



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 11:31 PM UTC

PDB ID : 7X08 / pdb_00007x08
EMDB ID : EMD-32920
Title : S protein of SARS-CoV-2 in complex with 2G1
Authors : Guo, Y.Y.; Zhang, Y.Y.; Zhou, Q.
Deposited on : 2022-02-21
Resolution : 2.70 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

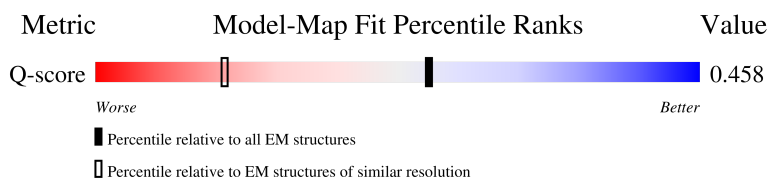
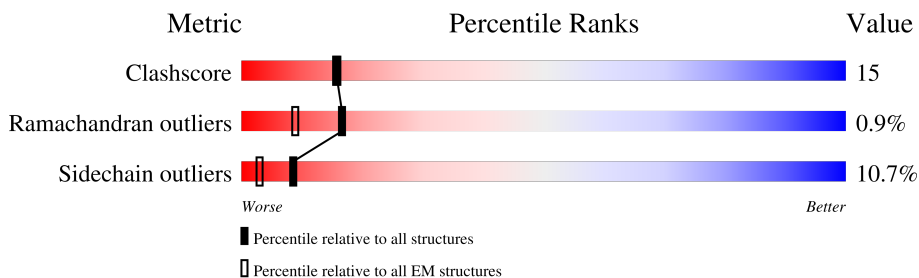
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.70 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	10327 (2.20 - 3.20)

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	452	

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Mol	Chain	Length	Quality of chain
2	I	452	
2	J	452	
3	L	216	
3	M	216	
3	N	216	
4	D	2	
4	E	2	
4	F	2	
4	G	2	
4	K	2	
4	O	2	
4	P	2	
4	Q	2	
4	R	2	
4	S	2	
4	T	2	
4	U	2	
4	V	2	
4	W	2	
4	X	2	
4	Y	2	
4	Z	2	
4	a	2	
4	b	2	
4	c	2	

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Mol	Chain	Length	Quality of chain	
4	d	2	50%	
			50%	50%
4	e	2	50%	
			50%	50%
4	f	2	50%	
			50%	50%
4	g	2	50%	
			50%	50%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 36396 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	1099	Total	C	N	O	S	0	0
			8595	5483	1436	1636	40		
1	B	1099	Total	C	N	O	S	0	0
			8595	5483	1436	1636	40		
1	C	1099	Total	C	N	O	S	0	0
			8595	5483	1436	1636	40		

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	817	PRO	PHE	engineered mutation	UNP P0DTC2
A	892	PRO	ALA	engineered mutation	UNP P0DTC2
A	899	PRO	ALA	engineered mutation	UNP P0DTC2
A	942	PRO	ALA	engineered mutation	UNP P0DTC2
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	817	PRO	PHE	engineered mutation	UNP P0DTC2
B	892	PRO	ALA	engineered mutation	UNP P0DTC2
B	899	PRO	ALA	engineered mutation	UNP P0DTC2
B	942	PRO	ALA	engineered mutation	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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
C	817	PRO	PHE	engineered mutation	UNP P0DTC2
C	892	PRO	ALA	engineered mutation	UNP P0DTC2
C	899	PRO	ALA	engineered mutation	UNP P0DTC2
C	942	PRO	ALA	engineered mutation	UNP P0DTC2
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 2G1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	214	Total	C	N	O	S	0	0
			1603	1016	268	311	8		
2	I	214	Total	C	N	O	S	0	0
			1603	1016	268	311	8		
2	J	214	Total	C	N	O	S	0	0
			1603	1016	268	311	8		

- Molecule 3 is a protein called light chain of 2G1.

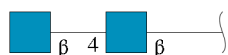
Mol	Chain	Residues	Atoms					AltConf	Trace
3	L	211	Total	C	N	O	S	0	0
			1550	964	260	321	5		
3	M	211	Total	C	N	O	S	0	0
			1550	964	260	321	5		

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	N	211	Total	C	N	O	S	0	0
			1550	964	260	321	5		

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



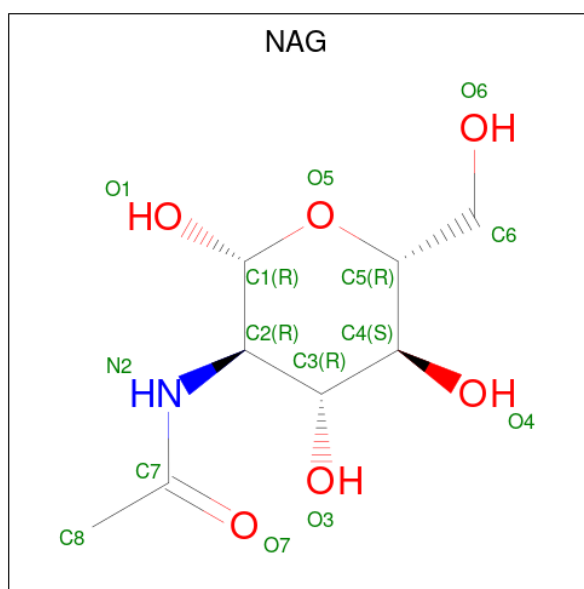
Mol	Chain	Residues	Atoms				AltConf	Trace
4	D	2	Total	C	N	O	0	0
			28	16	2	10		
4	E	2	Total	C	N	O	0	0
			28	16	2	10		
4	F	2	Total	C	N	O	0	0
			28	16	2	10		
4	G	2	Total	C	N	O	0	0
			28	16	2	10		
4	K	2	Total	C	N	O	0	0
			28	16	2	10		
4	O	2	Total	C	N	O	0	0
			28	16	2	10		
4	P	2	Total	C	N	O	0	0
			28	16	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	U	2	Total	C	N	O	0	0
			28	16	2	10		
4	V	2	Total	C	N	O	0	0
			28	16	2	10		
4	W	2	Total	C	N	O	0	0
			28	16	2	10		
4	X	2	Total	C	N	O	0	0
			28	16	2	10		
4	Y	2	Total	C	N	O	0	0
			28	16	2	10		

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Mol	Chain	Residues	Atoms				AltConf	Trace
4	Z	2	Total	C	N	O	0	0
			28	16	2	10		
4	a	2	Total	C	N	O	0	0
			28	16	2	10		
4	b	2	Total	C	N	O	0	0
			28	16	2	10		
4	c	2	Total	C	N	O	0	0
			28	16	2	10		
4	d	2	Total	C	N	O	0	0
			28	16	2	10		
4	e	2	Total	C	N	O	0	0
			28	16	2	10		
4	f	2	Total	C	N	O	0	0
			28	16	2	10		
4	g	2	Total	C	N	O	0	0
			28	16	2	10		

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



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

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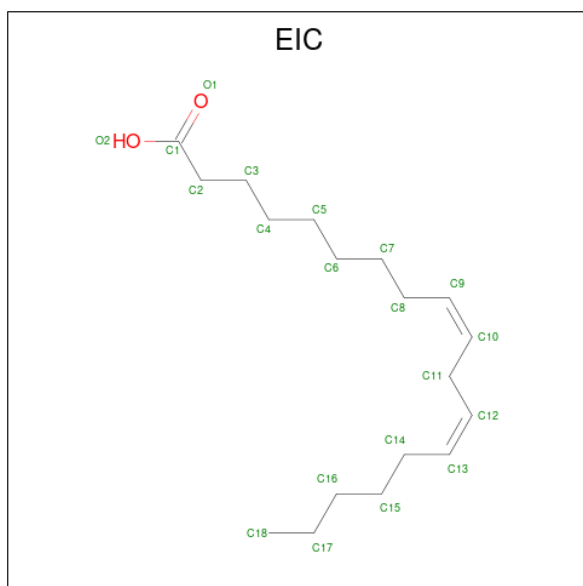
Mol	Chain	Residues	Atoms				AltConf
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	B	1	Total	C	N	O	0
			14	8	1	5	
5	B	1	Total	C	N	O	0
			14	8	1	5	
5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

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

- Molecule 6 is LINOLEIC ACID (CCD ID: EIC) (formula: $C_{18}H_{32}O_2$) (labeled as "Ligand of Interest" by depositor).

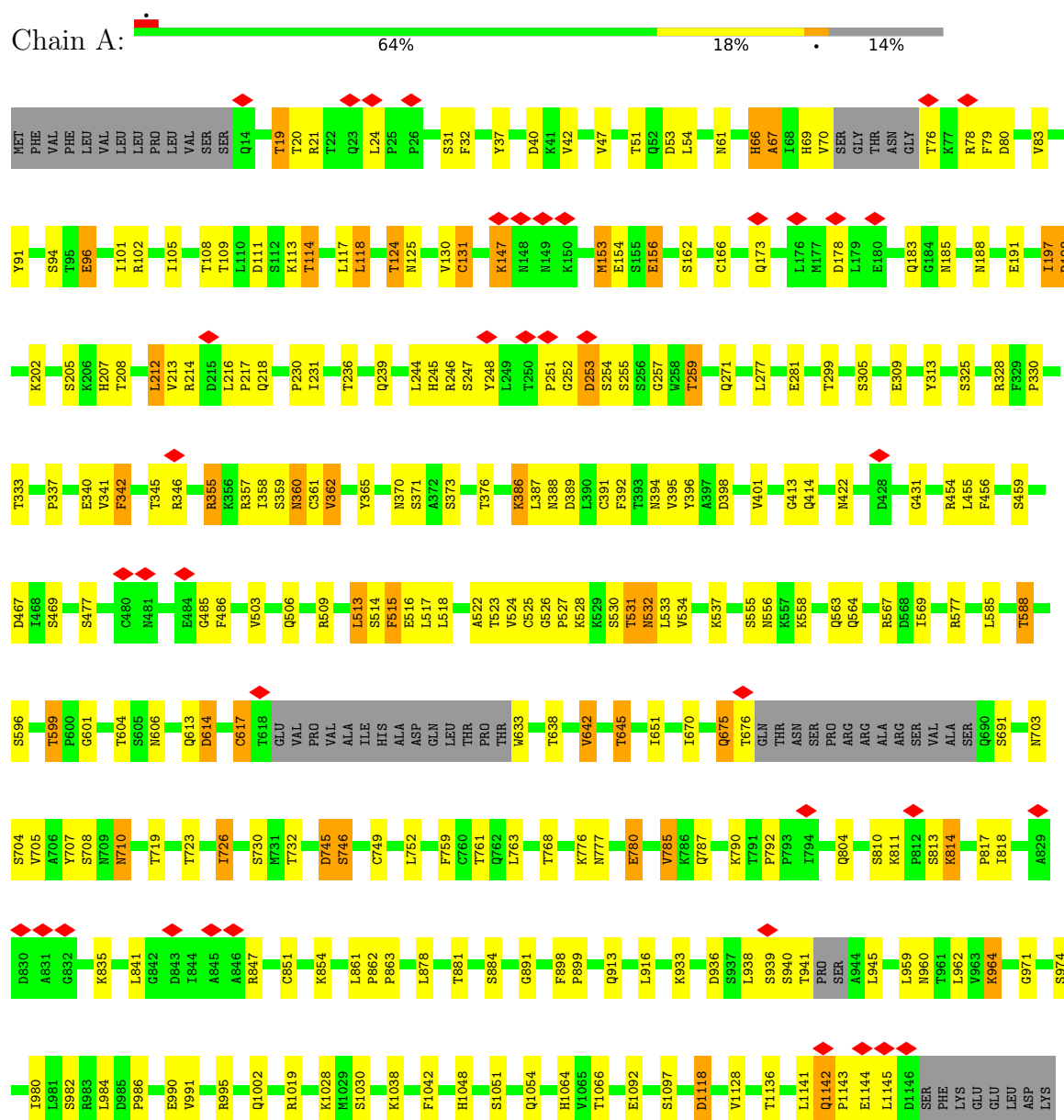


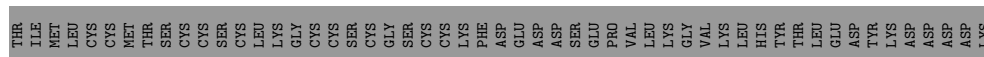
Mol	Chain	Residues	Atoms			AltConf
6	A	1	Total	C	O	0
			20	18	2	
6	A	1	Total	C	O	0
			20	18	2	
6	B	1	Total	C	O	0
			20	18	2	

3 Residue-property plots

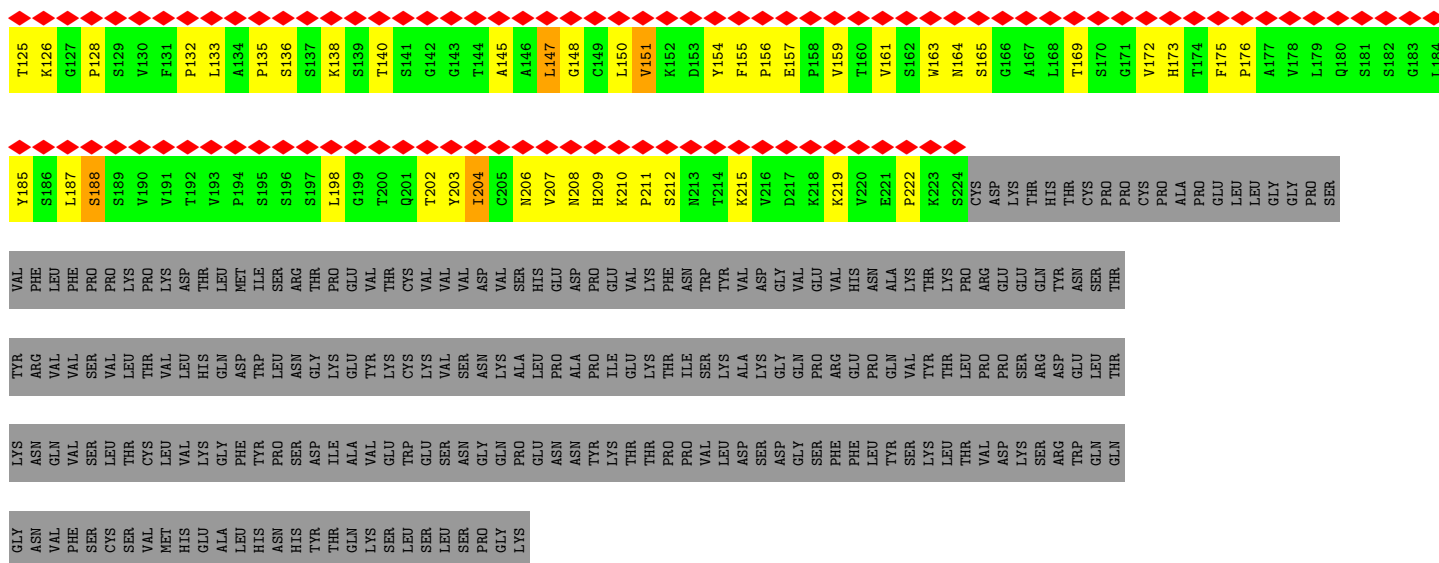
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: Spike glycoprotein

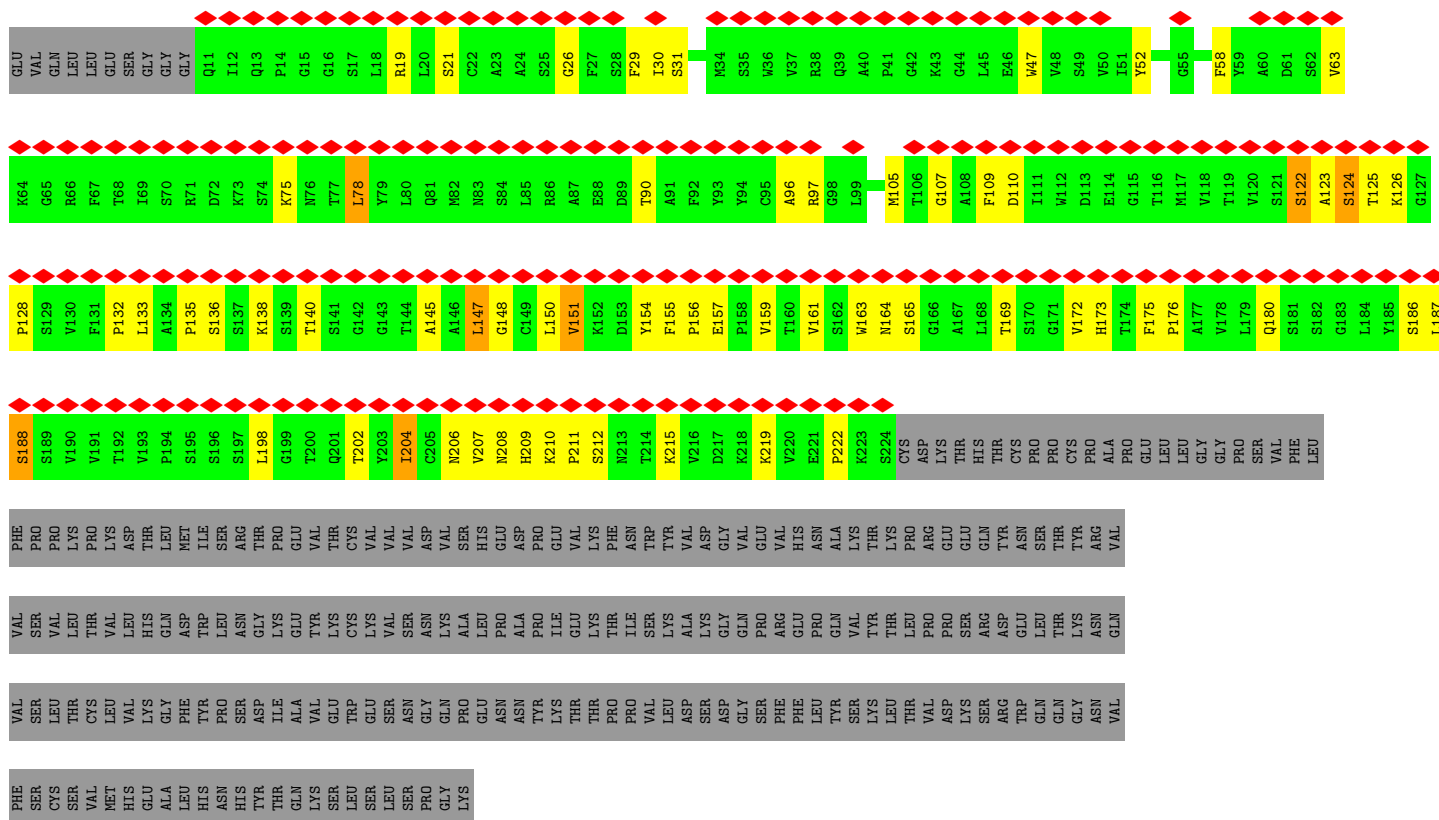
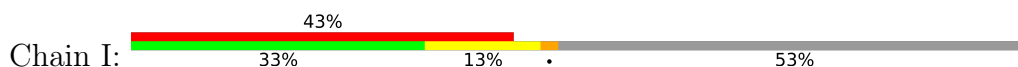




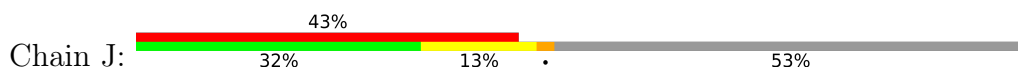
D61												S62												V63												K64												G65												R66												F67												T68												Q69												I70												L71												O72												U73												E74												S75												M76												Y77												L78												Y79												L80												Q81												M82												N83												S84												L85												R86												A87												E88												D89												T90												A91												F92												Y93												Y94												C95												A96												R97												G98												L99												M100												T106												G107												A108												F109												D110												I111												W112												D113												E114												G115												T116												M117												V118												T119												V120												S121												A122												A123												A124											
GLU												VAL												GLN												LEU												GLU												SER												GLY												GLY												Q11												T12												Q13												P14												G15												G16												S17												L18												R19												L20												S21												C22												A23												A24												S25												C26												F27												S28												F29												L30												S31												N32												N33												S35												N36												V37												R38												Q39												A40												P41												O42												K43												L44												L45												E46												W47												V48												S49												V50												T51												S52												S53												O54												S55												S56												T57												F58												V59												A60																																			

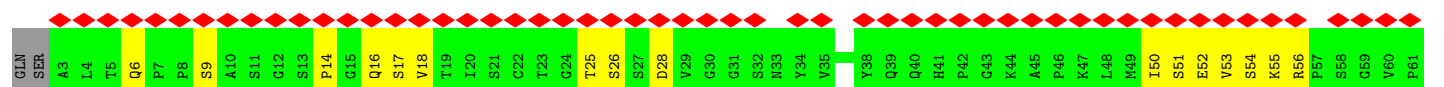


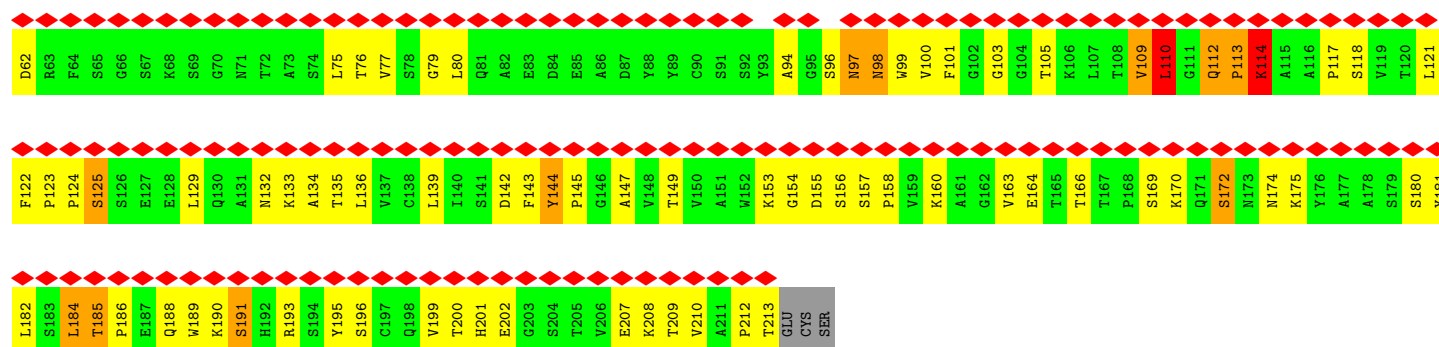
- Molecule 2: heavy chain of 2G1



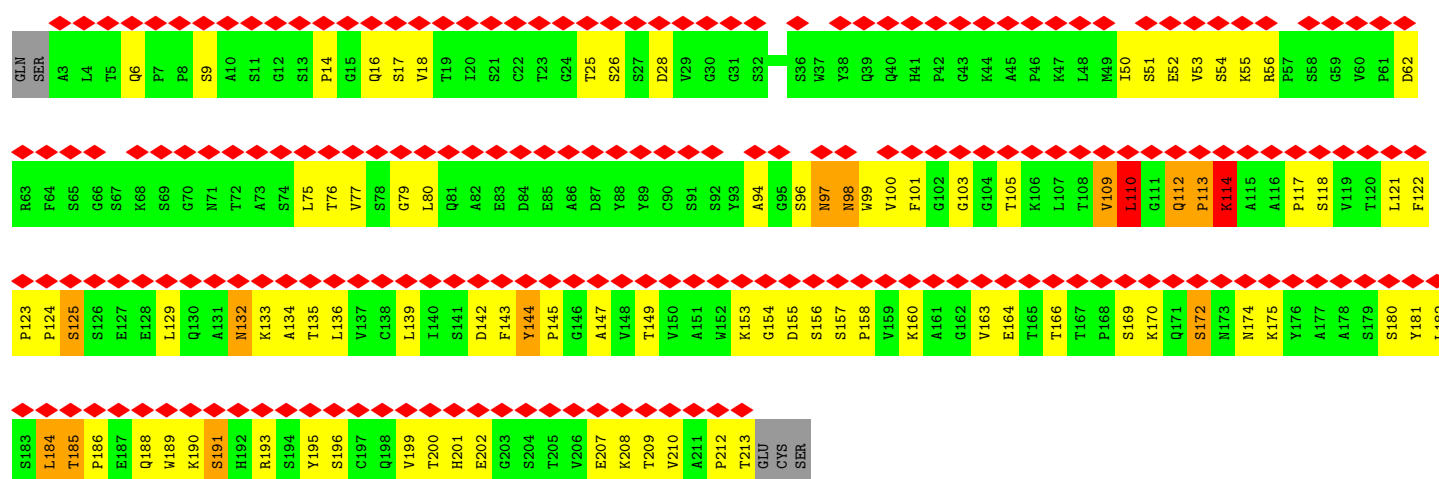
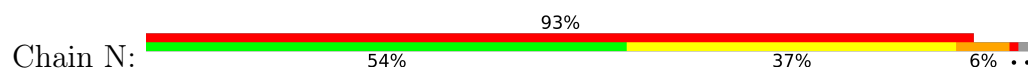
- Molecule 2: heavy chain of 2G1







- Molecule 3: light chain of 2G1



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



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



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



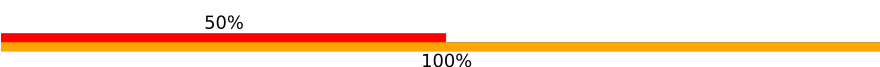


- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:  50% 50%

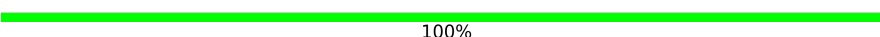


- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:  50% 100%



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

Chain O:  100%



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

Chain P:  50% 50% 50%

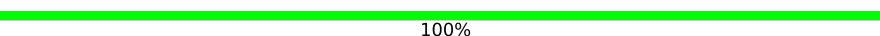


- Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Q:  100% 100%



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

Chain R:  100%



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



- 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



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	349830	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	0.225	Depositor
Minimum map value	-0.112	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.025	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	0.40	0/8797	0.55	3/11975 (0.0%)
1	B	0.40	0/8797	0.55	4/11975 (0.0%)
1	C	0.40	0/8797	0.55	5/11975 (0.0%)
2	H	0.38	0/1641	0.64	1/2229 (0.0%)
2	I	0.38	0/1641	0.64	1/2229 (0.0%)
2	J	0.38	0/1641	0.64	1/2229 (0.0%)
3	L	0.40	0/1589	0.60	0/2169
3	M	0.40	0/1589	0.60	0/2169
3	N	0.40	0/1589	0.60	0/2169
All	All	0.40	0/36081	0.57	15/49119 (0.0%)

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	63	VAL	N-CA-C	-7.96	106.15	113.71
2	I	63	VAL	N-CA-C	-7.94	106.17	113.71
2	H	63	VAL	N-CA-C	-7.93	106.18	113.71
1	A	891	GLY	CA-C-N	-5.68	114.12	120.14
1	A	891	GLY	C-N-CA	-5.68	114.12	120.14
1	C	517	LEU	N-CA-C	5.65	117.77	109.24
1	B	515	PHE	N-CA-C	5.41	115.51	107.88
1	B	847	ARG	N-CA-C	-5.40	107.70	114.56
1	C	847	ARG	N-CA-C	-5.39	107.71	114.56
1	A	847	ARG	N-CA-C	-5.38	107.72	114.56
1	B	520	ALA	CA-C-N	-5.37	114.39	119.76
1	B	520	ALA	C-N-CA	-5.37	114.39	119.76
1	C	515	PHE	N-CA-C	5.30	115.54	108.38
1	C	520	ALA	CA-C-N	-5.27	114.28	119.92
1	C	520	ALA	C-N-CA	-5.27	114.28	119.92

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	8595	0	8352	186	0
1	B	8595	0	8351	183	0
1	C	8595	0	8352	174	0
2	H	1603	0	1584	73	0
2	I	1603	0	1584	71	0
2	J	1603	0	1584	71	0
3	L	1550	0	1490	105	0
3	M	1550	0	1490	107	0
3	N	1550	0	1490	110	0
4	D	28	0	25	1	0
4	E	28	0	25	0	0
4	F	28	0	25	1	0
4	G	28	0	25	0	0
4	K	28	0	25	1	0
4	O	28	0	25	0	0
4	P	28	0	25	0	0
4	Q	28	0	25	1	0
4	R	28	0	25	0	0
4	S	28	0	25	0	0
4	T	28	0	26	1	0
4	U	28	0	26	6	0
4	V	28	0	25	2	0
4	W	28	0	26	2	0
4	X	28	0	26	1	0
4	Y	28	0	26	6	0
4	Z	28	0	25	2	0
4	a	28	0	25	1	0
4	b	28	0	26	2	0
4	c	28	0	26	1	0
4	d	28	0	26	6	0
4	e	28	0	25	2	0
4	f	28	0	25	1	0
4	g	28	0	26	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	140	0	130	14	0
5	B	140	0	130	15	0
5	C	140	0	130	15	0
6	A	40	0	62	9	0
6	B	20	0	31	4	0
All	All	36396	0	35369	1029	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 15.

