



## Full wwPDB EM Validation Report ⓘ

Nov 22, 2022 – 01:45 AM JST

PDB ID : 7DX5  
EMDB ID : EMD-30896  
Title : S protein of SARS-CoV-2 bound with PD of ACE2 in the conformation 2 (1 up RBD and 1 PD bound)  
Authors : Yan, R.H.; Zhang, Y.Y.; Li, Y.N.; Ye, F.F.; Guo, Y.Y.; Xia, L.; Zhong, X.Y.; Chi, X.M.; Zhou, Q.  
Deposited on : 2021-01-18  
Resolution : 3.30 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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

EMDB validation analysis : 0.0.1.dev43  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.3

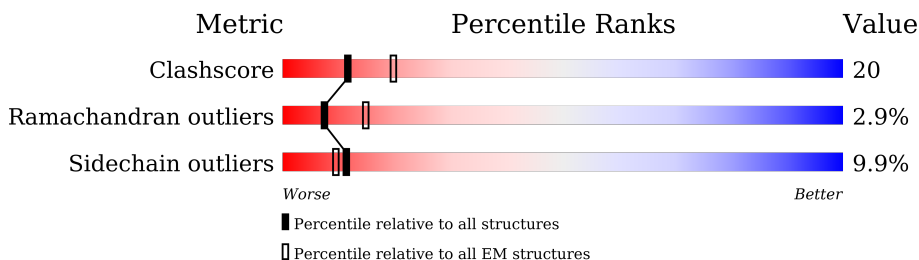
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1283	
1	B	1283	
1	C	1283	
2	D	817	
3	E	2	
3	F	2	
3	G	2	
3	H	2	

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Mol	Chain	Length	Quality of chain
3	I	2	50% 50%
3	J	2	50% 50%
3	K	2	50% 50%
3	L	2	100% 100%
3	M	2	50% 100%
3	N	2	50% 50%
3	O	2	50% 50%
3	P	2	100%
3	Q	2	50% 100%
3	R	2	100% 100%
3	S	2	50% 50%
3	T	2	50% 50%
3	U	2	50% 50%
3	V	2	100%
3	W	2	50% 50%
3	X	2	100%
3	Y	2	100%
3	Z	2	100% 50%
3	a	2	50% 50%
3	b	2	100% 100%
3	c	2	100% 100%
3	d	2	50% 50%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	NAG	B	1407	-	-	X	-

## 2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 29045 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
			Total	C	N	O	S		
1	A	1007	7872	5025	1310	1501	36	0	0
1	B	971	7584	4843	1262	1445	34	0	0
1	C	971	7584	4843	1262	1445	34	0	0

There are 36 discrepancies between the modelled and reference sequences:

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

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

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

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

There are 13 discrepancies between the modelled and reference sequences:

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

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



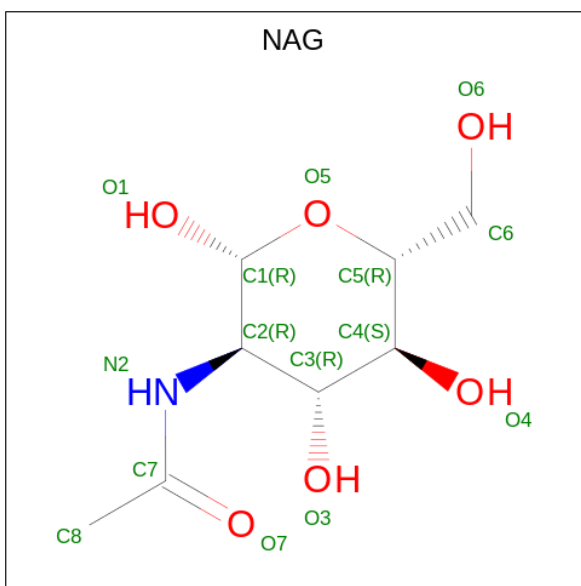
Mol	Chain	Residues	Atoms				AltConf	Trace
3	E	2	Total 28	C 16	N 2	O 10	0	0
3	F	2	Total 28	C 16	N 2	O 10	0	0
3	G	2	Total 28	C 16	N 2	O 10	0	0
3	H	2	Total 28	C 16	N 2	O 10	0	0
3	I	2	Total 28	C 16	N 2	O 10	0	0
3	J	2	Total 28	C 16	N 2	O 10	0	0
3	K	2	Total 28	C 16	N 2	O 10	0	0
3	L	2	Total 28	C 16	N 2	O 10	0	0
3	M	2	Total 28	C 16	N 2	O 10	0	0
3	N	2	Total 28	C 16	N 2	O 10	0	0
3	O	2	Total 28	C 16	N 2	O 10	0	0
3	P	2	Total 28	C 16	N 2	O 10	0	0
3	Q	2	Total 28	C 16	N 2	O 10	0	0
3	R	2	Total 28	C 16	N 2	O 10	0	0
3	S	2	Total 28	C 16	N 2	O 10	0	0
3	T	2	Total 28	C 16	N 2	O 10	0	0
3	U	2	Total 28	C 16	N 2	O 10	0	0
3	V	2	Total 28	C 16	N 2	O 10	0	0
3	W	2	Total 28	C 16	N 2	O 10	0	0
3	X	2	Total 28	C 16	N 2	O 10	0	0
3	Y	2	Total 28	C 16	N 2	O 10	0	0
3	Z	2	Total 28	C 16	N 2	O 10	0	0

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Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	a	2	Total 28	C 16	N 2	O 10	0	0
3	b	2	Total 28	C 16	N 2	O 10	0	0
3	c	2	Total 28	C 16	N 2	O 10	0	0
3	d	2	Total 28	C 16	N 2	O 10	0	0

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



Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
4	A	1	Total 126	C 72	N 9	O 45	0
4	A	1	Total 126	C 72	N 9	O 45	0
4	A	1	Total 126	C 72	N 9	O 45	0
4	A	1	Total 126	C 72	N 9	O 45	0
4	A	1	Total 126	C 72	N 9	O 45	0
4	A	1	Total 126	C 72	N 9	O 45	0
4	A	1	Total 126	C 72	N 9	O 45	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
4	A	1	Total 126	C 72	N 9	O 45	0
4	A	1	Total 126	C 72	N 9	O 45	0
4	B	1	Total 168	C 96	N 12	O 60	0
4	B	1	Total 168	C 96	N 12	O 60	0
4	B	1	Total 168	C 96	N 12	O 60	0
4	B	1	Total 168	C 96	N 12	O 60	0
4	B	1	Total 168	C 96	N 12	O 60	0
4	B	1	Total 168	C 96	N 12	O 60	0
4	B	1	Total 168	C 96	N 12	O 60	0
4	B	1	Total 168	C 96	N 12	O 60	0
4	B	1	Total 168	C 96	N 12	O 60	0
4	B	1	Total 168	C 96	N 12	O 60	0
4	B	1	Total 168	C 96	N 12	O 60	0
4	B	1	Total 168	C 96	N 12	O 60	0
4	B	1	Total 168	C 96	N 12	O 60	0
4	C	1	Total 112	C 64	N 8	O 40	0
4	C	1	Total 112	C 64	N 8	O 40	0
4	C	1	Total 112	C 64	N 8	O 40	0
4	C	1	Total 112	C 64	N 8	O 40	0
4	C	1	Total 112	C 64	N 8	O 40	0
4	C	1	Total 112	C 64	N 8	O 40	0
4	C	1	Total 112	C 64	N 8	O 40	0

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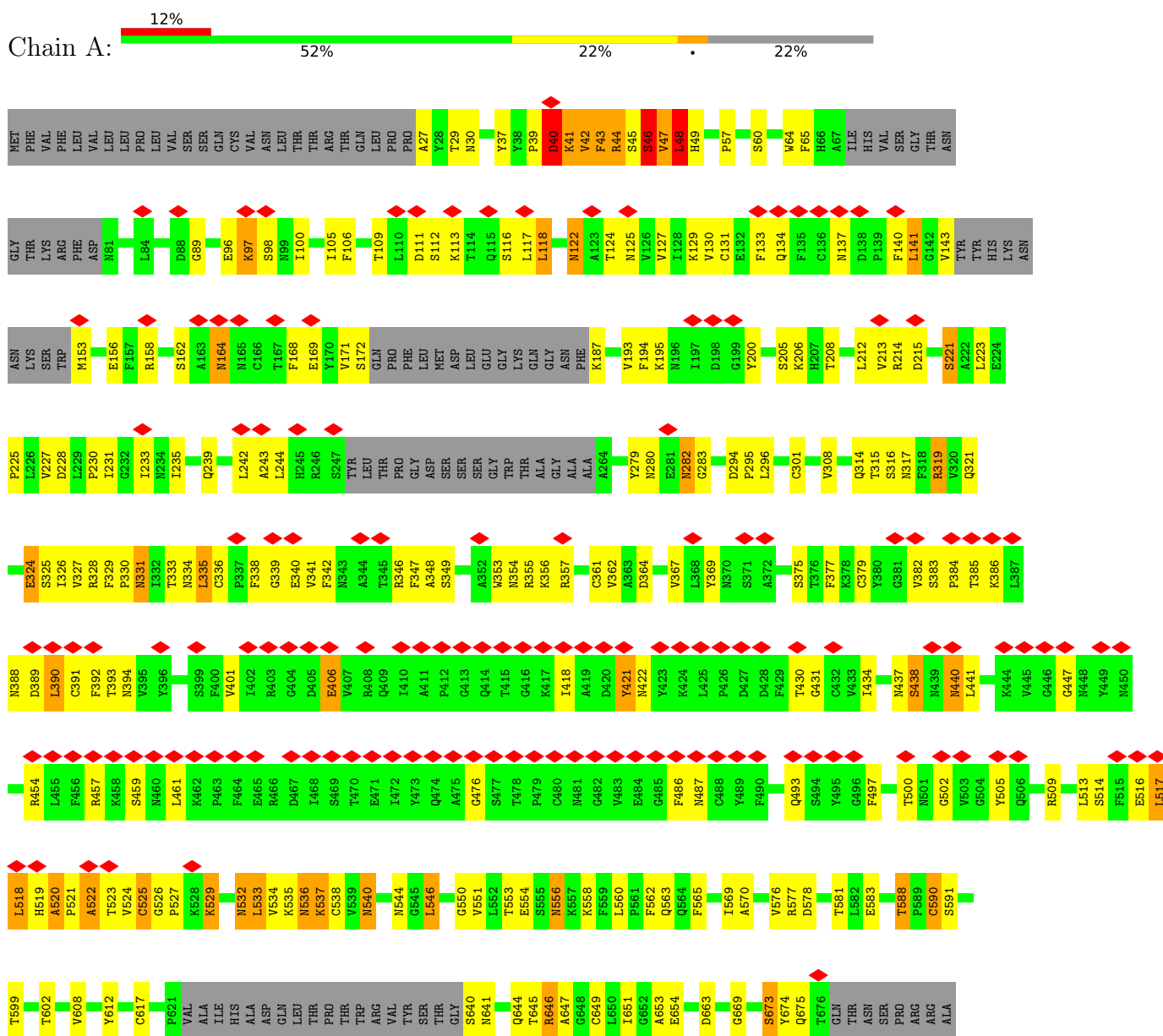
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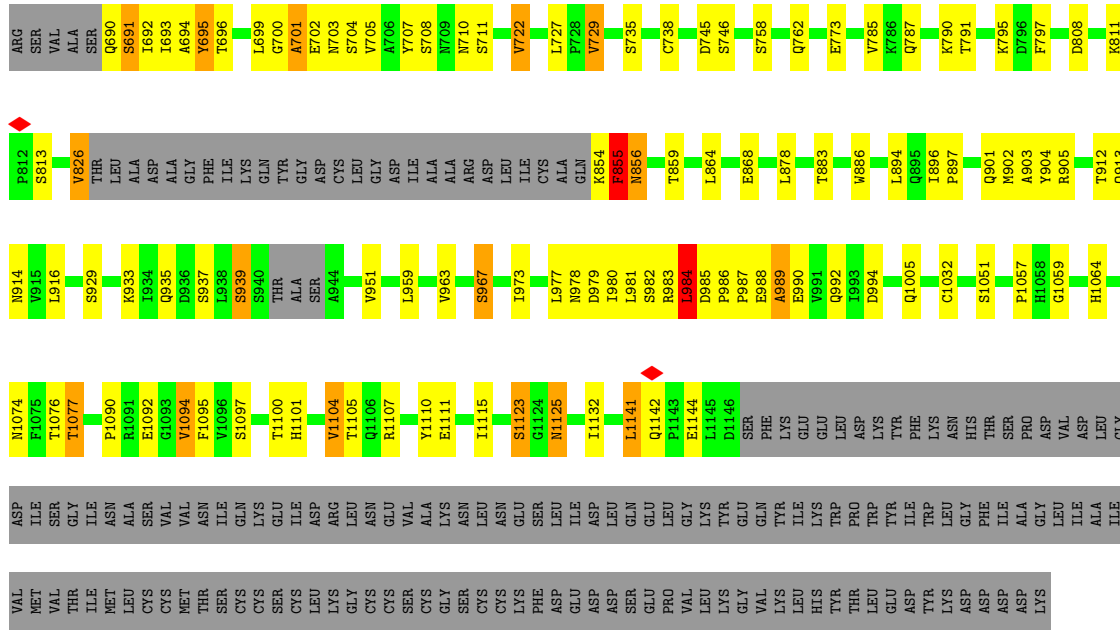
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
4	C	1	112	64	8	40	0
4	D	1	14	8	1	5	0

### 3 Residue-property plots

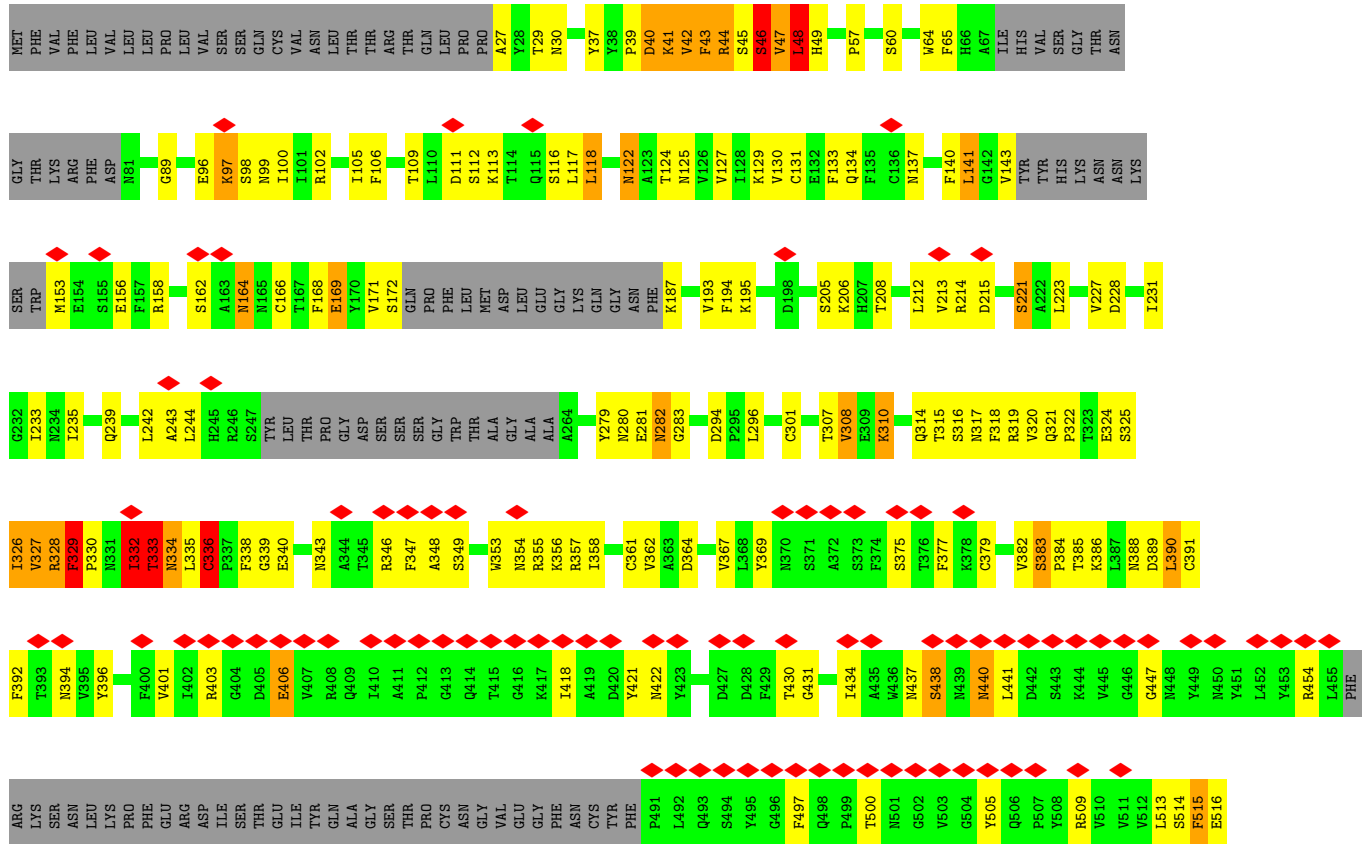
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

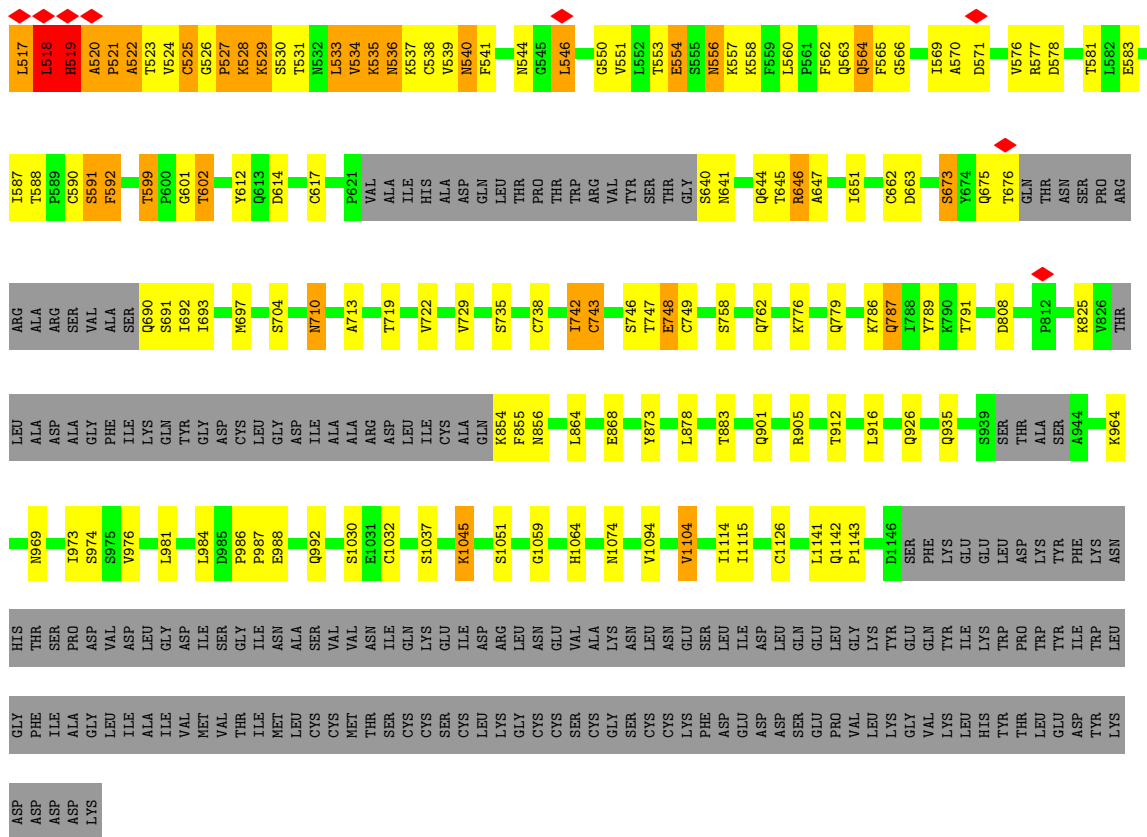
#### • Molecule 1: Spike glycoprotein



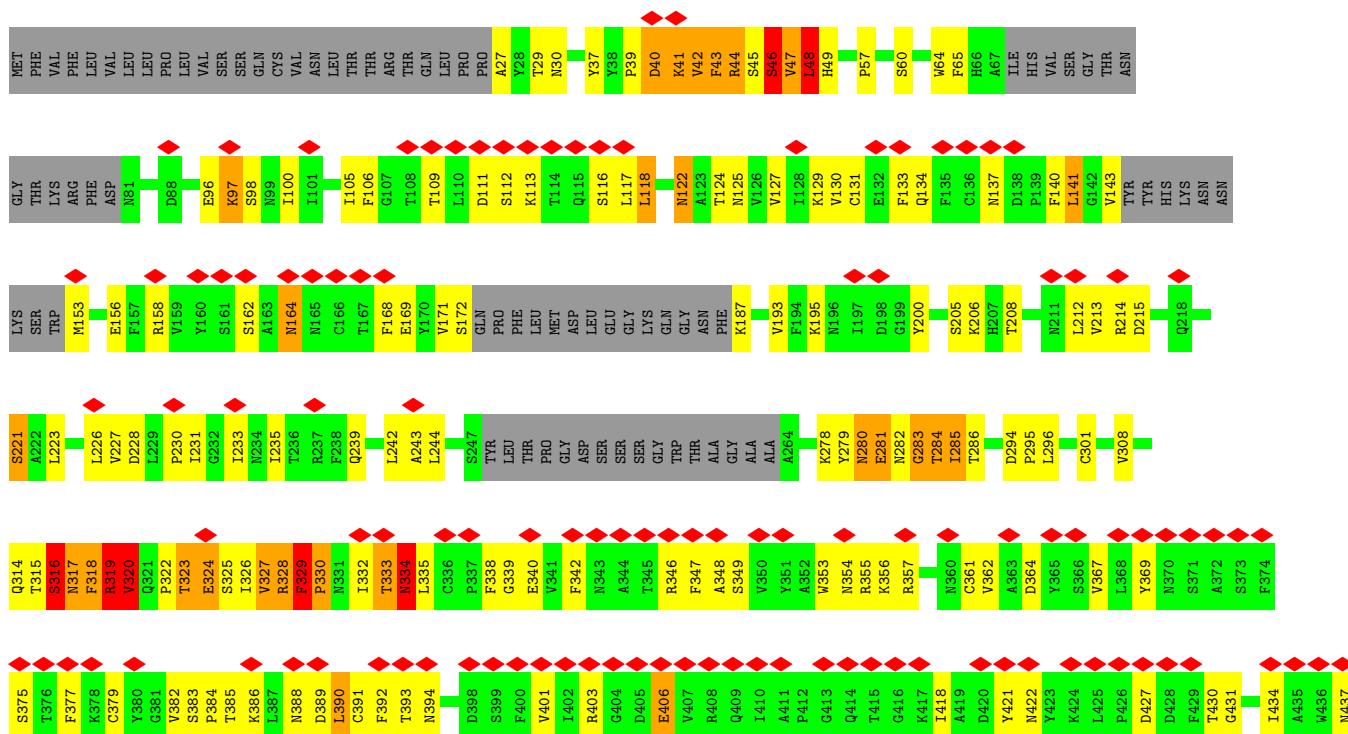


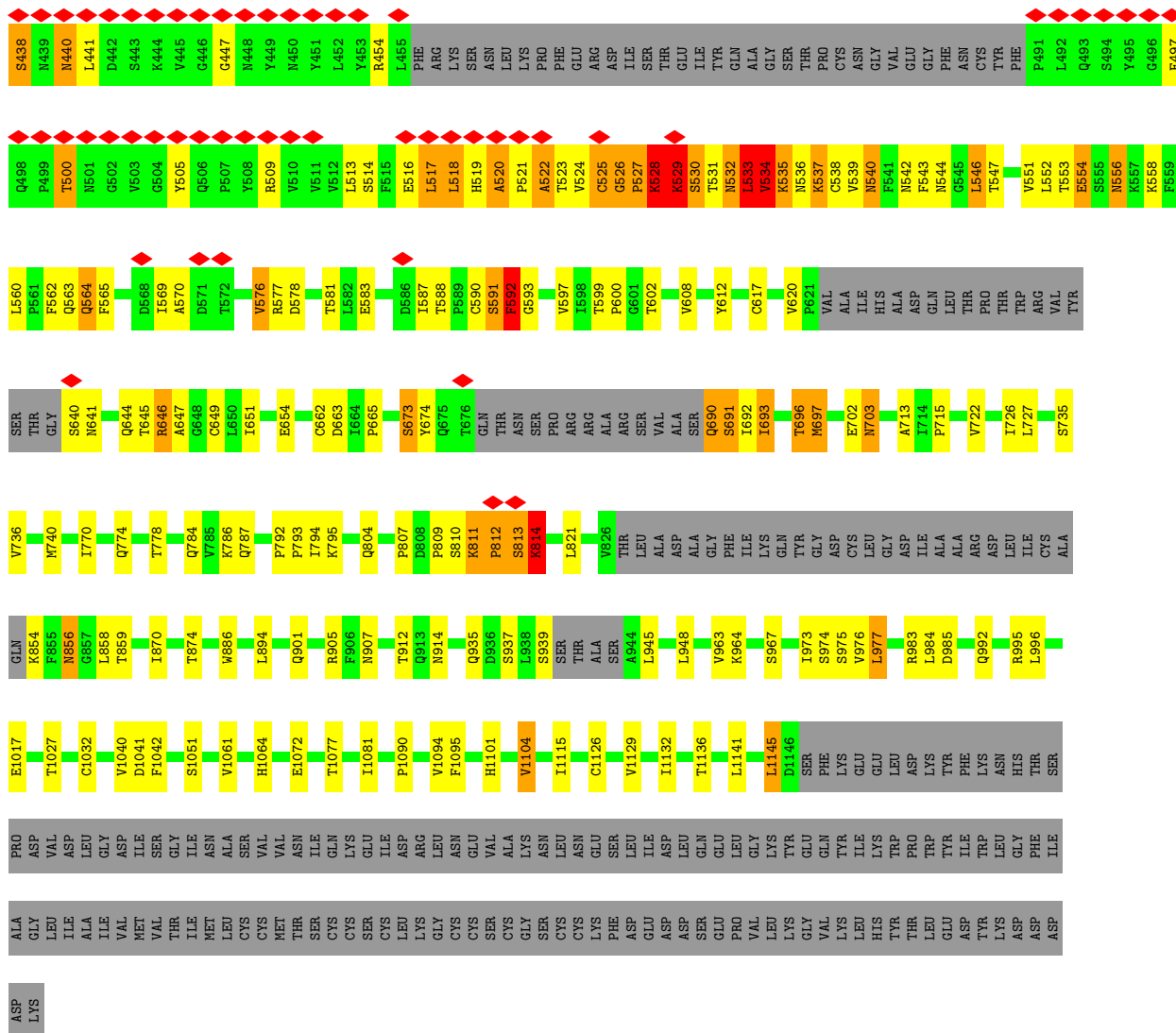
• Molecule 1: Spike glycoprotein



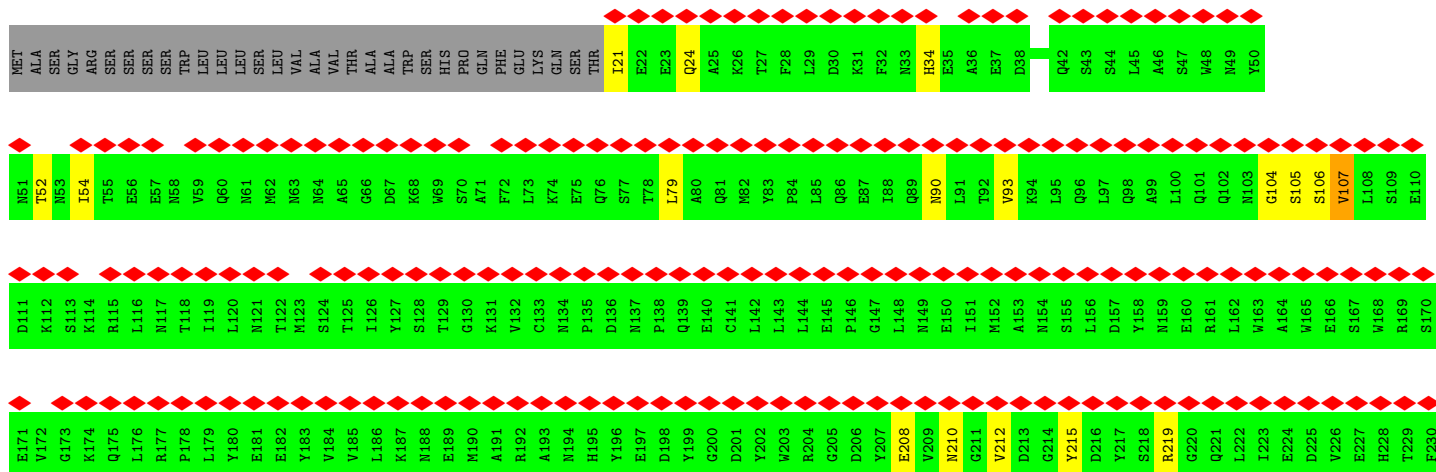


● Molecule 1: Spike glycoprotein





• Molecule 2: Angiotensin-converting enzyme 2





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

Chain G:  100%



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

Chain H:  50%  
50%



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

Chain I:  50%  
50%



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

Chain J:  50%  
50%



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

Chain K:  50%  
50%



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

Chain L:  100%  
100%





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



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



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



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



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



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



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



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



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



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



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



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



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

Chain Y:  100%



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

Chain Z:  100%



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

Chain a:  100%



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

Chain b:  100%



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

Chain c:  100%



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

Chain d:  100%



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	98516	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.141	Depositor
Minimum map value	-0.074	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	313.056, 313.056, 313.056	wwPDB
Map dimensions	288, 288, 288	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.087, 1.087, 1.087	Depositor

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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	0.59	0/8048	0.56	0/10947
1	B	0.58	0/7751	0.55	0/10544
1	C	0.58	0/7751	0.54	0/10544
2	D	0.35	0/4994	0.50	0/6785
All	All	0.55	0/28544	0.54	0/38820

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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	7872	0	7671	375	0
1	B	7584	0	7403	354	0
1	C	7584	0	7404	449	0
2	D	4857	0	4624	67	0
3	E	28	0	25	0	0
3	F	28	0	25	3	0
3	G	28	0	25	0	0
3	H	28	0	25	1	0
3	I	28	0	25	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	J	28	0	25	0	0
3	K	28	0	25	0	0
3	L	28	0	25	0	0
3	M	28	0	25	0	0
3	N	28	0	25	0	0
3	O	28	0	25	0	0
3	P	28	0	25	1	0
3	Q	28	0	25	0	0
3	R	28	0	25	0	0
3	S	28	0	25	3	0
3	T	28	0	25	1	0
3	U	28	0	25	0	0
3	V	28	0	25	0	0
3	W	28	0	25	1	0
3	X	28	0	25	2	0
3	Y	28	0	25	0	0
3	Z	28	0	25	0	0
3	a	28	0	25	0	0
3	b	28	0	25	0	0
3	c	28	0	25	0	0
3	d	28	0	25	0	0
4	A	126	0	117	4	0
4	B	168	0	154	15	0
4	C	112	0	104	4	0
4	D	14	0	13	0	0
All	All	29045	0	28140	1121	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 20.

All (1121) 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)
1:A:41:LYS:HD2	1:C:562:PHE:CD2	1.46	1.48
4:B:1411:NAG:O4	4:B:1412:NAG:C1	1.63	1.45
1:C:333:THR:HG21	1:C:361:CYS:C	1.36	1.44
1:C:329:PHE:CE2	1:C:528:LYS:HG2	1.56	1.39
1:C:329:PHE:CZ	1:C:528:LYS:HG2	1.60	1.36
1:B:431:GLY:HA2	1:B:515:PHE:CE1	1.59	1.34
1:A:703:ASN:HB2	1:B:787:GLN:OE1	1.28	1.31
1:A:536:ASN:O	1:A:537:LYS:CG	1.81	1.26

