H:213:HIS:CD2	2:H:215:PRO:HD2	2.51	0.45
2:I:184:GLN:OE1	2:I:190:SER:OG	2.31	0.45
1:A:596:SER:OG	1:A:613:GLN:OE1	2.34	0.45
1:A:1141:LEU:O	1:A:1144:GLU:HB2	2.16	0.45
1:B:353:TRP:O	1:B:466:ARG:NH1	2.50	0.45
3:N:34:GLY:HA2	3:N:48:ILE:O	2.16	0.45
6:B:1305:NAG:H5	6:B:1306:NAG:O7	2.16	0.45
1:C:99:ASN:ND2	1:C:99:ASN:N	2.65	0.45
1:C:1141:LEU:O	1:C:1144:GLU:HB2	2.16	0.45
2:H:158:TYR:OH	2:H:191:LEU:HD23	2.17	0.45
2:H:184:GLN:OE1	2:H:190:SER:OG	2.31	0.45
2:J:158:TYR:OH	2:J:191:LEU:HD23	2.17	0.45
1:A:1048:HIS:HA	1:A:1066:THR:HG22	1.98	0.45
1:B:391:CYS:HA	1:B:525:CYS:HA	1.98	0.45
1:C:617:CYS:HB3	1:C:633:TRP:CE2	2.50	0.45
2:J:37:ILE:HG12	2:J:47:TRP:HA	1.99	0.45
3:N:140:TYR:CB	3:N:141:PRO:CD	2.94	0.45
1:A:144:TYR:CD1	1:A:144:TYR:O	2.70	0.45
1:A:279:TYR:HA	1:A:285:ILE:HA	1.99	0.45
1:B:149:ASN:C	1:B:151:SER:N	2.73	0.45
1:C:532:ASN:N	1:C:532:ASN:HD22	2.15	0.45
2:I:158:TYR:OH	2:I:191:LEU:HD23	2.17	0.45
3:M:108:ARG:NH1	3:M:109:THR:OG1	2.50	0.45
3:N:108:ARG:NH1	3:N:109:THR:OG1	2.50	0.45
1:B:47:VAL:O	1:B:278:LYS:HA	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:726:ILE:HD12	1:B:945:LEU:HD22	1.99	0.44
1:B:938:LEU:O	1:B:940:SER:N	2.49	0.44
2:H:114:ASP:OD1	2:H:114:ASP:N	2.50	0.44
2:I:143:SER:OG	3:M:118:PHE:CE1	2.60	0.44
1:C:47:VAL:O	1:C:278:LYS:HA	2.17	0.44
2:H:182:VAL:HG21	3:L:160:GLN:CD	2.42	0.44
3:L:142:ARG:C	3:L:144:ALA:H	2.26	0.44
2:J:11:LEU:CD1	2:J:159:PHE:HZ	2.10	0.44
1:A:358:ILE:HD13	7:A:1311:EIC:H162	1.98	0.44
1:C:353:TRP:O	1:C:466:ARG:NH1	2.50	0.44
1:B:144:TYR:O	1:B:144:TYR:CD1	2.70	0.44
1:B:532:ASN:N	1:B:532:ASN:HD22	2.14	0.44
2:H:125:SER:C	2:H:127:ALA:N	2.69	0.44
2:I:37:ILE:HG12	2:I:47:TRP:HA	1.99	0.44
6:A:1305:NAG:C8	6:A:1305:NAG:C3	2.87	0.44
1:B:785:VAL:HG23	1:B:787:GLN:H	1.83	0.44
6:B:1313:NAG:H61	6:B:1314:NAG:O7	2.18	0.44
2:H:37:ILE:HG12	2:H:47:TRP:HA	1.99	0.44
2:I:11:LEU:C	2:I:11:LEU:CD2	2.85	0.44
2:I:135:PHE:HE2	3:M:124:GLN:HG3	1.72	0.44
1:A:98:SER:C	1:A:99:ASN:CG	2.86	0.44
6:A:1309:NAG:H61	6:A:1310:NAG:O7	2.18	0.44
1:B:293:LEU:C	1:B:293:LEU:HD22	2.43	0.44
1:B:383:SER:OG	1:C:985:ASP:OD1	2.35	0.44
1:C:109:THR:HA	1:C:237:ARG:HH21	1.82	0.44
3:L:108:ARG:NH1	3:L:109:THR:OG1	2.50	0.44
3:L:140:TYR:CB	3:L:141:PRO:CD	2.94	0.44
1:A:532:ASN:HD22	1:A:532:ASN:N	2.14	0.44
1:B:145:TYR:C	1:B:147:LYS:N	2.73	0.44
1:B:287:ASP:OD1	1:B:306:PHE:HE2	2.00	0.44
1:B:971:GLY:O	1:B:995:ARG:NH1	2.47	0.44
1:C:135:PHE:HA	1:C:160:TYR:HA	2.00	0.44
1:C:291:CYS:C	1:C:293:LEU:H	2.25	0.44
6:C:1313:NAG:H61	6:C:1314:NAG:O7	2.18	0.44
2:I:143:SER:CA	3:M:116:PHE:HB3	2.40	0.44
3:N:142:ARG:C	3:N:144:ALA:H	2.26	0.44
1:A:391:CYS:HA	1:A:525:CYS:HA	1.98	0.44
1:C:144:TYR:O	1:C:144:TYR:CD1	2.70	0.44
1:C:431:GLY:HA2	1:C:515:PHE:CZ	2.53	0.44
1:C:452:LEU:HD13	4:F:2:NAG:H83	1.98	0.44
1:C:726:ILE:HD12	1:C:945:LEU:HD22	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:167:TRP:HD1	2:J:176:VAL:HG13	1.83	0.44
1:A:99:ASN:ND2	1:A:99:ASN:N	2.64	0.44
1:A:135:PHE:HA	1:A:160:TYR:HA	2.00	0.44
1:A:431:GLY:HA2	1:A:515:PHE:CZ	2.53	0.44
1:A:971:GLY:O	1:A:995:ARG:NH1	2.47	0.44
2:I:142:LYS:HG3	3:M:117:ILE:O	2.18	0.44
2:I:167:TRP:HD1	2:I:176:VAL:HG13	1.83	0.44
3:M:142:ARG:C	3:M:144:ALA:H	2.26	0.44
2:J:184:GLN:OE1	2:J:190:SER:OG	2.31	0.44
2:J:208:ILE:HG23	2:J:223:LYS:HD2	2.00	0.44
1:A:726:ILE:HD12	1:A:945:LEU:HD22	1.99	0.43
1:C:23:GLN:O	1:C:24:LEU:CB	2.51	0.43
1:C:98:SER:C	1:C:99:ASN:CG	2.86	0.43
1:C:785:VAL:HG23	1:C:787:GLN:H	1.83	0.43
2:H:208:ILE:HG23	2:H:223:LYS:HD2	2.00	0.43
1:A:383:SER:OG	1:B:985:ASP:OD1	2.26	0.43
1:A:395:VAL:HG21	1:A:524:VAL:HG21	1.99	0.43
1:A:785:VAL:HG23	1:A:787:GLN:H	1.83	0.43
1:B:291:CYS:C	1:B:293:LEU:H	2.25	0.43
1:B:431:GLY:HA2	1:B:515:PHE:CZ	2.53	0.43
1:C:149:ASN:C	1:C:151:SER:N	2.73	0.43
2:J:142:LYS:HE3	3:N:119:PRO:CD	2.49	0.43
1:A:109:THR:HA	1:A:237:ARG:HH21	1.82	0.43
1:C:279:TYR:HA	1:C:285:ILE:HA	1.99	0.43
1:C:1142:GLN:N	1:C:1143:PRO:HD2	2.33	0.43
2:H:167:TRP:HD1	2:H:176:VAL:HG13	1.83	0.43
2:J:11:LEU:HD12	2:J:159:PHE:HE2	1.71	0.43
2:H:168:ASN:OD1	2:H:208:ILE:HG13	2.19	0.43
2:I:208:ILE:HG23	2:I:223:LYS:HD2	2.00	0.43
2:J:91:THR:HA	2:J:122:VAL:O	2.18	0.43
1:A:275:PHE:CE1	1:A:290:ASP:CB	2.96	0.43
1:A:339:GLY:CA	4:P:1:NAG:C8	2.66	0.43
1:B:109:THR:HA	1:B:237:ARG:HH21	1.82	0.43
1:C:395:VAL:HG21	1:C:524:VAL:HG21	1.99	0.43
2:J:142:LYS:HG3	3:N:117:ILE:O	2.19	0.43
4:O:1:NAG:H62	4:O:2:NAG:H82	1.99	0.43
1:A:614:ASP:OD2	1:B:854:LYS:HE3	2.19	0.43
2:I:155:VAL:HG13	2:I:191:LEU:HG	2.01	0.43
2:I:182:VAL:HG21	3:M:160:GLN:CD	2.42	0.43
2:J:143:SER:CA	3:N:116:PHE:HB3	2.40	0.43
2:J:155:VAL:HG13	2:J:191:LEU:HG	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:98:SER:C	1:B:99:ASN:CG	2.86	0.43
2:H:91:THR:HA	2:H:122:VAL:O	2.18	0.43
2:J:168:ASN:OD1	2:J:208:ILE:HG13	2.19	0.43
1:A:353:TRP:O	1:A:466:ARG:NH1	2.50	0.43
1:C:95:THR:HG21	1:C:187:LYS:NZ	2.34	0.43
2:I:11:LEU:HD11	2:I:159:PHE:CE2	2.48	0.43
3:M:105:GLU:HG2	3:M:173:TYR:OH	2.19	0.43
2:J:182:VAL:HG21	3:N:160:GLN:CD	2.42	0.43
1:B:279:TYR:HA	1:B:285:ILE:HA	1.99	0.43
2:I:91:THR:HA	2:I:122:VAL:O	2.18	0.43
1:A:980:ILE:O	1:A:984:LEU:HB2	2.19	0.43
2:H:160:PRO:HD2	2:H:213:HIS:CE1	2.54	0.43
2:H:191:LEU:HD12	2:H:192:SER:N	2.34	0.43
2:I:160:PRO:HD2	2:I:213:HIS:CE1	2.54	0.43
3:N:82:ASP:O	3:N:86:TYR:OH	2.30	0.43
1:A:293:LEU:C	1:A:293:LEU:HD13	2.44	0.42
1:B:1142:GLN:N	1:B:1143:PRO:HD2	2.34	0.42
1:C:980:ILE:O	1:C:984:LEU:HB2	2.19	0.42
6:C:1307:NAG:H3	6:C:1307:NAG:H83	1.96	0.42
2:J:160:PRO:HD2	2:J:213:HIS:CE1	2.54	0.42
3:N:105:GLU:HG2	3:N:173:TYR:OH	2.19	0.42
1:C:191:GLU:O	1:C:205:SER:HA	2.19	0.42
1:A:191:GLU:O	1:A:205:SER:HA	2.19	0.42
1:B:135:PHE:HA	1:B:160:TYR:HA	2.00	0.42
1:C:130:VAL:HG21	1:C:231:ILE:HG23	2.01	0.42
1:C:563:GLN:O	1:C:577:ARG:NH1	2.53	0.42
2:H:142:LYS:HG3	3:L:117:ILE:O	2.18	0.42
1:A:147:LYS:O	1:A:150:LYS:N	2.49	0.42
1:B:913:GLN:H	1:B:913:GLN:HG3	1.63	0.42
1:C:37:TYR:OH	1:C:54:LEU:O	2.31	0.42
2:I:11:LEU:HD12	2:I:159:PHE:HE2	1.71	0.42
2:I:135:PHE:HD1	3:M:123:GLU:OE1	2.02	0.42
1:A:588:THR:HG21	1:B:841:LEU:HD12	2.02	0.42
1:A:1038:LYS:HA	1:A:1038:LYS:HD3	1.90	0.42
1:B:563:GLN:O	1:B:577:ARG:NH1	2.53	0.42
1:B:980:ILE:O	1:B:984:LEU:HB2	2.19	0.42
1:C:675:GLN:HE21	1:C:675:GLN:HB3	1.62	0.42
7:C:1315:EIC:H112	7:C:1315:EIC:H142	1.65	0.42
2:J:1:GLU:HB3	2:J:2:VAL:H	1.51	0.42
2:H:202:LEU:HB3	2:H:226:PRO:HG3	2.02	0.42
1:A:498:GLN:HE21	1:A:498:GLN:HB2	1.61	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:95:THR:HG21	1:B:187:LYS:NZ	2.34	0.42
1:B:746:SER:HB3	1:B:749:CYS:HB3	2.02	0.42
1:C:752:LEU:HD21	1:C:990:GLU:OE2	2.20	0.42
2:H:142:LYS:HE3	3:L:119:PRO:CD	2.49	0.42
2:I:191:LEU:HD12	2:I:192:SER:N	2.34	0.42
2:I:222:LYS:HD2	2:I:222:LYS:HA	1.92	0.42
2:J:135:PHE:HD1	3:N:123:GLU:OE1	2.02	0.42
1:A:95:THR:HG21	1:A:187:LYS:NZ	2.34	0.42
1:A:96:GLU:HB2	1:A:263:ALA:HB2	2.01	0.42
1:A:746:SER:HB3	1:A:749:CYS:HB3	2.02	0.42
1:A:1142:GLN:N	1:A:1143:PRO:HD2	2.34	0.42
1:C:98:SER:HB2	1:C:99:ASN:H	1.63	0.42
1:C:328:ARG:NH1	1:C:531:THR:O	2.50	0.42
1:C:1038:LYS:HA	1:C:1038:LYS:HD3	1.90	0.42
2:H:129:THR:HA	2:H:160:PRO:HG3	2.02	0.42
3:L:105:GLU:HG2	3:L:173:TYR:OH	2.19	0.42
2:I:11:LEU:CD1	2:I:159:PHE:HZ	2.11	0.42
1:B:130:VAL:HG21	1:B:231:ILE:HG23	2.01	0.42
1:B:191:GLU:O	1:B:205:SER:HA	2.19	0.42
1:C:96:GLU:HB2	1:C:263:ALA:HB2	2.01	0.42
2:H:155:VAL:HG13	2:H:191:LEU:HG	2.00	0.42
1:A:328:ARG:NH1	1:A:531:THR:O	2.50	0.42
1:A:703:ASN:OD1	1:A:704:SER:N	2.53	0.42
1:B:482:GLY:O	3:N:60:SER:OG	2.30	0.42
2:H:179:PHE:CD2	3:L:176:SER:HB3	2.54	0.42
2:I:168:ASN:OD1	2:I:208:ILE:HG13	2.19	0.42
2:I:179:PHE:CD2	3:M:176:SER:HB3	2.54	0.42
2:J:191:LEU:HD12	2:J:192:SER:N	2.34	0.42
1:A:463:PRO:CB	1:B:198:ASP:OD1	2.32	0.41
1:B:145:TYR:HB2	1:B:153:MET:HA	1.99	0.41
3:L:181:LEU:HA	3:L:181:LEU:HD23	1.81	0.41
2:J:129:THR:HA	2:J:160:PRO:HG3	2.02	0.41
1:A:291:CYS:O	1:A:292:ALA:C	2.62	0.41
1:B:113:LYS:HE2	1:B:113:LYS:HB2	1.84	0.41
1:C:537:LYS:HB3	1:C:537:LYS:HE2	1.70	0.41
1:C:703:ASN:OD1	1:C:704:SER:N	2.53	0.41
1:A:563:GLN:O	1:A:577:ARG:NH1	2.53	0.41
1:B:122:ASN:CG	1:B:123:ALA:H	2.28	0.41
1:B:164:ASN:OD1	1:B:164:ASN:N	2.53	0.41
1:B:290:ASP:O	1:B:293:LEU:HB3	2.20	0.41
1:B:291:CYS:O	1:B:293:LEU:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:43:PHE:CD1	1:C:43:PHE:C	2.98	0.41
2:I:212:ASN:HB3	2:I:219:LYS:CE	2.49	0.41
1:A:130:VAL:HG21	1:A:231:ILE:HG23	2.01	0.41
1:A:532:ASN:N	1:A:532:ASN:ND2	2.69	0.41
1:B:37:TYR:OH	1:B:54:LEU:O	2.31	0.41
1:B:149:ASN:O	1:B:151:SER:N	2.54	0.41
1:B:569:ILE:HD11	1:C:964:LYS:HB3	2.01	0.41
1:B:703:ASN:OD1	1:B:704:SER:N	2.53	0.41
1:C:818:ILE:HB	1:C:1054:GLN:HE21	1.86	0.41
3:L:139:PHE:HE1	3:L:174:SER:N	2.18	0.41
2:J:213:HIS:HD2	2:J:215:PRO:HD2	1.86	0.41
1:A:43:PHE:CD1	1:A:43:PHE:C	2.98	0.41
1:A:122:ASN:CG	1:A:123:ALA:H	2.28	0.41
1:A:164:ASN:OD1	1:A:164:ASN:N	2.53	0.41
1:A:752:LEU:HD21	1:A:990:GLU:OE2	2.20	0.41
1:B:96:GLU:HB2	1:B:263:ALA:HB2	2.01	0.41
1:B:533:LEU:HD12	1:B:533:LEU:HA	1.91	0.41
1:C:278:LYS:O	1:C:285:ILE:HG23	2.20	0.41
2:H:135:PHE:HD1	3:L:123:GLU:OE1	2.03	0.41
1:A:124:THR:C	1:A:125:ASN:HD22	2.20	0.41
1:B:818:ILE:HB	1:B:1054:GLN:HE21	1.86	0.41
1:B:959:LEU:HD23	1:B:959:LEU:HA	1.86	0.41
1:C:564:GLN:HE21	1:C:564:GLN:HB2	1.67	0.41
1:C:759:PHE:O	1:C:763:LEU:HG	2.21	0.41
2:J:179:PHE:CD2	3:N:176:SER:HB3	2.55	0.41
2:J:202:LEU:HB3	2:J:226:PRO:HG3	2.02	0.41
3:N:139:PHE:HE1	3:N:174:SER:N	2.18	0.41
3:N:142:ARG:O	3:N:144:ALA:N	2.47	0.41
1:A:938:LEU:HD23	1:A:938:LEU:HA	1.90	0.41
1:B:48:LEU:HD12	1:B:278:LYS:HB3	2.03	0.41
1:A:459:SER:CB	4:W:2:NAG:H81	2.49	0.41
1:B:48:LEU:CD1	1:B:278:LYS:CB	2.98	0.41
1:C:145:TYR:C	1:C:147:LYS:H	2.29	0.41
1:C:452:LEU:CD1	4:F:2:NAG:H83	2.51	0.41
1:C:746:SER:HB3	1:C:749:CYS:HB3	2.02	0.41
2:I:129:THR:HA	2:I:160:PRO:HG3	2.02	0.41
1:A:145:TYR:C	1:A:147:LYS:H	2.29	0.41
1:A:715:PRO:HA	1:A:1072:GLU:HA	2.03	0.41
1:A:818:ILE:HB	1:A:1054:GLN:HE21	1.85	0.41
1:B:425:LEU:HD23	1:B:425:LEU:HA	1.93	0.41
1:B:555:SER:C	1:B:556:ASN:HD22	2.29	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:752:LEU:HD21	1:B:990:GLU:OE2	2.20	0.41
1:C:555:SER:C	1:C:556:ASN:HD22	2.29	0.41
1:C:959:LEU:HD23	1:C:959:LEU:HA	1.85	0.41
3:L:39:LYS:NZ	3:L:81:GLU:O	2.37	0.41
2:I:114:ASP:OD1	2:I:114:ASP:N	2.50	0.41
2:I:125:SER:OG	2:I:159:PHE:CE1	2.50	0.41
2:I:207:TYR:H	2:I:223:LYS:HE3	1.86	0.41
2:I:213:HIS:HD2	2:I:215:PRO:HD2	1.86	0.41
3:M:139:PHE:HE1	3:M:174:SER:N	2.18	0.41
3:M:181:LEU:HA	3:M:181:LEU:HD23	1.82	0.41
1:A:759:PHE:O	1:A:763:LEU:HG	2.21	0.41
1:A:884:SER:OG	1:A:893:ALA:HB1	2.21	0.41
1:A:1028:LYS:NZ	1:A:1042:PHE:O	2.53	0.41
1:B:537:LYS:HB3	1:B:537:LYS:HE2	1.70	0.41
1:B:884:SER:OG	1:B:893:ALA:HB1	2.21	0.41
1:C:862:PRO:HA	1:C:863:PRO:HD3	1.97	0.41
2:H:128:SER:C	2:H:129:THR:CG2	2.87	0.41
2:H:213:HIS:HD2	2:H:215:PRO:HD2	1.86	0.41
1:A:353:TRP:CD1	1:A:353:TRP:H	2.38	0.40
1:B:278:LYS:O	1:B:278:LYS:HG3	2.20	0.40
1:C:290:ASP:O	1:C:293:LEU:HB3	2.22	0.40
1:C:1028:LYS:NZ	1:C:1042:PHE:O	2.53	0.40
2:I:202:LEU:HB3	2:I:226:PRO:HG3	2.02	0.40
1:B:145:TYR:C	1:B:147:LYS:H	2.29	0.40
1:B:353:TRP:H	1:B:353:TRP:CD1	2.39	0.40
1:B:1028:LYS:NZ	1:B:1042:PHE:O	2.52	0.40
1:C:330:PRO:HD2	1:C:525:CYS:SG	2.62	0.40
2:J:211:VAL:O	2:J:219:LYS:HA	2.22	0.40
2:J:212:ASN:HB3	2:J:219:LYS:CE	2.49	0.40
1:A:149:ASN:O	1:A:151:SER:N	2.54	0.40
1:A:555:SER:C	1:A:556:ASN:HD22	2.29	0.40
1:B:43:PHE:CD1	1:B:43:PHE:C	2.98	0.40
1:B:155:SER:C	1:B:156:GLU:CG	2.95	0.40
1:B:293:LEU:O	1:B:294:ASP:CB	2.69	0.40
2:H:49:SER:HB3	2:H:70:ILE:HD11	2.03	0.40
3:M:39:LYS:NZ	3:M:81:GLU:O	2.37	0.40
1:A:358:ILE:HD13	7:A:1311:EIC:C16	2.52	0.40
1:B:826:VAL:HB	1:B:1057:PRO:HG2	2.04	0.40
1:C:884:SER:OG	1:C:893:ALA:HB1	2.21	0.40
2:H:214:LYS:HD3	2:H:214:LYS:HA	1.90	0.40
2:J:207:TYR:H	2:J:223:LYS:HE3	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:155:SER:C	1:A:156:GLU:CG	2.95	0.40
1:A:330:PRO:HD2	1:A:525:CYS:SG	2.62	0.40
2:H:33:TYR:N	2:H:100:GLY:HA3	2.36	0.40
2:H:207:TYR:H	2:H:223:LYS:HE3	1.86	0.40
2:I:49:SER:HB3	2:I:70:ILE:HD11	2.04	0.40
2:I:161:GLU:HG3	2:I:189:TYR:CE2	2.57	0.40
3:N:39:LYS:NZ	3:N:81:GLU:O	2.37	0.40
3:N:116:PHE:CE2	3:N:137:ASN:HB2	2.51	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	1067/1283 (83%)	977 (92%)	77 (7%)	13 (1%)	10	34
1	B	1067/1283 (83%)	977 (92%)	80 (8%)	10 (1%)	14	41
1	C	1067/1283 (83%)	978 (92%)	79 (7%)	10 (1%)	14	41
2	H	226/267 (85%)	206 (91%)	14 (6%)	6 (3%)	4	15
2	I	226/267 (85%)	206 (91%)	14 (6%)	6 (3%)	4	15
2	J	226/267 (85%)	206 (91%)	14 (6%)	6 (3%)	4	15
3	L	212/257 (82%)	187 (88%)	21 (10%)	4 (2%)	6	22
3	M	212/257 (82%)	187 (88%)	21 (10%)	4 (2%)	6	22
3	N	212/257 (82%)	187 (88%)	21 (10%)	4 (2%)	6	22
All	All	4515/5421 (83%)	4111 (91%)	341 (8%)	63 (1%)	11	30

All (63) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	23	GLN
1	A	24	LEU
1	A	145	TYR
1	B	23	GLN
1	B	24	LEU
1	B	145	TYR
1	C	23	GLN
1	C	24	LEU
1	C	145	TYR
2	H	127	ALA
2	H	128	SER
2	H	129	THR
3	L	138	ASN
2	I	127	ALA
2	I	128	SER
2	I	129	THR
3	M	138	ASN
2	J	127	ALA
2	J	128	SER
2	J	129	THR
3	N	138	ASN
1	A	122	ASN
1	A	292	ALA
1	B	122	ASN
1	C	122	ASN
1	A	939	SER
1	B	939	SER
1	C	939	SER
1	A	96	GLU
1	A	150	LYS
1	A	284	THR
1	B	96	GLU
1	B	150	LYS
1	B	284	THR
1	C	96	GLU
1	C	150	LYS
1	C	284	THR
2	H	102	GLU
2	I	102	GLU
2	J	102	GLU
1	A	291	CYS
1	A	936	ASP
1	B	294	ASP

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Mol	Chain	Res	Type
1	B	936	ASP
1	C	936	ASP
2	H	126	SER
3	L	139	PHE
3	L	140	TYR
3	L	143	GLU
2	I	126	SER
3	M	139	PHE
3	M	140	TYR
3	M	143	GLU
2	J	126	SER
3	N	139	PHE
3	N	140	TYR
3	N	143	GLU
2	H	103	LEU
2	I	103	LEU
2	J	103	LEU
1	A	294	ASP
1	C	294	ASP
1	A	295	PRO

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	941/1122 (84%)	838 (89%)	103 (11%)	6	21
1	B	941/1122 (84%)	837 (89%)	104 (11%)	6	20
1	C	941/1122 (84%)	838 (89%)	103 (11%)	6	21
2	H	189/221 (86%)	176 (93%)	13 (7%)	14	41
2	I	189/221 (86%)	176 (93%)	13 (7%)	14	41
2	J	189/221 (86%)	176 (93%)	13 (7%)	14	41
3	L	187/221 (85%)	179 (96%)	8 (4%)	26	60
3	M	187/221 (85%)	179 (96%)	8 (4%)	26	60

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	N	187/221 (85%)	179 (96%)	8 (4%)	26	60
All	All	3951/4692 (84%)	3578 (91%)	373 (9%)	10	27

All (373) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	VAL
1	A	24	LEU
1	A	45	SER
1	A	46	SER
1	A	48	LEU
1	A	96	GLU
1	A	97	LYS
1	A	98	SER
1	A	99	ASN
1	A	100	ILE
1	A	121	ASN
1	A	144	TYR
1	A	145	TYR
1	A	146	HIS
1	A	147	LYS
1	A	148	ASN
1	A	149	ASN
1	A	150	LYS
1	A	155	SER
1	A	276	LEU
1	A	278	LYS
1	A	282	ASN
1	A	290	ASP
1	A	293	LEU
1	A	299	THR
1	A	305	SER
1	A	325	SER
1	A	333	THR
1	A	345	THR
1	A	366	SER
1	A	370	ASN
1	A	373	SER
1	A	375	SER
1	A	378	LYS
1	A	393	THR
1	A	399	SER

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Mol	Chain	Res	Type
1	A	443	SER
1	A	445	VAL
1	A	459	SER
1	A	469	SER
1	A	471	GLU
1	A	480	CYS
1	A	493	GLN
1	A	503	VAL
1	A	514	SER
1	A	516	GLU
1	A	528	LYS
1	A	530	SER
1	A	531	THR
1	A	532	ASN
1	A	534	VAL
1	A	558	LYS
1	A	569	ILE
1	A	588	THR
1	A	599	THR
1	A	604	THR
1	A	606	ASN
1	A	614	ASP
1	A	617	CYS
1	A	638	THR
1	A	642	VAL
1	A	645	THR
1	A	675	GLN
1	A	676	THR
1	A	691	SER
1	A	705	VAL
1	A	708	SER
1	A	710	ASN
1	A	719	THR
1	A	723	THR
1	A	726	ILE
1	A	730	SER
1	A	732	THR
1	A	745	ASP
1	A	746	SER
1	A	761	THR
1	A	768	THR
1	A	780	GLU

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Mol	Chain	Res	Type
1	A	785	VAL
1	A	790	LYS
1	A	810	SER
1	A	814	LYS
1	A	854	LYS
1	A	861	LEU
1	A	878	LEU
1	A	881	THR
1	A	884	SER
1	A	913	GLN
1	A	916	LEU
1	A	933	LYS
1	A	962	LEU
1	A	964	LYS
1	A	974	SER
1	A	982	SER
1	A	991	VAL
1	A	1002	GLN
1	A	1030	SER
1	A	1092	GLU
1	A	1097	SER
1	A	1118	ASP
1	A	1128	VAL
1	A	1136	THR
1	A	1142	GLN
1	B	16	VAL
1	B	24	LEU
1	B	45	SER
1	B	46	SER
1	B	48	LEU
1	B	96	GLU
1	B	97	LYS
1	B	98	SER
1	B	99	ASN
1	B	100	ILE
1	B	121	ASN
1	B	144	TYR
1	B	145	TYR
1	B	146	HIS
1	B	147	LYS
1	B	148	ASN
1	B	149	ASN

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Mol	Chain	Res	Type
1	B	150	LYS
1	B	155	SER
1	B	224	GLU
1	B	276	LEU
1	B	278	LYS
1	B	282	ASN
1	B	293	LEU
1	B	299	THR
1	B	301	CYS
1	B	305	SER
1	B	325	SER
1	B	333	THR
1	B	345	THR
1	B	366	SER
1	B	370	ASN
1	B	373	SER
1	B	375	SER
1	B	378	LYS
1	B	393	THR
1	B	399	SER
1	B	443	SER
1	B	445	VAL
1	B	459	SER
1	B	469	SER
1	B	471	GLU
1	B	480	CYS
1	B	493	GLN
1	B	503	VAL
1	B	514	SER
1	B	516	GLU
1	B	528	LYS
1	B	530	SER
1	B	531	THR
1	B	532	ASN
1	B	534	VAL
1	B	558	LYS
1	B	569	ILE
1	B	588	THR
1	B	599	THR
1	B	604	THR
1	B	606	ASN
1	B	614	ASP

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Mol	Chain	Res	Type
1	B	617	CYS
1	B	638	THR
1	B	642	VAL
1	B	645	THR
1	B	675	GLN
1	B	676	THR
1	B	691	SER
1	B	705	VAL
1	B	708	SER
1	B	710	ASN
1	B	719	THR
1	B	723	THR
1	B	726	ILE
1	B	730	SER
1	B	732	THR
1	B	745	ASP
1	B	746	SER
1	B	761	THR
1	B	768	THR
1	B	780	GLU
1	B	785	VAL
1	B	790	LYS
1	B	810	SER
1	B	814	LYS
1	B	854	LYS
1	B	861	LEU
1	B	878	LEU
1	B	881	THR
1	B	884	SER
1	B	913	GLN
1	B	916	LEU
1	B	933	LYS
1	B	962	LEU
1	B	964	LYS
1	B	974	SER
1	B	982	SER
1	B	991	VAL
1	B	1002	GLN
1	B	1030	SER
1	B	1092	GLU
1	B	1097	SER
1	B	1118	ASP

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Mol	Chain	Res	Type
1	B	1128	VAL
1	B	1136	THR
1	B	1142	GLN
1	C	16	VAL
1	C	24	LEU
1	C	45	SER
1	C	46	SER
1	C	48	LEU
1	C	96	GLU
1	C	97	LYS
1	C	98	SER
1	C	99	ASN
1	C	100	ILE
1	C	121	ASN
1	C	144	TYR
1	C	145	TYR
1	C	146	HIS
1	C	147	LYS
1	C	148	ASN
1	C	149	ASN
1	C	150	LYS
1	C	155	SER
1	C	224	GLU
1	C	276	LEU
1	C	278	LYS
1	C	282	ASN
1	C	293	LEU
1	C	299	THR
1	C	305	SER
1	C	325	SER
1	C	333	THR
1	C	345	THR
1	C	366	SER
1	C	370	ASN
1	C	373	SER
1	C	375	SER
1	C	378	LYS
1	C	393	THR
1	C	399	SER
1	C	443	SER
1	C	445	VAL
1	C	459	SER

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Mol	Chain	Res	Type
1	C	469	SER
1	C	471	GLU
1	C	480	CYS
1	C	493	GLN
1	C	503	VAL
1	C	514	SER
1	C	516	GLU
1	C	528	LYS
1	C	530	SER
1	C	531	THR
1	C	532	ASN
1	C	534	VAL
1	C	558	LYS
1	C	569	ILE
1	C	588	THR
1	C	599	THR
1	C	604	THR
1	C	606	ASN
1	C	614	ASP
1	C	617	CYS
1	C	638	THR
1	C	642	VAL
1	C	645	THR
1	C	675	GLN
1	C	676	THR
1	C	691	SER
1	C	705	VAL
1	C	708	SER
1	C	710	ASN
1	C	719	THR
1	C	723	THR
1	C	726	ILE
1	C	730	SER
1	C	732	THR
1	C	745	ASP
1	C	746	SER
1	C	761	THR
1	C	768	THR
1	C	780	GLU
1	C	785	VAL
1	C	790	LYS
1	C	810	SER

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Mol	Chain	Res	Type
1	C	814	LYS
1	C	854	LYS
1	C	861	LEU
1	C	878	LEU
1	C	881	THR
1	C	884	SER
1	C	913	GLN
1	C	916	LEU
1	C	933	LYS
1	C	962	LEU
1	C	964	LYS
1	C	974	SER
1	C	982	SER
1	C	991	VAL
1	C	1002	GLN
1	C	1030	SER
1	C	1092	GLU
1	C	1097	SER
1	C	1118	ASP
1	C	1128	VAL
1	C	1136	THR
1	C	1142	GLN
2	H	125	SER
2	H	126	SER
2	H	129	THR
2	H	130	LYS
2	H	151	LEU
2	H	155	VAL
2	H	169	SER
2	H	173	THR
2	H	177	HIS
2	H	192	SER
2	H	208	ILE
2	H	210	ASN
2	H	216	SER
3	L	107	LYS
3	L	108	ARG
3	L	114	SER
3	L	131	SER
3	L	142	ARG
3	L	159	SER
3	L	176	SER

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Mol	Chain	Res	Type
3	L	202	SER
2	I	125	SER
2	I	126	SER
2	I	129	THR
2	I	130	LYS
2	I	151	LEU
2	I	155	VAL
2	I	169	SER
2	I	173	THR
2	I	177	HIS
2	I	192	SER
2	I	208	ILE
2	I	210	ASN
2	I	216	SER
3	M	107	LYS
3	M	108	ARG
3	M	114	SER
3	M	131	SER
3	M	142	ARG
3	M	159	SER
3	M	176	SER
3	M	202	SER
2	J	125	SER
2	J	126	SER
2	J	129	THR
2	J	130	LYS
2	J	151	LEU
2	J	155	VAL
2	J	169	SER
2	J	173	THR
2	J	177	HIS
2	J	192	SER
2	J	208	ILE
2	J	210	ASN
2	J	216	SER
3	N	107	LYS
3	N	108	ARG
3	N	114	SER
3	N	131	SER
3	N	142	ARG
3	N	159	SER
3	N	176	SER

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Mol	Chain	Res	Type
3	N	202	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (130) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	GLN
1	A	69	HIS
1	A	87	ASN
1	A	99	ASN
1	A	125	ASN
1	A	149	ASN
1	A	196	ASN
1	A	271	GLN
1	A	314	GLN
1	A	317	ASN
1	A	448	ASN
1	A	450	ASN
1	A	493	GLN
1	A	498	GLN
1	A	532	ASN
1	A	540	ASN
1	A	544	ASN
1	A	556	ASN
1	A	564	GLN
1	A	606	ASN
1	A	613	GLN
1	A	655	HIS
1	A	675	GLN
1	A	710	ASN
1	A	751	ASN
1	A	764	ASN
1	A	804	GLN
1	A	836	GLN
1	A	925	ASN
1	A	955	ASN
1	A	1005	GLN
1	A	1011	GLN
1	A	1023	ASN
1	A	1036	GLN
1	A	1054	GLN
1	A	1064	HIS
1	A	1106	GLN

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Mol	Chain	Res	Type
1	A	1125	ASN
1	B	14	GLN
1	B	69	HIS
1	B	87	ASN
1	B	99	ASN
1	B	121	ASN
1	B	125	ASN
1	B	149	ASN
1	B	196	ASN
1	B	271	GLN
1	B	314	GLN
1	B	317	ASN
1	B	448	ASN
1	B	450	ASN
1	B	493	GLN
1	B	498	GLN
1	B	532	ASN
1	B	540	ASN
1	B	544	ASN
1	B	556	ASN
1	B	564	GLN
1	B	606	ASN
1	B	613	GLN
1	B	655	HIS
1	B	675	GLN
1	B	710	ASN
1	B	751	ASN
1	B	764	ASN
1	B	804	GLN
1	B	836	GLN
1	B	925	ASN
1	B	935	GLN
1	B	955	ASN
1	B	1011	GLN
1	B	1023	ASN
1	B	1036	GLN
1	B	1054	GLN
1	B	1064	HIS
1	B	1106	GLN
1	B	1125	ASN
1	C	14	GLN
1	C	69	HIS

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Mol	Chain	Res	Type
1	C	87	ASN
1	C	99	ASN
1	C	125	ASN
1	C	149	ASN
1	C	196	ASN
1	C	271	GLN
1	C	314	GLN
1	C	317	ASN
1	C	448	ASN
1	C	450	ASN
1	C	493	GLN
1	C	498	GLN
1	C	532	ASN
1	C	540	ASN
1	C	544	ASN
1	C	556	ASN
1	C	564	GLN
1	C	606	ASN
1	C	613	GLN
1	C	655	HIS
1	C	675	GLN
1	C	710	ASN
1	C	751	ASN
1	C	764	ASN
1	C	804	GLN
1	C	872	GLN
1	C	925	ASN
1	C	935	GLN
1	C	955	ASN
1	C	1005	GLN
1	C	1011	GLN
1	C	1023	ASN
1	C	1036	GLN
1	C	1054	GLN
1	C	1064	HIS
1	C	1125	ASN
2	H	77	ASN
2	H	217	ASN
3	L	6	GLN
3	L	79	GLN
3	L	91	HIS
2	I	77	ASN

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Mol	Chain	Res	Type
2	I	217	ASN
3	M	6	GLN
3	M	79	GLN
3	M	91	HIS
2	J	77	ASN
2	J	217	ASN
3	N	6	GLN
3	N	79	GLN
3	N	91	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

55 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	NAG	D	1	1,4	14,14,15	0.77	1 (7%)	17,19,21	1.08	2 (11%)
4	NAG	D	2	4	14,14,15	0.71	1 (7%)	17,19,21	0.63	0
5	NAG	E	1	1,5	14,14,15	0.50	0	17,19,21	0.60	0
5	NAG	E	2	5	14,14,15	0.29	0	17,19,21	0.53	0
5	NAG	E	3	5	14,14,15	0.28	0	17,19,21	0.64	1 (5%)
4	NAG	F	1	1,4	14,14,15	0.25	0	17,19,21	0.59	0
4	NAG	F	2	4	14,14,15	0.28	0	17,19,21	0.64	0
4	NAG	G	1	1,4	14,14,15	0.45	0	17,19,21	0.81	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	G	2	4	14,14,15	0.84	1 (7%)	17,19,21	0.60	0
4	NAG	K	1	1,4	14,14,15	0.89	1 (7%)	17,19,21	2.37	3 (17%)
4	NAG	K	2	4	14,14,15	0.41	0	17,19,21	0.51	0
4	NAG	O	1	1,4	14,14,15	1.10	1 (7%)	17,19,21	0.63	0
4	NAG	O	2	4	14,14,15	2.24	2 (14%)	17,19,21	1.02	2 (11%)
4	NAG	P	1	1,4	14,14,15	0.83	1 (7%)	17,19,21	0.57	0
4	NAG	P	2	4	14,14,15	2.97	3 (21%)	17,19,21	1.58	4 (23%)
4	NAG	Q	1	1,4	14,14,15	0.29	0	17,19,21	0.63	0
4	NAG	Q	2	4	14,14,15	0.53	0	17,19,21	0.49	0
4	NAG	R	1	1,4	14,14,15	0.69	1 (7%)	17,19,21	0.71	0
4	NAG	R	2	4	14,14,15	0.41	0	17,19,21	1.48	3 (17%)
4	NAG	S	1	1,4	14,14,15	0.66	1 (7%)	17,19,21	0.68	0
4	NAG	S	2	4	14,14,15	0.28	0	17,19,21	0.68	0
4	NAG	T	1	1,4	14,14,15	0.76	1 (7%)	17,19,21	1.08	2 (11%)
4	NAG	T	2	4	14,14,15	0.72	1 (7%)	17,19,21	0.62	0
5	NAG	U	1	1,5	14,14,15	0.48	0	17,19,21	0.60	0
5	NAG	U	2	5	14,14,15	0.31	0	17,19,21	0.53	0
5	NAG	U	3	5	14,14,15	0.29	0	17,19,21	0.65	1 (5%)
4	NAG	V	1	1,4	14,14,15	0.25	0	17,19,21	0.59	0
4	NAG	V	2	4	14,14,15	0.28	0	17,19,21	0.64	1 (5%)
4	NAG	W	1	1,4	14,14,15	0.44	0	17,19,21	0.82	1 (5%)
4	NAG	W	2	4	14,14,15	0.84	1 (7%)	17,19,21	0.59	0
4	NAG	X	1	1,4	14,14,15	0.89	1 (7%)	17,19,21	2.37	3 (17%)
4	NAG	X	2	4	14,14,15	0.41	0	17,19,21	0.51	0
4	NAG	Y	1	1,4	14,14,15	1.10	1 (7%)	17,19,21	0.63	0
4	NAG	Y	2	4	14,14,15	2.26	2 (14%)	17,19,21	1.01	2 (11%)
4	NAG	Z	1	1,4	14,14,15	0.28	0	17,19,21	0.64	0
4	NAG	Z	2	4	14,14,15	0.51	0	17,19,21	0.48	0
4	NAG	a	1	1,4	14,14,15	0.69	1 (7%)	17,19,21	0.69	0
4	NAG	a	2	4	14,14,15	0.28	0	17,19,21	0.68	0
4	NAG	b	1	1,4	14,14,15	0.77	1 (7%)	17,19,21	1.08	2 (11%)
4	NAG	b	2	4	14,14,15	0.70	1 (7%)	17,19,21	0.62	0
5	NAG	c	1	1,5	14,14,15	0.51	0	17,19,21	0.60	0
5	NAG	c	2	5	14,14,15	0.31	0	17,19,21	0.53	0
5	NAG	c	3	5	14,14,15	0.29	0	17,19,21	0.64	1 (5%)
4	NAG	d	1	1,4	14,14,15	0.24	0	17,19,21	0.60	0
4	NAG	d	2	4	14,14,15	0.27	0	17,19,21	0.64	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	e	1	1,4	14,14,15	0.45	0	17,19,21	0.81	1 (5%)
4	NAG	e	2	4	14,14,15	0.84	1 (7%)	17,19,21	0.60	0
4	NAG	f	1	1,4	14,14,15	0.89	1 (7%)	17,19,21	2.37	3 (17%)
4	NAG	f	2	4	14,14,15	0.40	0	17,19,21	0.51	0
4	NAG	g	1	1,4	14,14,15	1.10	1 (7%)	17,19,21	0.62	0
4	NAG	g	2	4	14,14,15	2.25	2 (14%)	17,19,21	1.01	2 (11%)
4	NAG	h	1	1,4	14,14,15	0.27	0	17,19,21	0.63	0
4	NAG	h	2	4	14,14,15	0.52	0	17,19,21	0.49	0
4	NAG	i	1	1,4	14,14,15	0.69	1 (7%)	17,19,21	0.68	0
4	NAG	i	2	4	14,14,15	0.29	0	17,19,21	0.69	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	D	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	D	2	4	-	2/6/23/26	0/1/1/1
5	NAG	E	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	E	2	5	-	2/6/23/26	0/1/1/1
5	NAG	E	3	5	-	2/6/23/26	0/1/1/1
4	NAG	F	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	F	2	4	-	0/6/23/26	0/1/1/1
4	NAG	G	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	G	2	4	-	2/6/23/26	0/1/1/1
4	NAG	K	1	1,4	-	6/6/23/26	0/1/1/1
4	NAG	K	2	4	-	2/6/23/26	0/1/1/1
4	NAG	O	1	1,4	-	1/6/23/26	0/1/1/1
4	NAG	O	2	4	-	2/6/23/26	0/1/1/1
4	NAG	P	1	1,4	-	1/6/23/26	0/1/1/1
4	NAG	P	2	4	-	1/6/23/26	0/1/1/1
4	NAG	Q	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	Q	2	4	-	2/6/23/26	0/1/1/1
4	NAG	R	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	R	2	4	-	6/6/23/26	0/1/1/1
4	NAG	S	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	S	2	4	-	4/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	T	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	T	2	4	-	2/6/23/26	0/1/1/1
5	NAG	U	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	U	2	5	-	2/6/23/26	0/1/1/1
5	NAG	U	3	5	-	2/6/23/26	0/1/1/1
4	NAG	V	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	V	2	4	-	0/6/23/26	0/1/1/1
4	NAG	W	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	W	2	4	-	2/6/23/26	0/1/1/1
4	NAG	X	1	1,4	-	6/6/23/26	0/1/1/1
4	NAG	X	2	4	-	2/6/23/26	0/1/1/1
4	NAG	Y	1	1,4	-	1/6/23/26	0/1/1/1
4	NAG	Y	2	4	-	2/6/23/26	0/1/1/1
4	NAG	Z	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	Z	2	4	-	2/6/23/26	0/1/1/1
4	NAG	a	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	a	2	4	-	4/6/23/26	0/1/1/1
4	NAG	b	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	b	2	4	-	2/6/23/26	0/1/1/1
5	NAG	c	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	c	2	5	-	2/6/23/26	0/1/1/1
5	NAG	c	3	5	-	2/6/23/26	0/1/1/1
4	NAG	d	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	d	2	4	-	0/6/23/26	0/1/1/1
4	NAG	e	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	e	2	4	-	2/6/23/26	0/1/1/1
4	NAG	f	1	1,4	-	6/6/23/26	0/1/1/1
4	NAG	f	2	4	-	2/6/23/26	0/1/1/1
4	NAG	g	1	1,4	-	1/6/23/26	0/1/1/1
4	NAG	g	2	4	-	2/6/23/26	0/1/1/1
4	NAG	h	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	h	2	4	-	2/6/23/26	0/1/1/1
4	NAG	i	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	i	2	4	-	4/6/23/26	0/1/1/1