All (1029) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:110:LEU:HB3	3:N:144:TYR:CE2	1.69	1.28
3:M:110:LEU:HB3	3:M:144:TYR:CE2	1.69	1.26
3:L:110:LEU:HB3	3:L:144:TYR:CE2	1.69	1.26
3:N:144:TYR:HB3	3:N:145:PRO:CD	1.71	1.20
3:N:9:SER:CB	3:N:147:ALA:HB2	1.73	1.19
4:c:1:NAG:HO4	4:c:2:NAG:C1	1.47	1.19
3:M:144:TYR:HB3	3:M:145:PRO:CD	1.71	1.19
3:L:144:TYR:HB3	3:L:145:PRO:CD	1.71	1.19
3:L:9:SER:CB	3:L:147:ALA:HB2	1.73	1.17
3:M:9:SER:CB	3:M:147:ALA:HB2	1.73	1.17
3:N:9:SER:HB3	3:N:147:ALA:CB	1.76	1.16
3:L:9:SER:HB3	3:L:147:ALA:CB	1.76	1.15
3:M:9:SER:HB3	3:M:147:ALA:CB	1.76	1.15
3:M:110:LEU:CB	3:M:144:TYR:HE2	1.60	1.14
3:L:110:LEU:CB	3:L:144:TYR:HE2	1.60	1.14
3:N:110:LEU:CB	3:N:144:TYR:HE2	1.60	1.13
1:C:67:ALA:HA	1:C:78:ARG:O	1.50	1.12
1:B:67:ALA:HA	1:B:78:ARG:O	1.50	1.11
1:A:485:GLY:HA2	2:H:52:TYR:CD2	1.86	1.10
1:A:67:ALA:HA	1:A:78:ARG:O	1.50	1.10
1:B:485:GLY:HA2	2:I:52:TYR:CD2	1.86	1.10
1:C:485:GLY:HA2	2:J:52:TYR:CD2	1.86	1.09
3:L:9:SER:CB	3:L:147:ALA:CB	2.32	1.07
3:L:110:LEU:CB	3:L:144:TYR:CE2	2.35	1.07
3:L:144:TYR:HB3	3:L:145:PRO:HD3	1.08	1.06
3:N:144:TYR:HB3	3:N:145:PRO:HD3	1.08	1.06
3:M:144:TYR:HB3	3:M:145:PRO:HD3	1.08	1.06
3:N:112:GLN:HB3	3:N:113:PRO:HD3	1.37	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:9:SER:CB	3:M:147:ALA:CB	2.32	1.05
4:T:1:NAG:HO4	4:T:2:NAG:C1	1.57	1.05
3:L:112:GLN:HB3	3:L:113:PRO:HD3	1.37	1.05
3:N:110:LEU:CB	3:N:144:TYR:CE2	2.35	1.04
3:N:9:SER:CB	3:N:147:ALA:CB	2.32	1.04
3:M:110:LEU:CB	3:M:144:TYR:CE2	2.35	1.03
3:M:112:GLN:HB3	3:M:113:PRO:HD3	1.37	1.03
3:L:110:LEU:HB3	3:L:144:TYR:CD2	1.94	1.02
1:A:124:THR:HG21	5:A:1302:NAG:C8	1.91	1.01
3:M:110:LEU:HB3	3:M:144:TYR:CD2	1.94	1.01
1:B:355:ARG:HH21	1:B:355:ARG:HG3	1.26	1.01
3:M:9:SER:HB3	3:M:147:ALA:HB2	1.02	1.00
1:C:124:THR:HG21	5:C:1302:NAG:C8	1.91	1.00
3:N:110:LEU:HB3	3:N:144:TYR:CD2	1.94	1.00
1:B:124:THR:HG21	5:B:1302:NAG:C8	1.90	1.00
3:L:9:SER:HB3	3:L:147:ALA:HB2	1.02	0.99
1:C:131:CYS:HB3	1:C:166:CYS:HA	1.42	0.98
1:A:131:CYS:HB3	1:A:166:CYS:HA	1.42	0.98
3:N:9:SER:HB3	3:N:147:ALA:HB2	1.02	0.98
1:C:355:ARG:HH21	1:C:355:ARG:HG3	1.26	0.97
1:B:131:CYS:HB3	1:B:166:CYS:HA	1.42	0.97
1:A:355:ARG:HH21	1:A:355:ARG:HG3	1.26	0.96
2:H:175:PHE:CE1	3:L:139:LEU:HD23	2.01	0.95
2:I:175:PHE:CE1	3:M:139:LEU:HD23	2.01	0.94
2:J:175:PHE:CE1	3:N:139:LEU:HD23	2.01	0.94
4:d:1:NAG:HO4	4:d:2:NAG:C1	1.71	0.94
4:X:1:NAG:HO4	4:X:2:NAG:C1	1.58	0.93
4:U:1:NAG:H62	4:U:2:NAG:C7	1.99	0.93
1:B:388:ASN:HB2	1:B:527:PRO:HD2	1.50	0.92
4:Y:1:NAG:HO4	4:Y:2:NAG:C1	1.80	0.92
1:B:1144:GLU:C	1:B:1145:LEU:HD23	1.95	0.92
1:C:1144:GLU:C	1:C:1145:LEU:HD23	1.95	0.92
1:A:1144:GLU:C	1:A:1145:LEU:HD23	1.95	0.91
4:W:1:NAG:HO4	4:W:2:NAG:C1	1.78	0.91
4:d:1:NAG:H62	4:d:2:NAG:C7	1.99	0.91
4:Y:1:NAG:H62	4:Y:2:NAG:C7	1.99	0.91
3:M:112:GLN:HB3	3:M:113:PRO:CD	2.03	0.89
3:N:112:GLN:CB	3:N:113:PRO:CD	2.51	0.89
3:L:112:GLN:CB	3:L:113:PRO:CD	2.51	0.89
3:L:112:GLN:HB3	3:L:113:PRO:CD	2.03	0.89
3:M:112:GLN:CB	3:M:113:PRO:CD	2.51	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:940:SER:O	1:C:941:THR:OG1	1.91	0.88
1:A:940:SER:O	1:A:941:THR:OG1	1.91	0.88
1:B:940:SER:O	1:B:941:THR:OG1	1.91	0.88
3:N:112:GLN:HB3	3:N:113:PRO:CD	2.03	0.88
1:A:485:GLY:CA	2:H:52:TYR:CE2	2.58	0.87
1:C:485:GLY:CA	2:J:52:TYR:CE2	2.58	0.87
1:C:485:GLY:HA2	2:J:52:TYR:CE2	2.10	0.86
1:B:485:GLY:CA	2:I:52:TYR:CE2	2.58	0.86
1:B:124:THR:HG21	5:B:1302:NAG:H82	1.58	0.86
1:B:485:GLY:HA2	2:I:52:TYR:CE2	2.10	0.86
3:M:144:TYR:CB	3:M:145:PRO:CD	2.54	0.86
4:g:1:NAG:HO4	4:g:2:NAG:C1	1.88	0.85
1:C:485:GLY:HA2	2:J:52:TYR:HD2	1.42	0.85
1:A:485:GLY:HA2	2:H:52:TYR:CE2	2.10	0.85
1:A:124:THR:HG21	5:A:1302:NAG:H82	1.58	0.84
1:C:124:THR:HG21	5:C:1302:NAG:H82	1.58	0.84
1:A:485:GLY:HA2	2:H:52:TYR:HD2	1.42	0.84
3:L:110:LEU:HD13	3:L:114:LYS:HD2	1.60	0.83
3:M:110:LEU:HD13	3:M:114:LYS:HD2	1.60	0.83
1:A:370:ASN:CG	2:J:29:PHE:HE1	1.87	0.83
1:A:388:ASN:HB2	1:A:527:PRO:HD2	1.60	0.82
1:C:388:ASN:HB2	1:C:527:PRO:HD2	1.60	0.82
4:U:1:NAG:HO4	4:U:2:NAG:C1	1.89	0.82
4:b:1:NAG:HO4	4:b:2:NAG:C1	1.91	0.82
3:N:110:LEU:HD13	3:N:114:LYS:HD2	1.60	0.82
1:B:485:GLY:HA2	2:I:52:TYR:HD2	1.42	0.82
3:N:144:TYR:CB	3:N:145:PRO:CD	2.54	0.82
1:A:431:GLY:HA3	1:A:513:LEU:O	1.81	0.81
1:B:431:GLY:HA3	1:B:513:LEU:O	1.81	0.81
3:M:94:ALA:HB3	3:M:98:ASN:HB2	1.63	0.80
3:N:94:ALA:HB3	3:N:98:ASN:HB2	1.64	0.80
1:C:422:ASN:HD21	1:C:454:ARG:H	1.29	0.80
1:C:431:GLY:HA3	1:C:513:LEU:O	1.81	0.80
1:A:131:CYS:HB3	1:A:166:CYS:CA	2.13	0.79
3:L:94:ALA:HB3	3:L:98:ASN:HB2	1.64	0.79
5:A:1309:NAG:H3	5:A:1309:NAG:C8	2.13	0.79
5:B:1309:NAG:H3	5:B:1309:NAG:C8	2.13	0.78
1:C:131:CYS:HB3	1:C:166:CYS:CA	2.13	0.78
3:N:112:GLN:CB	3:N:113:PRO:HD3	2.14	0.78
5:C:1309:NAG:H3	5:C:1309:NAG:C8	2.13	0.78
3:L:144:TYR:CB	3:L:145:PRO:CD	2.54	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:124:THR:HG21	5:B:1302:NAG:H83	1.65	0.78
1:B:131:CYS:HB3	1:B:166:CYS:CA	2.13	0.78
3:L:112:GLN:CB	3:L:113:PRO:HD3	2.14	0.78
1:A:599:THR:HG23	1:A:601:GLY:H	1.49	0.77
1:B:388:ASN:HB2	1:B:527:PRO:CD	2.13	0.77
1:A:124:THR:HG21	5:A:1302:NAG:H83	1.65	0.77
1:A:345:THR:HG23	1:A:346:ARG:H	1.49	0.77
1:B:24:LEU:HB2	1:B:78:ARG:NH2	2.00	0.77
1:B:422:ASN:HD21	1:B:454:ARG:H	1.29	0.77
1:C:599:THR:HG23	1:C:601:GLY:H	1.50	0.77
1:A:24:LEU:HB2	1:A:78:ARG:NH2	2.00	0.77
6:A:1312:EIC:H31	1:B:374:PHE:HE2	1.49	0.76
1:A:422:ASN:HD21	1:A:454:ARG:H	1.29	0.76
1:C:24:LEU:HB2	1:C:78:ARG:NH2	2.00	0.76
1:B:599:THR:HG23	1:B:601:GLY:H	1.50	0.76
1:C:124:THR:HG21	5:C:1302:NAG:H83	1.65	0.76
2:J:58:PHE:CE2	3:N:97:ASN:ND2	2.54	0.76
1:C:370:ASN:CG	2:I:29:PHE:HE1	1.93	0.76
2:I:58:PHE:CE2	3:M:97:ASN:ND2	2.54	0.75
1:B:389:ASP:OD1	1:B:528:LYS:HD2	1.86	0.75
2:H:58:PHE:CE2	3:L:97:ASN:ND2	2.54	0.75
1:C:358:ILE:HB	1:C:395:VAL:CG1	2.17	0.75
3:L:110:LEU:CA	3:L:144:TYR:HE2	2.00	0.75
2:J:107:GLY:O	3:N:99:TRP:HH2	1.70	0.75
1:B:124:THR:CG2	5:B:1302:NAG:C8	2.65	0.74
3:N:110:LEU:CA	3:N:144:TYR:HE2	2.00	0.74
2:H:107:GLY:O	3:L:99:TRP:HH2	1.70	0.74
1:B:358:ILE:HB	1:B:395:VAL:CG1	2.17	0.74
1:A:1144:GLU:O	1:A:1145:LEU:HD23	1.88	0.74
1:C:124:THR:CG2	5:C:1302:NAG:C8	2.65	0.74
1:B:485:GLY:C	2:I:52:TYR:CE2	2.66	0.74
2:I:107:GLY:O	3:M:99:TRP:HH2	1.70	0.74
5:C:1309:NAG:H3	5:C:1309:NAG:H82	1.71	0.73
1:A:485:GLY:C	2:H:52:TYR:CE2	2.66	0.73
3:M:110:LEU:CA	3:M:144:TYR:HE2	2.00	0.73
1:C:67:ALA:CA	1:C:78:ARG:O	2.34	0.73
1:C:485:GLY:C	2:J:52:TYR:CE2	2.66	0.73
1:B:355:ARG:HG3	1:B:355:ARG:NH2	1.98	0.73
1:A:358:ILE:HB	1:A:395:VAL:CG1	2.17	0.73
1:A:124:THR:CG2	5:A:1302:NAG:C8	2.65	0.73
5:B:1309:NAG:H3	5:B:1309:NAG:H82	1.71	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:d:1:NAG:H62	4:d:2:NAG:C8	2.19	0.72
1:A:67:ALA:CA	1:A:78:ARG:O	2.34	0.72
1:A:69:HIS:HA	1:A:76:THR:O	1.89	0.72
1:A:1142:GLN:N	1:A:1142:GLN:OE1	2.21	0.72
1:B:1142:GLN:N	1:B:1142:GLN:OE1	2.21	0.72
1:C:1142:GLN:OE1	1:C:1142:GLN:N	2.21	0.72
1:A:124:THR:CG2	5:A:1302:NAG:H82	2.20	0.72
1:A:69:HIS:C	1:A:70:VAL:HG23	2.15	0.72
1:B:69:HIS:HA	1:B:76:THR:O	1.89	0.72
1:C:355:ARG:HG3	1:C:355:ARG:NH2	1.98	0.72
1:A:388:ASN:HB2	1:A:527:PRO:CD	2.20	0.72
1:C:388:ASN:HB2	1:C:527:PRO:CD	2.19	0.72
1:C:1144:GLU:O	1:C:1145:LEU:HD23	1.88	0.72
1:A:485:GLY:CA	2:H:52:TYR:CD2	2.70	0.71
1:B:1144:GLU:O	1:B:1145:LEU:HD23	1.88	0.71
4:U:1:NAG:H62	4:U:2:NAG:C8	2.19	0.71
5:A:1309:NAG:H3	5:A:1309:NAG:H82	1.70	0.71
1:C:69:HIS:C	1:C:70:VAL:HG23	2.15	0.71
3:N:110:LEU:CD1	3:N:114:LYS:HD2	2.20	0.71
4:Y:1:NAG:H62	4:Y:2:NAG:C8	2.19	0.71
1:B:124:THR:CG2	5:B:1302:NAG:H82	2.20	0.71
1:C:69:HIS:HA	1:C:76:THR:O	1.89	0.71
1:B:69:HIS:C	1:B:70:VAL:HG23	2.15	0.71
1:A:358:ILE:HB	1:A:395:VAL:HG12	1.72	0.70
1:C:124:THR:CG2	5:C:1302:NAG:H82	2.20	0.70
1:C:358:ILE:HB	1:C:395:VAL:HG12	1.72	0.70
3:L:110:LEU:CD1	3:L:114:LYS:HD2	2.20	0.70
2:J:47:TRP:CE3	3:N:98:ASN:O	2.45	0.70
1:B:370:ASN:CG	2:H:29:PHE:HE1	1.99	0.70
3:M:110:LEU:CD1	3:M:114:LYS:HD2	2.20	0.70
2:H:47:TRP:CE3	3:L:98:ASN:O	2.45	0.70
2:I:47:TRP:CE3	3:M:98:ASN:O	2.45	0.69
1:A:131:CYS:CB	1:A:166:CYS:HA	2.20	0.69
1:C:131:CYS:CB	1:C:166:CYS:HA	2.20	0.69
1:B:358:ILE:HB	1:B:395:VAL:HG12	1.72	0.69
1:B:67:ALA:CA	1:B:78:ARG:O	2.34	0.69
1:B:131:CYS:CB	1:B:166:CYS:HA	2.21	0.69
1:B:246:ARG:NH2	1:B:254:SER:O	2.27	0.68
1:A:355:ARG:HG3	1:A:355:ARG:NH2	1.98	0.68
3:N:100:VAL:HG22	3:N:101:PHE:H	1.59	0.68
3:L:100:VAL:HG22	3:L:101:PHE:H	1.59	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:246:ARG:NH2	1:A:254:SER:O	2.27	0.67
1:A:358:ILE:CG1	1:A:395:VAL:HG12	2.24	0.67
1:C:804:GLN:O	1:C:818:ILE:HG12	1.94	0.67
1:B:358:ILE:CG1	1:B:395:VAL:HG12	2.24	0.67
1:C:246:ARG:NH2	1:C:254:SER:O	2.27	0.67
1:B:456:PHE:HZ	2:I:30:ILE:HD11	1.60	0.67
1:B:1144:GLU:OE2	1:B:1144:GLU:HA	1.94	0.67
1:C:358:ILE:CG1	1:C:395:VAL:HG12	2.24	0.67
1:A:1144:GLU:OE2	1:A:1144:GLU:HA	1.95	0.67
1:B:388:ASN:CB	1:B:527:PRO:HD2	2.25	0.67
3:M:100:VAL:HG22	3:M:101:PHE:H	1.59	0.67
2:J:124:SER:OG	2:J:125:THR:N	2.27	0.66
1:A:456:PHE:HZ	2:H:30:ILE:HD11	1.60	0.66
1:C:456:PHE:HZ	2:J:30:ILE:HD11	1.60	0.65
1:C:70:VAL:N	1:C:76:THR:O	2.29	0.65
2:H:124:SER:OG	2:H:125:THR:N	2.27	0.65
3:N:98:ASN:O	3:N:99:TRP:HB2	1.95	0.65
1:B:389:ASP:OD1	1:B:528:LYS:CD	2.44	0.65
1:C:1144:GLU:HA	1:C:1144:GLU:OE2	1.94	0.65
2:H:47:TRP:CZ3	3:L:98:ASN:O	2.50	0.65
1:B:776:LYS:O	1:B:780:GLU:HG2	1.97	0.65
3:L:98:ASN:O	3:L:99:TRP:HB2	1.95	0.65
3:N:6:GLN:HE21	3:N:103:GLY:H	1.45	0.64
1:C:124:THR:CG2	5:C:1302:NAG:H83	2.28	0.64
2:J:47:TRP:CZ3	3:N:98:ASN:O	2.50	0.64
2:J:124:SER:O	2:J:155:PHE:CD2	2.51	0.64
1:C:776:LYS:O	1:C:780:GLU:HG2	1.97	0.64
2:I:47:TRP:CZ3	3:M:98:ASN:O	2.50	0.64
3:M:98:ASN:O	3:M:99:TRP:HB2	1.95	0.64
6:A:1312:EIC:H31	1:B:374:PHE:CE2	2.30	0.64
2:I:208:ASN:HB3	2:I:215:LYS:HE2	1.79	0.64
2:I:124:SER:OG	2:I:125:THR:N	2.27	0.64
1:A:776:LYS:O	1:A:780:GLU:HG2	1.97	0.64
2:H:124:SER:O	2:H:155:PHE:CD2	2.51	0.64
3:M:6:GLN:HE21	3:M:103:GLY:H	1.45	0.64
2:H:208:ASN:HB3	2:H:215:LYS:HE2	1.79	0.63
2:H:175:PHE:CE1	3:L:139:LEU:CD2	2.81	0.63
3:L:6:GLN:HE21	3:L:103:GLY:H	1.45	0.63
2:I:133:LEU:HD11	2:I:150:LEU:HB2	1.80	0.63
2:I:107:GLY:C	3:M:99:TRP:HH2	2.07	0.63
3:M:124:PRO:HD3	3:M:136:LEU:HD22	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:133:LEU:HD11	2:H:150:LEU:HB2	1.80	0.63
2:H:161:VAL:HG22	2:H:207:VAL:HG22	1.81	0.63
3:M:125:SER:O	3:M:129:LEU:HG	1.99	0.63
2:J:133:LEU:HD11	2:J:150:LEU:HB2	1.80	0.63
3:N:125:SER:O	3:N:129:LEU:HG	1.99	0.63
2:I:124:SER:O	2:I:155:PHE:CD2	2.51	0.63
2:J:208:ASN:HB3	2:J:215:LYS:HE2	1.79	0.63
6:B:1311:EIC:H52	1:C:374:PHE:HE2	1.64	0.63
3:L:124:PRO:HD3	3:L:136:LEU:HD22	1.80	0.63
1:C:456:PHE:CZ	2:J:30:ILE:HD11	2.34	0.62
1:A:124:THR:CG2	5:A:1302:NAG:H83	2.28	0.62
2:H:107:GLY:C	3:L:99:TRP:HH2	2.07	0.62
2:J:107:GLY:C	3:N:99:TRP:HH2	2.07	0.62
3:N:145:PRO:HG2	3:N:201:HIS:CE1	2.34	0.62
1:A:456:PHE:CZ	2:H:30:ILE:HD11	2.34	0.62
3:N:124:PRO:HD3	3:N:136:LEU:HD22	1.80	0.62
3:L:145:PRO:HG2	3:L:201:HIS:CE1	2.34	0.62
2:J:175:PHE:CE1	3:N:139:LEU:CD2	2.81	0.62
1:B:111:ASP:OD2	1:B:113:LYS:NZ	2.33	0.62
2:J:161:VAL:HG22	2:J:207:VAL:HG22	1.81	0.62
1:A:345:THR:HG23	1:A:346:ARG:N	2.15	0.62
1:C:253:ASP:OD1	1:C:253:ASP:N	2.31	0.62
1:B:456:PHE:CZ	2:I:30:ILE:HD11	2.34	0.62
2:I:31:SER:HA	2:I:105:MET:HE2	1.82	0.62
4:U:1:NAG:H62	4:U:2:NAG:H82	1.82	0.62
1:B:745:ASP:OD1	1:B:745:ASP:N	2.32	0.62
3:L:136:LEU:HB2	3:L:182:LEU:HB3	1.82	0.62
4:Y:1:NAG:H62	4:Y:2:NAG:H82	1.82	0.62
1:A:745:ASP:N	1:A:745:ASP:OD1	2.32	0.61
3:M:145:PRO:HG2	3:M:201:HIS:CE1	2.35	0.61
3:L:125:SER:O	3:L:129:LEU:HG	1.99	0.61
1:C:111:ASP:OD2	1:C:113:LYS:NZ	2.33	0.61
1:A:111:ASP:OD2	1:A:113:LYS:NZ	2.33	0.61
1:B:102:ARG:NH2	1:B:154:GLU:OE1	2.33	0.61
1:B:940:SER:C	1:B:941:THR:HG1	2.03	0.61
1:C:156:GLU:OE1	1:C:246:ARG:NH1	2.34	0.61
1:A:253:ASP:OD1	1:A:253:ASP:N	2.31	0.61
1:B:156:GLU:OE1	1:B:246:ARG:NH1	2.34	0.61
4:d:1:NAG:H62	4:d:2:NAG:H82	1.82	0.61
3:N:100:VAL:HG22	3:N:101:PHE:N	2.16	0.61
1:C:813:SER:C	1:C:814:LYS:HD2	2.26	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:31:SER:HA	2:H:105:MET:HE2	1.82	0.61
2:I:161:VAL:HG22	2:I:207:VAL:HG22	1.81	0.61
2:H:175:PHE:CZ	3:L:139:LEU:HD23	2.36	0.61
3:N:136:LEU:HB2	3:N:182:LEU:HB3	1.82	0.61
1:A:156:GLU:OE1	1:A:246:ARG:NH1	2.34	0.61
1:B:124:THR:CG2	5:B:1302:NAG:H83	2.28	0.61
1:B:813:SER:C	1:B:814:LYS:HD2	2.26	0.61
3:M:100:VAL:HG22	3:M:101:PHE:N	2.16	0.61
3:M:136:LEU:HB2	3:M:182:LEU:HB3	1.82	0.60
1:C:389:ASP:OD1	1:C:528:LYS:HE3	2.01	0.60
1:A:102:ARG:NH2	1:A:154:GLU:OE1	2.33	0.60
1:B:485:GLY:CA	2:I:52:TYR:CD2	2.70	0.60
1:A:813:SER:C	1:A:814:LYS:HD2	2.26	0.60
1:C:102:ARG:NH2	1:C:154:GLU:OE1	2.34	0.60
1:C:745:ASP:OD1	1:C:745:ASP:N	2.32	0.60
2:J:31:SER:HA	2:J:105:MET:HE2	1.82	0.60
3:L:51:SER:OG	3:L:52:GLU:N	2.34	0.60
2:I:175:PHE:CZ	3:M:139:LEU:HD23	2.36	0.60
2:J:175:PHE:CZ	3:N:139:LEU:HD23	2.36	0.60
6:B:1311:EIC:H62	1:C:377:PHE:CE1	2.36	0.60
1:B:253:ASP:OD1	1:B:253:ASP:N	2.31	0.60
1:A:940:SER:C	1:A:941:THR:HG1	2.01	0.60
3:L:100:VAL:HG22	3:L:101:PHE:N	2.15	0.60
1:C:485:GLY:CA	2:J:52:TYR:CD2	2.70	0.60
4:K:1:NAG:H62	4:K:2:NAG:H82	1.84	0.60
1:B:814:LYS:HD2	1:B:814:LYS:N	2.18	0.59
3:L:17:SER:HA	3:L:77:VAL:O	2.02	0.59
3:L:112:GLN:HB2	3:L:113:PRO:CD	2.32	0.59
2:I:175:PHE:CE1	3:M:139:LEU:CD2	2.81	0.59
3:M:17:SER:HA	3:M:77:VAL:O	2.02	0.59
3:N:112:GLN:HB2	3:N:113:PRO:CD	2.32	0.59
1:C:814:LYS:HD2	1:C:814:LYS:N	2.18	0.59
3:M:110:LEU:HD11	3:M:114:LYS:HE2	1.85	0.59
3:N:17:SER:HA	3:N:77:VAL:O	2.02	0.59
3:N:110:LEU:HD11	3:N:114:LYS:HE2	1.84	0.59
1:A:69:HIS:O	1:A:70:VAL:HG23	2.03	0.59
1:A:814:LYS:HD2	1:A:814:LYS:N	2.17	0.59
1:B:70:VAL:N	1:B:76:THR:O	2.29	0.59
1:C:69:HIS:O	1:C:70:VAL:HG23	2.03	0.59
3:L:110:LEU:HD11	3:L:114:LYS:HE2	1.84	0.59
1:B:69:HIS:O	1:B:70:VAL:HG23	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:VAL:N	1:A:76:THR:O	2.29	0.58
1:A:370:ASN:ND2	2:J:29:PHE:HE1	2.01	0.58
1:C:91:TYR:OH	1:C:191:GLU:OE1	2.20	0.58
1:C:777:ASN:OD1	1:C:1019:ARG:NH1	2.31	0.58
2:H:188:SER:HB2	3:L:181:TYR:OH	2.04	0.58
2:J:188:SER:HB2	3:N:181:TYR:OH	2.04	0.58
1:C:393:THR:HG21	1:C:519:HIS:O	2.02	0.58
1:B:358:ILE:CB	1:B:395:VAL:HG12	2.34	0.58
2:I:188:SER:HB2	3:M:181:TYR:OH	2.04	0.58
3:M:153:LYS:HG2	3:M:154:GLY:O	2.03	0.58
3:M:117:PRO:HD3	3:M:201:HIS:HD2	1.69	0.58
4:U:1:NAG:C6	4:U:2:NAG:C7	2.80	0.58
2:I:157:GLU:H	2:I:157:GLU:CD	2.12	0.57
3:N:51:SER:OG	3:N:52:GLU:N	2.34	0.57
2:H:157:GLU:CD	2:H:157:GLU:H	2.12	0.57
1:C:358:ILE:CB	1:C:395:VAL:HG12	2.34	0.57
3:L:117:PRO:HD3	3:L:201:HIS:HD2	1.69	0.57
1:A:811:LYS:HB2	1:A:813:SER:O	2.04	0.57
1:B:124:THR:OG1	1:B:125:ASN:OD1	2.22	0.57
1:B:391:CYS:HB3	1:B:522:ALA:HB3	1.85	0.57
3:N:153:LYS:HG2	3:N:154:GLY:O	2.03	0.57
1:A:358:ILE:CB	1:A:395:VAL:HG12	2.34	0.57
1:B:811:LYS:HB2	1:B:813:SER:O	2.04	0.57
3:L:153:LYS:HG2	3:L:154:GLY:O	2.03	0.57
1:A:124:THR:OG1	1:A:125:ASN:OD1	2.22	0.57
3:M:112:GLN:HB2	3:M:113:PRO:CD	2.32	0.57
3:N:25:THR:OG1	3:N:26:SER:N	2.37	0.57
1:C:811:LYS:O	1:C:814:LYS:NZ	2.38	0.57
3:N:9:SER:OG	3:N:147:ALA:CB	2.52	0.57
3:N:117:PRO:HD3	3:N:201:HIS:HD2	1.69	0.57
1:B:91:TYR:OH	1:B:191:GLU:OE1	2.20	0.57
2:J:157:GLU:CD	2:J:157:GLU:H	2.12	0.57
1:B:777:ASN:OD1	1:B:1019:ARG:NH1	2.32	0.57
3:L:9:SER:OG	3:L:147:ALA:CB	2.52	0.57
3:L:25:THR:OG1	3:L:26:SER:N	2.37	0.57
1:A:811:LYS:O	1:A:814:LYS:NZ	2.38	0.56
1:C:66:HIS:O	1:C:67:ALA:HB2	2.05	0.56
1:C:124:THR:OG1	1:C:125:ASN:OD1	2.22	0.56
1:C:811:LYS:HB2	1:C:813:SER:O	2.04	0.56
4:F:2:NAG:H3	4:F:2:NAG:H83	1.87	0.56
1:A:777:ASN:OD1	1:A:1019:ARG:NH1	2.32	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:485:GLY:CA	2:I:52:TYR:HE2	2.15	0.56
1:C:519:HIS:O	1:C:520:ALA:HB3	2.05	0.56
3:M:9:SER:CB	3:M:147:ALA:HB1	2.33	0.56
3:M:9:SER:OG	3:M:147:ALA:CB	2.52	0.56
1:C:388:ASN:CB	1:C:527:PRO:HD2	2.33	0.56
2:J:122:SER:O	2:J:123:ALA:HB3	2.06	0.56
1:A:361:CYS:O	1:A:524:VAL:O	2.24	0.56
1:B:105:ILE:HG22	1:B:118:LEU:HD12	1.88	0.56
1:B:811:LYS:O	1:B:814:LYS:NZ	2.38	0.56
3:N:207:GLU:OE1	3:N:209:THR:OG1	2.24	0.56
4:a:2:NAG:H3	4:a:2:NAG:H83	1.87	0.56
1:C:337:PRO:HB2	1:C:340:GLU:HG2	1.88	0.56
3:L:207:GLU:OE1	3:L:209:THR:OG1	2.24	0.56
1:A:388:ASN:CB	1:A:527:PRO:HD2	2.33	0.55
2:I:208:ASN:HD22	2:I:210:LYS:HE3	1.72	0.55
3:M:207:GLU:OE1	3:M:209:THR:OG1	2.24	0.55
2:H:128:PRO:HB2	2:H:151:VAL:HG23	1.88	0.55
1:A:370:ASN:ND2	2:J:29:PHE:CE1	2.74	0.55
2:I:122:SER:O	2:I:123:ALA:HB3	2.06	0.55
2:I:175:PHE:CD1	3:M:139:LEU:HD23	2.41	0.55
3:M:163:VAL:HA	3:M:181:TYR:O	2.07	0.55
1:A:341:VAL:C	1:A:342:PHE:HD1	2.14	0.55
1:C:105:ILE:HG22	1:C:118:LEU:HD12	1.88	0.55
2:J:175:PHE:CD1	3:N:139:LEU:HD23	2.41	0.55
1:B:66:HIS:O	1:B:67:ALA:HB2	2.05	0.55
1:B:960:ASN:O	1:B:964:LYS:HG3	2.06	0.55
2:H:122:SER:O	2:H:123:ALA:HB3	2.06	0.55
1:A:91:TYR:OH	1:A:191:GLU:OE1	2.20	0.55
1:B:212:LEU:HD22	1:B:217:PRO:HG3	1.89	0.55
3:N:110:LEU:HA	3:N:144:TYR:HE2	1.71	0.55
3:N:163:VAL:HA	3:N:181:TYR:O	2.07	0.55
1:A:360:ASN:HA	1:A:523:THR:O	2.07	0.55
1:C:941:THR:HG22	1:C:941:THR:O	2.06	0.55
2:I:128:PRO:HB2	2:I:151:VAL:HG23	1.88	0.55
3:M:51:SER:OG	3:M:52:GLU:N	2.34	0.55
1:A:61:ASN:OD1	5:A:1301:NAG:H82	2.07	0.55
3:L:163:VAL:HA	3:L:181:TYR:O	2.07	0.55
1:A:212:LEU:HD22	1:A:217:PRO:HG3	1.89	0.55
1:A:485:GLY:CA	2:H:52:TYR:HE2	2.15	0.55
2:J:128:PRO:HB2	2:J:151:VAL:HG23	1.88	0.55
3:N:94:ALA:HB3	3:N:98:ASN:CB	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:f:2:NAG:H3	4:f:2:NAG:H83	1.87	0.55
2:J:208:ASN:HD22	2:J:210:LYS:HE3	1.72	0.55
6:A:1312:EIC:H91	1:B:387:LEU:HD13	1.89	0.54
1:B:941:THR:HG22	1:B:941:THR:O	2.06	0.54
3:M:110:LEU:CB	3:M:144:TYR:CD2	2.77	0.54
1:A:105:ILE:HG22	1:A:118:LEU:HD12	1.88	0.54
1:A:337:PRO:HB2	1:A:340:GLU:HG2	1.89	0.54
1:A:341:VAL:C	1:A:342:PHE:CD1	2.86	0.54
1:A:804:GLN:O	1:A:818:ILE:HG12	2.07	0.54
1:C:339:GLY:O	1:C:343:ASN:HB3	2.08	0.54
3:L:9:SER:CB	3:L:147:ALA:HB1	2.33	0.54
3:M:110:LEU:HA	3:M:144:TYR:HE2	1.71	0.54
1:A:66:HIS:O	1:A:67:ALA:HB2	2.05	0.54
1:A:514:SER:O	1:A:515:PHE:HB3	2.05	0.54
1:C:960:ASN:O	1:C:964:LYS:HG3	2.06	0.54
3:L:97:ASN:OD1	3:L:97:ASN:N	2.39	0.54
3:N:9:SER:OG	3:N:147:ALA:HB1	2.07	0.54
1:B:337:PRO:HB2	1:B:340:GLU:HG2	1.89	0.54
1:B:804:GLN:O	1:B:818:ILE:HG12	2.07	0.54
3:M:25:THR:OG1	3:M:26:SER:N	2.37	0.54
3:N:97:ASN:OD1	3:N:97:ASN:N	2.39	0.54
1:A:1142:GLN:HB2	1:A:1143:PRO:HD3	1.89	0.54
1:B:1142:GLN:HB2	1:B:1143:PRO:HD3	1.89	0.54
2:H:175:PHE:CD1	3:L:139:LEU:HD23	2.41	0.54
2:H:208:ASN:HD22	2:H:210:LYS:HE3	1.72	0.54
6:A:1312:EIC:H182	1:B:358:ILE:HD12	1.89	0.54
1:C:188:ASN:ND2	1:C:207:HIS:HE1	2.05	0.54
3:M:16:GLN:O	3:M:79:GLY:N	2.37	0.54
1:A:960:ASN:O	1:A:964:LYS:HG3	2.06	0.54
1:C:61:ASN:OD1	5:C:1301:NAG:H82	2.07	0.54
1:C:1142:GLN:HB2	1:C:1143:PRO:HD3	1.89	0.54
2:H:148:GLY:HA2	2:H:163:TRP:HZ2	1.73	0.54
3:L:9:SER:OG	3:L:147:ALA:HB1	2.07	0.54
3:L:110:LEU:HA	3:L:144:TYR:HE2	1.71	0.54
3:M:97:ASN:N	3:M:97:ASN:OD1	2.39	0.54
1:A:153:MET:HE2	5:A:1303:NAG:HN2	1.73	0.54
1:A:941:THR:O	1:A:941:THR:HG22	2.06	0.54
1:B:153:MET:HE2	5:B:1303:NAG:HN2	1.72	0.54
2:J:135:PRO:HG3	2:J:147:LEU:HD23	1.89	0.54
1:B:188:ASN:ND2	1:B:207:HIS:HE1	2.05	0.54
1:C:392:PHE:CD1	1:C:517:LEU:HD21	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:9:SER:OG	3:M:147:ALA:HB1	2.07	0.54
1:A:365:TYR:HB2	6:A:1311:EIC:H51	1.90	0.54
1:B:61:ASN:OD1	5:B:1301:NAG:H82	2.07	0.54
4:Z:2:NAG:H3	4:Z:2:NAG:H83	1.90	0.54
2:H:135:PRO:HG3	2:H:147:LEU:HD23	1.89	0.53
3:L:94:ALA:HB3	3:L:98:ASN:CB	2.37	0.53
2:I:135:PRO:HG3	2:I:147:LEU:HD23	1.89	0.53
4:V:2:NAG:H83	4:V:2:NAG:H3	1.90	0.53
1:C:212:LEU:HD22	1:C:217:PRO:HG3	1.89	0.53
4:e:2:NAG:H83	4:e:2:NAG:H3	1.90	0.53
3:N:9:SER:CB	3:N:147:ALA:HB1	2.33	0.53
1:A:188:ASN:ND2	1:A:207:HIS:HE1	2.05	0.53
1:A:818:ILE:HB	1:A:1054:GLN:HE21	1.73	0.53
1:C:940:SER:C	1:C:941:THR:HG1	2.03	0.53
1:B:393:THR:OG1	1:B:516:GLU:HB2	2.07	0.53
2:I:148:GLY:HA2	2:I:163:TRP:HZ2	1.73	0.53
2:J:148:GLY:HA2	2:J:163:TRP:HZ2	1.73	0.53
4:d:1:NAG:C6	4:d:2:NAG:C7	2.80	0.53
1:A:515:PHE:CD1	1:A:515:PHE:C	2.86	0.53
1:B:1118:ASP:N	1:B:1118:ASP:OD1	2.42	0.53
1:C:1118:ASP:OD1	1:C:1118:ASP:N	2.42	0.53
2:I:123:ALA:O	2:I:124:SER:OG	2.25	0.53
3:M:188:GLN:HA	3:M:191:SER:HB3	1.91	0.53
1:C:153:MET:HE2	5:C:1303:NAG:HN2	1.72	0.53
3:L:135:THR:HA	3:L:182:LEU:O	2.09	0.53
1:A:342:PHE:CD1	1:A:342:PHE:N	2.77	0.53
1:C:360:ASN:HA	1:C:523:THR:O	2.09	0.53
2:H:125:THR:OG1	2:H:156:PRO:CG	2.57	0.53
3:M:94:ALA:HB3	3:M:98:ASN:CB	2.37	0.53
1:C:485:GLY:CA	2:J:52:TYR:HE2	2.15	0.52
3:M:135:THR:HA	3:M:182:LEU:O	2.09	0.52
2:J:125:THR:OG1	2:J:156:PRO:CG	2.57	0.52
3:N:135:THR:HA	3:N:182:LEU:O	2.09	0.52
1:B:188:ASN:HD22	1:B:207:HIS:HE1	1.57	0.52
2:I:125:THR:OG1	2:I:156:PRO:CG	2.57	0.52
1:C:188:ASN:HD22	1:C:207:HIS:HE1	1.57	0.52
3:M:109:VAL:O	3:M:109:VAL:HG13	2.09	0.52
1:A:188:ASN:HD22	1:A:207:HIS:HE1	1.58	0.52
1:C:361:CYS:O	1:C:524:VAL:O	2.28	0.52
2:H:132:PRO:O	3:L:125:SER:HB3	2.10	0.52
3:L:109:VAL:O	3:L:109:VAL:HG13	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:841:LEU:HD12	1:C:588:THR:HG21	1.91	0.52
1:A:1142:GLN:N	1:A:1143:PRO:CD	2.73	0.52
1:B:713:ALA:HB3	1:C:894:LEU:HB3	1.92	0.52
3:N:110:LEU:HA	3:N:144:TYR:CE2	2.45	0.52
1:B:486:PHE:N	2:I:52:TYR:CE2	2.78	0.52
3:L:110:LEU:HA	3:L:144:TYR:CE2	2.45	0.52
1:A:486:PHE:N	2:H:52:TYR:CE2	2.78	0.51
1:C:390:LEU:HD13	1:C:517:LEU:HD22	1.92	0.51
2:H:138:LYS:HD2	3:L:210:VAL:HG13	1.92	0.51
2:J:132:PRO:O	3:N:125:SER:HB3	2.10	0.51
1:A:792:PRO:HG3	1:C:707:TYR:HB3	1.92	0.51
1:B:361:CYS:O	1:B:524:VAL:O	2.27	0.51
1:C:370:ASN:ND2	2:I:29:PHE:HE1	2.07	0.51
3:L:188:GLN:HA	3:L:191:SER:HB3	1.91	0.51
1:C:1142:GLN:N	1:C:1143:PRO:CD	2.73	0.51
3:N:50:ILE:HD13	3:N:75:LEU:HD11	1.92	0.51
4:Y:1:NAG:C6	4:Y:2:NAG:C7	2.80	0.51
3:L:16:GLN:O	3:L:79:GLY:N	2.37	0.51
1:B:355:ARG:HH21	1:B:355:ARG:CG	2.08	0.51
1:B:1142:GLN:N	1:B:1143:PRO:CD	2.73	0.51
1:C:19:THR:O	1:C:20:THR:OG1	2.27	0.51
1:C:818:ILE:HB	1:C:1054:GLN:HE21	1.76	0.51
3:M:110:LEU:HA	3:M:144:TYR:CE2	2.45	0.51
3:N:188:GLN:HA	3:N:191:SER:HB3	1.91	0.51
2:J:138:LYS:HD2	3:N:210:VAL:HG13	1.92	0.51
1:B:642:VAL:HG13	1:B:651:ILE:HG12	1.93	0.51
2:I:132:PRO:O	3:M:125:SER:HB3	2.10	0.51
3:M:50:ILE:HD13	3:M:75:LEU:HD11	1.92	0.51
3:N:109:VAL:O	3:N:109:VAL:HG13	2.09	0.51
1:B:835:LYS:HD3	1:B:851:CYS:SG	2.51	0.51
1:C:486:PHE:N	2:J:52:TYR:CE2	2.78	0.51
3:L:50:ILE:HD13	3:L:75:LEU:HD11	1.92	0.51
1:A:309:GLU:O	1:A:313:TYR:OH	2.27	0.51
1:A:898:PHE:HB3	1:A:899:PRO:HD3	1.93	0.51
1:B:804:GLN:NE2	4:Z:1:NAG:O6	2.44	0.51
3:L:110:LEU:CB	3:L:144:TYR:CD2	2.77	0.51
1:A:213:VAL:HG23	1:A:214:ARG:HG2	1.93	0.50
1:A:804:GLN:NE2	4:V:1:NAG:O6	2.44	0.50
1:C:642:VAL:HG13	1:C:651:ILE:HG12	1.93	0.50
1:B:358:ILE:HG13	1:B:395:VAL:HG12	1.94	0.50
2:I:138:LYS:HD2	3:M:210:VAL:HG13	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1118:ASP:OD1	1:A:1118:ASP:N	2.42	0.50
3:L:110:LEU:HB2	3:L:144:TYR:CE2	2.38	0.50
2:I:164:ASN:ND2	2:I:202:THR:O	2.45	0.50
2:J:164:ASN:ND2	2:J:202:THR:O	2.45	0.50
3:N:28:ASP:OD1	3:N:28:ASP:N	2.45	0.50
3:N:110:LEU:CA	3:N:144:TYR:CE2	2.88	0.50
1:A:835:LYS:HD3	1:A:851:CYS:SG	2.51	0.50
1:B:32:PHE:CD2	1:B:218:GLN:HG2	2.47	0.50
1:C:358:ILE:HG13	1:C:395:VAL:HG12	1.94	0.50
1:C:835:LYS:HD3	1:C:851:CYS:SG	2.51	0.50
3:N:110:LEU:HB2	3:N:144:TYR:CE2	2.38	0.50
1:A:370:ASN:CG	2:J:29:PHE:CE1	2.78	0.50
1:A:804:GLN:O	1:A:817:PRO:HD2	2.12	0.50
1:B:213:VAL:HG23	1:B:214:ARG:HG2	1.93	0.50
1:B:454:ARG:NH2	1:B:467:ASP:O	2.43	0.50
1:A:645:THR:CG2	1:A:670:ILE:HG13	2.42	0.50
2:H:176:PRO:HB2	3:L:166:THR:HG21	1.94	0.50
1:B:645:THR:CG2	1:B:670:ILE:HG13	2.42	0.50
1:C:804:GLN:NE2	4:e:1:NAG:O6	2.44	0.50
2:I:107:GLY:O	3:M:99:TRP:CH2	2.60	0.50
3:M:110:LEU:HB2	3:M:144:TYR:CE2	2.38	0.50
3:N:121:LEU:HD21	3:N:136:LEU:HD12	1.94	0.50
1:A:69:HIS:CE1	1:A:70:VAL:HG22	2.47	0.49
1:C:32:PHE:CD2	1:C:218:GLN:HG2	2.47	0.49
1:C:213:VAL:HG23	1:C:214:ARG:HG2	1.93	0.49
1:C:710:ASN:C	1:C:710:ASN:HD22	2.20	0.49
2:H:164:ASN:ND2	2:H:202:THR:O	2.45	0.49
1:A:32:PHE:CD2	1:A:218:GLN:HG2	2.47	0.49
1:C:69:HIS:CE1	1:C:70:VAL:HG22	2.47	0.49
1:A:710:ASN:HD22	1:A:710:ASN:C	2.20	0.49
1:A:1145:LEU:HD23	1:A:1145:LEU:N	2.26	0.49
2:J:128:PRO:HD3	2:J:209:HIS:HD1	1.77	0.49
1:B:392:PHE:CD1	1:B:517:LEU:HD21	2.48	0.49
1:C:79:PHE:CZ	1:C:244:LEU:HD13	2.48	0.49
1:A:362:VAL:HG22	1:A:526:GLY:O	2.13	0.49
1:A:567:ARG:HD2	1:B:42:VAL:HG11	1.95	0.49
1:B:898:PHE:HB3	1:B:899:PRO:HD3	1.94	0.49
1:C:1145:LEU:HD23	1:C:1145:LEU:N	2.26	0.49
2:J:58:PHE:CD2	3:N:97:ASN:ND2	2.64	0.49
1:A:79:PHE:CZ	1:A:244:LEU:HD13	2.48	0.49
1:B:69:HIS:CE1	1:B:70:VAL:HG22	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:128:PRO:HD3	2:H:209:HIS:HD1	1.78	0.49
3:M:121:LEU:HD21	3:M:136:LEU:HD12	1.94	0.49
3:M:109:VAL:O	3:M:109:VAL:HG22	2.13	0.49
2:J:176:PRO:HB2	3:N:166:THR:HG21	1.94	0.49
1:A:117:LEU:HD13	1:A:130:VAL:HG22	1.95	0.49
1:B:109:THR:OG1	1:B:114:THR:OG1	2.31	0.49
1:B:198:ASP:N	1:B:198:ASP:OD1	2.46	0.49
1:B:1145:LEU:HD23	1:B:1145:LEU:N	2.26	0.49
2:I:128:PRO:HD3	2:I:209:HIS:HD1	1.78	0.49
1:A:42:VAL:HG11	1:C:567:ARG:HD2	1.95	0.48
1:C:645:THR:CG2	1:C:670:ILE:HG13	2.42	0.48
3:L:201:HIS:CE1	3:L:202:GLU:HG2	2.48	0.48
1:C:370:ASN:ND2	2:I:29:PHE:CE1	2.81	0.48
3:L:28:ASP:N	3:L:28:ASP:OD1	2.45	0.48
3:N:109:VAL:O	3:N:109:VAL:HG22	2.13	0.48
1:A:396:TYR:CZ	1:B:230:PRO:HG3	2.49	0.48
1:B:360:ASN:HA	1:B:523:THR:O	2.14	0.48
3:N:201:HIS:CE1	3:N:202:GLU:HG2	2.48	0.48
1:A:198:ASP:OD1	1:A:198:ASP:N	2.46	0.48
1:A:642:VAL:HG13	1:A:651:ILE:HG12	1.93	0.48
1:C:109:THR:OG1	1:C:114:THR:OG1	2.31	0.48
1:C:117:LEU:HD13	1:C:130:VAL:HG22	1.95	0.48
3:L:172:SER:O	3:L:174:ASN:ND2	2.47	0.48
2:I:176:PRO:HB2	3:M:166:THR:HG21	1.94	0.48
3:M:28:ASP:OD1	3:M:28:ASP:N	2.45	0.48
1:C:454:ARG:NH2	1:C:467:ASP:O	2.43	0.48
3:L:121:LEU:HD21	3:L:136:LEU:HD12	1.94	0.48
3:N:193:ARG:O	3:N:212:PRO:HD2	2.13	0.48
1:B:391:CYS:HB3	1:B:522:ALA:CB	2.43	0.48
1:B:710:ASN:C	1:B:710:ASN:HD22	2.20	0.48
1:C:533:LEU:HD21	1:C:585:LEU:HD11	1.96	0.48
1:A:358:ILE:HG13	1:A:395:VAL:HG12	1.94	0.48
1:A:533:LEU:HD21	1:A:585:LEU:HD11	1.96	0.48
2:H:159:VAL:HG22	2:H:209:HIS:CD2	2.49	0.48
3:L:109:VAL:O	3:L:109:VAL:HG22	2.13	0.48
3:L:190:LYS:NZ	3:L:213:THR:OG1	2.47	0.48
3:L:193:ARG:O	3:L:212:PRO:HD2	2.13	0.48
2:I:159:VAL:HG22	2:I:209:HIS:CD2	2.49	0.48
3:N:110:LEU:CB	3:N:144:TYR:CD2	2.77	0.48
1:A:109:THR:OG1	1:A:114:THR:OG1	2.31	0.48
1:B:309:GLU:O	1:B:313:TYR:OH	2.27	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:58:PHE:CD2	3:L:97:ASN:ND2	2.64	0.48
3:M:201:HIS:CE1	3:M:202:GLU:HG2	2.48	0.48
1:B:117:LEU:HD13	1:B:130:VAL:HG22	1.95	0.47
1:B:360:ASN:HA	1:B:523:THR:HB	1.95	0.47
1:C:309:GLU:O	1:C:313:TYR:OH	2.27	0.47
3:M:190:LYS:NZ	3:M:213:THR:OG1	2.47	0.47
3:M:193:ARG:O	3:M:212:PRO:HD2	2.13	0.47
2:J:159:VAL:HG22	2:J:209:HIS:CD2	2.49	0.47
3:N:190:LYS:NZ	3:N:213:THR:OG1	2.47	0.47
1:B:533:LEU:HD21	1:B:585:LEU:HD11	1.96	0.47
1:C:388:ASN:HB2	1:C:527:PRO:CG	2.44	0.47
2:J:140:THR:HG23	2:J:145:ALA:HB2	1.96	0.47
3:N:110:LEU:HB2	3:N:144:TYR:HE2	1.67	0.47
3:N:172:SER:O	3:N:174:ASN:ND2	2.47	0.47
1:B:388:ASN:CB	1:B:527:PRO:CD	2.89	0.47
5:C:1306:NAG:H83	5:C:1306:NAG:O3	2.15	0.47
2:J:156:PRO:HB2	2:J:209:HIS:NE2	2.29	0.47
1:A:342:PHE:HD1	1:A:342:PHE:N	2.11	0.47
1:A:1051:SER:OG	1:A:1064:HIS:HD2	1.97	0.47
1:B:79:PHE:CZ	1:B:244:LEU:HD13	2.48	0.47
1:B:358:ILE:CB	1:B:395:VAL:CG1	2.91	0.47
5:B:1306:NAG:H83	5:B:1306:NAG:O3	2.15	0.47
1:A:69:HIS:HD2	1:A:259:THR:OG1	1.98	0.47
2:H:140:THR:HG23	2:H:145:ALA:HB2	1.97	0.47
3:M:172:SER:O	3:M:174:ASN:ND2	2.47	0.47
1:A:245:HIS:HB2	1:A:259:THR:HG22	1.97	0.47
1:A:341:VAL:HG12	1:A:341:VAL:O	2.13	0.47
1:B:197:ILE:HD12	1:B:202:LYS:HD2	1.97	0.47
1:B:455:LEU:HD21	1:C:370:ASN:HB3	1.95	0.47
1:C:197:ILE:HD12	1:C:202:LYS:HD2	1.96	0.47
1:B:370:ASN:ND2	2:H:29:PHE:HE1	2.13	0.47
1:B:818:ILE:HB	1:B:1054:GLN:HE21	1.79	0.47
1:B:986:PRO:O	1:B:990:GLU:HG3	2.15	0.47
1:C:986:PRO:O	1:C:990:GLU:HG3	2.15	0.47
5:C:1309:NAG:H3	5:C:1309:NAG:H83	1.96	0.47
3:N:123:PRO:HA	3:N:136:LEU:HD13	1.97	0.47
1:A:130:VAL:HG21	1:A:231:ILE:HG22	1.97	0.47
3:M:154:GLY:O	3:M:156:SER:N	2.48	0.47
3:N:164:GLU:O	3:N:180:SER:HA	2.15	0.47
1:C:386:LYS:HE3	1:C:386:LYS:HB3	1.73	0.47
1:A:147:LYS:HE3	1:A:147:LYS:HB3	1.58	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:413:GLY:O	1:B:414:GLN:NE2	2.48	0.47
1:B:1051:SER:OG	1:B:1064:HIS:HD2	1.97	0.47
1:C:37:TYR:OH	1:C:54:LEU:O	2.25	0.47
1:C:1051:SER:OG	1:C:1064:HIS:HD2	1.97	0.47
3:M:56:ARG:HH12	3:M:62:ASP:HA	1.80	0.47
2:J:123:ALA:O	2:J:124:SER:OG	2.26	0.47
1:A:19:THR:O	1:A:20:THR:OG1	2.27	0.46
1:A:197:ILE:HD12	1:A:202:LYS:HD2	1.96	0.46
1:A:413:GLY:O	1:A:414:GLN:NE2	2.48	0.46
5:A:1306:NAG:O3	5:A:1306:NAG:H83	2.15	0.46
3:N:154:GLY:O	3:N:156:SER:N	2.48	0.46
1:B:69:HIS:HD2	1:B:259:THR:OG1	1.97	0.46
1:B:245:HIS:HB2	1:B:259:THR:HG22	1.97	0.46
1:B:617:CYS:HB3	1:B:633:TRP:CE2	2.50	0.46
1:B:938:LEU:C	1:B:940:SER:N	2.73	0.46
1:C:245:HIS:HB2	1:C:259:THR:HG22	1.97	0.46
1:C:898:PHE:N	1:C:899:PRO:CD	2.77	0.46
3:L:56:ARG:HH12	3:L:62:ASP:HA	1.80	0.46
2:I:140:THR:HG23	2:I:145:ALA:HB2	1.97	0.46
3:N:52:GLU:O	3:N:54:SER:N	2.49	0.46
1:A:401:VAL:HG22	1:A:509:ARG:HG2	1.97	0.46
1:C:130:VAL:HG21	1:C:231:ILE:HG22	1.97	0.46
1:C:198:ASP:OD1	1:C:198:ASP:N	2.46	0.46
3:L:123:PRO:HA	3:L:136:LEU:HD13	1.97	0.46
3:L:164:GLU:O	3:L:180:SER:HA	2.15	0.46
2:I:156:PRO:HB2	2:I:209:HIS:NE2	2.29	0.46
1:C:413:GLY:O	1:C:414:GLN:NE2	2.48	0.46
1:C:617:CYS:HB3	1:C:633:TRP:CE2	2.50	0.46
1:C:69:HIS:HD2	1:C:259:THR:OG1	1.98	0.46
2:H:156:PRO:HB2	2:H:209:HIS:NE2	2.30	0.46
4:Q:1:NAG:H62	4:Q:2:NAG:H82	1.96	0.46
1:B:69:HIS:CG	1:B:70:VAL:HG23	2.50	0.46
3:L:154:GLY:O	3:L:156:SER:N	2.48	0.46
2:I:136:SER:HB3	2:I:138:LYS:HG2	1.98	0.46
1:A:986:PRO:O	1:A:990:GLU:HG3	2.15	0.46
1:C:69:HIS:CG	1:C:70:VAL:HG23	2.50	0.46
3:L:52:GLU:O	3:L:54:SER:N	2.49	0.46
1:A:388:ASN:HB2	1:A:527:PRO:CG	2.44	0.46
3:M:52:GLU:O	3:M:54:SER:N	2.49	0.46
2:J:136:SER:HB3	2:J:138:LYS:HG2	1.98	0.46
1:A:707:TYR:HB3	1:B:792:PRO:HG3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:69:HIS:C	1:B:70:VAL:CG2	2.86	0.46
1:B:388:ASN:HB2	1:B:527:PRO:CG	2.45	0.46
1:B:518:LEU:HD13	1:B:518:LEU:N	2.30	0.46
6:B:1311:EIC:H142	6:B:1311:EIC:H112	1.65	0.46
1:C:1141:LEU:O	1:C:1144:GLU:HB2	2.16	0.46
3:L:133:LYS:HD2	3:L:133:LYS:HA	1.70	0.46
2:I:209:HIS:CD2	2:I:211:PRO:HD2	2.51	0.46
2:J:209:HIS:CD2	2:J:211:PRO:HD2	2.51	0.45
3:N:16:GLN:O	3:N:79:GLY:N	2.37	0.45
1:A:21:ARG:HH11	1:A:79:PHE:HB3	1.82	0.45
1:A:938:LEU:O	1:A:940:SER:N	2.50	0.45
1:B:938:LEU:O	1:B:940:SER:N	2.49	0.45
1:C:244:LEU:HA	1:C:244:LEU:HD12	1.74	0.45
1:C:401:VAL:HG22	1:C:509:ARG:HG2	1.97	0.45
1:C:1048:HIS:HA	1:C:1066:THR:HG22	1.98	0.45
2:H:96:ALA:HB1	2:H:109:PHE:HB3	1.99	0.45
3:N:52:GLU:OE2	3:N:55:LYS:NZ	2.43	0.45
1:A:971:GLY:O	1:A:995:ARG:NH1	2.47	0.45
5:C:1309:NAG:C8	5:C:1309:NAG:C3	2.87	0.45
2:H:209:HIS:CD2	2:H:211:PRO:HD2	2.51	0.45
3:M:145:PRO:HG2	3:M:201:HIS:HE1	1.80	0.45
1:A:596:SER:OG	1:A:613:GLN:OE1	2.34	0.45
1:A:1048:HIS:HA	1:A:1066:THR:HG22	1.98	0.45
6:B:1311:EIC:H52	1:C:374:PHE:CE2	2.49	0.45
3:M:123:PRO:HA	3:M:136:LEU:HD13	1.97	0.45
3:M:164:GLU:O	3:M:180:SER:HA	2.15	0.45
3:N:153:LYS:HE2	3:N:154:GLY:C	2.42	0.45
4:U:1:NAG:H5	4:U:2:NAG:O7	2.16	0.45
1:A:617:CYS:HB3	1:A:633:TRP:CE2	2.50	0.45
1:C:362:VAL:HG22	1:C:526:GLY:O	2.16	0.45
1:C:596:SER:OG	1:C:613:GLN:OE1	2.34	0.45
1:C:938:LEU:C	1:C:940:SER:N	2.73	0.45
3:M:52:GLU:OE2	3:M:55:LYS:NZ	2.43	0.45
3:N:56:ARG:HH12	3:N:62:ASP:HA	1.80	0.45
1:A:938:LEU:C	1:A:940:SER:N	2.73	0.45
1:B:401:VAL:HG22	1:B:509:ARG:HG2	1.97	0.45
1:C:83:VAL:HG22	1:C:239:GLN:NE2	2.32	0.45
3:L:96:SER:C	3:L:98:ASN:H	2.25	0.45
3:N:14:PRO:HA	3:N:80:LEU:HB2	1.98	0.45
1:A:69:HIS:CG	1:A:70:VAL:HG23	2.50	0.45
1:A:1141:LEU:O	1:A:1144:GLU:HB2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:394:ASN:O	1:B:515:PHE:HA	2.17	0.45
2:J:154:TYR:OH	2:J:187:LEU:HD23	2.17	0.45
4:Y:1:NAG:H5	4:Y:2:NAG:O7	2.16	0.45
1:A:355:ARG:HH21	1:A:355:ARG:CG	2.08	0.45
1:C:358:ILE:CB	1:C:395:VAL:CG1	2.91	0.45
2:H:154:TYR:OH	2:H:187:LEU:HD23	2.17	0.45
3:L:52:GLU:OE2	3:L:55:LYS:NZ	2.43	0.45
2:I:180:GLN:OE1	2:I:186:SER:OG	2.31	0.45
3:N:145:PRO:HG2	3:N:201:HIS:HE1	1.80	0.45
1:B:596:SER:OG	1:B:613:GLN:OE1	2.34	0.45
1:B:1141:LEU:O	1:B:1144:GLU:HB2	2.17	0.45
1:C:21:ARG:HH11	1:C:79:PHE:HB3	1.81	0.45
3:M:14:PRO:HA	3:M:80:LEU:HB2	1.98	0.45
3:M:153:LYS:HE2	3:M:154:GLY:C	2.42	0.45
4:D:1:NAG:H62	4:D:2:NAG:H82	1.99	0.45
4:d:1:NAG:H5	4:d:2:NAG:O7	2.16	0.45
1:A:83:VAL:HG22	1:A:239:GLN:NE2	2.32	0.45
1:B:130:VAL:HG21	1:B:231:ILE:HG22	1.97	0.45
1:B:1048:HIS:HA	1:B:1066:THR:HG22	1.98	0.45
2:H:26:GLY:O	2:H:97:ARG:NH2	2.50	0.45
3:L:14:PRO:HA	3:L:80:LEU:HB2	1.99	0.45
3:L:145:PRO:HG2	3:L:201:HIS:HE1	1.80	0.45
3:N:18:VAL:O	3:N:76:THR:HA	2.17	0.45
1:A:69:HIS:C	1:A:70:VAL:CG2	2.86	0.44
1:A:117:LEU:HD13	1:A:130:VAL:CG2	2.47	0.44
1:C:428:ASP:OD1	1:C:428:ASP:N	2.50	0.44
3:M:18:VAL:O	3:M:76:THR:HA	2.17	0.44
1:A:370:ASN:HB3	1:C:455:LEU:HD21	2.00	0.44
1:A:532:ASN:HD22	1:A:532:ASN:N	2.14	0.44
1:B:355:ARG:HG3	1:B:398:ASP:OD1	2.18	0.44
1:C:532:ASN:N	1:C:532:ASN:HD22	2.15	0.44
3:L:196:SER:HB2	3:L:208:LYS:O	2.17	0.44
2:I:21:SER:HA	2:I:78:LEU:O	2.17	0.44
1:A:818:ILE:HB	1:A:1054:GLN:NE2	2.32	0.44
1:B:130:VAL:HG21	1:B:231:ILE:CG2	2.48	0.44
1:C:726:ILE:HD12	1:C:945:LEU:HD22	1.99	0.44
1:C:938:LEU:O	1:C:940:SER:N	2.50	0.44
3:M:196:SER:HB2	3:M:208:LYS:O	2.17	0.44
1:A:96:GLU:OE1	1:A:101:ILE:HD12	2.18	0.44
1:A:455:LEU:HD21	1:B:370:ASN:HB3	1.98	0.44
1:A:726:ILE:HD12	1:A:945:LEU:HD22	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:96:GLU:OE1	1:C:101:ILE:HD12	2.18	0.44
5:C:1305:NAG:O7	5:C:1305:NAG:O3	2.32	0.44
2:I:154:TYR:OH	2:I:187:LEU:HD23	2.17	0.44
3:N:193:ARG:HD2	3:N:193:ARG:HA	1.67	0.44
1:A:130:VAL:HG21	1:A:231:ILE:CG2	2.48	0.44
1:A:394:ASN:O	1:A:515:PHE:HA	2.18	0.44
1:B:83:VAL:HG22	1:B:239:GLN:NE2	2.32	0.44
1:B:147:LYS:HE3	1:B:147:LYS:HB3	1.58	0.44
1:B:355:ARG:NH2	1:B:355:ARG:CG	2.73	0.44
1:B:370:ASN:ND2	2:H:29:PHE:CE1	2.86	0.44
1:C:117:LEU:HD13	1:C:130:VAL:CG2	2.47	0.44
1:C:785:VAL:HG23	1:C:787:GLN:H	1.83	0.44
2:H:136:SER:HB3	2:H:138:LYS:HG2	1.98	0.44
2:H:163:TRP:HD1	2:H:172:VAL:HG13	1.83	0.44
3:L:153:LYS:HE2	3:L:154:GLY:C	2.42	0.44
2:I:26:GLY:O	2:I:97:ARG:NH2	2.50	0.44
3:M:96:SER:C	3:M:98:ASN:H	2.25	0.44
2:J:180:GLN:OE1	2:J:186:SER:OG	2.31	0.44
4:b:1:NAG:H61	4:b:2:NAG:O7	2.18	0.44
1:B:21:ARG:HH11	1:B:79:PHE:HB3	1.81	0.44
1:B:532:ASN:N	1:B:532:ASN:HD22	2.14	0.44
1:B:726:ILE:HD12	1:B:945:LEU:HD22	1.99	0.44
2:I:110:ASP:OD1	2:I:110:ASP:N	2.46	0.44
3:M:110:LEU:HB2	3:M:144:TYR:HE2	1.67	0.44
3:N:112:GLN:HB2	3:N:113:PRO:HD2	2.00	0.44
3:N:170:LYS:HB3	3:N:170:LYS:HE2	1.79	0.44
4:g:1:NAG:H61	4:g:2:NAG:O7	2.18	0.44
1:A:358:ILE:CB	1:A:395:VAL:CG1	2.91	0.44
1:B:971:GLY:O	1:B:995:ARG:NH1	2.47	0.44
1:C:252:GLY:HA3	1:C:257:GLY:N	2.33	0.44
2:H:204:ILE:HG23	2:H:219:LYS:HD2	2.00	0.44
2:I:96:ALA:HB1	2:I:109:PHE:HB3	1.98	0.44
2:J:21:SER:HA	2:J:78:LEU:O	2.17	0.44
4:W:1:NAG:H61	4:W:2:NAG:O7	2.18	0.44
2:H:125:THR:OG1	2:H:156:PRO:HG3	2.18	0.44
3:M:112:GLN:HB2	3:M:113:PRO:HD2	2.00	0.44
2:J:26:GLY:O	2:J:97:ARG:NH2	2.50	0.44
1:A:517:LEU:C	1:A:518:LEU:HG	2.43	0.44
1:B:117:LEU:HD13	1:B:130:VAL:CG2	2.47	0.44
2:H:107:GLY:O	3:L:99:TRP:CH2	2.60	0.44
2:I:204:ILE:HG23	2:I:219:LYS:HD2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:125:THR:HA	2:J:155:PHE:HB3	2.00	0.44
3:N:96:SER:C	3:N:98:ASN:H	2.25	0.44
3:N:196:SER:HB2	3:N:208:LYS:O	2.17	0.44
1:B:785:VAL:HG23	1:B:787:GLN:H	1.83	0.43
1:C:503:VAL:HA	1:C:506:GLN:HG3	2.00	0.43
2:H:21:SER:HA	2:H:78:LEU:O	2.17	0.43
3:L:18:VAL:O	3:L:76:THR:HA	2.17	0.43
2:J:96:ALA:HB1	2:J:109:PHE:HB3	1.99	0.43
2:J:204:ILE:HG23	2:J:219:LYS:HD2	2.00	0.43
1:A:785:VAL:HG23	1:A:787:GLN:H	1.83	0.43
1:B:503:VAL:HA	1:B:506:GLN:HG3	2.00	0.43
1:C:355:ARG:HG3	1:C:398:ASP:OD1	2.18	0.43
3:M:9:SER:HB2	3:M:147:ALA:HB2	1.87	0.43
1:A:387:LEU:HD13	6:A:1311:EIC:H91	2.01	0.43
1:A:392:PHE:CD1	1:A:517:LEU:HD21	2.53	0.43
1:A:1142:GLN:N	1:A:1143:PRO:HD2	2.33	0.43
5:A:1305:NAG:O7	5:A:1305:NAG:O3	2.32	0.43
1:C:130:VAL:HG21	1:C:231:ILE:CG2	2.48	0.43
1:C:971:GLY:O	1:C:995:ARG:NH1	2.47	0.43
3:M:193:ARG:HA	3:M:193:ARG:HD2	1.67	0.43
5:A:1309:NAG:H3	5:A:1309:NAG:H83	1.96	0.43
1:B:362:VAL:HG22	1:B:526:GLY:O	2.18	0.43
5:B:1309:NAG:C8	5:B:1309:NAG:C3	2.87	0.43
2:H:123:ALA:O	2:H:124:SER:OG	2.26	0.43
1:A:370:ASN:OD1	1:A:370:ASN:N	2.49	0.43
1:A:454:ARG:NH2	1:A:467:ASP:O	2.43	0.43
1:B:96:GLU:OE1	1:B:101:ILE:HD12	2.18	0.43
1:B:252:GLY:HA3	1:B:257:GLY:N	2.33	0.43
1:A:355:ARG:HG3	1:A:398:ASP:OD1	2.18	0.43
1:A:503:VAL:HA	1:A:506:GLN:HG3	2.00	0.43
2:H:75:LYS:HE3	2:H:75:LYS:HB3	1.87	0.43
3:L:110:LEU:CA	3:L:144:TYR:CE2	2.88	0.43
3:L:124:PRO:HG2	3:L:134:ALA:HB1	2.01	0.43
3:M:185:THR:HG23	3:M:188:GLN:HB2	2.01	0.43
1:C:153:MET:CE	5:C:1303:NAG:HN2	2.32	0.43
2:J:156:PRO:HD2	2:J:209:HIS:CE1	2.54	0.43
1:A:396:TYR:OH	1:B:230:PRO:HG3	2.19	0.43
1:B:19:THR:O	1:B:20:THR:OG1	2.27	0.43
1:C:1142:GLN:N	1:C:1143:PRO:HD2	2.34	0.43
2:H:151:VAL:HG13	2:H:187:LEU:HG	2.00	0.43
3:L:96:SER:C	3:L:98:ASN:N	2.76	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:163:TRP:HD1	2:I:172:VAL:HG13	1.83	0.43
2:I:164:ASN:OD1	2:I:204:ILE:HG13	2.19	0.43
2:J:163:TRP:HD1	2:J:172:VAL:HG13	1.83	0.43
2:J:187:LEU:HD12	2:J:188:SER:N	2.34	0.43
1:A:1038:LYS:HA	1:A:1038:LYS:HD3	1.90	0.42
1:B:370:ASN:CG	2:H:29:PHE:CE1	2.90	0.42
1:C:913:GLN:H	1:C:913:GLN:HG3	1.63	0.42
2:H:122:SER:C	2:H:124:SER:H	2.27	0.42
2:H:164:ASN:OD1	2:H:204:ILE:HG13	2.19	0.42
3:L:185:THR:HG23	3:L:188:GLN:HB2	2.01	0.42
3:L:193:ARG:HD2	3:L:193:ARG:HA	1.67	0.42
2:I:125:THR:HA	2:I:155:PHE:HB3	2.00	0.42
3:M:121:LEU:HD23	3:M:122:PHE:N	2.34	0.42
3:N:121:LEU:HD23	3:N:122:PHE:N	2.34	0.42
1:A:153:MET:CE	5:A:1303:NAG:HN2	2.32	0.42
1:A:252:GLY:HA3	1:A:257:GLY:N	2.33	0.42
1:B:980:ILE:O	1:B:984:LEU:HB2	2.19	0.42
1:C:980:ILE:O	1:C:984:LEU:HB2	2.19	0.42
2:H:125:THR:HA	2:H:155:PHE:HB3	2.00	0.42
3:L:112:GLN:HB2	3:L:113:PRO:HD2	2.00	0.42
1:A:614:ASP:OD2	1:B:854:LYS:HE3	2.19	0.42
1:A:980:ILE:O	1:A:984:LEU:HB2	2.19	0.42
1:C:394:ASN:O	1:C:515:PHE:HA	2.19	0.42
1:C:804:GLN:O	1:C:817:PRO:HD2	2.20	0.42
2:J:151:VAL:HG13	2:J:187:LEU:HG	2.01	0.42
1:A:563:GLN:O	1:A:577:ARG:NH1	2.53	0.42
1:A:588:THR:HG21	1:B:841:LEU:HD12	2.02	0.42
1:B:1142:GLN:N	1:B:1143:PRO:HD2	2.33	0.42
1:C:370:ASN:CG	2:I:29:PHE:CE1	2.84	0.42
2:I:151:VAL:HG13	2:I:187:LEU:HG	2.00	0.42
2:I:187:LEU:HD12	2:I:188:SER:N	2.34	0.42
1:A:752:LEU:HD21	1:A:990:GLU:OE2	2.20	0.42
1:B:177:MET:HE3	1:B:177:MET:HB3	1.87	0.42
1:C:746:SER:HB3	1:C:749:CYS:HB3	2.02	0.42
2:I:125:THR:OG1	2:I:156:PRO:HG3	2.18	0.42
2:I:156:PRO:HD2	2:I:209:HIS:CE1	2.54	0.42
3:M:96:SER:C	3:M:98:ASN:N	2.77	0.42
3:M:186:PRO:HA	3:M:189:TRP:HB3	2.02	0.42
1:A:78:ARG:HD2	1:A:78:ARG:HA	1.79	0.42
1:C:563:GLN:O	1:C:577:ARG:NH1	2.53	0.42
2:J:125:THR:OG1	2:J:156:PRO:HG3	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:96:SER:C	3:N:98:ASN:N	2.76	0.42
3:N:142:ASP:HA	3:N:175:LYS:HG3	2.01	0.42
1:A:360:ASN:HA	1:A:523:THR:HB	2.02	0.42
1:A:386:LYS:HE3	1:A:386:LYS:HB3	1.73	0.42
1:B:746:SER:HB3	1:B:749:CYS:HB3	2.02	0.42
1:C:344:ALA:HB3	1:C:347:PHE:CE1	2.55	0.42
2:I:138:LYS:HD2	3:M:210:VAL:CG1	2.50	0.42
3:M:142:ASP:HA	3:M:175:LYS:HG3	2.01	0.42
2:J:122:SER:C	2:J:124:SER:H	2.27	0.42
3:N:155:ASP:OD1	3:N:193:ARG:N	2.53	0.42
1:A:537:LYS:HB3	1:A:537:LYS:HE2	1.70	0.42
1:B:370:ASN:OD1	1:B:370:ASN:N	2.49	0.42
3:M:133:LYS:HD2	3:M:133:LYS:HA	1.70	0.42
2:J:125:THR:OG1	2:J:156:PRO:HG2	2.20	0.42
3:N:185:THR:HG23	3:N:188:GLN:HB2	2.01	0.42
1:A:328:ARG:NH1	1:A:531:THR:O	2.50	0.42
1:A:675:GLN:HE21	1:A:675:GLN:HB3	1.62	0.42
2:H:125:THR:OG1	2:H:156:PRO:HG2	2.20	0.42
3:L:186:PRO:HA	3:L:189:TRP:HB3	2.02	0.42
1:B:703:ASN:OD1	1:B:704:SER:N	2.53	0.42
1:C:66:HIS:HB2	1:C:67:ALA:H	1.60	0.42
2:H:156:PRO:HD2	2:H:209:HIS:CE1	2.54	0.42
3:L:142:ASP:HA	3:L:175:LYS:HG3	2.01	0.42
3:L:143:PHE:O	3:L:144:TYR:C	2.62	0.42
3:L:154:GLY:HA2	3:L:195:TYR:CD1	2.55	0.42
3:L:155:ASP:OD1	3:L:193:ARG:N	2.53	0.42
2:I:198:LEU:HB3	2:I:222:PRO:HG3	2.02	0.42
3:M:124:PRO:HG2	3:M:134:ALA:HB1	2.01	0.42
2:J:138:LYS:HD2	3:N:210:VAL:CG1	2.50	0.42
1:B:328:ARG:NH1	1:B:531:THR:O	2.50	0.41
3:M:52:GLU:HG3	3:M:55:LYS:HD2	2.02	0.41
3:M:110:LEU:HD11	3:M:114:LYS:CE	2.50	0.41
3:N:143:PHE:O	3:N:144:TYR:C	2.62	0.41
3:N:188:GLN:O	3:N:195:TYR:OH	2.38	0.41
1:A:703:ASN:OD1	1:A:704:SER:N	2.53	0.41
1:B:569:ILE:HD11	1:C:964:LYS:HB3	2.02	0.41
1:B:804:GLN:O	1:B:817:PRO:HD2	2.20	0.41
1:B:1038:LYS:HA	1:B:1038:LYS:HD3	1.90	0.41
1:C:959:LEU:HD23	1:C:959:LEU:HA	1.86	0.41
2:J:164:ASN:OD1	2:J:204:ILE:HG13	2.19	0.41
1:B:37:TYR:OH	1:B:54:LEU:O	2.25	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:563:GLN:O	1:B:577:ARG:NH1	2.53	0.41
2:H:187:LEU:HD12	2:H:188:SER:N	2.34	0.41
2:H:198:LEU:HB3	2:H:222:PRO:HG3	2.02	0.41
3:M:143:PHE:O	3:M:144:TYR:C	2.62	0.41
3:M:155:ASP:OD1	3:M:193:ARG:N	2.53	0.41
3:M:170:LYS:HE2	3:M:170:LYS:HB3	1.79	0.41
2:J:107:GLY:O	3:N:99:TRP:CH2	2.60	0.41
3:N:133:LYS:HD2	3:N:133:LYS:HA	1.70	0.41
6:A:1312:EIC:C18	1:B:358:ILE:HD12	2.50	0.41
1:B:513:LEU:HD12	1:B:513:LEU:HA	1.78	0.41
1:C:533:LEU:HD12	1:C:533:LEU:HA	1.91	0.41
3:M:105:THR:O	3:M:105:THR:OG1	2.38	0.41
3:M:136:LEU:HD23	3:M:184:LEU:HD11	2.02	0.41
2:J:208:ASN:HB3	2:J:215:LYS:CE	2.49	0.41
1:A:959:LEU:HD23	1:A:959:LEU:HA	1.86	0.41
1:B:532:ASN:N	1:B:532:ASN:ND2	2.69	0.41
1:C:392:PHE:CE1	1:C:517:LEU:HD21	2.55	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
3:L:105:THR:O	3:L:105:THR:OG1	2.38	0.41
3:L:121:LEU:HD23	3:L:122:PHE:N	2.34	0.41
3:L:170:LYS:HB3	3:L:170:LYS:HE2	1.79	0.41
3:L:190:LYS:NZ	3:L:212:PRO:HB2	2.36	0.41
2:I:122:SER:C	2:I:124:SER:H	2.27	0.41
3:M:154:GLY:HA2	3:M:195:TYR:CD1	2.55	0.41
3:N:124:PRO:HG2	3:N:134:ALA:HB1	2.01	0.41
1:A:78:ARG:HG3	1:A:80:ASP:OD2	2.21	0.41
1:A:759:PHE:O	1:A:763:LEU:HG	2.21	0.41
1:B:153:MET:CE	5:B:1303:NAG:HN2	2.32	0.41
1:B:752:LEU:HD21	1:B:990:GLU:OE2	2.20	0.41
2:H:138:LYS:HD2	3:L:210:VAL:CG1	2.50	0.41
2:I:209:HIS:HD2	2:I:211:PRO:HD2	1.86	0.41
2:J:198:LEU:HB3	2:J:222:PRO:HG3	2.02	0.41
3:N:154:GLY:HA2	3:N:195:TYR:CD1	2.55	0.41
1:A:147:LYS:HD3	1:A:248:TYR:CE1	2.56	0.41
3:N:132:ASN:OD1	3:N:132:ASN:N	2.54	0.41
1:A:230:PRO:HG3	1:C:396:TYR:CZ	2.55	0.41
1:B:759:PHE:O	1:B:763:LEU:HG	2.21	0.41
1:C:395:VAL:HG21	1:C:524:VAL:HG21	2.03	0.41
3:M:9:SER:HB3	3:M:147:ALA:HB1	1.88	0.41
1:B:715:PRO:HA	1:B:1072:GLU:HA	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:78:ARG:HA	1:C:78:ARG:HD2	1.80	0.41
1:C:147:LYS:HB3	1:C:147:LYS:HE3	1.58	0.41
1:C:355:ARG:HH21	1:C:355:ARG:CG	2.09	0.41
1:C:752:LEU:HD21	1:C:990:GLU:OE2	2.20	0.41
2:H:208:ASN:HB3	2:H:215:LYS:CE	2.49	0.41
3:L:52:GLU:HG3	3:L:55:LYS:HD2	2.02	0.41
3:L:132:ASN:OD1	3:L:132:ASN:N	2.54	0.41
3:L:136:LEU:HD23	3:L:184:LEU:HD11	2.02	0.41
3:M:154:GLY:O	3:M:155:ASP:C	2.64	0.41
3:M:158:PRO:HB2	3:M:160:LYS:NZ	2.36	0.41
2:J:203:TYR:H	2:J:219:LYS:HE3	1.86	0.41
3:N:52:GLU:HG3	3:N:55:LYS:HD2	2.02	0.41
3:N:105:THR:O	3:N:105:THR:OG1	2.38	0.41
1:A:555:SER:C	1:A:556:ASN:HD22	2.29	0.41
1:A:564:GLN:HE21	1:A:564:GLN:HB2	1.67	0.41
1:A:862:PRO:HA	1:A:863:PRO:HD3	1.97	0.41
2:I:75:LYS:HE3	2:I:75:LYS:HB3	1.87	0.41
3:M:190:LYS:HA	3:M:190:LYS:HD2	1.75	0.41
1:A:391:CYS:HB3	1:A:522:ALA:HB3	2.03	0.40
1:A:746:SER:HB3	1:A:749:CYS:HB3	2.02	0.40
1:A:1028:LYS:NZ	1:A:1042:PHE:O	2.53	0.40
6:A:1312:EIC:H52	1:B:377:PHE:CE1	2.56	0.40
1:B:78:ARG:HA	1:B:78:ARG:HD2	1.79	0.40
1:B:938:LEU:HD23	1:B:938:LEU:HA	1.91	0.40
1:B:1028:LYS:NZ	1:B:1042:PHE:O	2.52	0.40
1:C:513:LEU:HA	1:C:513:LEU:HD12	1.79	0.40
1:C:555:SER:C	1:C:556:ASN:HD22	2.29	0.40
3:L:154:GLY:O	3:L:155:ASP:C	2.64	0.40
3:N:158:PRO:HB2	3:N:160:LYS:NZ	2.36	0.40
1:B:78:ARG:HG3	1:B:80:ASP:OD2	2.21	0.40
1:B:854:LYS:HZ3	1:B:854:LYS:HG2	1.75	0.40
5:B:1305:NAG:O7	5:B:1305:NAG:O3	2.32	0.40
3:M:190:LYS:NZ	3:M:212:PRO:HB2	2.36	0.40
2:J:194:PRO:O	2:J:197:SER:OG	2.37	0.40
3:N:9:SER:HB2	3:N:147:ALA:HB2	1.87	0.40
6:A:1311:EIC:H72	6:A:1311:EIC:H42	1.88	0.40
1:B:148:ASN:OD1	1:B:148:ASN:N	2.55	0.40
1:B:486:PHE:HB2	2:I:52:TYR:OH	2.21	0.40
1:C:130:VAL:O	1:C:130:VAL:HG12	2.21	0.40
2:H:148:GLY:HA2	2:H:163:TRP:CZ2	2.56	0.40
3:N:154:GLY:O	3:N:155:ASP:C	2.64	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:186:PRO:HA	3:N:189:TRP:HB3	2.01	0.40
1:A:37:TYR:OH	1:A:54:LEU:O	2.25	0.40
1:A:486:PHE:HB2	2:H:52:TYR:OH	2.22	0.40
2:H:203:TYR:H	2:H:219:LYS:HE3	1.86	0.40
2:I:19:ARG:HE	2:I:19:ARG:HB2	1.71	0.40
2:I:207:VAL:O	2:I:215:LYS:HA	2.22	0.40
3:N:136:LEU:HD23	3:N:184:LEU:HD11	2.02	0.40
3:N:190:LYS:NZ	3:N:212:PRO:HB2	2.36	0.40
3:N:190:LYS:HD2	3:N:190:LYS:HA	1.75	0.40
1:A:330:PRO:HD2	1:A:525:CYS:SG	2.62	0.40
1:B:330:PRO:HD2	1:B:525:CYS:SG	2.62	0.40
5:B:1309:NAG:H3	5:B:1309:NAG:H83	1.96	0.40
1:C:826:VAL:HB	1:C:1057:PRO:HG2	2.04	0.40
1:C:1028:LYS:NZ	1:C:1042:PHE:O	2.53	0.40
2:H:157:GLU:HG3	2:H:185:TYR:CE2	2.57	0.40
2:H:207:VAL:O	2:H:215:LYS:HA	2.22	0.40
2:J:75:LYS:HB3	2:J:75:LYS:HE3	1.87	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	1089/1283 (85%)	1011 (93%)	72 (7%)	6 (1%)	21	44
1	B	1089/1283 (85%)	1011 (93%)	73 (7%)	5 (0%)	24	48
1	C	1089/1283 (85%)	1013 (93%)	71 (6%)	5 (0%)	24	48
2	H	212/452 (47%)	185 (87%)	26 (12%)	1 (0%)	24	48
2	I	212/452 (47%)	185 (87%)	26 (12%)	1 (0%)	24	48
2	J	212/452 (47%)	185 (87%)	26 (12%)	1 (0%)	24	48
3	L	209/216 (97%)	172 (82%)	29 (14%)	8 (4%)	2	5

