



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 07:59 AM UTC

PDB ID : 8GTQ / pdb_00008gtq
EMDB ID : EMD-34263
Title : cryo-EM structure of Omicron BA.5 S protein in complex with S2L20
Authors : Xia, X.Y.; Zhang, Y.Y.; Chi, X.M.; Huang, B.D.; Wu, L.S.; Zhou, Q.
Deposited on : 2022-09-08
Resolution : 3.10 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

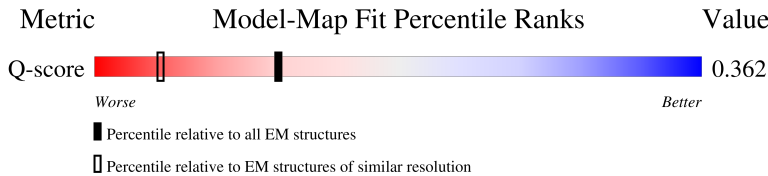
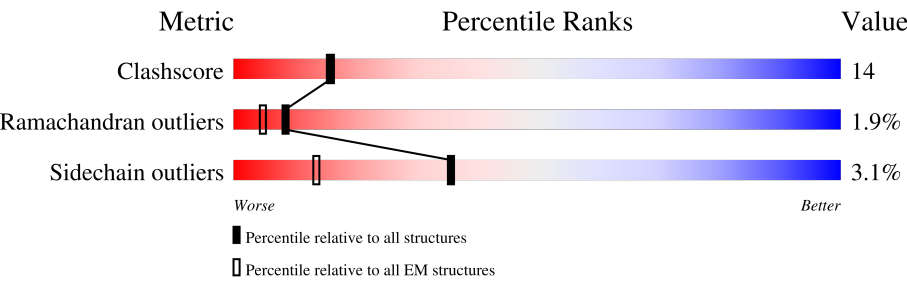
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.10 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.



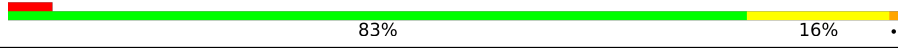
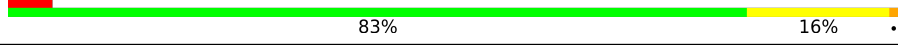
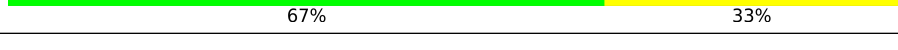
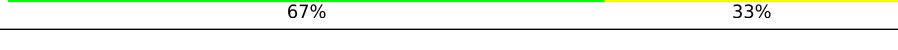
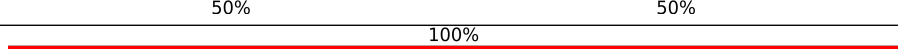
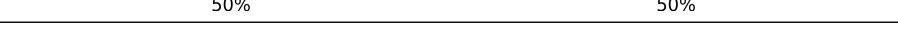
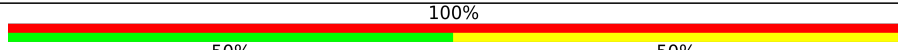
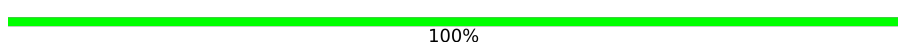
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14724 (2.60 - 3.60)

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	1271	11% 64% 14% • 19%
1	B	1271	13% 63% 15% • 19%
1	C	1271	12% 63% 15% • 19%
2	H	121	• 72% 22% 5% •

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Mol	Chain	Length	Quality of chain
2	I	121	
2	J	121	
3	L	107	
3	M	107	
3	N	107	
4	D	3	
4	Q	3	
4	X	3	
5	E	2	
5	F	2	
5	G	2	
5	K	2	
5	O	2	
5	P	2	
5	R	2	
5	S	2	
5	T	2	
5	U	2	
5	V	2	
5	W	2	
5	Y	2	
5	Z	2	
5	a	2	
5	b	2	
5	c	2	

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Mol	Chain	Length	Quality of chain
5	d	2	 100%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 30519 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	1025	Total	C	N	O	S	0	0
			8043	5154	1338	1514	37		
1	B	1025	Total	C	N	O	S	0	0
			8043	5154	1338	1514	37		
1	C	1025	Total	C	N	O	S	0	0
			8043	5154	1338	1514	37		

There are 108 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	19	ILE	THR	variant	UNP P0DTC2
A	?	-	HIS	deletion	UNP P0DTC2
A	?	-	VAL	deletion	UNP P0DTC2
A	142	ASP	GLY	variant	UNP P0DTC2
A	213	GLY	VAL	variant	UNP P0DTC2
A	339	ASP	GLY	variant	UNP P0DTC2
A	371	PHE	SER	variant	UNP P0DTC2
A	373	PRO	SER	variant	UNP P0DTC2
A	375	PHE	SER	variant	UNP P0DTC2
A	376	ALA	THR	variant	UNP P0DTC2
A	405	ASN	ASP	variant	UNP P0DTC2
A	408	SER	ARG	variant	UNP P0DTC2
A	417	ASN	LYS	variant	UNP P0DTC2
A	440	LYS	ASN	variant	UNP P0DTC2
A	452	ARG	LEU	variant	UNP P0DTC2
A	477	ASN	SER	variant	UNP P0DTC2
A	478	LYS	THR	variant	UNP P0DTC2
A	484	ALA	GLU	variant	UNP P0DTC2
A	486	VAL	PHE	variant	UNP P0DTC2
A	498	ARG	GLN	variant	UNP P0DTC2
A	501	TYR	ASN	variant	UNP P0DTC2
A	505	HIS	TYR	variant	UNP P0DTC2
A	614	GLY	ASP	variant	UNP P0DTC2
A	655	TYR	HIS	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	679	LYS	ASN	variant	UNP P0DTC2
A	681	HIS	PRO	variant	UNP P0DTC2
A	764	LYS	ASN	variant	UNP P0DTC2
A	796	TYR	ASP	variant	UNP P0DTC2
A	817	PRO	PHE	variant	UNP P0DTC2
A	892	PRO	ALA	variant	UNP P0DTC2
A	899	PRO	ALA	variant	UNP P0DTC2
A	942	PRO	ALA	variant	UNP P0DTC2
A	954	HIS	GLN	variant	UNP P0DTC2
A	969	LYS	ASN	variant	UNP P0DTC2
A	986	PRO	LYS	variant	UNP P0DTC2
A	987	PRO	VAL	variant	UNP P0DTC2
B	19	ILE	THR	variant	UNP P0DTC2
B	?	-	HIS	deletion	UNP P0DTC2
B	?	-	VAL	deletion	UNP P0DTC2
B	142	ASP	GLY	variant	UNP P0DTC2
B	213	GLY	VAL	variant	UNP P0DTC2
B	339	ASP	GLY	variant	UNP P0DTC2
B	371	PHE	SER	variant	UNP P0DTC2
B	373	PRO	SER	variant	UNP P0DTC2
B	375	PHE	SER	variant	UNP P0DTC2
B	376	ALA	THR	variant	UNP P0DTC2
B	405	ASN	ASP	variant	UNP P0DTC2
B	408	SER	ARG	variant	UNP P0DTC2
B	417	ASN	LYS	variant	UNP P0DTC2
B	440	LYS	ASN	variant	UNP P0DTC2
B	452	ARG	LEU	variant	UNP P0DTC2
B	477	ASN	SER	variant	UNP P0DTC2
B	478	LYS	THR	variant	UNP P0DTC2
B	484	ALA	GLU	variant	UNP P0DTC2
B	486	VAL	PHE	variant	UNP P0DTC2
B	498	ARG	GLN	variant	UNP P0DTC2
B	501	TYR	ASN	variant	UNP P0DTC2
B	505	HIS	TYR	variant	UNP P0DTC2
B	614	GLY	ASP	variant	UNP P0DTC2
B	655	TYR	HIS	variant	UNP P0DTC2
B	679	LYS	ASN	variant	UNP P0DTC2
B	681	HIS	PRO	variant	UNP P0DTC2
B	764	LYS	ASN	variant	UNP P0DTC2
B	796	TYR	ASP	variant	UNP P0DTC2
B	817	PRO	PHE	variant	UNP P0DTC2
B	892	PRO	ALA	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	899	PRO	ALA	variant	UNP P0DTC2
B	942	PRO	ALA	variant	UNP P0DTC2
B	954	HIS	GLN	variant	UNP P0DTC2
B	969	LYS	ASN	variant	UNP P0DTC2
B	986	PRO	LYS	variant	UNP P0DTC2
B	987	PRO	VAL	variant	UNP P0DTC2
C	19	ILE	THR	variant	UNP P0DTC2
C	?	-	HIS	deletion	UNP P0DTC2
C	?	-	VAL	deletion	UNP P0DTC2
C	142	ASP	GLY	variant	UNP P0DTC2
C	213	GLY	VAL	variant	UNP P0DTC2
C	339	ASP	GLY	variant	UNP P0DTC2
C	371	PHE	SER	variant	UNP P0DTC2
C	373	PRO	SER	variant	UNP P0DTC2
C	375	PHE	SER	variant	UNP P0DTC2
C	376	ALA	THR	variant	UNP P0DTC2
C	405	ASN	ASP	variant	UNP P0DTC2
C	408	SER	ARG	variant	UNP P0DTC2
C	417	ASN	LYS	variant	UNP P0DTC2
C	440	LYS	ASN	variant	UNP P0DTC2
C	452	ARG	LEU	variant	UNP P0DTC2
C	477	ASN	SER	variant	UNP P0DTC2
C	478	LYS	THR	variant	UNP P0DTC2
C	484	ALA	GLU	variant	UNP P0DTC2
C	486	VAL	PHE	variant	UNP P0DTC2
C	498	ARG	GLN	variant	UNP P0DTC2
C	501	TYR	ASN	variant	UNP P0DTC2
C	505	HIS	TYR	variant	UNP P0DTC2
C	614	GLY	ASP	variant	UNP P0DTC2
C	655	TYR	HIS	variant	UNP P0DTC2
C	679	LYS	ASN	variant	UNP P0DTC2
C	681	HIS	PRO	variant	UNP P0DTC2
C	764	LYS	ASN	variant	UNP P0DTC2
C	796	TYR	ASP	variant	UNP P0DTC2
C	817	PRO	PHE	variant	UNP P0DTC2
C	892	PRO	ALA	variant	UNP P0DTC2
C	899	PRO	ALA	variant	UNP P0DTC2
C	942	PRO	ALA	variant	UNP P0DTC2
C	954	HIS	GLN	variant	UNP P0DTC2
C	969	LYS	ASN	variant	UNP P0DTC2
C	986	PRO	LYS	variant	UNP P0DTC2
C	987	PRO	VAL	variant	UNP P0DTC2

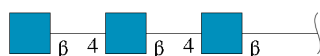
- Molecule 2 is a protein called heavy chain of S2L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	121	Total	C	N	O	S	0	0
			948	600	163	181	4		
2	I	121	Total	C	N	O	S	0	0
			948	600	163	181	4		
2	J	121	Total	C	N	O	S	0	0
			948	600	163	181	4		

- Molecule 3 is a protein called light chain of S2L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	L	107	Total	C	N	O	S	0	0
			832	529	134	165	4		
3	M	107	Total	C	N	O	S	0	0
			832	529	134	165	4		
3	N	107	Total	C	N	O	S	0	0
			832	529	134	165	4		

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



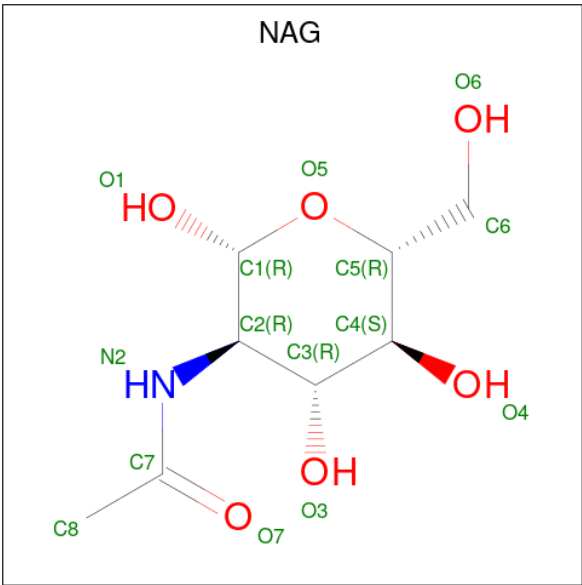
Mol	Chain	Residues	Atoms				AltConf	Trace
4	D	3	Total	C	N	O	0	0
			42	24	3	15		
4	Q	3	Total	C	N	O	0	0
			42	24	3	15		
4	X	3	Total	C	N	O	0	0
			42	24	3	15		

- Molecule 5 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
5	E	2	Total	C	N	O	0	0
			28	16	2	10		
5	F	2	Total	C	N	O	0	0
			28	16	2	10		
5	G	2	Total	C	N	O	0	0
			28	16	2	10		
5	K	2	Total	C	N	O	0	0
			28	16	2	10		
5	O	2	Total	C	N	O	0	0
			28	16	2	10		
5	P	2	Total	C	N	O	0	0
			28	16	2	10		
5	R	2	Total	C	N	O	0	0
			28	16	2	10		
5	S	2	Total	C	N	O	0	0
			28	16	2	10		
5	T	2	Total	C	N	O	0	0
			28	16	2	10		
5	U	2	Total	C	N	O	0	0
			28	16	2	10		
5	V	2	Total	C	N	O	0	0
			28	16	2	10		
5	W	2	Total	C	N	O	0	0
			28	16	2	10		
5	Y	2	Total	C	N	O	0	0
			28	16	2	10		
5	Z	2	Total	C	N	O	0	0
			28	16	2	10		
5	a	2	Total	C	N	O	0	0
			28	16	2	10		
5	b	2	Total	C	N	O	0	0
			28	16	2	10		
5	c	2	Total	C	N	O	0	0
			28	16	2	10		
5	d	2	Total	C	N	O	0	0
			28	16	2	10		

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



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

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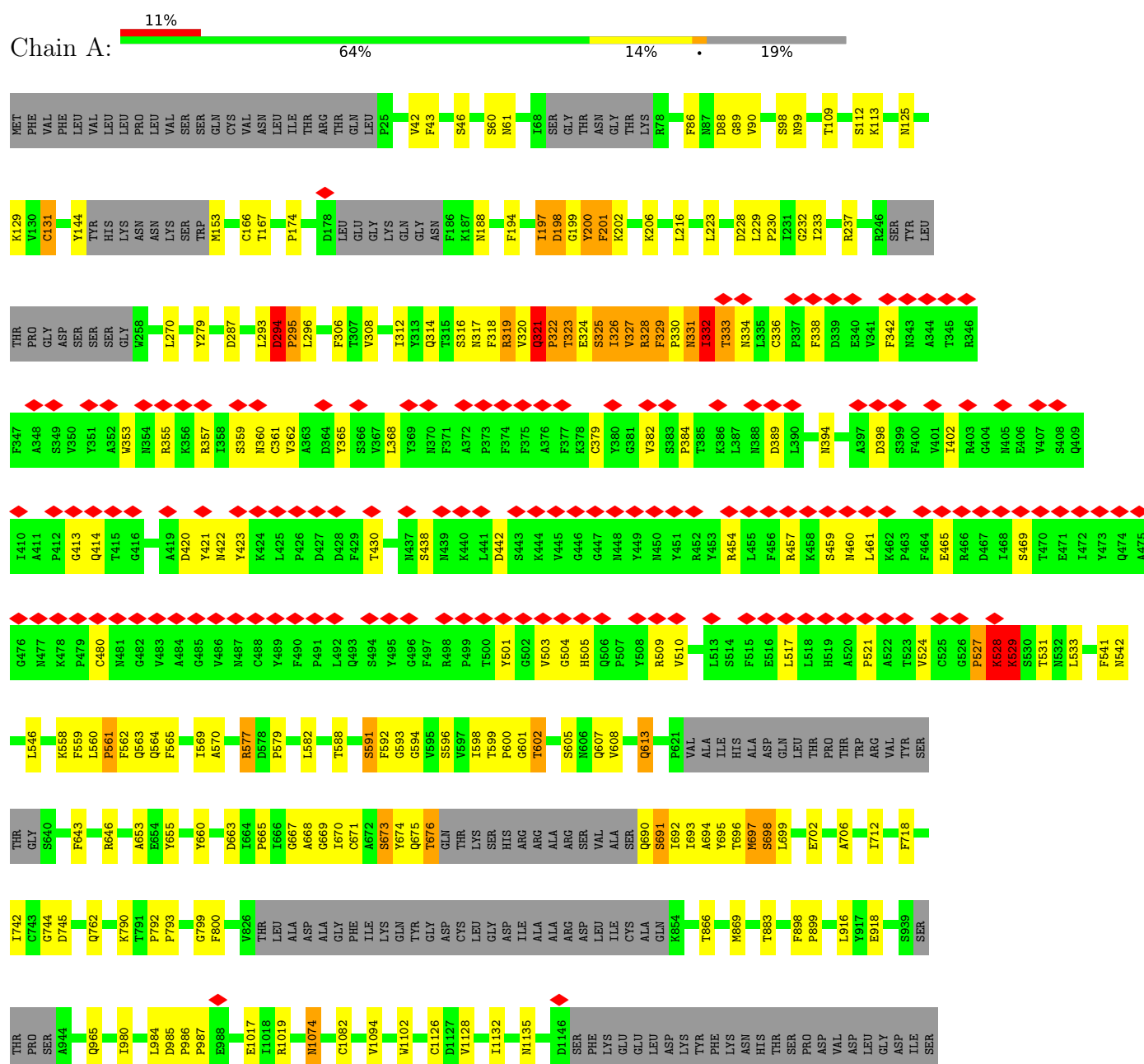
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Mol	Chain	Residues	Atoms				AltConf
6	B	1	Total	C	N	O	0
			14	8	1	5	
6	B	1	Total	C	N	O	0
			14	8	1	5	
6	B	1	Total	C	N	O	0
			14	8	1	5	
6	B	1	Total	C	N	O	0
			14	8	1	5	
6	B	1	Total	C	N	O	0
			14	8	1	5	
6	B	1	Total	C	N	O	0
			14	8	1	5	
6	C	1	Total	C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

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



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

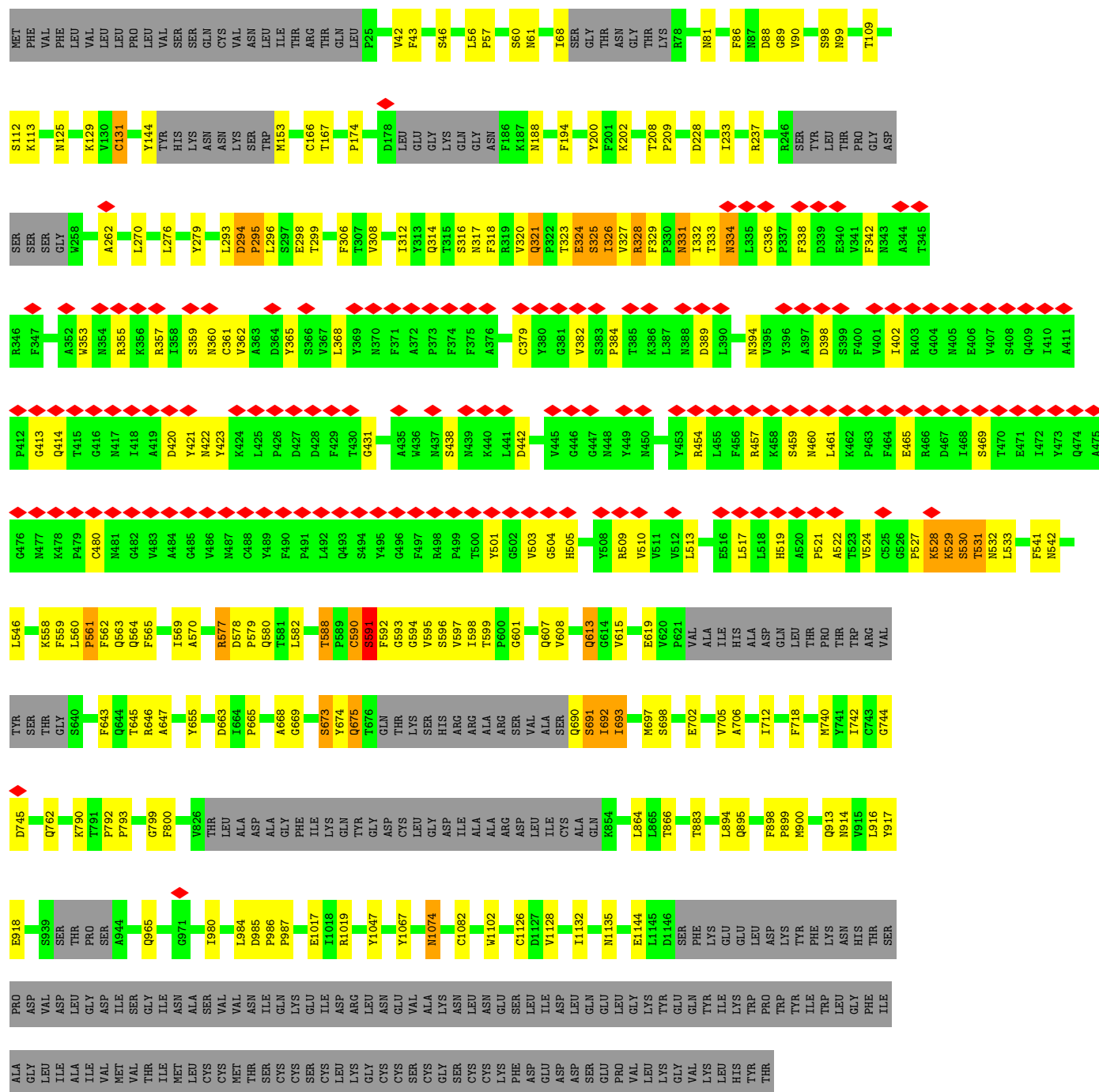
Chain B: 13% 63% 15% 9%



LEU
LYS
GLY
VAL
LEU
LYS
LEU
HIS
THR

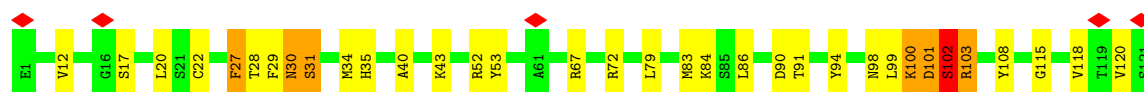
• Molecule 1: Spike glycoprotein

Chain C: 



• Molecule 2: heavy chain of S2L20

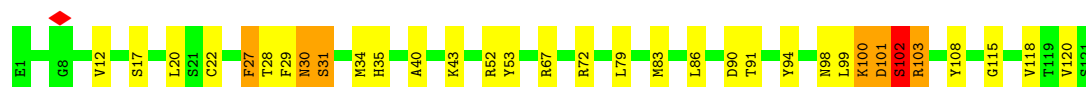
Chain H: 



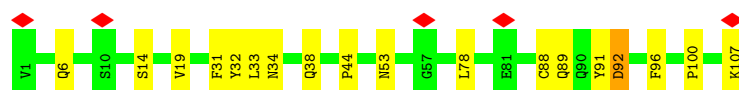
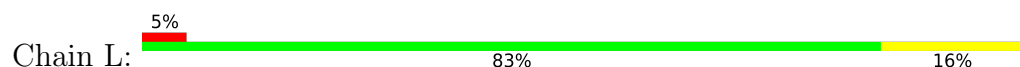
- Molecule 2: heavy chain of S2L20



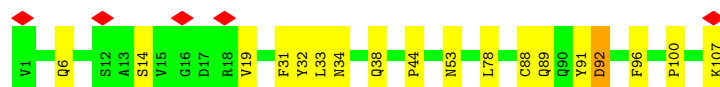
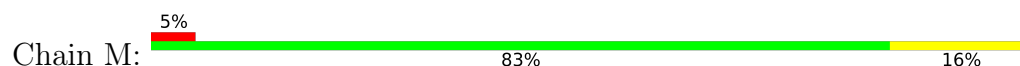
- Molecule 2: heavy chain of S2L20



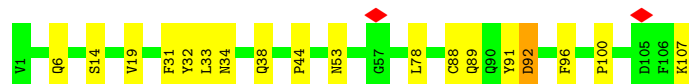
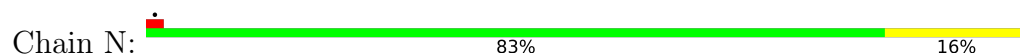
- Molecule 3: light chain of S2L20



- Molecule 3: light chain of S2L20



- Molecule 3: light chain of S2L20



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

Chain Q:  67% 33%



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

Chain X:  67% 33%

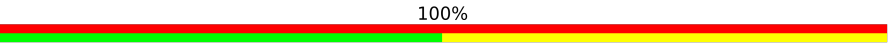


- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:  50% 50%



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

Chain F:  50% 100% 50%



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

Chain G:  50% 50%



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

Chain K:  50% 50%



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

Chain O:  100%



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

Chain P:  100%



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

Chain R:  100%



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

Chain S:  100%
50% 50%



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

Chain T:  50% 50%



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

Chain U:  50% 50%

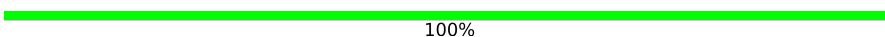


- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain V:  100%



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

Chain W:  100%



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

Chain Y:  50% 50%



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

Chain Z:  50% 100% 50%



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

Chain a:  50% 50%



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

Chain b:  50% 50%



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

Chain c:  100%



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

Chain d:  100%

MOL
MOL2

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	162448	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	4.058	Depositor
Minimum map value	-2.412	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.089	Depositor
Recommended contour level	0.3	Depositor
Map size ($\text{\AA}$)	344.64, 344.64, 344.64	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.077, 1.077, 1.077	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.52	0/8235	0.66	5/11204 (0.0%)
1	B	0.55	3/8235 (0.0%)	0.68	5/11204 (0.0%)
1	C	0.52	0/8235	0.66	7/11204 (0.1%)
2	H	0.45	0/971	0.59	1/1312 (0.1%)
2	I	0.45	0/971	0.59	1/1312 (0.1%)
2	J	0.45	0/971	0.59	1/1312 (0.1%)
3	L	0.37	0/854	0.55	1/1161 (0.1%)
3	M	0.37	0/854	0.55	1/1161 (0.1%)
3	N	0.37	0/854	0.55	1/1161 (0.1%)
All	All	0.51	3/30180 (0.0%)	0.65	23/41031 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	857	GLY	C-O	-6.40	1.15	1.24
1	B	858	LEU	CA-C	-5.95	1.44	1.52
1	B	858	LEU	C-O	-5.89	1.16	1.24

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	588	THR	N-CA-C	-7.86	100.10	110.40
1	C	588	THR	CA-C-N	-6.23	113.87	120.66
1	C	588	THR	C-N-CA	-6.23	113.87	120.66
1	B	588	THR	N-CA-C	-5.58	103.14	110.39
3	M	53	ASN	N-CA-C	5.57	118.45	107.98
3	N	53	ASN	N-CA-C	5.56	118.44	107.98
3	L	53	ASN	N-CA-C	5.55	118.41	107.98
2	J	31	SER	N-CA-C	-5.47	106.51	114.12
1	C	86	PHE	CA-C-N	5.47	131.98	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	86	PHE	C-N-CA	5.47	131.98	121.54
1	B	86	PHE	CA-C-N	5.45	131.96	121.54
1	B	86	PHE	C-N-CA	5.45	131.96	121.54
1	A	86	PHE	CA-C-N	5.45	131.95	121.54
1	A	86	PHE	C-N-CA	5.45	131.95	121.54
2	I	31	SER	N-CA-C	-5.44	106.55	114.12
2	H	31	SER	N-CA-C	-5.43	106.57	114.12
1	A	697	MET	N-CA-C	5.25	117.48	110.35
1	B	480	CYS	CA-C-N	5.07	129.60	122.46
1	B	480	CYS	C-N-CA	5.07	129.60	122.46
1	C	480	CYS	CA-C-N	5.05	129.58	122.46
1	C	480	CYS	C-N-CA	5.05	129.58	122.46
1	A	480	CYS	CA-C-N	5.04	129.57	122.46
1	A	480	CYS	C-N-CA	5.04	129.57	122.46

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	8043	0	7846	271	0
1	B	8043	0	7846	320	0
1	C	8043	0	7847	249	0
2	H	948	0	904	33	0
2	I	948	0	904	35	0
2	J	948	0	904	33	0
3	L	832	0	797	13	0
3	M	832	0	797	13	0
3	N	832	0	797	13	0
4	D	42	0	37	0	0
4	Q	42	0	37	0	0
4	X	42	0	37	0	0
5	E	28	0	25	3	0
5	F	28	0	25	0	0
5	G	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	K	28	0	25	0	0
5	O	28	0	25	1	0
5	P	28	0	25	0	0
5	R	28	0	25	0	0
5	S	28	0	25	0	0
5	T	28	0	25	0	0
5	U	28	0	25	0	0
5	V	28	0	25	1	0
5	W	28	0	25	0	0
5	Y	28	0	25	3	0
5	Z	28	0	25	0	0
5	a	28	0	25	0	0
5	b	28	0	25	0	0
5	c	28	0	25	1	0
5	d	28	0	25	0	0
6	A	140	0	129	6	0
6	B	140	0	129	7	0
6	C	140	0	129	7	0
All	All	30519	0	29590	864	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 14.