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:333:THR:CG2	1:C:362:VAL:HG23	1.66	1.25
1:B:367:VAL:CG2	4:B:1407:NAG:H83	1.65	1.24
1:A:41:LYS:CD	1:C:562:PHE:HD2	1.50	1.23
1:C:329:PHE:CE2	1:C:528:LYS:CG	2.22	1.22
1:A:536:ASN:O	1:A:537:LYS:HG2	1.11	1.22
1:A:486:PHE:CE1	2:D:79:LEU:HD22	1.75	1.20
1:C:536:ASN:HA	1:C:551:VAL:CG1	1.72	1.19
1:C:536:ASN:HA	1:C:551:VAL:HG13	1.20	1.16
1:B:367:VAL:HG21	4:B:1407:NAG:H83	1.21	1.16
1:A:340:GLU:OE2	1:A:356:LYS:HE2	1.47	1.14
1:A:565:PHE:O	1:B:42:VAL:HA	1.48	1.13
1:C:654:GLU:HG3	1:C:693:ILE:HG22	1.17	1.12
1:B:340:GLU:OE2	1:B:356:LYS:HE2	1.47	1.12
1:C:280:ASN:OD1	1:C:286:THR:HG21	1.48	1.12
1:A:41:LYS:HG2	1:C:519:HIS:HD1	1.10	1.12
1:A:654:GLU:HG3	1:A:693:ILE:HG22	1.20	1.11
1:A:41:LYS:CD	1:C:562:PHE:CD2	2.29	1.11
1:B:392:PHE:HE2	1:B:517:LEU:HB2	1.13	1.10
1:C:340:GLU:OE2	1:C:356:LYS:HE2	1.47	1.10
1:C:333:THR:HG22	1:C:362:VAL:HG23	1.29	1.10
1:C:523:THR:HG22	1:C:524:VAL:H	0.98	1.09
1:B:748:GLU:HG3	1:B:981:LEU:HD21	1.32	1.09
1:A:523:THR:HG22	1:A:524:VAL:H	0.98	1.08
1:A:392:PHE:HB3	1:A:517:LEU:HD21	1.35	1.08
1:A:520:ALA:HB1	1:A:521:PRO:HD2	1.35	1.08
1:B:332:ILE:HG22	1:B:362:VAL:HG22	1.35	1.08
1:A:533:LEU:CD2	1:A:535:LYS:HE3	1.84	1.08
1:C:520:ALA:HB1	1:C:521:PRO:HD2	1.35	1.07
1:C:662:CYS:HB2	1:C:697:MET:HE3	1.33	1.07
1:B:523:THR:HG22	1:B:524:VAL:H	1.20	1.07
1:C:333:THR:CG2	1:C:361:CYS:C	2.24	1.06
1:A:41:LYS:HG2	1:C:519:HIS:ND1	1.71	1.05
1:B:392:PHE:CE2	1:B:517:LEU:HD12	1.91	1.05
1:B:367:VAL:HG21	4:B:1407:NAG:C8	1.87	1.04
1:C:329:PHE:CD2	1:C:528:LYS:HG2	1.92	1.04
1:C:392:PHE:HB3	1:C:517:LEU:CD2	1.88	1.04
1:C:329:PHE:CZ	1:C:528:LYS:CG	2.38	1.04
1:C:392:PHE:HB3	1:C:517:LEU:HD21	1.34	1.04
1:A:392:PHE:HB3	1:A:517:LEU:CD2	1.88	1.03
1:B:392:PHE:HD2	1:B:517:LEU:HA	1.23	1.03
1:C:333:THR:HG22	1:C:362:VAL:CG2	1.88	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:523:THR:HG22	1:C:524:VAL:N	1.73	1.03
1:C:333:THR:HG21	1:C:361:CYS:O	1.55	1.03
1:C:536:ASN:CA	1:C:551:VAL:HG13	1.88	1.02
1:A:329:PHE:HB3	1:A:330:PRO:HD2	1.41	1.02
1:B:328:ARG:HG2	1:B:578:ASP:OD1	1.58	1.02
1:B:403:ARG:NH1	1:B:505:TYR:HE1	1.58	1.01
1:C:403:ARG:NH1	1:C:505:TYR:HE1	1.58	1.01
1:B:517:LEU:HD22	1:C:983:ARG:NE	1.76	1.01
1:B:44:ARG:O	1:B:283:GLY:HA2	1.61	1.00
4:B:1411:NAG:C4	4:B:1412:NAG:C1	2.38	1.00
1:A:41:LYS:HD2	1:C:562:PHE:CE2	1.96	1.00
1:A:392:PHE:CB	1:A:517:LEU:HD21	1.91	1.00
1:A:523:THR:HG22	1:A:524:VAL:N	1.73	0.99
1:B:332:ILE:HG22	1:B:362:VAL:CG2	1.92	0.99
1:B:748:GLU:CG	1:B:981:LEU:HD21	1.91	0.99
1:C:333:THR:HG23	1:C:334:ASN:H	1.23	0.99
1:B:523:THR:HG22	1:B:524:VAL:N	1.74	0.99
1:B:357:ARG:NH2	1:C:230:PRO:HG3	1.77	0.98
1:C:329:PHE:HB3	1:C:330:PRO:HD2	1.44	0.98
1:C:392:PHE:CB	1:C:517:LEU:HD21	1.91	0.98
1:C:811:LYS:HB2	1:C:812:PRO:CD	1.91	0.98
1:A:44:ARG:O	1:A:283:GLY:HA2	1.61	0.98
1:C:329:PHE:CE1	1:C:528:LYS:HG2	1.99	0.98
1:A:486:PHE:CE1	2:D:79:LEU:CD2	2.47	0.98
2:D:302:TRP:CH2	2:D:423:LEU:HD11	1.99	0.98
1:C:654:GLU:HG3	1:C:693:ILE:CG2	1.94	0.98
1:B:520:ALA:HB1	1:B:521:PRO:HD2	1.43	0.97
1:C:329:PHE:CE2	1:C:528:LYS:CB	2.48	0.97
1:C:329:PHE:CE2	1:C:528:LYS:HB2	1.98	0.97
1:A:346:ARG:NH2	1:A:347:PHE:O	1.98	0.97
1:A:295:PRO:HB2	1:A:608:VAL:HG11	1.44	0.97
1:A:523:THR:CG2	1:A:524:VAL:H	1.77	0.97
1:A:41:LYS:HB3	1:C:563:GLN:HA	1.44	0.96
1:B:346:ARG:NH2	1:B:347:PHE:O	1.98	0.96
1:C:523:THR:CG2	1:C:524:VAL:H	1.77	0.96
1:C:280:ASN:CG	1:C:286:THR:HG21	1.85	0.96
1:C:346:ARG:NH2	1:C:347:PHE:O	1.98	0.96
1:C:328:ARG:HG2	1:C:578:ASP:OD1	1.66	0.96
1:B:403:ARG:NH1	1:B:505:TYR:CE1	2.33	0.95
1:C:403:ARG:NH1	1:C:505:TYR:CE1	2.33	0.95
1:B:392:PHE:CE2	1:B:517:LEU:HB2	2.01	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:392:PHE:CD2	1:B:517:LEU:HA	2.01	0.95
1:A:980:ILE:O	1:A:984:LEU:HB2	1.67	0.95
1:A:985:ASP:HB2	1:A:987:PRO:HD2	1.49	0.95
1:C:528:LYS:O	1:C:529:LYS:HE3	1.67	0.94
1:A:703:ASN:OD1	1:B:789:TYR:HE1	1.50	0.94
2:D:302:TRP:HH2	2:D:423:LEU:HD11	1.34	0.93
1:B:329:PHE:CE1	1:B:544:ASN:HA	2.03	0.92
1:A:533:LEU:HD21	1:A:535:LYS:HG3	1.52	0.92
1:C:811:LYS:HB2	1:C:812:PRO:HD2	1.50	0.92
1:A:505:TYR:CD2	2:D:353:LYS:O	2.23	0.92
1:C:333:THR:HG23	1:C:362:VAL:HG23	1.50	0.92
1:B:392:PHE:HE2	1:B:517:LEU:CB	1.83	0.91
1:B:327:VAL:O	1:B:530:SER:HB2	1.70	0.91
1:C:333:THR:HG21	1:C:362:VAL:N	1.85	0.91
1:C:329:PHE:CD2	1:C:528:LYS:CB	2.54	0.91
1:B:386:LYS:HZ2	1:C:985:ASP:HB3	1.35	0.91
1:A:319:ARG:HH21	1:A:319:ARG:HG3	1.35	0.90
1:B:326:ILE:HD13	1:B:327:VAL:N	1.86	0.90
1:C:327:VAL:O	1:C:530:SER:HA	1.70	0.90
1:B:431:GLY:CA	1:B:515:PHE:CE1	2.53	0.89
1:A:476:GLY:CA	2:D:24:GLN:HE21	1.85	0.89
1:A:486:PHE:HE1	2:D:79:LEU:CD2	1.84	0.89
1:C:538:CYS:HB2	1:C:590:CYS:SG	2.13	0.89
1:A:533:LEU:HD21	1:A:535:LYS:HE3	1.54	0.89
1:C:333:THR:CG2	1:C:362:VAL:CG2	2.47	0.89
1:B:570:ALA:HB2	1:C:963:VAL:HG12	1.54	0.89
1:B:551:VAL:HB	1:B:588:THR:HG23	1.56	0.88
1:B:390:LEU:CD1	1:B:517:LEU:HD11	2.03	0.87
1:B:45:SER:O	1:B:47:VAL:HG22	1.75	0.87
1:A:41:LYS:CE	1:C:562:PHE:HD2	1.87	0.86
1:C:393:THR:O	1:C:523:THR:HG21	1.75	0.86
1:B:517:LEU:CD2	1:C:983:ARG:NE	2.39	0.86
2:D:335:ASP:HB3	2:D:361:CYS:SG	2.16	0.86
1:A:729:VAL:HG13	1:A:1059:GLY:HA2	1.57	0.86
1:B:46:SER:HA	1:B:279:TYR:O	1.76	0.86
1:B:569:ILE:HG22	1:C:964:LYS:HE2	1.58	0.86
1:A:46:SER:HA	1:A:279:TYR:O	1.76	0.85
2:D:105:SER:O	2:D:106:SER:OG	1.93	0.85
1:A:45:SER:O	1:A:47:VAL:HG22	1.75	0.85
1:A:520:ALA:HB1	1:A:521:PRO:CD	2.06	0.85
1:B:569:ILE:HG13	1:C:47:VAL:HG11	1.58	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:392:PHE:CD2	1:C:517:LEU:HD21	2.11	0.85
1:A:392:PHE:CD2	1:A:517:LEU:HD21	2.11	0.84
1:C:45:SER:O	1:C:47:VAL:HG22	1.75	0.84
1:C:520:ALA:HB1	1:C:521:PRO:CD	2.06	0.84
1:A:393:THR:O	1:A:523:THR:HG21	1.76	0.84
1:B:390:LEU:HD11	1:B:517:LEU:HD11	1.57	0.84
1:C:324:GLU:OE1	1:C:324:GLU:N	2.09	0.84
1:C:516:GLU:O	1:C:517:LEU:HD22	1.78	0.84
1:C:329:PHE:CZ	1:C:528:LYS:HD3	2.13	0.83
1:A:230:PRO:HB2	1:C:357:ARG:CZ	2.09	0.83
1:B:517:LEU:HD22	1:C:983:ARG:CZ	2.08	0.83
1:C:329:PHE:CD2	1:C:528:LYS:CG	2.57	0.83
1:A:516:GLU:O	1:A:517:LEU:HD22	1.78	0.83
1:B:431:GLY:HA2	1:B:515:PHE:HE1	1.04	0.83
1:C:538:CYS:CB	1:C:590:CYS:SG	2.67	0.83
1:A:486:PHE:CZ	2:D:79:LEU:HD22	2.13	0.83
1:A:703:ASN:OD1	1:B:789:TYR:CE1	2.32	0.83
1:B:357:ARG:HH22	1:C:230:PRO:HG3	1.40	0.83
1:B:523:THR:CG2	1:B:524:VAL:H	1.90	0.83
1:C:662:CYS:HB2	1:C:697:MET:CE	2.09	0.83
1:B:901:GLN:HE21	1:B:905:ARG:HE	1.26	0.82
1:C:328:ARG:NE	1:C:533:LEU:HD22	1.94	0.82
1:C:322:PRO:HA	1:C:538:CYS:O	1.79	0.82
1:A:983:ARG:O	1:A:984:LEU:HD23	1.80	0.82
1:B:571:ASP:HB2	1:C:967:SER:CB	2.09	0.82
1:A:42:VAL:N	1:C:563:GLN:HG2	1.95	0.82
1:C:280:ASN:HB2	1:C:284:THR:O	1.80	0.81
1:A:329:PHE:CE1	1:A:544:ASN:HA	2.16	0.81
1:C:901:GLN:HE21	1:C:905:ARG:HE	1.27	0.81
1:A:654:GLU:HG3	1:A:693:ILE:CG2	2.09	0.81
1:B:396:TYR:HE2	1:C:200:TYR:HH	0.82	0.81
1:C:329:PHE:HB3	1:C:330:PRO:CD	2.08	0.81
1:C:329:PHE:CZ	1:C:528:LYS:CD	2.64	0.80
1:A:334:ASN:O	1:A:362:VAL:HB	1.81	0.80
1:B:319:ARG:NH2	1:C:740:MET:SD	2.55	0.80
1:C:318:PHE:CZ	1:C:620:VAL:O	2.35	0.80
1:B:748:GLU:N	1:B:748:GLU:OE2	2.14	0.79
1:B:521:PRO:O	1:B:564:GLN:HG3	1.82	0.79
1:A:41:LYS:C	1:C:563:GLN:HG2	2.03	0.79
1:B:328:ARG:CG	1:B:578:ASP:OD1	2.31	0.79
1:A:707:TYR:HB2	1:B:883:THR:HG23	1.65	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:392:PHE:O	1:C:523:THR:HB	1.83	0.79
1:C:532:ASN:O	1:C:533:LEU:HD23	1.82	0.79
1:B:325:SER:HA	1:B:540:ASN:O	1.83	0.78
1:B:396:TYR:HE2	1:C:200:TYR:OH	1.63	0.78
1:B:390:LEU:HD23	1:B:391:CYS:H	1.48	0.78
1:A:392:PHE:O	1:A:523:THR:HB	1.83	0.78
1:B:332:ILE:CG2	1:B:362:VAL:HG22	2.13	0.78
1:B:520:ALA:HB1	1:B:521:PRO:CD	2.13	0.78
1:C:329:PHE:CB	1:C:330:PRO:HD2	2.14	0.78
1:C:531:THR:HG22	1:C:532:ASN:H	1.48	0.78
1:C:390:LEU:HD23	1:C:391:CYS:H	1.49	0.77
1:A:335:LEU:HA	1:A:362:VAL:HB	1.67	0.77
1:A:529:LYS:HA	1:A:529:LYS:NZ	1.98	0.77
1:A:979:ASP:O	1:A:983:ARG:HG3	1.84	0.77
1:B:361:CYS:SG	1:B:524:VAL:HG21	2.25	0.77
1:B:396:TYR:OH	1:C:230:PRO:HB3	1.85	0.77
1:A:361:CYS:SG	1:A:524:VAL:HG21	2.25	0.76
1:B:332:ILE:CG2	1:B:362:VAL:CG2	2.63	0.76
1:A:476:GLY:HA2	2:D:24:GLN:HE21	1.50	0.76
2:D:302:TRP:HH2	2:D:423:LEU:CD1	1.98	0.76
1:A:703:ASN:CB	1:B:787:GLN:OE1	2.23	0.76
1:A:390:LEU:HD23	1:A:391:CYS:H	1.49	0.76
1:A:41:LYS:HG2	1:C:519:HIS:CE1	2.20	0.76
1:A:529:LYS:HA	1:A:529:LYS:HZ1	1.51	0.76
1:A:533:LEU:CD2	1:A:535:LYS:HG3	2.15	0.76
1:A:529:LYS:HA	1:A:529:LYS:CE	2.16	0.76
1:A:963:VAL:HG12	1:C:570:ALA:HB1	1.67	0.76
1:B:571:ASP:HB2	1:C:967:SER:HB3	1.66	0.76
1:A:476:GLY:HA3	2:D:24:GLN:HE21	1.50	0.76
1:A:565:PHE:O	1:B:42:VAL:CA	2.32	0.76
1:A:533:LEU:HD22	1:A:535:LYS:HE3	1.66	0.75
1:A:826:VAL:HG13	1:A:1057:PRO:HG2	1.68	0.75
1:B:392:PHE:CE2	1:B:517:LEU:CD1	2.68	0.75
1:C:329:PHE:CD2	1:C:528:LYS:HB2	2.19	0.75
1:C:361:CYS:SG	1:C:524:VAL:HG21	2.25	0.75
1:C:735:SER:OG	1:C:859:THR:CG2	2.34	0.75
1:A:422:ASN:HD21	1:A:454:ARG:H	1.32	0.75
1:A:980:ILE:O	1:A:984:LEU:CB	2.35	0.75
1:A:1125:ASN:H	1:A:1125:ASN:HD22	1.33	0.75
1:B:392:PHE:CZ	1:B:517:LEU:HD12	2.22	0.75
1:B:47:VAL:O	1:B:49:HIS:N	2.20	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:47:VAL:O	1:C:49:HIS:N	2.20	0.74
1:C:403:ARG:HH11	1:C:505:TYR:HE1	1.33	0.74
1:B:329:PHE:HE1	1:B:544:ASN:HA	1.49	0.74
1:C:536:ASN:HA	1:C:551:VAL:HG11	1.66	0.74
1:A:326:ILE:HD12	1:A:533:LEU:HA	1.69	0.74
1:C:422:ASN:HD21	1:C:454:ARG:H	1.32	0.74
1:B:392:PHE:CE2	1:B:517:LEU:CB	2.65	0.74
1:B:422:ASN:HD21	1:B:454:ARG:H	1.32	0.74
2:D:335:ASP:CB	2:D:361:CYS:SG	2.75	0.74
1:A:47:VAL:O	1:A:49:HIS:N	2.20	0.74
1:B:335:LEU:HA	1:B:362:VAL:HB	1.69	0.74
1:B:743:CYS:SG	1:B:749:CYS:C	2.66	0.74
1:B:324:GLU:O	1:B:539:VAL:HG22	1.86	0.73
1:C:280:ASN:CG	1:C:286:THR:CG2	2.56	0.73
1:A:987:PRO:HB2	1:A:988:GLU:OE2	1.88	0.73
1:B:569:ILE:CG1	1:C:47:VAL:CG1	2.67	0.73
1:A:319:ARG:HG3	1:A:319:ARG:NH2	2.03	0.73
1:B:391:CYS:HA	1:B:525:CYS:HB3	1.71	0.73
1:C:328:ARG:NH2	1:C:543:PHE:CZ	2.55	0.73
1:C:531:THR:HG22	1:C:532:ASN:N	2.04	0.73
1:B:357:ARG:NH2	1:C:230:PRO:CG	2.52	0.73
1:B:973:ILE:HG12	1:B:992:GLN:HE21	1.53	0.73
1:B:403:ARG:HH11	1:B:505:TYR:HE1	1.32	0.72
1:B:570:ALA:CB	1:C:963:VAL:HG12	2.18	0.72
1:A:392:PHE:HD2	1:A:517:LEU:HD21	1.53	0.72
1:B:1142:GLN:HG3	1:B:1143:PRO:HD3	1.71	0.72
1:C:406:GLU:CD	1:C:418:ILE:HG13	2.10	0.72
1:B:406:GLU:CD	1:B:418:ILE:HG13	2.10	0.72
1:C:328:ARG:CZ	1:C:543:PHE:CZ	2.73	0.72
1:B:388:ASN:OD1	1:B:527:PRO:CD	2.37	0.72
1:C:391:CYS:HA	1:C:525:CYS:HB3	1.71	0.72
1:A:391:CYS:HA	1:A:525:CYS:HB3	1.71	0.72
1:A:41:LYS:CE	1:C:562:PHE:CD2	2.69	0.71
1:A:790:LYS:NZ	1:C:702:GLU:OE2	2.20	0.71
1:B:569:ILE:HG12	1:C:47:VAL:HG12	1.70	0.71
1:A:406:GLU:CD	1:A:418:ILE:HG13	2.10	0.71
1:C:392:PHE:HD2	1:C:517:LEU:HD21	1.53	0.71
1:A:41:LYS:H	1:C:519:HIS:CE1	2.09	0.71
1:A:536:ASN:O	1:A:537:LYS:HG3	1.87	0.71
4:B:1411:NAG:H4	4:B:1412:NAG:C1	2.21	0.71
1:C:333:THR:HG23	1:C:334:ASN:N	2.04	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:335:LEU:O	1:B:335:LEU:HD12	1.90	0.71
1:B:390:LEU:CD1	1:B:517:LEU:CD1	2.68	0.70
1:A:340:GLU:OE2	1:A:356:LYS:CE	2.35	0.70
1:A:536:ASN:C	1:A:537:LYS:HG2	2.09	0.70
1:A:124:THR:HG21	4:A:1402:NAG:HN2	1.56	0.70
1:C:329:PHE:CB	1:C:330:PRO:CD	2.69	0.70
1:C:329:PHE:CG	1:C:528:LYS:HG2	2.26	0.70
1:A:45:SER:OG	1:A:46:SER:N	2.25	0.70
1:C:124:THR:HG21	4:C:1402:NAG:HN2	1.56	0.70
1:B:390:LEU:HD13	1:B:517:LEU:CD1	2.21	0.70
1:C:340:GLU:OE2	1:C:356:LYS:CE	2.35	0.70
1:A:41:LYS:CA	1:C:563:GLN:HG2	2.21	0.70
1:A:988:GLU:O	1:A:990:GLU:N	2.25	0.70
1:A:187:LYS:N	1:A:212:LEU:O	2.25	0.69
1:C:187:LYS:N	1:C:212:LEU:O	2.25	0.69
1:C:945:LEU:HD12	1:C:948:LEU:HD12	1.74	0.69
1:B:124:THR:HG21	4:B:1402:NAG:HN2	1.56	0.69
1:C:45:SER:OG	1:C:46:SER:N	2.25	0.69
1:C:333:THR:OG1	1:C:334:ASN:ND2	2.25	0.69
1:C:329:PHE:CD1	1:C:528:LYS:HG2	2.28	0.69
1:B:431:GLY:CA	1:B:515:PHE:HE1	1.94	0.69
1:C:335:LEU:HD12	1:C:335:LEU:N	2.07	0.69
1:B:324:GLU:O	1:B:539:VAL:CG2	2.40	0.69
1:B:187:LYS:N	1:B:212:LEU:O	2.25	0.69
1:B:986:PRO:HB2	1:B:987:PRO:HD3	1.74	0.69
1:C:532:ASN:C	1:C:533:LEU:HD23	2.13	0.69
1:B:44:ARG:O	1:B:283:GLY:CA	2.40	0.69
1:B:45:SER:OG	1:B:46:SER:N	2.25	0.69
1:A:325:SER:HA	1:A:540:ASN:O	1.93	0.69
1:B:569:ILE:CG2	1:C:964:LYS:HE2	2.21	0.69
1:A:551:VAL:HB	1:A:588:THR:HG23	1.75	0.68
1:A:41:LYS:N	1:C:519:HIS:CE1	2.62	0.68
1:A:200:TYR:OH	1:C:394:ASN:ND2	2.21	0.68
1:A:43:PHE:CE1	1:A:283:GLY:HA3	2.29	0.68
1:B:43:PHE:CE1	1:B:283:GLY:HA3	2.29	0.68
1:B:321:GLN:OE1	1:B:321:GLN:HA	1.93	0.68
1:B:551:VAL:HB	1:B:588:THR:CG2	2.22	0.68
1:B:388:ASN:OD1	1:B:527:PRO:HD2	1.94	0.67
1:B:571:ASP:HB2	1:C:967:SER:HB2	1.77	0.67
1:A:392:PHE:CG	1:A:517:LEU:HD21	2.29	0.67
1:B:533:LEU:HD12	1:B:533:LEU:C	2.15	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:340:GLU:OE2	1:B:356:LYS:CE	2.35	0.67
1:C:392:PHE:CG	1:C:517:LEU:HD21	2.29	0.67
1:A:37:TYR:O	1:A:39:PRO:HD3	1.95	0.67
1:A:329:PHE:HB3	1:A:330:PRO:CD	2.22	0.67
1:C:333:THR:OG1	1:C:361:CYS:CA	2.43	0.67
1:A:187:LYS:HG2	1:A:213:VAL:HA	1.77	0.67
1:B:396:TYR:OH	1:C:230:PRO:CB	2.43	0.67
1:B:1045:LYS:NZ	1:C:786:LYS:HE3	2.09	0.67
1:C:37:TYR:O	1:C:39:PRO:HD3	1.95	0.67
1:A:41:LYS:HE3	1:C:562:PHE:CD2	2.30	0.66
1:A:536:ASN:C	1:A:537:LYS:CG	2.59	0.66
1:C:335:LEU:HA	1:C:362:VAL:HB	1.77	0.66
1:B:431:GLY:HA2	1:B:515:PHE:CD1	2.27	0.66
1:B:569:ILE:HD12	1:B:569:ILE:H	1.60	0.66
1:C:96:GLU:OE1	1:C:98:SER:N	2.28	0.66
1:C:187:LYS:HG2	1:C:213:VAL:HA	1.78	0.66
1:A:325:SER:CB	1:A:540:ASN:HB3	2.26	0.66
1:B:332:ILE:O	1:B:333:THR:HG23	1.96	0.66
1:B:390:LEU:HD12	1:C:983:ARG:HB3	1.75	0.66
1:C:522:ALA:O	1:C:523:THR:OG1	2.14	0.66
1:B:96:GLU:OE1	1:B:98:SER:N	2.28	0.66
1:A:529:LYS:HA	1:A:529:LYS:HE2	1.76	0.66
1:B:691:SER:O	1:B:692:ILE:HG13	1.96	0.66
1:C:280:ASN:CB	1:C:286:THR:CG2	2.73	0.66
1:A:963:VAL:CG1	1:C:570:ALA:HB1	2.26	0.65
1:B:187:LYS:HG2	1:B:213:VAL:HA	1.78	0.65
1:C:811:LYS:CB	1:C:812:PRO:CD	2.66	0.65
1:A:96:GLU:OE1	1:A:98:SER:N	2.28	0.65
1:A:388:ASN:OD1	1:A:527:PRO:CD	2.43	0.65
1:C:535:LYS:HD3	1:C:554:GLU:OE2	1.97	0.65
1:A:533:LEU:HD21	1:A:535:LYS:CG	2.26	0.65
1:B:719:THR:HA	1:B:926:GLN:HE22	1.60	0.65
1:A:522:ALA:O	1:A:523:THR:OG1	2.14	0.65
1:B:569:ILE:CG1	1:C:47:VAL:HG12	2.26	0.65
1:A:388:ASN:OD1	1:A:527:PRO:HD2	1.97	0.65
1:B:37:TYR:O	1:B:39:PRO:HD3	1.95	0.65
1:B:390:LEU:CD1	1:C:983:ARG:HB3	2.26	0.65
1:B:392:PHE:CD2	1:B:517:LEU:CA	2.78	0.65
1:C:392:PHE:HD2	1:C:517:LEU:CD2	2.09	0.65
1:A:569:ILE:HD12	1:A:569:ILE:H	1.60	0.65
1:A:745:ASP:HB2	1:C:319:ARG:NH1	2.12	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:316:SER:OG	1:C:317:ASN:N	2.30	0.65
1:C:569:ILE:H	1:C:569:ILE:HD12	1.60	0.65
1:C:690:GLN:O	1:C:691:SER:HB3	1.97	0.65
1:C:333:THR:CG2	1:C:362:VAL:N	2.54	0.64
1:C:335:LEU:O	1:C:361:CYS:HB2	1.97	0.64
1:C:391:CYS:CA	1:C:525:CYS:HB3	2.24	0.64
2:D:310:GLU:OE1	2:D:421:ILE:HD11	1.97	0.64
1:A:493:GLN:OE1	2:D:34:HIS:CB	2.45	0.64
1:A:41:LYS:CB	1:C:519:HIS:HE1	2.11	0.64
1:A:392:PHE:HD2	1:A:517:LEU:CD2	2.09	0.64
1:A:533:LEU:CD2	1:A:535:LYS:CE	2.70	0.64
1:B:544:ASN:HD21	1:B:564:GLN:NE2	1.95	0.64
1:A:325:SER:HB2	1:A:540:ASN:HB3	1.79	0.64
1:A:985:ASP:OD1	1:A:988:GLU:HB2	1.97	0.64
1:A:385:THR:HG1	1:A:386:LYS:HZ3	1.46	0.64
1:A:44:ARG:O	1:A:283:GLY:CA	2.40	0.64
1:A:43:PHE:CE1	1:A:282:ASN:O	2.52	0.63
1:A:985:ASP:CB	1:A:987:PRO:HD2	2.26	0.63
1:A:669:GLY:N	1:B:864:LEU:O	2.30	0.63
2:D:302:TRP:CZ3	2:D:423:LEU:HD11	2.34	0.63
1:A:326:ILE:CD1	1:A:533:LEU:HA	2.28	0.63
1:C:333:THR:OG1	1:C:361:CYS:N	2.31	0.63
2:D:335:ASP:N	2:D:361:CYS:SG	2.72	0.63
1:B:391:CYS:CA	1:B:525:CYS:HB3	2.24	0.63
1:A:321:GLN:HA	1:A:321:GLN:OE1	1.97	0.63
1:B:396:TYR:OH	1:C:230:PRO:HG3	1.98	0.63
1:B:571:ASP:CB	1:C:967:SER:HB2	2.29	0.63
1:A:117:LEU:HD12	1:A:118:LEU:H	1.64	0.63
1:A:654:GLU:CG	1:A:693:ILE:HG22	2.14	0.62
1:A:700:GLY:O	1:A:701:ALA:O	2.17	0.62
1:B:117:LEU:HD12	1:B:118:LEU:H	1.64	0.62
1:C:323:THR:N	1:C:538:CYS:O	2.32	0.62
1:A:43:PHE:HE1	1:A:282:ASN:O	1.83	0.62
1:B:43:PHE:CE1	1:B:282:ASN:O	2.51	0.62
1:B:43:PHE:HE1	1:B:282:ASN:O	1.83	0.62
1:B:520:ALA:CB	1:B:521:PRO:HD2	2.23	0.62
1:A:808:ASP:HB3	1:A:811:LYS:HD2	1.82	0.62
1:B:329:PHE:CD1	1:B:544:ASN:HA	2.35	0.62
1:C:811:LYS:HB2	1:C:812:PRO:HD3	1.80	0.62
1:C:813:SER:O	1:C:814:LYS:HE2	2.00	0.62
1:A:516:GLU:O	1:A:517:LEU:CD2	2.48	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:124:THR:OG1	1:B:125:ASN:N	2.32	0.62
1:A:391:CYS:CA	1:A:525:CYS:HB3	2.24	0.62
1:A:457:ARG:NH1	1:A:459:SER:O	2.33	0.62
1:C:96:GLU:OE1	1:C:97:LYS:N	2.32	0.62
1:C:117:LEU:HD12	1:C:118:LEU:H	1.64	0.62
1:C:318:PHE:HB3	1:C:592:PHE:O	1.98	0.62
1:C:516:GLU:O	1:C:517:LEU:CD2	2.48	0.62
1:A:124:THR:OG1	1:A:125:ASN:N	2.32	0.62
1:B:334:ASN:H	1:B:334:ASN:ND2	1.96	0.62
1:A:534:VAL:HG23	1:A:534:VAL:O	2.00	0.61
1:A:96:GLU:OE1	1:A:97:LYS:N	2.32	0.61
1:A:988:GLU:C	1:A:990:GLU:H	2.02	0.61
1:B:96:GLU:OE1	1:B:97:LYS:N	2.32	0.61
1:A:1077:THR:HG22	1:A:1095:PHE:O	2.01	0.61
1:B:327:VAL:O	1:B:530:SER:CB	2.46	0.61
1:A:521:PRO:O	1:A:522:ALA:HB2	2.01	0.61
1:C:295:PRO:HB3	1:C:597:VAL:HG22	1.82	0.61
1:C:281:GLU:OE2	1:C:281:GLU:N	2.33	0.61
1:C:328:ARG:CZ	1:C:543:PHE:HZ	2.13	0.61
1:A:357:ARG:HH12	1:A:394:ASN:HD21	1.49	0.61
1:C:521:PRO:O	1:C:522:ALA:HB2	2.01	0.61
1:C:319:ARG:CG	1:C:319:ARG:HH21	2.14	0.61
1:A:523:THR:HG22	1:A:524:VAL:HG12	1.83	0.61
1:C:556:ASN:HD22	1:C:556:ASN:H	1.49	0.61
1:A:327:VAL:O	1:A:328:ARG:HG2	2.01	0.60
1:B:569:ILE:CG1	1:C:47:VAL:HG11	2.24	0.60
1:A:617:CYS:H	1:A:644:GLN:HE22	1.49	0.60
1:B:320:VAL:HG23	1:B:591:SER:O	2.00	0.60
1:C:576:VAL:HG22	1:C:587:ILE:HD11	1.84	0.60
1:A:406:GLU:OE1	1:A:418:ILE:HG12	2.02	0.60
1:B:617:CYS:H	1:B:644:GLN:HE22	1.49	0.60
1:C:124:THR:OG1	1:C:125:ASN:N	2.32	0.60
1:C:523:THR:HG22	1:C:524:VAL:HG12	1.83	0.60
1:C:525:CYS:O	1:C:526:GLY:O	2.18	0.60
1:C:587:ILE:HG22	1:C:587:ILE:O	2.02	0.60
1:B:308:VAL:O	1:B:601:GLY:HA2	2.02	0.60
1:B:320:VAL:HG21	1:B:591:SER:HB2	1.84	0.60
1:B:310:LYS:HB2	1:B:310:LYS:HZ2	1.66	0.60
1:B:388:ASN:OD1	1:B:527:PRO:HD3	2.00	0.60
1:C:406:GLU:OE1	1:C:418:ILE:HG12	2.02	0.60
1:A:392:PHE:HB3	1:A:517:LEU:HD22	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:40:ASP:HB2	1:C:519:HIS:CE1	2.36	0.60
1:B:406:GLU:OE1	1:B:418:ILE:HG12	2.02	0.60
1:B:556:ASN:H	1:B:556:ASN:HD22	1.49	0.60
1:C:357:ARG:HH12	1:C:394:ASN:HD21	1.49	0.60
1:C:280:ASN:HB2	1:C:286:THR:CG2	2.32	0.60
1:C:318:PHE:CG	1:C:319:ARG:N	2.70	0.60
1:C:319:ARG:HH21	1:C:319:ARG:HG2	1.66	0.60
1:A:556:ASN:HD22	1:A:556:ASN:H	1.49	0.60
2:D:212:VAL:HG21	2:D:565:PRO:HG3	1.84	0.60
1:A:532:ASN:N	1:A:532:ASN:OD1	2.32	0.59
1:C:319:ARG:O	1:C:320:VAL:HG13	2.02	0.59
1:C:322:PRO:CA	1:C:538:CYS:O	2.50	0.59
1:B:164:ASN:OD1	1:B:164:ASN:N	2.35	0.59
1:B:541:PHE:CZ	1:B:587:ILE:HD13	2.37	0.59
1:C:617:CYS:H	1:C:644:GLN:HE22	1.49	0.59
1:A:141:LEU:HB2	1:A:156:GLU:HB2	1.85	0.59
1:B:325:SER:CA	1:B:540:ASN:O	2.49	0.59
1:B:523:THR:CG2	1:B:524:VAL:N	2.46	0.59
1:B:645:THR:HG22	1:B:647:ALA:H	1.66	0.59
1:C:206:LYS:NZ	1:C:221:SER:OG	2.35	0.59
1:B:529:LYS:HE3	1:B:529:LYS:O	2.01	0.59
1:C:333:THR:HG22	1:C:362:VAL:HG22	1.80	0.59
1:B:357:ARG:HH12	1:B:394:ASN:HD21	1.49	0.59
1:B:406:GLU:CD	1:B:418:ILE:CG1	2.71	0.59
1:C:406:GLU:CD	1:C:418:ILE:CG1	2.71	0.59
1:C:645:THR:HG22	1:C:647:ALA:H	1.66	0.59
1:A:645:THR:HG22	1:A:647:ALA:H	1.66	0.59
2:D:302:TRP:CH2	2:D:423:LEU:CD1	2.78	0.59
1:A:41:LYS:CB	1:C:519:HIS:CE1	2.86	0.59
1:A:230:PRO:CB	1:C:357:ARG:CZ	2.81	0.59
1:A:722:VAL:HA	1:A:1064:HIS:O	2.03	0.59
1:B:738:CYS:O	1:B:742:ILE:HG13	2.03	0.59
1:C:141:LEU:HB2	1:C:156:GLU:HB2	1.85	0.59
1:C:333:THR:OG1	1:C:361:CYS:HA	2.02	0.59
1:C:811:LYS:CB	1:C:812:PRO:HD2	2.28	0.59
1:A:565:PHE:CZ	1:B:42:VAL:HG22	2.38	0.58
1:B:206:LYS:NZ	1:B:221:SER:OG	2.35	0.58
1:A:325:SER:CA	1:A:540:ASN:O	2.52	0.58
1:B:438:SER:O	1:B:438:SER:OG	2.21	0.58
1:C:280:ASN:HB2	1:C:286:THR:HG23	1.84	0.58
1:A:978:ASN:O	1:A:982:SER:HB3	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:591:SER:C	1:C:592:PHE:HD1	2.07	0.58
1:A:325:SER:HB2	1:A:540:ASN:O	2.03	0.58
1:A:983:ARG:HB2	1:C:382:VAL:HB	1.85	0.58
2:D:368:ASP:HA	2:D:371:THR:HG22	1.85	0.58
1:A:206:LYS:NZ	1:A:221:SER:OG	2.35	0.58
1:C:391:CYS:SG	1:C:523:THR:O	2.61	0.58
1:A:476:GLY:HA3	2:D:24:GLN:NE2	2.17	0.58
1:B:141:LEU:HB2	1:B:156:GLU:HB2	1.85	0.58
4:B:1405:NAG:H83	4:B:1405:NAG:H3	1.86	0.58
1:C:47:VAL:O	1:C:47:VAL:HG23	2.04	0.58
1:C:338:PHE:O	1:C:340:GLU:N	2.37	0.58
3:W:2:NAG:H3	3:W:2:NAG:H83	1.86	0.58
1:A:164:ASN:OD1	1:A:164:ASN:N	2.35	0.58
4:A:1405:NAG:H3	4:A:1405:NAG:H83	1.86	0.58
1:B:570:ALA:CB	1:C:963:VAL:CG1	2.82	0.58
1:A:406:GLU:CD	1:A:418:ILE:CG1	2.71	0.58
1:A:901:GLN:HE21	1:A:905:ARG:HE	1.50	0.58
1:A:361:CYS:SG	1:A:524:VAL:CG2	2.92	0.57
4:C:1405:NAG:H3	4:C:1405:NAG:H83	1.86	0.57
1:A:230:PRO:HB2	1:C:357:ARG:NH2	2.20	0.57
1:B:47:VAL:O	1:B:47:VAL:HG23	2.04	0.57
1:C:164:ASN:OD1	1:C:164:ASN:N	2.35	0.57
1:C:295:PRO:HB2	1:C:608:VAL:HG11	1.86	0.57
1:A:48:LEU:HD13	1:A:48:LEU:H	1.69	0.57
1:A:338:PHE:O	1:A:340:GLU:N	2.37	0.57
1:B:361:CYS:SG	1:B:524:VAL:CG2	2.92	0.57
1:C:48:LEU:HD13	1:C:48:LEU:H	1.69	0.57
1:C:654:GLU:CG	1:C:693:ILE:CG2	2.77	0.57
1:C:735:SER:OG	1:C:859:THR:HG23	2.04	0.57
1:A:391:CYS:SG	1:A:523:THR:O	2.61	0.57
1:B:336:CYS:SG	1:B:358:ILE:CG2	2.93	0.57
1:A:41:LYS:O	1:A:42:VAL:HB	2.05	0.57
1:A:47:VAL:O	1:A:47:VAL:HG23	2.04	0.57
1:B:48:LEU:HD13	1:B:48:LEU:H	1.69	0.57
1:B:901:GLN:NE2	1:B:905:ARG:HE	1.99	0.57
1:C:663:ASP:OD2	1:C:673:SER:OG	2.22	0.57
1:C:43:PHE:CE1	1:C:283:GLY:HA3	2.40	0.57
1:C:227:VAL:HG12	1:C:228:ASP:N	2.20	0.57
1:C:361:CYS:SG	1:C:524:VAL:CG2	2.92	0.57
1:C:388:ASN:O	1:C:527:PRO:HD2	2.05	0.57
1:A:45:SER:O	1:A:279:TYR:HB2	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:41:LYS:O	1:B:42:VAL:HB	2.04	0.57
1:B:45:SER:O	1:B:279:TYR:HB2	2.05	0.57
1:B:675:GLN:HB3	1:B:693:ILE:HD11	1.87	0.57
1:C:41:LYS:O	1:C:42:VAL:HB	2.05	0.57
1:C:342:PHE:HB3	3:S:1:NAG:H82	1.87	0.57
1:C:392:PHE:HB3	1:C:517:LEU:HD22	1.82	0.57
3:X:2:NAG:H83	3:X:2:NAG:H3	1.87	0.57
1:B:338:PHE:O	1:B:340:GLU:N	2.37	0.57
1:C:804:GLN:HE21	1:C:935:GLN:HE22	1.52	0.57
1:A:105:ILE:HG12	1:A:239:GLN:HB2	1.87	0.56
1:B:591:SER:O	1:B:592:PHE:HB3	2.05	0.56
1:C:43:PHE:HE1	1:C:283:GLY:HA3	1.70	0.56
1:A:29:THR:HG22	1:A:30:ASN:H	1.70	0.56
1:A:663:ASP:OD2	1:A:673:SER:OG	2.22	0.56
1:B:357:ARG:HH21	1:C:230:PRO:HG3	1.69	0.56
1:B:390:LEU:HD23	1:B:391:CYS:N	2.19	0.56
1:B:663:ASP:OD2	1:B:673:SER:OG	2.22	0.56
1:C:690:GLN:O	1:C:690:GLN:HG3	2.04	0.56
1:A:227:VAL:HG12	1:A:228:ASP:N	2.20	0.56
1:A:813:SER:O	1:A:813:SER:OG	2.18	0.56
1:B:227:VAL:HG12	1:B:228:ASP:N	2.20	0.56
1:B:521:PRO:O	1:B:522:ALA:HB2	2.05	0.56
1:C:519:HIS:ND1	1:C:519:HIS:O	2.38	0.56
2:D:54:ILE:HD12	2:D:341:LYS:HG3	1.88	0.56
2:D:425:SER:HB3	2:D:427:ASP:OD1	2.06	0.56
1:B:515:PHE:CD1	1:B:515:PHE:N	2.73	0.56
1:C:318:PHE:O	1:C:319:ARG:CB	2.53	0.56
1:A:295:PRO:CB	1:A:608:VAL:HG11	2.28	0.56
1:A:406:GLU:OE1	1:A:418:ILE:CG1	2.54	0.56
1:B:533:LEU:HD12	1:B:534:VAL:O	2.06	0.56
1:B:1045:LYS:HZ2	1:C:786:LYS:HE3	1.69	0.56
1:A:563:GLN:O	1:A:577:ARG:NH1	2.38	0.56
1:A:654:GLU:O	1:A:693:ILE:HA	2.05	0.56
1:A:699:LEU:HD22	1:B:873:TYR:CZ	2.40	0.56
2:D:335:ASP:N	2:D:335:ASP:OD1	2.39	0.56
1:B:29:THR:HG22	1:B:30:ASN:H	1.70	0.56
1:C:563:GLN:O	1:C:577:ARG:NH1	2.38	0.56
1:A:563:GLN:OE1	1:B:43:PHE:HD1	1.89	0.56
1:A:565:PHE:CE2	1:B:42:VAL:HG22	2.41	0.56
1:A:988:GLU:C	1:A:990:GLU:N	2.57	0.56
1:B:563:GLN:O	1:B:577:ARG:NH1	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:105:ILE:HG12	1:C:239:GLN:HB2	1.87	0.56
1:C:406:GLU:OE1	1:C:418:ILE:CG1	2.54	0.56
1:A:57:PRO:O	1:A:60:SER:OG	2.24	0.56
1:B:329:PHE:CE2	1:B:528:LYS:HG3	2.41	0.56
1:A:978:ASN:ND2	1:C:547:THR:HG22	2.21	0.56
1:A:45:SER:HA	1:A:280:ASN:O	2.06	0.55
1:B:105:ILE:HG12	1:B:239:GLN:HB2	1.87	0.55
2:D:231:GLU:HA	2:D:234:LYS:HD3	1.88	0.55
1:C:530:SER:O	1:C:531:THR:OG1	2.21	0.55
1:C:600:PRO:HD3	1:C:692:ILE:HD11	1.88	0.55
1:A:43:PHE:CG	1:A:44:ARG:N	2.74	0.55
1:B:43:PHE:CG	1:B:44:ARG:N	2.74	0.55
1:B:318:PHE:O	1:B:592:PHE:HA	2.07	0.55
1:B:406:GLU:OE1	1:B:418:ILE:CG1	2.54	0.55
1:B:517:LEU:HD23	1:B:517:LEU:O	2.06	0.55
1:C:674:TYR:HA	1:C:691:SER:O	2.06	0.55
3:I:2:NAG:H3	3:I:2:NAG:H83	1.87	0.55
1:A:519:HIS:O	1:A:519:HIS:ND1	2.38	0.55
1:A:967:SER:O	1:A:967:SER:OG	2.24	0.55
1:C:556:ASN:HD22	1:C:556:ASN:N	2.05	0.55
1:B:529:LYS:HE3	1:B:529:LYS:C	2.27	0.55
1:A:347:PHE:CE1	1:A:509:ARG:HD3	2.42	0.55
1:A:392:PHE:HA	1:A:517:LEU:HD11	1.89	0.55
1:A:486:PHE:CZ	2:D:79:LEU:CD2	2.84	0.55
1:B:57:PRO:O	1:B:60:SER:OG	2.24	0.55
1:B:347:PHE:CE1	1:B:509:ARG:HD3	2.42	0.55
1:C:531:THR:CG2	1:C:532:ASN:H	2.19	0.55
1:B:357:ARG:HH21	1:C:230:PRO:CG	2.19	0.55
1:C:347:PHE:CE1	1:C:509:ARG:HD3	2.42	0.55
1:C:392:PHE:CD2	1:C:517:LEU:CD2	2.85	0.55
3:F:1:NAG:H61	3:F:2:NAG:HN2	1.71	0.55
1:A:342:PHE:HB3	3:F:1:NAG:H82	1.87	0.55
1:C:29:THR:HG22	1:C:30:ASN:H	1.71	0.55
1:C:295:PRO:HB3	1:C:597:VAL:CG2	2.35	0.55
1:A:556:ASN:HD22	1:A:556:ASN:N	2.05	0.55
1:B:45:SER:HA	1:B:280:ASN:O	2.06	0.55
1:B:676:THR:HB	1:B:693:ILE:HG21	1.88	0.55
3:S:1:NAG:H61	3:S:2:NAG:HN2	1.72	0.55
1:C:385:THR:HG1	1:C:386:LYS:HZ3	1.49	0.54
1:A:41:LYS:HB2	1:C:519:HIS:HE1	1.71	0.54
1:C:43:PHE:CG	1:C:44:ARG:N	2.74	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:886:TRP:HH2	1:A:904:TYR:HD2	1.56	0.54
1:A:43:PHE:O	1:A:44:ARG:HG3	2.08	0.54
1:A:388:ASN:OD1	1:A:527:PRO:HD3	2.08	0.54
1:C:392:PHE:HA	1:C:517:LEU:HD11	1.89	0.54
1:B:43:PHE:O	1:B:44:ARG:HG3	2.08	0.54
1:B:326:ILE:HD11	1:B:328:ARG:HD2	1.89	0.54
1:A:41:LYS:CG	1:C:519:HIS:CE1	2.90	0.54
1:A:111:ASP:OD1	1:A:134:GLN:NE2	2.41	0.54
1:A:476:GLY:CA	2:D:24:GLN:NE2	2.65	0.54
1:C:43:PHE:O	1:C:44:ARG:HG3	2.08	0.54
1:C:111:ASP:OD1	1:C:134:GLN:NE2	2.41	0.54
1:A:699:LEU:HD22	1:B:873:TYR:CE2	2.42	0.54
1:B:1142:GLN:HG3	1:B:1143:PRO:CD	2.37	0.54
1:C:390:LEU:HD23	1:C:391:CYS:N	2.19	0.54
1:B:390:LEU:HD11	1:C:983:ARG:HD3	1.89	0.54
1:C:438:SER:O	1:C:438:SER:OG	2.21	0.54
1:C:100:ILE:O	1:C:242:LEU:HA	2.08	0.53
2:D:538:PRO:HD2	2:D:541:LYS:HD2	1.88	0.53
1:B:310:LYS:HA	1:B:599:THR:O	2.08	0.53
1:A:538:CYS:HG	1:A:590:CYS:HG	0.55	0.53
1:B:748:GLU:HG2	1:B:981:LEU:HD21	1.83	0.53
1:B:100:ILE:O	1:B:242:LEU:HA	2.08	0.53
1:B:748:GLU:HG3	1:B:981:LEU:CD2	2.23	0.53
1:C:537:LYS:O	1:C:538:CYS:C	2.47	0.53
1:A:100:ILE:O	1:A:242:LEU:HA	2.08	0.53
1:A:505:TYR:CG	2:D:353:LYS:O	2.62	0.53
1:B:111:ASP:OD1	1:B:134:GLN:NE2	2.41	0.53
1:A:64:TRP:HD1	1:A:65:PHE:N	2.07	0.53
2:D:52:THR:OG1	2:D:332:MET:SD	2.66	0.53
1:A:894:LEU:HB3	1:C:713:ALA:HB3	1.90	0.53
1:B:556:ASN:HD22	1:B:556:ASN:N	2.05	0.53
1:C:280:ASN:CB	1:C:286:THR:HG23	2.39	0.53
1:C:592:PHE:N	1:C:592:PHE:CD1	2.76	0.53
1:B:544:ASN:O	1:B:544:ASN:ND2	2.41	0.53
1:C:528:LYS:O	1:C:529:LYS:CE	2.49	0.53
1:A:421:TYR:HA	1:A:461:LEU:HG	1.90	0.53
1:A:1141:LEU:HD12	1:C:1141:LEU:HD11	1.90	0.53
1:B:326:ILE:HD13	1:B:327:VAL:H	1.72	0.53
1:B:396:TYR:OH	1:C:230:PRO:CG	2.57	0.53
1:B:1104:VAL:HG22	1:B:1115:ILE:HG12	1.91	0.53
2:D:90:ASN:HB3	2:D:93:VAL:HG12	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:2:NAG:H3	3:H:2:NAG:H83	1.90	0.53
1:A:476:GLY:H	1:A:487:ASN:HB3	1.74	0.52
1:C:57:PRO:O	1:C:60:SER:OG	2.24	0.52
1:A:529:LYS:CE	1:A:529:LYS:CA	2.86	0.52
1:B:675:GLN:O	1:B:690:GLN:HG3	2.08	0.52
1:C:338:PHE:C	1:C:340:GLU:H	2.13	0.52
1:A:338:PHE:C	1:A:340:GLU:H	2.13	0.52
1:A:544:ASN:O	1:A:544:ASN:ND2	2.41	0.52
1:B:48:LEU:N	1:B:48:LEU:CD1	2.73	0.52
1:B:310:LYS:NZ	1:B:310:LYS:CB	2.73	0.52
1:C:520:ALA:CB	1:C:521:PRO:CD	2.79	0.52
1:C:318:PHE:O	1:C:319:ARG:HG2	2.10	0.52
1:A:328:ARG:HD3	1:A:578:ASP:OD1	2.09	0.52
1:C:1101:HIS:CD2	3:X:1:NAG:H5	2.45	0.52
1:B:536:ASN:O	1:B:537:LYS:HG2	2.09	0.52
2:D:394:ASN:HB2	2:D:562:LYS:HD2	1.92	0.52
1:A:694:ALA:O	1:A:695:TYR:HB3	2.10	0.52
1:B:64:TRP:HD1	1:B:65:PHE:N	2.07	0.52
1:B:338:PHE:C	1:B:340:GLU:H	2.13	0.52
1:B:390:LEU:HD22	1:B:517:LEU:HD12	1.92	0.52
1:C:403:ARG:NH1	1:C:505:TYR:CD1	2.78	0.52
1:A:901:GLN:NE2	1:A:905:ARG:HH21	2.08	0.51
1:A:319:ARG:NH2	1:A:319:ARG:CG	2.73	0.51
1:C:48:LEU:CD1	1:C:48:LEU:N	2.73	0.51
1:A:493:GLN:OE1	2:D:34:HIS:HB3	2.10	0.51
1:A:745:ASP:HB2	1:C:319:ARG:HH12	1.75	0.51
1:B:379:CYS:HB3	1:B:382:VAL:O	2.10	0.51
1:C:64:TRP:HD1	1:C:65:PHE:N	2.07	0.51
1:C:319:ARG:CG	1:C:319:ARG:NH2	2.73	0.51
1:C:324:GLU:O	1:C:539:VAL:HG23	2.11	0.51
2:D:104:GLY:O	2:D:107:VAL:HG22	2.10	0.51
1:A:505:TYR:CE2	2:D:354:GLY:HA3	2.45	0.51
2:D:245:ARG:NH1	2:D:603:PHE:O	2.42	0.51
1:A:131:CYS:H	1:A:133:PHE:HE1	1.59	0.51
1:B:348:ALA:HB2	1:B:354:ASN:ND2	2.26	0.51
1:C:715:PRO:HA	1:C:1072:GLU:HA	1.92	0.51
1:A:379:CYS:HB3	1:A:382:VAL:O	2.10	0.51
1:C:325:SER:HB2	1:C:540:ASN:HB3	1.93	0.51
1:A:41:LYS:CD	1:A:41:LYS:N	2.73	0.51
1:A:390:LEU:HD23	1:A:391:CYS:N	2.19	0.51
1:C:379:CYS:HB3	1:C:382:VAL:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:854:LYS:O	1:A:854:LYS:HG2	2.11	0.51
1:B:403:ARG:NH1	1:B:505:TYR:CD1	2.78	0.51
1:C:285:ILE:HG22	1:C:286:THR:N	2.25	0.51
1:B:328:ARG:HH11	1:B:533:LEU:HD22	1.75	0.51
1:C:335:LEU:N	1:C:335:LEU:CD1	2.73	0.51
1:A:41:LYS:CA	1:C:519:HIS:HE1	2.24	0.51
1:A:48:LEU:N	1:A:48:LEU:CD1	2.73	0.51
1:A:106:PHE:HB3	1:A:235:ILE:HD13	1.93	0.51
1:A:705:VAL:HB	1:B:883:THR:HG21	1.93	0.51
1:B:321:GLN:OE1	1:B:322:PRO:HD2	2.10	0.51
1:C:131:CYS:H	1:C:133:PHE:HE1	1.59	0.50
1:A:438:SER:O	1:A:438:SER:OG	2.21	0.50
1:B:310:LYS:HB2	1:B:310:LYS:NZ	2.26	0.50
1:C:348:ALA:HB2	1:C:354:ASN:ND2	2.26	0.50
2:D:342:ALA:O	2:D:343:VAL:C	2.50	0.50
1:C:544:ASN:ND2	1:C:544:ASN:O	2.41	0.50
1:C:804:GLN:HE21	1:C:935:GLN:NE2	2.08	0.50
2:D:433:GLU:O	2:D:437:ASN:ND2	2.44	0.50
1:A:129:LYS:HG2	1:A:133:PHE:HZ	1.76	0.50
1:B:131:CYS:H	1:B:133:PHE:HE1	1.59	0.50
1:A:520:ALA:CB	1:A:521:PRO:CD	2.79	0.50
1:B:326:ILE:CG2	1:B:541:PHE:CB	2.90	0.50
1:B:550:GLY:HA2	1:B:590:CYS:SG	2.52	0.50
1:B:367:VAL:CG2	4:B:1407:NAG:C8	2.55	0.50
1:A:41:LYS:HA	1:C:563:GLN:HG2	1.90	0.50
1:C:327:VAL:HG11	1:C:528:LYS:HE2	1.94	0.50
1:C:329:PHE:CE2	1:C:528:LYS:CD	2.91	0.50
1:C:674:TYR:CD1	1:C:691:SER:O	2.64	0.50
1:C:1032:CYS:O	1:C:1051:SER:HB2	2.11	0.50
1:B:401:VAL:HG22	1:B:509:ARG:HG2	1.94	0.50
1:B:535:LYS:HE2	1:B:554:GLU:CD	2.31	0.50
2:D:208:GLU:OE2	2:D:219:ARG:NH1	2.44	0.50
3:P:1:NAG:H62	3:P:2:NAG:H2	1.93	0.50
1:A:502:GLY:O	1:A:505:TYR:HB2	2.12	0.50
1:C:401:VAL:HG22	1:C:509:ARG:HG2	1.94	0.50
1:C:807:PRO:O	1:C:809:PRO:HD3	2.12	0.50
1:C:1090:PRO:HD3	1:C:1095:PHE:CE2	2.47	0.50
2:D:335:ASP:CA	2:D:361:CYS:SG	3.00	0.50
1:A:348:ALA:HB2	1:A:354:ASN:ND2	2.26	0.49
1:C:591:SER:C	1:C:592:PHE:CD1	2.86	0.49
1:B:316:SER:OG	1:B:317:ASN:N	2.44	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:329:PHE:HE2	1:B:528:LYS:HG3	1.76	0.49
1:C:130:VAL:HB	1:C:168:PHE:HB3	1.93	0.49
1:A:122:ASN:OD1	1:A:122:ASN:N	2.46	0.49
1:A:977:LEU:O	1:A:981:LEU:HG	2.12	0.49
1:B:106:PHE:HB3	1:B:235:ILE:HD13	1.93	0.49
1:B:431:GLY:HA3	1:B:513:LEU:O	2.12	0.49
1:B:41:LYS:CD	1:B:41:LYS:N	2.73	0.49
1:B:517:LEU:HD22	1:C:983:ARG:CD	2.41	0.49
1:B:520:ALA:CB	1:B:521:PRO:CD	2.85	0.49
1:C:535:LYS:CD	1:C:554:GLU:OE2	2.60	0.49
1:C:106:PHE:HB3	1:C:235:ILE:HD13	1.93	0.49
1:C:318:PHE:O	1:C:319:ARG:HB2	2.12	0.49
1:A:130:VAL:HB	1:A:168:PHE:HB3	1.93	0.49
1:A:735:SER:HB3	1:A:859:THR:HG22	1.94	0.49
1:B:122:ASN:OD1	1:B:122:ASN:N	2.46	0.49
1:C:171:VAL:HG12	1:C:172:SER:H	1.78	0.49
1:A:401:VAL:HG22	1:A:509:ARG:HG2	1.94	0.49
1:B:367:VAL:HG21	4:B:1407:NAG:H81	1.90	0.49
1:C:129:LYS:HG2	1:C:133:PHE:HZ	1.77	0.49
1:C:431:GLY:HA3	1:C:513:LEU:O	2.12	0.49
1:A:231:ILE:HB	1:A:233:ILE:HG22	1.95	0.49
1:B:129:LYS:HG2	1:B:133:PHE:HZ	1.76	0.49
1:B:130:VAL:HB	1:B:168:PHE:HB3	1.93	0.49
1:C:122:ASN:N	1:C:122:ASN:OD1	2.46	0.49
1:C:524:VAL:HG22	1:C:525:CYS:N	2.27	0.49
1:A:171:VAL:HG12	1:A:172:SER:H	1.78	0.49
1:A:334:ASN:O	1:A:362:VAL:CB	2.56	0.49
1:A:896:ILE:HG13	1:A:897:PRO:HD2	1.95	0.49
1:B:212:LEU:HD23	1:B:215:ASP:HB2	1.95	0.49
1:C:212:LEU:HD23	1:C:215:ASP:HB2	1.95	0.49
1:C:231:ILE:HB	1:C:233:ILE:HG22	1.95	0.49
1:B:171:VAL:HG12	1:B:172:SER:H	1.78	0.48
1:B:231:ILE:HB	1:B:233:ILE:HG22	1.95	0.48
1:B:524:VAL:HG22	1:B:525:CYS:N	2.27	0.48
1:B:675:GLN:HB3	1:B:693:ILE:CD1	2.42	0.48
1:C:41:LYS:N	1:C:41:LYS:CD	2.73	0.48
1:A:41:LYS:CD	1:C:562:PHE:CE2	2.78	0.48
1:A:41:LYS:HB2	1:C:519:HIS:CE1	2.47	0.48
1:C:552:LEU:HD23	1:C:587:ILE:HG12	1.96	0.48
1:B:517:LEU:HD21	1:C:983:ARG:NE	2.24	0.48
1:C:437:ASN:OD1	1:C:438:SER:N	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:978:ASN:HD22	1:C:547:THR:HG22	1.77	0.48
1:B:437:ASN:OD1	1:B:438:SER:N	2.46	0.48
1:C:328:ARG:NH2	1:C:543:PHE:HZ	2.03	0.48
1:A:335:LEU:HD12	1:A:335:LEU:H	1.78	0.48
1:A:392:PHE:CD2	1:A:517:LEU:CD2	2.85	0.48
1:A:437:ASN:OD1	1:A:438:SER:N	2.46	0.48
1:A:533:LEU:HD21	1:A:535:LYS:CE	2.34	0.48
1:A:538:CYS:HG	1:A:590:CYS:CB	2.20	0.48
1:A:935:GLN:O	1:A:939:SER:HB3	2.14	0.48
1:B:592:PHE:CD1	1:B:592:PHE:C	2.87	0.48
1:C:516:GLU:C	1:C:517:LEU:CD2	2.82	0.48
1:C:576:VAL:CG2	1:C:587:ILE:HD11	2.43	0.48
2:D:564:GLU:HB3	2:D:568:LEU:HD23	1.94	0.48
1:A:675:GLN:O	1:A:690:GLN:NE2	2.35	0.48
1:B:388:ASN:CG	1:B:527:PRO:HD2	2.34	0.48
1:A:212:LEU:HD23	1:A:215:ASP:HB2	1.95	0.48
1:A:361:CYS:O	1:A:524:VAL:HG23	2.13	0.48
1:A:431:GLY:HA3	1:A:513:LEU:O	2.12	0.48
1:A:886:TRP:CH2	1:A:904:TYR:HD2	2.31	0.48
1:B:557:LYS:HD2	1:C:43:PHE:HE2	1.78	0.48
1:C:1104:VAL:HG22	1:C:1115:ILE:HG12	1.95	0.48
1:B:544:ASN:HD21	1:B:564:GLN:HE22	1.61	0.48
1:B:710:ASN:N	1:B:710:ASN:HD22	2.11	0.48
1:A:46:SER:O	1:A:47:VAL:HG13	2.14	0.47
1:A:505:TYR:CE2	2:D:353:LYS:C	2.87	0.47
1:B:46:SER:O	1:B:47:VAL:HG13	2.14	0.47
1:C:361:CYS:O	1:C:524:VAL:HG23	2.13	0.47
1:A:524:VAL:HG22	1:A:525:CYS:N	2.27	0.47
1:B:560:LEU:O	1:B:562:PHE:N	2.47	0.47
1:C:280:ASN:CB	1:C:286:THR:HG21	2.42	0.47
1:B:361:CYS:O	1:B:524:VAL:HG23	2.13	0.47
1:C:560:LEU:O	1:C:562:PHE:N	2.47	0.47
1:A:516:GLU:C	1:A:517:LEU:CD2	2.82	0.47
1:B:326:ILE:CG2	1:B:541:PHE:HB3	2.45	0.47
1:B:392:PHE:HE2	1:B:517:LEU:CD1	2.16	0.47
1:B:566:GLY:HA2	1:C:43:PHE:HB3	1.96	0.47
1:C:227:VAL:HG12	1:C:228:ASP:H	1.79	0.47
1:C:46:SER:O	1:C:47:VAL:HG13	2.14	0.47
1:C:726:ILE:HG12	1:C:1061:VAL:HG22	1.97	0.47
1:A:486:PHE:HE1	2:D:79:LEU:CD1	2.27	0.47
1:B:227:VAL:HG12	1:B:228:ASP:H	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:367:VAL:HG22	4:B:1407:NAG:H83	1.82	0.47
1:C:328:ARG:NE	1:C:578:ASP:OD1	2.47	0.47
1:C:369:TYR:CE2	1:C:384:PRO:HB2	2.50	0.47
2:D:421:ILE:HG13	2:D:421:ILE:O	2.14	0.47
1:A:550:GLY:HA2	1:A:590:CYS:SG	2.55	0.47
1:B:328:ARG:HA	1:B:530:SER:HB2	1.97	0.47
1:B:640:SER:OG	1:B:641:ASN:N	2.48	0.47
2:D:425:SER:C	2:D:427:ASP:H	2.19	0.47
1:A:653:ALA:HA	1:A:692:ILE:O	2.14	0.47
1:B:364:ASP:O	1:B:367:VAL:HG12	2.15	0.47
1:B:569:ILE:HG13	1:C:47:VAL:CG1	2.28	0.47
1:C:524:VAL:C	1:C:525:CYS:SG	2.93	0.47
1:C:973:ILE:HG12	1:C:992:GLN:HE21	1.79	0.47
1:A:227:VAL:HG12	1:A:228:ASP:H	1.79	0.47
1:B:327:VAL:O	1:B:530:SER:HA	2.14	0.47
1:B:517:LEU:CD1	1:C:983:ARG:HD3	2.45	0.47
1:B:524:VAL:C	1:B:525:CYS:SG	2.93	0.47
1:B:562:PHE:CE2	1:C:41:LYS:HD2	2.50	0.47
1:B:713:ALA:HB3	1:C:894:LEU:HB3	1.97	0.47
1:C:535:LYS:O	1:C:536:ASN:HB2	2.15	0.47
2:D:333:LEU:O	2:D:362:THR:HG22	2.15	0.47
1:B:369:TYR:CE2	1:B:384:PRO:HB2	2.50	0.46
1:B:562:PHE:HE2	1:C:41:LYS:HD2	1.79	0.46
1:C:329:PHE:CG	1:C:330:PRO:HD2	2.50	0.46
1:C:364:ASP:O	1:C:367:VAL:HG12	2.15	0.46
1:C:804:GLN:HG3	1:C:935:GLN:HE22	1.80	0.46
1:A:640:SER:OG	1:A:641:ASN:N	2.48	0.46
1:B:729:VAL:HG13	1:B:1059:GLY:HA2	1.98	0.46
1:A:369:TYR:CE2	1:A:384:PRO:HB2	2.50	0.46
1:A:393:THR:HA	1:A:523:THR:HB	1.97	0.46
1:A:1105:THR:HG22	1:A:1111:GLU:H	1.80	0.46
1:A:524:VAL:C	1:A:525:CYS:SG	2.93	0.46
1:C:640:SER:OG	1:C:641:ASN:N	2.48	0.46
1:A:29:THR:HG22	1:A:30:ASN:N	2.31	0.46
1:B:326:ILE:HD11	1:B:328:ARG:CD	2.45	0.46
1:B:367:VAL:HG23	4:B:1407:NAG:H83	1.82	0.46
1:B:385:THR:HG1	1:B:386:LYS:HZ3	1.59	0.46
1:C:977:LEU:HD12	1:C:996:LEU:HD12	1.98	0.46
1:B:328:ARG:O	1:B:329:PHE:CD1	2.69	0.46
1:A:983:ARG:O	1:A:984:LEU:CD2	2.60	0.46
1:B:327:VAL:O	1:B:530:SER:CA	2.64	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:578:ASP:OD2	1:B:581:THR:HG22	2.16	0.46
1:A:447:GLY:HA2	1:A:497:PHE:O	2.16	0.46
1:B:390:LEU:CD2	1:B:517:LEU:HD11	2.45	0.46
1:C:41:LYS:N	1:C:41:LYS:HD3	2.31	0.46
1:C:531:THR:CG2	1:C:532:ASN:N	2.73	0.46
1:A:41:LYS:N	1:A:41:LYS:HD3	2.31	0.46
1:B:710:ASN:HD22	1:B:710:ASN:H	1.62	0.46
1:B:825:LYS:HB3	1:B:825:LYS:HE2	1.79	0.46
1:C:393:THR:HA	1:C:523:THR:HB	1.98	0.46
1:C:447:GLY:HA2	1:C:497:PHE:O	2.16	0.46
1:A:45:SER:O	1:A:279:TYR:CB	2.64	0.46
1:A:535:LYS:O	1:A:536:ASN:HB2	2.16	0.46
1:A:912:THR:OG1	1:A:914:ASN:ND2	2.48	0.46
1:B:45:SER:O	1:B:279:TYR:CB	2.64	0.46
1:B:127:VAL:HG11	4:B:1402:NAG:H61	1.98	0.46
1:B:517:LEU:CD2	1:C:983:ARG:CD	2.93	0.46
1:C:322:PRO:O	1:C:324:GLU:N	2.49	0.46
2:D:560:LEU:HD22	2:D:564:GLU:HG3	1.98	0.46
1:B:390:LEU:CD2	1:B:517:LEU:CD1	2.94	0.45
1:B:758:SER:O	1:B:762:GLN:HG3	2.16	0.45
1:B:1032:CYS:O	1:B:1051:SER:HB2	2.16	0.45
1:B:1045:LYS:HZ1	1:C:786:LYS:HE3	1.80	0.45
1:C:377:PHE:CD2	1:C:434:ILE:HG12	2.51	0.45
1:C:500:THR:O	1:C:500:THR:OG1	2.31	0.45
1:A:225:PRO:CG	1:C:562:PHE:CZ	3.00	0.45
1:A:364:ASP:O	1:A:367:VAL:HG12	2.15	0.45
1:A:903:ALA:HB1	1:A:913:GLN:HG2	1.98	0.45
1:B:377:PHE:CD2	1:B:434:ILE:HG12	2.51	0.45
1:A:1094:VAL:HG22	1:A:1107:ARG:HG2	1.98	0.45
1:B:722:VAL:HA	1:B:1064:HIS:O	2.16	0.45
2:D:52:THR:HA	2:D:342:ALA:HB1	1.98	0.45
1:C:578:ASP:OD2	1:C:581:THR:HG22	2.16	0.45
1:B:447:GLY:HA2	1:B:497:PHE:O	2.16	0.45
1:B:646:ARG:O	1:B:646:ARG:HG3	2.17	0.45
1:C:325:SER:CB	1:C:540:ASN:HB3	2.47	0.45
1:C:590:CYS:O	1:C:592:PHE:HD1	2.00	0.45
1:A:113:LYS:O	1:A:113:LYS:NZ	2.31	0.45
1:A:127:VAL:HG11	4:A:1402:NAG:H61	1.98	0.45
1:A:325:SER:HB3	1:A:540:ASN:HB3	1.98	0.45
1:A:329:PHE:CD1	1:A:544:ASN:HA	2.52	0.45
1:A:476:GLY:HA2	2:D:24:GLN:NE2	2.26	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:486:PHE:CE1	2:D:79:LEU:HD21	2.48	0.45
1:B:41:LYS:N	1:B:41:LYS:HD3	2.31	0.45
1:B:587:ILE:O	1:B:587:ILE:HG22	2.17	0.45
1:C:646:ARG:HG3	1:C:646:ARG:O	2.17	0.45
2:D:208:GLU:OE1	2:D:210:ASN:ND2	2.50	0.45
1:A:560:LEU:O	1:A:562:PHE:N	2.47	0.45
1:B:29:THR:HG22	1:B:30:ASN:N	2.31	0.45
1:C:117:LEU:HD12	1:C:118:LEU:N	2.30	0.45
1:C:153:MET:N	1:C:153:MET:SD	2.90	0.45
1:C:328:ARG:HE	1:C:533:LEU:HD22	1.78	0.45
1:C:527:PRO:HG2	1:C:528:LYS:H	1.82	0.45
1:A:316:SER:OG	1:A:317:ASN:N	2.48	0.45
1:A:377:PHE:CD2	1:A:434:ILE:HG12	2.51	0.45
1:B:614:ASP:OD2	1:C:854:LYS:HD2	2.16	0.45
1:A:187:LYS:HE3	1:A:213:VAL:HG12	1.99	0.45
1:A:854:LYS:O	1:A:855:PHE:CD1	2.70	0.45
1:A:153:MET:SD	1:A:153:MET:N	2.90	0.45
1:A:1090:PRO:HD3	1:A:1095:PHE:CE2	2.51	0.45
1:B:153:MET:SD	1:B:153:MET:N	2.90	0.45
1:C:48:LEU:HD13	1:C:48:LEU:N	2.32	0.45
1:C:127:VAL:HG11	4:C:1402:NAG:H61	1.98	0.45
1:C:323:THR:HG21	1:C:537:LYS:HE2	1.99	0.45
1:A:440:ASN:ND2	1:A:441:LEU:HG	2.32	0.44
1:A:529:LYS:NZ	1:A:529:LYS:CA	2.73	0.44
1:A:565:PHE:CZ	1:B:42:VAL:CG2	2.99	0.44
1:A:578:ASP:OD2	1:A:581:THR:HG22	2.16	0.44
1:A:984:LEU:HD22	1:A:984:LEU:HA	1.80	0.44
1:C:279:TYR:HA	1:C:285:ILE:HA	1.98	0.44
1:C:317:ASN:N	1:C:317:ASN:ND2	2.65	0.44
1:C:333:THR:CG2	1:C:334:ASN:H	2.06	0.44
1:C:534:VAL:HG11	1:C:537:LYS:HZ2	1.82	0.44
1:C:537:LYS:NZ	1:C:537:LYS:CB	2.80	0.44
2:D:431:ASP:OD1	2:D:431:ASP:N	2.44	0.44
1:B:326:ILE:HG22	1:B:541:PHE:HB3	1.98	0.44
1:C:134:GLN:HB3	1:C:162:SER:HB2	2.00	0.44
1:C:535:LYS:HG3	1:C:552:LEU:O	2.17	0.44
1:A:225:PRO:HG2	1:C:562:PHE:CE1	2.52	0.44
1:B:328:ARG:NH1	1:B:533:LEU:HD22	2.32	0.44
1:B:518:LEU:O	1:B:519:HIS:CG	2.71	0.44
1:B:529:LYS:C	1:B:529:LYS:CE	2.85	0.44
1:C:43:PHE:HZ	1:C:282:ASN:O	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1141:LEU:O	1:C:1145:LEU:HD12	2.16	0.44
1:A:41:LYS:HA	1:C:563:GLN:CG	2.47	0.44
1:A:538:CYS:SG	1:A:590:CYS:CB	3.05	0.44
1:A:856:ASN:OD1	1:A:856:ASN:N	2.50	0.44
1:C:1040:VAL:O	1:C:1041:ASP:HB2	2.17	0.44
1:B:322:PRO:HB3	1:B:538:CYS:SG	2.57	0.44
1:B:1045:LYS:NZ	1:C:786:LYS:CE	2.79	0.44
1:C:1081:ILE:HG12	1:C:1095:PHE:CE2	2.53	0.44
1:B:140:PHE:CG	1:B:244:LEU:HD11	2.53	0.44
1:B:335:LEU:C	1:B:362:VAL:O	2.55	0.44
1:C:334:ASN:ND2	1:C:361:CYS:HA	2.33	0.44
1:A:117:LEU:HD12	1:A:118:LEU:N	2.30	0.44
1:B:383:SER:OG	1:C:985:ASP:OD2	2.32	0.44
1:B:392:PHE:CE2	1:B:517:LEU:CA	3.01	0.44
1:B:662:CYS:HB2	1:B:697:MET:CE	2.48	0.44
2:D:356:PHE:HB3	2:D:379:ILE:HD12	1.98	0.44
1:A:294:ASP:OD1	1:A:294:ASP:N	2.50	0.44
1:A:335:LEU:C	1:A:362:VAL:O	2.56	0.44
1:A:546:LEU:HD11	1:A:565:PHE:CG	2.53	0.44
1:B:134:GLN:HB3	1:B:162:SER:HB2	2.00	0.44
1:B:187:LYS:HE3	1:B:213:VAL:HG12	1.99	0.44
1:B:334:ASN:ND2	1:B:334:ASN:N	2.60	0.44
1:C:527:PRO:O	1:C:528:LYS:HB2	2.16	0.44
1:A:493:GLN:OE1	2:D:34:HIS:CG	2.70	0.43
1:C:141:LEU:O	1:C:243:ALA:HA	2.18	0.43
1:C:440:ASN:ND2	1:C:441:LEU:HG	2.32	0.43
2:D:313:LYS:HA	2:D:316:VAL:HG12	2.00	0.43
1:C:187:LYS:HE3	1:C:213:VAL:HG12	1.99	0.43
1:A:1104:VAL:HG22	1:A:1115:ILE:HG12	2.00	0.43
1:B:99:ASN:O	1:B:102:ARG:NE	2.35	0.43
1:B:127:VAL:HG21	4:B:1402:NAG:H5	2.01	0.43
1:B:592:PHE:CD1	1:B:592:PHE:O	2.71	0.43
4:B:1411:NAG:O4	4:B:1412:NAG:O5	2.28	0.43
1:C:140:PHE:CG	1:C:244:LEU:HD11	2.53	0.43
1:A:612:TYR:HE1	1:A:651:ILE:HD12	1.84	0.43
1:A:646:ARG:O	1:A:646:ARG:HG3	2.17	0.43
1:A:959:LEU:HD23	1:A:959:LEU:HA	1.78	0.43
1:A:979:ASP:O	1:A:983:ARG:CG	2.60	0.43
1:B:294:ASP:N	1:B:294:ASP:OD1	2.50	0.43
1:C:546:LEU:HD11	1:C:565:PHE:CG	2.53	0.43
3:S:1:NAG:H61	3:S:2:NAG:N2	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:VAL:HG21	1:A:231:ILE:HD12	2.00	0.43
1:A:563:GLN:CD	1:B:43:PHE:HA	2.39	0.43
1:A:1097:SER:HA	1:A:1101:HIS:O	2.19	0.43
1:B:986:PRO:CB	1:B:987:PRO:HD3	2.45	0.43
1:C:294:ASP:OD1	1:C:294:ASP:N	2.50	0.43
1:C:323:THR:HG22	1:C:324:GLU:HG2	2.01	0.43
1:C:393:THR:O	1:C:523:THR:CG2	2.58	0.43
1:C:590:CYS:O	1:C:592:PHE:CD1	2.70	0.43
1:A:134:GLN:HB3	1:A:162:SER:HB2	2.00	0.43
1:A:325:SER:CB	1:A:540:ASN:O	2.65	0.43
1:A:390:LEU:O	1:A:525:CYS:HB3	2.18	0.43
1:A:535:LYS:O	1:A:536:ASN:CB	2.66	0.43
1:A:986:PRO:HA	1:A:989:ALA:HB3	1.99	0.43
1:B:141:LEU:O	1:B:243:ALA:HA	2.18	0.43
1:B:324:GLU:O	1:B:539:VAL:HG23	2.16	0.43
1:B:987:PRO:HG3	1:C:427:ASP:OD2	2.18	0.43
1:C:130:VAL:HG21	1:C:231:ILE:HD12	2.00	0.43
1:C:552:LEU:CD2	1:C:587:ILE:HG12	2.48	0.43
1:A:141:LEU:O	1:A:243:ALA:HA	2.18	0.43
1:A:795:LYS:HB3	1:A:797:PHE:CE2	2.54	0.43
1:B:569:ILE:O	1:B:570:ALA:HB3	2.19	0.43
1:C:212:LEU:HD12	1:C:212:LEU:HA	1.78	0.43
1:B:130:VAL:HG21	1:B:231:ILE:HD12	2.00	0.43
1:B:557:LYS:HD2	1:C:43:PHE:CE2	2.53	0.43
1:C:29:THR:HG22	1:C:30:ASN:N	2.31	0.43
1:C:912:THR:OG1	1:C:914:ASN:ND2	2.51	0.43
1:A:140:PHE:CG	1:A:244:LEU:HD11	2.53	0.43
1:B:117:LEU:HD12	1:B:118:LEU:N	2.30	0.43
1:C:131:CYS:HB3	1:C:164:ASN:O	2.19	0.43
3:F:1:NAG:H61	3:F:2:NAG:N2	2.33	0.43
1:B:546:LEU:HD11	1:B:565:PHE:CG	2.53	0.43
1:C:285:ILE:CG2	1:C:286:THR:N	2.81	0.43
1:C:333:THR:CG2	1:C:361:CYS:O	2.45	0.43
1:C:390:LEU:O	1:C:525:CYS:HB3	2.18	0.43
1:C:516:GLU:C	1:C:517:LEU:HD23	2.39	0.43
1:C:722:VAL:HA	1:C:1064:HIS:O	2.19	0.42
1:A:1032:CYS:O	1:A:1051:SER:HB2	2.18	0.42
1:B:440:ASN:ND2	1:B:441:LEU:HG	2.32	0.42
1:A:569:ILE:O	1:A:570:ALA:HB3	2.19	0.42
1:B:27:ALA:HB3	1:B:64:TRP:HB3	2.01	0.42
1:B:332:ILE:CG2	1:B:362:VAL:HG21	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:517:LEU:HD11	1:C:983:ARG:HD3	1.99	0.42
1:C:792:PRO:O	1:C:795:LYS:NZ	2.52	0.42
1:C:1027:THR:HG22	1:C:1042:PHE:HZ	1.83	0.42
1:A:112:SER:O	1:A:113:LYS:HB3	2.20	0.42
1:A:502:GLY:HA3	2:D:354:GLY:O	2.20	0.42
1:A:516:GLU:C	1:A:517:LEU:HD23	2.39	0.42
1:A:523:THR:CG2	1:A:524:VAL:N	2.46	0.42
1:C:995:ARG:HE	1:C:995:ARG:HB3	1.66	0.42
1:A:41:LYS:HA	1:C:562:PHE:CE2	2.54	0.42
1:B:524:VAL:CG2	1:B:525:CYS:N	2.83	0.42
1:C:317:ASN:HB3	1:C:593:GLY:O	2.20	0.42
1:A:565:PHE:O	1:B:43:PHE:N	2.53	0.42
1:B:48:LEU:HD13	1:B:48:LEU:N	2.32	0.42
1:B:390:LEU:O	1:B:525:CYS:HB3	2.18	0.42
1:B:392:PHE:HD2	1:B:517:LEU:CA	2.08	0.42
1:B:612:TYR:HE1	1:B:651:ILE:HD12	1.84	0.42
1:C:127:VAL:HG21	4:C:1402:NAG:H5	2.01	0.42
1:C:529:LYS:HD3	1:C:529:LYS:HA	1.80	0.42
1:A:27:ALA:HB3	1:A:64:TRP:HB3	2.01	0.42
1:A:316:SER:C	1:A:317:ASN:ND2	2.73	0.42
1:A:933:LYS:HB2	1:A:933:LYS:HE3	1.86	0.42
1:A:982:SER:OG	1:A:983:ARG:N	2.53	0.42
1:B:131:CYS:HB3	1:B:164:ASN:O	2.19	0.42
1:C:654:GLU:CG	1:C:693:ILE:HG22	2.12	0.42
3:T:1:NAG:H3	3:T:1:NAG:H83	2.02	0.42
1:A:131:CYS:HB3	1:A:164:ASN:O	2.19	0.42
1:A:406:GLU:CG	1:A:418:ILE:HG13	2.50	0.42
1:A:690:GLN:HB2	1:A:691:SER:H	1.69	0.42
1:C:316:SER:C	1:C:317:ASN:ND2	2.73	0.42
1:C:523:THR:CG2	1:C:524:VAL:N	2.46	0.42
1:C:569:ILE:O	1:C:570:ALA:HB3	2.19	0.42
1:C:736:VAL:HG23	1:C:858:LEU:HD23	2.02	0.42
2:D:425:SER:C	2:D:427:ASP:N	2.73	0.42
1:A:973:ILE:HG23	1:A:992:GLN:NE2	2.35	0.42
1:B:319:ARG:HH22	1:C:740:MET:CG	2.33	0.42
1:C:281:GLU:N	1:C:281:GLU:CD	2.73	0.42
1:C:612:TYR:HE1	1:C:651:ILE:HD12	1.84	0.42
1:C:793:PRO:HG2	1:C:794:ILE:HD12	2.00	0.42
1:C:856:ASN:O	1:C:856:ASN:ND2	2.48	0.42
1:A:326:ILE:HD13	1:A:534:VAL:H	1.85	0.41
1:A:524:VAL:CG2	1:A:525:CYS:N	2.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:529:LYS:HE2	1:A:529:LYS:CA	2.45	0.41
1:A:674:TYR:CD1	1:A:691:SER:O	2.73	0.41
1:A:758:SER:O	1:A:762:GLN:HG3	2.19	0.41
1:B:329:PHE:CG	1:B:330:PRO:HD2	2.55	0.41
1:C:393:THR:H	1:C:517:LEU:HD22	1.85	0.41
1:C:544:ASN:OD1	1:C:564:GLN:NE2	2.44	0.41
1:C:735:SER:OG	1:C:859:THR:HG22	2.17	0.41
1:B:112:SER:O	1:B:113:LYS:HB3	2.20	0.41
1:B:212:LEU:HD12	1:B:212:LEU:HA	1.78	0.41
1:B:529:LYS:C	1:B:529:LYS:NZ	2.73	0.41
1:C:784:GLN:HE21	1:C:784:GLN:HB3	1.63	0.41
1:A:388:ASN:CG	1:A:527:PRO:HD2	2.41	0.41
1:B:325:SER:O	1:B:327:VAL:HG23	2.19	0.41
1:B:517:LEU:HD13	1:C:983:ARG:HD2	2.00	0.41
1:C:27:ALA:HB3	1:C:64:TRP:HB3	2.01	0.41
1:C:325:SER:HB2	1:C:540:ASN:O	2.20	0.41
1:C:392:PHE:CA	1:C:517:LEU:HD21	2.49	0.41
1:C:524:VAL:CG2	1:C:525:CYS:N	2.83	0.41
1:C:617:CYS:HB2	1:C:649:CYS:HB2	1.87	0.41
1:A:393:THR:H	1:A:517:LEU:HD22	1.85	0.41
1:A:864:LEU:HD13	1:C:665:PRO:CB	2.50	0.41
1:B:307:THR:HA	1:B:602:THR:OG1	2.20	0.41
1:C:406:GLU:CG	1:C:418:ILE:HG13	2.50	0.41
1:C:696:THR:O	1:C:697:MET:C	2.56	0.41
1:C:985:ASP:OD1	1:C:985:ASP:N	2.46	0.41
1:A:193:VAL:HG23	1:A:223:LEU:CD2	2.51	0.41
1:A:617:CYS:HB2	1:A:649:CYS:HB2	1.87	0.41
1:B:48:LEU:H	1:B:48:LEU:CD1	2.32	0.41
1:B:776:LYS:HE3	1:B:776:LYS:HB3	1.65	0.41
1:C:521:PRO:O	1:C:522:ALA:CB	2.66	0.41
1:C:703:ASN:C	1:C:703:ASN:HD22	2.24	0.41
1:A:127:VAL:HG21	4:A:1402:NAG:H5	2.01	0.41
1:A:654:GLU:O	1:A:693:ILE:CA	2.69	0.41
1:B:45:SER:OG	1:B:281:GLU:HA	2.21	0.41
1:B:535:LYS:O	1:B:537:LYS:HG3	2.20	0.41
2:D:212:VAL:HG23	2:D:215:TYR:HB2	2.02	0.41
1:A:1123:SER:O	1:A:1123:SER:OG	2.39	0.41
1:C:45:SER:O	1:C:47:VAL:N	2.54	0.41
1:C:326:ILE:C	1:C:327:VAL:HG23	2.41	0.41
1:C:821:LEU:HD22	1:C:939:SER:HB3	2.03	0.41
1:C:973:ILE:HG23	1:C:992:GLN:NE2	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:330:PRO:O	1:A:331:ASN:O	2.39	0.41
1:A:486:PHE:HE1	2:D:79:LEU:HD21	1.77	0.41
1:A:855:PHE:HB3	1:A:856:ASN:H	1.69	0.41
1:B:193:VAL:HG23	1:B:223:LEU:CD2	2.51	0.41
1:B:213:VAL:HG23	1:B:214:ARG:N	2.36	0.41
1:C:112:SER:O	1:C:113:LYS:HB3	2.20	0.41
1:C:193:VAL:HG23	1:C:223:LEU:CD2	2.51	0.41
1:C:200:TYR:CE1	1:C:230:PRO:HB3	2.56	0.41
1:C:907:ASN:HD22	1:C:907:ASN:HA	1.64	0.41
1:C:984:LEU:HD23	1:C:984:LEU:HA	1.91	0.41
2:D:105:SER:C	2:D:106:SER:HG	2.02	0.41
1:A:505:TYR:CD2	2:D:353:LYS:C	2.93	0.41
1:B:338:PHE:C	1:B:340:GLU:N	2.75	0.41
1:C:542:ASN:HA	1:C:546:LEU:O	2.21	0.41
2:D:21:ILE:HD12	2:D:21:ILE:HA	1.97	0.41
1:B:89:GLY:HA2	1:B:194:PHE:O	2.21	0.40
1:C:347:PHE:CD1	1:C:509:ARG:HD3	2.56	0.40
1:C:740:MET:HE2	1:C:740:MET:HB2	1.81	0.40
1:C:870:ILE:O	1:C:874:THR:HG23	2.21	0.40
1:A:227:VAL:CG1	1:A:228:ASP:N	2.84	0.40
1:A:864:LEU:HD13	1:C:665:PRO:HB2	2.04	0.40
1:A:1051:SER:OG	1:A:1064:HIS:ND1	2.46	0.40
1:B:347:PHE:CD1	1:B:509:ARG:HD3	2.56	0.40
1:B:392:PHE:CE2	1:B:517:LEU:CG	3.03	0.40
1:B:984:LEU:HD23	1:B:988:GLU:HB3	2.03	0.40
1:C:213:VAL:HG23	1:C:214:ARG:N	2.36	0.40
1:C:770:ILE:O	1:C:774:GLN:HG2	2.21	0.40
2:D:294:THR:HG23	2:D:365:THR:HA	2.03	0.40
1:A:89:GLY:HA2	1:A:194:PHE:O	2.22	0.40
1:A:213:VAL:HG23	1:A:214:ARG:N	2.36	0.40
1:A:505:TYR:CE2	2:D:353:LYS:O	2.73	0.40
1:A:886:TRP:HH2	1:A:904:TYR:CD2	2.35	0.40
1:B:127:VAL:HG22	1:B:171:VAL:HG13	2.04	0.40
2:D:411:SER:OG	2:D:543:ASP:OD1	2.38	0.40
1:A:187:LYS:N	1:A:187:LYS:HE2	2.37	0.40
1:A:212:LEU:HD12	1:A:212:LEU:HA	1.78	0.40
1:A:340:GLU:HG3	1:A:341:VAL:N	2.37	0.40
1:A:486:PHE:CE1	2:D:79:LEU:HD13	2.56	0.40
1:A:521:PRO:O	1:A:522:ALA:CB	2.66	0.40
1:A:1105:THR:HG21	1:A:1110:TYR:CD1	2.57	0.40
1:B:166:CYS:HB3	1:B:169:GLU:OE1	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:187:LYS:N	1:B:187:LYS:HE2	2.37	0.40
1:A:45:SER:O	1:A:47:VAL:N	2.54	0.40
1:A:708:SER:OG	1:A:711:SER:HB2	2.22	0.40
1:C:226:LEU:HB3	1:C:227:VAL:HG23	2.03	0.40
1:C:693:ILE:H	1:C:693:ILE:HG13	1.82	0.40
1:C:854:LYS:HE2	1:C:854:LYS:HB3	1.88	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	989/1283 (77%)	871 (88%)	92 (9%)	26 (3%)	5	27
1	B	951/1283 (74%)	826 (87%)	96 (10%)	29 (3%)	4	24
1	C	951/1283 (74%)	807 (85%)	101 (11%)	43 (4%)	2	15
2	D	593/817 (73%)	563 (95%)	28 (5%)	2 (0%)	41	71
All	All	3484/4666 (75%)	3067 (88%)	317 (9%)	100 (3%)	7	24