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	M	209/216 (97%)	172 (82%)	29 (14%)	8 (4%)	2	5
3	N	209/216 (97%)	172 (82%)	29 (14%)	8 (4%)	2	5
All	All	4530/5853 (77%)	4106 (91%)	381 (8%)	43 (1%)	16	35

All (43) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	67	ALA
1	B	67	ALA
1	C	67	ALA
3	L	53	VAL
3	L	112	GLN
3	L	144	TYR
3	M	53	VAL
3	M	112	GLN
3	M	144	TYR
3	N	53	VAL
3	N	112	GLN
3	N	144	TYR
1	A	360	ASN
1	B	360	ASN
1	C	360	ASN
1	A	939	SER
1	B	939	SER
1	C	939	SER
2	H	124	SER
2	I	124	SER
2	J	124	SER
3	L	110	LEU
3	L	114	LYS
3	M	109	VAL
3	M	110	LEU
3	M	114	LYS
3	N	110	LEU
3	N	114	LYS
1	A	936	ASP
1	B	936	ASP
1	C	936	ASP
3	L	109	VAL
3	N	109	VAL
1	A	515	PHE

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Mol	Chain	Res	Type
3	L	98	ASN
3	L	113	PRO
3	M	98	ASN
3	M	113	PRO
3	N	98	ASN
3	N	113	PRO
1	A	251	PRO
1	B	251	PRO
1	C	251	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	959/1125 (85%)	847 (88%)	112 (12%)	5	13
1	B	959/1125 (85%)	847 (88%)	112 (12%)	5	13
1	C	959/1125 (85%)	846 (88%)	113 (12%)	5	13
2	H	180/398 (45%)	167 (93%)	13 (7%)	13	32
2	I	180/398 (45%)	167 (93%)	13 (7%)	13	32
2	J	180/398 (45%)	167 (93%)	13 (7%)	13	32
3	L	175/180 (97%)	160 (91%)	15 (9%)	10	25
3	M	175/180 (97%)	160 (91%)	15 (9%)	10	25
3	N	175/180 (97%)	160 (91%)	15 (9%)	10	25
All	All	3942/5109 (77%)	3521 (89%)	421 (11%)	8	16

All (421) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	THR
1	A	31	SER
1	A	40	ASP
1	A	47	VAL
1	A	51	THR

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Mol	Chain	Res	Type
1	A	53	ASP
1	A	66	HIS
1	A	94	SER
1	A	96	GLU
1	A	108	THR
1	A	114	THR
1	A	118	LEU
1	A	124	THR
1	A	131	CYS
1	A	147	LYS
1	A	153	MET
1	A	156	GLU
1	A	162	SER
1	A	173	GLN
1	A	178	ASP
1	A	183	GLN
1	A	185	ASN
1	A	197	ILE
1	A	198	ASP
1	A	205	SER
1	A	208	THR
1	A	212	LEU
1	A	216	LEU
1	A	236	THR
1	A	247	SER
1	A	253	ASP
1	A	255	SER
1	A	259	THR
1	A	271	GLN
1	A	277	LEU
1	A	281	GLU
1	A	299	THR
1	A	305	SER
1	A	325	SER
1	A	333	THR
1	A	342	PHE
1	A	355	ARG
1	A	357	ARG
1	A	359	SER
1	A	362	VAL
1	A	371	SER
1	A	373	SER

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Mol	Chain	Res	Type
1	A	376	THR
1	A	386	LYS
1	A	389	ASP
1	A	459	SER
1	A	469	SER
1	A	477	SER
1	A	513	LEU
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
1	A	785	VAL
1	A	790	LYS

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Mol	Chain	Res	Type
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	19	THR
1	B	31	SER
1	B	40	ASP
1	B	47	VAL
1	B	51	THR
1	B	53	ASP
1	B	66	HIS
1	B	94	SER
1	B	96	GLU
1	B	108	THR
1	B	114	THR
1	B	118	LEU
1	B	124	THR
1	B	131	CYS
1	B	147	LYS
1	B	153	MET
1	B	156	GLU
1	B	162	SER
1	B	173	GLN

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Mol	Chain	Res	Type
1	B	178	ASP
1	B	183	GLN
1	B	185	ASN
1	B	197	ILE
1	B	198	ASP
1	B	205	SER
1	B	208	THR
1	B	212	LEU
1	B	216	LEU
1	B	236	THR
1	B	247	SER
1	B	253	ASP
1	B	255	SER
1	B	259	THR
1	B	271	GLN
1	B	277	LEU
1	B	281	GLU
1	B	299	THR
1	B	305	SER
1	B	325	SER
1	B	333	THR
1	B	355	ARG
1	B	357	ARG
1	B	359	SER
1	B	362	VAL
1	B	371	SER
1	B	373	SER
1	B	376	THR
1	B	386	LYS
1	B	389	ASP
1	B	459	SER
1	B	469	SER
1	B	477	SER
1	B	513	LEU
1	B	516	GLU
1	B	518	LEU
1	B	528	LYS
1	B	530	SER
1	B	531	THR
1	B	532	ASN
1	B	534	VAL
1	B	558	LYS

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Mol	Chain	Res	Type
1	B	569	ILE
1	B	588	THR
1	B	599	THR
1	B	604	THR
1	B	606	ASN
1	B	614	ASP
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

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Mol	Chain	Res	Type
1	B	991	VAL
1	B	1002	GLN
1	B	1030	SER
1	B	1092	GLU
1	B	1097	SER
1	B	1118	ASP
1	B	1128	VAL
1	B	1136	THR
1	B	1142	GLN
1	C	19	THR
1	C	31	SER
1	C	40	ASP
1	C	47	VAL
1	C	51	THR
1	C	53	ASP
1	C	66	HIS
1	C	94	SER
1	C	96	GLU
1	C	108	THR
1	C	114	THR
1	C	118	LEU
1	C	124	THR
1	C	131	CYS
1	C	147	LYS
1	C	153	MET
1	C	156	GLU
1	C	162	SER
1	C	173	GLN
1	C	178	ASP
1	C	183	GLN
1	C	185	ASN
1	C	197	ILE
1	C	198	ASP
1	C	205	SER
1	C	208	THR
1	C	212	LEU
1	C	216	LEU
1	C	236	THR
1	C	247	SER
1	C	253	ASP
1	C	255	SER
1	C	259	THR

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Mol	Chain	Res	Type
1	C	271	GLN
1	C	277	LEU
1	C	281	GLU
1	C	299	THR
1	C	305	SER
1	C	325	SER
1	C	333	THR
1	C	355	ARG
1	C	357	ARG
1	C	359	SER
1	C	362	VAL
1	C	371	SER
1	C	373	SER
1	C	376	THR
1	C	386	LYS
1	C	389	ASP
1	C	459	SER
1	C	469	SER
1	C	477	SER
1	C	513	LEU
1	C	516	GLU
1	C	518	LEU
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

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Mol	Chain	Res	Type
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
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	894	LEU
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	78	LEU
2	H	90	THR
2	H	122	SER
2	H	126	LYS

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Mol	Chain	Res	Type
2	H	147	LEU
2	H	151	VAL
2	H	165	SER
2	H	169	THR
2	H	173	HIS
2	H	188	SER
2	H	204	ILE
2	H	206	ASN
2	H	212	SER
3	L	97	ASN
3	L	110	LEU
3	L	114	LYS
3	L	118	SER
3	L	125	SER
3	L	132	ASN
3	L	149	THR
3	L	157	SER
3	L	169	SER
3	L	172	SER
3	L	184	LEU
3	L	185	THR
3	L	191	SER
3	L	199	VAL
3	L	200	THR
2	I	78	LEU
2	I	90	THR
2	I	122	SER
2	I	126	LYS
2	I	147	LEU
2	I	151	VAL
2	I	165	SER
2	I	169	THR
2	I	173	HIS
2	I	188	SER
2	I	204	ILE
2	I	206	ASN
2	I	212	SER
3	M	97	ASN
3	M	110	LEU
3	M	114	LYS
3	M	118	SER
3	M	125	SER

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Mol	Chain	Res	Type
3	M	132	ASN
3	M	149	THR
3	M	157	SER
3	M	169	SER
3	M	172	SER
3	M	184	LEU
3	M	185	THR
3	M	191	SER
3	M	199	VAL
3	M	200	THR
2	J	78	LEU
2	J	90	THR
2	J	122	SER
2	J	126	LYS
2	J	147	LEU
2	J	151	VAL
2	J	165	SER
2	J	169	THR
2	J	173	HIS
2	J	188	SER
2	J	204	ILE
2	J	206	ASN
2	J	212	SER
3	N	97	ASN
3	N	110	LEU
3	N	114	LYS
3	N	118	SER
3	N	125	SER
3	N	132	ASN
3	N	149	THR
3	N	157	SER
3	N	169	SER
3	N	172	SER
3	N	184	LEU
3	N	185	THR
3	N	191	SER
3	N	199	VAL
3	N	200	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (133) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	69	HIS
1	A	183	GLN
1	A	188	ASN
1	A	207	HIS
1	A	218	GLN
1	A	239	GLN
1	A	314	GLN
1	A	317	ASN
1	A	360	ASN
1	A	414	GLN
1	A	422	ASN
1	A	450	ASN
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
1	A	1125	ASN
1	B	69	HIS
1	B	183	GLN
1	B	188	ASN
1	B	207	HIS
1	B	218	GLN
1	B	239	GLN
1	B	314	GLN

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Mol	Chain	Res	Type
1	B	317	ASN
1	B	360	ASN
1	B	414	GLN
1	B	422	ASN
1	B	450	ASN
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	925	ASN
1	B	955	ASN
1	B	1005	GLN
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	C	69	HIS
1	C	183	GLN
1	C	188	ASN
1	C	207	HIS
1	C	218	GLN
1	C	239	GLN
1	C	314	GLN
1	C	317	ASN
1	C	360	ASN
1	C	414	GLN
1	C	422	ASN
1	C	450	ASN
1	C	532	ASN
1	C	540	ASN
1	C	544	ASN

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Mol	Chain	Res	Type
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	955	ASN
1	C	1011	GLN
1	C	1023	ASN
1	C	1036	GLN
1	C	1054	GLN
1	C	1064	HIS
1	C	1106	GLN
1	C	1125	ASN
2	H	81	GLN
2	H	213	ASN
3	L	6	GLN
3	L	40	GLN
3	L	41	HIS
3	L	71	ASN
3	L	98	ASN
3	L	112	GLN
3	L	174	ASN
3	L	198	GLN
2	I	81	GLN
2	I	213	ASN
3	M	6	GLN
3	M	40	GLN
3	M	41	HIS
3	M	71	ASN
3	M	98	ASN
3	M	112	GLN
2	J	81	GLN
2	J	213	ASN
3	N	6	GLN
3	N	40	GLN

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Mol	Chain	Res	Type
3	N	41	HIS
3	N	71	ASN
3	N	98	ASN
3	N	112	GLN
3	N	174	ASN
3	N	198	GLN

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 ⓘ

48 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	4,1	14,14,15	1.10	1 (7%)	17,19,21	0.62	0
4	NAG	D	2	4	14,14,15	2.25	2 (14%)	17,19,21	1.02	2 (11%)
4	NAG	E	1	4,1	14,14,15	0.30	0	17,19,21	0.63	0
4	NAG	E	2	4	14,14,15	0.53	0	17,19,21	0.49	0
4	NAG	F	1	4,1	14,14,15	0.68	1 (7%)	17,19,21	0.70	0
4	NAG	F	2	4	14,14,15	0.44	0	17,19,21	1.49	3 (17%)
4	NAG	G	1	4,1	14,14,15	0.68	1 (7%)	17,19,21	0.68	0
4	NAG	G	2	4	14,14,15	0.28	0	17,19,21	0.68	0
4	NAG	K	1	4,1	14,14,15	1.10	1 (7%)	17,19,21	0.63	0
4	NAG	K	2	4	14,14,15	2.26	2 (14%)	17,19,21	1.02	2 (11%)
4	NAG	O	1	4,1	14,14,15	0.30	0	17,19,21	0.64	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	O	2	4	14,14,15	0.53	0	17,19,21	0.49	0
4	NAG	P	1	4,1	14,14,15	0.68	1 (7%)	17,19,21	0.68	0
4	NAG	P	2	4	14,14,15	0.28	0	17,19,21	0.68	0
4	NAG	Q	1	4,1	14,14,15	1.09	1 (7%)	17,19,21	0.63	0
4	NAG	Q	2	4	14,14,15	2.25	2 (14%)	17,19,21	1.02	2 (11%)
4	NAG	R	1	4,1	14,14,15	0.29	0	17,19,21	0.63	0
4	NAG	R	2	4	14,14,15	0.51	0	17,19,21	0.49	0
4	NAG	S	1	4,1	14,14,15	0.67	1 (7%)	17,19,21	0.68	0
4	NAG	S	2	4	14,14,15	0.29	0	17,19,21	0.68	0
4	NAG	T	1	4,1	14,14,15	0.43	0	17,19,21	1.16	2 (11%)
4	NAG	T	2	4	14,14,15	0.42	0	17,19,21	1.15	2 (11%)
4	NAG	U	1	4,1	14,14,15	0.29	0	17,19,21	0.57	0
4	NAG	U	2	4	14,14,15	0.41	0	17,19,21	1.15	2 (11%)
4	NAG	V	1	4,1	14,14,15	0.35	0	17,19,21	0.74	0
4	NAG	V	2	4	14,14,15	0.32	0	17,19,21	1.39	2 (11%)
4	NAG	W	1	4,1	14,14,15	0.24	0	17,19,21	0.70	1 (5%)
4	NAG	W	2	4	14,14,15	0.17	0	17,19,21	0.49	0
4	NAG	X	1	4,1	14,14,15	0.43	0	17,19,21	1.15	2 (11%)
4	NAG	X	2	4	14,14,15	0.42	0	17,19,21	1.17	2 (11%)
4	NAG	Y	1	4,1	14,14,15	0.29	0	17,19,21	0.57	0
4	NAG	Y	2	4	14,14,15	0.43	0	17,19,21	1.15	2 (11%)
4	NAG	Z	1	4,1	14,14,15	0.35	0	17,19,21	0.74	0
4	NAG	Z	2	4	14,14,15	0.31	0	17,19,21	1.40	2 (11%)
4	NAG	a	1	4,1	14,14,15	0.68	1 (7%)	17,19,21	0.71	0
4	NAG	a	2	4	14,14,15	0.42	0	17,19,21	1.49	3 (17%)
4	NAG	b	1	4,1	14,14,15	0.24	0	17,19,21	0.70	1 (5%)
4	NAG	b	2	4	14,14,15	0.16	0	17,19,21	0.48	0
4	NAG	c	1	4,1	14,14,15	0.42	0	17,19,21	1.16	2 (11%)
4	NAG	c	2	4	14,14,15	0.43	0	17,19,21	1.17	2 (11%)
4	NAG	d	1	4,1	14,14,15	0.28	0	17,19,21	0.56	0
4	NAG	d	2	4	14,14,15	0.44	0	17,19,21	1.15	2 (11%)
4	NAG	e	1	4,1	14,14,15	0.35	0	17,19,21	0.74	0
4	NAG	e	2	4	14,14,15	0.31	0	17,19,21	1.40	2 (11%)
4	NAG	f	1	4,1	14,14,15	0.68	1 (7%)	17,19,21	0.70	0
4	NAG	f	2	4	14,14,15	0.43	0	17,19,21	1.49	3 (17%)
4	NAG	g	1	4,1	14,14,15	0.25	0	17,19,21	0.69	1 (5%)
4	NAG	g	2	4	14,14,15	0.16	0	17,19,21	0.48	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	4,1	-	1/6/23/26	0/1/1/1
4	NAG	D	2	4	-	2/6/23/26	0/1/1/1
4	NAG	E	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	E	2	4	-	2/6/23/26	0/1/1/1
4	NAG	F	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	F	2	4	-	6/6/23/26	0/1/1/1
4	NAG	G	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	G	2	4	-	4/6/23/26	0/1/1/1
4	NAG	K	1	4,1	-	1/6/23/26	0/1/1/1
4	NAG	K	2	4	-	2/6/23/26	0/1/1/1
4	NAG	O	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	O	2	4	-	2/6/23/26	0/1/1/1
4	NAG	P	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	P	2	4	-	4/6/23/26	0/1/1/1
4	NAG	Q	1	4,1	-	1/6/23/26	0/1/1/1
4	NAG	Q	2	4	-	2/6/23/26	0/1/1/1
4	NAG	R	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	R	2	4	-	2/6/23/26	0/1/1/1
4	NAG	S	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	S	2	4	-	4/6/23/26	0/1/1/1
4	NAG	T	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	T	2	4	-	0/6/23/26	0/1/1/1
4	NAG	U	1	4,1	-	5/6/23/26	0/1/1/1
4	NAG	U	2	4	-	0/6/23/26	0/1/1/1
4	NAG	V	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	V	2	4	-	4/6/23/26	0/1/1/1
4	NAG	W	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	W	2	4	-	0/6/23/26	0/1/1/1
4	NAG	X	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	X	2	4	-	0/6/23/26	0/1/1/1
4	NAG	Y	1	4,1	-	5/6/23/26	0/1/1/1
4	NAG	Y	2	4	-	0/6/23/26	0/1/1/1
4	NAG	Z	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	Z	2	4	-	4/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	a	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	a	2	4	-	6/6/23/26	0/1/1/1
4	NAG	b	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	b	2	4	-	0/6/23/26	0/1/1/1
4	NAG	c	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	c	2	4	-	0/6/23/26	0/1/1/1
4	NAG	d	1	4,1	-	5/6/23/26	0/1/1/1
4	NAG	d	2	4	-	0/6/23/26	0/1/1/1
4	NAG	e	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	e	2	4	-	4/6/23/26	0/1/1/1
4	NAG	f	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	f	2	4	-	6/6/23/26	0/1/1/1
4	NAG	g	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	g	2	4	-	0/6/23/26	0/1/1/1

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	K	2	NAG	O5-C1	-6.81	1.32	1.43
4	D	2	NAG	O5-C1	-6.81	1.32	1.43
4	Q	2	NAG	O5-C1	-6.76	1.32	1.43
4	Q	2	NAG	C1-C2	-4.91	1.45	1.52
4	K	2	NAG	C1-C2	-4.86	1.45	1.52
4	D	2	NAG	C1-C2	-4.85	1.45	1.52
4	K	1	NAG	O5-C1	-4.03	1.36	1.43
4	D	1	NAG	O5-C1	-4.01	1.37	1.43
4	Q	1	NAG	O5-C1	-3.97	1.37	1.43
4	G	1	NAG	O5-C1	-2.48	1.39	1.43
4	P	1	NAG	O5-C1	-2.47	1.39	1.43
4	S	1	NAG	O5-C1	-2.43	1.39	1.43
4	a	1	NAG	O5-C1	-2.26	1.39	1.43
4	F	1	NAG	O5-C1	-2.23	1.39	1.43
4	f	1	NAG	O5-C1	-2.22	1.40	1.43

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	f	2	NAG	C2-N2-C7	4.76	129.28	122.90
4	a	2	NAG	C2-N2-C7	4.71	129.22	122.90
4	F	2	NAG	C2-N2-C7	4.70	129.20	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	Z	2	NAG	C2-N2-C7	4.55	128.99	122.90
4	e	2	NAG	C2-N2-C7	4.55	128.99	122.90
4	V	2	NAG	C2-N2-C7	4.52	128.96	122.90
4	K	2	NAG	C1-C2-N2	2.78	114.81	110.43
4	D	2	NAG	C1-C2-N2	2.77	114.80	110.43
4	Q	2	NAG	C1-C2-N2	2.75	114.76	110.43
4	e	2	NAG	C1-C2-N2	2.63	114.58	110.43
4	a	2	NAG	C1-C2-N2	2.59	114.52	110.43
4	V	2	NAG	C1-C2-N2	2.59	114.51	110.43
4	F	2	NAG	C1-C2-N2	2.58	114.50	110.43
4	Z	2	NAG	C1-C2-N2	2.57	114.48	110.43
4	f	2	NAG	C1-C2-N2	2.56	114.46	110.43
4	Q	2	NAG	C1-O5-C5	2.55	115.60	112.19
4	D	2	NAG	C1-O5-C5	2.51	115.56	112.19
4	K	2	NAG	C1-O5-C5	2.48	115.51	112.19
4	c	1	NAG	C8-C7-N2	2.41	120.11	116.12
4	X	2	NAG	C8-C7-N2	2.38	120.07	116.12
4	c	2	NAG	C8-C7-N2	2.38	120.06	116.12
4	U	2	NAG	C8-C7-N2	2.37	120.04	116.12
4	X	1	NAG	C8-C7-N2	2.36	120.03	116.12
4	d	2	NAG	C8-C7-N2	2.35	120.02	116.12
4	Y	2	NAG	C8-C7-N2	2.35	120.01	116.12
4	T	1	NAG	C8-C7-N2	2.34	120.00	116.12
4	T	2	NAG	C8-C7-N2	2.34	120.00	116.12
4	T	1	NAG	C2-N2-C7	-2.16	120.00	122.90
4	X	2	NAG	C2-N2-C7	-2.16	120.01	122.90
4	c	2	NAG	C2-N2-C7	-2.16	120.01	122.90
4	T	2	NAG	C2-N2-C7	-2.15	120.02	122.90
4	d	2	NAG	C2-N2-C7	-2.13	120.04	122.90
4	X	1	NAG	C2-N2-C7	-2.13	120.04	122.90
4	b	1	NAG	C1-O5-C5	2.13	115.04	112.19
4	U	2	NAG	C2-N2-C7	-2.12	120.05	122.90
4	F	2	NAG	C1-O5-C5	2.12	115.03	112.19
4	a	2	NAG	C1-O5-C5	2.12	115.02	112.19
4	c	1	NAG	C2-N2-C7	-2.11	120.07	122.90
4	W	1	NAG	C1-O5-C5	2.10	115.00	112.19
4	Y	2	NAG	C2-N2-C7	-2.10	120.08	122.90
4	f	2	NAG	C1-O5-C5	2.10	115.00	112.19
4	g	1	NAG	C1-O5-C5	2.06	114.95	112.19

There are no chirality outliers.

All (96) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	U	1	NAG	O5-C5-C6-O6
4	Y	1	NAG	O5-C5-C6-O6
4	d	1	NAG	O5-C5-C6-O6
4	D	2	NAG	O5-C5-C6-O6
4	K	2	NAG	O5-C5-C6-O6
4	Q	2	NAG	O5-C5-C6-O6
4	G	1	NAG	O5-C5-C6-O6
4	P	1	NAG	O5-C5-C6-O6
4	S	1	NAG	O5-C5-C6-O6
4	G	1	NAG	C4-C5-C6-O6
4	P	1	NAG	C4-C5-C6-O6
4	S	1	NAG	C4-C5-C6-O6
4	U	1	NAG	C4-C5-C6-O6
4	Y	1	NAG	C4-C5-C6-O6
4	d	1	NAG	C4-C5-C6-O6
4	U	1	NAG	C8-C7-N2-C2
4	Y	1	NAG	C8-C7-N2-C2
4	d	1	NAG	C8-C7-N2-C2
4	D	2	NAG	C4-C5-C6-O6
4	K	2	NAG	C4-C5-C6-O6
4	Q	2	NAG	C4-C5-C6-O6
4	F	2	NAG	C8-C7-N2-C2
4	F	2	NAG	O7-C7-N2-C2
4	U	1	NAG	O7-C7-N2-C2
4	V	2	NAG	C8-C7-N2-C2
4	V	2	NAG	O7-C7-N2-C2
4	Y	1	NAG	O7-C7-N2-C2
4	Z	2	NAG	C8-C7-N2-C2
4	Z	2	NAG	O7-C7-N2-C2
4	a	2	NAG	C8-C7-N2-C2
4	a	2	NAG	O7-C7-N2-C2
4	d	1	NAG	O7-C7-N2-C2
4	e	2	NAG	C8-C7-N2-C2
4	e	2	NAG	O7-C7-N2-C2
4	f	2	NAG	C8-C7-N2-C2
4	f	2	NAG	O7-C7-N2-C2
4	V	1	NAG	C4-C5-C6-O6
4	Z	1	NAG	C4-C5-C6-O6
4	e	1	NAG	C4-C5-C6-O6
4	F	1	NAG	C4-C5-C6-O6
4	a	1	NAG	C4-C5-C6-O6
4	f	1	NAG	C4-C5-C6-O6
4	V	1	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	Z	1	NAG	O5-C5-C6-O6
4	e	1	NAG	O5-C5-C6-O6
4	F	1	NAG	O5-C5-C6-O6
4	a	1	NAG	O5-C5-C6-O6
4	f	1	NAG	O5-C5-C6-O6
4	G	2	NAG	C4-C5-C6-O6
4	P	2	NAG	C4-C5-C6-O6
4	S	2	NAG	C4-C5-C6-O6
4	G	2	NAG	O5-C5-C6-O6
4	P	2	NAG	O5-C5-C6-O6
4	S	2	NAG	O5-C5-C6-O6
4	W	1	NAG	C4-C5-C6-O6
4	b	1	NAG	C4-C5-C6-O6
4	g	1	NAG	C4-C5-C6-O6
4	W	1	NAG	O5-C5-C6-O6
4	g	1	NAG	O5-C5-C6-O6
4	b	1	NAG	O5-C5-C6-O6
4	U	1	NAG	C3-C2-N2-C7
4	Y	1	NAG	C3-C2-N2-C7
4	d	1	NAG	C3-C2-N2-C7
4	E	2	NAG	C4-C5-C6-O6
4	R	2	NAG	C4-C5-C6-O6
4	O	2	NAG	C4-C5-C6-O6
4	E	2	NAG	O5-C5-C6-O6
4	O	2	NAG	O5-C5-C6-O6
4	R	2	NAG	O5-C5-C6-O6
4	G	2	NAG	C3-C2-N2-C7
4	P	2	NAG	C3-C2-N2-C7
4	S	2	NAG	C3-C2-N2-C7
4	a	2	NAG	C4-C5-C6-O6
4	F	2	NAG	C4-C5-C6-O6
4	f	2	NAG	C4-C5-C6-O6
4	Q	1	NAG	O5-C5-C6-O6
4	D	1	NAG	O5-C5-C6-O6
4	K	1	NAG	O5-C5-C6-O6
4	F	2	NAG	O5-C5-C6-O6
4	f	2	NAG	O5-C5-C6-O6
4	a	2	NAG	O5-C5-C6-O6
4	F	2	NAG	C1-C2-N2-C7
4	G	2	NAG	C1-C2-N2-C7
4	P	2	NAG	C1-C2-N2-C7
4	S	2	NAG	C1-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
4	V	2	NAG	C1-C2-N2-C7
4	Z	2	NAG	C1-C2-N2-C7
4	a	2	NAG	C1-C2-N2-C7
4	e	2	NAG	C1-C2-N2-C7
4	f	2	NAG	C1-C2-N2-C7
4	F	2	NAG	C3-C2-N2-C7
4	V	2	NAG	C3-C2-N2-C7
4	Z	2	NAG	C3-C2-N2-C7
4	a	2	NAG	C3-C2-N2-C7
4	e	2	NAG	C3-C2-N2-C7
4	f	2	NAG	C3-C2-N2-C7

There are no ring outliers.