All (864) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:1409:NAG:O4	6:C:1410:NAG:C1	1.63	1.45
6:B:1409:NAG:O4	6:B:1410:NAG:C1	1.63	1.44
6:A:1409:NAG:O4	6:A:1410:NAG:C1	1.63	1.43
1:A:332:ILE:CD1	1:A:362:VAL:HG21	1.58	1.31
1:A:389:ASP:OD1	1:A:528:LYS:HB3	1.32	1.27
1:C:308:VAL:O	1:C:601:GLY:HA2	1.35	1.26
1:B:858:LEU:O	1:B:859:THR:HG22	1.40	1.20
1:B:308:VAL:H	1:B:602:THR:CG2	1.52	1.20
1:A:167:THR:HG22	1:C:357:ARG:NH2	1.56	1.17
1:B:332:ILE:HG23	1:B:362:VAL:HG21	1.28	1.16
1:A:521:PRO:HG2	1:B:200:TYR:CE2	1.85	1.11
1:B:529:LYS:HA	1:B:529:LYS:HE3	1.24	1.11
1:A:329:PHE:HB3	1:A:330:PRO:HD2	1.31	1.10
1:A:197:ILE:HD11	1:A:202:LYS:HD2	1.30	1.10
1:C:326:ILE:CD1	1:C:533:LEU:HA	1.83	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:357:ARG:HH22	1:B:167:THR:HG22	1.17	1.08
1:B:312:ILE:HG12	1:B:598:ILE:HG12	1.28	1.07
1:C:332:ILE:HG23	1:C:362:VAL:HG21	1.10	1.07
1:B:308:VAL:HB	1:B:602:THR:HG22	1.36	1.06
1:A:521:PRO:CG	1:B:200:TYR:CE2	2.40	1.04
1:B:308:VAL:H	1:B:602:THR:HG21	1.21	1.04
1:A:321:GLN:HB3	1:A:322:PRO:HD2	1.35	1.03
1:C:312:ILE:HG12	1:C:598:ILE:HG12	1.40	1.03
1:B:737:ASP:HB3	1:B:857:GLY:HA3	1.40	1.03
1:A:312:ILE:HG12	1:A:598:ILE:HG12	1.41	1.02
1:C:326:ILE:HD11	1:C:533:LEU:HA	1.02	1.02
1:A:332:ILE:HD13	1:A:362:VAL:HG21	1.03	1.02
1:B:308:VAL:N	1:B:602:THR:CG2	2.21	1.01
6:A:1409:NAG:C4	6:A:1410:NAG:C1	2.38	1.01
6:C:1409:NAG:C4	6:C:1410:NAG:C1	2.38	1.01
1:A:329:PHE:O	1:A:579:PRO:HB2	1.59	1.00
1:A:1017:GLU:HG2	1:B:1019:ARG:HH22	1.25	1.00
1:B:332:ILE:CG2	1:B:362:VAL:HG21	1.90	1.00
6:B:1409:NAG:C4	6:B:1410:NAG:C1	2.38	1.00
1:B:527:PRO:O	1:B:528:LYS:NZ	1.95	1.00
1:A:357:ARG:NH2	1:B:167:THR:HG22	1.76	0.98
1:A:1019:ARG:NH2	1:C:1017:GLU:HG2	1.77	0.98
1:B:308:VAL:HB	1:B:602:THR:CG2	1.93	0.97
1:A:1017:GLU:HG2	1:B:1019:ARG:NH2	1.79	0.97
1:C:389:ASP:OD1	1:C:528:LYS:HG2	1.65	0.96
1:B:858:LEU:O	1:B:859:THR:CG2	2.13	0.96
1:A:294:ASP:HB2	1:A:295:PRO:CD	1.94	0.95
1:B:663:ASP:OD2	1:B:673:SER:HB3	1.64	0.95
1:B:324:GLU:HG3	1:B:325:SER:H	1.30	0.94
1:A:329:PHE:HB3	1:A:330:PRO:CD	1.97	0.94
1:C:324:GLU:HG3	1:C:325:SER:H	1.32	0.94
1:C:532:ASN:OD1	1:C:533:LEU:N	1.99	0.94
1:C:308:VAL:HG11	1:C:599:THR:HG21	1.50	0.94
1:B:1017:GLU:HG2	1:C:1019:ARG:HH22	1.31	0.93
1:C:663:ASP:OD2	1:C:673:SER:HB3	1.68	0.93
1:A:1019:ARG:HH22	1:C:1017:GLU:CG	1.82	0.93
1:A:294:ASP:HB2	1:A:295:PRO:HD3	1.51	0.93
1:B:308:VAL:O	1:B:602:THR:HG23	1.67	0.93
1:C:326:ILE:HD11	1:C:533:LEU:CA	1.96	0.93
1:A:671:CYS:HB2	1:A:695:TYR:CE2	2.04	0.92
1:C:332:ILE:HG23	1:C:362:VAL:CG2	2.00	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:308:VAL:H	1:B:602:THR:HG23	1.32	0.92
1:B:521:PRO:HG2	1:C:200:TYR:CE2	2.05	0.92
1:A:320:VAL:HG12	1:A:591:SER:O	1.68	0.91
1:B:312:ILE:HG12	1:B:598:ILE:CG1	1.98	0.91
1:B:521:PRO:CG	1:C:200:TYR:CE2	2.53	0.91
1:A:1017:GLU:CG	1:B:1019:ARG:HH22	1.83	0.91
1:B:112:SER:O	1:B:113:LYS:HG2	1.70	0.91
1:A:671:CYS:HB2	1:A:695:TYR:CZ	2.05	0.90
1:A:332:ILE:CD1	1:A:362:VAL:CG2	2.48	0.90
1:A:866:THR:CG2	1:C:646:ARG:HH21	1.83	0.90
1:A:866:THR:HG21	1:C:646:ARG:NH2	1.87	0.90
1:A:521:PRO:HG2	1:B:200:TYR:CZ	2.07	0.90
1:B:308:VAL:N	1:B:602:THR:HG21	1.80	0.89
1:C:530:SER:O	1:C:531:THR:OG1	1.90	0.89
1:C:112:SER:O	1:C:113:LYS:HG2	1.70	0.89
1:B:109:THR:HA	1:B:237:ARG:HH21	1.37	0.89
1:A:1019:ARG:HH22	1:C:1017:GLU:CD	1.81	0.89
1:B:1017:GLU:HG2	1:C:1019:ARG:NH2	1.88	0.89
1:A:112:SER:O	1:A:113:LYS:HG2	1.71	0.89
1:C:332:ILE:CG2	1:C:362:VAL:HG21	2.02	0.89
1:A:321:GLN:HB3	1:A:322:PRO:CD	2.03	0.89
1:C:109:THR:HA	1:C:237:ARG:HH21	1.38	0.88
1:C:582:LEU:HD11	5:Y:1:NAG:H83	1.55	0.88
1:A:109:THR:HA	1:A:237:ARG:HH21	1.37	0.88
1:A:762:GLN:HE22	1:C:965:GLN:NE2	1.70	0.88
1:B:308:VAL:N	1:B:602:THR:HG23	1.86	0.88
1:B:312:ILE:CG1	1:B:598:ILE:HG12	2.03	0.88
1:B:328:ARG:NH1	1:B:581:THR:HG23	1.89	0.88
1:C:308:VAL:O	1:C:601:GLY:CA	2.22	0.88
1:C:308:VAL:CG1	1:C:599:THR:HG21	2.04	0.87
1:A:332:ILE:HD13	1:A:362:VAL:CG2	1.99	0.87
1:A:329:PHE:C	1:A:579:PRO:HB2	1.98	0.87
1:A:1019:ARG:HH22	1:C:1017:GLU:HG2	1.31	0.86
1:A:389:ASP:OD1	1:A:528:LYS:HE3	1.76	0.86
1:C:294:ASP:HB2	1:C:295:PRO:CD	2.06	0.86
1:C:328:ARG:HG2	1:C:578:ASP:OD1	1.76	0.86
1:B:690:GLN:O	1:B:691:SER:OG	1.94	0.86
1:B:308:VAL:CA	1:B:602:THR:CG2	2.54	0.86
1:B:308:VAL:CB	1:B:602:THR:CG2	2.54	0.85
1:A:167:THR:CG2	1:C:357:ARG:NH2	2.39	0.84
1:B:329:PHE:O	1:B:580:GLN:HB2	1.76	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:737:ASP:CB	1:B:857:GLY:HA3	2.08	0.84
1:A:675:GLN:HG3	1:A:676:THR:N	1.91	0.84
1:A:866:THR:HG21	1:C:646:ARG:HH21	1.41	0.84
1:C:326:ILE:HG13	1:C:532:ASN:O	1.78	0.84
1:B:671:CYS:HB2	1:B:695:TYR:CE1	2.13	0.83
1:B:308:VAL:C	1:B:602:THR:HG23	2.03	0.82
1:B:1017:GLU:CG	1:C:1019:ARG:HH22	1.91	0.82
1:A:197:ILE:HD11	1:A:202:LYS:CD	2.09	0.82
1:A:389:ASP:OD1	1:A:528:LYS:CB	2.23	0.82
1:B:646:ARG:NH2	1:C:866:THR:CG2	2.42	0.82
1:B:672:ALA:HA	1:B:693:ILE:O	1.80	0.81
1:A:322:PRO:O	1:A:323:THR:OG1	1.97	0.81
1:B:332:ILE:CG2	1:B:362:VAL:CG2	2.59	0.81
1:A:198:ASP:OD2	1:A:199:GLY:N	2.11	0.80
1:B:328:ARG:HH12	1:B:581:THR:HG23	1.44	0.80
1:C:112:SER:O	1:C:113:LYS:CG	2.29	0.80
1:A:112:SER:O	1:A:113:LYS:CG	2.29	0.80
1:B:527:PRO:C	1:B:528:LYS:HZ2	1.90	0.79
1:A:965:GLN:NE2	1:B:762:GLN:HE22	1.79	0.79
1:B:112:SER:O	1:B:113:LYS:CG	2.29	0.79
1:A:198:ASP:OD1	1:A:200:TYR:HE1	1.63	0.79
1:B:521:PRO:HG2	1:C:200:TYR:CZ	2.17	0.79
1:B:308:VAL:CA	1:B:602:THR:HG23	2.13	0.78
1:A:663:ASP:OD2	1:A:673:SER:HB3	1.82	0.78
1:B:675:GLN:HG3	1:B:676:THR:H	1.49	0.78
1:C:46:SER:HA	1:C:279:TYR:O	1.85	0.77
1:B:333:THR:OG1	1:B:334:ASN:OD1	2.02	0.77
1:C:318:PHE:O	1:C:592:PHE:HA	1.85	0.77
1:B:46:SER:HA	1:B:279:TYR:O	1.85	0.77
2:J:103:ARG:HH21	2:J:103:ARG:HG3	1.49	0.77
1:A:200:TYR:HD1	1:A:200:TYR:H	1.32	0.77
1:B:671:CYS:O	1:B:694:ALA:HA	1.84	0.77
2:I:103:ARG:HH21	2:I:103:ARG:HG3	1.49	0.77
1:A:646:ARG:NH2	1:B:866:THR:CG2	2.48	0.77
1:B:659:SER:HB3	1:B:698:SER:HB3	1.66	0.77
1:A:200:TYR:HB2	1:A:229:LEU:O	1.84	0.76
1:A:319:ARG:HB2	1:A:319:ARG:CZ	2.15	0.76
1:B:659:SER:CB	1:B:698:SER:HB3	2.15	0.76
1:A:46:SER:HA	1:A:279:TYR:O	1.85	0.76
1:A:1017:GLU:CD	1:B:1019:ARG:HH22	1.93	0.76
2:H:103:ARG:HH21	2:H:103:ARG:HG3	1.49	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:167:THR:HG22	1:C:357:ARG:HH21	1.47	0.75
1:C:314:GLN:HA	1:C:596:SER:CB	2.16	0.74
2:J:94:TYR:O	2:J:115:GLY:HA2	1.87	0.74
1:C:333:THR:O	1:C:334:ASN:O	2.06	0.74
1:B:331:ASN:C	1:B:332:ILE:HG12	2.10	0.74
1:B:1128:VAL:CG2	1:C:918:GLU:HG2	2.18	0.74
1:C:389:ASP:OD1	1:C:528:LYS:CG	2.36	0.74
2:H:94:TYR:O	2:H:115:GLY:HA2	1.87	0.74
1:A:521:PRO:HG3	1:B:200:TYR:CE2	2.21	0.74
1:B:529:LYS:HE3	1:B:529:LYS:CA	1.97	0.74
1:A:660:TYR:O	1:A:698:SER:HB2	1.87	0.74
2:I:27:PHE:HD1	2:I:27:PHE:H	1.34	0.74
2:H:103:ARG:HG3	2:H:103:ARG:NH2	2.02	0.74
1:C:327:VAL:HB	1:C:530:SER:O	1.88	0.73
2:J:103:ARG:HG3	2:J:103:ARG:NH2	2.02	0.73
1:A:646:ARG:NH2	1:A:668:ALA:O	2.21	0.73
1:B:646:ARG:NH2	1:B:668:ALA:O	2.21	0.73
2:I:94:TYR:O	2:I:115:GLY:HA2	1.87	0.73
1:A:319:ARG:HB2	1:A:319:ARG:NH2	2.03	0.73
1:A:762:GLN:HE22	1:C:965:GLN:HE21	1.35	0.73
1:B:592:PHE:HD1	1:B:593:GLY:N	1.87	0.73
1:B:308:VAL:O	1:B:602:THR:CG2	2.36	0.72
2:H:27:PHE:HD1	2:H:27:PHE:H	1.34	0.72
2:J:27:PHE:HD1	2:J:27:PHE:H	1.34	0.72
2:I:103:ARG:HG3	2:I:103:ARG:NH2	2.02	0.72
1:A:201:PHE:O	1:A:202:LYS:HG3	1.90	0.72
6:A:1409:NAG:H4	6:A:1410:NAG:C1	2.21	0.71
1:B:319:ARG:HB2	1:B:319:ARG:NH2	2.04	0.71
1:C:312:ILE:HG12	1:C:598:ILE:CG1	2.19	0.70
1:A:667:GLY:HA2	1:B:864:LEU:CD1	2.21	0.70
1:A:667:GLY:HA2	1:B:864:LEU:HD12	1.72	0.70
1:B:324:GLU:HG3	1:B:325:SER:N	2.05	0.70
6:C:1409:NAG:H4	6:C:1410:NAG:C1	2.20	0.70
1:A:237:ARG:CZ	2:H:102:SER:OG	2.40	0.70
1:B:592:PHE:CD1	1:B:593:GLY:N	2.59	0.70
1:C:295:PRO:HG2	1:C:608:VAL:HG21	1.72	0.70
1:A:326:ILE:HD12	1:A:326:ILE:C	2.16	0.70
3:L:33:LEU:HA	3:L:89:GLN:O	1.93	0.69
1:A:663:ASP:OD2	1:A:673:SER:CB	2.39	0.69
1:C:328:ARG:CG	1:C:578:ASP:OD1	2.40	0.69
6:B:1409:NAG:H4	6:B:1410:NAG:C1	2.20	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:333:THR:O	1:C:334:ASN:C	2.35	0.69
1:B:533:LEU:CD2	1:B:535:LYS:HE3	2.22	0.69
1:A:287:ASP:HB3	1:A:306:PHE:HE2	1.56	0.69
1:A:328:ARG:O	1:A:329:PHE:HD1	1.76	0.69
1:B:965:GLN:NE2	1:C:762:GLN:HE22	1.90	0.69
1:C:237:ARG:CZ	2:J:102:SER:OG	2.40	0.69
1:B:237:ARG:CZ	2:I:102:SER:OG	2.40	0.69
1:B:668:ALA:H	1:C:864:LEU:HA	1.57	0.69
1:B:674:TYR:HA	1:B:691:SER:O	1.92	0.69
1:B:328:ARG:NH1	1:B:578:ASP:OD2	2.26	0.69
1:B:646:ARG:HH21	1:C:866:THR:HG22	1.55	0.69
1:B:858:LEU:O	1:B:859:THR:CB	2.41	0.68
3:N:33:LEU:HA	3:N:89:GLN:O	1.93	0.68
1:A:799:GLY:O	1:A:800:PHE:C	2.37	0.68
3:M:33:LEU:HA	3:M:89:GLN:O	1.93	0.68
1:A:329:PHE:CB	1:A:330:PRO:HD2	2.17	0.68
1:B:799:GLY:O	1:B:800:PHE:C	2.37	0.68
1:B:672:ALA:CB	1:B:693:ILE:O	2.42	0.68
1:A:308:VAL:CG1	1:A:599:THR:HG21	2.24	0.68
1:B:672:ALA:C	1:B:673:SER:OG	2.34	0.68
1:A:670:ILE:HG23	1:A:695:TYR:O	1.94	0.68
1:C:560:LEU:O	1:C:562:PHE:N	2.27	0.68
3:M:32:TYR:HB3	3:M:91:TYR:HB2	1.76	0.68
1:A:521:PRO:CG	1:B:200:TYR:HE2	2.01	0.67
1:A:560:LEU:O	1:A:562:PHE:N	2.27	0.67
3:L:31:PHE:CE1	3:L:32:TYR:CE1	2.83	0.67
3:N:32:TYR:HB3	3:N:91:TYR:HB2	1.76	0.67
1:B:560:LEU:O	1:B:562:PHE:N	2.27	0.67
1:C:799:GLY:O	1:C:800:PHE:C	2.37	0.67
1:A:198:ASP:OD1	1:A:200:TYR:CE1	2.46	0.67
1:A:670:ILE:HA	1:A:695:TYR:O	1.95	0.67
3:M:31:PHE:CE1	3:M:32:TYR:CE1	2.83	0.67
1:B:528:LYS:NZ	1:B:528:LYS:HB2	2.10	0.67
1:B:1017:GLU:CD	1:C:1019:ARG:HH22	2.03	0.67
3:N:31:PHE:CE1	3:N:32:TYR:CE1	2.83	0.67
1:B:333:THR:OG1	1:B:334:ASN:N	2.28	0.67
1:A:646:ARG:NH2	1:B:866:THR:HG21	2.09	0.66
1:A:646:ARG:HH21	1:B:866:THR:CG2	2.07	0.66
1:A:669:GLY:HA2	1:B:869:MET:HE1	1.76	0.66
1:B:529:LYS:HA	1:B:529:LYS:CE	2.15	0.66
1:B:294:ASP:N	1:B:294:ASP:OD1	2.27	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:31:PHE:CE1	3:L:32:TYR:CZ	2.84	0.66
3:N:31:PHE:CE1	3:N:32:TYR:CZ	2.84	0.66
1:A:318:PHE:O	1:A:593:GLY:N	2.28	0.66
1:A:674:TYR:HA	1:A:691:SER:O	1.96	0.66
1:B:533:LEU:CD2	1:B:535:LYS:CE	2.73	0.66
1:B:1128:VAL:HG23	1:C:918:GLU:HG2	1.77	0.66
1:C:323:THR:O	1:C:324:GLU:HB2	1.95	0.66
3:L:32:TYR:HB3	3:L:91:TYR:HB2	1.76	0.66
1:C:308:VAL:CG1	1:C:599:THR:CG2	2.74	0.66
1:C:582:LEU:HD11	5:Y:1:NAG:C8	2.25	0.66
1:B:528:LYS:HB2	1:B:528:LYS:HZ3	1.60	0.66
1:B:329:PHE:C	1:B:579:PRO:HB2	2.21	0.65
3:M:31:PHE:CE1	3:M:32:TYR:CZ	2.84	0.65
1:C:326:ILE:CG1	1:C:532:ASN:O	2.44	0.65
1:B:675:GLN:HB2	1:B:693:ILE:HD13	1.78	0.65
1:A:318:PHE:N	1:A:593:GLY:O	2.20	0.65
1:A:669:GLY:CA	1:B:869:MET:HE1	2.27	0.65
1:A:144:TYR:HB3	1:A:153:MET:HB3	1.79	0.65
1:B:144:TYR:HB3	1:B:153:MET:HB3	1.79	0.64
1:A:198:ASP:OD2	1:A:200:TYR:CD1	2.51	0.64
1:B:672:ALA:CA	1:B:693:ILE:O	2.45	0.64
1:B:675:GLN:HG3	1:B:676:THR:N	2.11	0.64
1:C:321:GLN:N	1:C:321:GLN:OE1	2.31	0.64
1:B:735:SER:O	1:B:858:LEU:C	2.41	0.64
1:B:736:VAL:HA	1:B:858:LEU:HA	1.79	0.64
1:C:530:SER:C	1:C:531:THR:HG1	1.99	0.64
1:B:646:ARG:NH2	1:C:866:THR:HG22	2.10	0.64
1:A:332:ILE:HD12	1:A:362:VAL:HG21	1.70	0.63
1:B:533:LEU:HD23	1:B:535:LYS:HE3	1.80	0.63
1:B:324:GLU:OE2	1:B:324:GLU:HA	1.99	0.63
1:C:321:GLN:CD	1:C:321:GLN:H	2.05	0.63
1:C:690:GLN:O	1:C:690:GLN:HG2	1.98	0.63
1:B:332:ILE:HG23	1:B:362:VAL:CG2	2.16	0.63
1:C:324:GLU:HG3	1:C:325:SER:N	2.05	0.63
2:I:29:PHE:O	2:I:31:SER:N	2.31	0.63
1:B:310:LYS:HG3	1:B:600:PRO:HA	1.79	0.63
1:B:329:PHE:HD1	1:B:330:PRO:HD2	1.63	0.63
2:H:29:PHE:O	2:H:31:SER:N	2.31	0.63
2:J:29:PHE:O	2:J:31:SER:N	2.31	0.63
1:C:692:ILE:O	1:C:692:ILE:HG23	2.00	0.62
1:A:321:GLN:CB	1:A:322:PRO:HD2	2.21	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:67:ARG:NH2	2:H:90:ASP:OD2	2.32	0.62
2:I:67:ARG:NH2	2:I:90:ASP:OD2	2.32	0.62
1:C:294:ASP:HB2	1:C:295:PRO:HD3	1.80	0.62
2:J:67:ARG:NH2	2:J:90:ASP:OD2	2.32	0.62
2:I:91:THR:HA	2:I:118:VAL:O	2.00	0.61
1:A:319:ARG:CG	1:A:319:ARG:HH21	2.13	0.61
1:C:144:TYR:HB3	1:C:153:MET:HB3	1.79	0.61
1:C:326:ILE:HG22	1:C:541:PHE:HA	1.83	0.61
2:J:91:THR:HA	2:J:118:VAL:O	2.00	0.61
1:C:582:LEU:CD1	5:Y:1:NAG:H83	2.28	0.61
1:A:319:ARG:HH21	1:A:319:ARG:HG3	1.64	0.61
1:A:324:GLU:O	1:A:325:SER:HB2	2.00	0.61
2:J:34:MET:HE3	2:J:98:ASN:HB2	1.82	0.61
1:B:314:GLN:HA	1:B:596:SER:CB	2.30	0.61
2:H:91:THR:HA	2:H:118:VAL:O	2.00	0.61
1:A:312:ILE:HG12	1:A:598:ILE:CG1	2.25	0.61
1:A:322:PRO:C	1:A:323:THR:HG1	2.05	0.61
1:A:308:VAL:N	1:A:602:THR:OG1	2.25	0.61
1:C:332:ILE:HG22	1:C:333:THR:N	2.15	0.61
1:A:333:THR:OG1	1:A:334:ASN:N	2.32	0.61
1:B:308:VAL:CB	1:B:602:THR:HG21	2.31	0.60
1:B:296:LEU:O	1:B:299:THR:N	2.34	0.60
1:C:296:LEU:O	1:C:299:THR:N	2.34	0.60
3:L:34:ASN:ND2	3:L:91:TYR:OH	2.35	0.60
1:B:706:ALA:CB	6:B:1409:NAG:H5	2.32	0.60
2:H:34:MET:HE3	2:H:98:ASN:HB2	1.82	0.60
1:B:856:ASN:N	1:B:856:ASN:OD1	2.34	0.60
1:C:316:SER:O	1:C:595:VAL:N	2.22	0.60
2:I:34:MET:HE3	2:I:98:ASN:HB2	1.82	0.60
1:C:294:ASP:CB	1:C:295:PRO:CD	2.78	0.60
2:I:99:LEU:O	2:I:101:ASP:N	2.35	0.60
1:A:1128:VAL:CG2	1:B:918:GLU:HG2	2.32	0.60
1:C:109:THR:HA	1:C:237:ARG:NH2	2.15	0.59
1:A:706:ALA:CB	6:A:1409:NAG:H5	2.32	0.59
1:B:109:THR:HA	1:B:237:ARG:NH2	2.15	0.59
3:M:34:ASN:ND2	3:M:91:TYR:OH	2.35	0.59
3:N:34:ASN:ND2	3:N:91:TYR:OH	2.34	0.59
1:B:702:GLU:OE2	1:C:790:LYS:NZ	2.33	0.59
1:C:706:ALA:CB	6:C:1409:NAG:H5	2.32	0.59
1:A:646:ARG:HH21	1:B:866:THR:HG22	1.67	0.59
1:B:324:GLU:OE2	2:I:84:LYS:HD2	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:99:LEU:O	2:H:101:ASP:N	2.35	0.59
1:B:1128:VAL:HG21	1:C:918:GLU:HG2	1.83	0.58
1:A:109:THR:HA	1:A:237:ARG:NH2	2.15	0.58
1:B:663:ASP:OD2	1:B:673:SER:CB	2.47	0.58
1:C:353:TRP:HZ3	1:C:355:ARG:HD2	1.69	0.58
1:B:353:TRP:HZ3	1:B:355:ARG:HD2	1.68	0.58
1:B:702:GLU:OE2	1:C:790:LYS:CE	2.51	0.58
2:J:99:LEU:O	2:J:101:ASP:N	2.35	0.58
1:A:527:PRO:C	1:A:529:LYS:H	2.12	0.58
1:A:965:GLN:HE21	1:B:762:GLN:HE22	1.52	0.58
1:B:521:PRO:HB2	1:C:200:TYR:HE2	1.68	0.58
1:B:521:PRO:CB	1:C:200:TYR:CE2	2.87	0.58
1:A:353:TRP:HZ3	1:A:355:ARG:HD2	1.68	0.58
1:B:319:ARG:HB2	1:B:319:ARG:CZ	2.34	0.58
1:B:521:PRO:HB2	1:C:200:TYR:CE2	2.39	0.58
1:A:389:ASP:HB3	1:A:528:LYS:HZ1	1.69	0.57
1:C:276:LEU:HD23	1:C:306:PHE:HE1	1.69	0.57
1:C:326:ILE:CD1	1:C:532:ASN:O	2.52	0.57
1:C:294:ASP:HB2	1:C:295:PRO:HD2	1.86	0.57
1:C:359:SER:OG	1:C:360:ASN:N	2.37	0.57
1:A:43:PHE:CE1	1:C:558:LYS:O	2.57	0.57
1:B:646:ARG:NH2	1:C:866:THR:HG21	2.19	0.57
1:A:582:LEU:HD11	5:E:1:NAG:C8	2.33	0.57
1:A:324:GLU:O	1:A:325:SER:CB	2.53	0.57
1:B:294:ASP:HB2	1:B:295:PRO:CD	2.35	0.57
3:M:14:SER:HB3	3:M:107:LYS:HE2	1.87	0.57
1:B:325:SER:HA	1:B:540:ASN:O	2.05	0.57
1:B:329:PHE:CD1	1:B:330:PRO:HD2	2.38	0.57
1:A:389:ASP:CG	1:A:528:LYS:HE3	2.29	0.57
2:J:29:PHE:CD2	2:J:30:ASN:N	2.72	0.56
3:N:14:SER:HB3	3:N:107:LYS:HE2	1.87	0.56
1:A:197:ILE:CD1	1:A:202:LYS:HE2	2.36	0.56
1:A:359:SER:OG	1:A:360:ASN:N	2.37	0.56
1:B:318:PHE:CZ	1:B:620:VAL:O	2.58	0.56
1:B:357:ARG:NH2	1:C:167:THR:HG22	2.20	0.56
1:C:320:VAL:HG13	1:C:590:CYS:SG	2.44	0.56
2:I:27:PHE:CD1	2:I:27:PHE:N	2.73	0.56
1:B:332:ILE:HG22	1:B:362:VAL:CG2	2.34	0.56
3:L:14:SER:HB3	3:L:107:LYS:HE2	1.87	0.56
1:B:522:ALA:HB2	1:C:200:TYR:OH	2.06	0.56
1:A:675:GLN:HG3	1:A:676:THR:H	1.69	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:308:VAL:O	1:B:602:THR:N	2.32	0.56
1:C:314:GLN:HA	1:C:596:SER:HB3	1.85	0.56
1:A:592:PHE:CE2	1:B:854:LYS:HG2	2.41	0.56
1:B:659:SER:HB2	1:B:698:SER:HB3	1.85	0.56
1:A:308:VAL:HG12	1:A:599:THR:HG21	1.87	0.56
1:C:312:ILE:CG1	1:C:598:ILE:HG12	2.26	0.56
2:I:29:PHE:CD2	2:I:30:ASN:N	2.72	0.56
1:A:592:PHE:CE1	1:B:857:GLY:HA2	2.41	0.56
1:B:735:SER:O	1:B:858:LEU:HA	2.06	0.56
1:A:321:GLN:CB	1:A:322:PRO:CD	2.76	0.56
1:A:866:THR:HG22	1:C:646:ARG:HH21	1.69	0.55
1:A:327:VAL:HG13	1:A:542:ASN:HB3	1.86	0.55
1:A:869:MET:HE1	1:C:669:GLY:CA	2.36	0.55
2:H:103:ARG:HH21	2:H:103:ARG:CG	2.18	0.55
1:A:314:GLN:HA	1:A:596:SER:CB	2.37	0.55
1:B:533:LEU:CD2	1:B:535:LYS:HE2	2.36	0.55
1:B:323:THR:OG1	1:B:324:GLU:N	2.34	0.55
1:A:230:PRO:CB	1:C:522:ALA:O	2.54	0.55
1:A:582:LEU:CD1	5:E:1:NAG:H83	2.36	0.55
1:B:295:PRO:O	1:B:298:GLU:HB3	2.07	0.55
1:C:308:VAL:HG12	1:C:599:THR:CG2	2.36	0.55
1:A:197:ILE:CD1	1:A:202:LYS:CE	2.85	0.55
1:B:695:TYR:CD1	1:B:695:TYR:C	2.85	0.55
1:C:294:ASP:OD1	1:C:295:PRO:HD2	2.06	0.55
1:C:646:ARG:NH2	1:C:668:ALA:O	2.39	0.55
1:B:592:PHE:CD1	1:B:592:PHE:C	2.86	0.54
1:B:735:SER:O	1:B:858:LEU:CA	2.55	0.54
1:B:319:ARG:CZ	1:B:319:ARG:CB	2.85	0.54
1:B:319:ARG:HH21	1:B:319:ARG:CG	2.19	0.54
2:H:29:PHE:CD2	2:H:30:ASN:N	2.72	0.54
1:A:332:ILE:HG23	1:A:333:THR:N	2.23	0.54
1:A:691:SER:OG	1:A:692:ILE:N	2.40	0.54
1:B:303:LEU:HD21	1:B:313:TYR:CD1	2.43	0.54
1:B:329:PHE:HB3	1:B:330:PRO:HD2	1.89	0.54
1:C:328:ARG:NH1	1:C:580:GLN:OE1	2.40	0.54
1:A:693:ILE:HG13	1:A:693:ILE:O	2.07	0.54
1:B:326:ILE:O	1:B:327:VAL:HG23	2.08	0.54
1:B:854:LYS:C	1:B:855:PHE:CD1	2.86	0.54
3:N:31:PHE:HE1	3:N:32:TYR:CE1	2.26	0.54
1:B:303:LEU:O	1:B:304:LYS:C	2.51	0.54
1:B:702:GLU:OE2	1:C:790:LYS:HE3	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:27:PHE:CD1	2:J:27:PHE:N	2.73	0.54
1:A:112:SER:OG	1:A:113:LYS:N	2.41	0.53
1:A:200:TYR:HB3	1:A:230:PRO:HA	1.90	0.53
1:A:332:ILE:O	1:A:333:THR:HG22	2.08	0.53
1:A:200:TYR:CB	1:A:229:LEU:O	2.56	0.53
1:A:329:PHE:CB	1:A:330:PRO:CD	2.70	0.53
1:B:533:LEU:HD23	1:B:535:LYS:CE	2.37	0.53
1:A:869:MET:HE1	1:C:669:GLY:HA2	1.88	0.53
1:C:318:PHE:O	1:C:592:PHE:CA	2.56	0.53
1:B:522:ALA:CB	1:C:200:TYR:OH	2.56	0.53
1:B:328:ARG:NH1	1:B:580:GLN:HB3	2.24	0.53
1:B:531:THR:HG22	1:B:532:ASN:N	2.22	0.53
1:C:112:SER:OG	1:C:113:LYS:N	2.41	0.53
3:L:31:PHE:HE1	3:L:32:TYR:CE1	2.26	0.53
3:M:31:PHE:HE1	3:M:32:TYR:CE1	2.26	0.52
1:A:316:SER:OG	1:A:317:ASN:N	2.42	0.52
1:A:671:CYS:O	1:A:694:ALA:HA	2.08	0.52
1:B:695:TYR:O	1:B:695:TYR:HD1	1.92	0.52
1:C:308:VAL:HG11	1:C:599:THR:CG2	2.32	0.52
1:B:112:SER:OG	1:B:113:LYS:N	2.41	0.52
1:B:310:LYS:CG	1:B:664:ILE:HD11	2.39	0.52
1:B:674:TYR:CE2	1:B:690:GLN:N	2.77	0.52
1:C:327:VAL:O	1:C:328:ARG:HD3	2.09	0.52
1:A:295:PRO:HD2	1:A:296:LEU:H	1.72	0.52
1:B:695:TYR:C	1:B:695:TYR:HD1	2.17	0.52
1:B:858:LEU:C	1:B:859:THR:HG22	2.22	0.52
3:M:6:GLN:NE2	3:M:88:CYS:SG	2.82	0.52
1:A:42:VAL:HA	1:C:565:PHE:O	2.10	0.52
1:A:201:PHE:O	1:A:202:LYS:CG	2.57	0.52
1:C:442:ASP:OD2	1:C:509:ARG:NE	2.41	0.52
3:L:6:GLN:NE2	3:L:88:CYS:SG	2.82	0.52
2:I:29:PHE:C	2:I:31:SER:H	2.18	0.52
1:C:316:SER:OG	1:C:317:ASN:N	2.42	0.52
3:N:6:GLN:NE2	3:N:88:CYS:SG	2.82	0.52
1:A:332:ILE:CG2	1:A:333:THR:N	2.73	0.52
1:A:918:GLU:HG2	1:C:1128:VAL:CG2	2.39	0.52
1:C:389:ASP:CG	1:C:528:LYS:HG2	2.34	0.52
2:H:29:PHE:C	2:H:31:SER:H	2.18	0.52
1:A:694:ALA:C	1:A:695:TYR:CD1	2.87	0.52
1:A:762:GLN:NE2	1:C:965:GLN:HE21	2.06	0.52
1:B:898:PHE:N	1:B:899:PRO:CD	2.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:92:ASP:N	3:M:92:ASP:OD1	2.43	0.52
1:B:359:SER:OG	1:B:360:ASN:N	2.37	0.52
1:A:197:ILE:CD1	1:A:202:LYS:CD	2.87	0.51
1:A:230:PRO:HB2	1:C:522:ALA:O	2.09	0.51
1:B:321:GLN:CD	1:B:321:GLN:H	2.18	0.51
1:B:454:ARG:NH2	1:B:469:SER:O	2.44	0.51
1:A:293:LEU:O	1:A:293:LEU:HG	2.09	0.51
1:A:319:ARG:NH2	1:A:319:ARG:CB	2.73	0.51
1:A:328:ARG:HG3	1:A:533:LEU:HD13	1.92	0.51
1:C:332:ILE:CG2	1:C:333:THR:N	2.73	0.51
1:A:898:PHE:N	1:A:899:PRO:CD	2.73	0.51
1:B:319:ARG:HH11	1:C:740:MET:HE2	1.75	0.51
1:C:454:ARG:NH2	1:C:469:SER:O	2.43	0.51
2:J:29:PHE:C	2:J:31:SER:H	2.18	0.51
1:B:1079:PRO:HB3	1:C:917:TYR:CE1	2.46	0.51
1:B:854:LYS:NZ	1:B:854:LYS:CB	2.73	0.51
1:A:671:CYS:CB	1:A:695:TYR:CZ	2.87	0.51
1:B:319:ARG:HH21	1:B:319:ARG:HG3	1.76	0.51
1:A:295:PRO:HG2	1:A:608:VAL:HG21	1.92	0.51
1:C:898:PHE:N	1:C:899:PRO:CD	2.73	0.51
1:B:316:SER:OG	1:B:317:ASN:N	2.42	0.51
1:B:737:ASP:N	1:B:857:GLY:O	2.43	0.51
1:A:308:VAL:HG11	1:A:599:THR:HG21	1.93	0.51
1:A:454:ARG:NH2	1:A:469:SER:O	2.43	0.51
1:C:314:GLN:HA	1:C:596:SER:HA	1.93	0.51
1:A:1128:VAL:HG23	1:B:918:GLU:HG2	1.93	0.50
1:B:318:PHE:CE1	1:B:620:VAL:O	2.64	0.50
1:C:276:LEU:HD23	1:C:306:PHE:CE1	2.46	0.50
1:C:295:PRO:CD	1:C:296:LEU:H	2.25	0.50
1:A:200:TYR:CD1	1:A:200:TYR:N	2.73	0.50
1:B:324:GLU:OE2	2:I:84:LYS:CD	2.60	0.50
1:C:318:PHE:O	1:C:593:GLY:N	2.44	0.50
1:A:319:ARG:CZ	1:A:319:ARG:CB	2.86	0.50
1:B:98:SER:OG	1:B:99:ASN:N	2.45	0.50
1:B:461:LEU:HB3	1:B:465:GLU:HB3	1.94	0.50
1:B:533:LEU:HD21	1:B:535:LYS:HE2	1.93	0.50
1:B:1094:VAL:HG23	1:C:900:MET:HE1	1.94	0.50
1:A:328:ARG:C	1:A:329:PHE:HD1	2.18	0.50
1:C:389:ASP:OD1	1:C:528:LYS:HA	2.11	0.50
3:L:92:ASP:OD1	3:L:92:ASP:N	2.43	0.50
1:A:332:ILE:HG23	1:A:333:THR:H	1.75	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:461:LEU:HB3	1:A:465:GLU:HB3	1.94	0.50
1:B:534:VAL:HG21	1:B:539:VAL:HG11	1.93	0.50
1:A:294:ASP:OD1	1:A:294:ASP:N	2.41	0.50
1:A:599:THR:C	1:A:601:GLY:H	2.20	0.50
1:B:326:ILE:C	1:B:327:VAL:HG23	2.37	0.50
1:B:690:GLN:C	1:B:691:SER:HG	2.07	0.50
1:A:98:SER:OG	1:A:99:ASN:N	2.45	0.50
2:I:100:LYS:O	2:I:100:LYS:HG2	2.12	0.50
1:A:442:ASP:OD2	1:A:509:ARG:NE	2.41	0.50
1:A:690:GLN:O	1:A:691:SER:HB2	2.12	0.50
2:J:100:LYS:O	2:J:100:LYS:HG2	2.12	0.50
2:J:40:ALA:HB3	2:J:43:LYS:HB2	1.94	0.49
1:B:694:ALA:O	1:B:695:TYR:HB3	2.12	0.49
1:C:461:LEU:HB3	1:C:465:GLU:HB3	1.94	0.49
1:C:675:GLN:HA	1:C:675:GLN:NE2	2.26	0.49
3:M:6:GLN:HG3	3:M:100:PRO:HD2	1.95	0.49
1:A:287:ASP:HB3	1:A:306:PHE:CE2	2.42	0.49
1:A:1094:VAL:HG23	1:B:900:MET:HE1	1.93	0.49
1:C:334:ASN:ND2	1:C:360:ASN:O	2.45	0.49
1:A:326:ILE:O	1:A:327:VAL:HG22	2.13	0.49
1:A:1128:VAL:HG21	1:B:918:GLU:HG2	1.93	0.49
1:B:328:ARG:HH22	1:B:580:GLN:CD	2.19	0.49
1:B:643:PHE:CE1	1:B:655:TYR:CD2	3.01	0.49
1:C:333:THR:C	1:C:334:ASN:O	2.55	0.49
2:H:17:SER:HA	2:H:83:MET:O	2.13	0.49
1:B:316:SER:O	1:B:595:VAL:N	2.28	0.49
1:C:320:VAL:HG12	1:C:591:SER:O	2.13	0.49
1:C:331:ASN:O	1:C:332:ILE:HD13	2.12	0.49
1:C:643:PHE:CE1	1:C:655:TYR:CD2	3.01	0.49
1:C:744:GLY:O	1:C:745:ASP:HB2	2.13	0.49
3:L:6:GLN:HG3	3:L:100:PRO:HD2	1.95	0.49
1:B:237:ARG:NH1	2:I:102:SER:OG	2.46	0.49
1:B:338:PHE:HB3	1:B:342:PHE:HD2	1.78	0.49
1:B:705:VAL:HG11	1:C:883:THR:OG1	2.13	0.49
1:C:690:GLN:O	1:C:691:SER:HB2	2.11	0.49
2:H:100:LYS:O	2:H:100:LYS:HG2	2.12	0.49
1:A:326:ILE:C	1:A:327:VAL:CG2	2.85	0.49
1:A:332:ILE:C	1:A:333:THR:CG2	2.86	0.49
1:C:338:PHE:HB3	1:C:342:PHE:HD2	1.78	0.49
1:A:866:THR:CG2	1:C:646:ARG:NH2	2.54	0.49
1:A:319:ARG:NH2	1:A:319:ARG:CG	2.73	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:668:ALA:H	1:B:864:LEU:HA	1.78	0.48
2:H:101:ASP:O	2:H:102:SER:CB	2.61	0.48
1:A:237:ARG:NH1	2:H:102:SER:OG	2.46	0.48
1:B:744:GLY:O	1:B:745:ASP:HB2	2.13	0.48
2:J:17:SER:HA	2:J:83:MET:O	2.13	0.48
1:A:694:ALA:O	1:A:695:TYR:HB3	2.13	0.48
1:B:442:ASP:OD2	1:B:509:ARG:NE	2.41	0.48
1:C:331:ASN:C	1:C:332:ILE:HG12	2.39	0.48
2:I:17:SER:HA	2:I:83:MET:O	2.13	0.48
1:A:430:THR:O	1:A:430:THR:OG1	2.31	0.48
1:A:643:PHE:CE1	1:A:655:TYR:CD2	3.01	0.48
1:C:98:SER:OG	1:C:99:ASN:N	2.45	0.48
1:C:326:ILE:HD11	1:C:532:ASN:O	2.13	0.48
2:H:40:ALA:HB3	2:H:43:LYS:HB2	1.94	0.48
2:J:52:ARG:O	2:J:72:ARG:NH1	2.44	0.48
1:A:199:GLY:O	1:A:232:GLY:N	2.35	0.48
1:A:600:PRO:HG2	1:A:674:TYR:CD1	2.48	0.48
3:N:92:ASP:OD1	3:N:92:ASP:N	2.43	0.48
1:A:744:GLY:O	1:A:745:ASP:HB2	2.13	0.48
2:J:101:ASP:O	2:J:102:SER:CB	2.62	0.48
1:A:323:THR:HG22	1:A:324:GLU:OE1	2.13	0.48
1:A:1019:ARG:NH2	1:C:1017:GLU:CG	2.52	0.48
1:B:202:LYS:NZ	1:B:228:ASP:OD2	2.47	0.48
1:A:501:TYR:HB3	1:A:505:HIS:HB2	1.96	0.48
1:B:916:LEU:C	1:B:916:LEU:HD23	2.39	0.48
2:I:52:ARG:O	2:I:72:ARG:NH1	2.44	0.48
1:B:1082:CYS:SG	1:B:1132:ILE:HD13	2.54	0.48
1:A:916:LEU:C	1:A:916:LEU:HD23	2.39	0.47
1:A:1082:CYS:SG	1:A:1132:ILE:HD13	2.54	0.47
3:N:6:GLN:HG3	3:N:100:PRO:HD2	1.95	0.47
1:B:564:GLN:O	1:B:577:ARG:HB3	2.14	0.47
1:C:237:ARG:NH1	2:J:102:SER:OG	2.46	0.47
1:C:916:LEU:C	1:C:916:LEU:HD23	2.39	0.47
2:H:27:PHE:CD1	2:H:27:PHE:N	2.73	0.47
1:A:167:THR:CG2	1:C:357:ARG:HH22	2.20	0.47
1:A:202:LYS:NZ	1:A:228:ASP:OD2	2.47	0.47
1:C:202:LYS:NZ	1:C:228:ASP:OD2	2.47	0.47
1:C:1082:CYS:SG	1:C:1132:ILE:HD13	2.54	0.47
2:I:101:ASP:O	2:I:102:SER:CB	2.62	0.47
1:A:318:PHE:O	1:A:592:PHE:HA	2.14	0.47
1:B:319:ARG:NH2	1:B:319:ARG:CB	2.75	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:501:TYR:HB3	1:C:505:HIS:HB2	1.96	0.47
1:A:338:PHE:HB3	1:A:342:PHE:HD2	1.78	0.47
1:A:600:PRO:HG2	1:A:674:TYR:HD1	1.78	0.47
1:B:326:ILE:O	1:B:327:VAL:CG2	2.63	0.47
1:B:674:TYR:CD2	1:B:690:GLN:N	2.83	0.47
1:B:715:PRO:HD3	1:C:894:LEU:CD1	2.45	0.47
1:C:420:ASP:OD1	1:C:421:TYR:N	2.42	0.47
1:A:564:GLN:O	1:A:577:ARG:HB3	2.14	0.47
2:J:103:ARG:HH21	2:J:103:ARG:CG	2.18	0.47
1:A:667:GLY:CA	1:B:864:LEU:HD12	2.44	0.47
1:A:670:ILE:CG2	1:A:695:TYR:O	2.62	0.47
1:B:501:TYR:HB3	1:B:505:HIS:HB2	1.96	0.47
1:B:1123:SER:OG	1:C:914:ASN:ND2	2.47	0.47
2:I:40:ALA:HB3	2:I:43:LYS:HB2	1.94	0.47
1:A:653:ALA:HA	1:A:692:ILE:O	2.14	0.47
1:B:854:LYS:NZ	1:B:854:LYS:HB3	2.30	0.47
1:A:201:PHE:C	1:A:202:LYS:HG3	2.39	0.47
1:A:599:THR:C	1:A:601:GLY:N	2.73	0.47
1:C:314:GLN:HA	1:C:596:SER:CA	2.44	0.47
1:A:328:ARG:O	1:A:329:PHE:CD1	2.62	0.46
1:B:675:GLN:CG	1:B:676:THR:H	2.18	0.46
1:C:237:ARG:NH1	2:J:108:TYR:HD1	2.14	0.46
1:A:706:ALA:HB1	6:A:1409:NAG:H5	1.97	0.46
1:B:324:GLU:OE2	2:I:84:LYS:HG3	2.15	0.46
1:B:327:VAL:O	1:B:327:VAL:HG12	2.15	0.46
1:B:529:LYS:O	1:B:530:SER:HB3	2.15	0.46
1:B:675:GLN:C	1:B:676:THR:HG23	2.39	0.46
1:A:232:GLY:HA2	1:C:519:HIS:CD2	2.50	0.46
1:B:521:PRO:HG3	1:C:200:TYR:CE2	2.46	0.46
1:C:607:GLN:O	1:C:608:VAL:HG13	2.15	0.46
1:A:582:LEU:HD11	5:E:1:NAG:H83	1.96	0.46
1:B:706:ALA:HB1	6:B:1409:NAG:H5	1.97	0.46
6:B:1409:NAG:O4	6:B:1410:NAG:O5	2.28	0.46
2:H:35:HIS:HE1	3:L:96:PHE:HE2	1.64	0.46
2:H:52:ARG:O	2:H:72:ARG:NH1	2.44	0.46
1:A:112:SER:C	1:A:113:LYS:HG2	2.39	0.46
1:B:328:ARG:HE	1:B:533:LEU:HD12	1.80	0.46
1:B:420:ASP:OD1	1:B:421:TYR:N	2.42	0.46
2:J:35:HIS:HE1	3:N:96:PHE:HE2	1.64	0.46
1:A:527:PRO:O	1:A:529:LYS:N	2.44	0.46
1:B:569:ILE:O	1:B:570:ALA:HB3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:569:ILE:O	1:C:570:ALA:HB3	2.16	0.46
1:A:607:GLN:O	1:A:608:VAL:HG13	2.15	0.46
1:B:237:ARG:NH1	2:I:108:TYR:HD1	2.14	0.46
1:B:314:GLN:HA	1:B:596:SER:HB2	1.98	0.46
1:B:607:GLN:O	1:B:608:VAL:HG13	2.15	0.46
1:B:671:CYS:HB2	1:B:695:TYR:HE1	1.75	0.46
1:C:312:ILE:HD12	1:C:665:PRO:O	2.15	0.46
1:A:200:TYR:CG	1:C:521:PRO:HG3	2.51	0.46
1:A:237:ARG:NH1	2:H:108:TYR:HD1	2.14	0.46
1:B:331:ASN:O	1:B:332:ILE:HD13	2.16	0.46
1:B:597:VAL:CG1	1:B:608:VAL:HB	2.45	0.46
1:C:564:GLN:O	1:C:577:ARG:HB3	2.14	0.46
1:A:420:ASP:OD1	1:A:421:TYR:N	2.42	0.46
1:B:296:LEU:C	1:B:298:GLU:N	2.73	0.46
1:B:318:PHE:O	1:B:592:PHE:HA	2.15	0.46
1:B:336:CYS:HB3	1:B:361:CYS:HB3	1.83	0.46
1:B:398:ASP:OD2	1:B:423:TYR:OH	2.32	0.46
1:A:89:GLY:HA2	1:A:194:PHE:O	2.17	0.45
1:B:319:ARG:NH2	1:B:319:ARG:CG	2.77	0.45
1:B:329:PHE:CB	1:B:330:PRO:HD2	2.46	0.45
2:H:83:MET:HE1	2:H:118:VAL:HG11	1.98	0.45
1:A:569:ILE:O	1:A:570:ALA:HB3	2.16	0.45
1:B:669:GLY:N	1:C:864:LEU:O	2.49	0.45
1:C:89:GLY:HA2	1:C:194:PHE:O	2.17	0.45
1:B:89:GLY:HA2	1:B:194:PHE:O	2.16	0.45
1:C:295:PRO:CG	1:C:296:LEU:N	2.79	0.45
1:A:542:ASN:HA	1:A:546:LEU:O	2.17	0.45
1:B:430:THR:O	1:B:430:THR:OG1	2.32	0.45
1:B:527:PRO:O	1:B:528:LYS:HG3	2.17	0.45
2:J:83:MET:HE1	2:J:118:VAL:HG11	1.98	0.45
1:A:60:SER:OG	1:A:61:ASN:N	2.50	0.45
1:A:394:ASN:OD1	1:A:394:ASN:N	2.49	0.45
1:A:438:SER:O	1:A:438:SER:OG	2.31	0.45
1:A:558:LYS:O	1:B:43:PHE:CE1	2.70	0.45
2:I:35:HIS:HE1	3:M:96:PHE:HE2	1.64	0.45
2:I:100:LYS:O	2:I:101:ASP:O	2.35	0.45
1:A:702:GLU:OE2	1:B:790:LYS:NZ	2.45	0.45
1:B:413:GLY:O	1:B:414:GLN:NE2	2.50	0.45
1:C:299:THR:OG1	1:C:597:VAL:HB	2.17	0.45
2:H:100:LYS:O	2:H:101:ASP:O	2.35	0.45
1:B:559:PHE:HE2	1:B:565:PHE:HA	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:323:THR:HG22	1:A:324:GLU:N	2.30	0.45
1:B:321:GLN:CD	1:B:321:GLN:N	2.73	0.45
1:B:331:ASN:O	1:B:332:ILE:HG12	2.15	0.45
1:B:1094:VAL:CG2	1:C:900:MET:HE1	2.47	0.45
1:C:398:ASP:OD2	1:C:423:TYR:OH	2.32	0.45
1:C:542:ASN:HA	1:C:546:LEU:O	2.17	0.45
1:C:559:PHE:HE2	1:C:565:PHE:HA	1.82	0.45
1:A:918:GLU:HG2	1:C:1128:VAL:HG23	1.99	0.45
1:A:986:PRO:HB2	1:A:987:PRO:HD3	1.99	0.45
1:B:328:ARG:O	1:B:329:PHE:CD2	2.70	0.45
1:B:328:ARG:NE	1:B:578:ASP:OD1	2.46	0.45
1:B:534:VAL:CG2	1:B:539:VAL:HG11	2.47	0.45
1:B:715:PRO:HD3	1:C:894:LEU:HD13	1.98	0.45
1:C:986:PRO:HB2	1:C:987:PRO:HD3	1.99	0.45
1:B:314:GLN:HA	1:B:596:SER:HA	1.98	0.44
1:A:270:LEU:O	2:H:53:TYR:OH	2.35	0.44
1:B:531:THR:CG2	1:B:532:ASN:N	2.80	0.44
1:B:854:LYS:O	1:B:855:PHE:CD1	2.70	0.44
1:C:60:SER:OG	1:C:61:ASN:N	2.50	0.44
1:C:413:GLY:O	1:C:414:GLN:NE2	2.50	0.44
1:A:312:ILE:CG1	1:A:598:ILE:HG12	2.30	0.44
1:A:528:LYS:HB3	1:A:528:LYS:HE3	1.80	0.44
1:B:60:SER:OG	1:B:61:ASN:N	2.50	0.44
1:C:327:VAL:HB	1:C:531:THR:OG1	2.18	0.44
1:A:197:ILE:HD11	1:A:202:LYS:CE	2.48	0.44
1:B:318:PHE:O	1:B:318:PHE:CD2	2.70	0.44
1:B:438:SER:O	1:B:438:SER:OG	2.31	0.44
1:B:542:ASN:HA	1:B:546:LEU:O	2.17	0.44
1:B:675:GLN:HB2	1:B:693:ILE:CD1	2.46	0.44
1:B:854:LYS:O	1:B:855:PHE:CG	2.70	0.44
1:C:365:TYR:O	1:C:368:LEU:HB2	2.17	0.44
1:C:706:ALA:HB1	6:C:1409:NAG:H5	1.97	0.44
2:J:103:ARG:HD2	2:J:103:ARG:HA	1.66	0.44
1:A:365:TYR:O	1:A:368:LEU:HB2	2.17	0.44
1:B:298:GLU:OE1	1:B:298:GLU:HA	2.16	0.44
1:B:718:PHE:CD1	1:B:718:PHE:C	2.96	0.44
1:B:986:PRO:HB2	1:B:987:PRO:HD3	1.99	0.44
1:C:422:ASN:HD21	1:C:454:ARG:H	1.66	0.44
1:B:565:PHE:O	1:C:42:VAL:HA	2.17	0.44
1:B:1126:CYS:SG	1:B:1132:ILE:HD13	2.58	0.44
1:C:293:LEU:HD12	1:C:293:LEU:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:712:ILE:O	1:C:1074:ASN:HA	2.18	0.44
1:A:699:LEU:HD22	1:B:873:TYR:OH	2.17	0.44
1:C:328:ARG:HB3	1:C:579:PRO:HD2	1.99	0.44
1:A:398:ASP:OD2	1:A:423:TYR:OH	2.32	0.44
1:A:527:PRO:C	1:A:529:LYS:N	2.76	0.44
1:B:365:TYR:O	1:B:368:LEU:HB2	2.17	0.44
1:B:854:LYS:CB	1:B:854:LYS:HZ2	2.30	0.44
1:C:613:GLN:H	1:C:613:GLN:HG2	1.48	0.44
2:H:101:ASP:O	2:H:102:SER:HB2	2.18	0.44
1:A:667:GLY:HA2	1:B:864:LEU:HD13	1.96	0.43
1:B:402:ILE:HD11	1:B:510:VAL:HG21	2.00	0.43
1:B:705:VAL:HG11	1:C:883:THR:CB	2.48	0.43
1:C:985:ASP:OD1	1:C:985:ASP:C	2.60	0.43
2:I:83:MET:HE1	2:I:118:VAL:HG11	1.98	0.43
2:I:101:ASP:O	2:I:102:SER:HB2	2.18	0.43
1:A:317:ASN:HA	1:A:594:GLY:HA2	1.98	0.43
1:A:702:GLU:OE2	1:B:790:LYS:CE	2.67	0.43
1:B:314:GLN:HA	1:B:596:SER:CA	2.49	0.43
1:C:402:ILE:HD11	1:C:510:VAL:HG21	2.00	0.43
2:I:29:PHE:C	2:I:31:SER:N	2.77	0.43
1:A:1126:CYS:SG	1:A:1132:ILE:HD13	2.58	0.43
1:B:270:LEU:O	2:I:53:TYR:OH	2.35	0.43
1:B:792:PRO:HA	1:B:793:PRO:HD3	1.91	0.43
1:A:541:PHE:CD1	1:A:541:PHE:C	2.97	0.43
1:A:718:PHE:CD1	1:A:718:PHE:C	2.96	0.43
1:A:985:ASP:OD1	1:A:985:ASP:C	2.60	0.43
1:C:328:ARG:HD2	1:C:328:ARG:HA	1.74	0.43
1:C:718:PHE:CD1	1:C:718:PHE:C	2.96	0.43
1:C:980:ILE:O	1:C:984:LEU:HB3	2.19	0.43
3:M:38:GLN:HB2	3:M:44:PRO:HB3	2.00	0.43
1:A:413:GLY:O	1:A:414:GLN:NE2	2.50	0.43
1:B:233:ILE:HD13	1:B:233:ILE:HA	1.87	0.43
1:B:318:PHE:O	1:B:318:PHE:CG	2.71	0.43
1:B:331:ASN:C	1:B:332:ILE:CG1	2.87	0.43
1:B:334:ASN:OD1	1:B:334:ASN:N	2.43	0.43
1:B:558:LYS:O	1:C:43:PHE:CE1	2.72	0.43
1:B:646:ARG:HH21	1:C:866:THR:CG2	2.16	0.43
1:B:712:ILE:O	1:B:1074:ASN:HA	2.18	0.43
3:L:38:GLN:HB2	3:L:44:PRO:HB3	2.00	0.43
5:O:1:NAG:H4	5:O:2:NAG:C7	2.49	0.43
1:A:336:CYS:HB3	1:A:361:CYS:HB3	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:402:ILE:HD11	1:A:510:VAL:HG21	2.00	0.43
1:A:592:PHE:CZ	1:B:854:LYS:HG2	2.53	0.43
1:A:712:ILE:O	1:A:1074:ASN:HA	2.18	0.43
1:B:985:ASP:C	1:B:985:ASP:OD1	2.60	0.43
1:C:318:PHE:HZ	1:C:619:GLU:O	2.00	0.43
1:C:541:PHE:CD1	1:C:541:PHE:C	2.97	0.43
2:H:29:PHE:C	2:H:31:SER:N	2.76	0.43
2:I:103:ARG:HA	2:I:103:ARG:HD2	1.66	0.43
2:J:100:LYS:O	2:J:101:ASP:O	2.35	0.43
1:A:233:ILE:HD13	1:A:233:ILE:HA	1.87	0.43
1:A:1094:VAL:CG2	1:B:900:MET:HE1	2.49	0.43
1:C:317:ASN:HA	1:C:594:GLY:HA2	2.01	0.43
1:C:332:ILE:CG2	1:C:362:VAL:CG2	2.81	0.43
1:C:1126:CYS:SG	1:C:1132:ILE:HD13	2.58	0.43
3:N:38:GLN:HB2	3:N:44:PRO:HB3	2.00	0.43
1:A:324:GLU:HG3	2:H:84:LYS:HD2	2.00	0.43
1:A:326:ILE:C	1:A:327:VAL:HG23	2.43	0.43
1:A:528:LYS:O	1:A:529:LYS:HG2	2.18	0.43
5:c:1:NAG:H4	5:c:2:NAG:C7	2.49	0.43
1:A:331:ASN:O	1:A:332:ILE:HG12	2.19	0.43
1:A:559:PHE:HE2	1:A:565:PHE:HA	1.82	0.43
1:B:457:ARG:NH1	1:B:460:ASN:O	2.52	0.43
1:B:541:PHE:CD1	1:B:541:PHE:C	2.97	0.43
1:B:695:TYR:CD1	1:B:695:TYR:O	2.70	0.43
1:B:980:ILE:O	1:B:984:LEU:HB3	2.18	0.43
1:C:379:CYS:HB2	1:C:384:PRO:HG3	2.01	0.43
2:H:12:VAL:HG11	2:H:86:LEU:HD12	2.01	0.43
1:A:422:ASN:HD21	1:A:454:ARG:H	1.66	0.42
1:A:613:GLN:H	1:A:613:GLN:HG2	1.48	0.42
2:I:103:ARG:HH21	2:I:103:ARG:CG	2.18	0.42
2:J:101:ASP:O	2:J:102:SER:HB2	2.18	0.42
1:A:188:ASN:OD1	1:A:188:ASN:N	2.52	0.42
1:B:613:GLN:H	1:B:613:GLN:HG2	1.48	0.42
1:C:188:ASN:OD1	1:C:188:ASN:N	2.52	0.42
1:C:295:PRO:HG2	1:C:296:LEU:N	2.34	0.42
1:A:333:THR:O	1:A:334:ASN:C	2.63	0.42
1:A:980:ILE:O	1:A:984:LEU:HB3	2.19	0.42
1:B:961:THR:HG21	1:C:762:GLN:NE2	2.34	0.42
1:C:295:PRO:CG	1:C:296:LEU:H	2.33	0.42
1:C:394:ASN:OD1	1:C:394:ASN:N	2.49	0.42
2:H:22:CYS:HB3	2:H:79:LEU:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:22:CYS:HB3	2:I:79:LEU:HB2	2.02	0.42
3:N:19:VAL:HG23	3:N:78:LEU:HD11	2.01	0.42
5:V:1:NAG:H4	5:V:2:NAG:C7	2.49	0.42
1:A:690:GLN:O	1:A:691:SER:CB	2.66	0.42
1:B:379:CYS:HB2	1:B:384:PRO:HG3	2.01	0.42
1:C:318:PHE:CE2	1:C:615:VAL:HG11	2.55	0.42
1:B:560:LEU:HB2	1:B:563:GLN:OE1	2.20	0.42
1:C:112:SER:C	1:C:113:LYS:HG2	2.39	0.42
1:C:336:CYS:HB3	1:C:361:CYS:HB3	1.83	0.42
1:C:898:PHE:HB3	1:C:899:PRO:HD3	2.01	0.42
2:I:12:VAL:HG11	2:I:86:LEU:HD12	2.01	0.42
1:A:669:GLY:O	1:A:696:THR:HA	2.19	0.42
1:A:792:PRO:HA	1:A:793:PRO:HD3	1.91	0.42
1:C:270:LEU:O	2:J:53:TYR:OH	2.35	0.42
1:C:607:GLN:C	1:C:608:VAL:HG13	2.45	0.42
1:C:129:LYS:HG2	1:C:131:CYS:SG	2.59	0.42
2:H:103:ARG:HD2	2:H:103:ARG:HA	1.66	0.42
3:L:19:VAL:HG23	3:L:78:LEU:HD11	2.01	0.42
1:A:129:LYS:HG2	1:A:131:CYS:SG	2.59	0.42
1:C:457:ARG:NH1	1:C:460:ASN:O	2.52	0.42
6:C:1409:NAG:O4	6:C:1410:NAG:O5	2.28	0.42
1:A:216:LEU:HD23	1:A:216:LEU:HA	1.92	0.42
1:B:188:ASN:OD1	1:B:188:ASN:N	2.52	0.42
1:B:607:GLN:C	1:B:608:VAL:HG13	2.45	0.42
1:C:81:ASN:OD1	1:C:81:ASN:N	2.51	0.42
1:C:560:LEU:HB2	1:C:563:GLN:OE1	2.20	0.42
1:A:389:ASP:HB3	1:A:528:LYS:NZ	2.35	0.42
1:A:457:ARG:NH1	1:A:460:ASN:O	2.52	0.42
1:A:918:GLU:HG2	1:C:1128:VAL:HG21	2.01	0.42
1:A:986:PRO:N	1:A:987:PRO:CD	2.83	0.42
1:B:129:LYS:HG2	1:B:131:CYS:SG	2.60	0.42
2:H:20:LEU:HD23	2:H:20:LEU:HA	1.92	0.42
2:H:91:THR:HB	2:H:120:VAL:H	1.85	0.42
2:J:22:CYS:HB3	2:J:79:LEU:HB2	2.02	0.42
2:J:91:THR:HB	2:J:120:VAL:H	1.85	0.42
1:A:295:PRO:HG2	1:A:608:VAL:CG2	2.50	0.41
1:B:112:SER:C	1:B:113:LYS:HG2	2.39	0.41
1:B:310:LYS:HG2	1:B:664:ILE:HD11	2.02	0.41
1:B:532:ASN:HD22	1:B:532:ASN:HA	1.67	0.41
1:B:1102:TRP:HB2	1:B:1135:ASN:ND2	2.36	0.41
1:C:327:VAL:N	1:C:531:THR:OG1	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1102:TRP:HB2	1:A:1135:ASN:ND2	2.35	0.41
1:B:898:PHE:HB3	1:B:899:PRO:HD3	2.01	0.41
2:J:20:LEU:HD23	2:J:20:LEU:HA	1.92	0.41
2:J:101:ASP:HB3	2:J:102:SER:H	1.46	0.41
1:A:607:GLN:C	1:A:608:VAL:HG13	2.45	0.41
1:B:1141:LEU:CD2	1:C:1144:GLU:OE1	2.68	0.41
1:C:459:SER:OG	1:C:460:ASN:N	2.52	0.41
1:B:672:ALA:O	1:B:673:SER:OG	2.37	0.41
1:A:379:CYS:HB2	1:A:384:PRO:HG3	2.01	0.41
1:B:986:PRO:N	1:B:987:PRO:CD	2.83	0.41
1:C:233:ILE:HD13	1:C:233:ILE:HA	1.87	0.41
1:C:438:SER:O	1:C:438:SER:OG	2.31	0.41
1:C:504:GLY:O	1:C:505:HIS:ND1	2.54	0.41
1:A:663:ASP:CG	1:A:673:SER:HB3	2.45	0.41
1:B:276:LEU:HD23	1:B:306:PHE:HE1	1.86	0.41
1:B:422:ASN:HD21	1:B:454:ARG:H	1.66	0.41
1:C:1102:TRP:HB2	1:C:1135:ASN:ND2	2.36	0.41
1:A:504:GLY:O	1:A:505:HIS:ND1	2.54	0.41
1:A:898:PHE:HB3	1:A:899:PRO:HD3	2.01	0.41
1:B:329:PHE:HB3	1:B:330:PRO:CD	2.48	0.41
1:B:459:SER:OG	1:B:460:ASN:N	2.52	0.41
1:C:327:VAL:CB	1:C:530:SER:O	2.64	0.41
1:C:431:GLY:HA3	1:C:513:LEU:O	2.21	0.41
1:C:693:ILE:H	1:C:693:ILE:HG13	1.54	0.41
1:A:312:ILE:HD12	1:A:665:PRO:O	2.20	0.41
1:A:560:LEU:HB2	1:A:563:GLN:OE1	2.20	0.41
1:A:694:ALA:C	1:A:695:TYR:HD1	2.29	0.41
1:B:68:ILE:HG21	1:B:262:ALA:HA	2.03	0.41
1:B:431:GLY:HA3	1:B:513:LEU:O	2.21	0.41
1:C:792:PRO:HA	1:C:793:PRO:HD3	1.91	0.41
2:I:91:THR:HB	2:I:120:VAL:H	1.85	0.41
2:J:12:VAL:HG11	2:J:86:LEU:HD12	2.01	0.41
1:B:527:PRO:HB2	1:B:528:LYS:H	1.72	0.41
1:B:607:GLN:HE21	1:B:607:GLN:HB3	1.69	0.41
1:B:1090:PRO:O	1:C:913:GLN:NE2	2.54	0.41
1:C:68:ILE:HD12	1:C:68:ILE:HA	1.92	0.41
1:C:125:ASN:HD21	6:C:1402:NAG:H5	1.86	0.41
1:C:208:THR:HA	1:C:209:PRO:HD3	1.95	0.41
1:C:986:PRO:N	1:C:987:PRO:CD	2.83	0.41
2:I:100:LYS:O	2:I:100:LYS:CG	2.69	0.41
3:M:19:VAL:HG23	3:M:78:LEU:HD11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:29:PHE:C	2:J:31:SER:N	2.77	0.41
1:B:308:VAL:C	1:B:602:THR:CG2	2.78	0.41
1:B:504:GLY:O	1:B:505:HIS:ND1	2.54	0.41
1:C:295:PRO:O	1:C:298:GLU:HB3	2.21	0.41
1:C:331:ASN:O	1:C:332:ILE:CD1	2.69	0.41
1:C:675:GLN:O	1:C:690:GLN:N	2.54	0.41
1:B:690:GLN:O	1:B:690:GLN:HG2	2.21	0.40
1:C:68:ILE:HG21	1:C:262:ALA:HA	2.03	0.40
1:A:43:PHE:CD1	1:C:559:PHE:HA	2.57	0.40
1:A:125:ASN:HD21	6:A:1402:NAG:H5	1.86	0.40
1:A:198:ASP:CG	1:A:200:TYR:CE1	2.98	0.40
1:A:790:LYS:NZ	1:C:702:GLU:OE2	2.53	0.40
1:B:125:ASN:HD21	6:B:1402:NAG:H5	1.86	0.40
1:B:320:VAL:O	1:B:320:VAL:HG13	2.20	0.40
1:B:534:VAL:O	1:B:534:VAL:HG23	2.22	0.40
1:C:607:GLN:HE21	1:C:607:GLN:HB3	1.69	0.40
1:A:565:PHE:O	1:B:42:VAL:HA	2.21	0.40
1:B:1047:TYR:HB2	1:B:1067:TYR:HB3	2.04	0.40
1:C:329:PHE:CE2	1:C:528:LYS:HD3	2.56	0.40
1:A:459:SER:OG	1:A:460:ASN:N	2.52	0.40
1:C:56:LEU:HA	1:C:57:PRO:HD3	1.96	0.40
1:C:334:ASN:OD1	1:C:334:ASN:N	2.53	0.40
1:A:206:LYS:HB3	1:A:223:LEU:HD23	2.04	0.40
1:A:883:THR:CB	1:C:705:VAL:HG11	2.51	0.40
1:B:607:GLN:O	1:B:608:VAL:CG1	2.70	0.40
1:B:712:ILE:HA	1:C:895:GLN:O	2.21	0.40
1:C:607:GLN:O	1:C:608:VAL:CG1	2.70	0.40
1:C:645:THR:HG23	1:C:647:ALA:H	1.86	0.40
1:C:1047:TYR:HB2	1:C:1067:TYR:HB3	2.04	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	1007/1271 (79%)	907 (90%)	79 (8%)	21 (2%)	5	25
1	B	1007/1271 (79%)	909 (90%)	79 (8%)	19 (2%)	6	27
1	C	1007/1271 (79%)	919 (91%)	71 (7%)	17 (2%)	7	30
2	H	119/121 (98%)	107 (90%)	8 (7%)	4 (3%)	3	16
2	I	119/121 (98%)	107 (90%)	8 (7%)	4 (3%)	3	16
2	J	119/121 (98%)	107 (90%)	8 (7%)	4 (3%)	3	16
3	L	105/107 (98%)	99 (94%)	6 (6%)	0	100	100
3	M	105/107 (98%)	99 (94%)	6 (6%)	0	100	100
3	N	105/107 (98%)	99 (94%)	6 (6%)	0	100	100
All	All	3693/4497 (82%)	3353 (91%)	271 (7%)	69 (2%)	8	27

