



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 23, 2024 – 02:05 AM EDT

PDB ID : 6SJJ  
Title : A new modulated crystal structure of ANS complex of St John's wort Hyp-1 protein with 36 protein molecules in the asymmetric unit of the supercell  
Authors : Smietanska, J.; Sliwiak, J.; Gilski, M.; Dauter, Z.; Strzalka, R.; Wolny, J.; Jaskolski, M.  
Deposited on : 2019-08-13  
Resolution : 2.30 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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/XrayValidationReportHelp>

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:

MolProbity : 4.02b-467  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 1.20.1  
EDS : 2.37.1  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.37.1

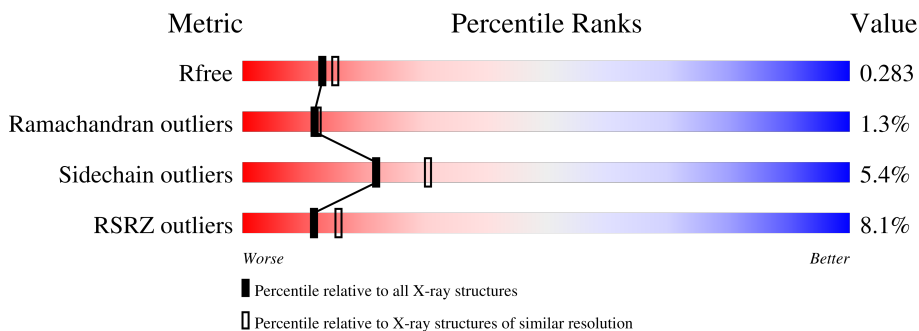
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	5042 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower 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 electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	163	18% (poor fit), 94% (0-1 outliers), 5% (2-3 outliers), 3% (not modelled)
1	B	163	6% (poor fit), 96% (0-1 outliers), 2% (2-3 outliers), 2% (not modelled)
1	C	163	9% (poor fit), 96% (0-1 outliers), 2% (2-3 outliers), 3% (not modelled)
1	D	163	13% (poor fit), 90% (0-1 outliers), 8% (2-3 outliers), 2% (not modelled)
1	E	163	5% (poor fit), 90% (0-1 outliers), 9% (2-3 outliers), 2% (not modelled)
1	F	163	18% (poor fit), 90% (0-1 outliers), 8% (2-3 outliers), 2% (not modelled)

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Mol	Chain	Length	Quality of chain
1	G	163	9% 94% 6% .
1	H	163	10% 93% 5% .
1	I	163	3% 93% 6% .
1	J	163	7% 94% 6% .
1	K	163	2% 93% 7% .
1	L	163	5% 91% 7% .
1	M	163	4% 96% . .
1	N	163	6% 99% . .
1	O	163	15% 93% 6% .
1	P	163	5% 94% . .
1	Q	163	4% 97% . .
1	R	163	9% 97% . .
1	S	163	5% 91% 7% .
1	T	163	4% 93% 6% .
1	U	163	18% 91% 5% . .
1	V	163	6% 94% . .
1	W	163	14% 93% 5% .
1	X	163	10% 93% . .
1	Y	163	10% 90% 7% .
1	Z	163	15% 90% 8% .
1	a	163	9% 92% 6% .
1	b	163	9% 92% 7% .
1	c	163	2% 96% . .
1	d	163	15% 91% 8% .
1	e	163	2% 91% 7% .

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Mol	Chain	Length	Quality of chain
1	f	163	
1	g	163	
1	h	163	
1	i	163	
1	j	163	

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
2	2AN	A	204	-	-	-	X
2	2AN	F	206	-	-	-	X
2	2AN	I	205	-	-	-	X
2	2AN	N	203	-	-	-	X
2	2AN	S	204	-	-	-	X
2	2AN	U	202	-	-	-	X
2	2AN	d	204	-	-	-	X
2	2AN	f	203	-	-	-	X
2	2AN	h	205	-	-	-	X
2	2AN	j	207	-	-	-	X
3	SO4	A	205	-	-	-	X
6	FLC	G	206	-	X	-	-

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 48343 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 PR-10 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	B	159	Total 1244	C 806	N 202	O 232	S 4	0	0	0
1	A	162	Total 1204	C 776	N 195	O 229	S 4	0	0	0
1	R	161	Total 1252	C 807	N 205	O 237	S 3	0	0	0
1	Q	162	Total 1266	C 821	N 204	O 237	S 4	0	0	0
1	P	159	Total 1249	C 808	N 202	O 236	S 3	0	0	0
1	O	161	Total 1215	C 780	N 200	O 231	S 4	0	0	0
1	N	163	Total 1265	C 815	N 204	O 243	S 3	0	0	0
1	M	162	Total 1271	C 822	N 205	O 240	S 4	0	0	0
1	L	160	Total 1256	C 813	N 203	O 236	S 4	0	0	0
1	K	162	Total 1266	C 822	N 204	O 237	S 3	0	0	0
1	J	163	Total 1257	C 809	N 204	O 241	S 3	0	0	0
1	I	161	Total 1253	C 811	N 204	O 234	S 4	0	0	0
1	H	160	Total 1232	C 793	N 201	O 234	S 4	0	0	0
1	G	162	Total 1232	C 799	N 202	O 227	S 4	0	0	0
1	F	159	Total 1188	C 760	N 197	O 227	S 4	0	0	0
1	E	161	Total 1250	C 810	N 203	O 235	S 2	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	D	159	1223	793	199	228	3	0	0	0
1	C	161	1235	801	203	228	3	0	0	0
1	f	161	1262	818	201	239	4	0	0	0
1	e	161	1253	810	203	236	4	0	0	0
1	d	162	1254	812	206	233	3	0	0	0
1	c	159	1248	808	202	234	4	0	0	0
1	b	161	1244	808	197	235	4	0	0	0
1	a	159	1224	790	198	232	4	0	0	0
1	Z	159	1218	782	199	233	4	0	0	0
1	Y	159	1227	791	201	231	4	0	0	0
1	X	159	1226	792	200	231	3	0	0	0
1	W	159	1220	789	201	226	4	0	0	0
1	V	159	1246	806	198	238	4	0	0	0
1	U	159	1218	787	199	228	4	0	0	0
1	T	161	1261	817	201	240	3	0	0	0
1	S	160	1253	813	204	232	4	0	0	0
1	j	159	1243	805	199	236	3	0	0	0
1	i	161	1250	808	204	234	4	0	0	0
1	h	162	1264	817	205	238	4	0	0	0
1	g	160	1257	815	203	235	4	0	0	0

There are 144 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-3	ASP	-	expression tag	UNP A0A160HRF0
B	-2	PRO	-	expression tag	UNP A0A160HRF0
B	-1	PHE	-	expression tag	UNP A0A160HRF0
B	0	THR	-	expression tag	UNP A0A160HRF0
A	-3	ASP	-	expression tag	UNP A0A160HRF0
A	-2	PRO	-	expression tag	UNP A0A160HRF0
A	-1	PHE	-	expression tag	UNP A0A160HRF0
A	0	THR	-	expression tag	UNP A0A160HRF0
R	-3	ASP	-	expression tag	UNP A0A160HRF0
R	-2	PRO	-	expression tag	UNP A0A160HRF0
R	-1	PHE	-	expression tag	UNP A0A160HRF0
R	0	THR	-	expression tag	UNP A0A160HRF0
Q	-3	ASP	-	expression tag	UNP A0A160HRF0
Q	-2	PRO	-	expression tag	UNP A0A160HRF0
Q	-1	PHE	-	expression tag	UNP A0A160HRF0
Q	0	THR	-	expression tag	UNP A0A160HRF0
P	-3	ASP	-	expression tag	UNP A0A160HRF0
P	-2	PRO	-	expression tag	UNP A0A160HRF0
P	-1	PHE	-	expression tag	UNP A0A160HRF0
P	0	THR	-	expression tag	UNP A0A160HRF0
O	-3	ASP	-	expression tag	UNP A0A160HRF0
O	-2	PRO	-	expression tag	UNP A0A160HRF0
O	-1	PHE	-	expression tag	UNP A0A160HRF0
O	0	THR	-	expression tag	UNP A0A160HRF0
N	-3	ASP	-	expression tag	UNP A0A160HRF0
N	-2	PRO	-	expression tag	UNP A0A160HRF0
N	-1	PHE	-	expression tag	UNP A0A160HRF0
N	0	THR	-	expression tag	UNP A0A160HRF0
M	-3	ASP	-	expression tag	UNP A0A160HRF0
M	-2	PRO	-	expression tag	UNP A0A160HRF0
M	-1	PHE	-	expression tag	UNP A0A160HRF0
M	0	THR	-	expression tag	UNP A0A160HRF0
L	-3	ASP	-	expression tag	UNP A0A160HRF0
L	-2	PRO	-	expression tag	UNP A0A160HRF0
L	-1	PHE	-	expression tag	UNP A0A160HRF0
L	0	THR	-	expression tag	UNP A0A160HRF0
K	-3	ASP	-	expression tag	UNP A0A160HRF0
K	-2	PRO	-	expression tag	UNP A0A160HRF0
K	-1	PHE	-	expression tag	UNP A0A160HRF0
K	0	THR	-	expression tag	UNP A0A160HRF0
J	-3	ASP	-	expression tag	UNP A0A160HRF0
J	-2	PRO	-	expression tag	UNP A0A160HRF0
J	-1	PHE	-	expression tag	UNP A0A160HRF0

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Chain	Residue	Modelled	Actual	Comment	Reference
J	0	THR	-	expression tag	UNP A0A160HRF0
I	-3	ASP	-	expression tag	UNP A0A160HRF0
I	-2	PRO	-	expression tag	UNP A0A160HRF0
I	-1	PHE	-	expression tag	UNP A0A160HRF0
I	0	THR	-	expression tag	UNP A0A160HRF0
H	-3	ASP	-	expression tag	UNP A0A160HRF0
H	-2	PRO	-	expression tag	UNP A0A160HRF0
H	-1	PHE	-	expression tag	UNP A0A160HRF0
H	0	THR	-	expression tag	UNP A0A160HRF0
G	-3	ASP	-	expression tag	UNP A0A160HRF0
G	-2	PRO	-	expression tag	UNP A0A160HRF0
G	-1	PHE	-	expression tag	UNP A0A160HRF0
G	0	THR	-	expression tag	UNP A0A160HRF0
F	-3	ASP	-	expression tag	UNP A0A160HRF0
F	-2	PRO	-	expression tag	UNP A0A160HRF0
F	-1	PHE	-	expression tag	UNP A0A160HRF0
F	0	THR	-	expression tag	UNP A0A160HRF0
E	-3	ASP	-	expression tag	UNP A0A160HRF0
E	-2	PRO	-	expression tag	UNP A0A160HRF0
E	-1	PHE	-	expression tag	UNP A0A160HRF0
E	0	THR	-	expression tag	UNP A0A160HRF0
D	-3	ASP	-	expression tag	UNP A0A160HRF0
D	-2	PRO	-	expression tag	UNP A0A160HRF0
D	-1	PHE	-	expression tag	UNP A0A160HRF0
D	0	THR	-	expression tag	UNP A0A160HRF0
C	-3	ASP	-	expression tag	UNP A0A160HRF0
C	-2	PRO	-	expression tag	UNP A0A160HRF0
C	-1	PHE	-	expression tag	UNP A0A160HRF0
C	0	THR	-	expression tag	UNP A0A160HRF0
f	-3	ASP	-	expression tag	UNP A0A160HRF0
f	-2	PRO	-	expression tag	UNP A0A160HRF0
f	-1	PHE	-	expression tag	UNP A0A160HRF0
f	0	THR	-	expression tag	UNP A0A160HRF0
e	-3	ASP	-	expression tag	UNP A0A160HRF0
e	-2	PRO	-	expression tag	UNP A0A160HRF0
e	-1	PHE	-	expression tag	UNP A0A160HRF0
e	0	THR	-	expression tag	UNP A0A160HRF0
d	-3	ASP	-	expression tag	UNP A0A160HRF0
d	-2	PRO	-	expression tag	UNP A0A160HRF0
d	-1	PHE	-	expression tag	UNP A0A160HRF0
d	0	THR	-	expression tag	UNP A0A160HRF0
c	-3	ASP	-	expression tag	UNP A0A160HRF0

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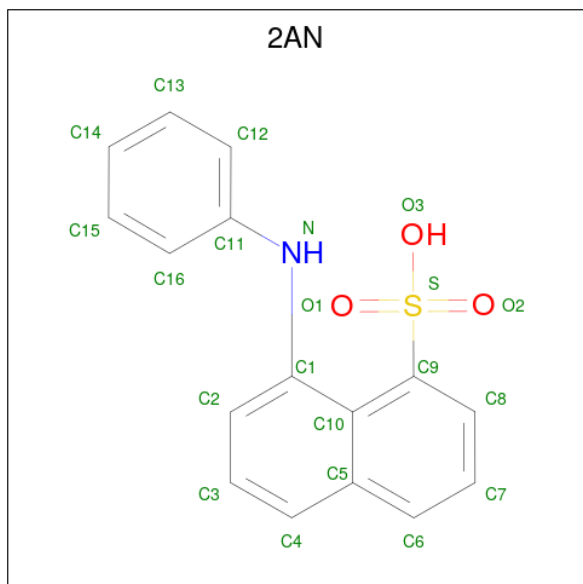
Chain	Residue	Modelled	Actual	Comment	Reference
c	-2	PRO	-	expression tag	UNP A0A160HRF0
c	-1	PHE	-	expression tag	UNP A0A160HRF0
c	0	THR	-	expression tag	UNP A0A160HRF0
b	-3	ASP	-	expression tag	UNP A0A160HRF0
b	-2	PRO	-	expression tag	UNP A0A160HRF0
b	-1	PHE	-	expression tag	UNP A0A160HRF0
b	0	THR	-	expression tag	UNP A0A160HRF0
a	-3	ASP	-	expression tag	UNP A0A160HRF0
a	-2	PRO	-	expression tag	UNP A0A160HRF0
a	-1	PHE	-	expression tag	UNP A0A160HRF0
a	0	THR	-	expression tag	UNP A0A160HRF0
Z	-3	ASP	-	expression tag	UNP A0A160HRF0
Z	-2	PRO	-	expression tag	UNP A0A160HRF0
Z	-1	PHE	-	expression tag	UNP A0A160HRF0
Z	0	THR	-	expression tag	UNP A0A160HRF0
Y	-3	ASP	-	expression tag	UNP A0A160HRF0
Y	-2	PRO	-	expression tag	UNP A0A160HRF0
Y	-1	PHE	-	expression tag	UNP A0A160HRF0
Y	0	THR	-	expression tag	UNP A0A160HRF0
X	-3	ASP	-	expression tag	UNP A0A160HRF0
X	-2	PRO	-	expression tag	UNP A0A160HRF0
X	-1	PHE	-	expression tag	UNP A0A160HRF0
X	0	THR	-	expression tag	UNP A0A160HRF0
W	-3	ASP	-	expression tag	UNP A0A160HRF0
W	-2	PRO	-	expression tag	UNP A0A160HRF0
W	-1	PHE	-	expression tag	UNP A0A160HRF0
W	0	THR	-	expression tag	UNP A0A160HRF0
V	-3	ASP	-	expression tag	UNP A0A160HRF0
V	-2	PRO	-	expression tag	UNP A0A160HRF0
V	-1	PHE	-	expression tag	UNP A0A160HRF0
V	0	THR	-	expression tag	UNP A0A160HRF0
U	-3	ASP	-	expression tag	UNP A0A160HRF0
U	-2	PRO	-	expression tag	UNP A0A160HRF0
U	-1	PHE	-	expression tag	UNP A0A160HRF0
U	0	THR	-	expression tag	UNP A0A160HRF0
T	-3	ASP	-	expression tag	UNP A0A160HRF0
T	-2	PRO	-	expression tag	UNP A0A160HRF0
T	-1	PHE	-	expression tag	UNP A0A160HRF0
T	0	THR	-	expression tag	UNP A0A160HRF0
S	-3	ASP	-	expression tag	UNP A0A160HRF0
S	-2	PRO	-	expression tag	UNP A0A160HRF0
S	-1	PHE	-	expression tag	UNP A0A160HRF0

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Chain	Residue	Modelled	Actual	Comment	Reference
S	0	THR	-	expression tag	UNP A0A160HRF0
j	-3	ASP	-	expression tag	UNP A0A160HRF0
j	-2	PRO	-	expression tag	UNP A0A160HRF0
j	-1	PHE	-	expression tag	UNP A0A160HRF0
j	0	THR	-	expression tag	UNP A0A160HRF0
i	-3	ASP	-	expression tag	UNP A0A160HRF0
i	-2	PRO	-	expression tag	UNP A0A160HRF0
i	-1	PHE	-	expression tag	UNP A0A160HRF0
i	0	THR	-	expression tag	UNP A0A160HRF0
h	-3	ASP	-	expression tag	UNP A0A160HRF0
h	-2	PRO	-	expression tag	UNP A0A160HRF0
h	-1	PHE	-	expression tag	UNP A0A160HRF0
h	0	THR	-	expression tag	UNP A0A160HRF0
g	-3	ASP	-	expression tag	UNP A0A160HRF0
g	-2	PRO	-	expression tag	UNP A0A160HRF0
g	-1	PHE	-	expression tag	UNP A0A160HRF0
g	0	THR	-	expression tag	UNP A0A160HRF0

- Molecule 2 is 8-ANILINO-1-NAPHTHALENE SULFONATE (three-letter code: 2AN) (formula: C<sub>16</sub>H<sub>13</sub>NO<sub>3</sub>S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
2	B	1	21	16	1	3	1	0	0
2	B	1	Total	C	N	O	S	0	0
			21	16	1	3	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	B	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	B	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	B	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	A	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	A	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	A	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	A	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	R	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	R	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	R	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	R	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	R	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	R	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	Q	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	Q	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	Q	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	P	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	P	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	P	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	P	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	O	1	Total	C	N	O	S	0	0
			21	16	1	3	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	O	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	O	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	N	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	N	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	N	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	N	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	M	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	M	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	M	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	L	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	L	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	L	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	L	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	K	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	K	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	K	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	J	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	J	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	J	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	I	1	Total	C	N	O	S	0	0
			21	16	1	3	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	I	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	I	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	I	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	I	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	I	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	H	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	H	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	H	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	H	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	G	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	G	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	G	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	G	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	G	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	F	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	F	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	F	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	F	1	Total	C	N	O	S	0	0
			21	16	1	3	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	F	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	E	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	E	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	E	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	E	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	D	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	D	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	D	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	D	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	C	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	C	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	C	1	Total	C	N	O	S	0	1
			21	16	1	3	1		
2	f	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	f	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	f	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	f	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	f	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	f	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	e	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	d	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	d	1	Total	C	N	O	S	0	0
			21	16	1	3	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	d	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	d	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	c	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	c	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	c	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	c	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	c	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	c	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	b	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	b	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	b	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	b	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	b	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	b	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	a	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	a	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	a	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	a	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	Z	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	Z	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	Z	1	Total	C	N	O	S	0	0
			21	16	1	3	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	Z	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	Z	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	Z	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	Y	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	Y	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	Y	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	Y	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	X	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	X	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	X	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	X	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	X	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	X	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	W	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	V	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	V	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	V	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	V	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	V	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	V	1	Total	C	N	O	S	0	0
			21	16	1	3	1		

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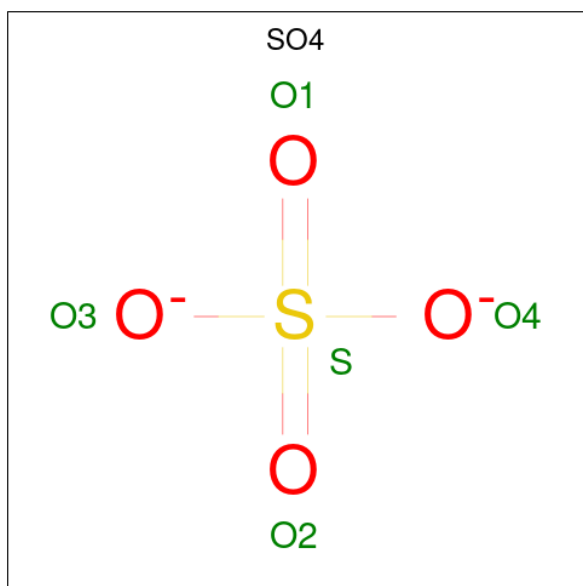
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	V	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	U	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	U	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	T	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	T	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	T	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	T	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	S	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	S	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	S	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	S	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	j	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	j	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	j	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	j	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	j	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	j	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	i	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	h	1	Total	C	N	O	S	0	0
			21	16	1	3	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	h	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	h	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	h	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	h	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	g	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	g	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	g	1	Total	C	N	O	S	0	0
			21	16	1	3	1		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	Q	1	Total	O	S	0	0
			5	4	1		
3	I	1	Total	O	S	0	0
			5	4	1		

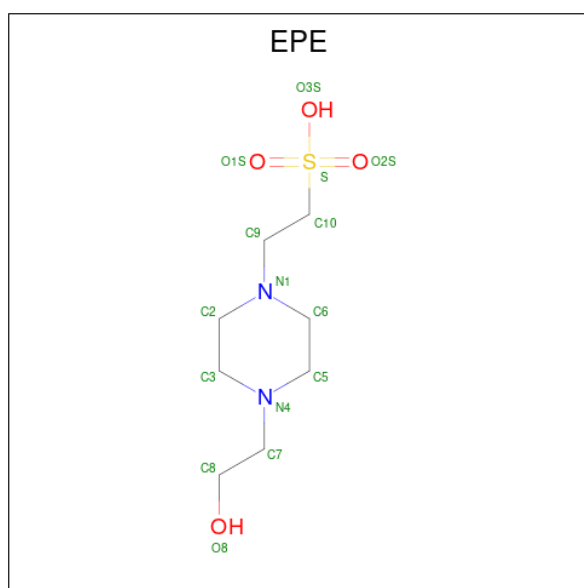
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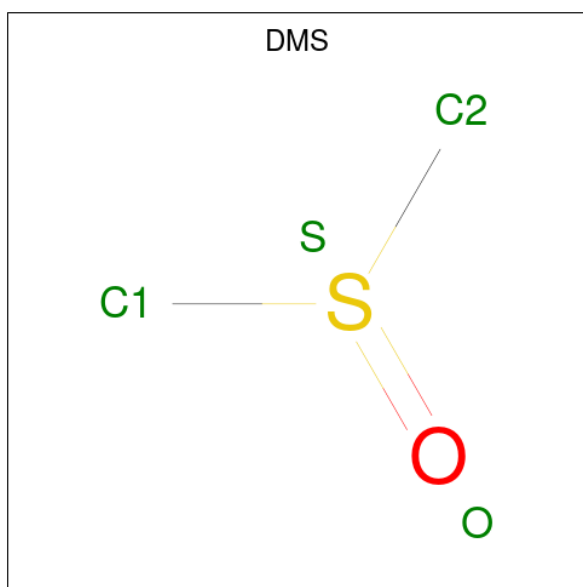
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	G	1	Total	O	S	0	0	
			5	4	1			
3	E	1	Total	O	S	0	0	
			5	4	1			
3	c	1	Total	O	S	0	0	
			5	4	1			
3	c	1	Total	O	S	0	0	
			5	4	1			
3	c	1	Total	O	S	0	0	
			5	4	1			
3	Y	1	Total	O	S	0	0	
			5	4	1			
3	g	1	Total	O	S	0	0	
			5	4	1			

- Molecule 4 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: C<sub>8</sub>H<sub>18</sub>N<sub>2</sub>O<sub>4</sub>S).



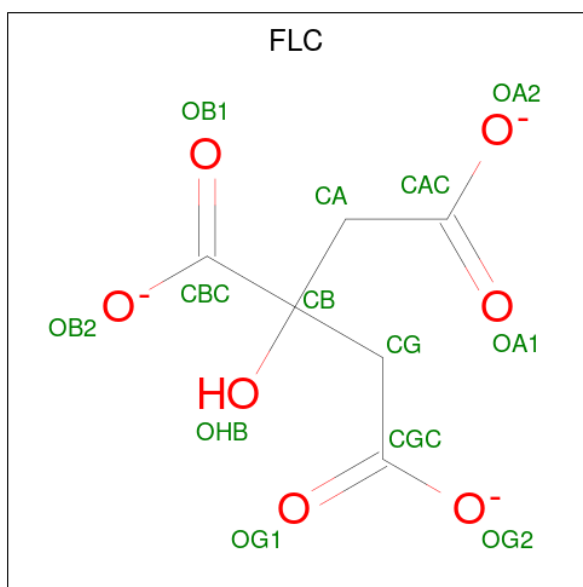
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	P	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

- Molecule 5 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C<sub>2</sub>H<sub>6</sub>OS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	N	1	Total	C	O	S	0	0
			4	2	1	1		
5	G	1	Total	C	O	S	0	0
			4	2	1	1		
5	X	1	Total	C	O	S	0	0
			4	2	1	1		

- Molecule 6 is CITRATE ANION (three-letter code: FLC) (formula:  $C_6H_5O_7$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	G	1	Total	C	O	0	0
			13	6	7		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	e	1	Total	C	O	0	0
			13	6	7		
6	a	1	Total	C	O	0	0
			13	6	7		
6	a	1	Total	C	O	0	0
			13	6	7		
6	j	1	Total	C	O	0	0
			13	6	7		
6	i	1	Total	C	O	0	0
			13	6	7		
6	i	1	Total	C	O	0	0
			13	6	7		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	5	Total	O	0	0
			5	5		
7	A	6	Total	O	0	0
			6	6		
7	R	3	Total	O	0	0
			3	3		
7	Q	1	Total	O	0	0
			1	1		
7	P	5	Total	O	0	0
			5	5		
7	O	4	Total	O	0	0
			4	4		
7	N	3	Total	O	0	0
			3	3		
7	M	1	Total	O	0	0
			1	1		
7	L	3	Total	O	0	0
			3	3		
7	K	6	Total	O	0	0
			6	6		
7	J	2	Total	O	0	0
			2	2		
7	I	5	Total	O	0	0
			5	5		
7	H	3	Total	O	0	0
			3	3		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	G	5	Total O 5 5	0	0
7	F	1	Total O 1 1	0	0
7	E	5	Total O 5 5	0	0
7	D	3	Total O 3 3	0	0
7	C	4	Total O 4 4	0	0
7	f	8	Total O 8 8	0	0
7	e	9	Total O 9 9	0	0
7	d	2	Total O 2 2	0	0
7	c	3	Total O 3 3	0	0
7	b	6	Total O 6 6	0	0
7	a	8	Total O 8 8	0	0
7	Z	4	Total O 4 4	0	0
7	Y	4	Total O 4 4	0	0
7	X	3	Total O 3 3	0	0
7	W	2	Total O 2 2	0	0
7	V	9	Total O 9 9	0	0
7	T	5	Total O 5 5	0	0
7	S	1	Total O 1 1	0	0
7	j	5	Total O 5 5	0	0
7	i	6	Total O 6 6	0	0
7	h	8	Total O 8 8	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	g	4	Total	O	0	0
			4	4		

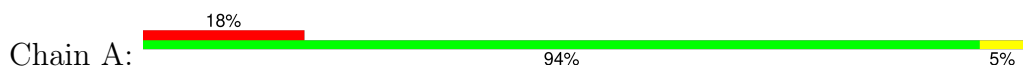
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron 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 dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). 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: PR-10 protein



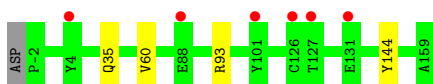
- Molecule 1: PR-10 protein



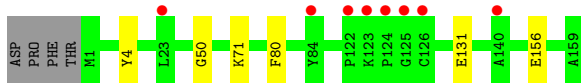
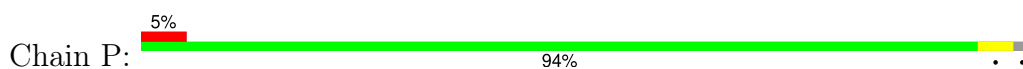
- Molecule 1: PR-10 protein



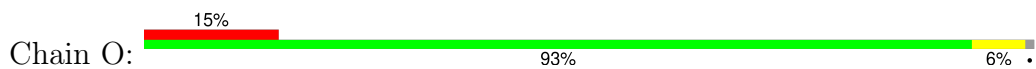
- Molecule 1: PR-10 protein



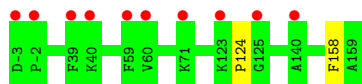
- Molecule 1: PR-10 protein



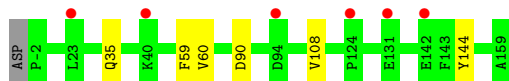
- Molecule 1: PR-10 protein



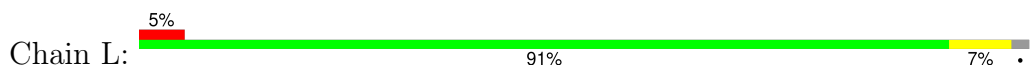
- Molecule 1: PR-10 protein



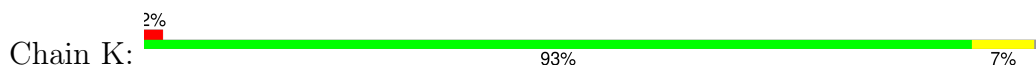
- Molecule 1: PR-10 protein



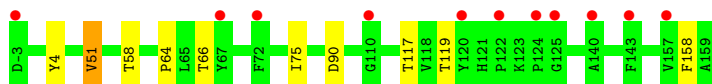
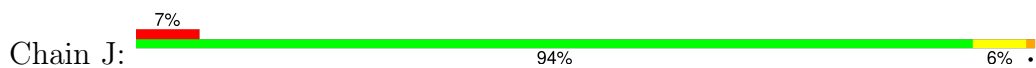
- Molecule 1: PR-10 protein



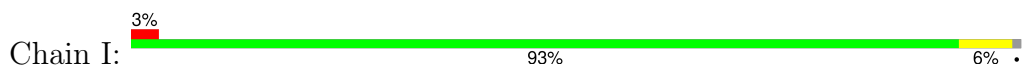
- Molecule 1: PR-10 protein



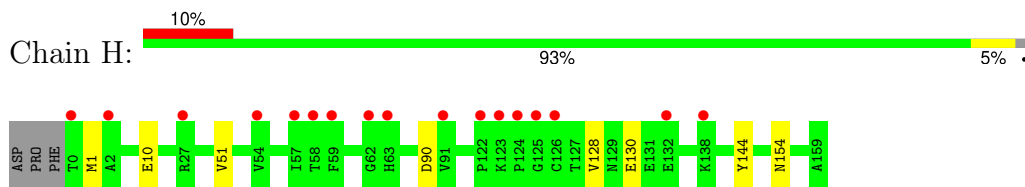
- Molecule 1: PR-10 protein



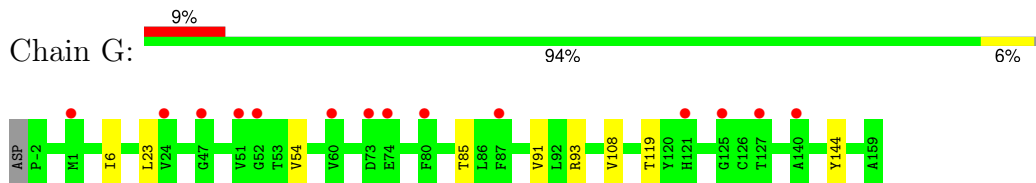
- Molecule 1: PR-10 protein



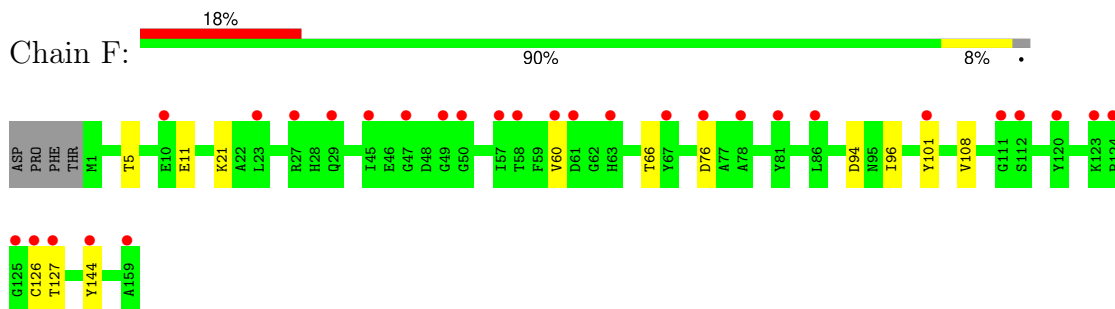
- Molecule 1: PR-10 protein



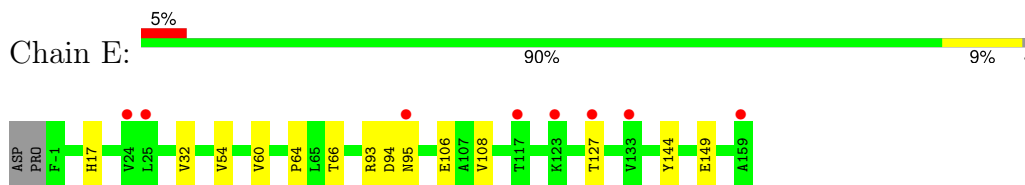
- Molecule 1: PR-10 protein



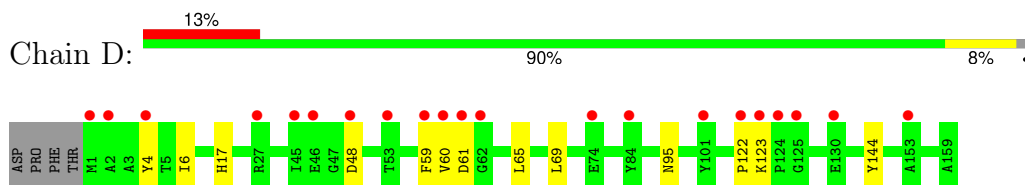
- Molecule 1: PR-10 protein



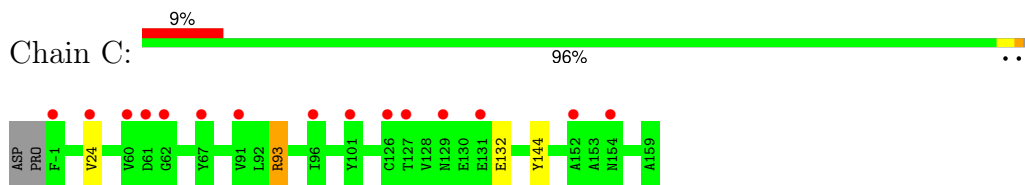
- Molecule 1: PR-10 protein



- Molecule 1: PR-10 protein

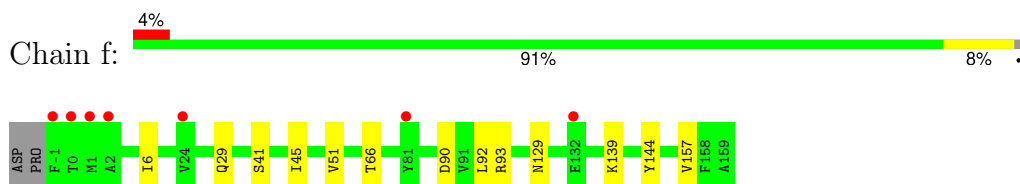


- Molecule 1: PR-10 protein

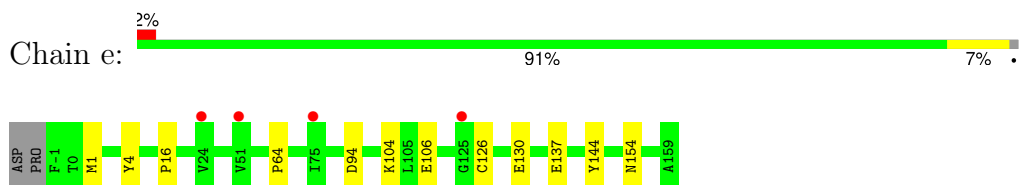


- Molecule 1: PR-10 protein

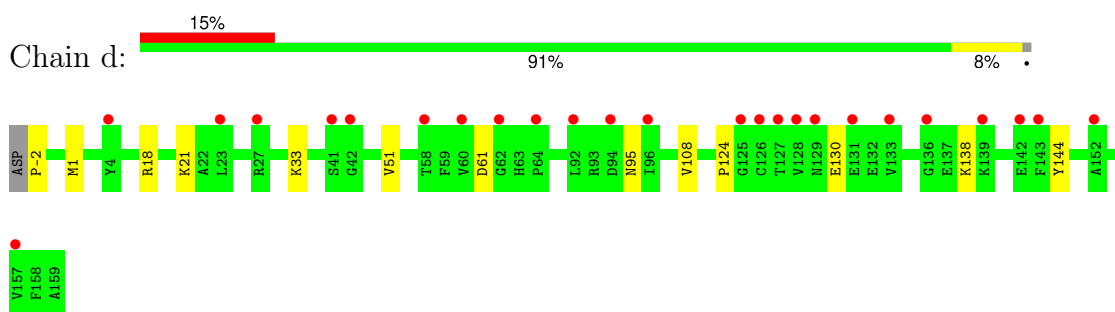




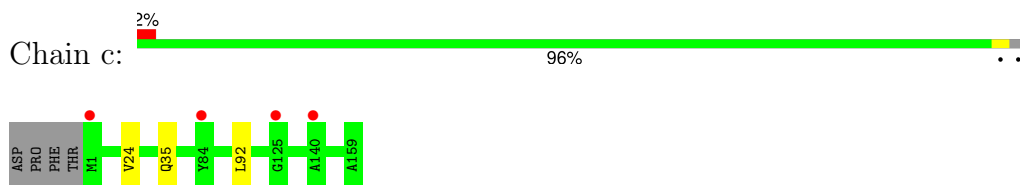
- Molecule 1: PR-10 protein



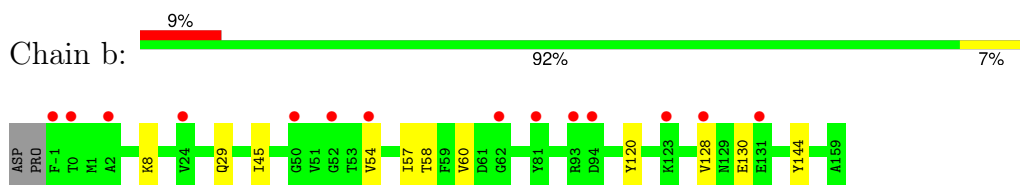
- Molecule 1: PR-10 protein



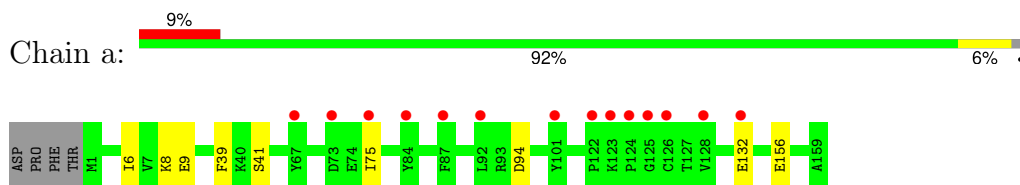
- Molecule 1: PR-10 protein



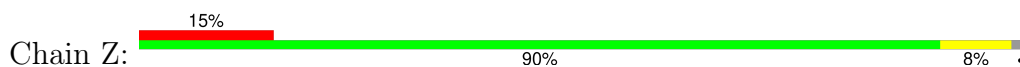
- Molecule 1: PR-10 protein

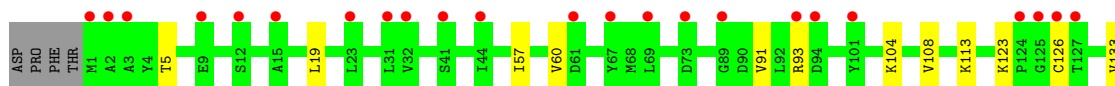


- Molecule 1: PR-10 protein

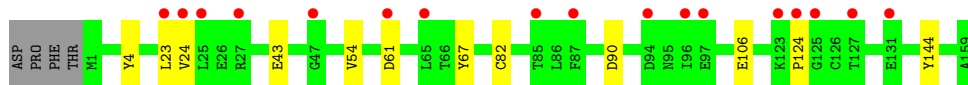


- Molecule 1: PR-10 protein

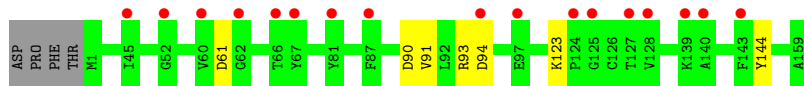




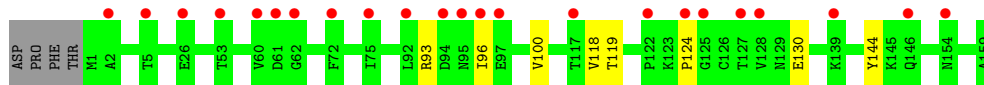
● Molecule 1: PR-10 protein



● Molecule 1: PR-10 protein



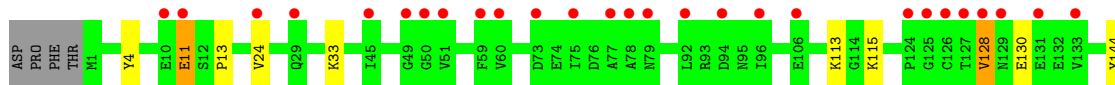
● Molecule 1: PR-10 protein



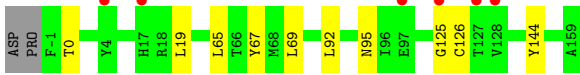
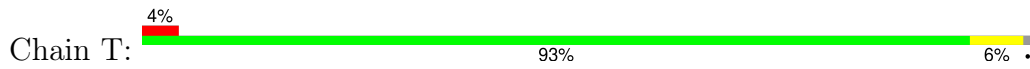
● Molecule 1: PR-10 protein