33 monomers are involved in 39 short contacts:

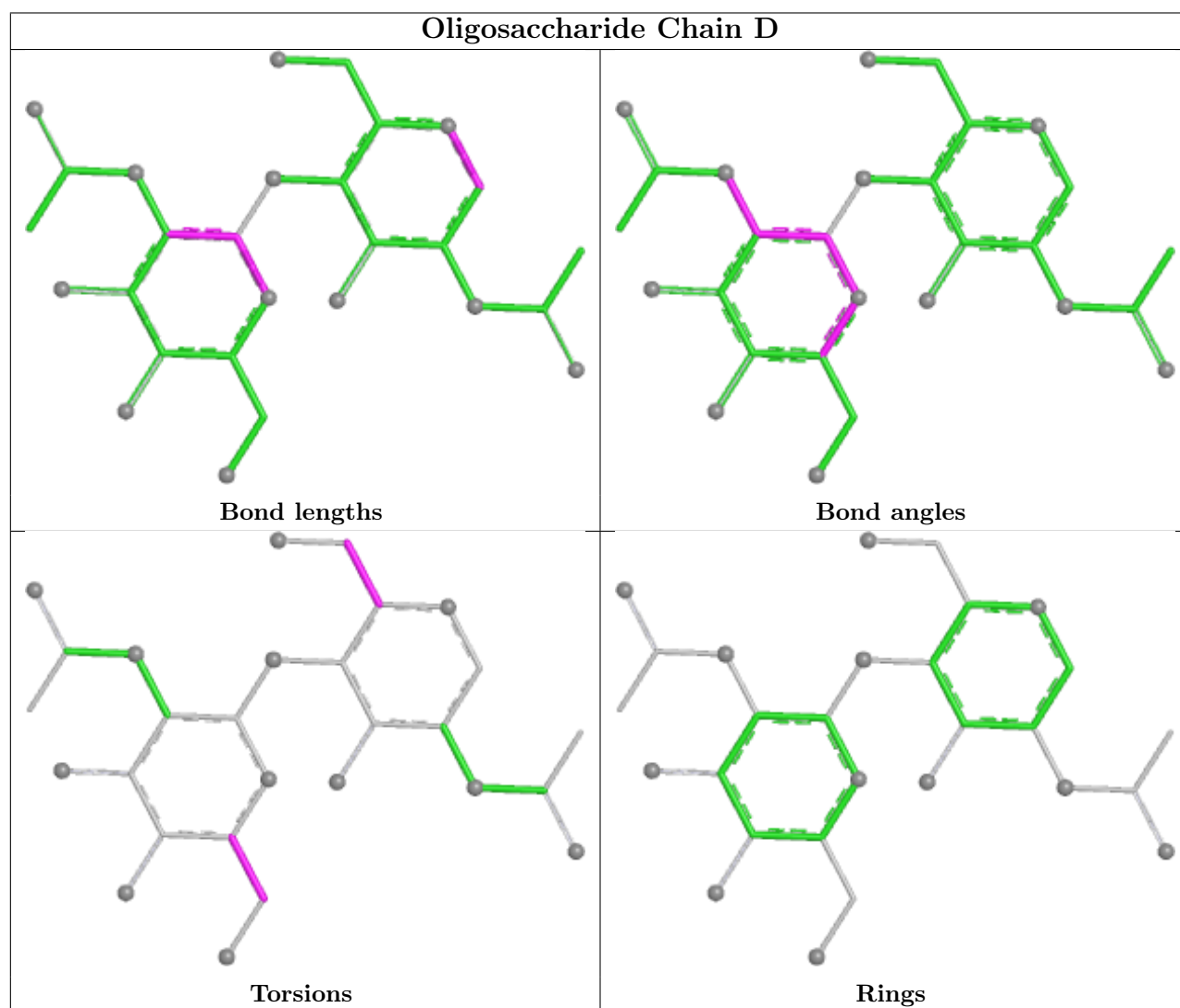
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	e	2	NAG	1	0
4	Q	1	NAG	1	0
4	a	2	NAG	1	0
4	V	2	NAG	1	0
4	U	2	NAG	6	0
4	g	2	NAG	2	0
4	X	1	NAG	1	0
4	W	2	NAG	2	0
4	F	2	NAG	1	0
4	T	2	NAG	1	0
4	d	1	NAG	6	0
4	Y	1	NAG	6	0
4	T	1	NAG	1	0
4	g	1	NAG	2	0
4	D	1	NAG	1	0
4	b	1	NAG	2	0
4	X	2	NAG	1	0
4	V	1	NAG	1	0
4	U	1	NAG	6	0
4	f	2	NAG	1	0
4	K	2	NAG	1	0
4	K	1	NAG	1	0
4	W	1	NAG	2	0
4	Z	2	NAG	1	0
4	d	2	NAG	6	0
4	Y	2	NAG	6	0

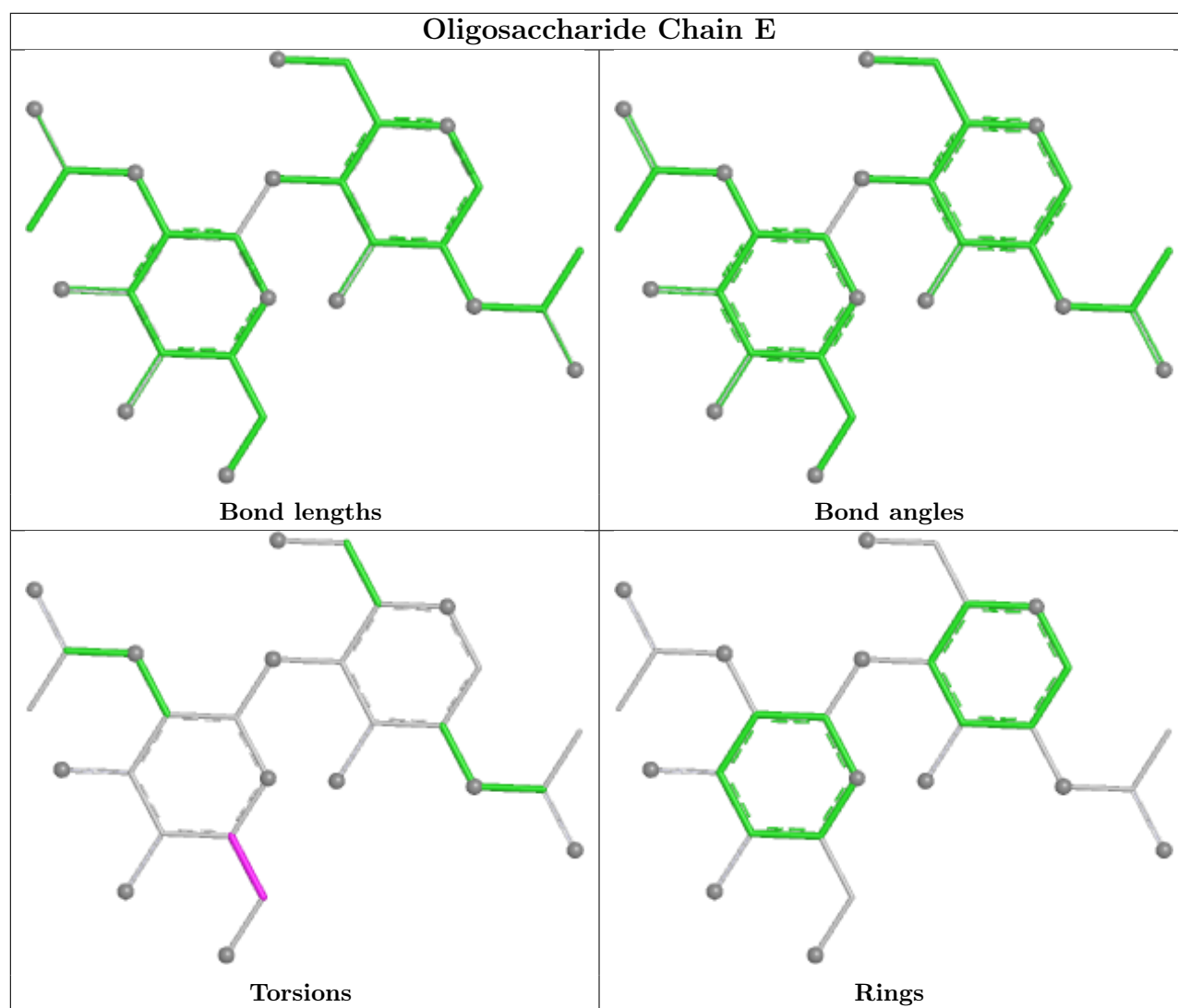
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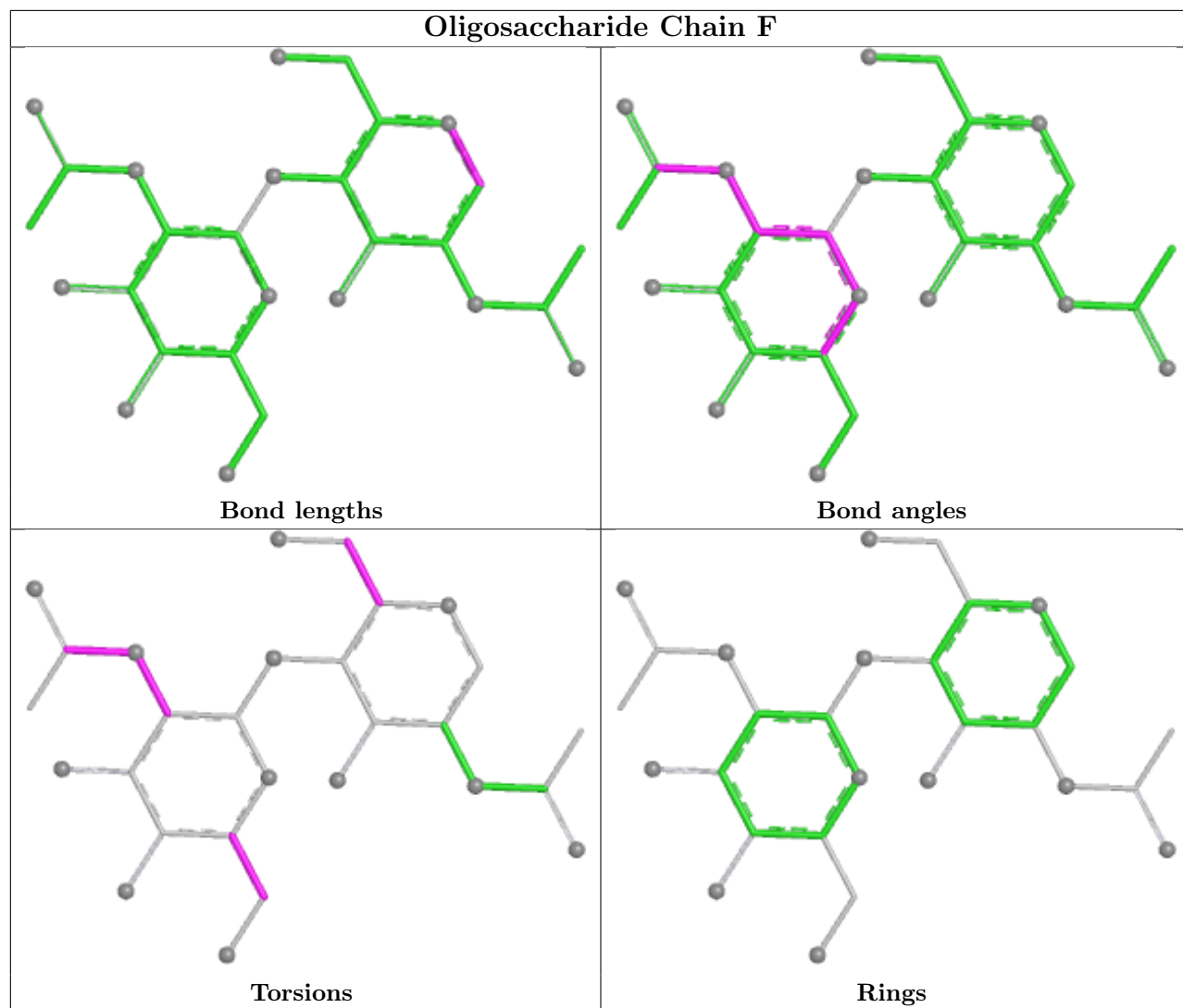
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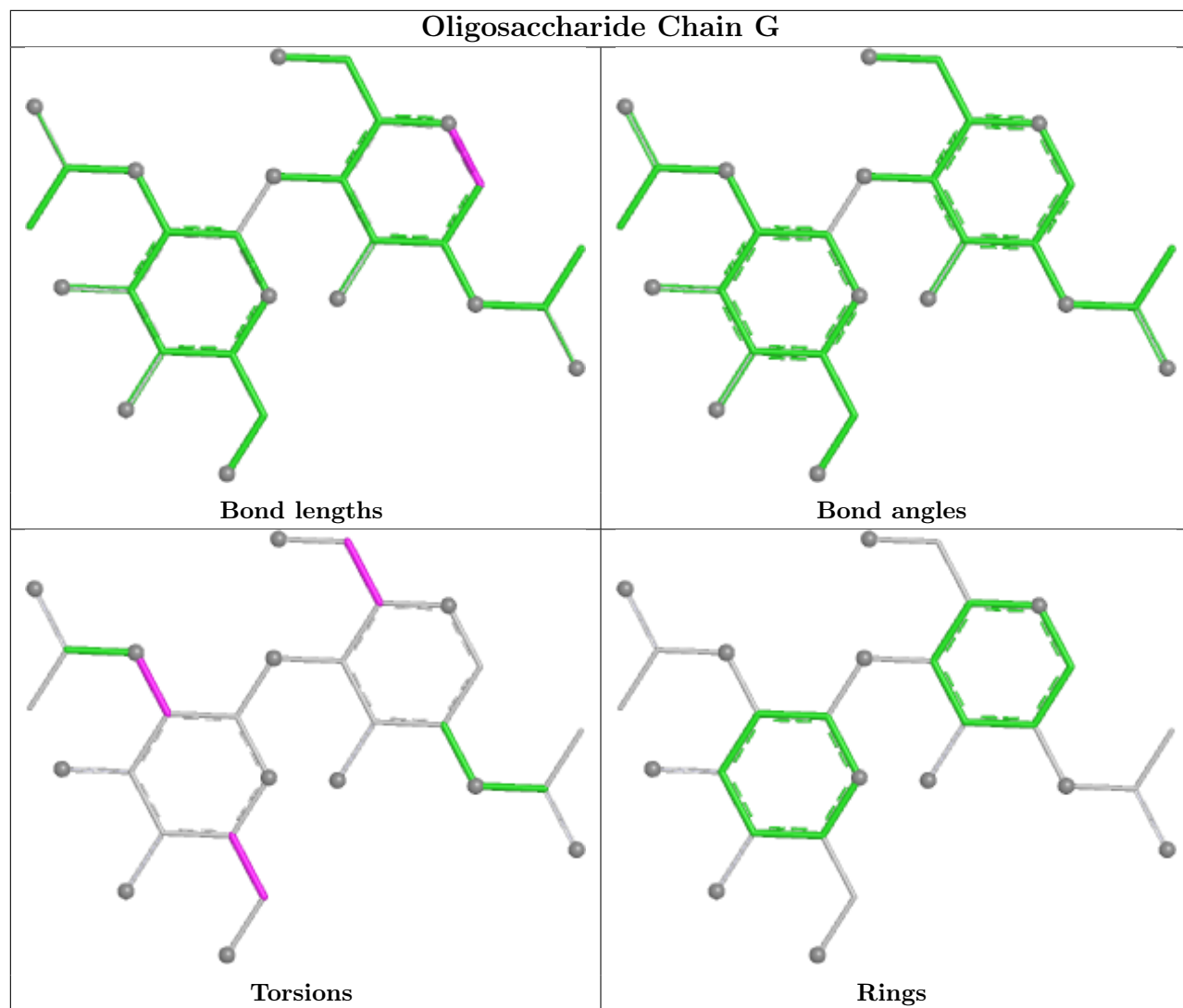
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	c	2	NAG	1	0
4	e	1	NAG	1	0
4	Q	2	NAG	1	0
4	c	1	NAG	1	0
4	D	2	NAG	1	0
4	Z	1	NAG	1	0
4	b	2	NAG	2	0

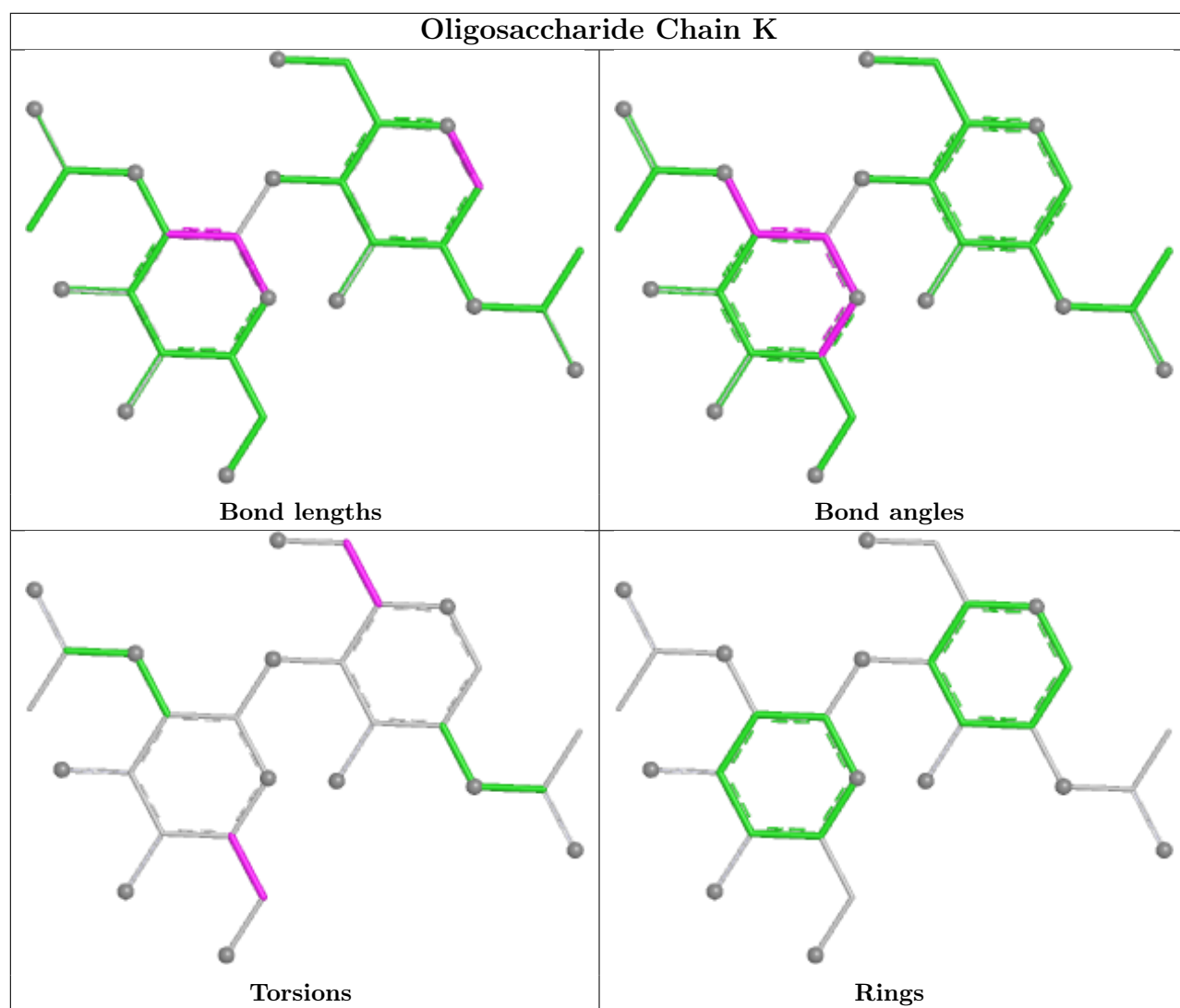
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