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	P	2	NAG	O5-C1	-7.66	1.30	1.43
4	P	2	NAG	C1-C2	-7.49	1.42	1.52
4	Y	2	NAG	O5-C1	-6.78	1.32	1.43
4	O	2	NAG	O5-C1	-6.75	1.32	1.43
4	g	2	NAG	O5-C1	-6.75	1.32	1.43
4	Y	2	NAG	C1-C2	-4.93	1.45	1.52
4	g	2	NAG	C1-C2	-4.91	1.45	1.52
4	O	2	NAG	C1-C2	-4.86	1.45	1.52
4	Y	1	NAG	O5-C1	-4.02	1.36	1.43
4	g	1	NAG	O5-C1	-4.01	1.37	1.43
4	O	1	NAG	O5-C1	-4.00	1.37	1.43
4	f	1	NAG	C1-C2	2.72	1.56	1.52
4	X	1	NAG	C1-C2	2.70	1.56	1.52
4	P	1	NAG	O5-C1	-2.68	1.39	1.43
4	K	1	NAG	C1-C2	2.67	1.56	1.52
4	b	1	NAG	O5-C1	-2.65	1.39	1.43
4	D	1	NAG	O5-C1	-2.65	1.39	1.43
4	W	2	NAG	C1-C2	2.63	1.55	1.52
4	e	2	NAG	C1-C2	2.62	1.55	1.52
4	T	1	NAG	O5-C1	-2.60	1.39	1.43
4	G	2	NAG	C1-C2	2.57	1.55	1.52
4	i	1	NAG	O5-C1	-2.50	1.39	1.43
4	a	1	NAG	O5-C1	-2.50	1.39	1.43
4	S	1	NAG	O5-C1	-2.41	1.39	1.43
4	T	2	NAG	C1-C2	2.38	1.55	1.52
4	D	2	NAG	C1-C2	2.32	1.55	1.52
4	b	2	NAG	C1-C2	2.31	1.55	1.52
4	R	1	NAG	O5-C1	-2.28	1.39	1.43
4	P	2	NAG	C2-N2	-2.01	1.42	1.46

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	K	1	NAG	C2-N2-C7	8.27	133.99	122.90
4	X	1	NAG	C2-N2-C7	8.25	133.96	122.90
4	f	1	NAG	C2-N2-C7	8.22	133.92	122.90
4	R	2	NAG	C2-N2-C7	4.70	129.21	122.90
4	f	1	NAG	C1-C2-N2	3.98	116.70	110.43
4	X	1	NAG	C1-C2-N2	3.96	116.67	110.43
4	K	1	NAG	C1-C2-N2	3.95	116.65	110.43
4	P	2	NAG	C1-C2-N2	3.53	115.99	110.43
4	P	2	NAG	O5-C1-C2	3.32	116.43	111.29
4	P	2	NAG	C1-O5-C5	3.27	116.57	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	Y	2	NAG	C1-C2-N2	2.79	114.83	110.43
4	O	2	NAG	C1-C2-N2	2.75	114.76	110.43
4	g	2	NAG	C1-C2-N2	2.70	114.68	110.43
4	R	2	NAG	C1-C2-N2	2.61	114.54	110.43
4	O	2	NAG	C1-O5-C5	2.57	115.63	112.19
4	g	2	NAG	C1-O5-C5	2.51	115.56	112.19
4	Y	2	NAG	C1-O5-C5	2.40	115.40	112.19
4	T	1	NAG	O4-C4-C3	-2.40	104.73	110.38
4	b	1	NAG	O4-C4-C3	-2.39	104.75	110.38
4	D	1	NAG	O4-C4-C3	-2.37	104.79	110.38
4	G	1	NAG	C1-O5-C5	2.33	115.30	112.19
4	W	1	NAG	C1-O5-C5	2.32	115.29	112.19
4	e	1	NAG	C1-O5-C5	2.31	115.28	112.19
4	P	2	NAG	C2-N2-C7	2.26	125.93	122.90
5	U	3	NAG	C1-O5-C5	2.24	115.18	112.19
4	f	1	NAG	C8-C7-N2	2.22	119.80	116.12
4	X	1	NAG	C8-C7-N2	2.22	119.80	116.12
5	c	3	NAG	C1-O5-C5	2.21	115.14	112.19
5	E	3	NAG	C1-O5-C5	2.19	115.12	112.19
4	K	1	NAG	C8-C7-N2	2.17	119.72	116.12
4	T	1	NAG	C3-C4-C5	2.13	114.09	110.23
4	b	1	NAG	C3-C4-C5	2.12	114.08	110.23
4	D	1	NAG	C3-C4-C5	2.11	114.05	110.23
4	R	2	NAG	C1-O5-C5	2.06	114.95	112.19
4	d	2	NAG	C1-O5-C5	2.03	114.91	112.19
4	V	2	NAG	C1-O5-C5	2.01	114.88	112.19

There are no chirality outliers.

All (109) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	K	2	NAG	O5-C5-C6-O6
4	O	2	NAG	O5-C5-C6-O6
4	X	2	NAG	O5-C5-C6-O6
4	Y	2	NAG	O5-C5-C6-O6
4	g	2	NAG	O5-C5-C6-O6
4	S	1	NAG	O5-C5-C6-O6
4	a	1	NAG	O5-C5-C6-O6
4	f	2	NAG	O5-C5-C6-O6
4	i	1	NAG	O5-C5-C6-O6
4	K	1	NAG	O5-C5-C6-O6
4	X	1	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	f	1	NAG	O5-C5-C6-O6
5	E	2	NAG	O5-C5-C6-O6
5	U	2	NAG	O5-C5-C6-O6
5	c	2	NAG	O5-C5-C6-O6
5	E	1	NAG	O5-C5-C6-O6
4	K	2	NAG	C4-C5-C6-O6
4	X	2	NAG	C4-C5-C6-O6
4	f	2	NAG	C4-C5-C6-O6
4	G	2	NAG	O5-C5-C6-O6
4	W	2	NAG	O5-C5-C6-O6
4	e	2	NAG	O5-C5-C6-O6
5	U	1	NAG	O5-C5-C6-O6
5	c	1	NAG	O5-C5-C6-O6
4	S	1	NAG	C4-C5-C6-O6
4	a	1	NAG	C4-C5-C6-O6
4	i	1	NAG	C4-C5-C6-O6
5	E	3	NAG	C4-C5-C6-O6
5	U	3	NAG	C4-C5-C6-O6
5	c	3	NAG	C4-C5-C6-O6
4	G	2	NAG	C4-C5-C6-O6
4	W	2	NAG	C4-C5-C6-O6
4	e	2	NAG	C4-C5-C6-O6
5	E	3	NAG	O5-C5-C6-O6
5	U	3	NAG	O5-C5-C6-O6
5	c	3	NAG	O5-C5-C6-O6
4	O	2	NAG	C4-C5-C6-O6
4	Y	2	NAG	C4-C5-C6-O6
4	g	2	NAG	C4-C5-C6-O6
5	E	1	NAG	C4-C5-C6-O6
5	U	1	NAG	C4-C5-C6-O6
5	c	1	NAG	C4-C5-C6-O6
4	K	1	NAG	C4-C5-C6-O6
4	X	1	NAG	C4-C5-C6-O6
4	f	1	NAG	C4-C5-C6-O6
4	W	1	NAG	O5-C5-C6-O6
4	G	1	NAG	O5-C5-C6-O6
4	e	1	NAG	O5-C5-C6-O6
5	E	2	NAG	C4-C5-C6-O6
5	U	2	NAG	C4-C5-C6-O6
5	c	2	NAG	C4-C5-C6-O6
4	K	1	NAG	C8-C7-N2-C2
4	K	1	NAG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
4	R	2	NAG	C8-C7-N2-C2
4	R	2	NAG	O7-C7-N2-C2
4	X	1	NAG	C8-C7-N2-C2
4	X	1	NAG	O7-C7-N2-C2
4	f	1	NAG	C8-C7-N2-C2
4	f	1	NAG	O7-C7-N2-C2
4	R	1	NAG	C4-C5-C6-O6
4	T	1	NAG	O5-C5-C6-O6
4	D	1	NAG	C4-C5-C6-O6
4	T	1	NAG	C4-C5-C6-O6
4	b	1	NAG	C4-C5-C6-O6
4	D	1	NAG	O5-C5-C6-O6
4	b	1	NAG	O5-C5-C6-O6
4	R	1	NAG	O5-C5-C6-O6
4	S	2	NAG	C4-C5-C6-O6
4	a	2	NAG	C4-C5-C6-O6
4	i	2	NAG	C4-C5-C6-O6
4	S	2	NAG	O5-C5-C6-O6
4	a	2	NAG	O5-C5-C6-O6
4	i	2	NAG	O5-C5-C6-O6
4	D	2	NAG	O5-C5-C6-O6
4	T	2	NAG	O5-C5-C6-O6
4	b	2	NAG	O5-C5-C6-O6
4	e	1	NAG	C4-C5-C6-O6
4	G	1	NAG	C4-C5-C6-O6
4	W	1	NAG	C4-C5-C6-O6
4	h	2	NAG	C4-C5-C6-O6
4	Q	2	NAG	C4-C5-C6-O6
4	Z	2	NAG	C4-C5-C6-O6
4	Q	2	NAG	O5-C5-C6-O6
4	Z	2	NAG	O5-C5-C6-O6
4	h	2	NAG	O5-C5-C6-O6
4	S	2	NAG	C3-C2-N2-C7
4	a	2	NAG	C3-C2-N2-C7
4	i	2	NAG	C3-C2-N2-C7
4	T	2	NAG	C4-C5-C6-O6
4	D	2	NAG	C4-C5-C6-O6
4	b	2	NAG	C4-C5-C6-O6
4	R	2	NAG	C4-C5-C6-O6
4	g	1	NAG	O5-C5-C6-O6
4	O	1	NAG	O5-C5-C6-O6
4	Y	1	NAG	O5-C5-C6-O6

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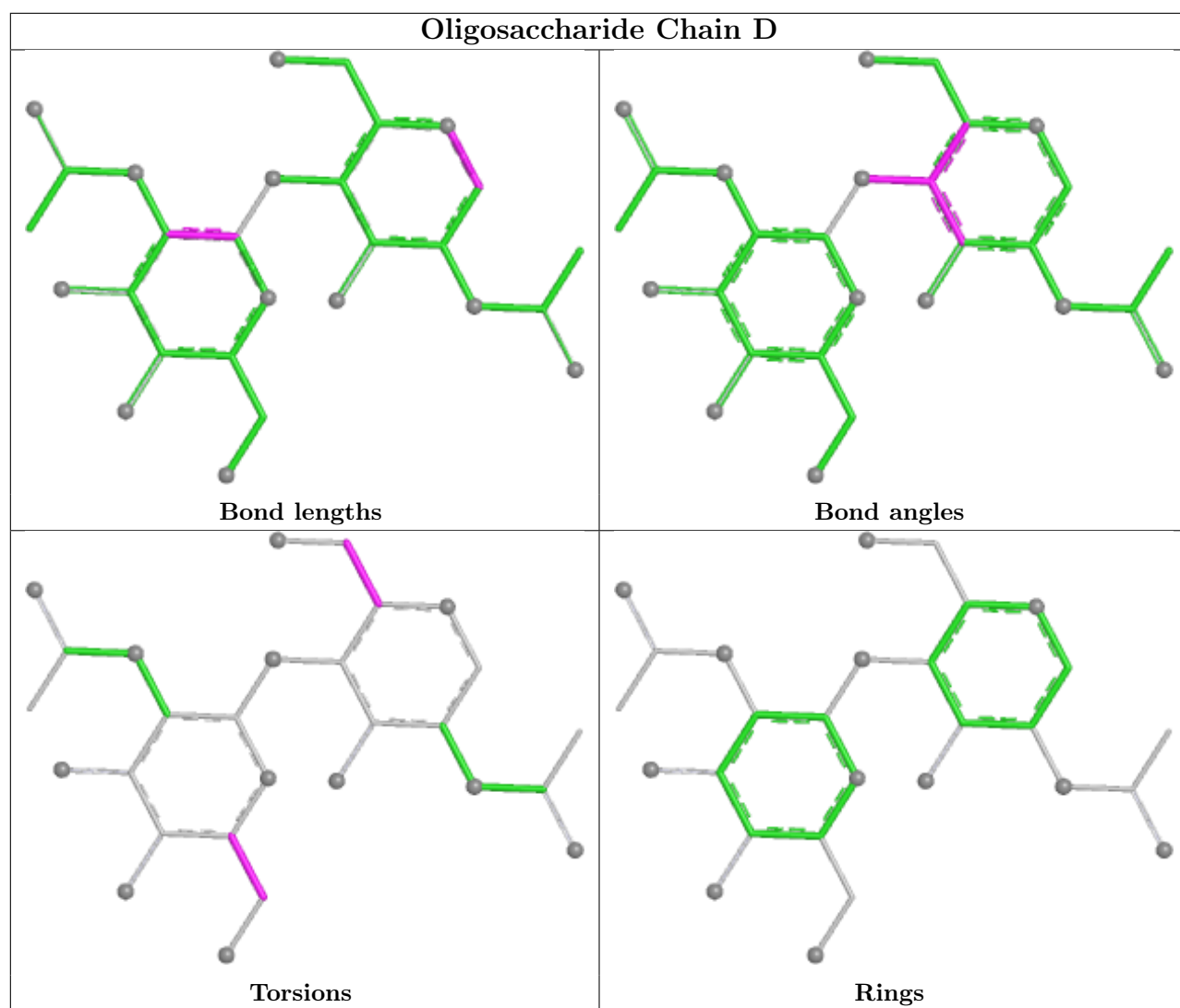
Mol	Chain	Res	Type	Atoms
4	R	2	NAG	O5-C5-C6-O6
4	K	1	NAG	C1-C2-N2-C7
4	R	2	NAG	C1-C2-N2-C7
4	S	2	NAG	C1-C2-N2-C7
4	X	1	NAG	C1-C2-N2-C7
4	a	2	NAG	C1-C2-N2-C7
4	f	1	NAG	C1-C2-N2-C7
4	i	2	NAG	C1-C2-N2-C7
4	P	1	NAG	C4-C5-C6-O6
4	K	1	NAG	C3-C2-N2-C7
4	P	2	NAG	C3-C2-N2-C7
4	R	2	NAG	C3-C2-N2-C7
4	X	1	NAG	C3-C2-N2-C7
4	f	1	NAG	C3-C2-N2-C7

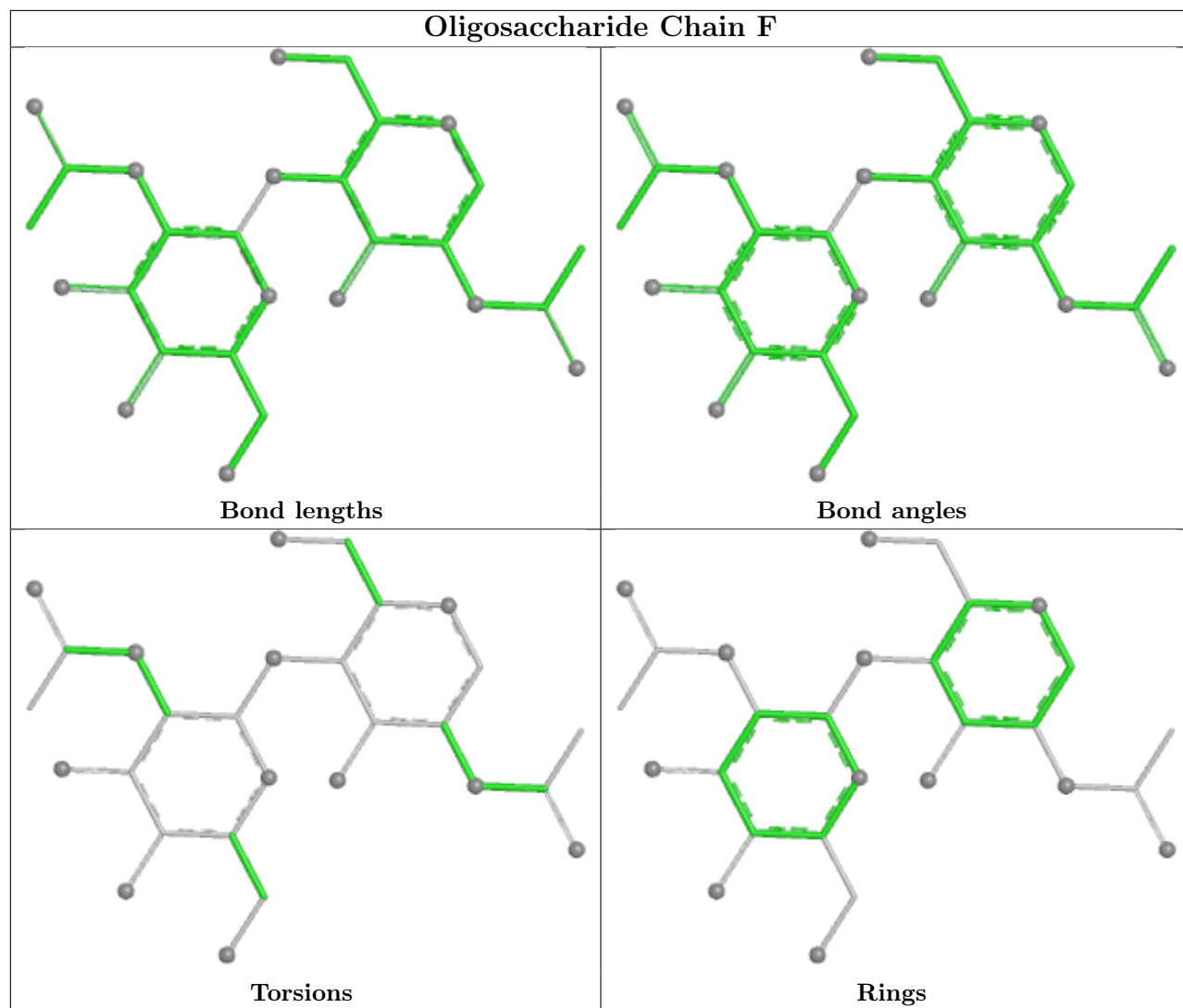
There are no ring outliers.

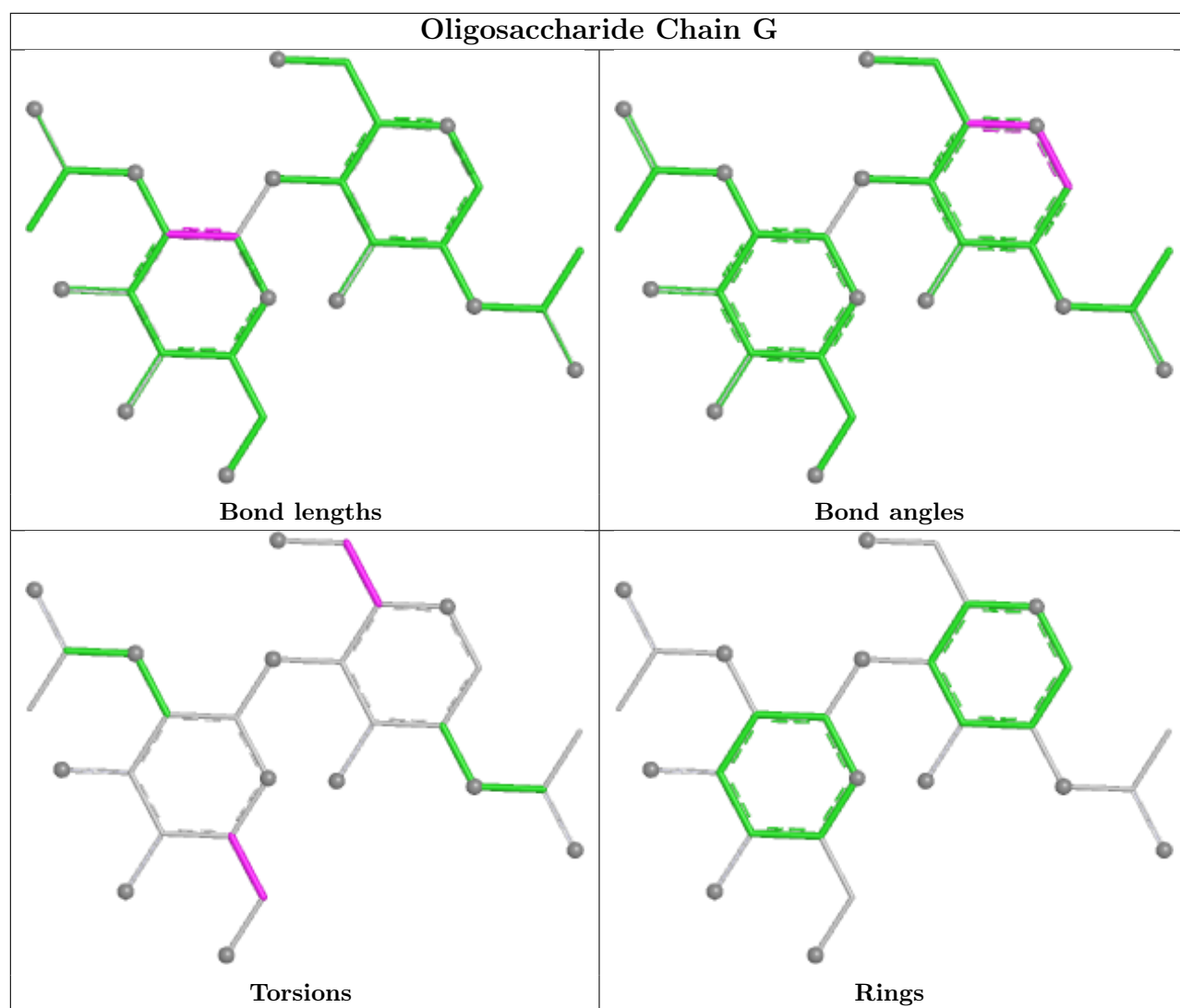
16 monomers are involved in 33 short contacts:

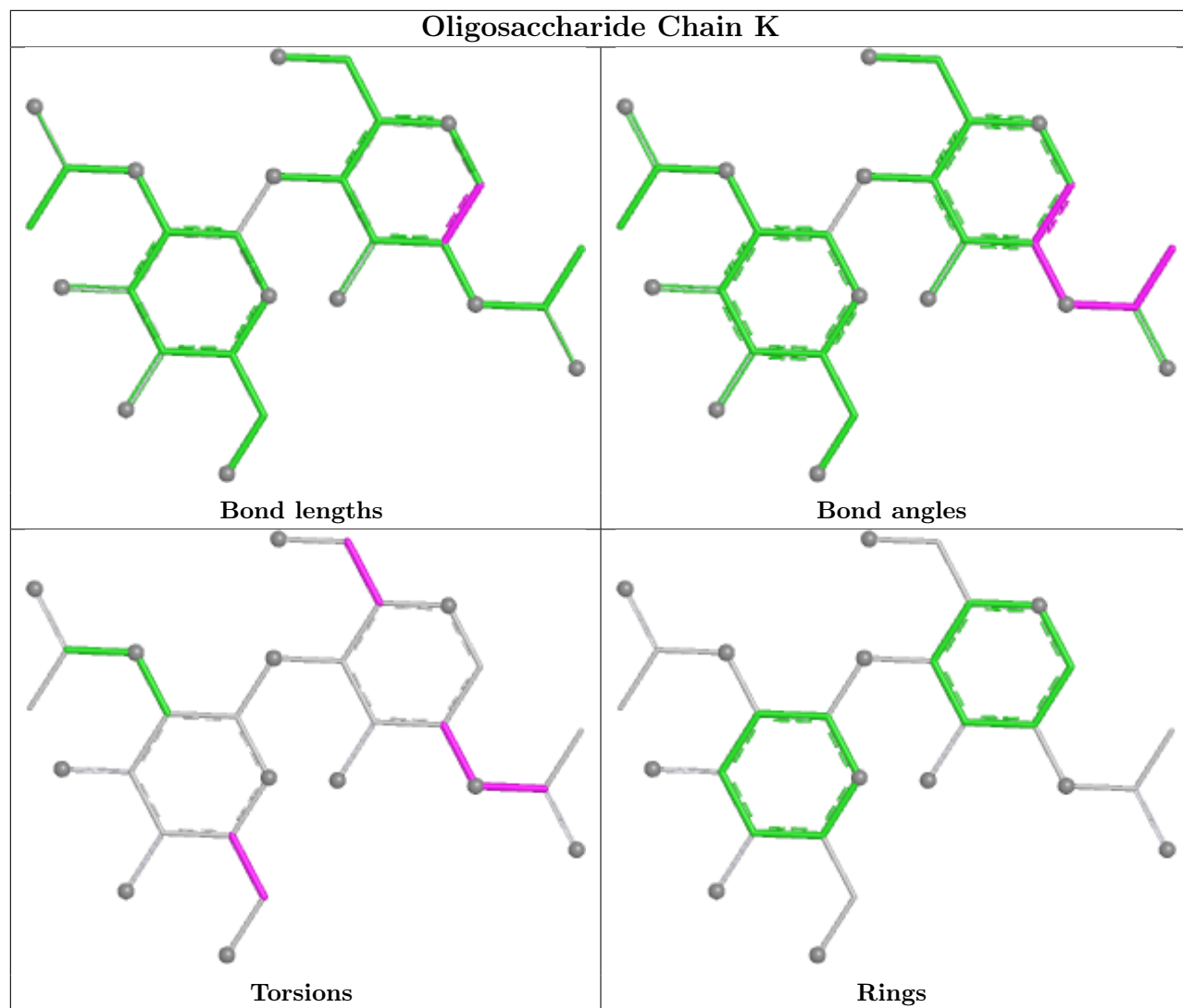
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	P	1	NAG	6	0
4	F	2	NAG	5	0
4	W	2	NAG	2	0
5	E	1	NAG	2	0
4	d	2	NAG	3	0
4	R	2	NAG	1	0
4	g	1	NAG	1	0
4	O	1	NAG	1	0
4	Y	2	NAG	1	0
4	e	1	NAG	1	0
5	U	1	NAG	2	0
4	g	2	NAG	1	0
4	O	2	NAG	1	0
4	V	2	NAG	6	0
4	Y	1	NAG	1	0
5	c	1	NAG	2	0

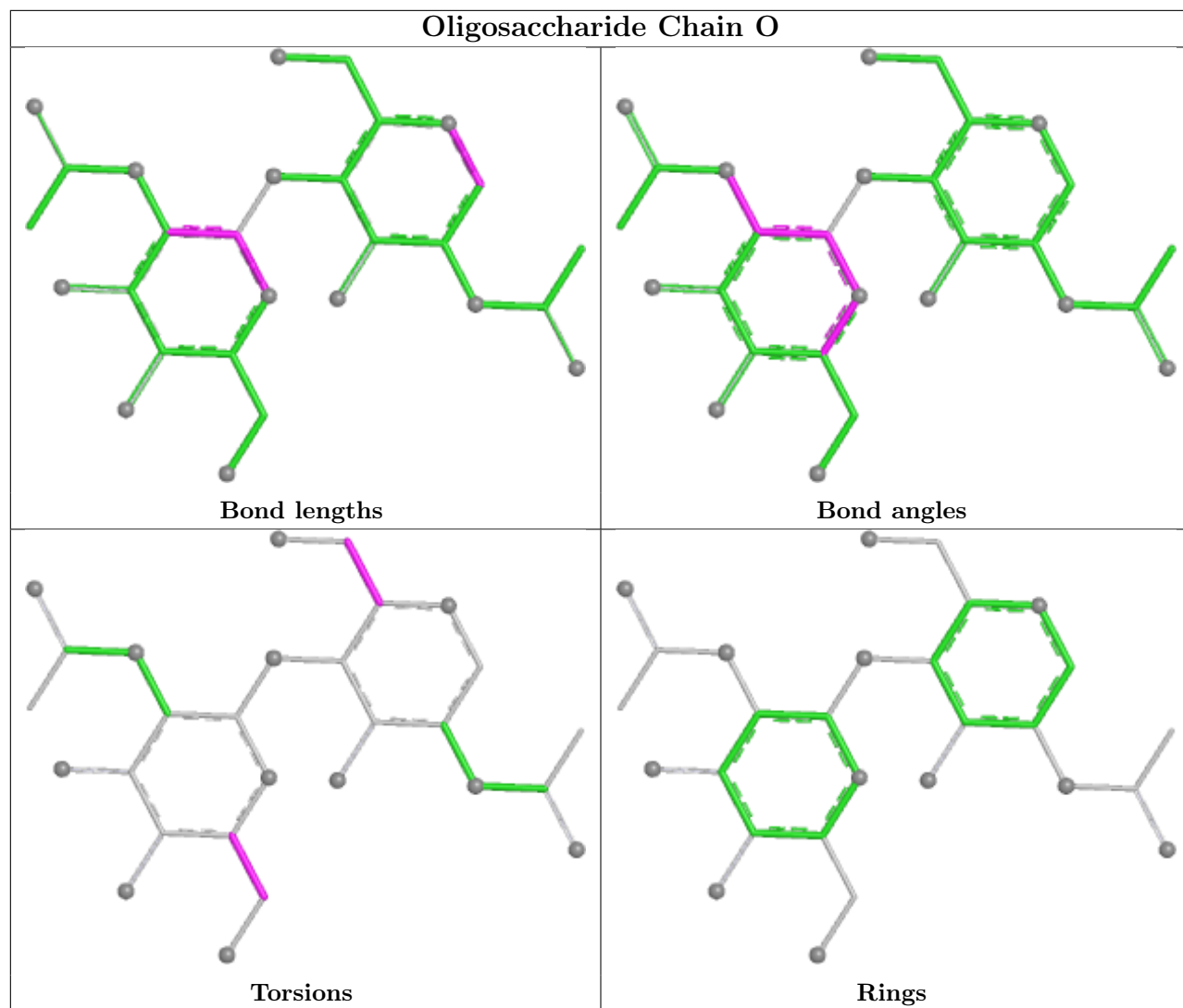
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