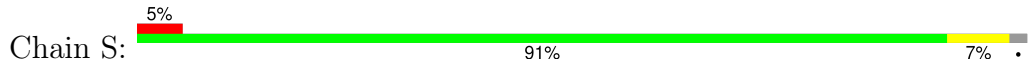
● Molecule 1: PR-10 protein



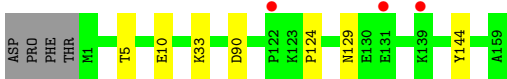
● Molecule 1: PR-10 protein



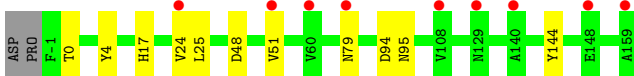
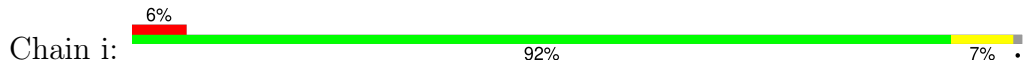
- Molecule 1: PR-10 protein



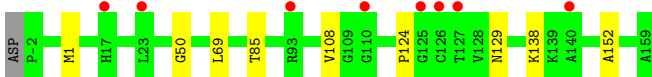
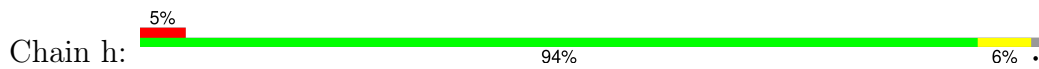
- Molecule 1: PR-10 protein



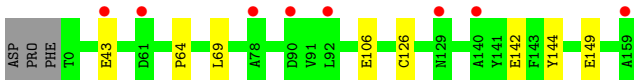
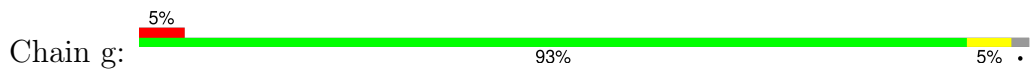
- Molecule 1: PR-10 protein



- Molecule 1: PR-10 protein



- Molecule 1: PR-10 protein



## 4 Data and refinement statistics i

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	145.85Å 145.85Å 385.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	31.58 – 2.30 31.58 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.3 (31.58-2.30) 99.3 (31.58-2.30)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.23 (at 2.29Å)	Xtrriage
Refinement program	REFMAC 5.8.0222	Depositor
R, $R_{free}$	0.226 , 0.255 0.273 , 0.283	Depositor DCC
$R_{free}$ test set	3979 reflections (1.11%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	57.8	Xtrriage
Anisotropy	0.131	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 54.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	0.064 for k,h,-l 0.054 for -k,-h,-l 0.084 for -h,-k,l	Xtrriage
Reported twinning fraction	0.241 for H, K, L 0.242 for K, H, -L 0.233 for -K, -H, -L 0.284 for h,-k,-l	Depositor
Outliers	18 of 357481 reflections (0.005%)	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	48343	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	70.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 74.65 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.4696e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FLC, SO4, 2AN, EPE, DMS

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.52	0/1233	0.82	0/1682
1	B	0.56	0/1273	0.87	0/1722
1	C	0.47	0/1263	0.75	0/1709
1	D	0.52	0/1252	0.84	0/1697
1	E	0.65	0/1279	0.88	0/1731
1	F	0.53	0/1215	0.82	0/1649
1	G	0.56	0/1262	0.79	0/1712
1	H	0.57	0/1261	0.82	0/1709
1	I	0.64	0/1282	0.83	0/1734
1	J	0.52	0/1287	0.88	0/1746
1	K	0.61	0/1297	0.86	0/1755
1	L	0.57	0/1285	0.83	0/1738
1	M	0.60	0/1301	0.83	0/1760
1	N	0.61	0/1295	0.94	0/1757
1	O	0.53	0/1242	0.80	0/1684
1	P	0.67	0/1278	0.94	0/1729
1	Q	0.54	0/1296	0.82	0/1753
1	R	0.61	0/1280	0.86	0/1732
1	S	0.60	0/1282	0.82	0/1733
1	T	0.63	0/1291	0.89	0/1747
1	U	0.51	0/1246	0.82	0/1690
1	V	0.62	0/1275	0.90	0/1726
1	W	0.53	0/1249	0.78	0/1689
1	X	0.56	0/1254	0.86	0/1697
1	Y	0.53	0/1256	0.80	0/1699
1	Z	0.55	0/1246	0.80	0/1687
1	a	0.58	0/1253	0.87	0/1695
1	b	0.52	0/1274	0.80	0/1727
1	c	0.62	0/1277	0.86	0/1725
1	d	0.50	0/1284	0.83	0/1735
1	e	0.61	0/1282	0.89	0/1734
1	f	0.63	0/1292	0.87	0/1748

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	g	0.53	0/1286	0.86	0/1738
1	h	0.59	0/1294	0.89	0/1749
1	i	0.62	0/1279	0.87	0/1730
1	j	0.70	0/1272	0.96	0/1722
All	All	0.58	0/45773	0.85	0/61970

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](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

## 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 X-ray entries followed by that with respect to entries of similar resolution.

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	160/163 (98%)	137 (86%)	20 (12%)	3 (2%)	8	7
1	B	157/163 (96%)	134 (85%)	21 (13%)	2 (1%)	12	12
1	C	159/163 (98%)	141 (89%)	16 (10%)	2 (1%)	12	12
1	D	157/163 (96%)	122 (78%)	30 (19%)	5 (3%)	4	2
1	E	159/163 (98%)	134 (84%)	21 (13%)	4 (2%)	5	4
1	F	157/163 (96%)	142 (90%)	12 (8%)	3 (2%)	8	7
1	G	160/163 (98%)	137 (86%)	22 (14%)	1 (1%)	25	31
1	H	158/163 (97%)	145 (92%)	13 (8%)	0	100	100
1	I	159/163 (98%)	143 (90%)	13 (8%)	3 (2%)	8	7

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	J	161/163 (99%)	138 (86%)	22 (14%)	1 (1%)	25	31
1	K	160/163 (98%)	148 (92%)	10 (6%)	2 (1%)	12	12
1	L	158/163 (97%)	142 (90%)	13 (8%)	3 (2%)	8	7
1	M	160/163 (98%)	145 (91%)	13 (8%)	2 (1%)	12	12
1	N	161/163 (99%)	144 (89%)	16 (10%)	1 (1%)	25	31
1	O	159/163 (98%)	140 (88%)	15 (9%)	4 (2%)	5	4
1	P	157/163 (96%)	137 (87%)	19 (12%)	1 (1%)	25	31
1	Q	160/163 (98%)	148 (92%)	11 (7%)	1 (1%)	25	31
1	R	159/163 (98%)	146 (92%)	13 (8%)	0	100	100
1	S	158/163 (97%)	146 (92%)	11 (7%)	1 (1%)	25	31
1	T	159/163 (98%)	141 (89%)	16 (10%)	2 (1%)	12	12
1	U	157/163 (96%)	136 (87%)	17 (11%)	4 (2%)	5	4
1	V	157/163 (96%)	146 (93%)	9 (6%)	2 (1%)	12	12
1	W	157/163 (96%)	134 (85%)	19 (12%)	4 (2%)	5	4
1	X	157/163 (96%)	139 (88%)	16 (10%)	2 (1%)	12	12
1	Y	157/163 (96%)	143 (91%)	12 (8%)	2 (1%)	12	12
1	Z	157/163 (96%)	134 (85%)	20 (13%)	3 (2%)	8	7
1	a	157/163 (96%)	140 (89%)	16 (10%)	1 (1%)	25	31
1	b	159/163 (98%)	142 (89%)	16 (10%)	1 (1%)	25	31
1	c	157/163 (96%)	145 (92%)	12 (8%)	0	100	100
1	d	160/163 (98%)	139 (87%)	17 (11%)	4 (2%)	5	4
1	e	159/163 (98%)	137 (86%)	20 (13%)	2 (1%)	12	12
1	f	159/163 (98%)	141 (89%)	15 (9%)	3 (2%)	8	7
1	g	158/163 (97%)	140 (89%)	18 (11%)	0	100	100
1	h	160/163 (98%)	144 (90%)	13 (8%)	3 (2%)	8	7
1	i	159/163 (98%)	145 (91%)	12 (8%)	2 (1%)	12	12
1	j	157/163 (96%)	144 (92%)	12 (8%)	1 (1%)	25	31
All	All	5705/5868 (97%)	5059 (89%)	571 (10%)	75 (1%)	12	12

5 of 75 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	76	ASP

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Mol	Chain	Res	Type
1	O	51	VAL
1	F	94	ASP
1	X	123	LYS
1	O	24	VAL

### 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 X-ray entries followed by that with respect to entries of similar resolution.

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	114/138 (83%)	109 (96%)	5 (4%)	28	39
1	B	130/138 (94%)	129 (99%)	1 (1%)	81	91
1	C	124/138 (90%)	121 (98%)	3 (2%)	49	66
1	D	123/138 (89%)	115 (94%)	8 (6%)	17	23
1	E	128/138 (93%)	118 (92%)	10 (8%)	12	16
1	F	114/138 (83%)	104 (91%)	10 (9%)	10	12
1	G	122/138 (88%)	114 (93%)	8 (7%)	16	22
1	H	125/138 (91%)	117 (94%)	8 (6%)	17	23
1	I	130/138 (94%)	123 (95%)	7 (5%)	22	30
1	J	128/138 (93%)	118 (92%)	10 (8%)	12	16
1	K	132/138 (96%)	123 (93%)	9 (7%)	16	21
1	L	132/138 (96%)	123 (93%)	9 (7%)	16	21
1	M	134/138 (97%)	130 (97%)	4 (3%)	41	57
1	N	131/138 (95%)	130 (99%)	1 (1%)	81	91
1	O	120/138 (87%)	115 (96%)	5 (4%)	30	42
1	P	131/138 (95%)	126 (96%)	5 (4%)	33	47
1	Q	132/138 (96%)	129 (98%)	3 (2%)	50	67
1	R	130/138 (94%)	127 (98%)	3 (2%)	50	67
1	S	131/138 (95%)	120 (92%)	11 (8%)	11	13
1	T	131/138 (95%)	123 (94%)	8 (6%)	18	25

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	U	123/138 (89%)	115 (94%)	8 (6%)	17	23
1	V	131/138 (95%)	128 (98%)	3 (2%)	50	67
1	W	121/138 (88%)	117 (97%)	4 (3%)	38	53
1	X	124/138 (90%)	119 (96%)	5 (4%)	31	44
1	Y	123/138 (89%)	113 (92%)	10 (8%)	11	15
1	Z	122/138 (88%)	112 (92%)	10 (8%)	11	14
1	a	123/138 (89%)	115 (94%)	8 (6%)	17	23
1	b	127/138 (92%)	117 (92%)	10 (8%)	12	15
1	c	130/138 (94%)	127 (98%)	3 (2%)	50	67
1	d	127/138 (92%)	118 (93%)	9 (7%)	14	19
1	e	129/138 (94%)	119 (92%)	10 (8%)	12	16
1	f	132/138 (96%)	122 (92%)	10 (8%)	13	16
1	g	132/138 (96%)	124 (94%)	8 (6%)	18	25
1	h	131/138 (95%)	125 (95%)	6 (5%)	27	38
1	i	129/138 (94%)	120 (93%)	9 (7%)	15	19
1	j	130/138 (94%)	124 (95%)	6 (5%)	27	38
All	All	4576/4968 (92%)	4329 (95%)	247 (5%)	22	30

5 of 247 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	f	90	ASP
1	j	90	ASP
1	b	45	ILE
1	j	10	GLU
1	h	108	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 36 such sidechains are listed below:

Mol	Chain	Res	Type
1	T	95	ASN
1	g	146	GLN
1	S	146	GLN
1	h	35	GLN
1	G	70	HIS

### 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](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

178 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
2	2AN	S	203	-	22,23,23	1.72	4 (18%)	29,33,33	1.08	2 (6%)
3	SO4	E	205	-	4,4,4	0.19	0	6,6,6	0.13	0
2	2AN	B	203	-	22,23,23	1.71	5 (22%)	29,33,33	1.53	4 (13%)
2	2AN	b	202	-	22,23,23	1.86	5 (22%)	29,33,33	1.24	3 (10%)
2	2AN	M	201	-	22,23,23	2.11	4 (18%)	29,33,33	2.09	9 (31%)
2	2AN	S	201	-	22,23,23	2.06	4 (18%)	29,33,33	1.84	4 (13%)
2	2AN	N	201	-	22,23,23	1.39	4 (18%)	29,33,33	1.22	2 (6%)
2	2AN	V	207	-	22,23,23	1.74	5 (22%)	29,33,33	0.90	1 (3%)
2	2AN	b	204	-	22,23,23	1.73	3 (13%)	29,33,33	1.11	2 (6%)
5	DMS	G	208	-	3,3,3	0.52	0	3,3,3	1.10	0
2	2AN	Q	202	-	22,23,23	1.80	4 (18%)	29,33,33	1.24	2 (6%)
2	2AN	L	203	-	22,23,23	1.60	4 (18%)	29,33,33	1.92	8 (27%)
2	2AN	X	201	-	22,23,23	2.00	5 (22%)	29,33,33	1.63	4 (13%)
2	2AN	V	204	-	22,23,23	1.74	5 (22%)	29,33,33	1.37	3 (10%)
6	FLC	i	202	-	12,12,12	1.34	2 (16%)	17,17,17	1.21	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	2AN	P	202	-	22,23,23	1.84	7 (31%)	29,33,33	1.96	10 (34%)
2	2AN	j	207	-	22,23,23	2.30	5 (22%)	29,33,33	1.13	2 (6%)
2	2AN	R	205	-	22,23,23	1.83	5 (22%)	29,33,33	1.36	2 (6%)
2	2AN	W	201	-	22,23,23	2.06	5 (22%)	29,33,33	1.63	5 (17%)
5	DMS	X	207	-	3,3,3	0.56	0	3,3,3	0.62	0
2	2AN	V	205	-	22,23,23	1.58	7 (31%)	29,33,33	1.65	6 (20%)
2	2AN	H	202	-	22,23,23	1.82	4 (18%)	29,33,33	1.55	5 (17%)
2	2AN	P	204	-	22,23,23	1.81	5 (22%)	29,33,33	1.51	3 (10%)
3	SO4	I	208	-	4,4,4	0.32	0	6,6,6	0.90	0
2	2AN	H	204	-	22,23,23	2.01	5 (22%)	29,33,33	1.41	2 (6%)
2	2AN	X	206	-	22,23,23	1.81	5 (22%)	29,33,33	0.90	2 (6%)
2	2AN	d	202	-	22,23,23	1.96	5 (22%)	29,33,33	1.41	2 (6%)
2	2AN	I	205	-	22,23,23	2.69	5 (22%)	29,33,33	1.61	7 (24%)
2	2AN	K	201	-	22,23,23	1.70	5 (22%)	29,33,33	1.79	7 (24%)
2	2AN	f	206	-	22,23,23	1.87	4 (18%)	29,33,33	1.28	2 (6%)
2	2AN	X	202	-	22,23,23	1.82	6 (27%)	29,33,33	1.33	2 (6%)
2	2AN	S	204	-	22,23,23	1.69	6 (27%)	29,33,33	2.56	4 (13%)
2	2AN	j	202	-	22,23,23	1.39	3 (13%)	29,33,33	1.99	8 (27%)
2	2AN	j	206	-	22,23,23	1.94	6 (27%)	29,33,33	1.36	3 (10%)
6	FLC	G	206	-	12,12,12	1.04	0	17,17,17	1.93	5 (29%)
2	2AN	j	204	-	22,23,23	1.68	5 (22%)	29,33,33	1.50	4 (13%)
2	2AN	b	206	-	22,23,23	2.33	5 (22%)	29,33,33	1.60	4 (13%)
2	2AN	F	202	-	22,23,23	2.04	4 (18%)	29,33,33	2.07	13 (44%)
2	2AN	V	201	-	22,23,23	1.83	5 (22%)	29,33,33	1.58	6 (20%)
2	2AN	a	204	-	22,23,23	1.90	5 (22%)	29,33,33	1.21	2 (6%)
2	2AN	L	202	-	22,23,23	1.76	4 (18%)	29,33,33	1.29	3 (10%)
2	2AN	A	202	-	22,23,23	2.07	7 (31%)	29,33,33	1.79	8 (27%)
2	2AN	Y	203	-	22,23,23	1.71	5 (22%)	29,33,33	1.54	6 (20%)
2	2AN	M	202	-	22,23,23	1.58	5 (22%)	29,33,33	2.09	9 (31%)
2	2AN	B	205	-	22,23,23	1.71	4 (18%)	29,33,33	1.31	4 (13%)
2	2AN	L	204	-	22,23,23	1.98	5 (22%)	29,33,33	1.55	6 (20%)
6	FLC	i	203	-	12,12,12	1.39	1 (8%)	17,17,17	2.32	5 (29%)
2	2AN	F	201	-	22,23,23	1.55	4 (18%)	29,33,33	1.45	6 (20%)
2	2AN	I	202	-	22,23,23	1.78	5 (22%)	29,33,33	1.36	4 (13%)
2	2AN	d	201	-	22,23,23	1.58	3 (13%)	29,33,33	1.59	5 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	2AN	a	201	-	22,23,23	1.98	5 (22%)	29,33,33	2.21	8 (27%)
2	2AN	U	202	-	22,23,23	1.79	5 (22%)	29,33,33	1.30	2 (6%)
4	EPE	P	205	-	15,15,15	2.10	1 (6%)	19,20,20	1.74	7 (36%)
2	2AN	V	206	-	22,23,23	1.71	4 (18%)	29,33,33	1.87	8 (27%)
2	2AN	G	201	-	22,23,23	1.71	4 (18%)	29,33,33	1.38	5 (17%)
2	2AN	Z	202	-	22,23,23	2.01	5 (22%)	29,33,33	1.55	5 (17%)
2	2AN	a	203	-	22,23,23	2.19	7 (31%)	29,33,33	1.51	3 (10%)
2	2AN	c	203	-	22,23,23	1.69	3 (13%)	29,33,33	1.19	2 (6%)
2	2AN	E	202	-	22,23,23	1.44	3 (13%)	29,33,33	1.68	7 (24%)
2	2AN	F	203	-	22,23,23	1.45	4 (18%)	29,33,33	1.36	4 (13%)
2	2AN	c	205	-	22,23,23	1.66	5 (22%)	29,33,33	1.09	2 (6%)
2	2AN	V	208	-	22,23,23	2.11	6 (27%)	29,33,33	3.43	10 (34%)
2	2AN	B	206	-	22,23,23	1.81	4 (18%)	29,33,33	0.96	1 (3%)
2	2AN	N	202	-	22,23,23	1.73	6 (27%)	29,33,33	1.59	6 (20%)
2	2AN	h	202	-	22,23,23	1.63	5 (22%)	29,33,33	1.68	6 (20%)
2	2AN	Y	204	-	22,23,23	1.68	4 (18%)	29,33,33	0.90	2 (6%)
2	2AN	P	201	-	22,23,23	1.68	3 (13%)	29,33,33	1.16	3 (10%)
2	2AN	G	203	-	22,23,23	1.39	4 (18%)	29,33,33	1.23	3 (10%)
2	2AN	e	201	-	22,23,23	2.01	6 (27%)	29,33,33	1.59	6 (20%)
6	FLC	a	206	-	12,12,12	1.15	0	17,17,17	1.43	3 (17%)
2	2AN	f	204	-	22,23,23	1.67	7 (31%)	29,33,33	1.35	2 (6%)
3	SO4	c	207	-	4,4,4	0.43	0	6,6,6	0.45	0
3	SO4	c	208	-	4,4,4	0.45	0	6,6,6	0.38	0
2	2AN	X	204	-	22,23,23	1.91	4 (18%)	29,33,33	1.41	5 (17%)
2	2AN	R	201	-	22,23,23	1.84	5 (22%)	29,33,33	1.00	1 (3%)
2	2AN	g	202	-	22,23,23	1.63	4 (18%)	29,33,33	1.86	7 (24%)
2	2AN	O	202	-	22,23,23	2.12	4 (18%)	29,33,33	1.29	4 (13%)
2	2AN	O	203	-	22,23,23	2.08	4 (18%)	29,33,33	1.52	3 (10%)
2	2AN	F	204	-	22,23,23	1.77	4 (18%)	29,33,33	1.29	4 (13%)
2	2AN	D	201	-	22,23,23	1.77	6 (27%)	29,33,33	1.56	5 (17%)
2	2AN	c	204	-	22,23,23	1.44	4 (18%)	29,33,33	1.52	4 (13%)
2	2AN	A	203	-	22,23,23	2.11	4 (18%)	29,33,33	1.39	4 (13%)
2	2AN	I	207	-	22,23,23	2.37	4 (18%)	29,33,33	1.69	10 (34%)
2	2AN	I	204	-	22,23,23	2.03	5 (22%)	29,33,33	1.43	4 (13%)
2	2AN	H	201	-	22,23,23	1.60	5 (22%)	29,33,33	1.38	3 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	2AN	R	202	-	22,23,23	2.09	8 (36%)	29,33,33	1.30	5 (17%)
2	2AN	C	203[A]	-	22,23,23	0.61	0	29,33,33	1.44	5 (17%)
2	2AN	V	202	-	22,23,23	1.48	5 (22%)	29,33,33	1.71	7 (24%)
3	SO4	Q	204	-	4,4,4	0.53	0	6,6,6	0.58	0
6	FLC	e	202	-	12,12,12	1.54	1 (8%)	17,17,17	1.85	3 (17%)
2	2AN	K	202	-	22,23,23	1.63	4 (18%)	29,33,33	1.10	4 (13%)
2	2AN	F	205	-	22,23,23	1.71	4 (18%)	29,33,33	1.27	3 (10%)
2	2AN	f	202	-	22,23,23	1.36	2 (9%)	29,33,33	1.52	4 (13%)
2	2AN	G	205	-	22,23,23	1.88	4 (18%)	29,33,33	1.19	3 (10%)
2	2AN	c	201	-	22,23,23	1.69	6 (27%)	29,33,33	1.52	4 (13%)
6	FLC	a	205	-	12,12,12	1.33	1 (8%)	17,17,17	1.47	5 (29%)
2	2AN	C	202	-	22,23,23	1.75	5 (22%)	29,33,33	1.02	1 (3%)
2	2AN	h	204	-	22,23,23	1.51	4 (18%)	29,33,33	1.58	2 (6%)
2	2AN	E	203	-	22,23,23	1.91	4 (18%)	29,33,33	1.87	8 (27%)
2	2AN	b	203	-	22,23,23	1.75	5 (22%)	29,33,33	1.06	2 (6%)
3	SO4	G	209	-	4,4,4	0.52	0	6,6,6	0.20	0
2	2AN	Q	203	-	22,23,23	2.14	5 (22%)	29,33,33	1.75	5 (17%)
2	2AN	a	202	-	22,23,23	1.96	4 (18%)	29,33,33	1.54	6 (20%)
2	2AN	c	206	-	22,23,23	1.35	3 (13%)	29,33,33	1.25	3 (10%)
2	2AN	Y	201	-	22,23,23	2.49	6 (27%)	29,33,33	2.18	12 (41%)
3	SO4	A	205	-	4,4,4	0.41	0	6,6,6	0.78	0
2	2AN	J	202	-	22,23,23	1.49	4 (18%)	29,33,33	0.99	2 (6%)
2	2AN	A	201	-	22,23,23	1.67	6 (27%)	29,33,33	1.40	6 (20%)
2	2AN	h	205	-	22,23,23	2.11	5 (22%)	29,33,33	1.30	2 (6%)
2	2AN	H	203	-	22,23,23	1.69	5 (22%)	29,33,33	1.29	2 (6%)
2	2AN	G	202	-	22,23,23	1.51	4 (18%)	29,33,33	1.62	5 (17%)
2	2AN	h	203	-	22,23,23	2.21	6 (27%)	29,33,33	1.84	8 (27%)
2	2AN	Z	204	-	22,23,23	1.78	4 (18%)	29,33,33	1.42	3 (10%)
2	2AN	G	204	-	22,23,23	2.05	5 (22%)	29,33,33	1.39	5 (17%)
2	2AN	T	204	-	22,23,23	2.27	5 (22%)	29,33,33	1.64	9 (31%)
2	2AN	j	201	-	22,23,23	1.66	4 (18%)	29,33,33	1.60	5 (17%)
2	2AN	X	203	-	22,23,23	1.79	5 (22%)	29,33,33	0.90	1 (3%)
2	2AN	j	203	-	22,23,23	1.71	6 (27%)	29,33,33	1.73	8 (27%)
2	2AN	T	202	-	22,23,23	2.00	4 (18%)	29,33,33	1.58	3 (10%)
5	DMS	N	206	-	3,3,3	0.50	0	3,3,3	0.85	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	2AN	h	201	-	22,23,23	2.23	4 (18%)	29,33,33	1.35	6 (20%)
6	FLC	j	208	-	12,12,12	2.27	1 (8%)	17,17,17	2.39	6 (35%)
2	2AN	E	204	-	22,23,23	2.09	6 (27%)	29,33,33	1.89	5 (17%)
2	2AN	B	204	-	22,23,23	1.60	4 (18%)	29,33,33	1.49	4 (13%)
2	2AN	M	203	-	22,23,23	1.87	7 (31%)	29,33,33	1.84	6 (20%)
2	2AN	B	202	-	22,23,23	1.65	3 (13%)	29,33,33	0.95	1 (3%)
2	2AN	h	206	-	22,23,23	2.03	4 (18%)	29,33,33	1.63	6 (20%)
2	2AN	R	204	-	22,23,23	2.16	4 (18%)	29,33,33	1.56	6 (20%)
2	2AN	D	202	-	22,23,23	1.81	6 (27%)	29,33,33	1.21	2 (6%)
3	SO4	c	209	-	4,4,4	0.49	0	6,6,6	0.62	0
2	2AN	K	203	-	22,23,23	1.74	4 (18%)	29,33,33	1.26	1 (3%)
2	2AN	b	205	-	22,23,23	2.00	5 (22%)	29,33,33	1.57	5 (17%)
2	2AN	D	204	-	22,23,23	2.40	5 (22%)	29,33,33	2.15	10 (34%)
2	2AN	N	204	-	22,23,23	1.56	5 (22%)	29,33,33	1.90	5 (17%)
2	2AN	f	203	-	22,23,23	1.81	5 (22%)	29,33,33	0.91	2 (6%)
2	2AN	S	202	-	22,23,23	1.85	4 (18%)	29,33,33	1.85	9 (31%)
2	2AN	N	205	-	22,23,23	2.42	7 (31%)	29,33,33	1.65	5 (17%)
2	2AN	d	204	-	22,23,23	1.64	4 (18%)	29,33,33	2.01	5 (17%)
2	2AN	F	206	-	22,23,23	1.88	5 (22%)	29,33,33	1.61	7 (24%)
2	2AN	X	205	-	22,23,23	2.06	5 (22%)	29,33,33	1.30	3 (10%)
2	2AN	j	205	-	22,23,23	1.80	4 (18%)	29,33,33	1.87	10 (34%)
2	2AN	c	202	-	22,23,23	2.14	5 (22%)	29,33,33	1.80	10 (34%)
2	2AN	N	203	-	22,23,23	1.97	5 (22%)	29,33,33	2.66	9 (31%)
2	2AN	Q	201	-	22,23,23	1.94	5 (22%)	29,33,33	1.73	6 (20%)
2	2AN	G	207	-	22,23,23	2.04	5 (22%)	29,33,33	1.05	1 (3%)
2	2AN	T	205	-	22,23,23	2.27	6 (27%)	29,33,33	2.23	10 (34%)
3	SO4	Y	205	-	4,4,4	0.31	0	6,6,6	0.63	0
2	2AN	f	201	-	22,23,23	2.07	6 (27%)	29,33,33	1.92	9 (31%)
2	2AN	f	205	-	22,23,23	1.68	4 (18%)	29,33,33	1.29	5 (17%)
2	2AN	A	204	-	22,23,23	1.81	5 (22%)	29,33,33	0.88	2 (6%)
2	2AN	i	201	-	22,23,23	1.75	4 (18%)	29,33,33	1.72	6 (20%)
2	2AN	b	201	-	22,23,23	1.78	4 (18%)	29,33,33	1.01	1 (3%)
2	2AN	C	201	-	22,23,23	1.64	5 (22%)	29,33,33	1.39	4 (13%)
3	SO4	g	204	-	4,4,4	0.60	0	6,6,6	0.47	0
2	2AN	Z	203	-	22,23,23	1.90	5 (22%)	29,33,33	1.64	7 (24%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	2AN	d	203	-	22,23,23	1.74	5 (22%)	29,33,33	0.92	1 (3%)
2	2AN	g	203	-	22,23,23	1.79	6 (27%)	29,33,33	1.55	4 (13%)
2	2AN	E	201	-	22,23,23	1.71	4 (18%)	29,33,33	1.14	2 (6%)
2	2AN	I	206	-	22,23,23	2.36	6 (27%)	29,33,33	1.81	7 (24%)
2	2AN	J	203	-	22,23,23	1.76	4 (18%)	29,33,33	1.63	6 (20%)
2	2AN	B	201	-	22,23,23	1.80	5 (22%)	29,33,33	2.02	12 (41%)
2	2AN	Z	205	-	22,23,23	1.63	4 (18%)	29,33,33	1.61	5 (17%)
2	2AN	I	201	-	22,23,23	1.32	3 (13%)	29,33,33	1.89	7 (24%)
2	2AN	U	201	-	22,23,23	1.94	5 (22%)	29,33,33	1.26	1 (3%)
2	2AN	T	203	-	22,23,23	1.60	5 (22%)	29,33,33	1.92	7 (24%)
2	2AN	L	201	-	22,23,23	1.62	5 (22%)	29,33,33	1.25	2 (6%)
2	2AN	J	201	-	22,23,23	1.48	3 (13%)	29,33,33	1.01	1 (3%)
2	2AN	Z	201	-	22,23,23	2.32	6 (27%)	29,33,33	1.60	8 (27%)
2	2AN	R	203	-	22,23,23	1.84	6 (27%)	29,33,33	1.36	3 (10%)
2	2AN	Y	202	-	22,23,23	1.85	6 (27%)	29,33,33	1.42	6 (20%)
2	2AN	V	203	-	22,23,23	1.97	6 (27%)	29,33,33	1.59	6 (20%)
2	2AN	T	201	-	22,23,23	1.77	7 (31%)	29,33,33	1.31	2 (6%)
2	2AN	D	203	-	22,23,23	1.87	6 (27%)	29,33,33	1.62	5 (17%)
2	2AN	Z	206	-	22,23,23	2.02	5 (22%)	29,33,33	1.73	6 (20%)
2	2AN	g	201	-	22,23,23	1.96	6 (27%)	29,33,33	1.75	8 (27%)
2	2AN	P	203	-	22,23,23	1.65	6 (27%)	29,33,33	1.57	4 (13%)
2	2AN	I	203	-	22,23,23	1.92	5 (22%)	29,33,33	1.26	3 (10%)
2	2AN	O	201	-	22,23,23	1.44	2 (9%)	29,33,33	1.42	3 (10%)