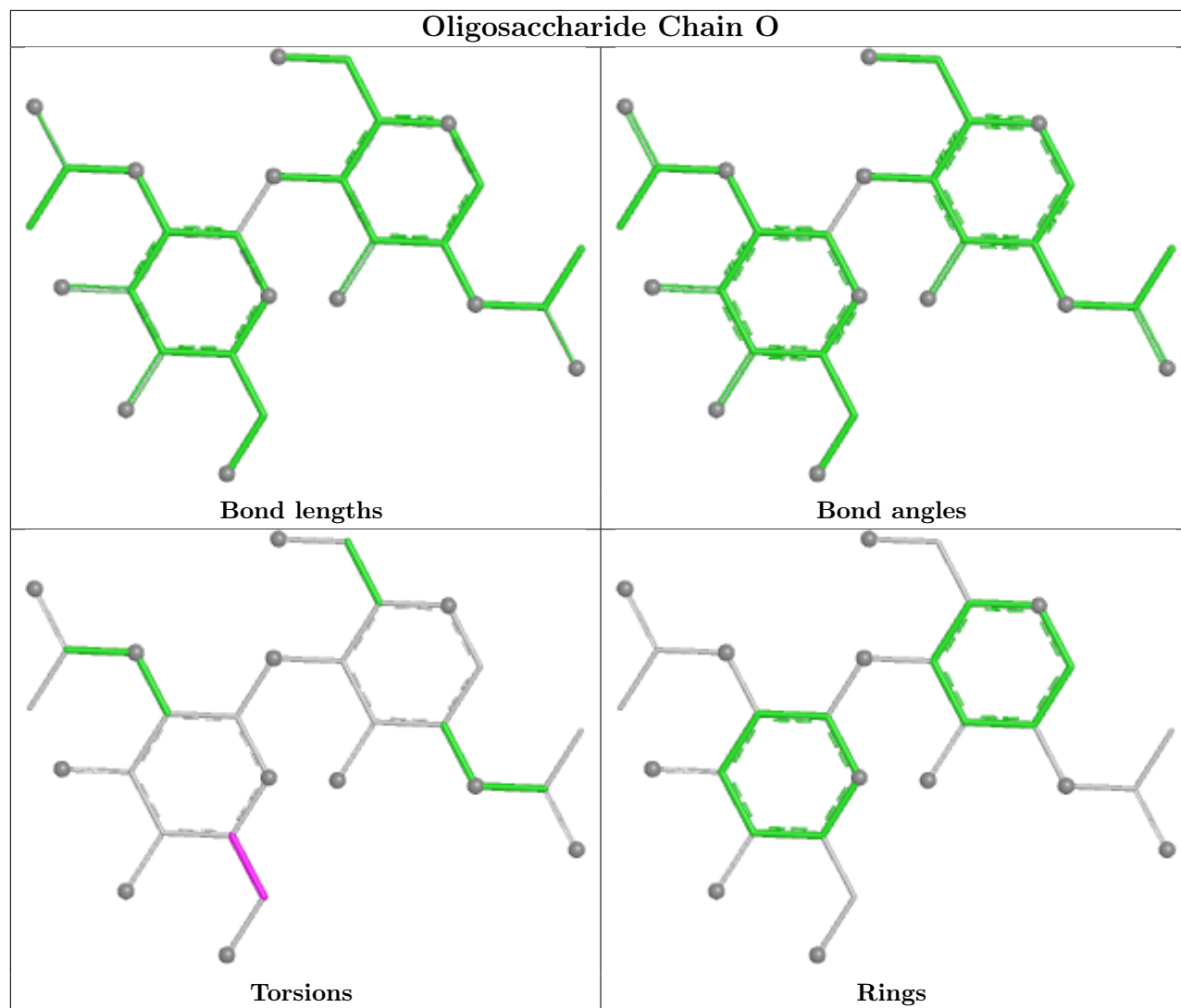


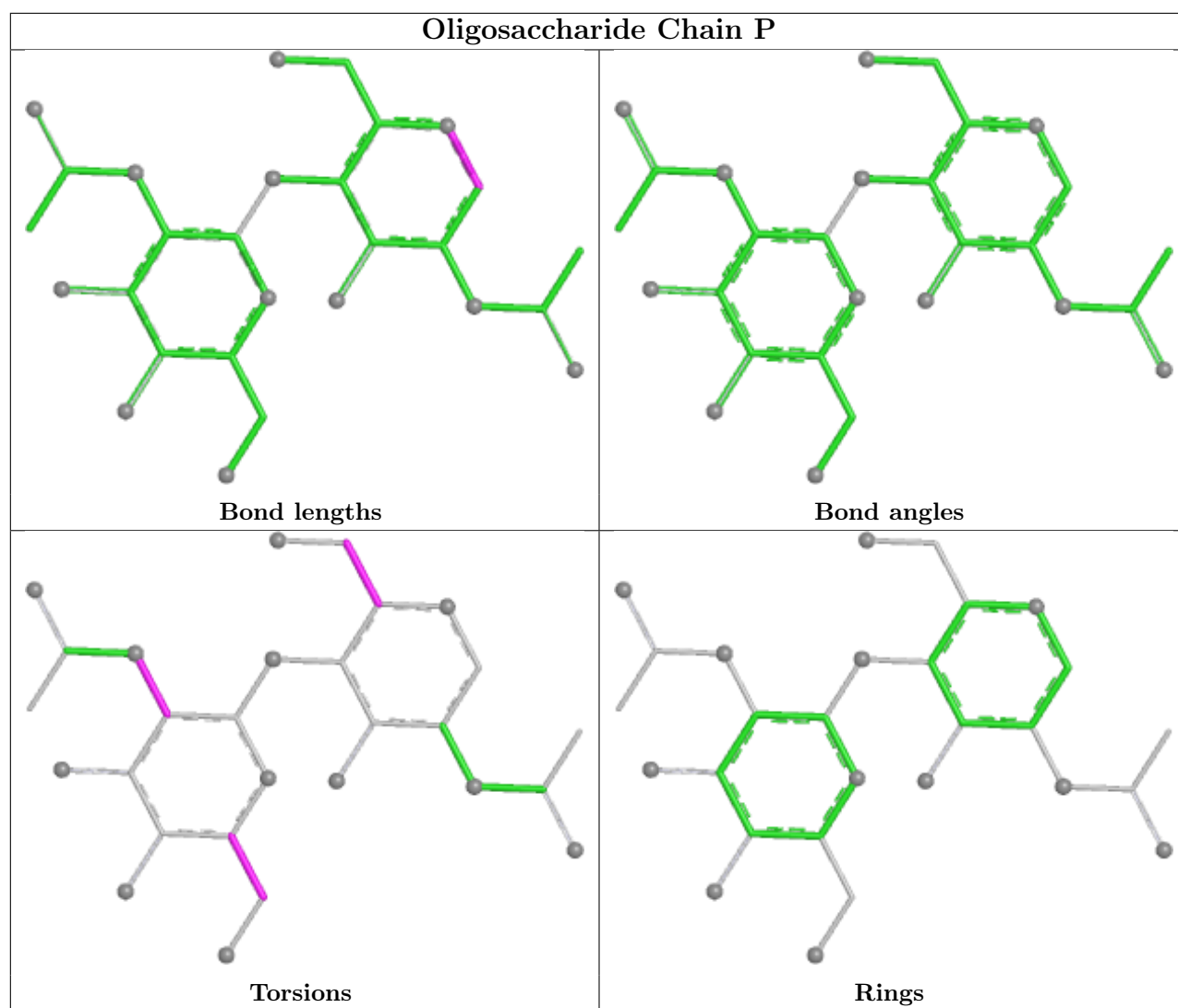


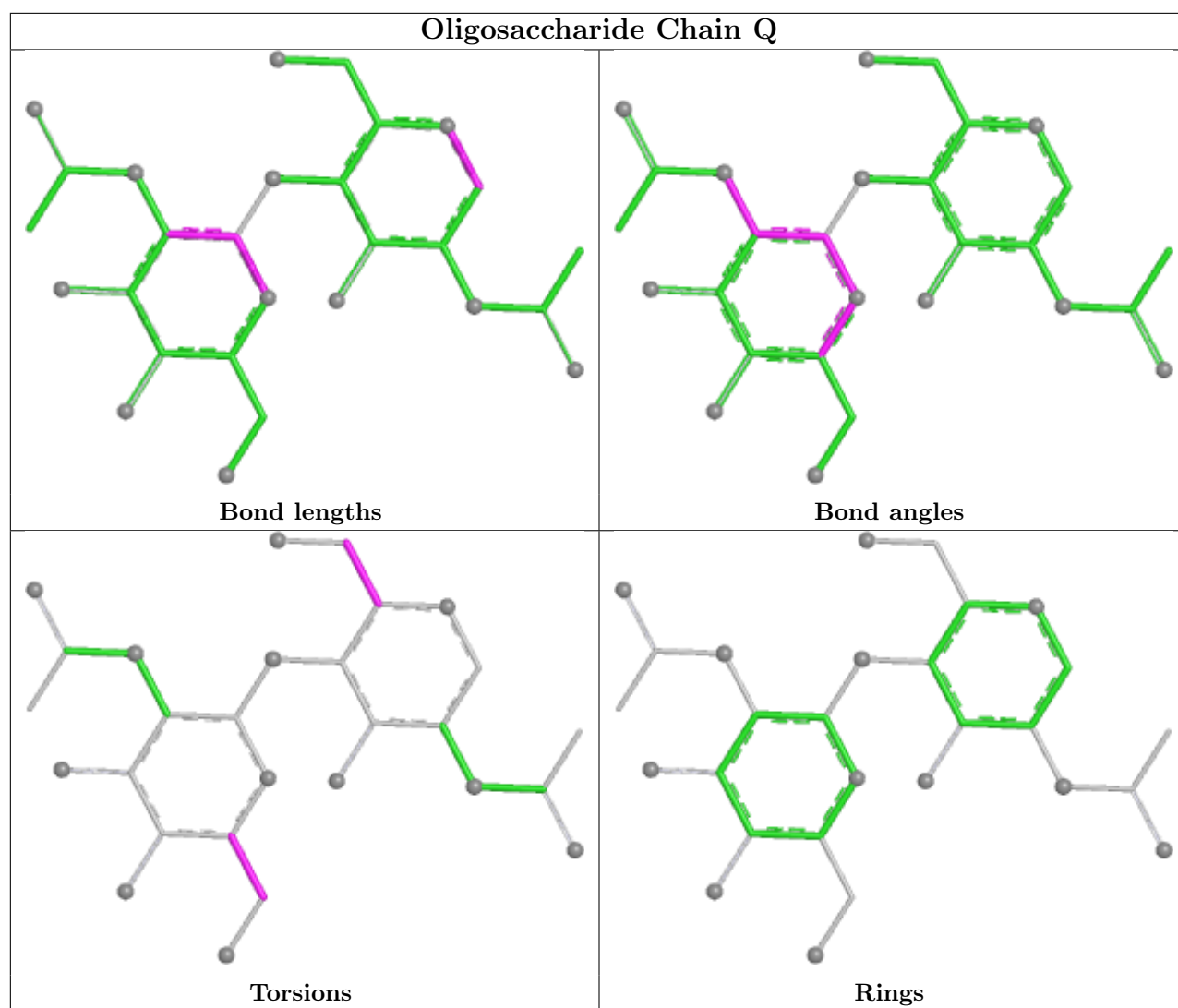


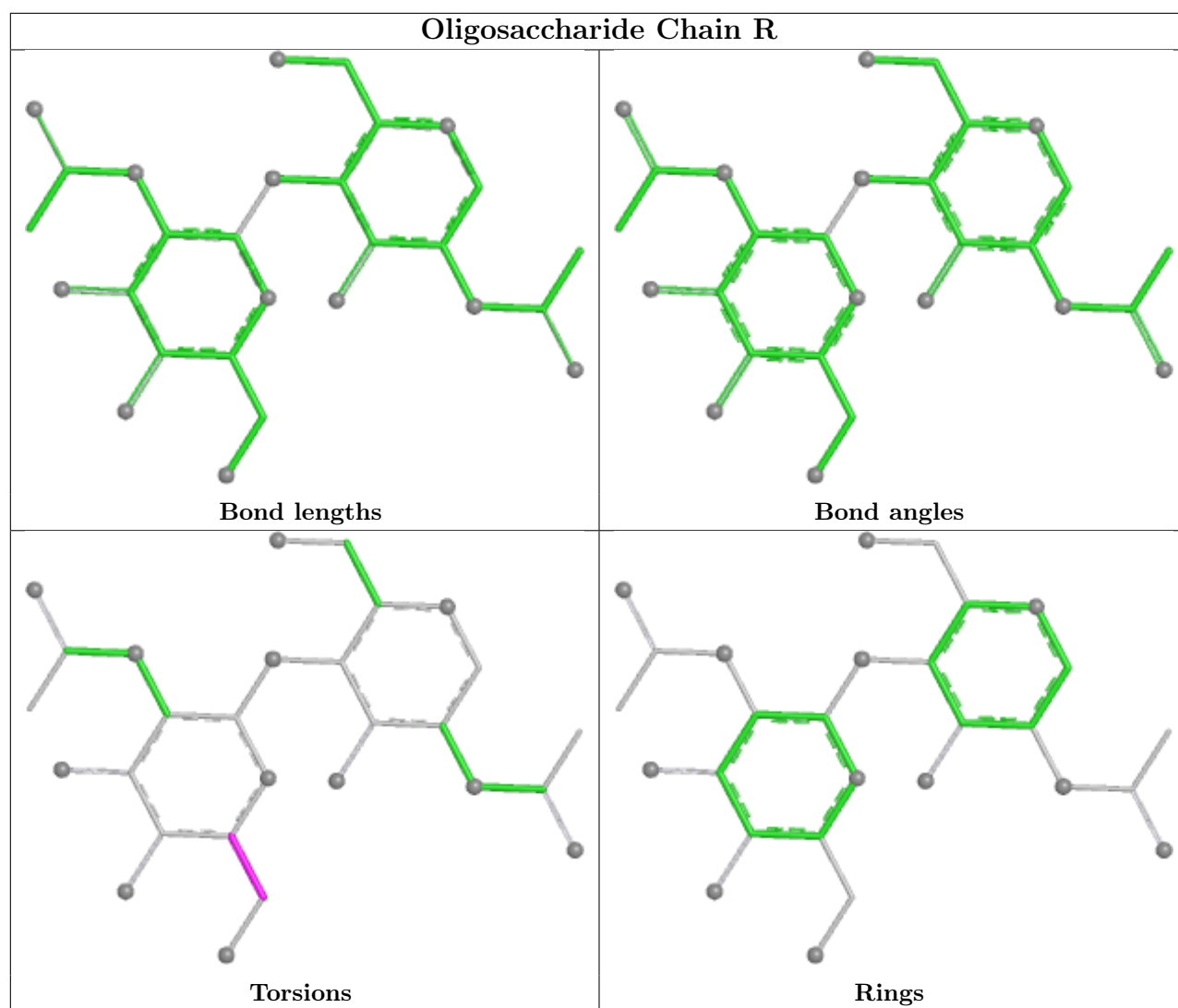


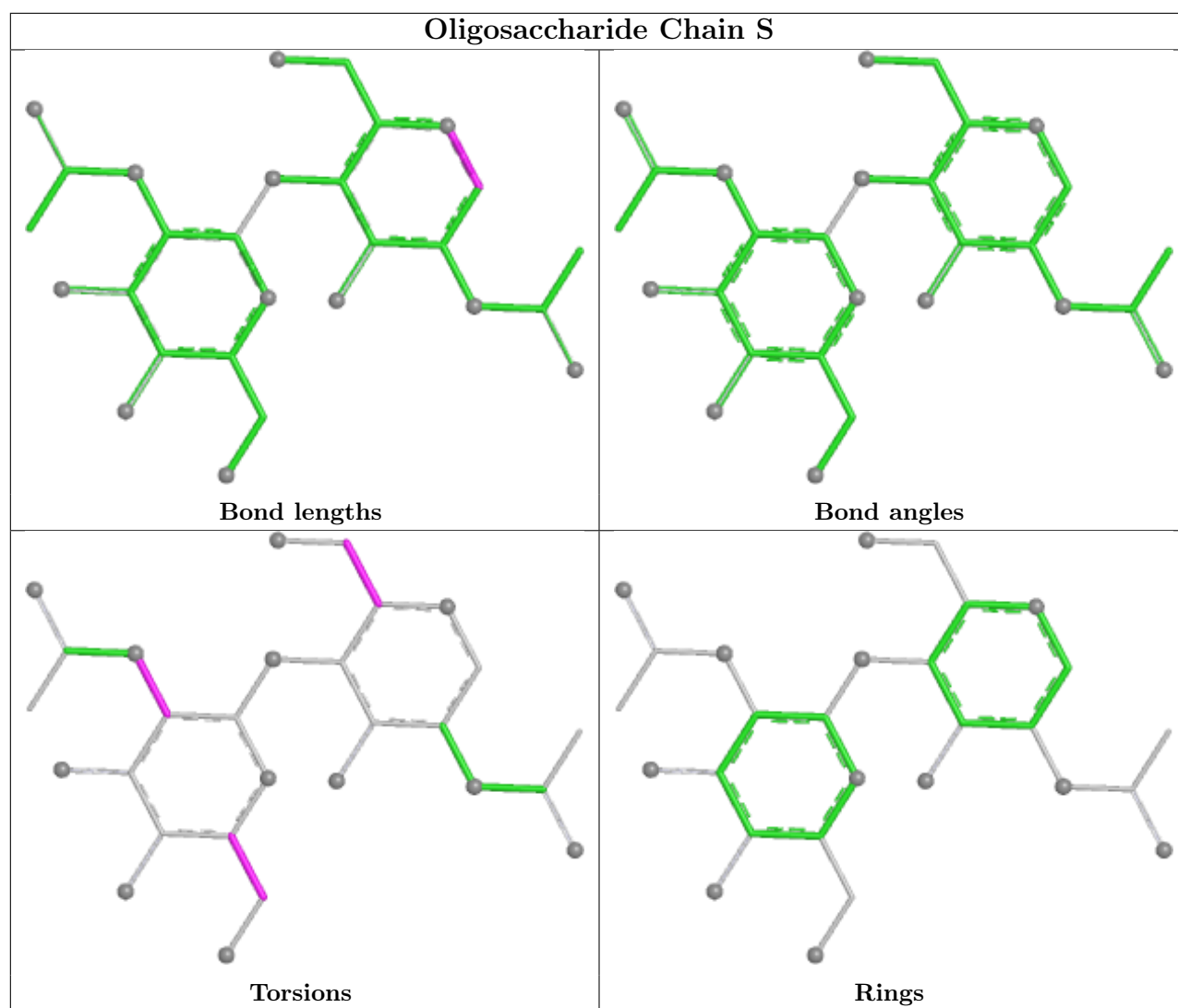


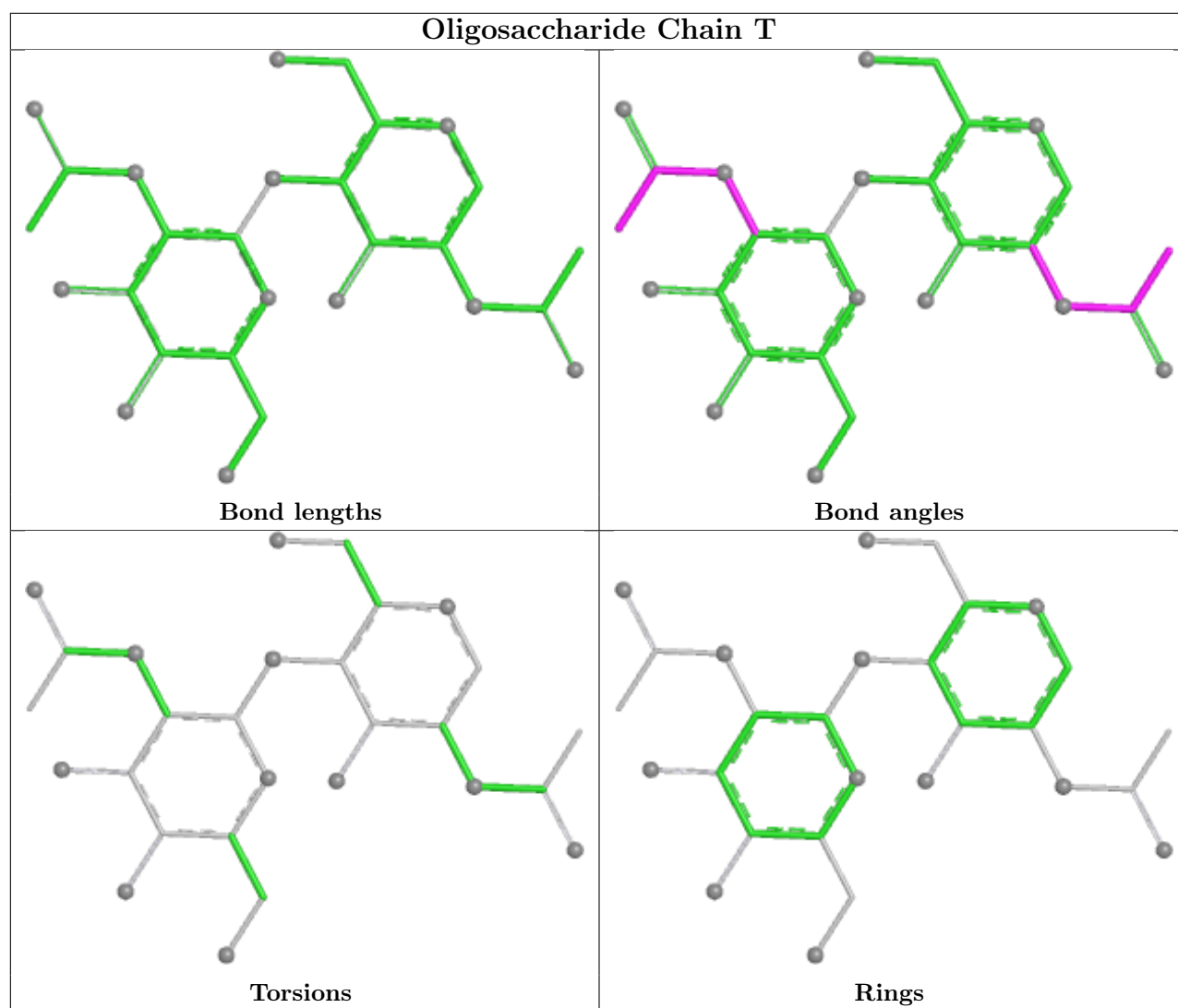


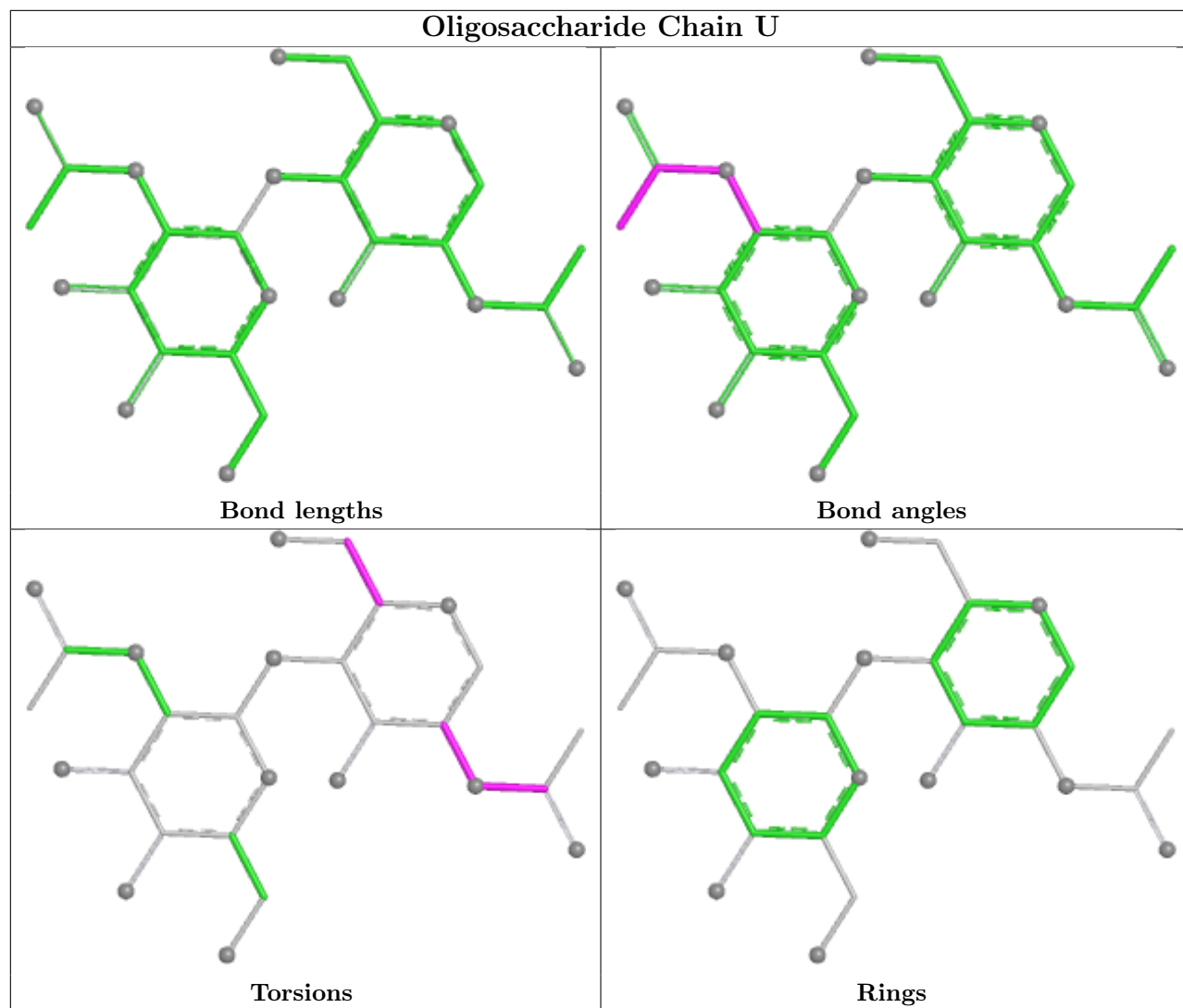


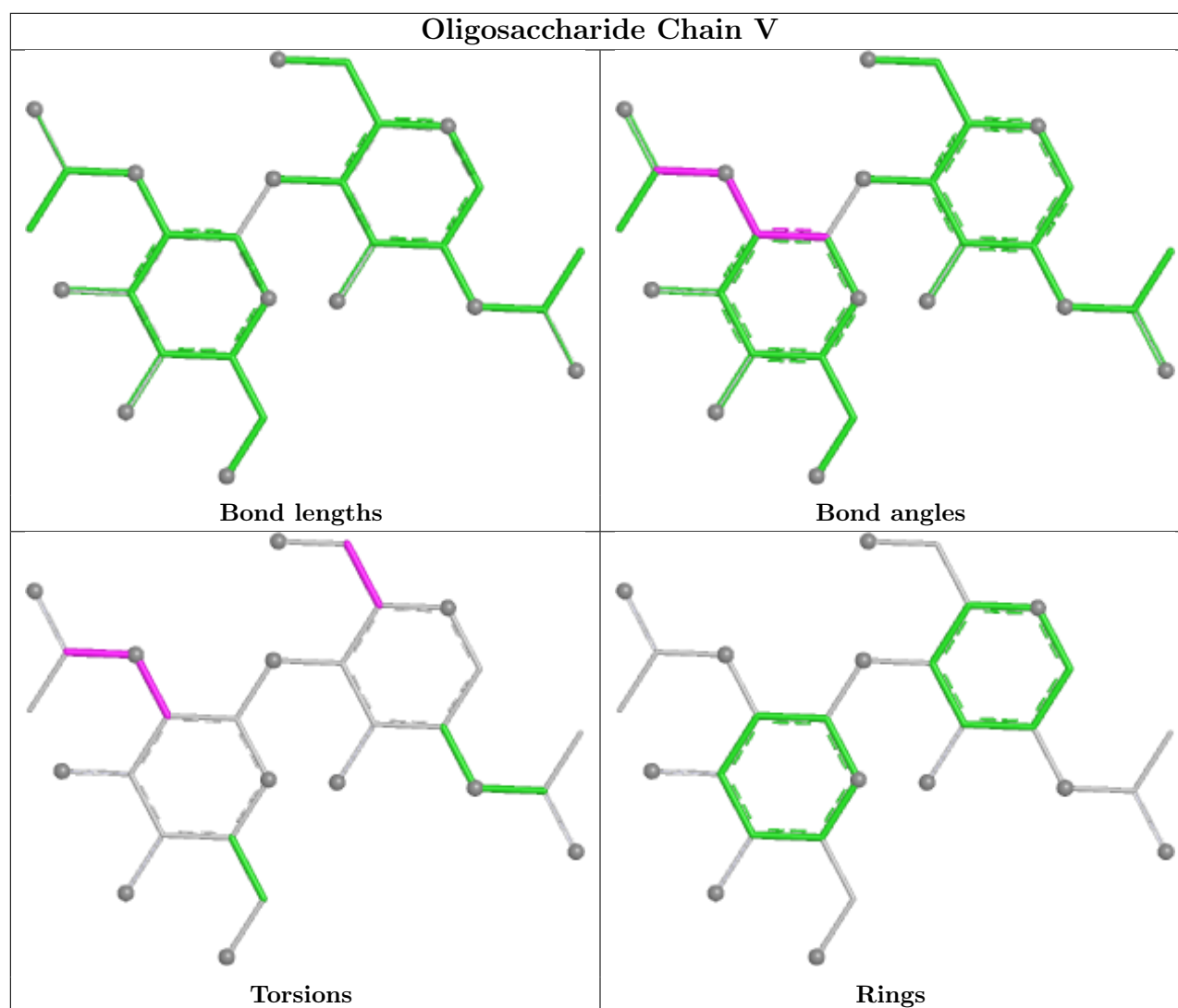


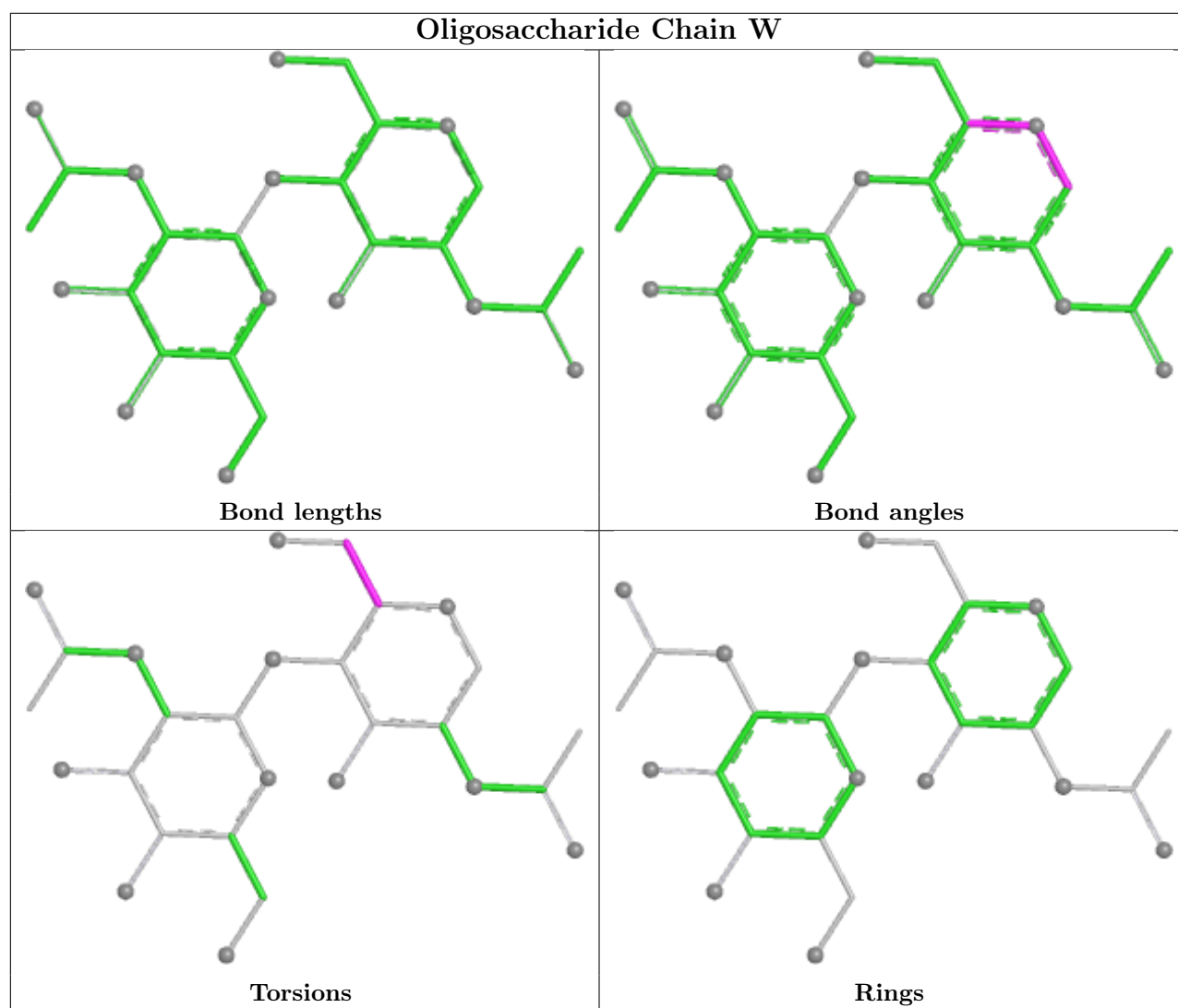


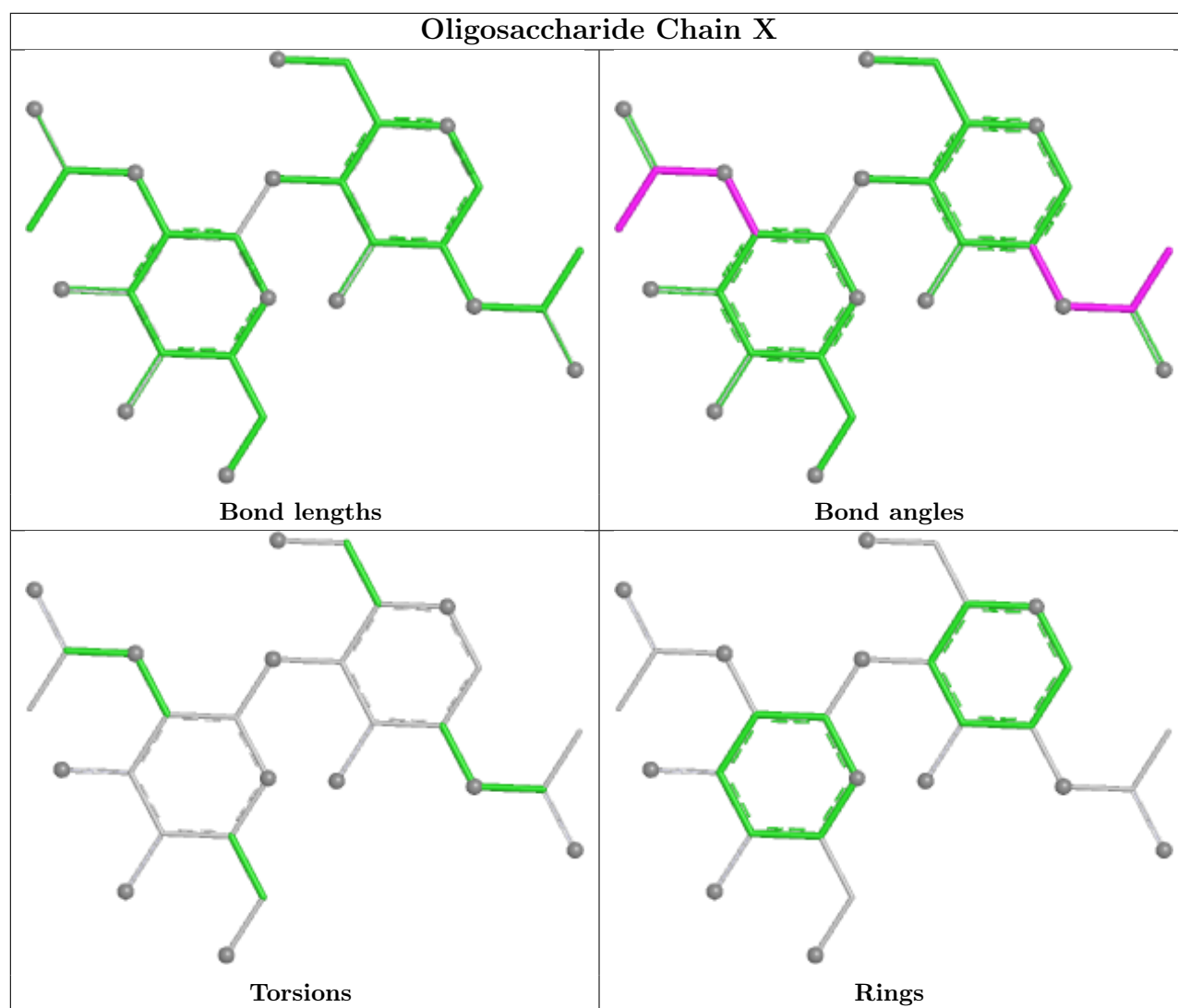


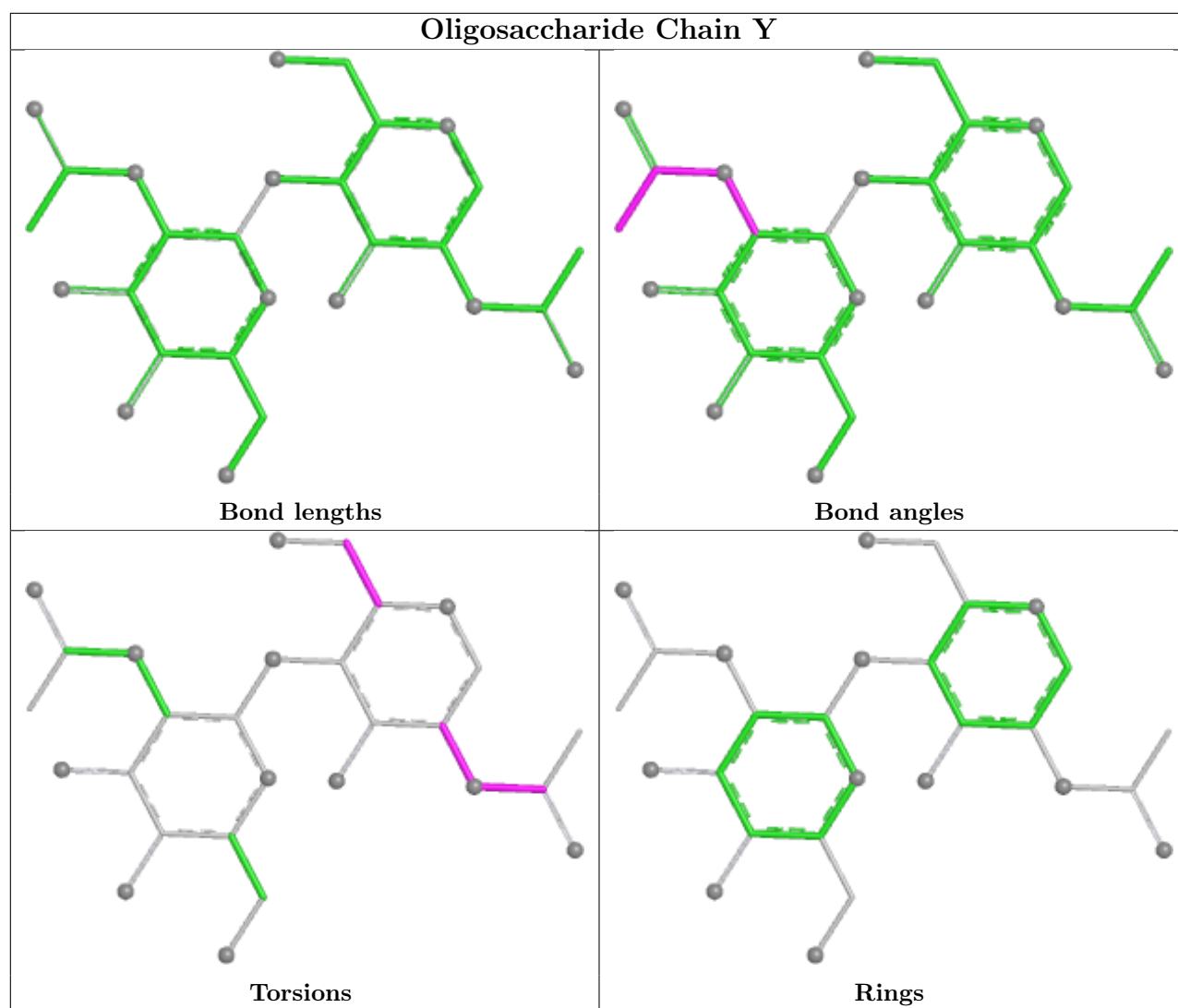


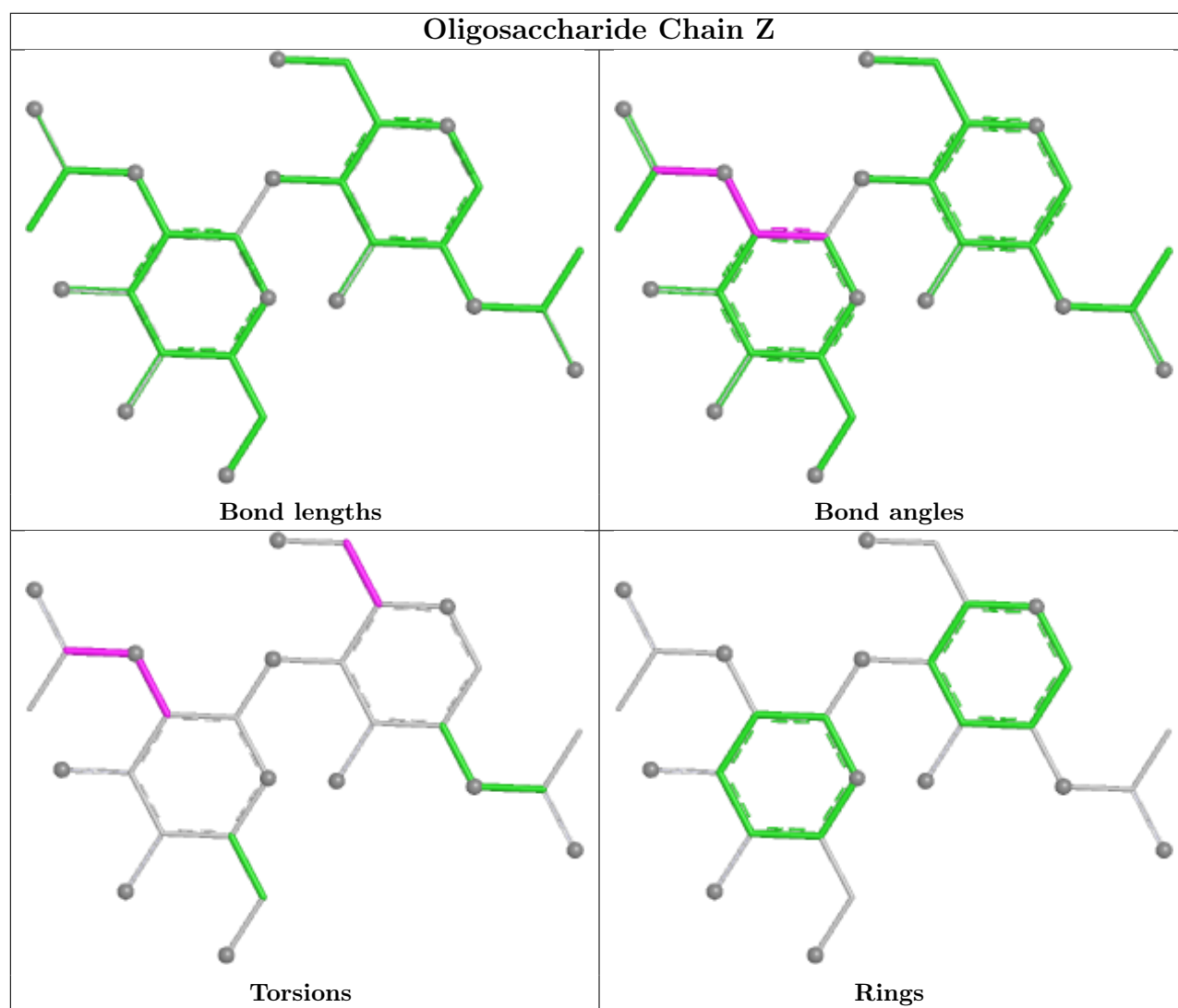


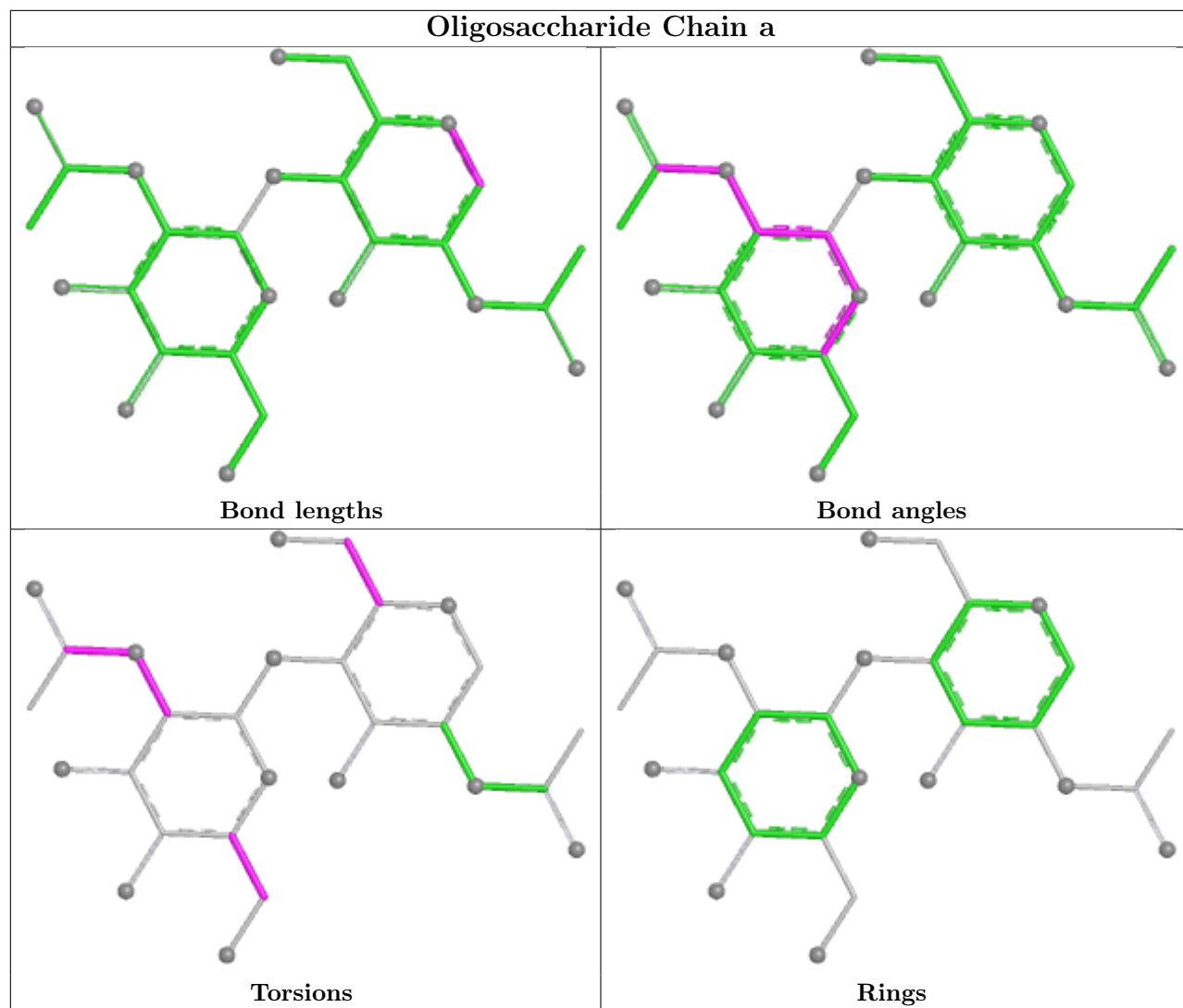


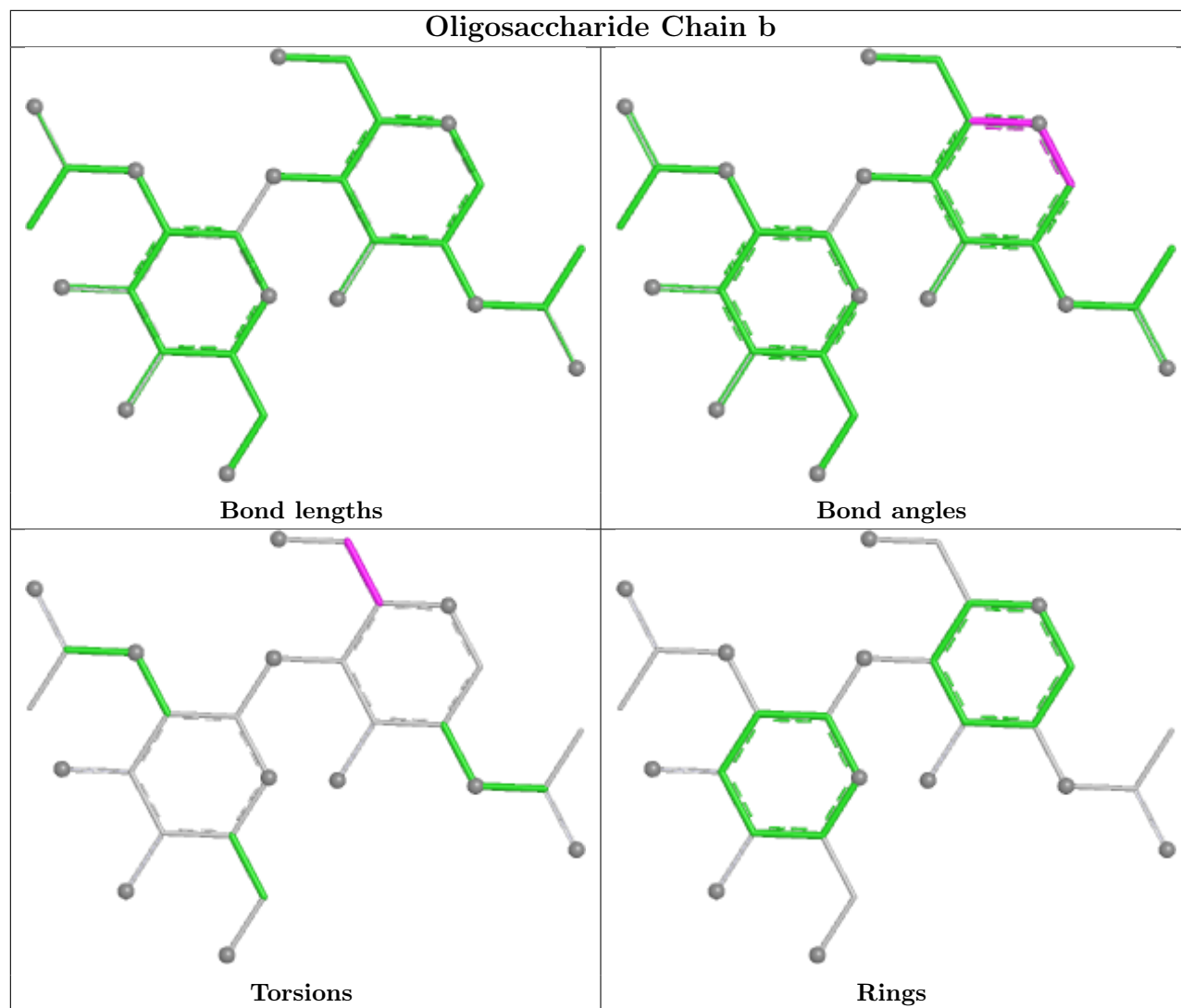


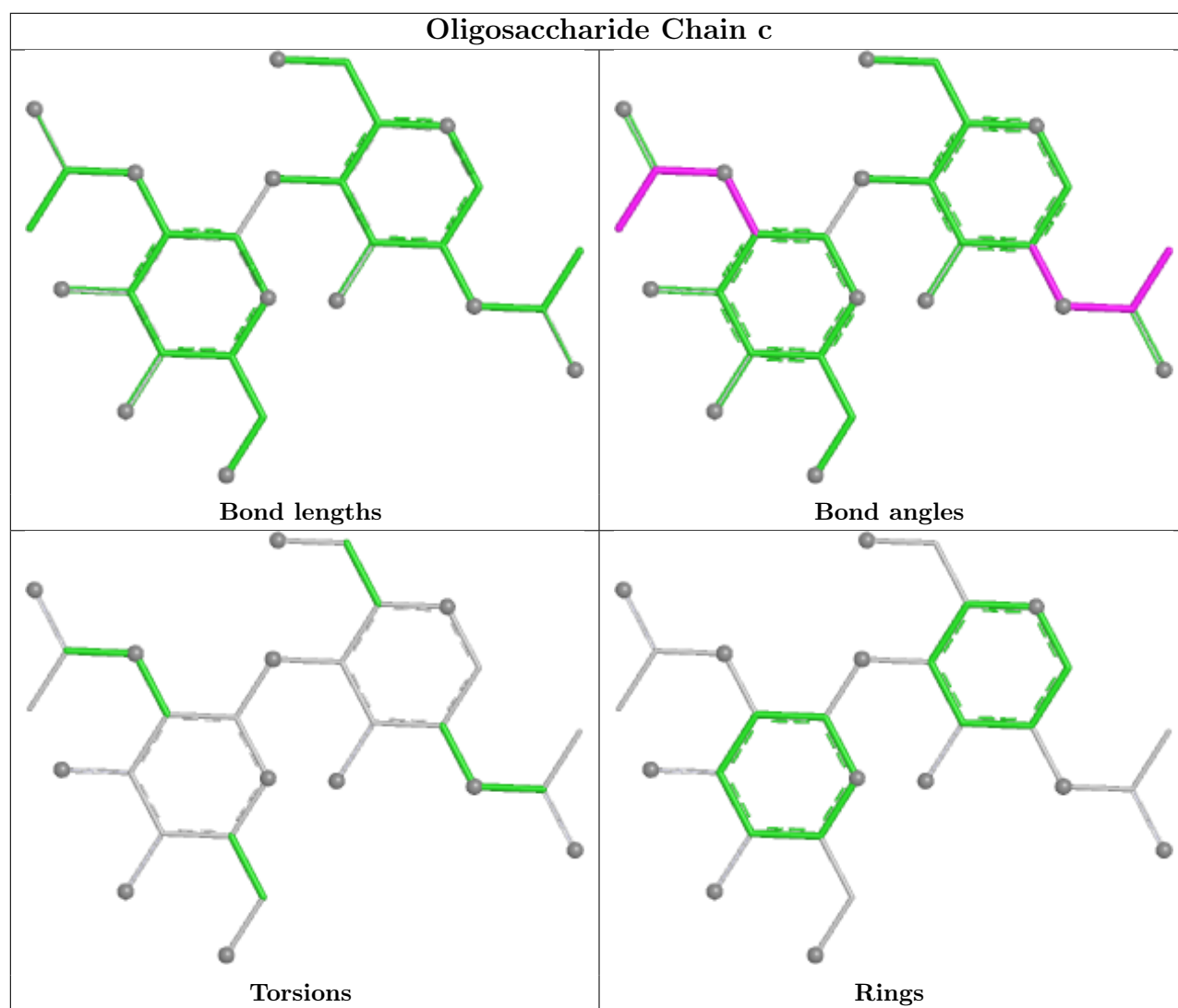


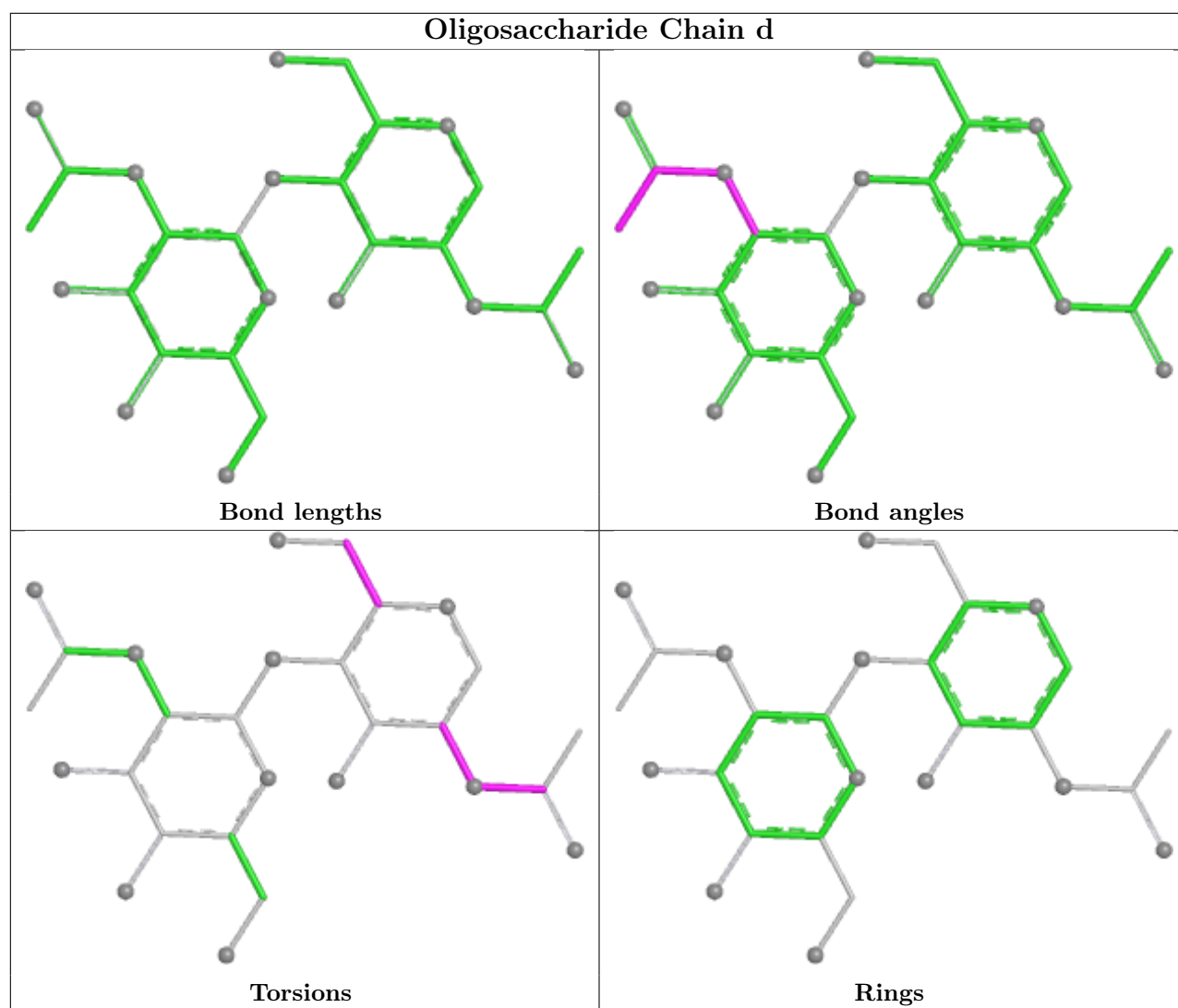


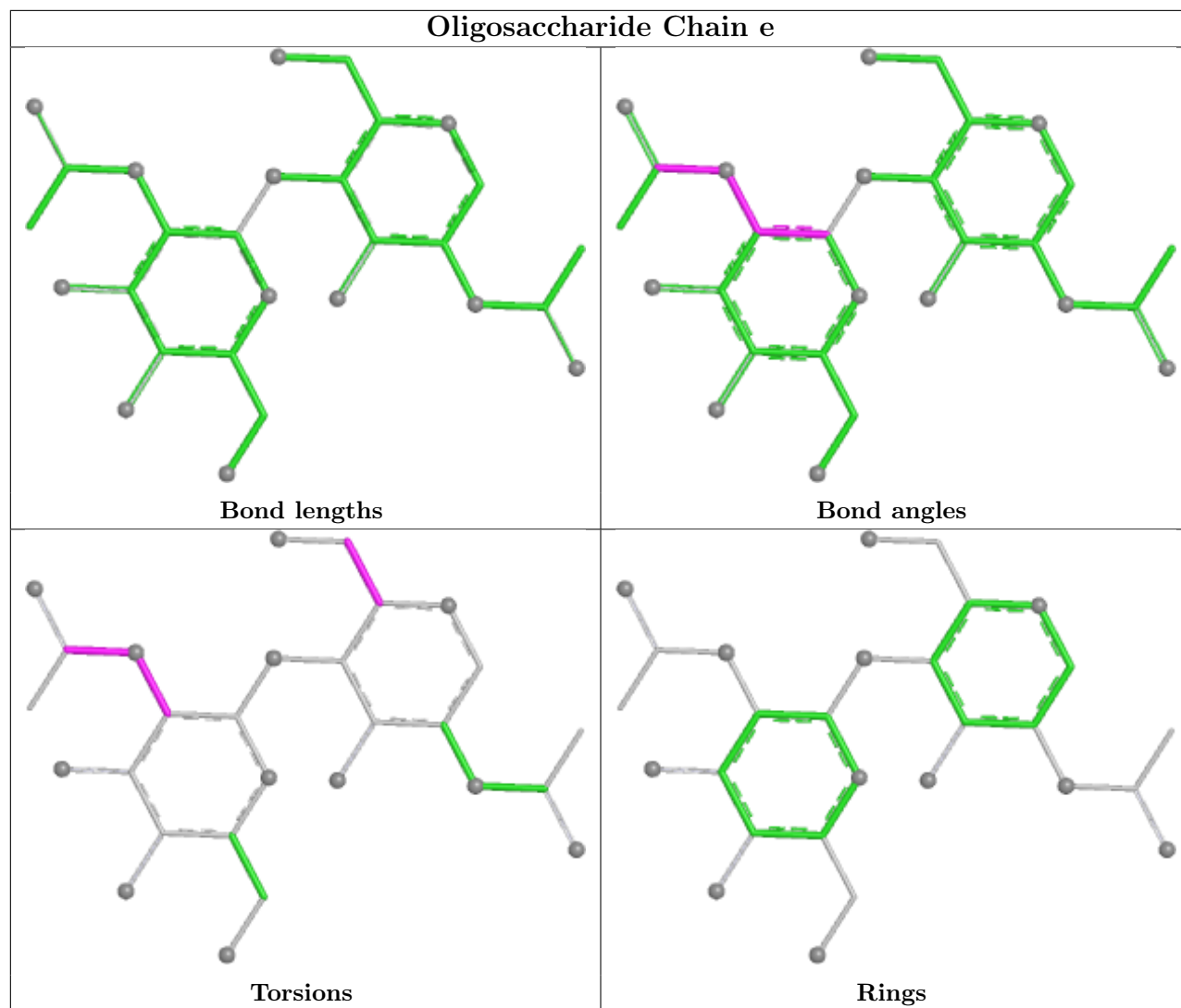


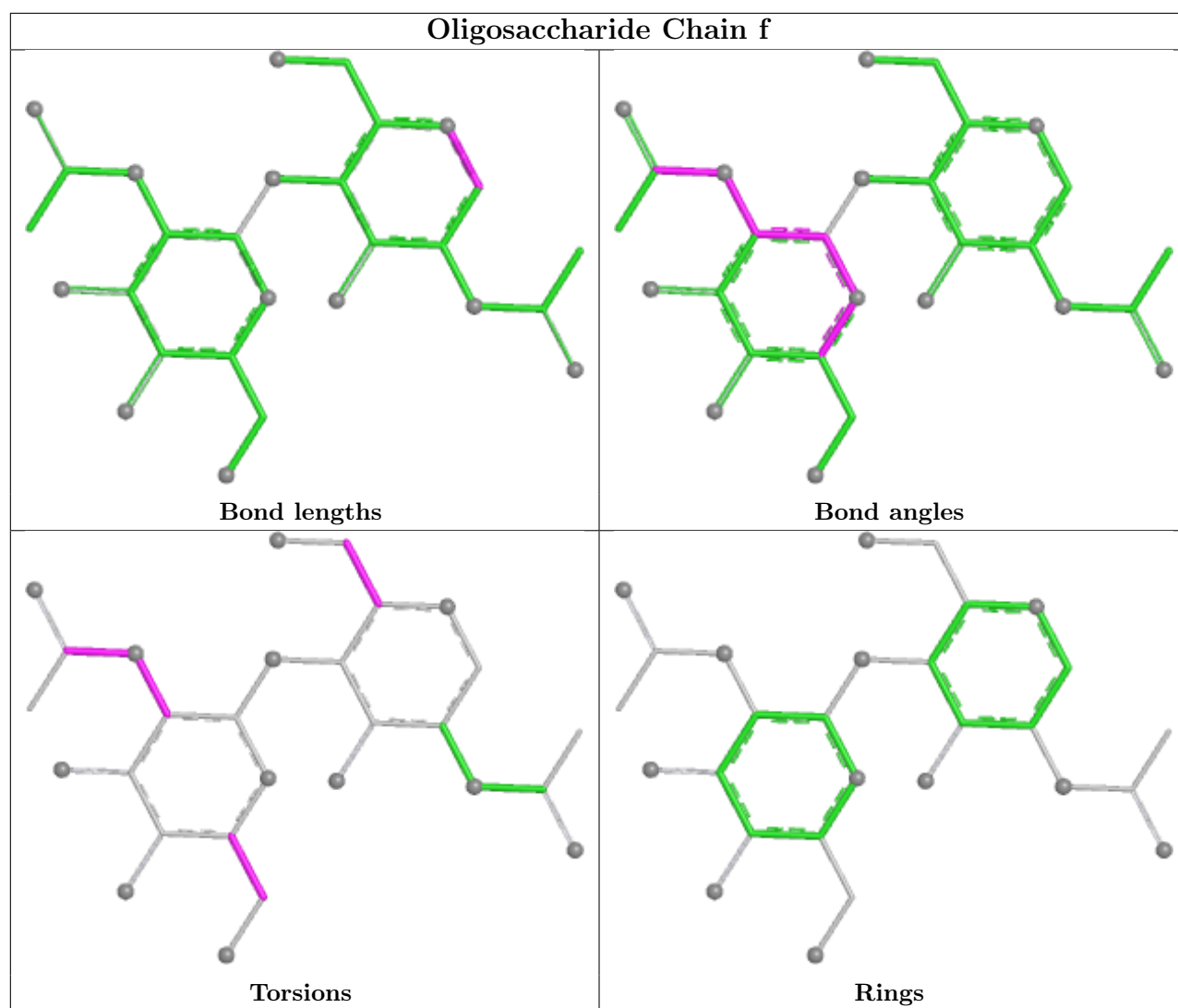


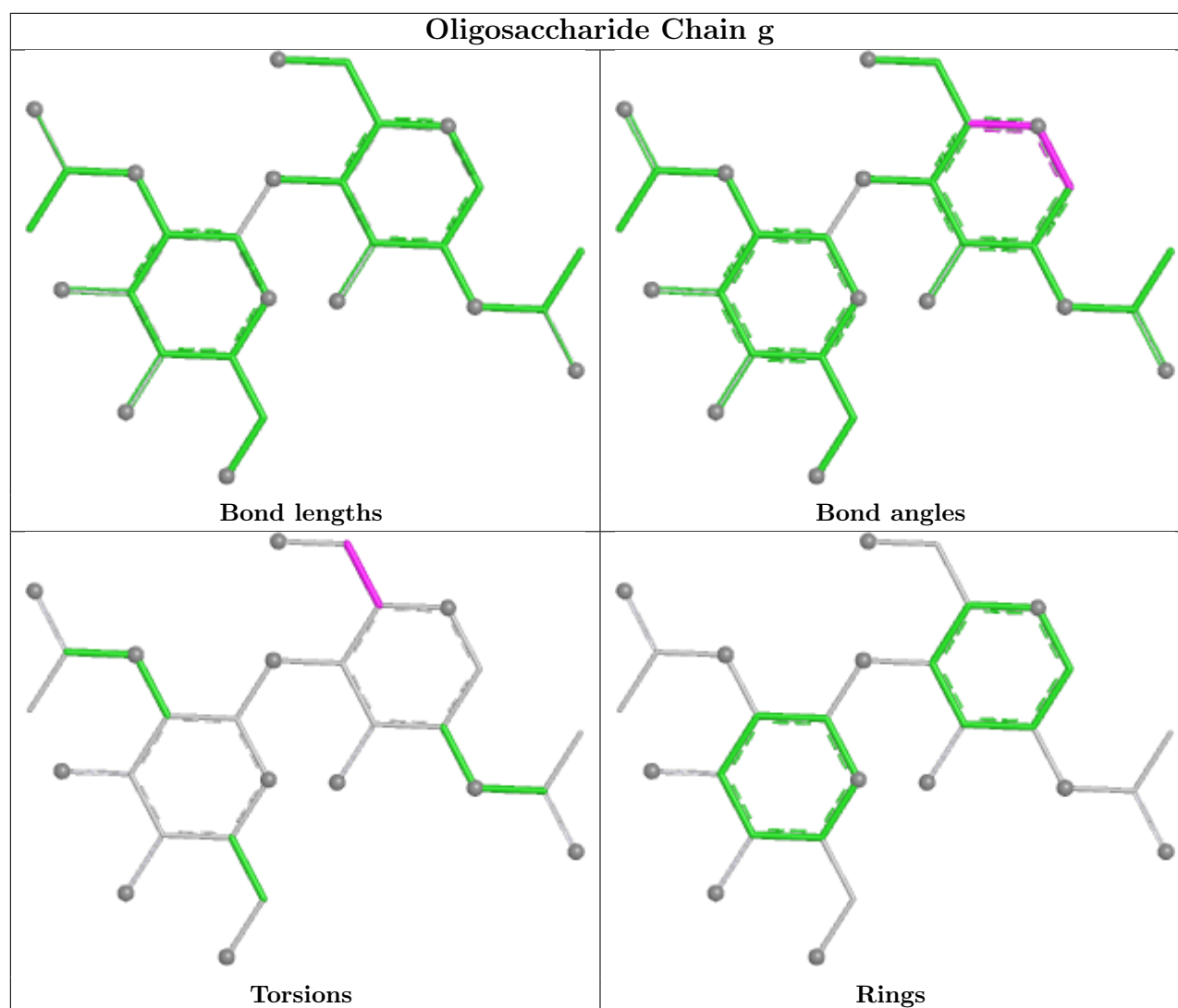












5.6 Ligand geometry [i](#)

33 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	$\# Z > 2$
5	NAG	A	1307	1	14,14,15	0.83	1 (7%)	17,19,21	0.57	0
5	NAG	B	1306	1	14,14,15	0.29	0	17,19,21	0.56	0
5	NAG	B	1310	1	14,14,15	0.51	0	17,19,21	0.37	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	B	1308	1	14,14,15	0.65	1 (7%)	17,19,21	0.78	1 (5%)
6	EIC	B	1311	-	19,19,19	0.58	0	19,19,19	0.95	0
5	NAG	A	1306	1	14,14,15	0.29	0	17,19,21	0.56	0
5	NAG	C	1301	1	14,14,15	0.21	0	17,19,21	0.40	0
5	NAG	A	1304	1	14,14,15	0.28	0	17,19,21	0.41	0
6	EIC	A	1312	-	19,19,19	0.58	0	19,19,19	0.96	1 (5%)
5	NAG	A	1301	1	14,14,15	0.20	0	17,19,21	0.40	0
5	NAG	B	1302	1	14,14,15	0.45	0	17,19,21	0.63	0
5	NAG	A	1310	1	14,14,15	0.50	0	17,19,21	0.36	0
5	NAG	B	1303	1	14,14,15	0.42	0	17,19,21	1.17	2 (11%)
5	NAG	C	1305	1	14,14,15	0.78	1 (7%)	17,19,21	0.64	0
6	EIC	A	1311	-	19,19,19	0.56	0	19,19,19	0.98	1 (5%)
5	NAG	B	1301	1	14,14,15	0.19	0	17,19,21	0.40	0
5	NAG	C	1309	1	14,14,15	0.28	0	17,19,21	0.56	0
5	NAG	C	1304	1	14,14,15	0.30	0	17,19,21	0.41	0
5	NAG	A	1302	1	14,14,15	0.44	0	17,19,21	0.64	0
5	NAG	B	1305	1	14,14,15	0.79	1 (7%)	17,19,21	0.64	0
5	NAG	B	1307	1	14,14,15	0.80	1 (7%)	17,19,21	0.59	0
5	NAG	A	1303	1	14,14,15	0.43	0	17,19,21	1.16	2 (11%)
5	NAG	B	1309	1	14,14,15	0.29	0	17,19,21	0.56	0
5	NAG	C	1306	1	14,14,15	0.29	0	17,19,21	0.57	0
5	NAG	C	1308	1	14,14,15	0.65	1 (7%)	17,19,21	0.77	1 (5%)
5	NAG	A	1308	1	14,14,15	0.67	1 (7%)	17,19,21	0.77	1 (5%)
5	NAG	C	1310	1	14,14,15	0.50	0	17,19,21	0.37	0
5	NAG	A	1305	1	14,14,15	0.79	1 (7%)	17,19,21	0.63	0
5	NAG	C	1307	1	14,14,15	0.42	0	17,19,21	1.15	2 (11%)
5	NAG	C	1302	1	14,14,15	0.45	0	17,19,21	0.64	0
5	NAG	A	1309	1	14,14,15	0.28	0	17,19,21	0.57	0
5	NAG	C	1303	1	14,14,15	0.43	0	17,19,21	1.16	2 (11%)
5	NAG	B	1304	1	14,14,15	0.30	0	17,19,21	0.42	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	A	1307	1	-	1/6/23/26	0/1/1/1
5	NAG	B	1306	1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	B	1310	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1308	1	-	2/6/23/26	0/1/1/1
6	EIC	B	1311	-	-	6/17/17/17	-
5	NAG	A	1306	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1301	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1304	1	-	2/6/23/26	0/1/1/1
6	EIC	A	1312	-	-	7/17/17/17	-
5	NAG	A	1301	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1302	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1310	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1303	1	-	0/6/23/26	0/1/1/1
5	NAG	C	1305	1	-	3/6/23/26	0/1/1/1
6	EIC	A	1311	-	-	11/17/17/17	-
5	NAG	B	1301	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1309	1	-	4/6/23/26	0/1/1/1
5	NAG	C	1304	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1302	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1305	1	-	3/6/23/26	0/1/1/1
5	NAG	B	1307	1	-	1/6/23/26	0/1/1/1
5	NAG	A	1303	1	-	0/6/23/26	0/1/1/1
5	NAG	B	1309	1	-	4/6/23/26	0/1/1/1
5	NAG	C	1306	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1308	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1308	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1310	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1305	1	-	3/6/23/26	0/1/1/1
5	NAG	C	1307	1	-	0/6/23/26	0/1/1/1
5	NAG	C	1302	1	-	3/6/23/26	0/1/1/1
5	NAG	A	1309	1	-	4/6/23/26	0/1/1/1
5	NAG	C	1303	1	-	0/6/23/26	0/1/1/1
5	NAG	B	1304	1	-	2/6/23/26	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1307	NAG	O5-C1	-2.69	1.39	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1307	NAG	O5-C1	-2.56	1.39	1.43
5	A	1305	NAG	C1-C2	2.22	1.55	1.52
5	B	1305	NAG	C1-C2	2.21	1.55	1.52
5	A	1308	NAG	C1-C2	2.14	1.55	1.52
5	C	1305	NAG	C1-C2	2.13	1.55	1.52
5	C	1308	NAG	C1-C2	2.09	1.55	1.52
5	B	1308	NAG	C1-C2	2.07	1.55	1.52

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	1303	NAG	C8-C7-N2	2.35	120.02	116.12
5	C	1307	NAG	C8-C7-N2	2.35	120.02	116.12
5	B	1303	NAG	C8-C7-N2	2.34	120.00	116.12
5	A	1303	NAG	C8-C7-N2	2.33	119.98	116.12
5	B	1308	NAG	C1-O5-C5	2.27	115.23	112.19
5	A	1308	NAG	C1-O5-C5	2.26	115.21	112.19
5	C	1308	NAG	C1-O5-C5	2.23	115.17	112.19
5	A	1303	NAG	C2-N2-C7	-2.17	120.00	122.90
5	B	1303	NAG	C2-N2-C7	-2.16	120.00	122.90
5	C	1303	NAG	C2-N2-C7	-2.16	120.01	122.90
5	C	1307	NAG	C2-N2-C7	-2.14	120.04	122.90
6	A	1311	EIC	O2-C1-C2	2.02	120.38	114.00
6	A	1312	EIC	O2-C1-C2	2.01	120.34	114.00

There are no chirality outliers.