All (100) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	48	LEU
1	A	331	ASN
1	A	518	LEU
1	A	691	SER
1	A	701	ALA
1	A	855	PHE
1	B	48	LEU
1	B	333	THR
1	B	518	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	519	HIS
1	B	520	ALA
1	C	48	LEU
1	C	323	THR
1	C	333	THR
1	C	334	ASN
1	C	518	LEU
1	C	526	GLY
1	C	532	ASN
1	C	814	LYS
1	A	41	LYS
1	A	46	SER
1	A	339	GLY
1	A	536	ASN
1	A	537	LYS
1	A	989	ALA
1	B	41	LYS
1	B	46	SER
1	B	339	GLY
1	B	526	GLY
1	B	534	VAL
1	B	742	ILE
1	B	743	CYS
1	C	41	LYS
1	C	46	SER
1	C	280	ASN
1	C	318	PHE
1	C	319	ARG
1	C	332	ILE
1	C	339	GLY
1	C	527	PRO
1	C	592	PHE
1	C	697	MET
1	C	810	SER
2	D	343	VAL
1	A	43	PHE
1	A	324	GLU
1	A	336	CYS
1	A	522	ALA
1	A	695	TYR
1	A	710	ASN
1	A	984	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	43	PHE
1	B	521	PRO
1	C	43	PHE
1	C	316	SER
1	C	522	ALA
1	C	528	LYS
1	C	691	SER
2	D	423	LEU
1	A	44	ARG
1	A	349	SER
1	A	520	ALA
1	B	44	ARG
1	B	349	SER
1	B	517	LEU
1	B	522	ALA
1	B	592	PHE
1	B	746	SER
1	C	44	ARG
1	C	329	PHE
1	C	349	SER
1	C	520	ALA
1	C	529	LYS
1	C	533	LEU
1	C	591	SER
1	C	813	SER
1	A	40	ASP
1	A	42	VAL
1	A	47	VAL
1	B	40	ASP
1	B	42	VAL
1	B	47	VAL
1	B	329	PHE
1	B	531	THR
1	C	40	ASP
1	C	42	VAL
1	C	47	VAL
1	C	283	GLY
1	C	330	PRO
1	C	812	PRO
1	B	527	PRO
1	C	285	ILE
1	C	320	VAL

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Mol	Chain	Res	Type
1	C	811	LYS
1	B	332	ILE
1	B	336	CYS
1	B	327	VAL
1	C	327	VAL
1	C	534	VAL
1	A	526	GLY

### 5.3.2 Protein sidechains [i](#)

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	882/1122 (79%)	779 (88%)	103 (12%)	5	21
1	B	850/1122 (76%)	749 (88%)	101 (12%)	5	21
1	C	850/1122 (76%)	754 (89%)	96 (11%)	6	22
2	D	525/721 (73%)	518 (99%)	7 (1%)	69	82
All	All	3107/4087 (76%)	2800 (90%)	307 (10%)	11	28

All (307) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	ASP
1	A	46	SER
1	A	48	LEU
1	A	97	LYS
1	A	109	THR
1	A	116	SER
1	A	118	LEU
1	A	122	ASN
1	A	137	ASN
1	A	141	LEU
1	A	143	VAL
1	A	158	ARG
1	A	164	ASN
1	A	169	GLU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	195	LYS
1	A	205	SER
1	A	208	THR
1	A	221	SER
1	A	282	ASN
1	A	296	LEU
1	A	301	CYS
1	A	308	VAL
1	A	314	GLN
1	A	315	THR
1	A	319	ARG
1	A	324	GLU
1	A	333	THR
1	A	335	LEU
1	A	353	TRP
1	A	355	ARG
1	A	375	SER
1	A	383	SER
1	A	389	ASP
1	A	390	LEU
1	A	406	GLU
1	A	421	TYR
1	A	430	THR
1	A	438	SER
1	A	440	ASN
1	A	500	THR
1	A	514	SER
1	A	517	LEU
1	A	518	LEU
1	A	525	CYS
1	A	529	LYS
1	A	532	ASN
1	A	533	LEU
1	A	540	ASN
1	A	546	LEU
1	A	553	THR
1	A	554	GLU
1	A	556	ASN
1	A	558	LYS
1	A	576	VAL
1	A	583	GLU
1	A	588	THR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	590	CYS
1	A	591	SER
1	A	599	THR
1	A	602	THR
1	A	646	ARG
1	A	673	SER
1	A	696	THR
1	A	702	GLU
1	A	704	SER
1	A	722	VAL
1	A	727	LEU
1	A	729	VAL
1	A	738	CYS
1	A	746	SER
1	A	773	GLU
1	A	785	VAL
1	A	787	GLN
1	A	791	THR
1	A	826	VAL
1	A	855	PHE
1	A	856	ASN
1	A	868	GLU
1	A	878	LEU
1	A	883	THR
1	A	902	MET
1	A	916	LEU
1	A	929	SER
1	A	937	SER
1	A	939	SER
1	A	951	VAL
1	A	967	SER
1	A	984	LEU
1	A	994	ASP
1	A	1005	GLN
1	A	1074	ASN
1	A	1076	THR
1	A	1077	THR
1	A	1092	GLU
1	A	1094	VAL
1	A	1100	THR
1	A	1104	VAL
1	A	1123	SER

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	1125	ASN
1	A	1132	ILE
1	A	1141	LEU
1	A	1142	GLN
1	A	1144	GLU
1	B	40	ASP
1	B	46	SER
1	B	48	LEU
1	B	97	LYS
1	B	109	THR
1	B	116	SER
1	B	118	LEU
1	B	122	ASN
1	B	137	ASN
1	B	141	LEU
1	B	143	VAL
1	B	158	ARG
1	B	164	ASN
1	B	169	GLU
1	B	195	LYS
1	B	205	SER
1	B	208	THR
1	B	221	SER
1	B	282	ASN
1	B	296	LEU
1	B	301	CYS
1	B	308	VAL
1	B	310	LYS
1	B	314	GLN
1	B	315	THR
1	B	326	ILE
1	B	328	ARG
1	B	329	PHE
1	B	332	ILE
1	B	333	THR
1	B	334	ASN
1	B	336	CYS
1	B	343	ASN
1	B	353	TRP
1	B	355	ARG
1	B	375	SER
1	B	383	SER

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	389	ASP
1	B	390	LEU
1	B	406	GLU
1	B	421	TYR
1	B	430	THR
1	B	438	SER
1	B	440	ASN
1	B	500	THR
1	B	514	SER
1	B	515	PHE
1	B	516	GLU
1	B	518	LEU
1	B	519	HIS
1	B	525	CYS
1	B	528	LYS
1	B	529	LYS
1	B	533	LEU
1	B	535	LYS
1	B	536	ASN
1	B	540	ASN
1	B	546	LEU
1	B	553	THR
1	B	554	GLU
1	B	556	ASN
1	B	558	LYS
1	B	564	GLN
1	B	576	VAL
1	B	583	GLU
1	B	591	SER
1	B	599	THR
1	B	602	THR
1	B	646	ARG
1	B	673	SER
1	B	704	SER
1	B	710	ASN
1	B	735	SER
1	B	747	THR
1	B	748	GLU
1	B	779	GLN
1	B	786	LYS
1	B	787	GLN
1	B	791	THR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	808	ASP
1	B	854	LYS
1	B	855	PHE
1	B	856	ASN
1	B	868	GLU
1	B	878	LEU
1	B	912	THR
1	B	916	LEU
1	B	935	GLN
1	B	964	LYS
1	B	969	ASN
1	B	974	SER
1	B	976	VAL
1	B	1030	SER
1	B	1037	SER
1	B	1045	LYS
1	B	1074	ASN
1	B	1094	VAL
1	B	1104	VAL
1	B	1114	ILE
1	B	1126	CYS
1	B	1141	LEU
1	C	40	ASP
1	C	46	SER
1	C	48	LEU
1	C	97	LYS
1	C	109	THR
1	C	116	SER
1	C	118	LEU
1	C	122	ASN
1	C	137	ASN
1	C	141	LEU
1	C	143	VAL
1	C	158	ARG
1	C	164	ASN
1	C	169	GLU
1	C	195	LYS
1	C	205	SER
1	C	208	THR
1	C	221	SER
1	C	278	LYS
1	C	281	GLU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	C	284	THR
1	C	296	LEU
1	C	301	CYS
1	C	308	VAL
1	C	314	GLN
1	C	315	THR
1	C	316	SER
1	C	317	ASN
1	C	319	ARG
1	C	320	VAL
1	C	324	GLU
1	C	328	ARG
1	C	329	PHE
1	C	334	ASN
1	C	353	TRP
1	C	355	ARG
1	C	375	SER
1	C	383	SER
1	C	389	ASP
1	C	390	LEU
1	C	406	GLU
1	C	421	TYR
1	C	430	THR
1	C	438	SER
1	C	440	ASN
1	C	500	THR
1	C	514	SER
1	C	517	LEU
1	C	518	LEU
1	C	525	CYS
1	C	528	LYS
1	C	529	LYS
1	C	530	SER
1	C	533	LEU
1	C	534	VAL
1	C	535	LYS
1	C	537	LYS
1	C	540	ASN
1	C	546	LEU
1	C	553	THR
1	C	554	GLU
1	C	556	ASN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	C	558	LYS
1	C	564	GLN
1	C	576	VAL
1	C	583	GLU
1	C	588	THR
1	C	592	PHE
1	C	599	THR
1	C	602	THR
1	C	646	ARG
1	C	673	SER
1	C	690	GLN
1	C	693	ILE
1	C	696	THR
1	C	703	ASN
1	C	727	LEU
1	C	778	THR
1	C	787	GLN
1	C	814	LYS
1	C	856	ASN
1	C	886	TRP
1	C	937	SER
1	C	974	SER
1	C	975	SER
1	C	976	VAL
1	C	977	LEU
1	C	1017	GLU
1	C	1077	THR
1	C	1094	VAL
1	C	1104	VAL
1	C	1126	CYS
1	C	1129	VAL
1	C	1132	ILE
1	C	1136	THR
1	C	1145	LEU
2	D	107	VAL
2	D	344	CYS
2	D	345	HIS
2	D	347	THR
2	D	361	CYS
2	D	423	LEU
2	D	425	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (94)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	134	GLN
1	A	137	ASN
1	A	188	ASN
1	A	239	GLN
1	A	317	ASN
1	A	354	ASN
1	A	360	ASN
1	A	394	ASN
1	A	422	ASN
1	A	440	ASN
1	A	498	GLN
1	A	540	ASN
1	A	556	ASN
1	A	580	GLN
1	A	644	GLN
1	A	658	ASN
1	A	703	ASN
1	A	762	GLN
1	A	787	GLN
1	A	901	GLN
1	A	914	ASN
1	A	919	ASN
1	A	926	GLN
1	A	955	ASN
1	A	969	ASN
1	A	978	ASN
1	A	992	GLN
1	A	1125	ASN
1	A	1142	GLN
1	B	134	GLN
1	B	137	ASN
1	B	188	ASN
1	B	239	GLN
1	B	317	ASN
1	B	334	ASN
1	B	354	ASN
1	B	360	ASN
1	B	394	ASN
1	B	422	ASN
1	B	440	ASN
1	B	498	GLN
1	B	540	ASN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	556	ASN
1	B	564	GLN
1	B	644	GLN
1	B	658	ASN
1	B	710	ASN
1	B	804	GLN
1	B	901	GLN
1	B	914	ASN
1	B	919	ASN
1	B	920	GLN
1	B	926	GLN
1	B	992	GLN
1	B	1054	GLN
1	C	134	GLN
1	C	137	ASN
1	C	188	ASN
1	C	239	GLN
1	C	317	ASN
1	C	334	ASN
1	C	354	ASN
1	C	360	ASN
1	C	394	ASN
1	C	422	ASN
1	C	440	ASN
1	C	498	GLN
1	C	519	HIS
1	C	540	ASN
1	C	556	ASN
1	C	644	GLN
1	C	658	ASN
1	C	703	ASN
1	C	784	GLN
1	C	804	GLN
1	C	901	GLN
1	C	907	ASN
1	C	914	ASN
1	C	926	GLN
1	C	935	GLN
1	C	969	ASN
1	C	992	GLN
1	C	1010	GLN
1	C	1071	GLN

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Mol	Chain	Res	Type
1	C	1101	HIS
1	C	1106	GLN
2	D	24	GLN
2	D	58	ASN
2	D	96	GLN
2	D	175	GLN
2	D	239	HIS
2	D	277	ASN
2	D	505	HIS
2	D	586	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

52 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	NAG	E	1	3,1	14,14,15	0.56	0	17,19,21	0.49	0
3	NAG	E	2	3	14,14,15	0.25	0	17,19,21	0.59	0
3	NAG	F	1	3,1	14,14,15	0.59	1 (7%)	17,19,21	0.57	0
3	NAG	F	2	3	14,14,15	0.32	0	17,19,21	0.46	0
3	NAG	G	1	3,1	14,14,15	0.32	0	17,19,21	0.61	0
3	NAG	G	2	3	14,14,15	0.52	0	17,19,21	0.47	0
3	NAG	H	1	3,1	14,14,15	0.38	0	17,19,21	0.72	0
3	NAG	H	2	3	14,14,15	0.28	0	17,19,21	1.32	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	NAG	I	1	3,1	14,14,15	0.69	1 (7%)	17,19,21	0.70	0
3	NAG	I	2	3	14,14,15	0.38	0	17,19,21	1.40	3 (17%)
3	NAG	J	1	3,1	14,14,15	0.70	1 (7%)	17,19,21	0.66	0
3	NAG	J	2	3	14,14,15	0.30	0	17,19,21	0.65	0
3	NAG	K	1	3,1	14,14,15	0.24	0	17,19,21	0.69	1 (5%)
3	NAG	K	2	3	14,14,15	0.17	0	17,19,21	0.48	0
3	NAG	L	1	3,1	14,14,15	0.55	0	17,19,21	0.50	0
3	NAG	L	2	3	14,14,15	0.25	0	17,19,21	0.58	0
3	NAG	M	1	3,1	14,14,15	0.32	0	17,19,21	0.40	0
3	NAG	M	2	3	14,14,15	0.37	0	17,19,21	0.37	0
3	NAG	N	1	3,1	14,14,15	0.35	0	17,19,21	1.13	1 (5%)
3	NAG	N	2	3	14,14,15	0.27	0	17,19,21	0.47	0
3	NAG	O	1	3,1	14,14,15	0.32	0	17,19,21	0.70	1 (5%)
3	NAG	O	2	3	14,14,15	0.20	0	17,19,21	0.40	0
3	NAG	P	1	3,1	14,14,15	0.75	1 (7%)	17,19,21	0.91	1 (5%)
3	NAG	P	2	3	14,14,15	0.32	0	17,19,21	0.69	1 (5%)
3	NAG	Q	1	3,1	14,14,15	0.22	0	17,19,21	0.44	0
3	NAG	Q	2	3	14,14,15	0.27	0	17,19,21	0.38	0
3	NAG	R	1	3,1	14,14,15	0.54	0	17,19,21	0.49	0
3	NAG	R	2	3	14,14,15	0.25	0	17,19,21	0.58	0
3	NAG	S	1	3,1	14,14,15	0.59	1 (7%)	17,19,21	0.56	0
3	NAG	S	2	3	14,14,15	0.30	0	17,19,21	0.46	0
3	NAG	T	1	3,1	14,14,15	0.23	0	17,19,21	1.36	1 (5%)
3	NAG	T	2	3	14,14,15	0.20	0	17,19,21	0.50	0
3	NAG	U	1	3,1	14,14,15	0.54	0	17,19,21	0.71	1 (5%)
3	NAG	U	2	3	14,14,15	0.37	0	17,19,21	0.47	0
3	NAG	V	1	3,1	14,14,15	0.37	0	17,19,21	0.40	0
3	NAG	V	2	3	14,14,15	0.21	0	17,19,21	0.74	0
3	NAG	W	1	3,1	14,14,15	0.38	0	17,19,21	0.49	0
3	NAG	W	2	3	14,14,15	0.54	0	17,19,21	1.30	1 (5%)
3	NAG	X	1	3,1	14,14,15	0.63	1 (7%)	17,19,21	0.43	0
3	NAG	X	2	3	14,14,15	0.34	0	17,19,21	1.36	2 (11%)
3	NAG	Y	1	3,1	14,14,15	0.40	0	17,19,21	0.45	0
3	NAG	Y	2	3	14,14,15	0.23	0	17,19,21	0.49	0
3	NAG	Z	1	2,3	14,14,15	0.62	1 (7%)	17,19,21	0.74	0
3	NAG	Z	2	3	14,14,15	0.54	0	17,19,21	0.36	0
3	NAG	a	1	2,3	14,14,15	0.42	0	17,19,21	0.65	0
3	NAG	a	2	3	14,14,15	0.28	0	17,19,21	0.69	1 (5%)
3	NAG	b	1	2,3	14,14,15	0.29	0	17,19,21	0.62	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	NAG	b	2	3	14,14,15	0.30	0	17,19,21	0.62	0
3	NAG	c	1	2,3	14,14,15	0.30	0	17,19,21	0.51	0
3	NAG	c	2	3	14,14,15	0.36	0	17,19,21	0.47	0
3	NAG	d	1	2,3	14,14,15	0.23	0	17,19,21	0.62	0
3	NAG	d	2	3	14,14,15	0.34	0	17,19,21	0.59	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	E	1	3,1	-	1/6/23/26	0/1/1/1
3	NAG	E	2	3	-	2/6/23/26	0/1/1/1
3	NAG	F	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	F	2	3	-	4/6/23/26	0/1/1/1
3	NAG	G	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	G	2	3	-	2/6/23/26	0/1/1/1
3	NAG	H	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	H	2	3	-	3/6/23/26	0/1/1/1
3	NAG	I	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	I	2	3	-	5/6/23/26	0/1/1/1
3	NAG	J	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	J	2	3	-	3/6/23/26	0/1/1/1
3	NAG	K	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	K	2	3	-	0/6/23/26	0/1/1/1
3	NAG	L	1	3,1	-	1/6/23/26	0/1/1/1
3	NAG	L	2	3	-	2/6/23/26	0/1/1/1
3	NAG	M	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	M	2	3	-	1/6/23/26	0/1/1/1
3	NAG	N	1	3,1	-	1/6/23/26	0/1/1/1
3	NAG	N	2	3	-	0/6/23/26	0/1/1/1
3	NAG	O	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	O	2	3	-	3/6/23/26	0/1/1/1
3	NAG	P	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	P	2	3	-	3/6/23/26	0/1/1/1
3	NAG	Q	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	Q	2	3	-	2/6/23/26	0/1/1/1

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

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	P	1	NAG	O5-C1	-2.70	1.39	1.43
3	J	1	NAG	O5-C1	-2.55	1.39	1.43
3	I	1	NAG	O5-C1	-2.32	1.40	1.43
3	Z	1	NAG	O5-C1	-2.17	1.40	1.43
3	X	1	NAG	O5-C1	-2.11	1.40	1.43
3	S	1	NAG	O5-C1	-2.07	1.40	1.43
3	F	1	NAG	O5-C1	-2.07	1.40	1.43

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	T	1	NAG	C2-N2-C7	4.68	129.57	122.90
3	I	2	NAG	C2-N2-C7	4.43	129.20	122.90
3	X	2	NAG	C2-N2-C7	4.37	129.13	122.90
3	H	2	NAG	C2-N2-C7	4.29	129.01	122.90
3	W	2	NAG	C2-N2-C7	4.25	128.95	122.90
3	N	1	NAG	C1-O5-C5	3.32	116.69	112.19
3	a	2	NAG	C1-O5-C5	2.46	115.52	112.19
3	I	2	NAG	C1-C2-N2	2.41	114.60	110.49
3	H	2	NAG	C1-C2-N2	2.36	114.52	110.49
3	P	1	NAG	O4-C4-C3	-2.34	104.93	110.35
3	O	1	NAG	C1-O5-C5	2.32	115.33	112.19
3	U	1	NAG	C1-O5-C5	2.29	115.29	112.19
3	X	2	NAG	C1-C2-N2	2.23	114.29	110.49
3	K	1	NAG	C1-O5-C5	2.10	115.04	112.19
3	I	2	NAG	C1-O5-C5	2.06	114.99	112.19
3	P	2	NAG	C1-O5-C5	2.04	114.95	112.19
3	d	2	NAG	C1-O5-C5	2.04	114.95	112.19

There are no chirality outliers.