All (69) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	294	ASP
1	A	322	PRO
1	A	323	THR
1	A	325	SER
1	A	331	ASN
1	A	561	PRO
1	B	325	SER
1	B	331	ASN
1	B	333	THR
1	B	527	PRO
1	B	528	LYS
1	B	530	SER
1	B	561	PRO
1	B	858	LEU
1	B	859	THR
1	C	331	ASN
1	C	334	ASN
1	C	527	PRO
1	C	528	LYS
1	C	529	LYS
1	C	530	SER
1	C	561	PRO
1	C	591	SER
2	H	30	ASN
2	H	101	ASP
2	H	102	SER

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Mol	Chain	Res	Type
2	I	30	ASN
2	I	101	ASP
2	I	102	SER
2	J	30	ASN
2	J	101	ASP
2	J	102	SER
1	A	174	PRO
1	A	327	VAL
1	A	332	ILE
1	A	529	LYS
1	A	691	SER
1	B	174	PRO
1	B	324	GLU
1	B	327	VAL
1	B	591	SER
1	C	174	PRO
1	C	324	GLU
1	A	88	ASP
1	A	198	ASP
1	A	295	PRO
1	A	329	PHE
1	A	528	LYS
1	A	591	SER
1	B	88	ASP
1	C	88	ASP
1	C	294	ASP
1	C	326	ILE
1	C	691	SER
2	H	100	LYS
2	I	100	LYS
2	J	100	LYS
1	B	531	THR
1	B	691	SER
1	C	295	PRO
1	A	321	GLN
1	C	531	THR
1	A	527	PRO
1	B	332	ILE
1	B	294	ASP
1	A	326	ILE
1	A	742	ILE
1	B	742	ILE

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Mol	Chain	Res	Type
1	C	742	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	896/1111 (81%)	866 (97%)	30 (3%)	33	63
1	B	896/1111 (81%)	866 (97%)	30 (3%)	33	63
1	C	896/1111 (81%)	871 (97%)	25 (3%)	38	66
2	H	98/98 (100%)	94 (96%)	4 (4%)	27	59
2	I	98/98 (100%)	94 (96%)	4 (4%)	27	59
2	J	98/98 (100%)	94 (96%)	4 (4%)	27	59
3	L	94/94 (100%)	93 (99%)	1 (1%)	65	78
3	M	94/94 (100%)	93 (99%)	1 (1%)	65	78
3	N	94/94 (100%)	93 (99%)	1 (1%)	65	78
All	All	3264/3909 (84%)	3164 (97%)	100 (3%)	36	64

All (100) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	90	VAL
1	A	131	CYS
1	A	166	CYS
1	A	197	ILE
1	A	200	TYR
1	A	201	PHE
1	A	294	ASP
1	A	319	ARG
1	A	321	GLN
1	A	328	ARG
1	A	332	ILE
1	A	333	THR
1	A	382	VAL

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Mol	Chain	Res	Type
1	A	503	VAL
1	A	517	LEU
1	A	524	VAL
1	A	528	LYS
1	A	529	LYS
1	A	531	THR
1	A	561	PRO
1	A	577	ARG
1	A	588	THR
1	A	602	THR
1	A	605	SER
1	A	613	GLN
1	A	673	SER
1	A	676	THR
1	A	697	MET
1	A	698	SER
1	A	1074	ASN
1	B	90	VAL
1	B	131	CYS
1	B	166	CYS
1	B	294	ASP
1	B	299	THR
1	B	303	LEU
1	B	319	ARG
1	B	321	GLN
1	B	332	ILE
1	B	333	THR
1	B	334	ASN
1	B	503	VAL
1	B	517	LEU
1	B	524	VAL
1	B	528	LYS
1	B	529	LYS
1	B	532	ASN
1	B	533	LEU
1	B	561	PRO
1	B	577	ARG
1	B	591	SER
1	B	602	THR
1	B	613	GLN
1	B	673	SER
1	B	674	TYR

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Mol	Chain	Res	Type
1	B	690	GLN
1	B	695	TYR
1	B	854	LYS
1	B	856	ASN
1	B	1074	ASN
1	C	90	VAL
1	C	131	CYS
1	C	166	CYS
1	C	321	GLN
1	C	325	SER
1	C	328	ARG
1	C	382	VAL
1	C	503	VAL
1	C	517	LEU
1	C	524	VAL
1	C	529	LYS
1	C	561	PRO
1	C	577	ARG
1	C	588	THR
1	C	590	CYS
1	C	591	SER
1	C	613	GLN
1	C	673	SER
1	C	674	TYR
1	C	675	GLN
1	C	692	ILE
1	C	693	ILE
1	C	697	MET
1	C	698	SER
1	C	1074	ASN
2	H	27	PHE
2	H	28	THR
2	H	102	SER
2	H	103	ARG
3	L	92	ASP
2	I	27	PHE
2	I	28	THR
2	I	102	SER
2	I	103	ARG
3	M	92	ASP
2	J	27	PHE
2	J	28	THR

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Mol	Chain	Res	Type
2	J	102	SER
2	J	103	ARG
3	N	92	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (63) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	ASN
1	A	164	ASN
1	A	173	GLN
1	A	317	ASN
1	A	414	GLN
1	A	422	ASN
1	A	450	ASN
1	A	536	ASN
1	A	606	ASN
1	A	607	GLN
1	A	690	GLN
1	A	824	ASN
1	A	949	GLN
1	A	965	GLN
1	A	1083	HIS
1	B	30	ASN
1	B	164	ASN
1	B	173	GLN
1	B	414	GLN
1	B	422	ASN
1	B	450	ASN
1	B	519	HIS
1	B	532	ASN
1	B	536	ASN
1	B	607	GLN
1	B	913	GLN
1	B	949	GLN
1	B	965	GLN
1	B	1083	HIS
1	C	30	ASN
1	C	164	ASN
1	C	173	GLN
1	C	414	GLN
1	C	422	ASN
1	C	450	ASN

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Mol	Chain	Res	Type
1	C	519	HIS
1	C	536	ASN
1	C	607	GLN
1	C	762	GLN
1	C	787	GLN
1	C	913	GLN
1	C	949	GLN
1	C	965	GLN
1	C	1083	HIS
2	H	35	HIS
2	H	39	GLN
2	H	74	ASN
3	L	34	ASN
3	L	38	GLN
3	L	79	GLN
2	I	35	HIS
2	I	39	GLN
2	I	74	ASN
3	M	6	GLN
3	M	34	ASN
3	M	38	GLN
3	M	79	GLN
2	J	35	HIS
2	J	39	GLN
2	J	74	ASN
3	N	34	ASN
3	N	38	GLN
3	N	79	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 ⓘ

45 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	NAG	D	1	1,4	14,14,15	0.24	0	17,19,21	0.60	0
4	NAG	D	2	4	14,14,15	0.40	0	17,19,21	0.68	1 (5%)
4	NAG	D	3	4	14,14,15	0.43	0	17,19,21	0.57	0
5	NAG	E	1	5,1	14,14,15	0.33	0	17,19,21	0.43	0
5	NAG	E	2	5	14,14,15	0.38	0	17,19,21	0.51	0
5	NAG	F	1	5,1	14,14,15	0.18	0	17,19,21	0.84	1 (5%)
5	NAG	F	2	5	14,14,15	0.26	0	17,19,21	0.54	0
5	NAG	G	1	5,1	14,14,15	0.35	0	17,19,21	1.18	1 (5%)
5	NAG	G	2	5	14,14,15	0.23	0	17,19,21	0.46	0
5	NAG	K	1	5,1	14,14,15	0.31	0	17,19,21	0.70	1 (5%)
5	NAG	K	2	5	14,14,15	0.23	0	17,19,21	0.42	0
5	NAG	O	1	5,1	14,14,15	0.71	1 (7%)	17,19,21	0.92	1 (5%)
5	NAG	O	2	5	14,14,15	0.36	0	17,19,21	0.75	1 (5%)
5	NAG	P	1	5,1	14,14,15	0.21	0	17,19,21	0.45	0
5	NAG	P	2	5	14,14,15	0.28	0	17,19,21	0.39	0
4	NAG	Q	1	1,4	14,14,15	0.24	0	17,19,21	0.59	0
4	NAG	Q	2	4	14,14,15	0.41	0	17,19,21	0.68	1 (5%)
4	NAG	Q	3	4	14,14,15	0.44	0	17,19,21	0.58	0
5	NAG	R	1	5,1	14,14,15	0.35	0	17,19,21	0.44	0
5	NAG	R	2	5	14,14,15	0.38	0	17,19,21	0.51	0
5	NAG	S	1	5,1	14,14,15	0.17	0	17,19,21	0.84	1 (5%)
5	NAG	S	2	5	14,14,15	0.25	0	17,19,21	0.54	0
5	NAG	T	1	5,1	14,14,15	0.35	0	17,19,21	1.18	1 (5%)
5	NAG	T	2	5	14,14,15	0.26	0	17,19,21	0.48	0
5	NAG	U	1	5,1	14,14,15	0.32	0	17,19,21	0.71	1 (5%)
5	NAG	U	2	5	14,14,15	0.24	0	17,19,21	0.40	0
5	NAG	V	1	5,1	14,14,15	0.70	1 (7%)	17,19,21	0.91	1 (5%)
5	NAG	V	2	5	14,14,15	0.37	0	17,19,21	0.74	1 (5%)
5	NAG	W	1	5,1	14,14,15	0.20	0	17,19,21	0.46	0
5	NAG	W	2	5	14,14,15	0.30	0	17,19,21	0.40	0
4	NAG	X	1	1,4	14,14,15	0.23	0	17,19,21	0.59	0
4	NAG	X	2	4	14,14,15	0.38	0	17,19,21	0.68	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	X	3	4	14,14,15	0.44	0	17,19,21	0.57	0
5	NAG	Y	1	5,1	14,14,15	0.33	0	17,19,21	0.44	0
5	NAG	Y	2	5	14,14,15	0.37	0	17,19,21	0.51	0
5	NAG	Z	1	5,1	14,14,15	0.18	0	17,19,21	0.83	1 (5%)
5	NAG	Z	2	5	14,14,15	0.25	0	17,19,21	0.55	0
5	NAG	a	1	5,1	14,14,15	0.37	0	17,19,21	1.19	1 (5%)
5	NAG	a	2	5	14,14,15	0.24	0	17,19,21	0.47	0
5	NAG	b	1	5,1	14,14,15	0.29	0	17,19,21	0.70	1 (5%)
5	NAG	b	2	5	14,14,15	0.23	0	17,19,21	0.42	0
5	NAG	c	1	5,1	14,14,15	0.70	1 (7%)	17,19,21	0.91	1 (5%)
5	NAG	c	2	5	14,14,15	0.36	0	17,19,21	0.73	1 (5%)
5	NAG	d	1	5,1	14,14,15	0.21	0	17,19,21	0.46	0
5	NAG	d	2	5	14,14,15	0.29	0	17,19,21	0.40	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	D	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	D	2	4	-	0/6/23/26	0/1/1/1
4	NAG	D	3	4	-	2/6/23/26	0/1/1/1
5	NAG	E	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	E	2	5	-	0/6/23/26	0/1/1/1
5	NAG	F	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	F	2	5	-	2/6/23/26	0/1/1/1
5	NAG	G	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	G	2	5	-	0/6/23/26	0/1/1/1
5	NAG	K	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	K	2	5	-	0/6/23/26	0/1/1/1
5	NAG	O	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	O	2	5	-	0/6/23/26	0/1/1/1
5	NAG	P	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	P	2	5	-	0/6/23/26	0/1/1/1
4	NAG	Q	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	Q	2	4	-	0/6/23/26	0/1/1/1
4	NAG	Q	3	4	-	2/6/23/26	0/1/1/1
5	NAG	R	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	R	2	5	-	0/6/23/26	0/1/1/1

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

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	O	1	NAG	O5-C1	-2.57	1.39	1.43
5	c	1	NAG	O5-C1	-2.56	1.39	1.43
5	V	1	NAG	O5-C1	-2.53	1.39	1.43

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	a	1	NAG	C1-O5-C5	3.41	116.76	112.19
5	T	1	NAG	C1-O5-C5	3.38	116.71	112.19
5	G	1	NAG	C1-O5-C5	3.36	116.69	112.19
5	S	1	NAG	C1-O5-C5	2.82	115.96	112.19
5	F	1	NAG	C1-O5-C5	2.81	115.96	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	Z	1	NAG	C1-O5-C5	2.80	115.94	112.19
5	c	1	NAG	O4-C4-C3	-2.36	104.82	110.38
5	O	1	NAG	O4-C4-C3	-2.36	104.82	110.38
5	V	1	NAG	O4-C4-C3	-2.32	104.91	110.38
4	X	2	NAG	C1-O5-C5	2.29	115.25	112.19
4	D	2	NAG	C1-O5-C5	2.28	115.24	112.19
4	Q	2	NAG	C1-O5-C5	2.27	115.22	112.19
5	U	1	NAG	C1-O5-C5	2.26	115.22	112.19
5	b	1	NAG	C1-O5-C5	2.25	115.21	112.19
5	K	1	NAG	C1-O5-C5	2.23	115.18	112.19
5	O	2	NAG	C1-O5-C5	2.15	115.07	112.19
5	V	2	NAG	C1-O5-C5	2.10	115.00	112.19
5	c	2	NAG	C1-O5-C5	2.06	114.95	112.19

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	1	NAG	O5-C5-C6-O6
4	D	3	NAG	O5-C5-C6-O6
4	Q	1	NAG	O5-C5-C6-O6
4	Q	3	NAG	O5-C5-C6-O6
4	X	1	NAG	O5-C5-C6-O6
4	X	3	NAG	O5-C5-C6-O6
5	F	2	NAG	O5-C5-C6-O6
5	S	2	NAG	O5-C5-C6-O6
5	Z	2	NAG	O5-C5-C6-O6
5	E	1	NAG	O5-C5-C6-O6
5	R	1	NAG	O5-C5-C6-O6
5	Y	1	NAG	O5-C5-C6-O6
4	D	3	NAG	C4-C5-C6-O6
4	Q	3	NAG	C4-C5-C6-O6
4	X	3	NAG	C4-C5-C6-O6
4	D	1	NAG	C4-C5-C6-O6
4	Q	1	NAG	C4-C5-C6-O6
4	X	1	NAG	C4-C5-C6-O6
5	F	2	NAG	C4-C5-C6-O6
5	S	2	NAG	C4-C5-C6-O6
5	Z	2	NAG	C4-C5-C6-O6
5	E	1	NAG	C4-C5-C6-O6
5	R	1	NAG	C4-C5-C6-O6
5	Y	1	NAG	C4-C5-C6-O6

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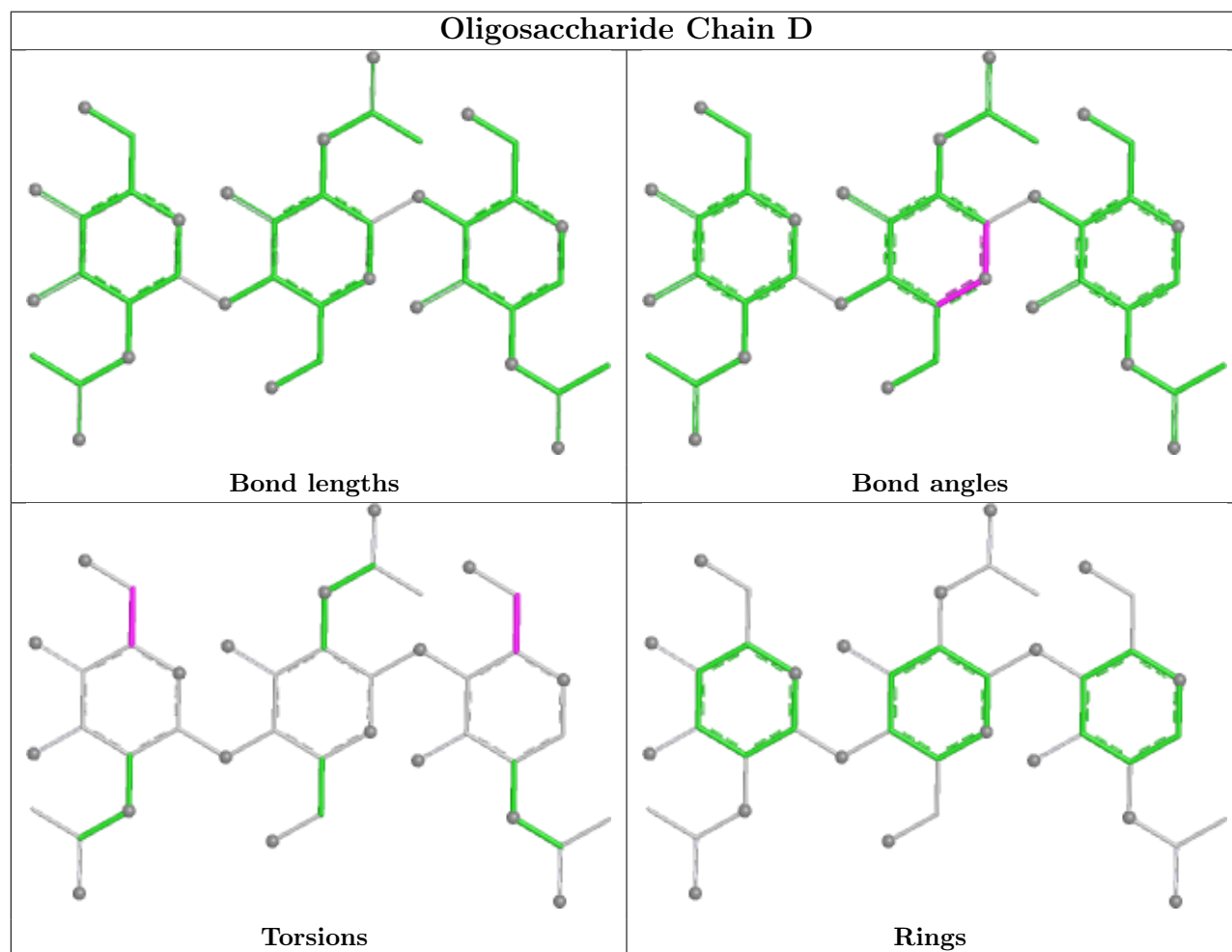
Mol	Chain	Res	Type	Atoms
5	Z	1	NAG	C4-C5-C6-O6

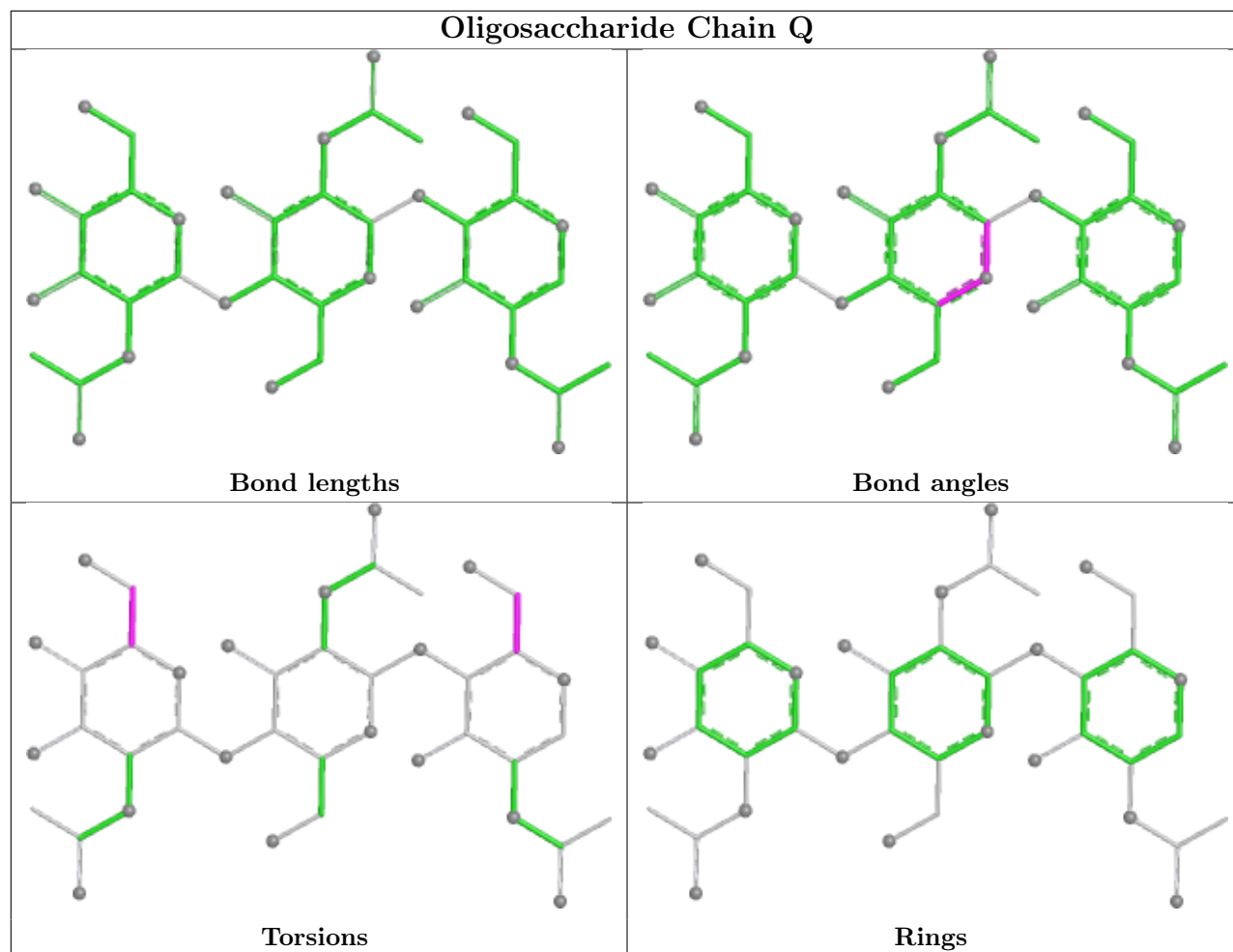
There are no ring outliers.

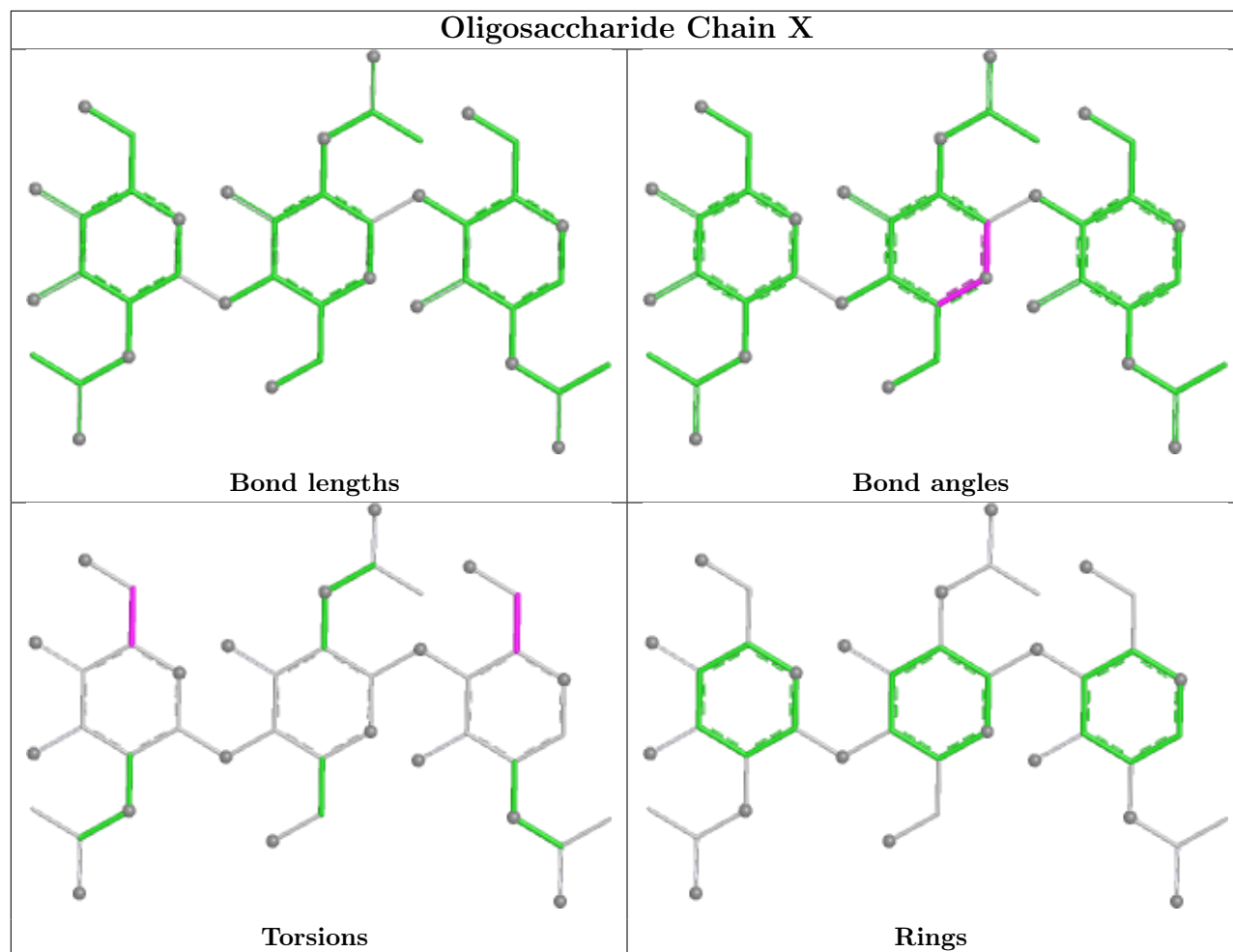
8 monomers are involved in 9 short contacts:

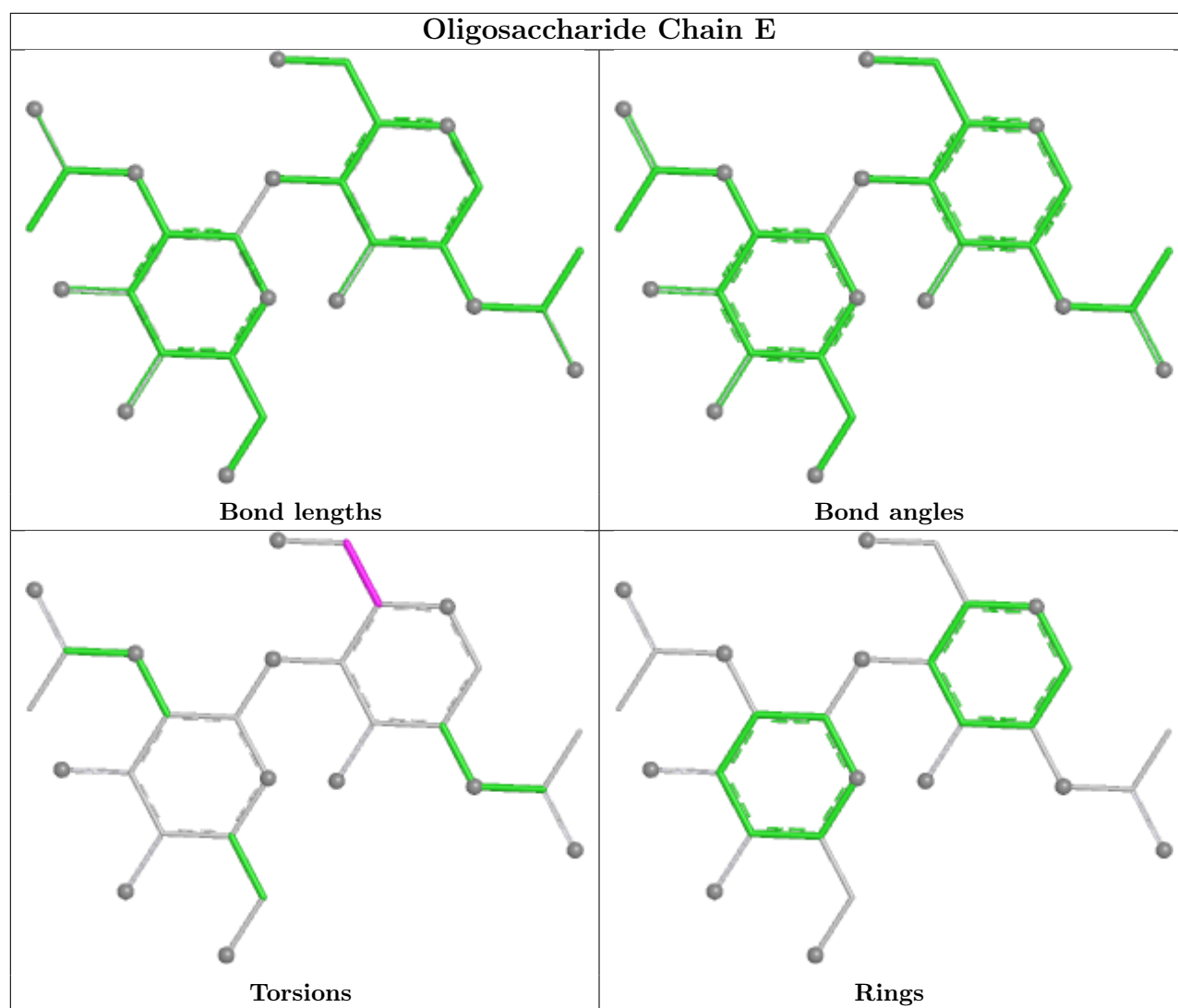
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	c	1	NAG	1	0
5	E	1	NAG	3	0
5	c	2	NAG	1	0
5	V	2	NAG	1	0
5	V	1	NAG	1	0
5	O	1	NAG	1	0
5	O	2	NAG	1	0
5	Y	1	NAG	3	0