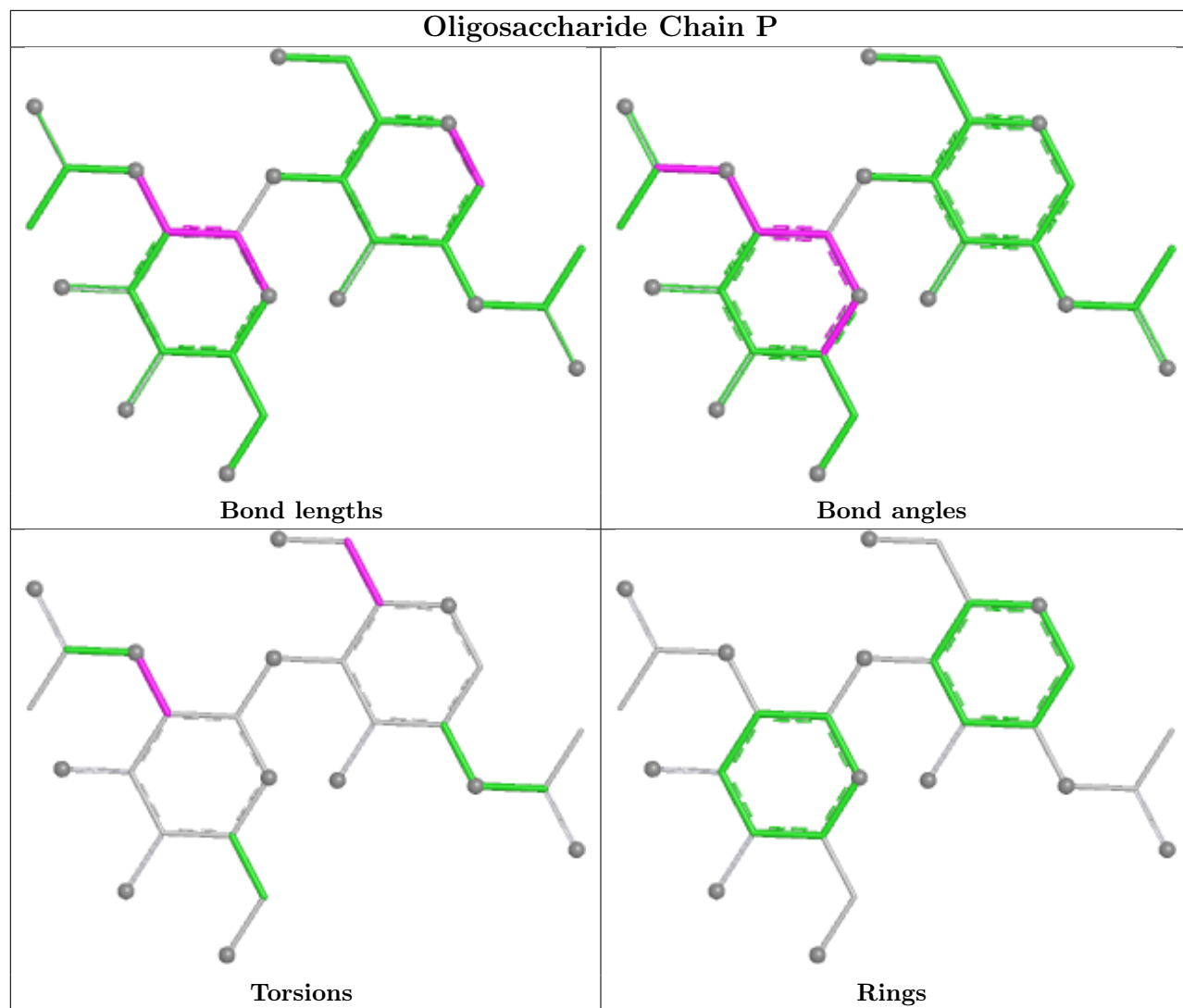


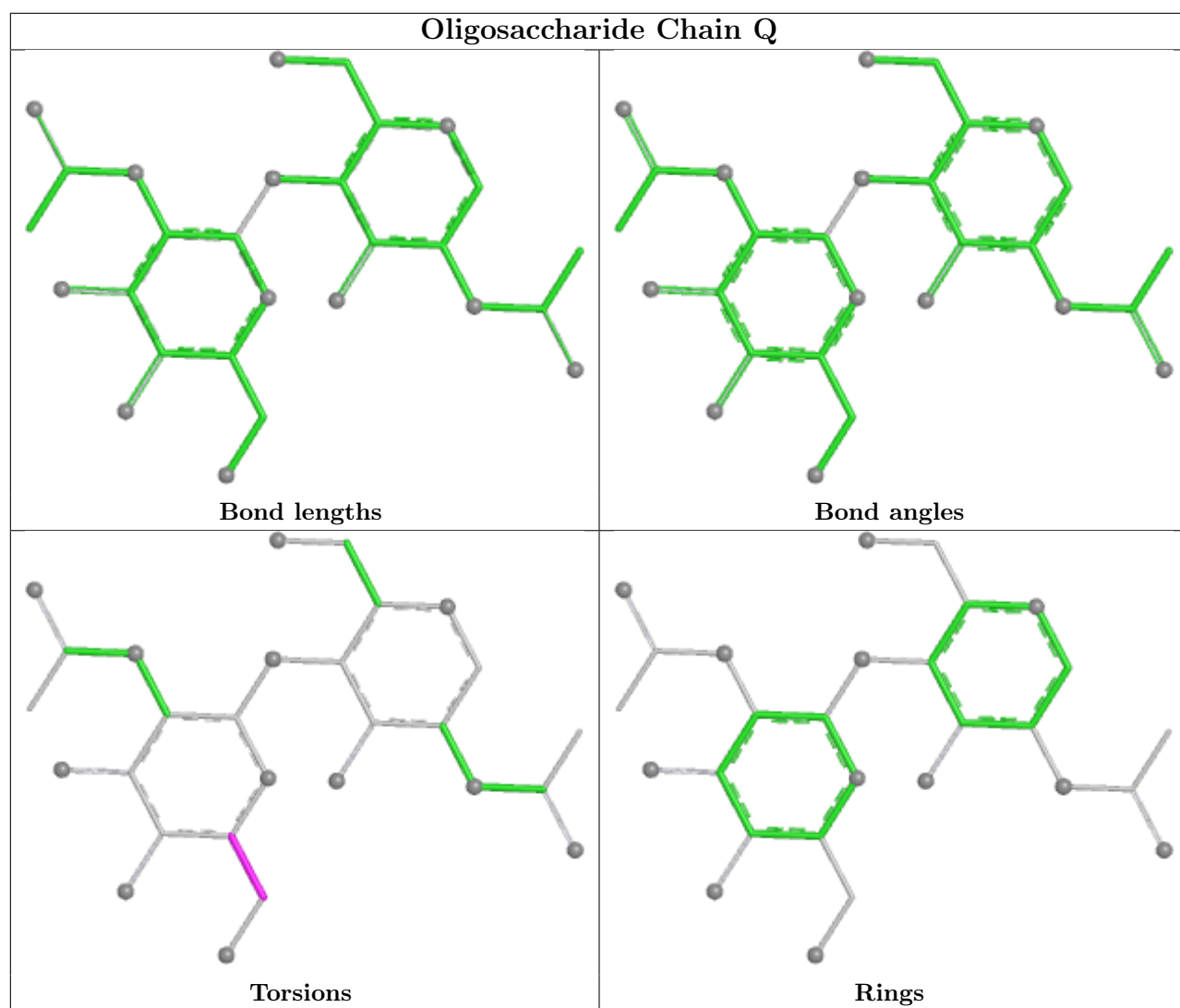


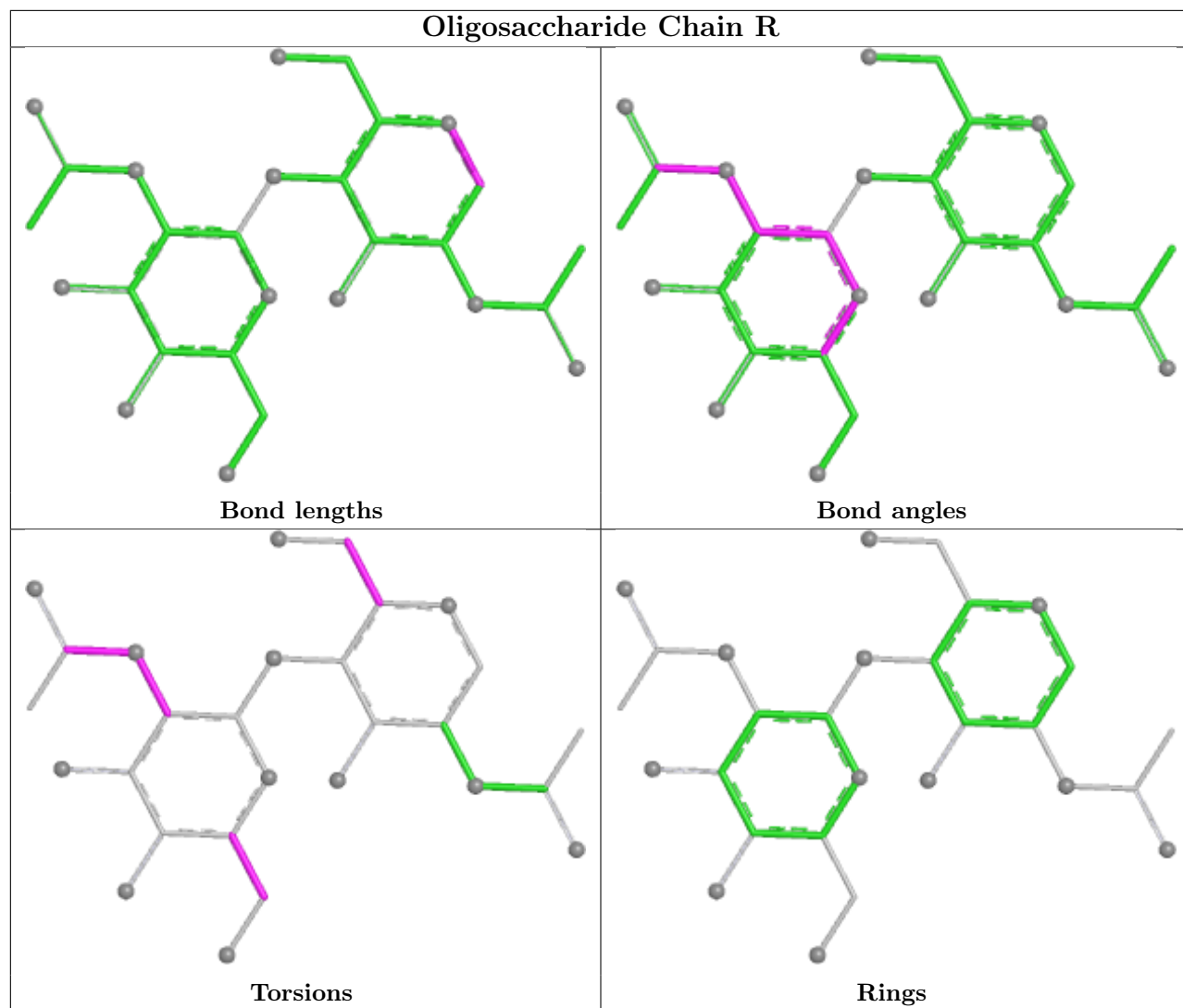


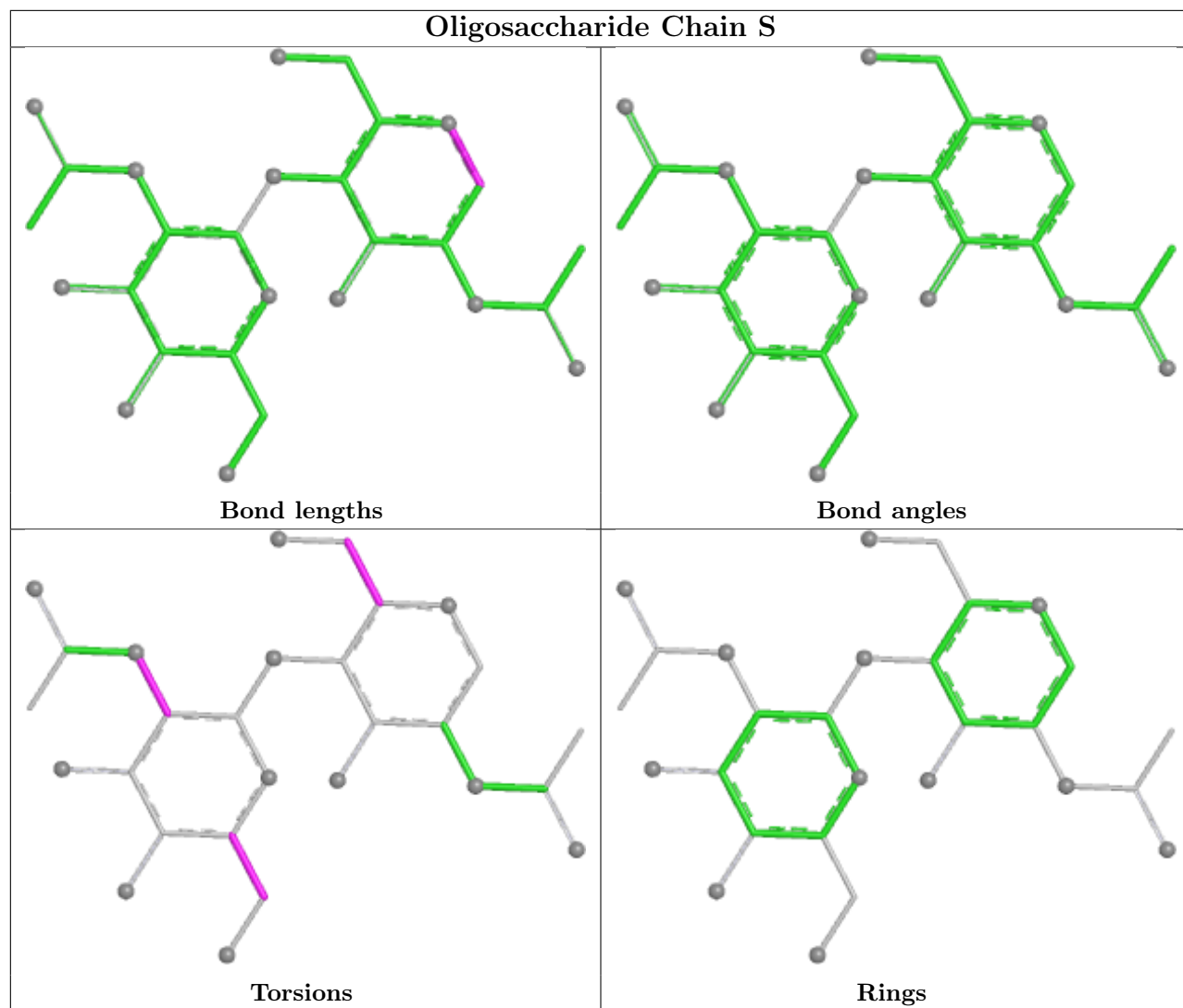


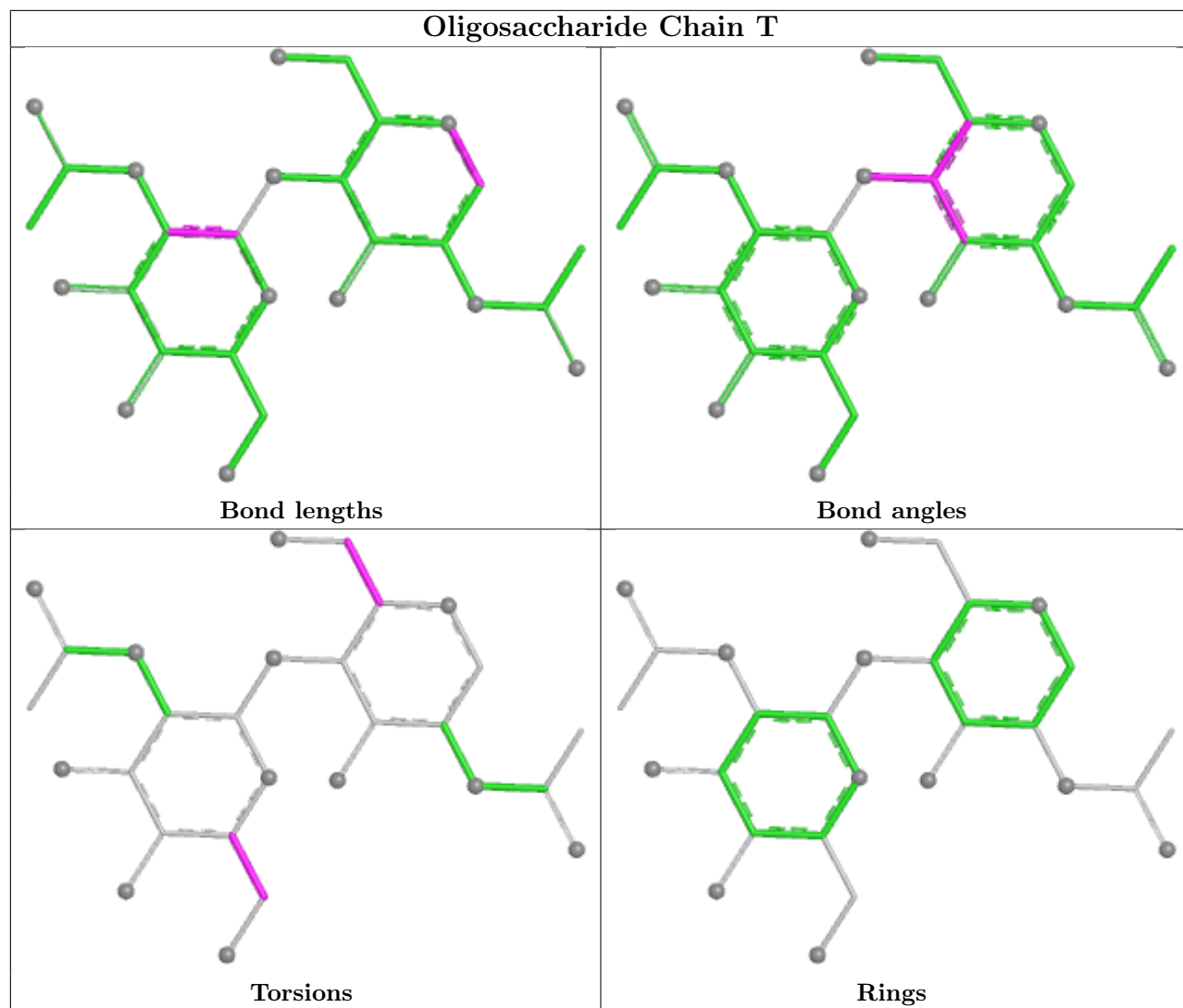


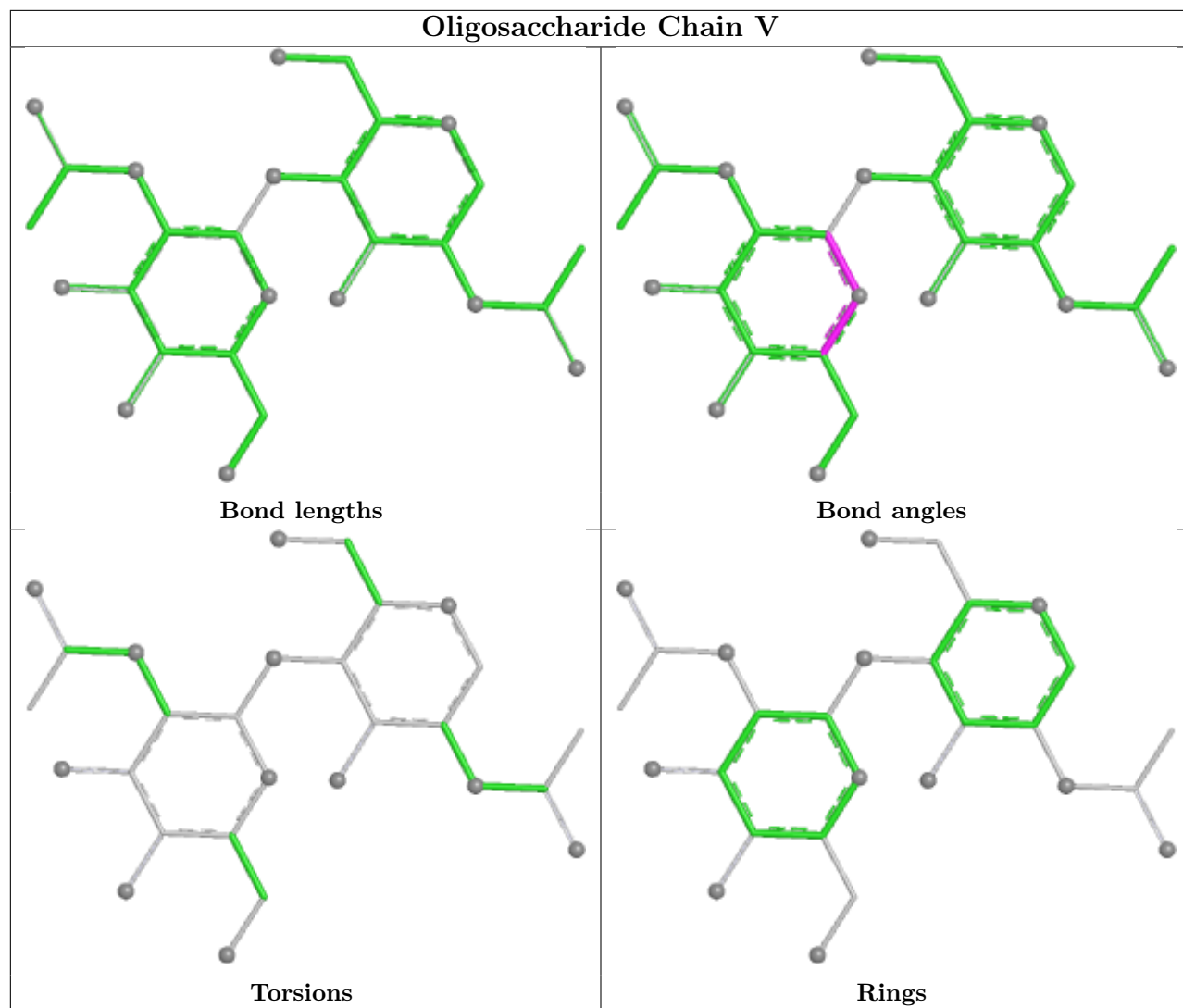


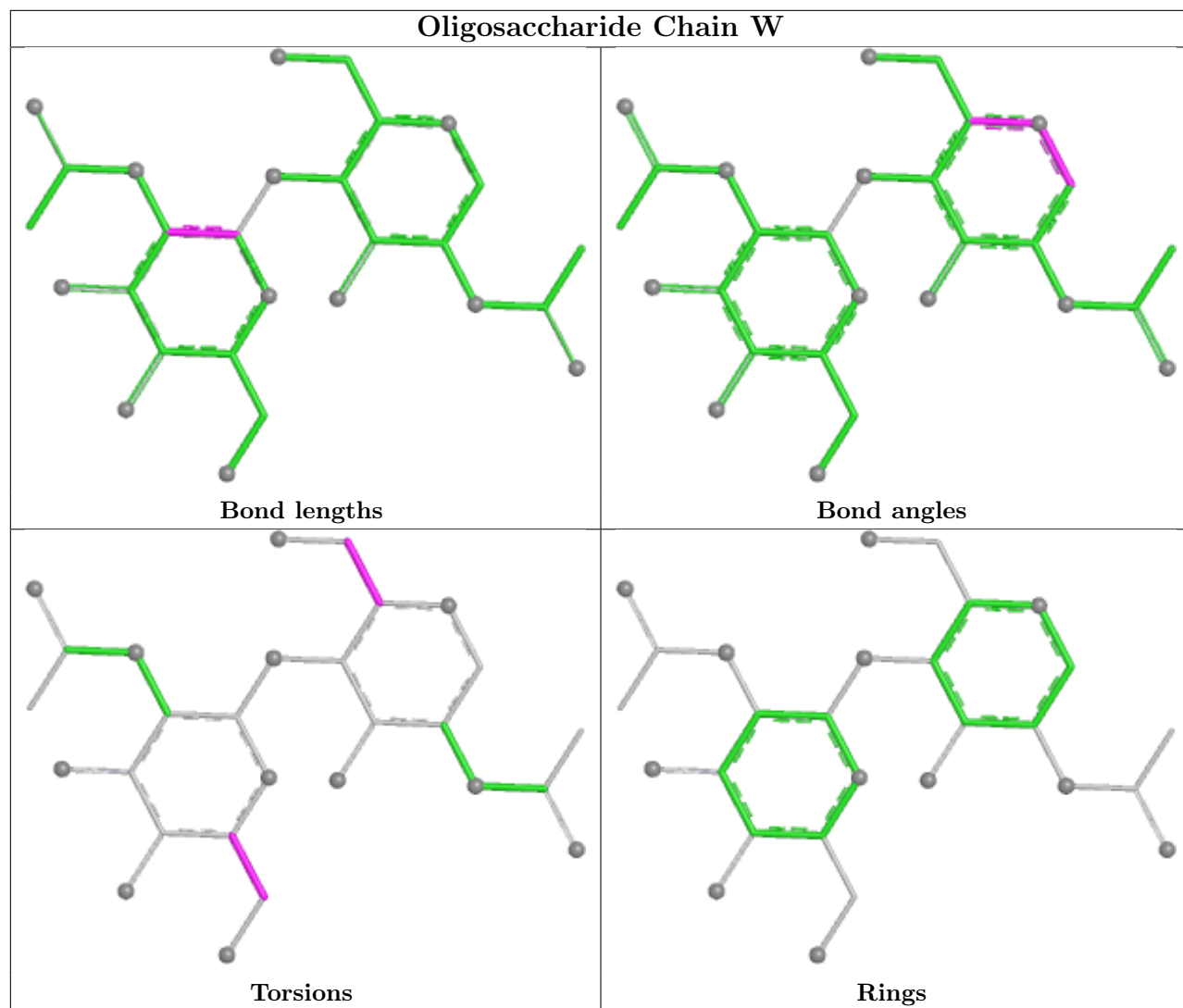


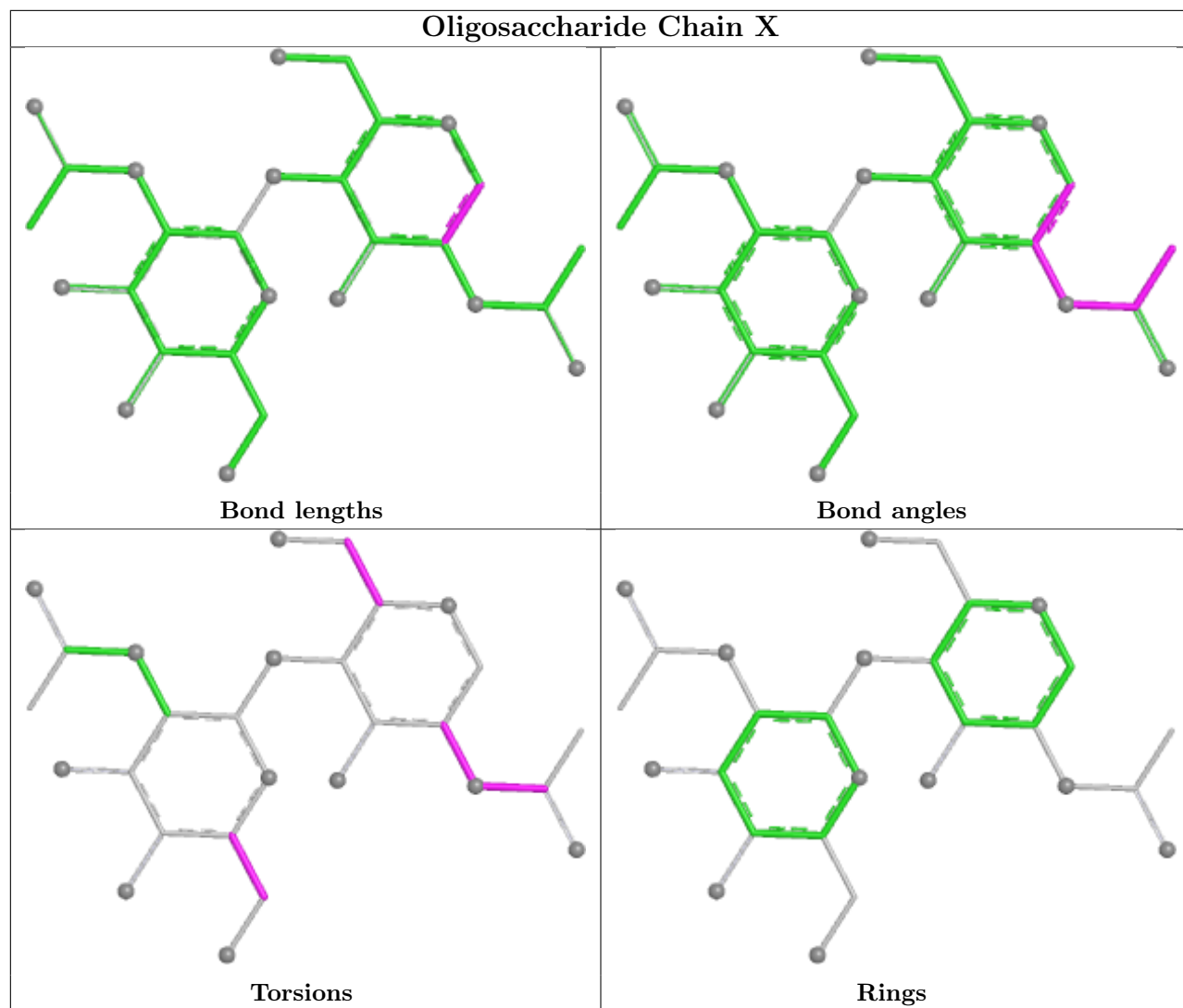


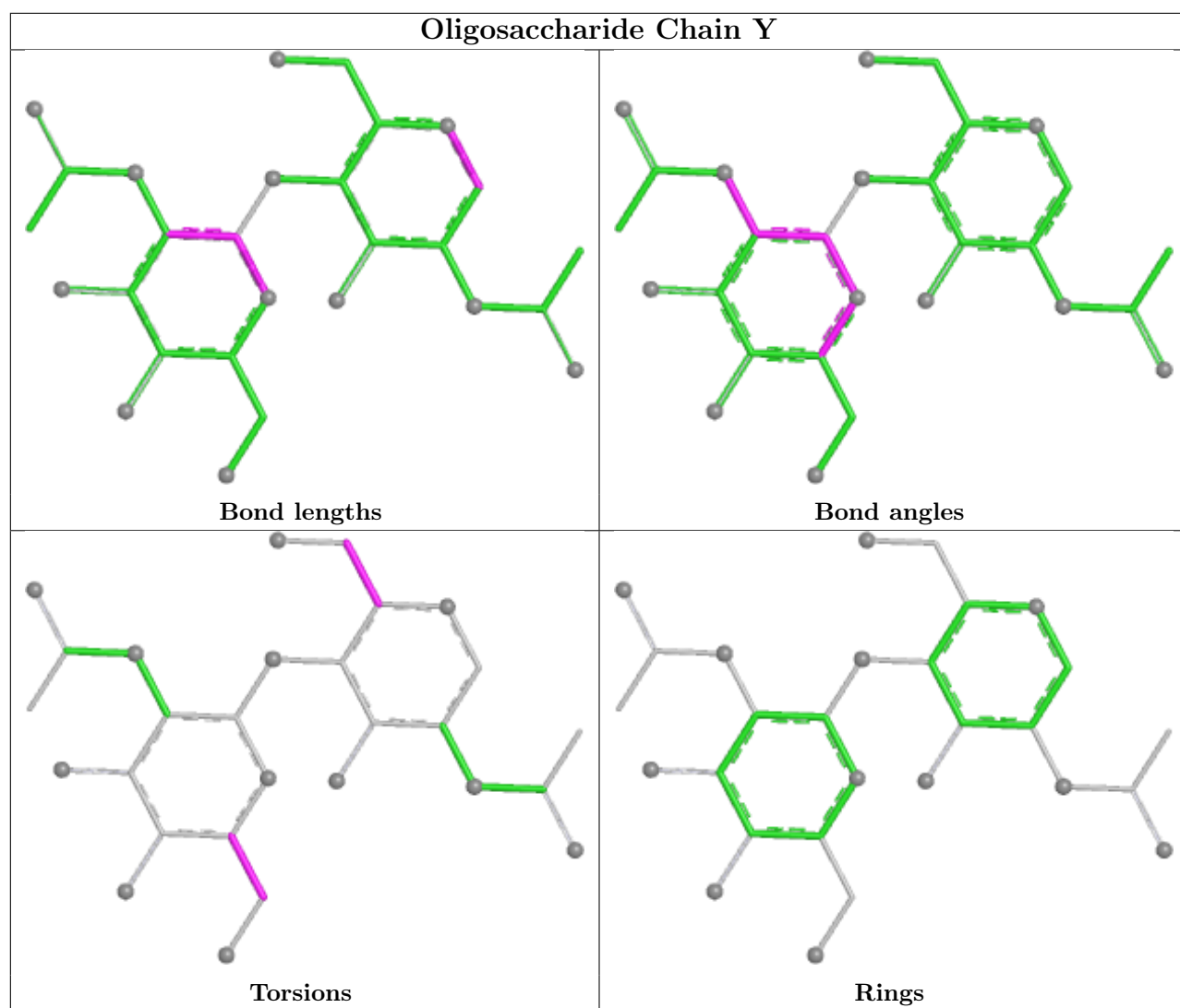


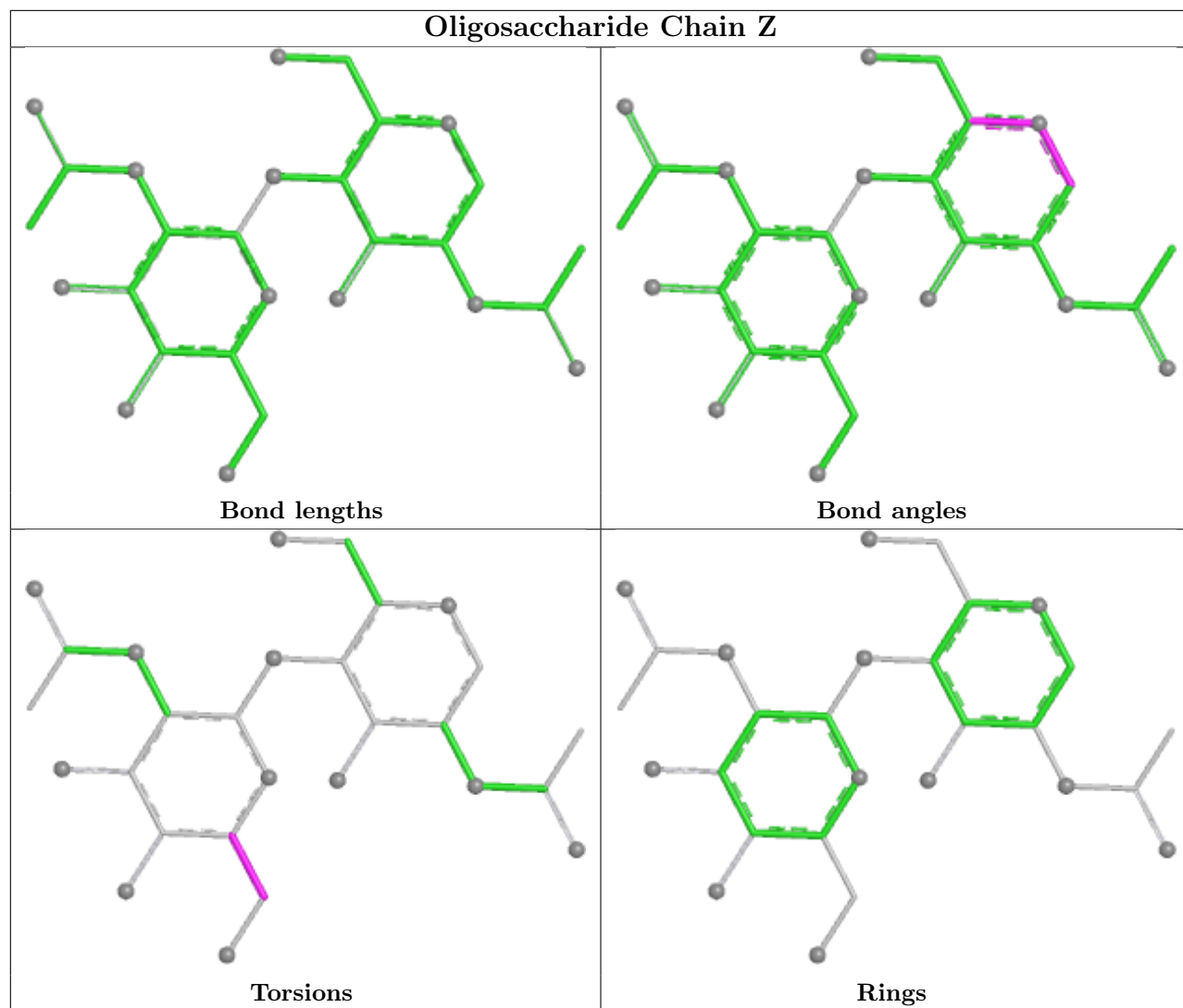


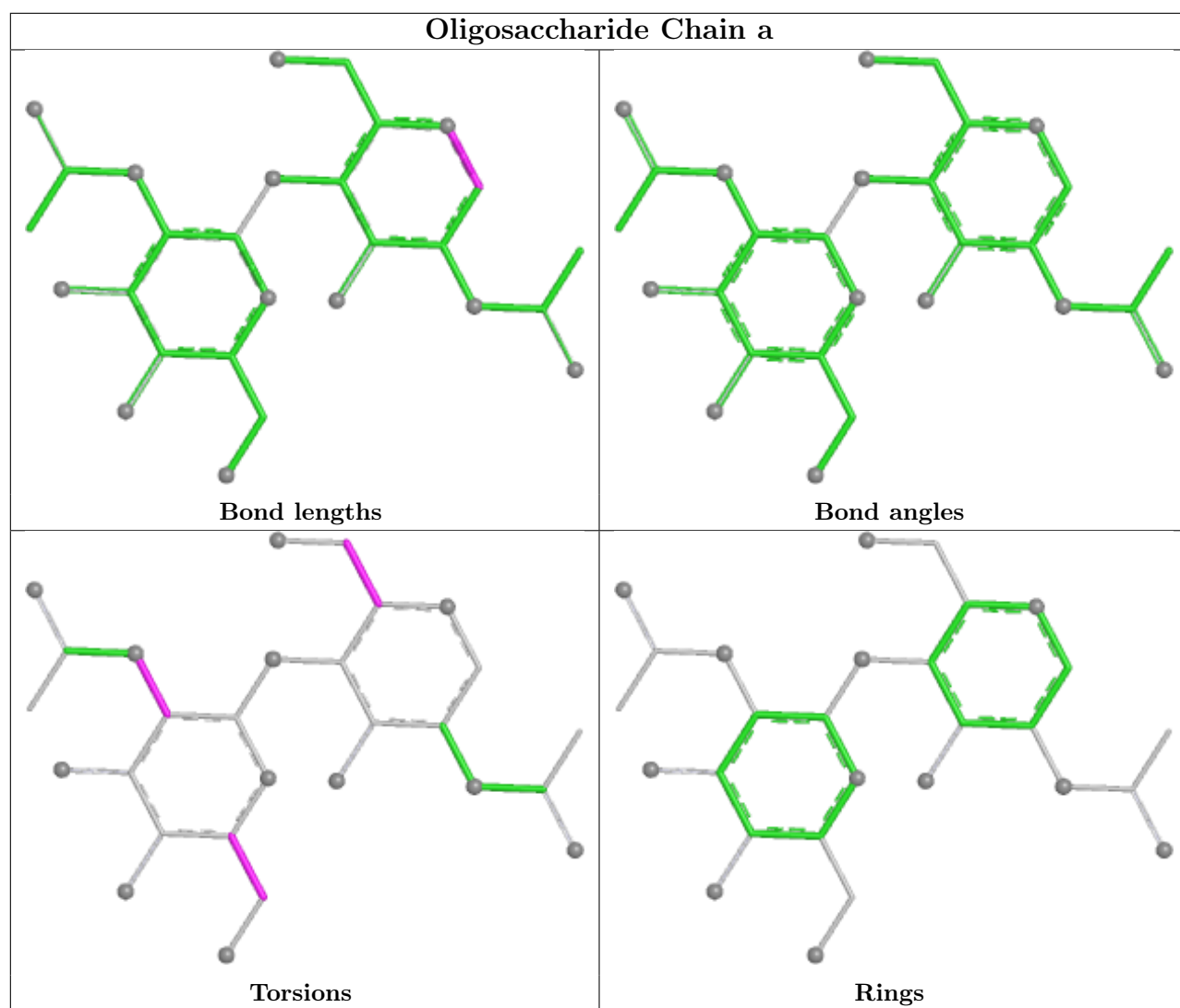


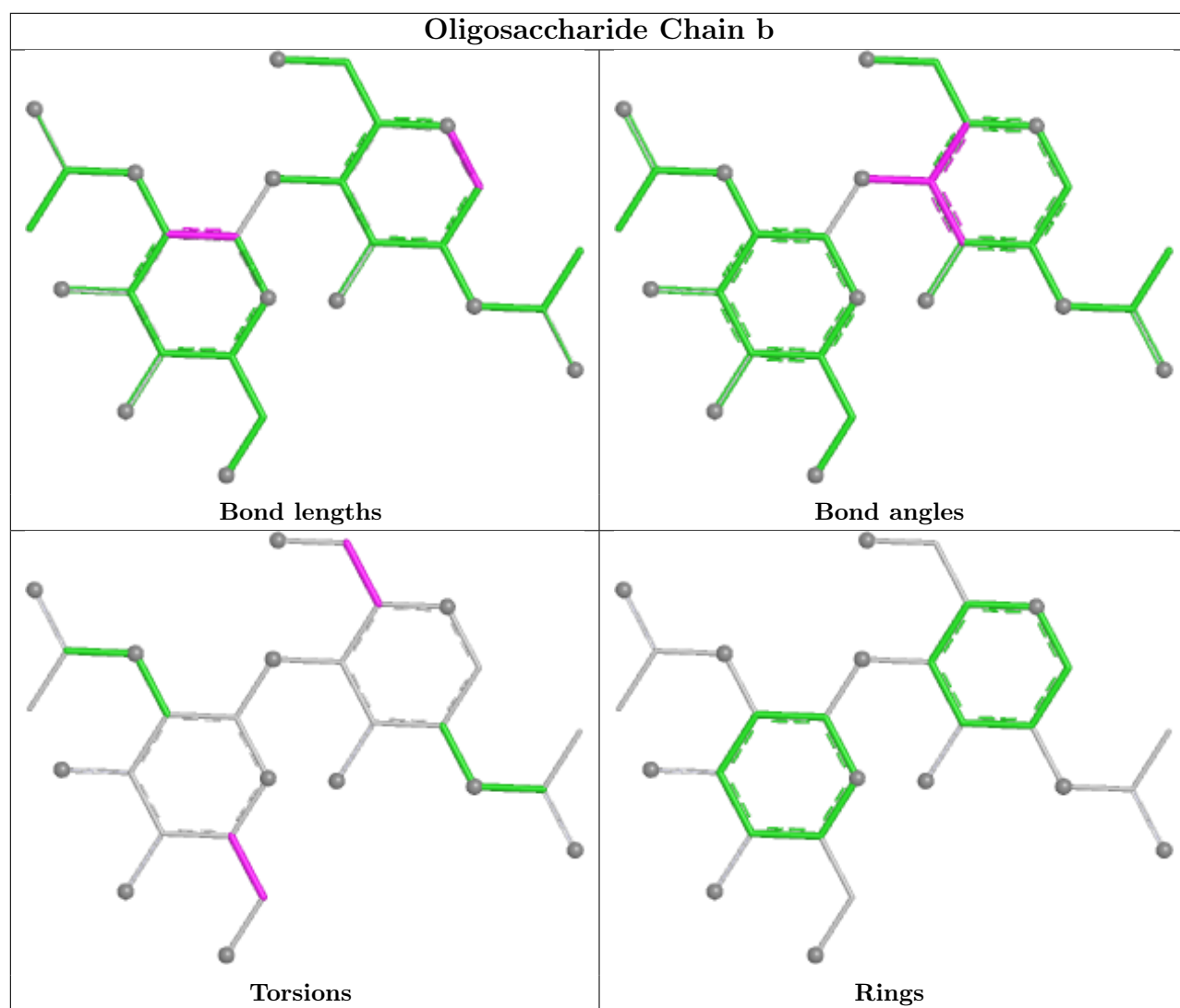


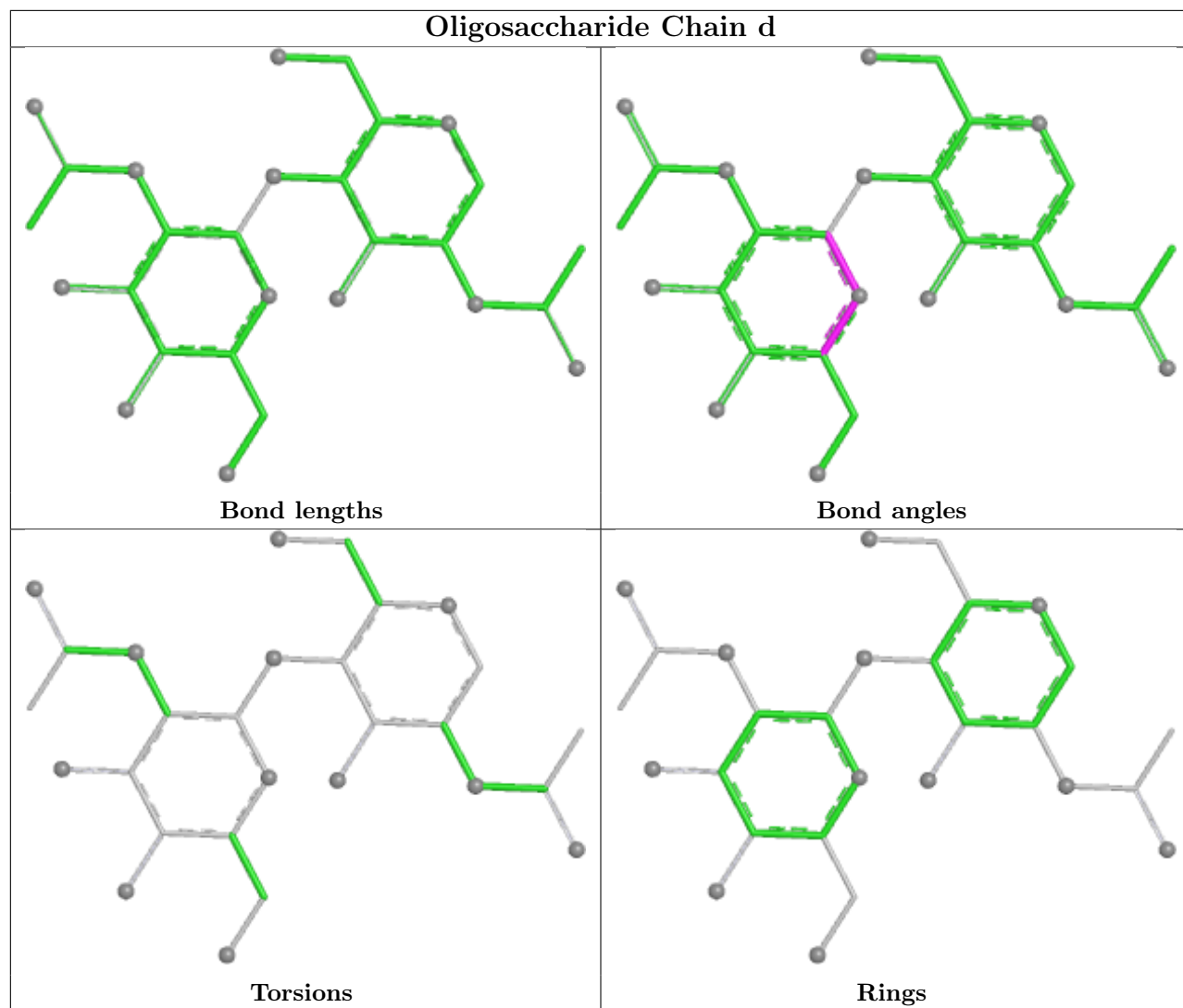


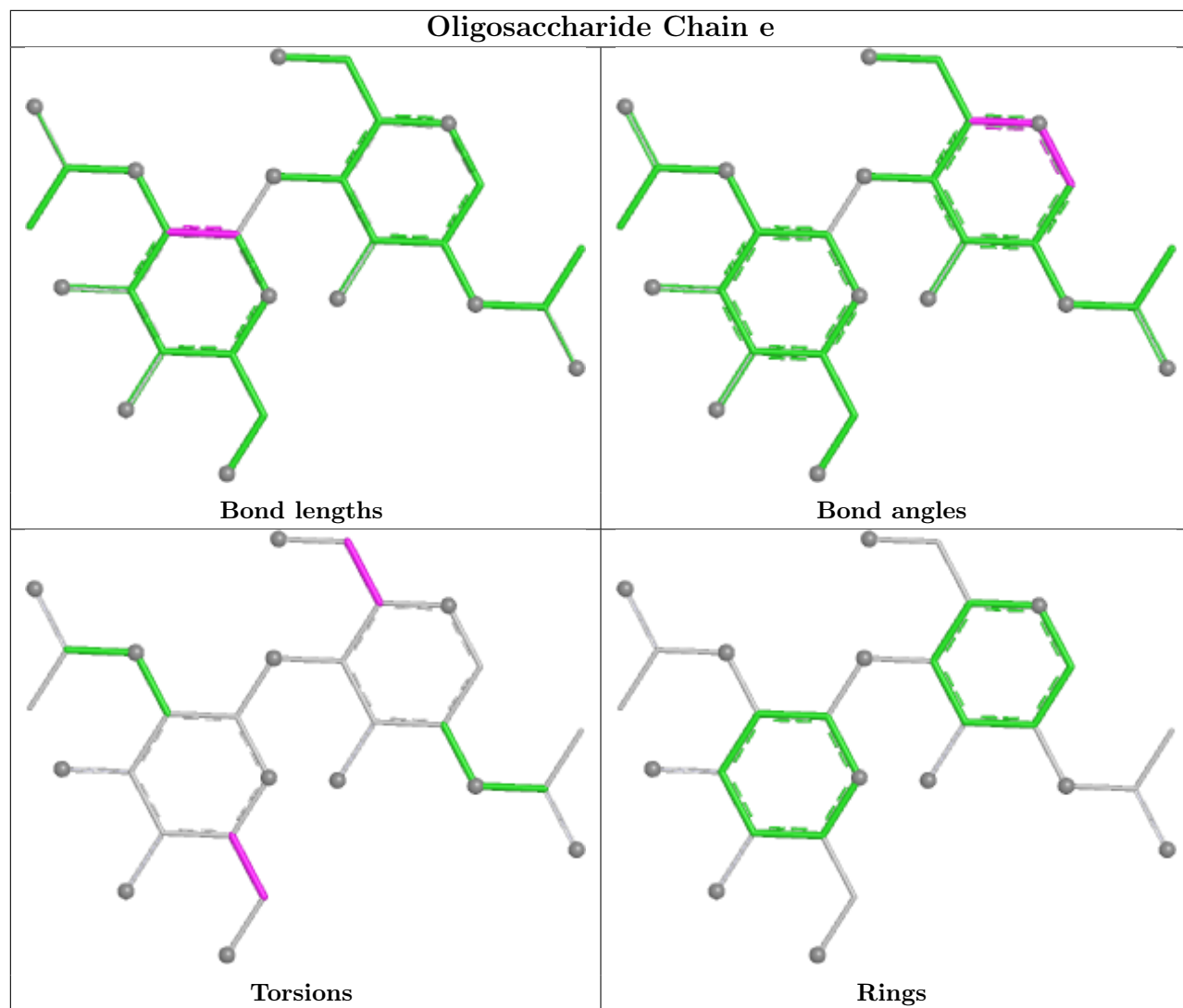


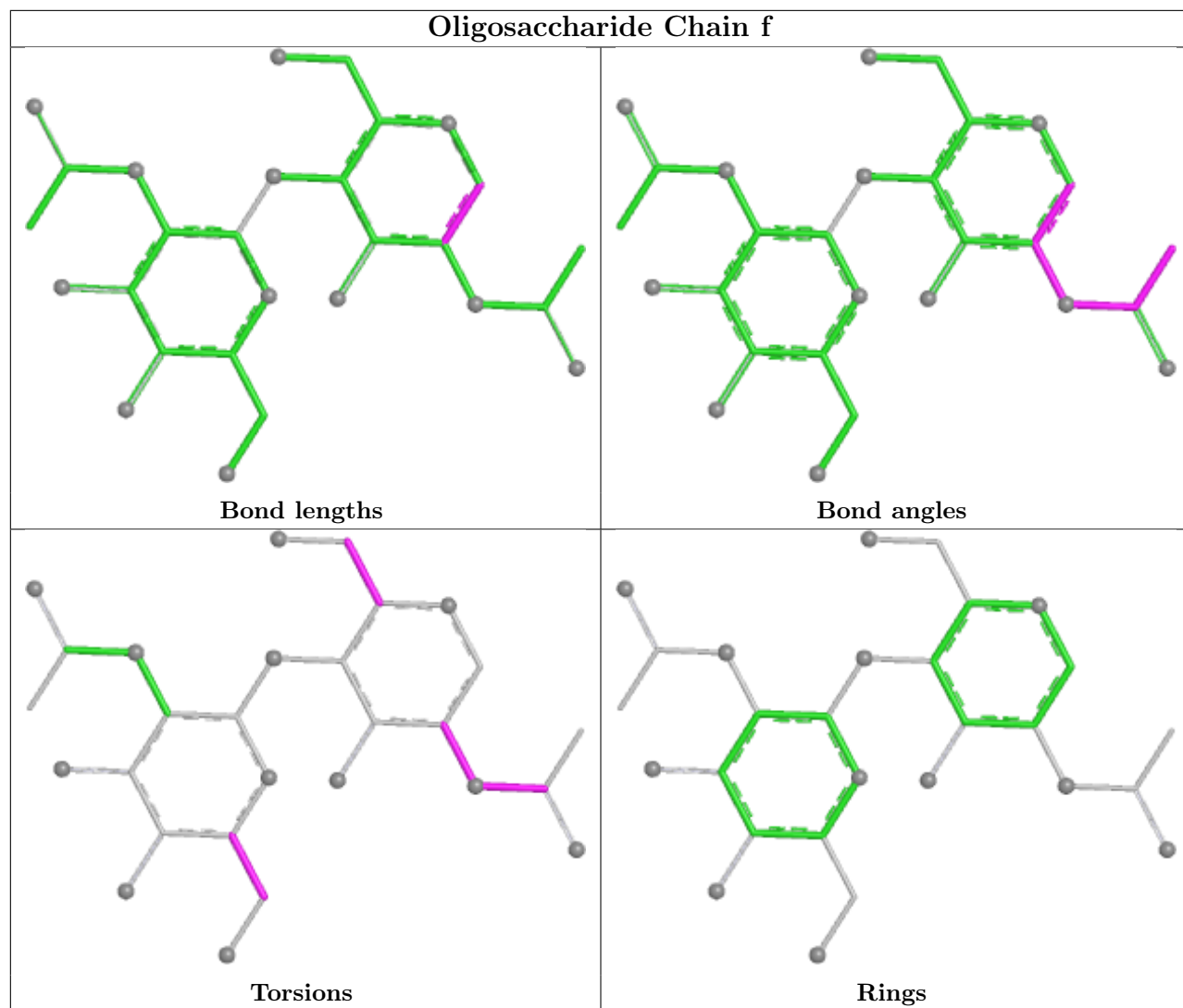


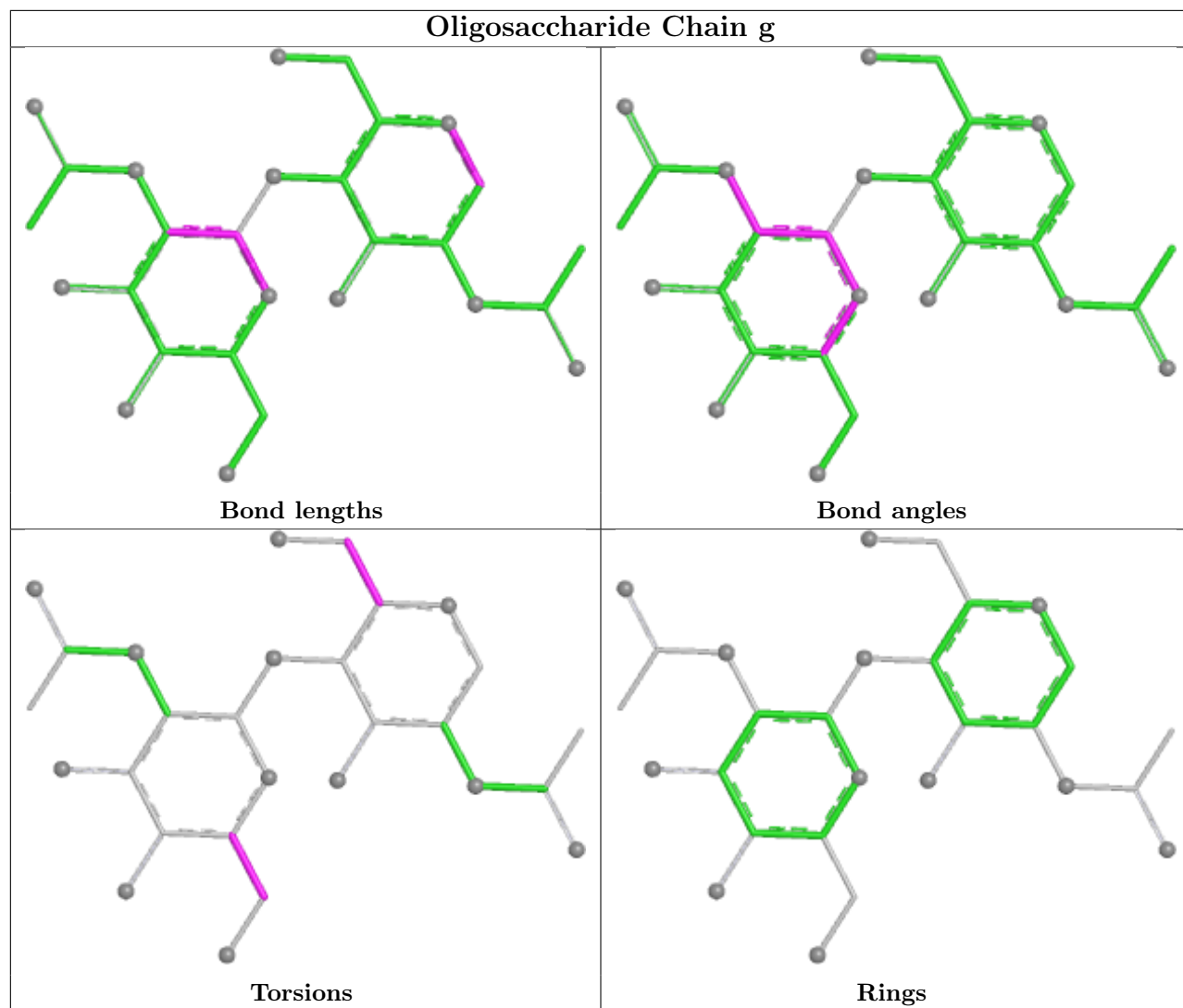


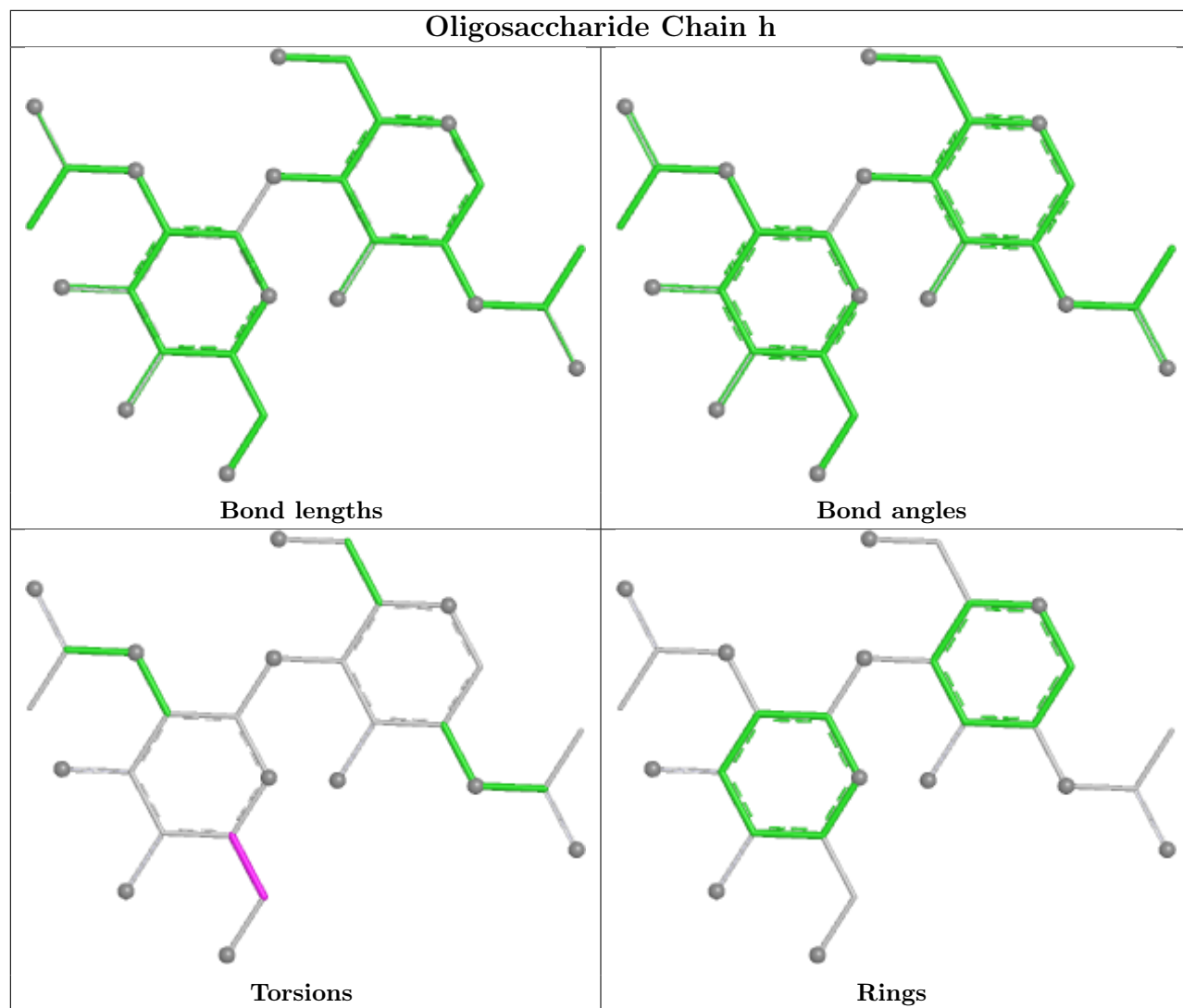


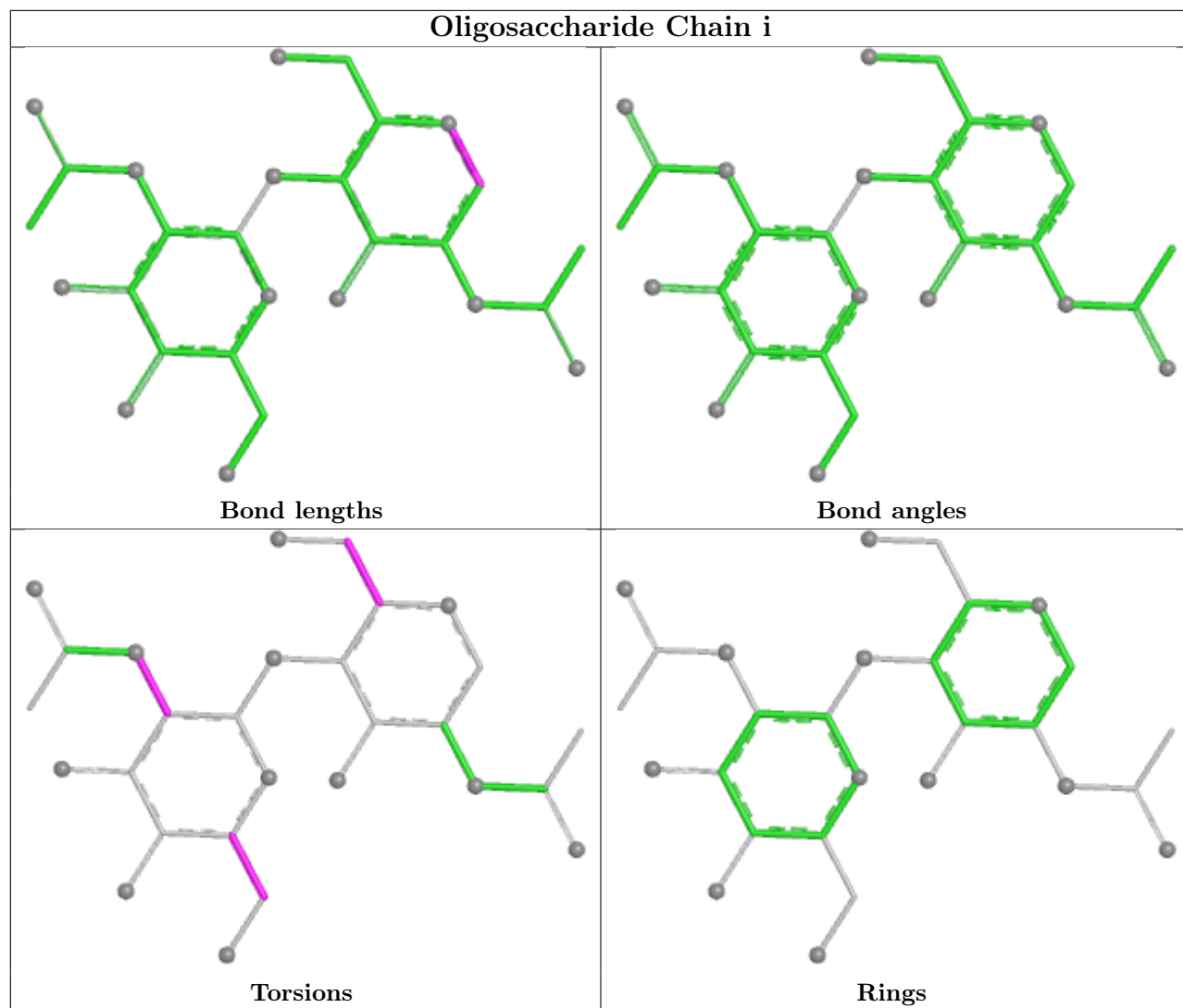


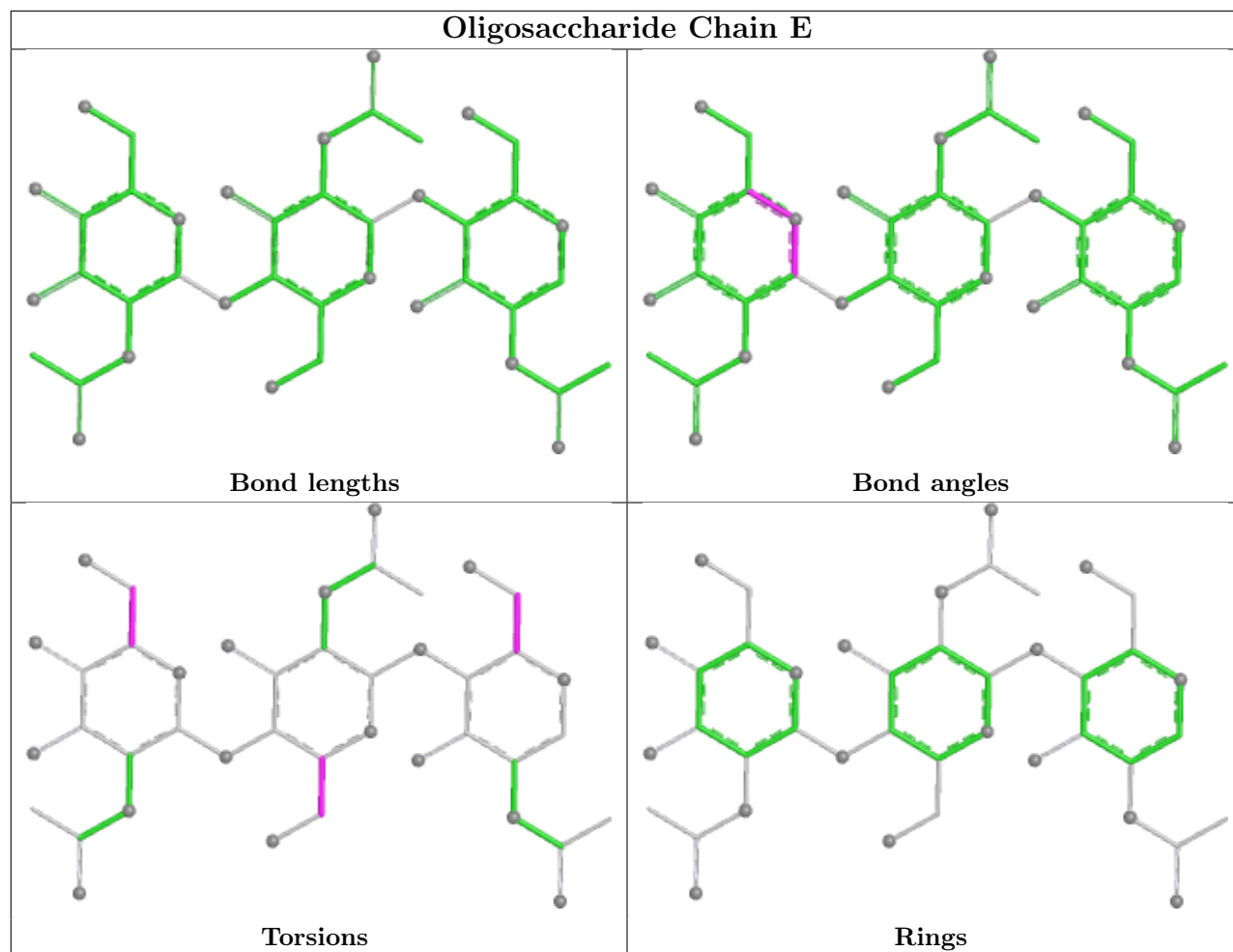


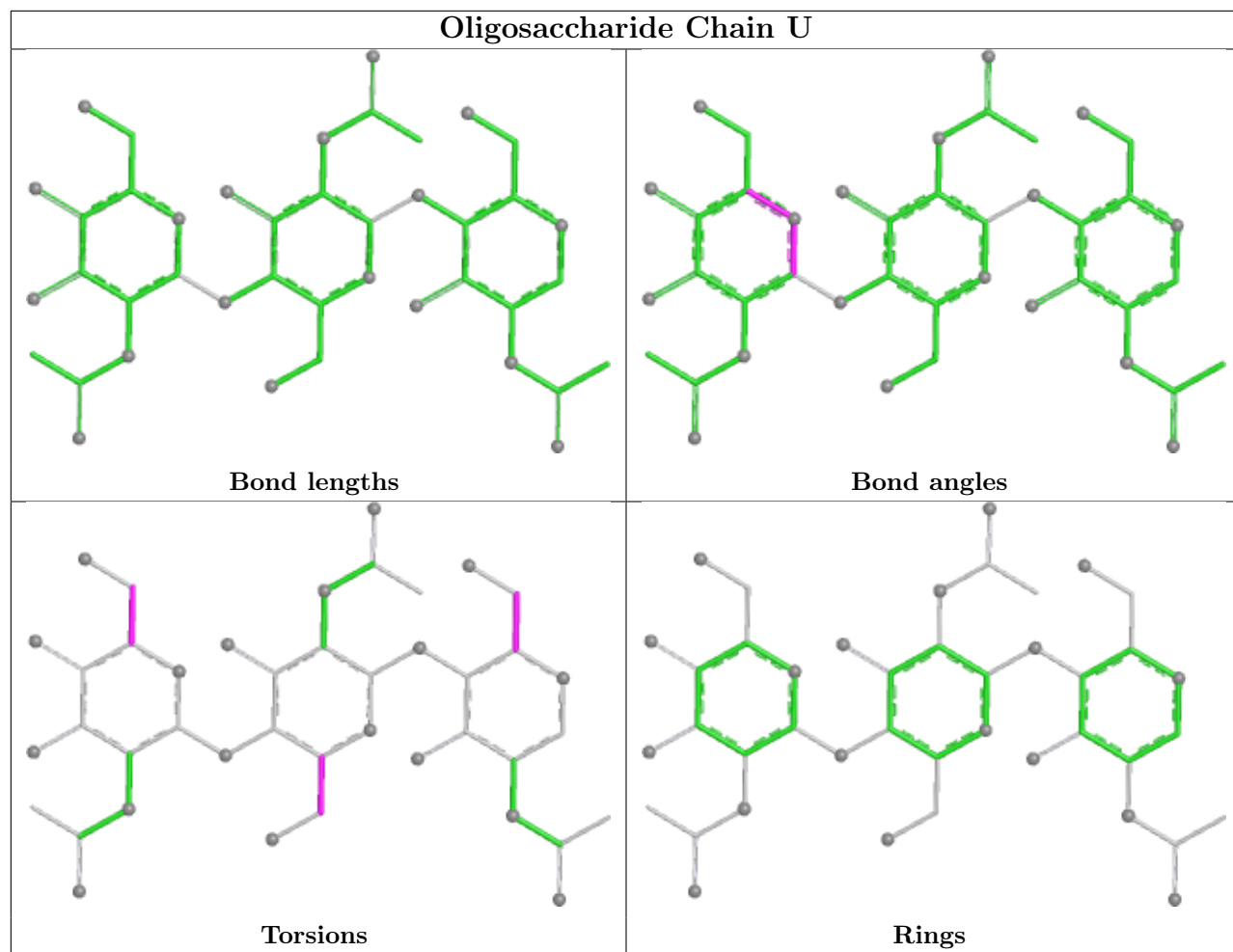


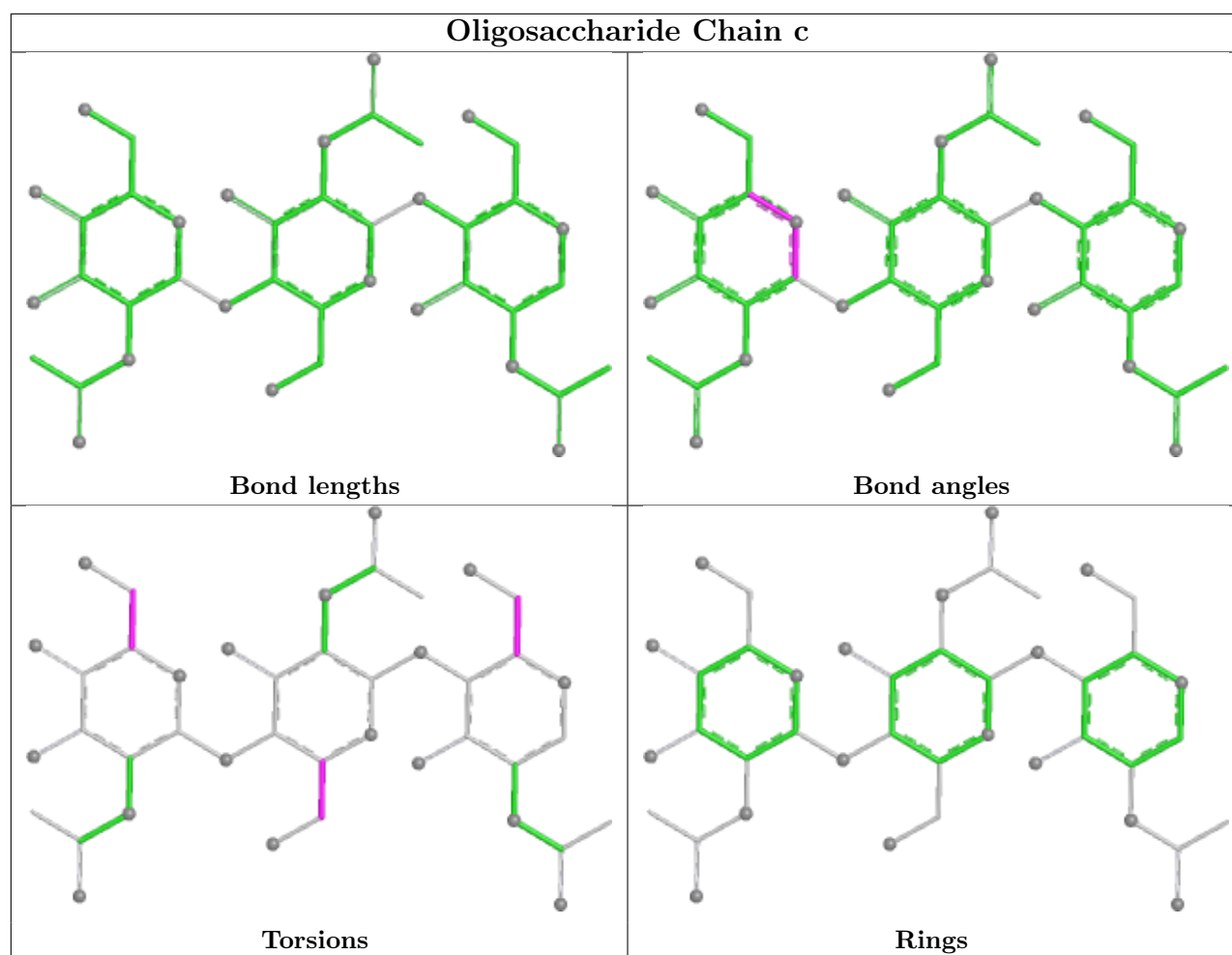












5.6 Ligand geometry [i](#)

41 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	$\# Z > 2$
6	NAG	A	1307	1	14,14,15	0.36	0	17,19,21	0.73	0
6	NAG	C	1310	-	14,14,15	0.32	0	17,19,21	1.41	2 (11%)
6	NAG	A	1303	1	14,14,15	0.29	0	17,19,21	0.58	0
6	NAG	B	1305	1	14,14,15	0.29	0	17,19,21	0.57	0
6	NAG	A	1308	-	14,14,15	0.31	0	17,19,21	1.40	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	NAG	A	1310	-	14,14,15	0.15	0	17,19,21	0.49	0
6	NAG	C	1313	1	14,14,15	0.25	0	17,19,21	0.69	1 (5%)
6	NAG	C	1312	-	14,14,15	0.44	0	17,19,21	1.49	3 (17%)
6	NAG	B	1314	-	14,14,15	0.15	0	17,19,21	0.49	0
6	NAG	A	1309	1	14,14,15	0.25	0	17,19,21	0.70	1 (5%)
7	EIC	A	1311	-	19,19,19	0.56	0	19,19,19	0.98	1 (5%)
6	NAG	A	1301	1	14,14,15	0.39	0	17,19,21	0.62	1 (5%)
6	NAG	C	1304	1	14,14,15	0.66	1 (7%)	17,19,21	0.76	1 (5%)
6	NAG	C	1311	1	14,14,15	0.67	1 (7%)	17,19,21	0.71	0
6	NAG	B	1302	1	14,14,15	0.83	1 (7%)	17,19,21	0.57	0
6	NAG	B	1303	-	14,14,15	2.97	2 (14%)	17,19,21	1.58	4 (23%)
6	NAG	B	1312	-	14,14,15	0.42	0	17,19,21	1.50	3 (17%)
6	NAG	C	1301	1	14,14,15	0.40	0	17,19,21	0.63	1 (5%)
7	EIC	C	1315	-	19,19,19	0.59	0	19,19,19	0.95	0
6	NAG	B	1304	1	14,14,15	0.66	1 (7%)	17,19,21	0.78	1 (5%)
6	NAG	B	1307	1	14,14,15	0.26	0	17,19,21	0.58	0
6	NAG	C	1309	1	14,14,15	0.36	0	17,19,21	0.73	0
6	NAG	C	1306	-	14,14,15	0.44	0	17,19,21	1.16	2 (11%)
6	NAG	B	1308	1	14,14,15	0.50	0	17,19,21	0.37	0
6	NAG	B	1310	-	14,14,15	0.31	0	17,19,21	1.40	2 (11%)
6	NAG	A	1305	1	14,14,15	0.28	0	17,19,21	0.56	0
6	NAG	B	1309	1	14,14,15	0.35	0	17,19,21	0.74	0
6	NAG	A	1304	-	14,14,15	0.42	0	17,19,21	1.15	2 (11%)
6	NAG	B	1306	-	14,14,15	0.43	0	17,19,21	1.15	2 (11%)
6	NAG	C	1307	1	14,14,15	0.29	0	17,19,21	0.56	0
6	NAG	A	1302	1	14,14,15	0.66	1 (7%)	17,19,21	0.77	1 (5%)
6	NAG	C	1305	1	14,14,15	0.27	0	17,19,21	0.58	0
6	NAG	C	1314	-	14,14,15	0.16	0	17,19,21	0.49	0
6	NAG	C	1303	-	14,14,15	2.99	3 (21%)	17,19,21	1.61	4 (23%)
6	NAG	B	1313	1	14,14,15	0.24	0	17,19,21	0.70	1 (5%)
6	NAG	C	1302	1	14,14,15	0.82	1 (7%)	17,19,21	0.58	0
6	NAG	C	1308	1	14,14,15	0.50	0	17,19,21	0.36	0
6	NAG	A	1306	1	14,14,15	0.51	0	17,19,21	0.36	0
6	NAG	B	1311	1	14,14,15	0.69	1 (7%)	17,19,21	0.70	0
6	NAG	B	1301	1	14,14,15	0.40	0	17,19,21	0.62	1 (5%)
7	EIC	B	1315	-	19,19,19	0.58	0	19,19,19	0.96	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
6	NAG	A	1307	1	-	2/6/23/26	0/1/1/1
6	NAG	C	1310	-	-	4/6/23/26	0/1/1/1
6	NAG	A	1303	1	-	5/6/23/26	0/1/1/1
6	NAG	B	1305	1	-	5/6/23/26	0/1/1/1
6	NAG	A	1308	-	-	4/6/23/26	0/1/1/1
6	NAG	A	1310	-	-	0/6/23/26	0/1/1/1
6	NAG	C	1313	1	-	2/6/23/26	0/1/1/1
6	NAG	C	1312	-	-	6/6/23/26	0/1/1/1
6	NAG	B	1314	-	-	0/6/23/26	0/1/1/1
6	NAG	A	1309	1	-	2/6/23/26	0/1/1/1
7	EIC	A	1311	-	-	11/17/17/17	-
6	NAG	A	1301	1	-	2/6/23/26	0/1/1/1
6	NAG	C	1304	1	-	2/6/23/26	0/1/1/1
6	NAG	C	1311	1	-	2/6/23/26	0/1/1/1
6	NAG	B	1302	1	-	1/6/23/26	0/1/1/1
6	NAG	B	1303	-	-	1/6/23/26	0/1/1/1
6	NAG	B	1312	-	-	6/6/23/26	0/1/1/1
6	NAG	C	1301	1	-	2/6/23/26	0/1/1/1
7	EIC	C	1315	-	-	6/17/17/17	-
6	NAG	B	1304	1	-	2/6/23/26	0/1/1/1
6	NAG	B	1307	1	-	4/6/23/26	0/1/1/1
6	NAG	C	1309	1	-	2/6/23/26	0/1/1/1
6	NAG	C	1306	-	-	0/6/23/26	0/1/1/1
6	NAG	B	1308	1	-	2/6/23/26	0/1/1/1
6	NAG	B	1310	-	-	4/6/23/26	0/1/1/1
6	NAG	A	1305	1	-	4/6/23/26	0/1/1/1
6	NAG	B	1309	1	-	2/6/23/26	0/1/1/1
6	NAG	A	1304	-	-	0/6/23/26	0/1/1/1
6	NAG	B	1306	-	-	0/6/23/26	0/1/1/1
6	NAG	C	1307	1	-	4/6/23/26	0/1/1/1
6	NAG	A	1302	1	-	2/6/23/26	0/1/1/1
6	NAG	C	1305	1	-	5/6/23/26	0/1/1/1
6	NAG	C	1314	-	-	0/6/23/26	0/1/1/1
6	NAG	C	1303	-	-	1/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	B	1313	1	-	2/6/23/26	0/1/1/1
6	NAG	C	1302	1	-	1/6/23/26	0/1/1/1
6	NAG	C	1308	1	-	2/6/23/26	0/1/1/1
6	NAG	A	1306	1	-	2/6/23/26	0/1/1/1
6	NAG	B	1311	1	-	2/6/23/26	0/1/1/1
6	NAG	B	1301	1	-	2/6/23/26	0/1/1/1
7	EIC	B	1315	-	-	7/17/17/17	-

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	1303	NAG	O5-C1	-7.75	1.30	1.43
6	B	1303	NAG	O5-C1	-7.72	1.30	1.43
6	B	1303	NAG	C1-C2	-7.49	1.42	1.52
6	C	1303	NAG	C1-C2	-7.48	1.42	1.52
6	B	1302	NAG	O5-C1	-2.67	1.39	1.43
6	C	1302	NAG	O5-C1	-2.63	1.39	1.43