All (100) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	b	1	NAG	C8-C7-N2-C2
3	b	1	NAG	O7-C7-N2-C2
3	b	2	NAG	C3-C2-N2-C7
3	b	2	NAG	C8-C7-N2-C2
3	b	2	NAG	O7-C7-N2-C2
3	T	2	NAG	O5-C5-C6-O6
3	V	1	NAG	O5-C5-C6-O6
3	U	2	NAG	O5-C5-C6-O6
3	E	2	NAG	O5-C5-C6-O6
3	J	1	NAG	O5-C5-C6-O6
3	L	2	NAG	O5-C5-C6-O6
3	P	1	NAG	O5-C5-C6-O6
3	R	2	NAG	O5-C5-C6-O6
3	d	2	NAG	O5-C5-C6-O6
3	Z	1	NAG	O5-C5-C6-O6
3	a	2	NAG	O5-C5-C6-O6
3	U	1	NAG	O5-C5-C6-O6
3	E	2	NAG	C4-C5-C6-O6
3	L	2	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	P	1	NAG	C4-C5-C6-O6
3	R	2	NAG	C4-C5-C6-O6
3	Q	1	NAG	C4-C5-C6-O6
3	U	1	NAG	C4-C5-C6-O6
3	P	2	NAG	O5-C5-C6-O6
3	a	1	NAG	O5-C5-C6-O6
3	J	1	NAG	C4-C5-C6-O6
3	V	1	NAG	C4-C5-C6-O6
3	a	2	NAG	C4-C5-C6-O6
3	U	2	NAG	C4-C5-C6-O6
3	W	2	NAG	O5-C5-C6-O6
3	Z	2	NAG	C4-C5-C6-O6
3	T	2	NAG	C4-C5-C6-O6
3	Q	2	NAG	O5-C5-C6-O6
3	P	2	NAG	C4-C5-C6-O6
3	H	2	NAG	C8-C7-N2-C2
3	H	2	NAG	O7-C7-N2-C2
3	I	2	NAG	C8-C7-N2-C2
3	I	2	NAG	O7-C7-N2-C2
3	O	2	NAG	C8-C7-N2-C2
3	O	2	NAG	O7-C7-N2-C2
3	T	1	NAG	C8-C7-N2-C2
3	T	1	NAG	O7-C7-N2-C2
3	W	2	NAG	C8-C7-N2-C2
3	W	2	NAG	O7-C7-N2-C2
3	X	2	NAG	C8-C7-N2-C2
3	X	2	NAG	O7-C7-N2-C2
3	d	2	NAG	C4-C5-C6-O6
3	I	1	NAG	C4-C5-C6-O6
3	W	2	NAG	C4-C5-C6-O6
3	a	1	NAG	C4-C5-C6-O6
3	T	1	NAG	O5-C5-C6-O6
3	H	1	NAG	C4-C5-C6-O6
3	Z	1	NAG	C4-C5-C6-O6
3	Z	2	NAG	O5-C5-C6-O6
3	T	1	NAG	C4-C5-C6-O6
3	Q	2	NAG	C4-C5-C6-O6
3	Q	1	NAG	O5-C5-C6-O6
3	J	2	NAG	O5-C5-C6-O6
3	H	1	NAG	O5-C5-C6-O6
3	I	1	NAG	O5-C5-C6-O6
3	X	1	NAG	O5-C5-C6-O6

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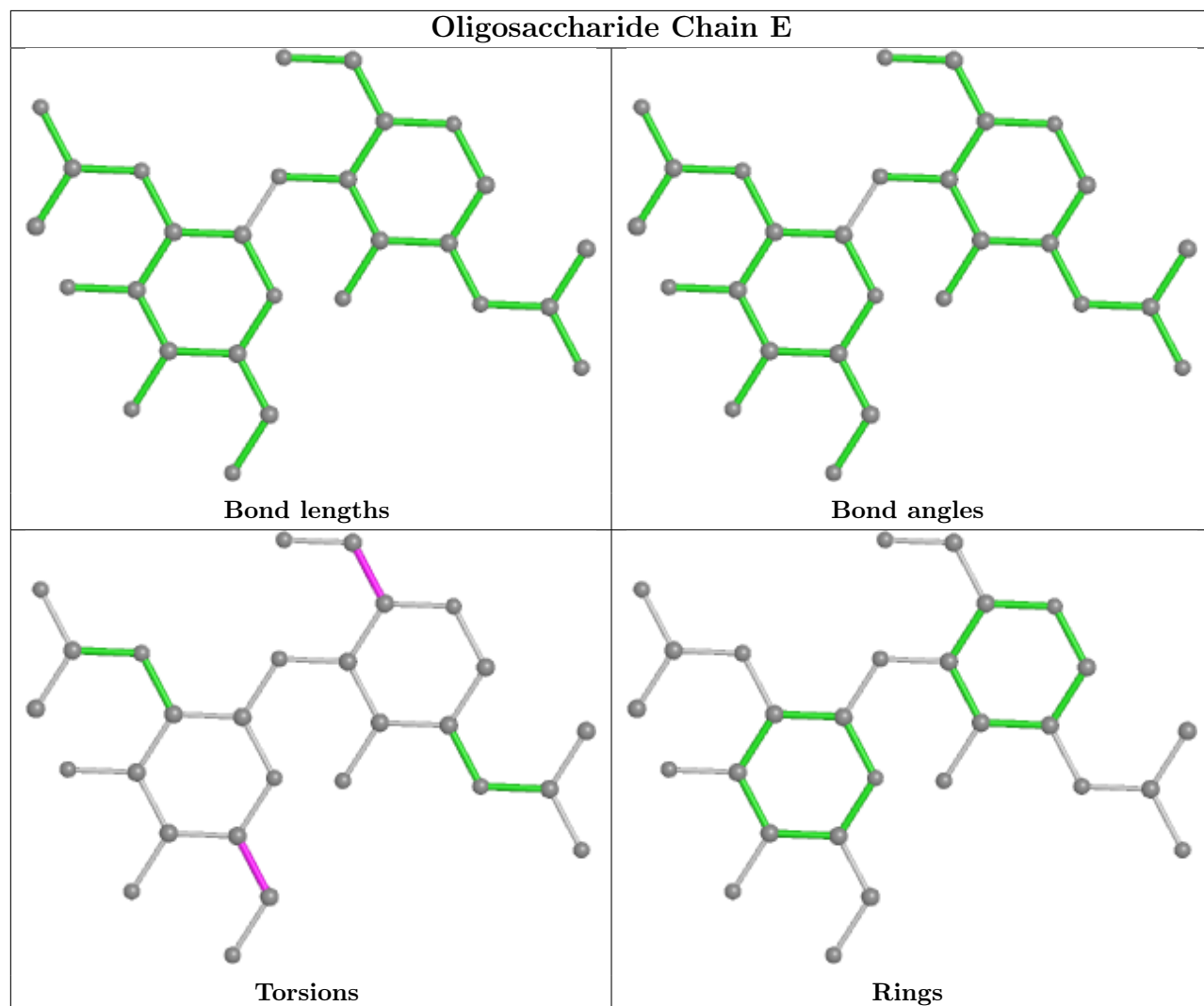
Mol	Chain	Res	Type	Atoms
3	J	2	NAG	C4-C5-C6-O6
3	X	1	NAG	C4-C5-C6-O6
3	K	1	NAG	C4-C5-C6-O6
3	K	1	NAG	O5-C5-C6-O6
3	b	2	NAG	C1-C2-N2-C7
3	F	2	NAG	C1-C2-N2-C7
3	X	2	NAG	O5-C5-C6-O6
3	S	2	NAG	C1-C2-N2-C7
3	O	2	NAG	O5-C5-C6-O6
3	E	1	NAG	O5-C5-C6-O6
3	L	1	NAG	O5-C5-C6-O6
3	R	1	NAG	O5-C5-C6-O6
3	O	1	NAG	C4-C5-C6-O6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

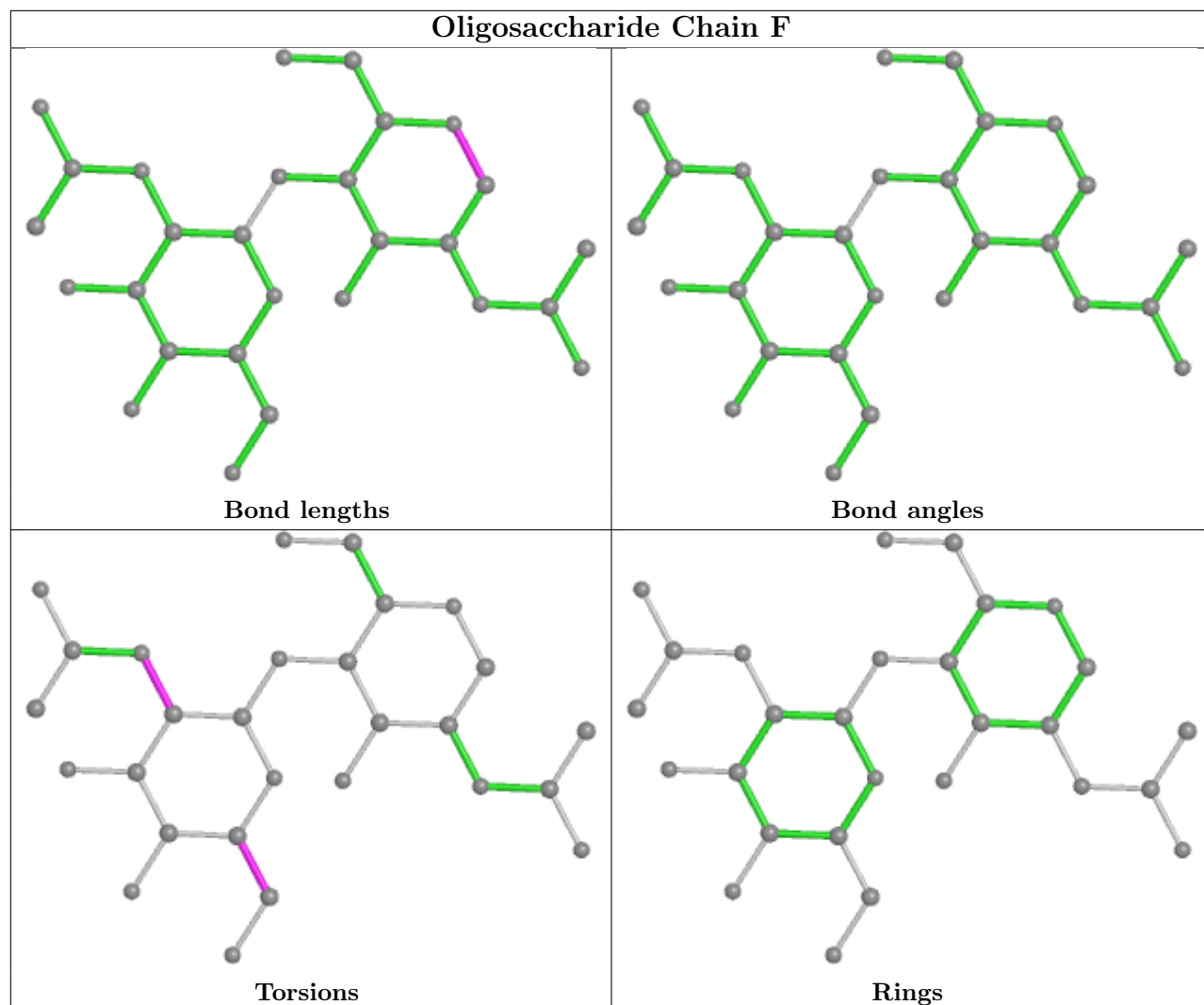
There are no ring outliers.

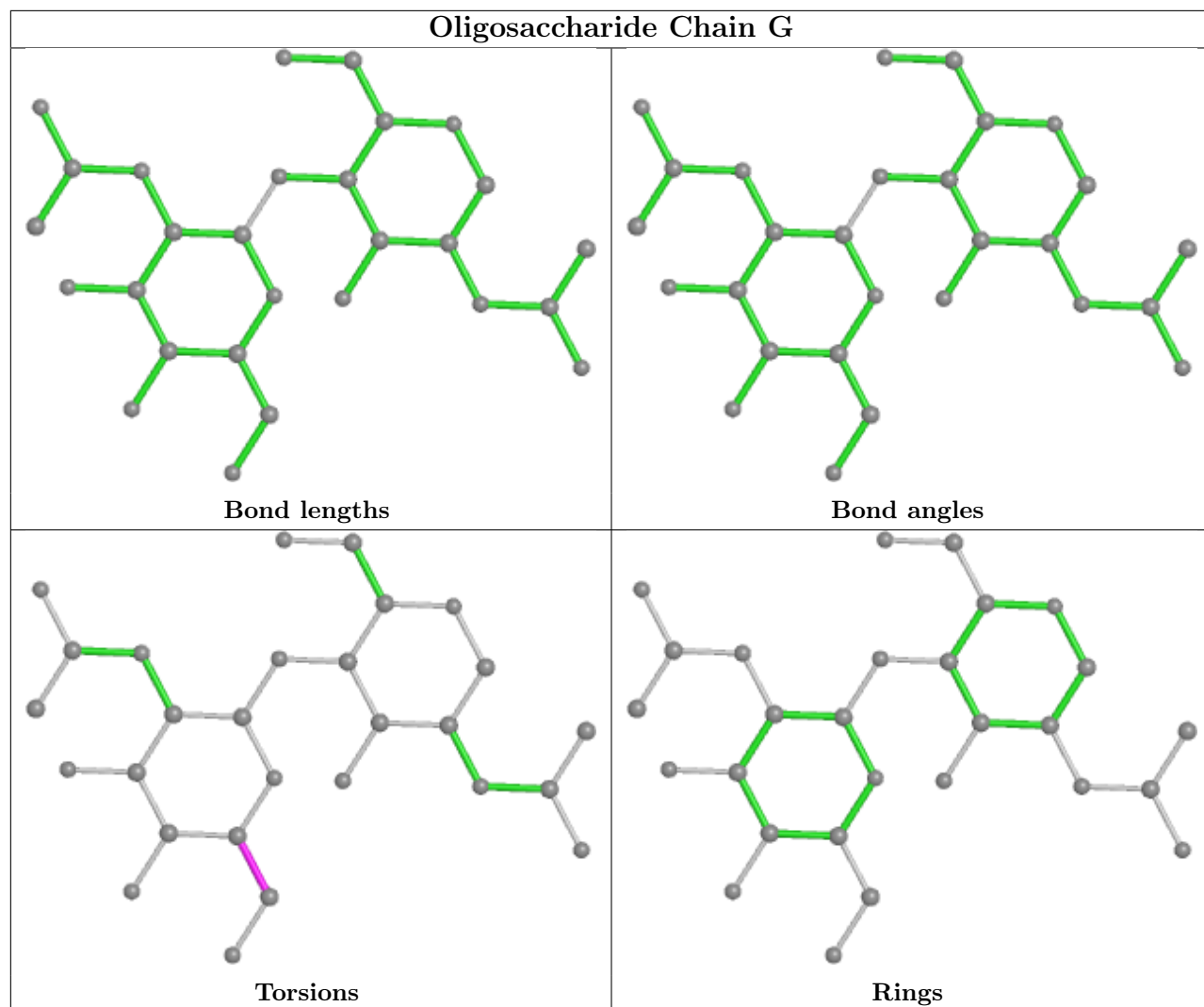
12 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	X	2	NAG	1	0
3	I	2	NAG	1	0
3	S	2	NAG	2	0
3	X	1	NAG	1	0
3	P	1	NAG	1	0
3	S	1	NAG	3	0
3	P	2	NAG	1	0
3	T	1	NAG	1	0
3	F	2	NAG	2	0
3	W	2	NAG	1	0
3	H	2	NAG	1	0
3	F	1	NAG	3	0

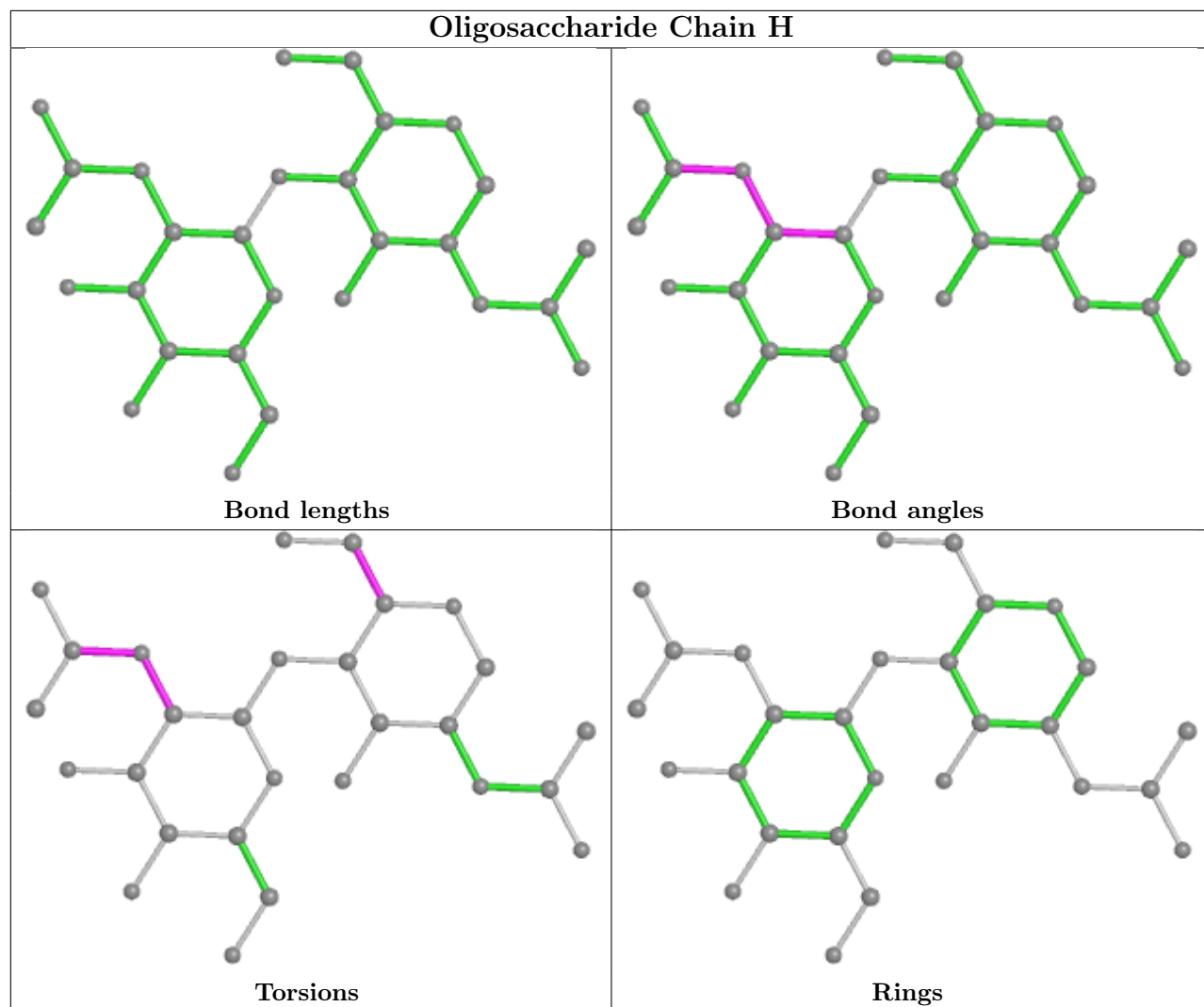
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