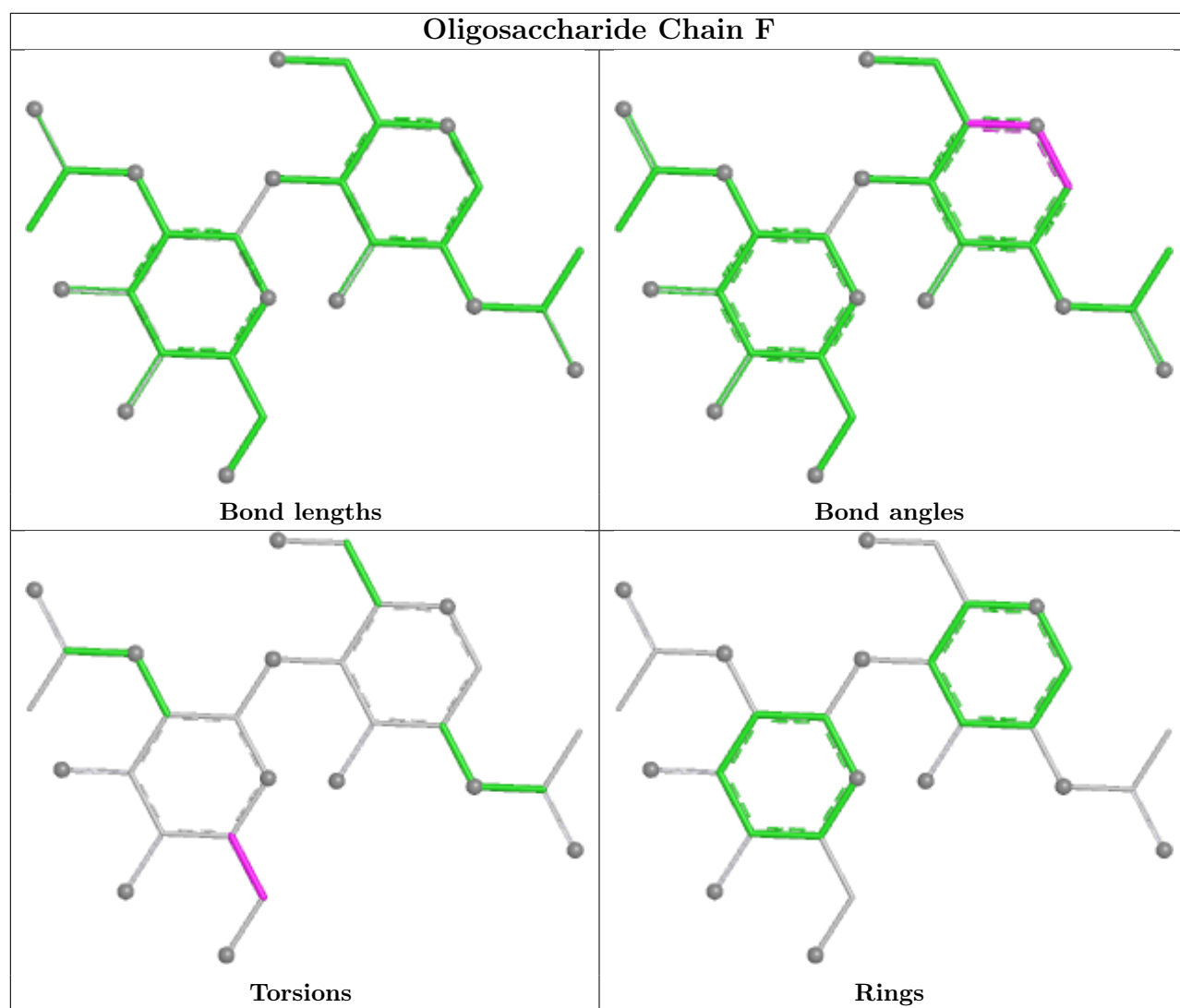
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