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
2	2AN	S	203	-	-	0/10/10/10	0/3/3/3
2	2AN	B	203	-	-	0/10/10/10	0/3/3/3
2	2AN	b	202	-	-	0/10/10/10	0/3/3/3
2	2AN	M	201	-	-	0/10/10/10	0/3/3/3
2	2AN	S	201	-	-	8/10/10/10	0/3/3/3
2	2AN	N	201	-	-	0/10/10/10	0/3/3/3
2	2AN	V	207	-	-	0/10/10/10	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	2AN	b	204	-	-	0/10/10/10	0/3/3/3
2	2AN	Q	202	-	-	0/10/10/10	0/3/3/3
2	2AN	L	203	-	-	2/10/10/10	0/3/3/3
2	2AN	X	201	-	-	0/10/10/10	0/3/3/3
2	2AN	V	204	-	-	0/10/10/10	0/3/3/3
6	FLC	i	202	-	-	8/16/16/16	-
2	2AN	P	202	-	-	2/10/10/10	0/3/3/3
2	2AN	j	207	-	-	0/10/10/10	0/3/3/3
2	2AN	R	205	-	-	0/10/10/10	0/3/3/3
2	2AN	W	201	-	-	6/10/10/10	0/3/3/3
2	2AN	V	205	-	-	2/10/10/10	0/3/3/3
2	2AN	H	202	-	-	2/10/10/10	0/3/3/3
2	2AN	P	204	-	-	1/10/10/10	0/3/3/3
2	2AN	H	204	-	-	2/10/10/10	0/3/3/3
2	2AN	X	206	-	-	2/10/10/10	0/3/3/3
2	2AN	d	202	-	-	6/10/10/10	0/3/3/3
2	2AN	I	205	-	-	6/10/10/10	0/3/3/3
2	2AN	K	201	-	-	4/10/10/10	0/3/3/3
2	2AN	f	206	-	-	1/10/10/10	0/3/3/3
2	2AN	X	202	-	-	0/10/10/10	0/3/3/3
2	2AN	S	204	-	-	8/10/10/10	0/3/3/3
2	2AN	j	202	-	-	1/10/10/10	0/3/3/3
2	2AN	j	206	-	-	0/10/10/10	0/3/3/3
6	FLC	G	206	-	-	14/16/16/16	-
2	2AN	j	204	-	-	5/10/10/10	0/3/3/3
2	2AN	b	206	-	-	7/10/10/10	0/3/3/3
2	2AN	F	202	-	-	8/10/10/10	0/3/3/3
2	2AN	V	201	-	-	2/10/10/10	0/3/3/3
2	2AN	a	204	-	-	0/10/10/10	0/3/3/3
2	2AN	L	202	-	-	0/10/10/10	0/3/3/3
2	2AN	A	202	-	-	2/10/10/10	0/3/3/3
2	2AN	Y	203	-	-	0/10/10/10	0/3/3/3
2	2AN	M	202	-	-	3/10/10/10	0/3/3/3
2	2AN	B	205	-	-	7/10/10/10	0/3/3/3
2	2AN	L	204	-	-	5/10/10/10	0/3/3/3
6	FLC	i	203	-	-	9/16/16/16	-
2	2AN	F	201	-	-	6/10/10/10	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	2AN	I	202	-	-	0/10/10/10	0/3/3/3
2	2AN	d	201	-	-	0/10/10/10	0/3/3/3
2	2AN	a	201	-	-	2/10/10/10	0/3/3/3
2	2AN	U	202	-	-	5/10/10/10	0/3/3/3
4	EPE	P	205	-	-	2/9/19/19	0/1/1/1
2	2AN	V	206	-	-	0/10/10/10	0/3/3/3
2	2AN	G	201	-	-	1/10/10/10	0/3/3/3
2	2AN	Z	202	-	-	0/10/10/10	0/3/3/3
2	2AN	a	203	-	-	0/10/10/10	0/3/3/3
2	2AN	c	203	-	-	3/10/10/10	0/3/3/3
2	2AN	E	202	-	-	1/10/10/10	0/3/3/3
2	2AN	F	203	-	-	0/10/10/10	0/3/3/3
2	2AN	c	205	-	-	0/10/10/10	0/3/3/3
2	2AN	V	208	-	-	4/10/10/10	0/3/3/3
2	2AN	B	206	-	-	1/10/10/10	0/3/3/3
2	2AN	N	202	-	-	1/10/10/10	0/3/3/3
2	2AN	h	202	-	-	0/10/10/10	0/3/3/3
2	2AN	Y	204	-	-	7/10/10/10	0/3/3/3
2	2AN	P	201	-	-	0/10/10/10	0/3/3/3
2	2AN	G	203	-	-	0/10/10/10	0/3/3/3
2	2AN	e	201	-	-	4/10/10/10	0/3/3/3
6	FLC	a	206	-	-	7/16/16/16	-
2	2AN	f	204	-	-	0/10/10/10	0/3/3/3
2	2AN	X	204	-	-	3/10/10/10	0/3/3/3
2	2AN	R	201	-	-	0/10/10/10	0/3/3/3
2	2AN	g	202	-	-	4/10/10/10	0/3/3/3
2	2AN	O	202	-	-	0/10/10/10	0/3/3/3
2	2AN	O	203	-	-	6/10/10/10	0/3/3/3
2	2AN	F	204	-	-	2/10/10/10	0/3/3/3
2	2AN	D	201	-	-	0/10/10/10	0/3/3/3
2	2AN	c	204	-	-	2/10/10/10	0/3/3/3
2	2AN	A	203	-	-	6/10/10/10	0/3/3/3
2	2AN	I	207	-	-	5/10/10/10	0/3/3/3
2	2AN	I	204	-	-	0/10/10/10	0/3/3/3
2	2AN	H	201	-	-	0/10/10/10	0/3/3/3
2	2AN	R	202	-	-	2/10/10/10	0/3/3/3
2	2AN	C	203[A]	-	-	7/10/10/10	0/3/3/3
2	2AN	V	202	-	-	1/10/10/10	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	FLC	e	202	-	-	11/16/16/16	-
2	2AN	K	202	-	-	0/10/10/10	0/3/3/3
2	2AN	F	205	-	-	3/10/10/10	0/3/3/3
2	2AN	f	202	-	-	1/10/10/10	0/3/3/3
2	2AN	G	205	-	-	6/10/10/10	0/3/3/3
2	2AN	c	201	-	-	2/10/10/10	0/3/3/3
6	FLC	a	205	-	-	9/16/16/16	-
2	2AN	C	202	-	-	0/10/10/10	0/3/3/3
2	2AN	h	204	-	-	0/10/10/10	0/3/3/3
2	2AN	E	203	-	-	3/10/10/10	0/3/3/3
2	2AN	b	203	-	-	6/10/10/10	0/3/3/3
2	2AN	Q	203	-	-	5/10/10/10	0/3/3/3
2	2AN	a	202	-	-	0/10/10/10	0/3/3/3
2	2AN	c	206	-	-	0/10/10/10	0/3/3/3
2	2AN	Y	201	-	-	0/10/10/10	0/3/3/3
2	2AN	J	202	-	-	0/10/10/10	0/3/3/3
2	2AN	A	201	-	-	0/10/10/10	0/3/3/3
2	2AN	h	205	-	-	0/10/10/10	0/3/3/3
2	2AN	H	203	-	-	6/10/10/10	0/3/3/3
2	2AN	G	202	-	-	2/10/10/10	0/3/3/3
2	2AN	h	203	-	-	3/10/10/10	0/3/3/3
2	2AN	Z	204	-	-	0/10/10/10	0/3/3/3
2	2AN	G	204	-	-	0/10/10/10	0/3/3/3
2	2AN	T	204	-	-	6/10/10/10	0/3/3/3
2	2AN	j	201	-	-	6/10/10/10	0/3/3/3
2	2AN	X	203	-	-	2/10/10/10	0/3/3/3
2	2AN	j	203	-	-	0/10/10/10	0/3/3/3
2	2AN	T	202	-	-	1/10/10/10	0/3/3/3
2	2AN	h	201	-	-	0/10/10/10	0/3/3/3
6	FLC	j	208	-	-	7/16/16/16	-
2	2AN	E	204	-	-	8/10/10/10	0/3/3/3
2	2AN	B	204	-	-	0/10/10/10	0/3/3/3
2	2AN	M	203	-	-	8/10/10/10	0/3/3/3
2	2AN	B	202	-	-	0/10/10/10	0/3/3/3
2	2AN	h	206	-	-	0/10/10/10	0/3/3/3
2	2AN	R	204	-	-	6/10/10/10	0/3/3/3
2	2AN	D	202	-	-	1/10/10/10	0/3/3/3
2	2AN	K	203	-	-	0/10/10/10	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	2AN	b	205	-	-	0/10/10/10	0/3/3/3
2	2AN	D	204	-	-	8/10/10/10	0/3/3/3
2	2AN	N	204	-	-	0/10/10/10	0/3/3/3
2	2AN	f	203	-	-	2/10/10/10	0/3/3/3
2	2AN	S	202	-	-	6/10/10/10	0/3/3/3
2	2AN	N	205	-	-	0/10/10/10	0/3/3/3
2	2AN	d	204	-	-	0/10/10/10	0/3/3/3
2	2AN	F	206	-	-	2/10/10/10	0/3/3/3
2	2AN	X	205	-	-	0/10/10/10	0/3/3/3
2	2AN	j	205	-	-	1/10/10/10	0/3/3/3
2	2AN	c	202	-	-	0/10/10/10	0/3/3/3
2	2AN	N	203	-	-	8/10/10/10	0/3/3/3
2	2AN	Q	201	-	-	1/10/10/10	0/3/3/3
2	2AN	G	207	-	-	0/10/10/10	0/3/3/3
2	2AN	T	205	-	-	5/10/10/10	0/3/3/3
2	2AN	f	201	-	-	0/10/10/10	0/3/3/3
2	2AN	f	205	-	-	0/10/10/10	0/3/3/3
2	2AN	A	204	-	-	4/10/10/10	0/3/3/3
2	2AN	i	201	-	-	3/10/10/10	0/3/3/3
2	2AN	b	201	-	-	0/10/10/10	0/3/3/3
2	2AN	C	201	-	-	1/10/10/10	0/3/3/3
2	2AN	Z	203	-	-	0/10/10/10	0/3/3/3
2	2AN	d	203	-	-	2/10/10/10	0/3/3/3
2	2AN	g	203	-	-	2/10/10/10	0/3/3/3
2	2AN	E	201	-	-	0/10/10/10	0/3/3/3
2	2AN	I	206	-	-	2/10/10/10	0/3/3/3
2	2AN	J	203	-	-	2/10/10/10	0/3/3/3
2	2AN	B	201	-	-	2/10/10/10	0/3/3/3
2	2AN	Z	205	-	-	0/10/10/10	0/3/3/3
2	2AN	I	201	-	-	2/10/10/10	0/3/3/3
2	2AN	U	201	-	-	6/10/10/10	0/3/3/3
2	2AN	T	203	-	-	0/10/10/10	0/3/3/3
2	2AN	L	201	-	-	0/10/10/10	0/3/3/3
2	2AN	J	201	-	-	0/10/10/10	0/3/3/3
2	2AN	Z	201	-	-	2/10/10/10	0/3/3/3
2	2AN	R	203	-	-	6/10/10/10	0/3/3/3
2	2AN	Y	202	-	-	6/10/10/10	0/3/3/3
2	2AN	V	203	-	-	1/10/10/10	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	2AN	T	201	-	-	0/10/10/10	0/3/3/3
2	2AN	D	203	-	-	6/10/10/10	0/3/3/3
2	2AN	Z	206	-	-	6/10/10/10	0/3/3/3
2	2AN	g	201	-	-	0/10/10/10	0/3/3/3
2	2AN	P	203	-	-	6/10/10/10	0/3/3/3
2	2AN	I	203	-	-	0/10/10/10	0/3/3/3
2	2AN	O	201	-	-	5/10/10/10	0/3/3/3

The worst 5 of 754 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	205	2AN	C1-C10	8.45	1.54	1.43
2	M	201	2AN	C1-C10	7.97	1.53	1.43
2	Y	201	2AN	C1-C10	7.65	1.53	1.43
2	j	207	2AN	C1-C10	7.55	1.52	1.43
4	P	205	EPE	C10-S	-7.51	1.67	1.77

The worst 5 of 780 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	V	208	2AN	C10-C1-N	11.92	137.79	120.39
2	S	204	2AN	C11-N-C1	-10.66	103.10	126.36
2	V	208	2AN	C2-C1-N	-7.89	103.51	123.47
2	E	204	2AN	C11-N-C1	-7.89	109.16	126.36
2	N	203	2AN	C2-C1-C10	7.18	126.86	120.21

There are no chirality outliers.

5 of 404 torsion outliers are listed below:

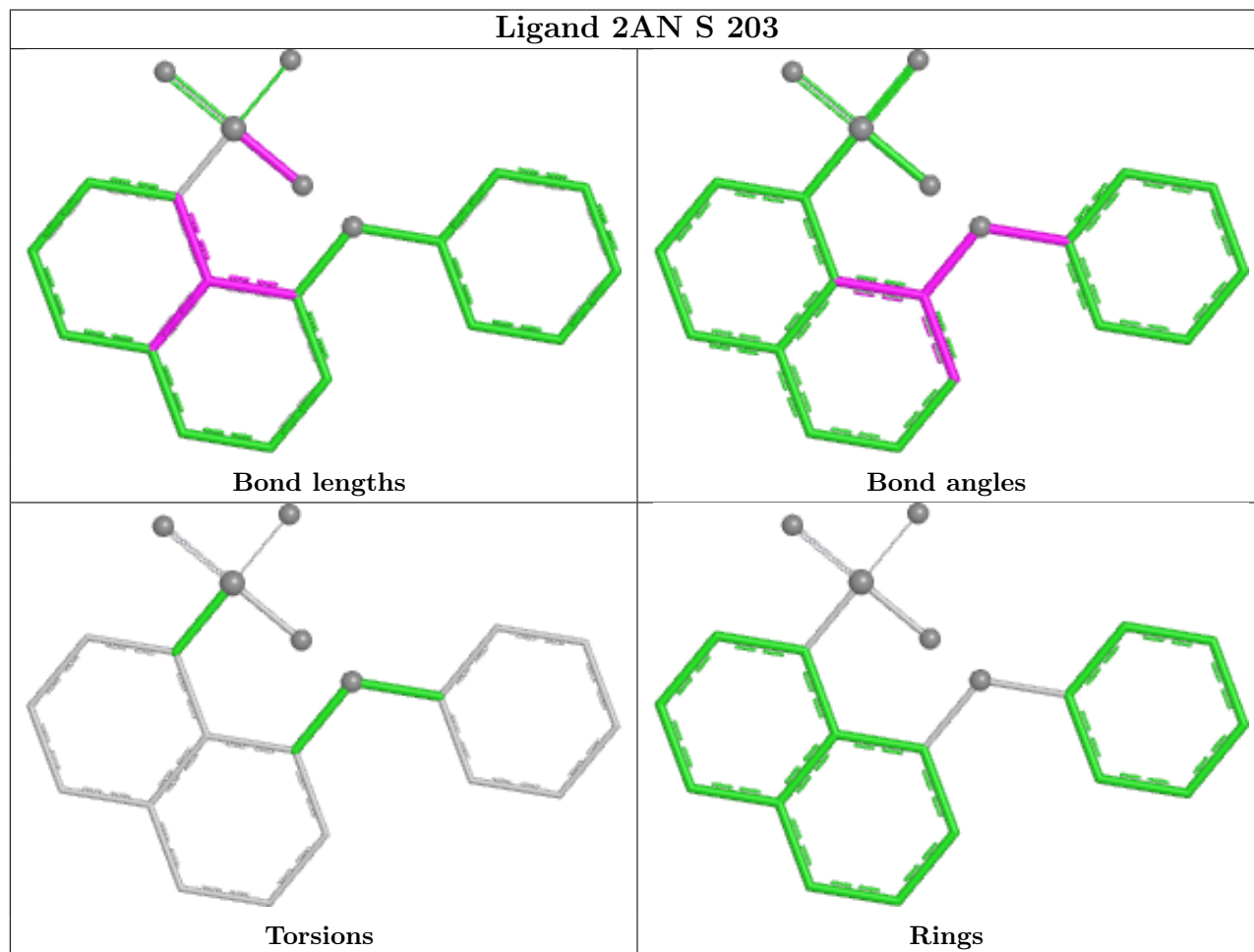
Mol	Chain	Res	Type	Atoms
2	B	205	2AN	C8-C9-S-O1
2	B	205	2AN	C10-C9-S-O1
2	B	205	2AN	C8-C9-S-O2
2	B	205	2AN	C8-C9-S-O3
2	B	205	2AN	C10-C9-S-O3

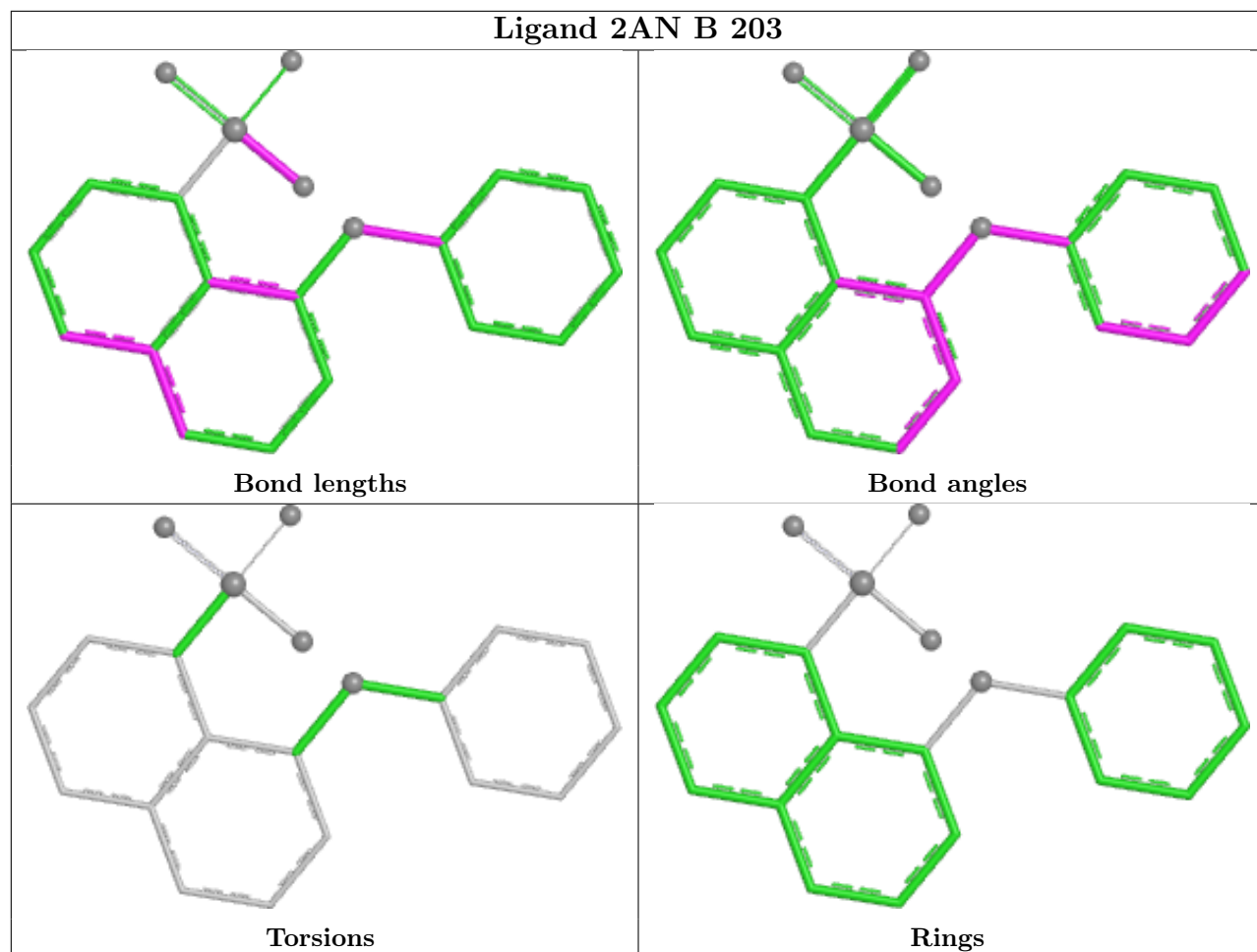
There are no ring outliers.

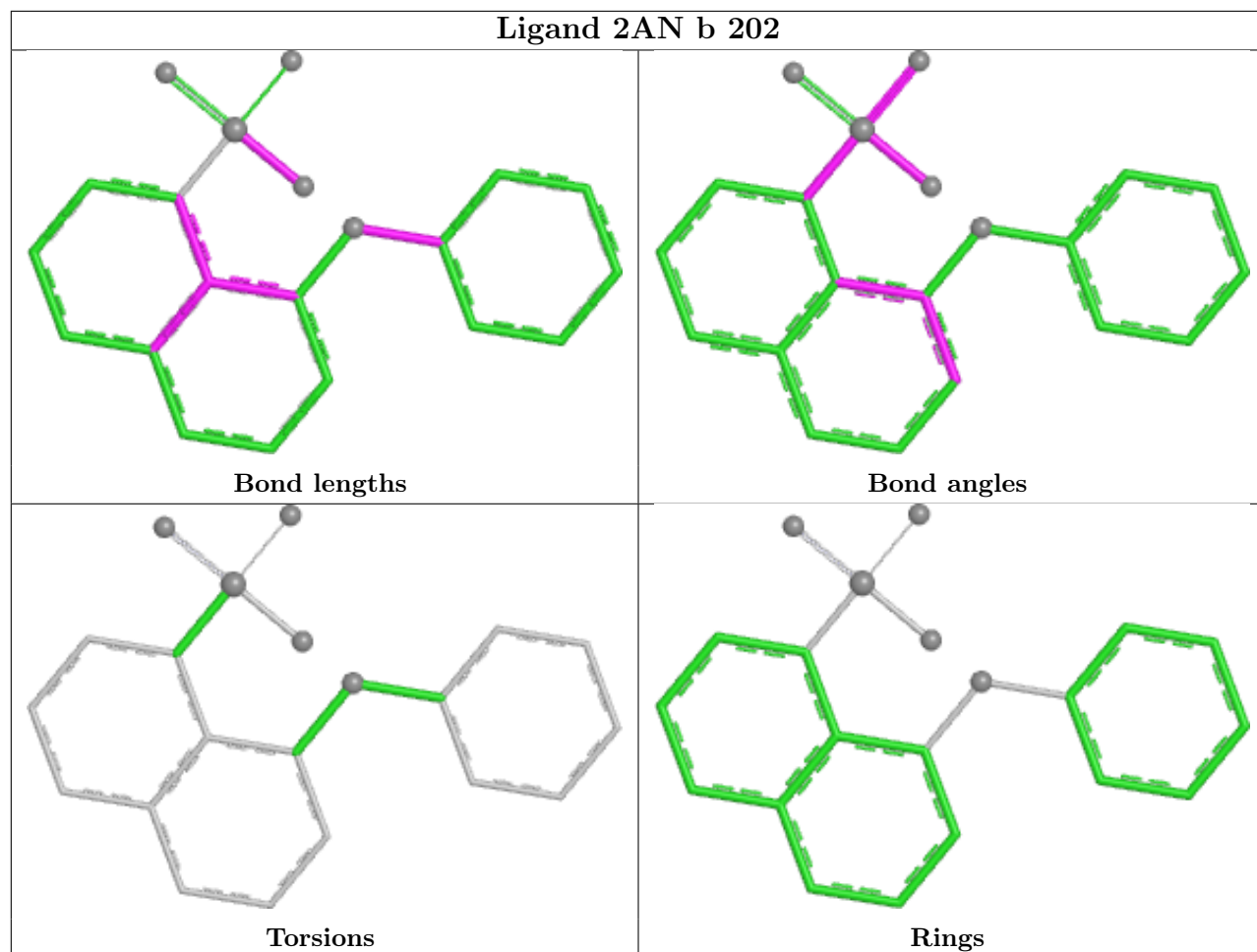
No monomer is involved in short contacts.

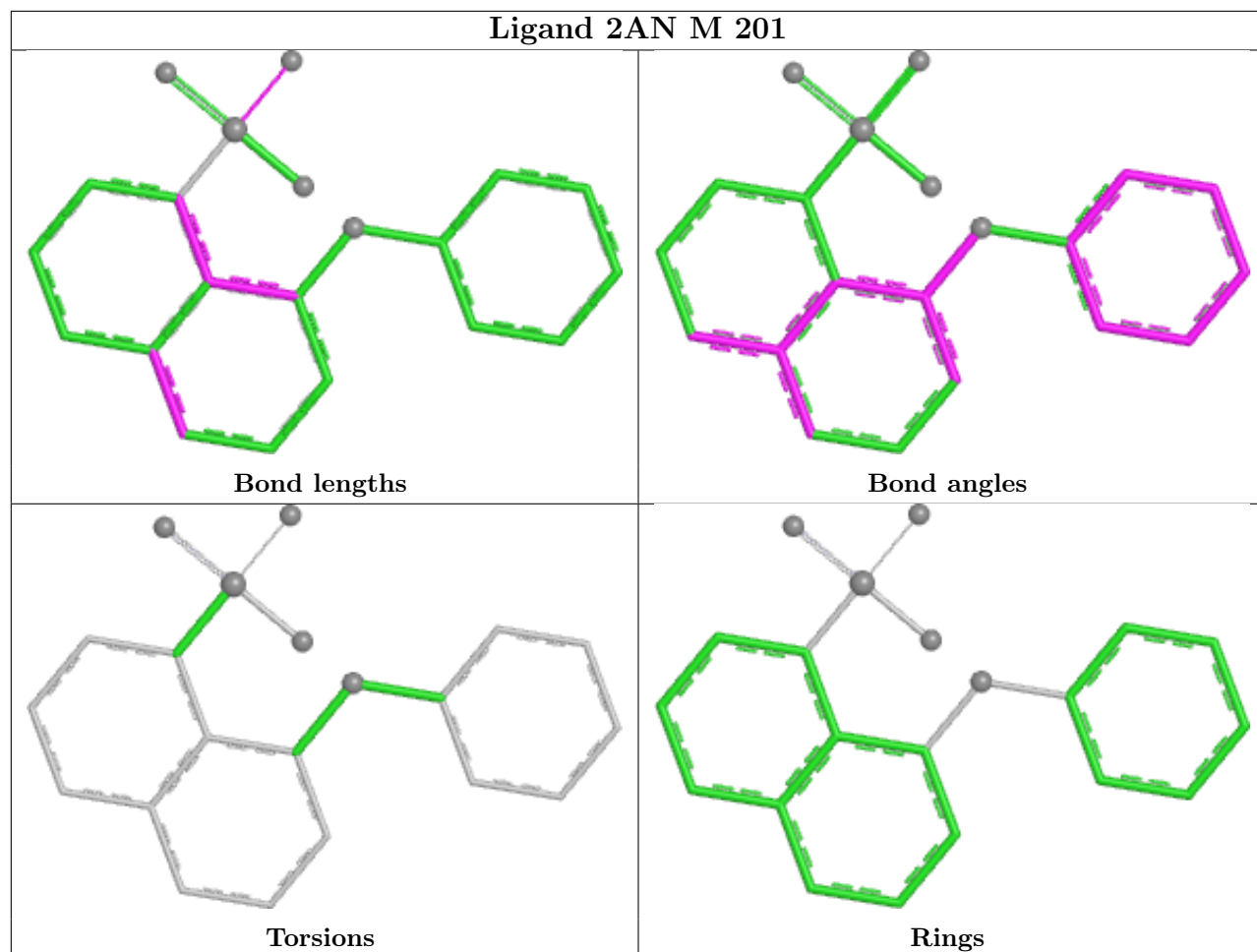
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

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.