All (84) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1306	NAG	C8-C7-N2-C2
5	A	1306	NAG	O7-C7-N2-C2
5	A	1309	NAG	C1-C2-N2-C7
5	A	1309	NAG	C8-C7-N2-C2
5	A	1309	NAG	O7-C7-N2-C2
5	B	1306	NAG	C8-C7-N2-C2
5	B	1306	NAG	O7-C7-N2-C2
5	B	1309	NAG	C1-C2-N2-C7
5	B	1309	NAG	C8-C7-N2-C2
5	B	1309	NAG	O7-C7-N2-C2
5	C	1306	NAG	C8-C7-N2-C2
5	C	1306	NAG	O7-C7-N2-C2
5	C	1309	NAG	C1-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
5	C	1309	NAG	C8-C7-N2-C2
5	C	1309	NAG	O7-C7-N2-C2
5	B	1302	NAG	C4-C5-C6-O6
5	C	1302	NAG	C4-C5-C6-O6
5	A	1302	NAG	C4-C5-C6-O6
5	B	1305	NAG	O5-C5-C6-O6
5	C	1305	NAG	O5-C5-C6-O6
5	A	1305	NAG	O5-C5-C6-O6
5	A	1302	NAG	O5-C5-C6-O6
5	B	1302	NAG	O5-C5-C6-O6
5	C	1302	NAG	O5-C5-C6-O6
5	A	1301	NAG	O5-C5-C6-O6
5	B	1301	NAG	O5-C5-C6-O6
5	C	1301	NAG	O5-C5-C6-O6
5	A	1310	NAG	C4-C5-C6-O6
5	B	1310	NAG	C4-C5-C6-O6
5	C	1310	NAG	C4-C5-C6-O6
5	A	1310	NAG	O5-C5-C6-O6
5	B	1310	NAG	O5-C5-C6-O6
5	C	1310	NAG	O5-C5-C6-O6
5	A	1308	NAG	O5-C5-C6-O6
5	B	1308	NAG	O5-C5-C6-O6
5	C	1308	NAG	O5-C5-C6-O6
5	B	1308	NAG	C4-C5-C6-O6
5	A	1309	NAG	O5-C5-C6-O6
5	B	1309	NAG	O5-C5-C6-O6
5	C	1309	NAG	O5-C5-C6-O6
5	A	1308	NAG	C4-C5-C6-O6
5	C	1308	NAG	C4-C5-C6-O6
5	A	1305	NAG	C4-C5-C6-O6
5	B	1305	NAG	C4-C5-C6-O6
5	C	1305	NAG	C4-C5-C6-O6
6	A	1311	EIC	C1-C2-C3-C4
5	A	1304	NAG	O5-C5-C6-O6
5	B	1304	NAG	O5-C5-C6-O6
5	C	1304	NAG	O5-C5-C6-O6
5	A	1304	NAG	C4-C5-C6-O6
5	B	1304	NAG	C4-C5-C6-O6
5	C	1304	NAG	C4-C5-C6-O6
6	B	1311	EIC	C4-C5-C6-C7
6	A	1311	EIC	C5-C6-C7-C8
6	A	1311	EIC	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
6	A	1311	EIC	C14-C15-C16-C17
6	A	1311	EIC	C6-C7-C8-C9
6	A	1311	EIC	C15-C16-C17-C18
6	B	1311	EIC	C2-C3-C4-C5
6	A	1312	EIC	C4-C5-C6-C7
6	A	1311	EIC	C10-C11-C12-C13
6	A	1312	EIC	C10-C11-C12-C13
6	B	1311	EIC	C5-C6-C7-C8
5	B	1301	NAG	C4-C5-C6-O6
5	C	1301	NAG	C4-C5-C6-O6
5	A	1301	NAG	C4-C5-C6-O6
6	A	1312	EIC	C15-C16-C17-C18
6	A	1312	EIC	C7-C8-C9-C10
6	B	1311	EIC	O1-C1-C2-C3
6	A	1311	EIC	C9-C10-C11-C12
6	B	1311	EIC	O2-C1-C2-C3
5	A	1307	NAG	C4-C5-C6-O6
6	A	1311	EIC	C4-C5-C6-C7
5	B	1307	NAG	C4-C5-C6-O6
5	A	1305	NAG	C3-C2-N2-C7
5	B	1305	NAG	C3-C2-N2-C7
5	C	1302	NAG	C3-C2-N2-C7
5	C	1305	NAG	C3-C2-N2-C7
6	A	1312	EIC	O1-C1-C2-C3
6	A	1312	EIC	O2-C1-C2-C3
6	B	1311	EIC	C7-C8-C9-C10
6	A	1312	EIC	C14-C15-C16-C17
6	A	1311	EIC	C7-C8-C9-C10
6	A	1311	EIC	C12-C13-C14-C15

There are no ring outliers.

21 monomers are involved in 57 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	1306	NAG	1	0
6	B	1311	EIC	4	0
5	A	1306	NAG	1	0
5	C	1301	NAG	1	0
6	A	1312	EIC	6	0
5	A	1301	NAG	1	0
5	B	1302	NAG	6	0
5	B	1303	NAG	2	0

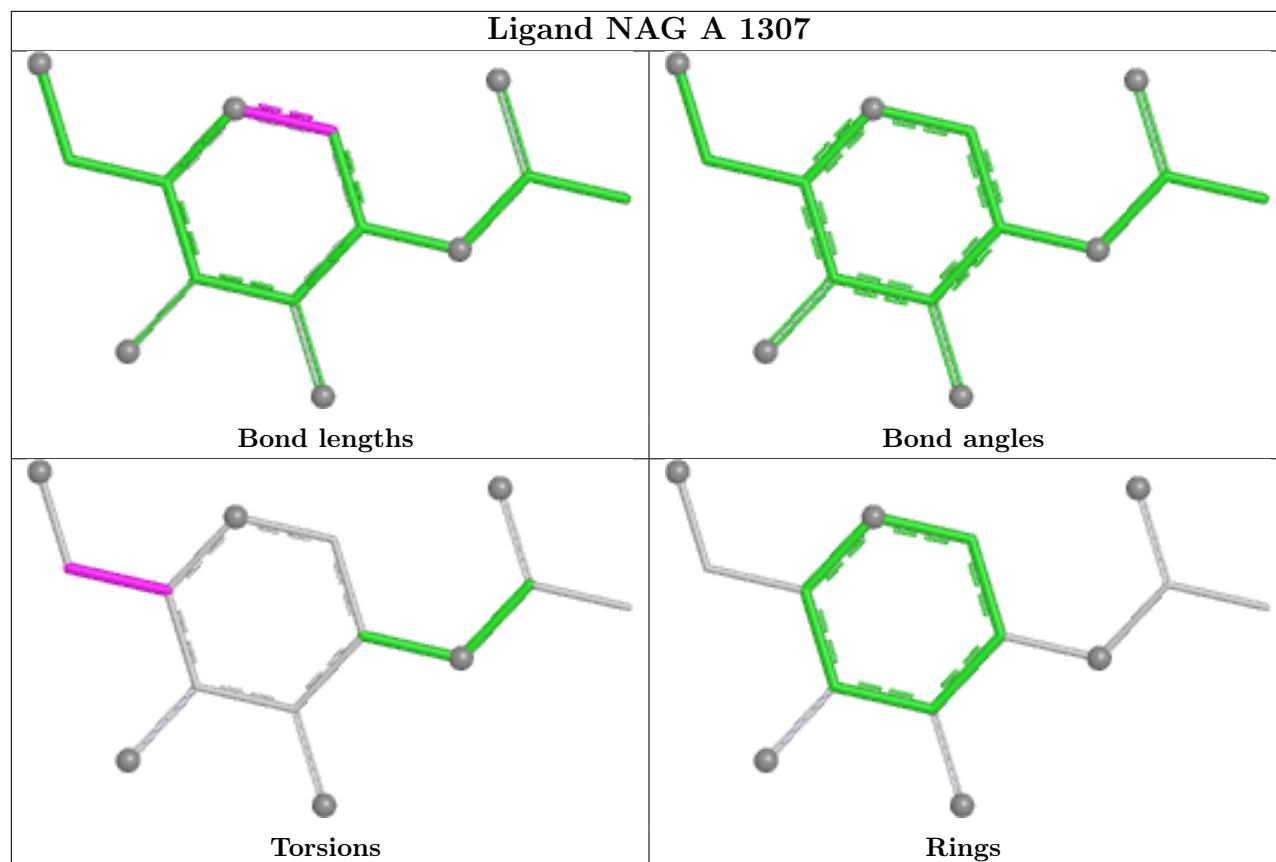
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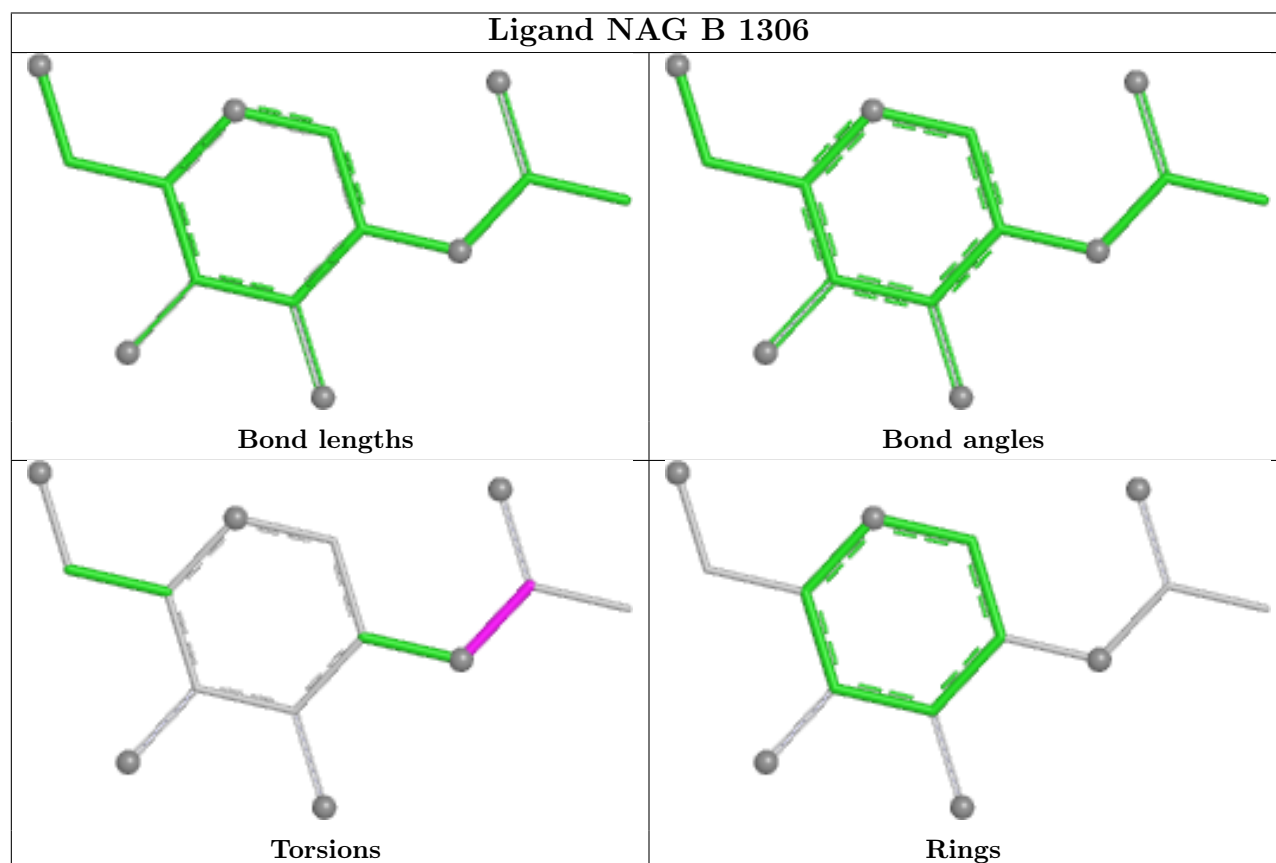
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	1305	NAG	1	0
6	A	1311	EIC	3	0
5	B	1301	NAG	1	0
5	C	1309	NAG	4	0
5	A	1302	NAG	6	0
5	B	1305	NAG	1	0
5	A	1303	NAG	2	0
5	B	1309	NAG	4	0
5	C	1306	NAG	1	0
5	A	1305	NAG	1	0
5	C	1302	NAG	6	0
5	A	1309	NAG	3	0
5	C	1303	NAG	2	0

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

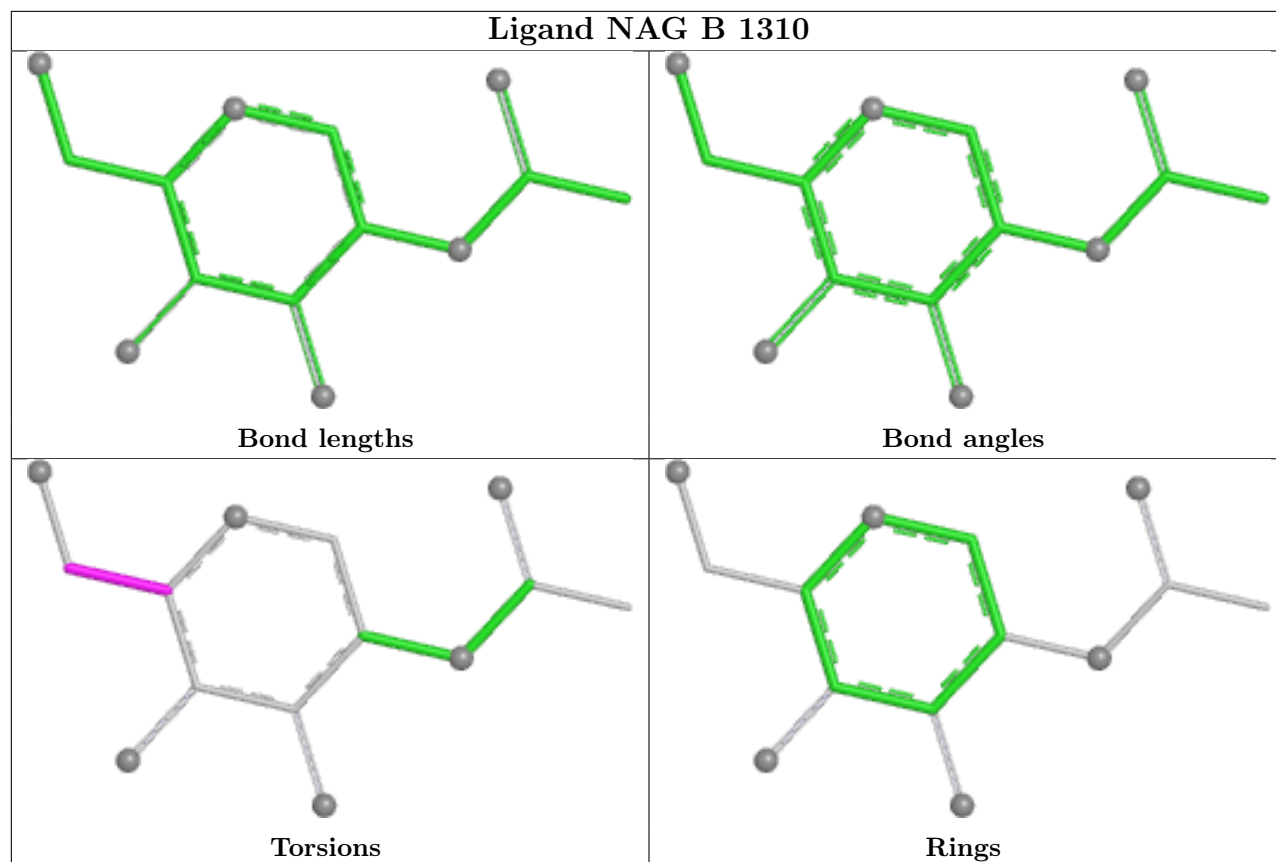
Ligand NAG A 1307



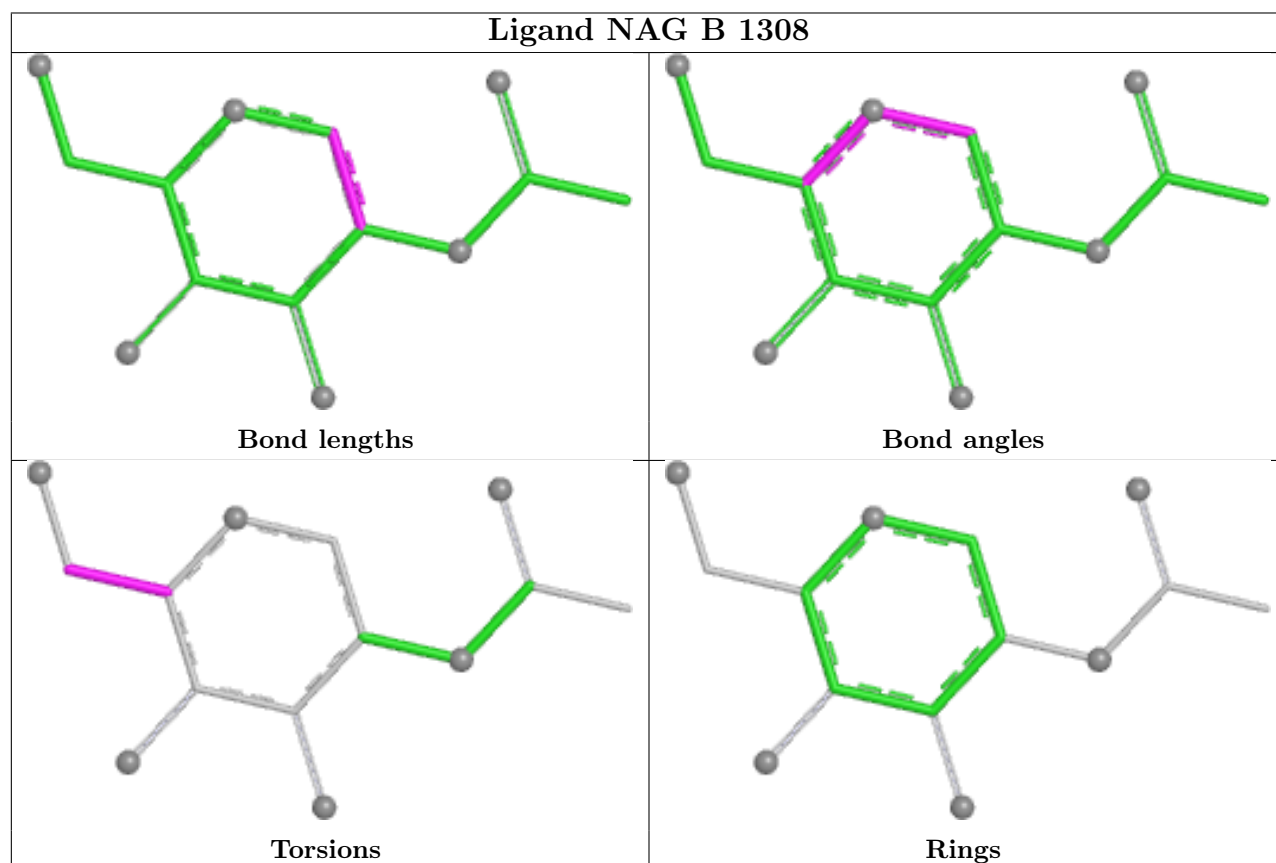
Ligand NAG B 1306

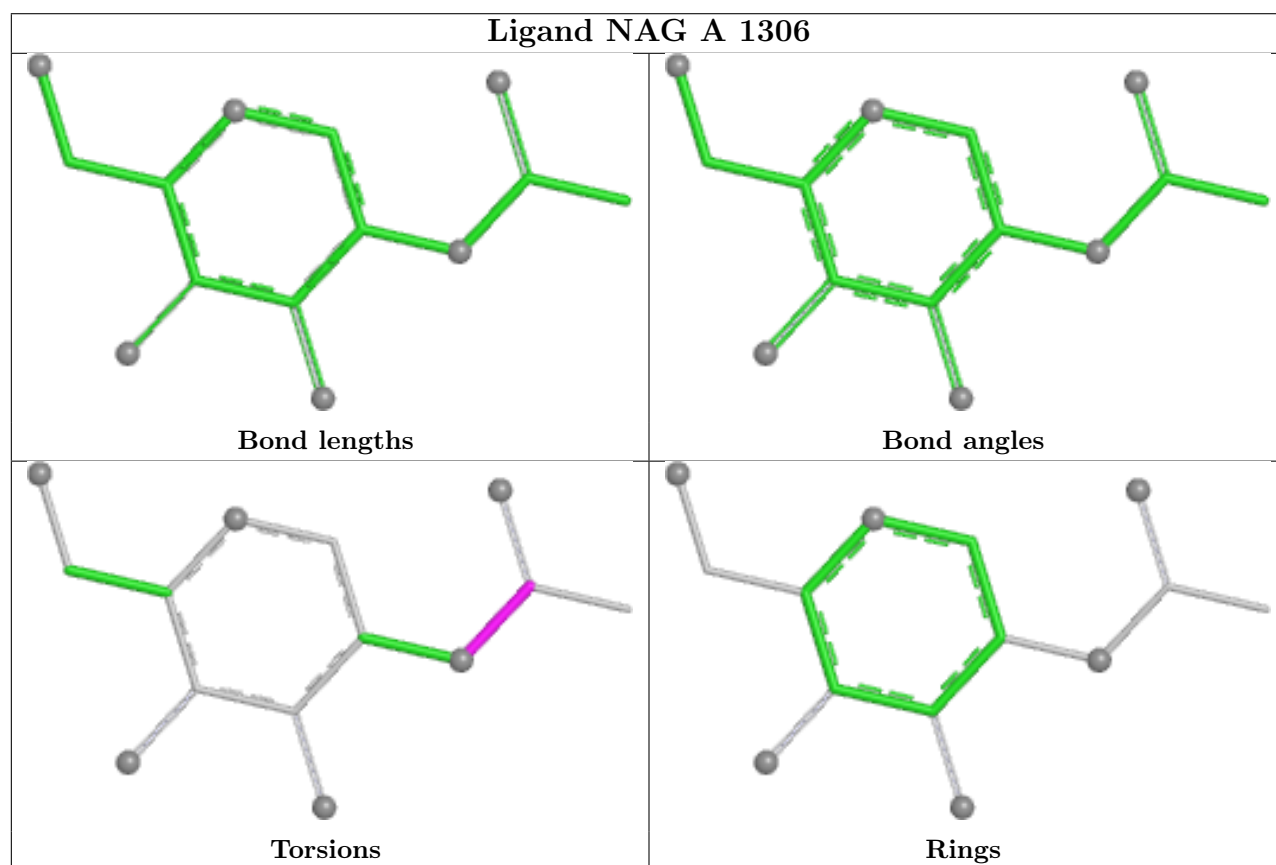
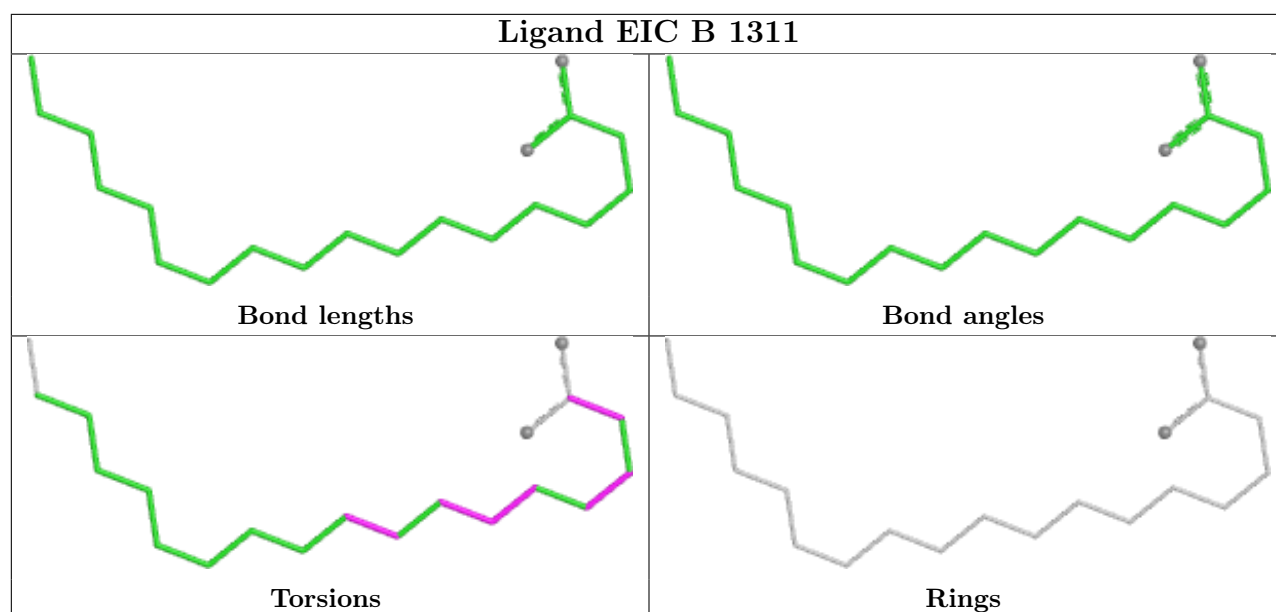


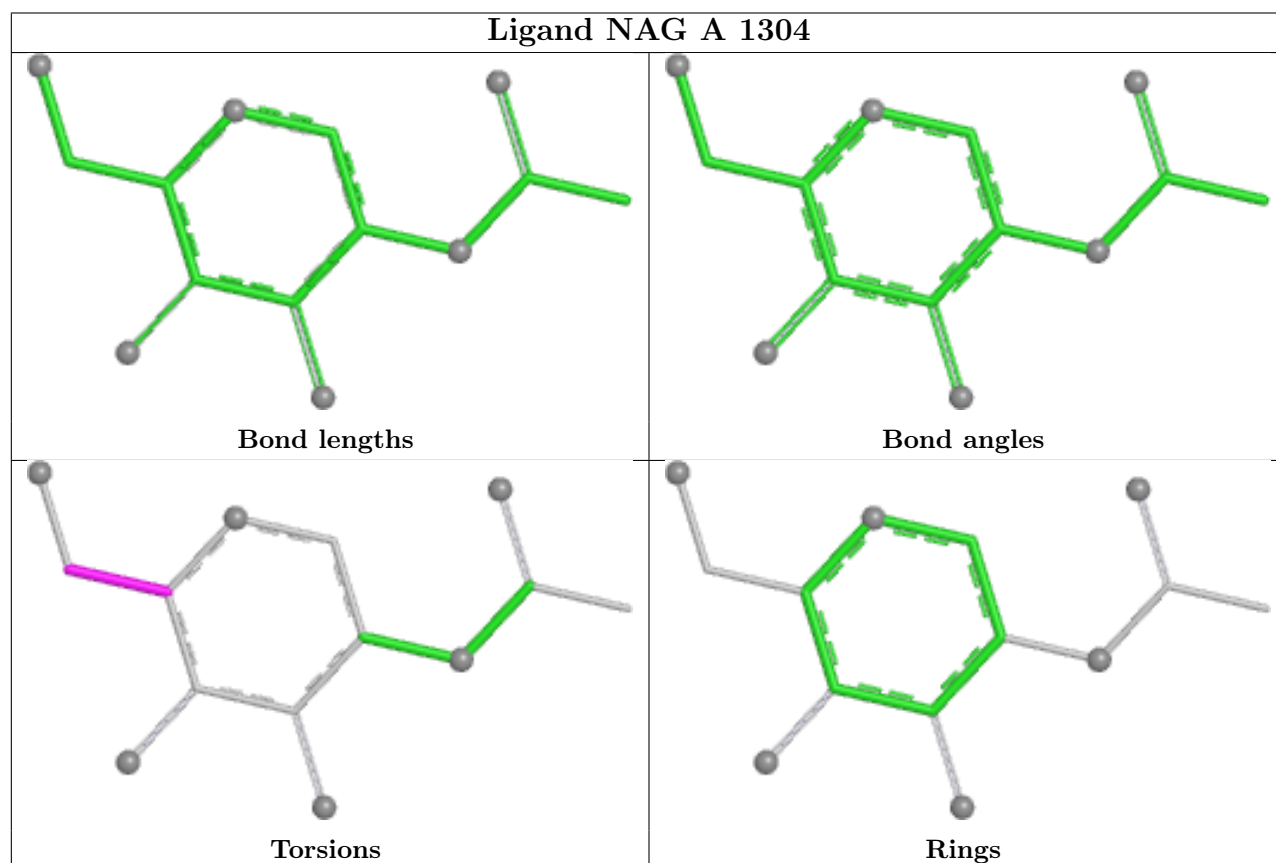
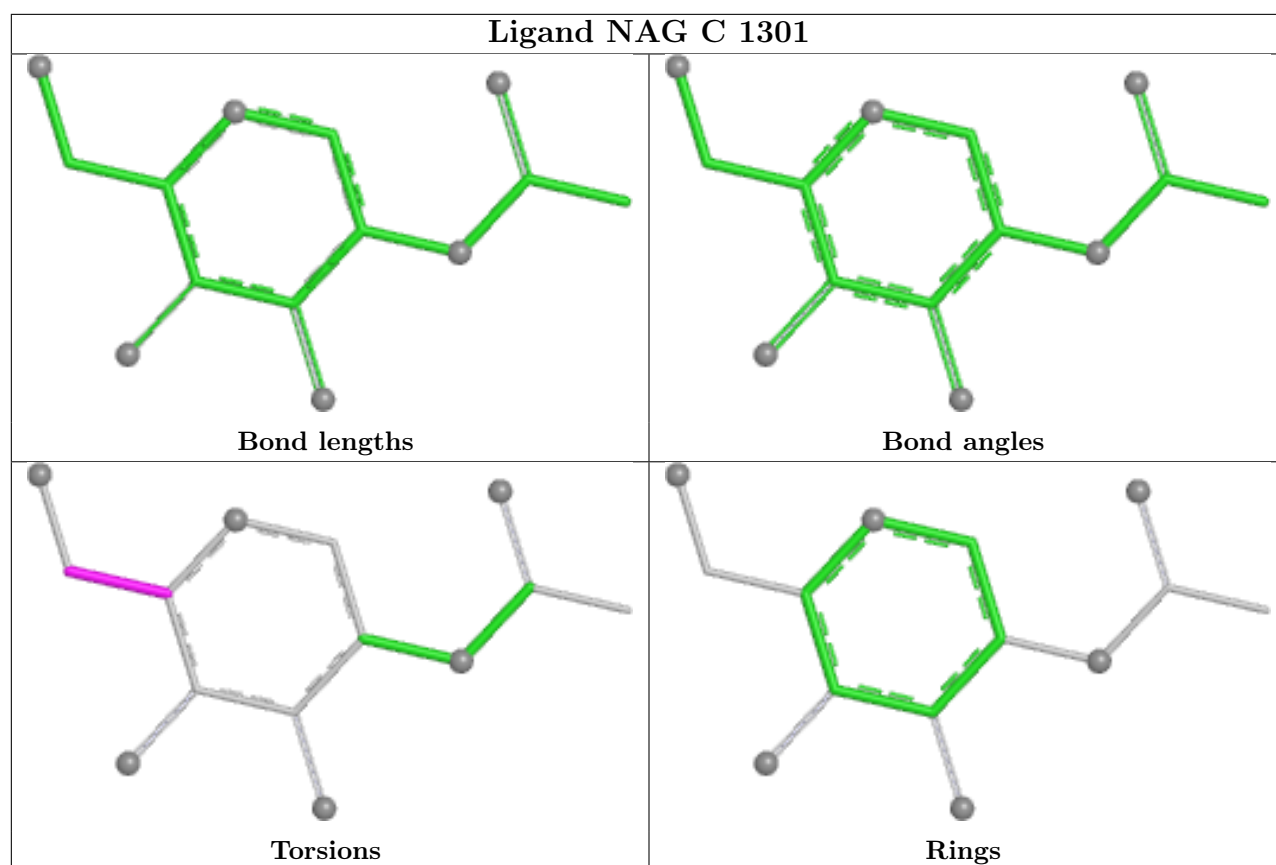
Ligand NAG B 1310

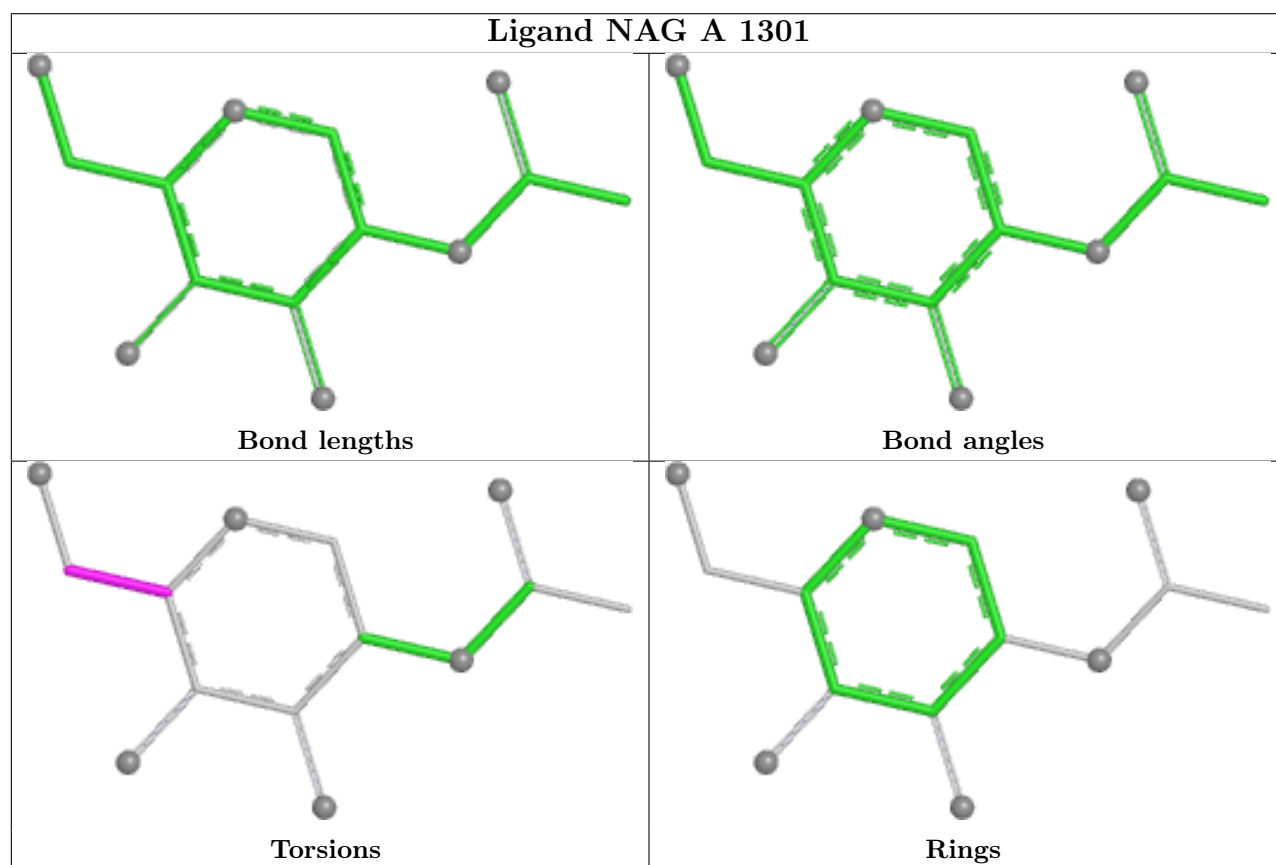
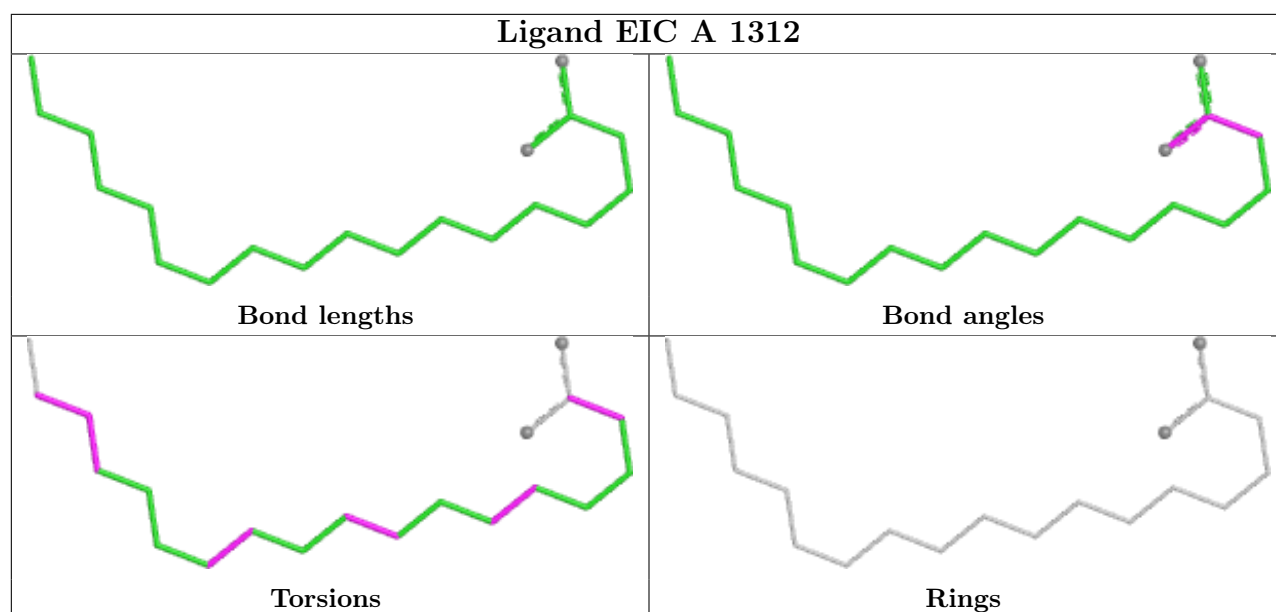