6	B	1311	NAG	O5-C1	-2.23	1.40	1.43
6	C	1311	NAG	O5-C1	-2.20	1.40	1.43
6	A	1302	NAG	C1-C2	2.16	1.55	1.52
6	C	1304	NAG	C1-C2	2.14	1.55	1.52
6	B	1304	NAG	C1-C2	2.11	1.55	1.52
6	C	1303	NAG	C2-N2	-2.10	1.42	1.46

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	1312	NAG	C2-N2-C7	4.77	129.29	122.90
6	C	1312	NAG	C2-N2-C7	4.72	129.23	122.90
6	B	1310	NAG	C2-N2-C7	4.57	129.03	122.90
6	C	1310	NAG	C2-N2-C7	4.57	129.03	122.90
6	A	1308	NAG	C2-N2-C7	4.57	129.03	122.90
6	C	1303	NAG	C1-C2-N2	3.64	116.16	110.43
6	B	1303	NAG	C1-C2-N2	3.58	116.08	110.43
6	C	1303	NAG	O5-C1-C2	3.35	116.48	111.29
6	B	1303	NAG	O5-C1-C2	3.35	116.47	111.29
6	C	1303	NAG	C1-O5-C5	3.27	116.57	112.19
6	B	1303	NAG	C1-O5-C5	3.15	116.41	112.19
6	C	1310	NAG	C1-C2-N2	2.60	114.53	110.43
6	B	1312	NAG	C1-C2-N2	2.60	114.53	110.43
6	C	1312	NAG	C1-C2-N2	2.59	114.52	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	1308	NAG	C1-C2-N2	2.58	114.50	110.43
6	B	1310	NAG	C1-C2-N2	2.56	114.47	110.43
6	C	1303	NAG	C2-N2-C7	2.38	126.09	122.90
6	A	1304	NAG	C8-C7-N2	2.38	120.06	116.12
6	C	1306	NAG	C8-C7-N2	2.37	120.04	116.12
6	B	1306	NAG	C8-C7-N2	2.34	120.00	116.12
6	B	1303	NAG	C2-N2-C7	2.27	125.94	122.90
6	B	1304	NAG	C1-O5-C5	2.27	115.23	112.19
6	A	1302	NAG	C1-O5-C5	2.25	115.21	112.19
6	C	1304	NAG	C1-O5-C5	2.20	115.13	112.19
6	C	1301	NAG	C1-O5-C5	2.14	115.06	112.19
6	C	1312	NAG	C1-O5-C5	2.14	115.05	112.19
6	B	1312	NAG	C1-O5-C5	2.13	115.05	112.19
6	A	1301	NAG	C1-O5-C5	2.13	115.04	112.19
6	C	1306	NAG	C2-N2-C7	-2.13	120.05	122.90
6	B	1313	NAG	C1-O5-C5	2.11	115.02	112.19
6	B	1301	NAG	C1-O5-C5	2.11	115.01	112.19
6	A	1309	NAG	C1-O5-C5	2.10	115.00	112.19
6	B	1306	NAG	C2-N2-C7	-2.09	120.09	122.90
6	A	1304	NAG	C2-N2-C7	-2.09	120.10	122.90
6	C	1313	NAG	C1-O5-C5	2.04	114.92	112.19
7	A	1311	EIC	O2-C1-C2	2.02	120.39	114.00

There are no chirality outliers.

All (113) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	1305	NAG	C1-C2-N2-C7
6	A	1305	NAG	C8-C7-N2-C2
6	A	1305	NAG	O7-C7-N2-C2
6	B	1307	NAG	C1-C2-N2-C7
6	B	1307	NAG	C8-C7-N2-C2
6	B	1307	NAG	O7-C7-N2-C2
6	C	1307	NAG	C1-C2-N2-C7
6	C	1307	NAG	C8-C7-N2-C2
6	C	1307	NAG	O7-C7-N2-C2
6	A	1303	NAG	O5-C5-C6-O6
6	B	1305	NAG	O5-C5-C6-O6
6	C	1305	NAG	O5-C5-C6-O6
6	A	1301	NAG	O5-C5-C6-O6
6	B	1301	NAG	O5-C5-C6-O6
6	C	1301	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
6	A	1303	NAG	C4-C5-C6-O6
6	B	1305	NAG	C4-C5-C6-O6
6	C	1305	NAG	C4-C5-C6-O6
6	A	1303	NAG	C8-C7-N2-C2
6	B	1305	NAG	C8-C7-N2-C2
6	C	1305	NAG	C8-C7-N2-C2
6	A	1301	NAG	C4-C5-C6-O6
6	B	1301	NAG	C4-C5-C6-O6
6	C	1301	NAG	C4-C5-C6-O6
6	A	1306	NAG	C4-C5-C6-O6
6	B	1308	NAG	C4-C5-C6-O6
6	C	1308	NAG	C4-C5-C6-O6
6	A	1306	NAG	O5-C5-C6-O6
6	B	1308	NAG	O5-C5-C6-O6
6	C	1308	NAG	O5-C5-C6-O6
6	A	1303	NAG	O7-C7-N2-C2
6	A	1308	NAG	C8-C7-N2-C2
6	A	1308	NAG	O7-C7-N2-C2
6	B	1305	NAG	O7-C7-N2-C2
6	B	1310	NAG	C8-C7-N2-C2
6	B	1310	NAG	O7-C7-N2-C2
6	B	1312	NAG	C8-C7-N2-C2
6	B	1312	NAG	O7-C7-N2-C2
6	C	1305	NAG	O7-C7-N2-C2
6	C	1310	NAG	C8-C7-N2-C2
6	C	1310	NAG	O7-C7-N2-C2
6	C	1312	NAG	C8-C7-N2-C2
6	C	1312	NAG	O7-C7-N2-C2
6	A	1302	NAG	O5-C5-C6-O6
6	B	1304	NAG	O5-C5-C6-O6
6	C	1304	NAG	O5-C5-C6-O6
6	A	1307	NAG	C4-C5-C6-O6
6	B	1309	NAG	C4-C5-C6-O6
6	C	1309	NAG	C4-C5-C6-O6
6	B	1311	NAG	C4-C5-C6-O6
6	C	1311	NAG	C4-C5-C6-O6
6	A	1305	NAG	O5-C5-C6-O6
6	B	1307	NAG	O5-C5-C6-O6
6	C	1307	NAG	O5-C5-C6-O6
6	A	1302	NAG	C4-C5-C6-O6
6	B	1304	NAG	C4-C5-C6-O6
6	C	1304	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
7	A	1311	EIC	C1-C2-C3-C4
6	A	1307	NAG	O5-C5-C6-O6
6	B	1309	NAG	O5-C5-C6-O6
6	C	1309	NAG	O5-C5-C6-O6
6	B	1311	NAG	O5-C5-C6-O6
6	C	1311	NAG	O5-C5-C6-O6
6	A	1309	NAG	C4-C5-C6-O6
6	C	1313	NAG	C4-C5-C6-O6
6	B	1313	NAG	C4-C5-C6-O6
6	C	1313	NAG	O5-C5-C6-O6
6	A	1309	NAG	O5-C5-C6-O6
6	B	1313	NAG	O5-C5-C6-O6
7	C	1315	EIC	C4-C5-C6-C7
7	A	1311	EIC	C5-C6-C7-C8
7	A	1311	EIC	C13-C14-C15-C16
7	A	1311	EIC	C14-C15-C16-C17
6	A	1303	NAG	C3-C2-N2-C7
6	B	1305	NAG	C3-C2-N2-C7
6	C	1305	NAG	C3-C2-N2-C7
7	A	1311	EIC	C6-C7-C8-C9
7	A	1311	EIC	C15-C16-C17-C18
7	C	1315	EIC	C2-C3-C4-C5
7	B	1315	EIC	C4-C5-C6-C7
7	A	1311	EIC	C10-C11-C12-C13
7	B	1315	EIC	C10-C11-C12-C13
7	C	1315	EIC	C5-C6-C7-C8
7	B	1315	EIC	C15-C16-C17-C18
6	B	1312	NAG	C4-C5-C6-O6
6	C	1312	NAG	C4-C5-C6-O6
7	B	1315	EIC	C7-C8-C9-C10
7	C	1315	EIC	O1-C1-C2-C3
6	B	1312	NAG	O5-C5-C6-O6
7	A	1311	EIC	C9-C10-C11-C12
6	A	1308	NAG	C1-C2-N2-C7
6	B	1310	NAG	C1-C2-N2-C7
6	B	1312	NAG	C1-C2-N2-C7
6	C	1310	NAG	C1-C2-N2-C7
6	C	1312	NAG	C1-C2-N2-C7
6	C	1312	NAG	O5-C5-C6-O6
7	A	1311	EIC	C4-C5-C6-C7
7	C	1315	EIC	O2-C1-C2-C3
6	C	1302	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
6	B	1302	NAG	C4-C5-C6-O6
6	A	1308	NAG	C3-C2-N2-C7
6	B	1303	NAG	C3-C2-N2-C7
6	B	1310	NAG	C3-C2-N2-C7
6	B	1312	NAG	C3-C2-N2-C7
6	C	1303	NAG	C3-C2-N2-C7
6	C	1310	NAG	C3-C2-N2-C7
6	C	1312	NAG	C3-C2-N2-C7
7	B	1315	EIC	O1-C1-C2-C3
7	B	1315	EIC	O2-C1-C2-C3
7	C	1315	EIC	C7-C8-C9-C10
7	B	1315	EIC	C14-C15-C16-C17
7	A	1311	EIC	C7-C8-C9-C10
7	A	1311	EIC	C12-C13-C14-C15

There are no ring outliers.