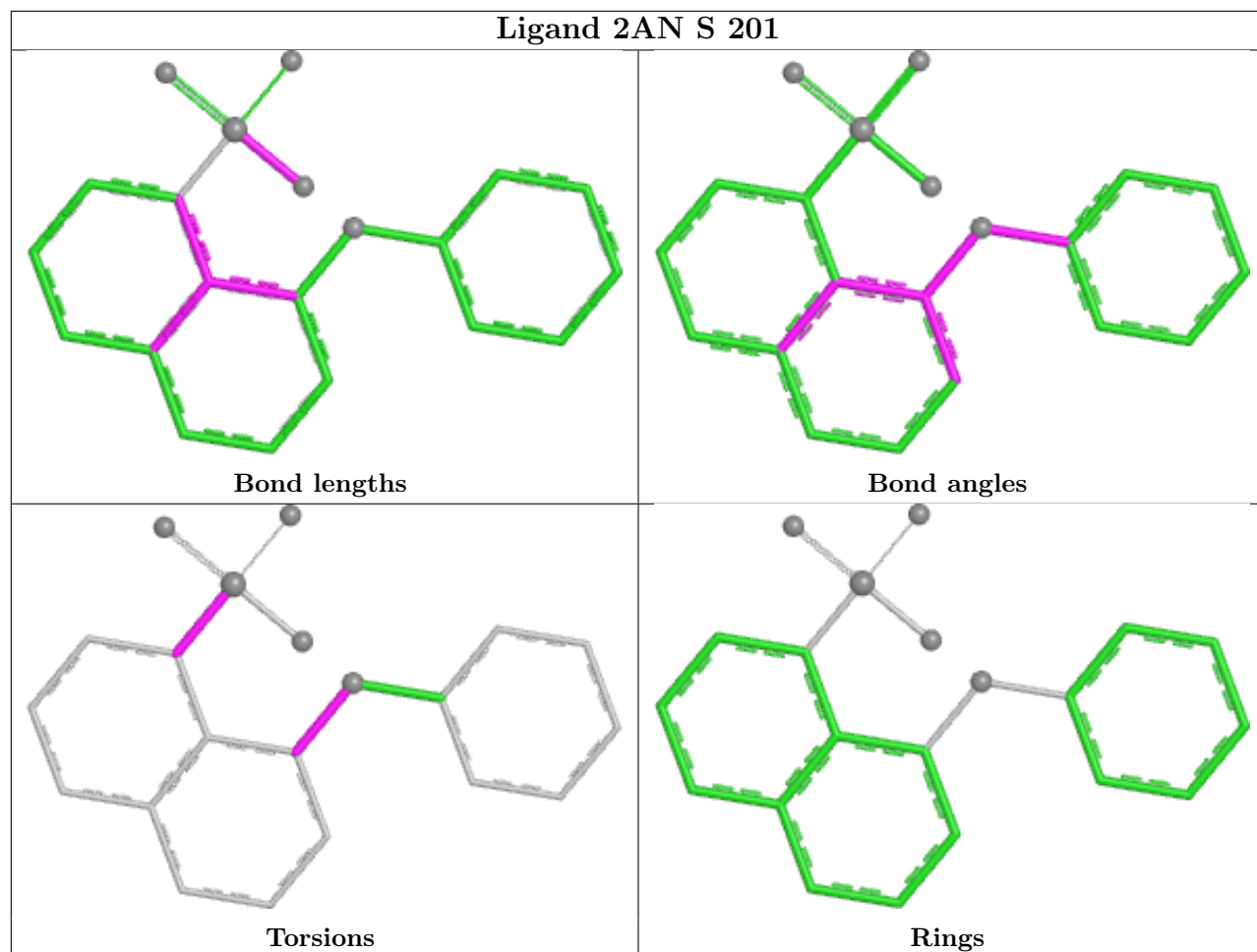


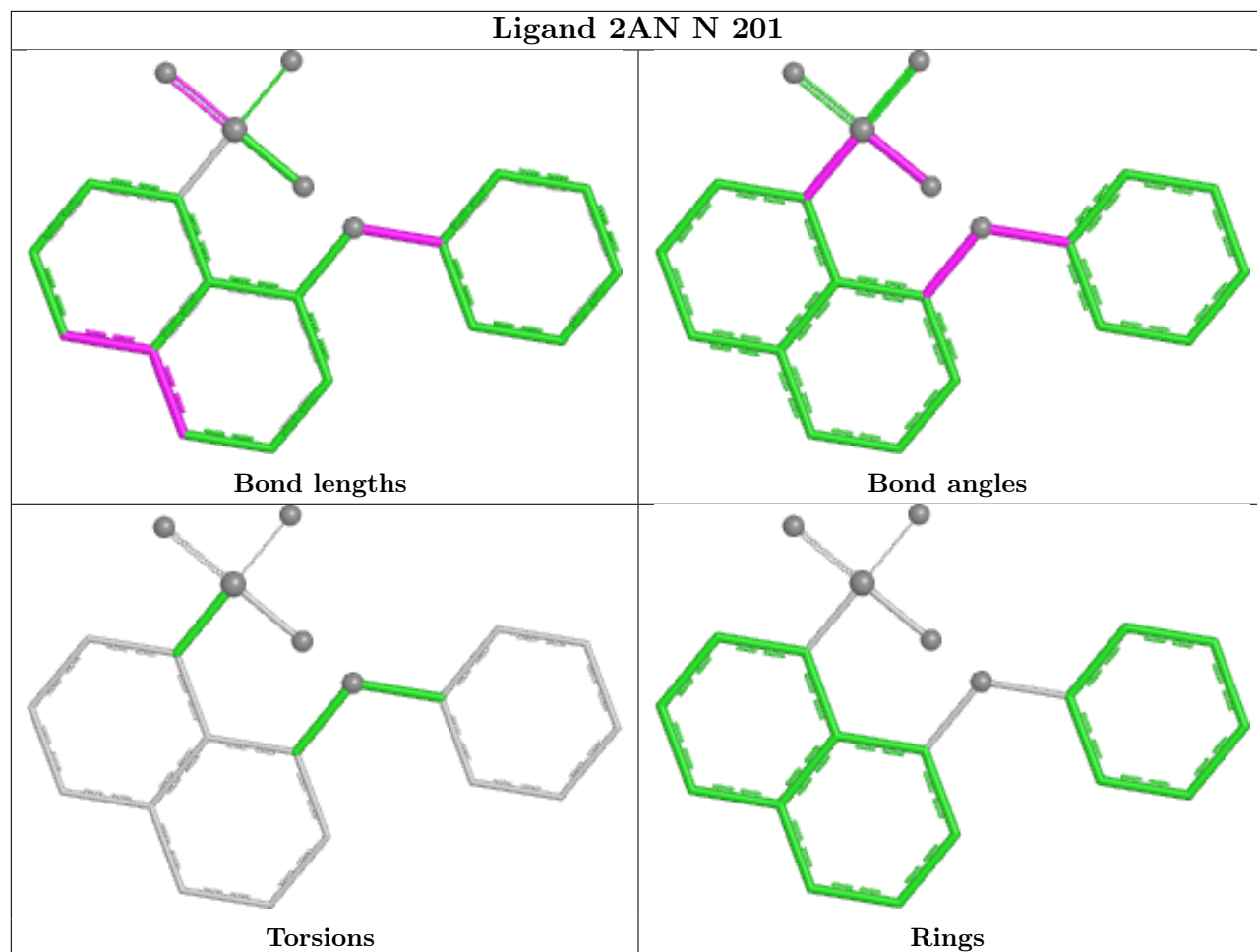


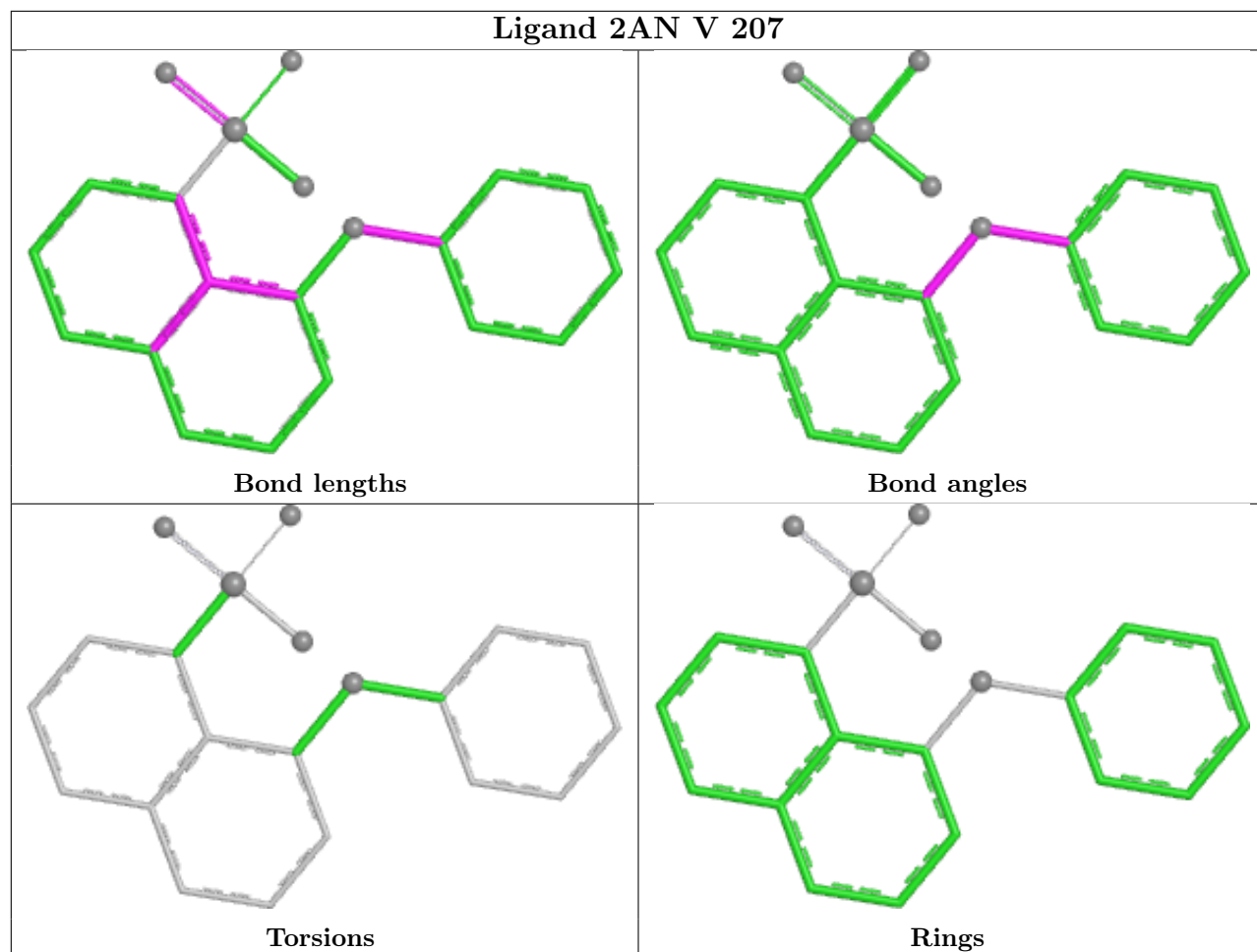


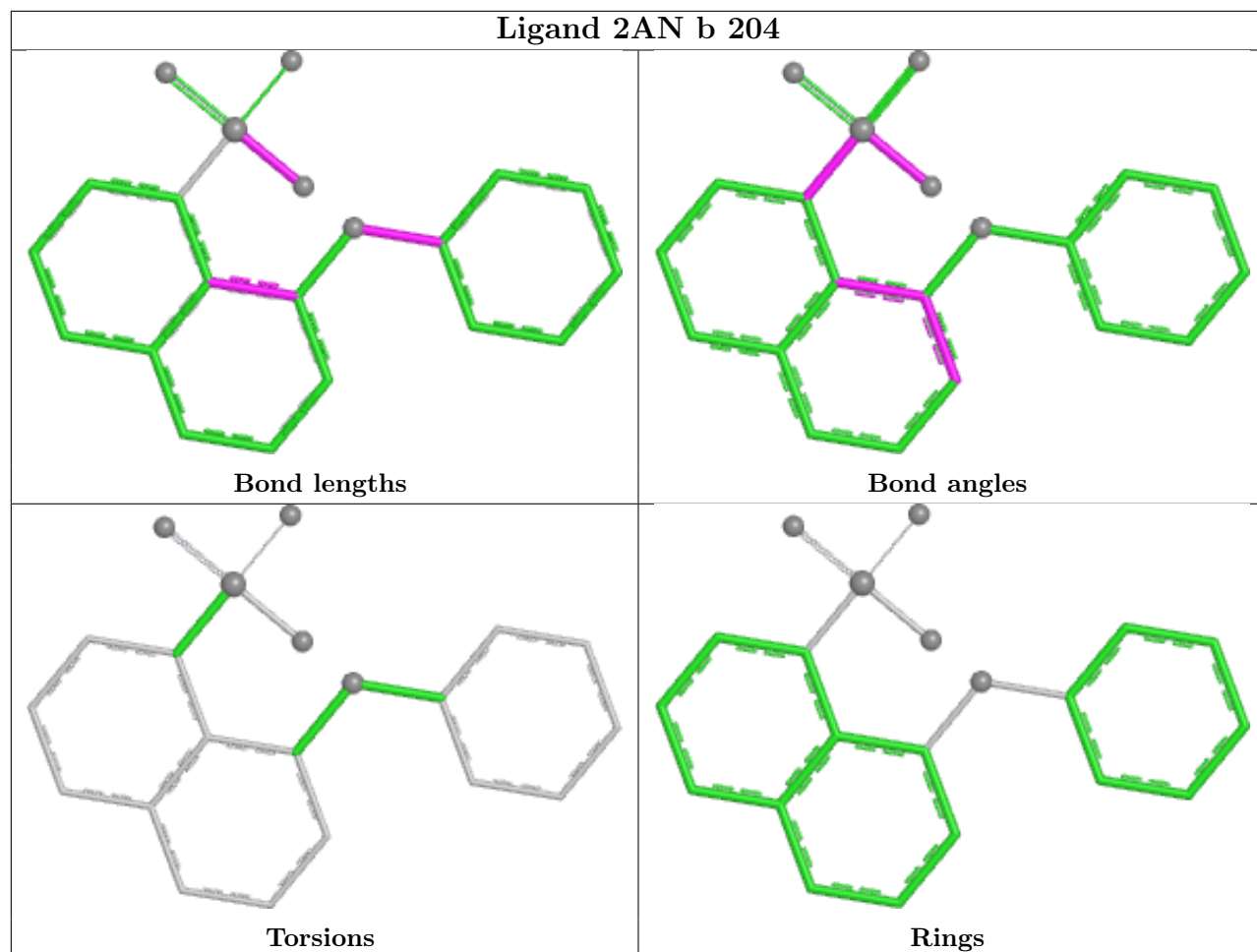


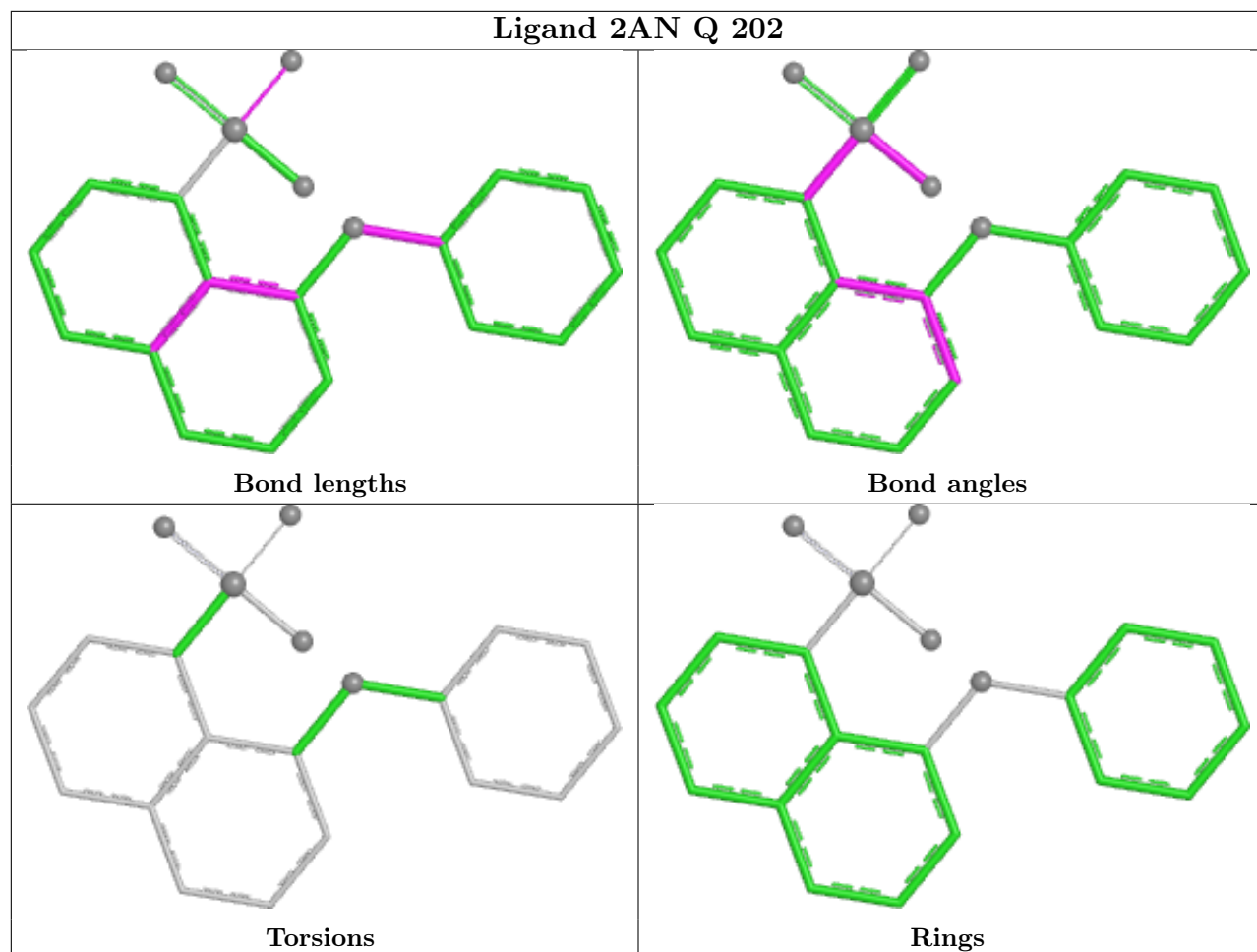


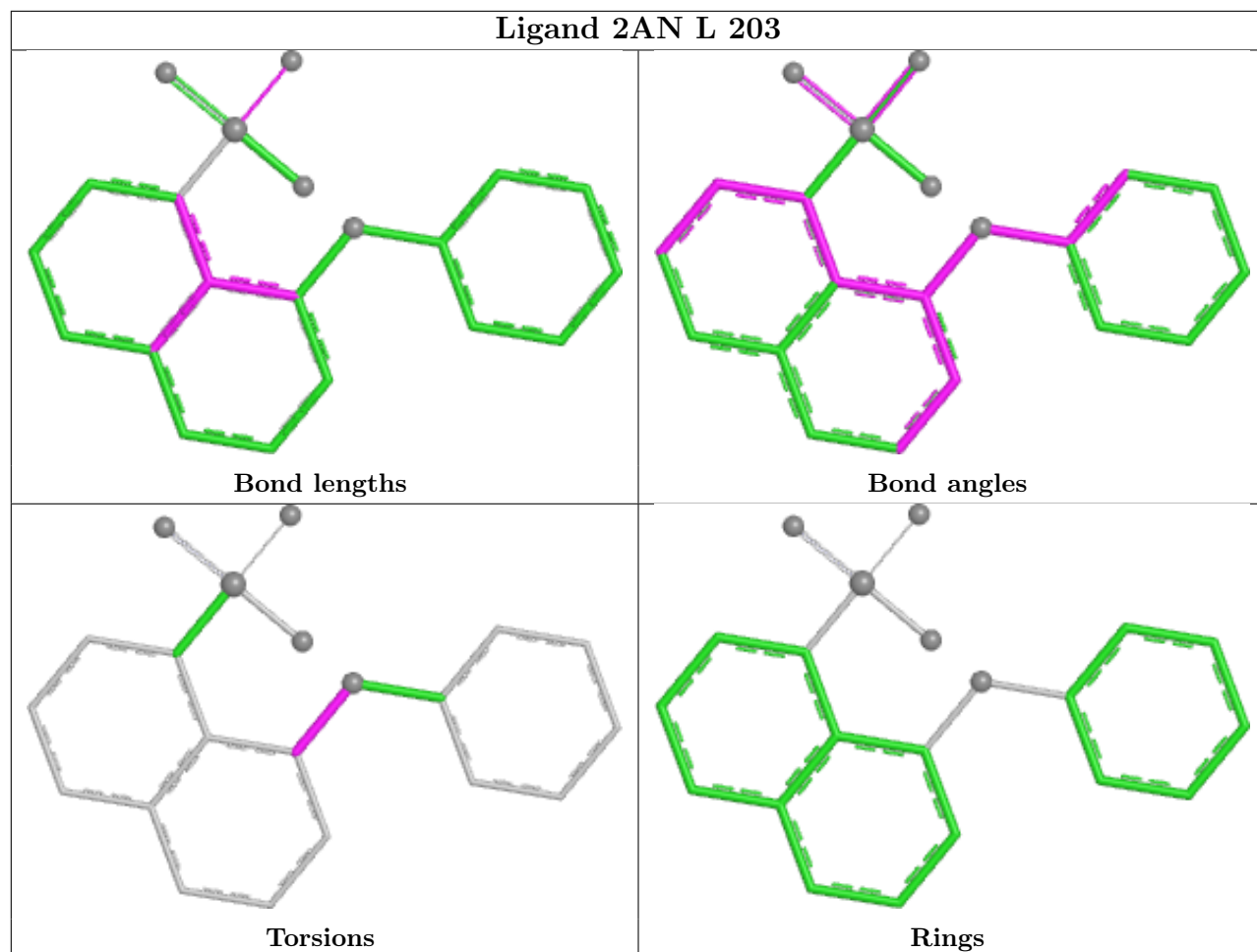


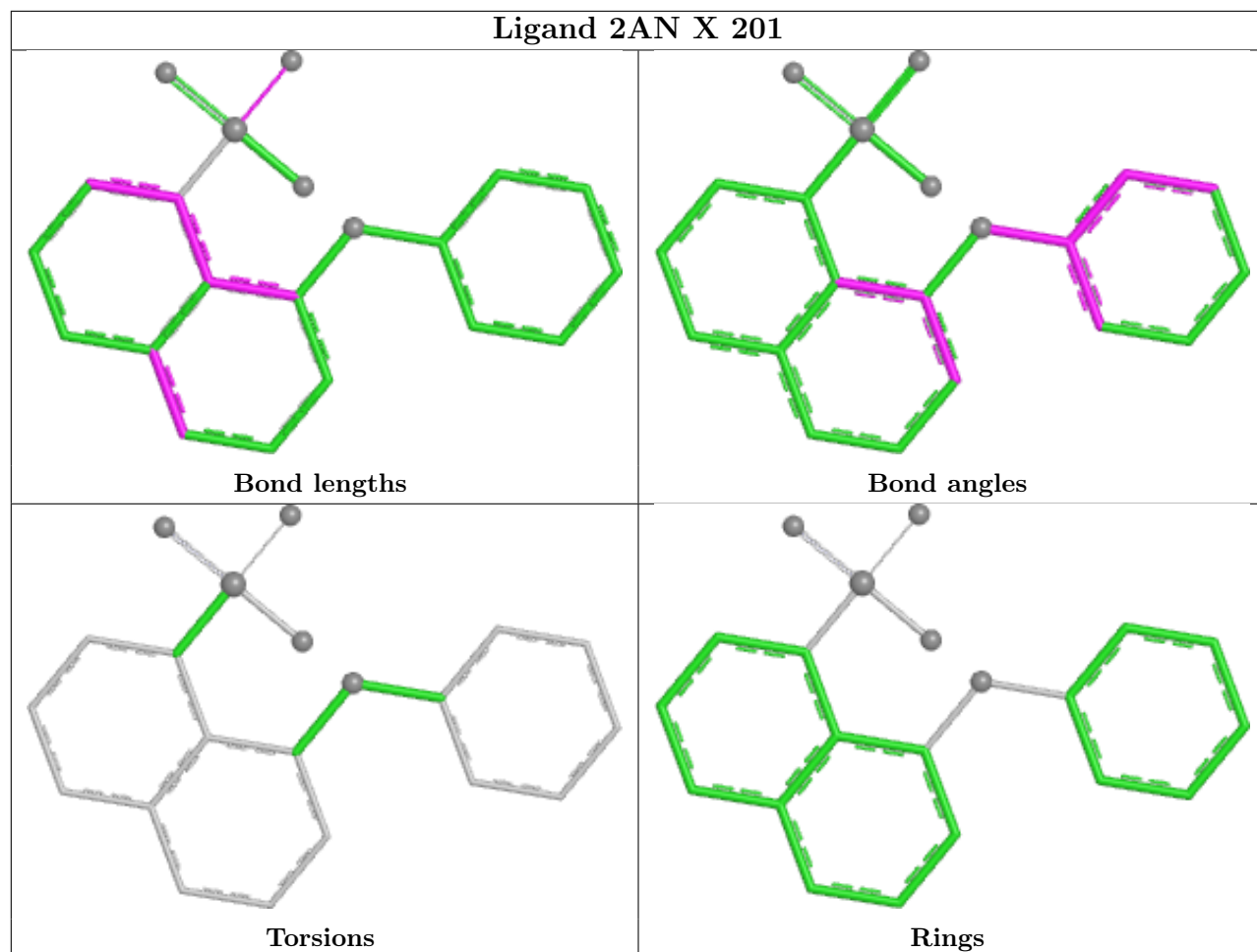


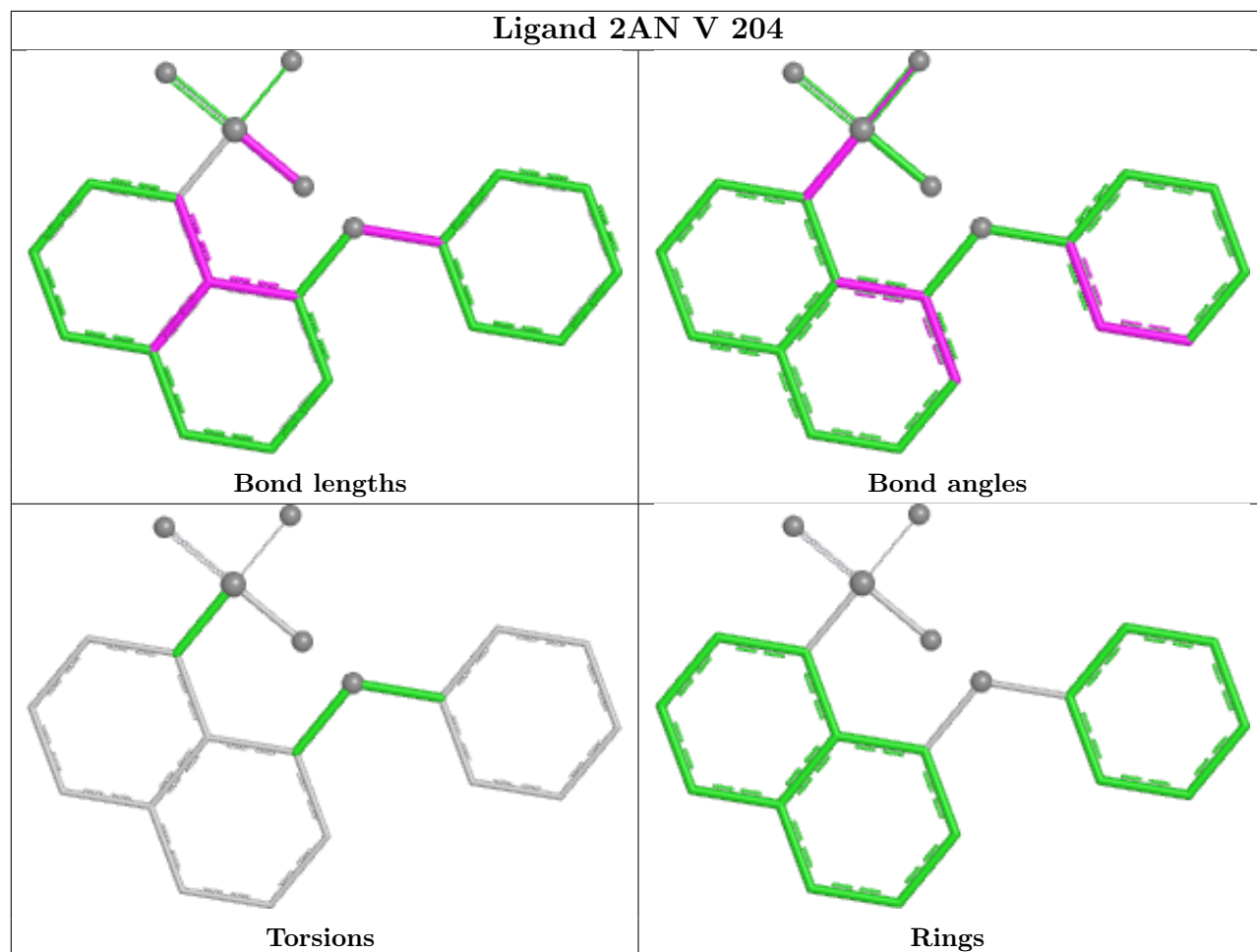




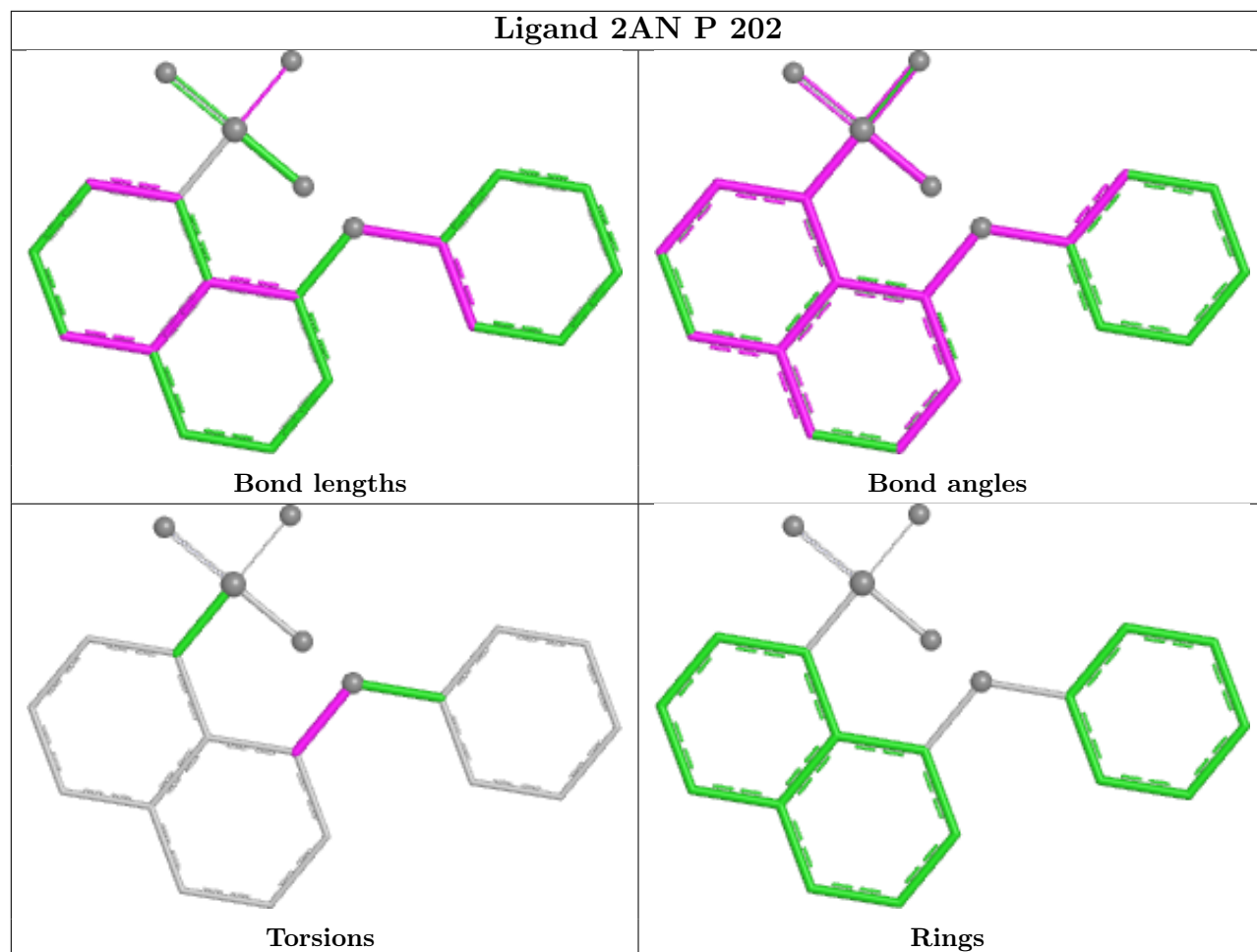


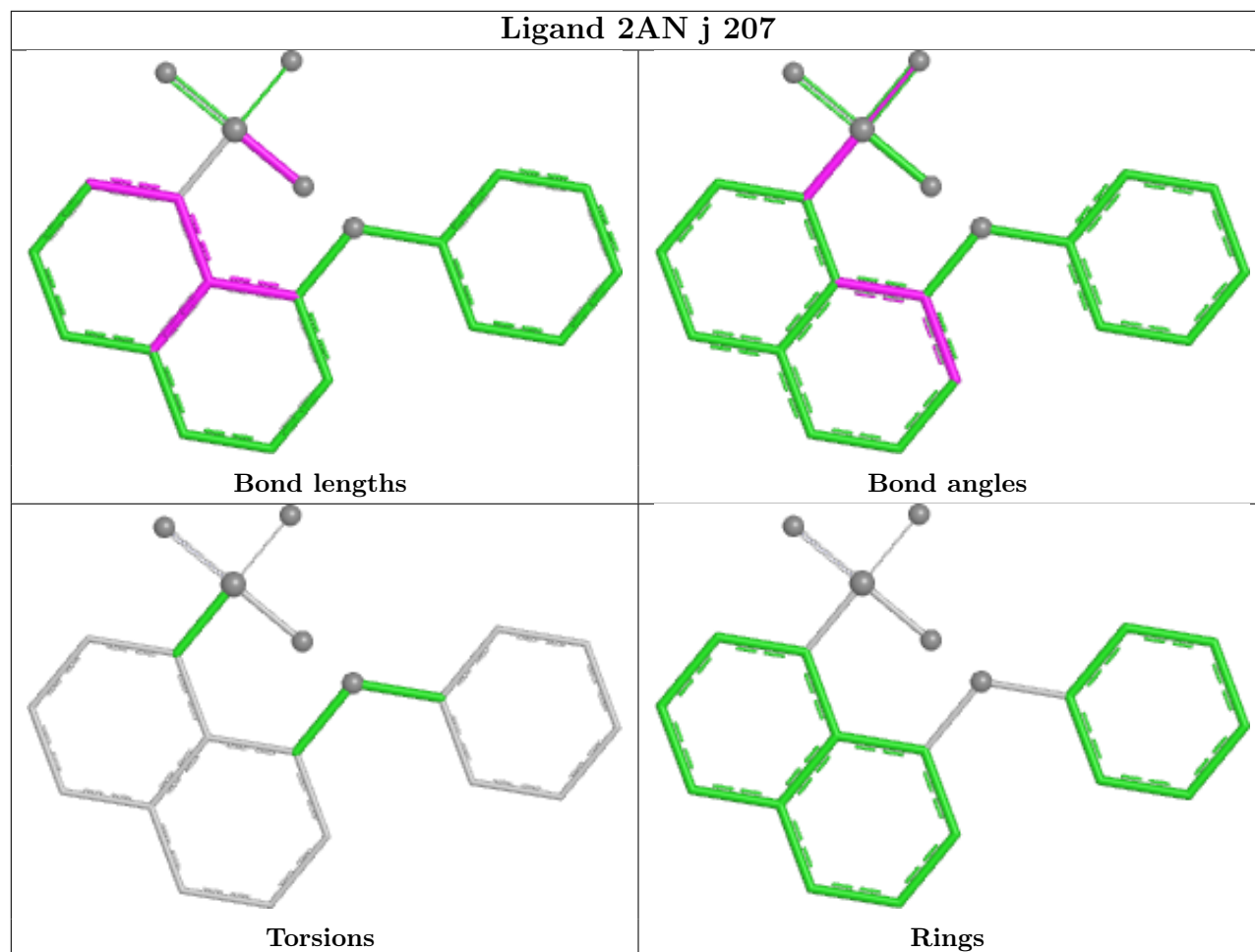


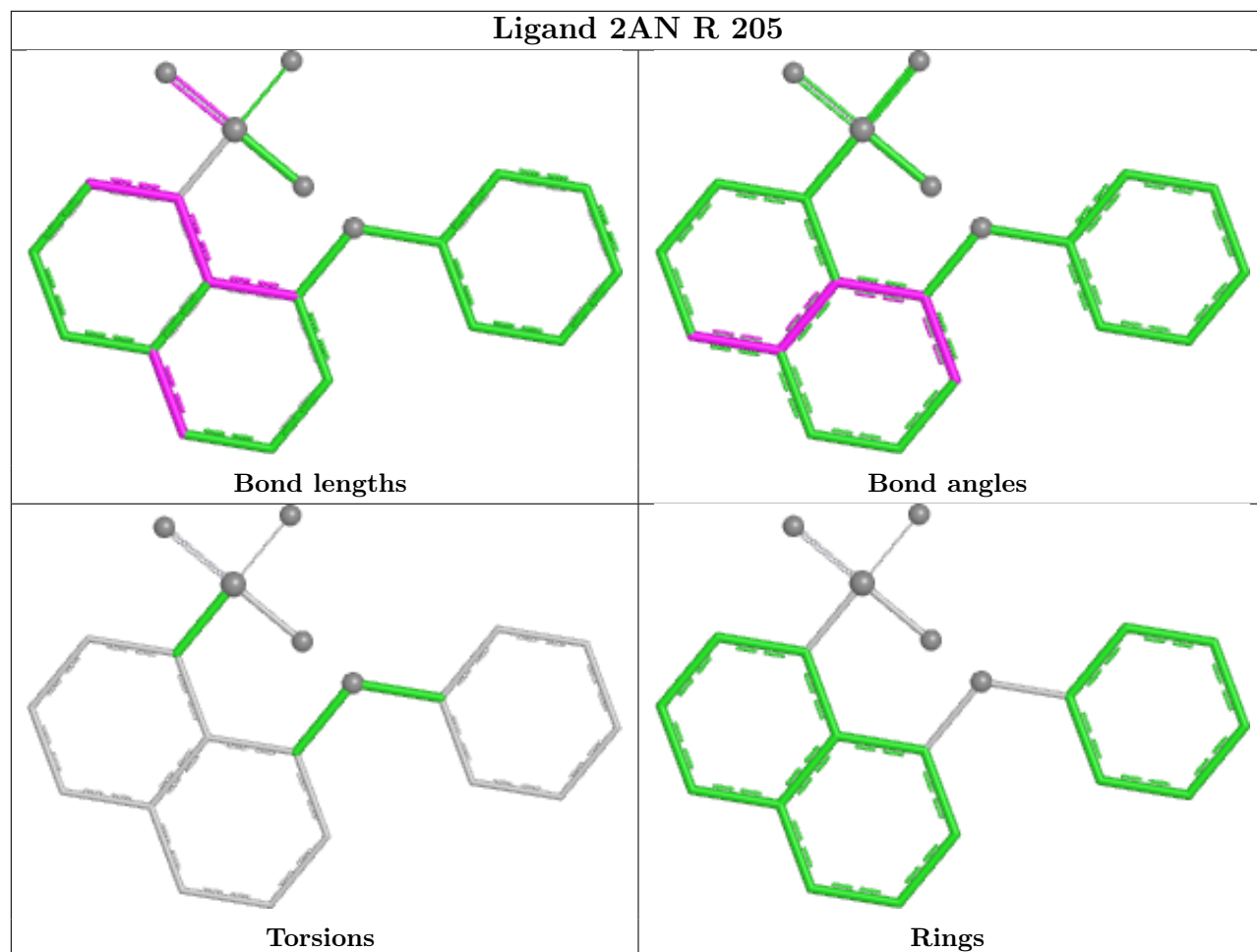