Ligand NAG B 1308

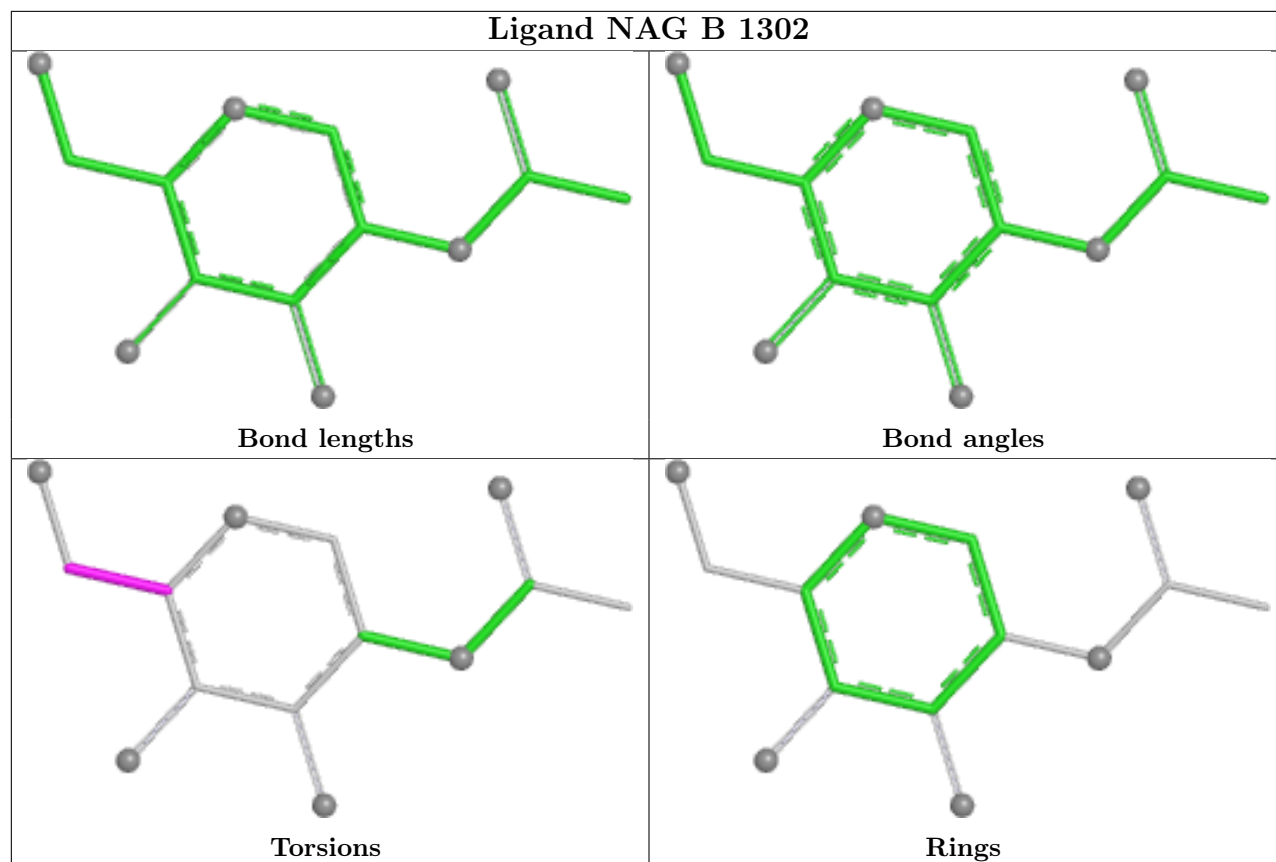




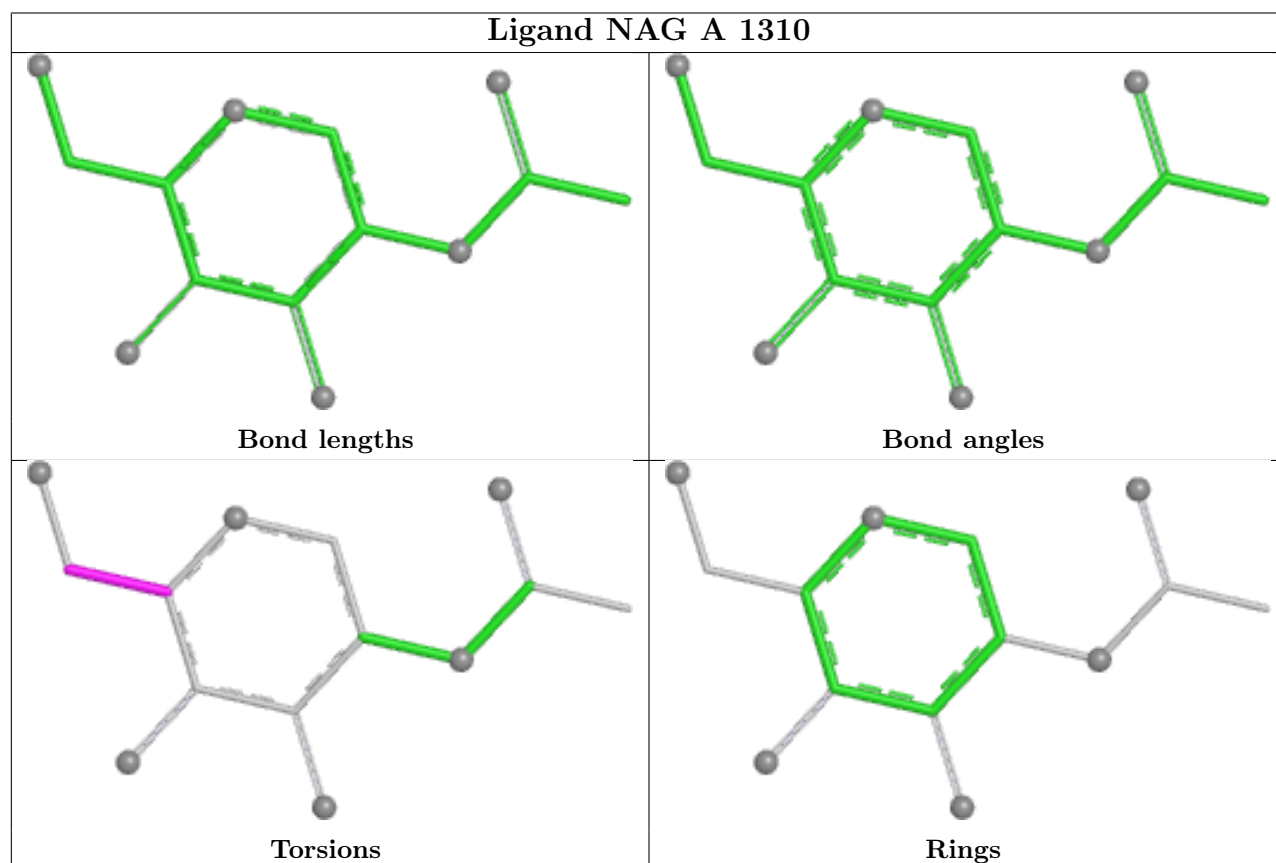




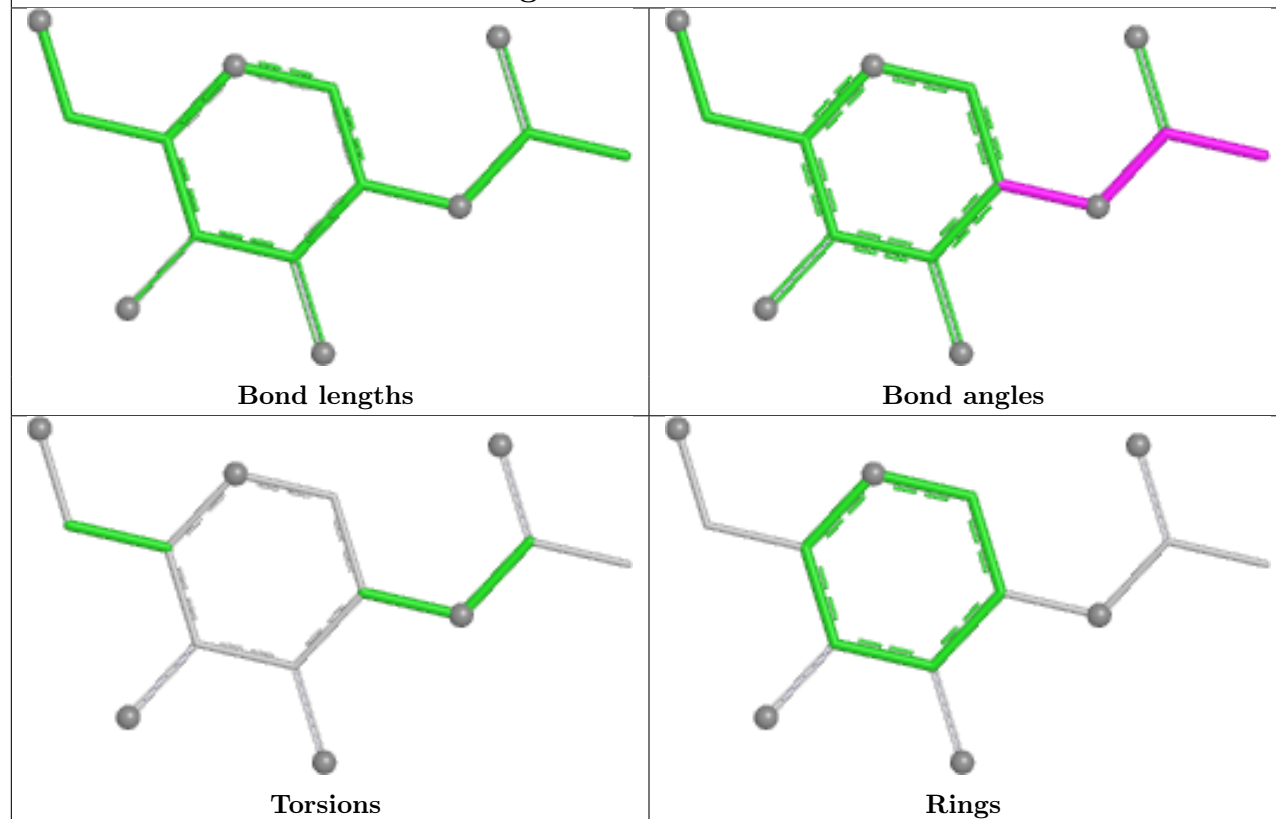
Ligand NAG B 1302



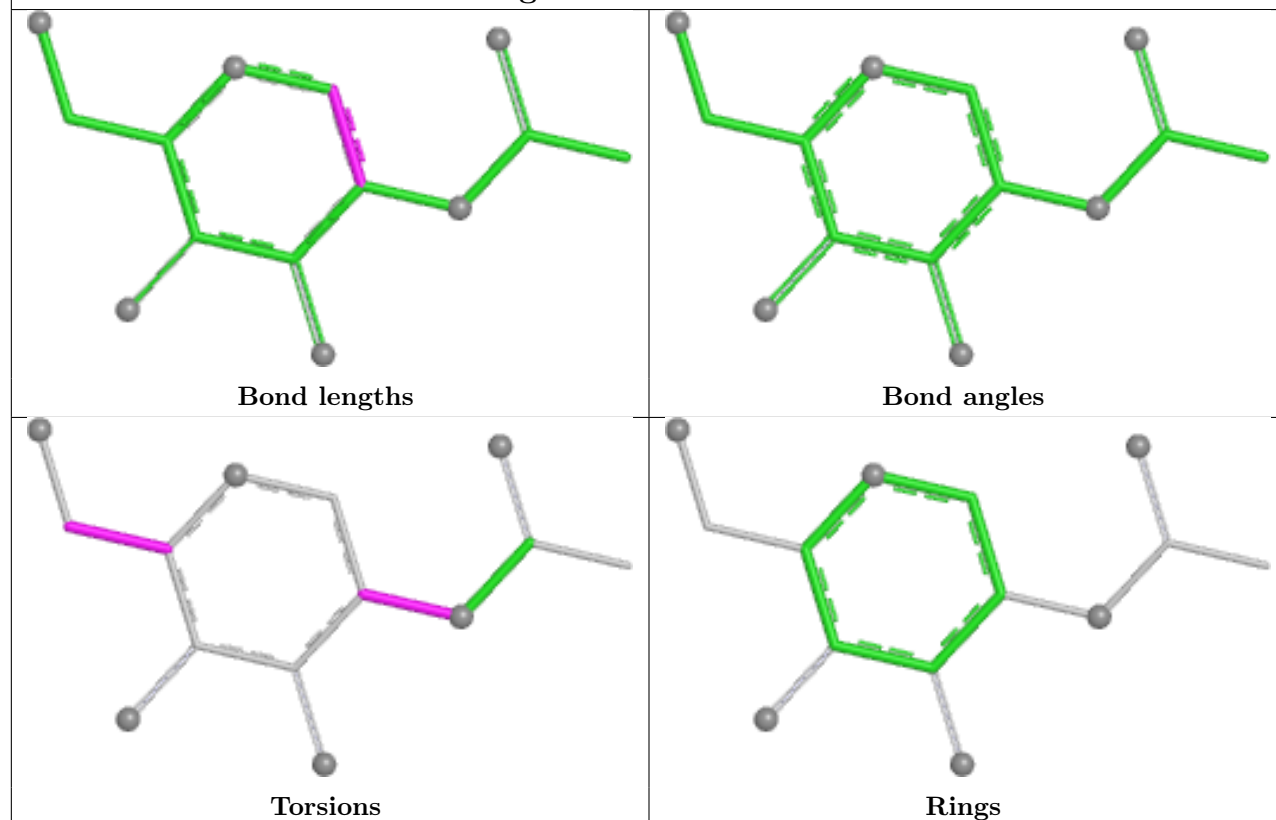
Ligand NAG A 1310

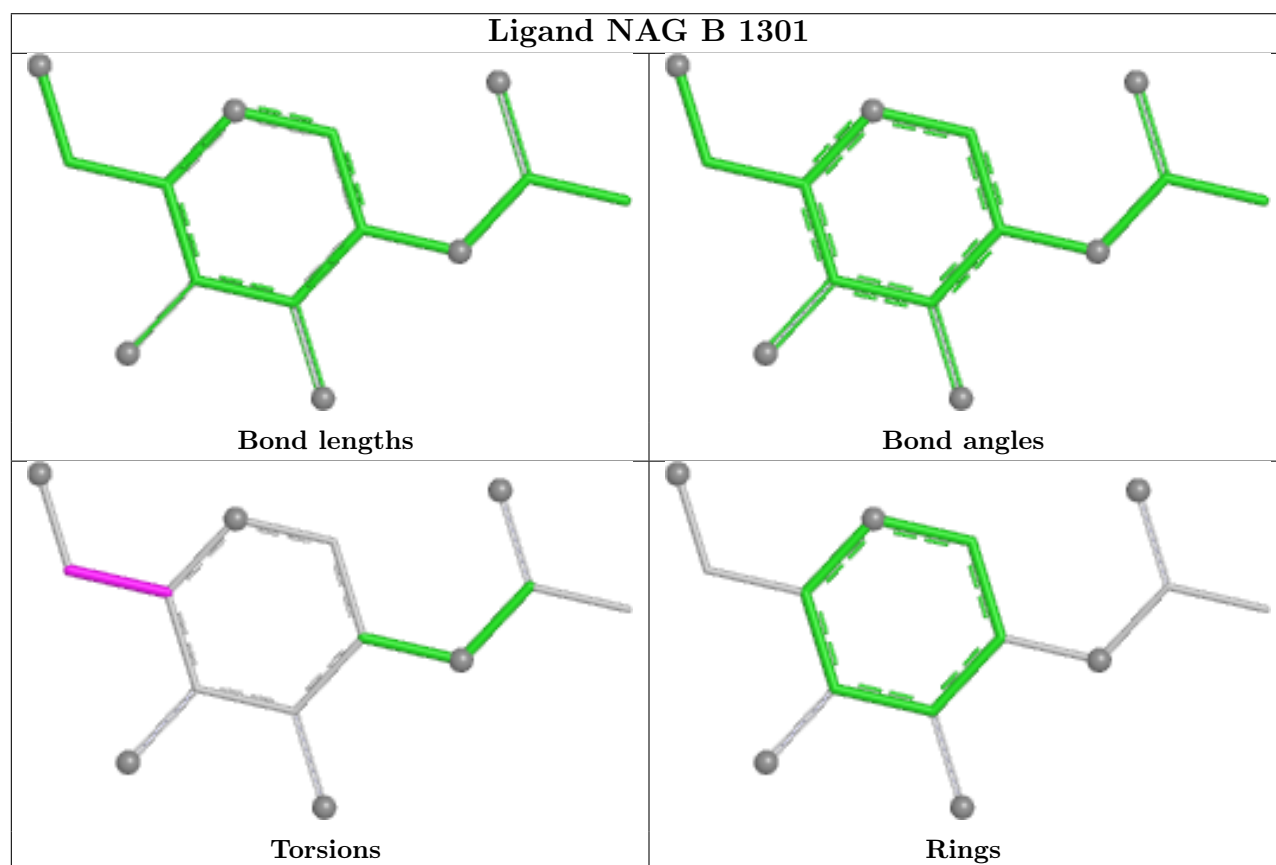
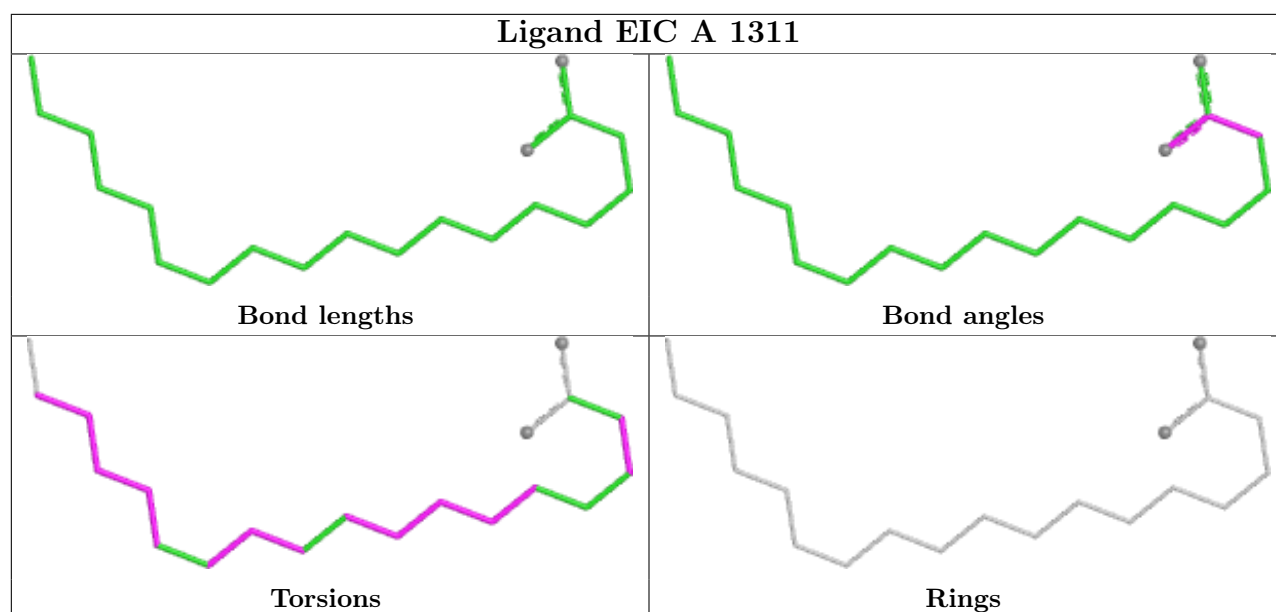


Ligand NAG B 1303

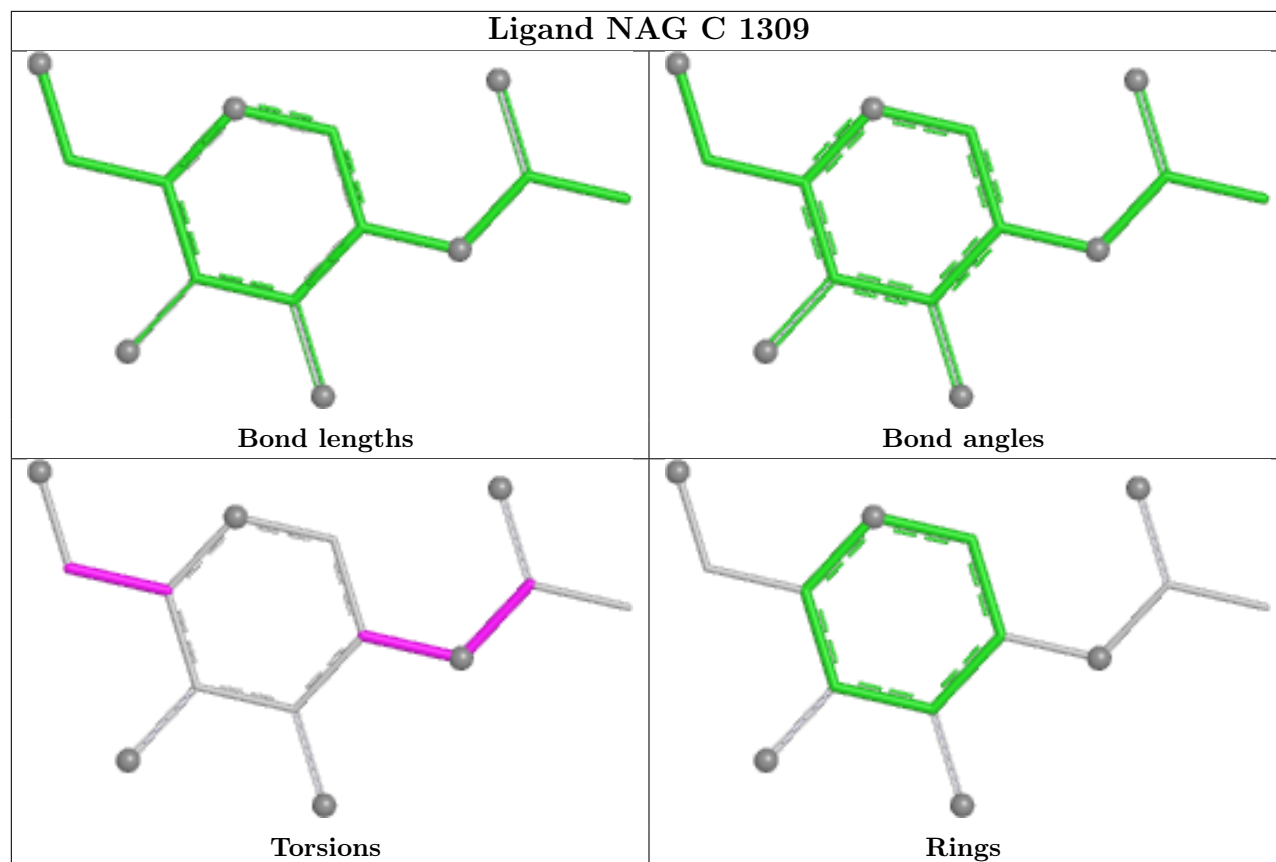


Ligand NAG C 1305

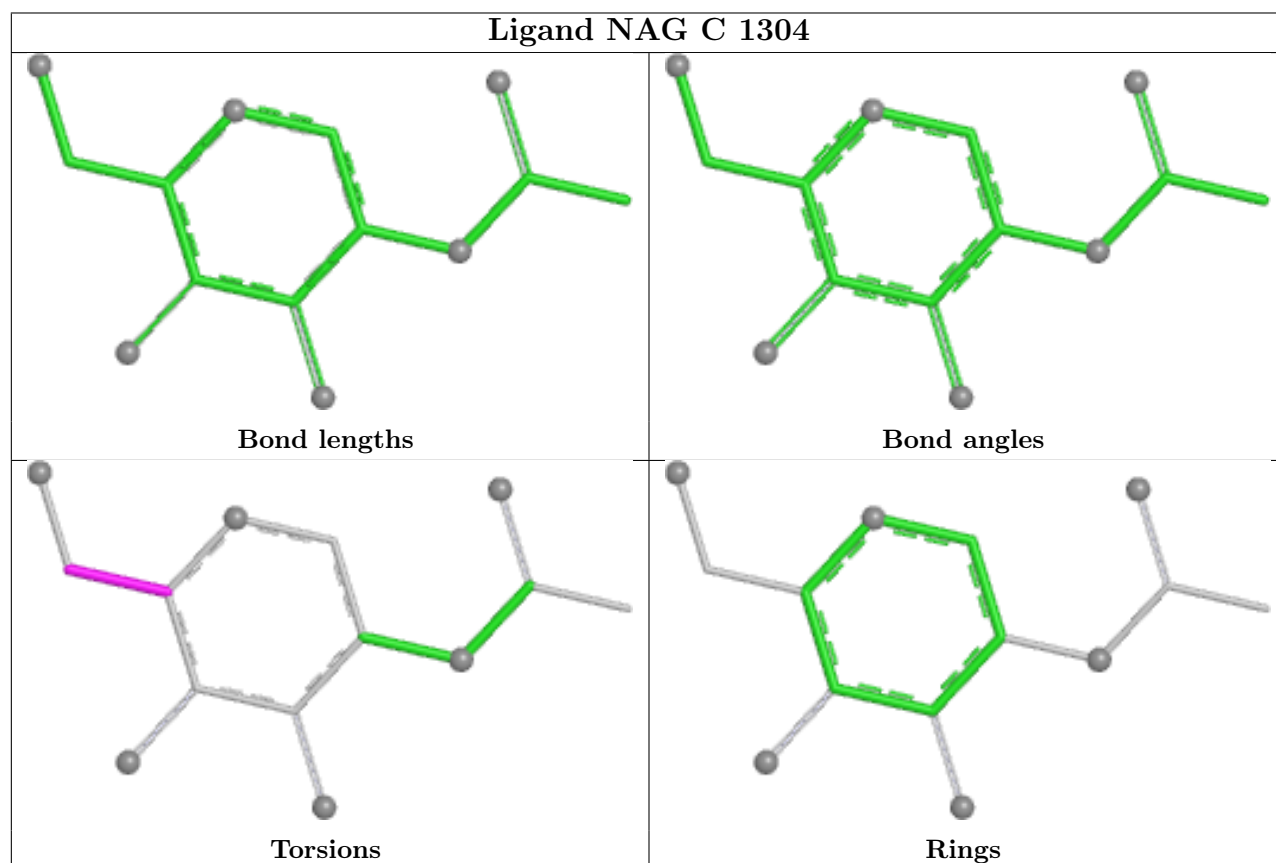




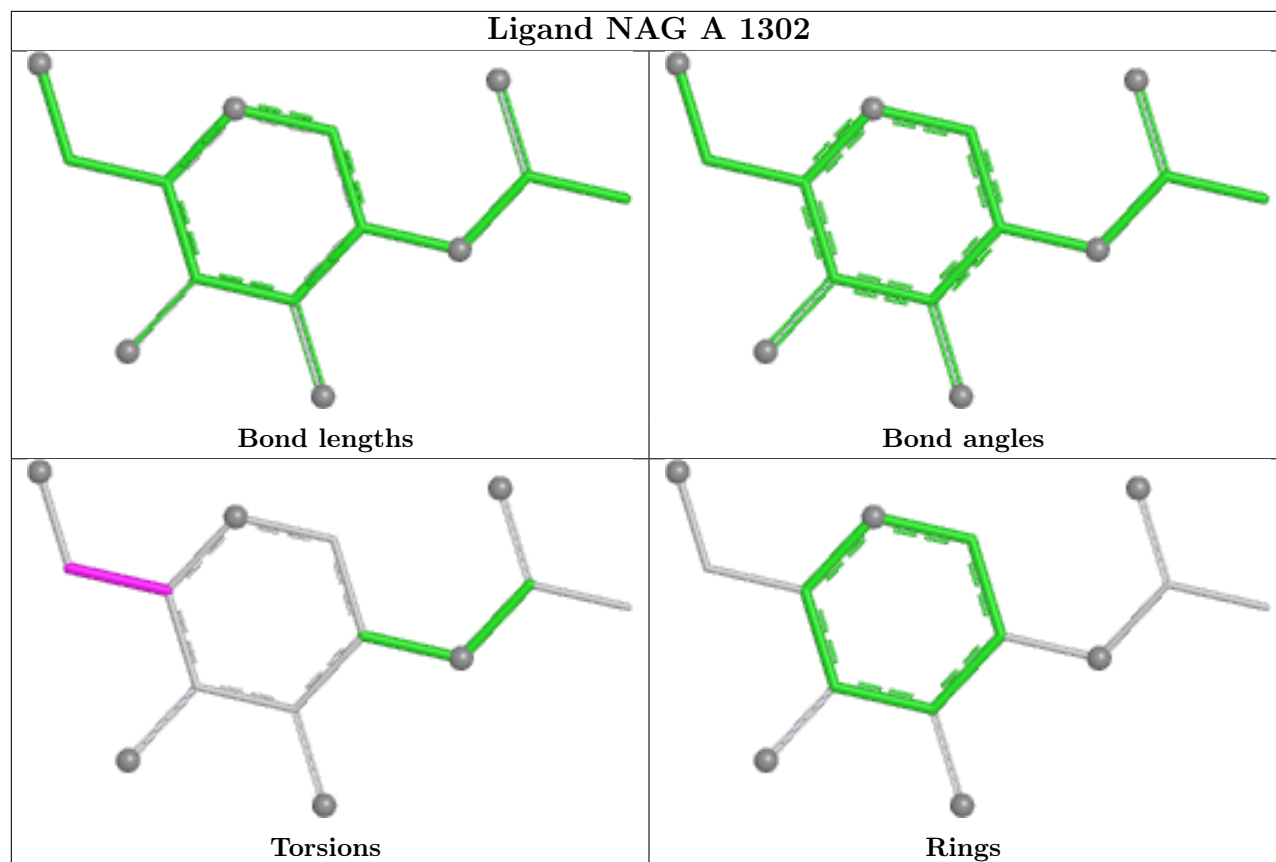
Ligand NAG C 1309



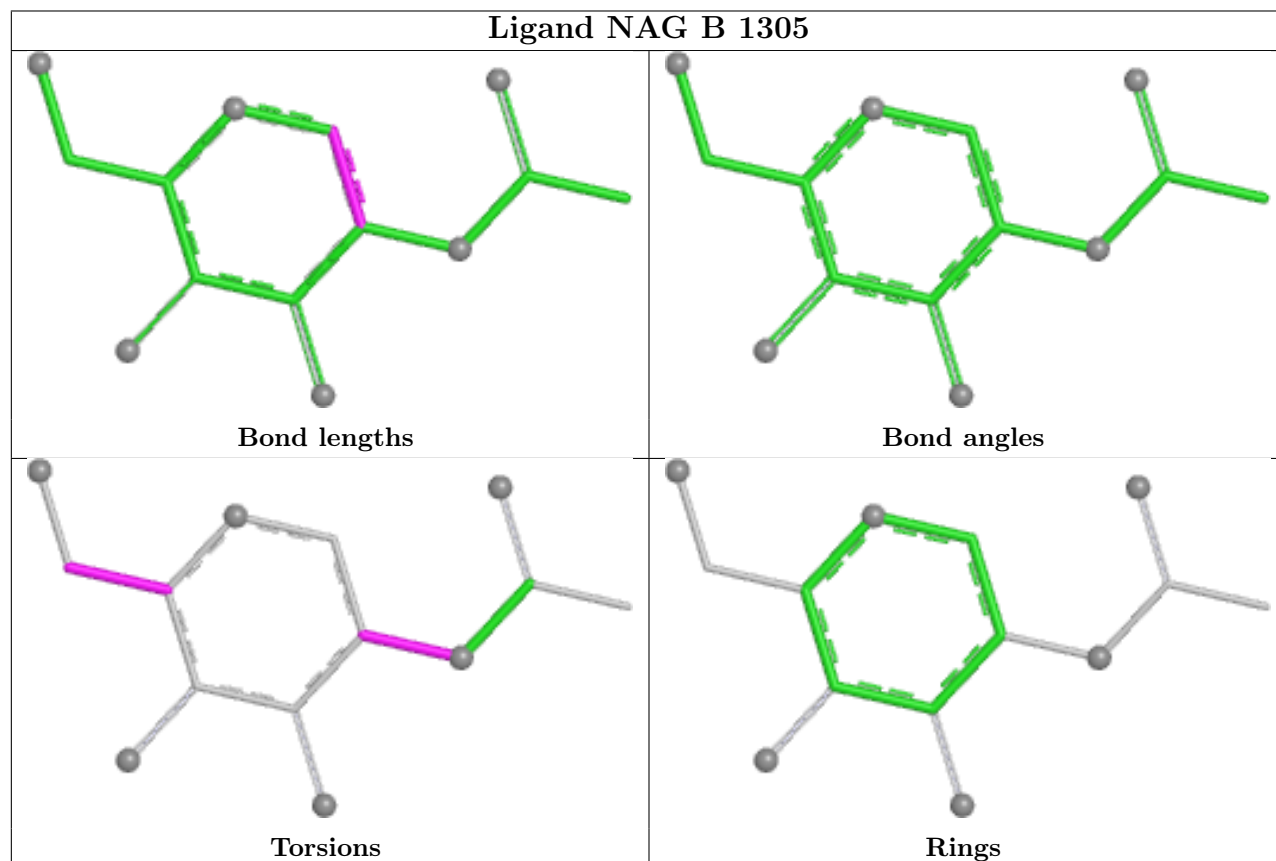
Ligand NAG C 1304



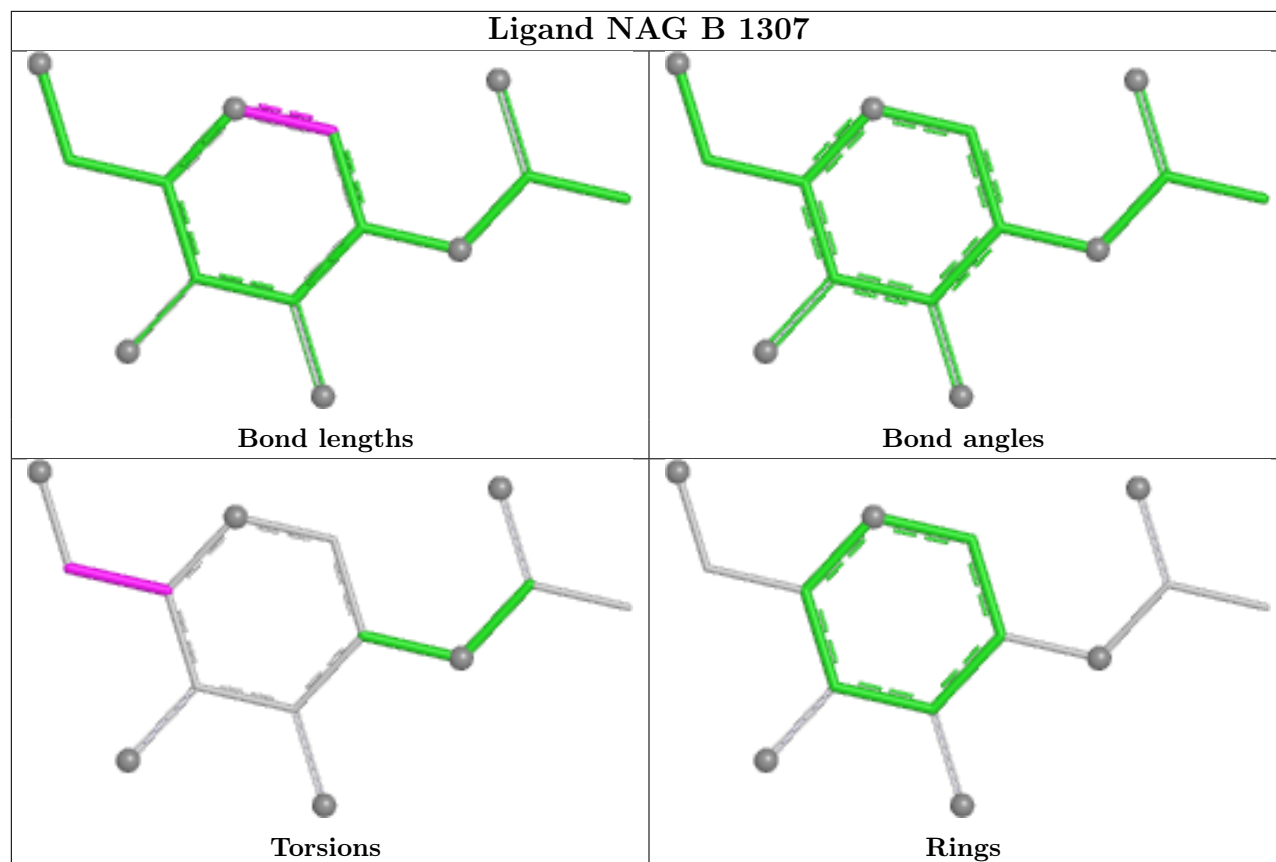
Ligand NAG A 1302



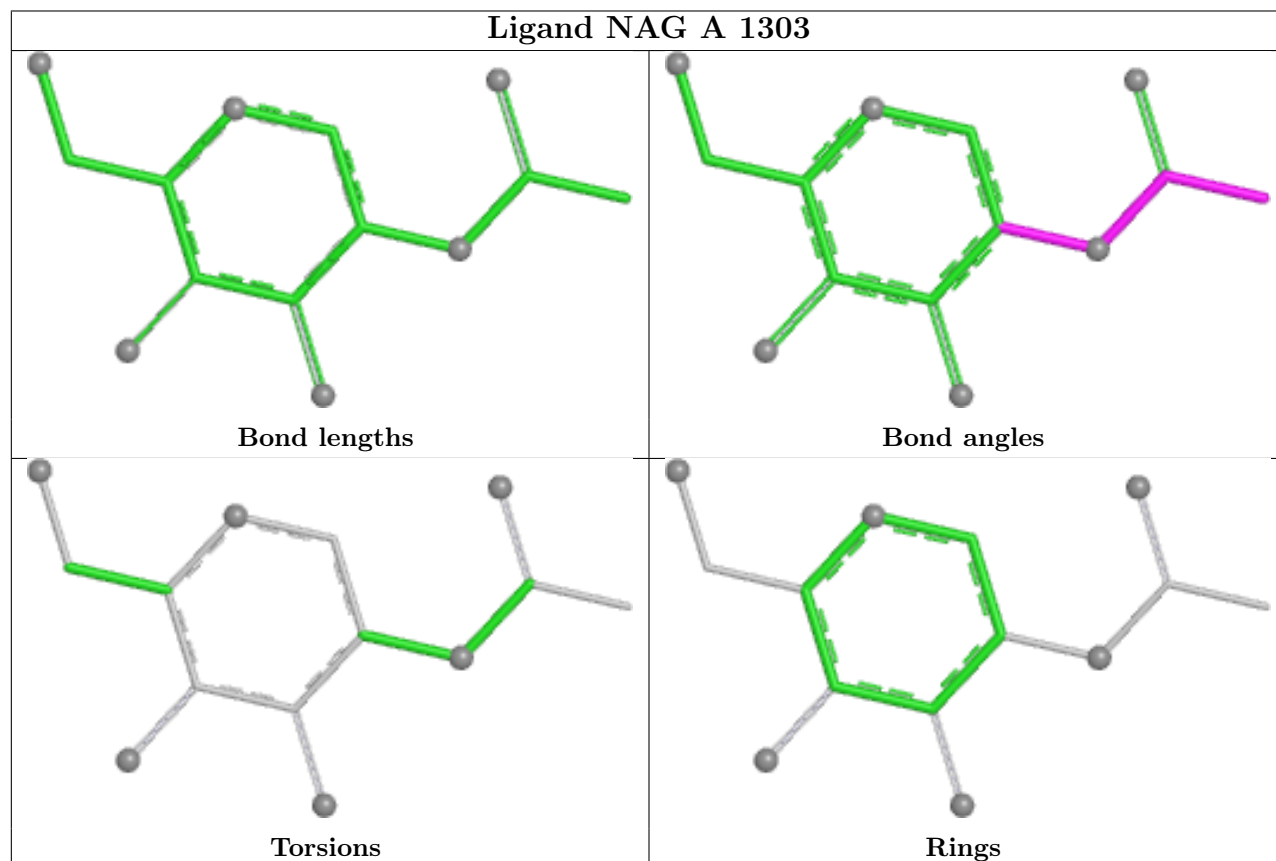
Ligand NAG B 1305



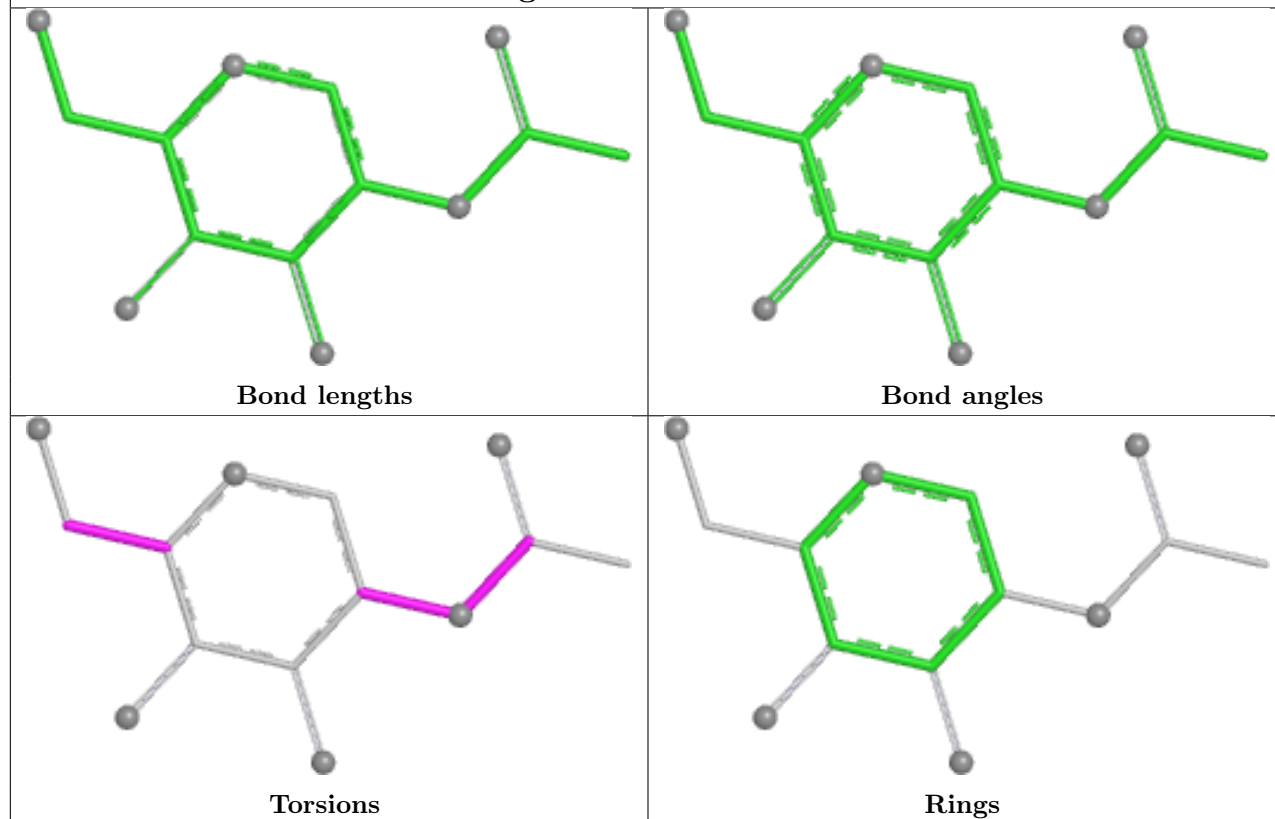
Ligand NAG B 1307



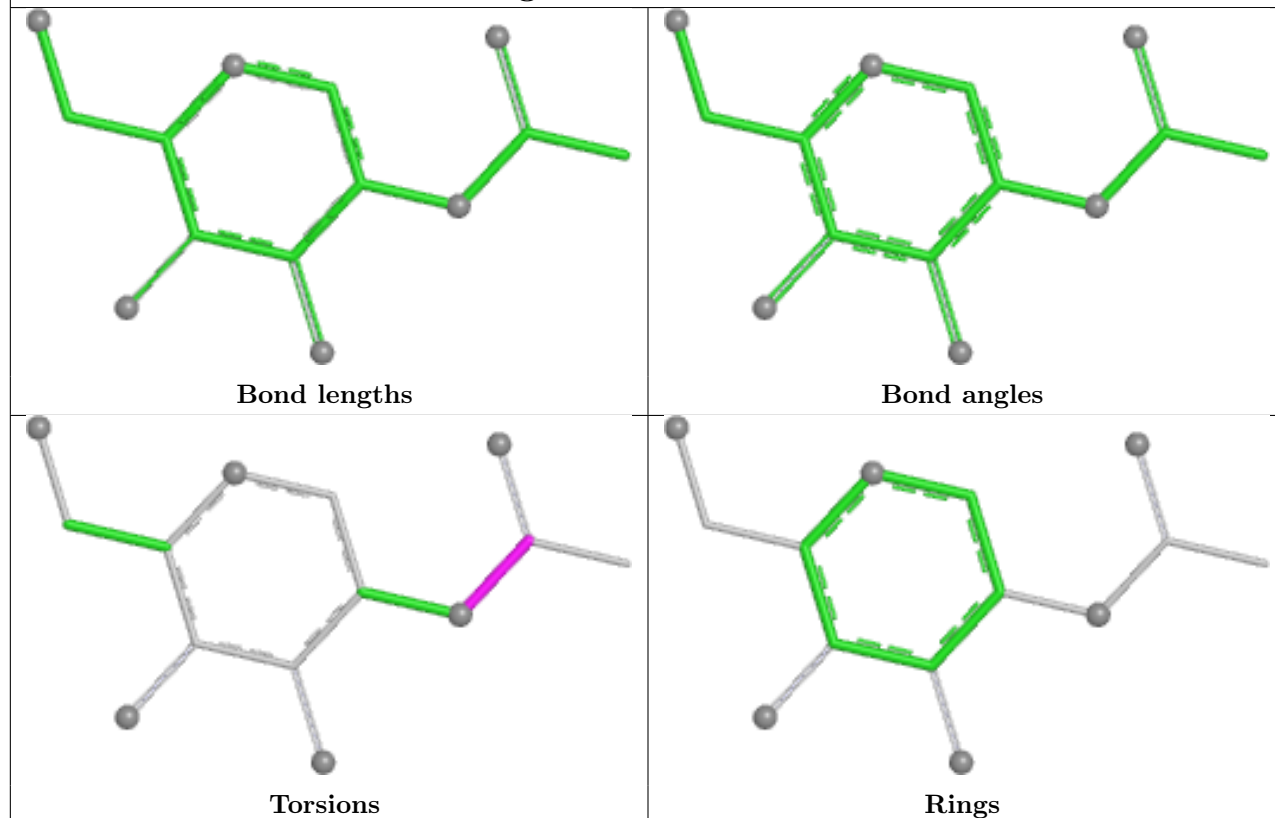
Ligand NAG A 1303

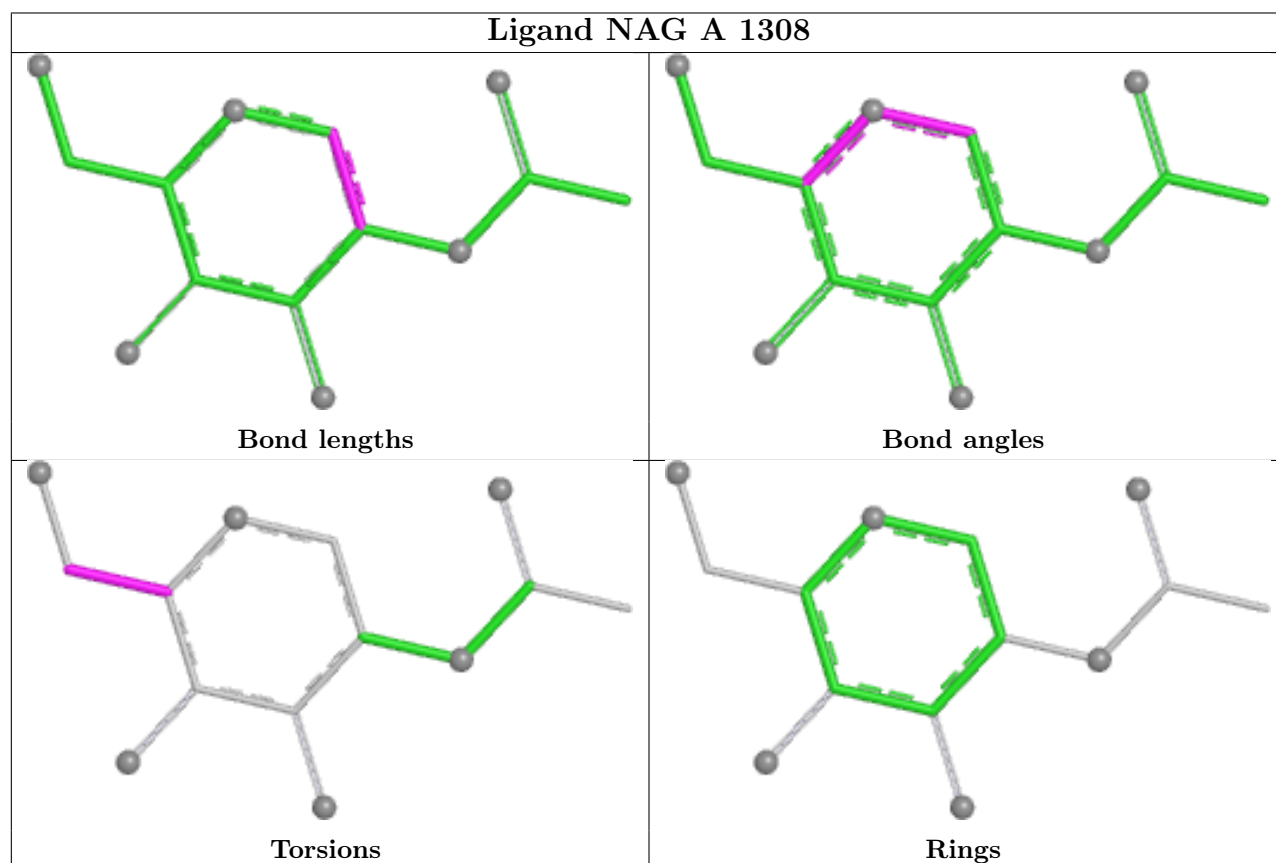
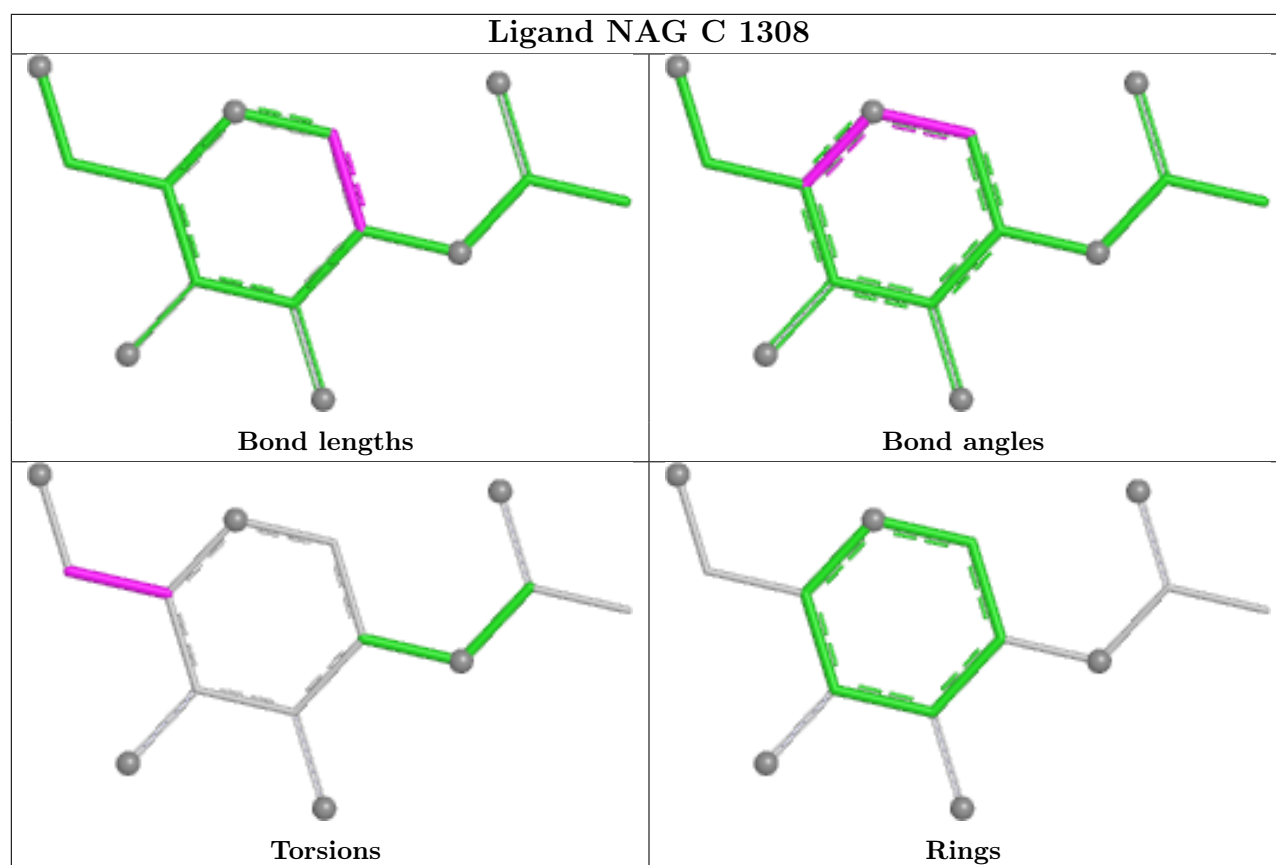