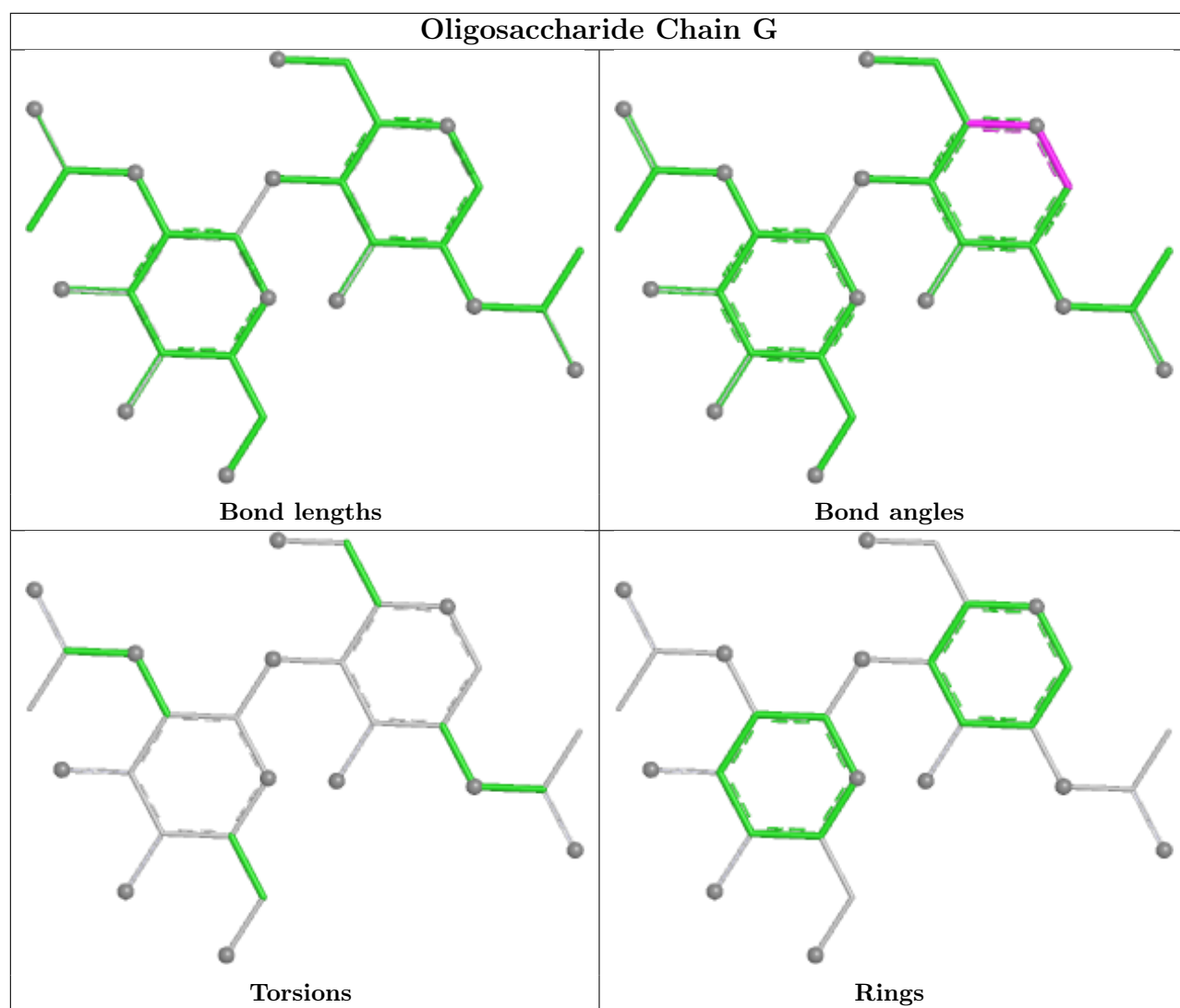


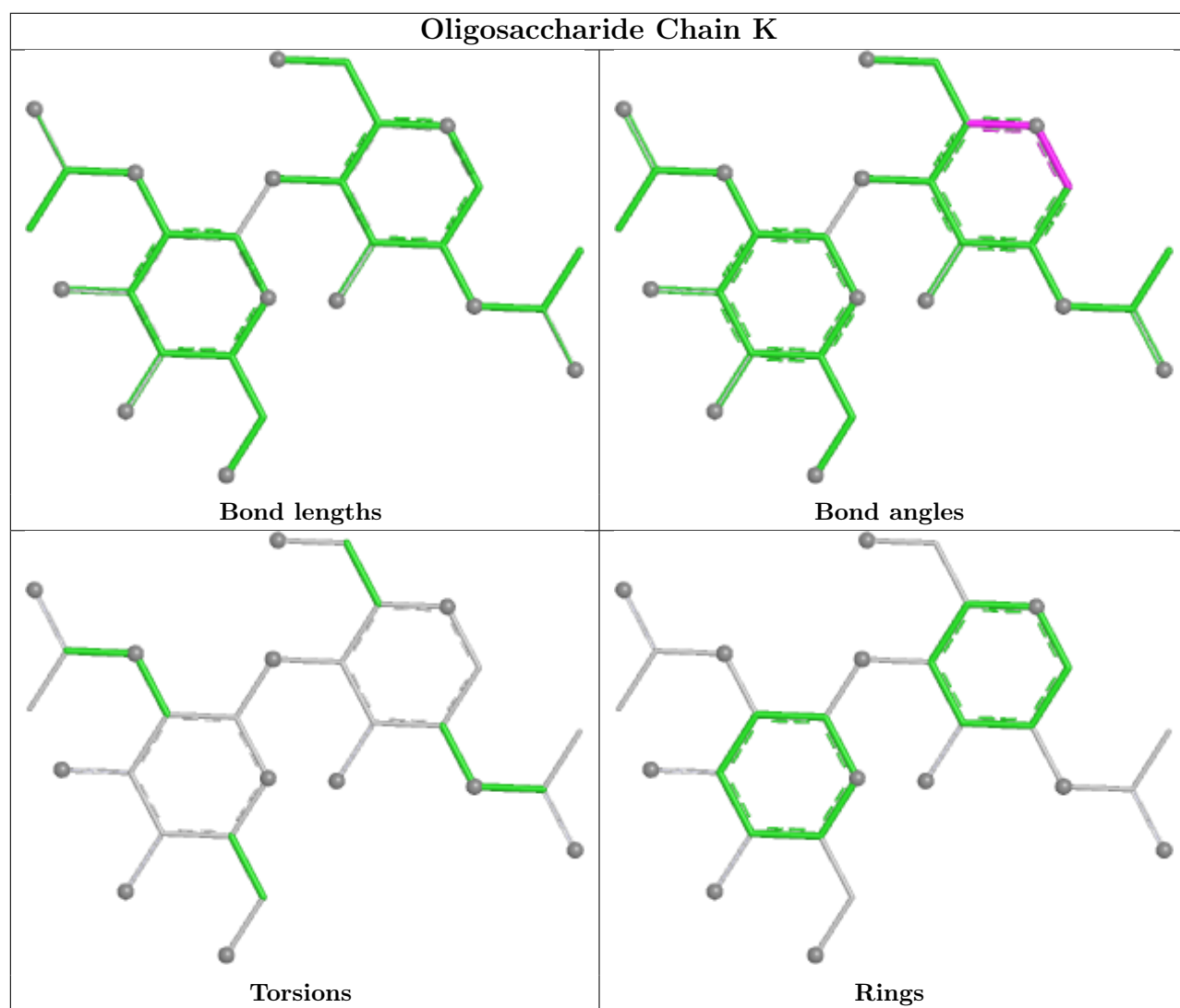


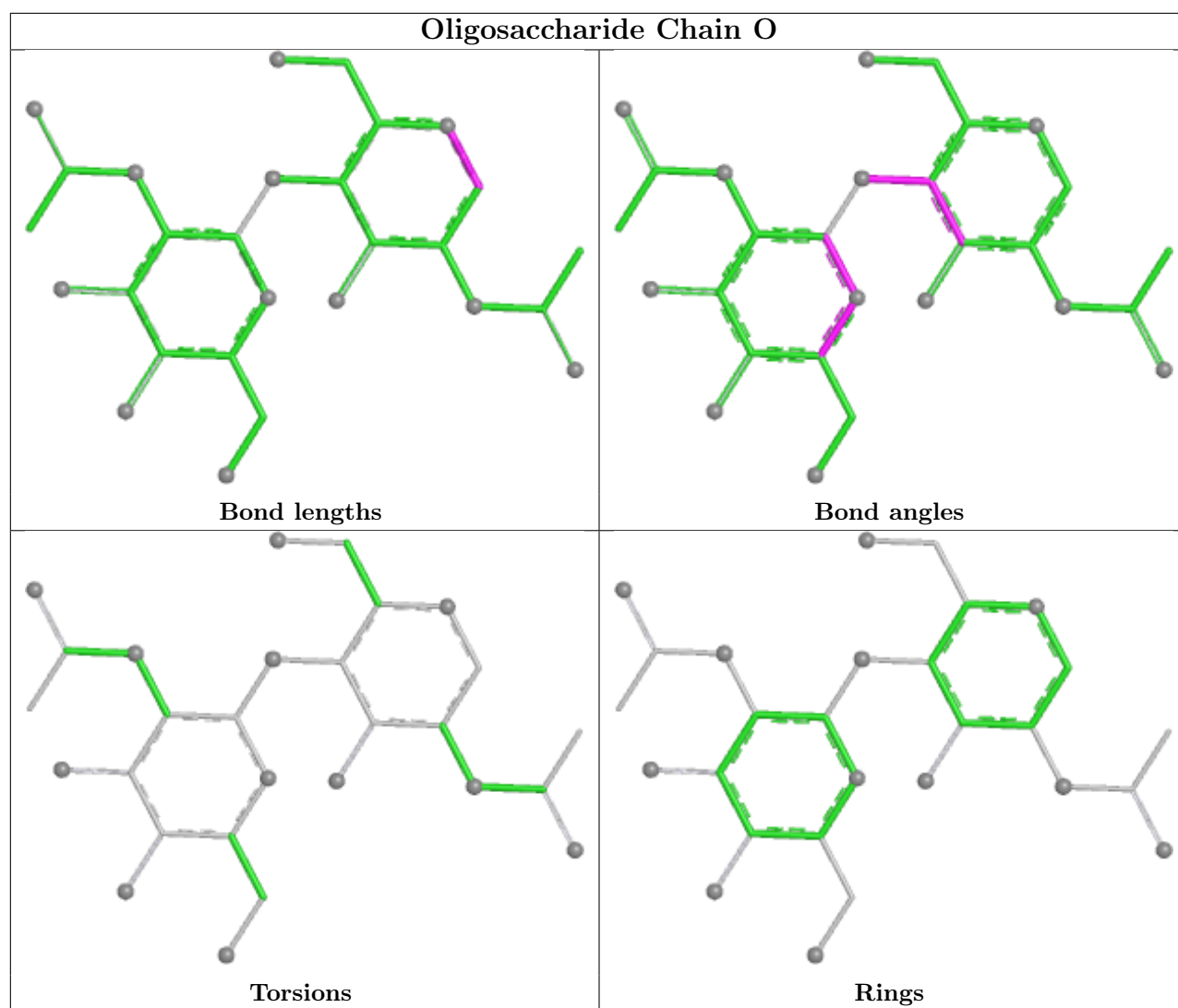


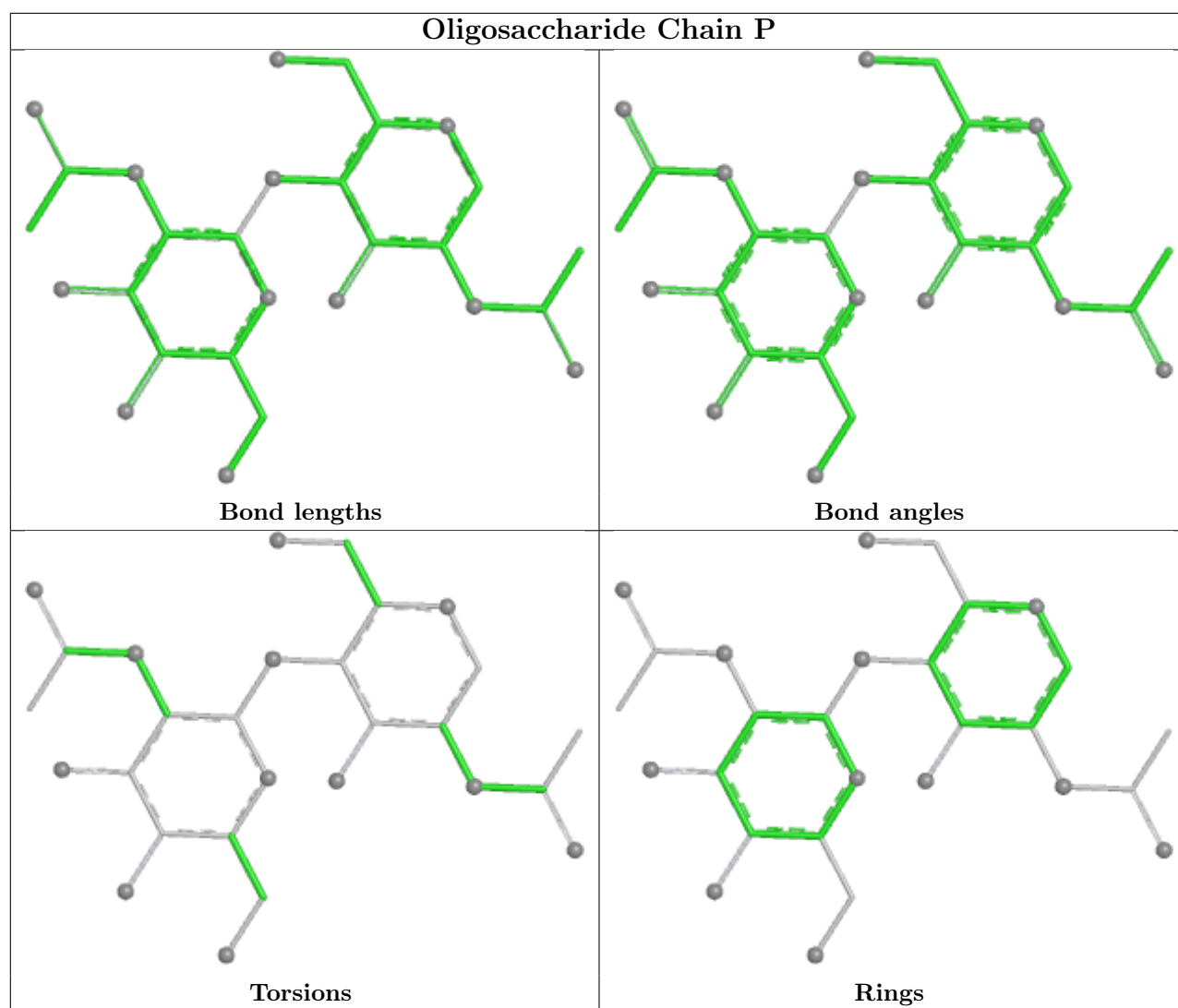


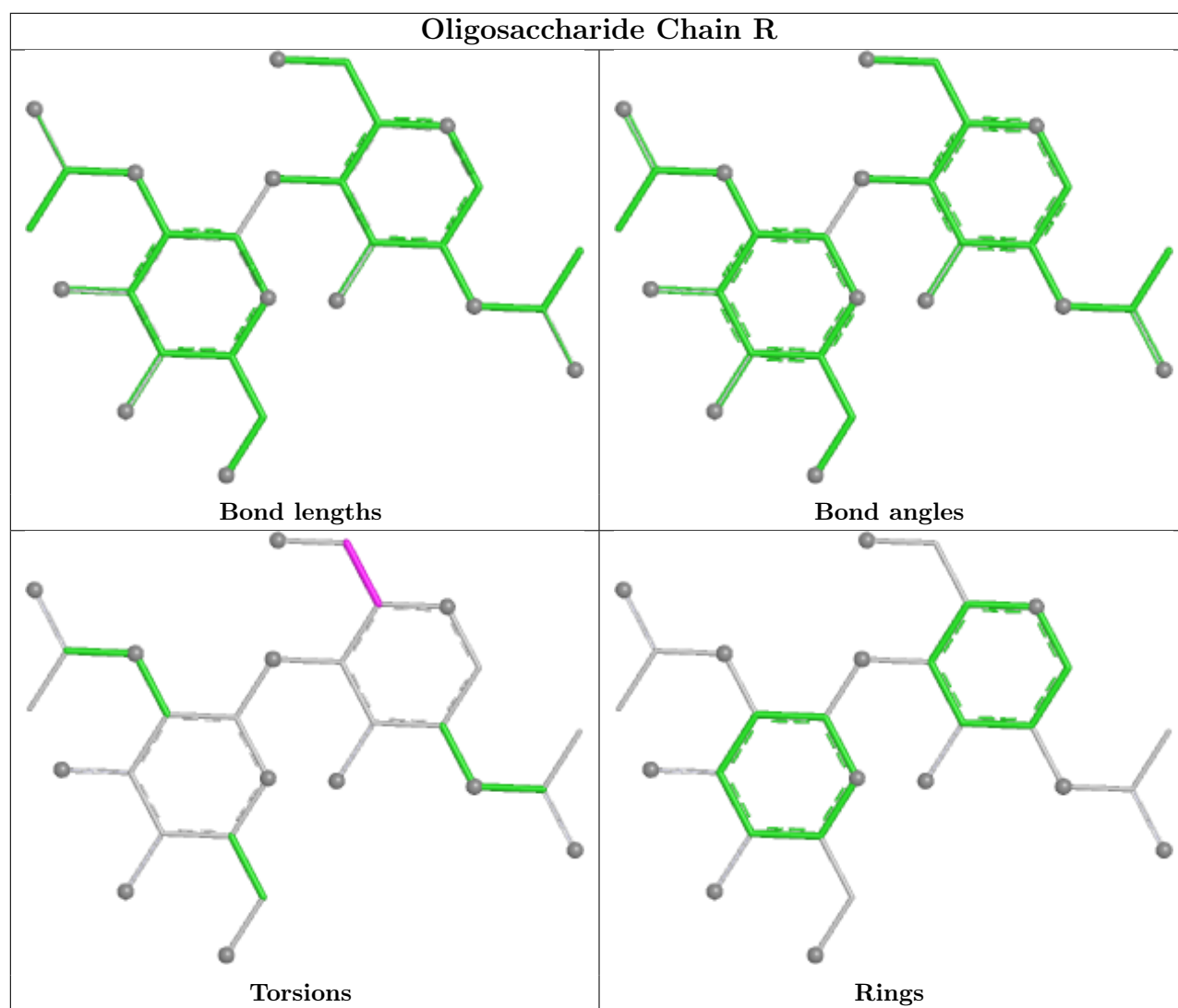


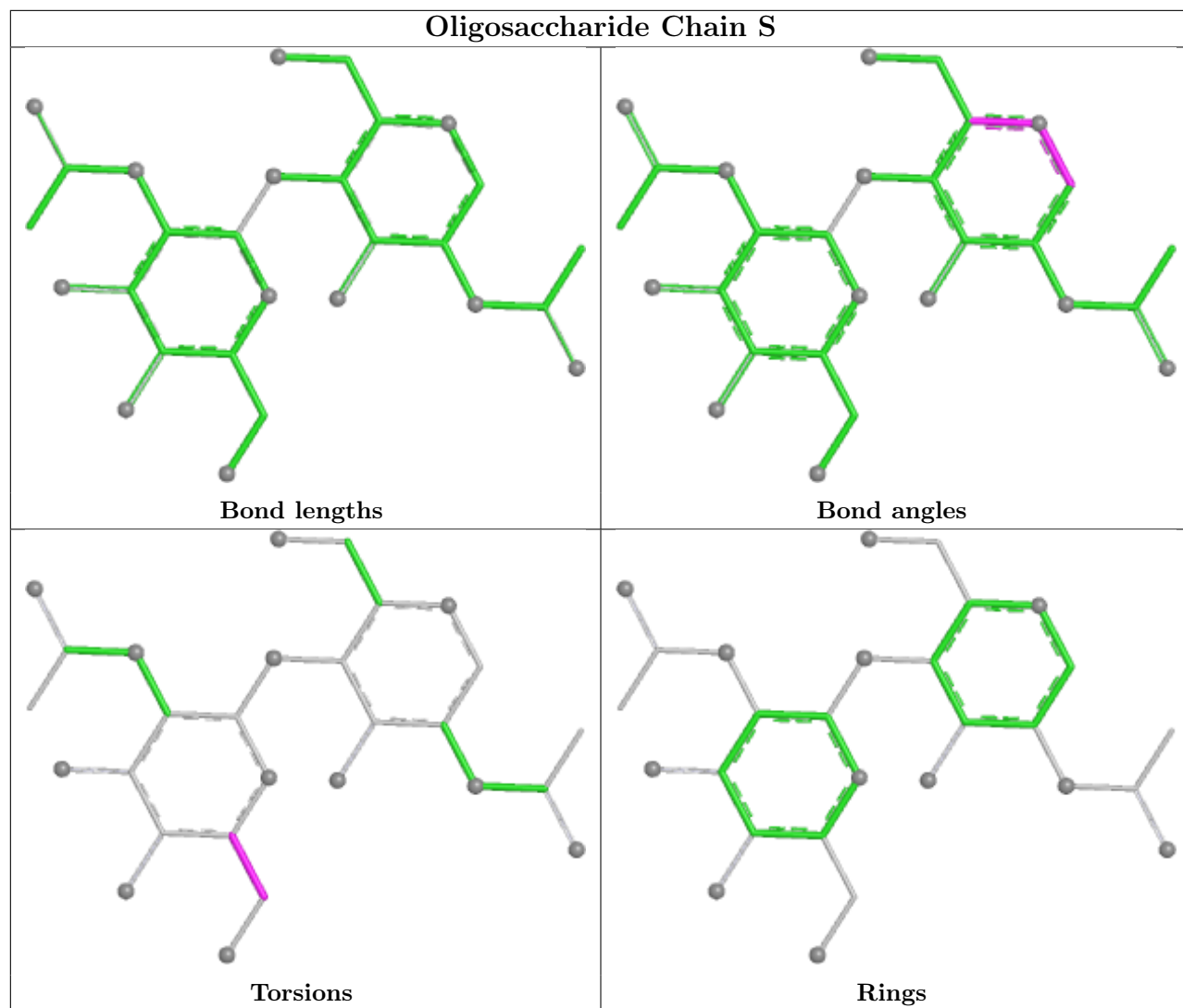


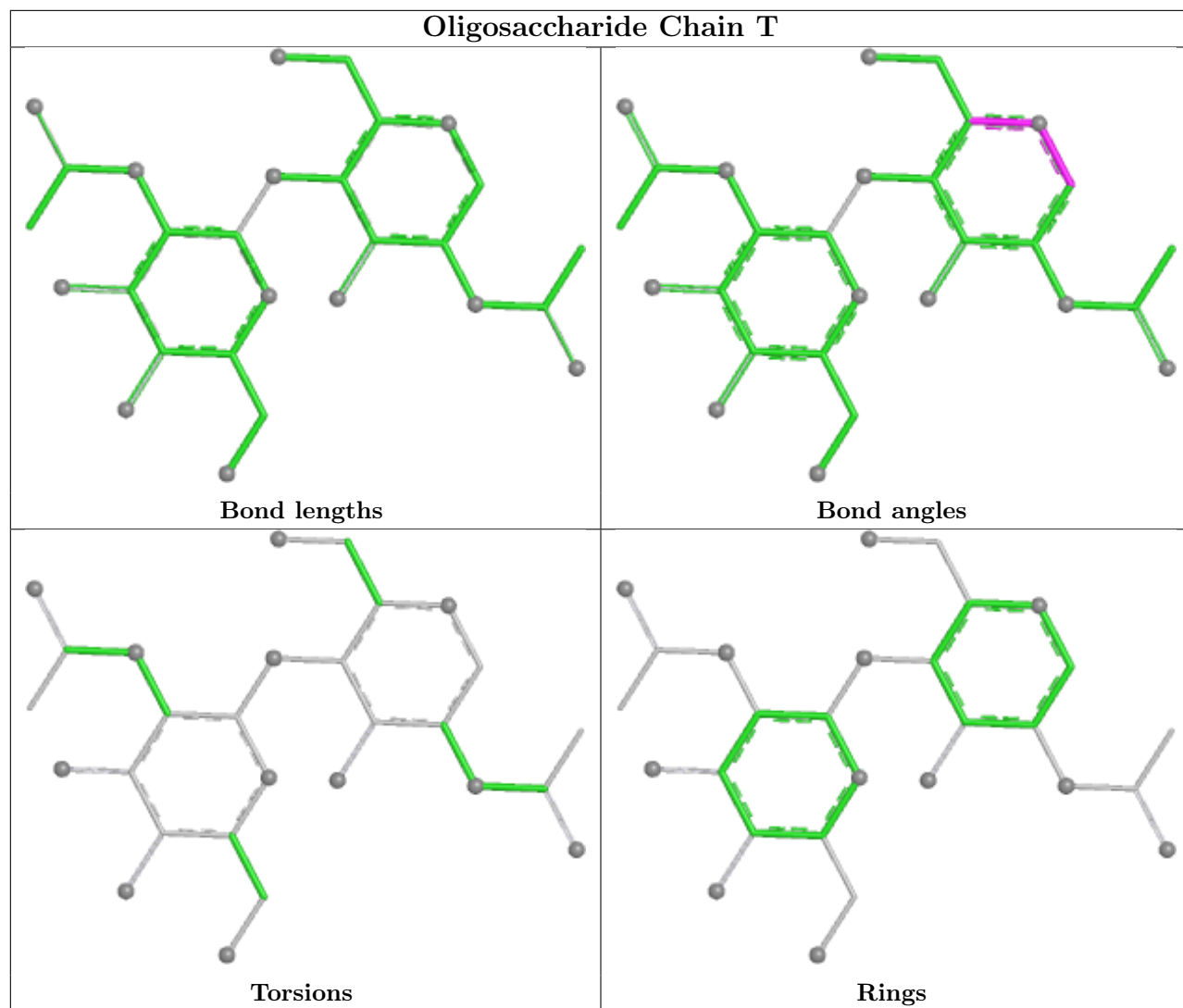


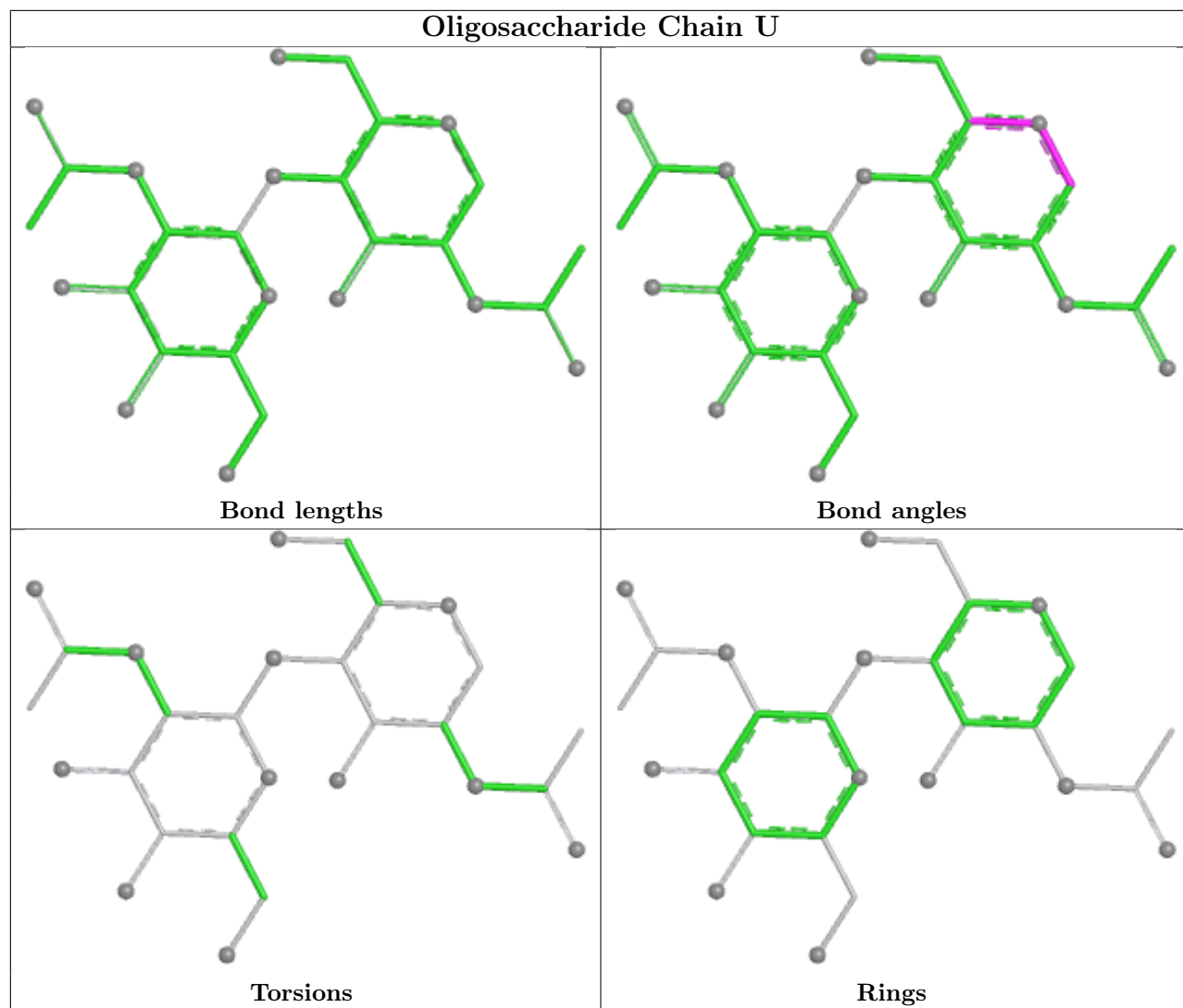


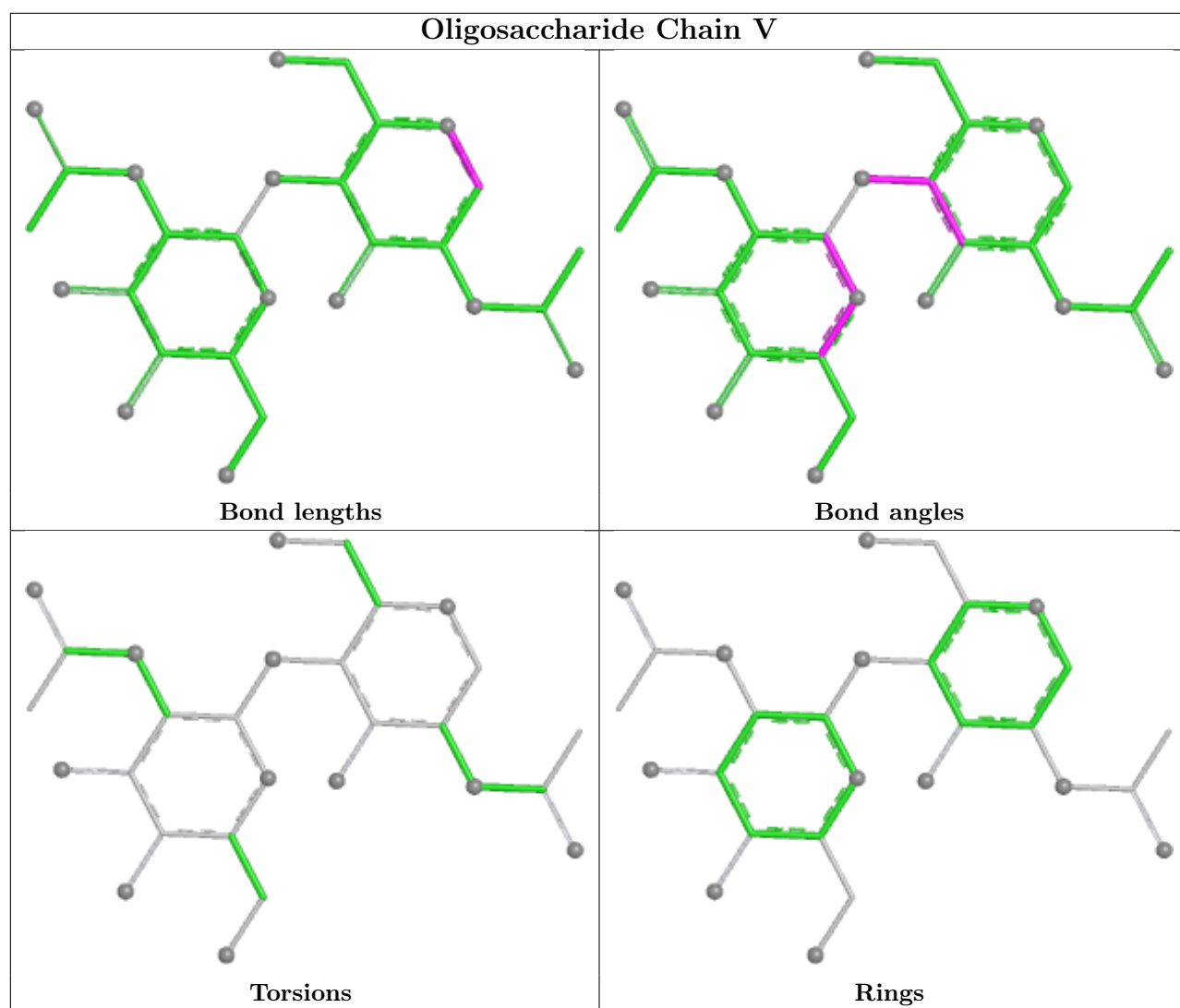


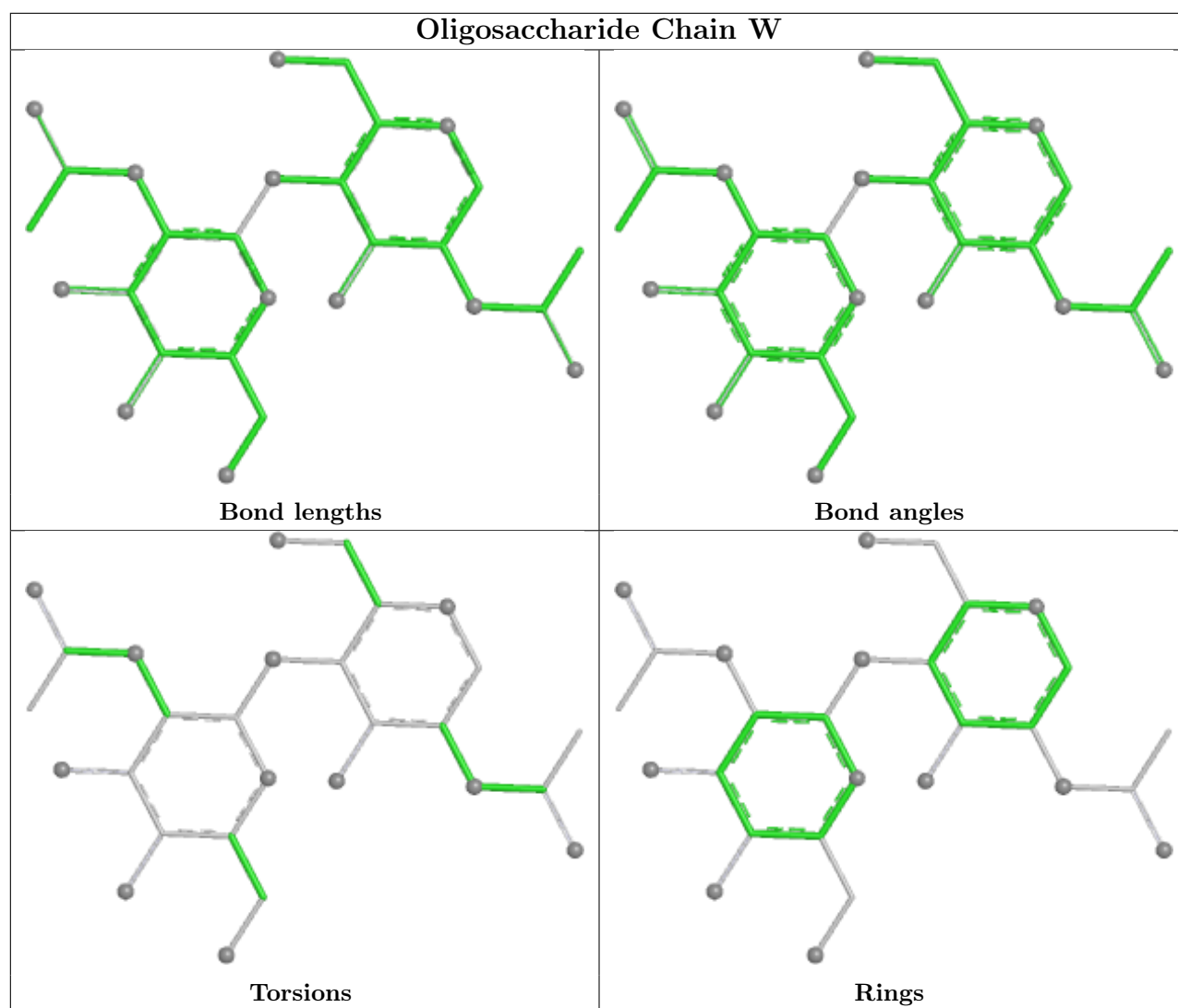


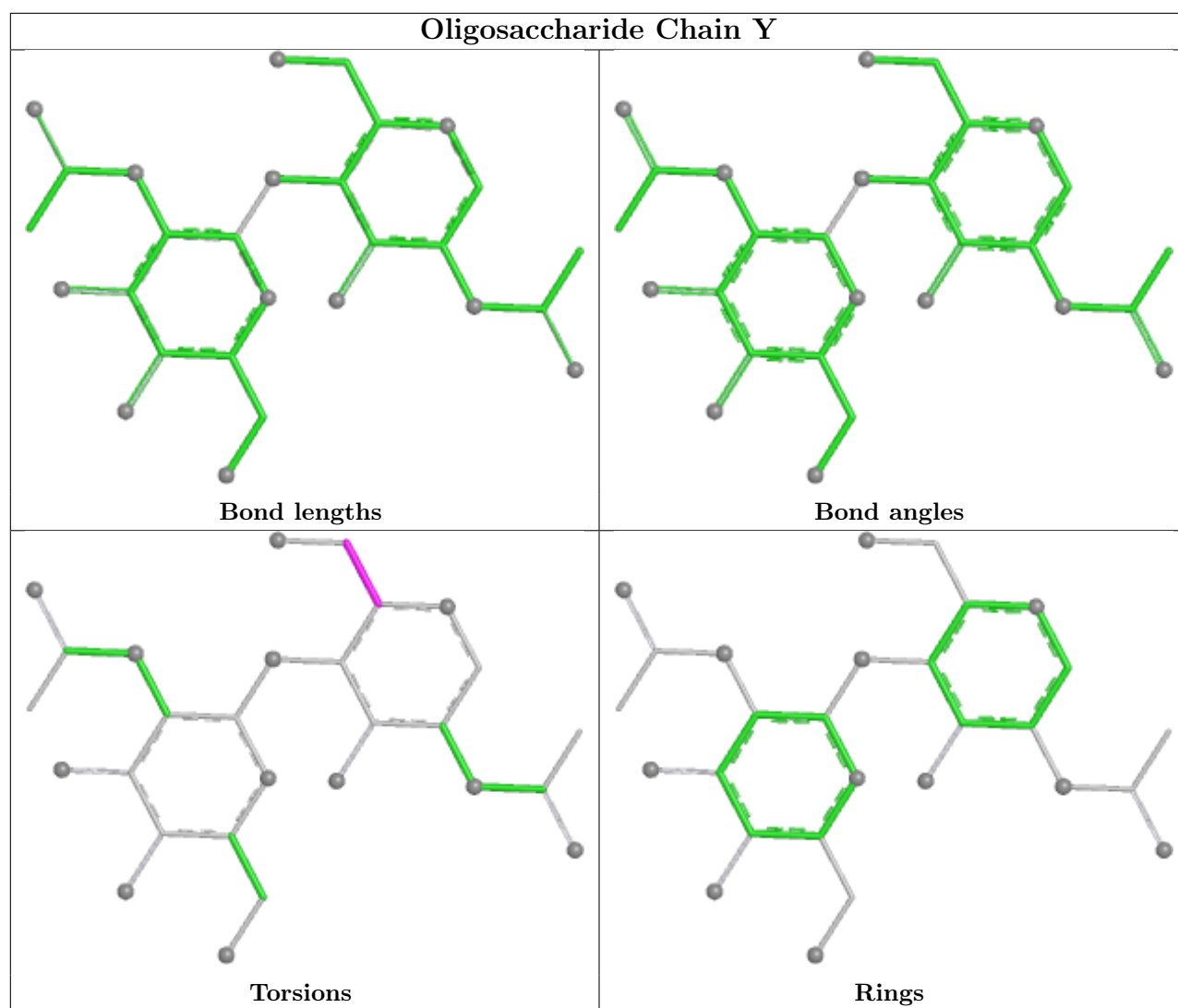


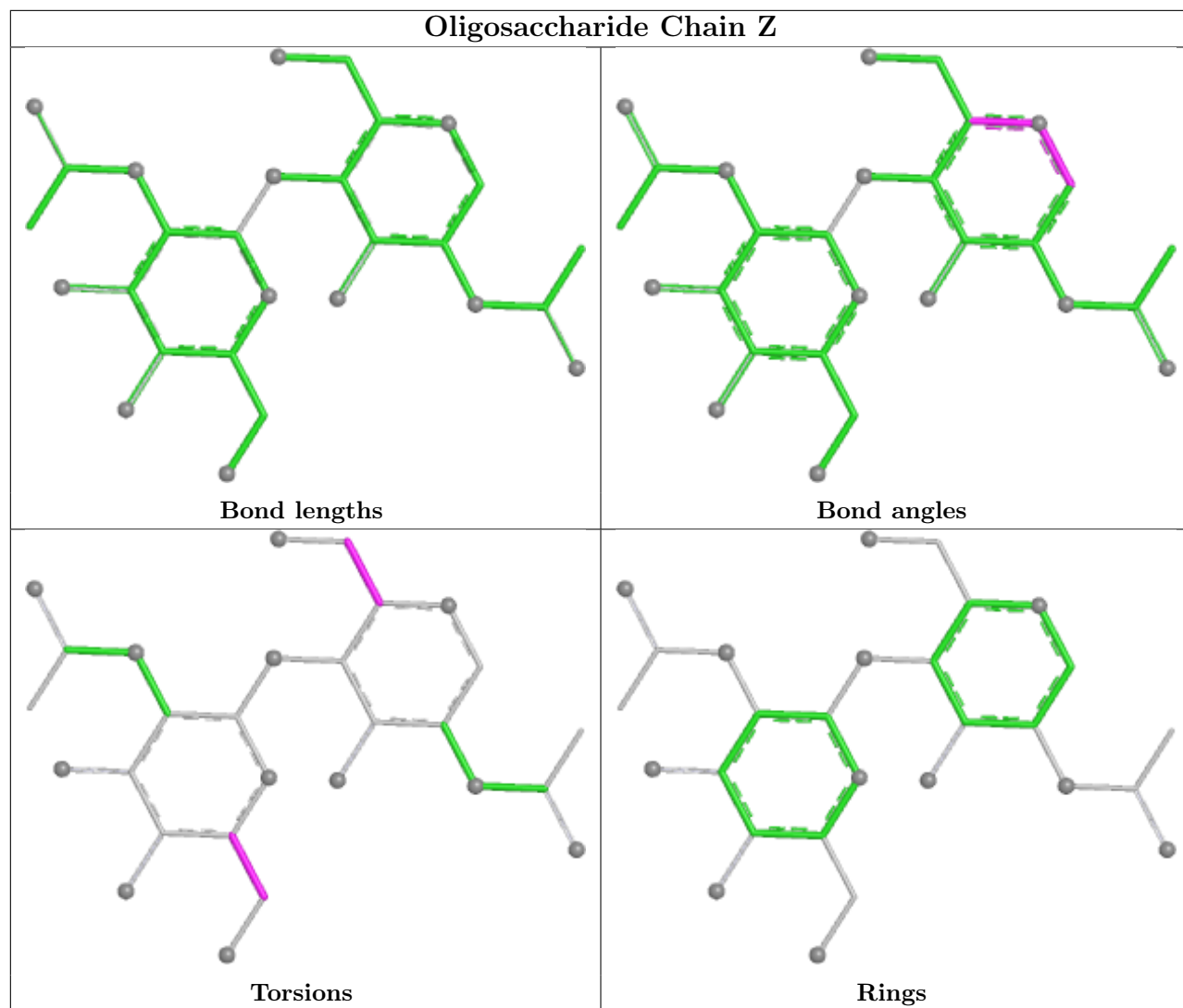


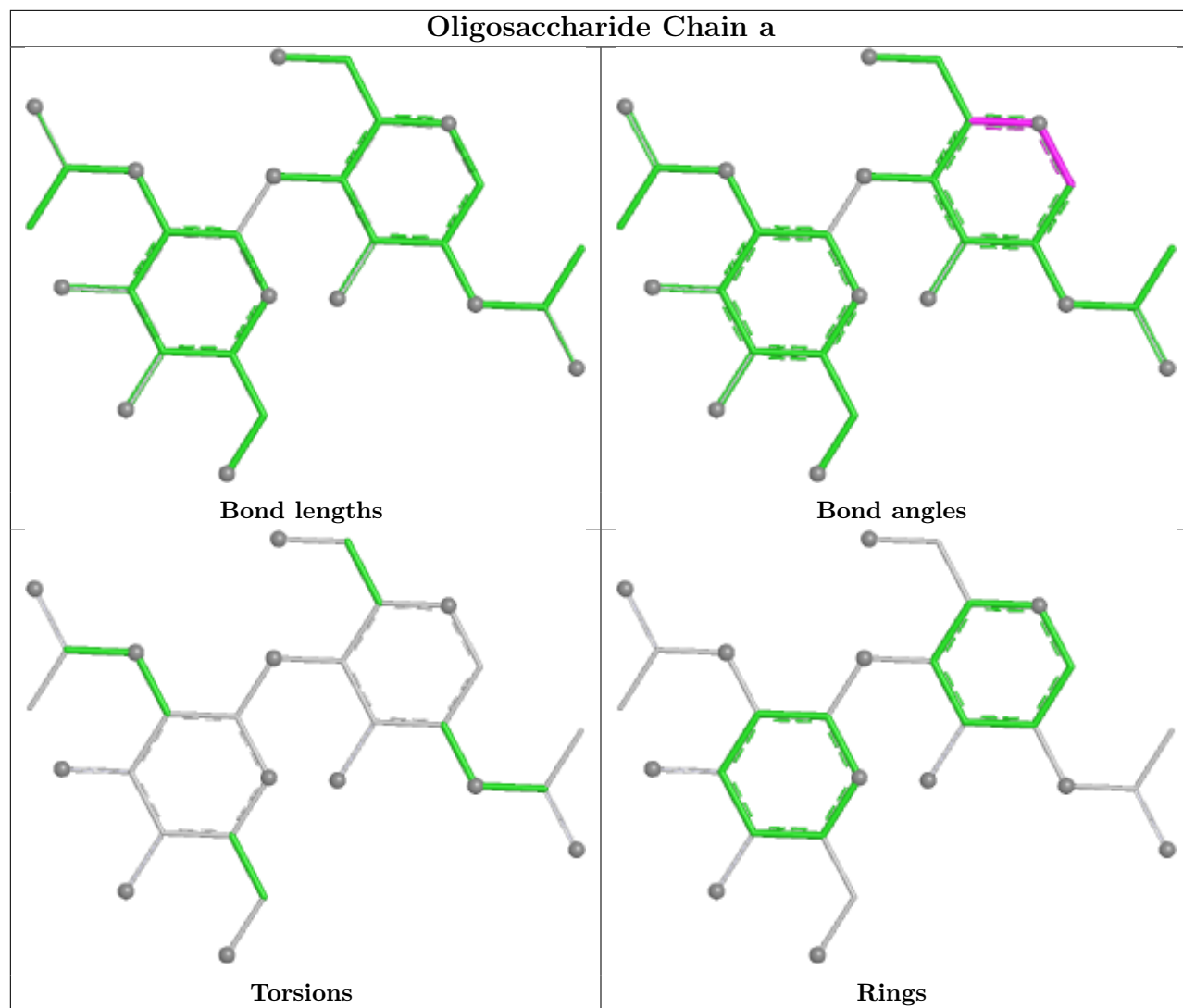


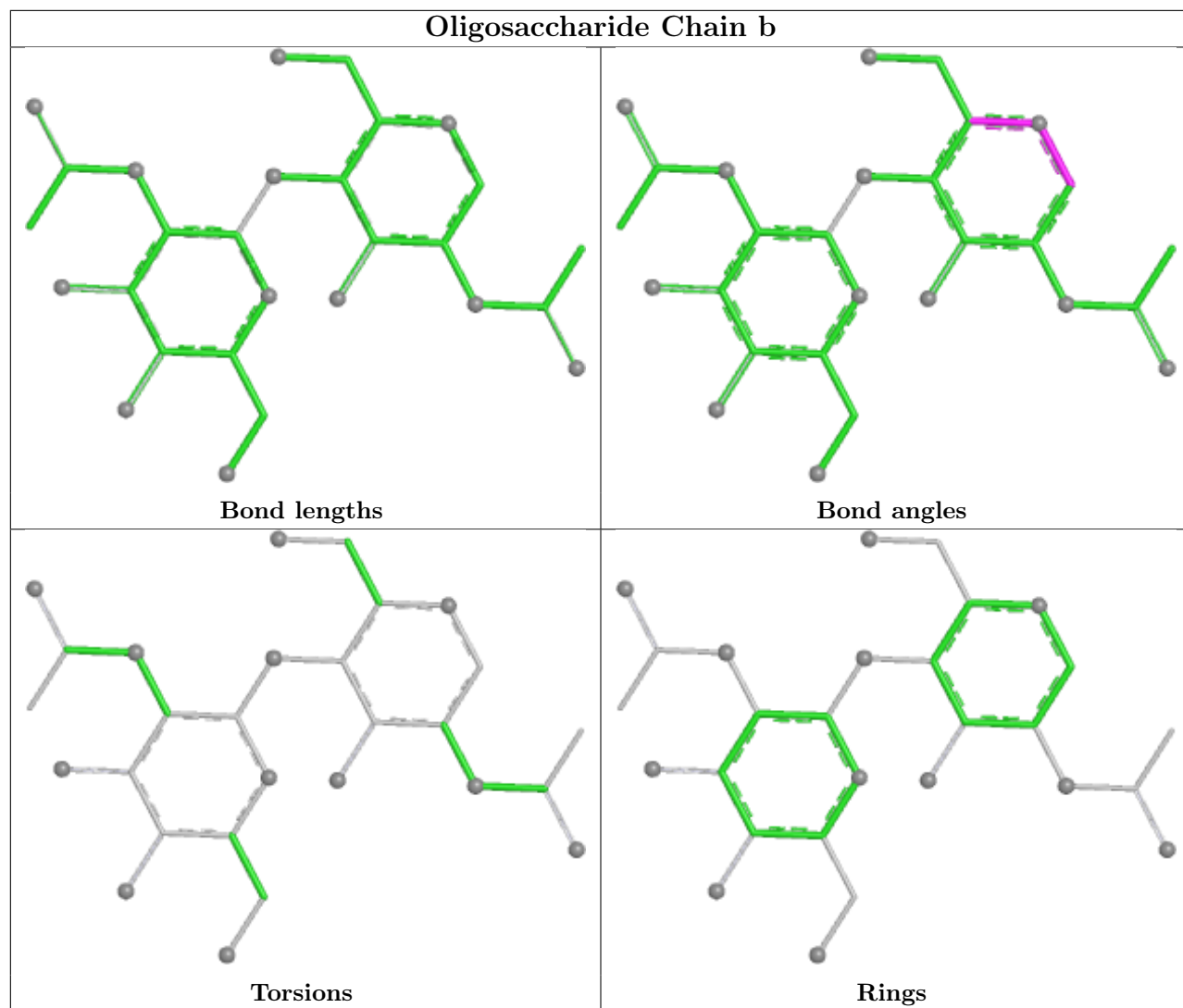


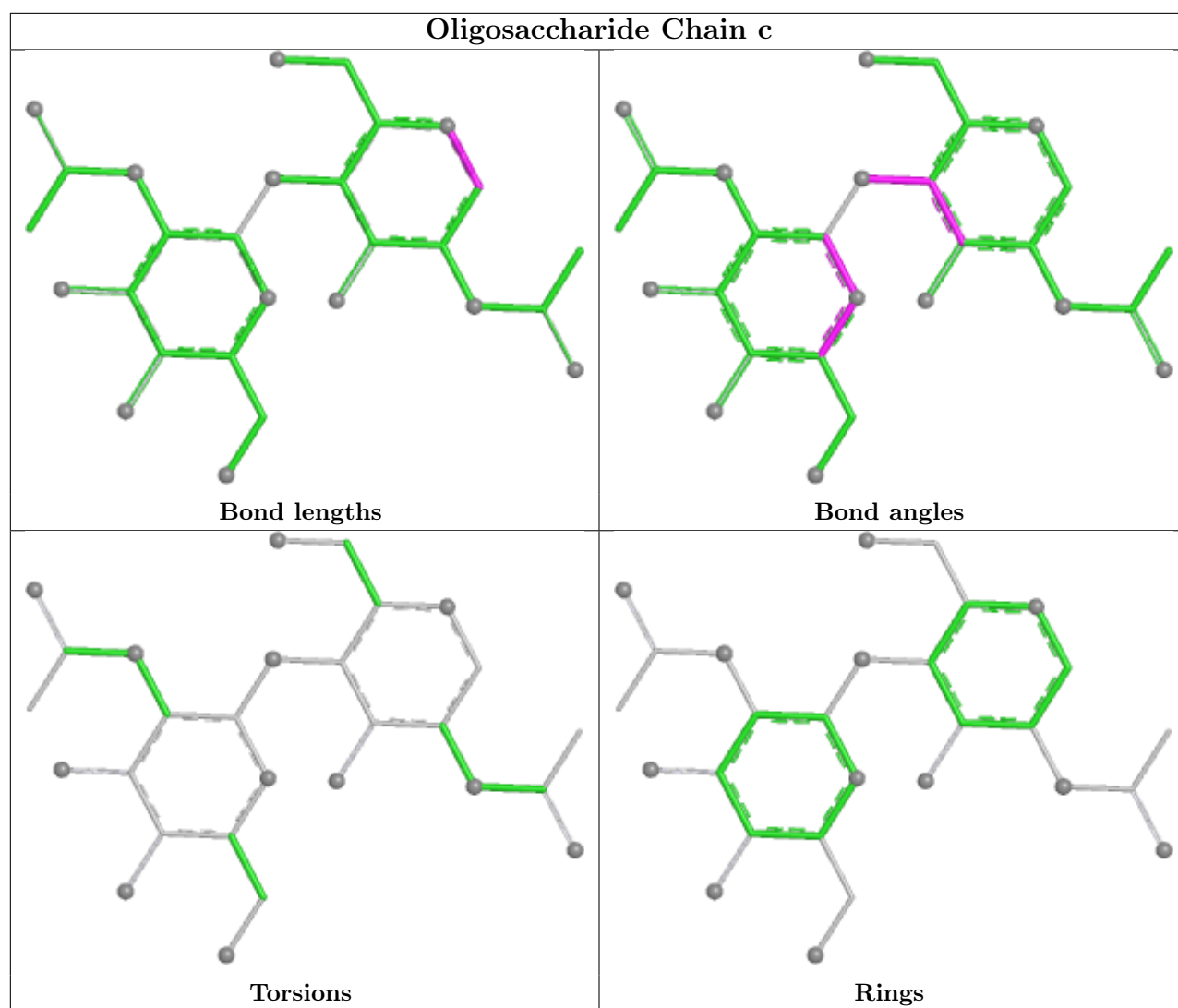


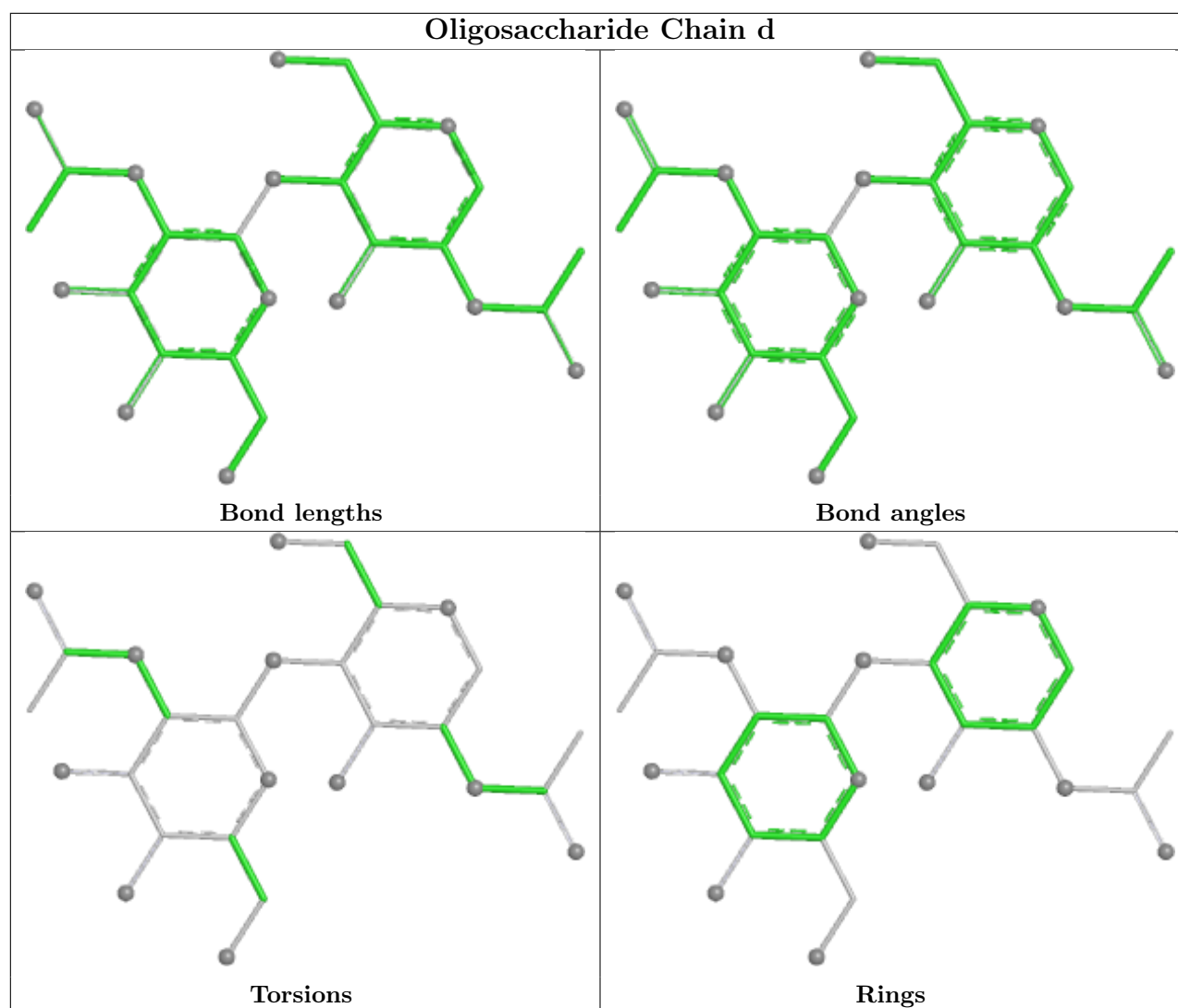












5.6 Ligand geometry [i](#)

30 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
6	NAG	B	1405	1	14,14,15	0.26	0	17,19,21	0.41	0
6	NAG	C	1402	1	14,14,15	0.22	0	17,19,21	0.67	1 (5%)
6	NAG	C	1410	-	14,14,15	0.38	0	17,19,21	0.43	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	NAG	C	1401	1	14,14,15	0.26	0	17,19,21	0.56	0
6	NAG	A	1408	1	14,14,15	0.29	0	17,19,21	0.42	0
6	NAG	A	1406	1	14,14,15	0.24	0	17,19,21	0.51	0
6	NAG	C	1407	1	14,14,15	0.34	0	17,19,21	0.41	0
6	NAG	B	1410	-	14,14,15	0.40	0	17,19,21	0.44	0
6	NAG	B	1404	1	14,14,15	0.30	0	17,19,21	0.46	0
6	NAG	B	1402	1	14,14,15	0.23	0	17,19,21	0.66	1 (5%)
6	NAG	B	1403	1	14,14,15	0.33	0	17,19,21	0.45	0
6	NAG	B	1409	1	14,14,15	0.42	0	17,19,21	1.12	2 (11%)
6	NAG	C	1403	1	14,14,15	0.33	0	17,19,21	0.46	0
6	NAG	B	1407	1	14,14,15	0.34	0	17,19,21	0.41	0
6	NAG	C	1408	1	14,14,15	0.30	0	17,19,21	0.41	0
6	NAG	A	1409	1	14,14,15	0.45	0	17,19,21	1.14	2 (11%)
6	NAG	B	1408	1	14,14,15	0.30	0	17,19,21	0.41	0
6	NAG	A	1402	1	14,14,15	0.22	0	17,19,21	0.67	1 (5%)
6	NAG	B	1401	1	14,14,15	0.26	0	17,19,21	0.56	0
6	NAG	A	1401	1	14,14,15	0.25	0	17,19,21	0.56	0
6	NAG	A	1405	1	14,14,15	0.27	0	17,19,21	0.41	0
6	NAG	C	1404	1	14,14,15	0.30	0	17,19,21	0.46	0
6	NAG	A	1410	-	14,14,15	0.36	0	17,19,21	0.43	0
6	NAG	B	1406	1	14,14,15	0.25	0	17,19,21	0.52	0
6	NAG	C	1409	1	14,14,15	0.44	0	17,19,21	1.13	2 (11%)
6	NAG	A	1404	1	14,14,15	0.30	0	17,19,21	0.46	0
6	NAG	C	1406	1	14,14,15	0.26	0	17,19,21	0.51	0
6	NAG	A	1407	1	14,14,15	0.34	0	17,19,21	0.41	0
6	NAG	C	1405	1	14,14,15	0.26	0	17,19,21	0.40	0
6	NAG	A	1403	1	14,14,15	0.33	0	17,19,21	0.45	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	B	1405	1	-	0/6/23/26	0/1/1/1
6	NAG	C	1402	1	-	2/6/23/26	0/1/1/1
6	NAG	C	1410	-	-	0/6/23/26	0/1/1/1
6	NAG	C	1401	1	-	2/6/23/26	0/1/1/1
6	NAG	A	1408	1	-	0/6/23/26	0/1/1/1
6	NAG	A	1406	1	-	0/6/23/26	0/1/1/1
6	NAG	C	1407	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	B	1410	-	-	0/6/23/26	0/1/1/1
6	NAG	B	1404	1	-	0/6/23/26	0/1/1/1
6	NAG	B	1402	1	-	2/6/23/26	0/1/1/1
6	NAG	B	1403	1	-	2/6/23/26	0/1/1/1
6	NAG	B	1409	1	-	0/6/23/26	0/1/1/1
6	NAG	C	1403	1	-	2/6/23/26	0/1/1/1
6	NAG	B	1407	1	-	0/6/23/26	0/1/1/1
6	NAG	C	1408	1	-	0/6/23/26	0/1/1/1
6	NAG	A	1409	1	-	0/6/23/26	0/1/1/1
6	NAG	B	1408	1	-	0/6/23/26	0/1/1/1
6	NAG	A	1402	1	-	2/6/23/26	0/1/1/1
6	NAG	B	1401	1	-	2/6/23/26	0/1/1/1
6	NAG	A	1401	1	-	2/6/23/26	0/1/1/1
6	NAG	A	1405	1	-	0/6/23/26	0/1/1/1
6	NAG	C	1404	1	-	0/6/23/26	0/1/1/1
6	NAG	A	1410	-	-	0/6/23/26	0/1/1/1
6	NAG	B	1406	1	-	0/6/23/26	0/1/1/1
6	NAG	C	1409	1	-	0/6/23/26	0/1/1/1
6	NAG	A	1404	1	-	0/6/23/26	0/1/1/1
6	NAG	C	1406	1	-	0/6/23/26	0/1/1/1
6	NAG	A	1407	1	-	0/6/23/26	0/1/1/1
6	NAG	C	1405	1	-	0/6/23/26	0/1/1/1
6	NAG	A	1403	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	1402	NAG	C1-O5-C5	2.42	115.43	112.19
6	C	1402	NAG	C1-O5-C5	2.39	115.39	112.19
6	B	1402	NAG	C1-O5-C5	2.36	115.35	112.19
6	B	1409	NAG	C8-C7-N2	2.26	119.87	116.12
6	A	1409	NAG	C8-C7-N2	2.25	119.85	116.12
6	C	1409	NAG	C2-N2-C7	-2.24	119.90	122.90
6	C	1409	NAG	C8-C7-N2	2.21	119.79	116.12
6	B	1409	NAG	C2-N2-C7	-2.18	119.98	122.90
6	A	1409	NAG	C2-N2-C7	-2.17	119.99	122.90

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	1402	NAG	O5-C5-C6-O6
6	B	1402	NAG	O5-C5-C6-O6
6	C	1402	NAG	O5-C5-C6-O6
6	A	1402	NAG	C4-C5-C6-O6
6	B	1402	NAG	C4-C5-C6-O6
6	C	1402	NAG	C4-C5-C6-O6
6	A	1403	NAG	O5-C5-C6-O6
6	B	1403	NAG	O5-C5-C6-O6
6	C	1403	NAG	O5-C5-C6-O6
6	A	1401	NAG	O5-C5-C6-O6
6	B	1401	NAG	O5-C5-C6-O6
6	C	1401	NAG	O5-C5-C6-O6
6	A	1403	NAG	C4-C5-C6-O6
6	B	1403	NAG	C4-C5-C6-O6
6	C	1403	NAG	C4-C5-C6-O6
6	A	1401	NAG	C4-C5-C6-O6
6	B	1401	NAG	C4-C5-C6-O6
6	C	1401	NAG	C4-C5-C6-O6

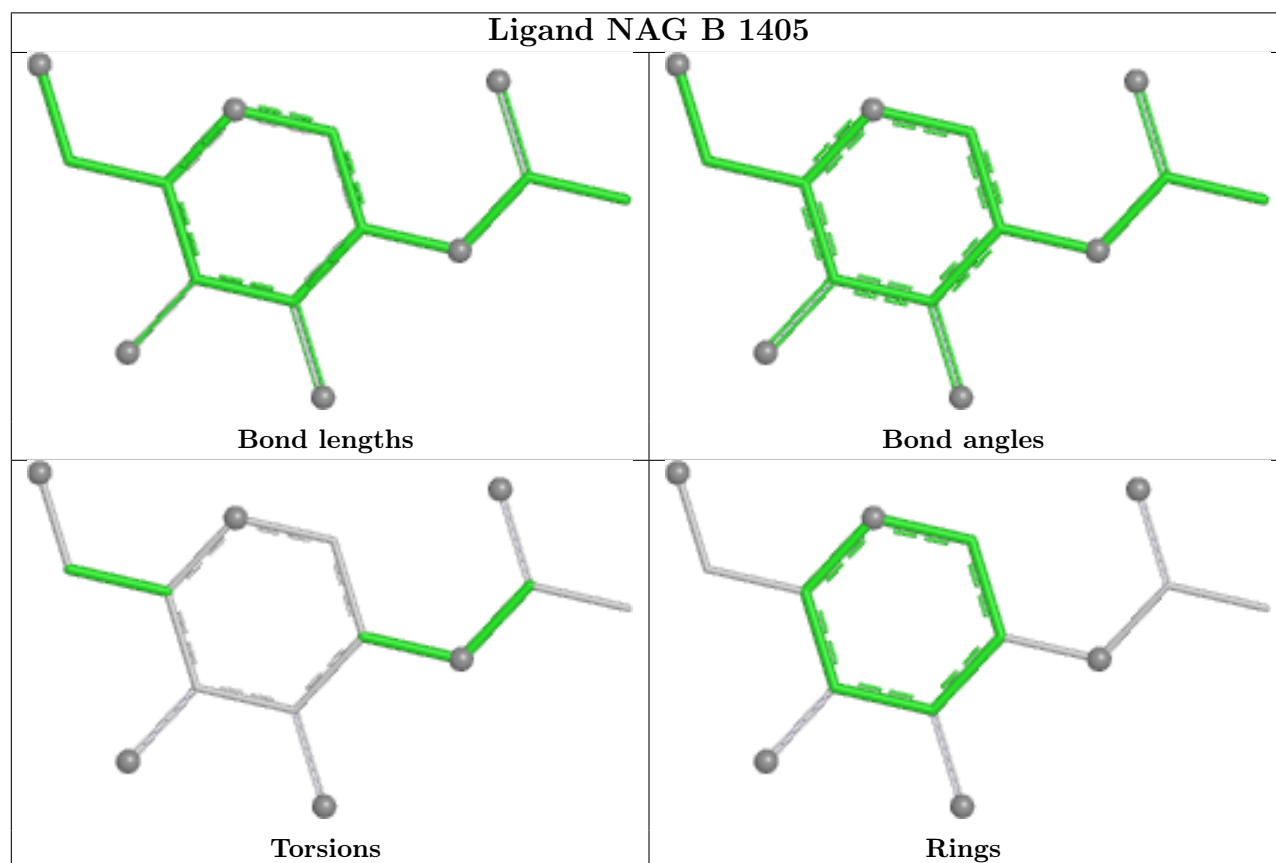
There are no ring outliers.

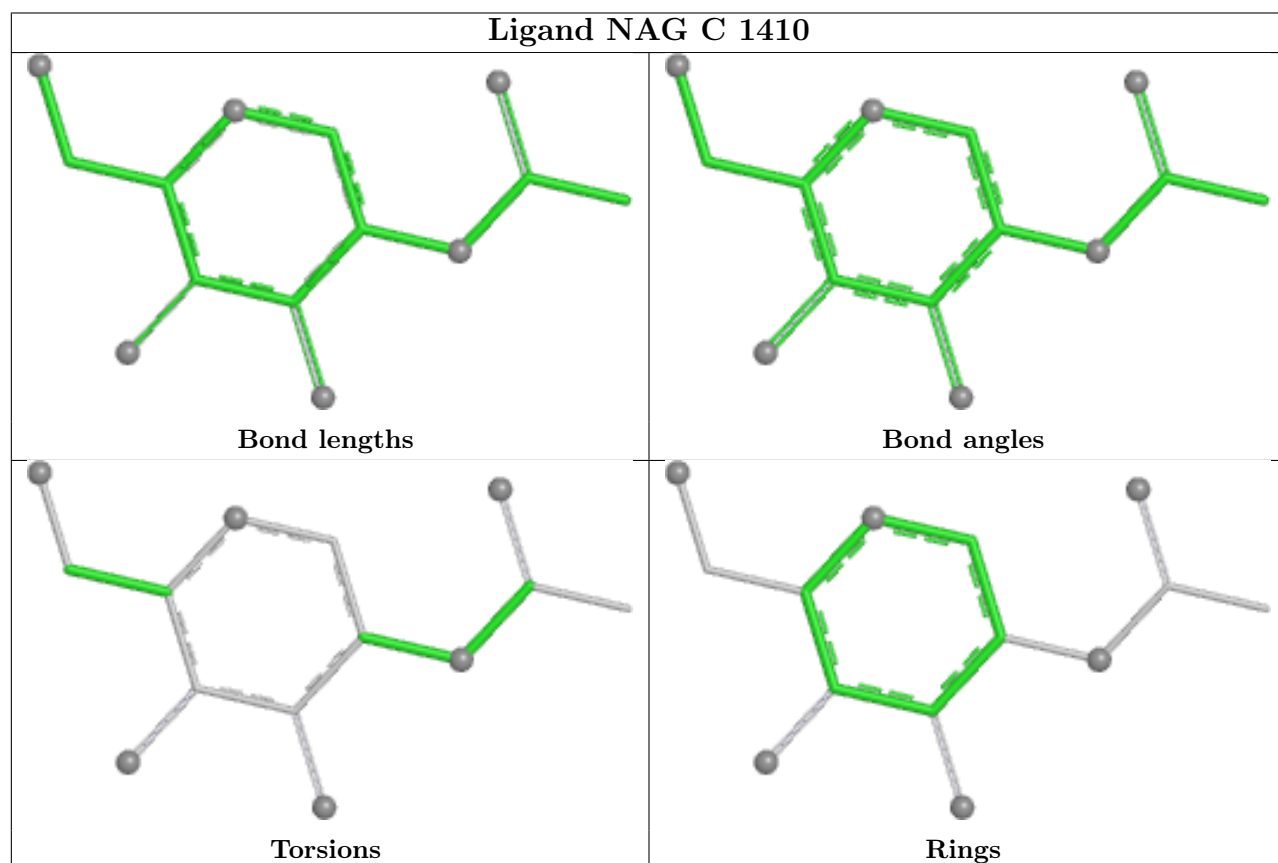
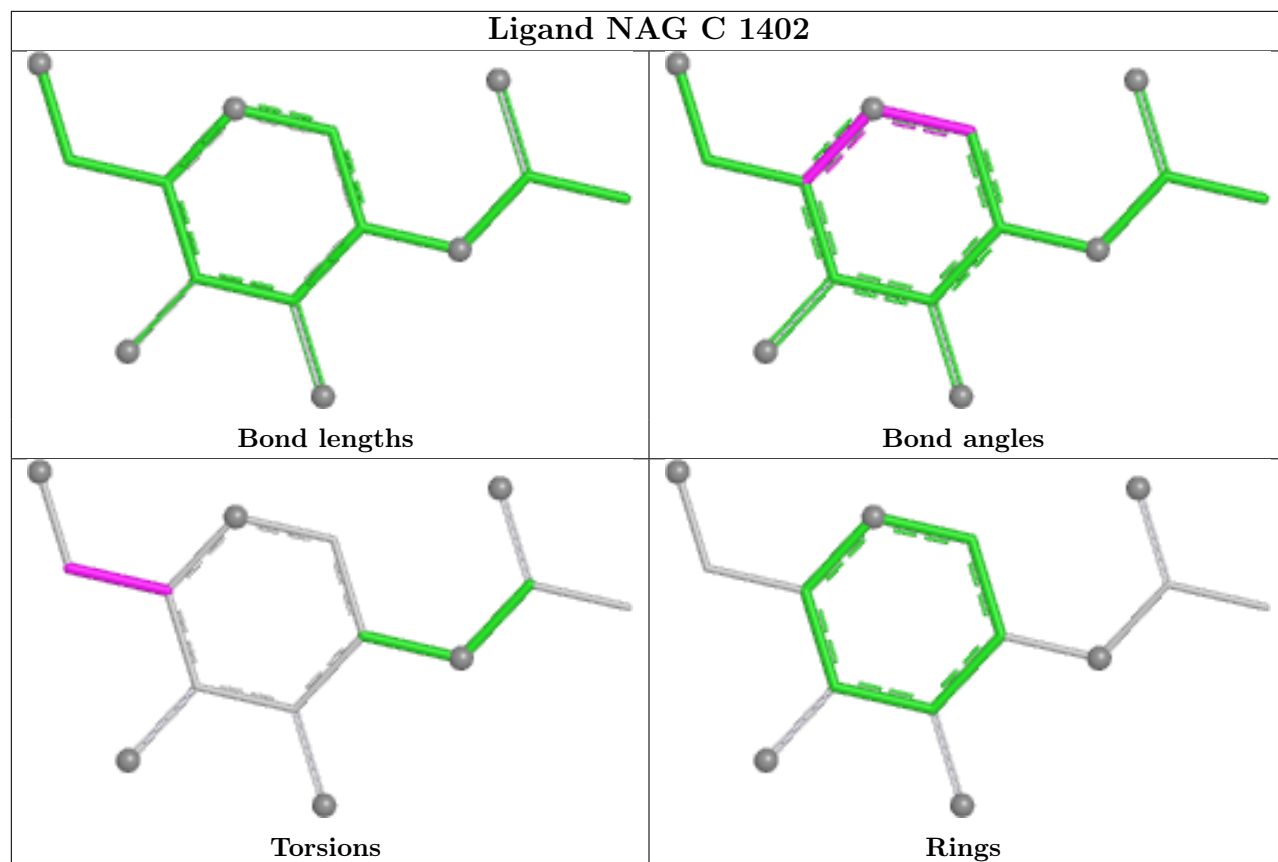
9 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	1402	NAG	1	0
6	C	1410	NAG	4	0
6	B	1410	NAG	4	0
6	B	1402	NAG	1	0
6	B	1409	NAG	6	0
6	A	1409	NAG	5	0
6	A	1402	NAG	1	0
6	A	1410	NAG	3	0
6	C	1409	NAG	6	0

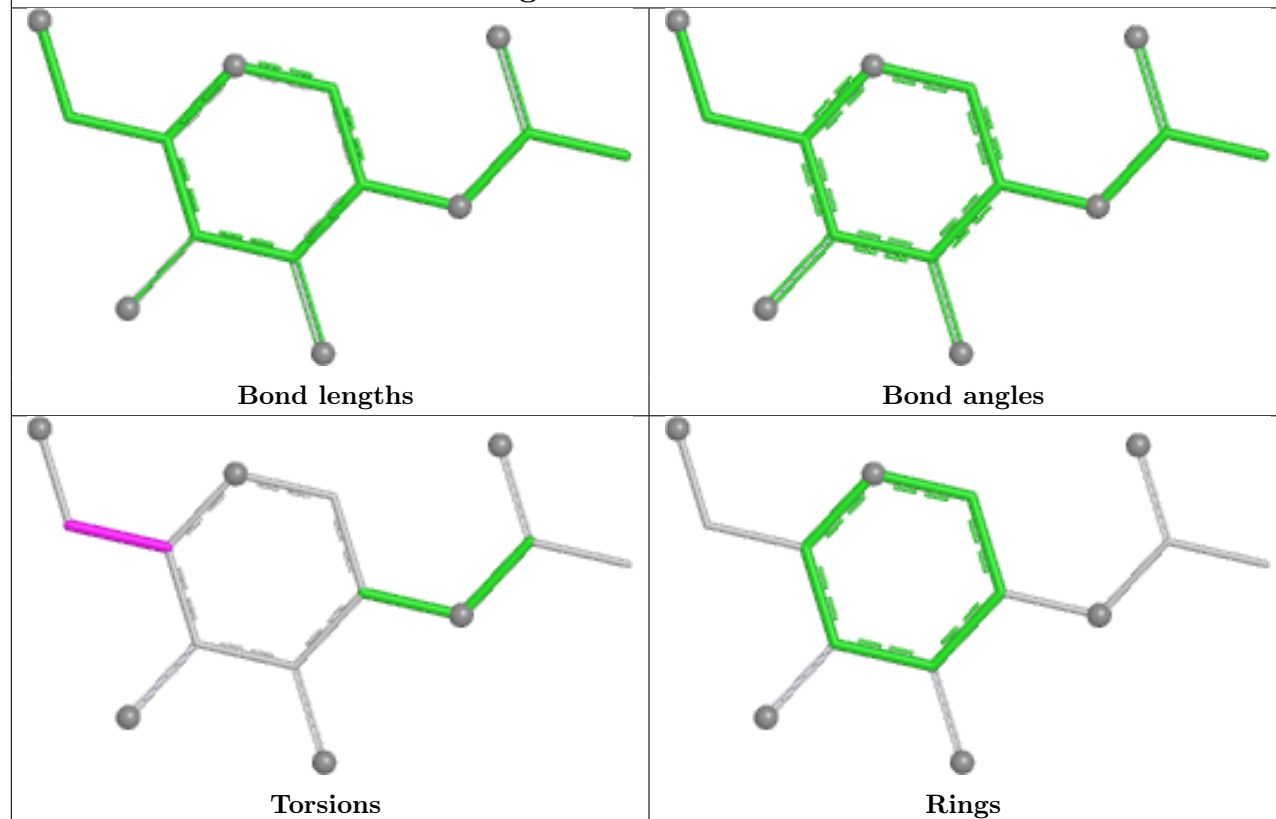
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier.