28 monomers are involved in 69 short contacts:

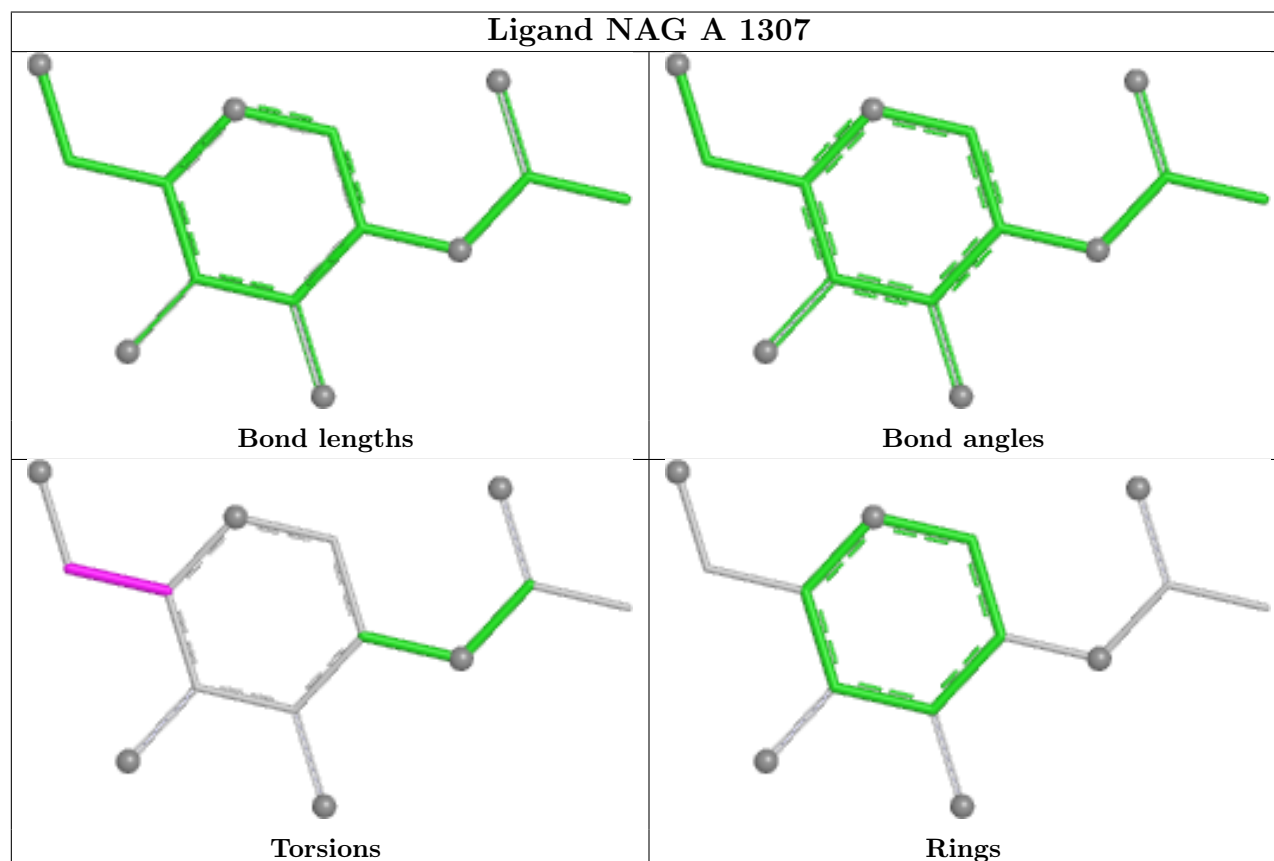
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1307	NAG	1	0
6	C	1310	NAG	1	0
6	A	1303	NAG	7	0
6	B	1305	NAG	7	0
6	A	1308	NAG	1	0
6	A	1310	NAG	3	0
6	C	1313	NAG	3	0
6	C	1312	NAG	1	0
6	B	1314	NAG	3	0
6	A	1309	NAG	3	0
7	A	1311	EIC	4	0
6	B	1302	NAG	5	0
6	B	1312	NAG	1	0
7	C	1315	EIC	2	0
6	B	1307	NAG	4	0
6	C	1309	NAG	1	0
6	C	1306	NAG	7	0
6	B	1310	NAG	1	0
6	A	1305	NAG	3	0
6	B	1309	NAG	1	0
6	A	1304	NAG	7	0
6	B	1306	NAG	7	0
6	C	1307	NAG	3	0

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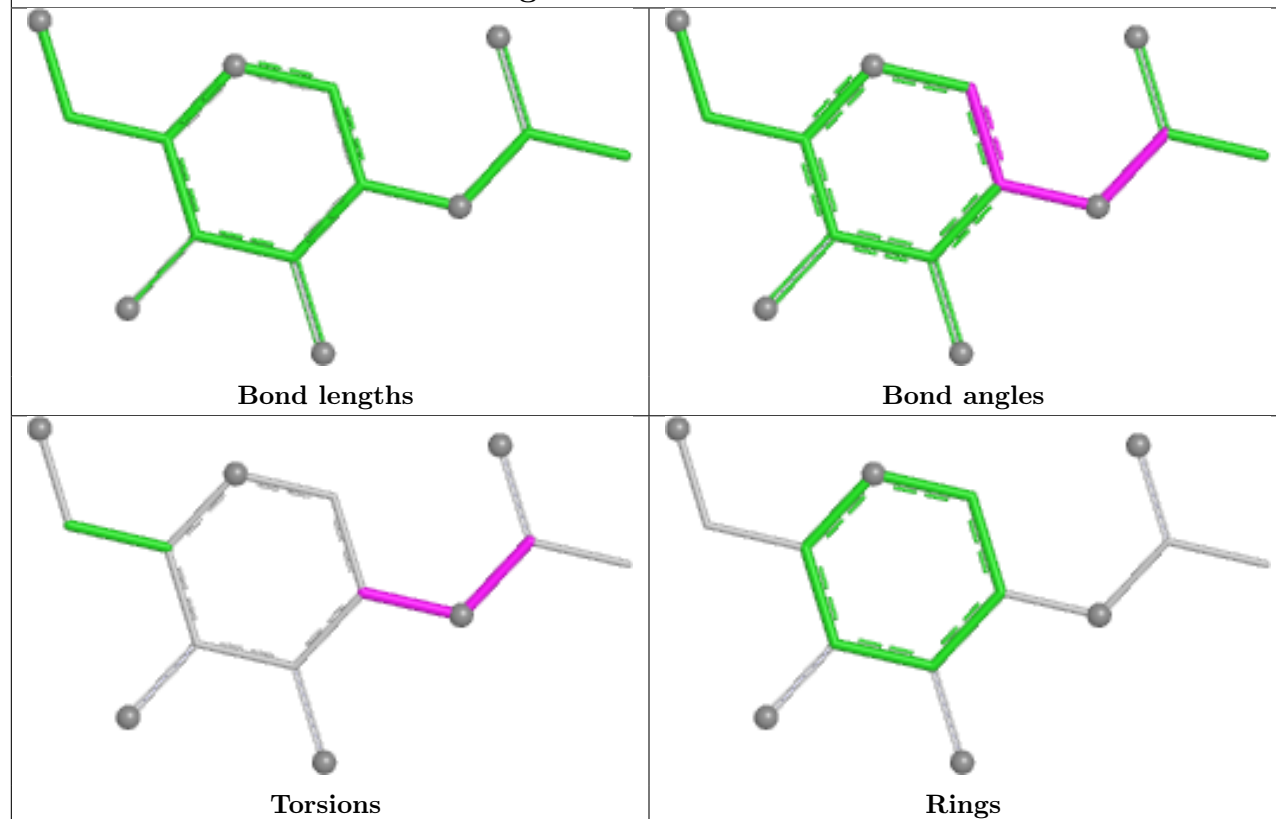
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	1305	NAG	7	0
6	C	1314	NAG	3	0
6	B	1313	NAG	3	0
6	C	1302	NAG	6	0
7	B	1315	EIC	4	0

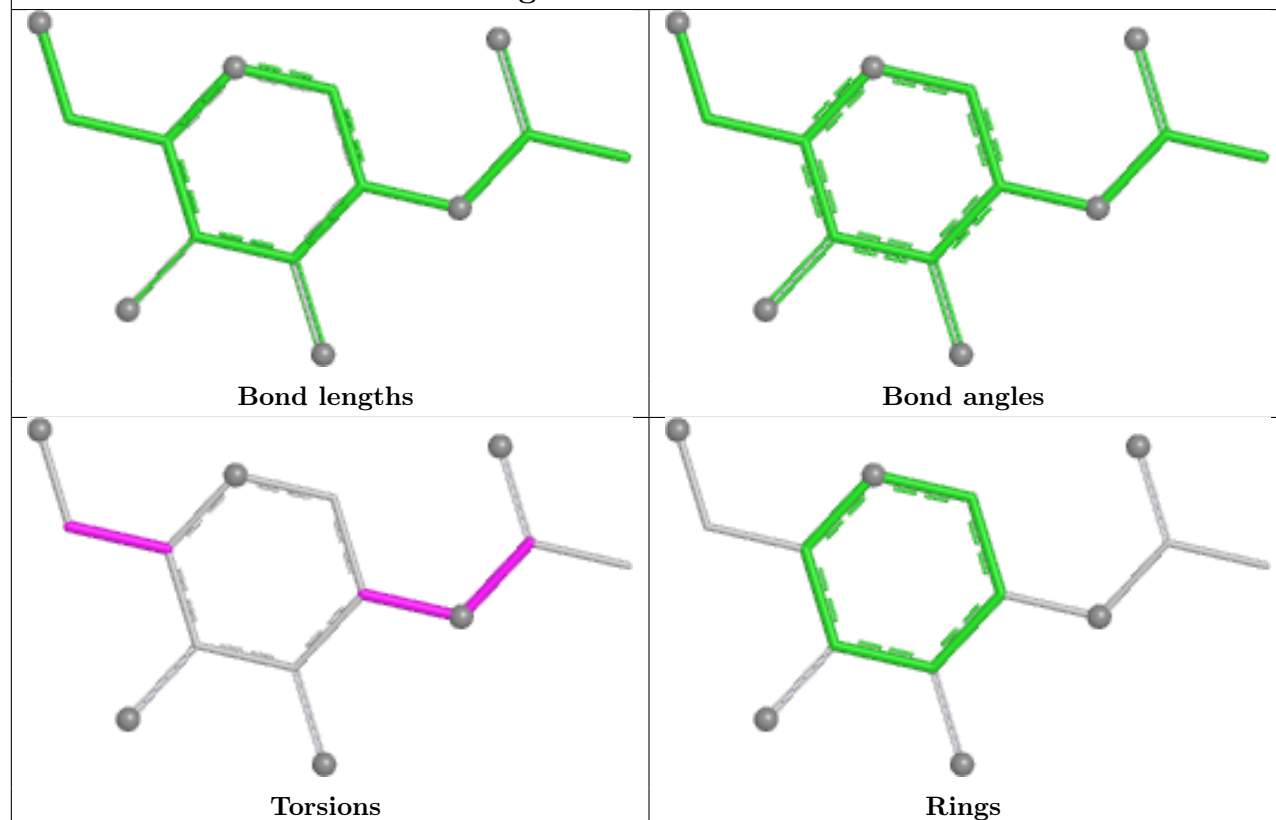
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



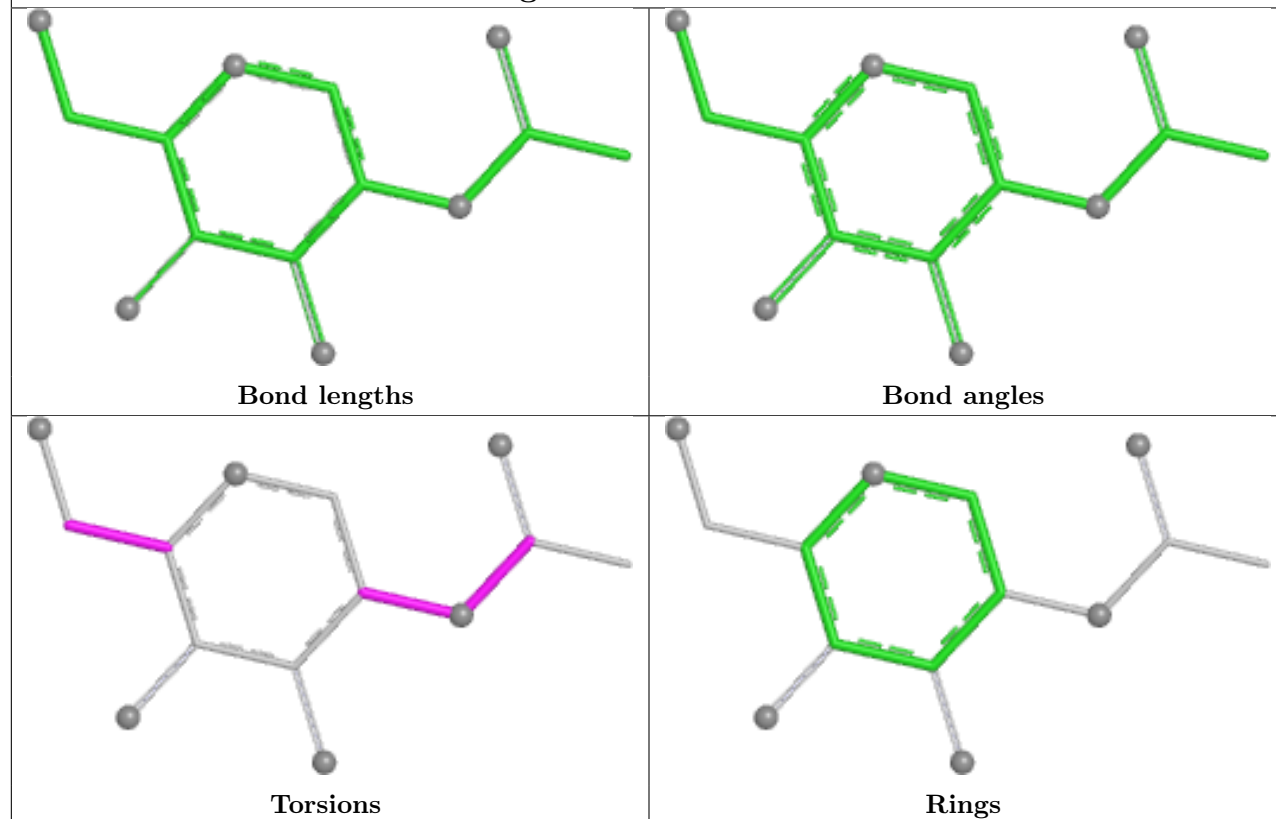
Ligand NAG C 1310



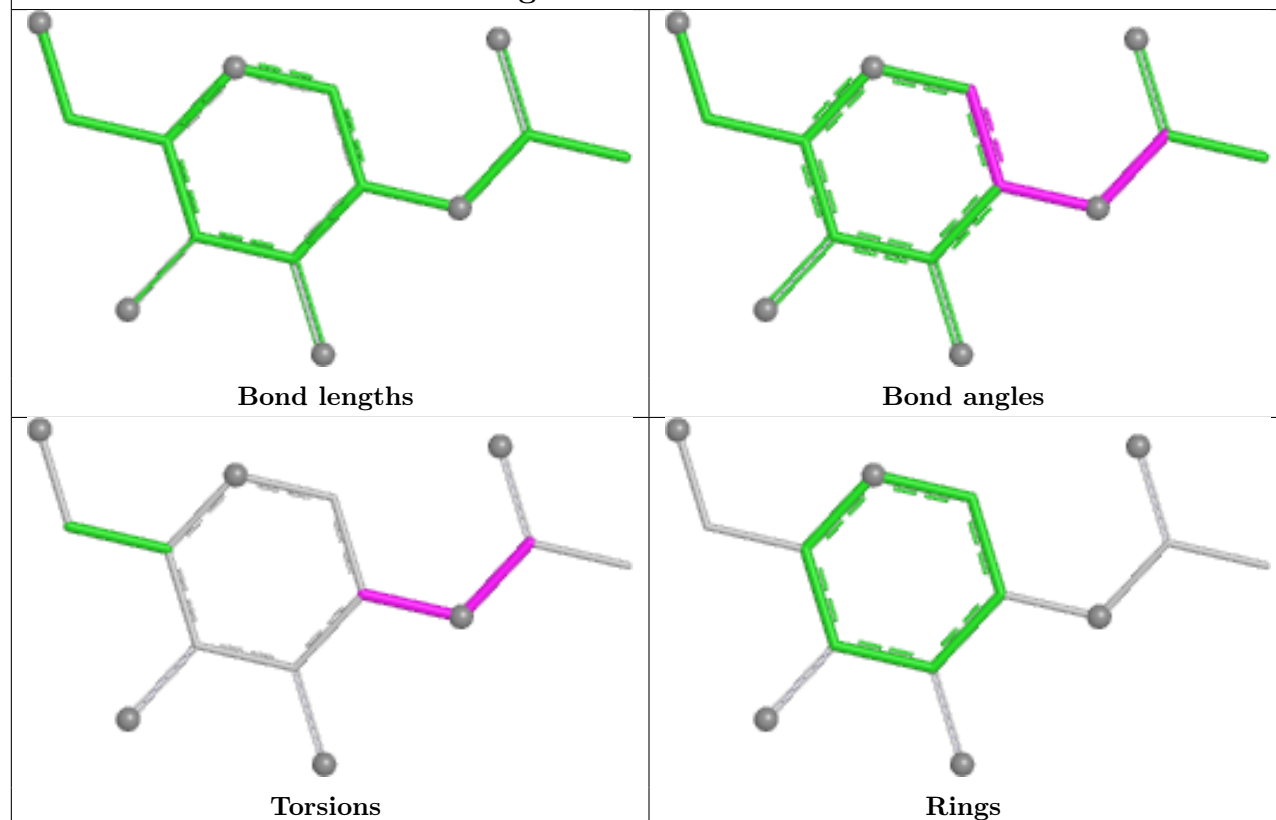
Ligand NAG A 1303



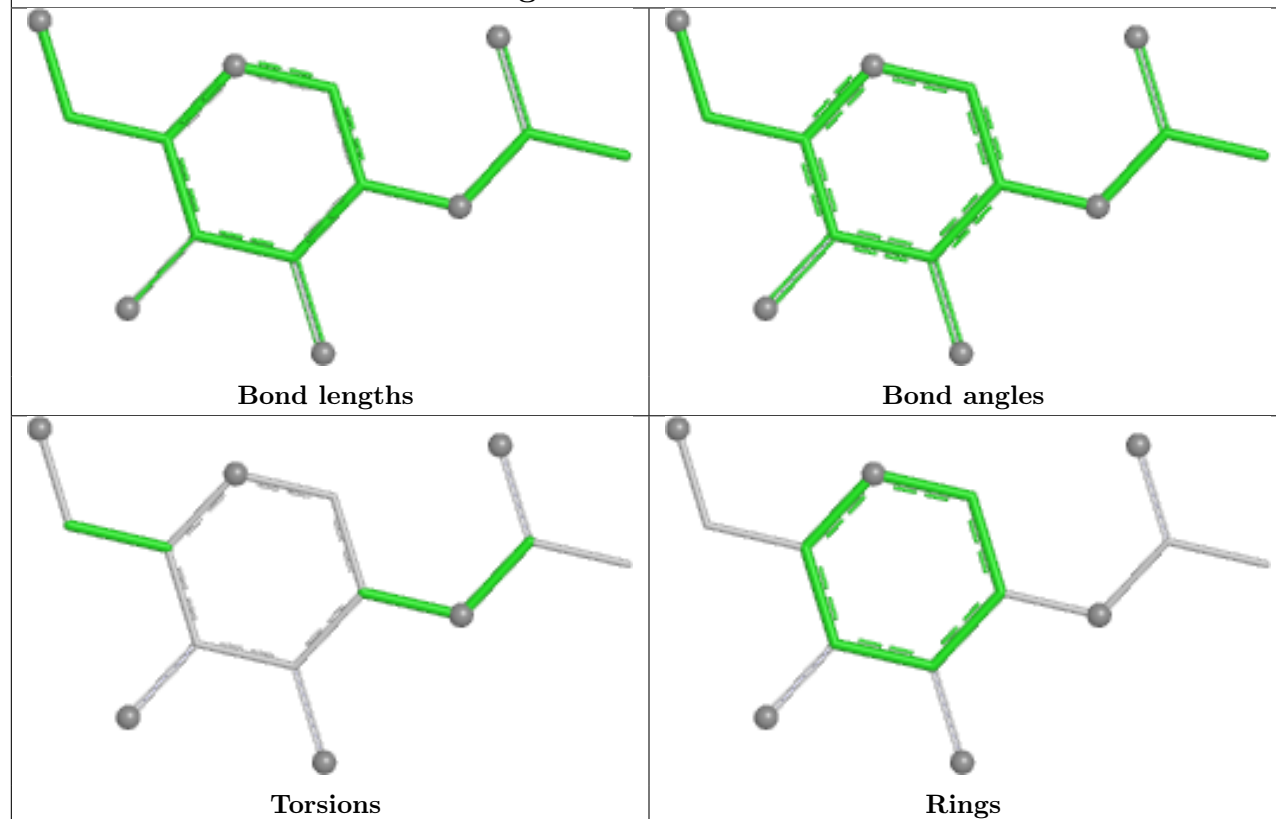
Ligand NAG B 1305



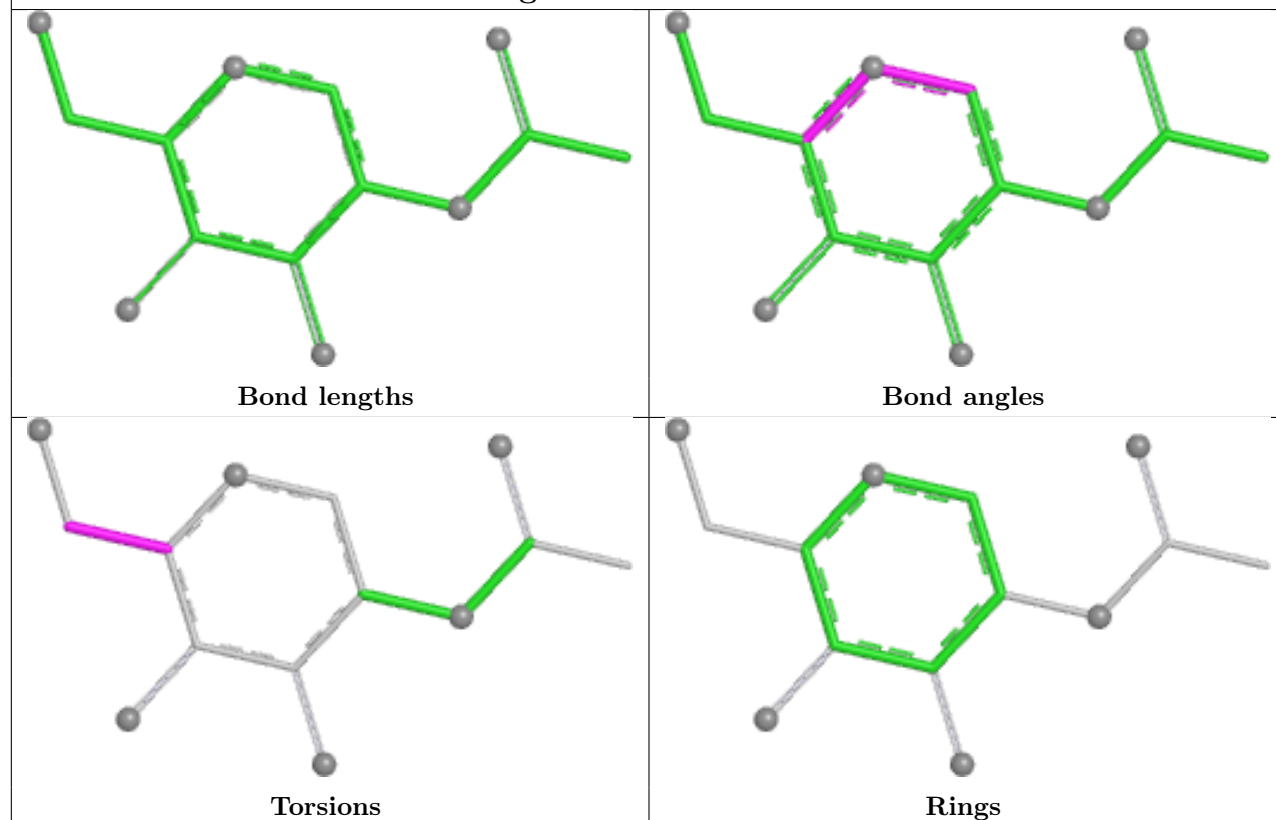
Ligand NAG A 1308



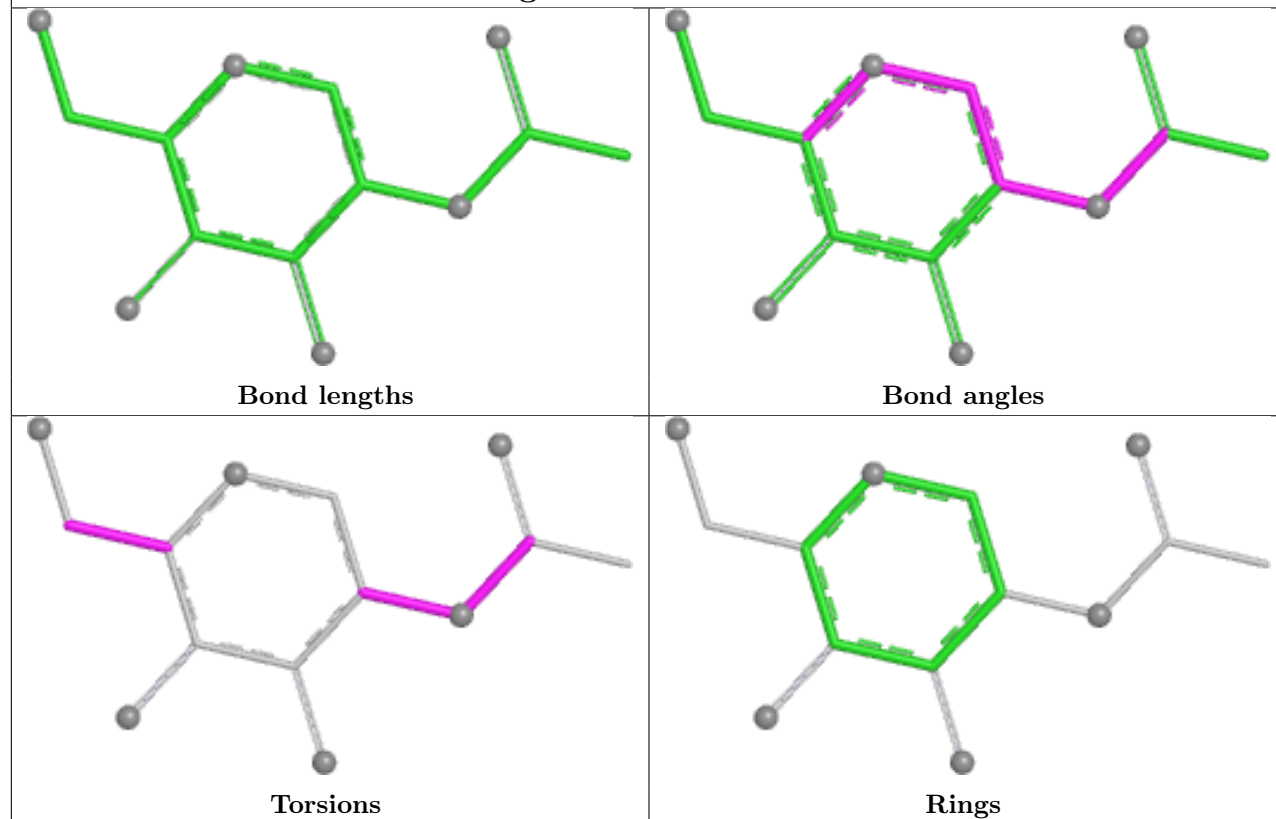
Ligand NAG A 1310



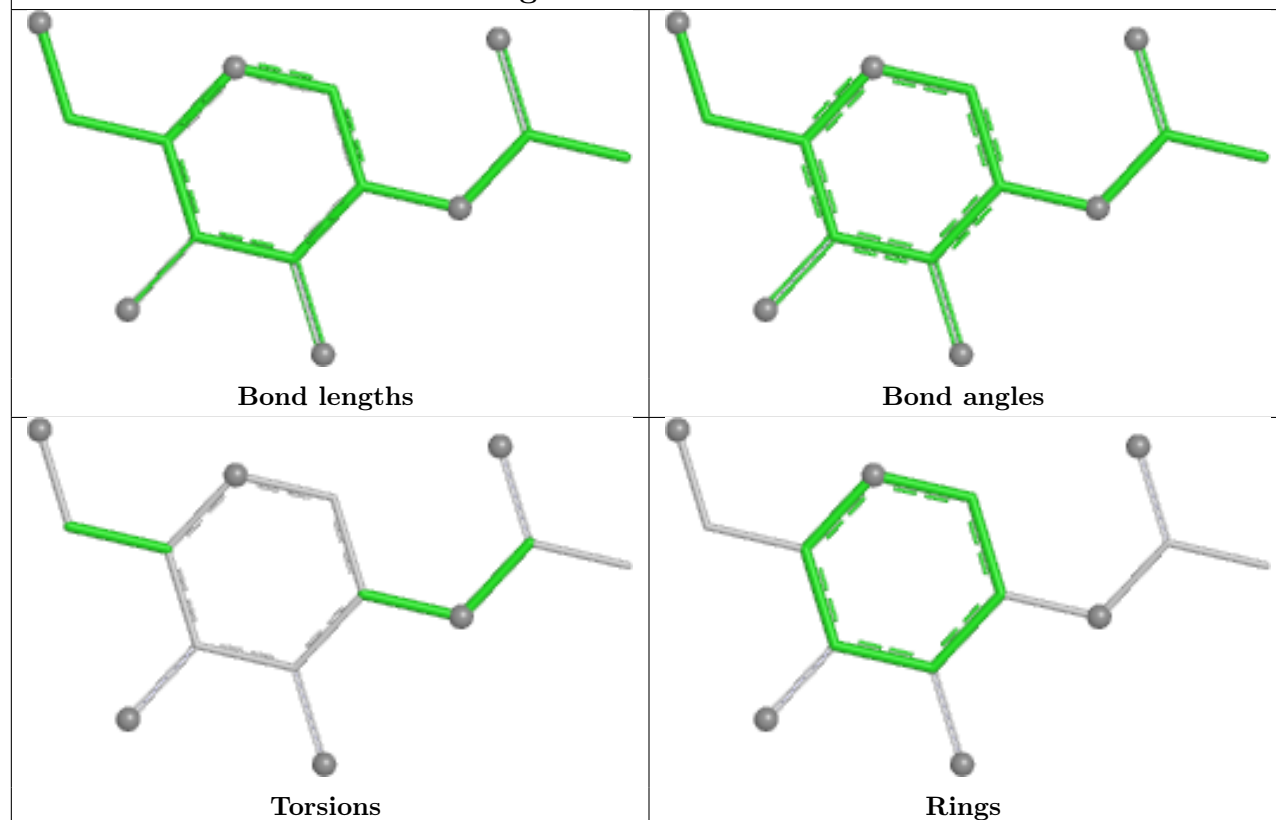
Ligand NAG C 1313

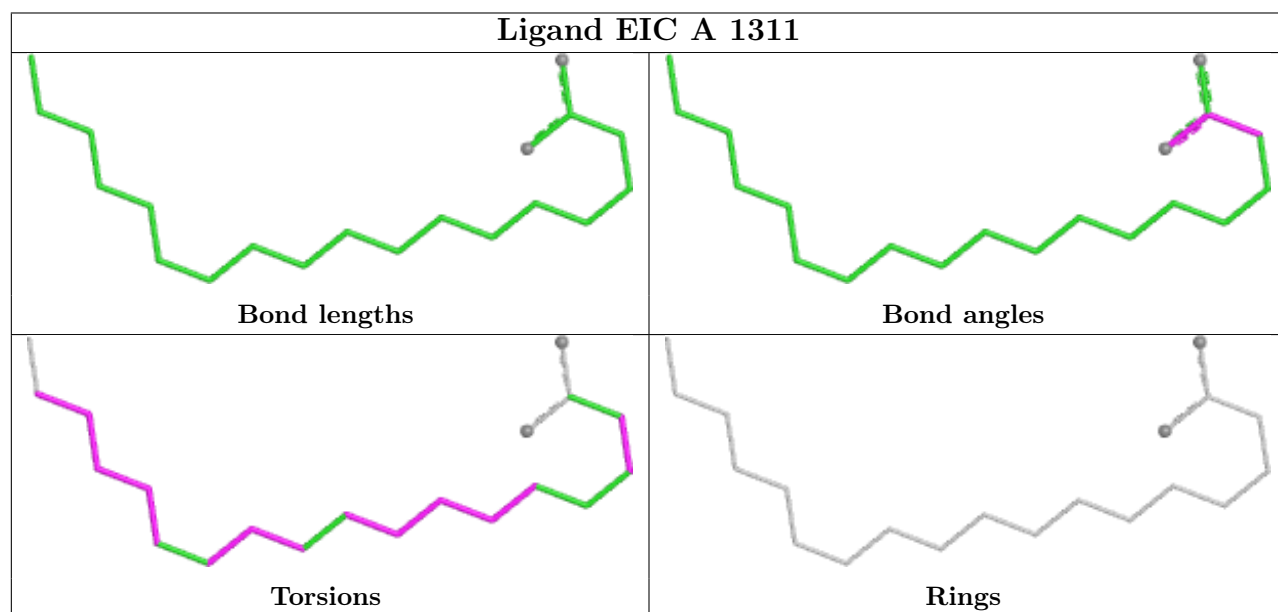
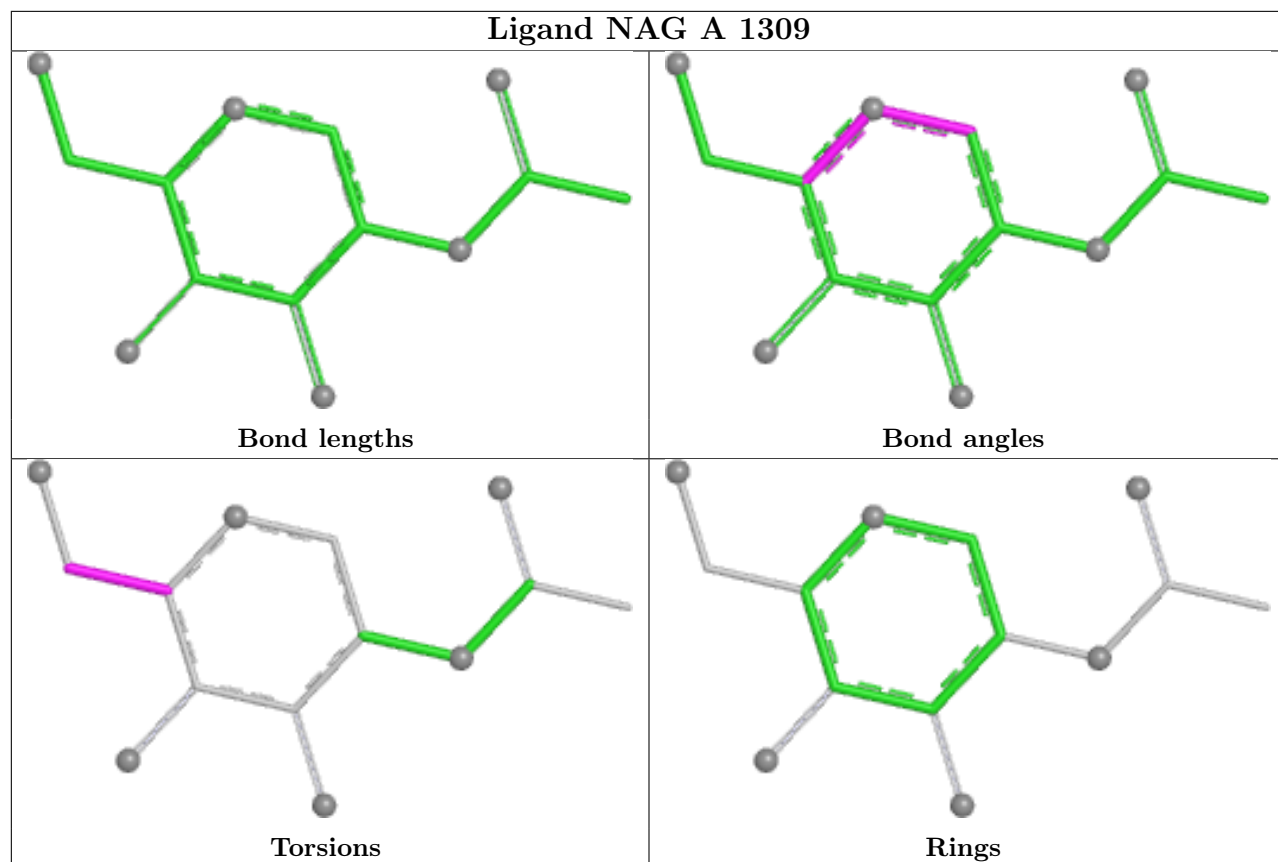