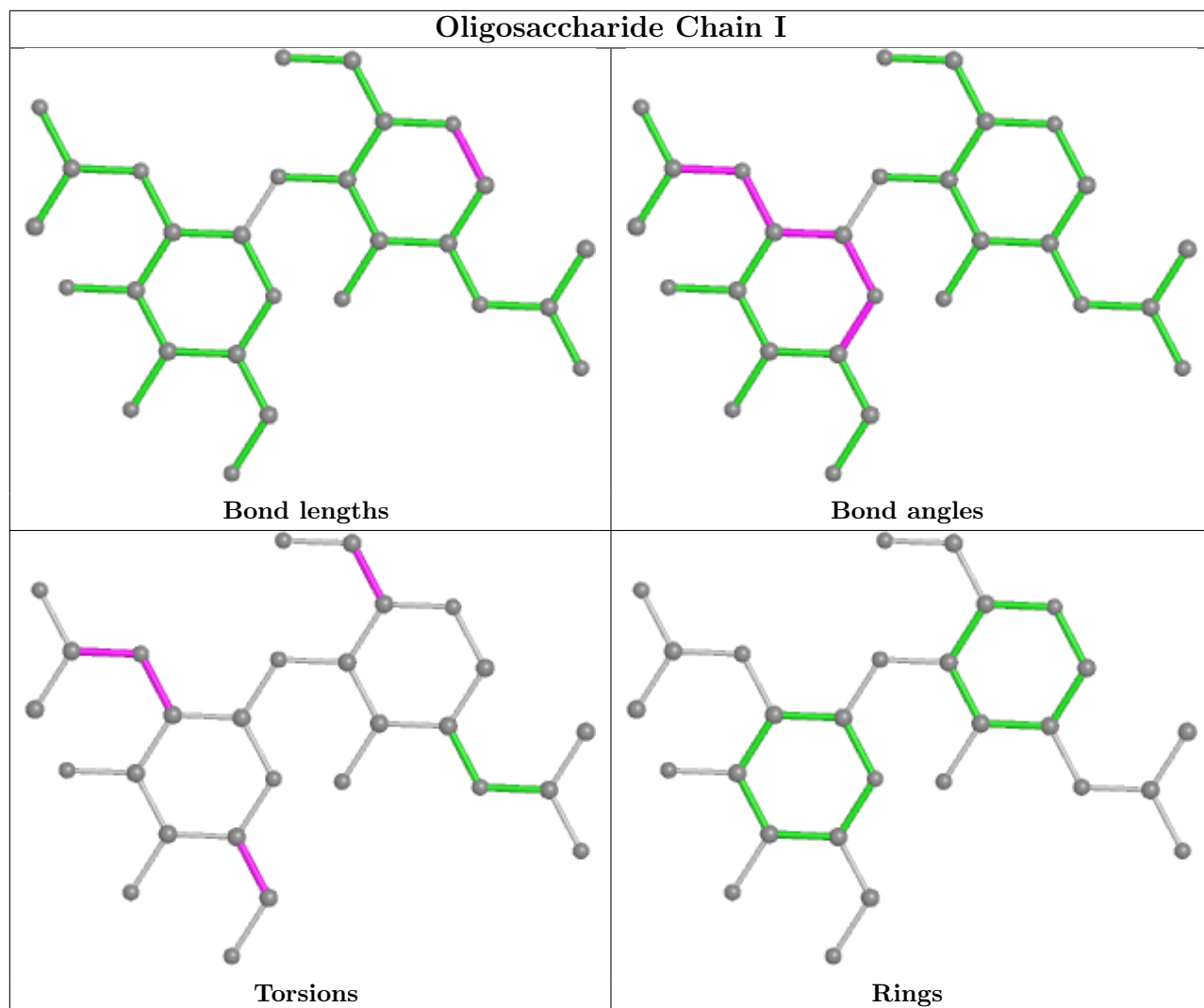


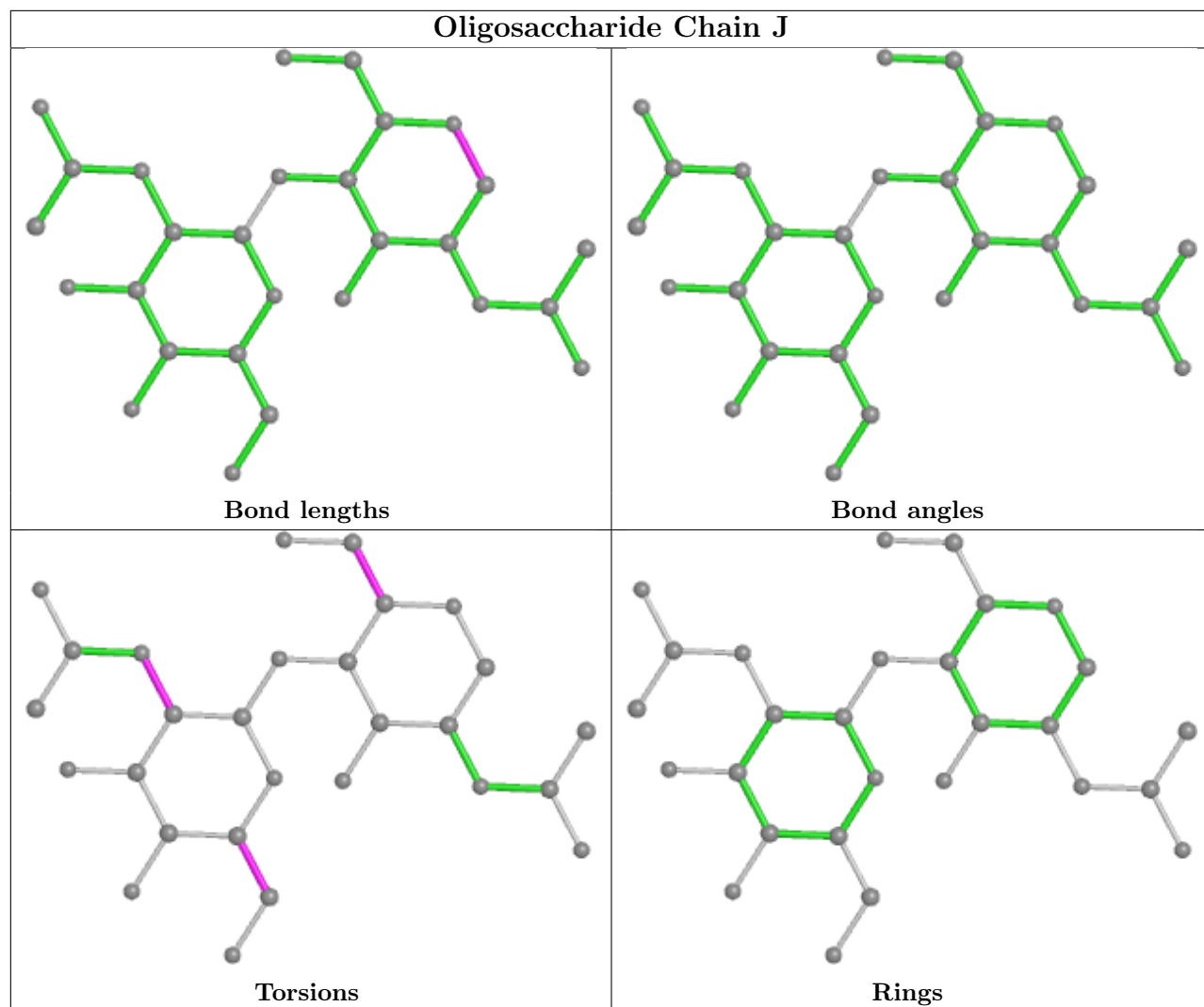


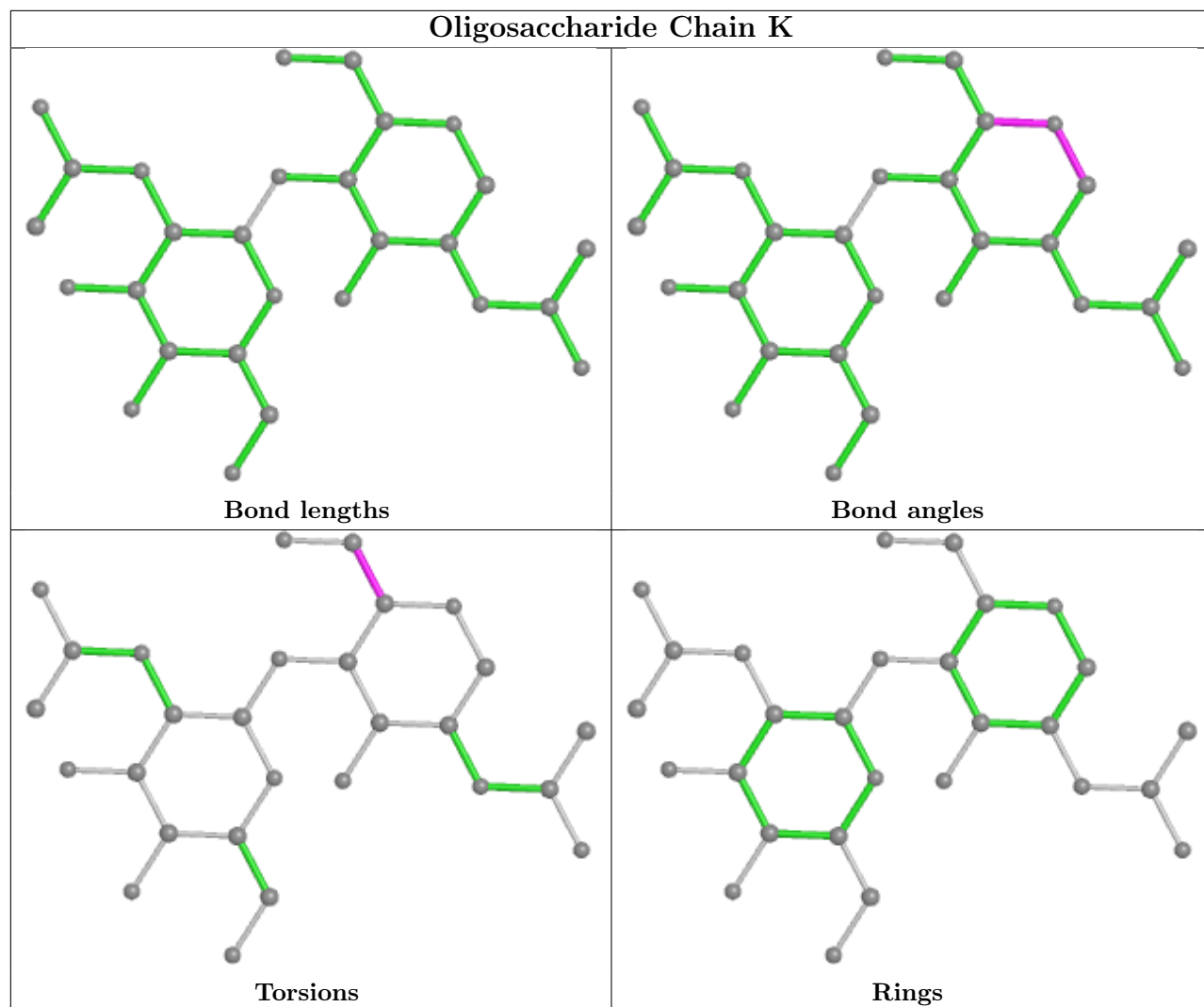


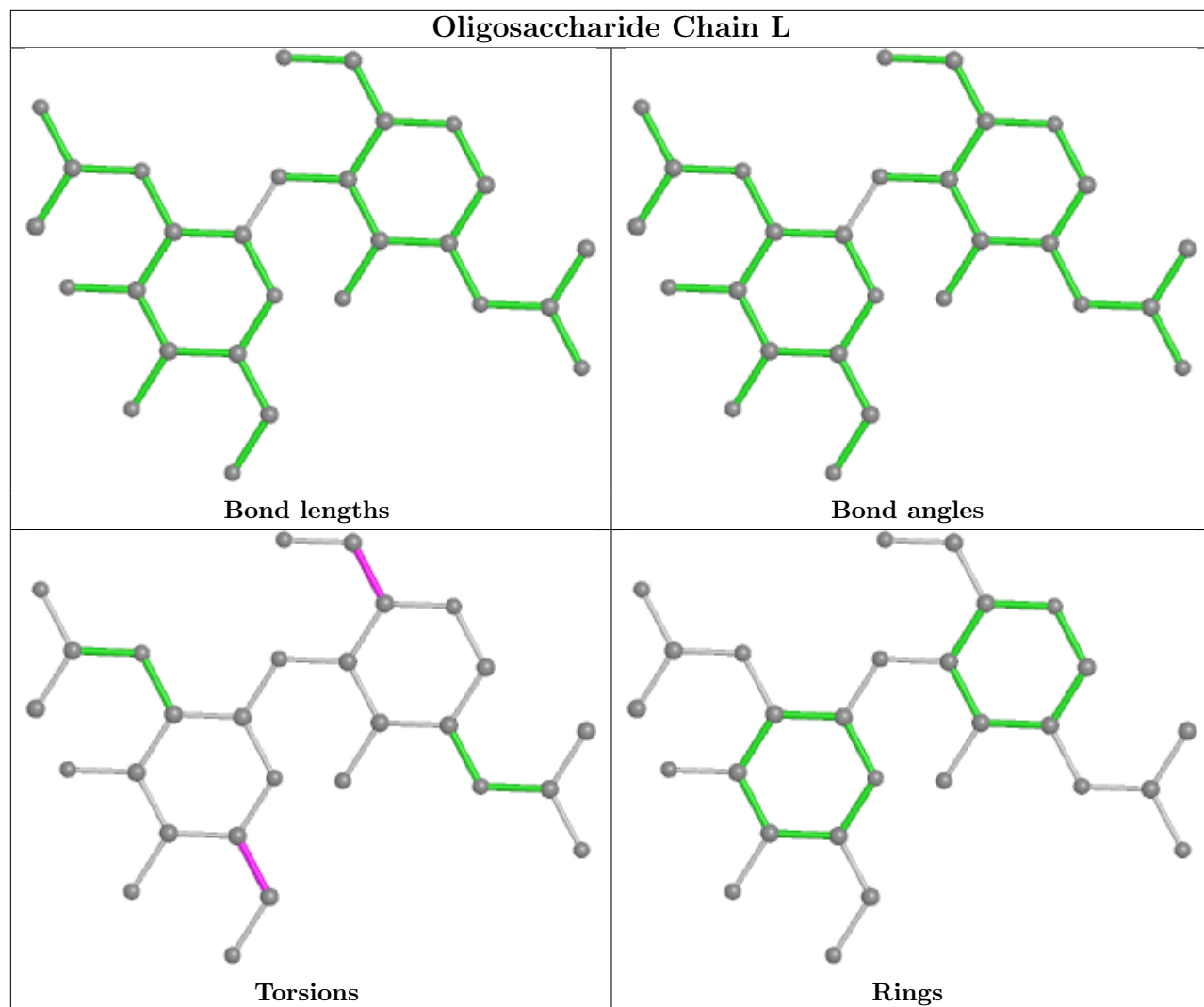


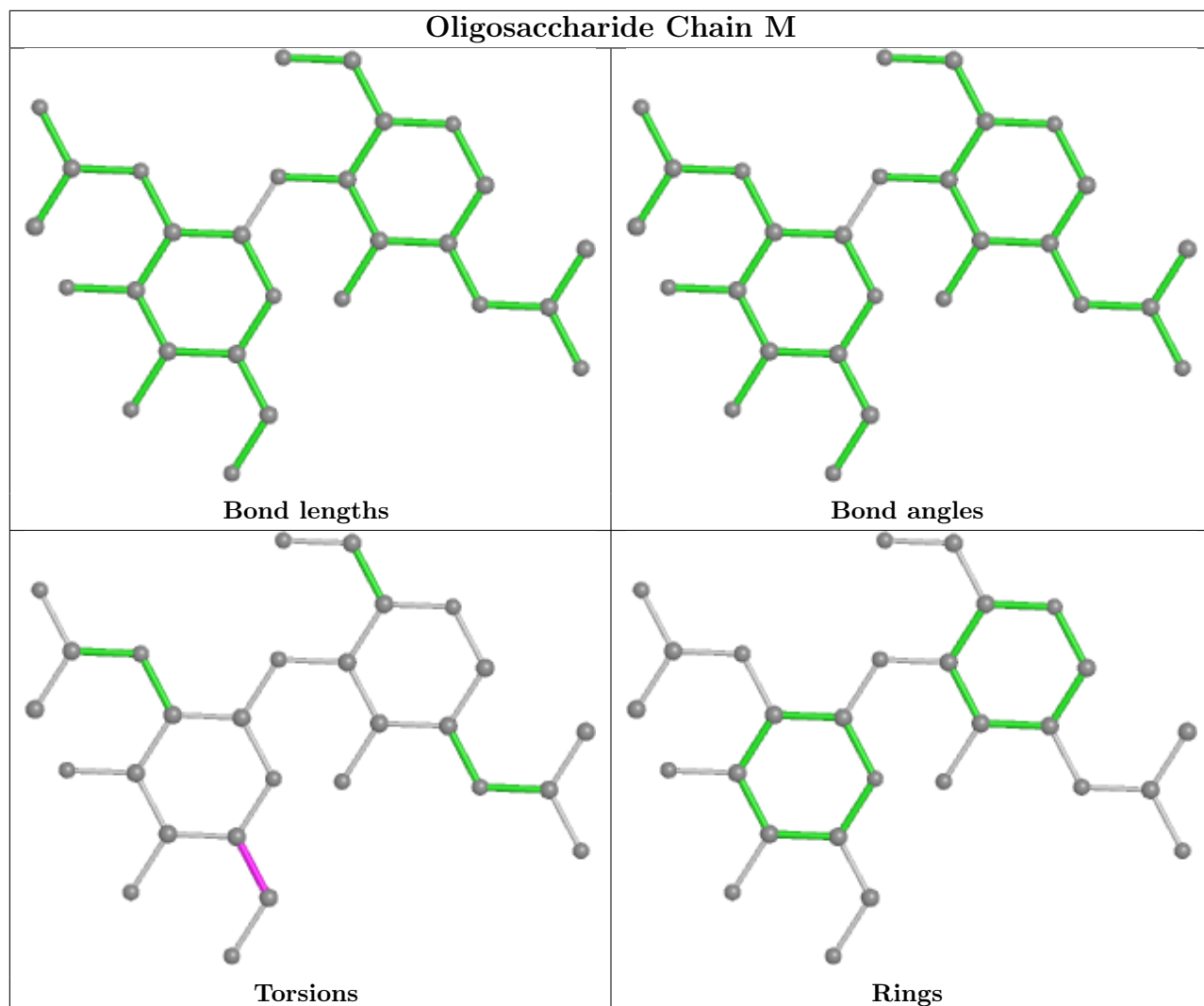


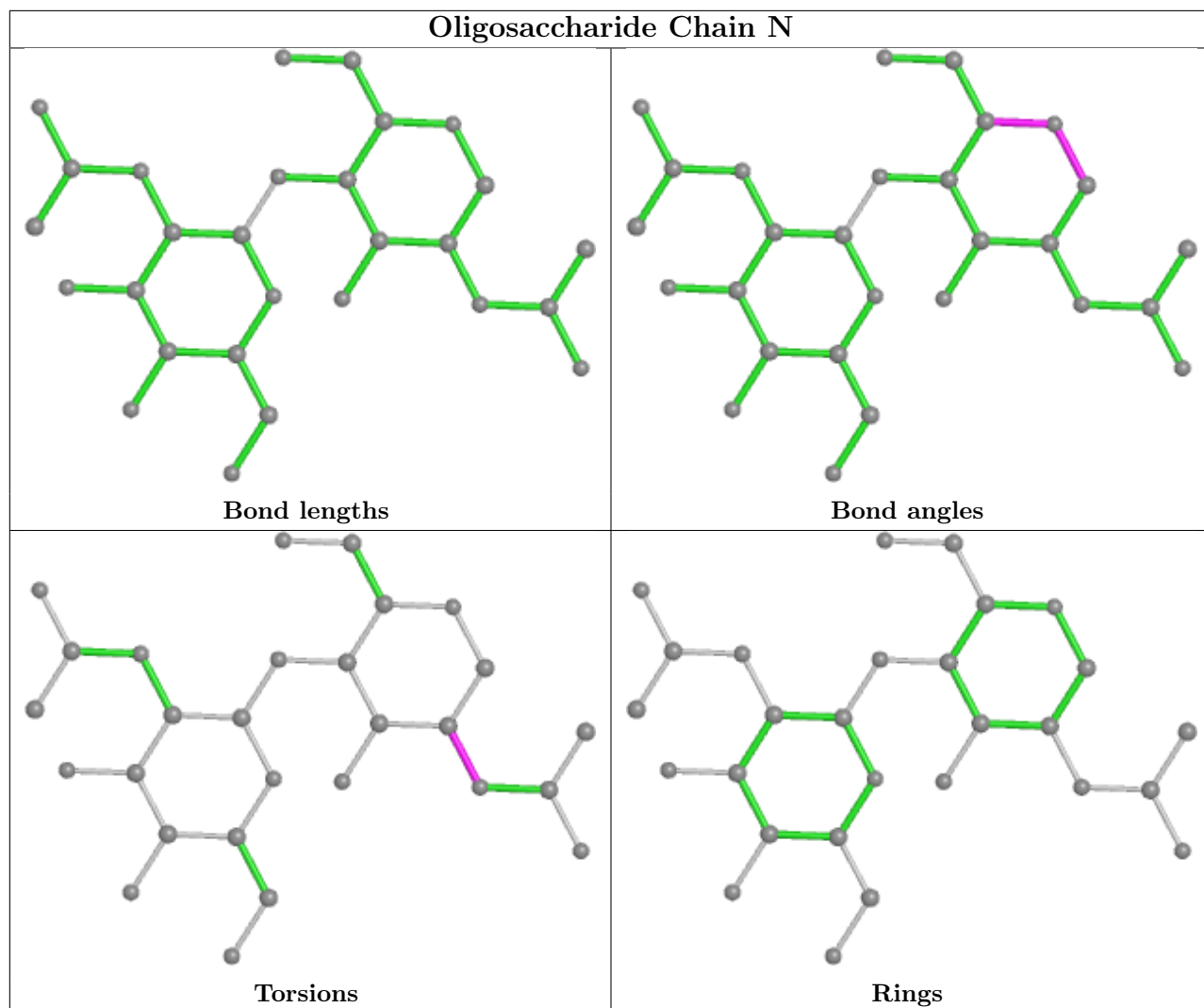


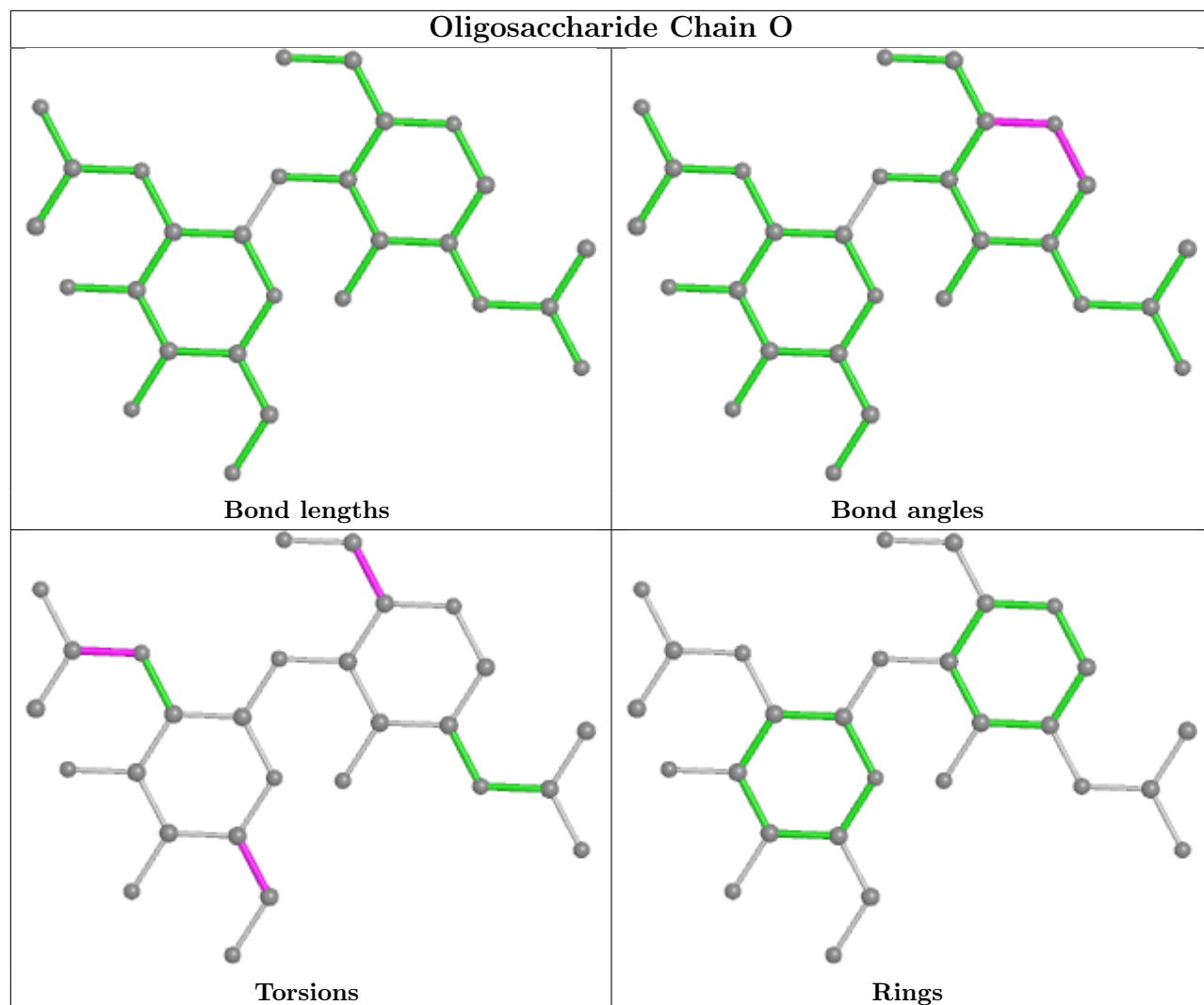




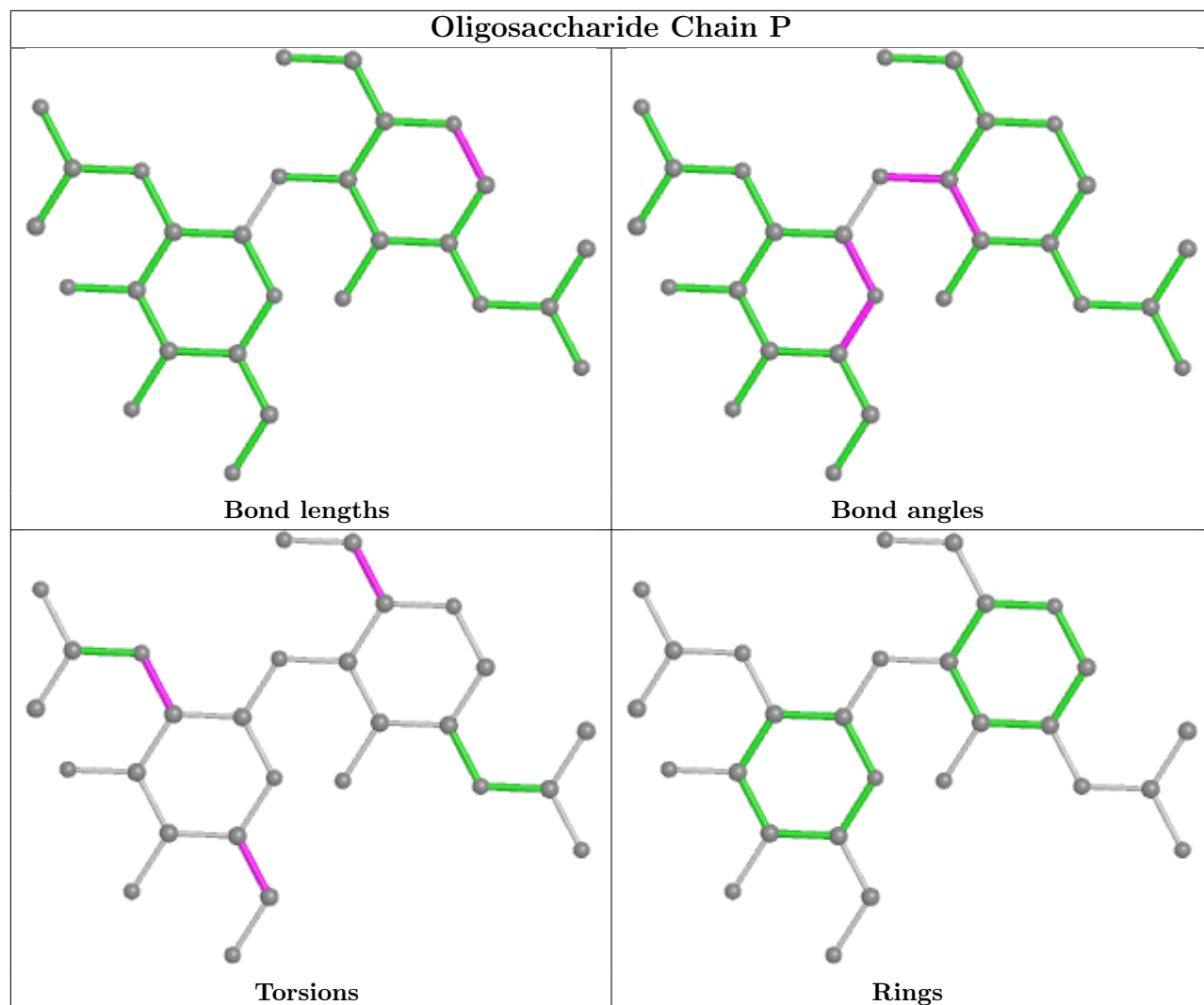


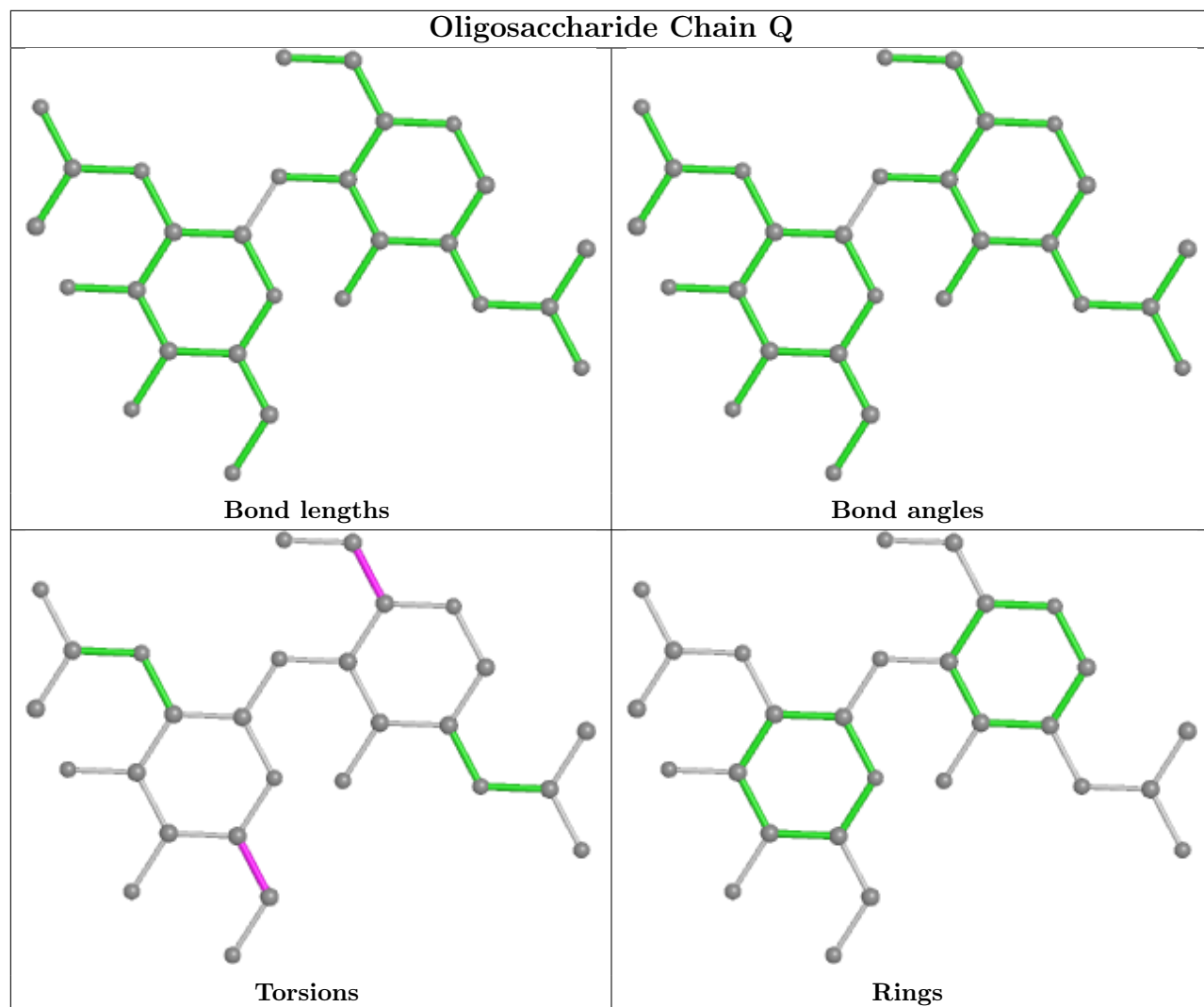


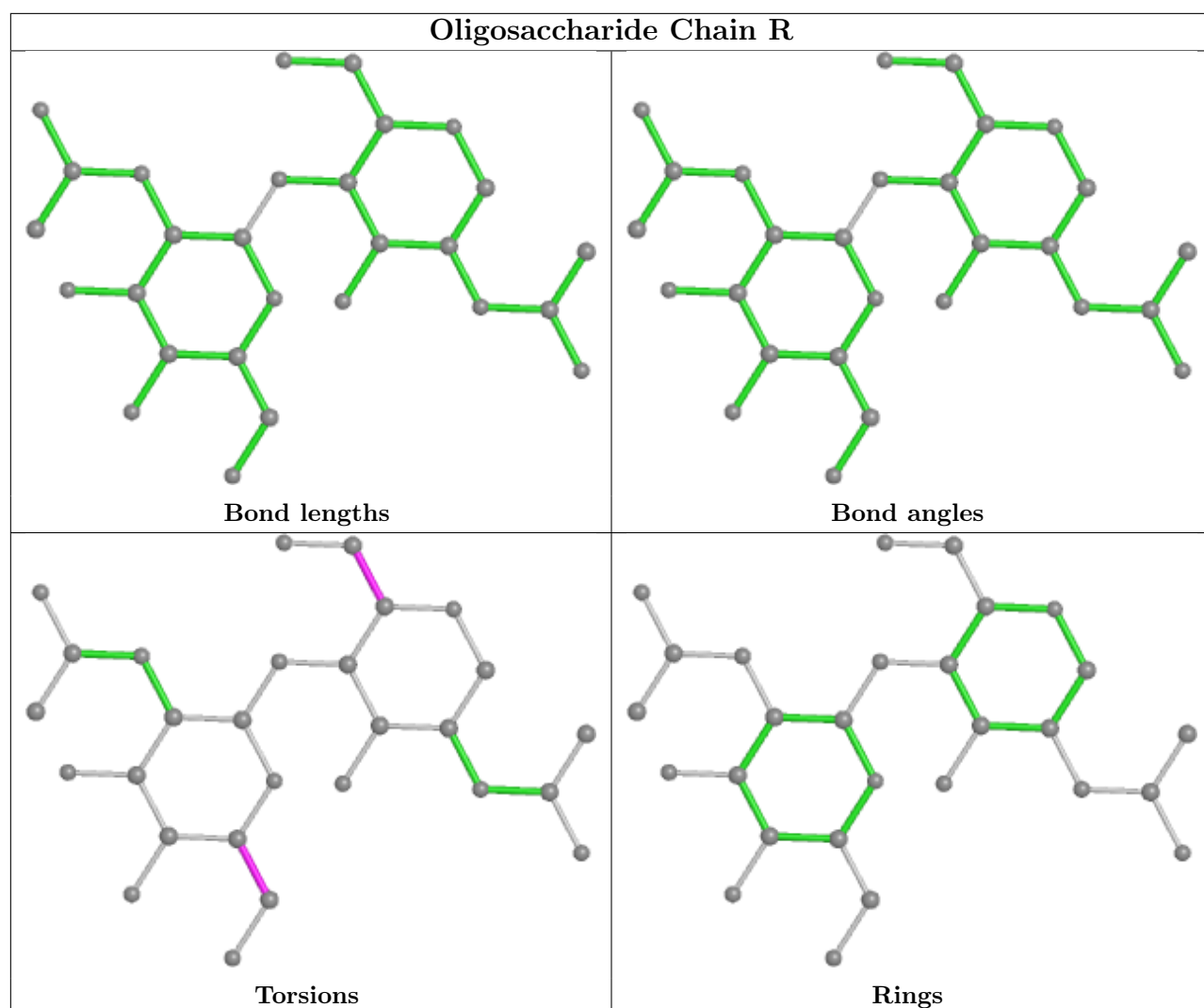


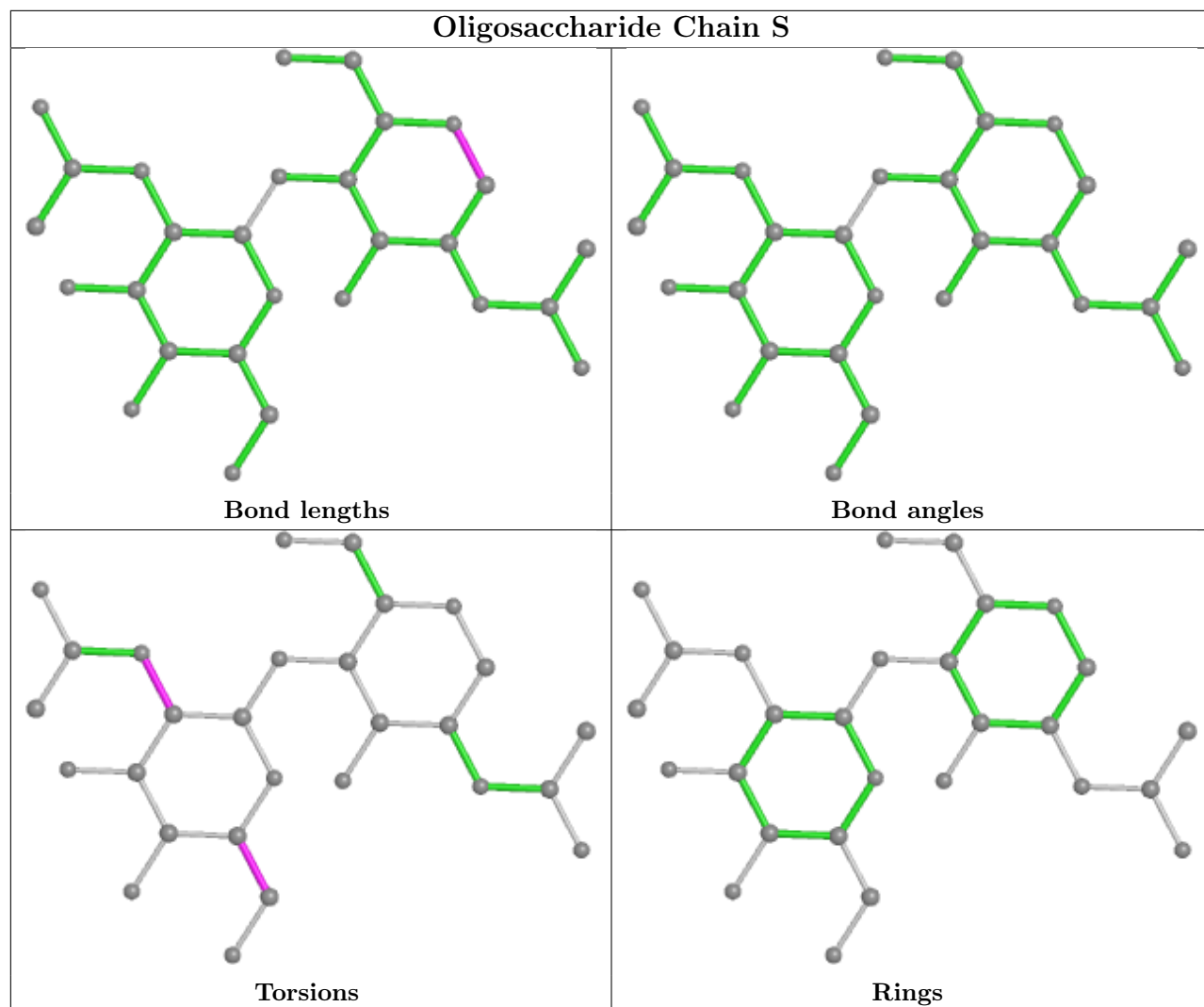


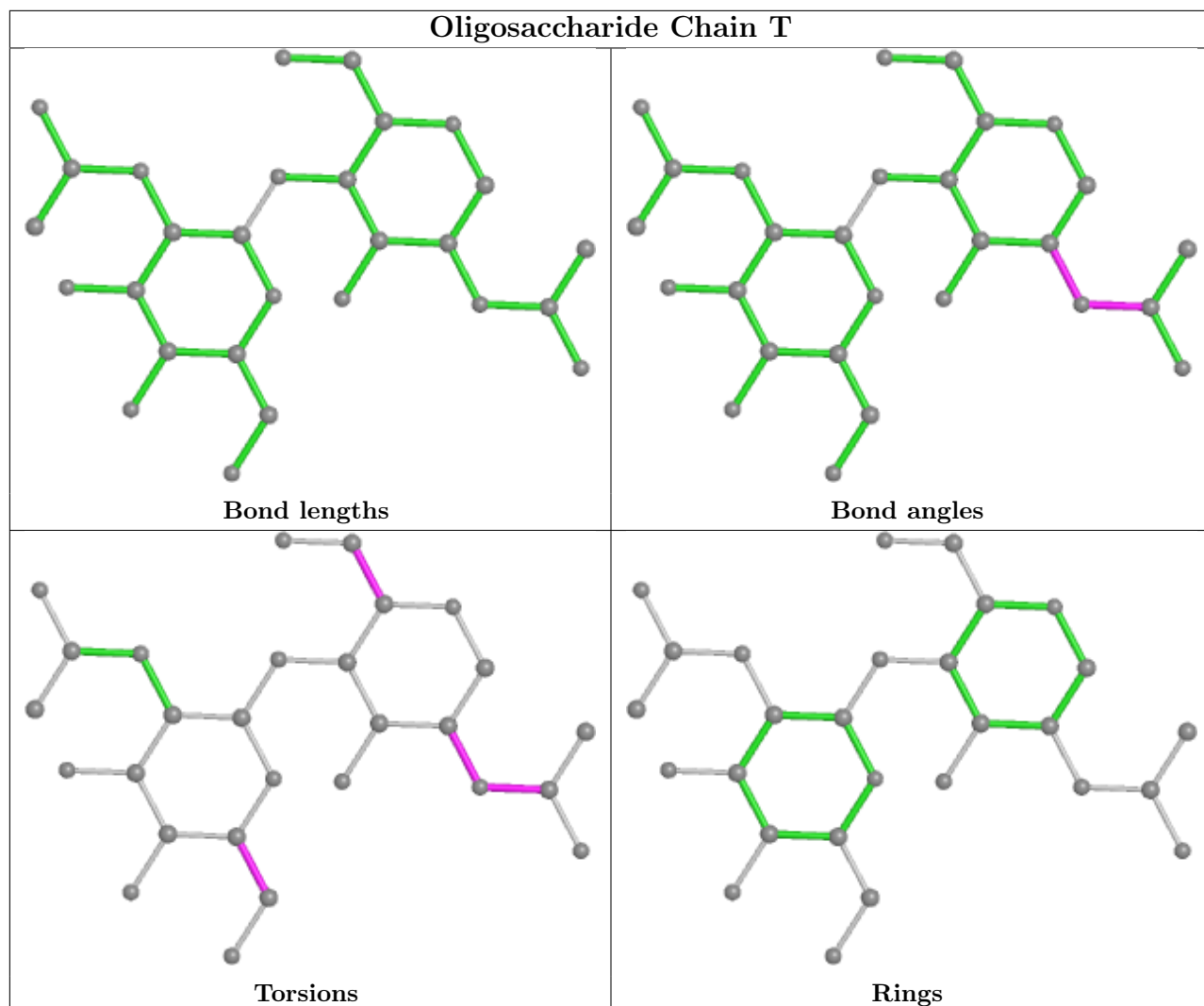


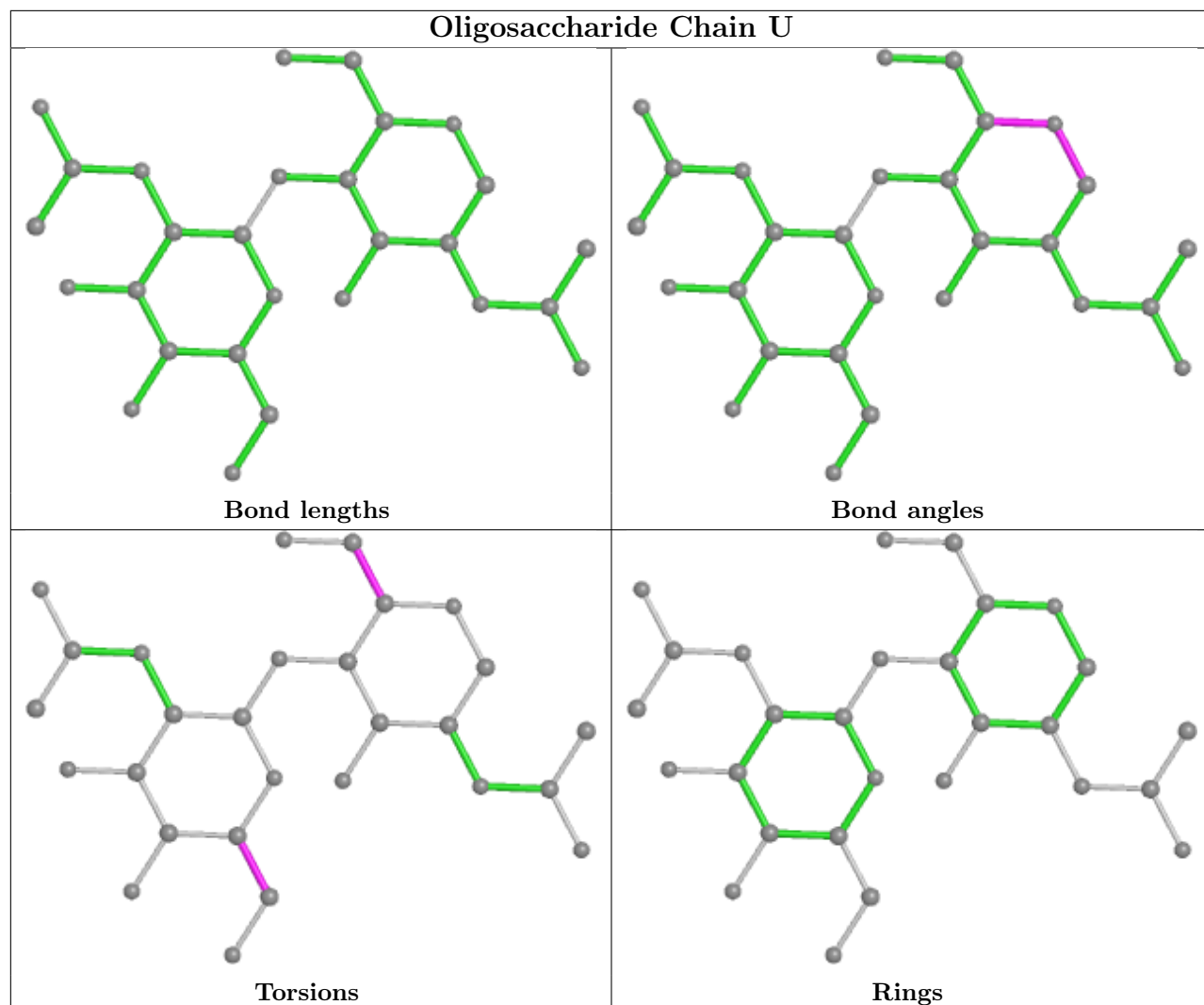


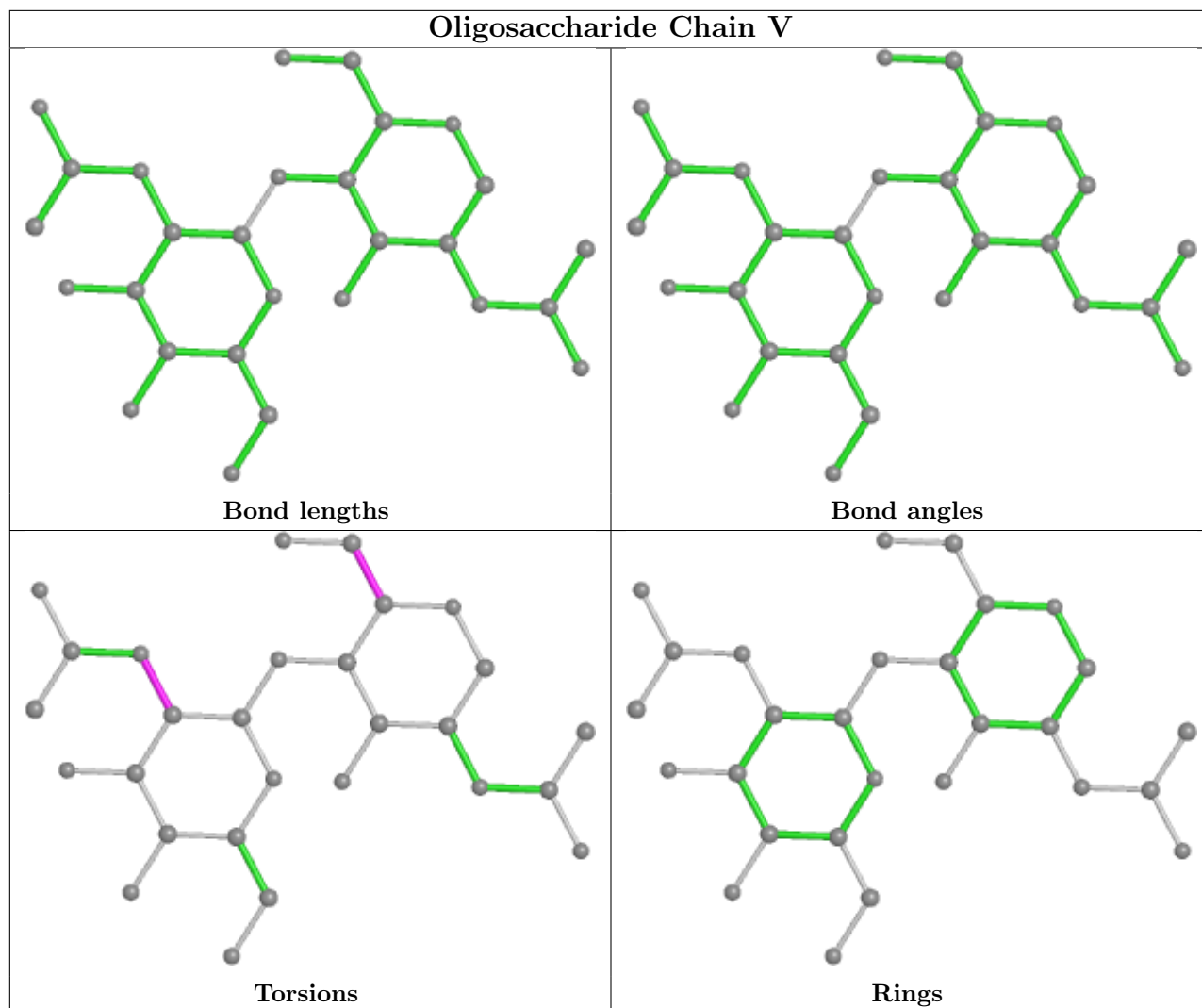


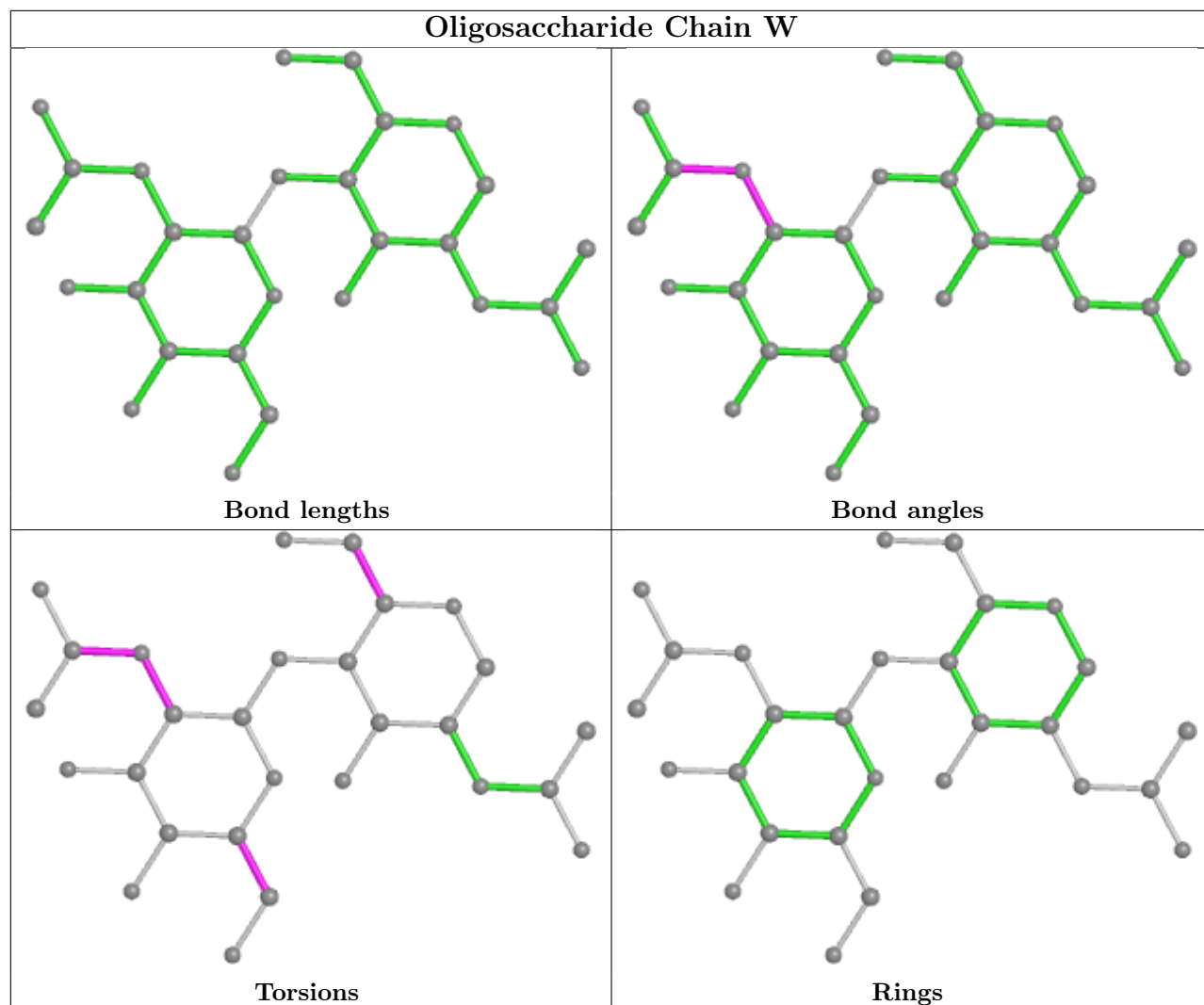




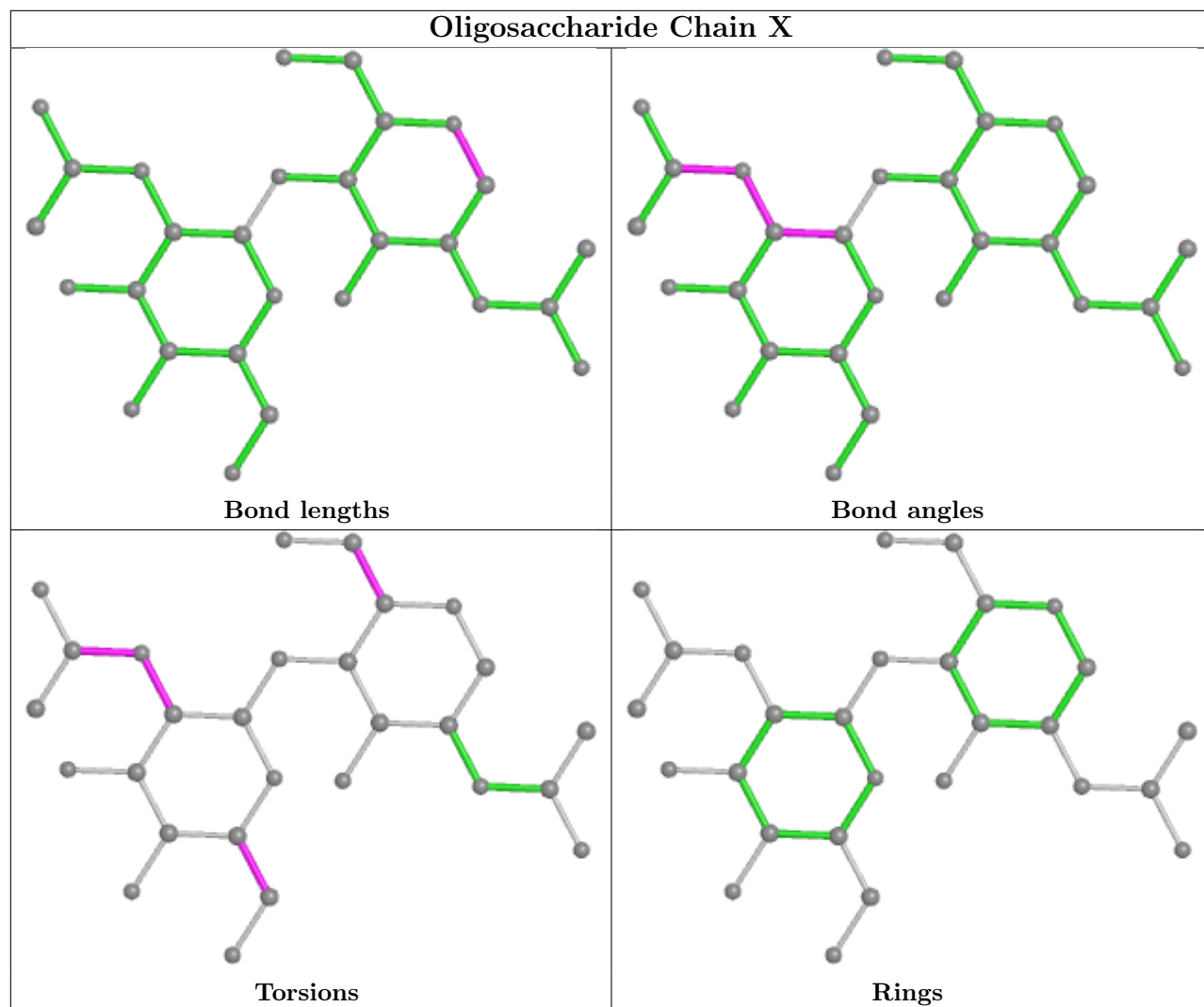


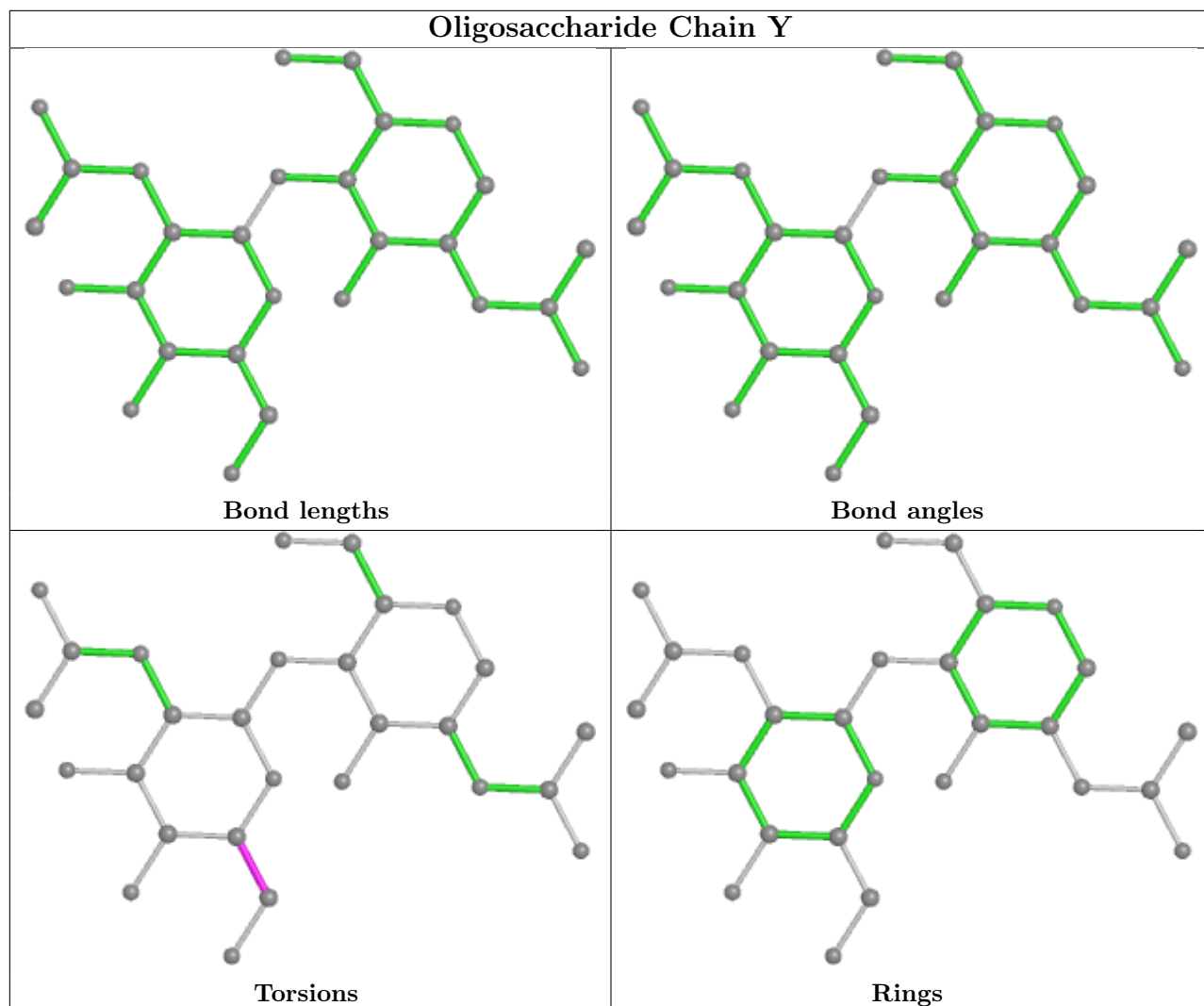


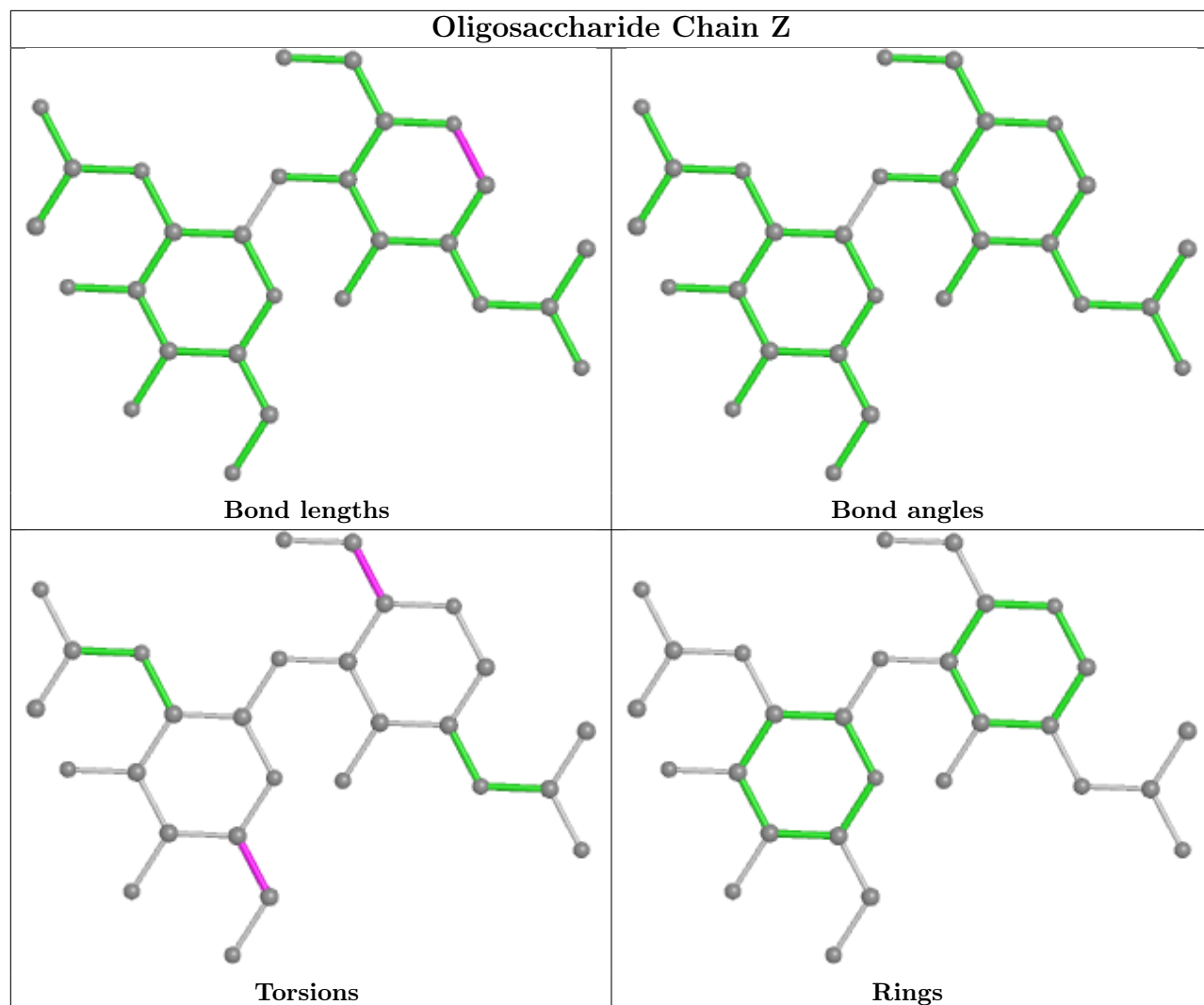


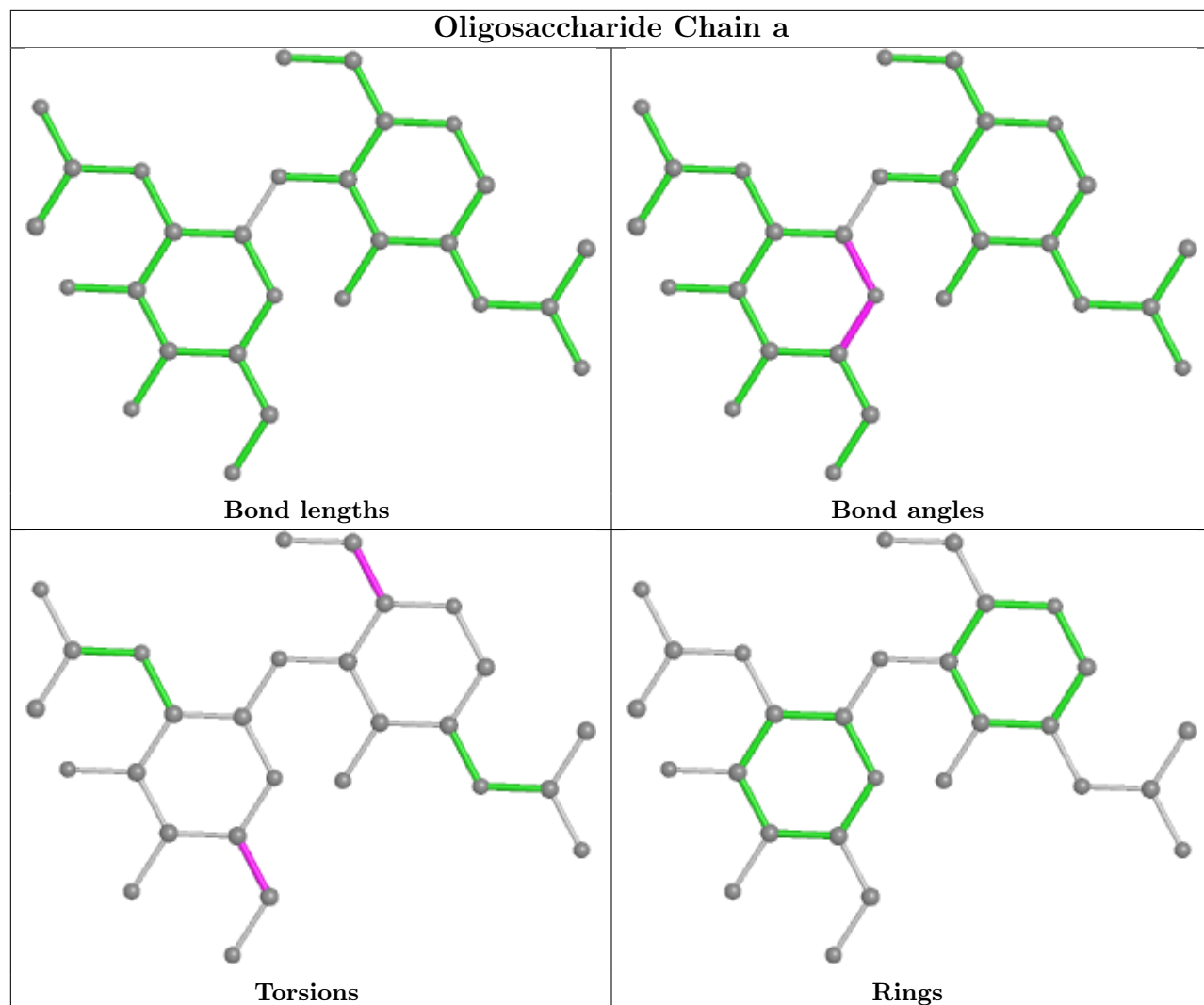


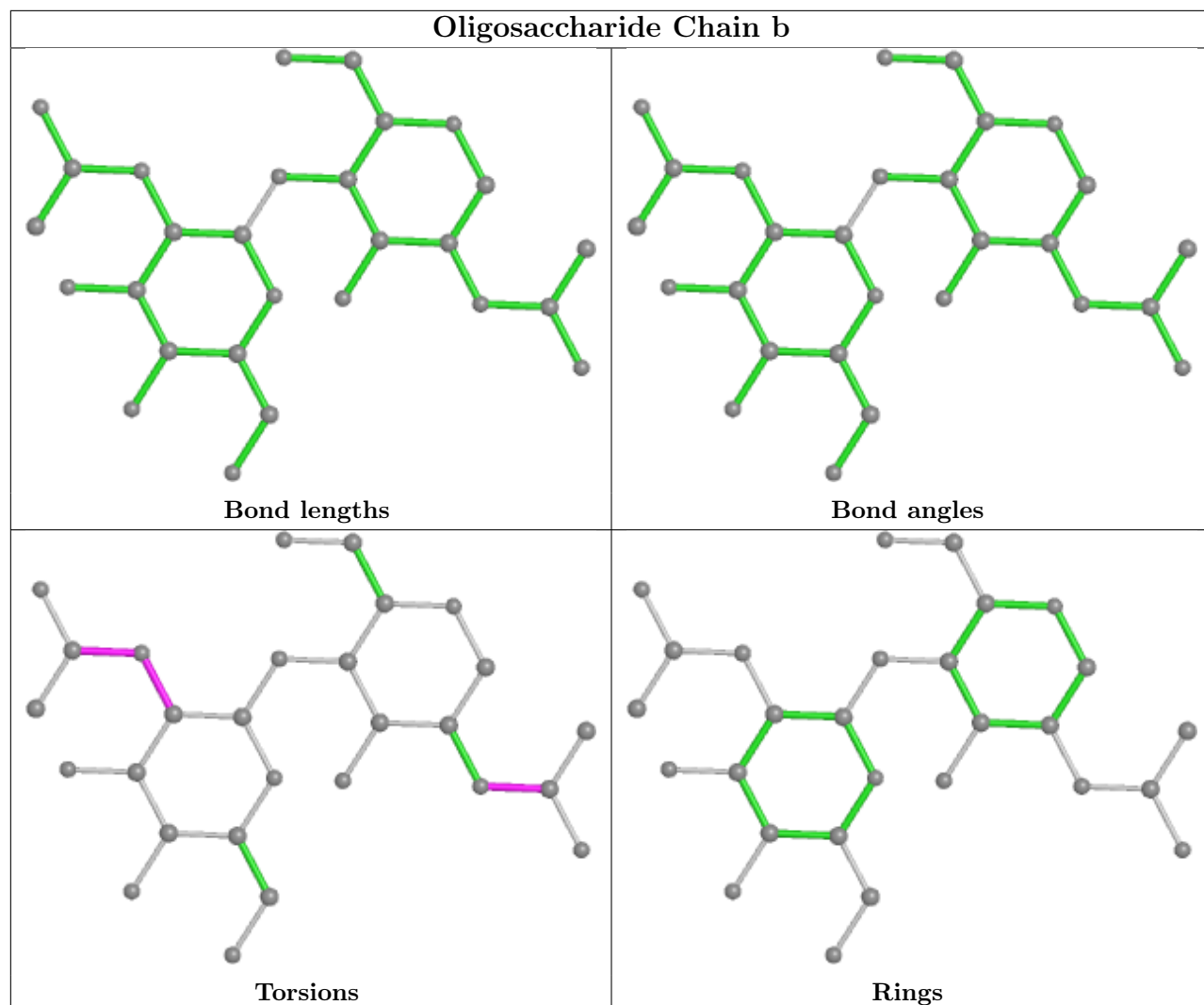


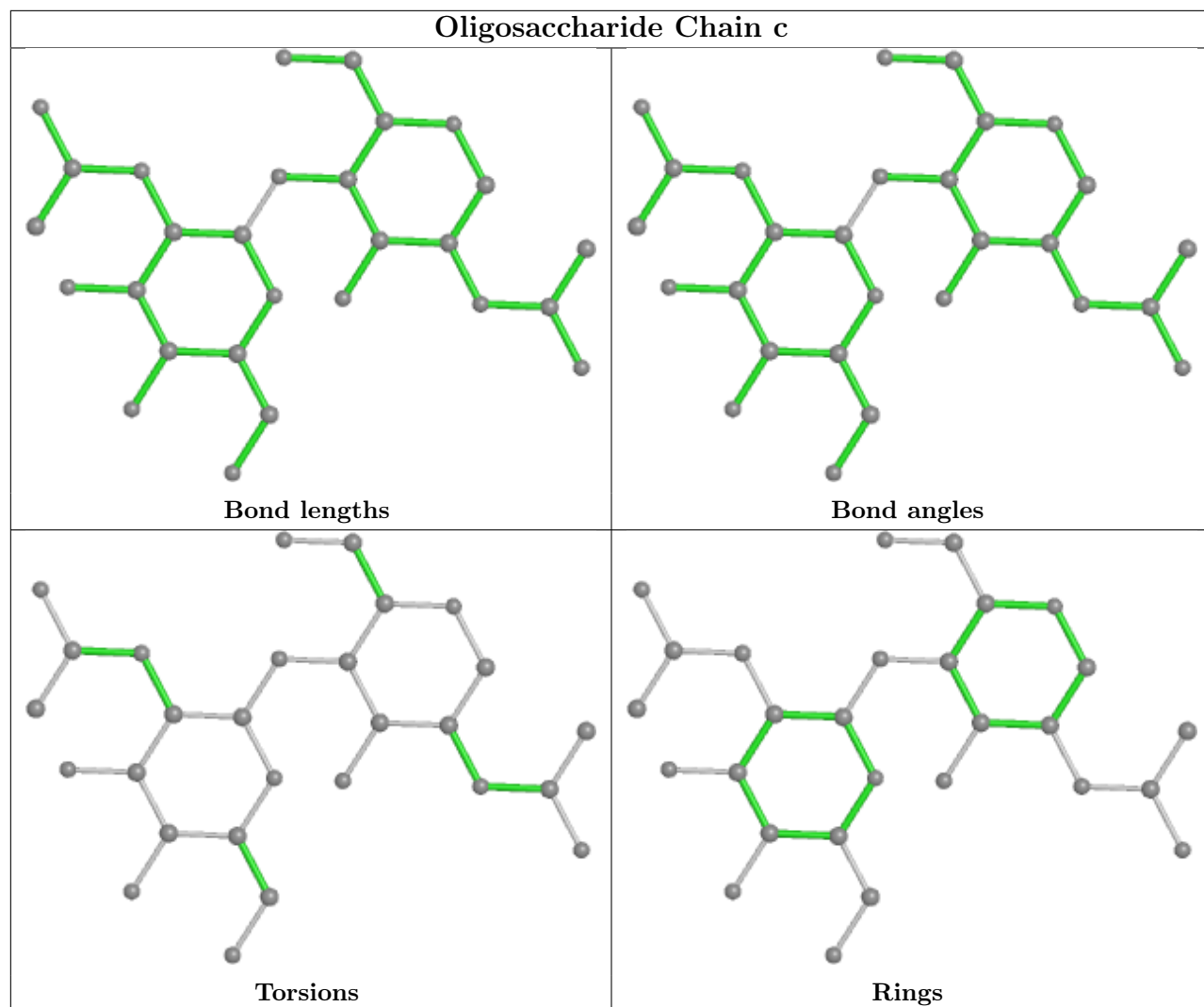


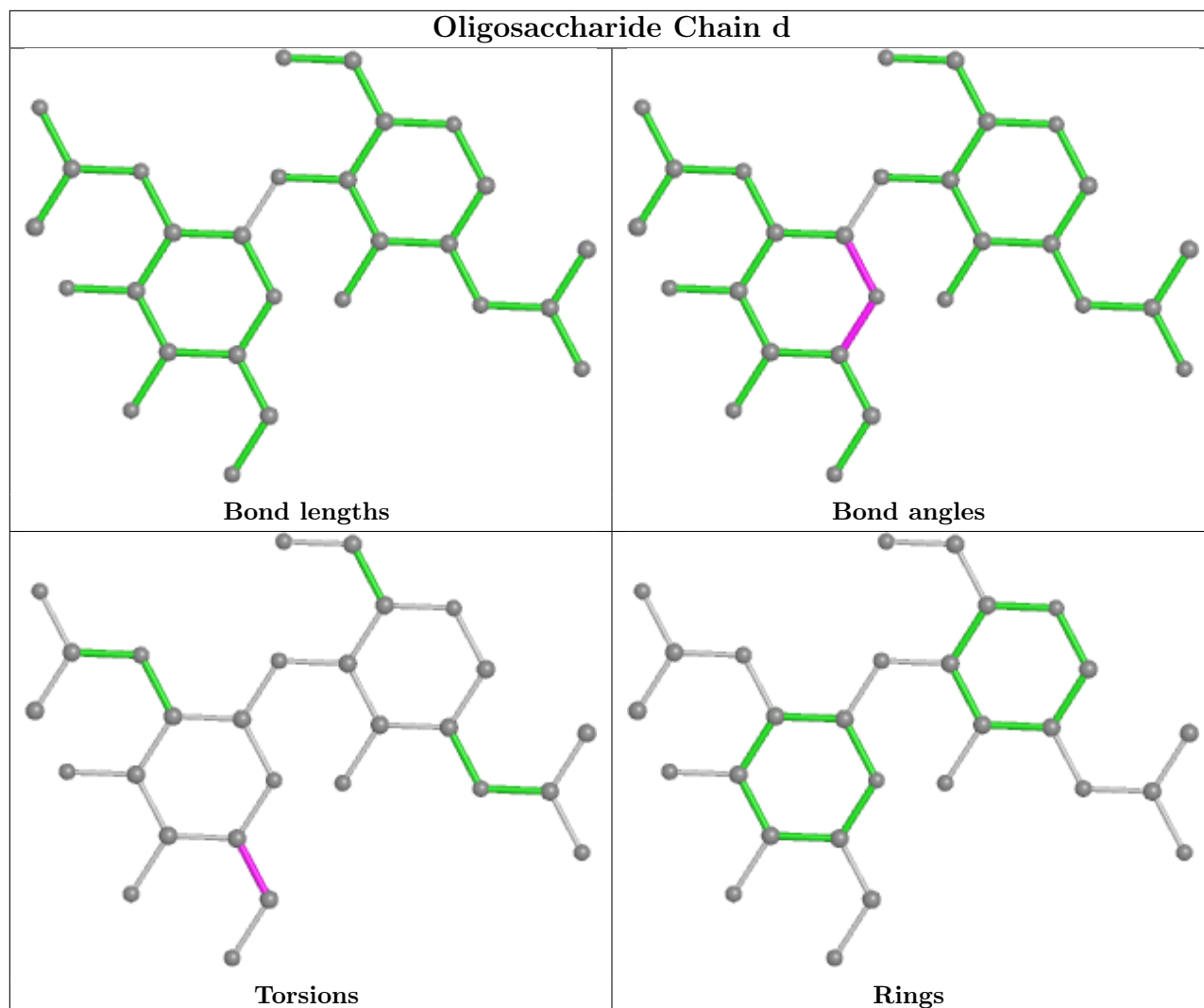












## 5.6 Ligand geometry [i](#)

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	$\# Z  > 2$
4	NAG	C	1405	1	14,14,15	0.57	0	17,19,21	1.26	1 (5%)
4	NAG	C	1404	1	14,14,15	0.47	0	17,19,21	0.53	0
4	NAG	C	1402	1	14,14,15	0.21	0	17,19,21	0.63	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	NAG	C	1401	1	14,14,15	0.31	0	17,19,21	0.34	0
4	NAG	A	1409	1	14,14,15	0.52	0	17,19,21	0.35	0
4	NAG	A	1403	1	14,14,15	0.22	0	17,19,21	0.41	0
4	NAG	A	1404	1	14,14,15	0.46	0	17,19,21	0.53	0
4	NAG	B	1409	1	14,14,15	0.22	0	17,19,21	0.49	0
4	NAG	B	1404	1	14,14,15	0.47	0	17,19,21	0.54	0
4	NAG	C	1407	1	14,14,15	0.24	0	17,19,21	0.50	0
4	NAG	B	1403	1	14,14,15	0.20	0	17,19,21	0.42	0
4	NAG	C	1408	1	14,14,15	0.33	0	17,19,21	0.39	0
4	NAG	C	1406	1	14,14,15	0.28	0	17,19,21	0.38	0
4	NAG	A	1402	1	14,14,15	0.22	0	17,19,21	0.64	0
4	NAG	B	1401	1	14,14,15	0.29	0	17,19,21	0.33	0
4	NAG	C	1403	1	14,14,15	0.21	0	17,19,21	0.42	0
4	NAG	A	1401	1	14,14,15	0.28	0	17,19,21	0.33	0
4	NAG	A	1405	1	14,14,15	0.56	0	17,19,21	1.26	1 (5%)
4	NAG	B	1411	1	14,14,15	0.42	0	17,19,21	1.16	2 (11%)
4	NAG	B	1408	1	14,14,15	0.29	0	17,19,21	0.38	0
4	NAG	B	1412	-	14,14,15	0.36	0	17,19,21	0.41	0
4	NAG	B	1402	1	14,14,15	0.22	0	17,19,21	0.63	0
4	NAG	A	1408	1	14,14,15	0.31	0	17,19,21	0.38	0
4	NAG	B	1407	-	14,14,15	0.29	0	17,19,21	0.62	0
4	NAG	A	1407	1	14,14,15	0.24	0	17,19,21	0.49	0
4	NAG	D	901	2	14,14,15	0.38	0	17,19,21	0.60	1 (5%)
4	NAG	B	1405	1	14,14,15	0.57	0	17,19,21	1.26	1 (5%)
4	NAG	A	1406	1	14,14,15	0.30	0	17,19,21	0.38	0
4	NAG	B	1410	1	14,14,15	0.31	0	17,19,21	0.38	0
4	NAG	B	1406	-	14,14,15	0.41	0	17,19,21	1.17	2 (11%)

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	C	1405	1	-	5/6/23/26	0/1/1/1
4	NAG	C	1404	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1402	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1401	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1409	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1403	1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	1404	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1409	1	-	1/6/23/26	0/1/1/1
4	NAG	B	1404	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1407	1	-	1/6/23/26	0/1/1/1
4	NAG	B	1403	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1408	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1406	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1402	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1401	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1403	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1401	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1405	1	-	5/6/23/26	0/1/1/1