The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

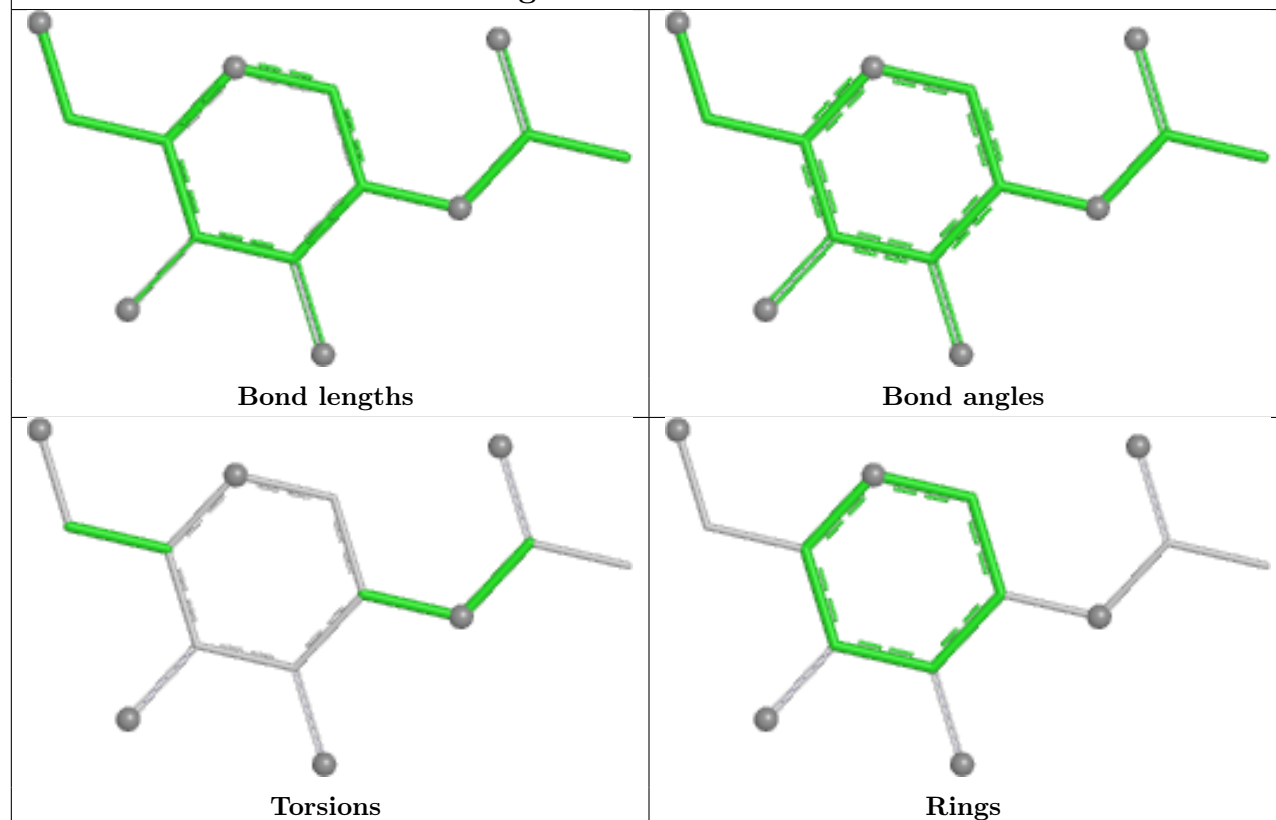




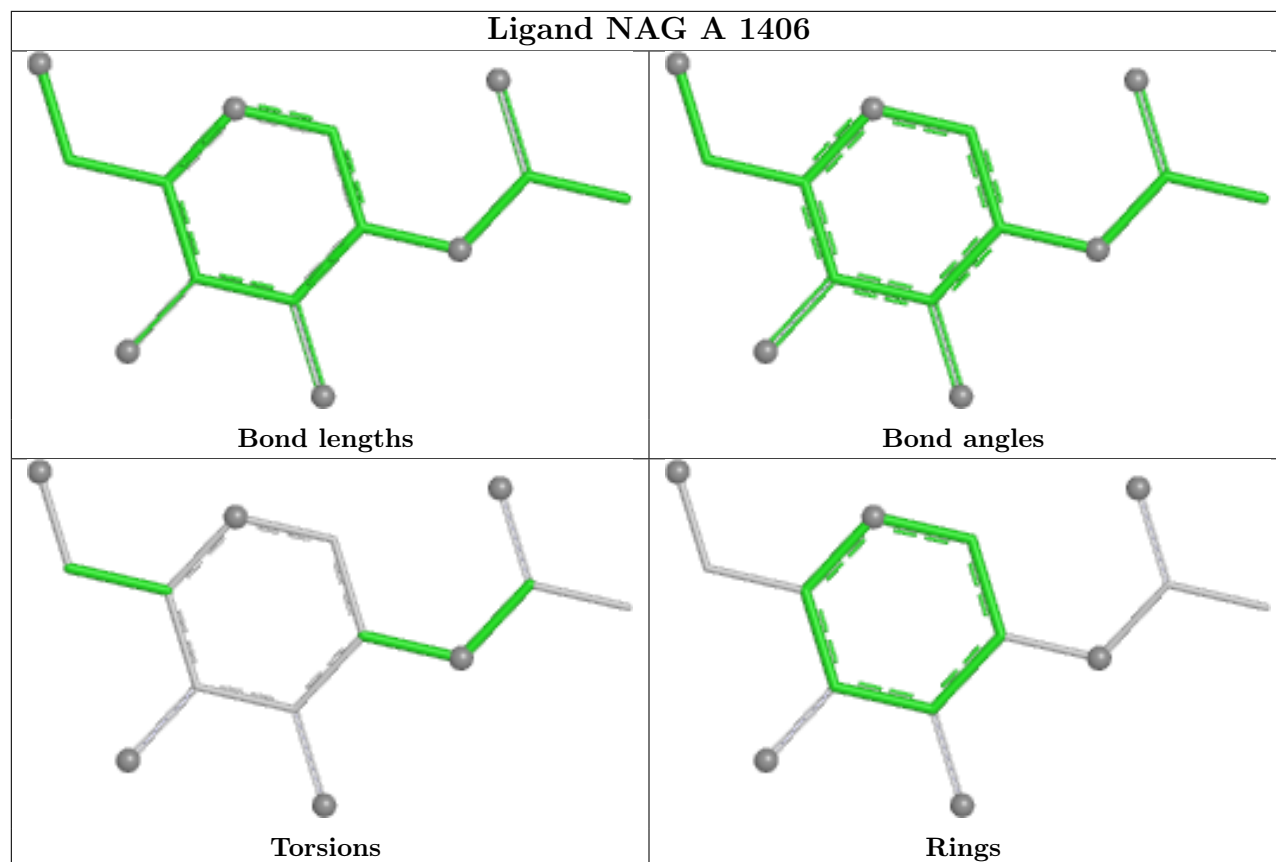
Ligand NAG C 1401



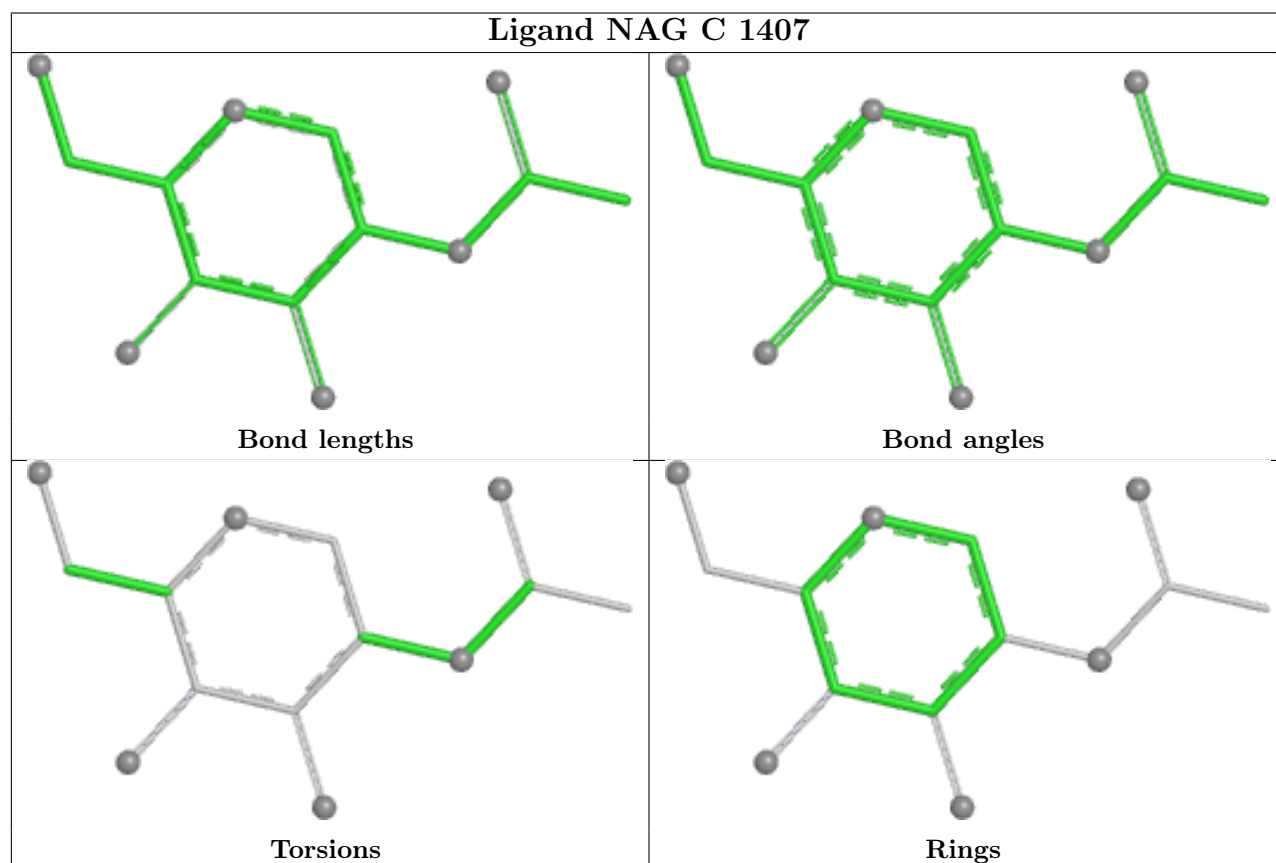
Ligand NAG A 1408



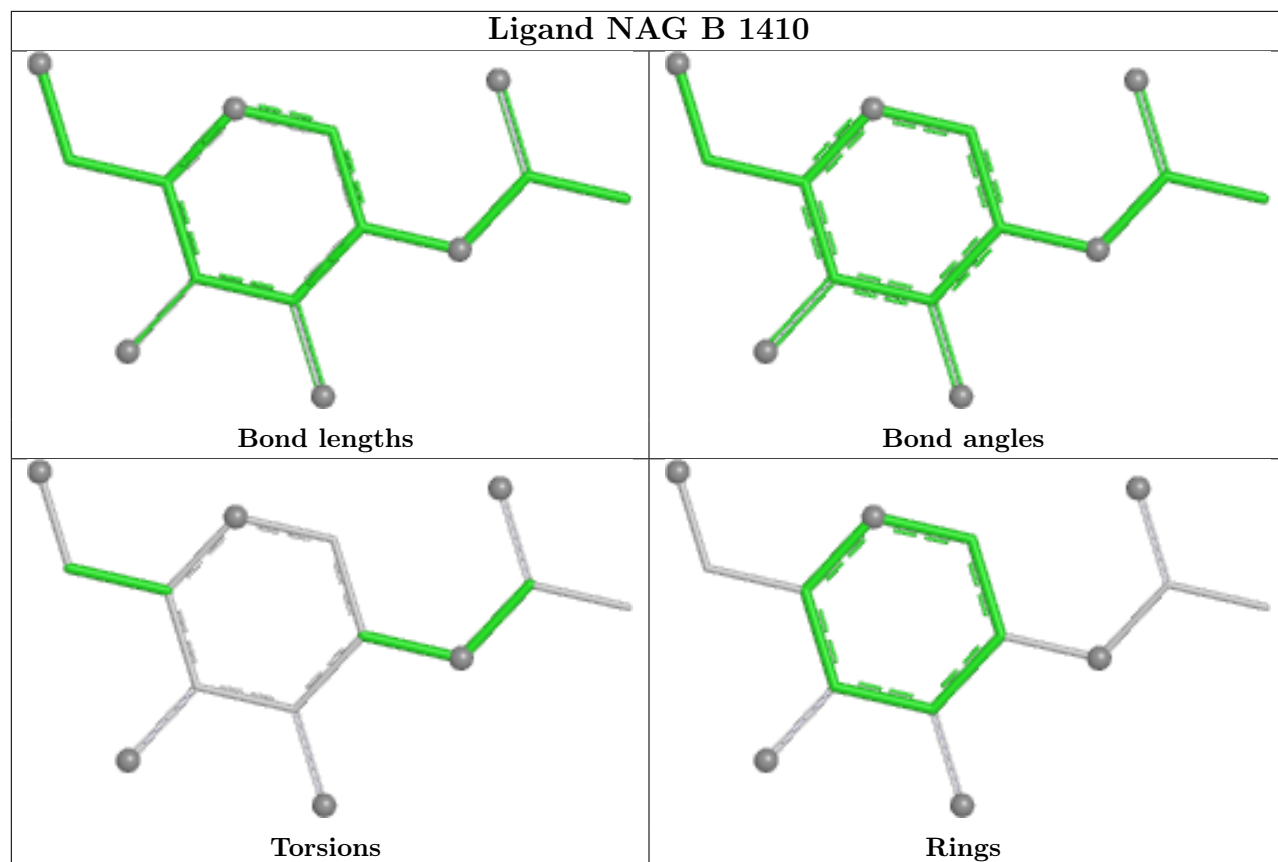
Ligand NAG A 1406



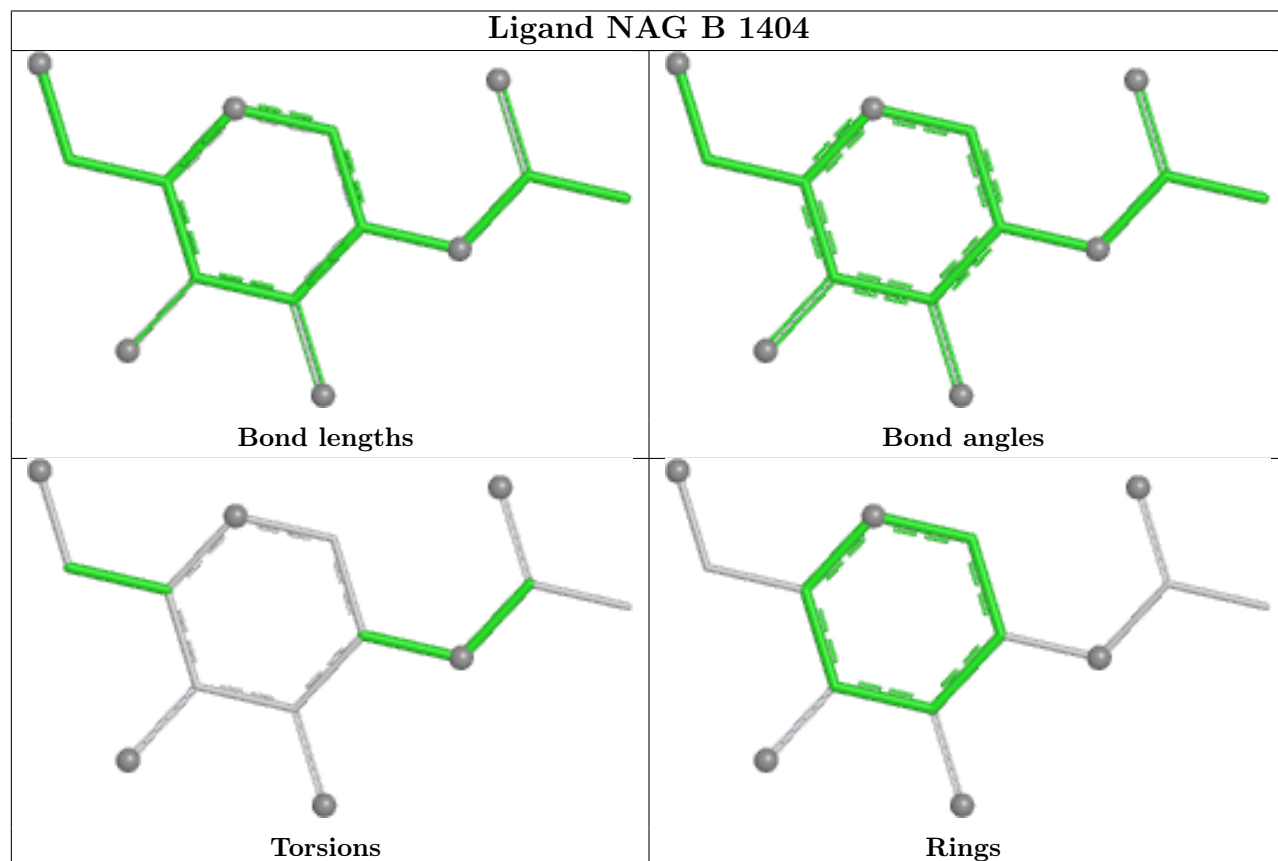
Ligand NAG C 1407



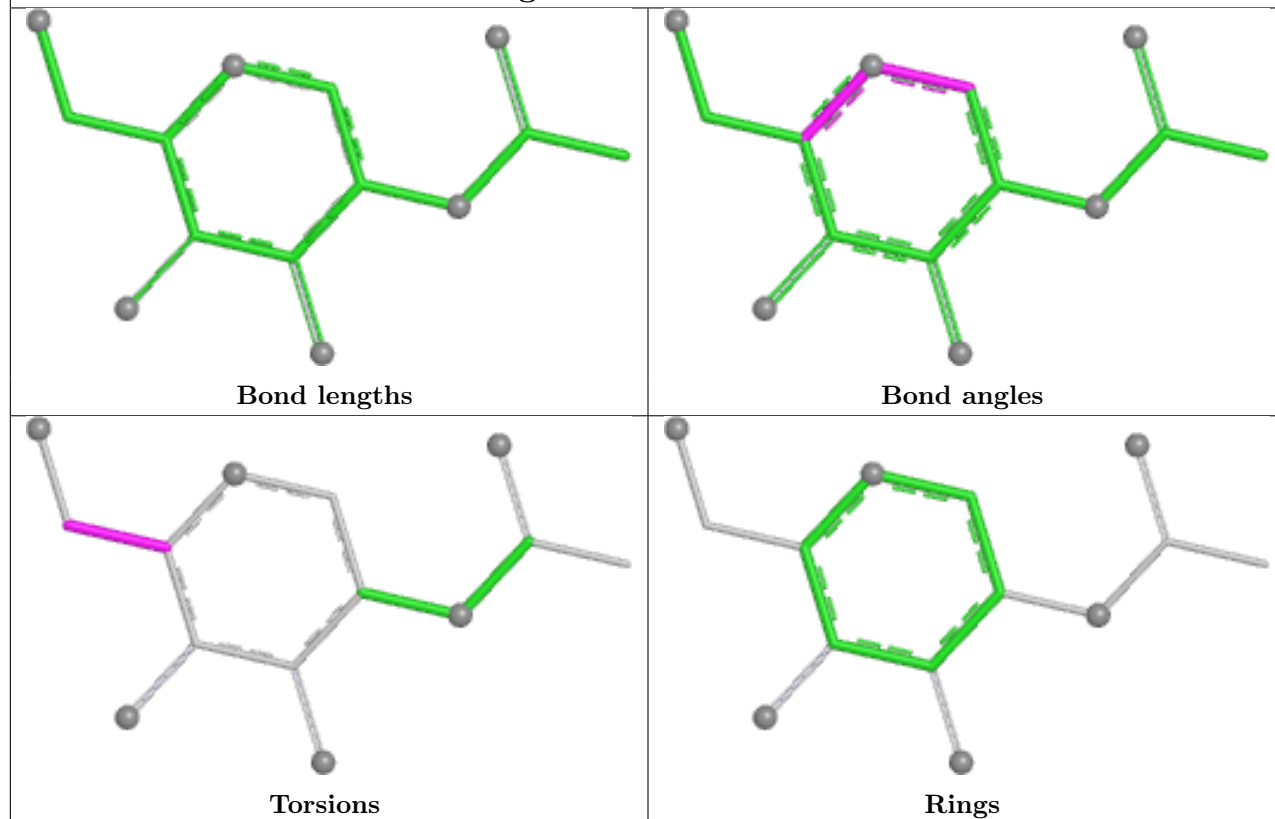
Ligand NAG B 1410



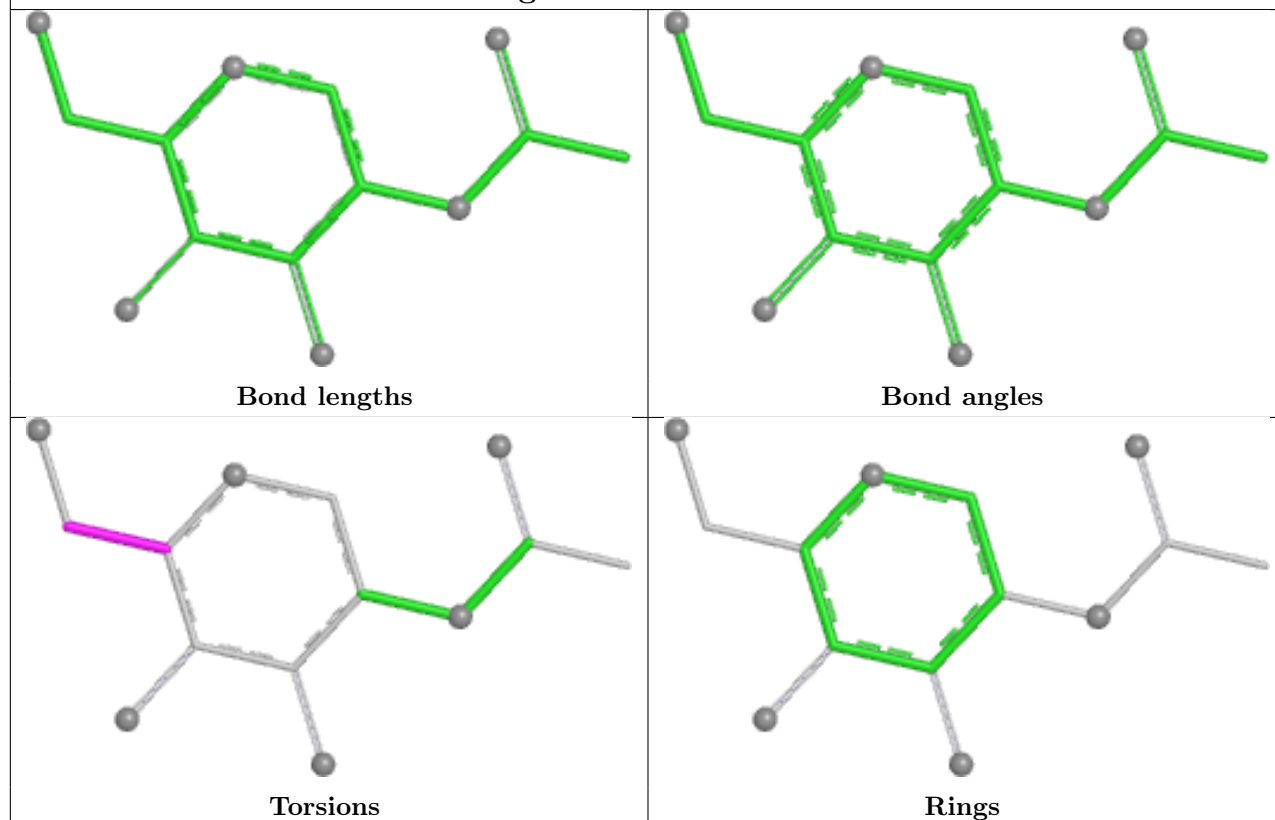
Ligand NAG B 1404



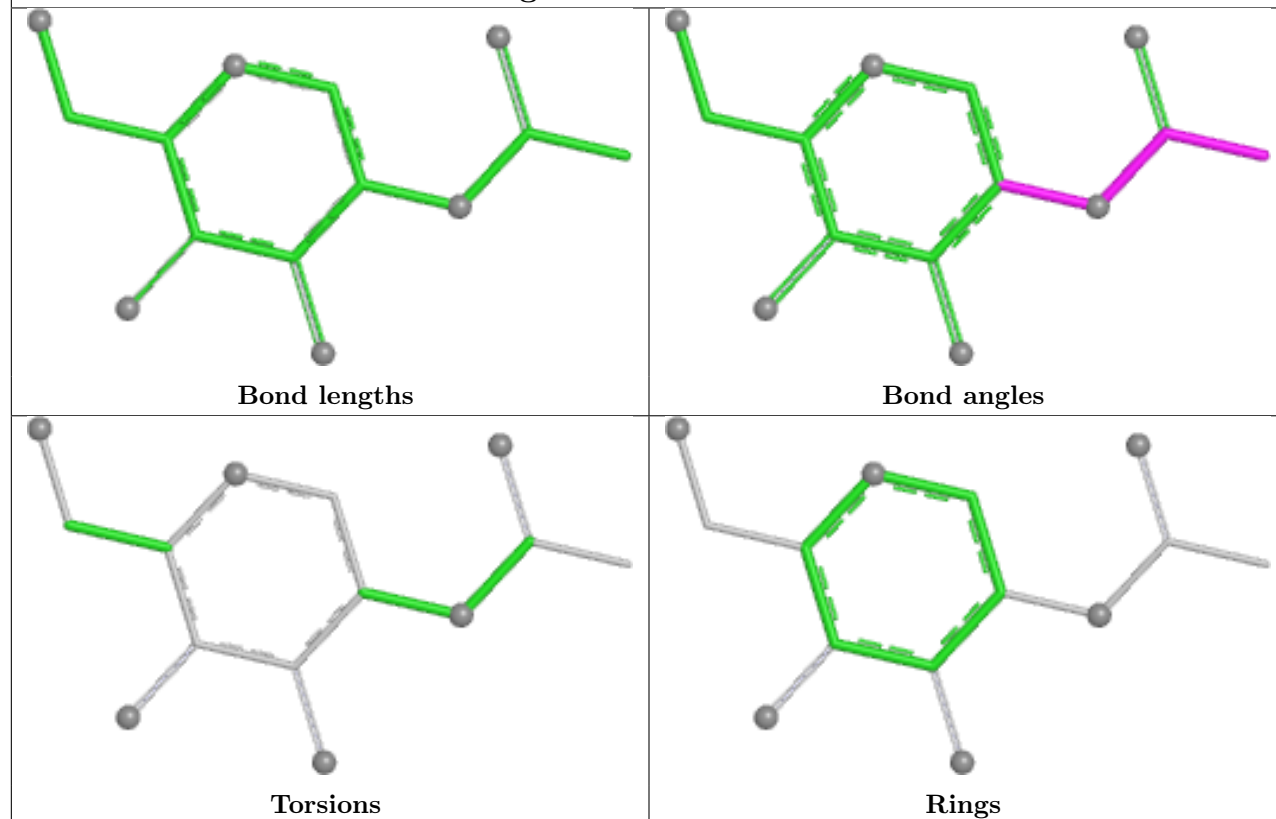
Ligand NAG B 1402



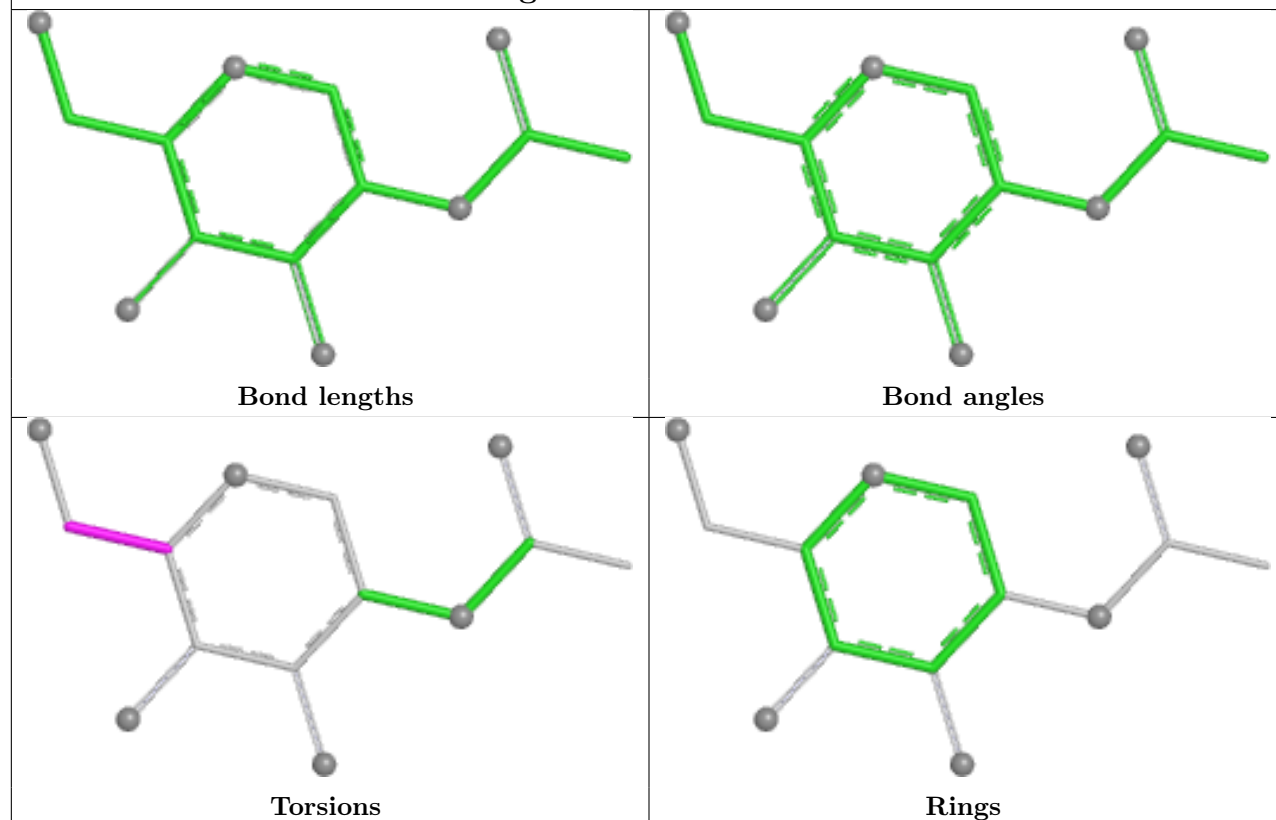
Ligand NAG B 1403



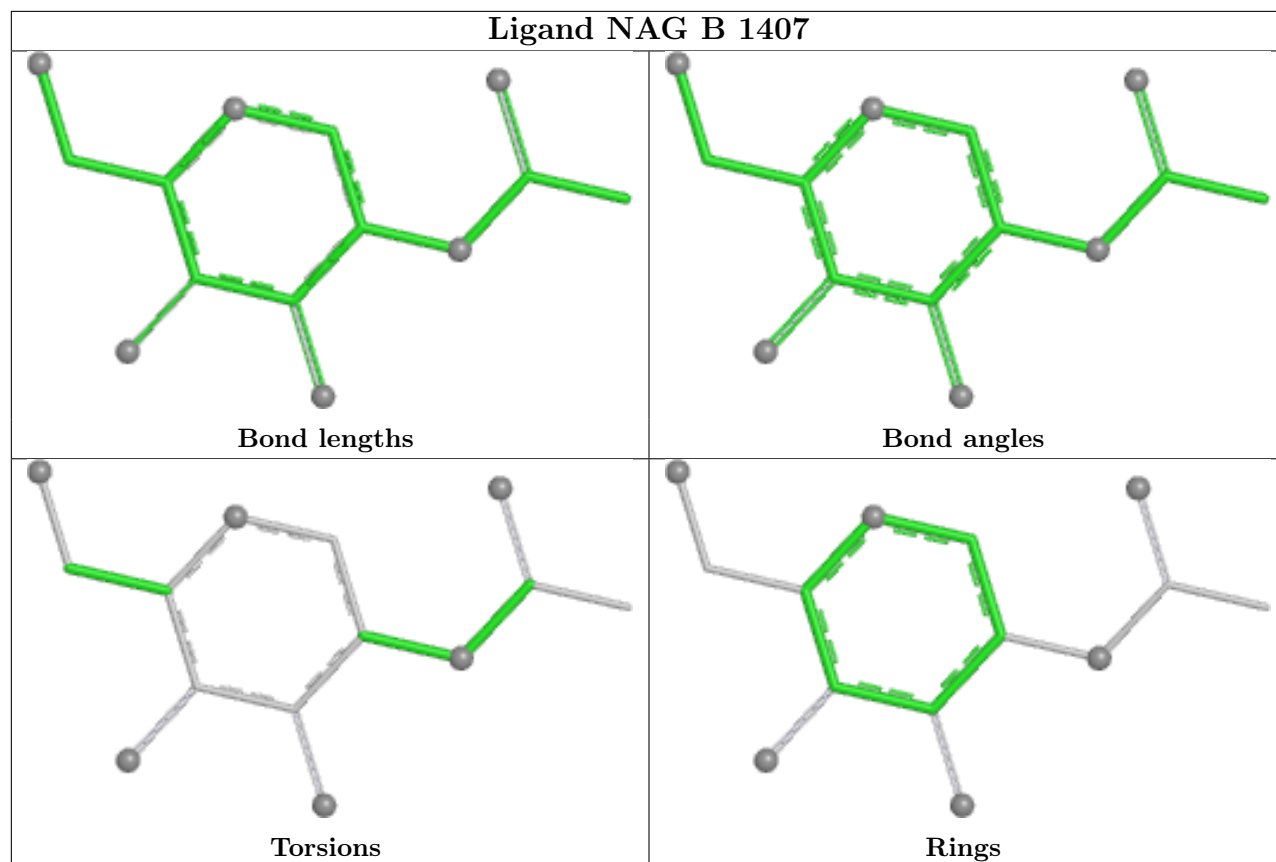
Ligand NAG B 1409



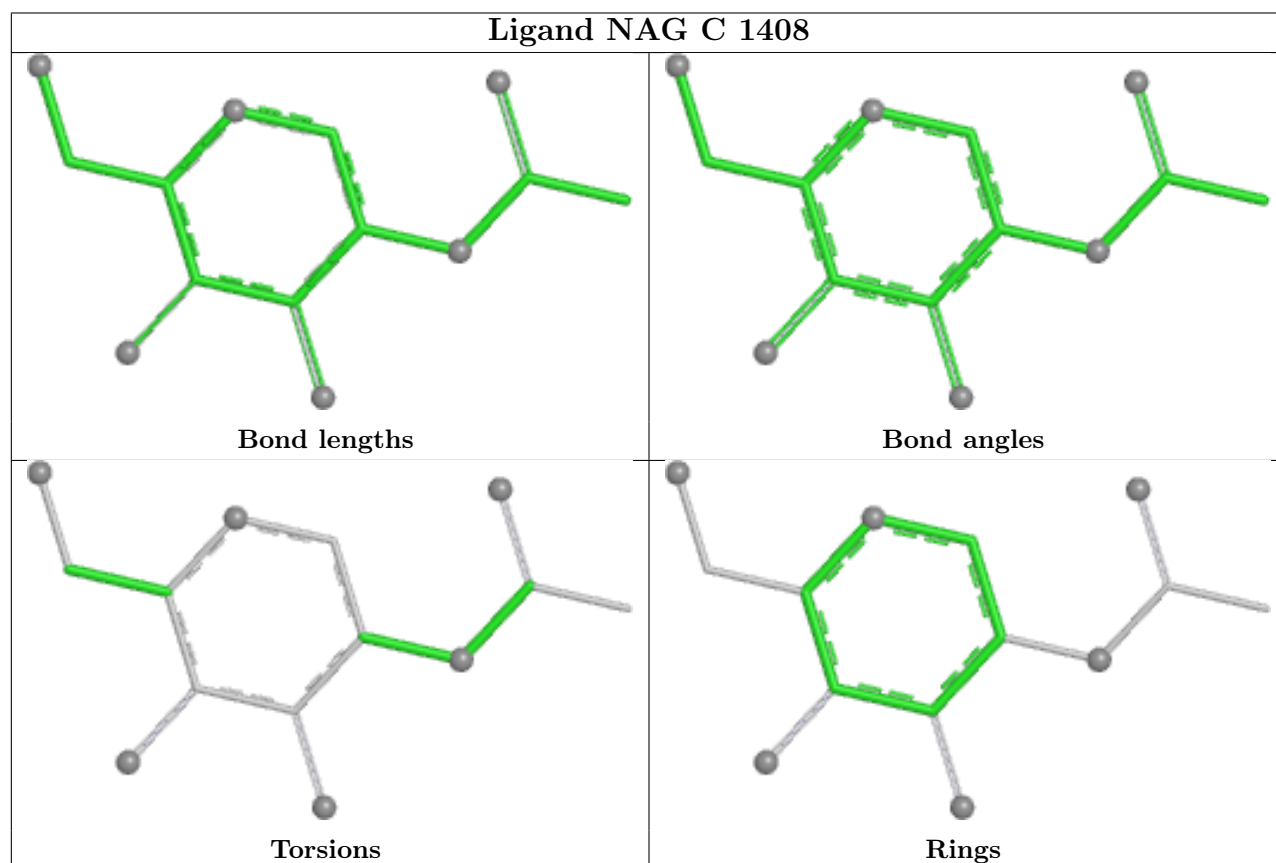
Ligand NAG C 1403



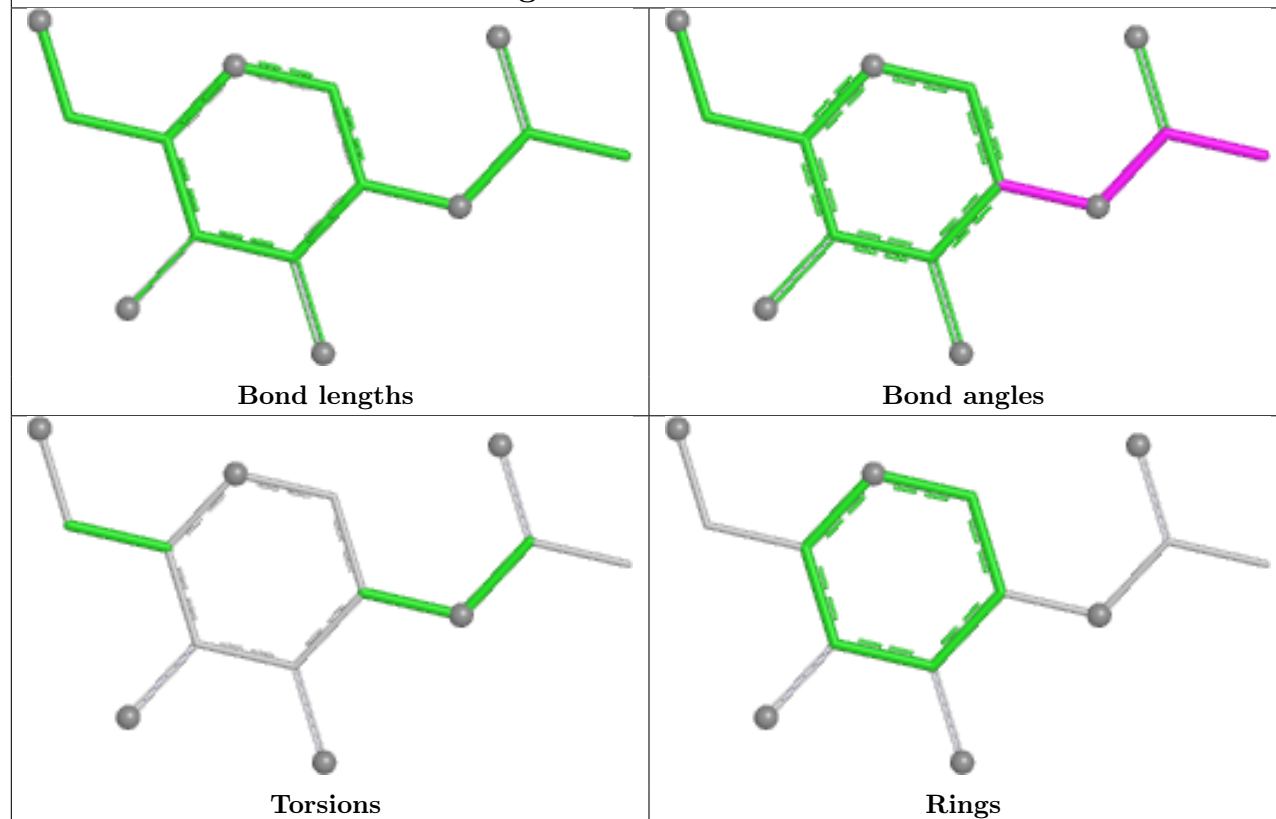
Ligand NAG B 1407



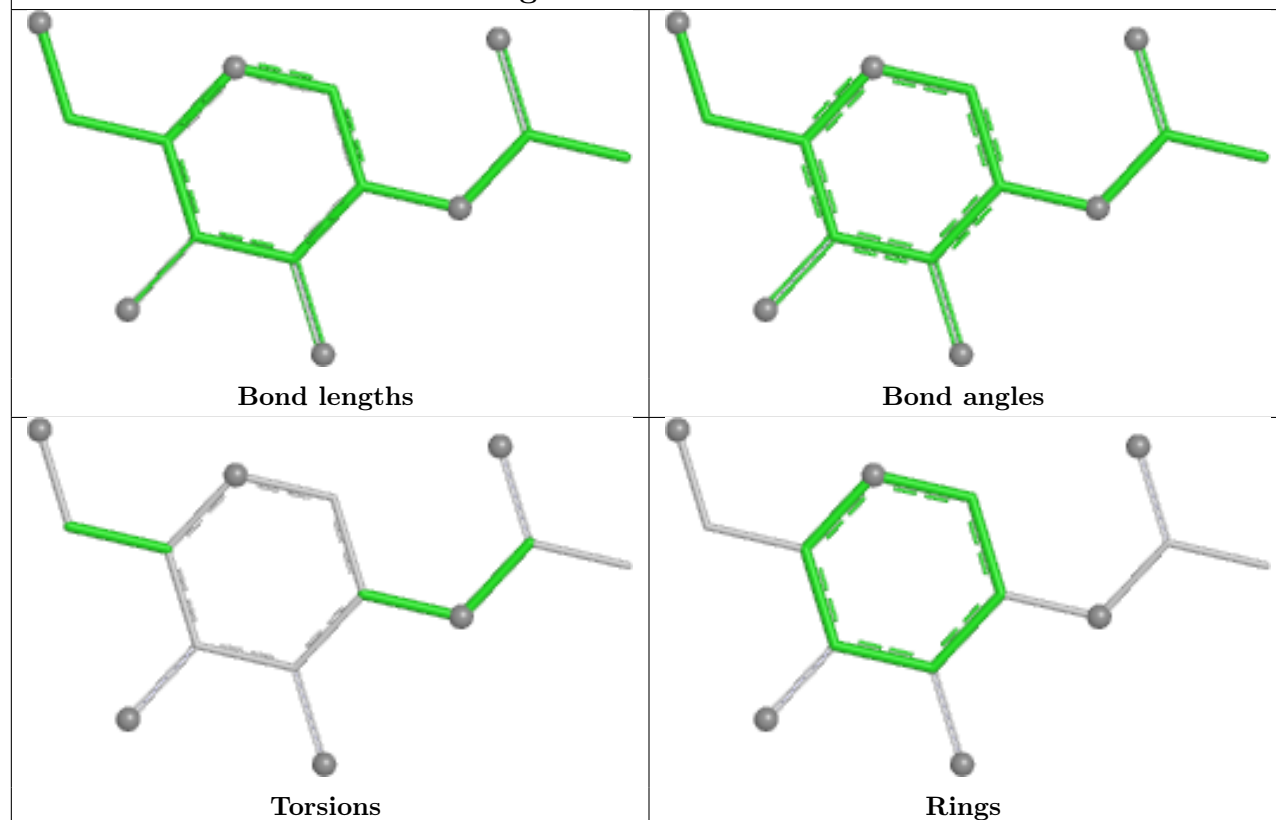
Ligand NAG C 1408