Ligand NAG C 1312

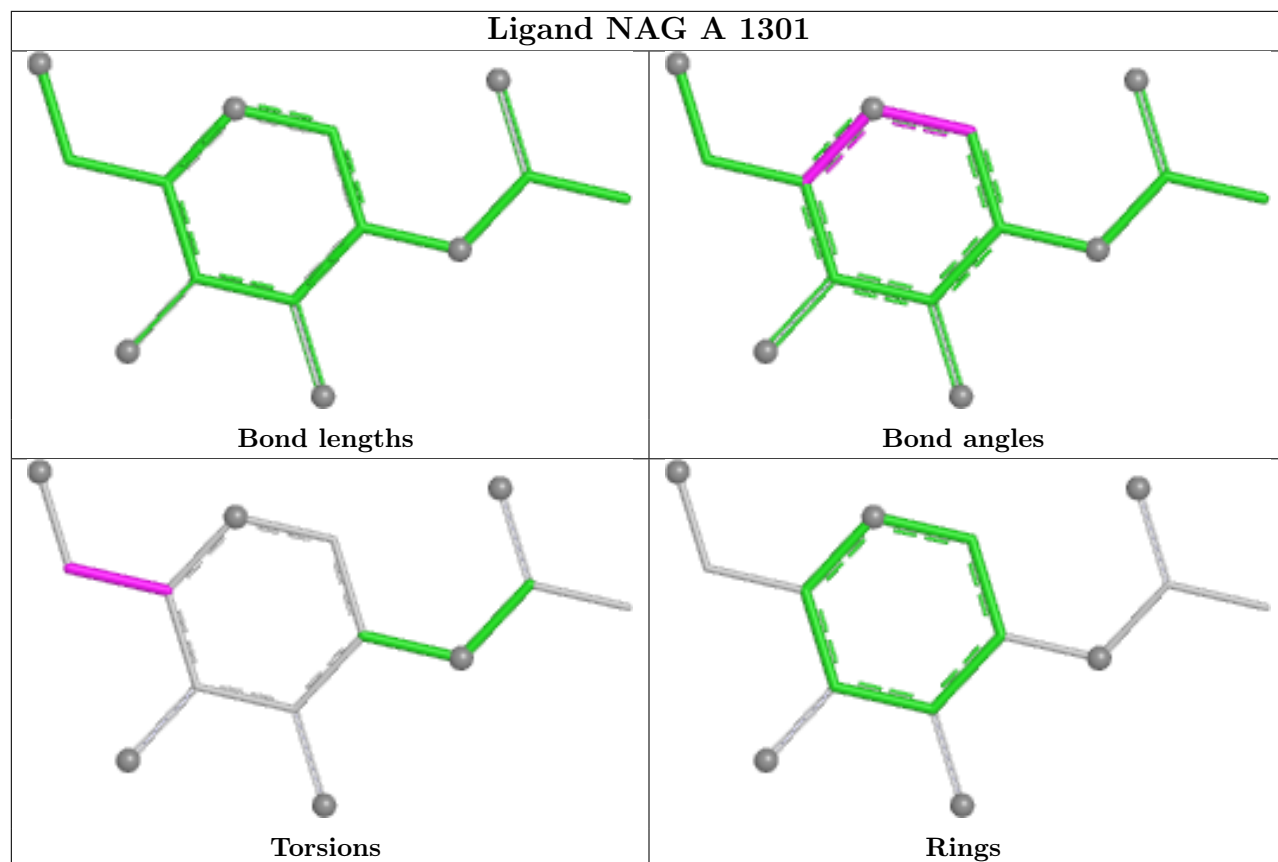


Ligand NAG B 1314

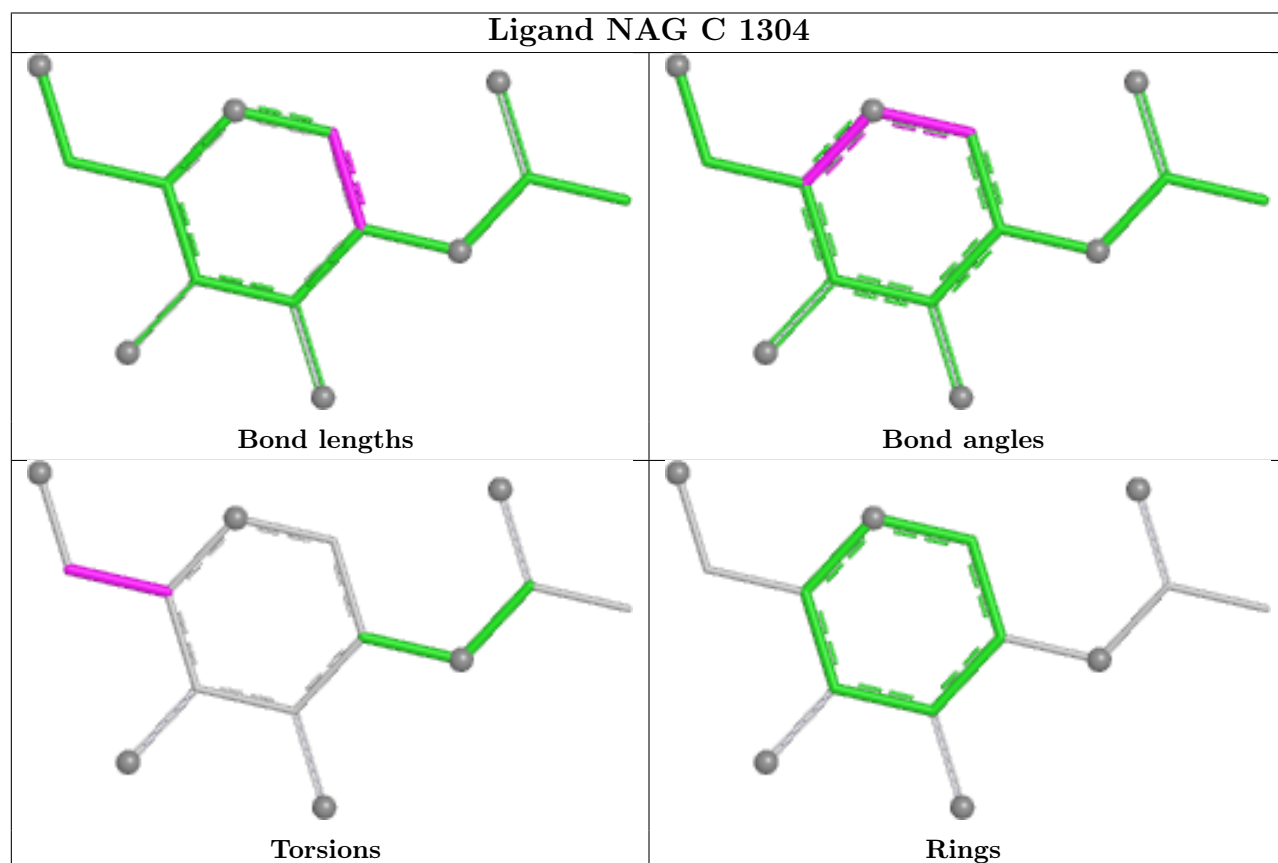




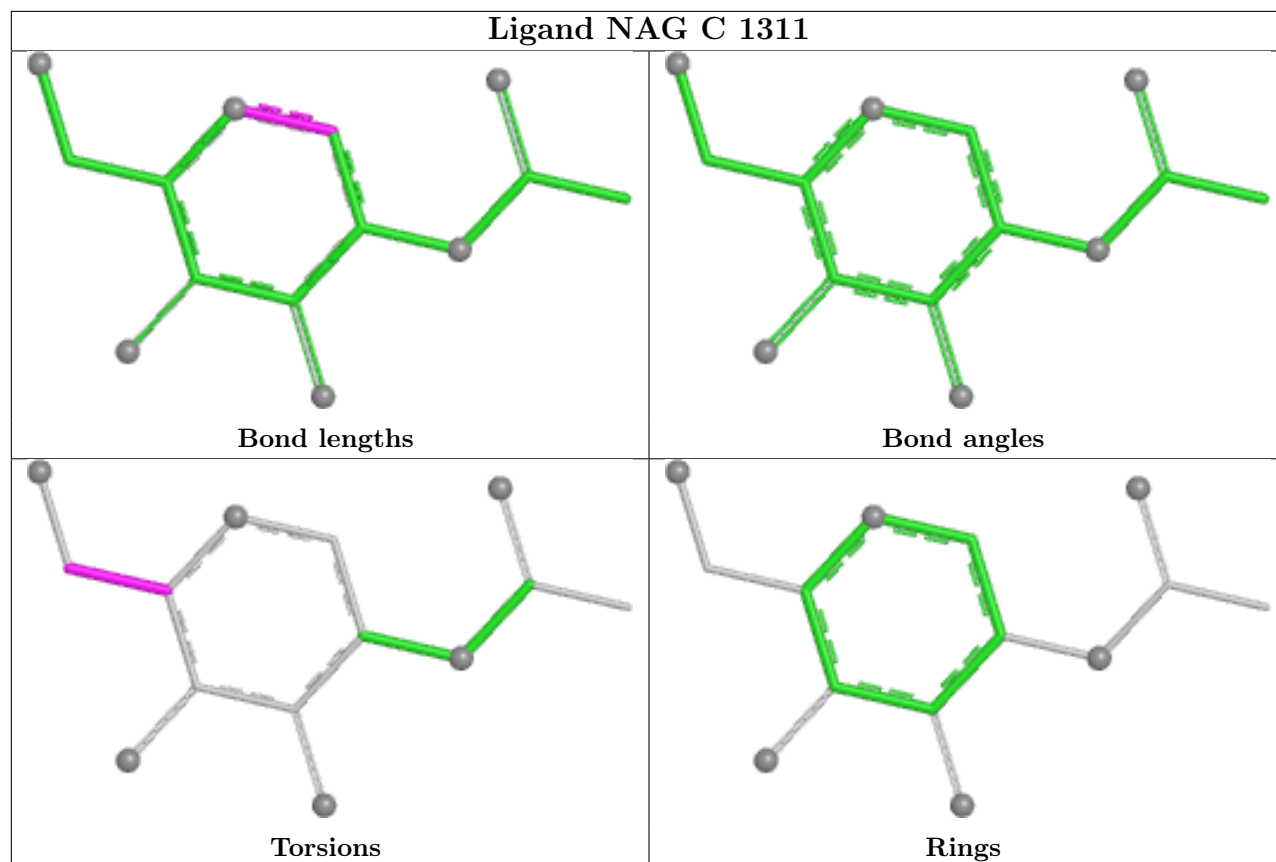
Ligand NAG A 1301



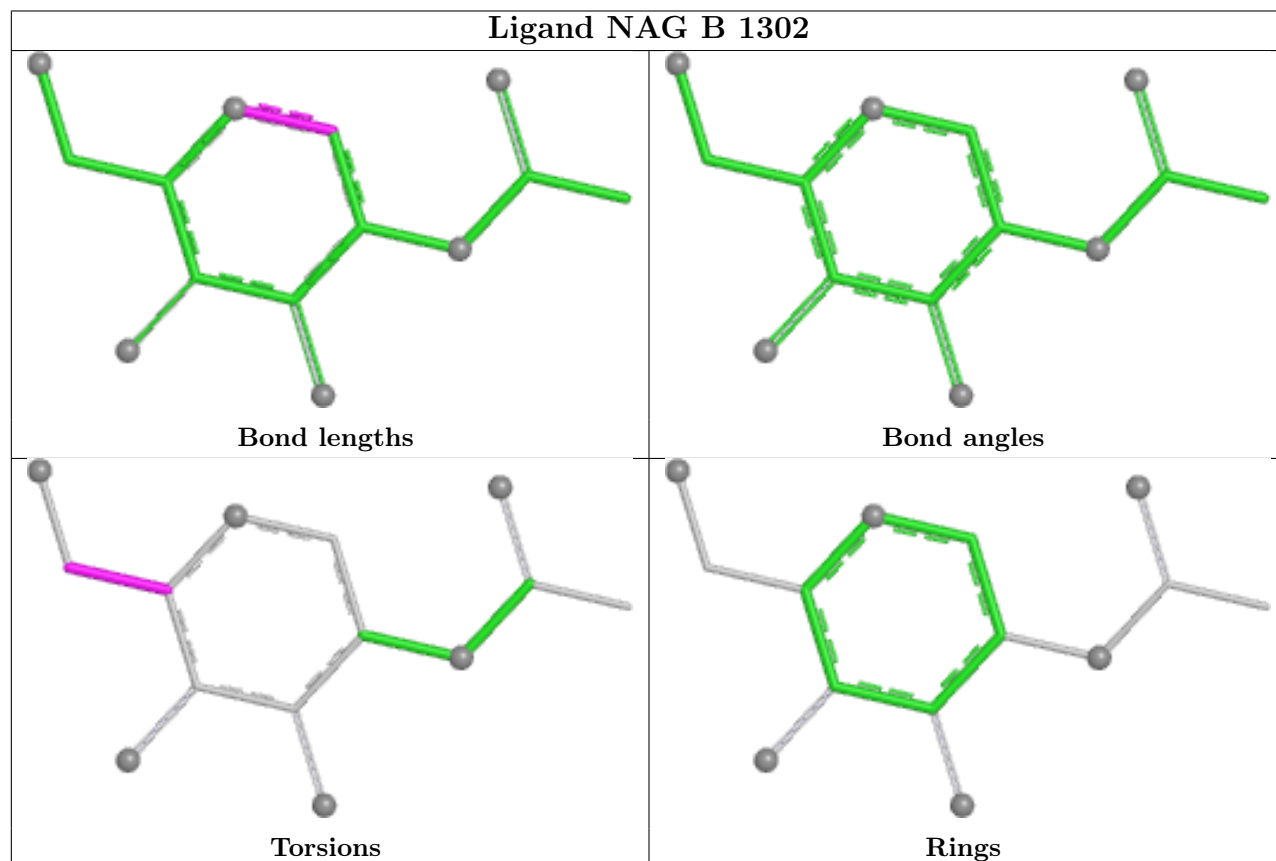
Ligand NAG C 1304



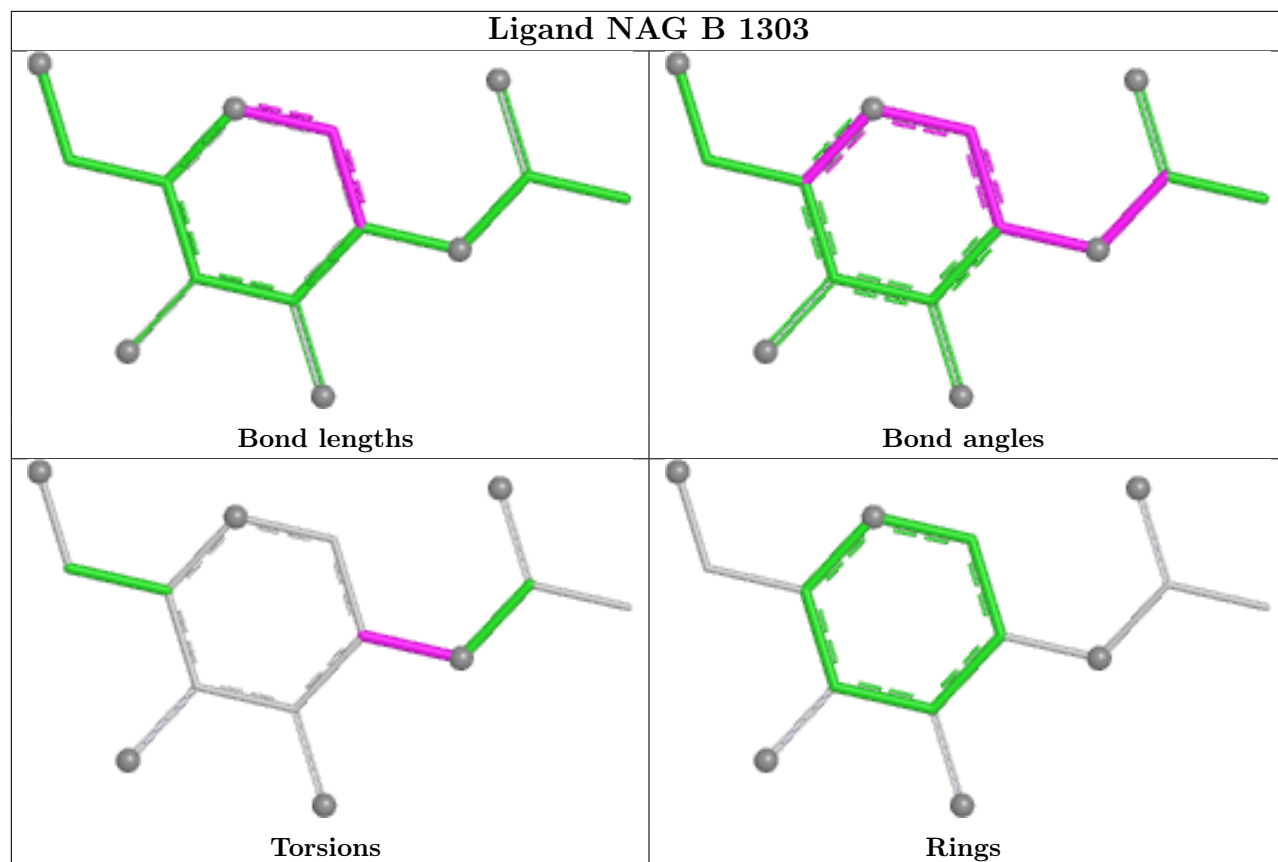
Ligand NAG C 1311



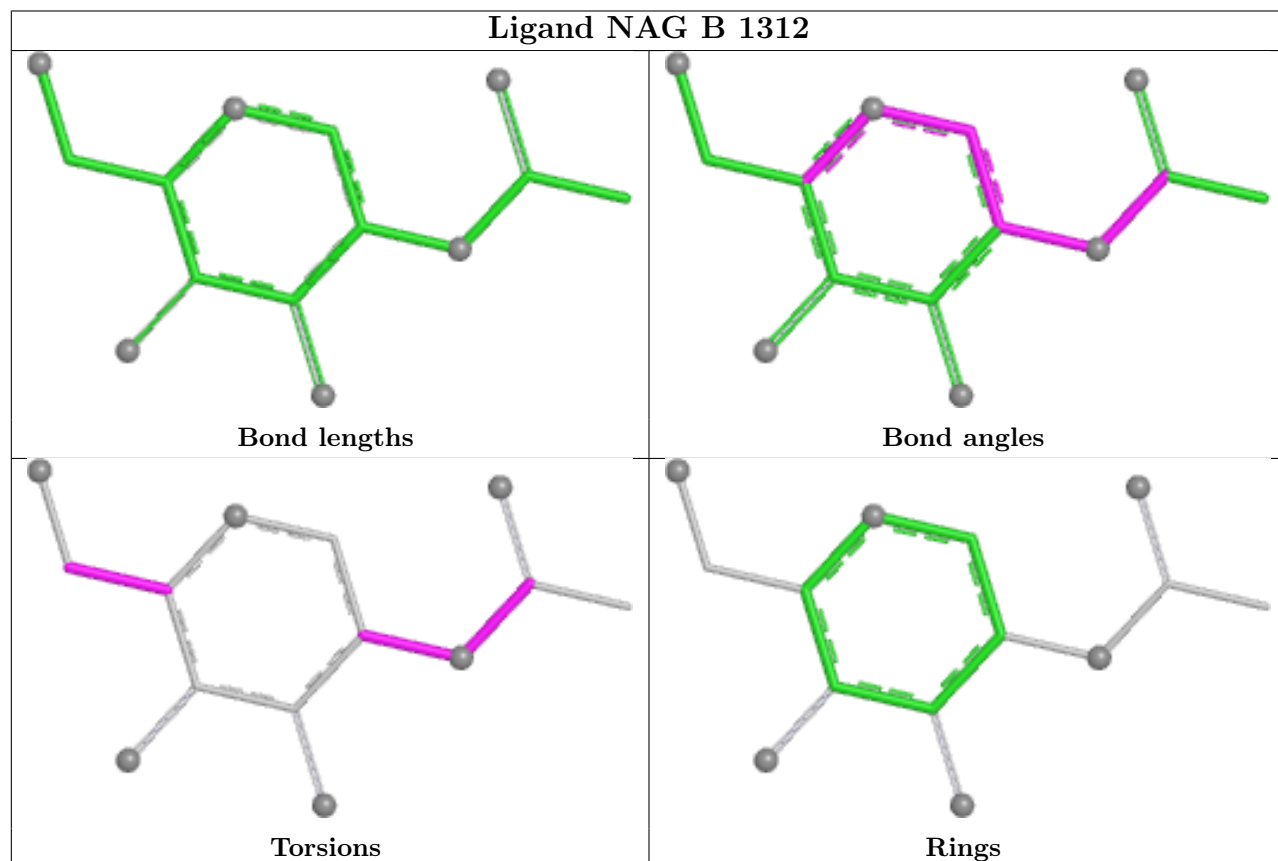
Ligand NAG B 1302



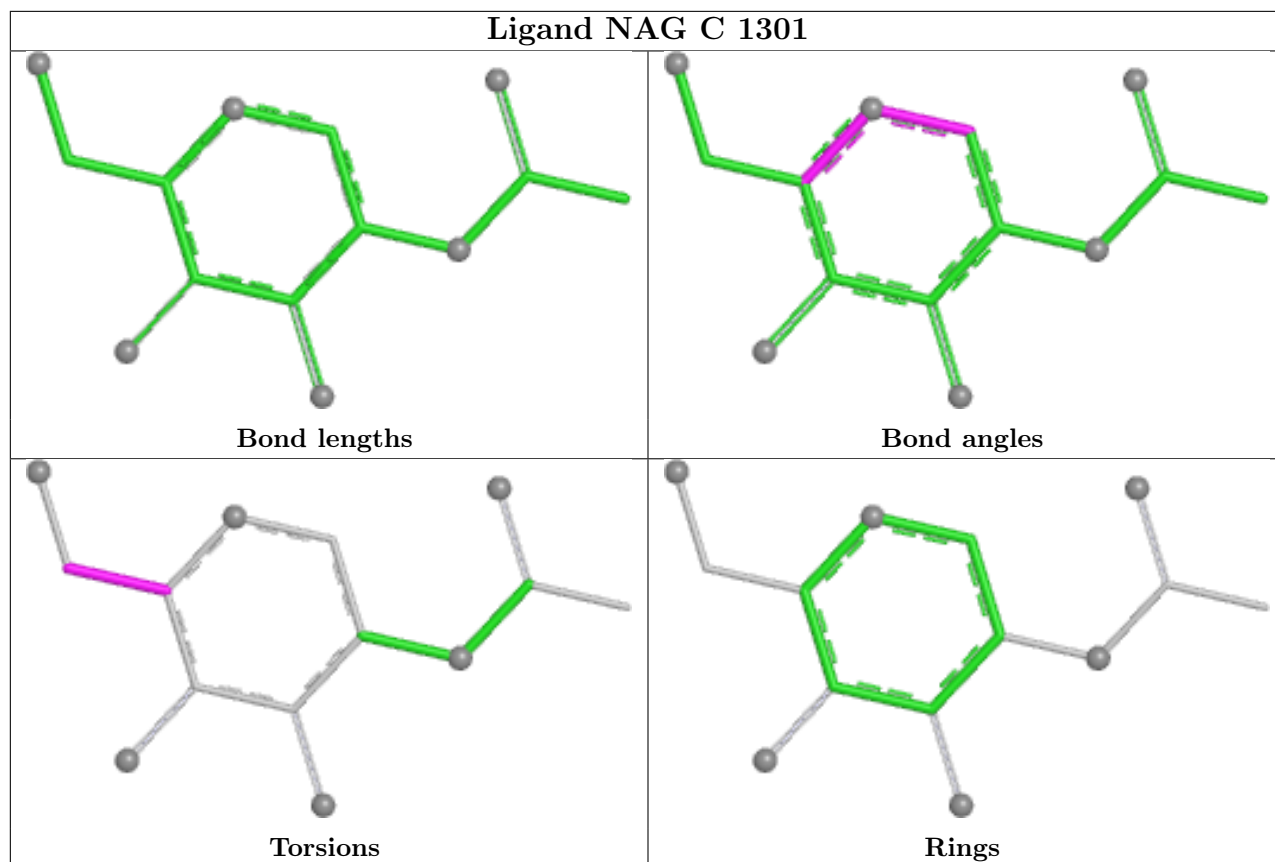
Ligand NAG B 1303



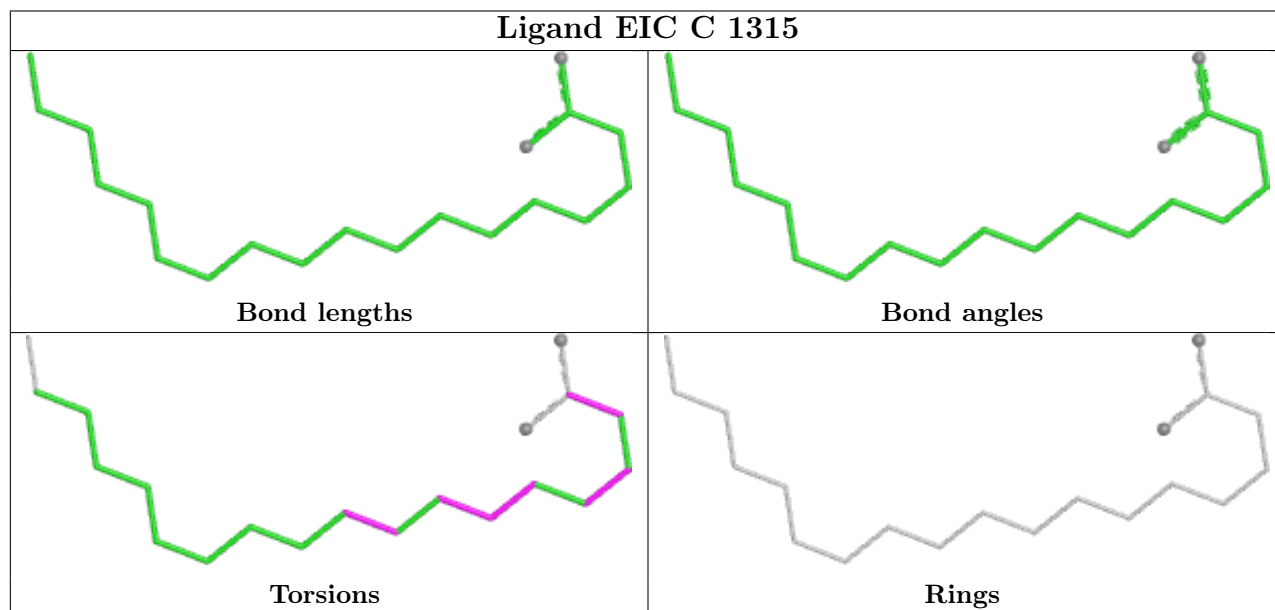
Ligand NAG B 1312

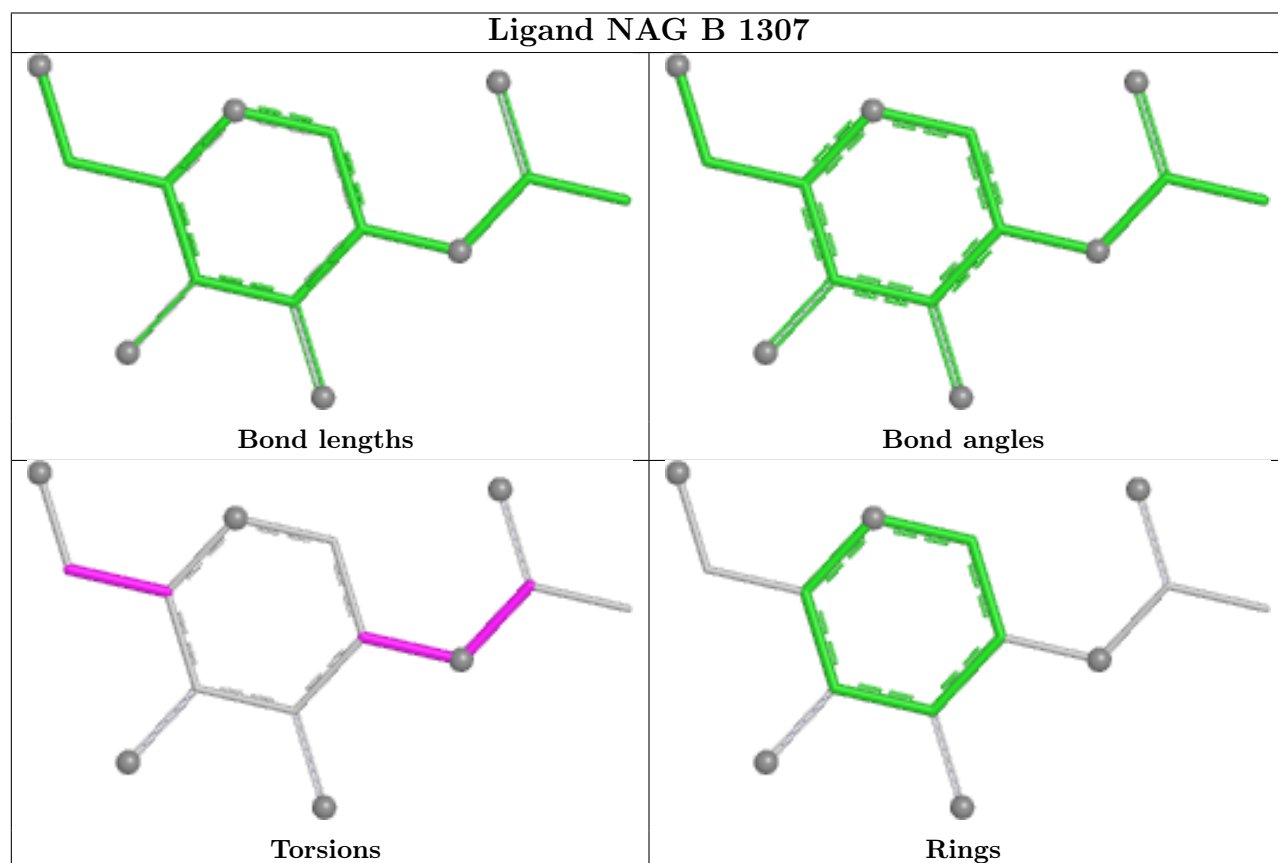
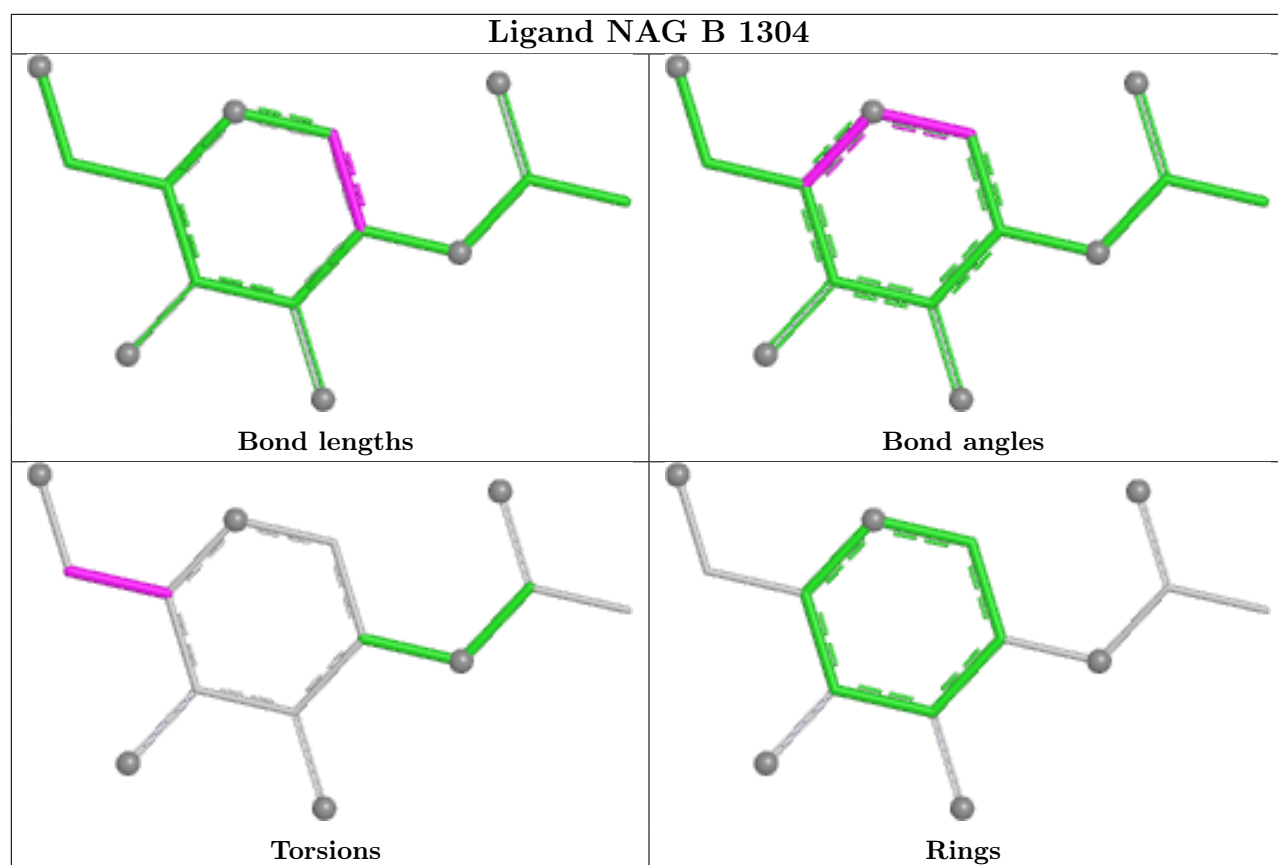