4	NAG	B	1411	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1408	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1412	-	-	0/6/23/26	0/1/1/1
4	NAG	B	1402	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1408	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1407	-	-	1/6/23/26	0/1/1/1
4	NAG	A	1407	1	-	1/6/23/26	0/1/1/1
4	NAG	D	901	2	-	2/6/23/26	0/1/1/1
4	NAG	B	1405	1	-	5/6/23/26	0/1/1/1
4	NAG	A	1406	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1410	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1406	-	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1405	NAG	C2-N2-C7	4.32	129.06	122.90
4	A	1405	NAG	C2-N2-C7	4.31	129.03	122.90
4	C	1405	NAG	C2-N2-C7	4.30	129.02	122.90
4	B	1406	NAG	C8-C7-N2	2.32	120.03	116.10
4	B	1411	NAG	C8-C7-N2	2.26	119.92	116.10
4	B	1411	NAG	C2-N2-C7	-2.06	119.97	122.90
4	D	901	NAG	C1-O5-C5	2.05	114.97	112.19
4	B	1406	NAG	C2-N2-C7	-2.02	120.02	122.90

There are no chirality outliers.

All (59) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1406	NAG	O5-C5-C6-O6
4	B	1408	NAG	O5-C5-C6-O6
4	C	1406	NAG	O5-C5-C6-O6
4	A	1401	NAG	O5-C5-C6-O6
4	B	1401	NAG	O5-C5-C6-O6
4	C	1401	NAG	O5-C5-C6-O6
4	A	1402	NAG	C4-C5-C6-O6
4	B	1402	NAG	C4-C5-C6-O6
4	C	1402	NAG	C4-C5-C6-O6
4	A	1402	NAG	O5-C5-C6-O6
4	A	1404	NAG	O5-C5-C6-O6
4	B	1402	NAG	O5-C5-C6-O6
4	B	1404	NAG	O5-C5-C6-O6
4	C	1402	NAG	O5-C5-C6-O6
4	C	1404	NAG	O5-C5-C6-O6
4	B	1405	NAG	O5-C5-C6-O6
4	C	1405	NAG	O5-C5-C6-O6
4	A	1405	NAG	O5-C5-C6-O6
4	A	1409	NAG	C4-C5-C6-O6
4	A	1408	NAG	O5-C5-C6-O6
4	B	1410	NAG	O5-C5-C6-O6
4	C	1408	NAG	O5-C5-C6-O6
4	A	1405	NAG	C4-C5-C6-O6
4	B	1405	NAG	C4-C5-C6-O6
4	C	1405	NAG	C4-C5-C6-O6
4	A	1405	NAG	C8-C7-N2-C2
4	A	1405	NAG	O7-C7-N2-C2
4	B	1405	NAG	C8-C7-N2-C2
4	B	1405	NAG	O7-C7-N2-C2
4	C	1405	NAG	C8-C7-N2-C2
4	C	1405	NAG	O7-C7-N2-C2
4	A	1409	NAG	O5-C5-C6-O6
4	A	1406	NAG	C4-C5-C6-O6
4	B	1408	NAG	C4-C5-C6-O6
4	C	1406	NAG	C4-C5-C6-O6
4	A	1404	NAG	C4-C5-C6-O6
4	C	1404	NAG	C4-C5-C6-O6
4	B	1404	NAG	C4-C5-C6-O6
4	D	901	NAG	O5-C5-C6-O6
4	A	1403	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	B	1403	NAG	O5-C5-C6-O6
4	C	1403	NAG	O5-C5-C6-O6
4	A	1403	NAG	C4-C5-C6-O6
4	B	1403	NAG	C4-C5-C6-O6
4	C	1403	NAG	C4-C5-C6-O6
4	A	1408	NAG	C4-C5-C6-O6
4	C	1408	NAG	C4-C5-C6-O6
4	B	1410	NAG	C4-C5-C6-O6
4	B	1401	NAG	C4-C5-C6-O6
4	A	1401	NAG	C4-C5-C6-O6
4	C	1401	NAG	C4-C5-C6-O6
4	D	901	NAG	C4-C5-C6-O6
4	A	1407	NAG	C1-C2-N2-C7
4	B	1409	NAG	C1-C2-N2-C7
4	C	1407	NAG	C1-C2-N2-C7
4	B	1407	NAG	C4-C5-C6-O6
4	A	1405	NAG	C3-C2-N2-C7
4	B	1405	NAG	C3-C2-N2-C7
4	C	1405	NAG	C3-C2-N2-C7

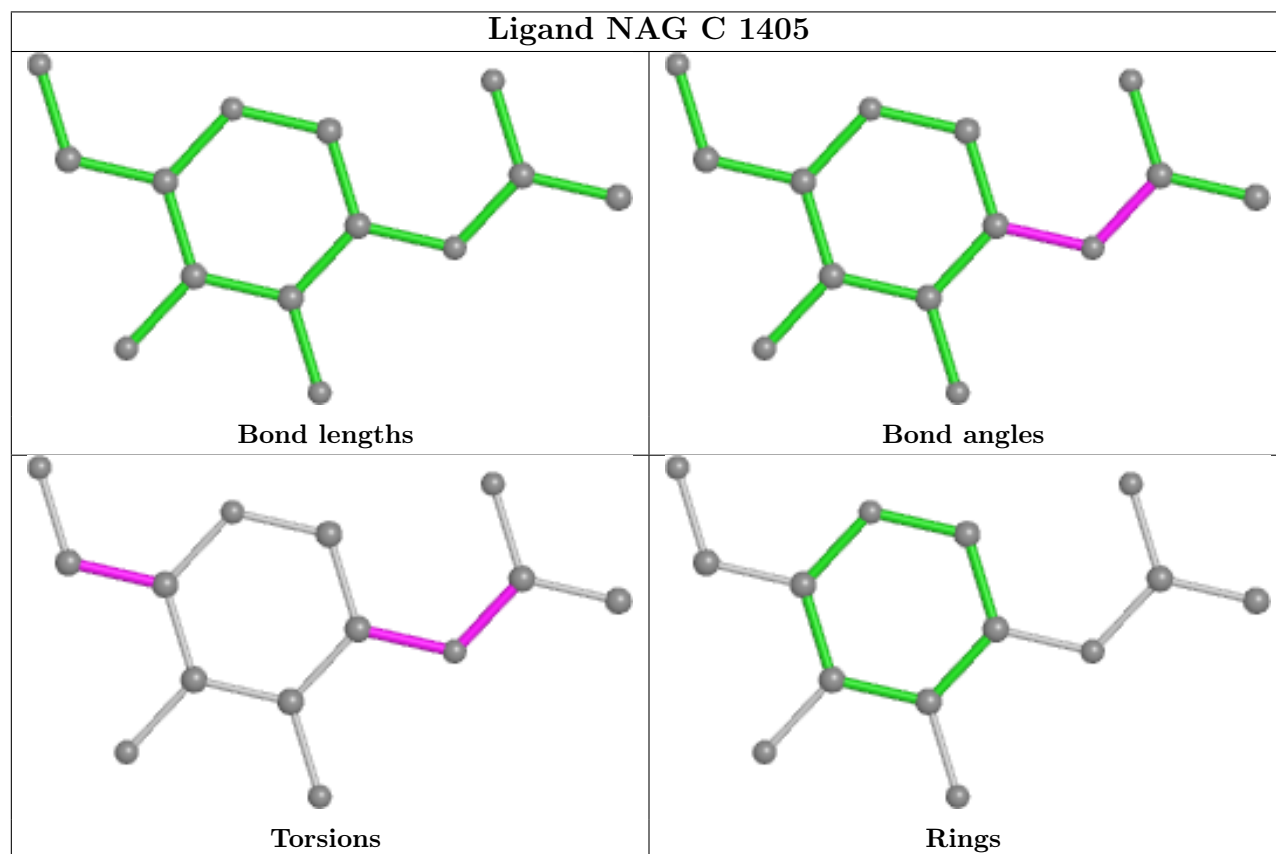
There are no ring outliers.

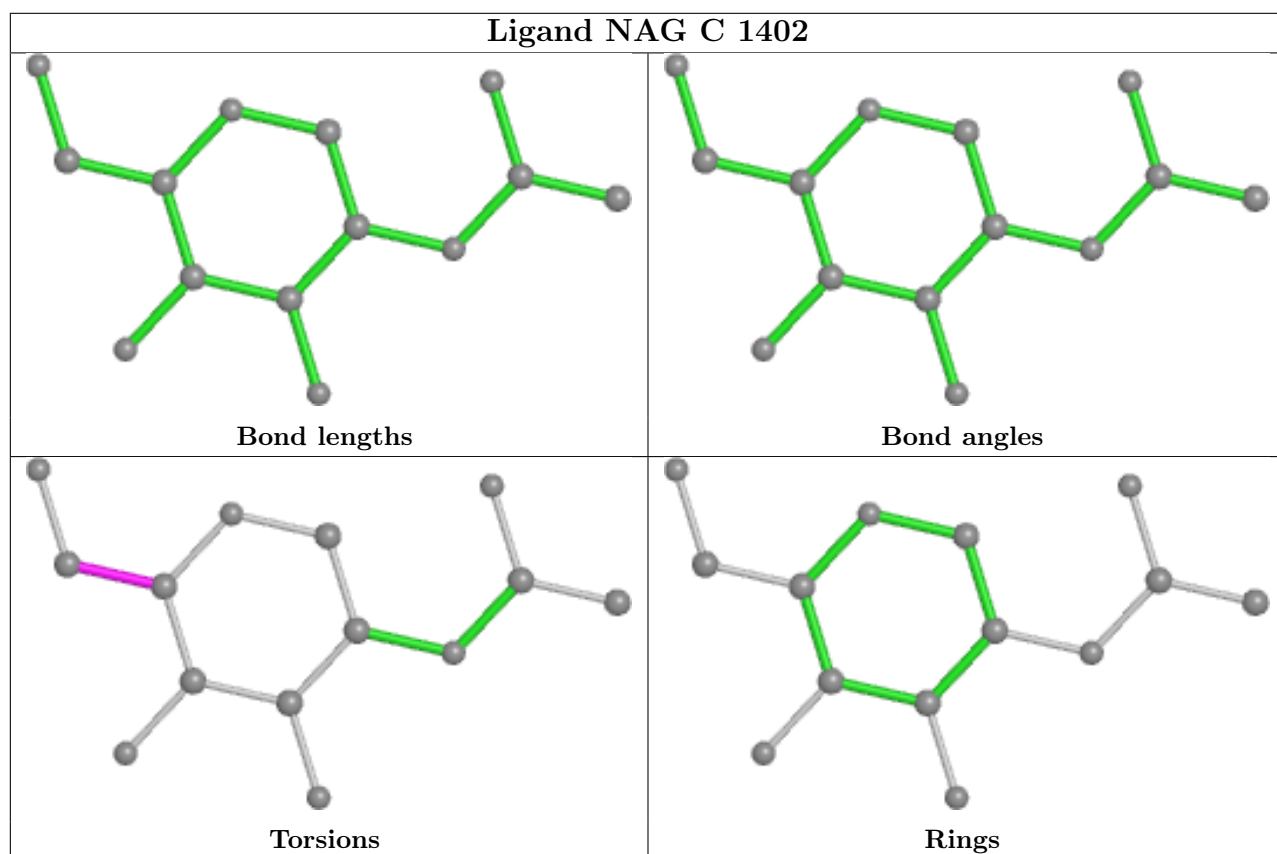
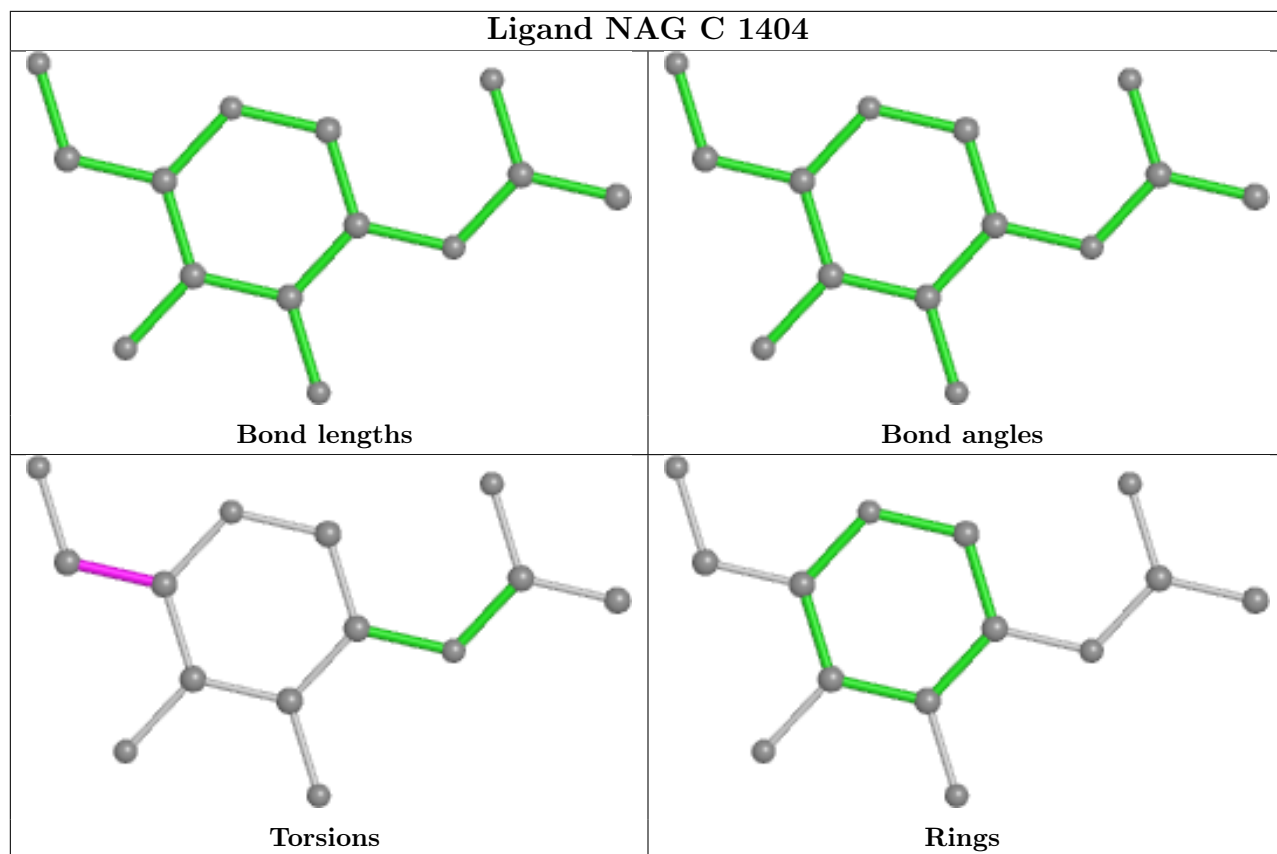
9 monomers are involved in 23 short contacts:

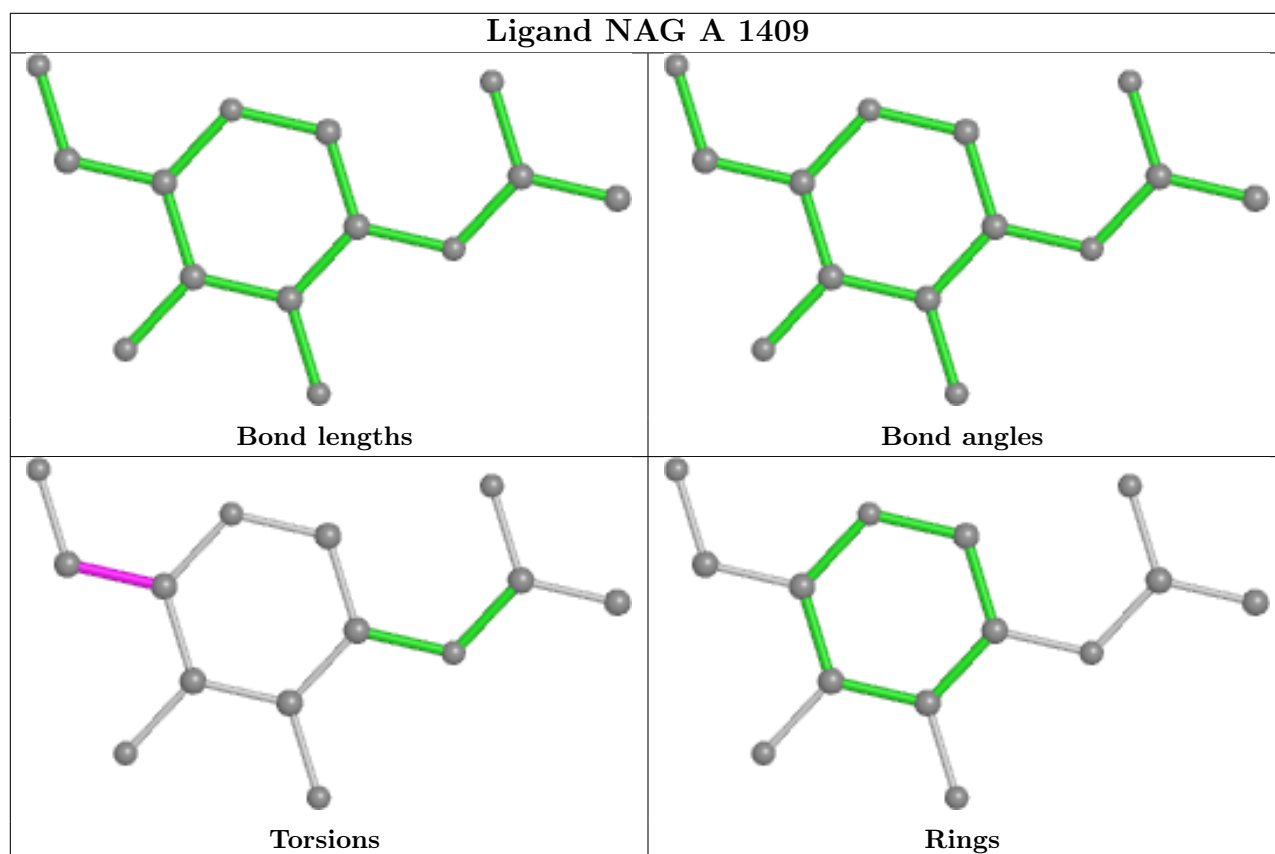
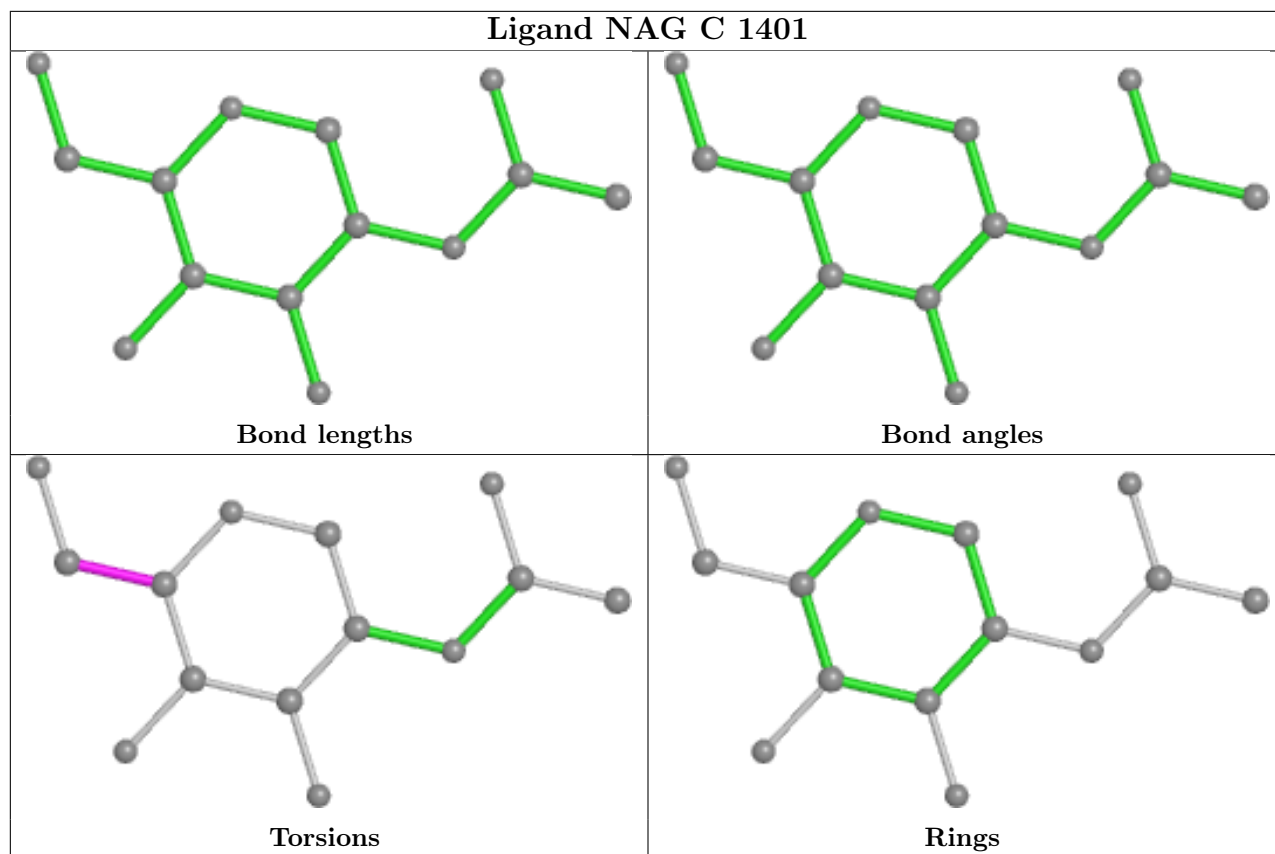
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	1405	NAG	1	0
4	C	1402	NAG	3	0
4	A	1402	NAG	3	0
4	A	1405	NAG	1	0
4	B	1411	NAG	4	0
4	B	1412	NAG	4	0
4	B	1402	NAG	3	0
4	B	1407	NAG	7	0
4	B	1405	NAG	1	0

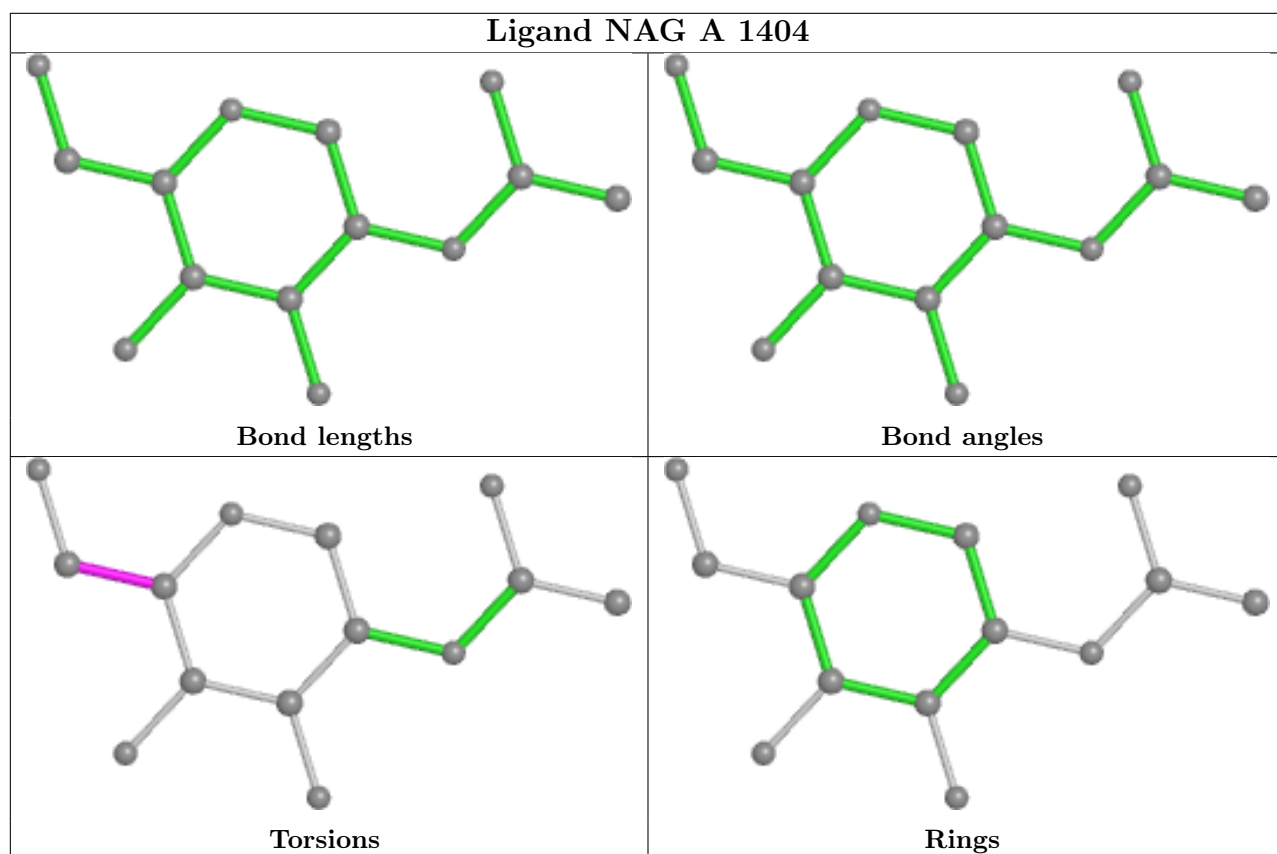
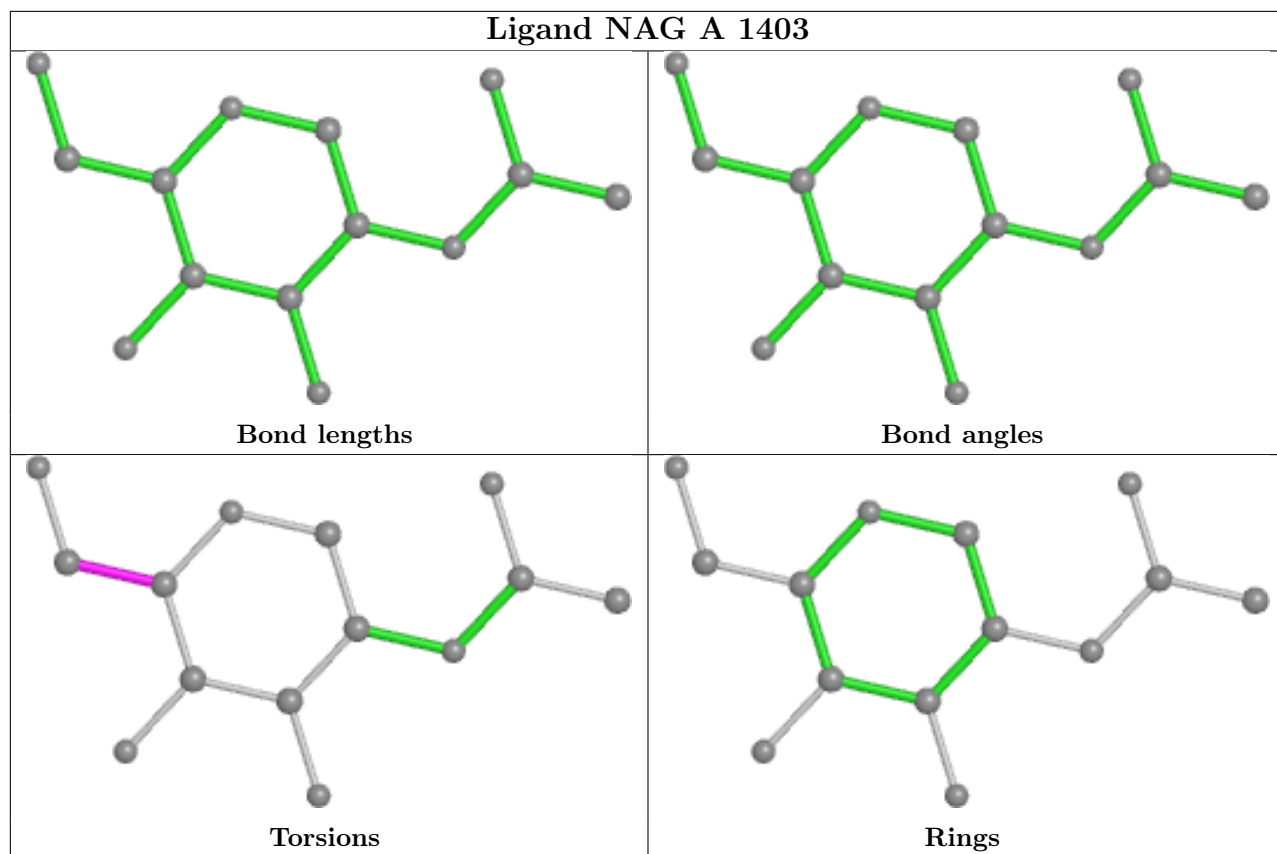
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

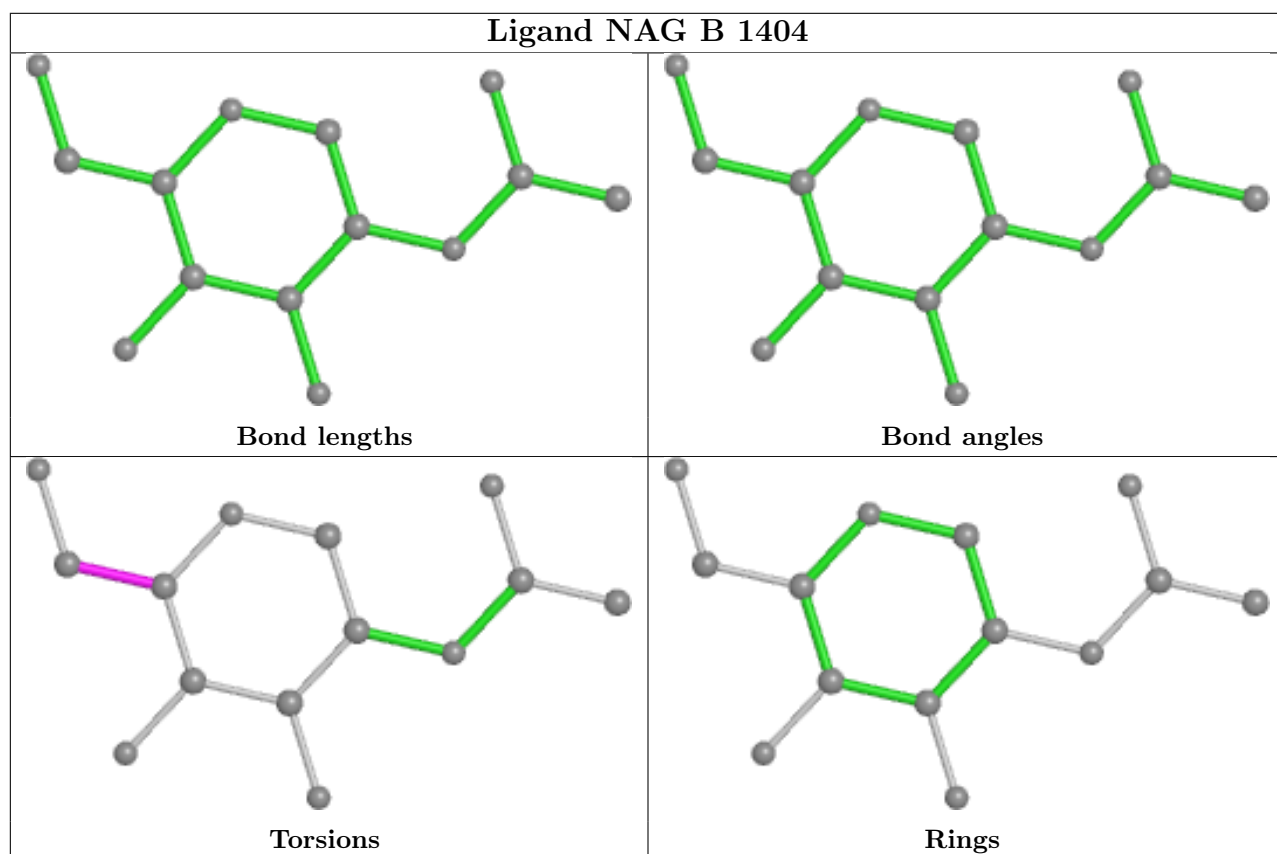
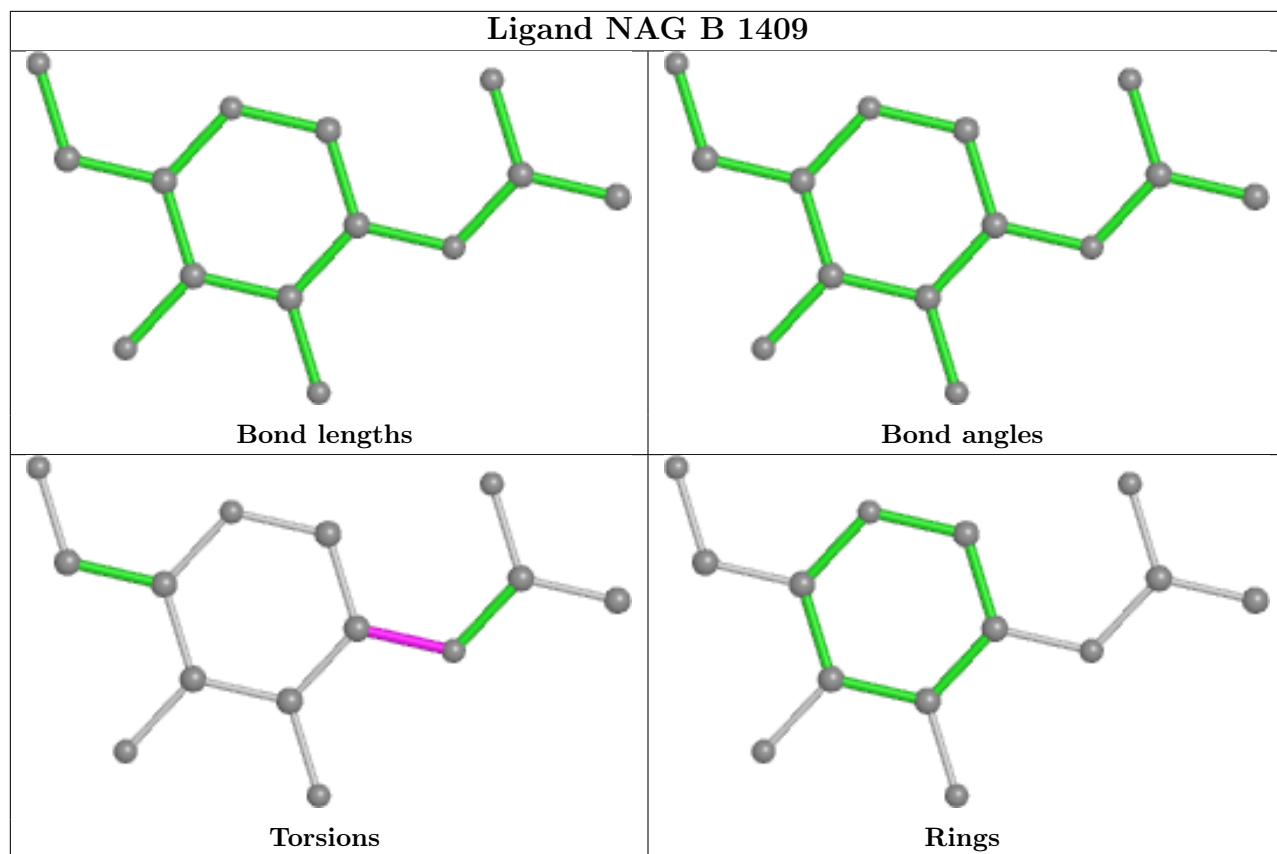
average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