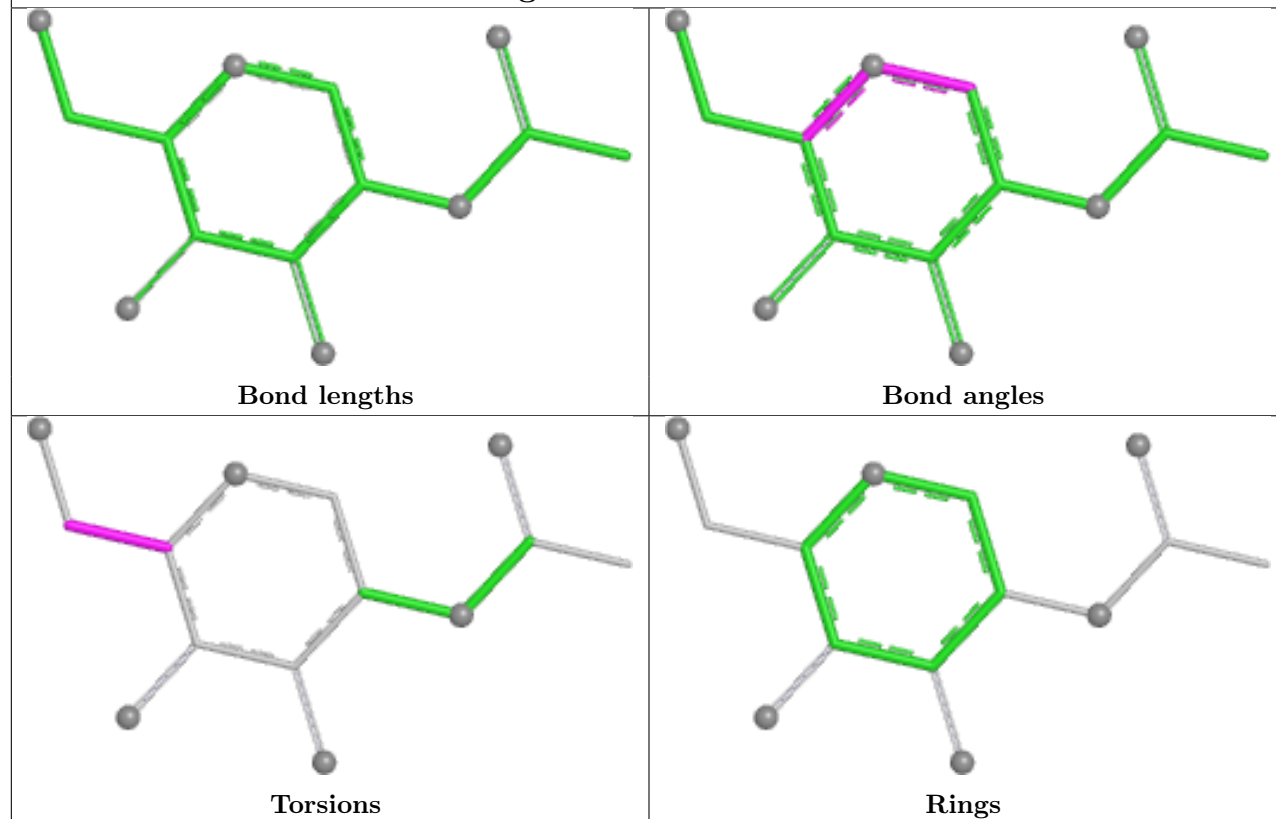
Ligand NAG A 1409



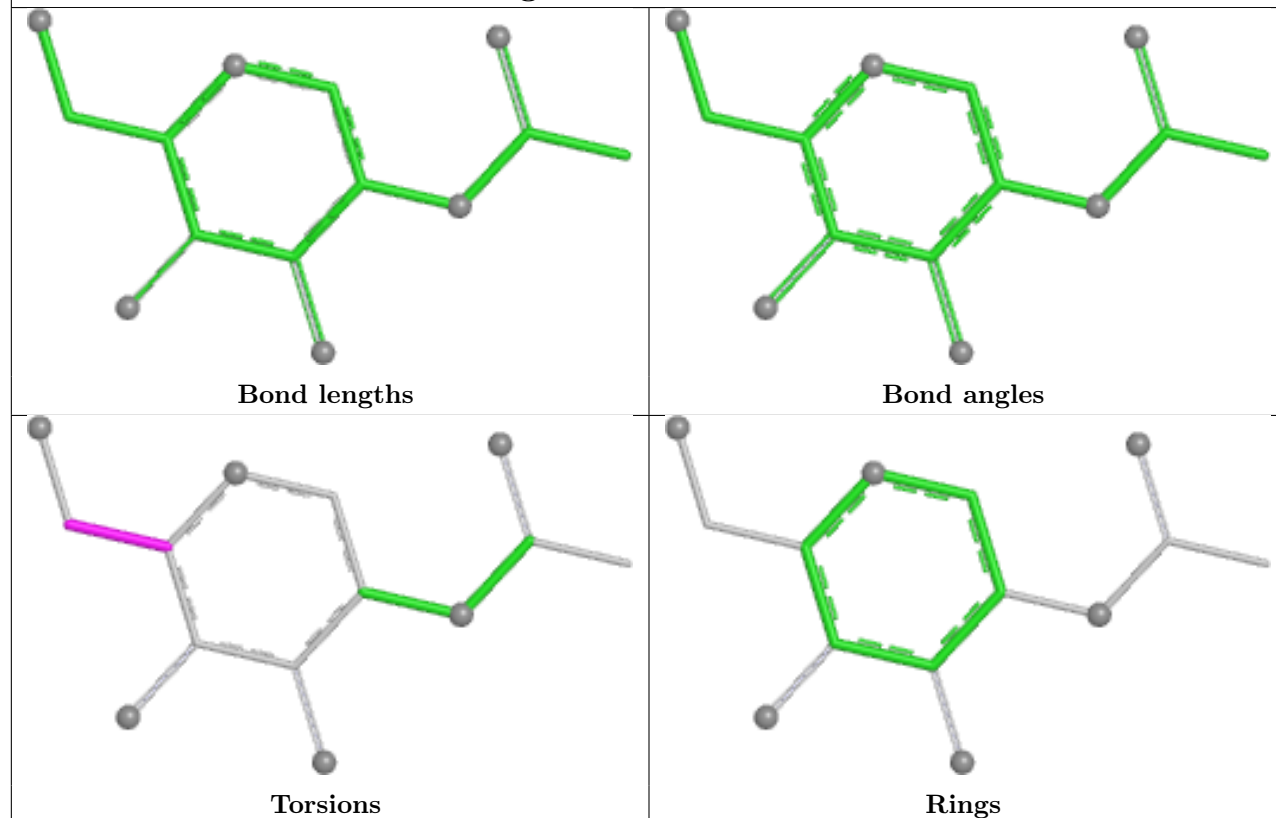
Ligand NAG B 1408



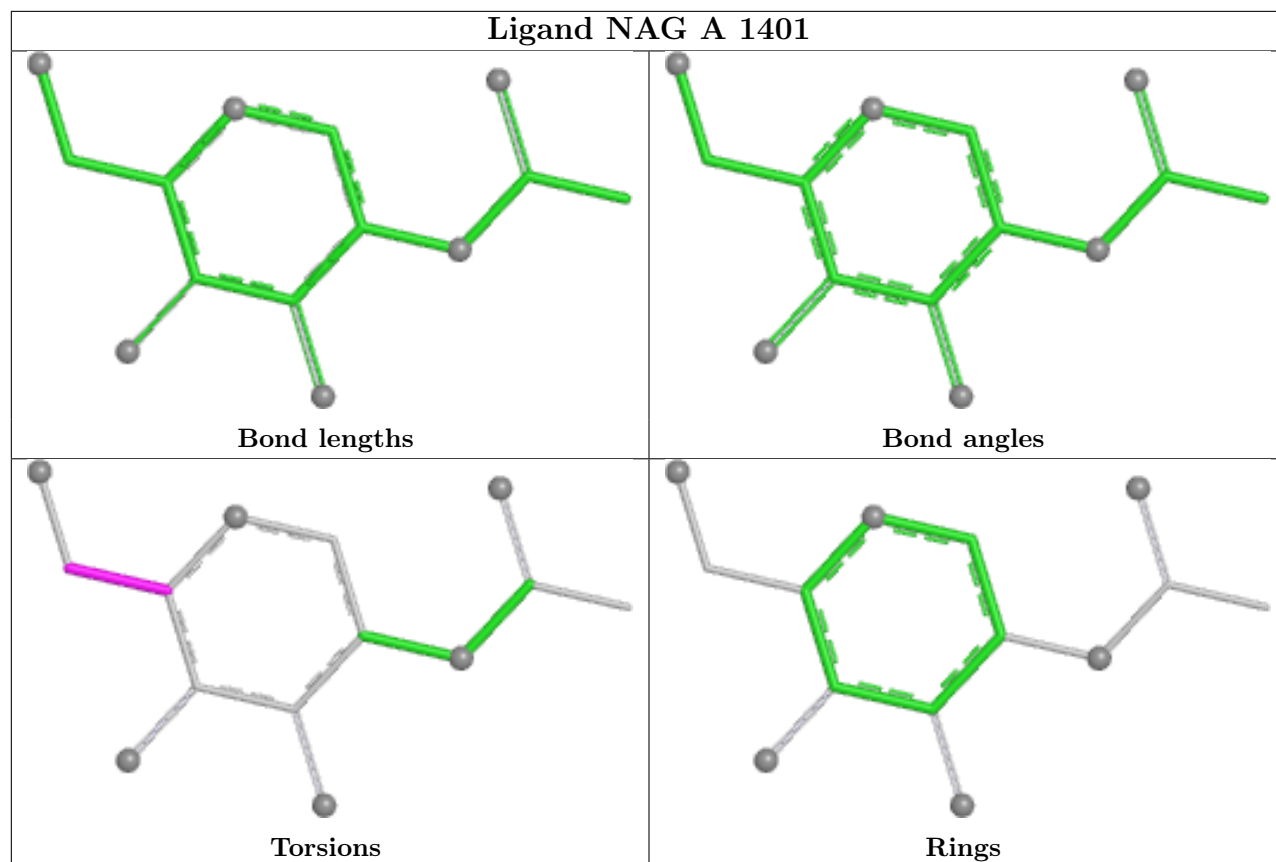
Ligand NAG A 1402



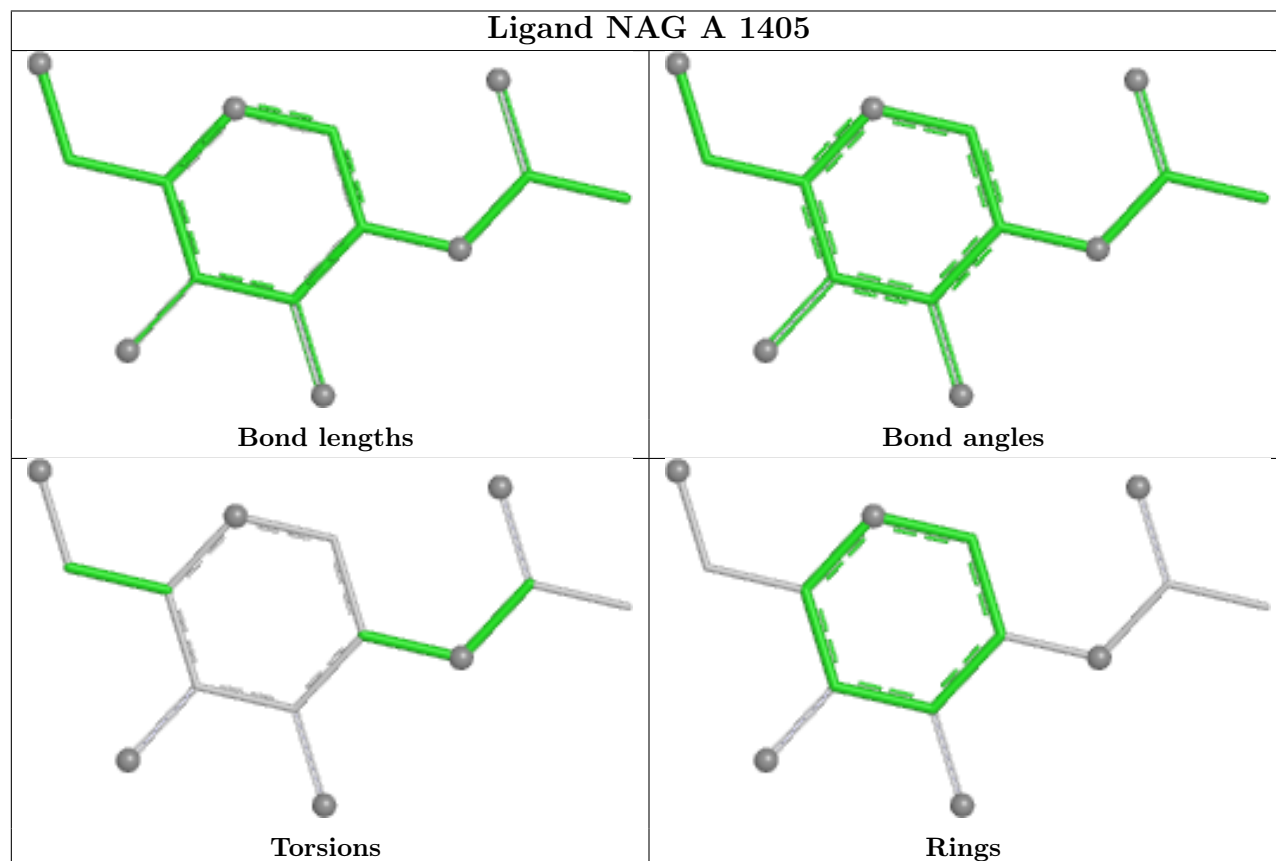
Ligand NAG B 1401



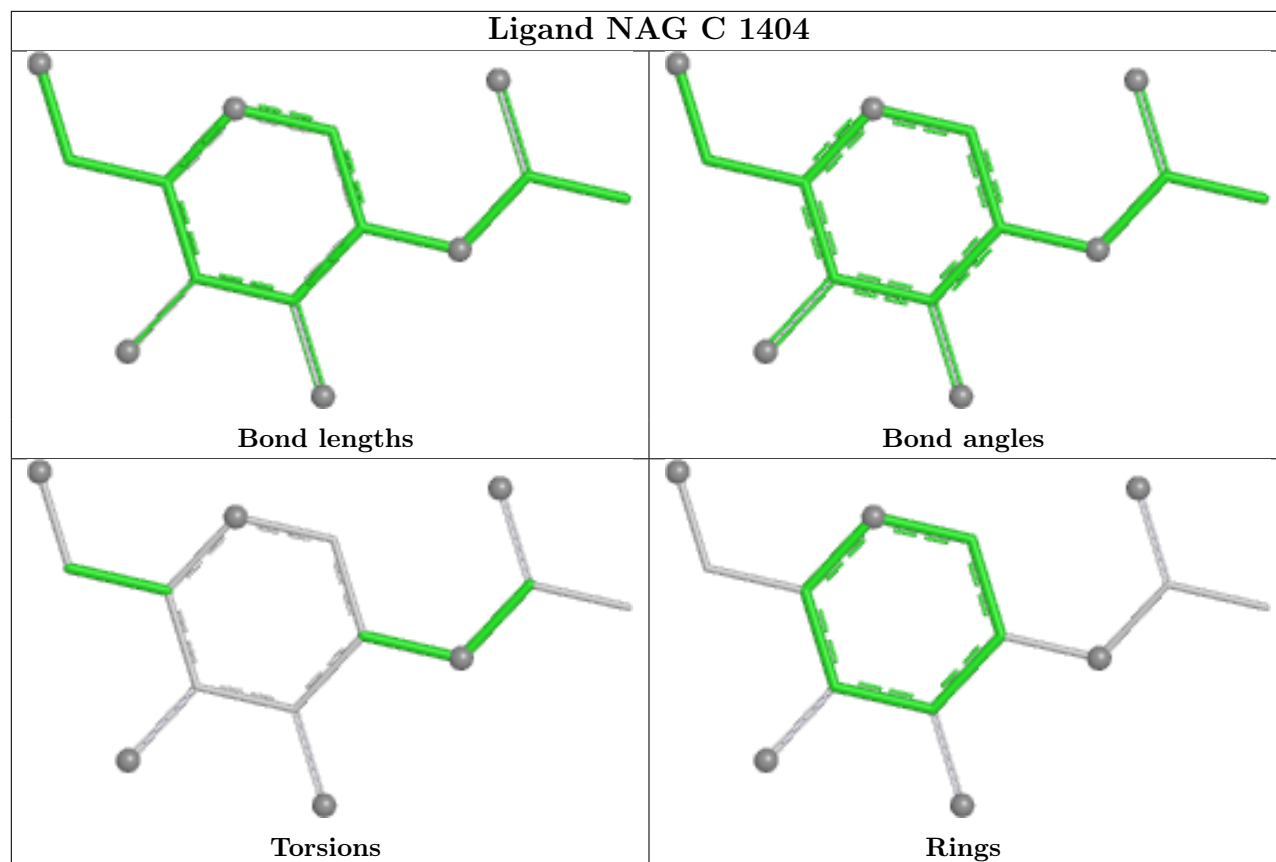
Ligand NAG A 1401



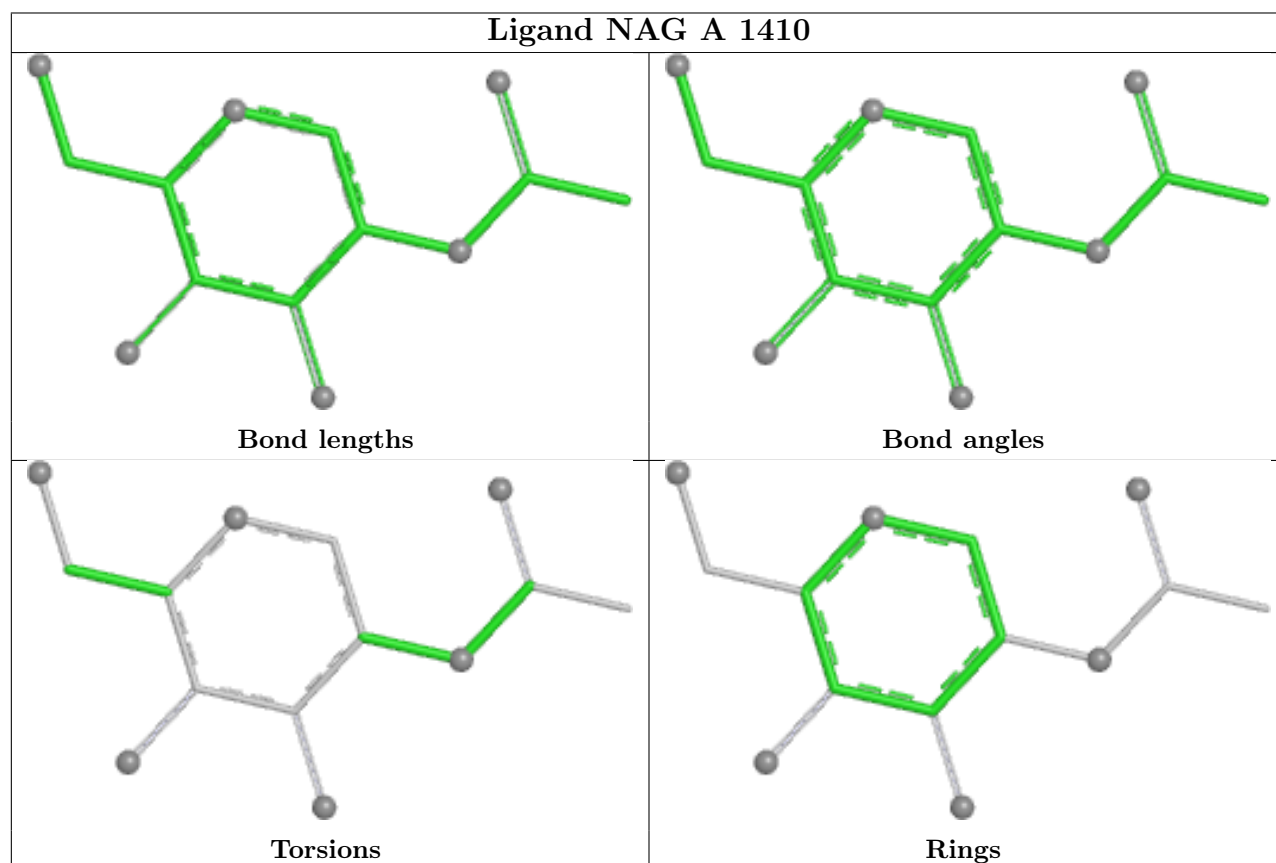
Ligand NAG A 1405



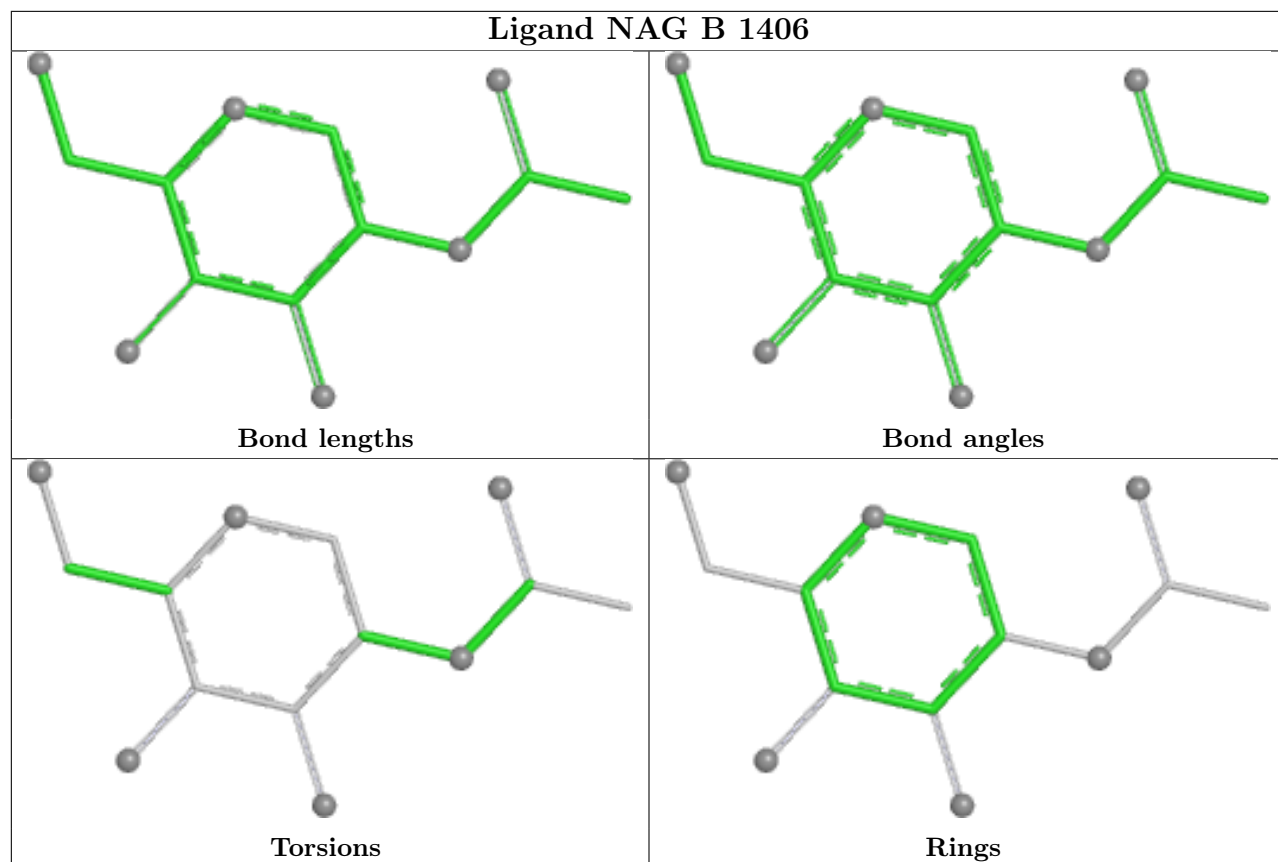
Ligand NAG C 1404



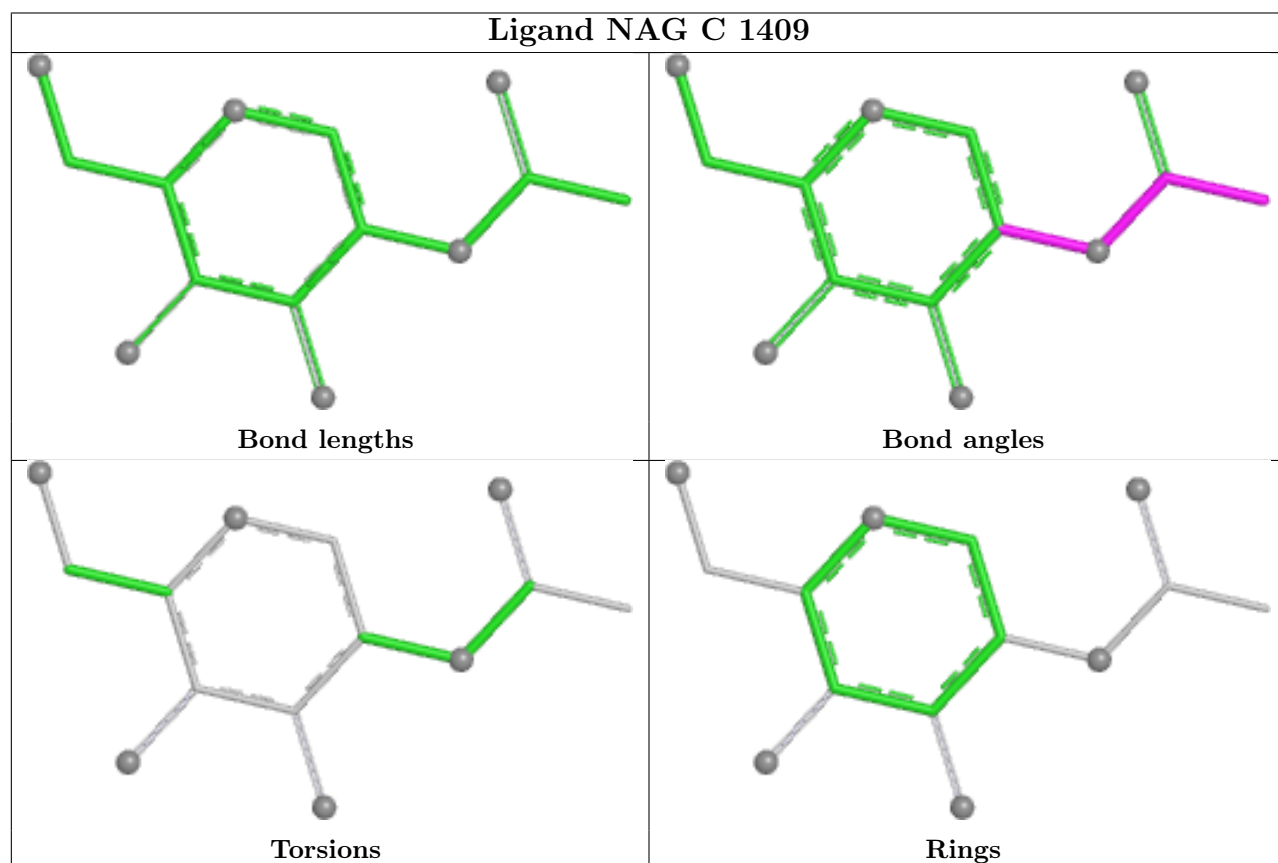
Ligand NAG A 1410



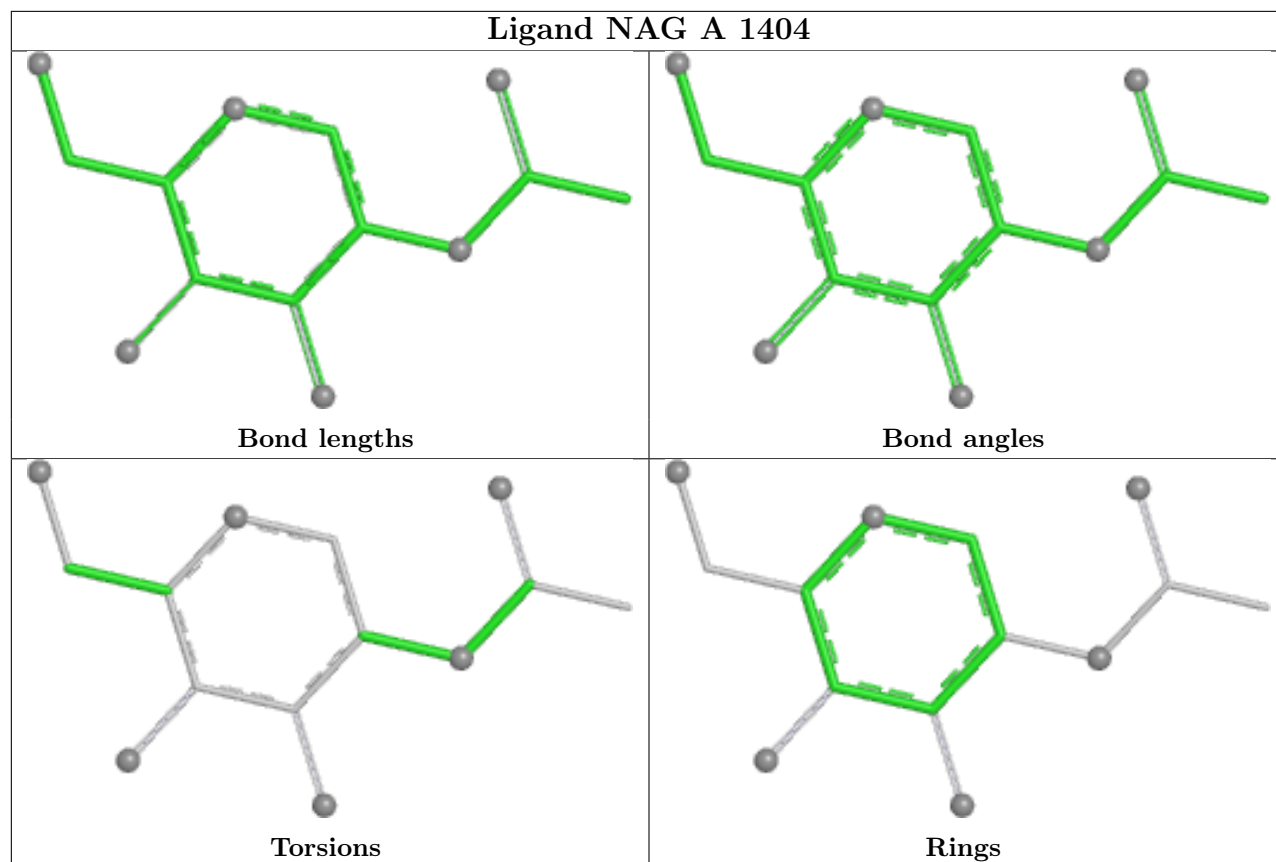
Ligand NAG B 1406



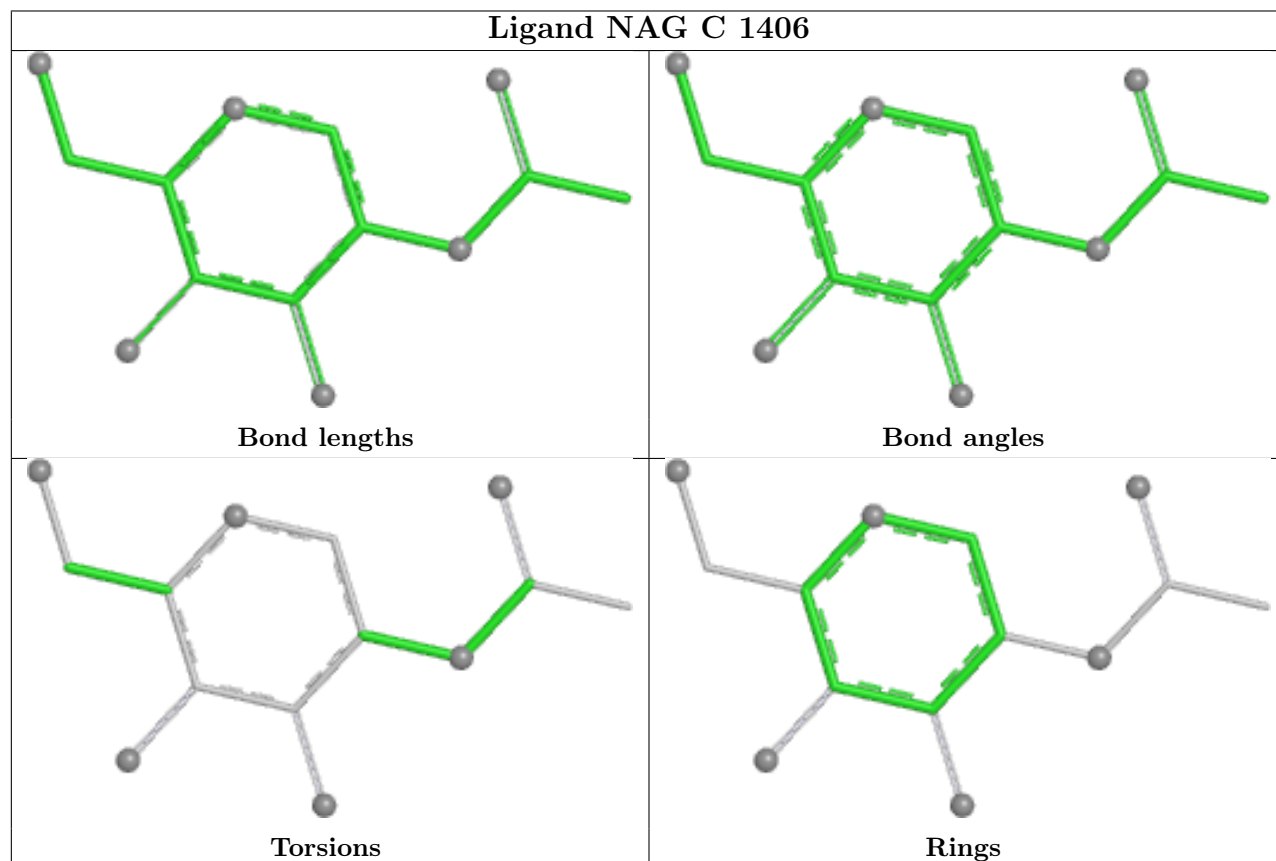
Ligand NAG C 1409



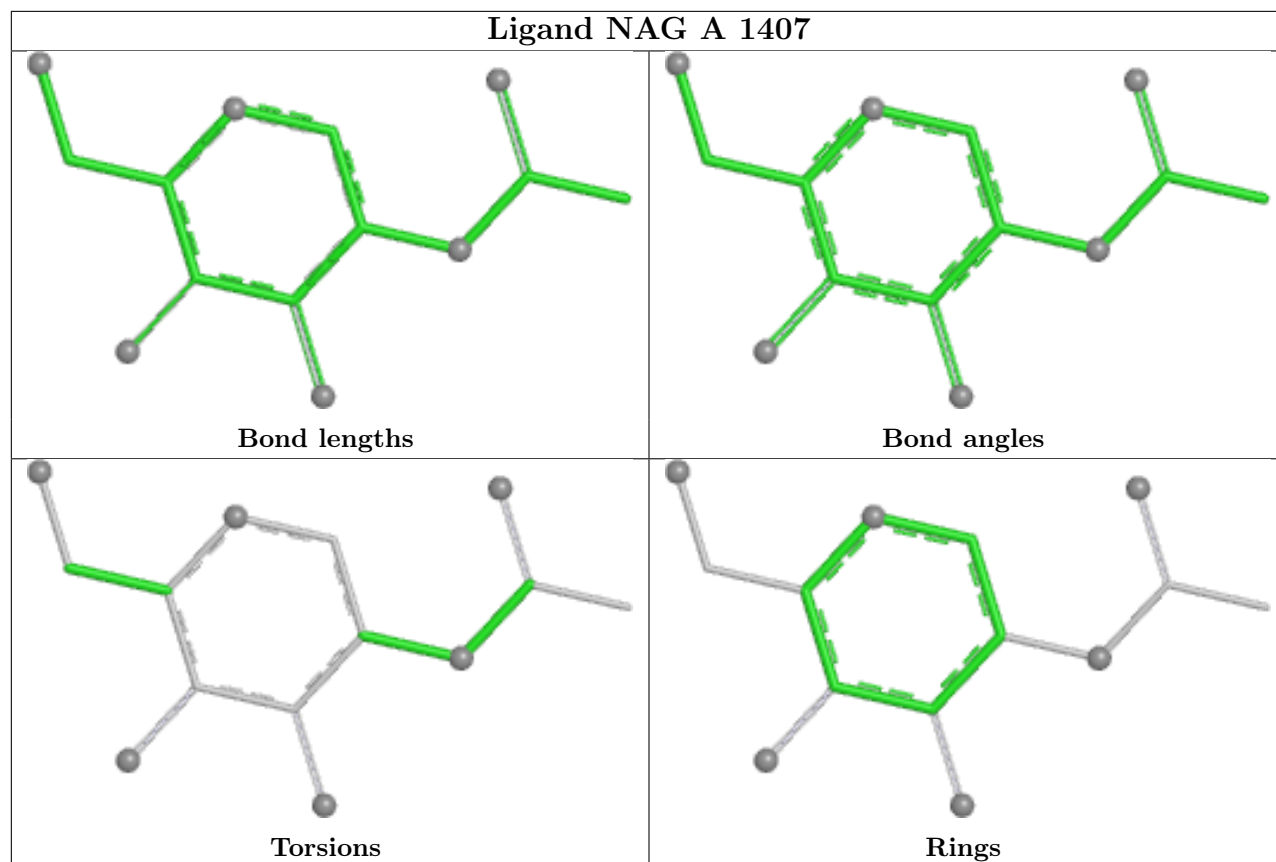
Ligand NAG A 1404



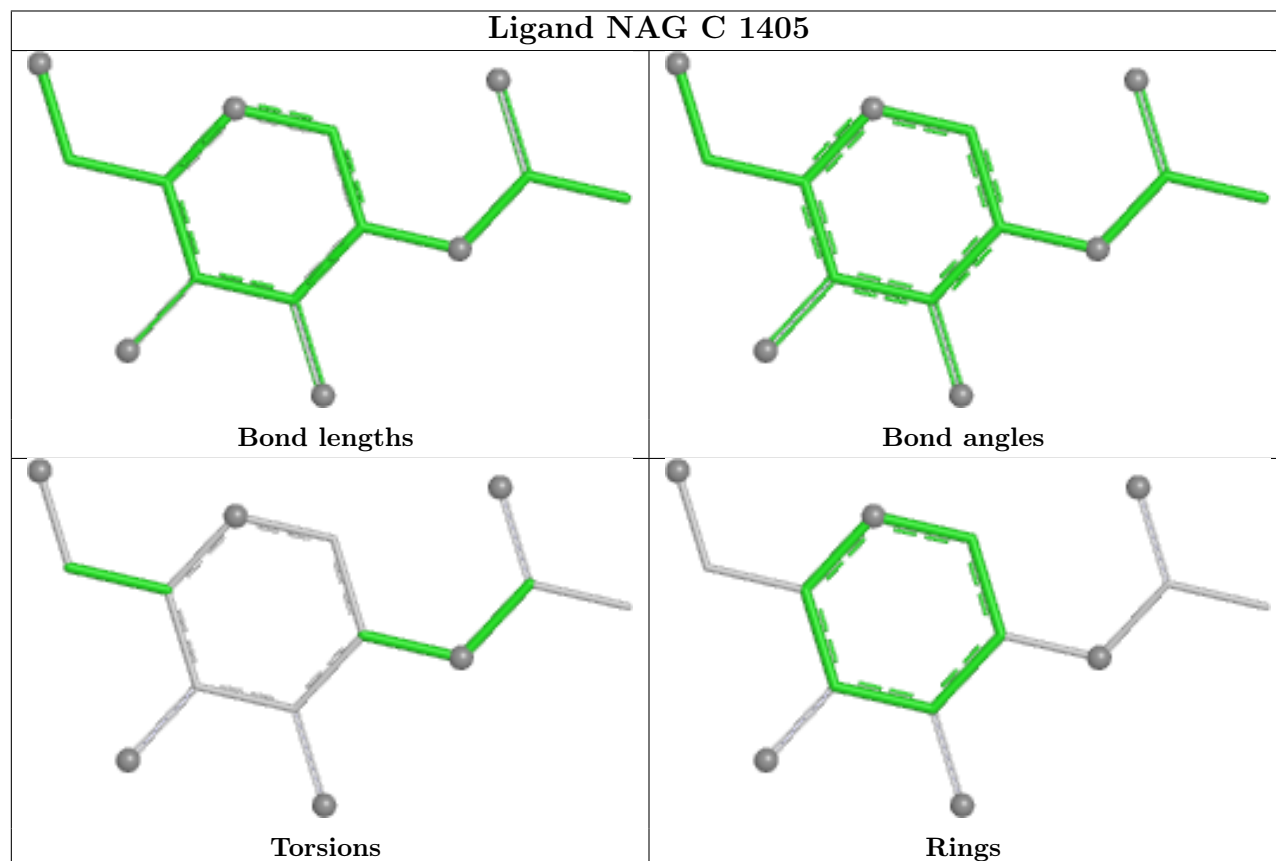
Ligand NAG C 1406

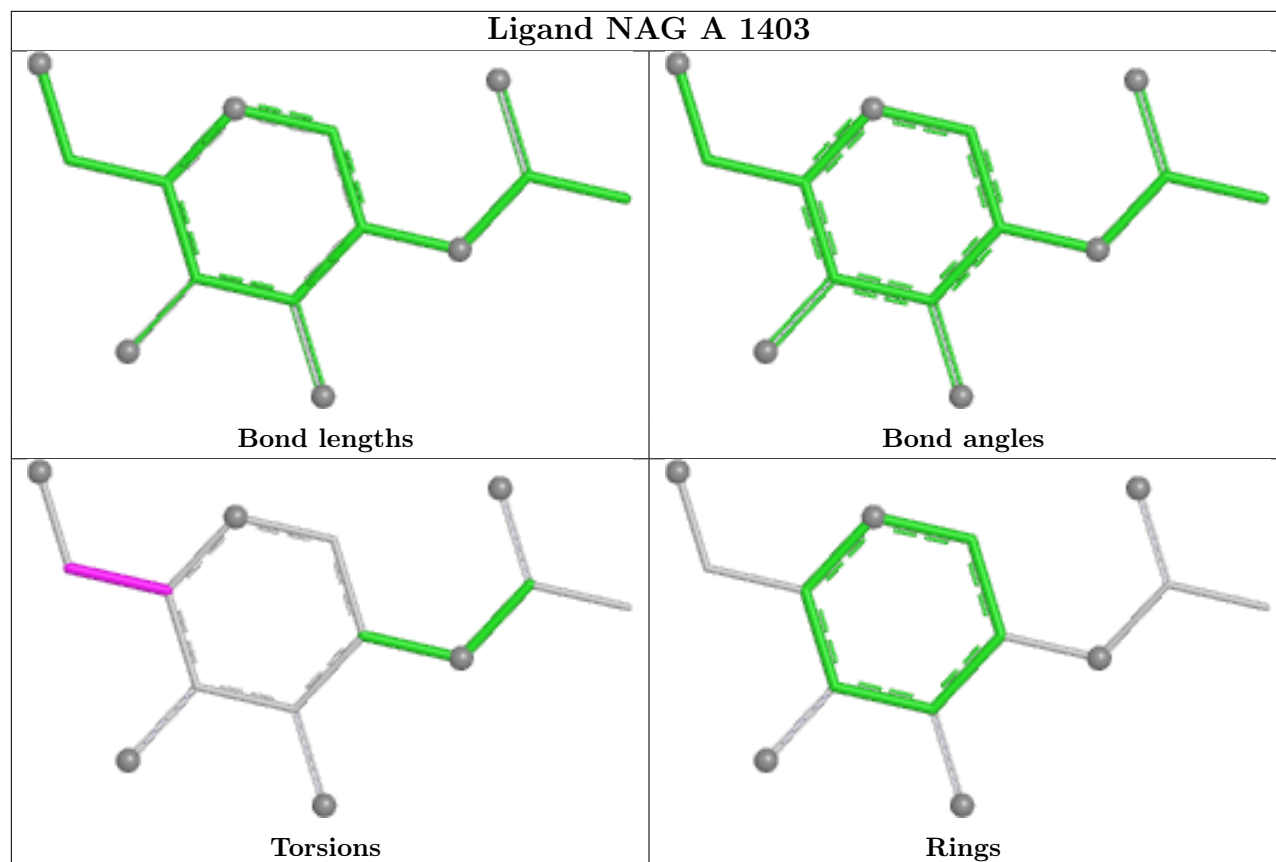


Ligand NAG A 1407



Ligand NAG C 1405





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.