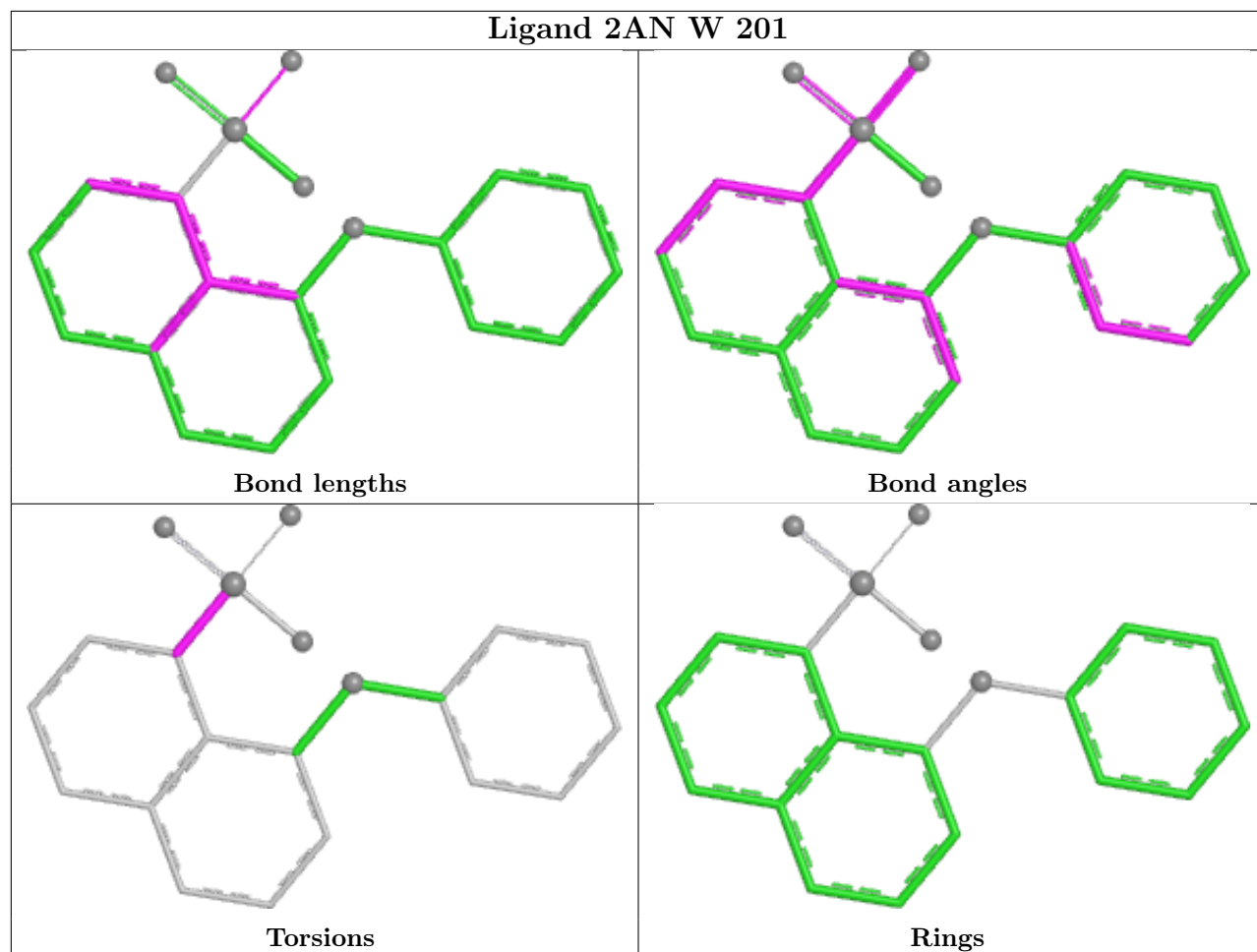


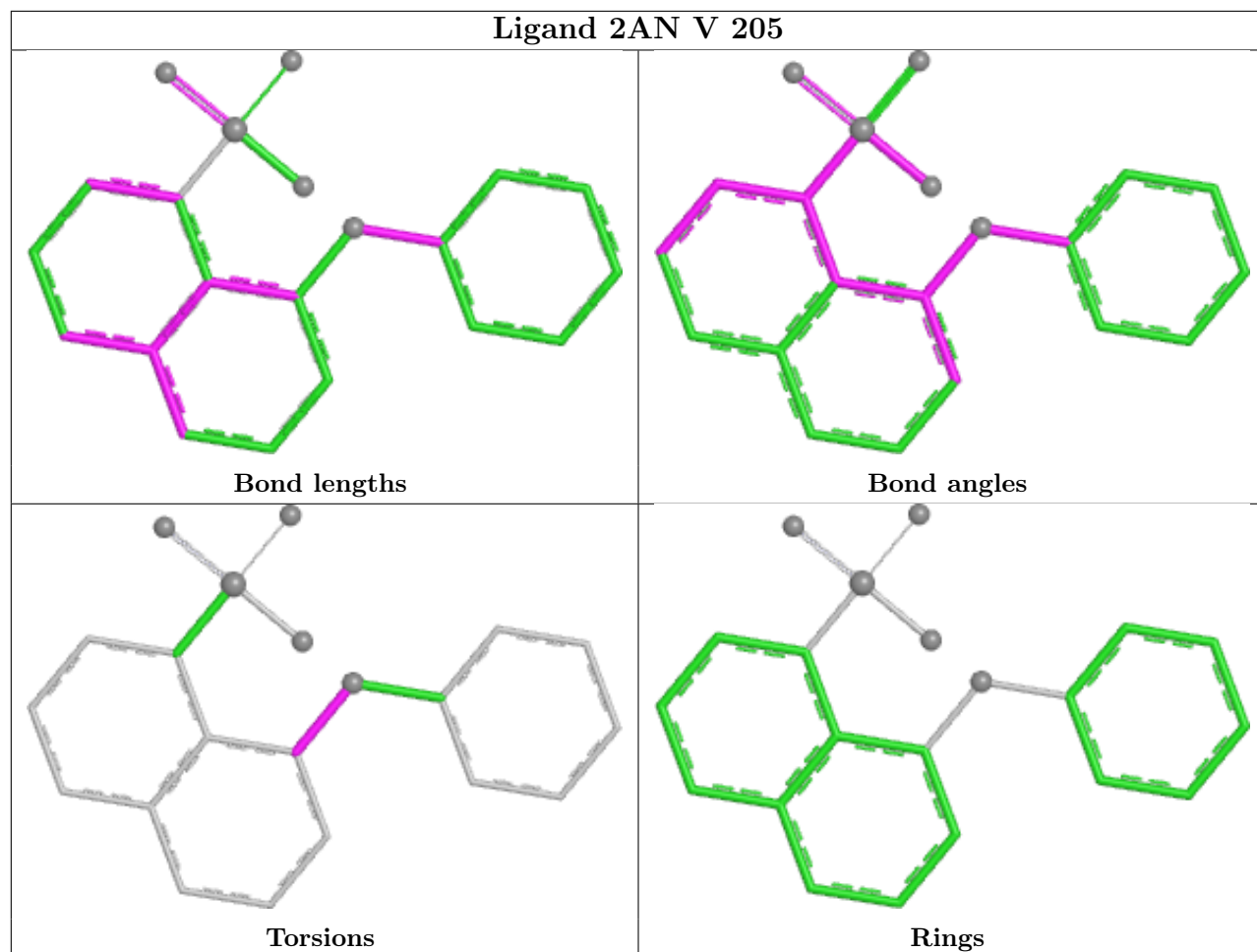


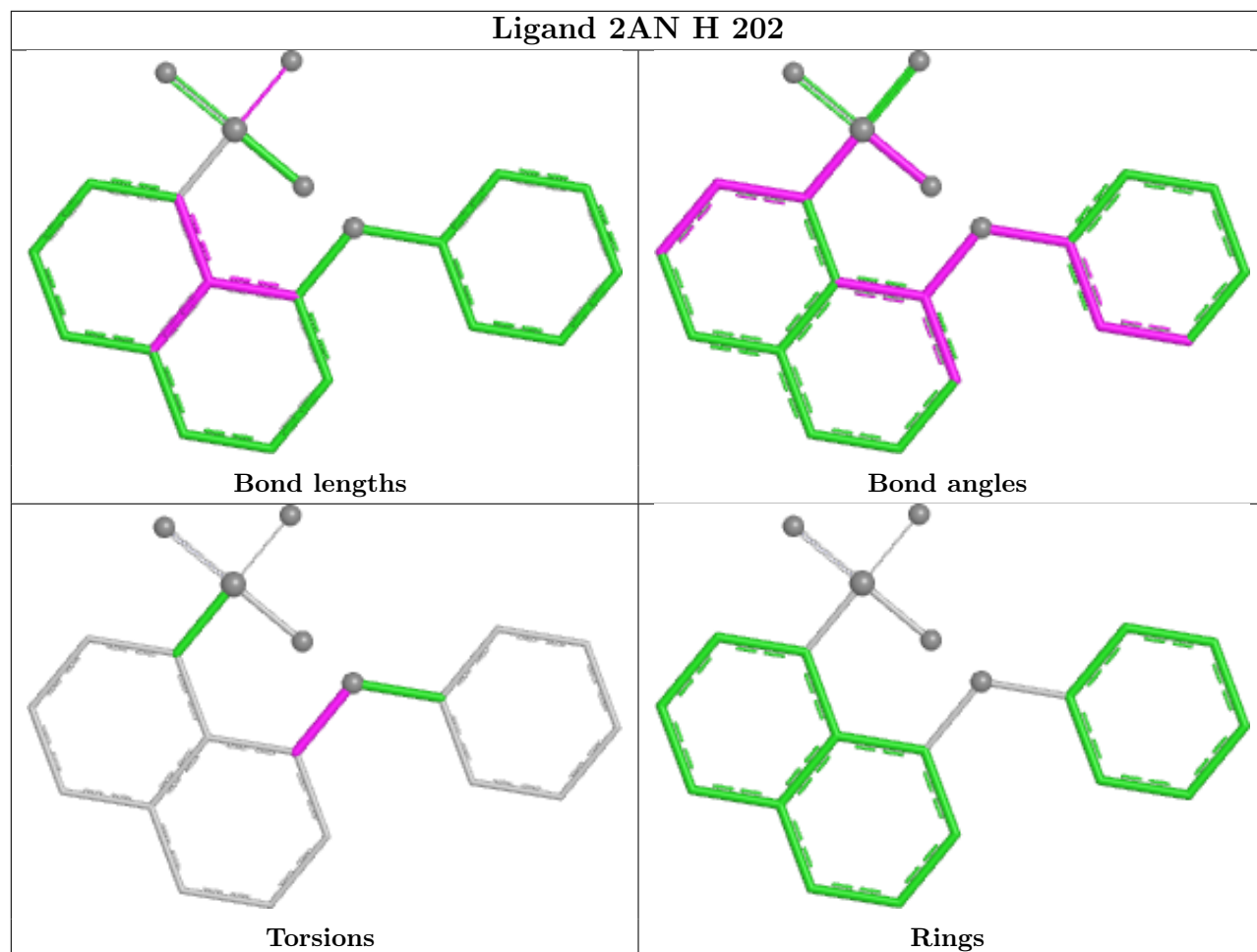


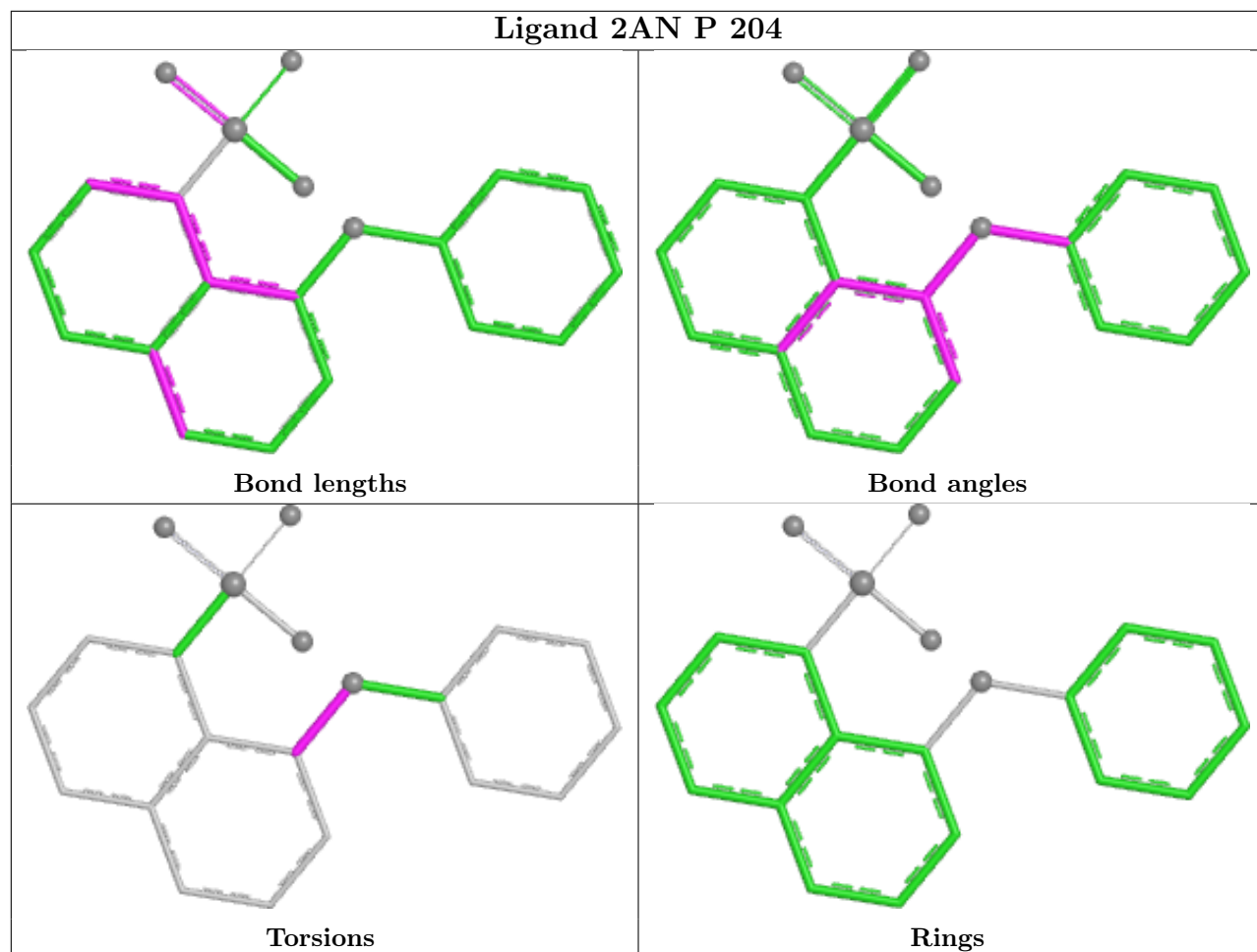


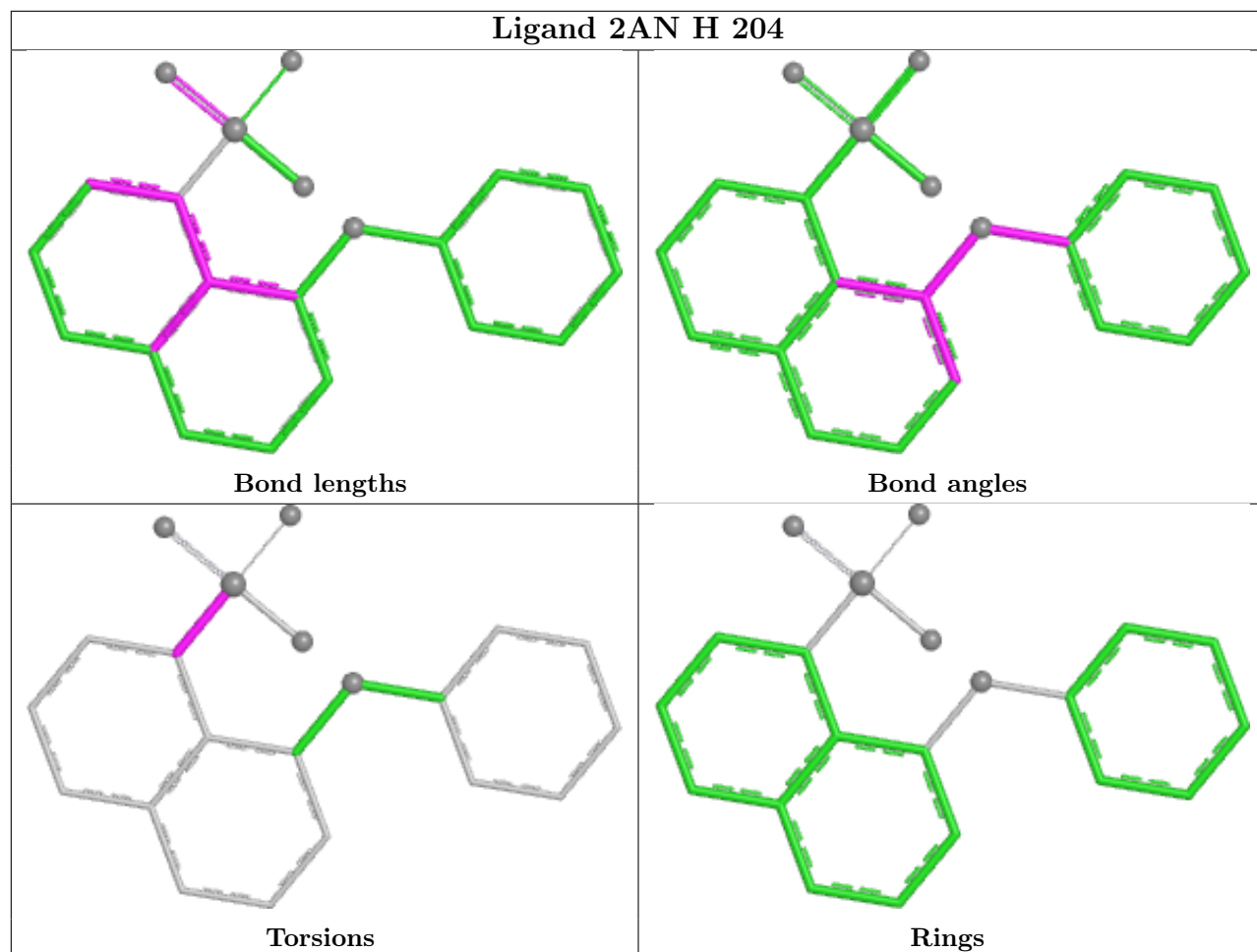




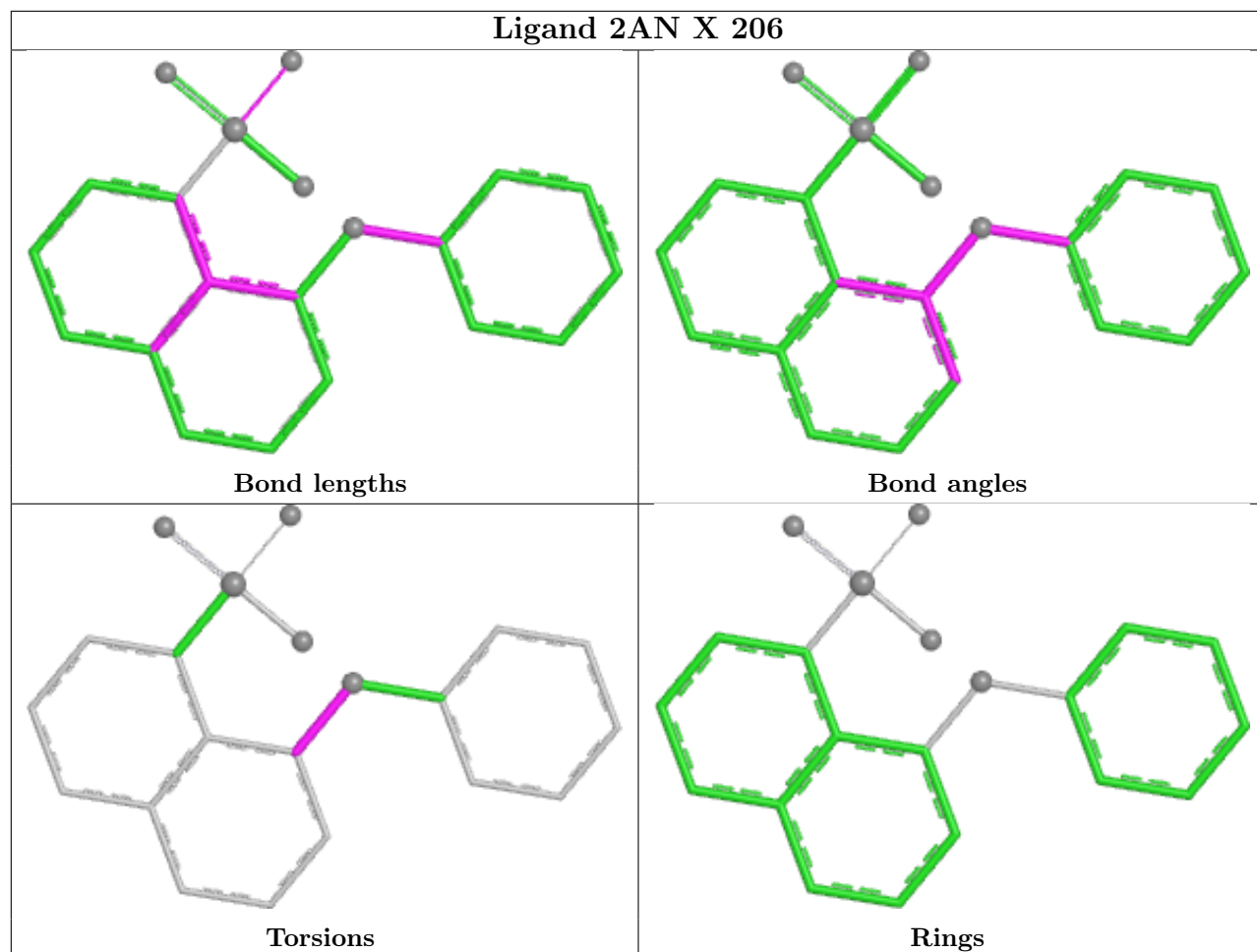


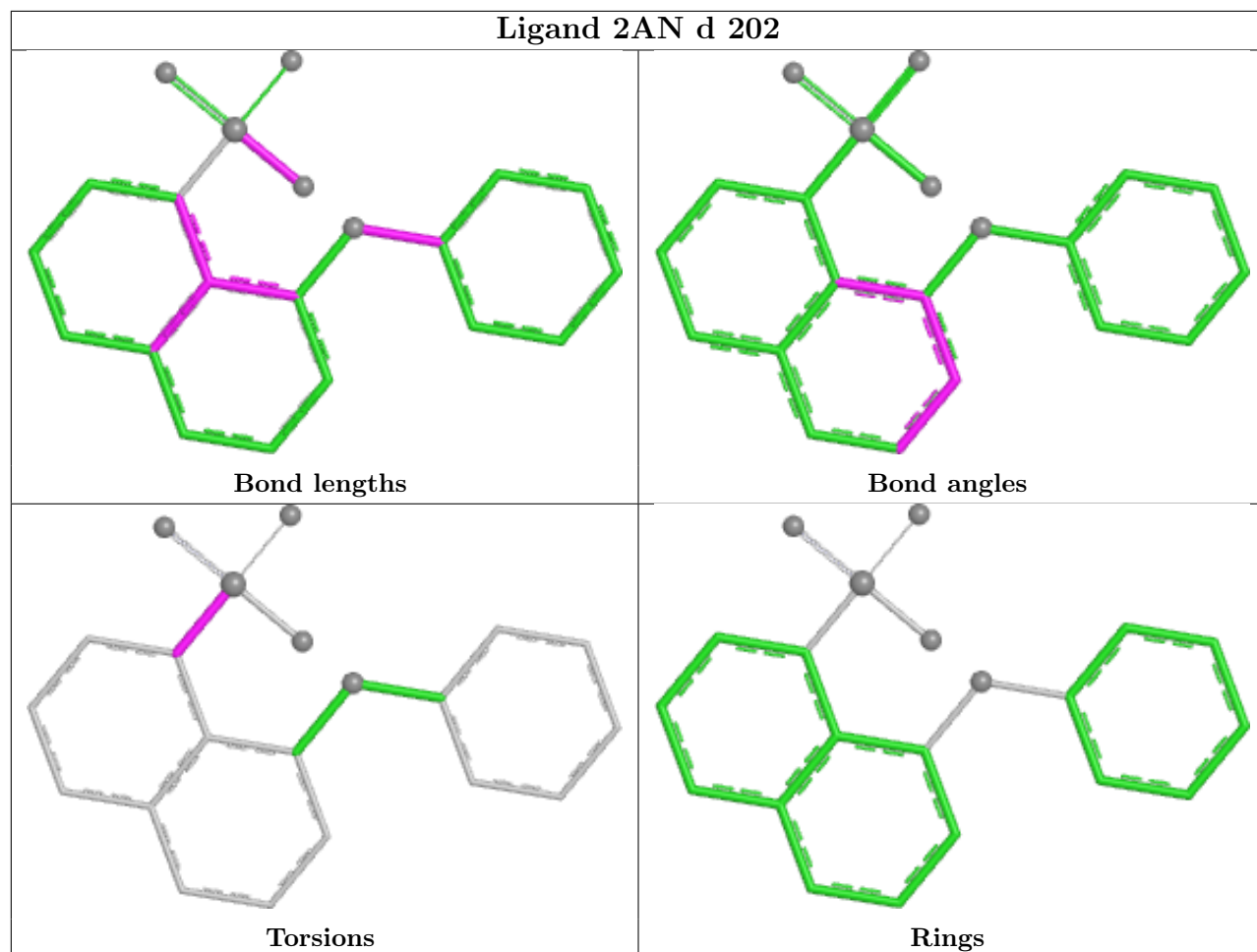


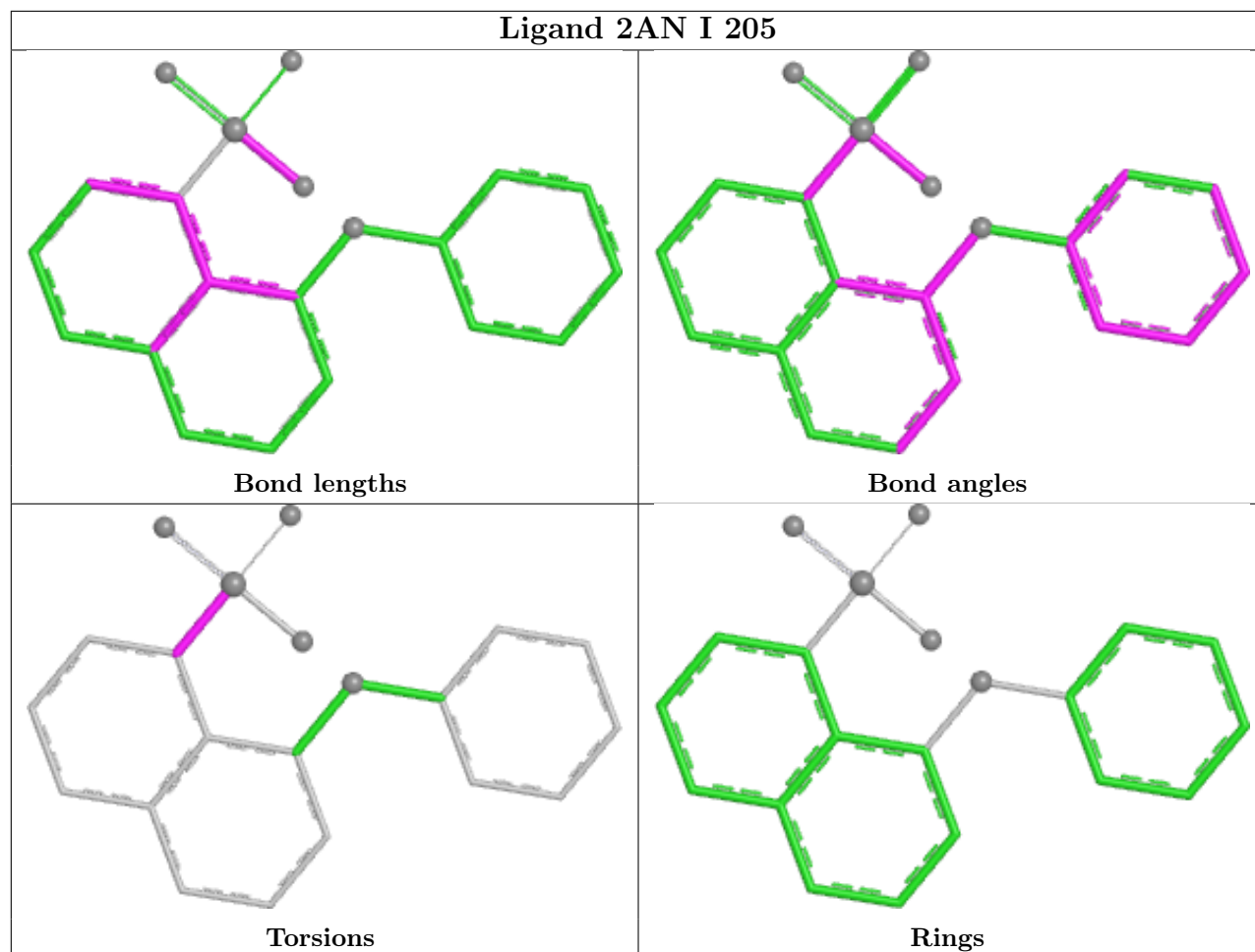


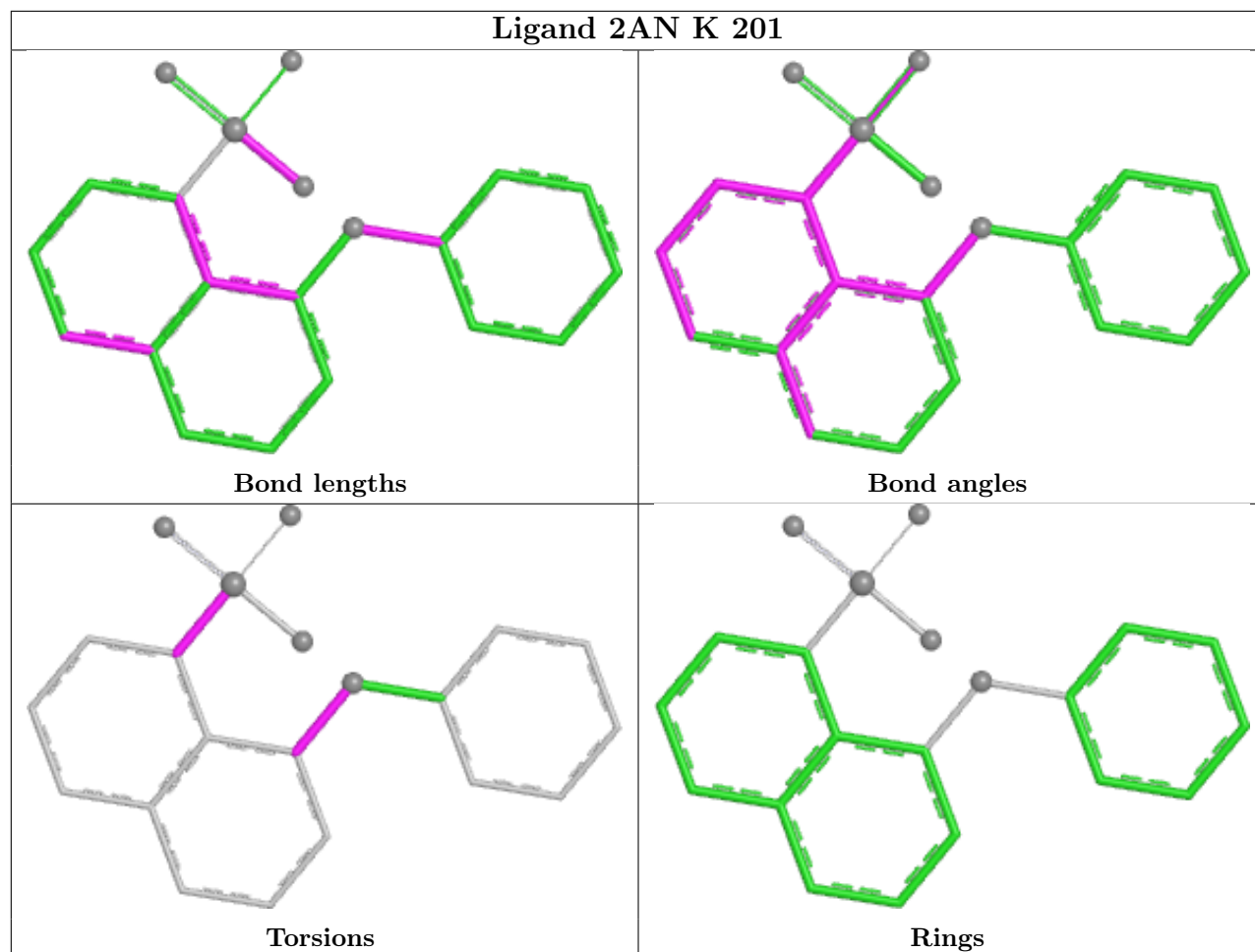


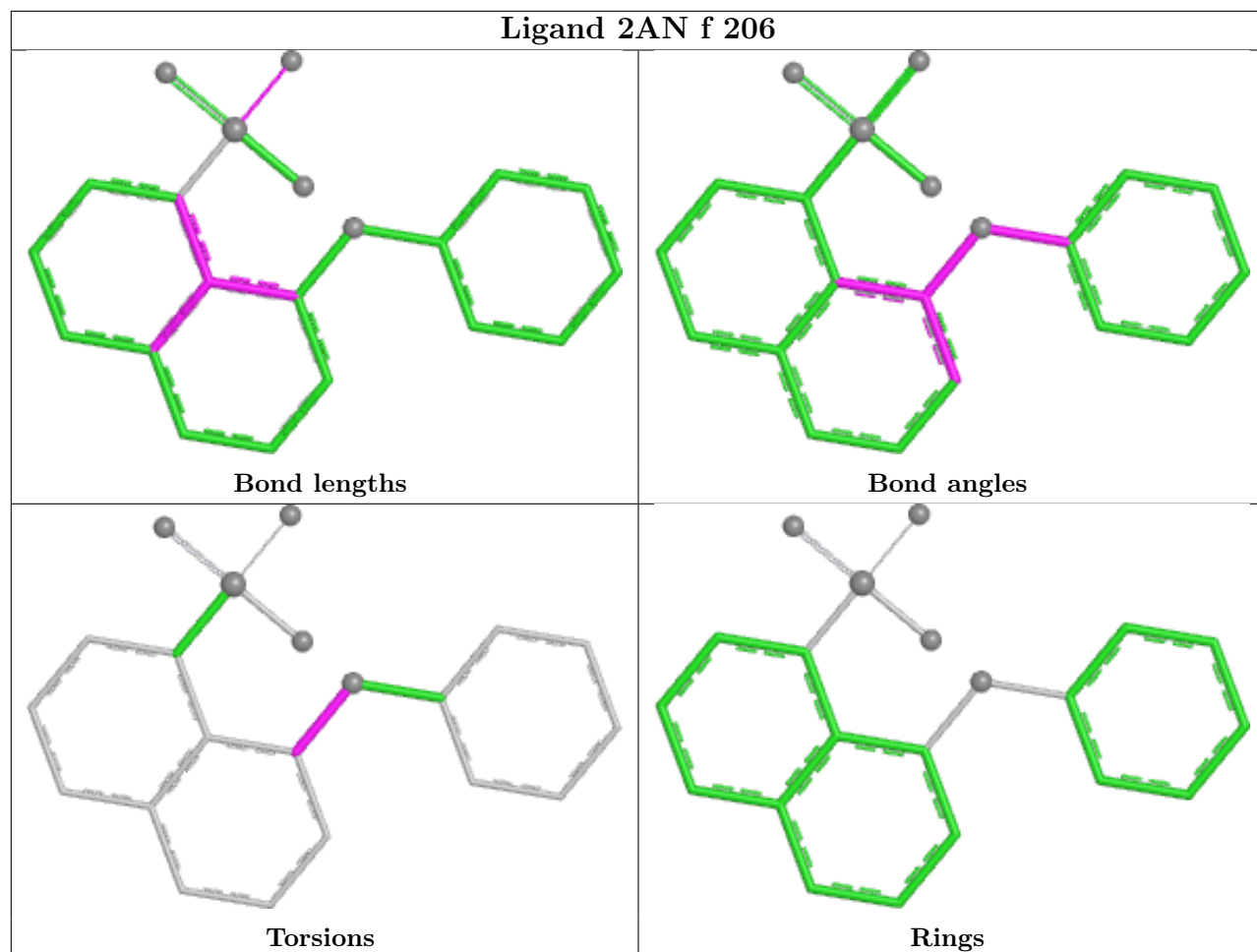


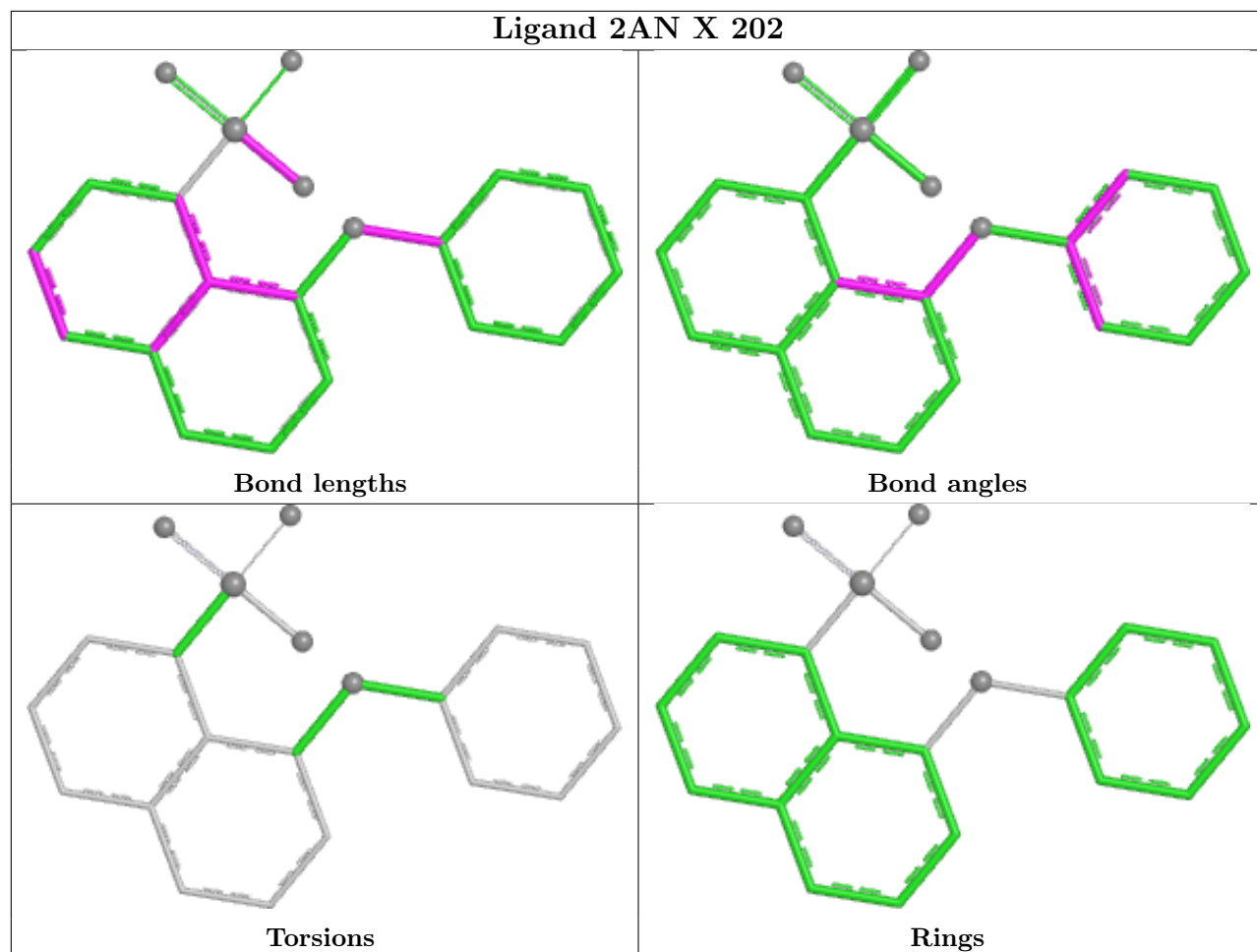