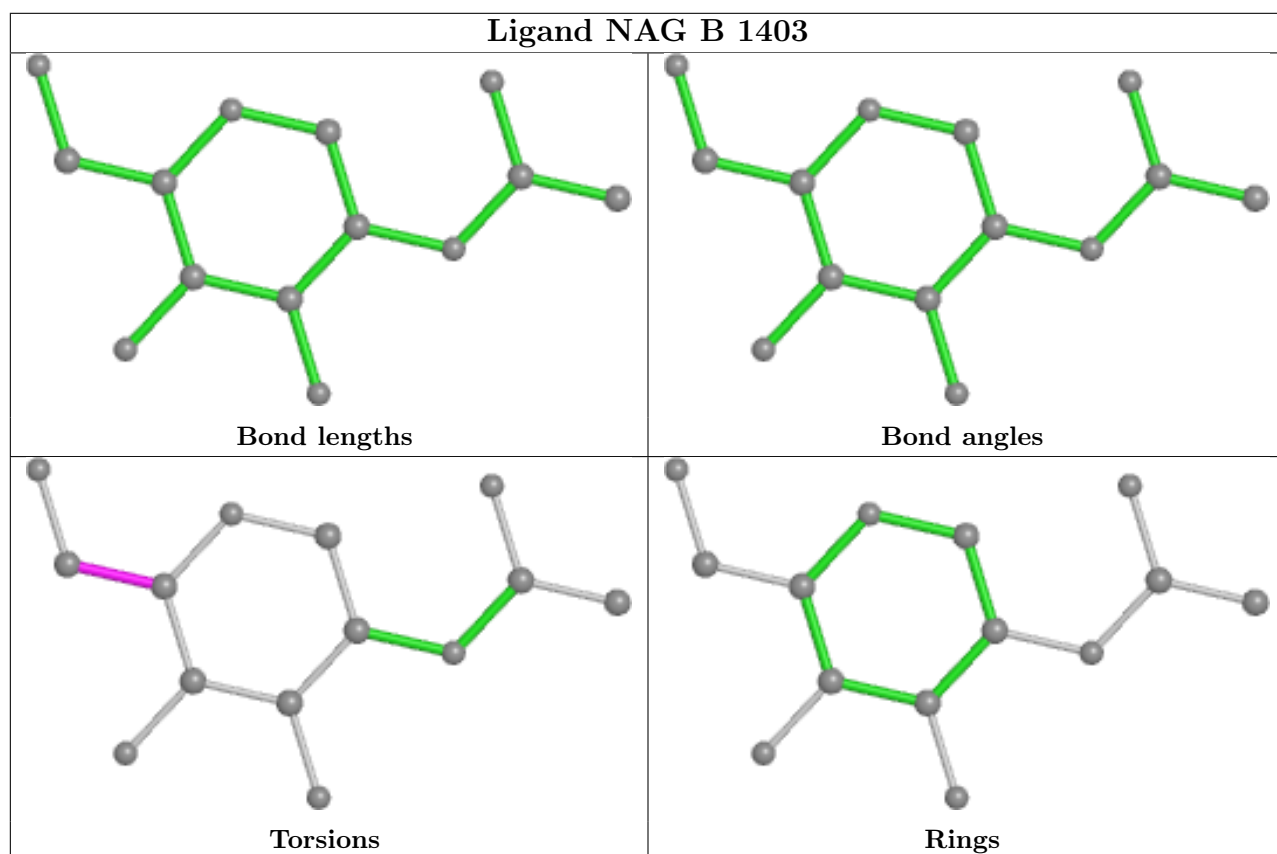
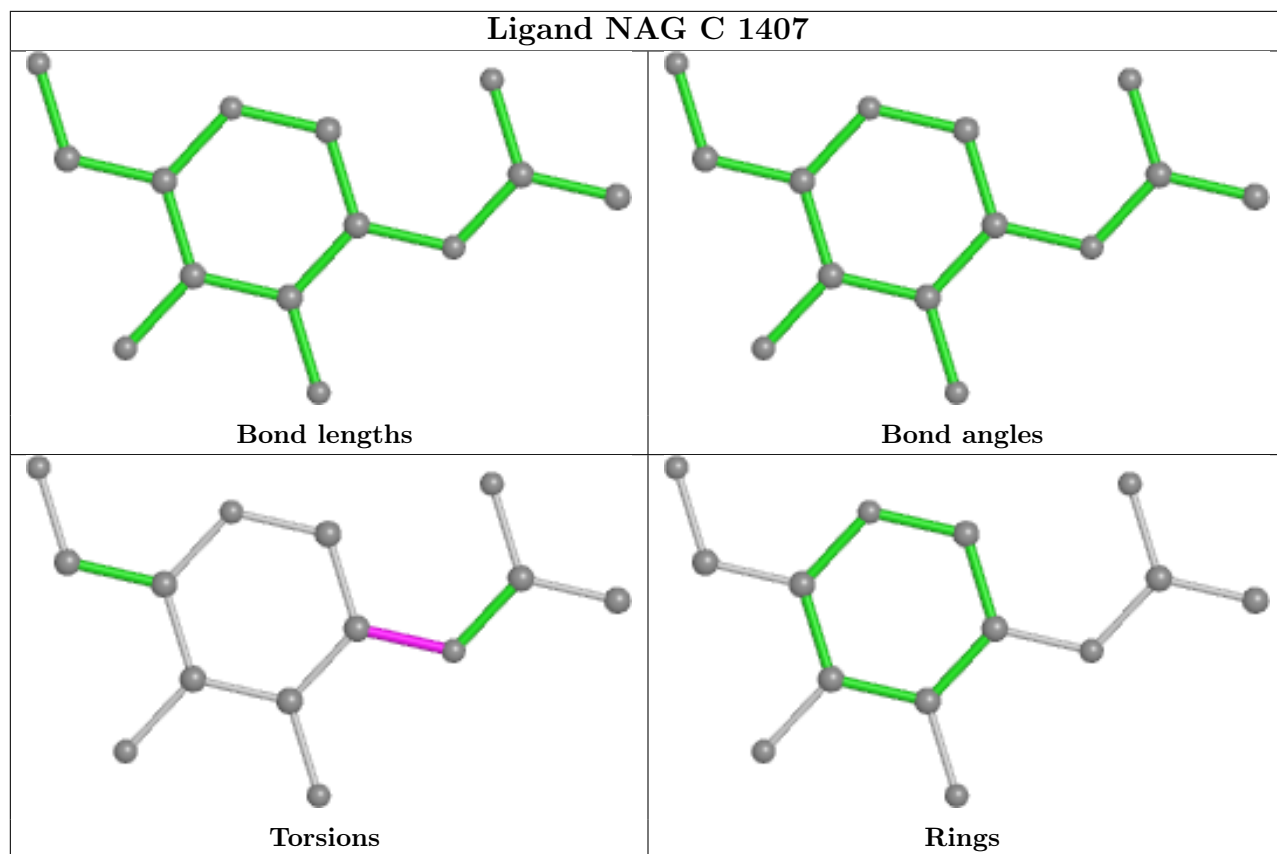


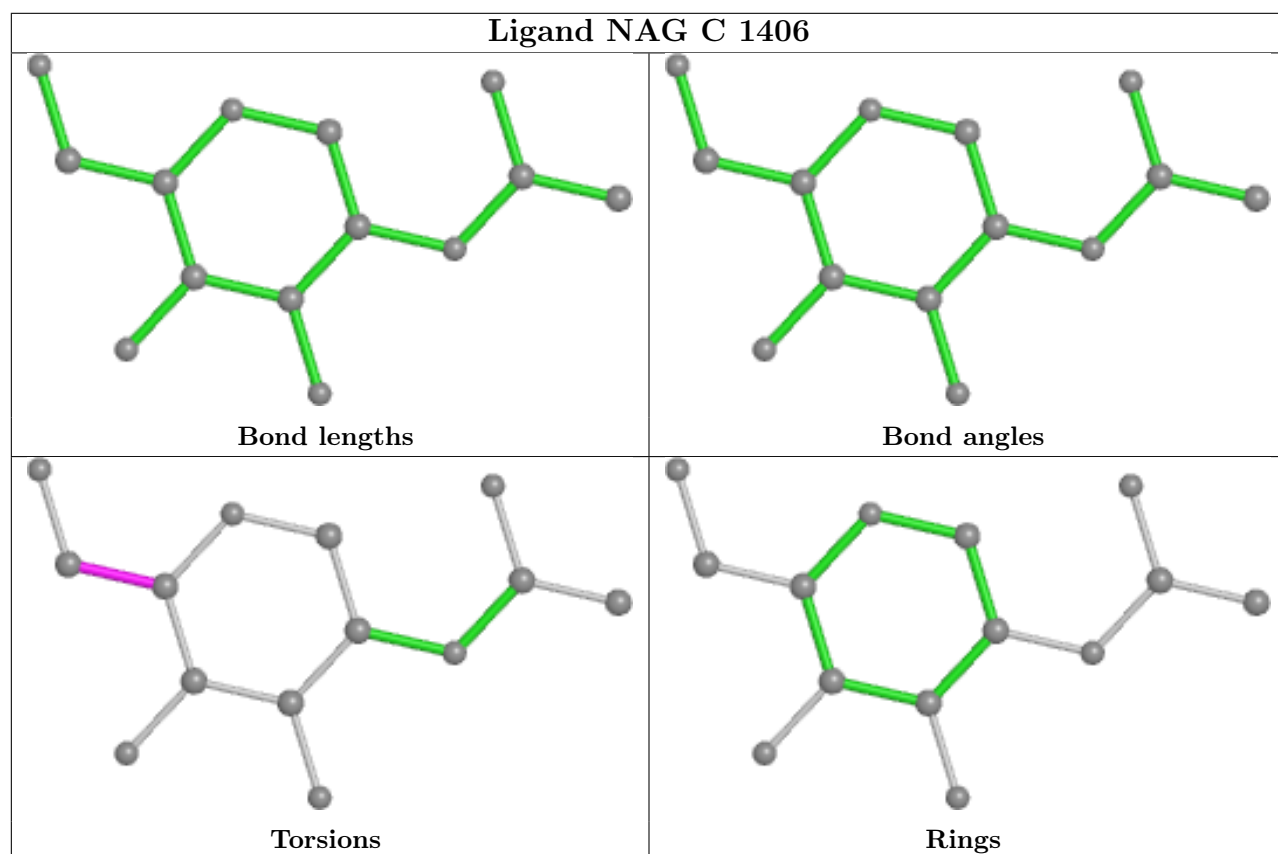
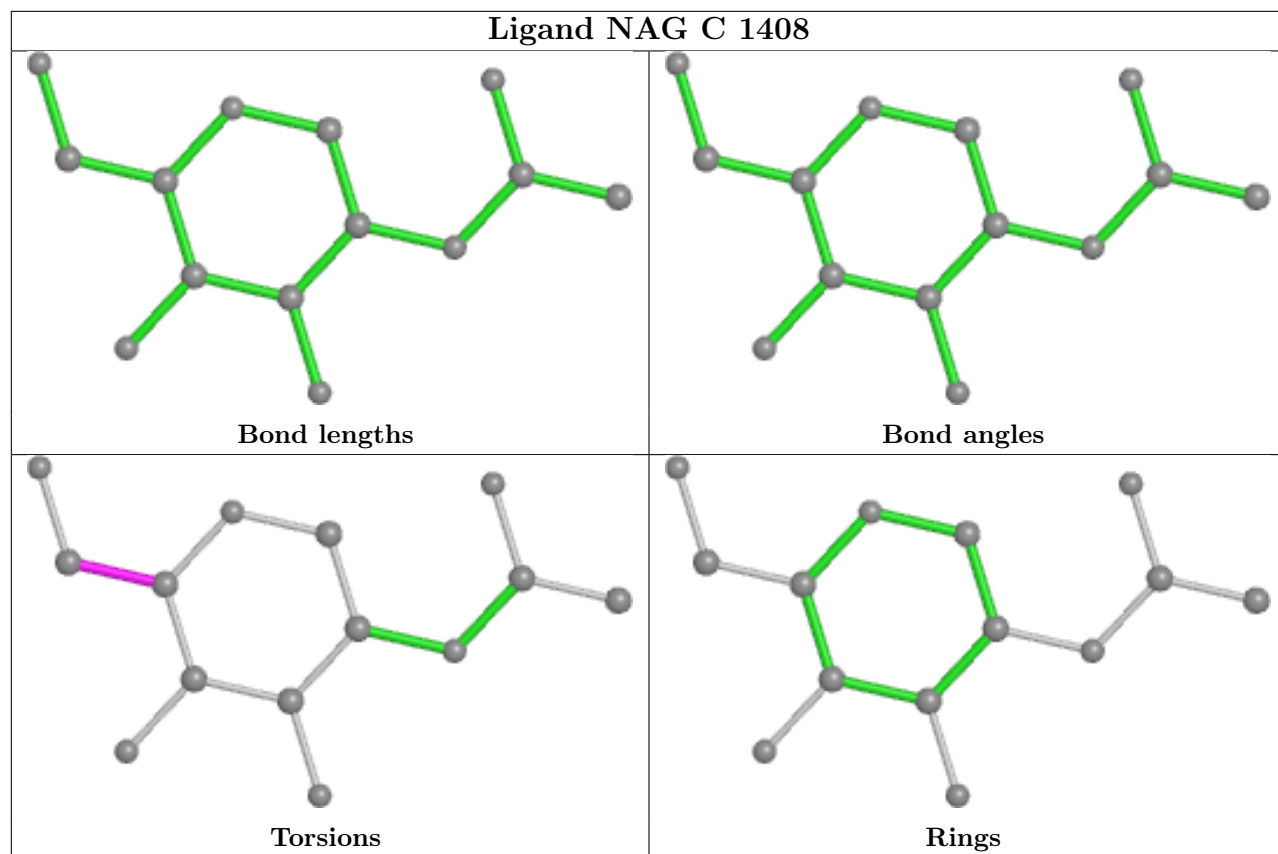


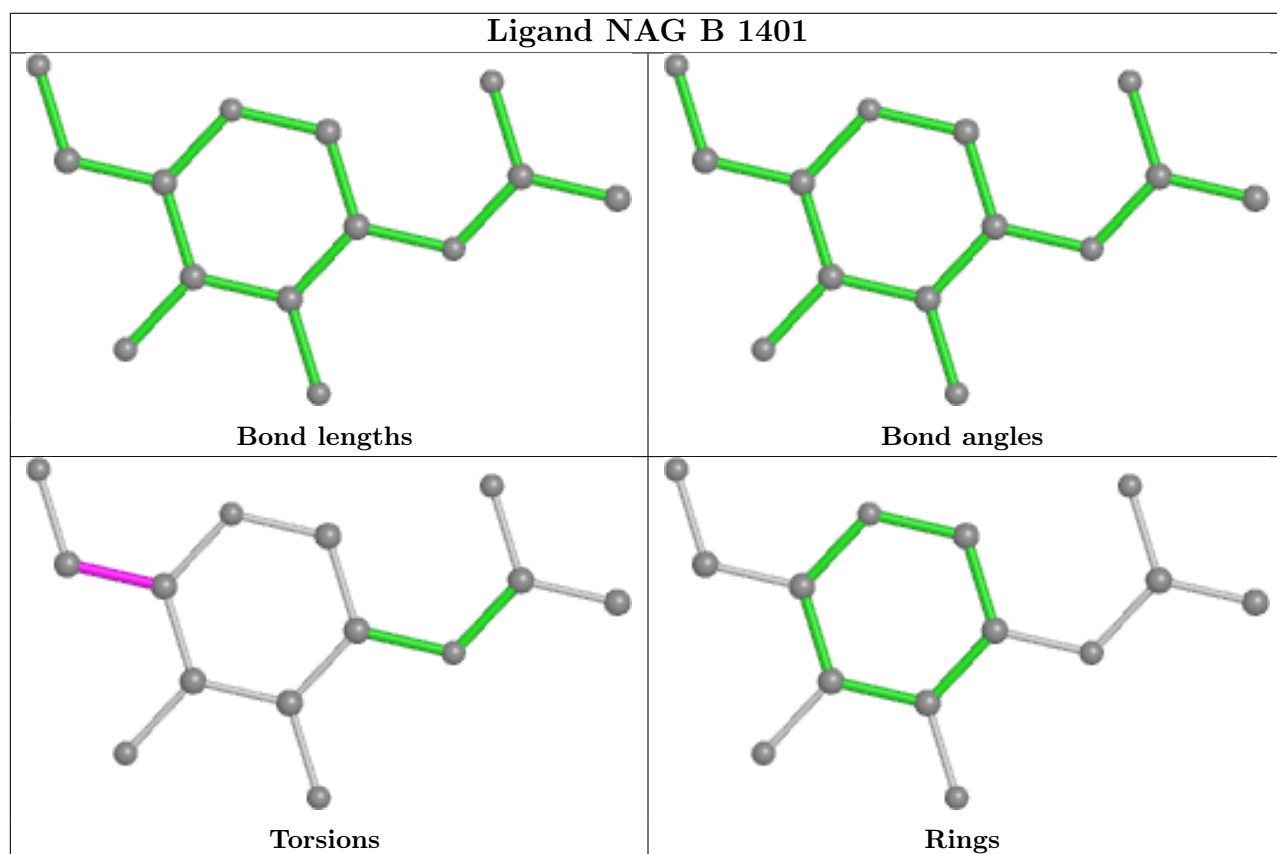
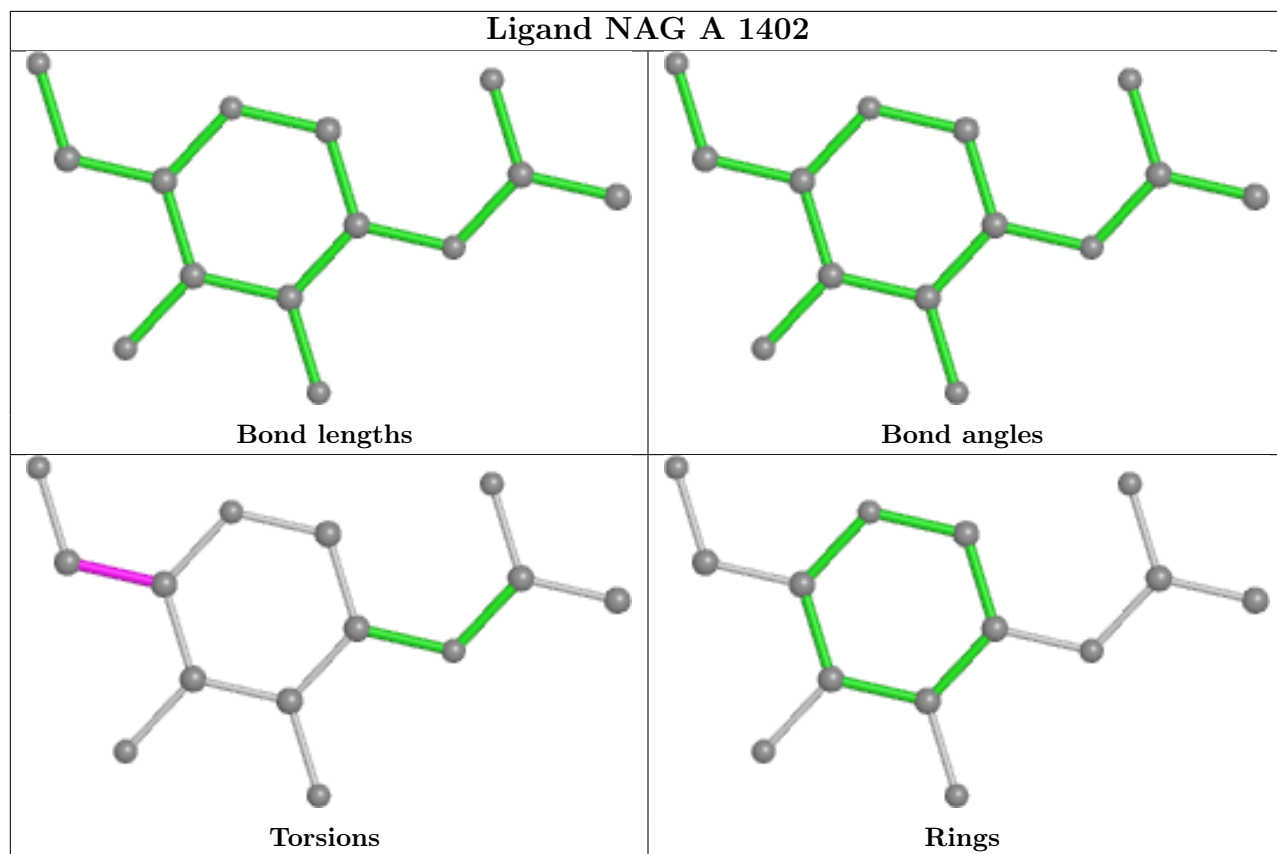


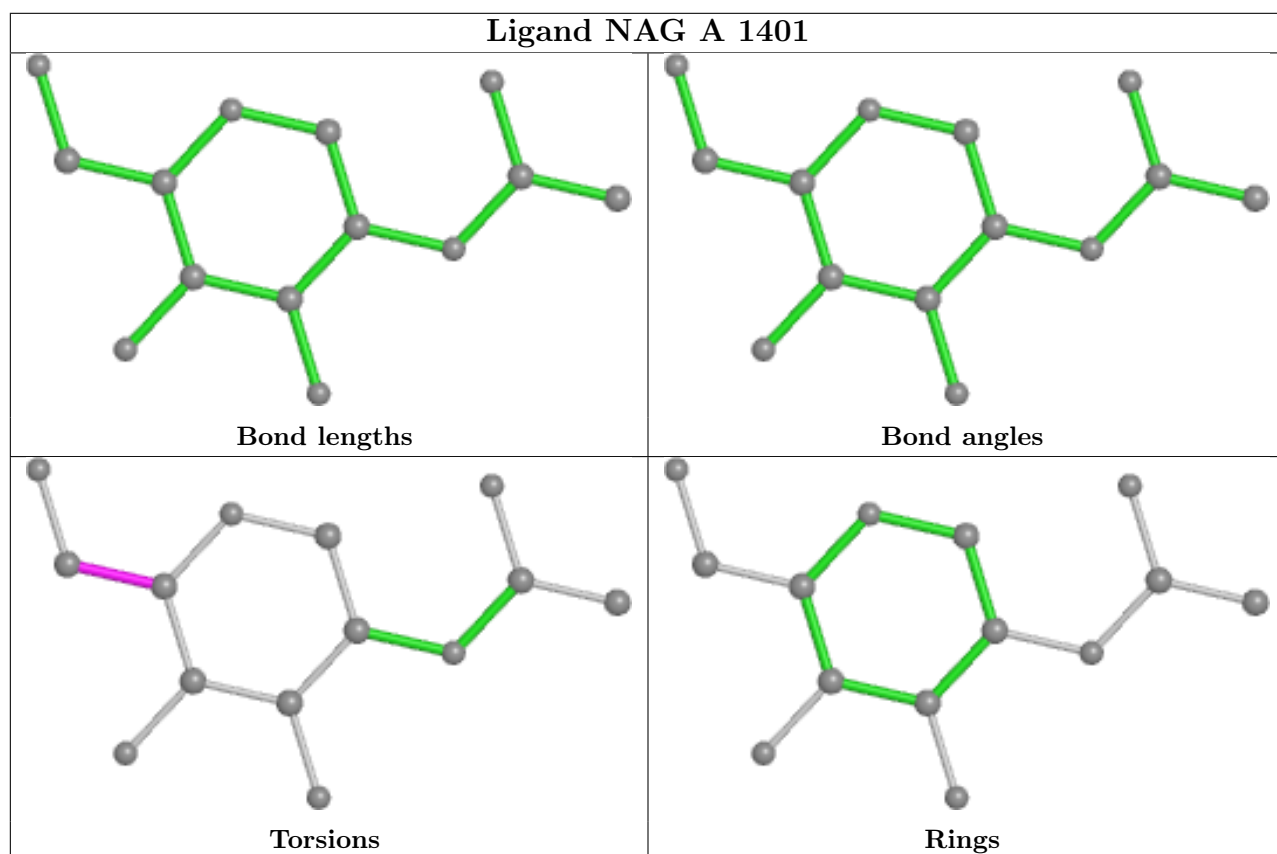
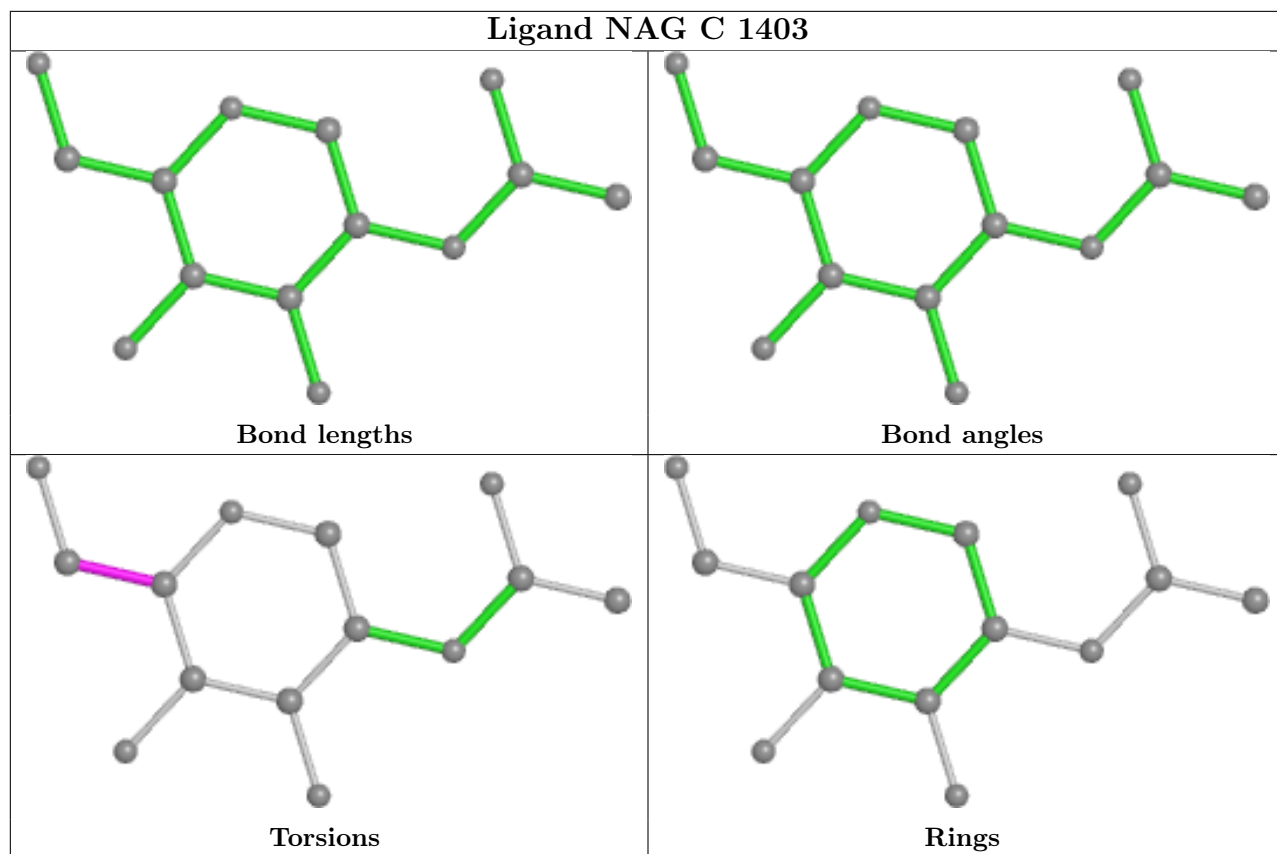


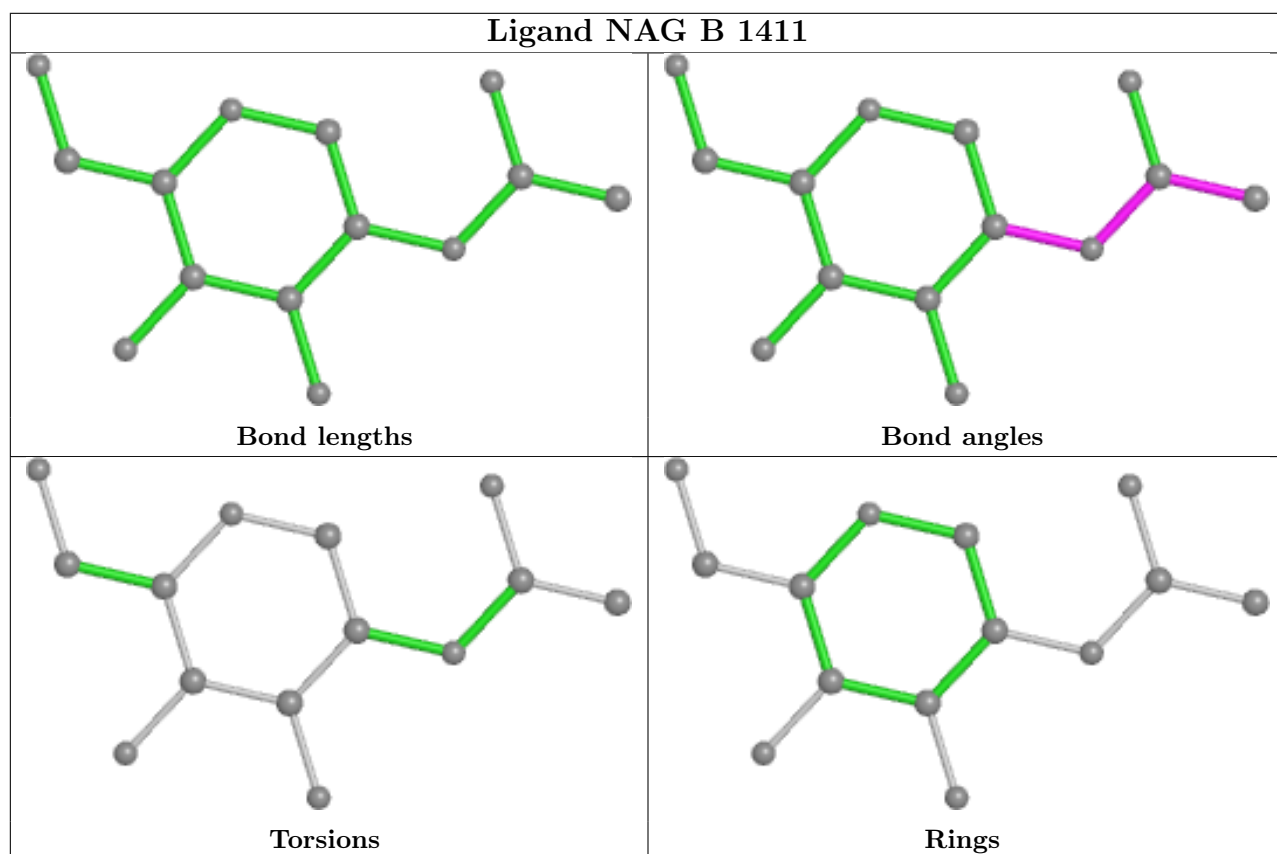
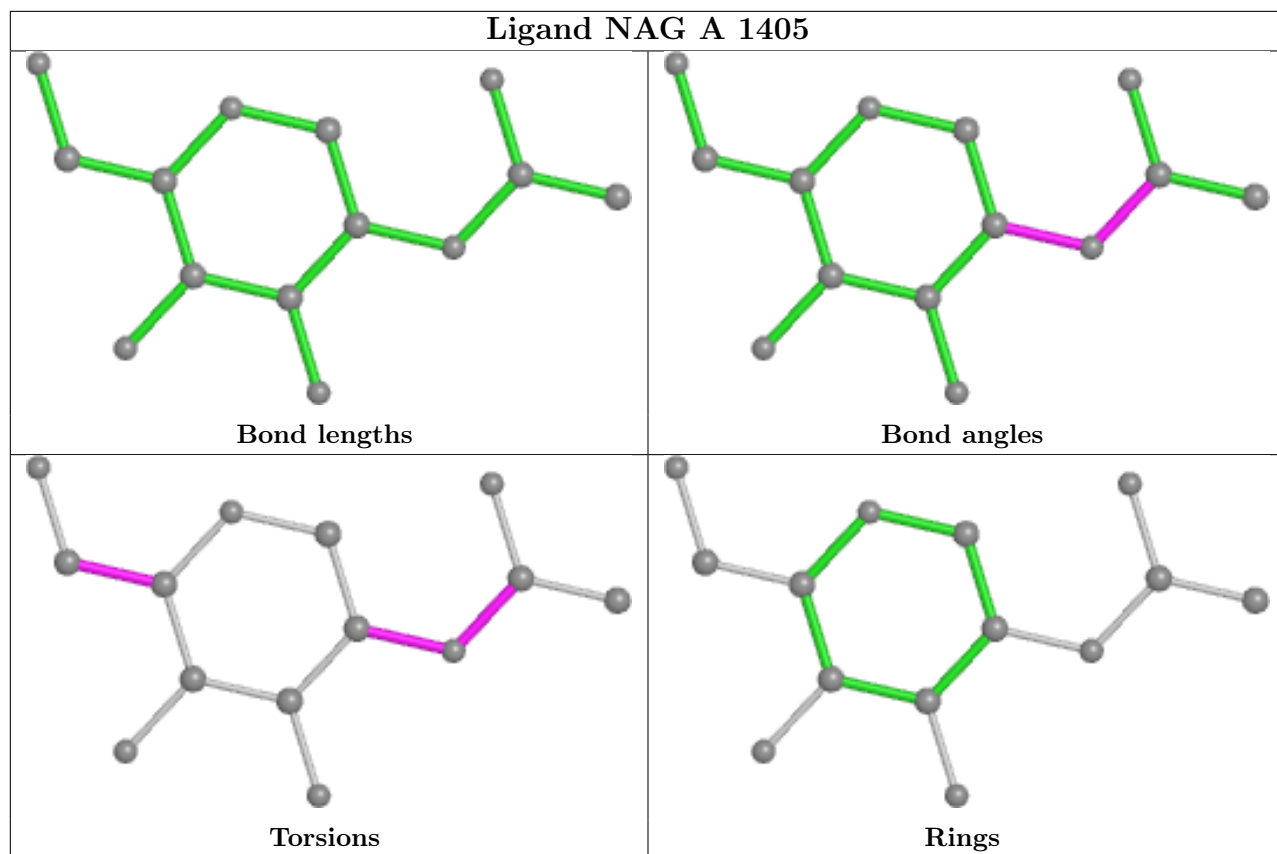


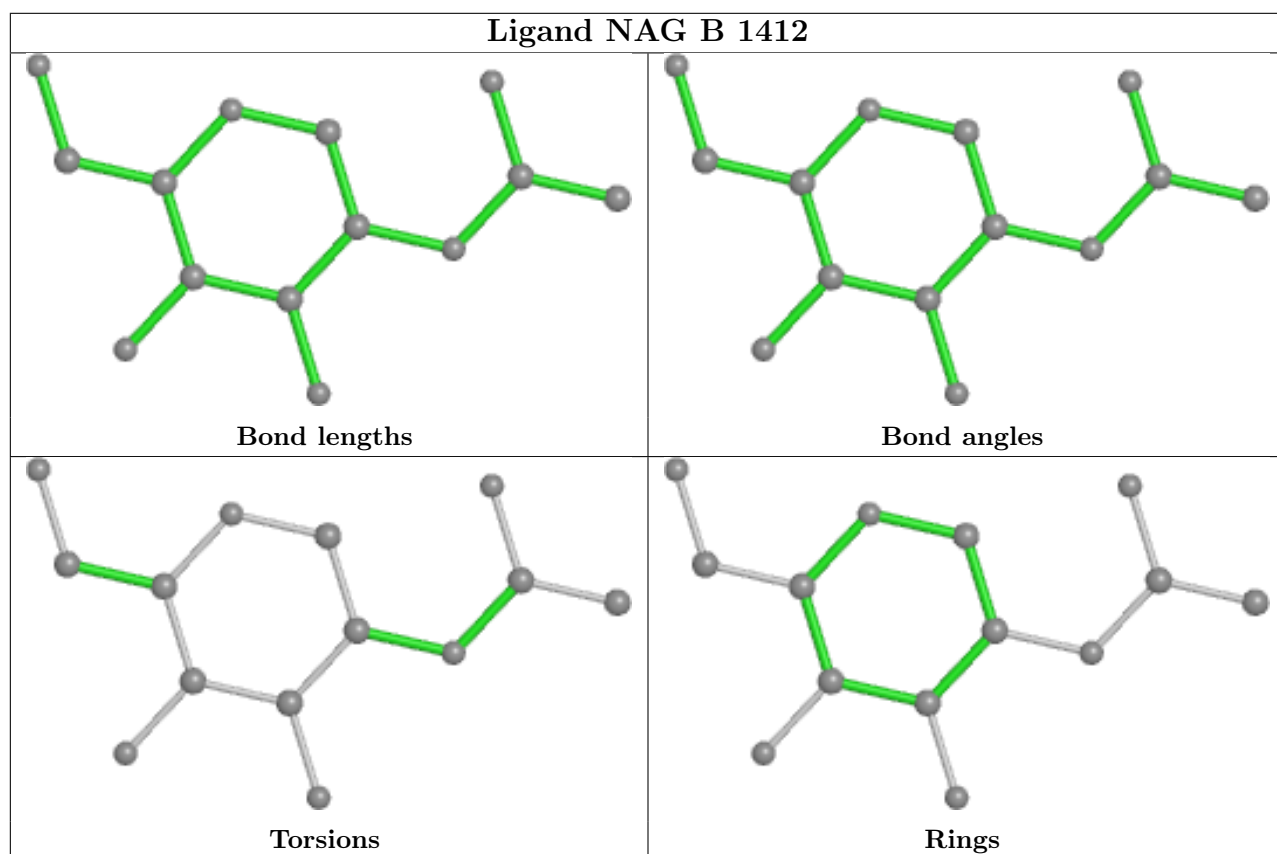
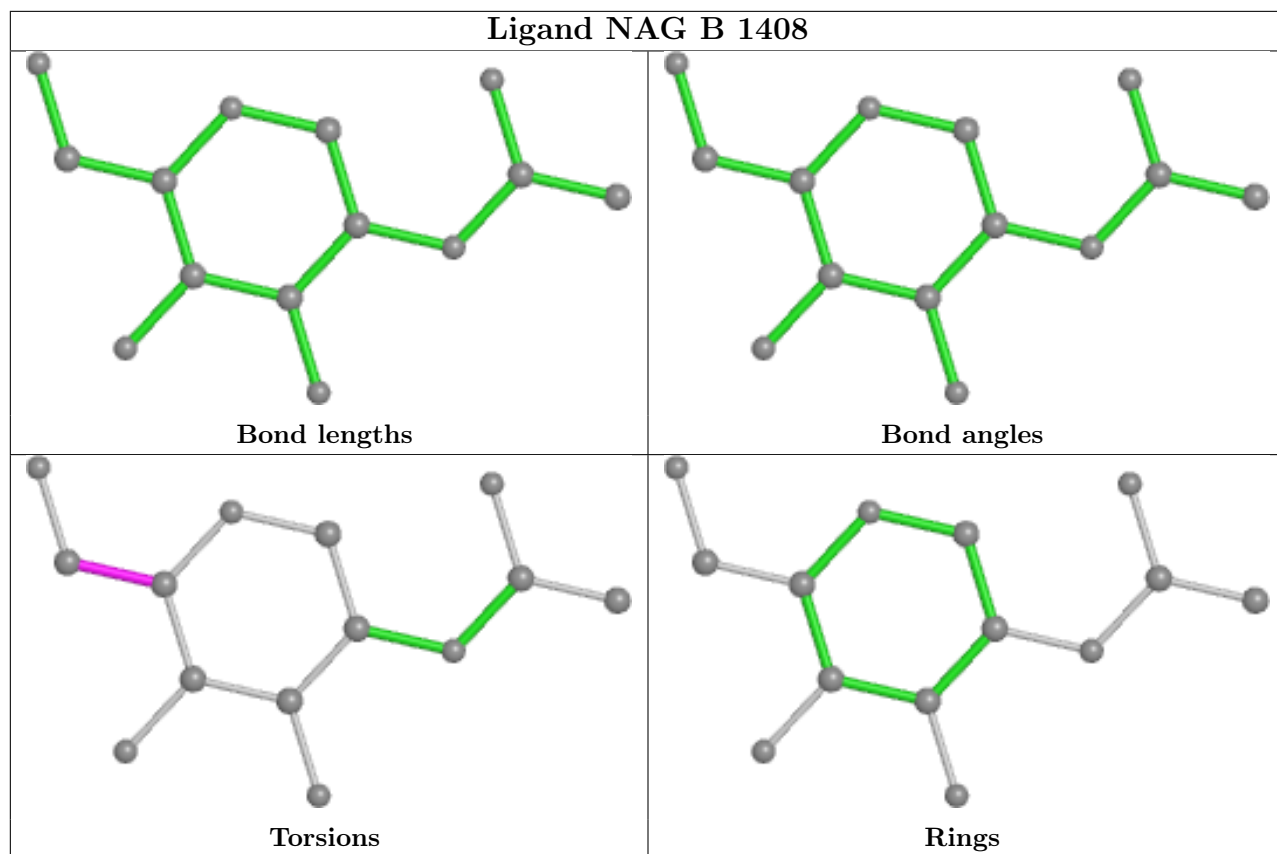


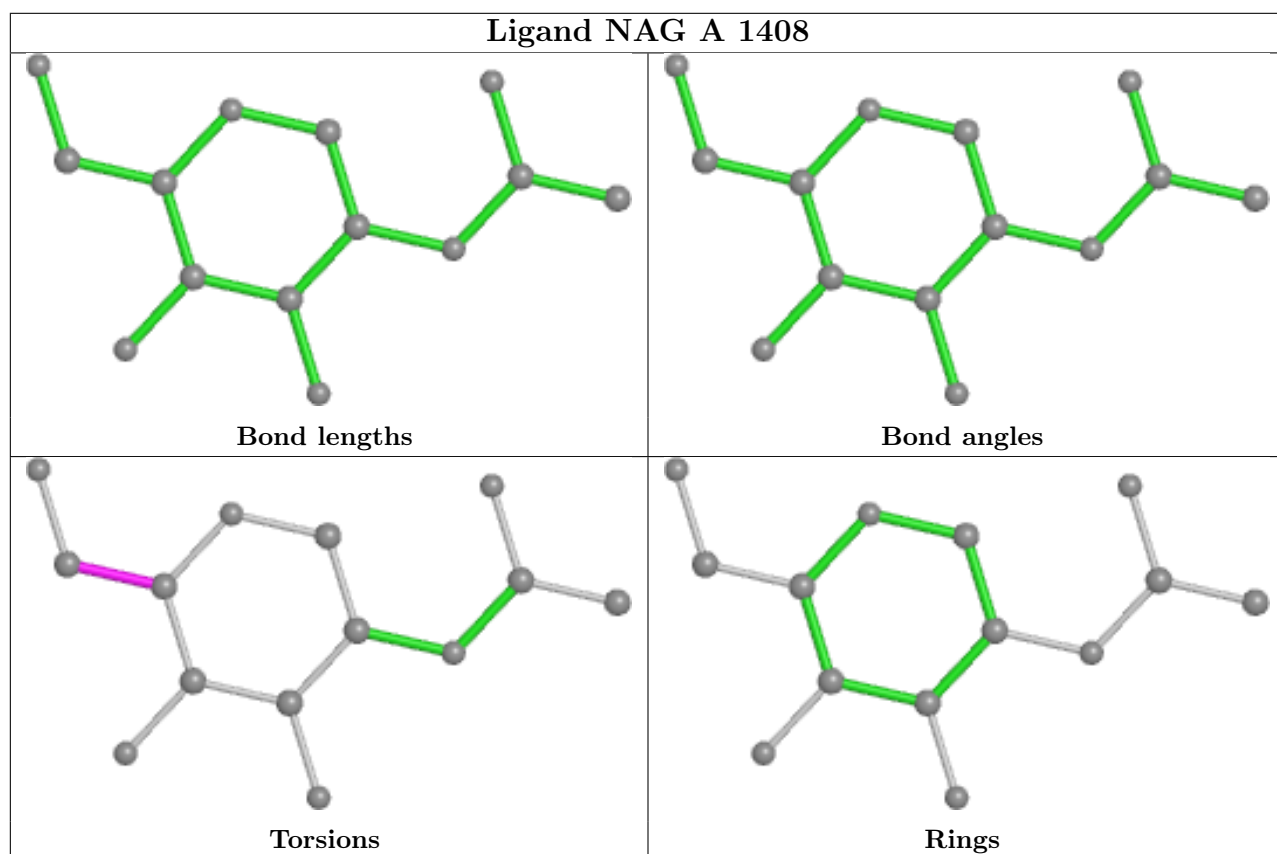
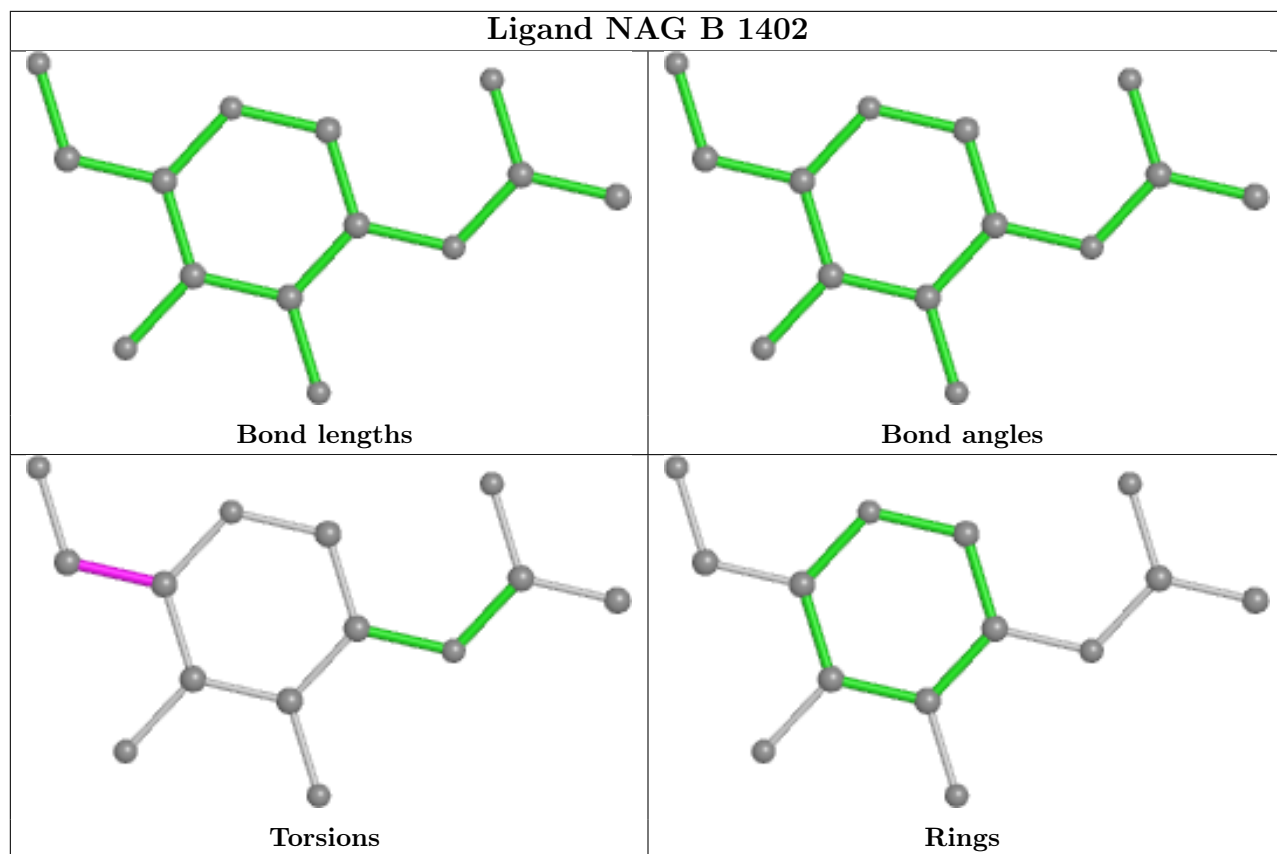