Ligand NAG B 1309

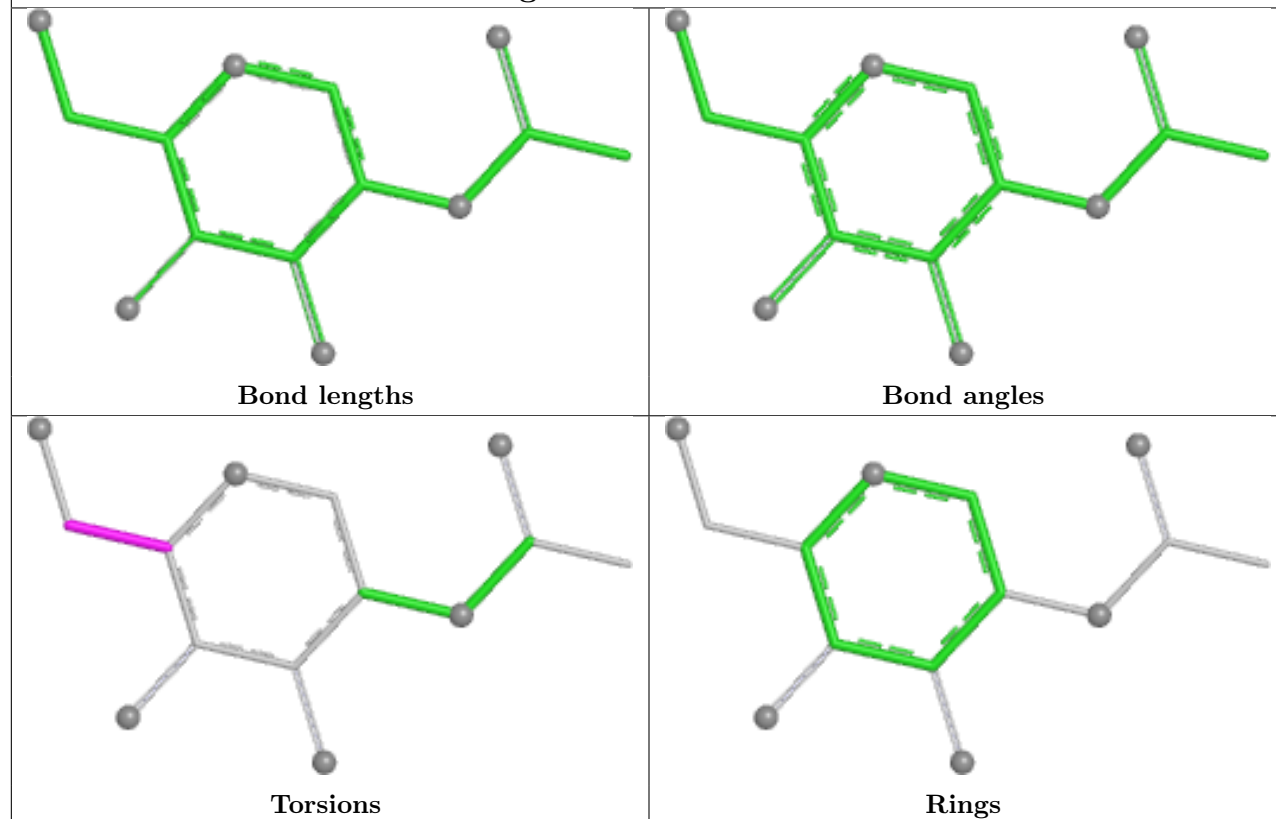


Ligand NAG C 1306

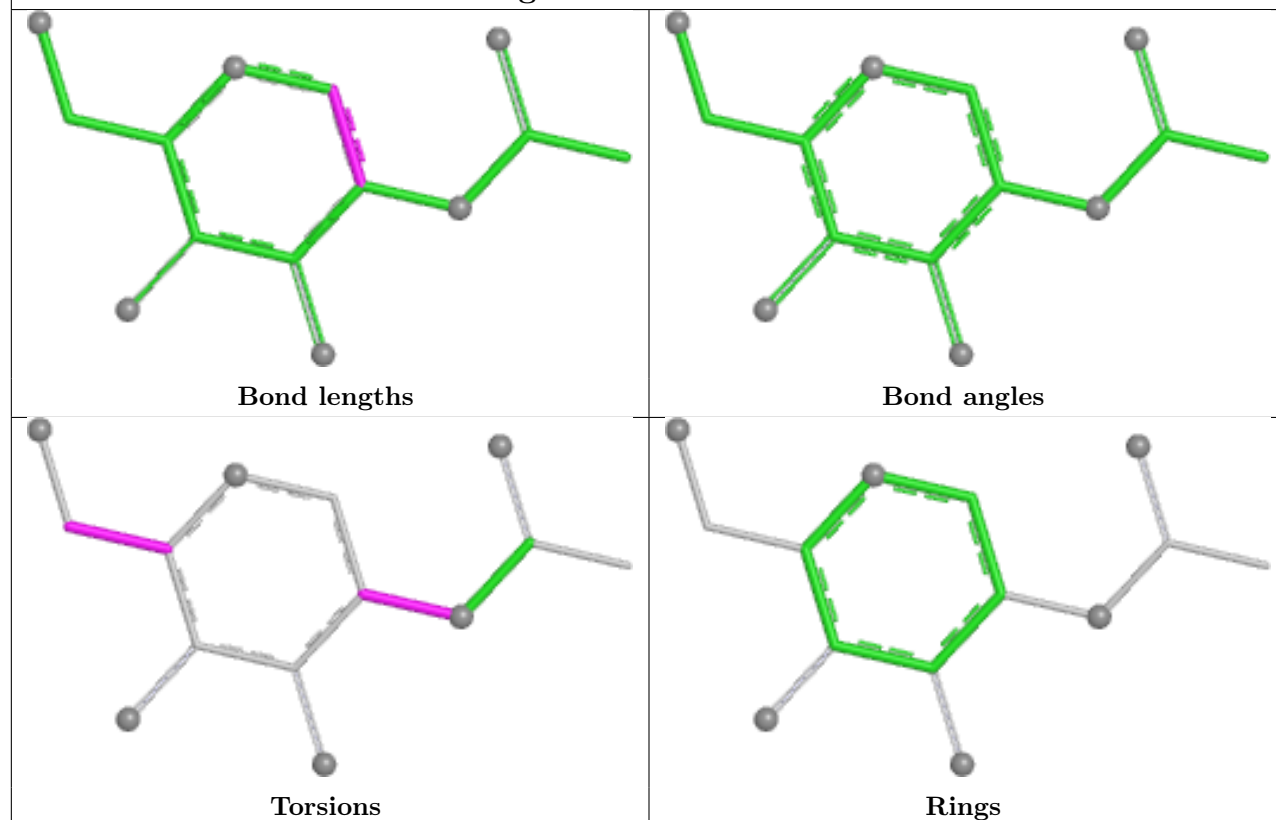




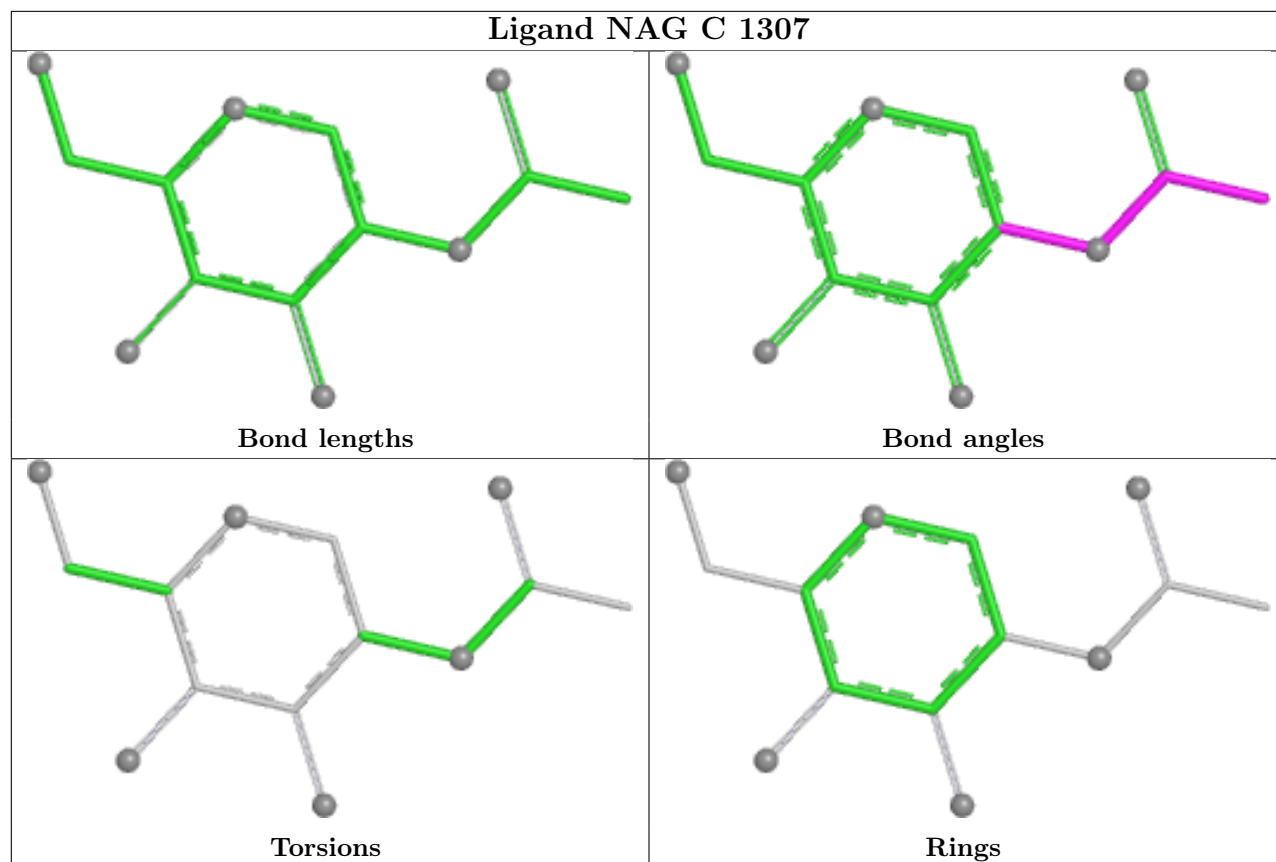
Ligand NAG C 1310



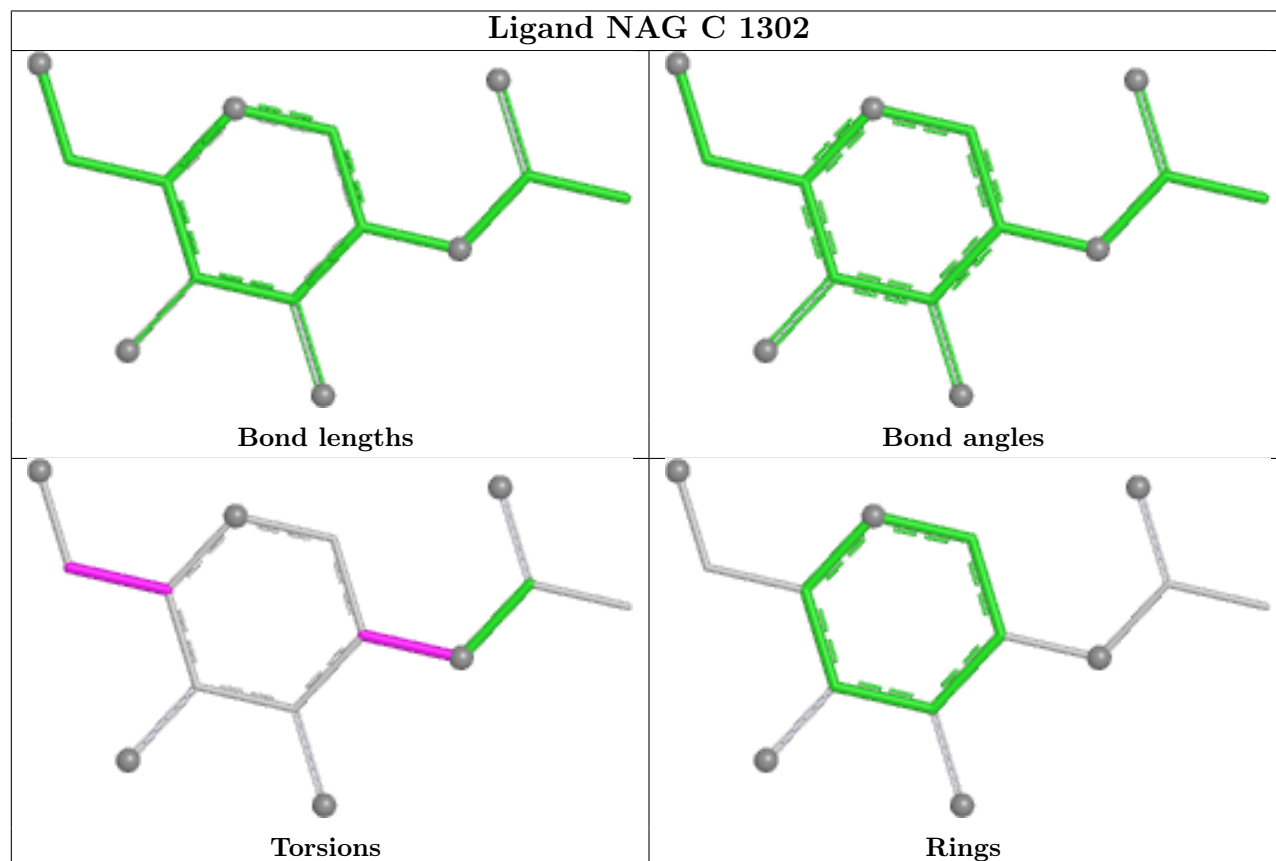
Ligand NAG A 1305



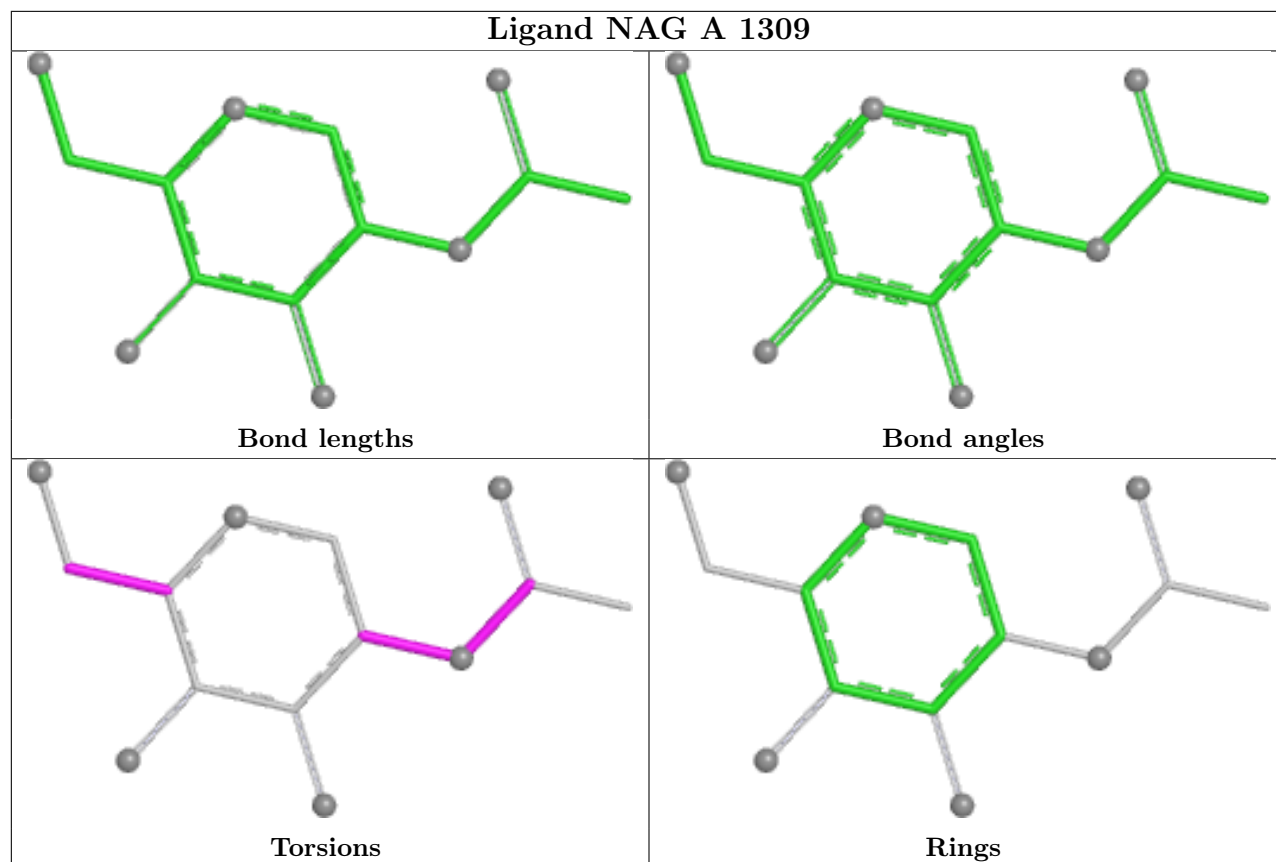
Ligand NAG C 1307



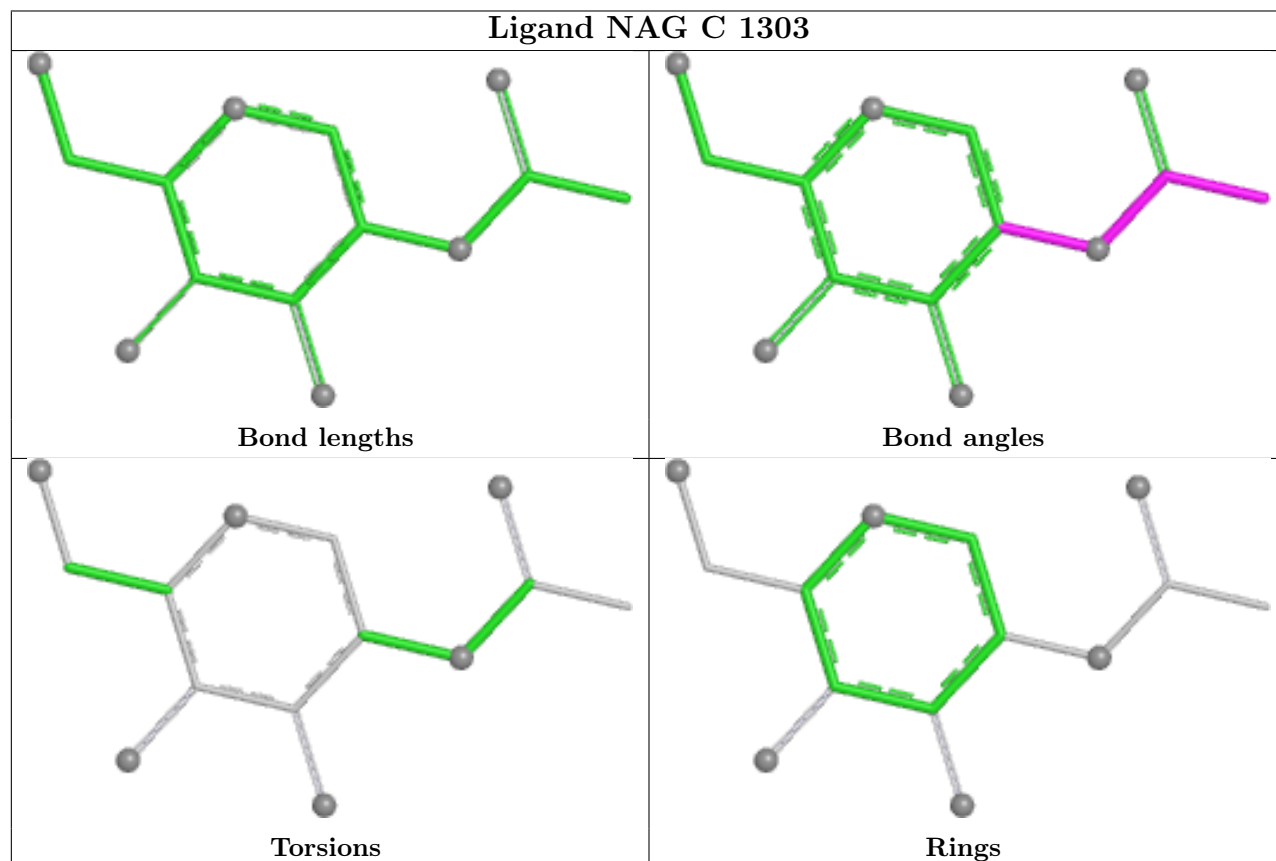
Ligand NAG C 1302

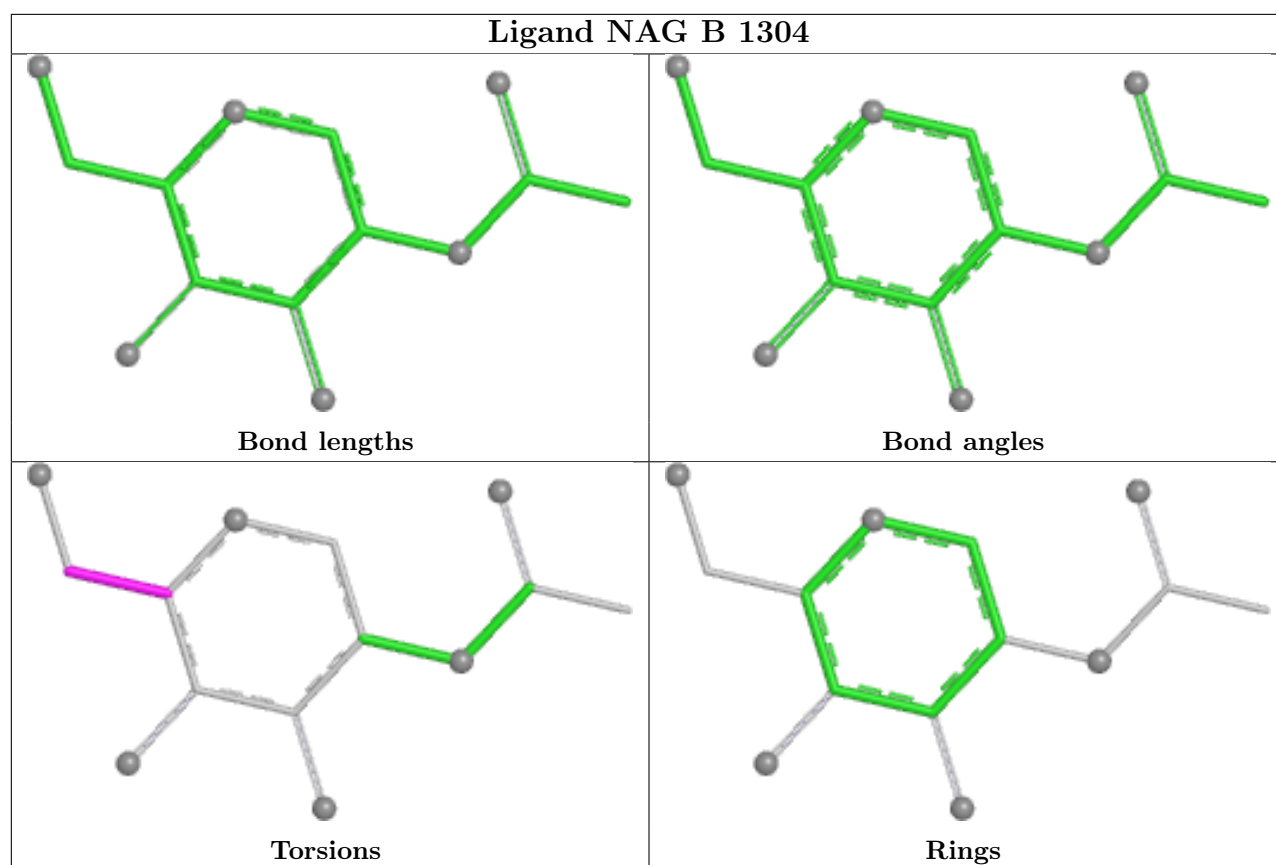


Ligand NAG A 1309



Ligand NAG C 1303





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

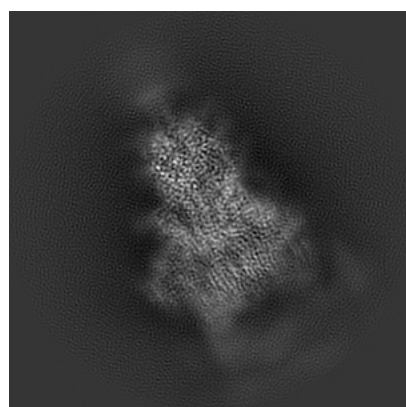
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-32920. These allow visual inspection of the internal detail of the map and identification of artifacts.

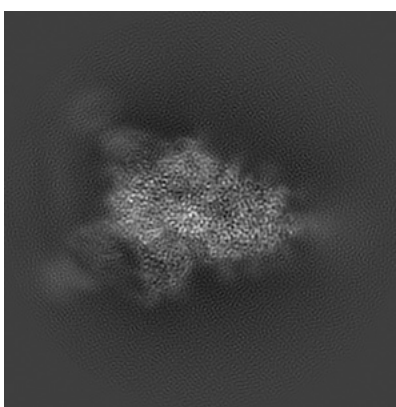
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

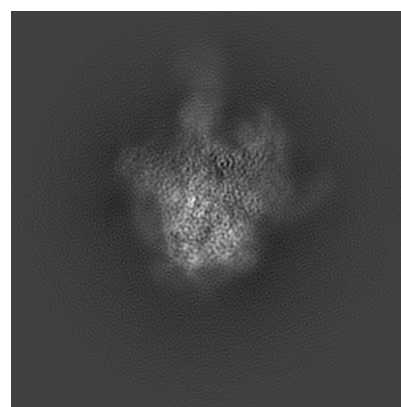
6.1.1 Primary map



X



Y

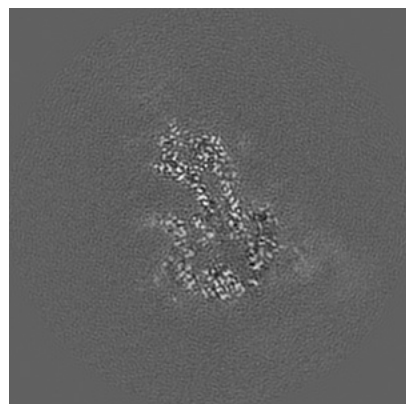


Z

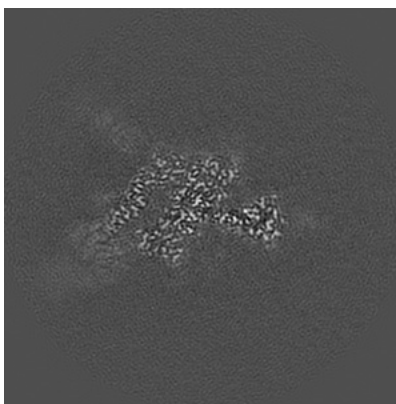
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

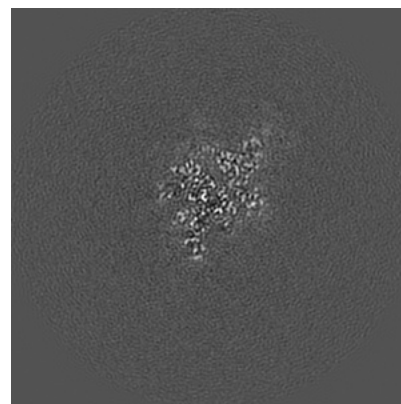
6.2.1 Primary map



X Index: 144



Y Index: 144

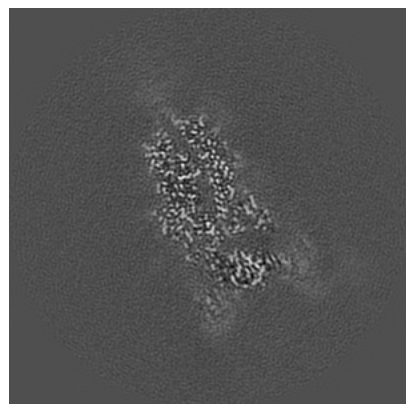


Z Index: 144

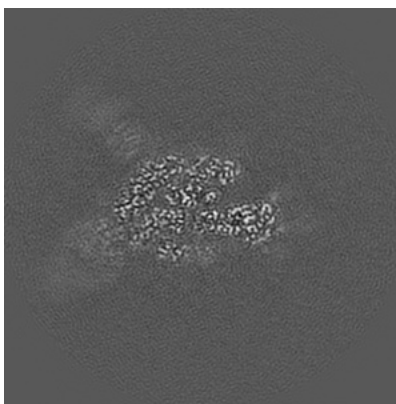
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

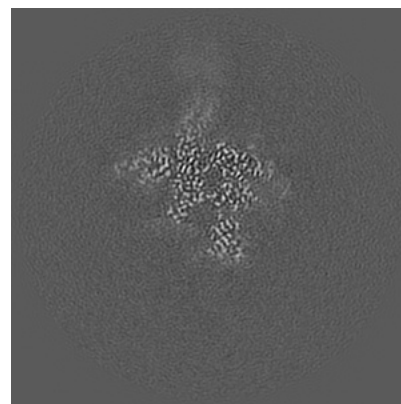
6.3.1 Primary map



X Index: 129



Y Index: 149

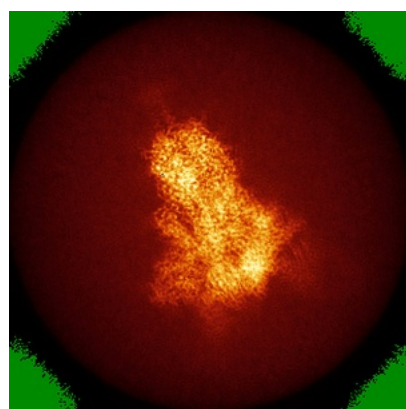


Z Index: 102

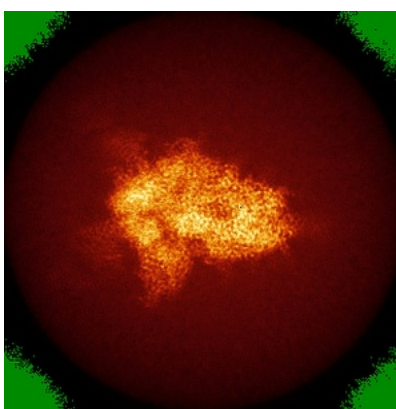
The images above show the largest variance slices of the map in three orthogonal directions.

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

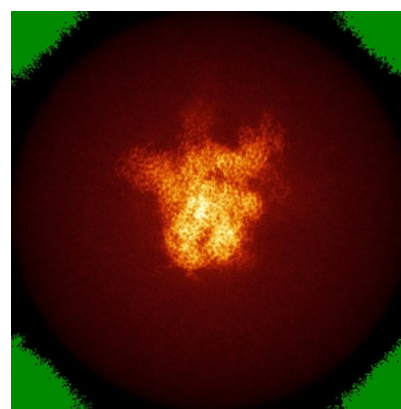
6.4.1 Primary map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views

This section was not generated.

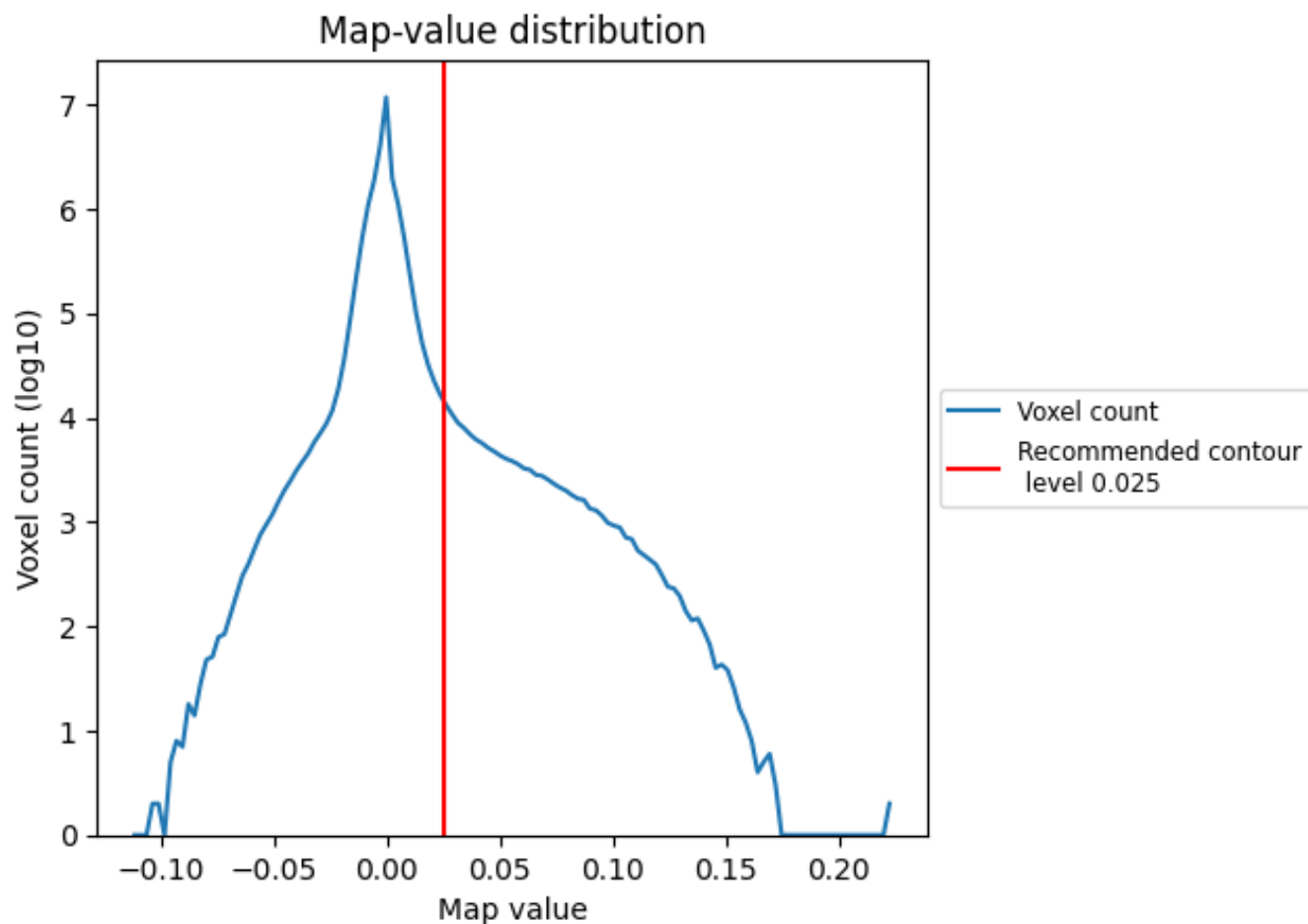
6.6 Mask visualisation

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

7 Map analysis [i](#)

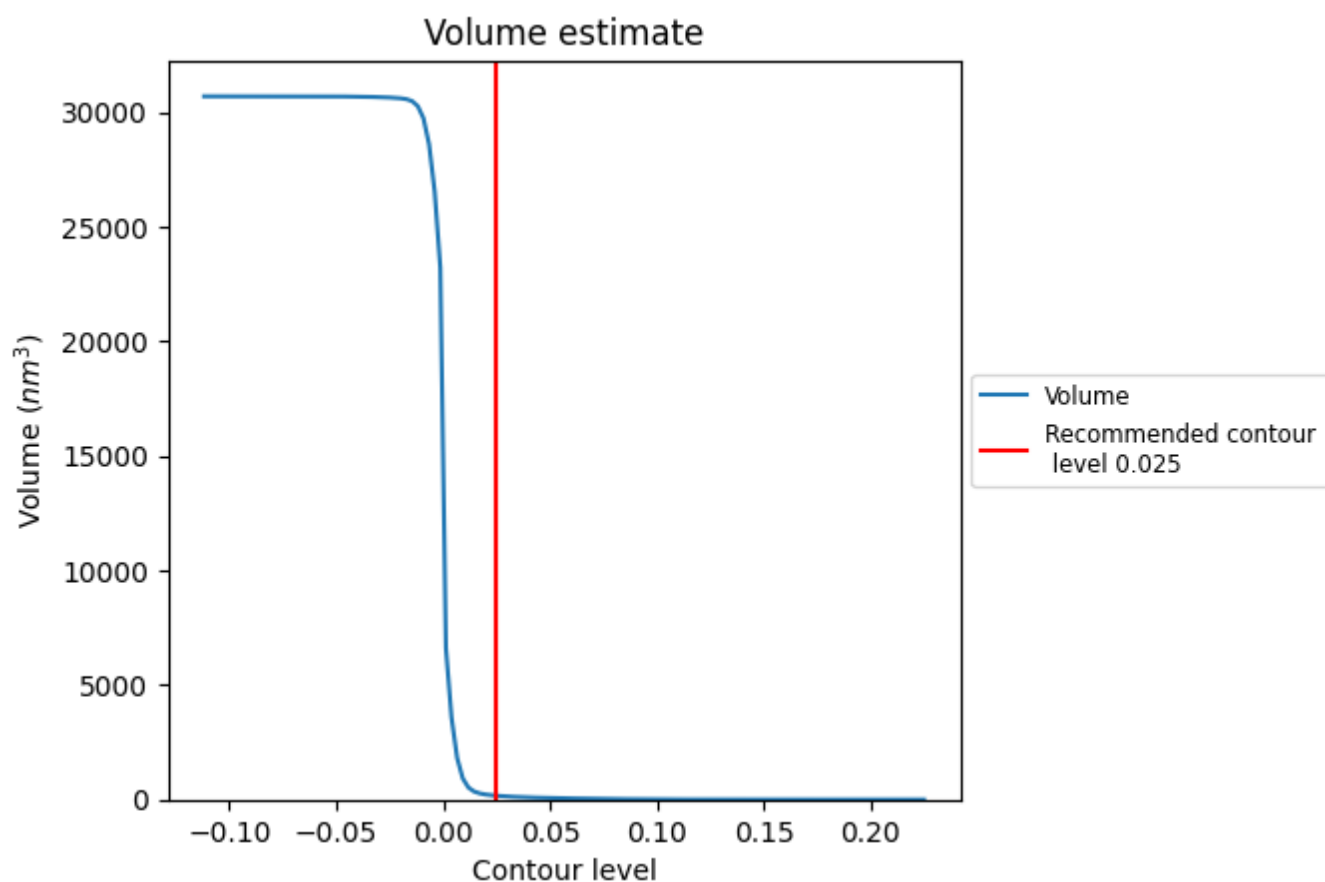
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

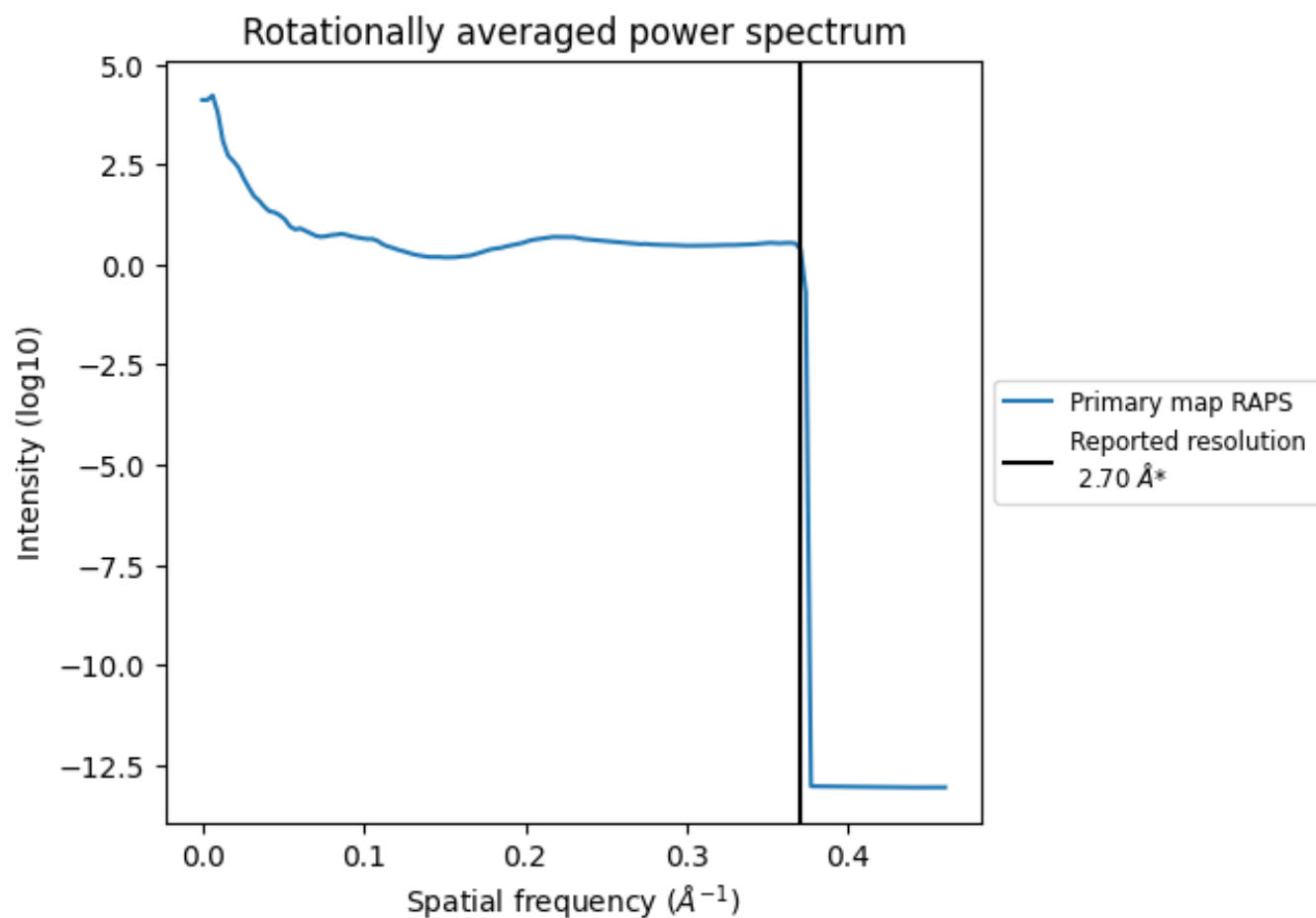
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 166 nm³; this corresponds to an approximate mass of 150 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 0.370 Å⁻¹

8 Fourier-Shell correlation

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

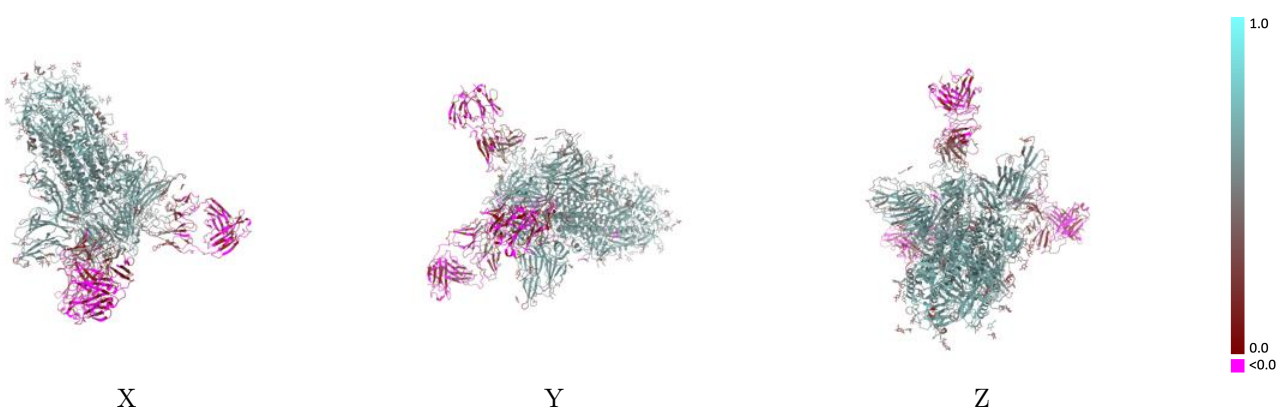
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-32920 and PDB model 7X08. Per-residue inclusion information can be found in section 3 on page 11.

9.1 Map-model overlay [i](#)

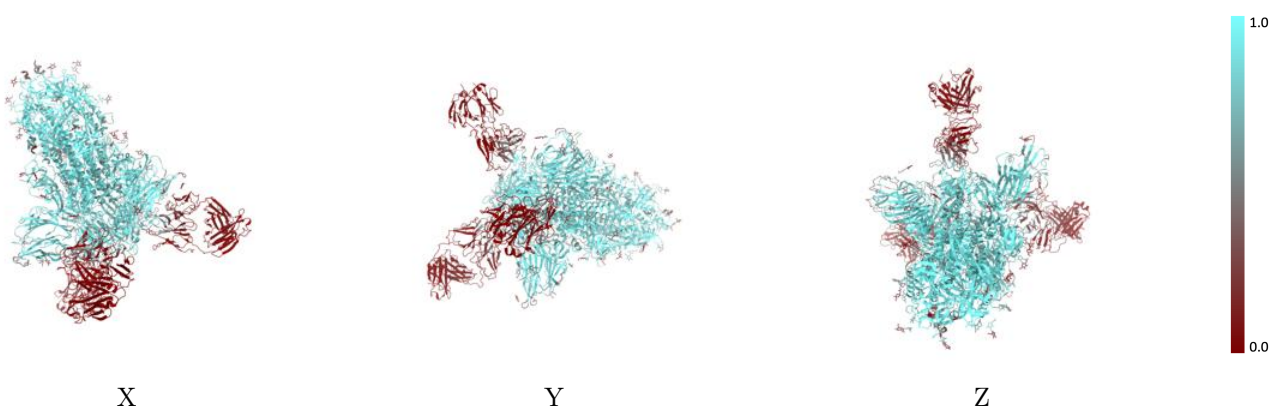
This section was not generated.

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



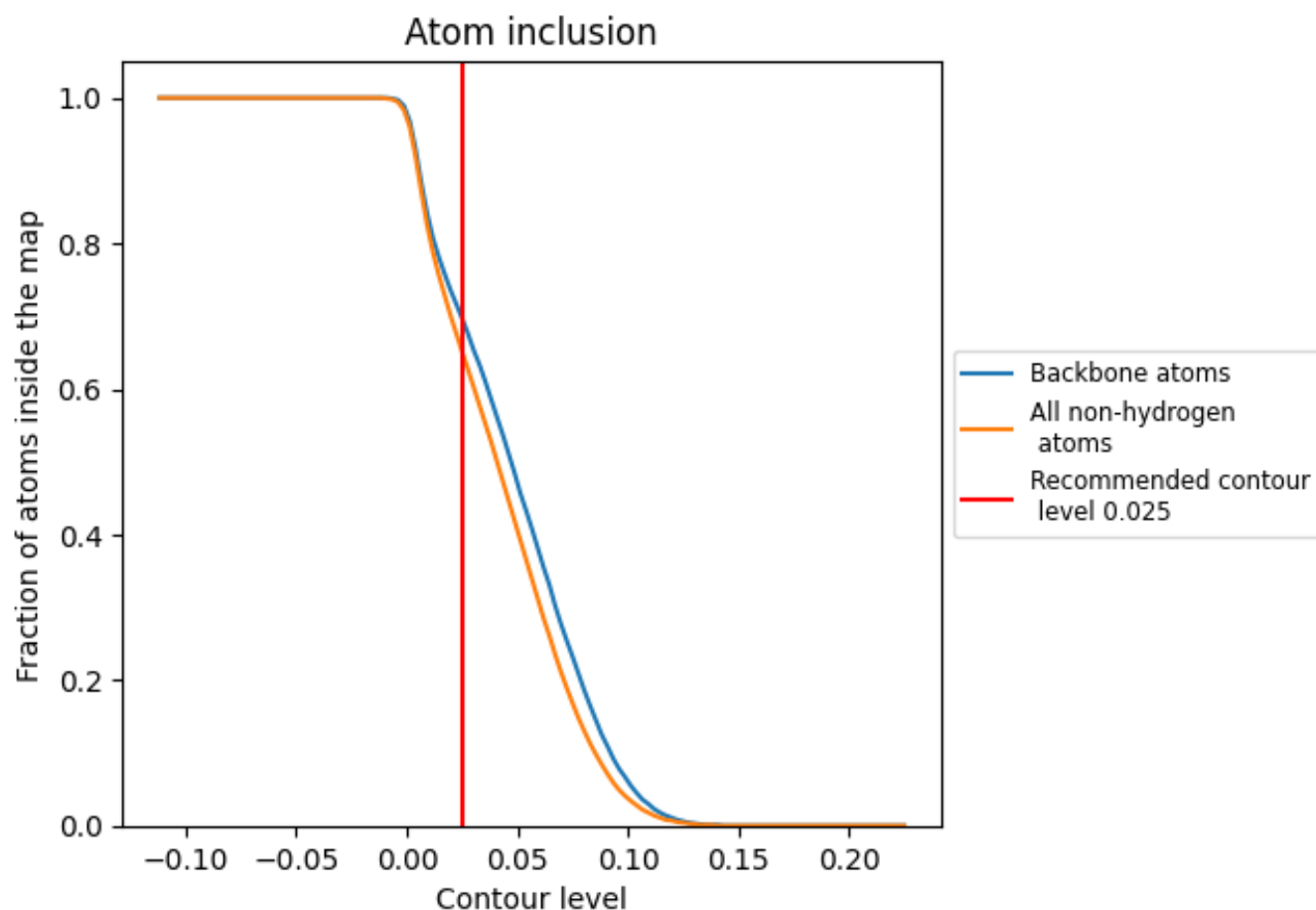
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.025).

9.4 Atom inclusion [i](#)



At the recommended contour level, 70% of all backbone atoms, 65% 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 (0.025) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6510	 0.4580
A	 0.8590	 0.5880
B	 0.8700	 0.5880
C	 0.8690	 0.5860
D	 0.2500	 0.2500
E	 0.6070	 0.4790
F	 0.3210	 0.5030
G	 0.5360	 0.4310
H	 0.0780	 0.1200
I	 0.0920	 0.1100
J	 0.0860	 0.1060
K	 0.2500	 0.2200
L	 0.0690	 0.1070
M	 0.0470	 0.1040
N	 0.0610	 0.0970
O	 0.6070	 0.4680
P	 0.4640	 0.3490
Q	 0.1430	 0.1640
R	 0.7140	 0.5060
S	 0.4640	 0.4080
T	 0.2860	 0.2750
U	 0.2860	 0.1200
V	 0.3930	 0.3170
W	 0.4290	 0.3570
X	 0.2500	 0.2390
Y	 0.4290	 0.3580
Z	 0.5360	 0.4500
a	 0.3210	 0.3630
b	 0.4290	 0.3930
c	 0.2860	 0.2180
d	 0.3210	 0.2290
e	 0.5710	 0.3330
f	 0.2500	 0.3990
g	 0.4290	 0.3100