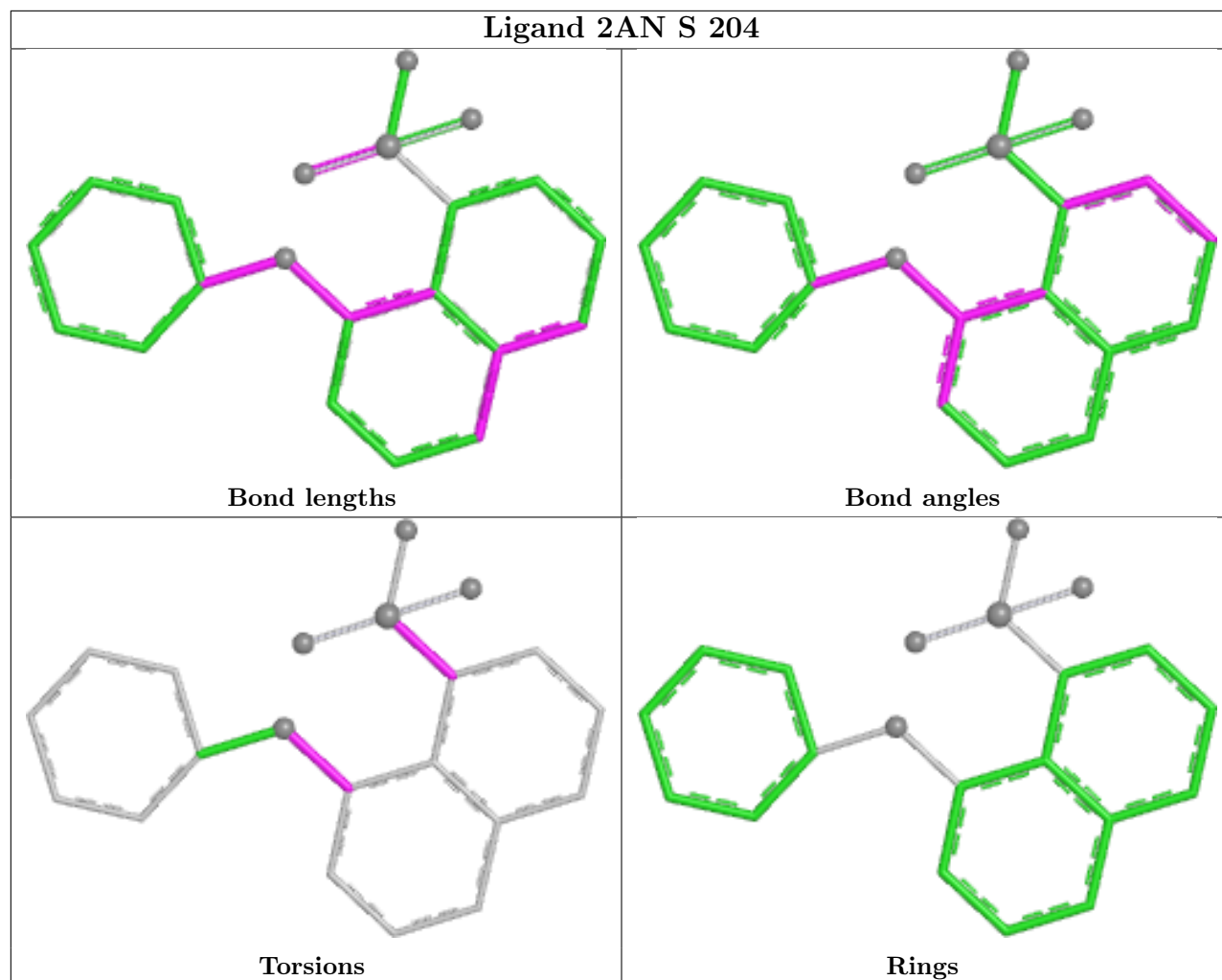


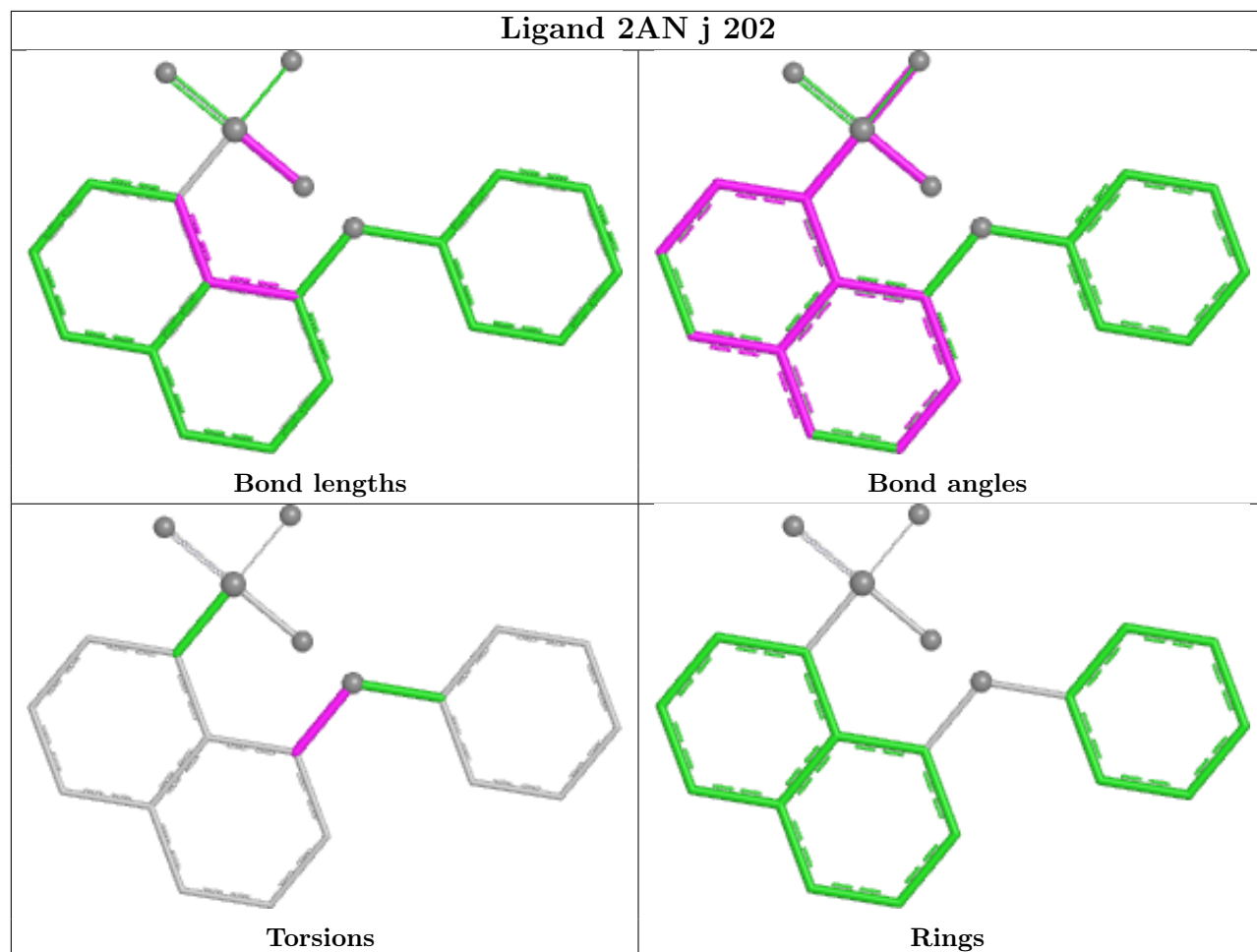




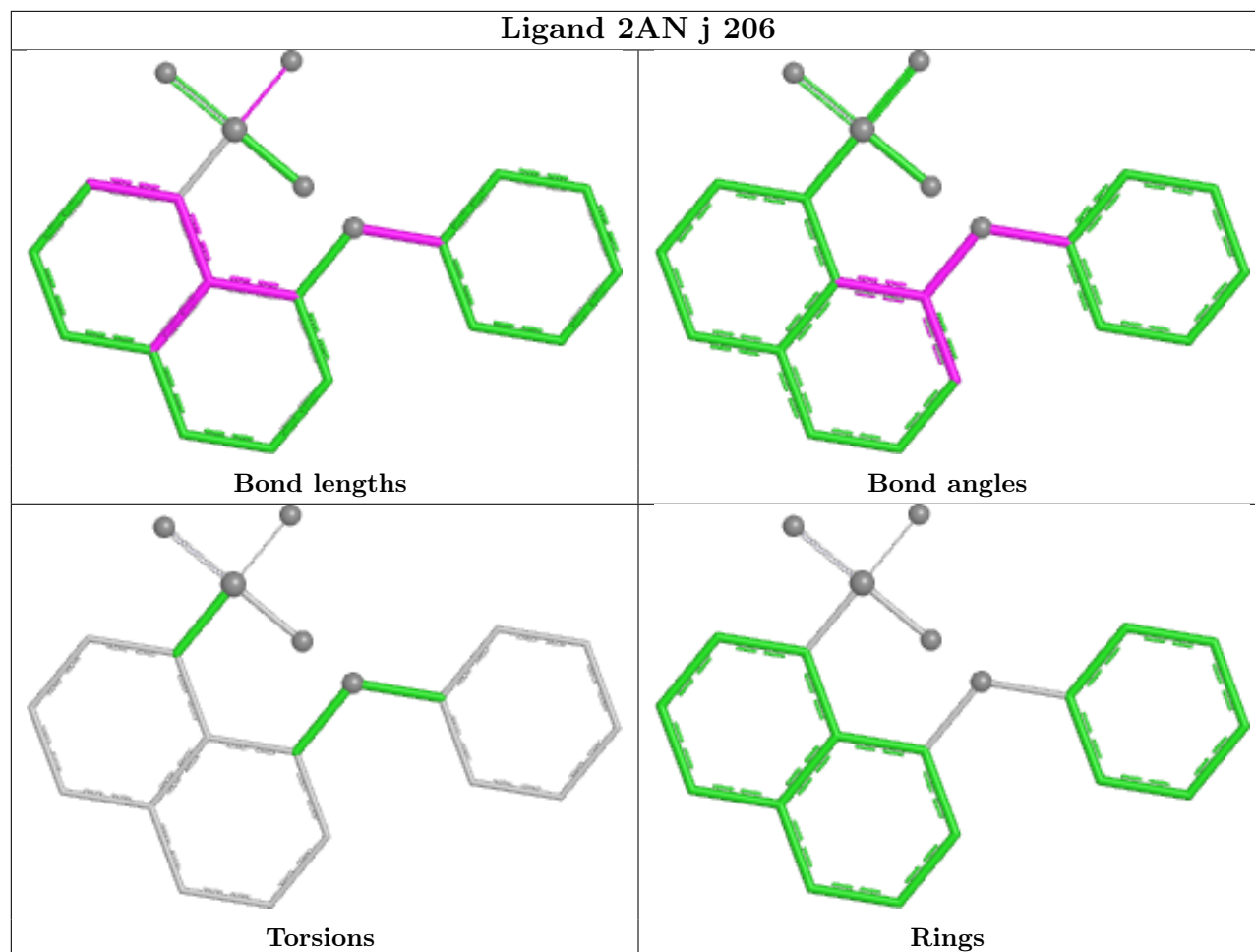


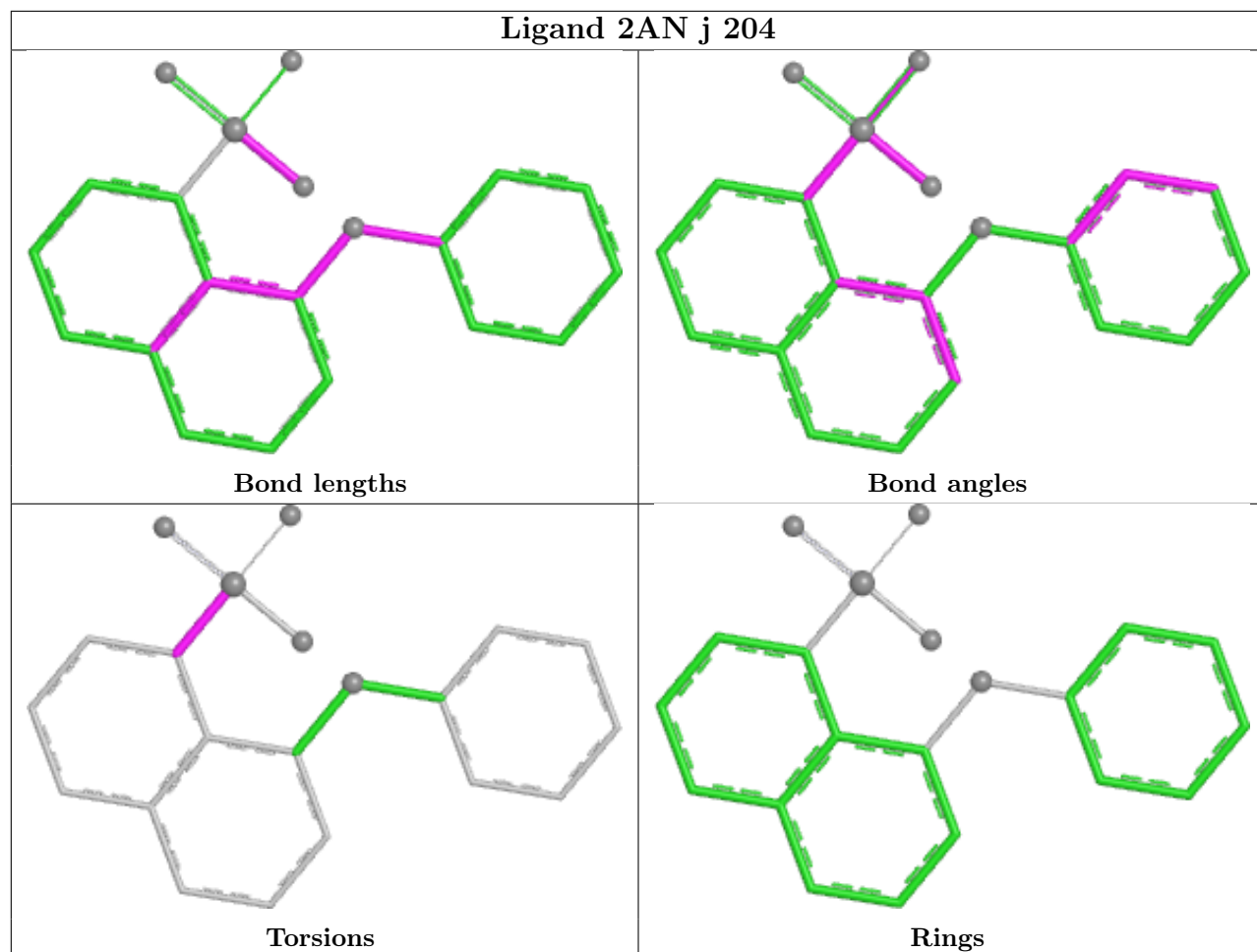


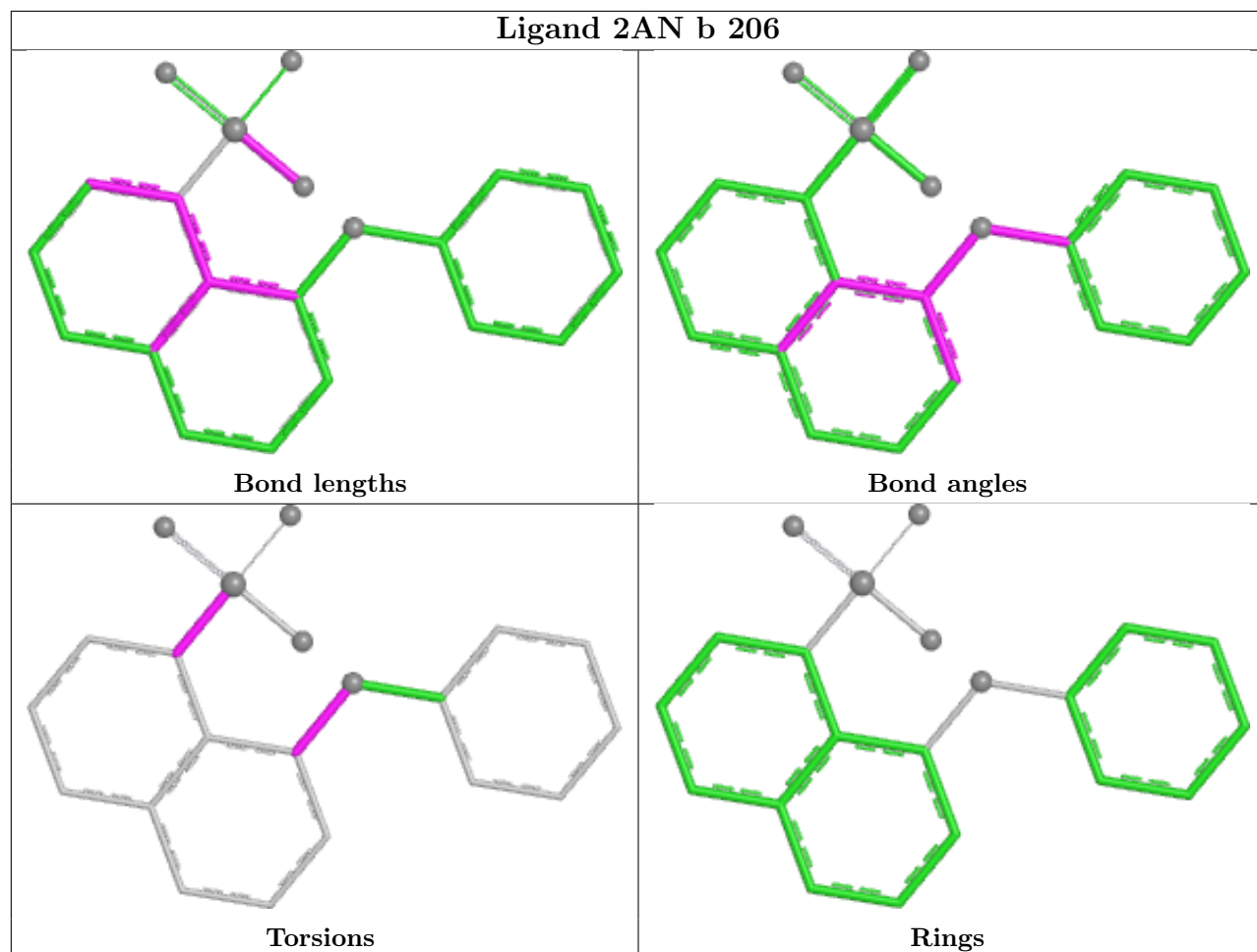


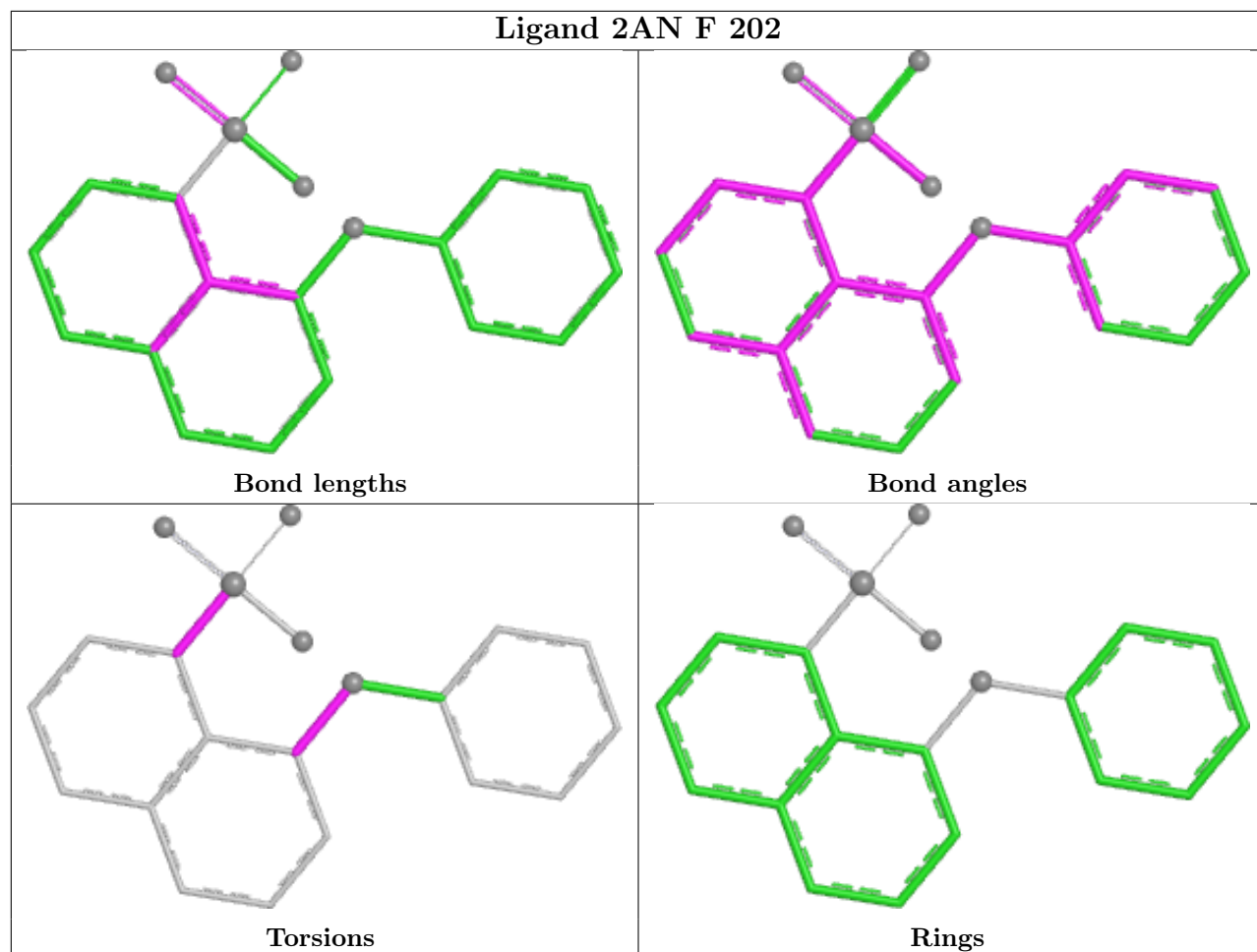


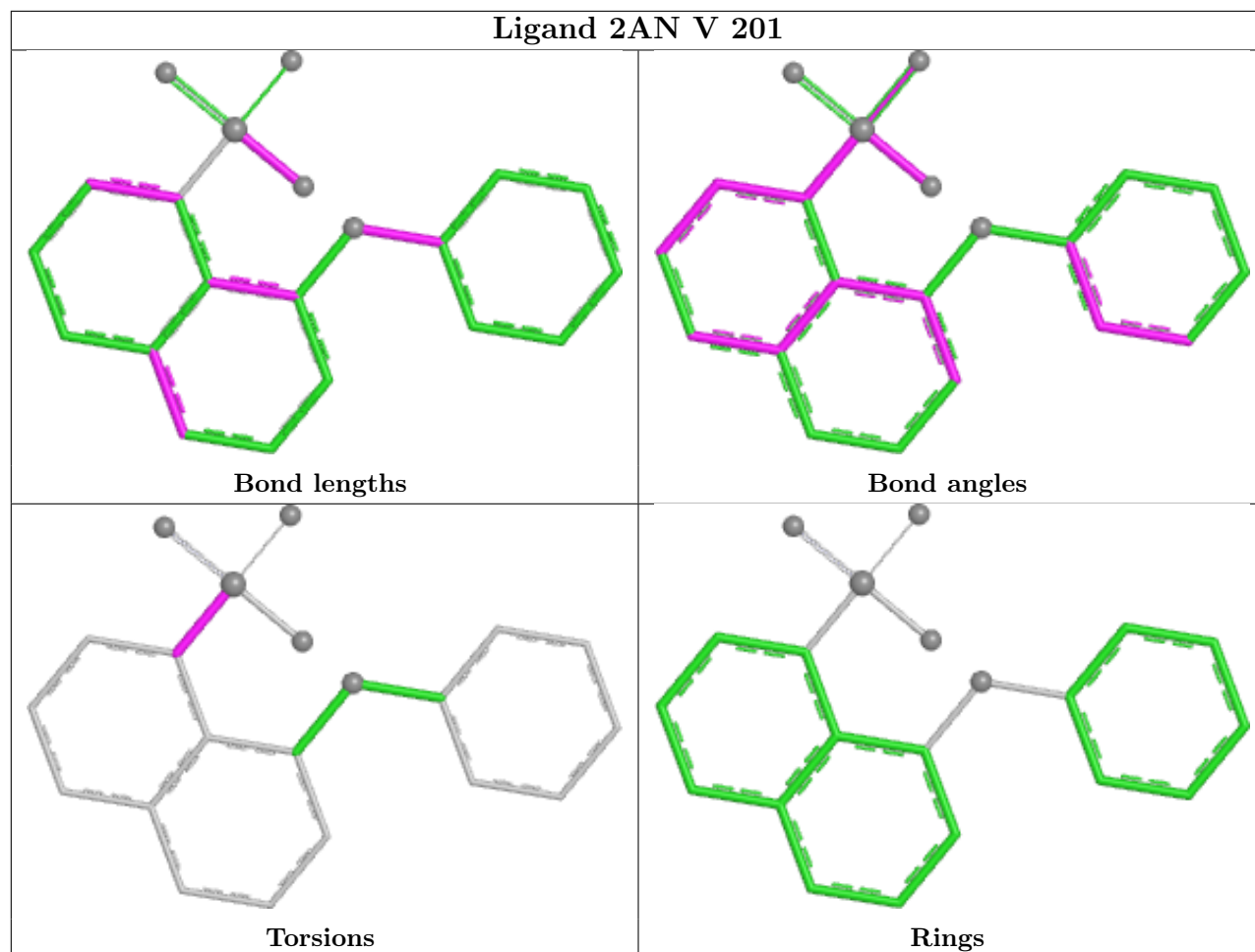


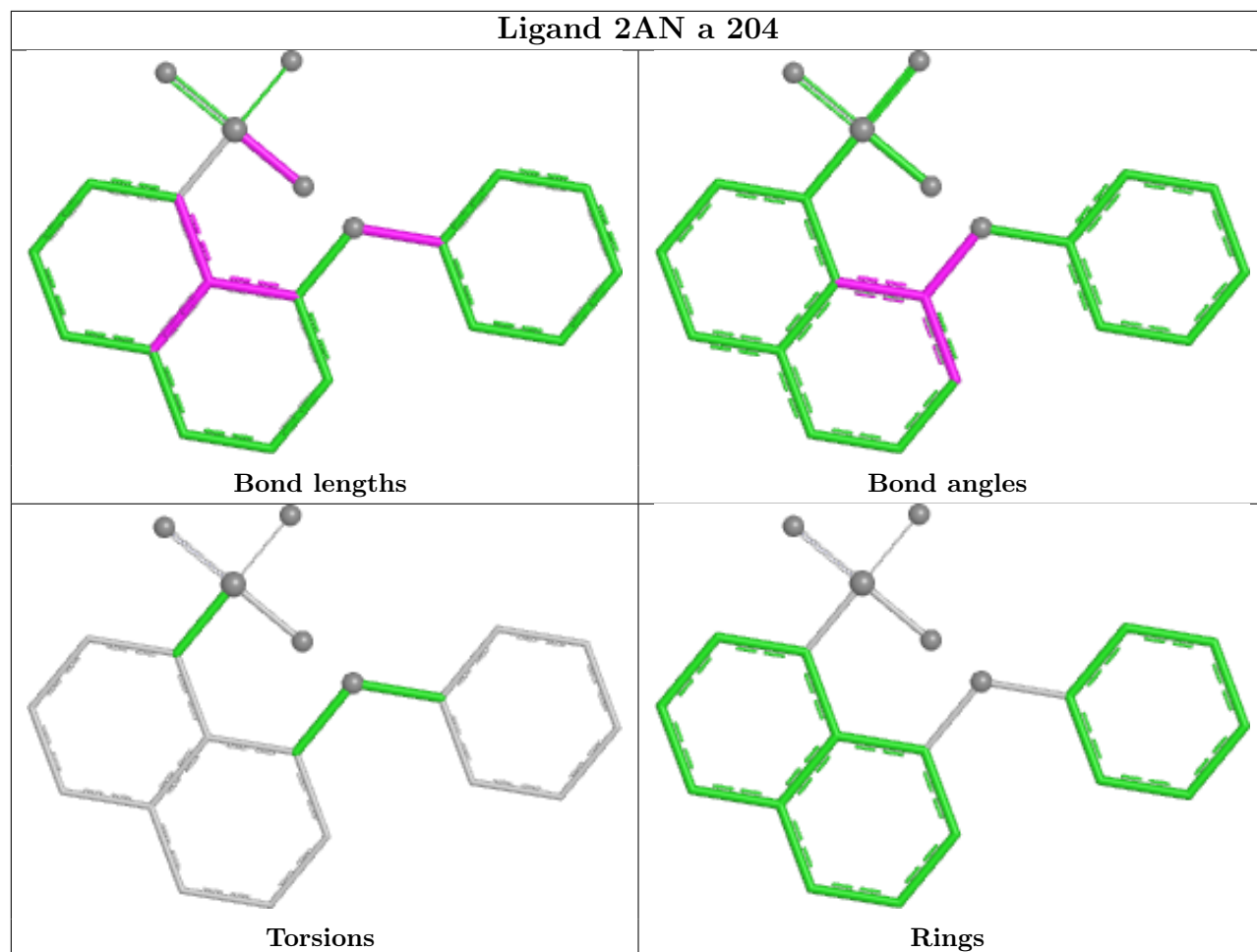


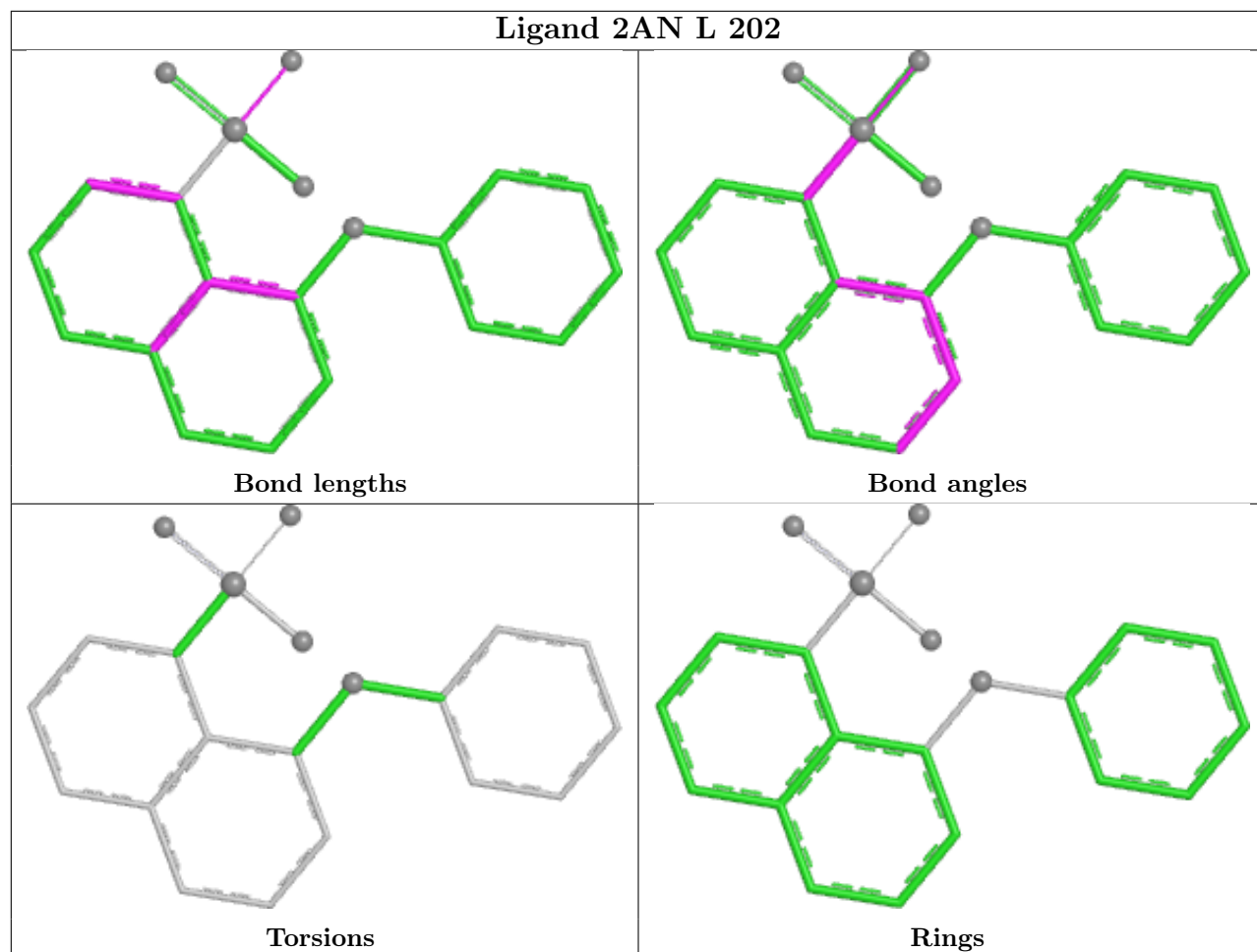


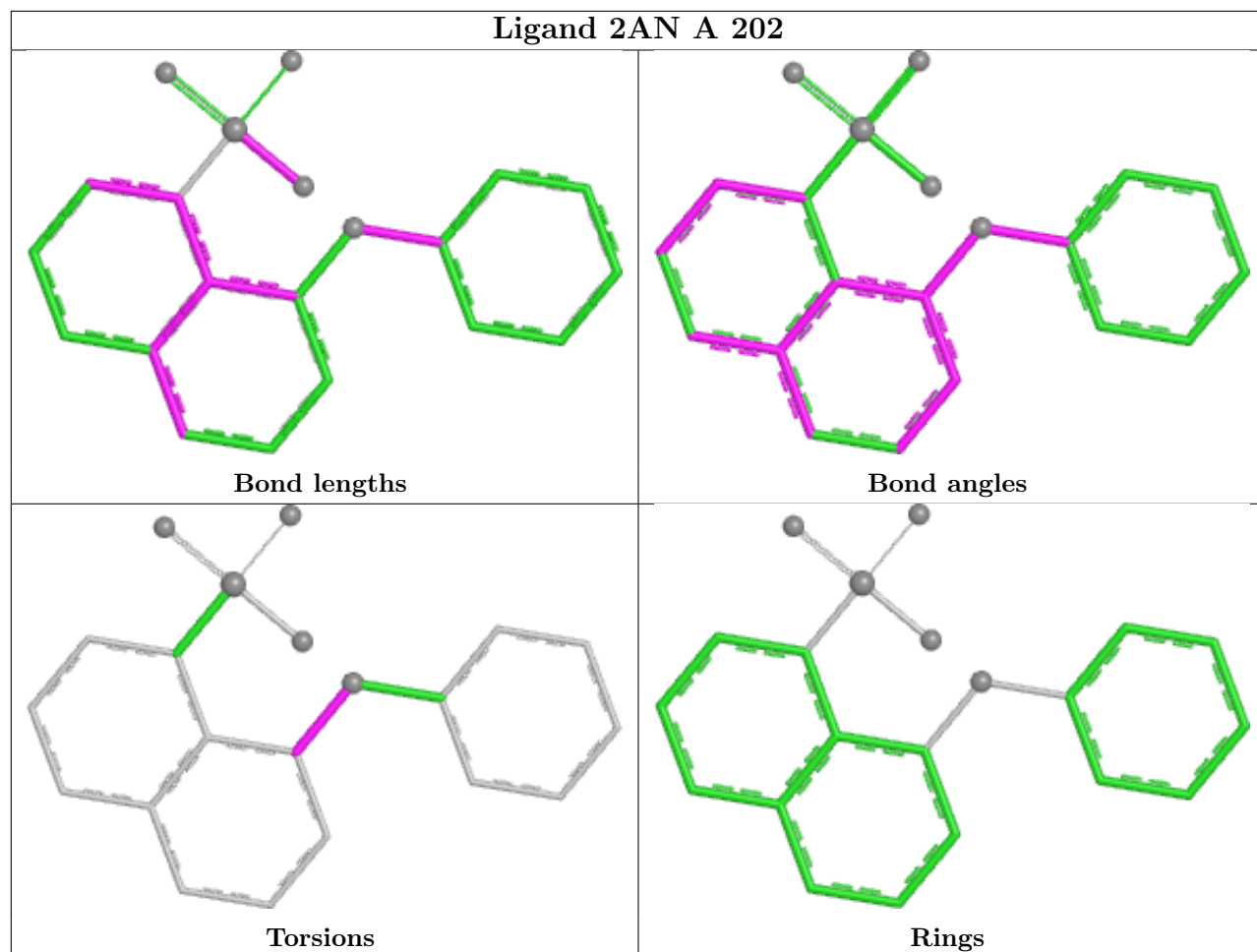




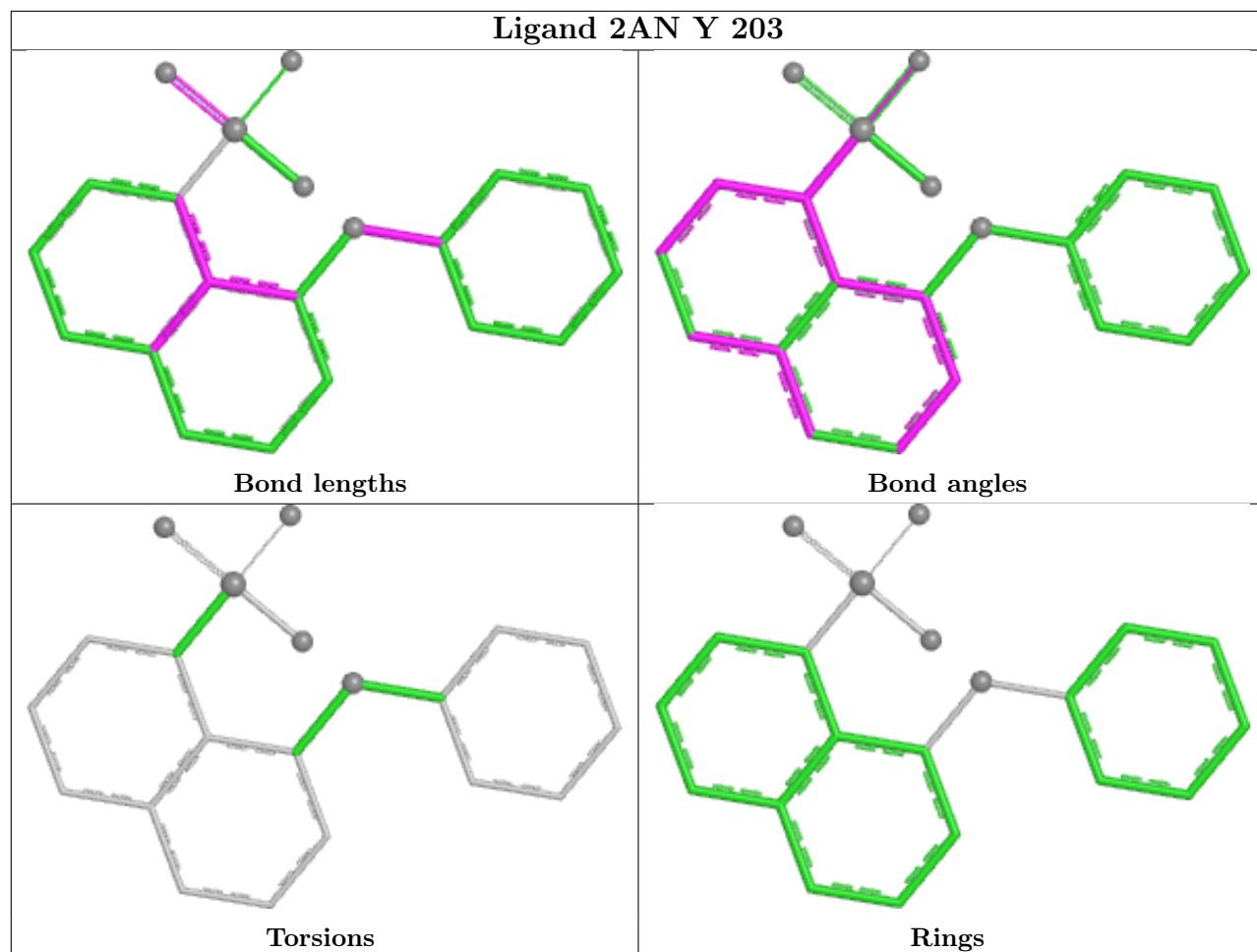