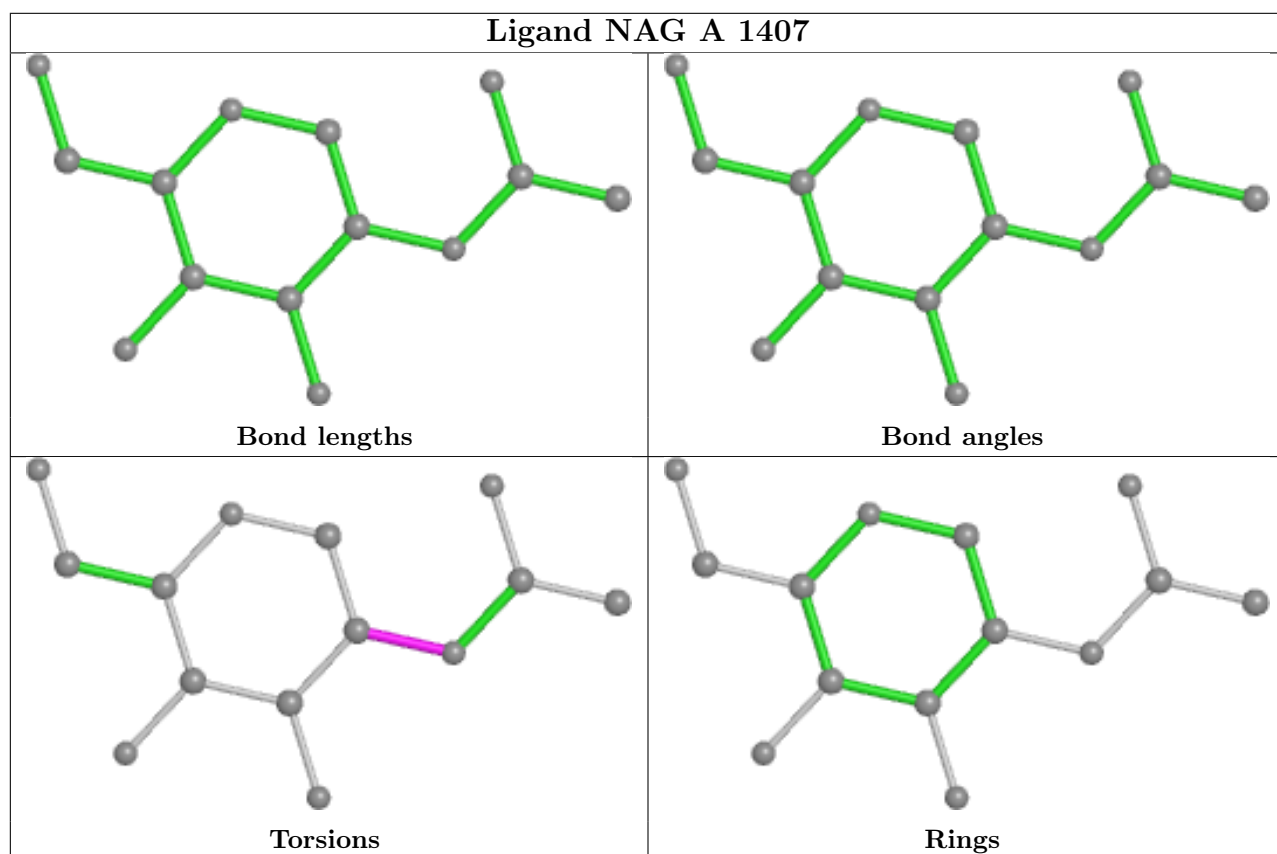
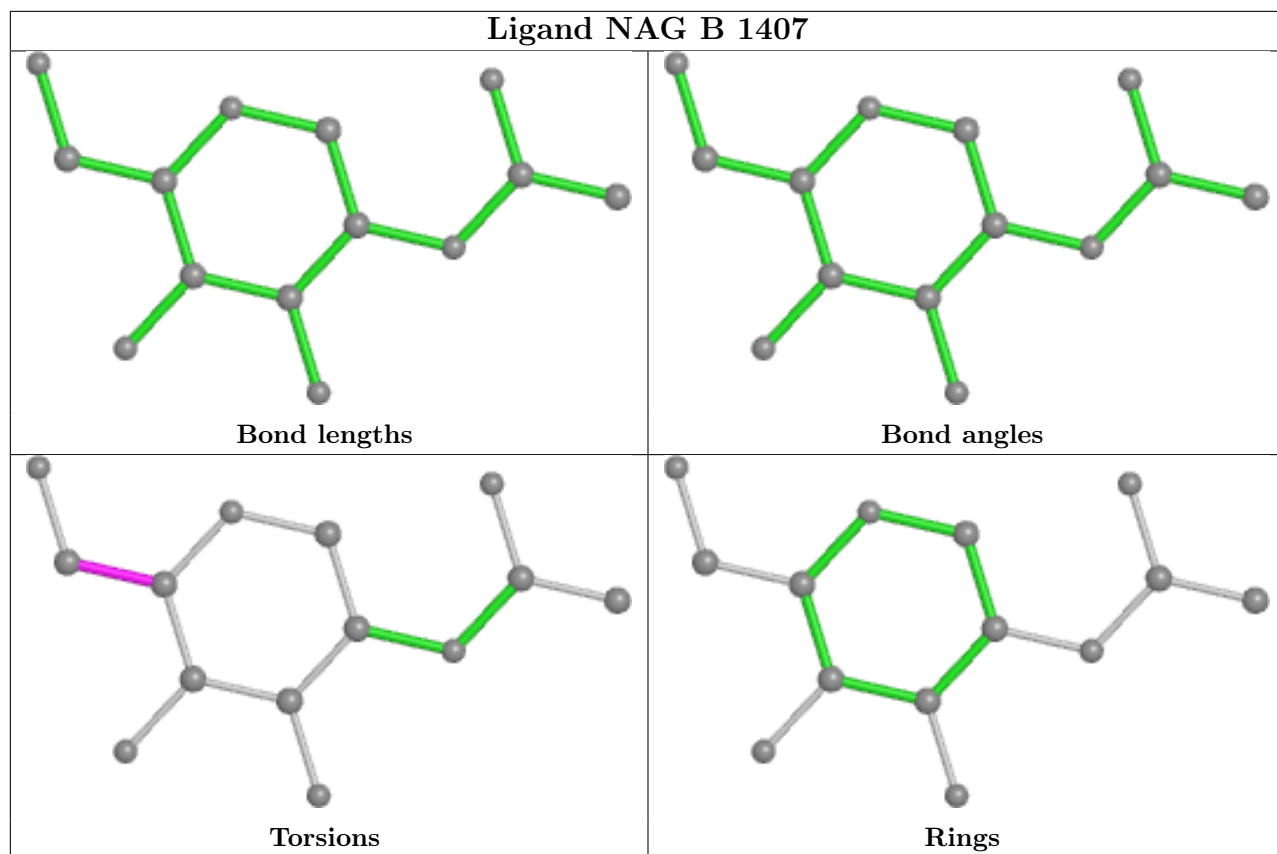




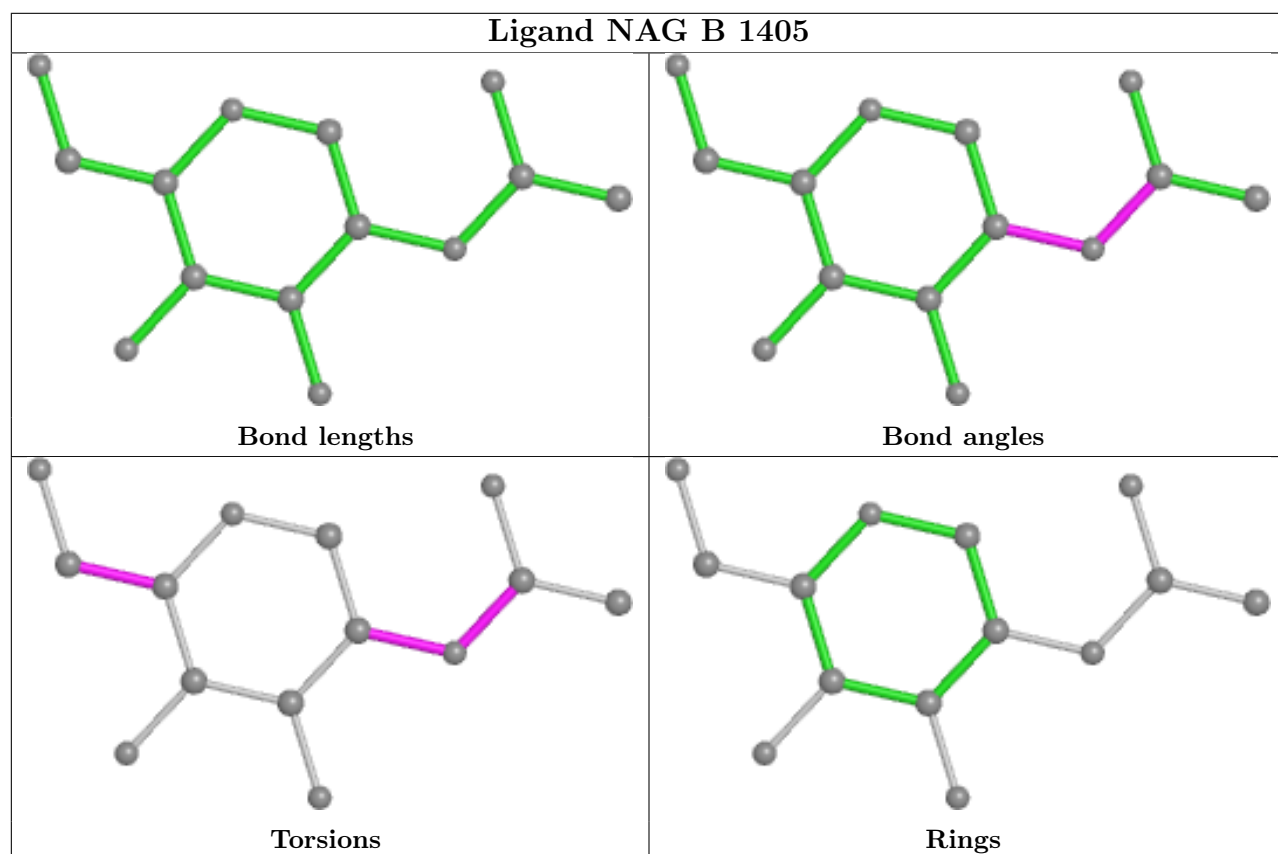
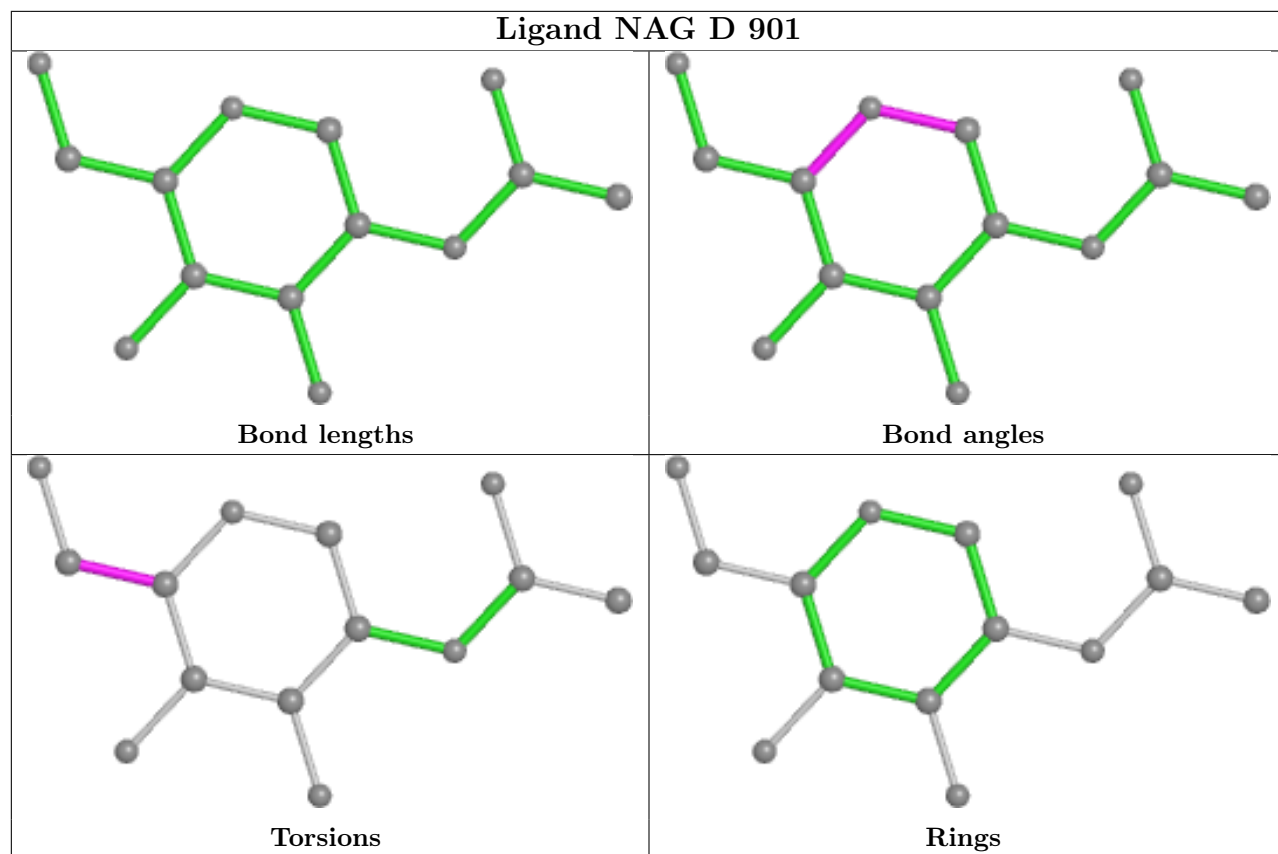


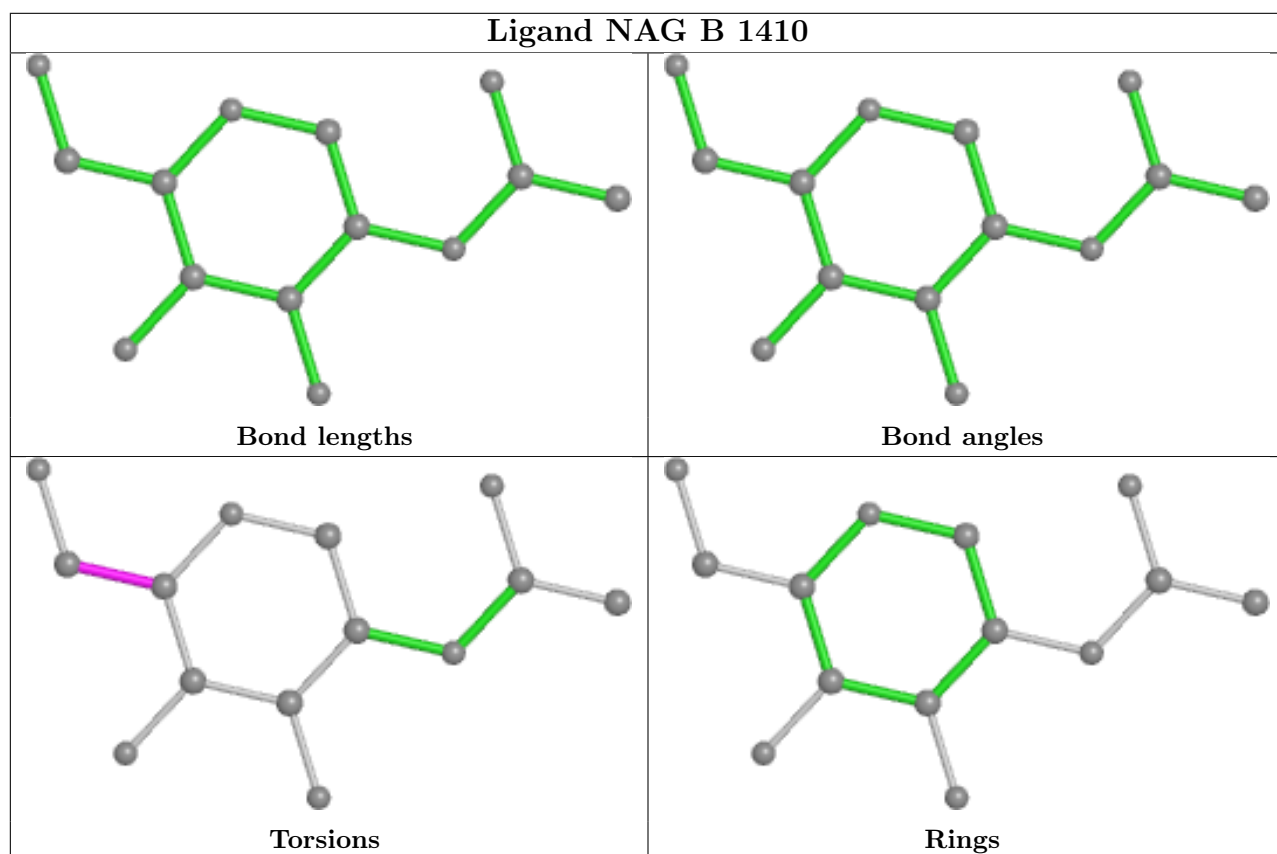
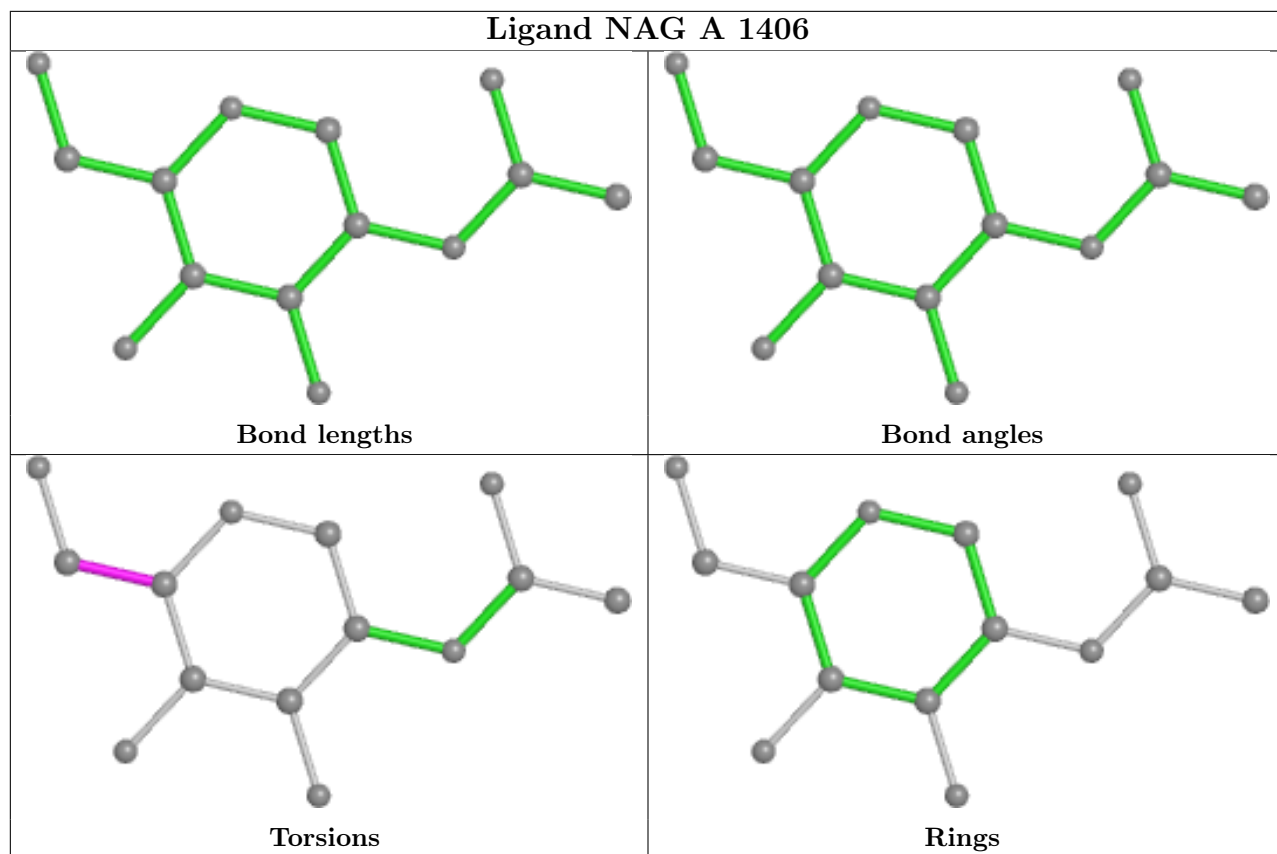


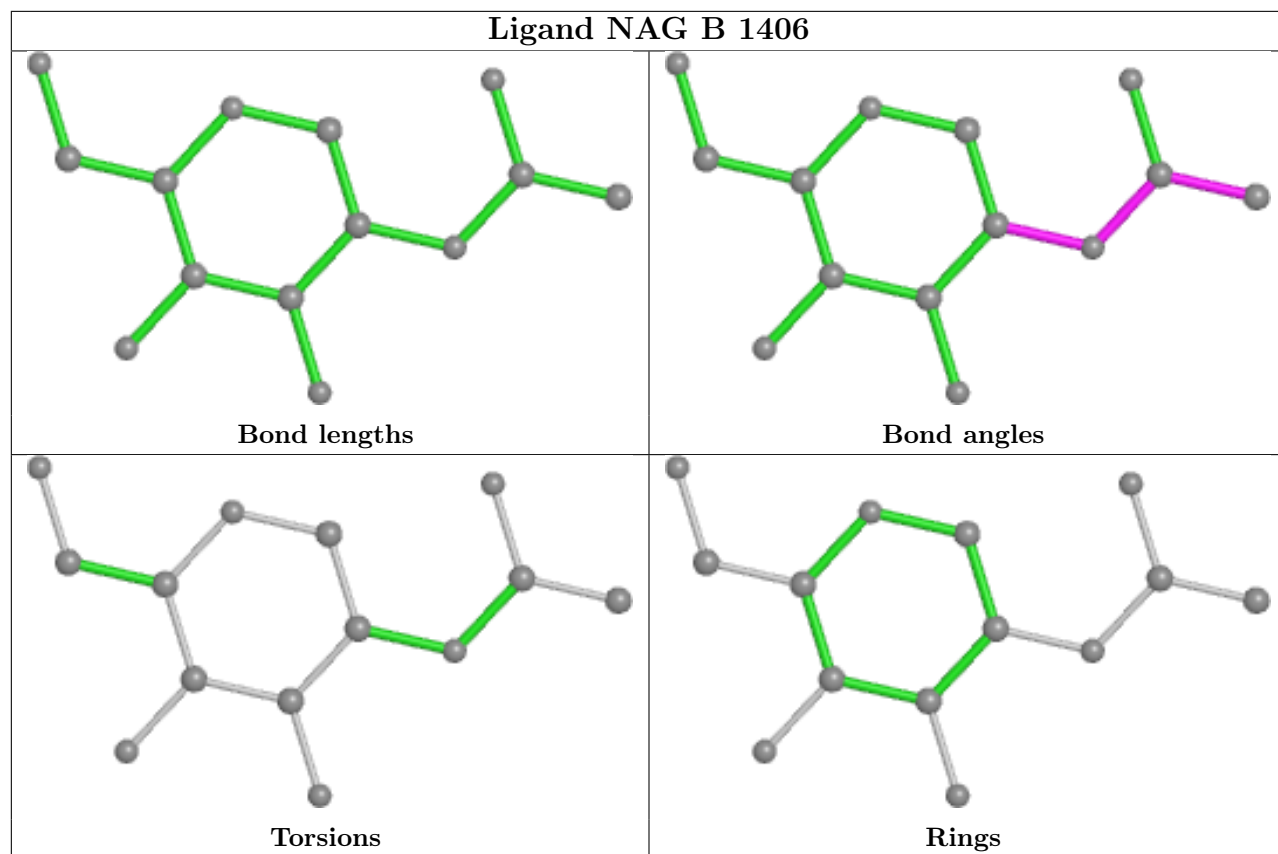












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

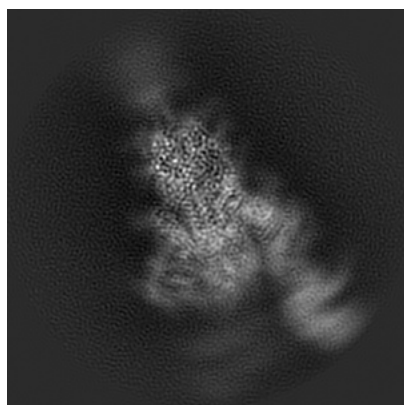
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-30896. These allow visual inspection of the internal detail of the map and identification of artifacts.

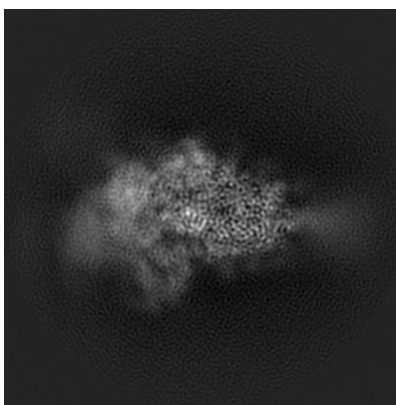
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

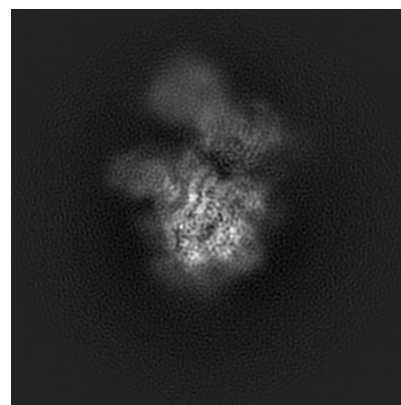
#### 6.1.1 Primary map



X



Y

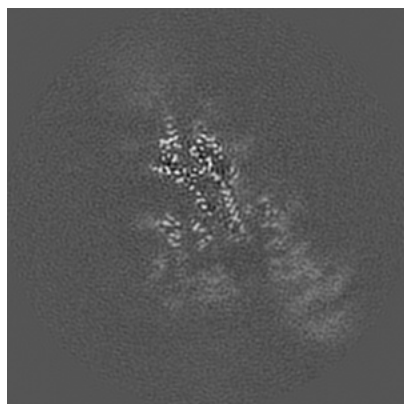


Z

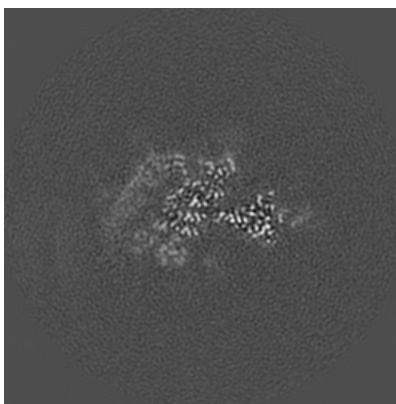
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

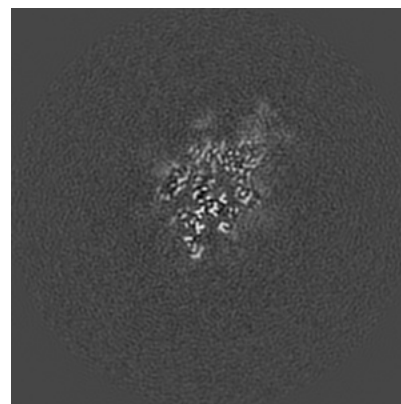
#### 6.2.1 Primary map



X Index: 144



Y Index: 144

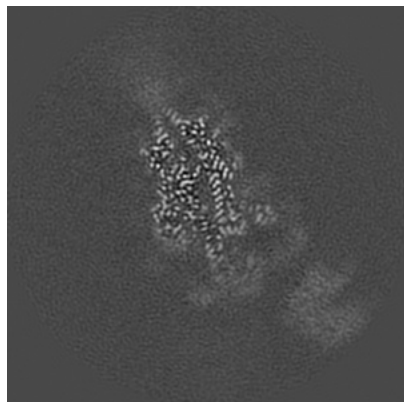


Z Index: 144

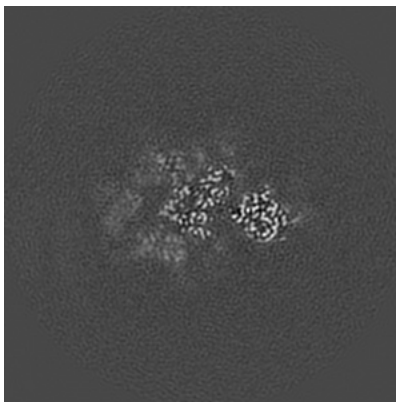
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

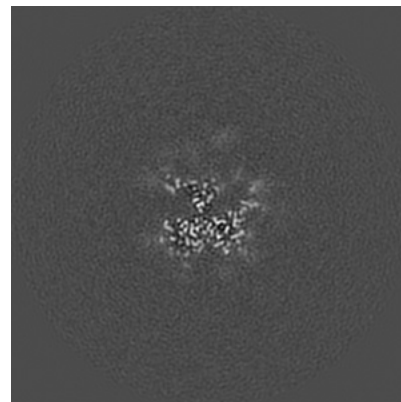
### 6.3.1 Primary map



X Index: 131



Y Index: 141

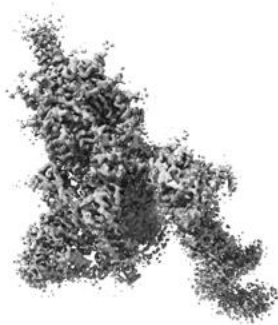


Z Index: 164

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

## 6.4 Orthogonal surface views [i](#)

### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

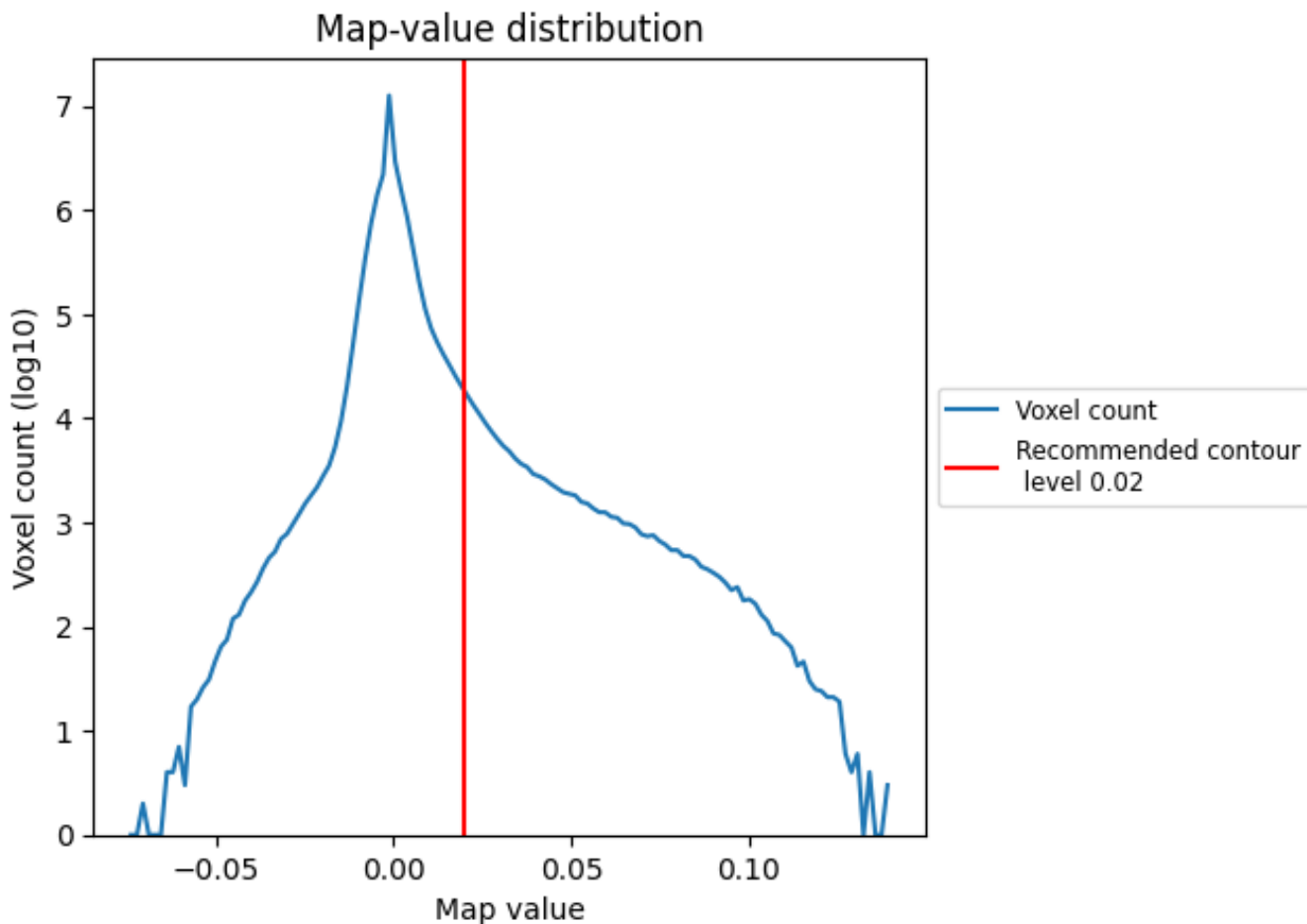
## 6.5 Mask visualisation

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

## 7 Map analysis [i](#)

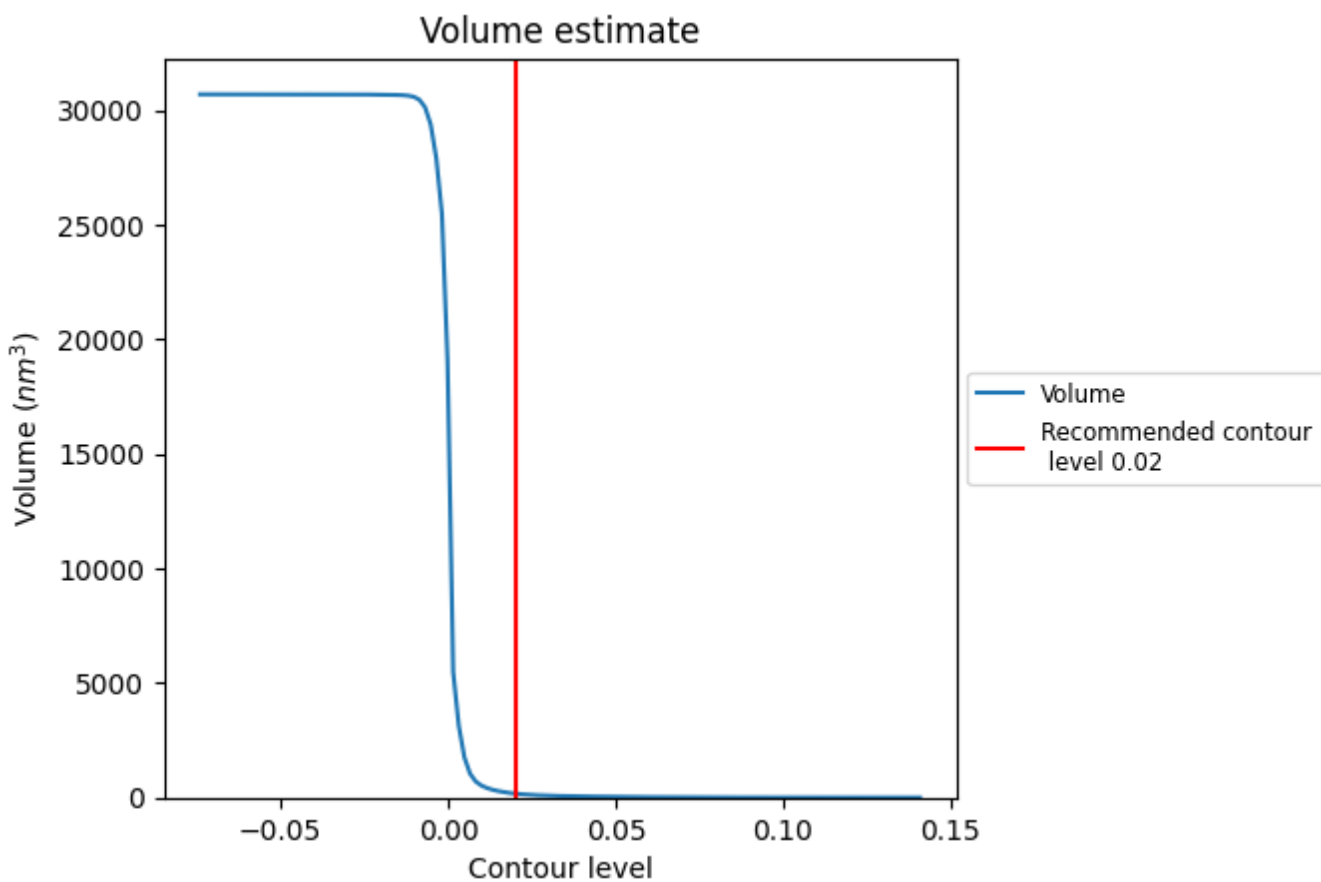
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



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

## 7.2 Volume estimate [i](#)

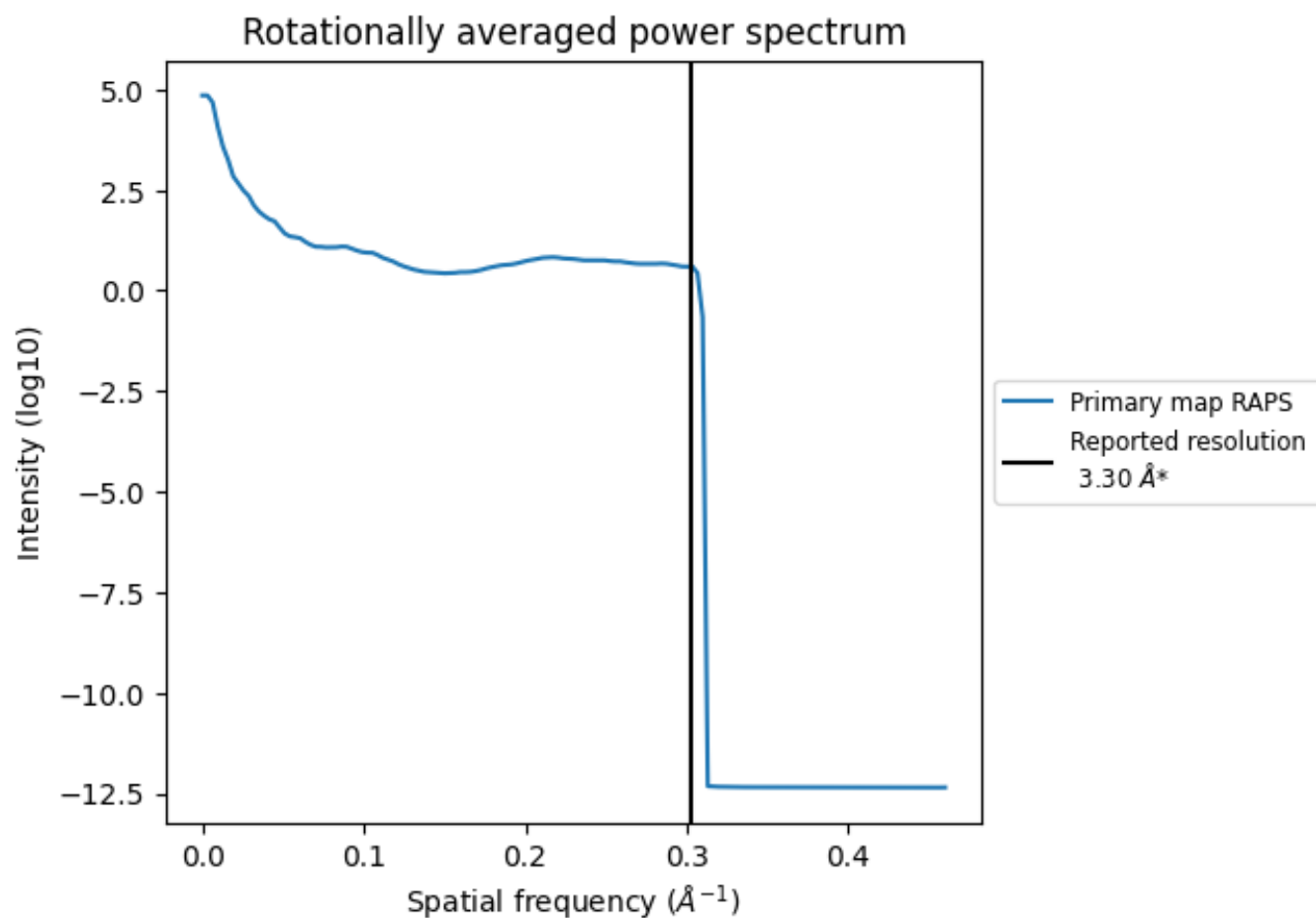


The volume at the recommended contour level is 172 nm<sup>3</sup>; this corresponds to an approximate mass of 156 kDa.

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 [i](#)



\*Reported resolution corresponds to spatial frequency of 0.303 Å<sup>-1</sup>

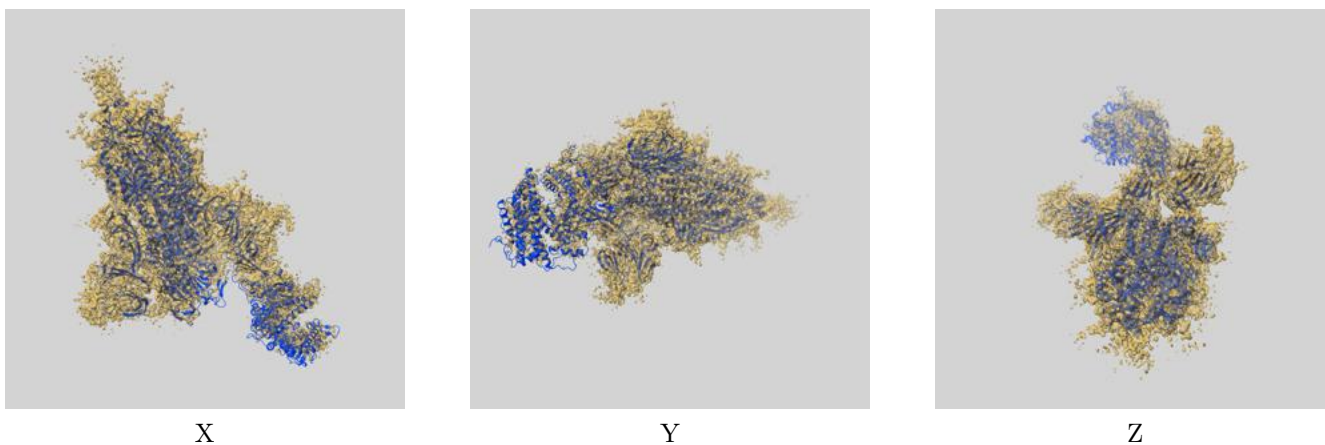
## 8 Fourier-Shell correlation

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

## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-30896 and PDB model 7DX5. Per-residue inclusion information can be found in section 3 on page 11.

### 9.1 Map-model overlay [i](#)



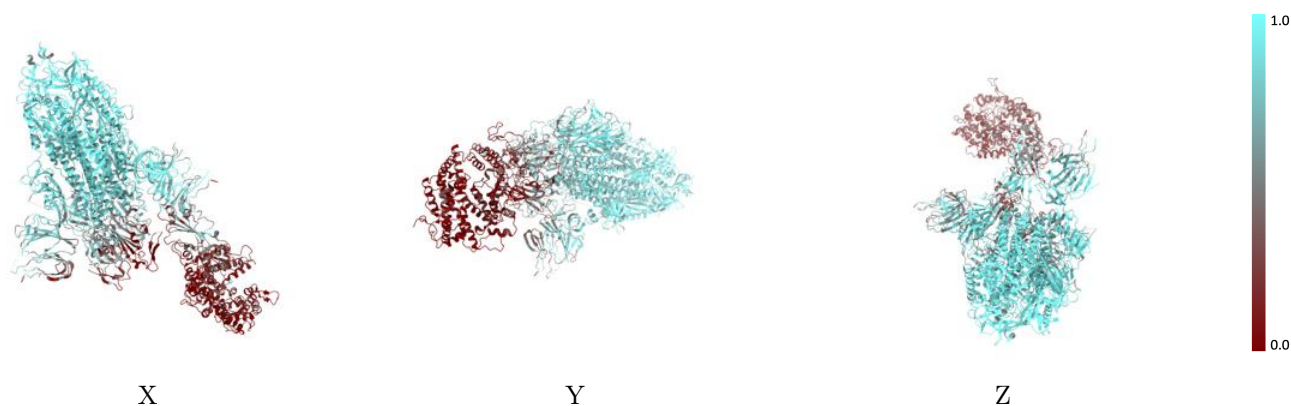
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



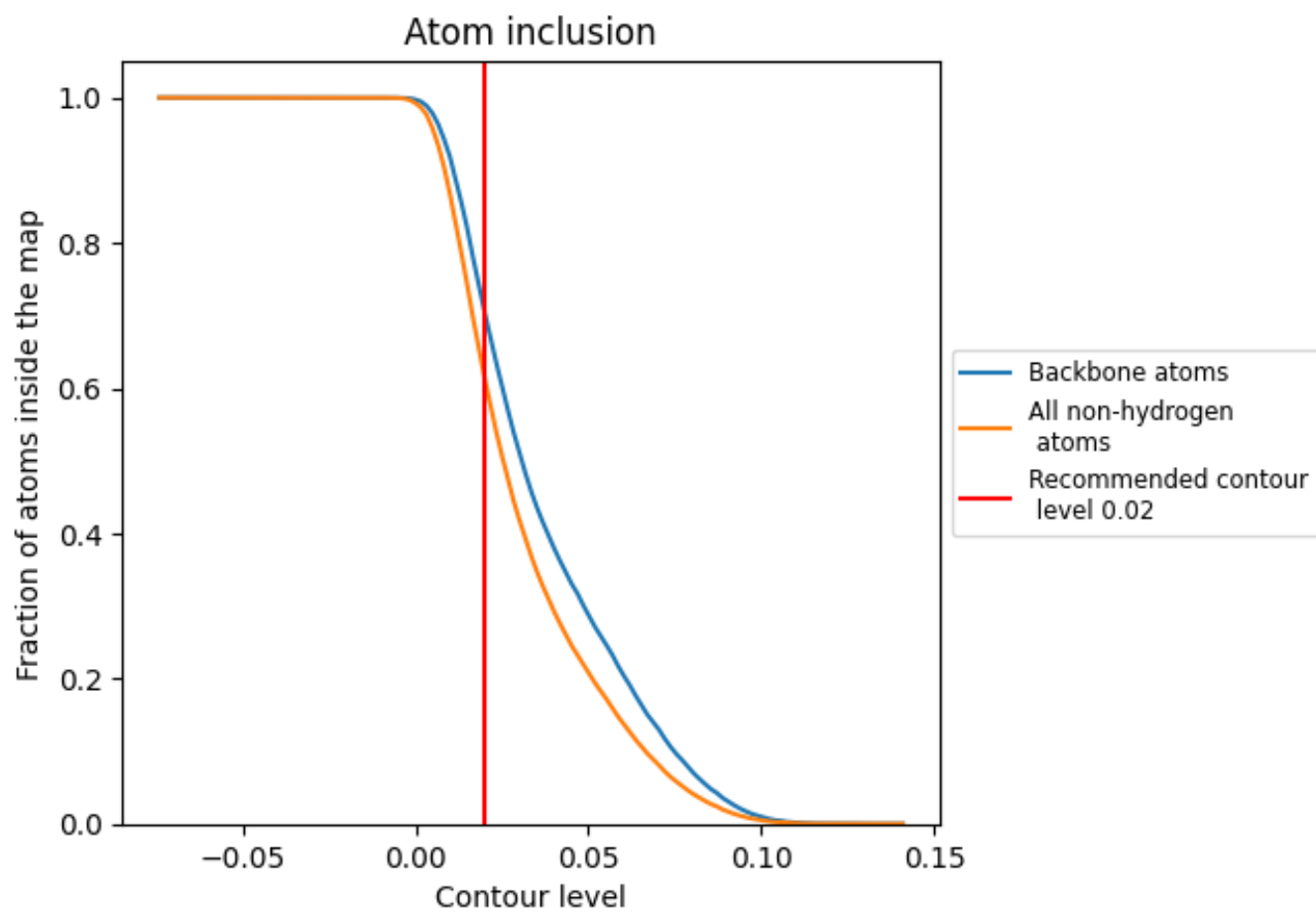
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



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































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 70% of all backbone atoms, 61% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6140	 0.3670
A	 0.7179	 0.4250
B	 0.7700	 0.4660
C	 0.7036	 0.4240
D	 0.0771	 0.0380
E	 0.5357	 0.2990
F	 0.2857	 0.1300
G	 0.7857	 0.5090
H	 0.5714	 0.3660
I	 0.5357	 0.4610
J	 0.8214	 0.5450
K	 0.7857	 0.4120
L	 0.0000	 -0.0530
M	 0.3929	 0.2360
N	 0.7500	 0.4480
O	 0.6071	 0.4310
P	 0.8214	 0.4590
Q	 0.6071	 0.3440
R	 0.0714	 0.1400
S	 0.1429	 -0.0580
T	 0.4286	 0.2840
U	 0.7500	 0.4870
V	 0.7500	 0.3810
W	 0.4643	 0.2670
X	 0.7500	 0.4510
Y	 0.6429	 0.3290
Z	 0.1429	 0.0050
a	 0.0000	 0.1120
b	 0.0000	 0.0070
c	 0.0000	 -0.0980
d	 0.0000	 0.1070