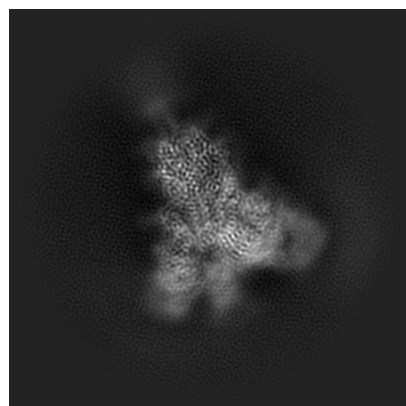
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-34263. These allow visual inspection of the internal detail of the map and identification of artifacts.

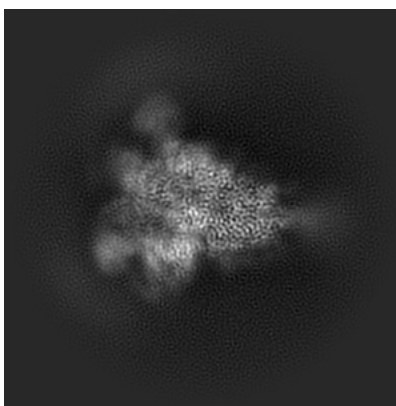
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

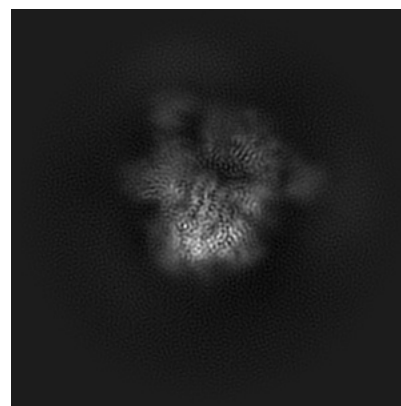
6.1.1 Primary map



X

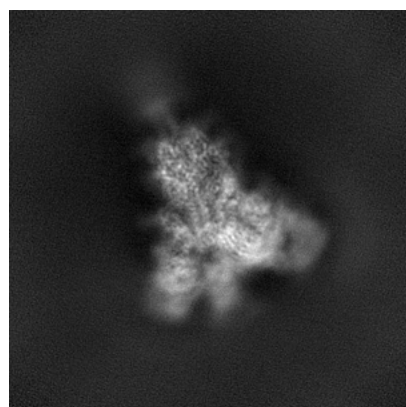


Y

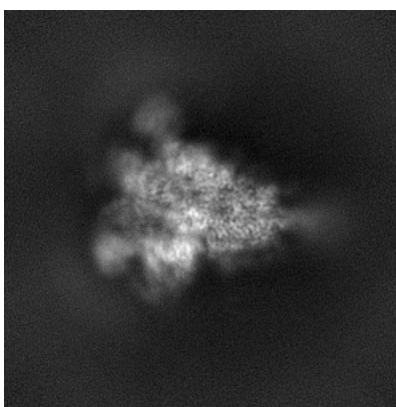


Z

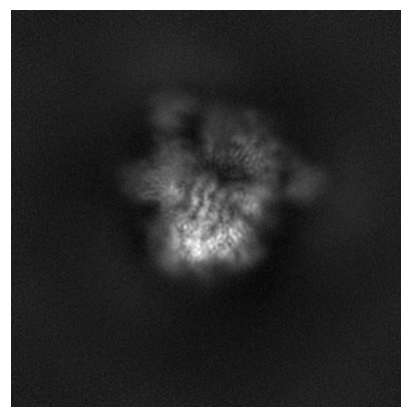
6.1.2 Raw map



X



Y

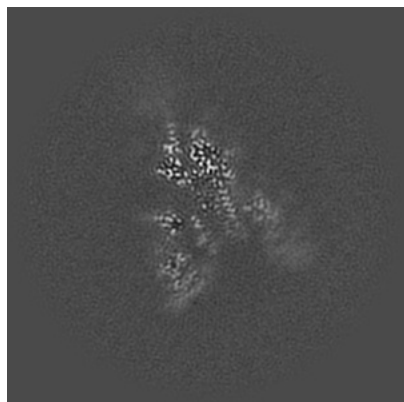


Z

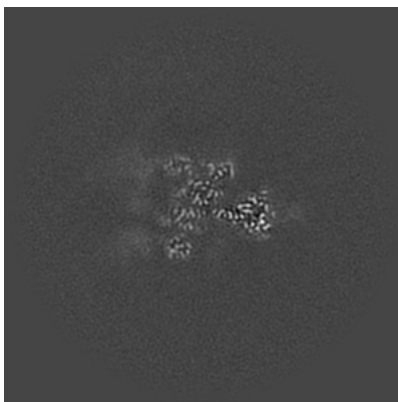
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

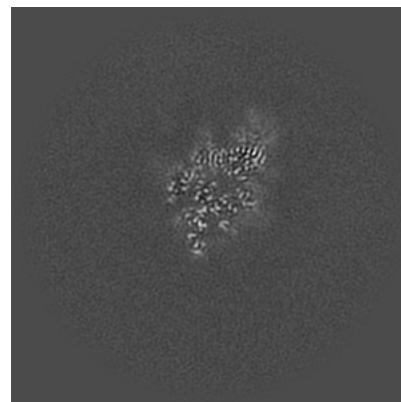
6.2.1 Primary map



X Index: 160

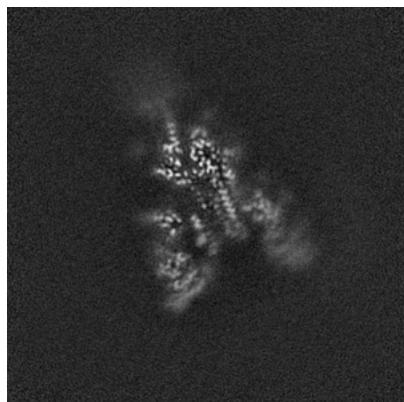


Y Index: 160

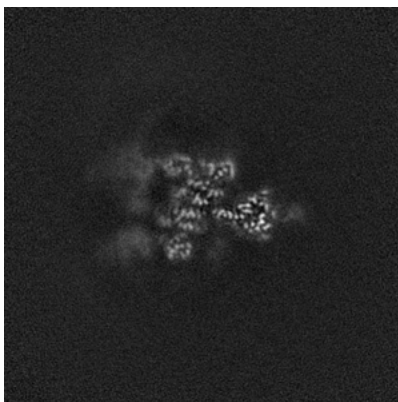


Z Index: 160

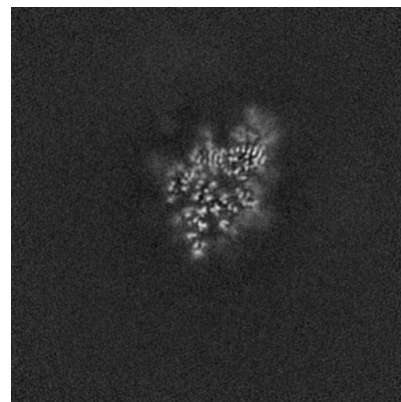
6.2.2 Raw map



X Index: 160



Y Index: 160

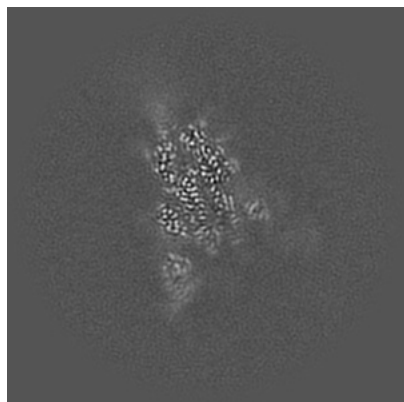


Z Index: 160

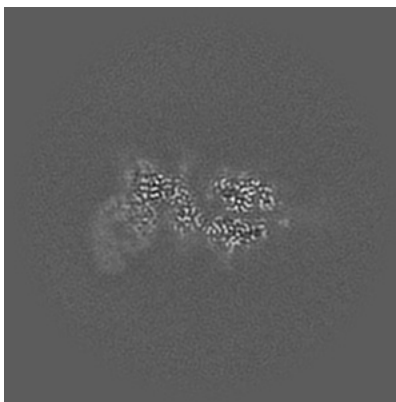
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

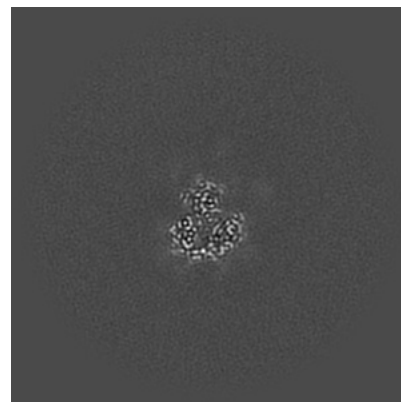
6.3.1 Primary map



X Index: 150

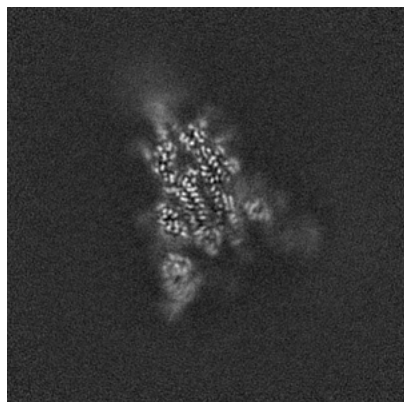


Y Index: 135

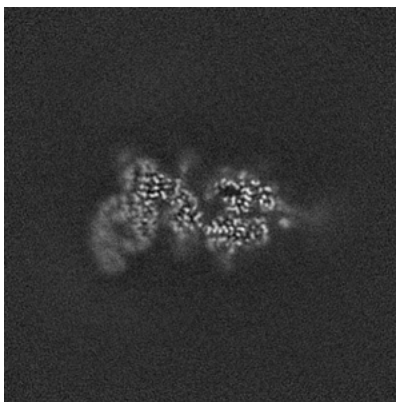


Z Index: 189

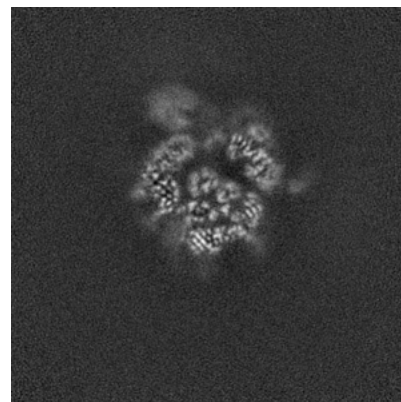
6.3.2 Raw map



X Index: 150



Y Index: 134

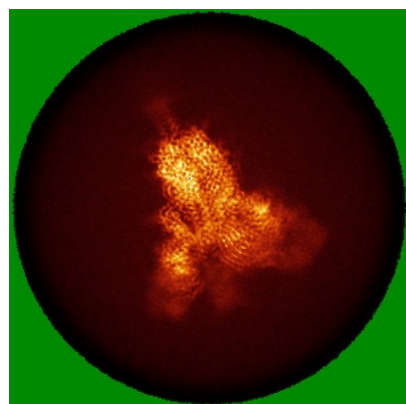


Z Index: 144

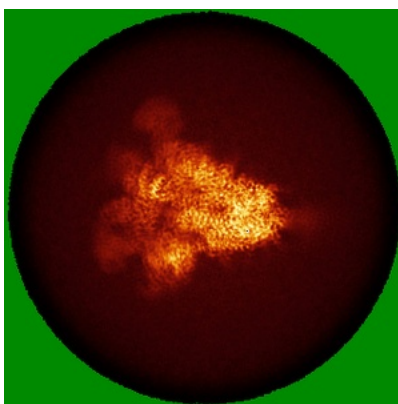
The images above show the largest variance slices of the map in three orthogonal directions.

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

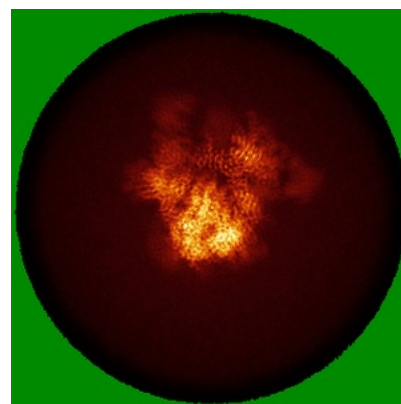
6.4.1 Primary map



X

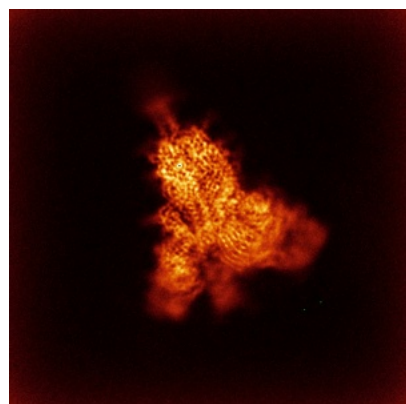


Y

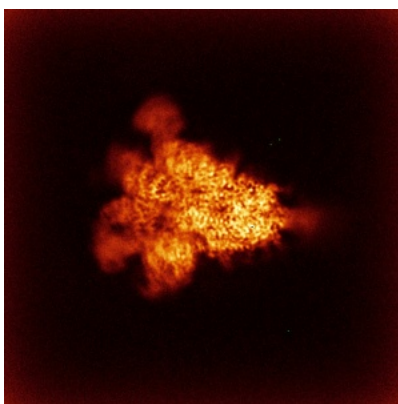


Z

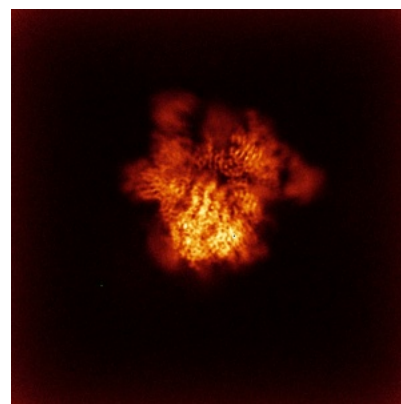
6.4.2 Raw map



X



Y

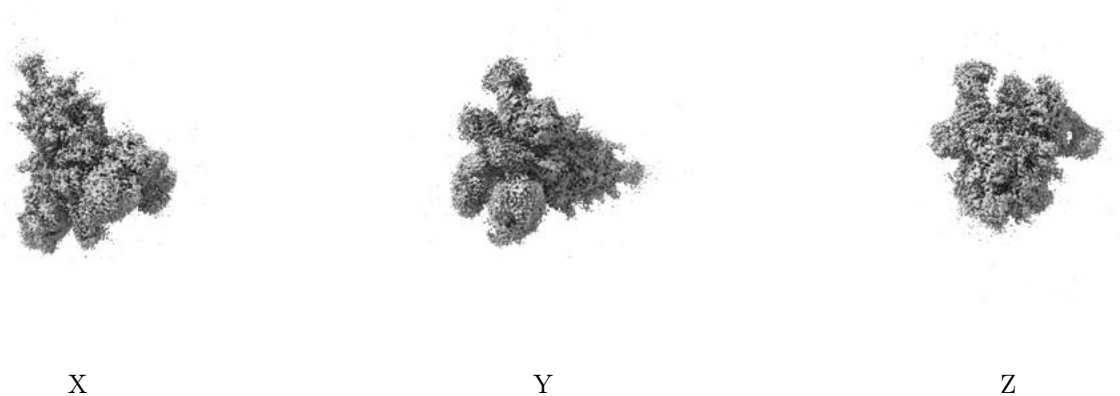


Z

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

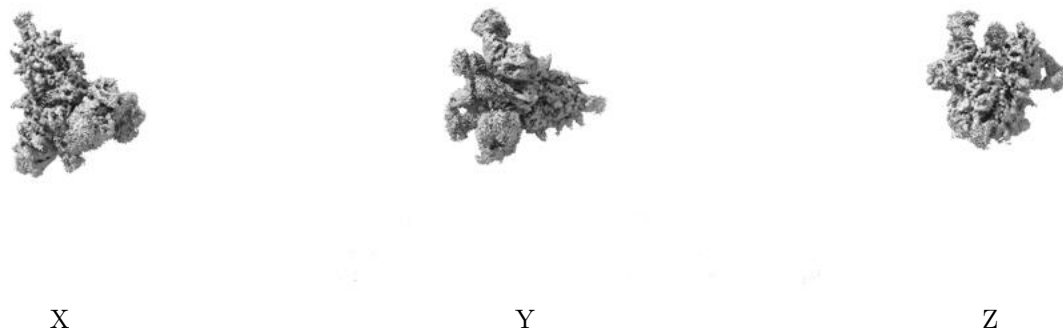
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.3. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

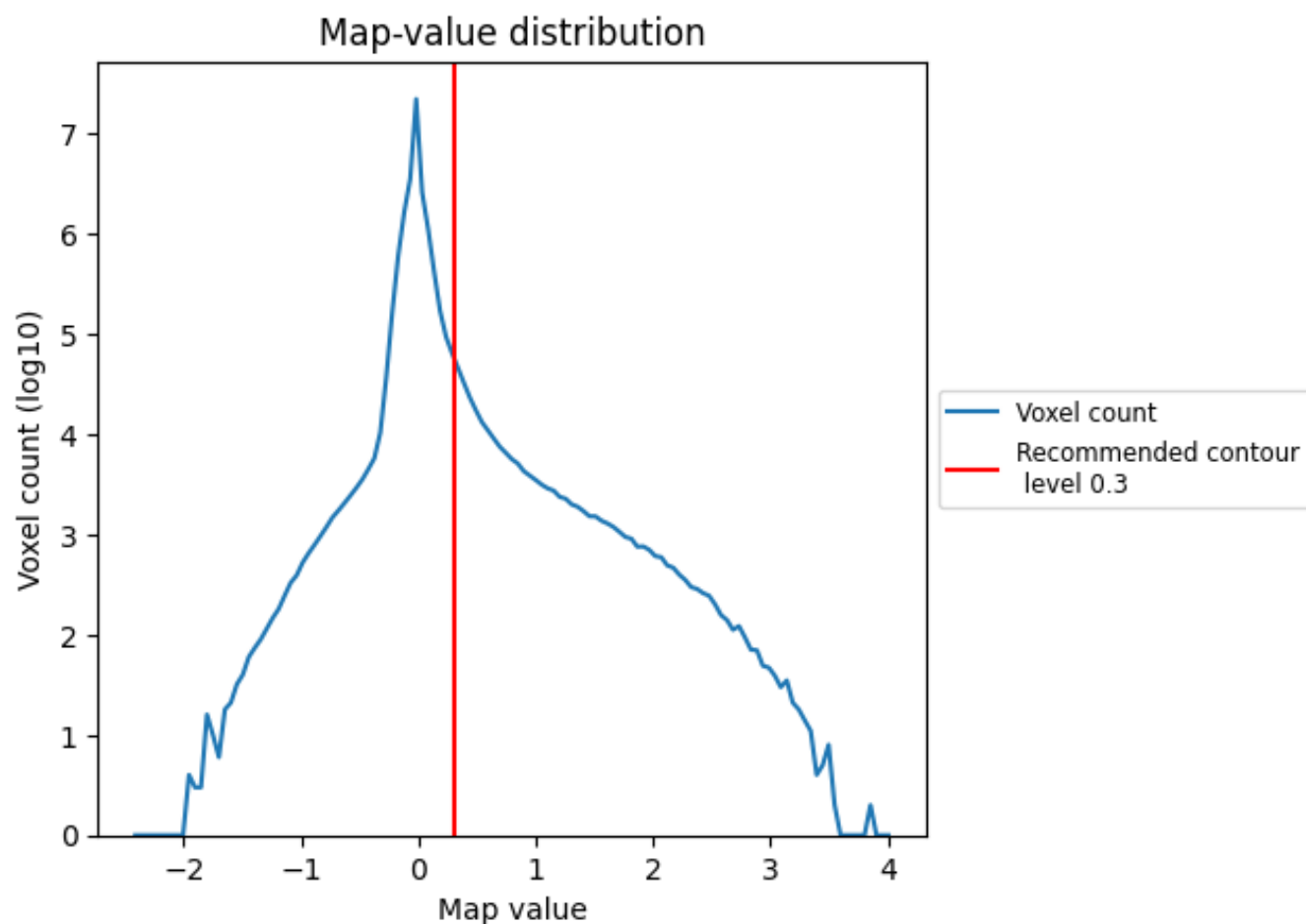
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

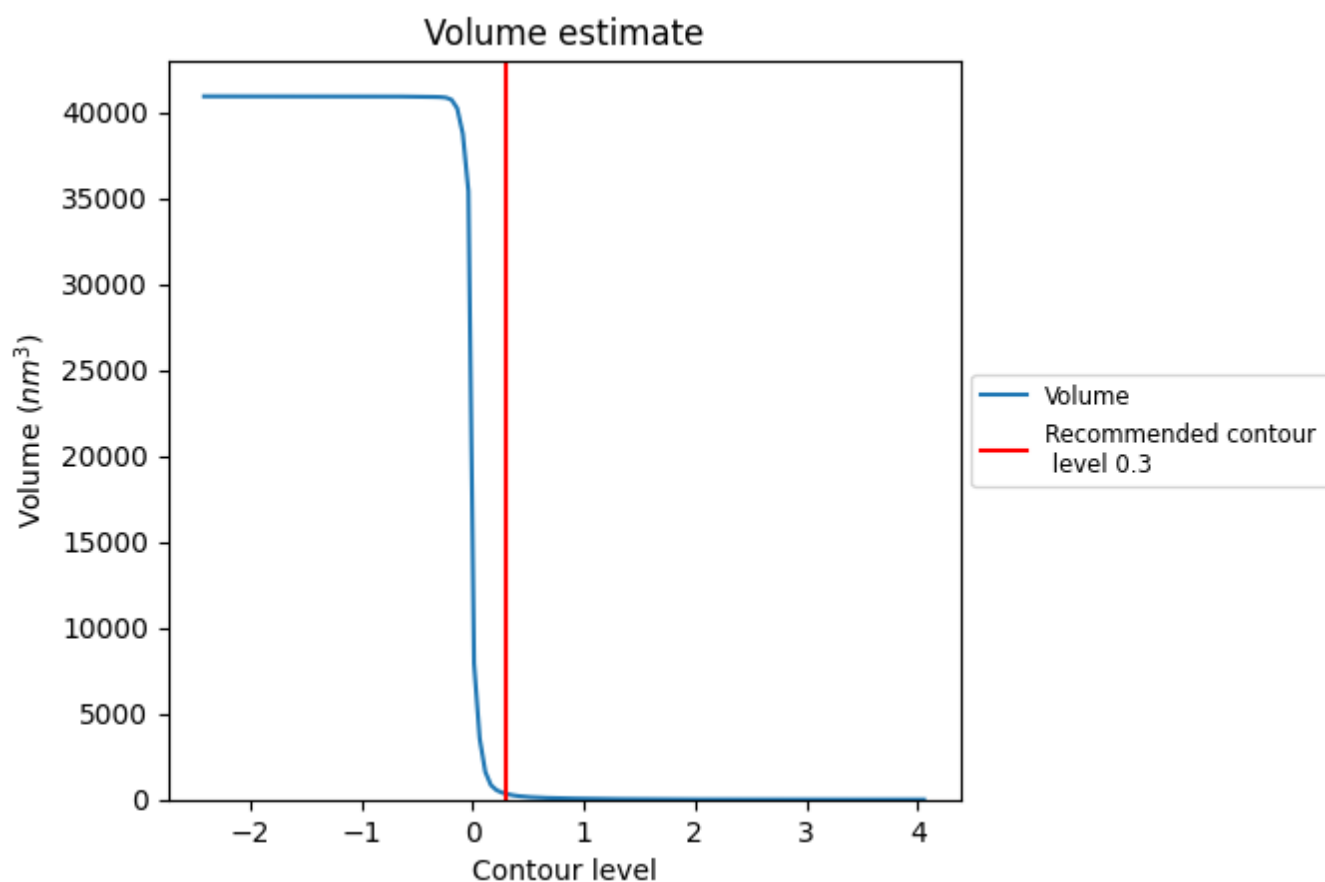
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

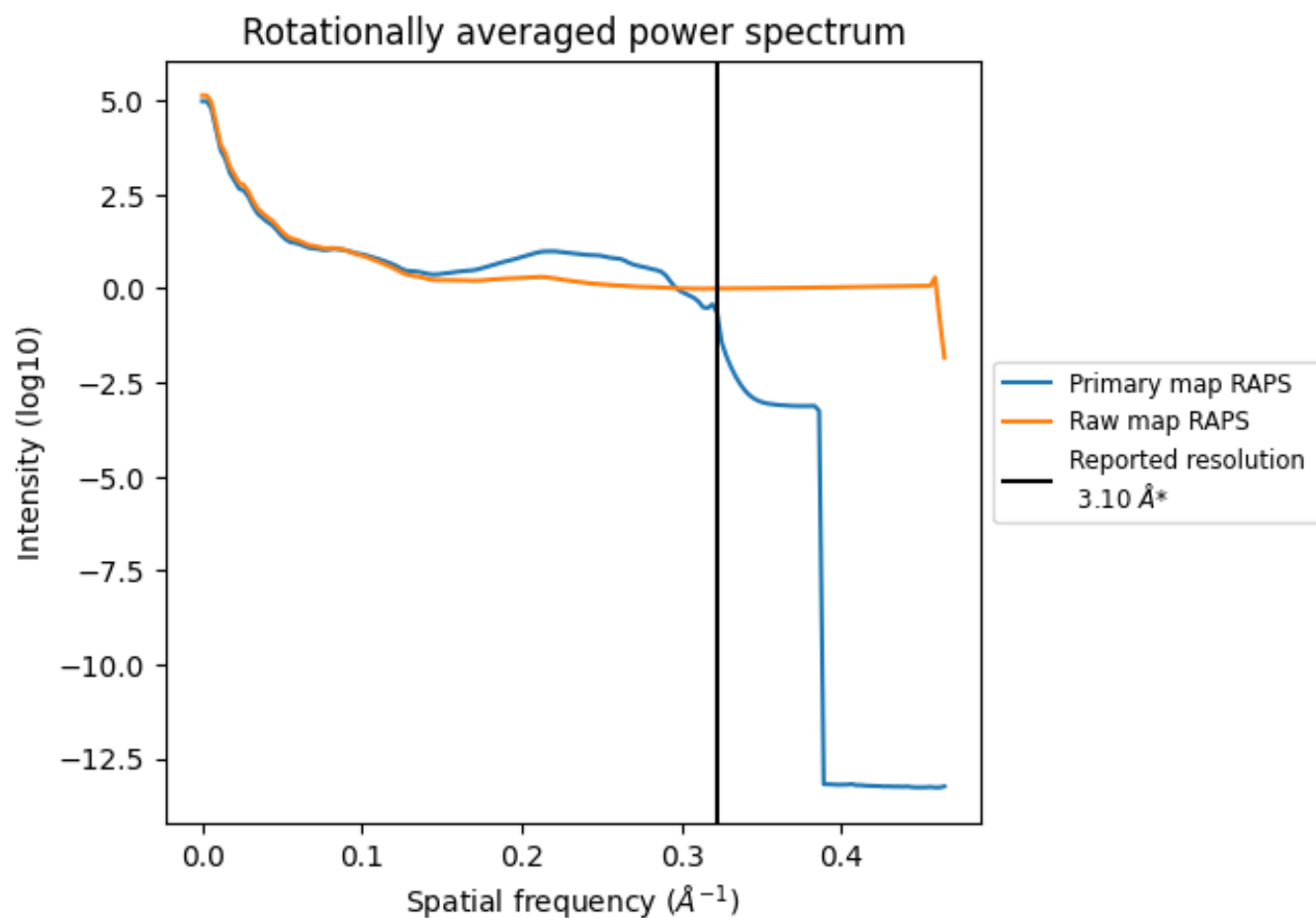
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 342 nm^3 ; this corresponds to an approximate mass of 309 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 ⓘ

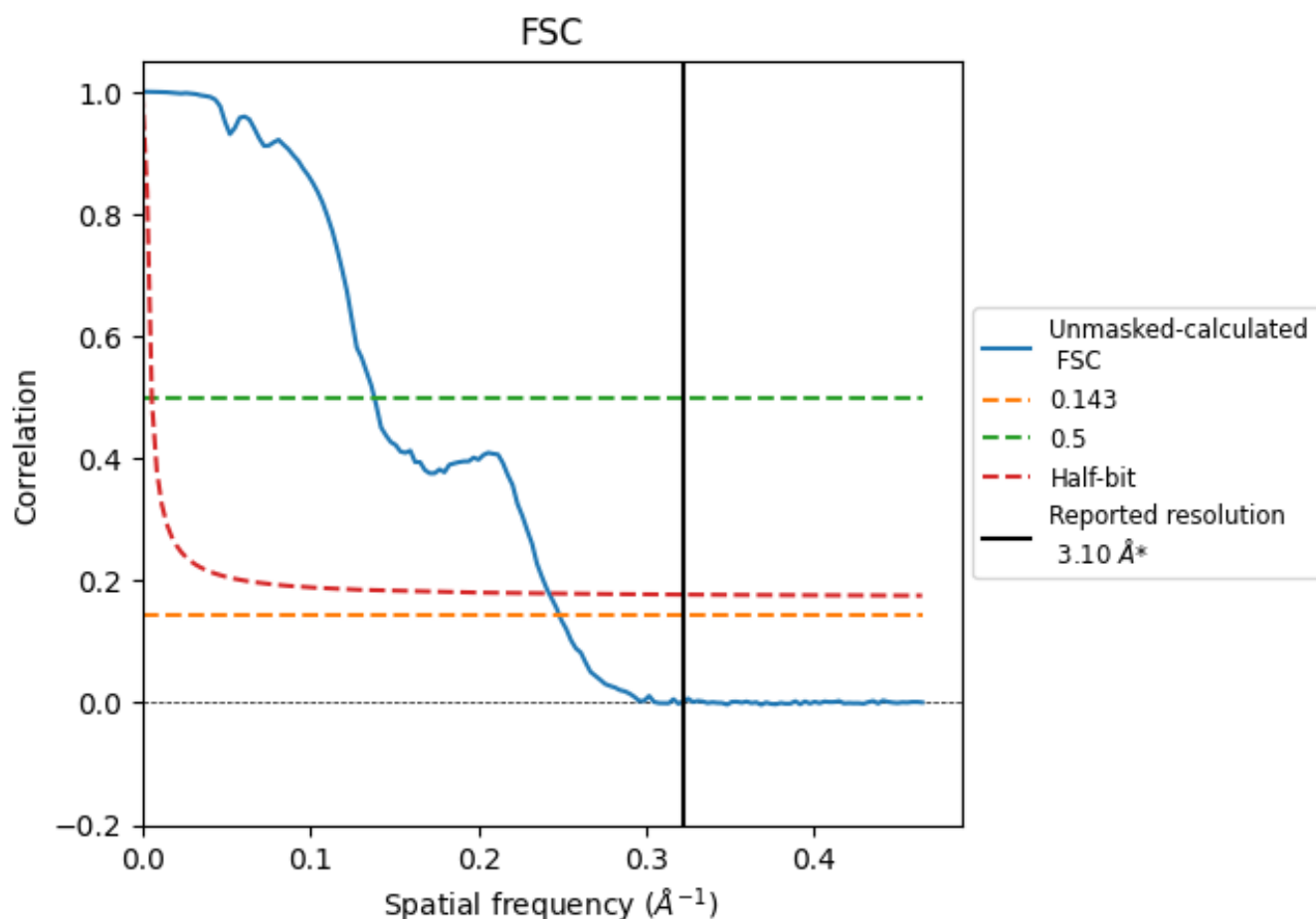


*Reported resolution corresponds to spatial frequency of 0.323 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.323 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

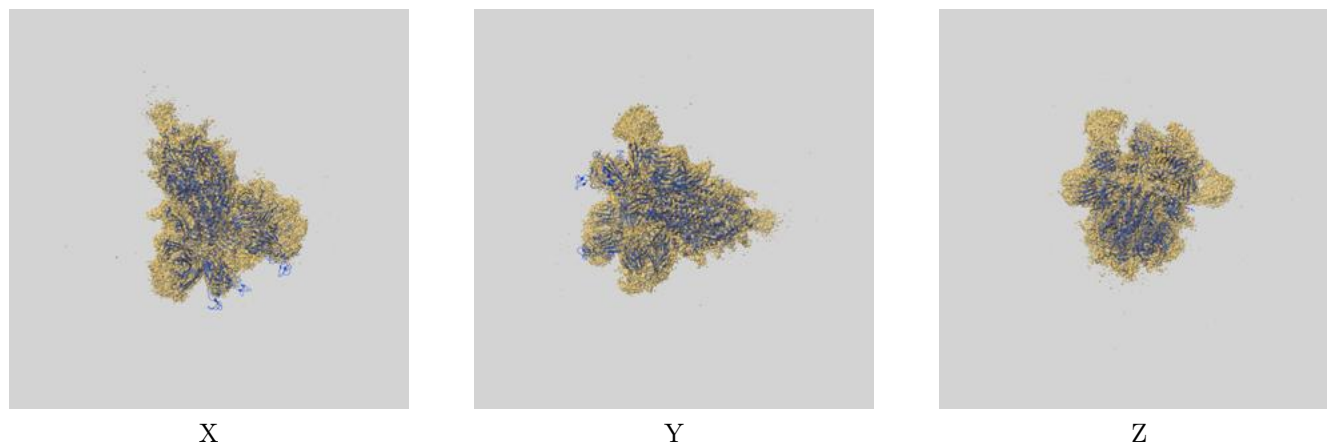
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.03	7.24	4.13

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.03 differs from the reported value 3.1 by more than 10 %

9 Map-model fit [i](#)

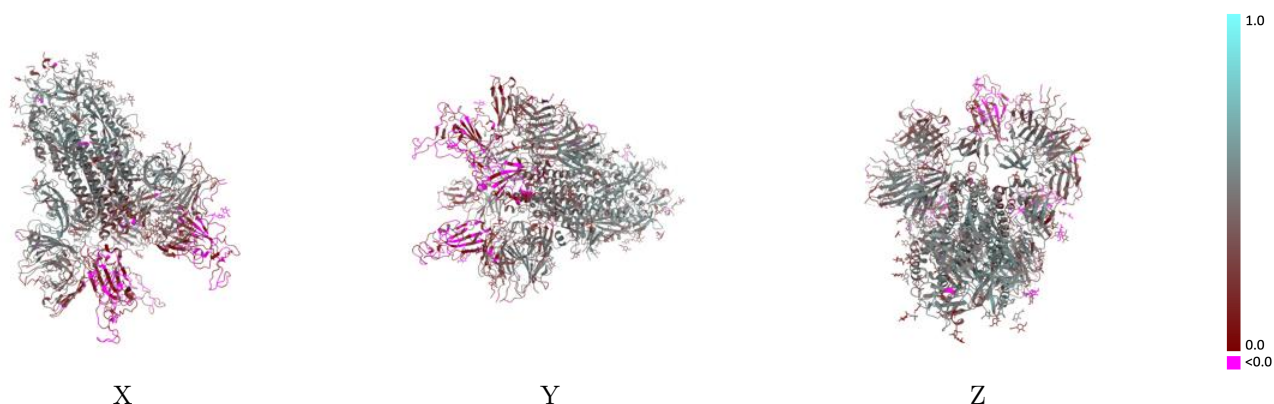
This section contains information regarding the fit between EMDB map EMD-34263 and PDB model 8GTQ. Per-residue inclusion information can be found in section [3](#) on page [12](#).

9.1 Map-model overlay [i](#)



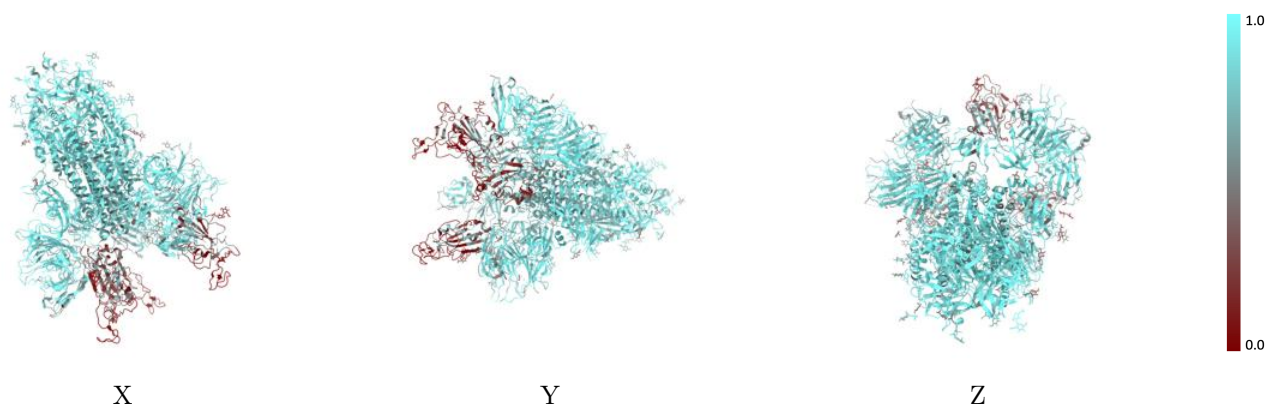
The images above show the 3D surface view of the map at the recommended contour level 0.3 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



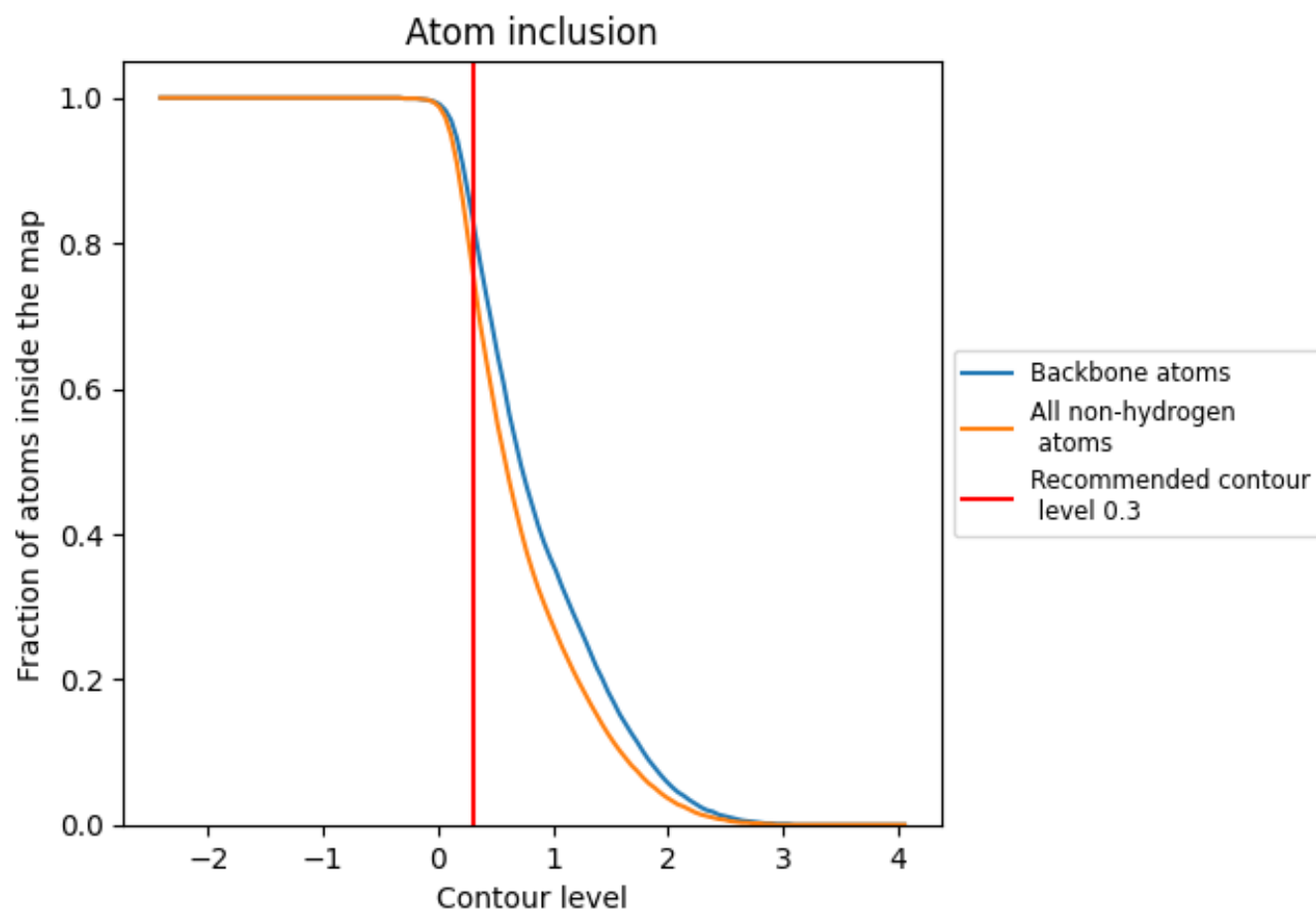
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.3).

9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 76% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7640	 0.3620
A	 0.7630	 0.3740
B	 0.7550	 0.3760
C	 0.7500	 0.3600
D	 0.5950	 0.2050
E	 0.6430	 0.2160
F	 0.0000	 -0.0100
G	 0.7860	 0.3910
H	 0.8390	 0.3590
I	 0.8700	 0.4000
J	 0.8440	 0.3830
K	 0.8210	 0.3570
L	 0.7980	 0.2710
M	 0.7730	 0.2970
N	 0.7680	 0.3000
O	 0.8570	 0.3790
P	 0.8930	 0.3690
Q	 0.5480	 0.2920
R	 0.6790	 0.3480
S	 0.0360	 -0.0910
T	 0.7140	 0.3110
U	 0.8930	 0.3660
V	 0.7500	 0.1820
W	 0.7500	 0.2730
X	 0.6190	 0.2430
Y	 0.6430	 0.2090
Z	 0.0000	 -0.1600
a	 0.7140	 0.2750
b	 0.7500	 0.3180
c	 0.7140	 0.2570
d	 0.7860	 0.3190