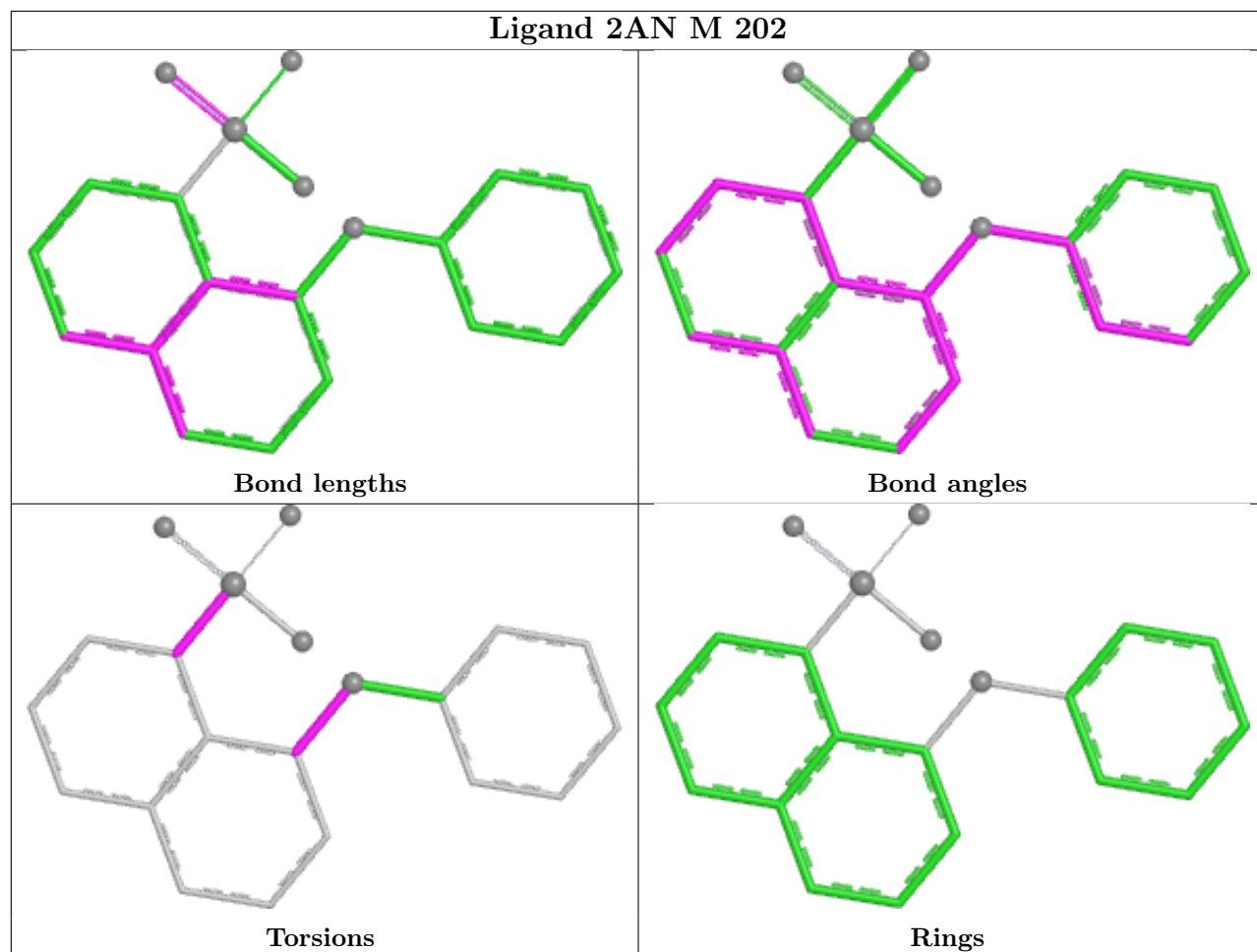


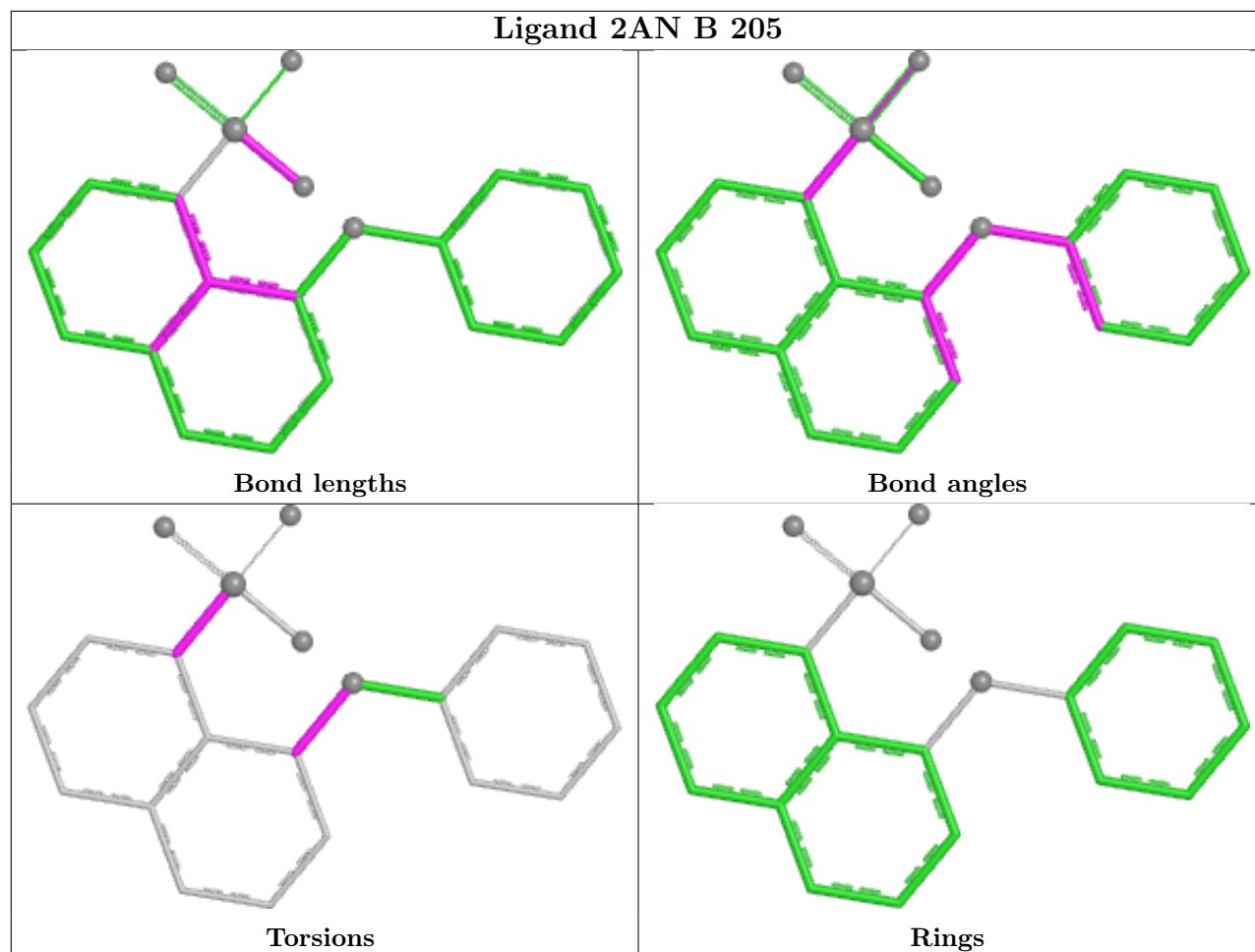


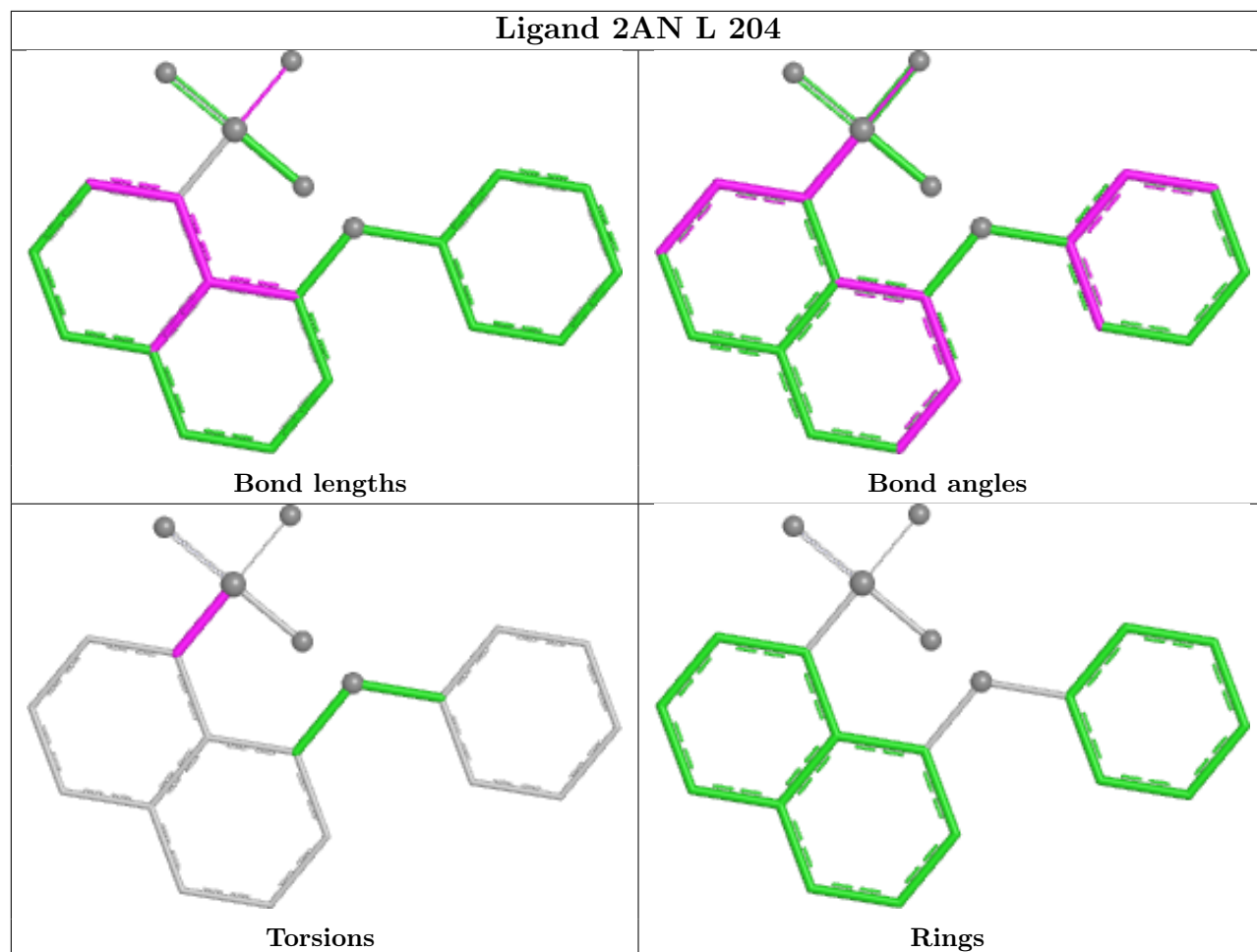


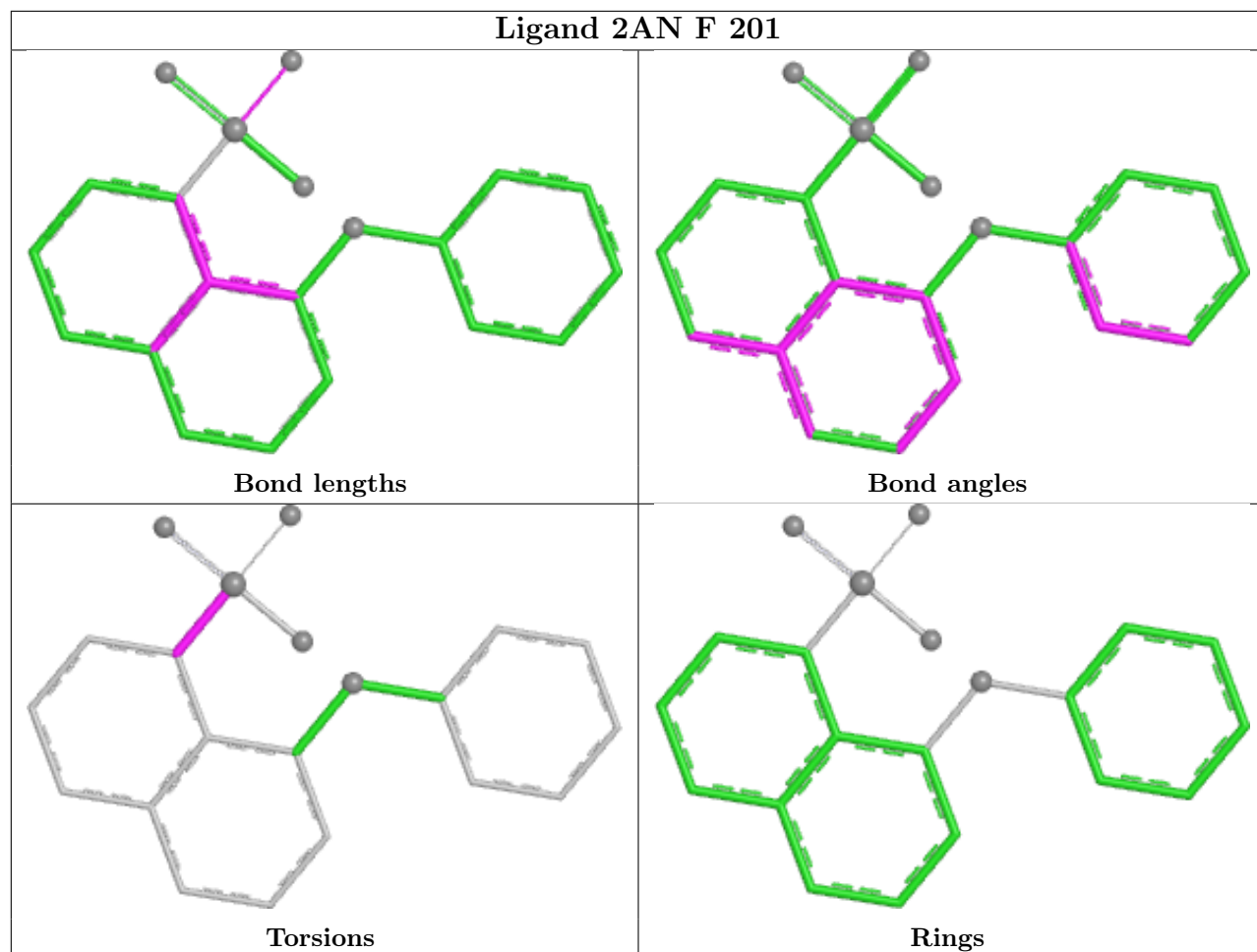


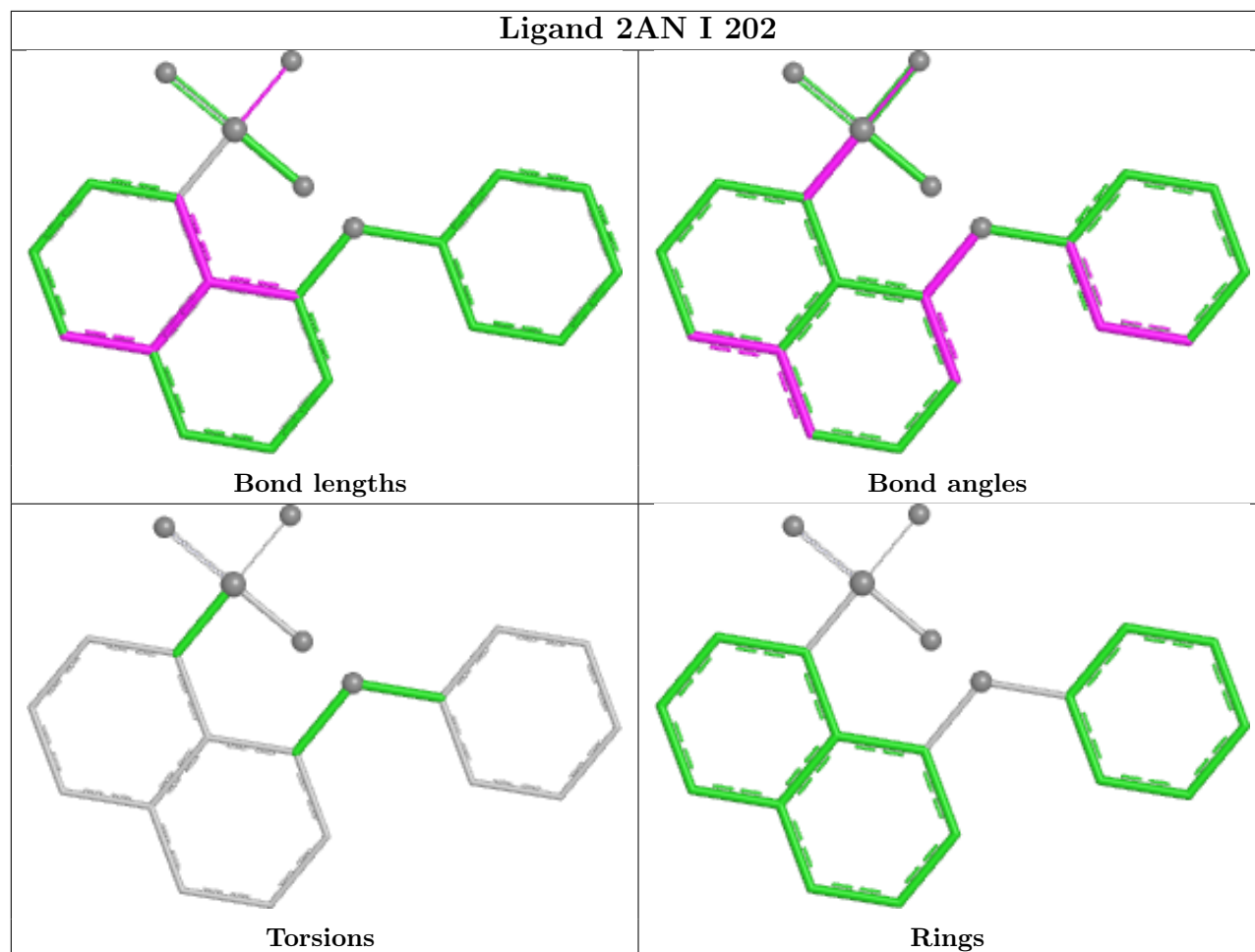


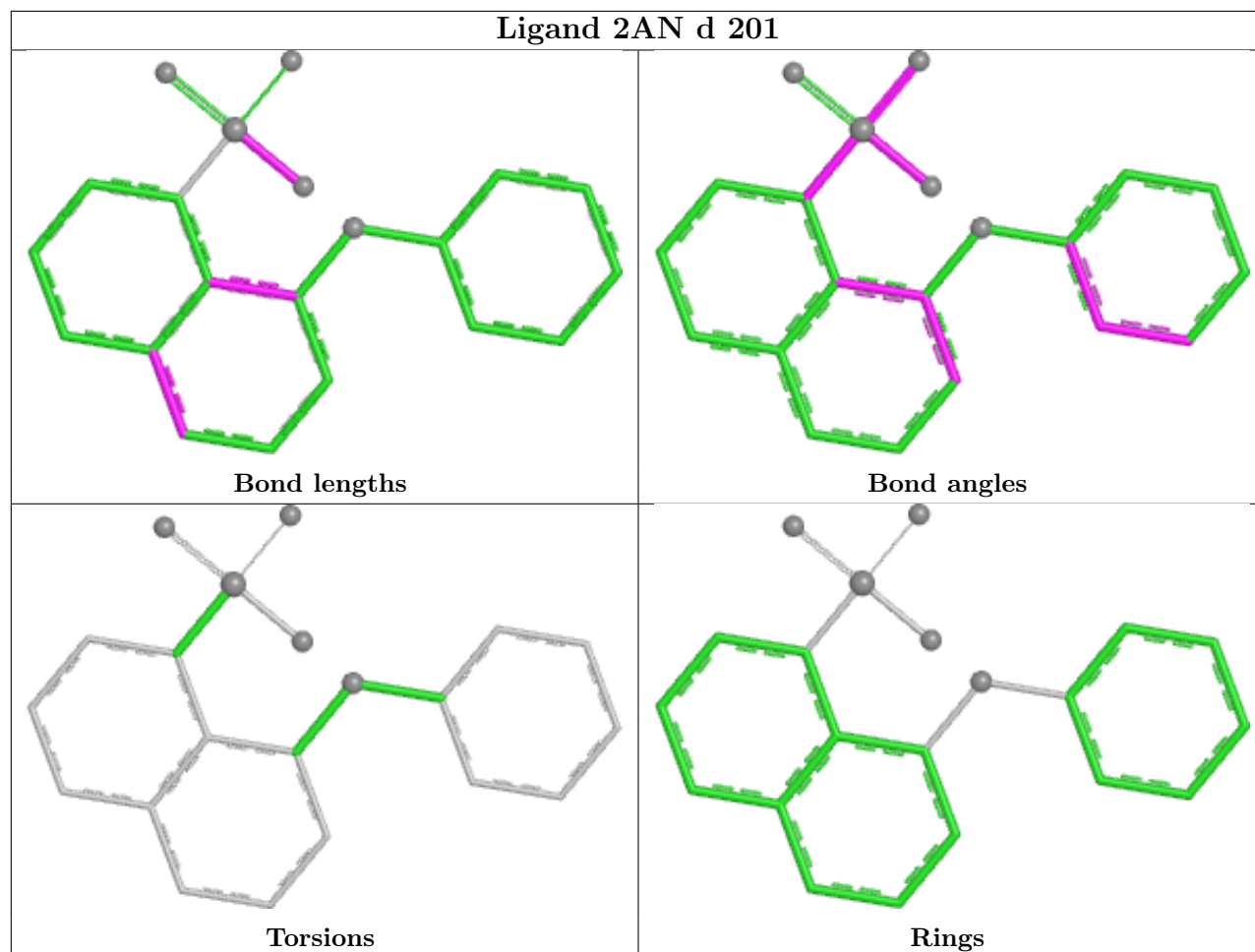


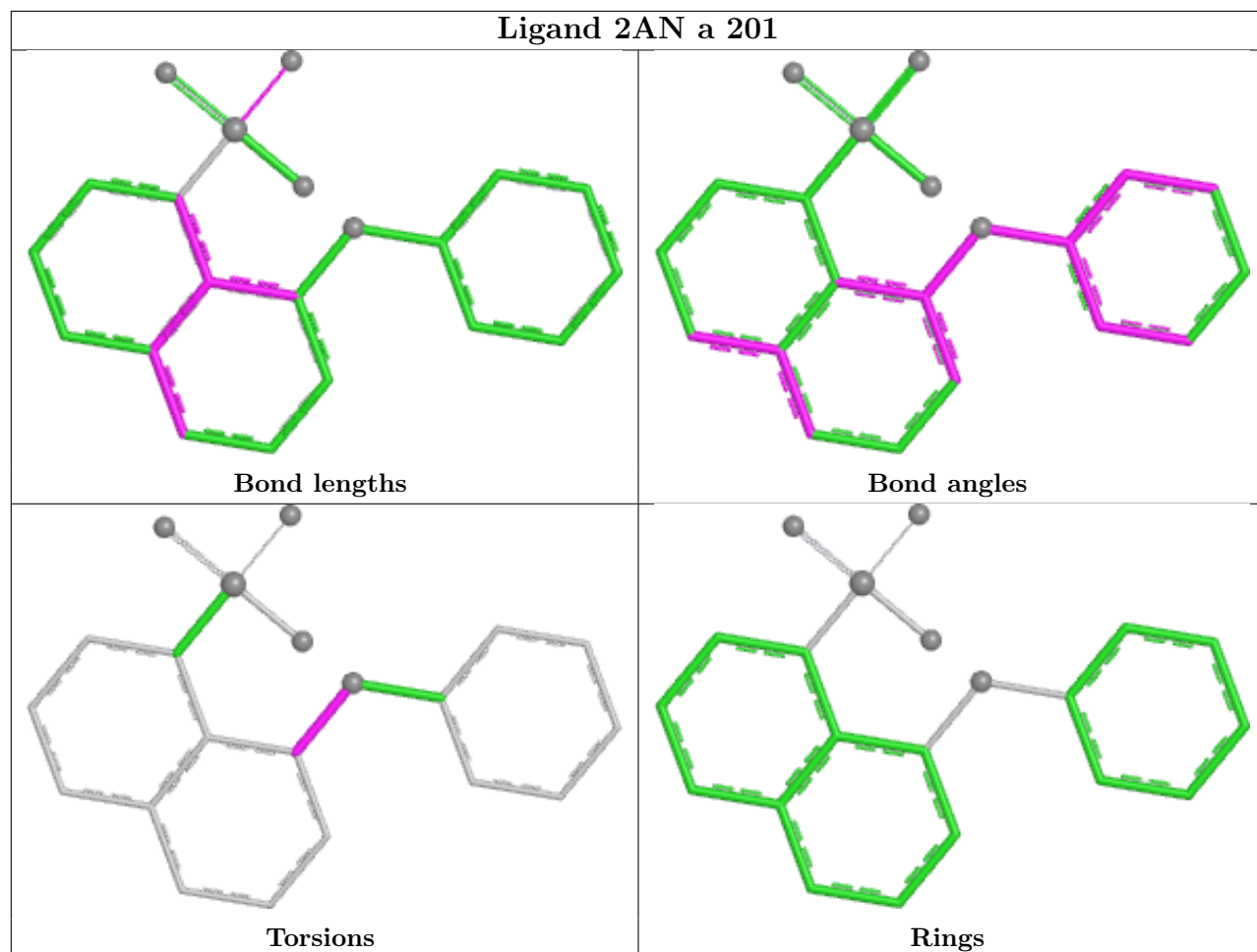




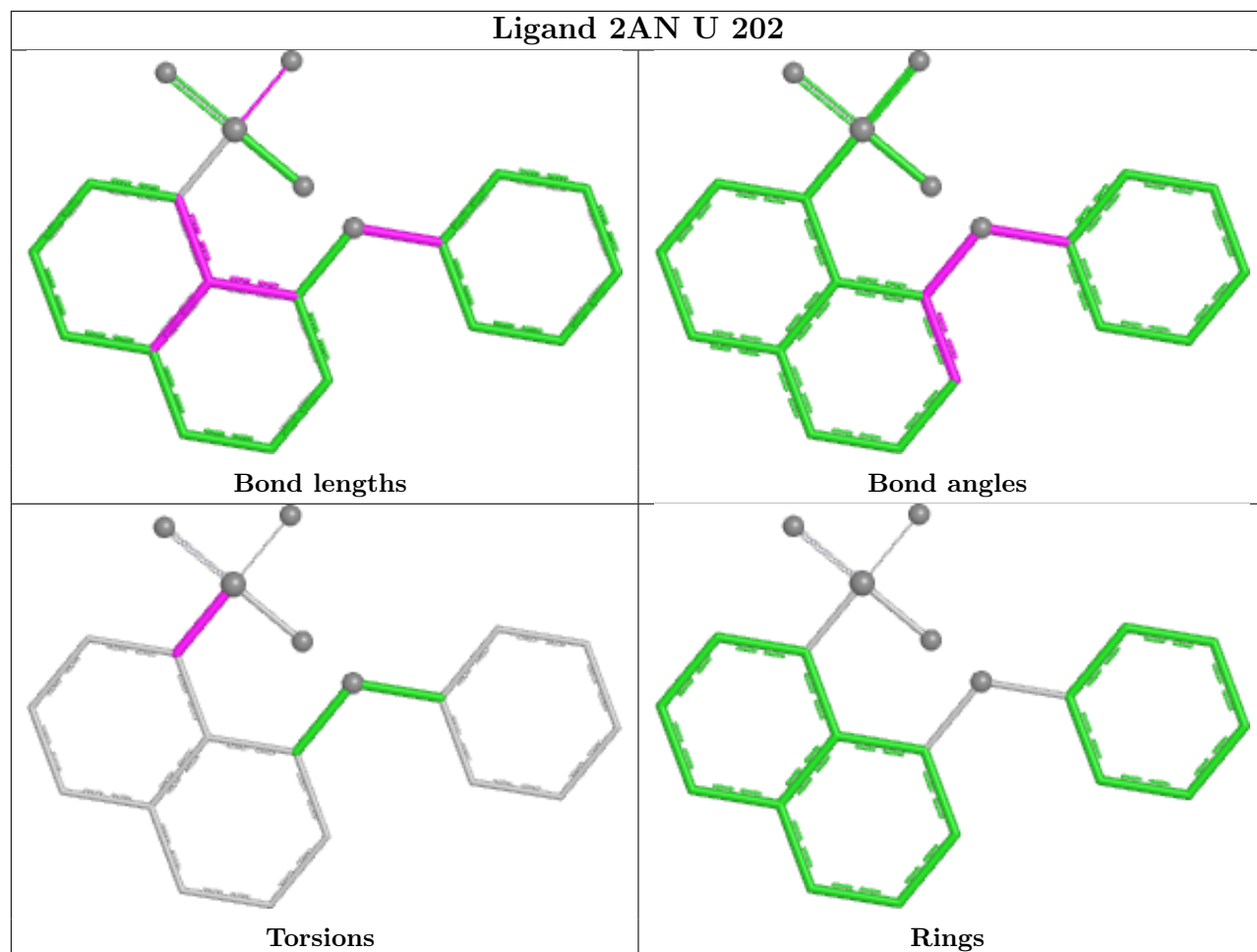


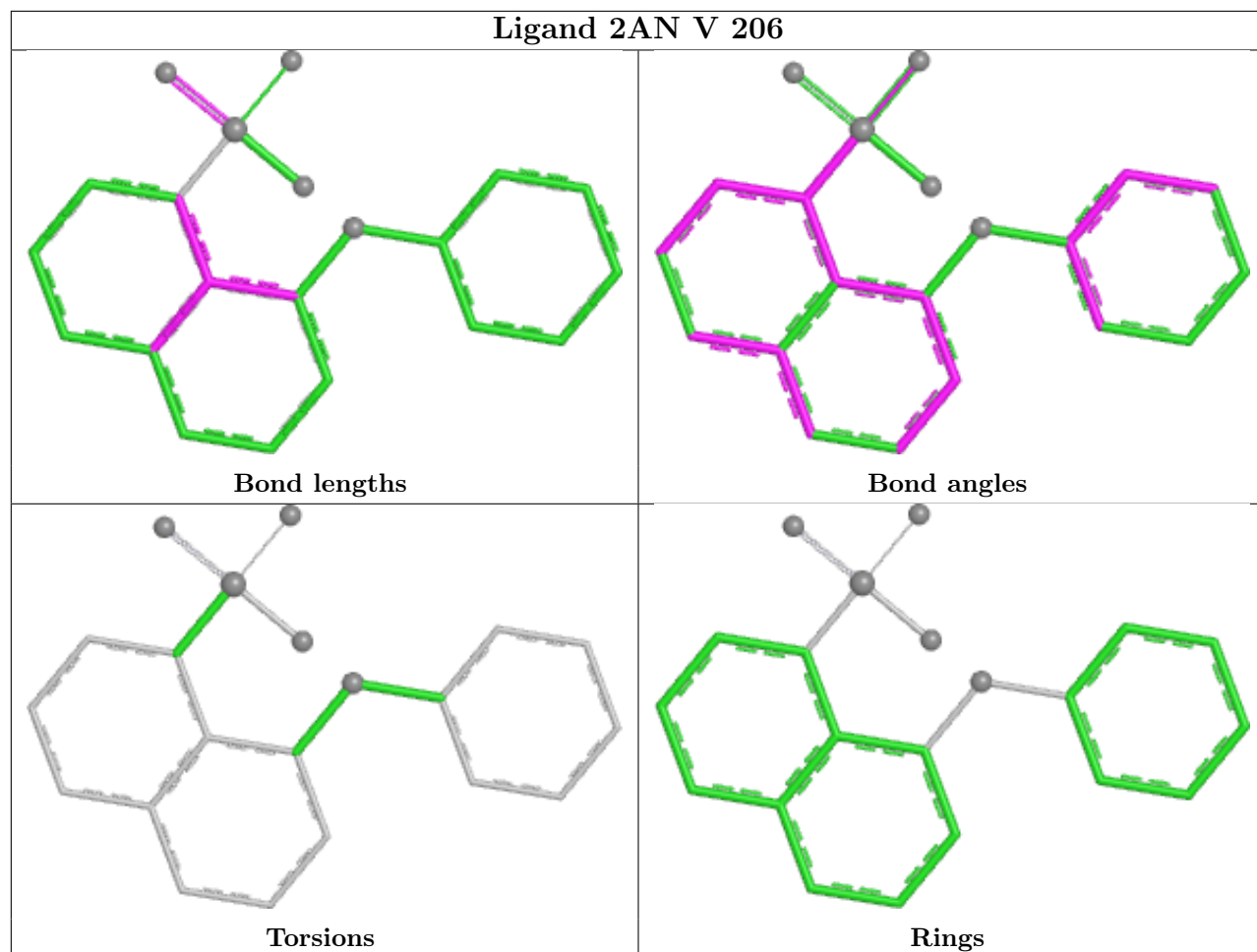


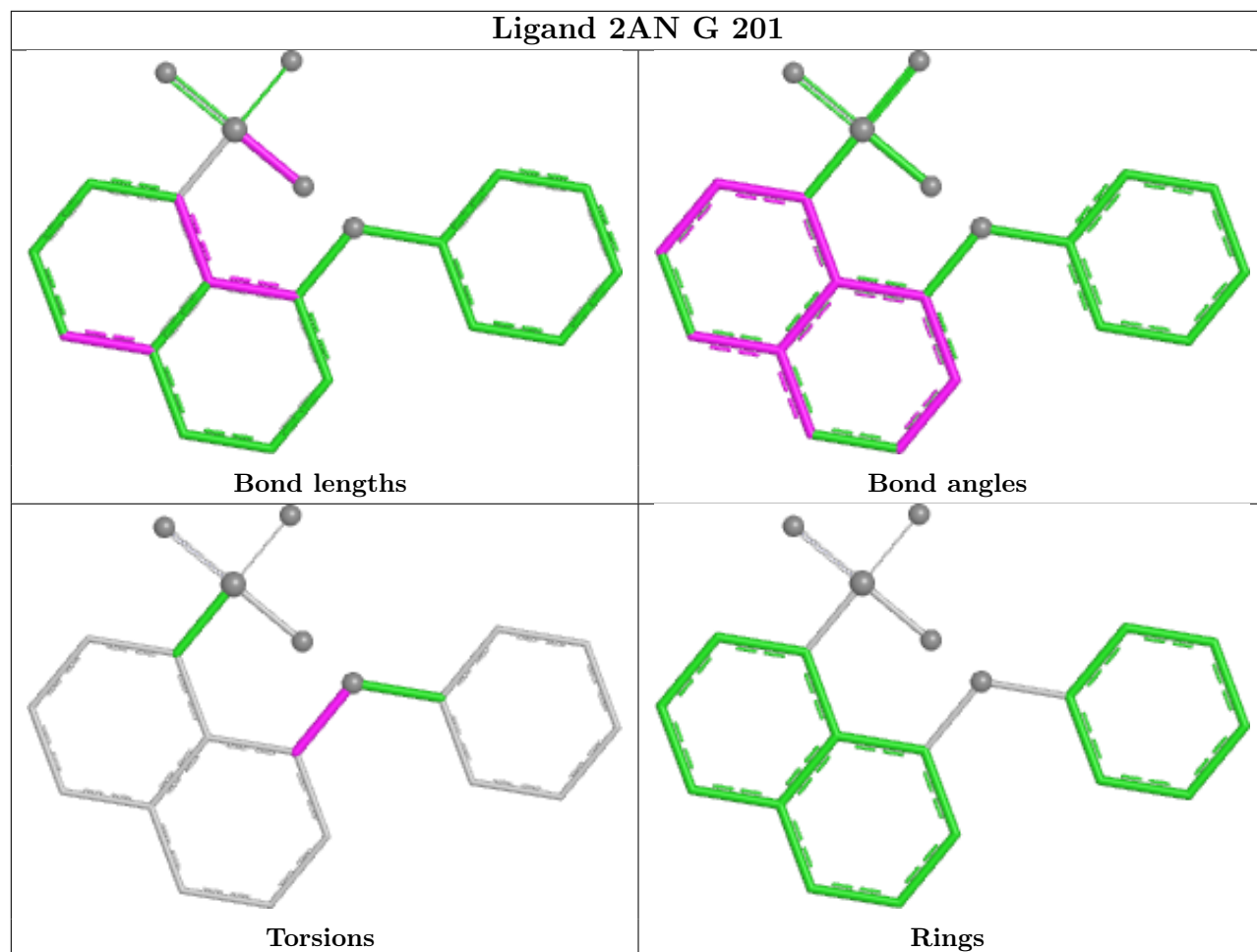


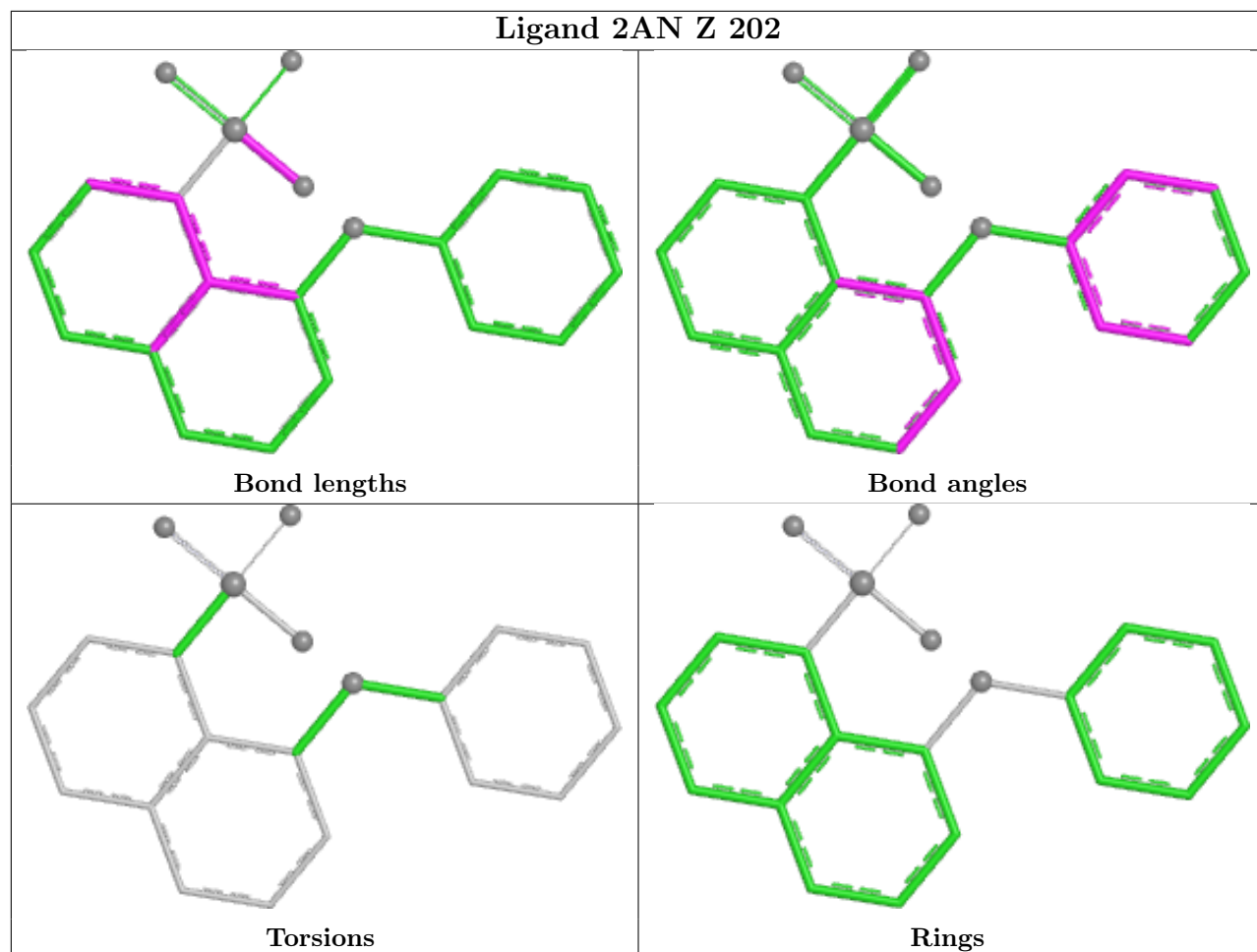