Ligand NAG C 1301

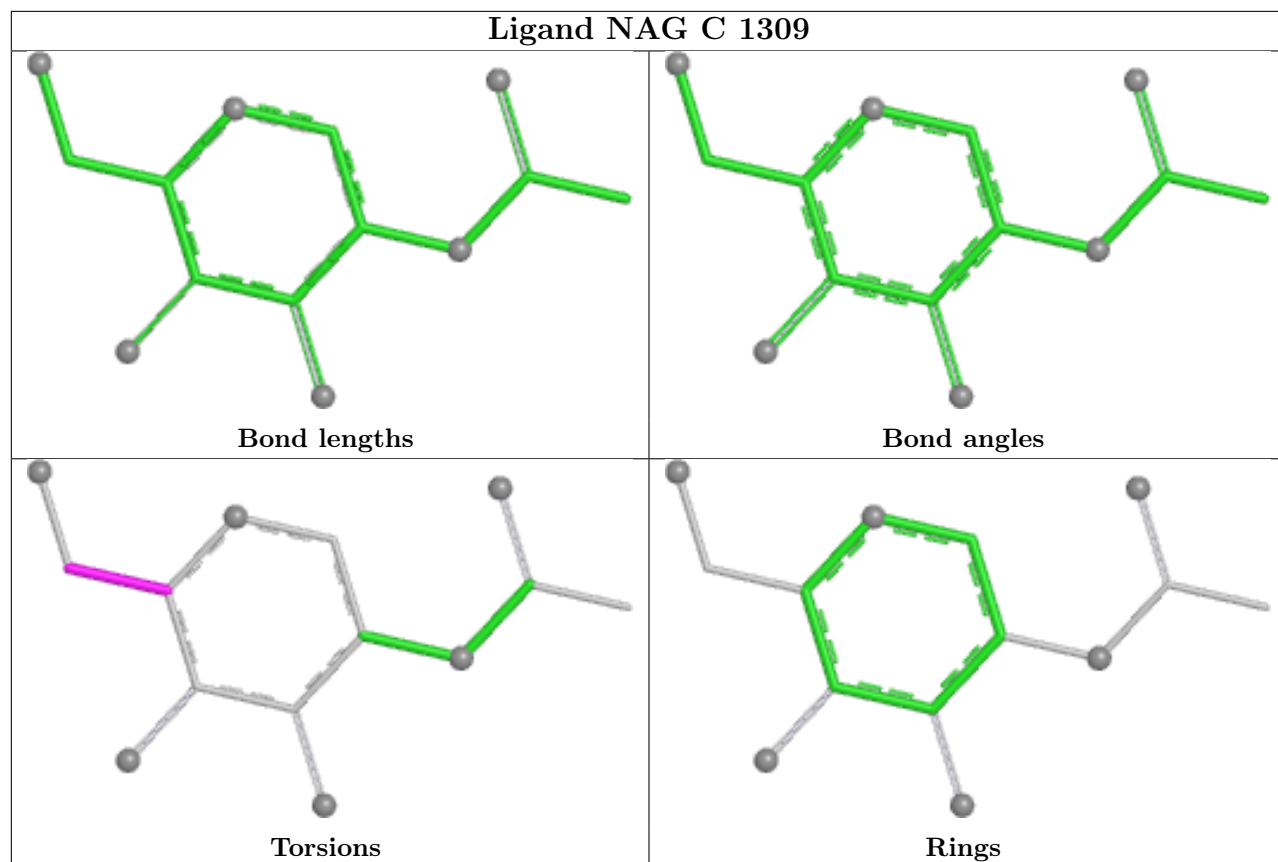


Ligand EIC C 1315

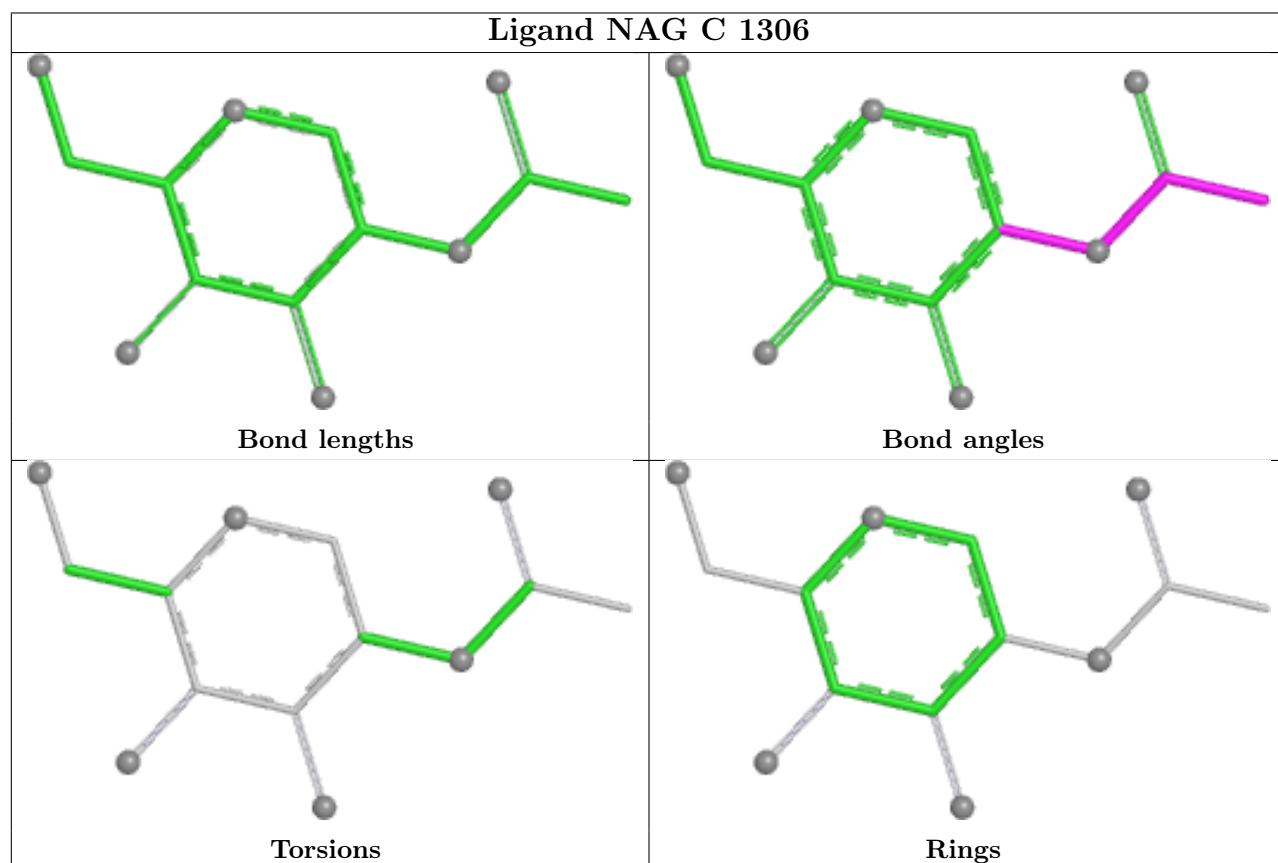




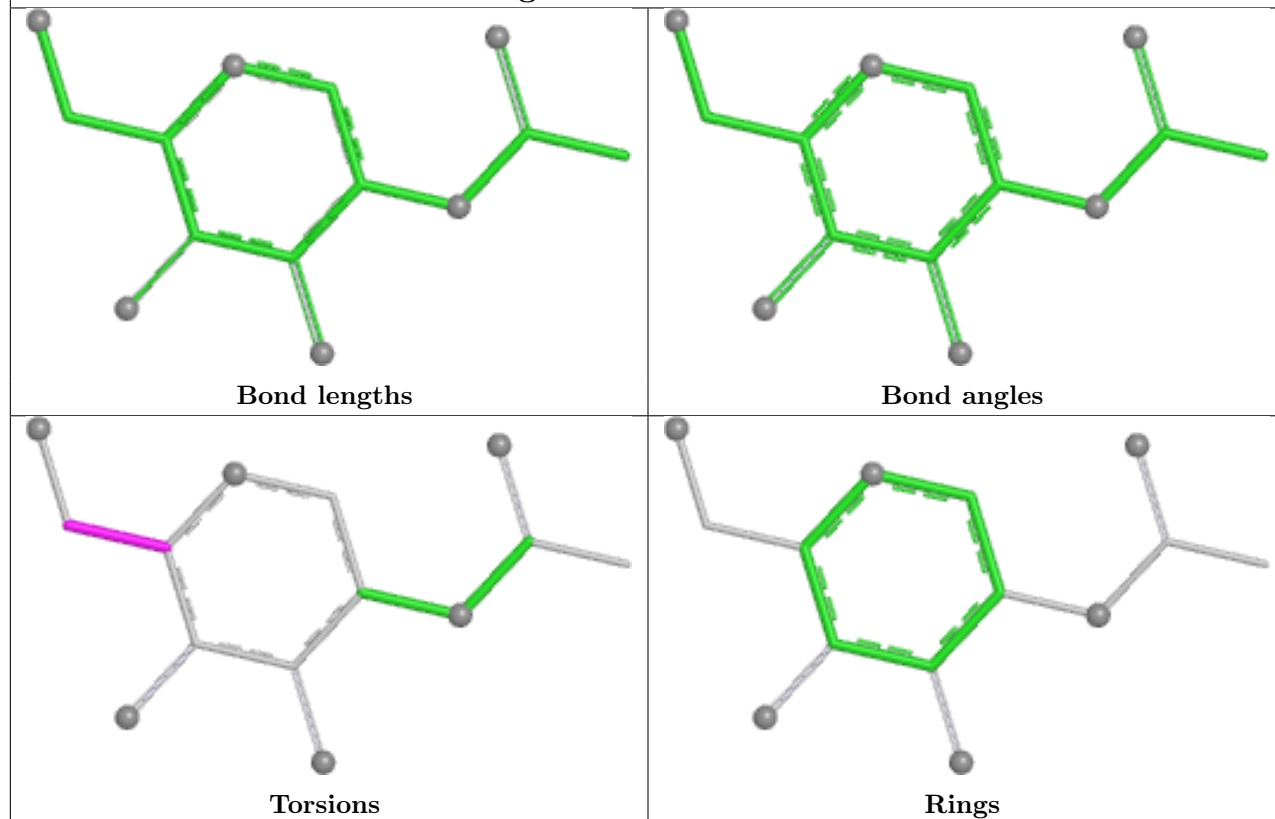
Ligand NAG C 1309



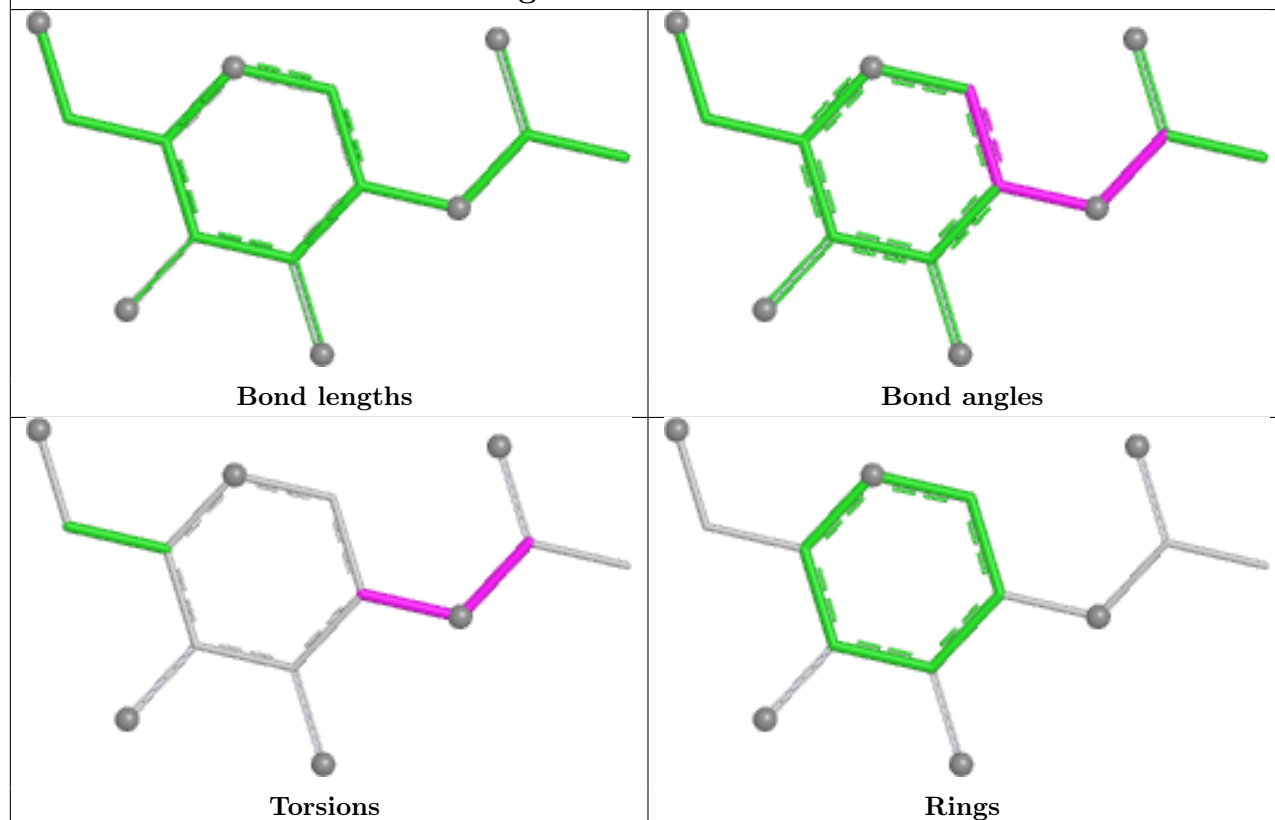
Ligand NAG C 1306



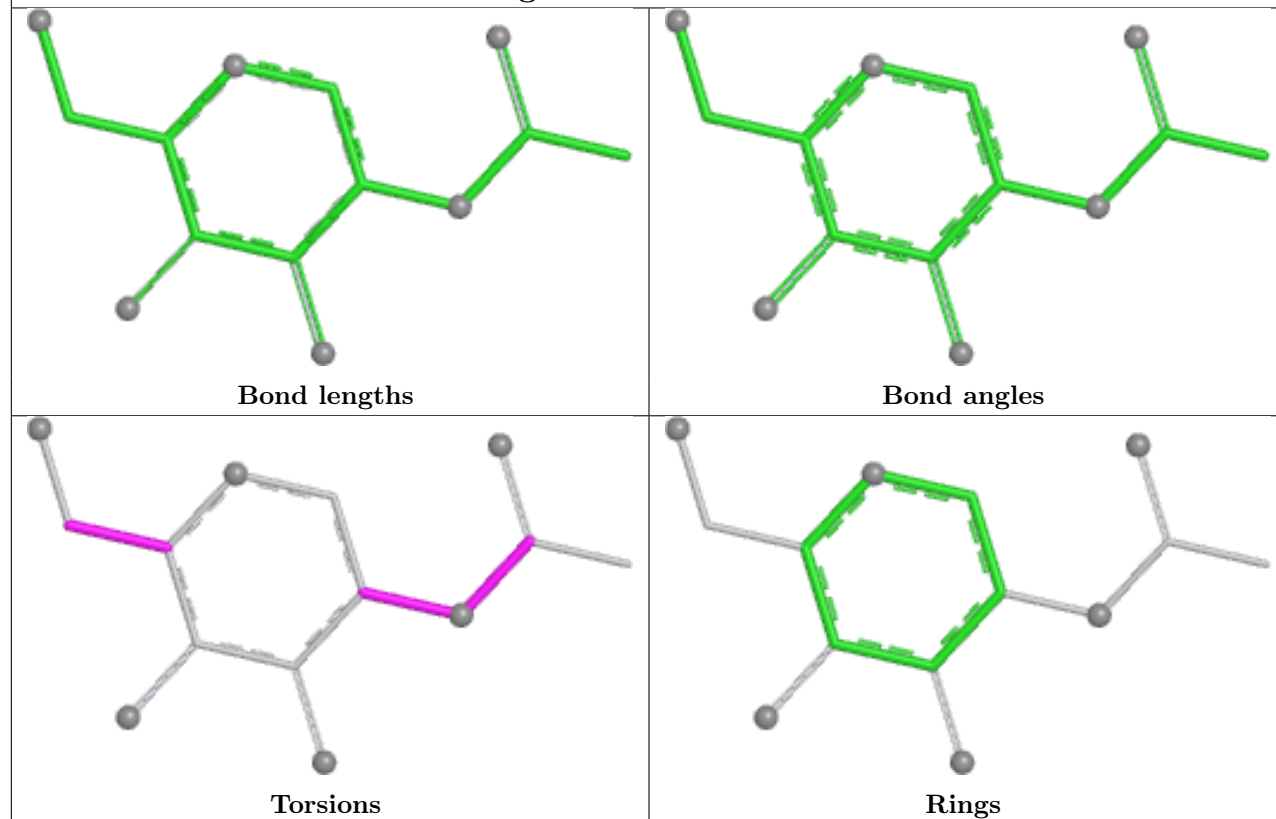
Ligand NAG B 1308



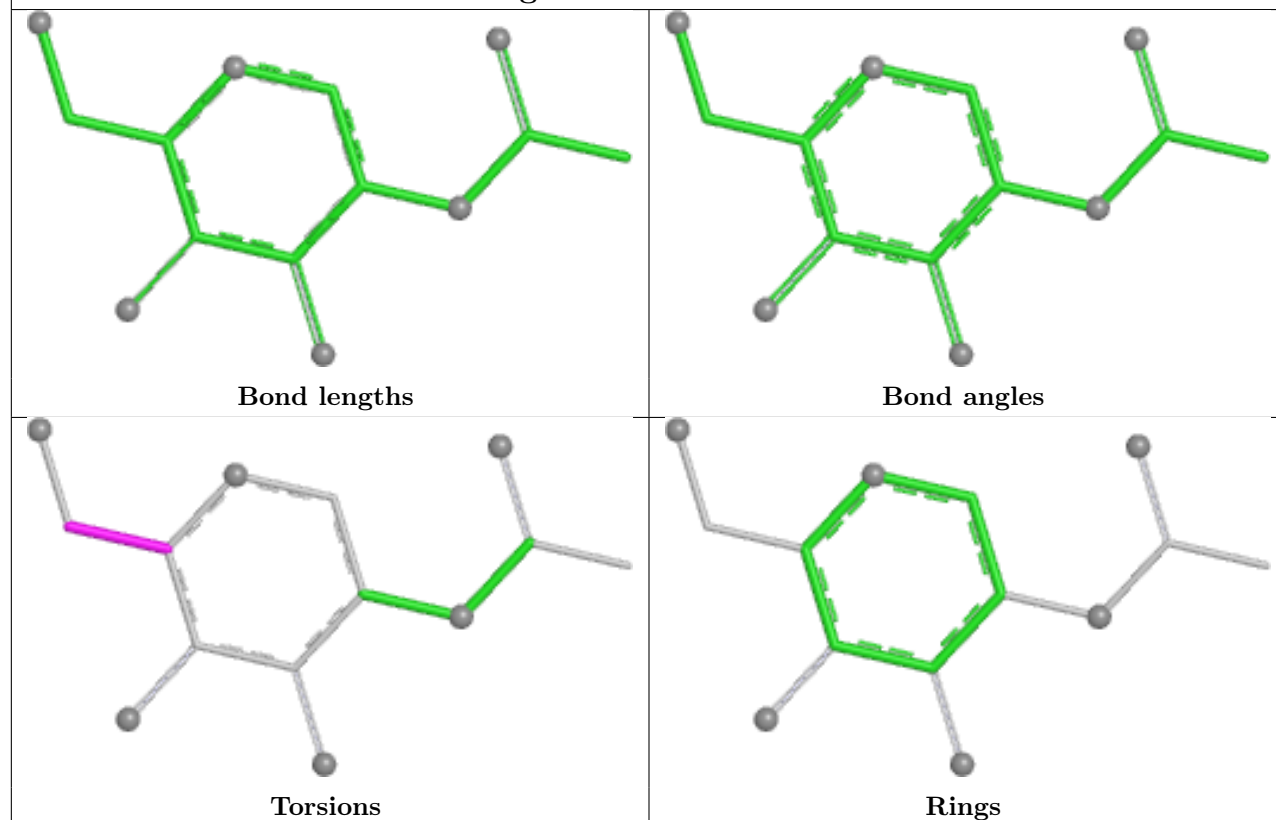
Ligand NAG B 1310



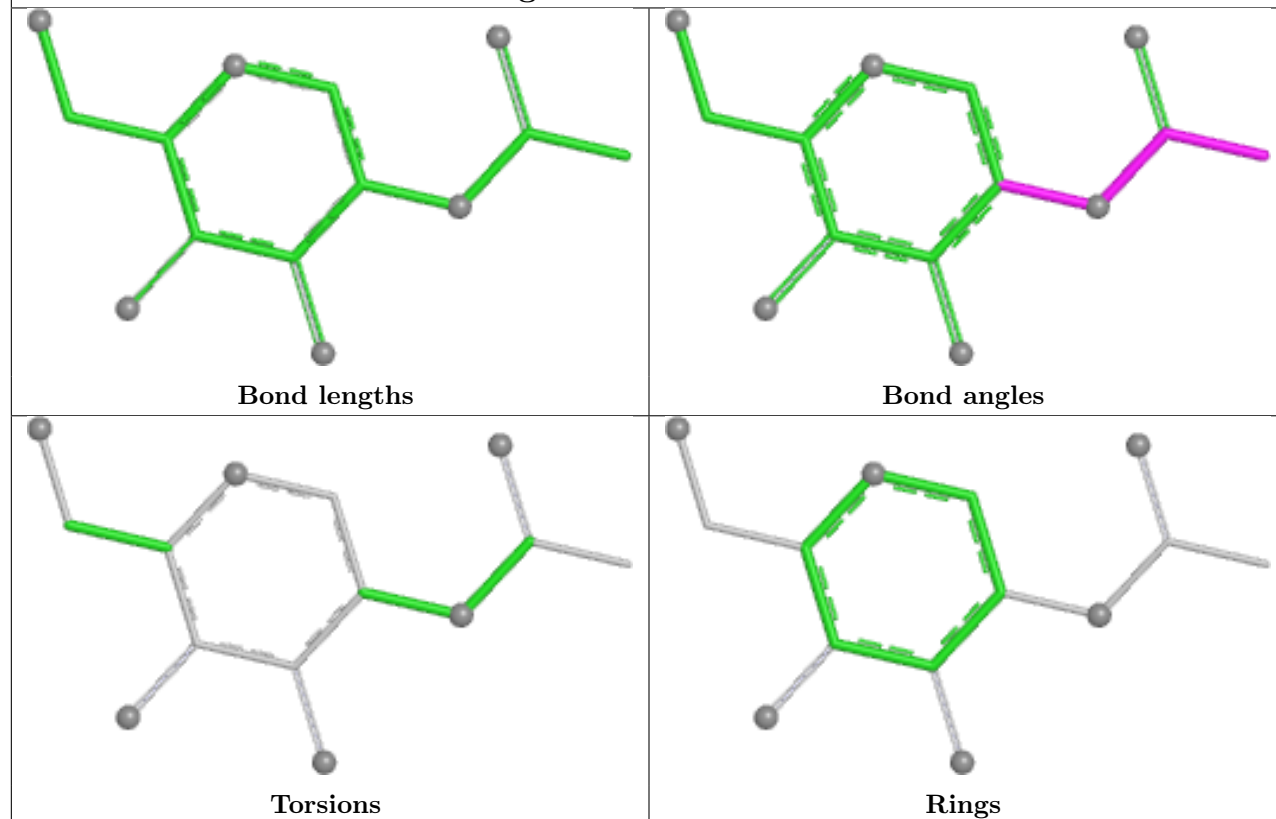
Ligand NAG A 1305



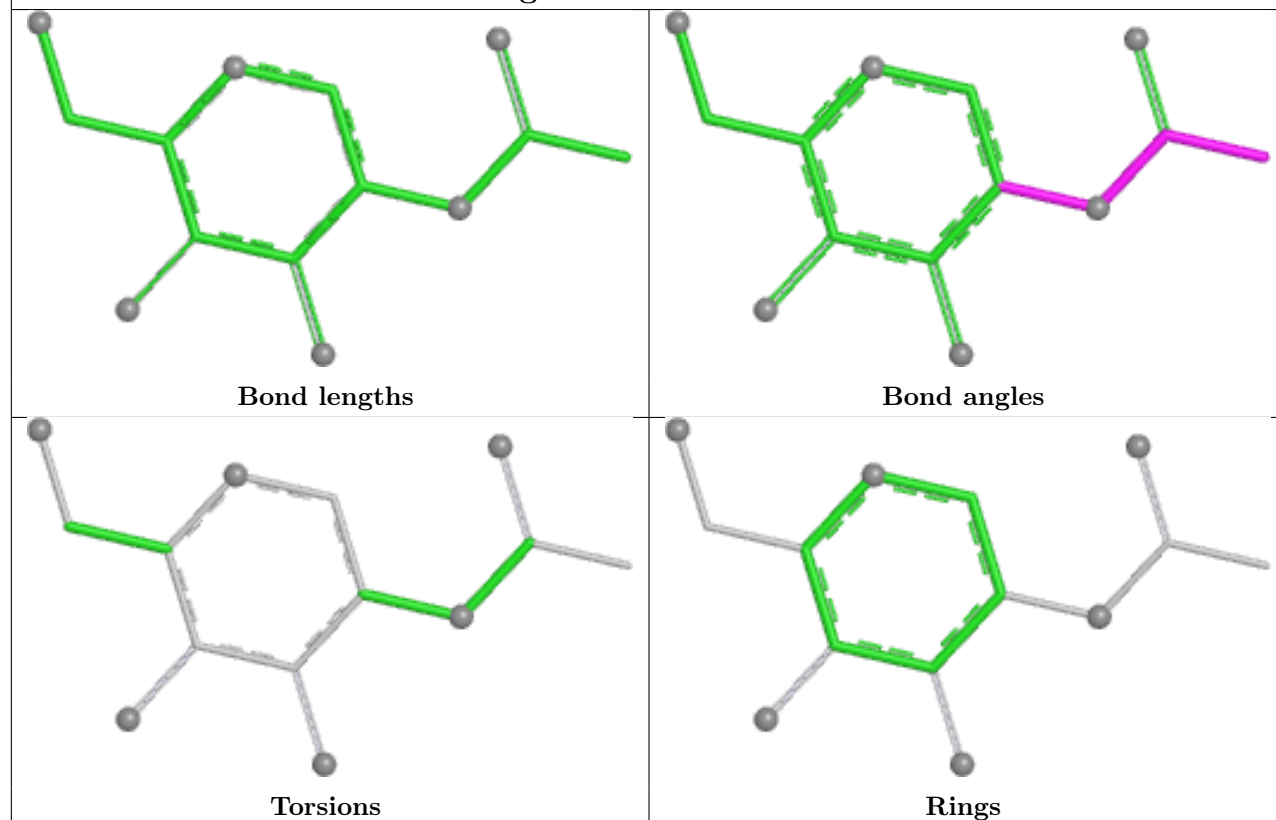
Ligand NAG B 1309



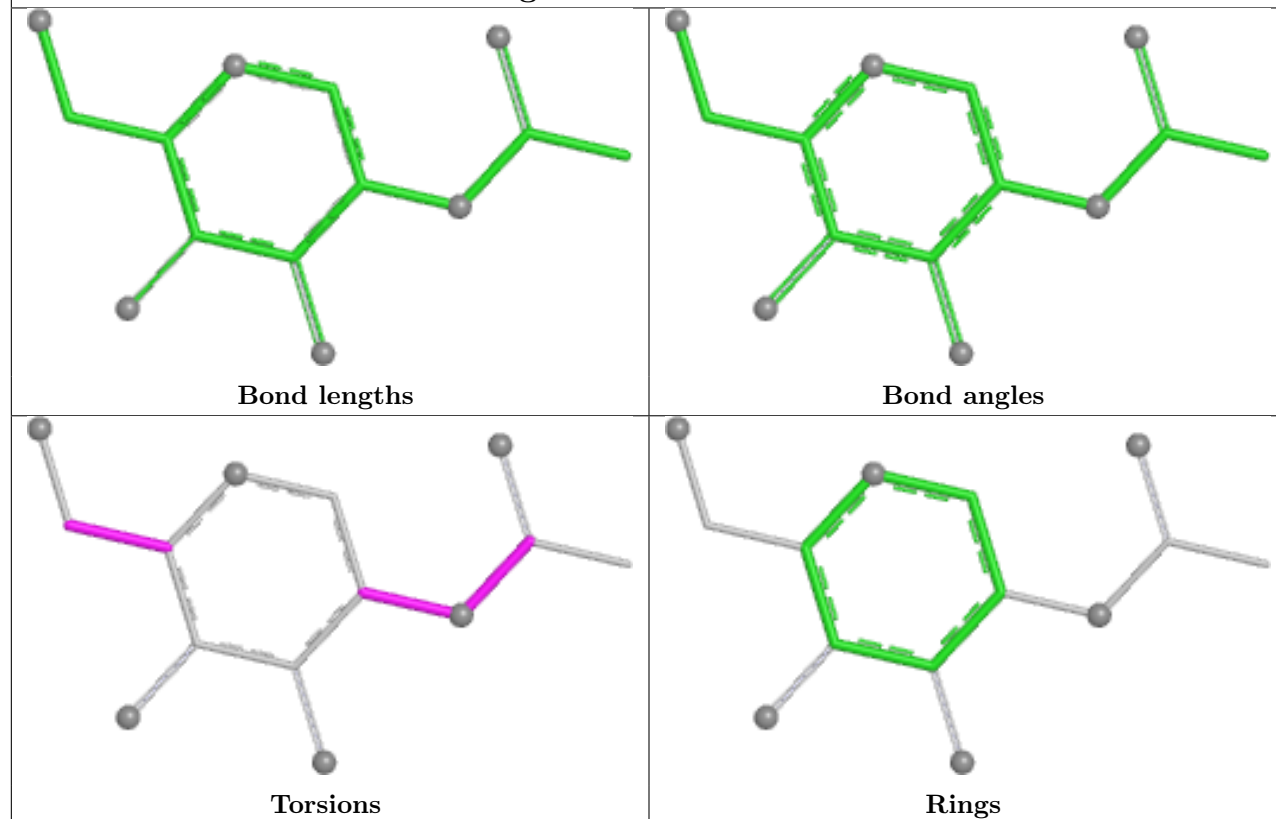
Ligand NAG A 1304



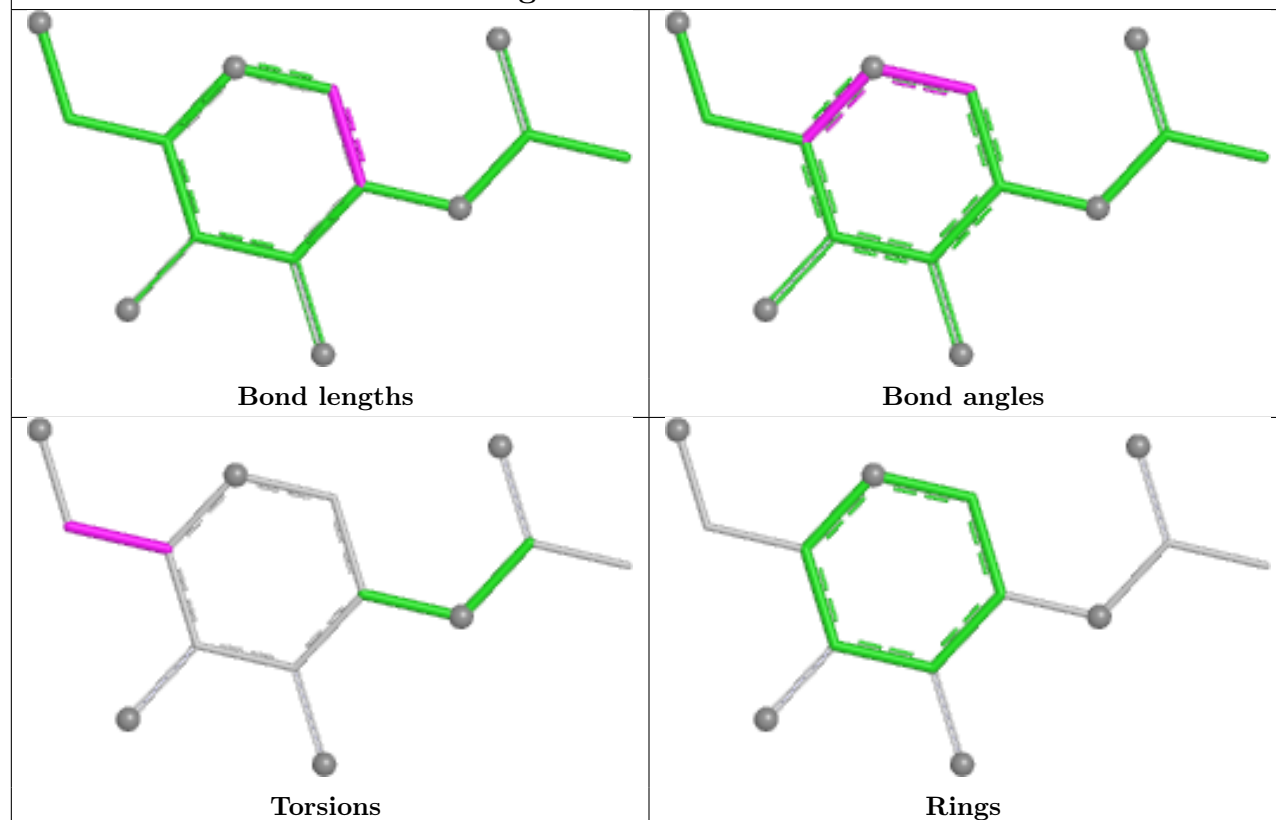
Ligand NAG B 1306



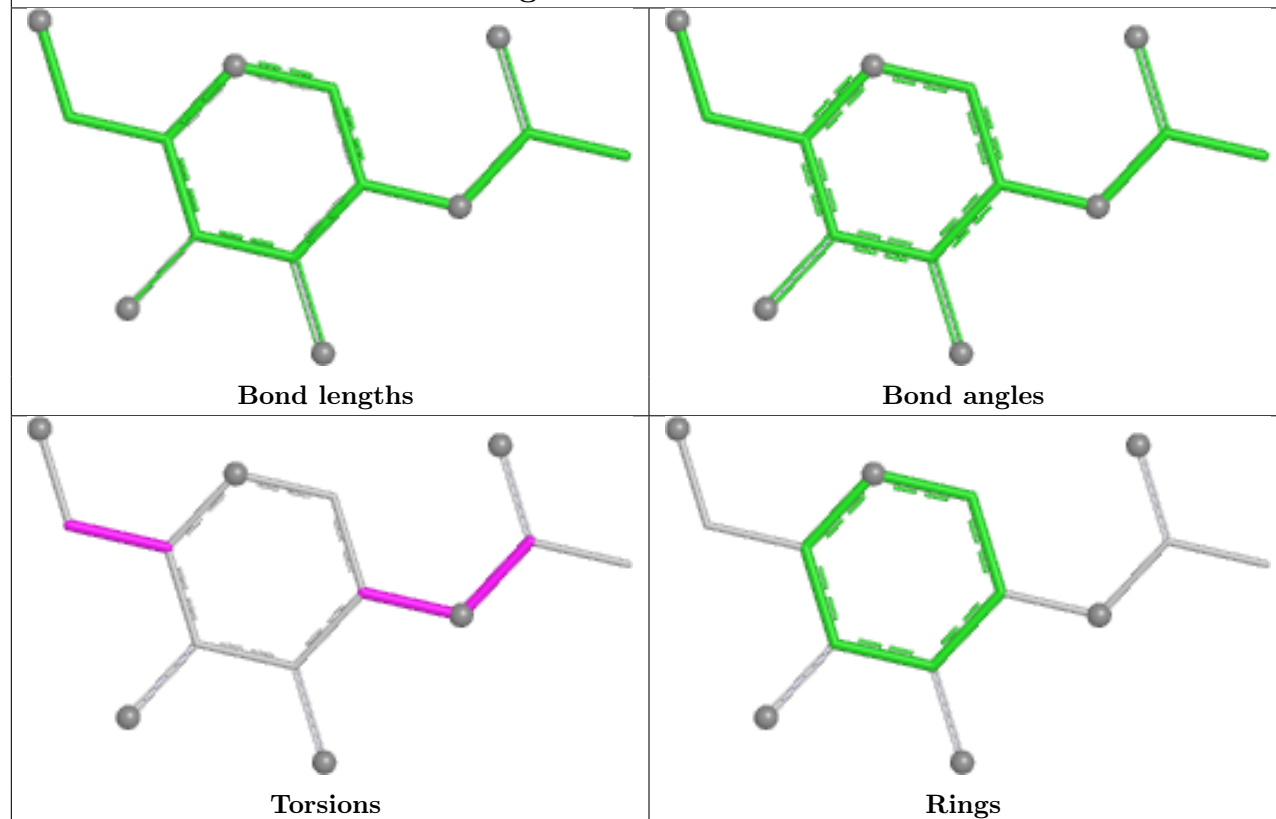
Ligand NAG C 1307



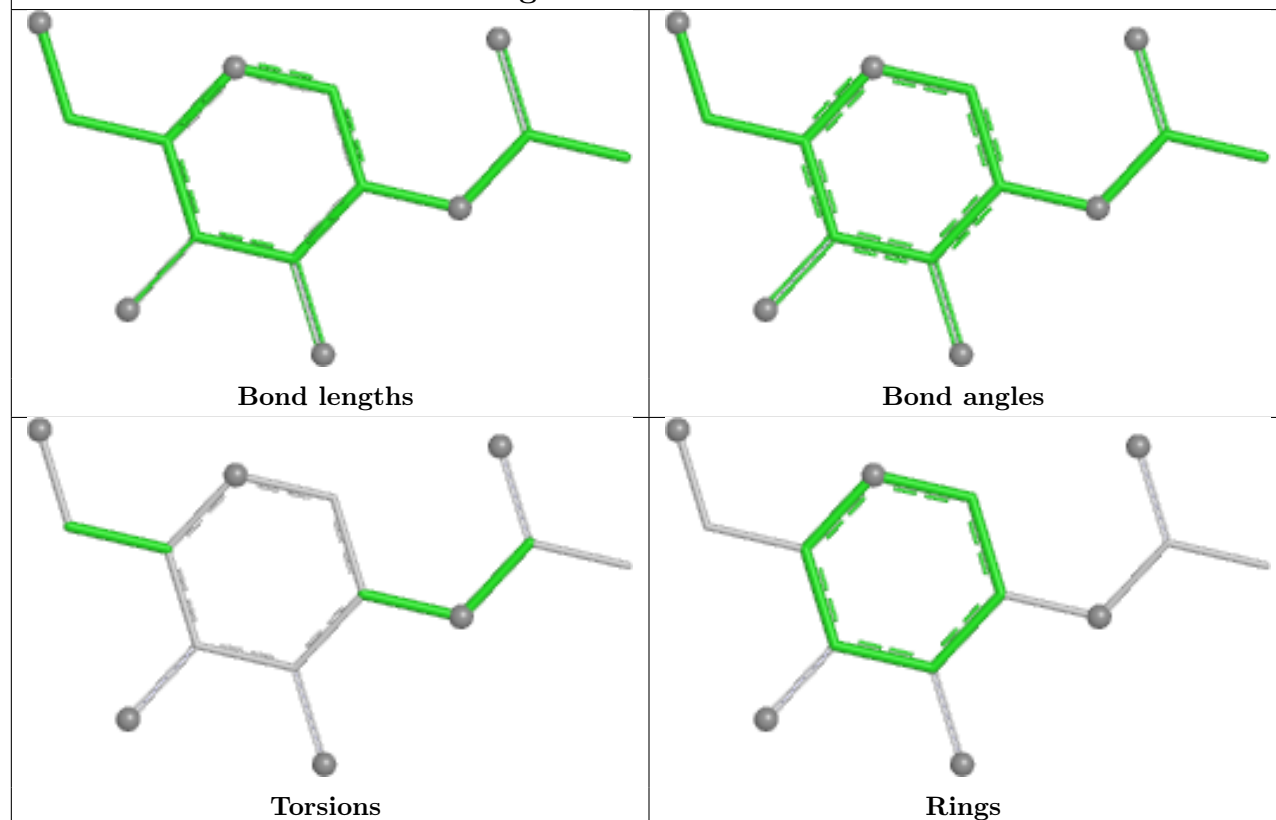
Ligand NAG A 1302



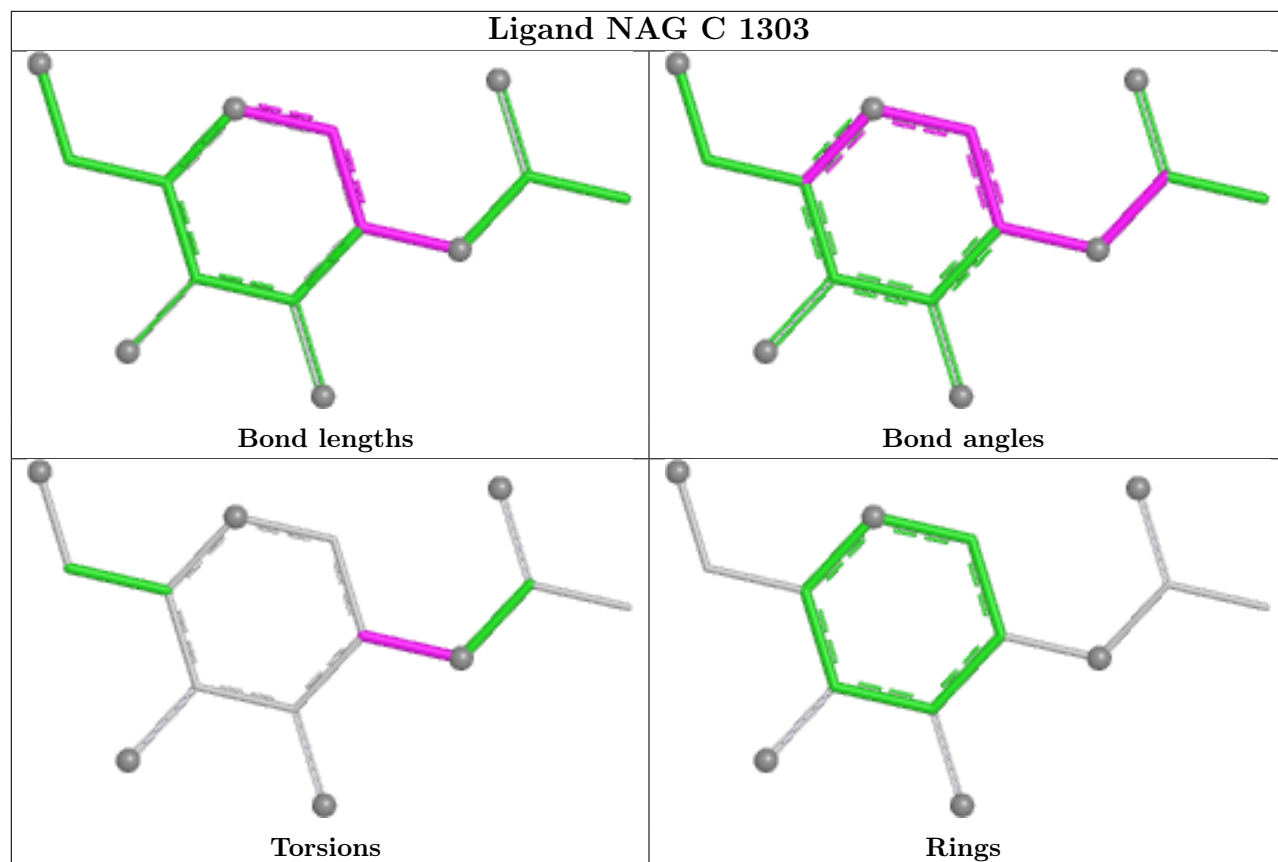
Ligand NAG C 1305



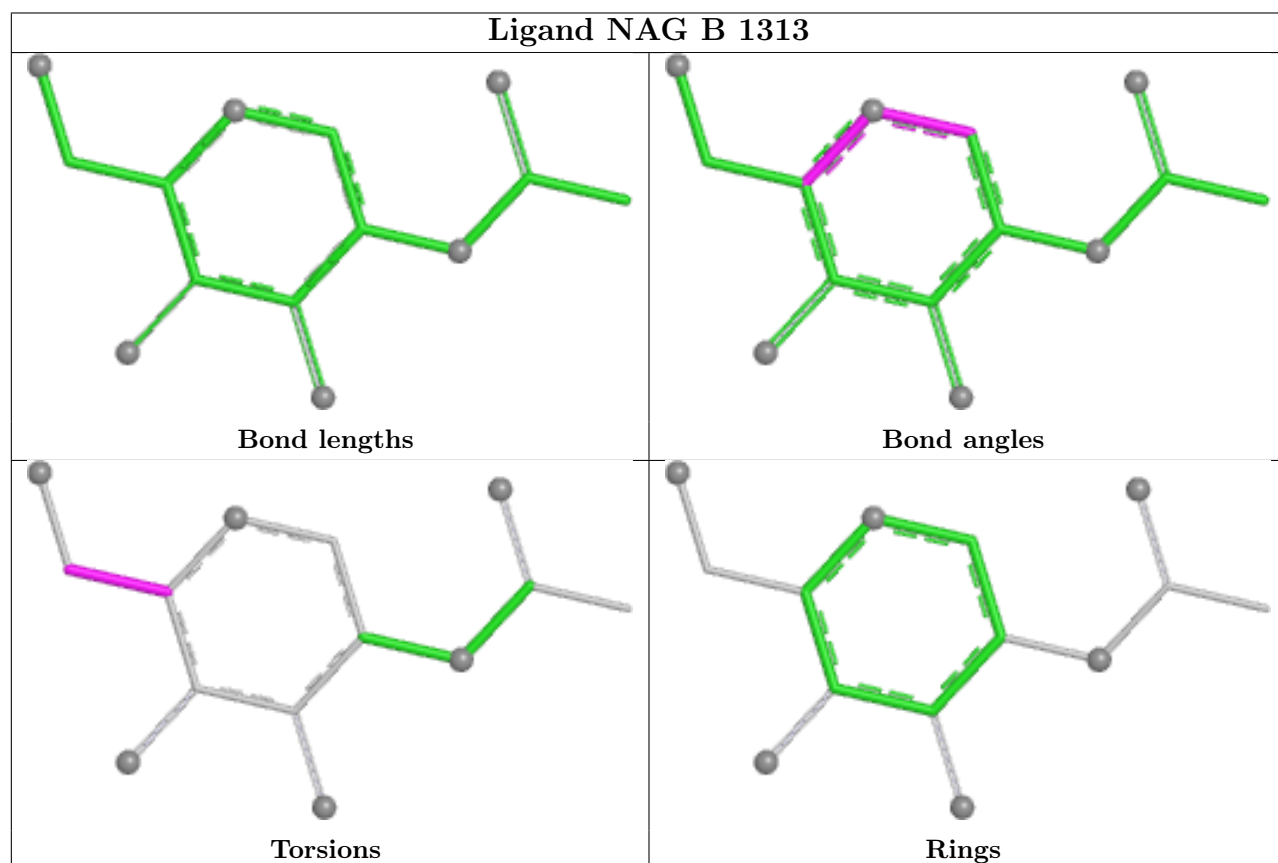
Ligand NAG C 1314



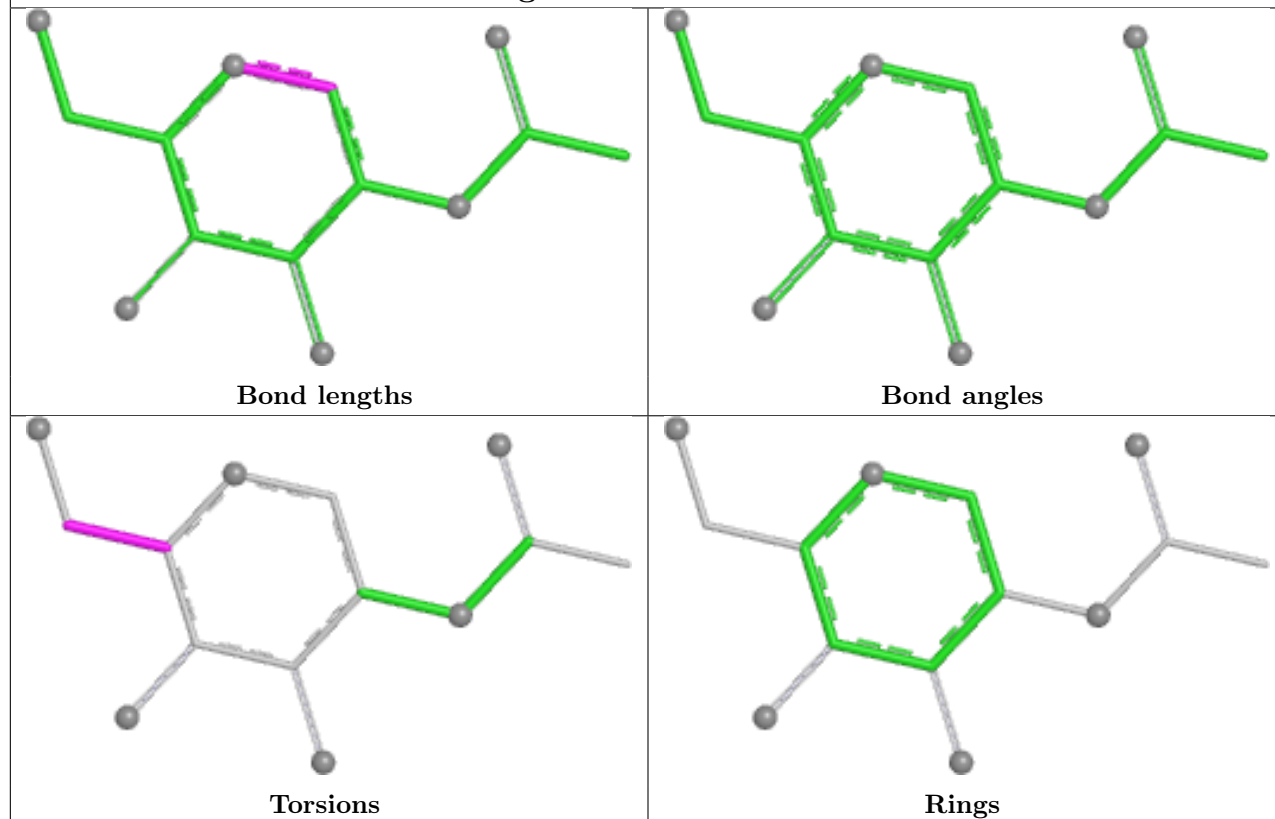
Ligand NAG C 1303



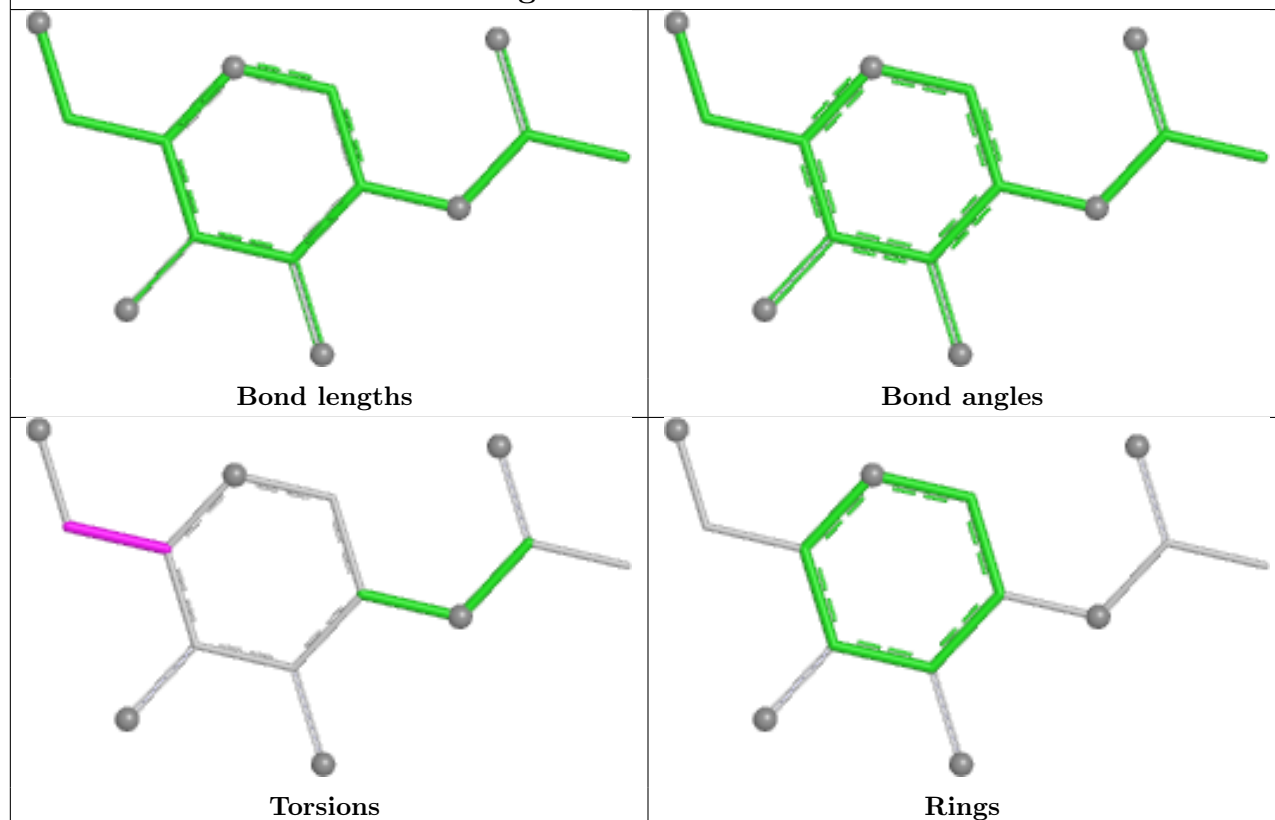
Ligand NAG B 1313



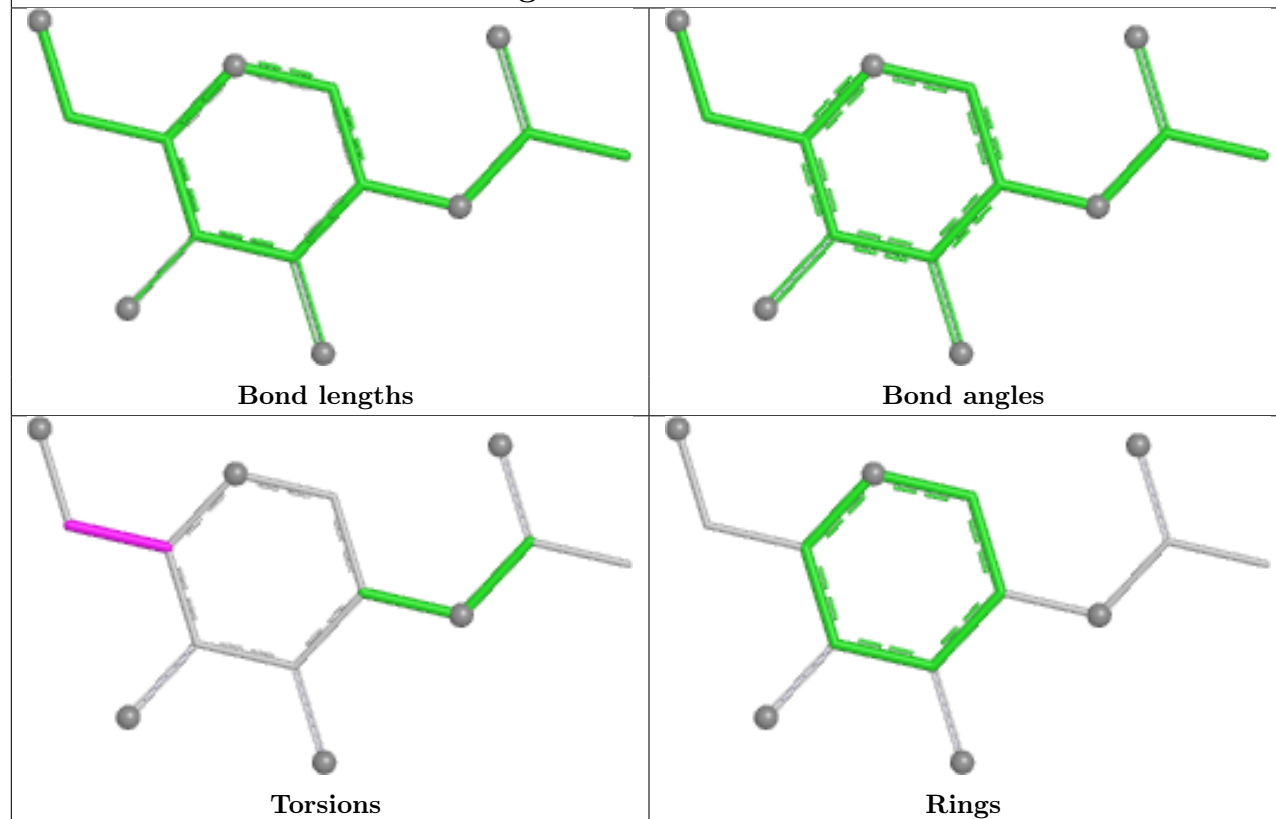
Ligand NAG C 1302



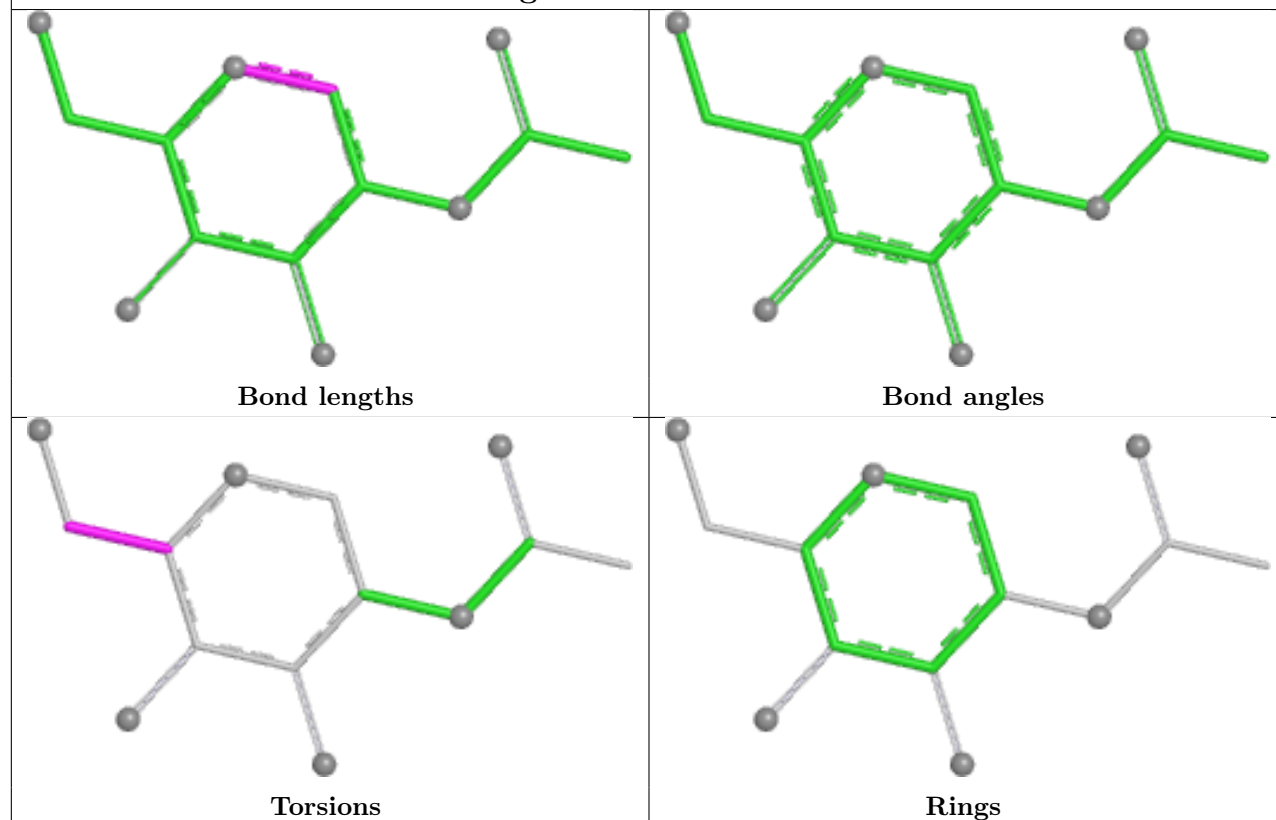
Ligand NAG C 1308

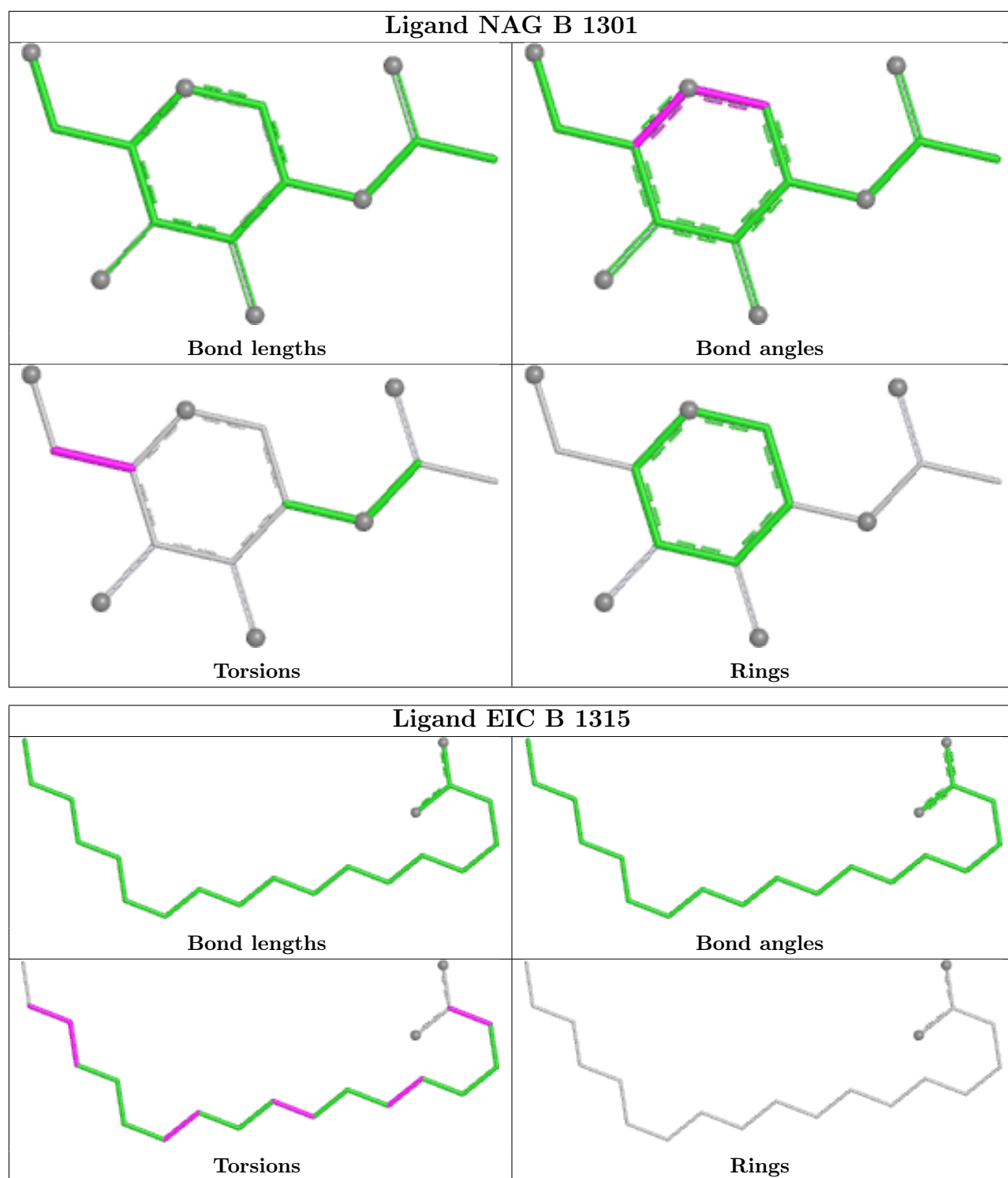


Ligand NAG A 1306



Ligand NAG B 1311





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

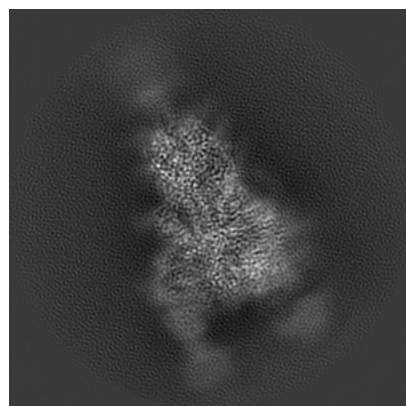
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-34872. These allow visual inspection of the internal detail of the map and identification of artifacts.

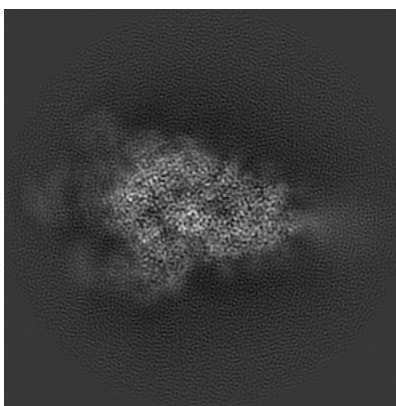
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

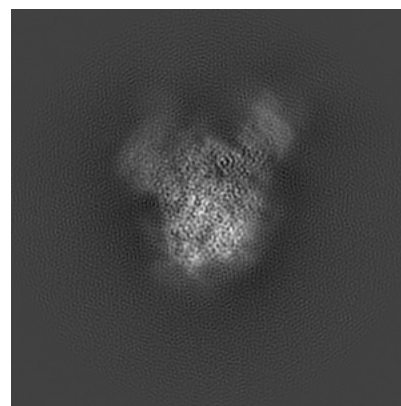
6.1.1 Primary map



X

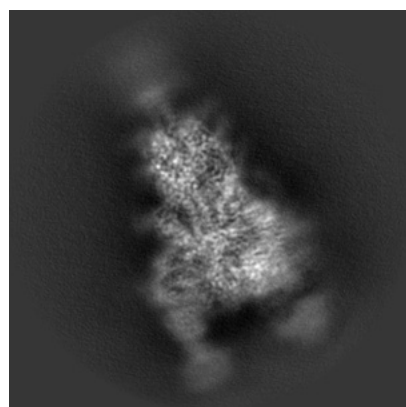


Y

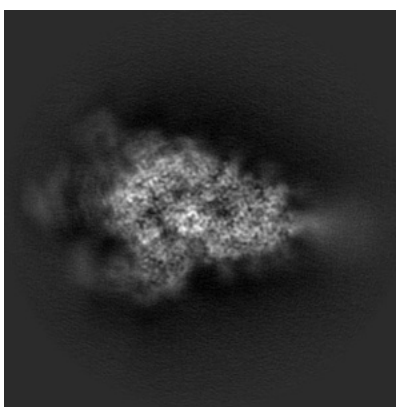


Z

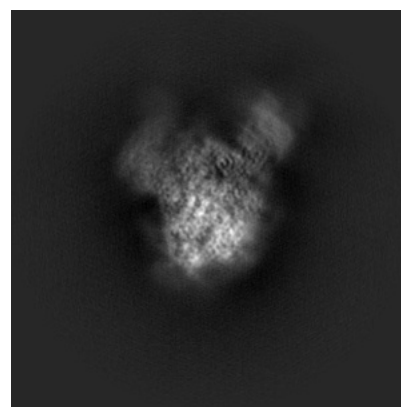
6.1.2 Raw map



X



Y

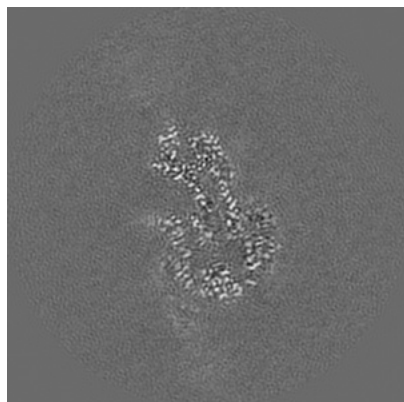


Z

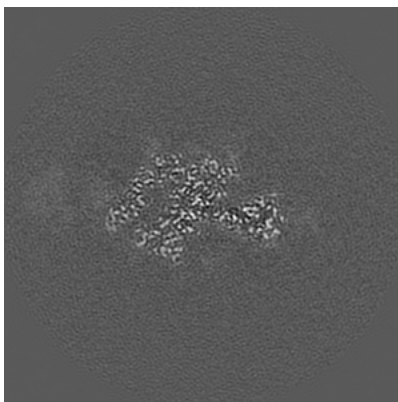
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

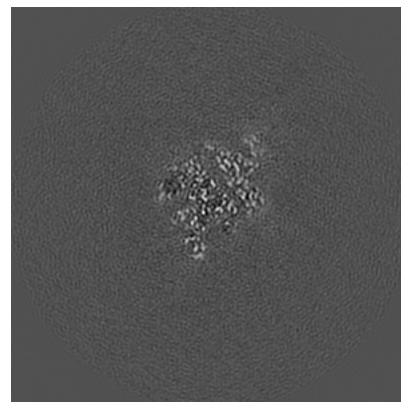
6.2.1 Primary map



X Index: 144

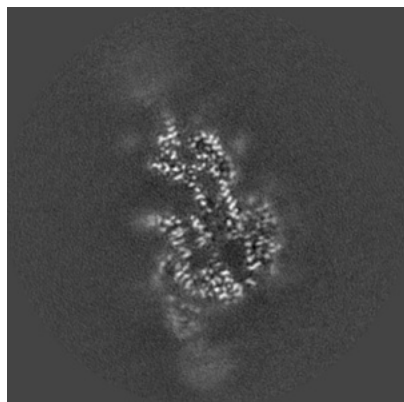


Y Index: 144

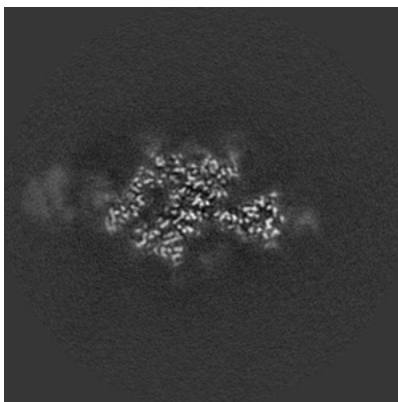


Z Index: 144

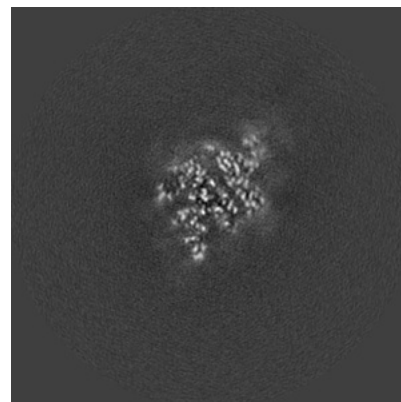
6.2.2 Raw map



X Index: 144



Y Index: 144

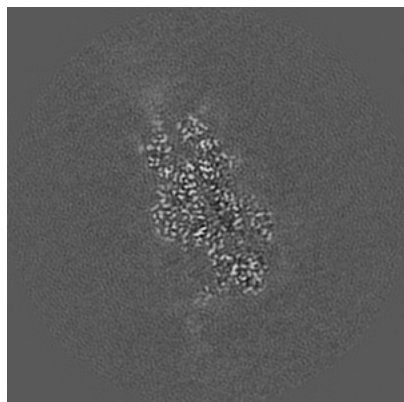


Z Index: 144

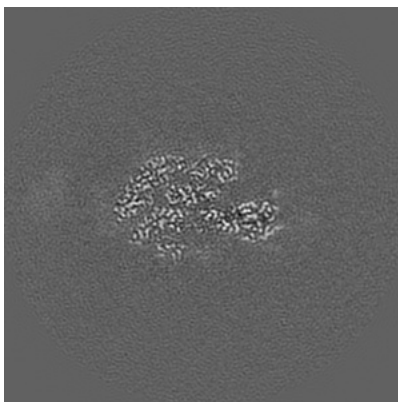
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

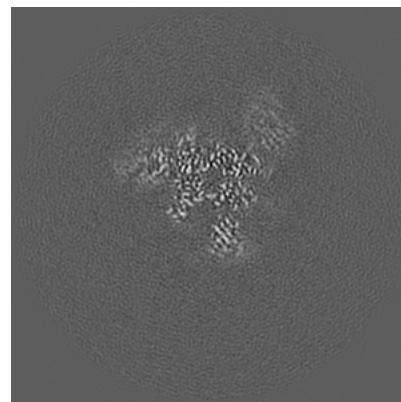
6.3.1 Primary map



X Index: 133

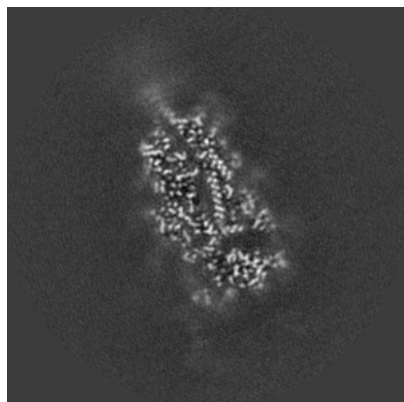


Y Index: 148

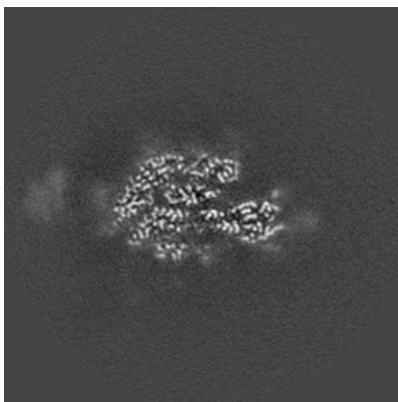


Z Index: 102

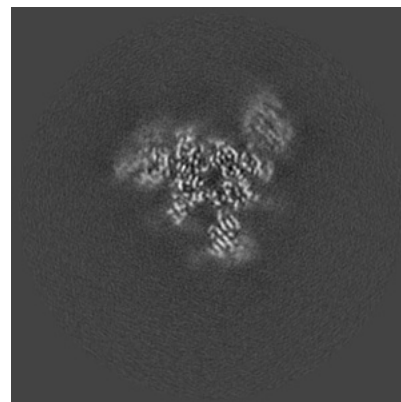
6.3.2 Raw map



X Index: 129



Y Index: 148

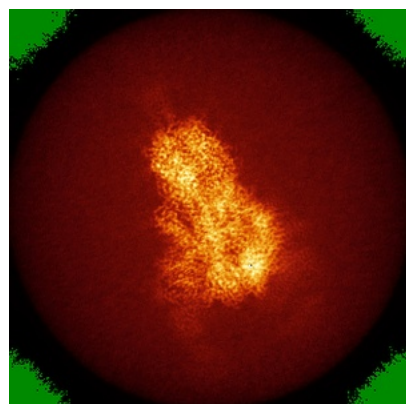


Z Index: 101

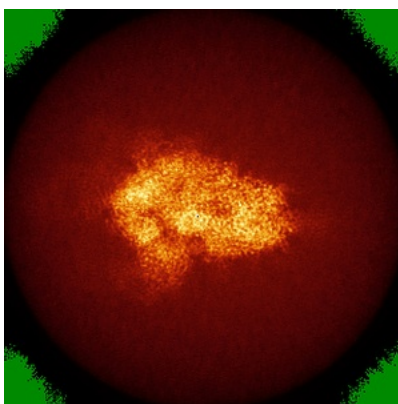
The images above show the largest variance slices of the map in three orthogonal directions.

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

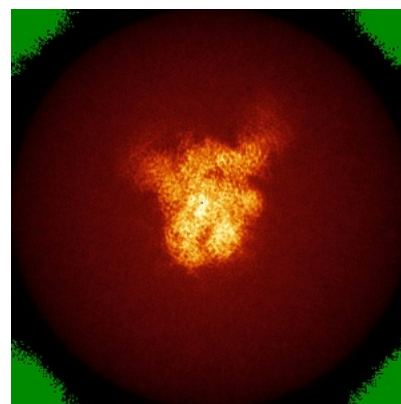
6.4.1 Primary map



X

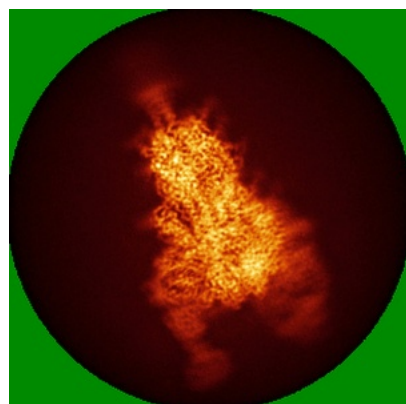


Y

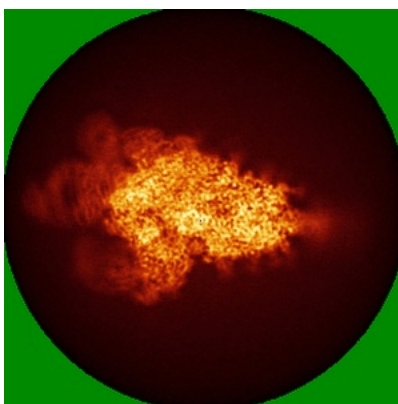


Z

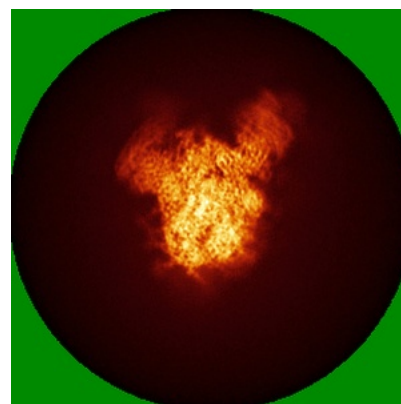
6.4.2 Raw map



X



Y

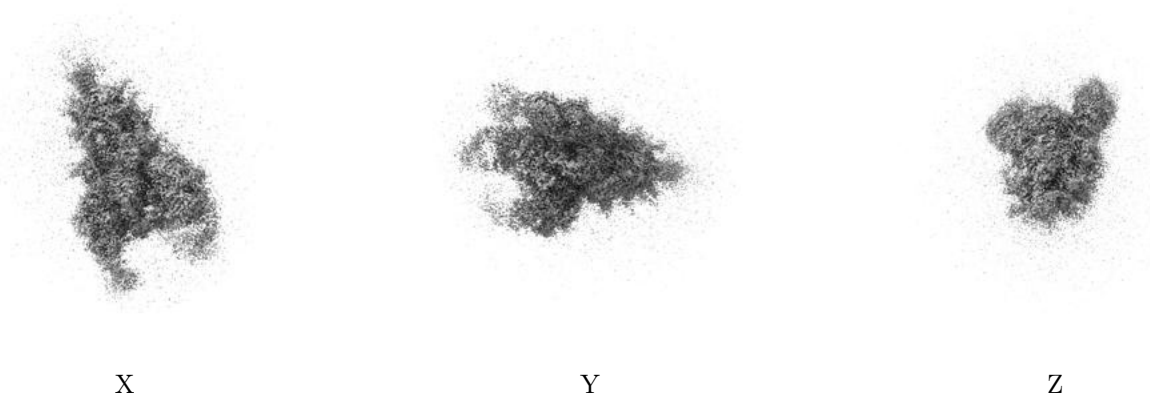


Z

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.

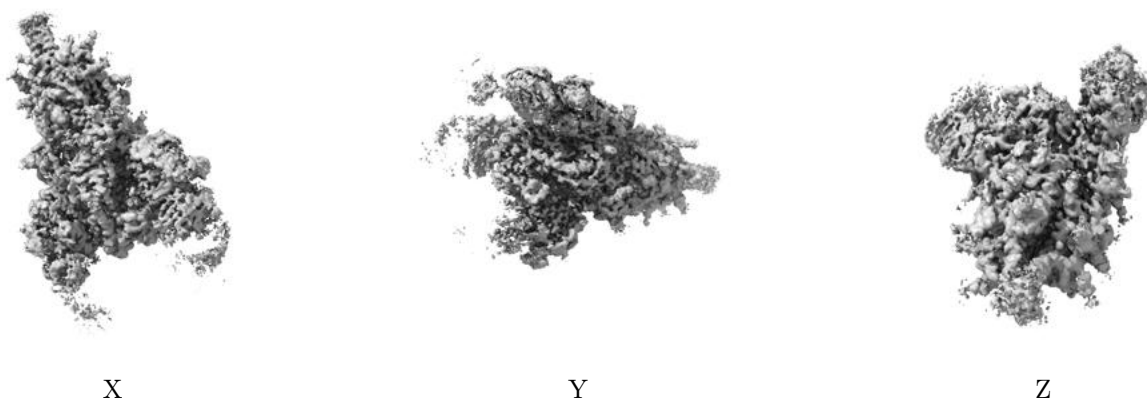
6.5 Orthogonal surface views [i](#)

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.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

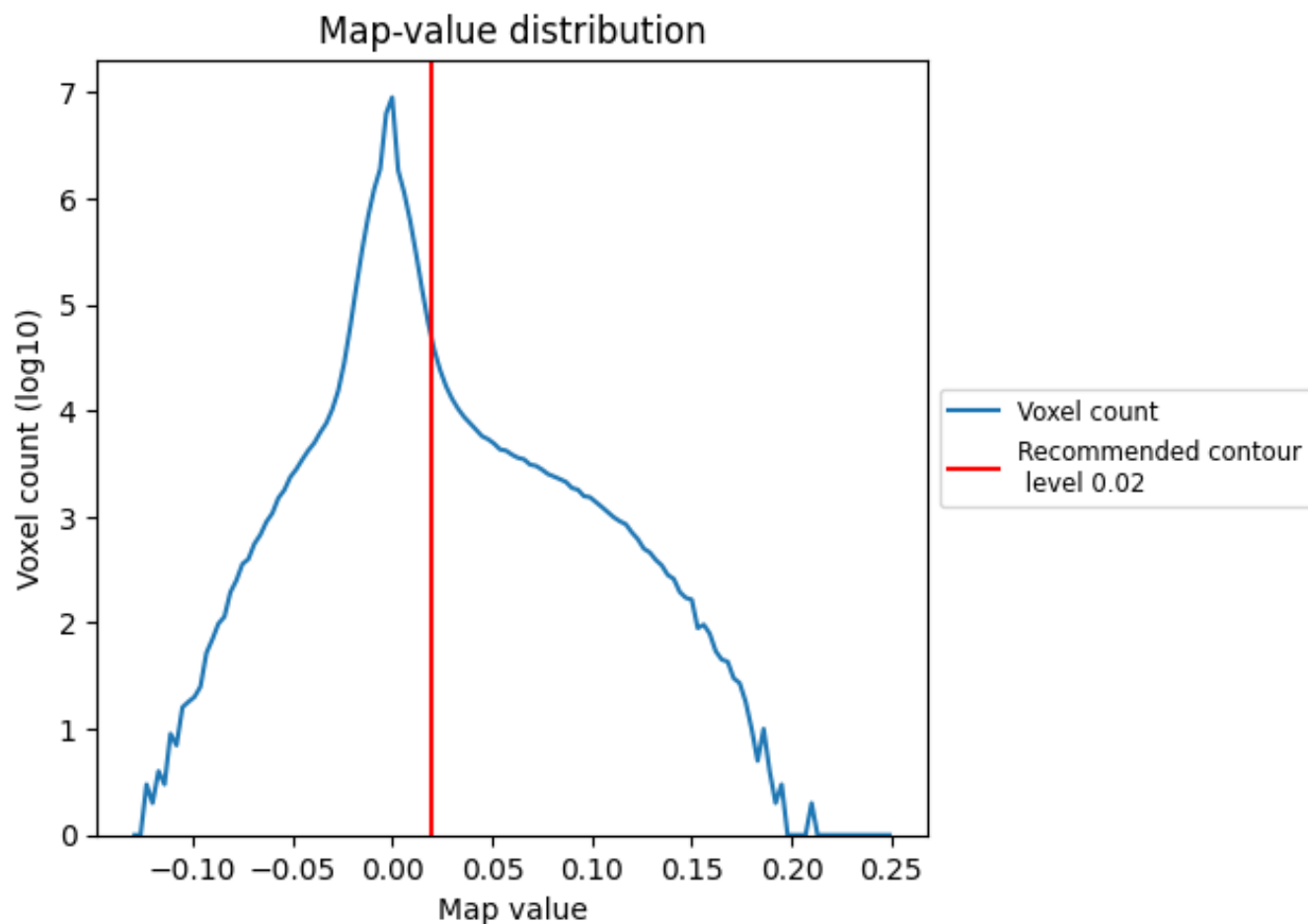
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

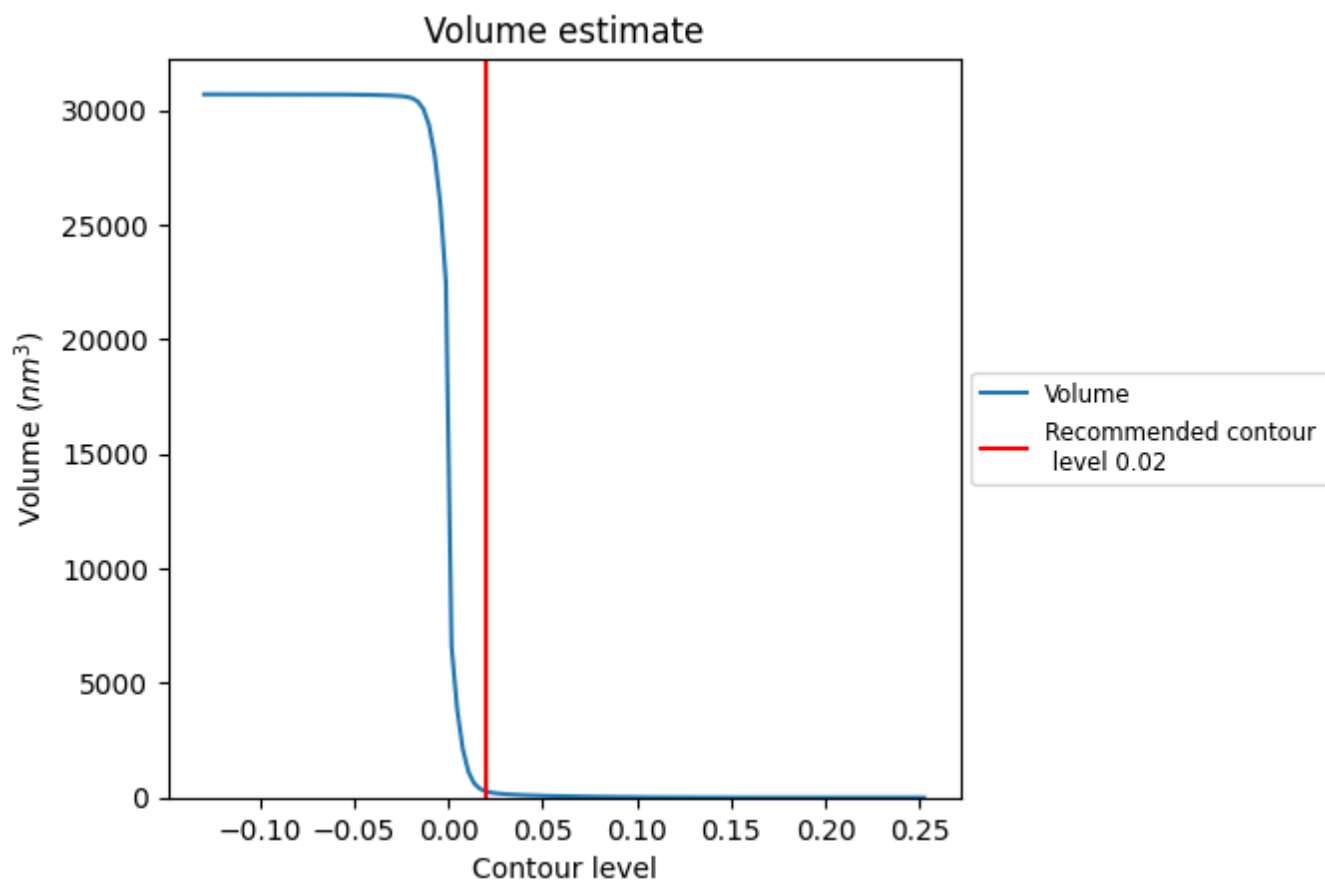
This section contains the results of statistical analysis of the map.

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.

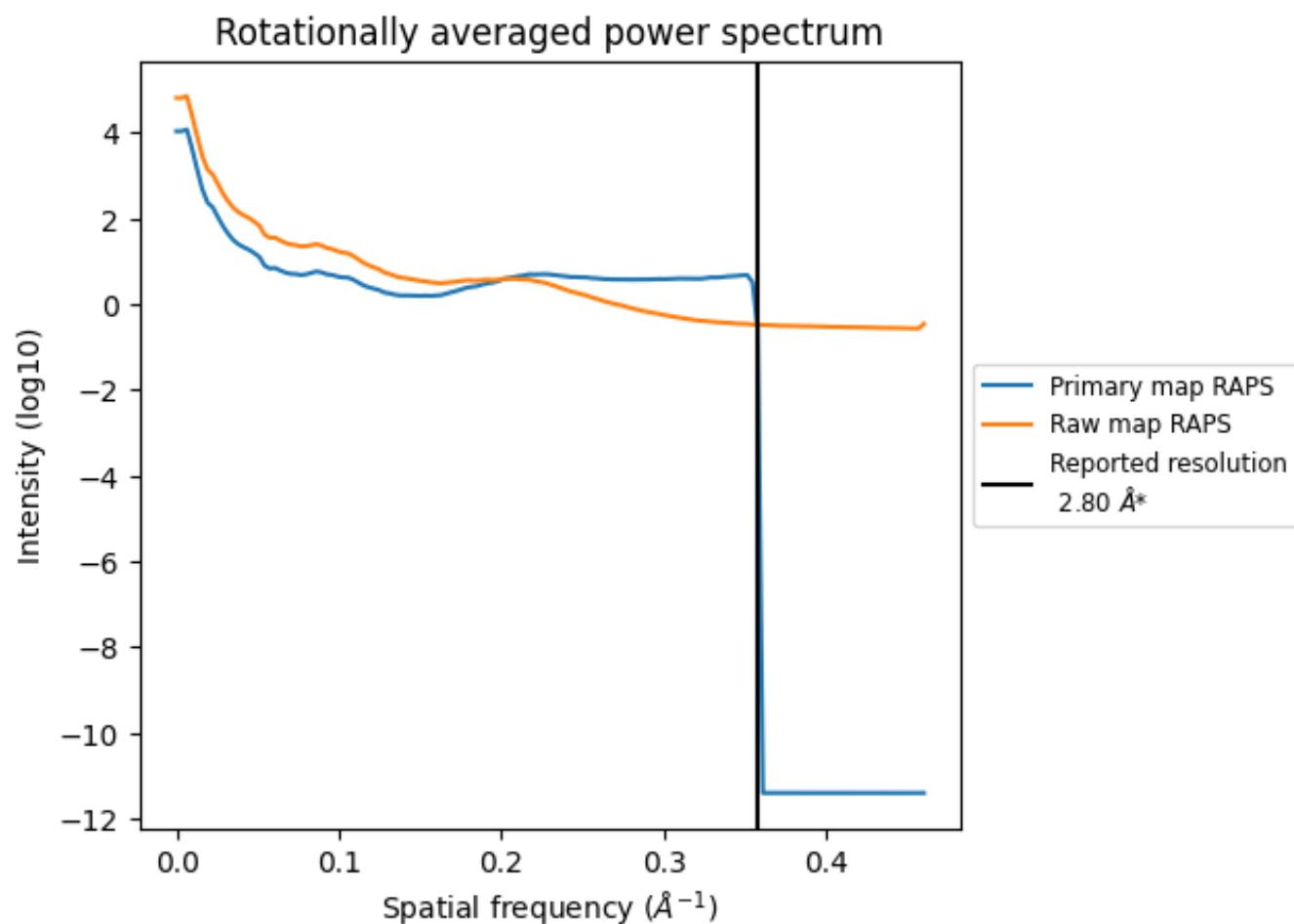
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 273 nm^3 ; this corresponds to an approximate mass of 247 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 ⓘ

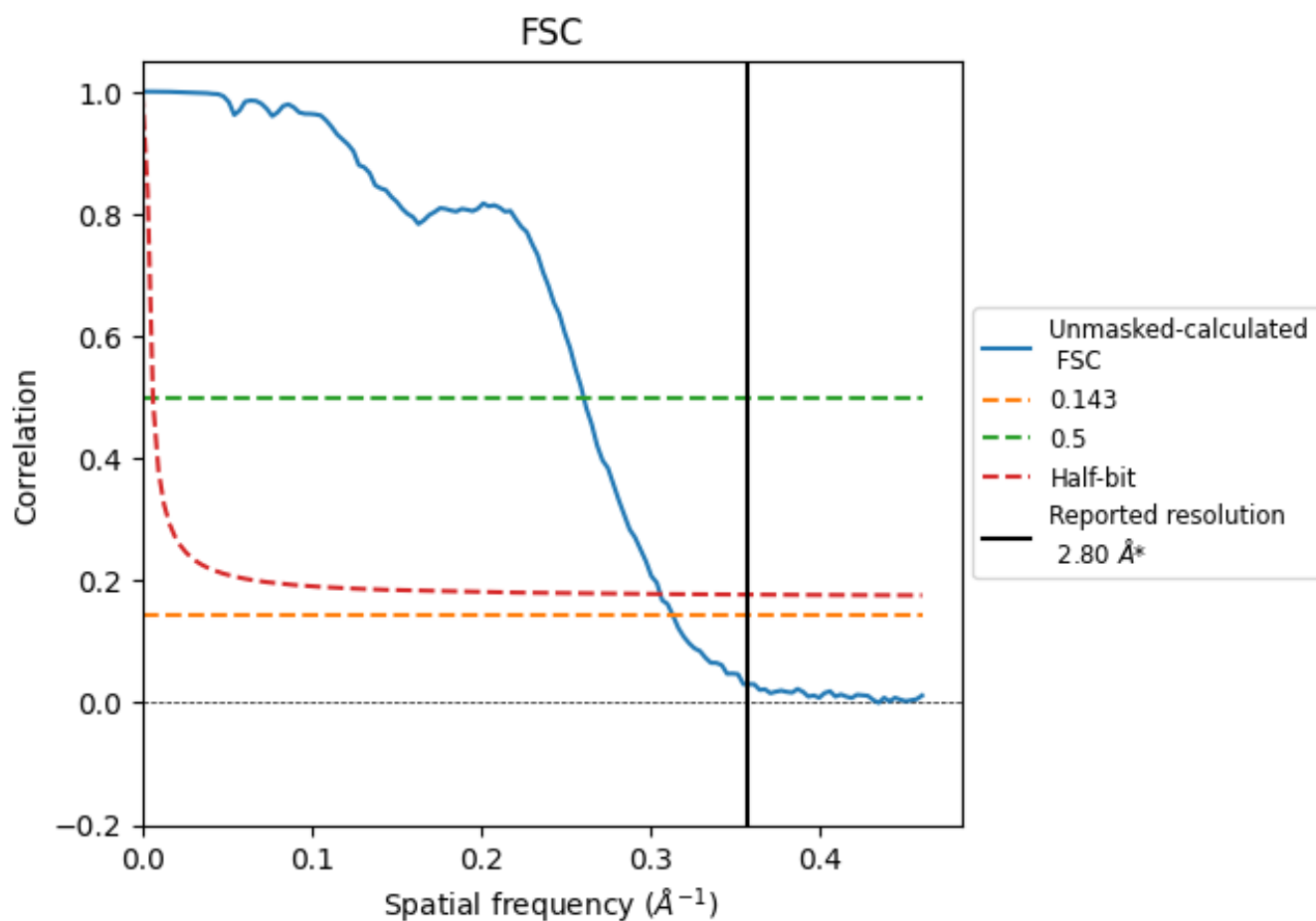


*Reported resolution corresponds to spatial frequency of 0.357 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.357 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

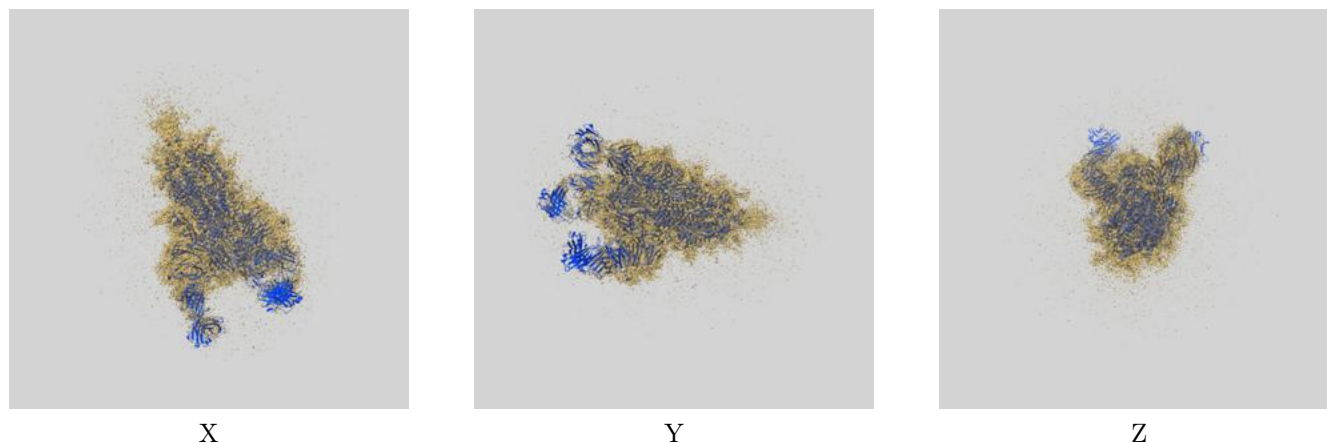
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.80	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.19	3.84	3.27

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.19 differs from the reported value 2.8 by more than 10 %

9 Map-model fit [i](#)

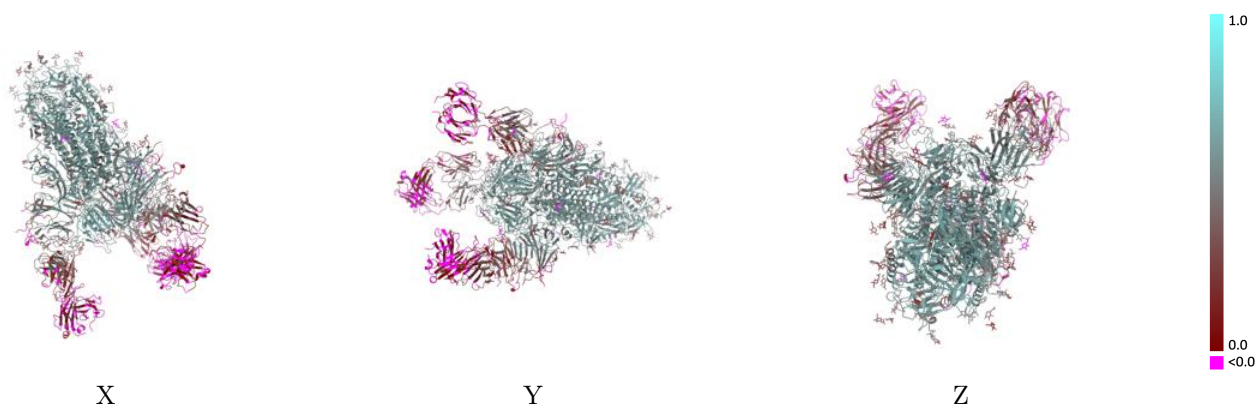
This section contains information regarding the fit between EMDB map EMD-34872 and PDB model 8HLC. Per-residue inclusion information can be found in section 3 on page 12.

9.1 Map-model overlay [i](#)



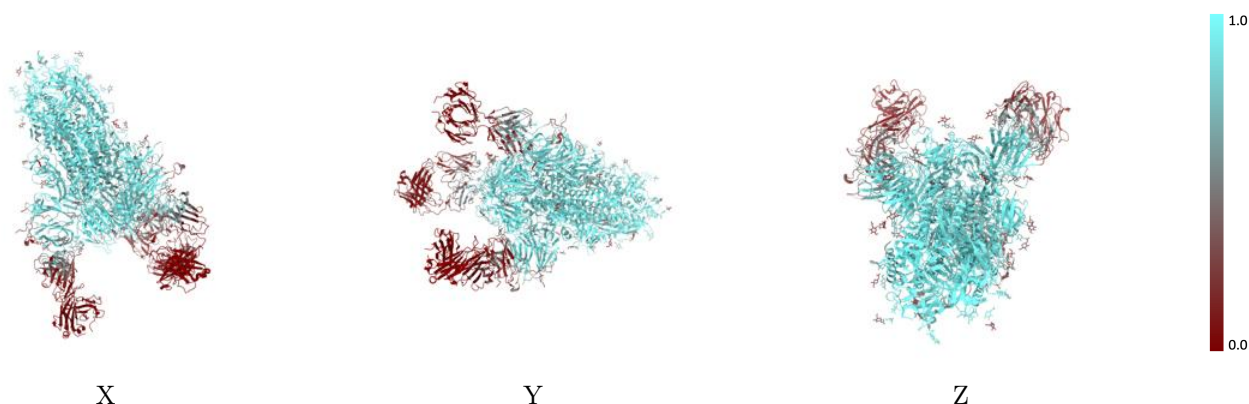
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



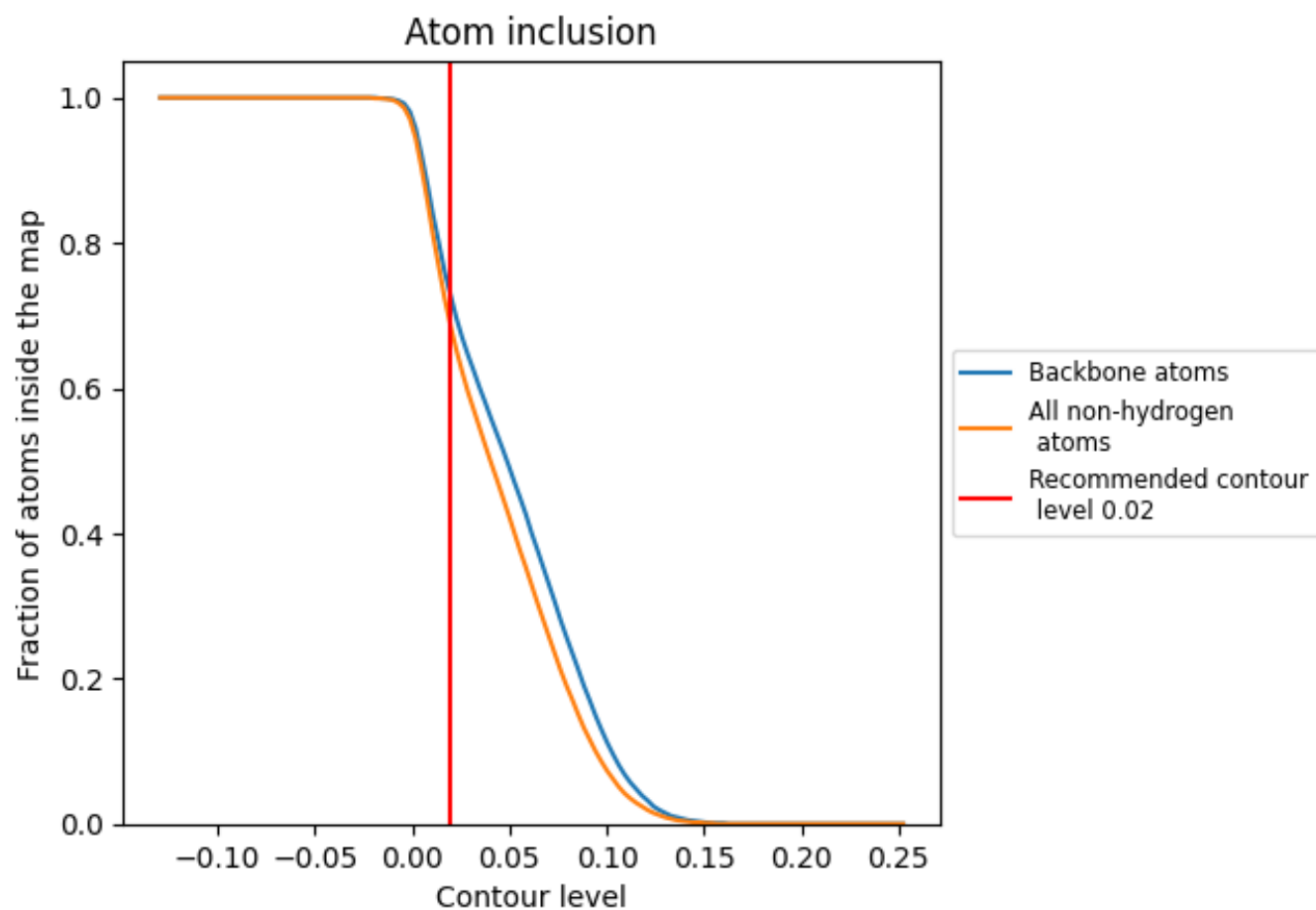
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 72% of all backbone atoms, 68% 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	 0.6830	 0.4310
A	 0.8930	 0.5480
B	 0.8870	 0.5420
C	 0.8740	 0.5270
D	 0.6070	 0.3990
E	 0.3090	 0.2320
F	 0.3570	 0.2730
G	 0.5360	 0.2820
H	 0.2550	 0.1820
I	 0.1770	 0.1590
J	 0.0920	 0.1240
K	 0.3210	 0.2010
L	 0.2550	 0.2020
M	 0.2000	 0.1850
N	 0.0950	 0.1320
O	 0.3570	 0.1460
P	 0.4290	 0.2080
Q	 0.7860	 0.5000
R	 0.5000	 0.3880
S	 0.8210	 0.3980
T	 0.4290	 0.2680
U	 0.3330	 0.2760
V	 0.3930	 0.1750
W	 0.6430	 0.3600
X	 0.3930	 0.1720
Y	 0.2500	 0.2620
Z	 0.8210	 0.4660
a	 0.8570	 0.4060
b	 0.5710	 0.2490
c	 0.2380	 0.1330
d	 0.2140	 0.0110
e	 0.5000	 0.2050
f	 0.2140	 0.1880
g	 0.2860	 0.0910
h	 0.7140	 0.4500
i	 0.7500	 0.3000