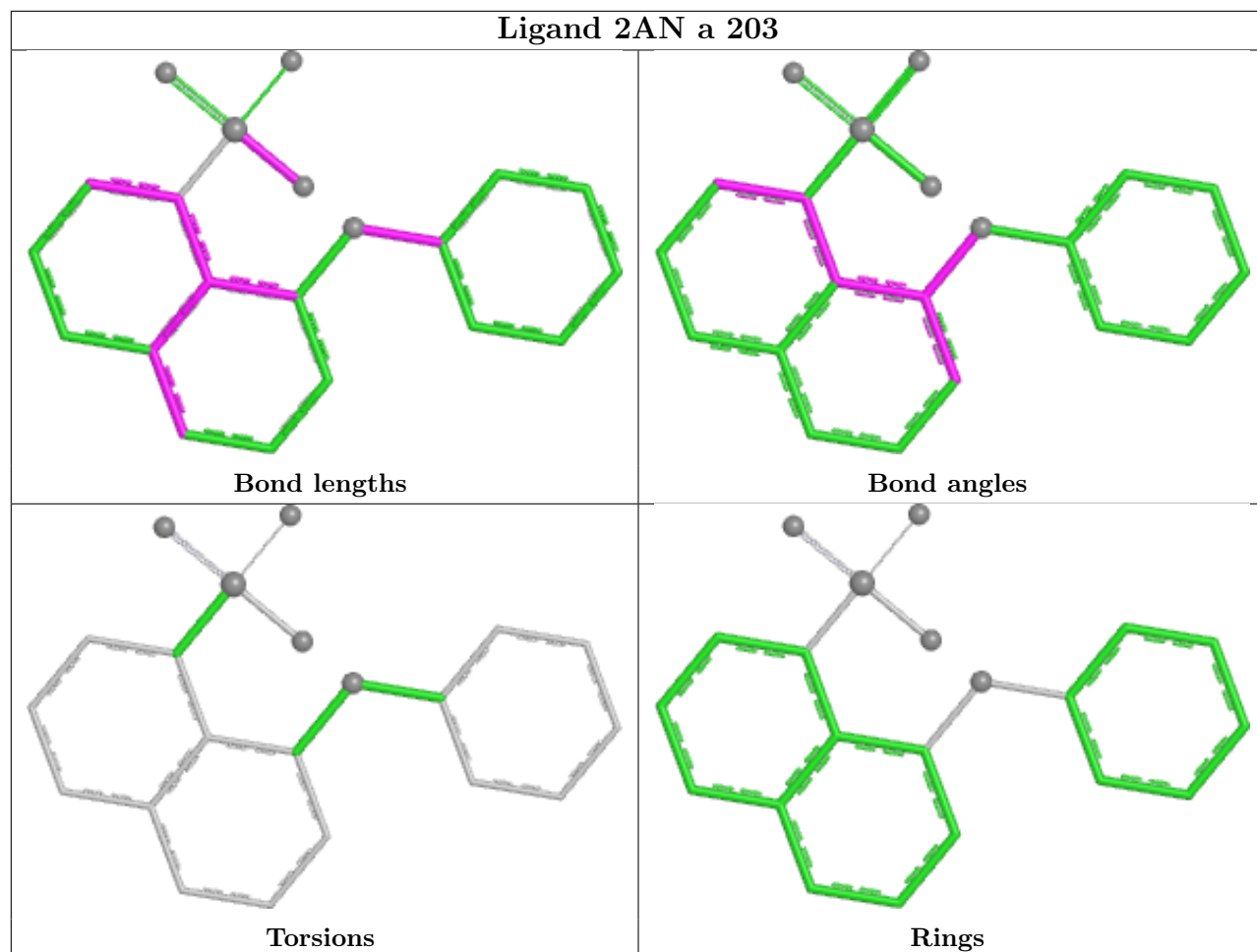


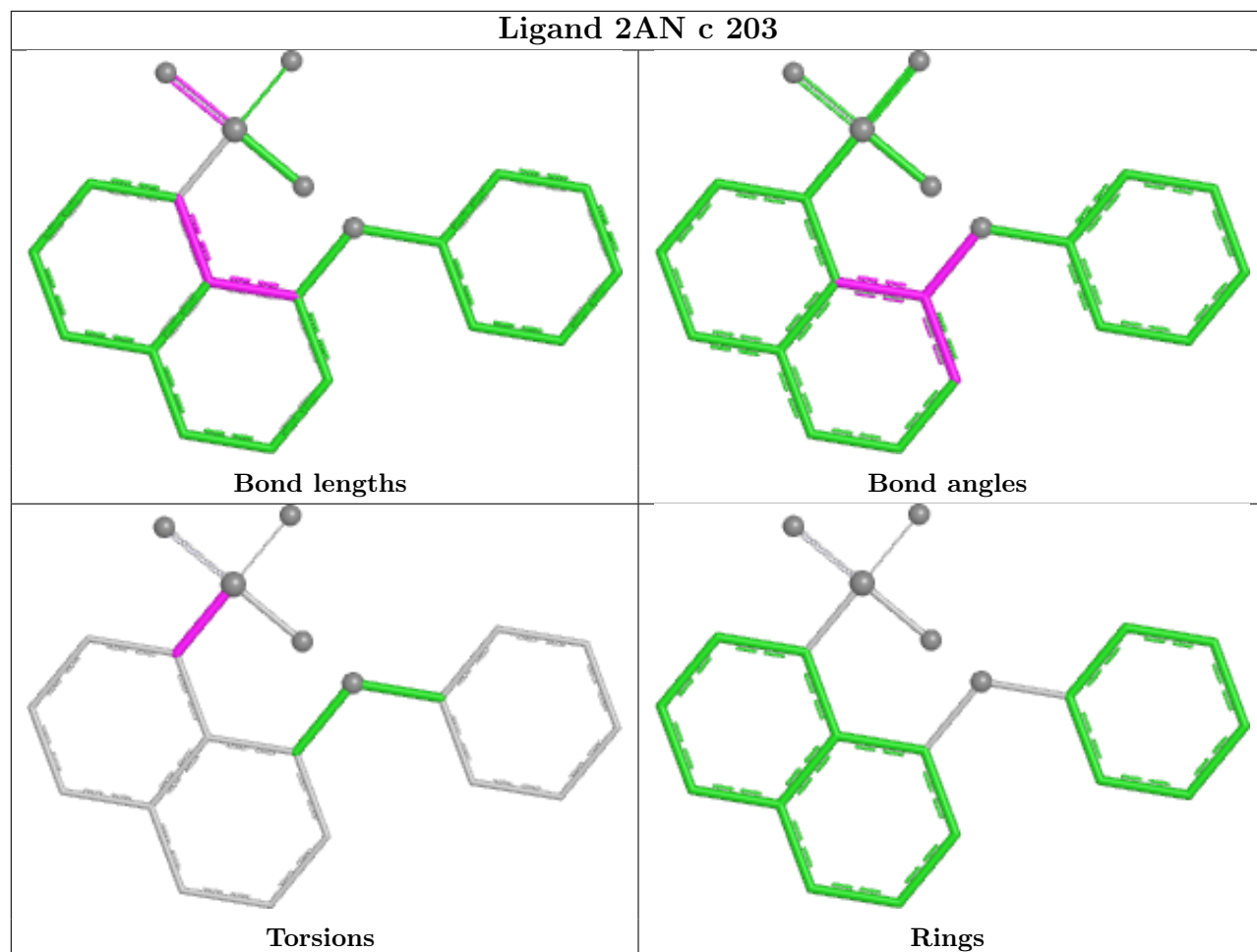


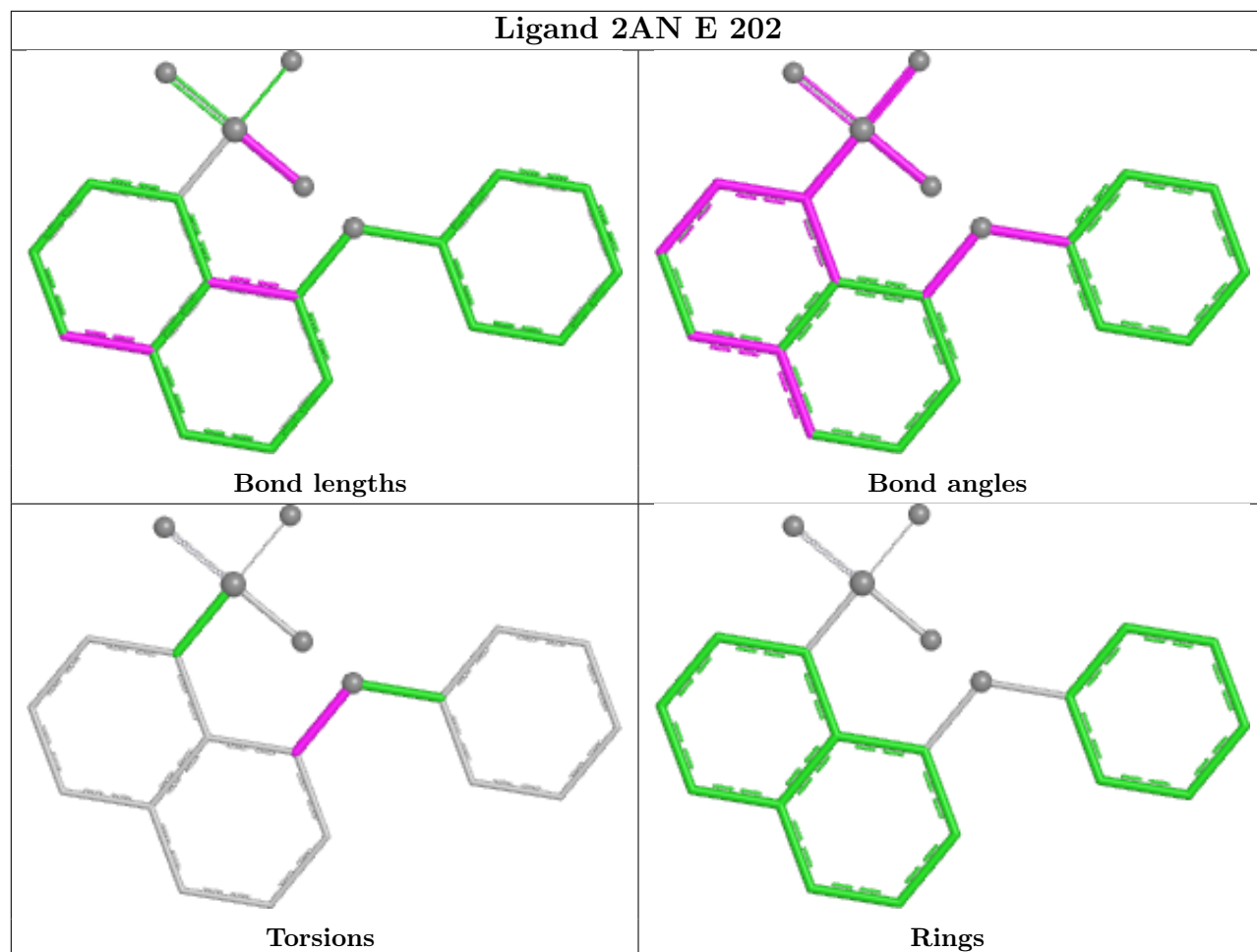


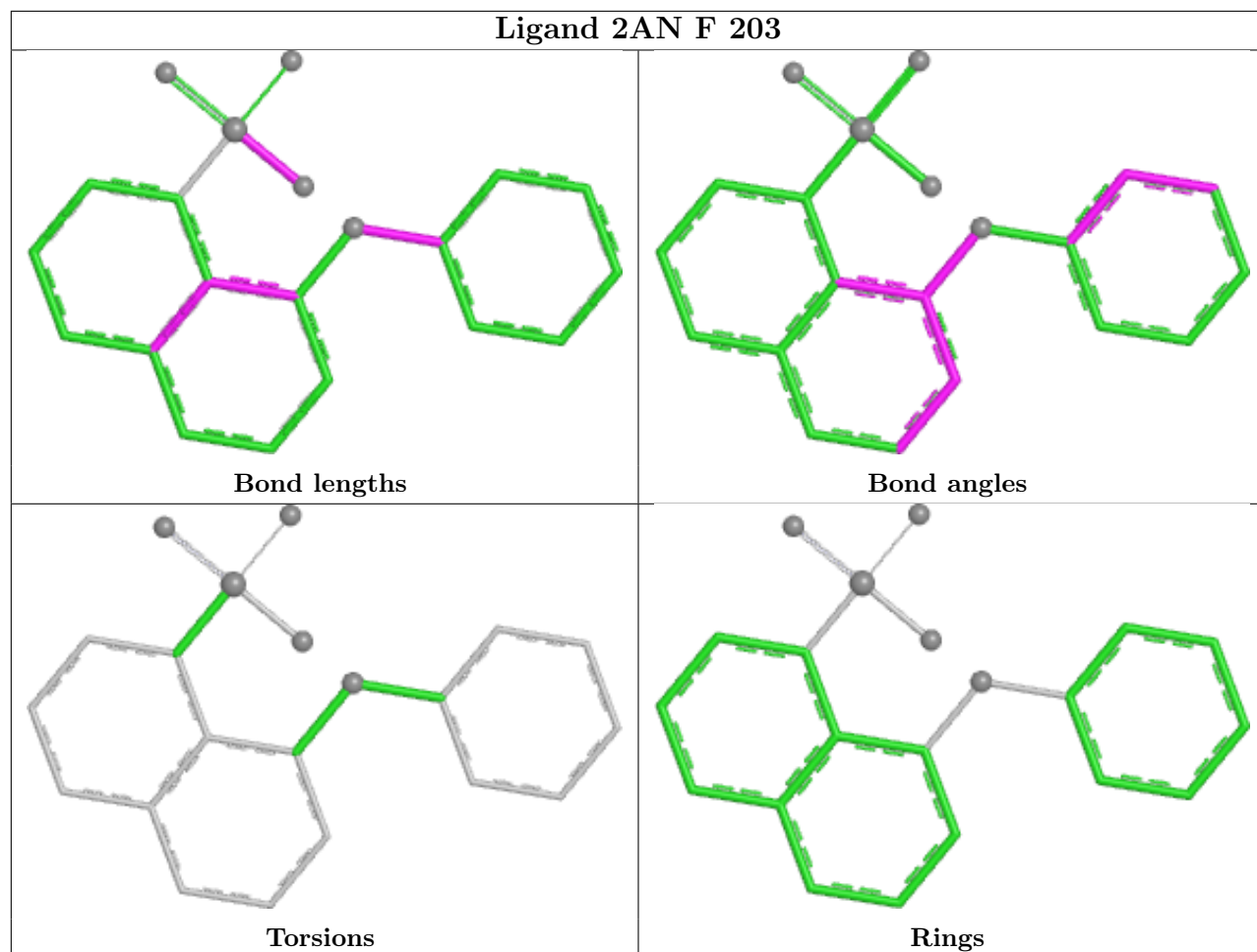




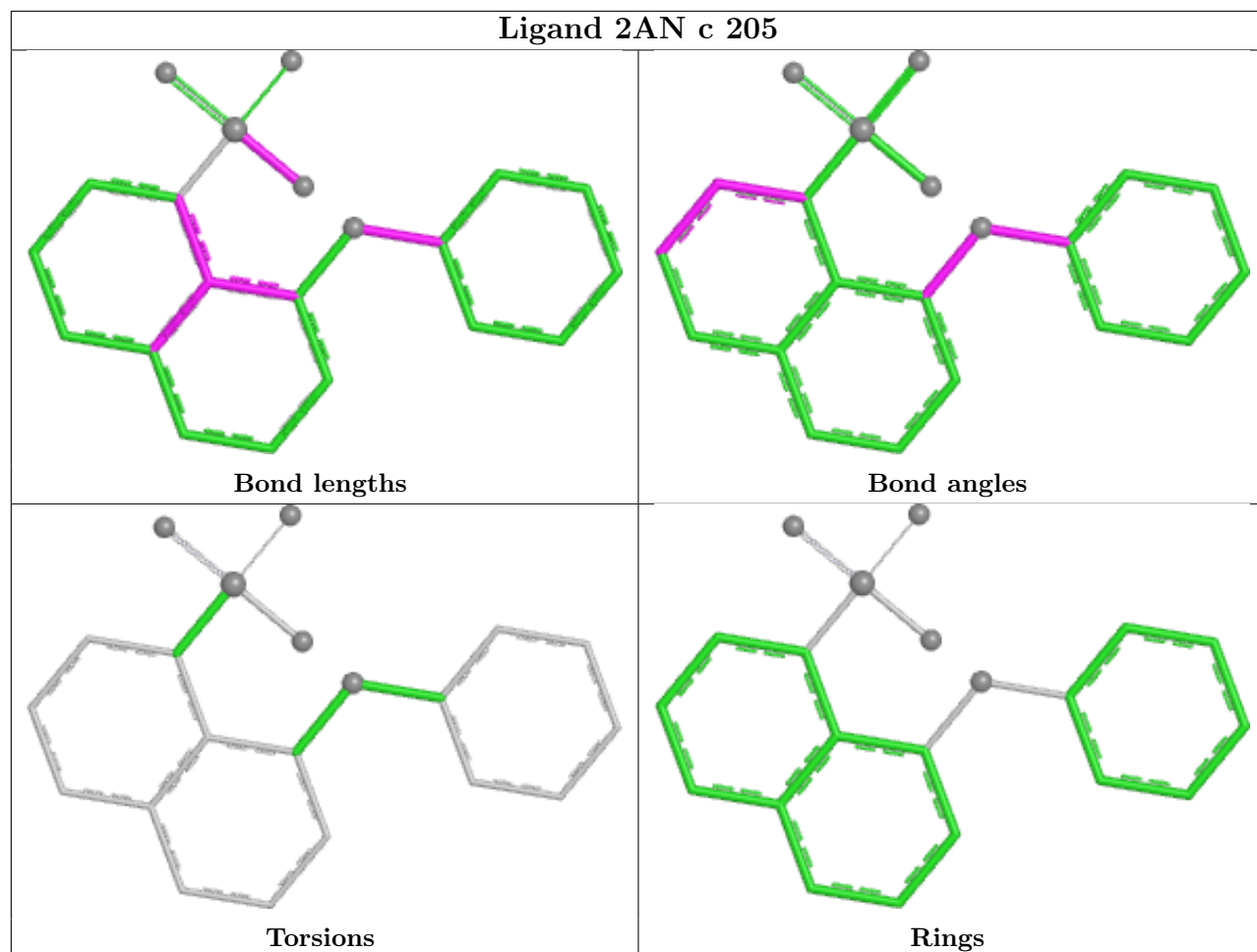


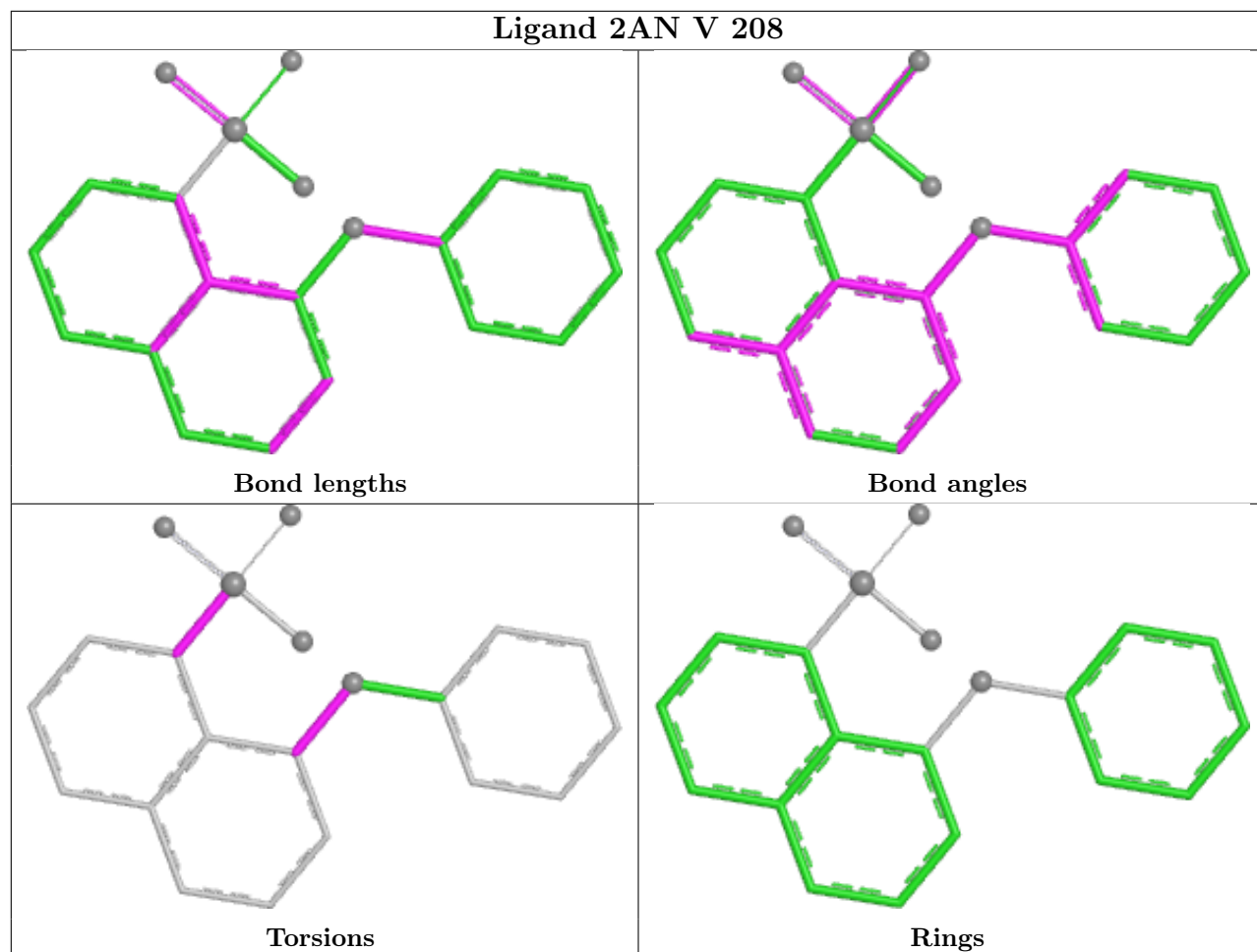


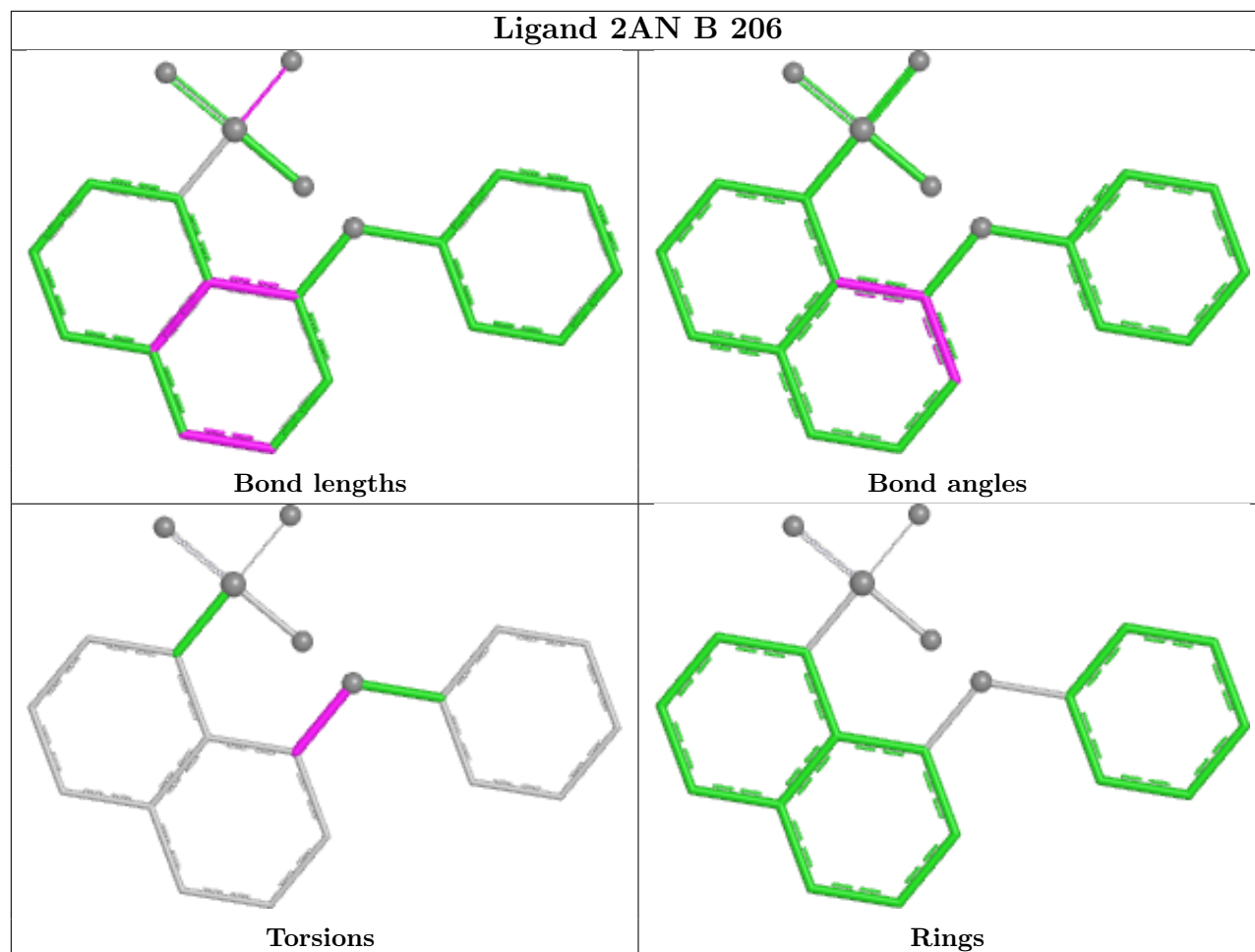


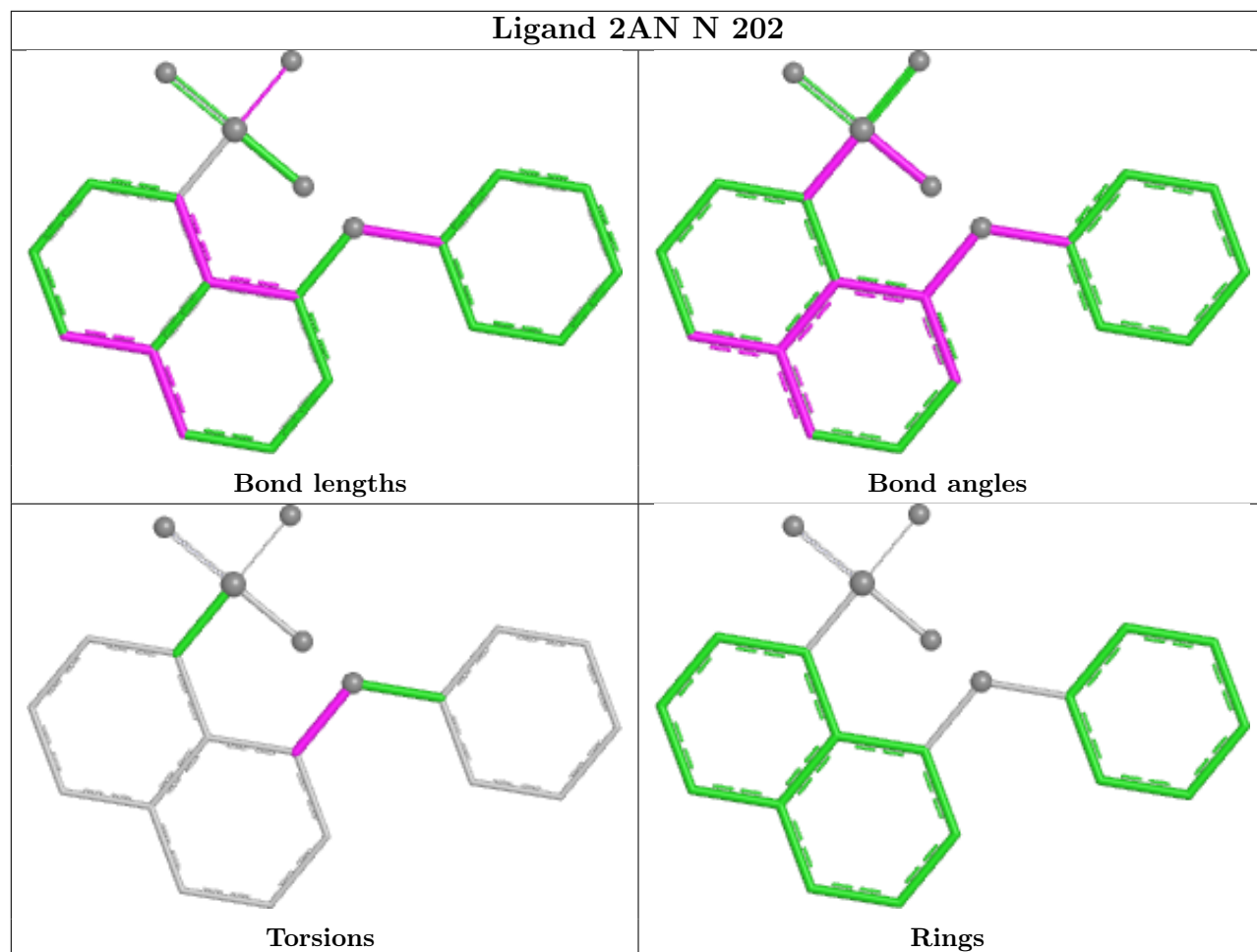


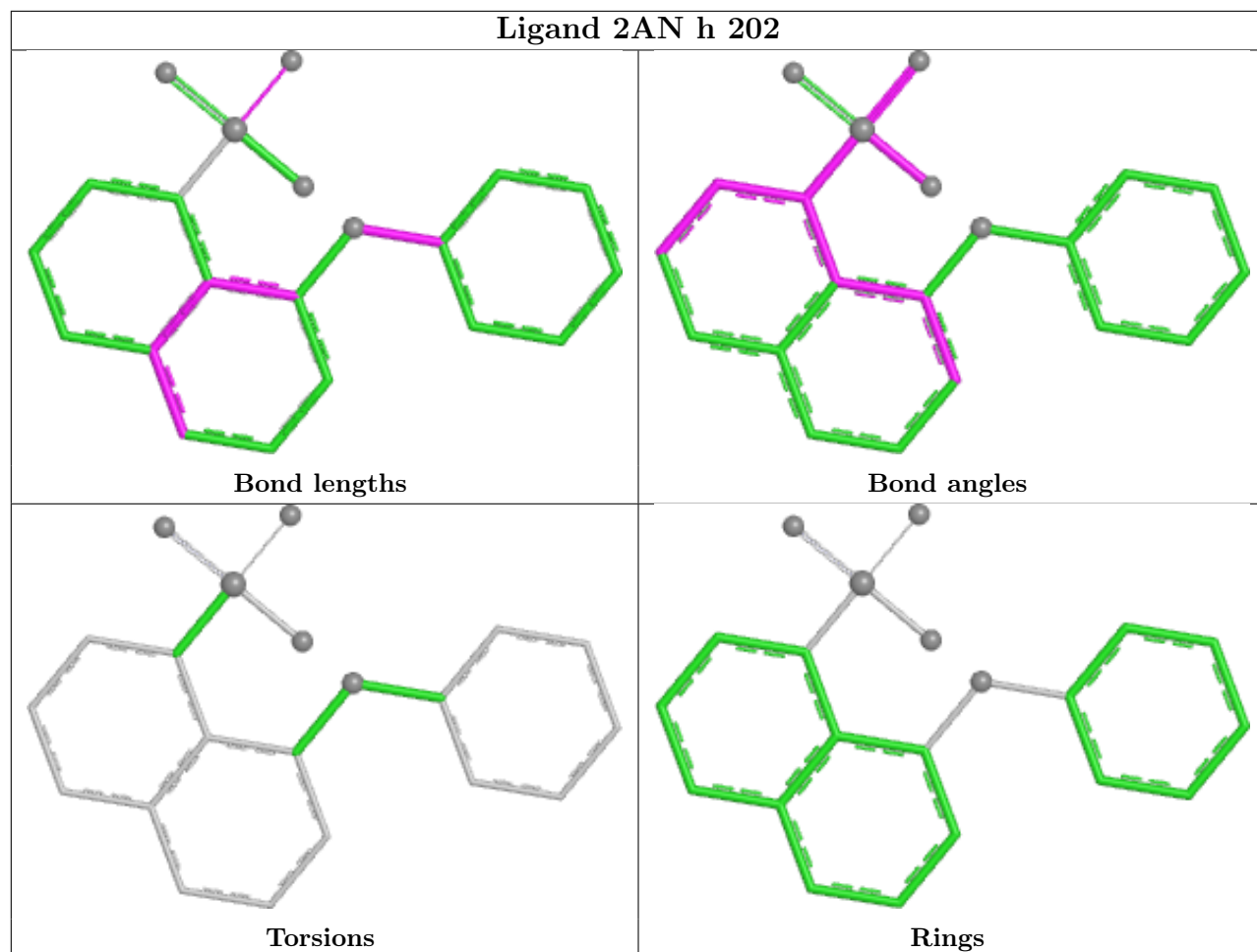


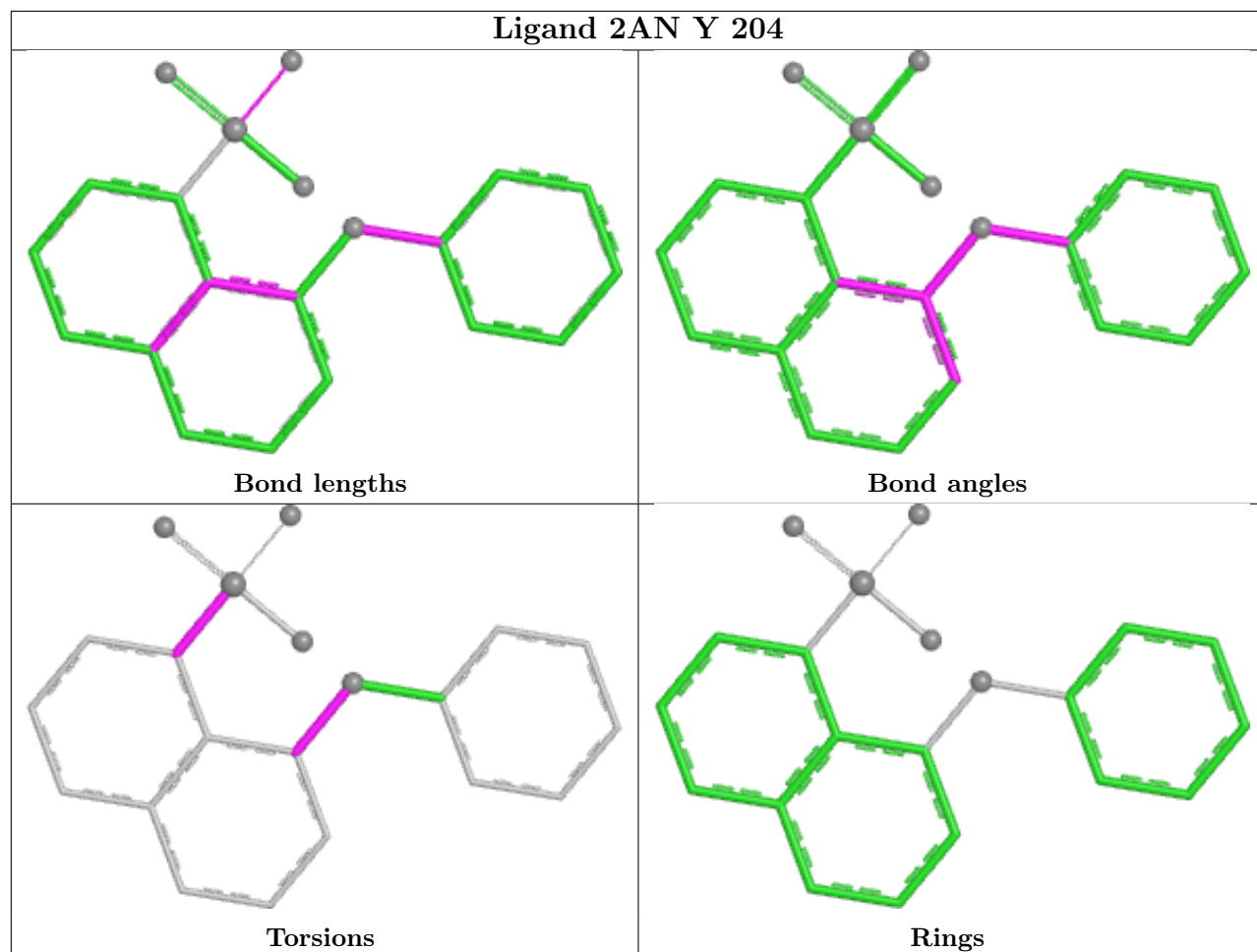


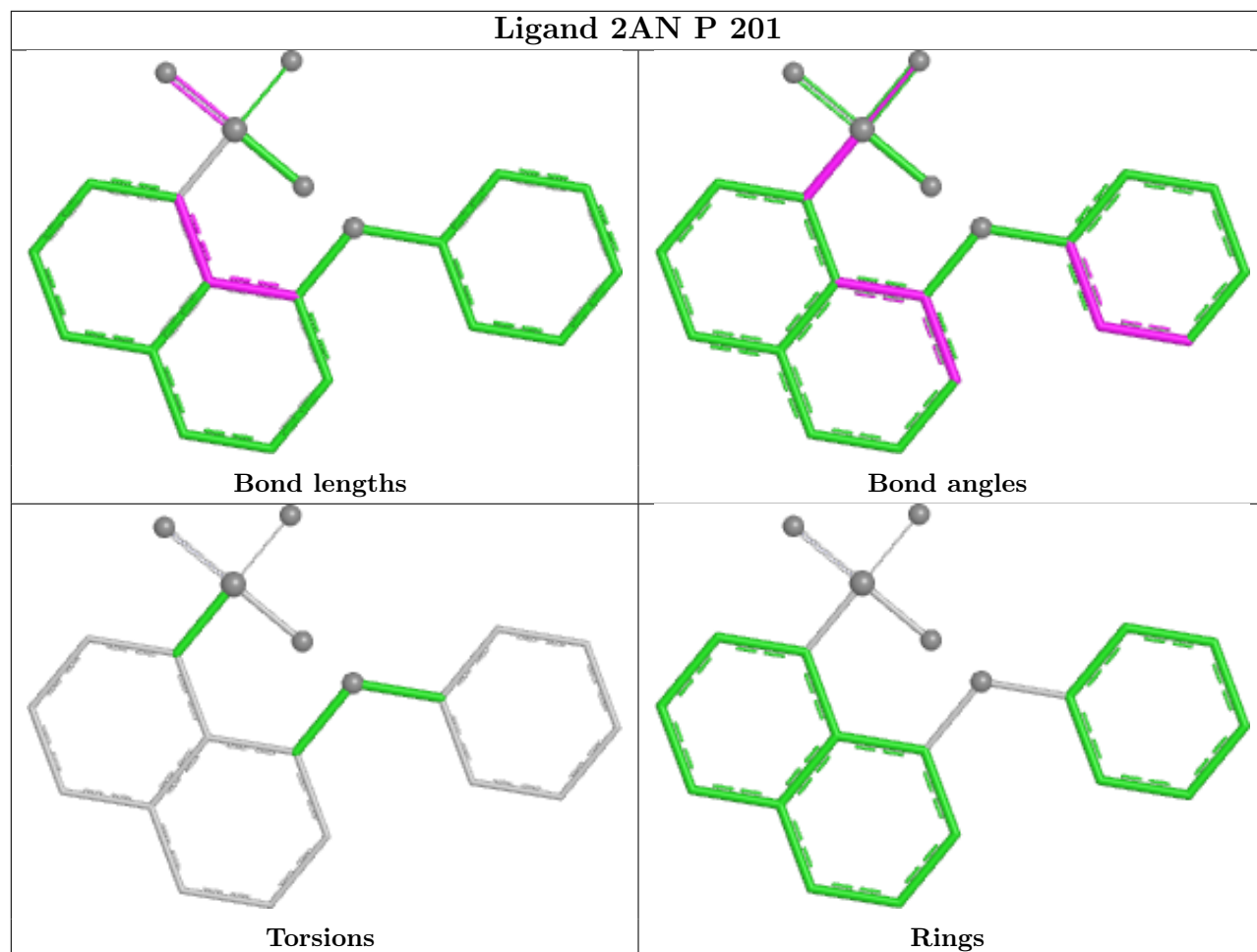


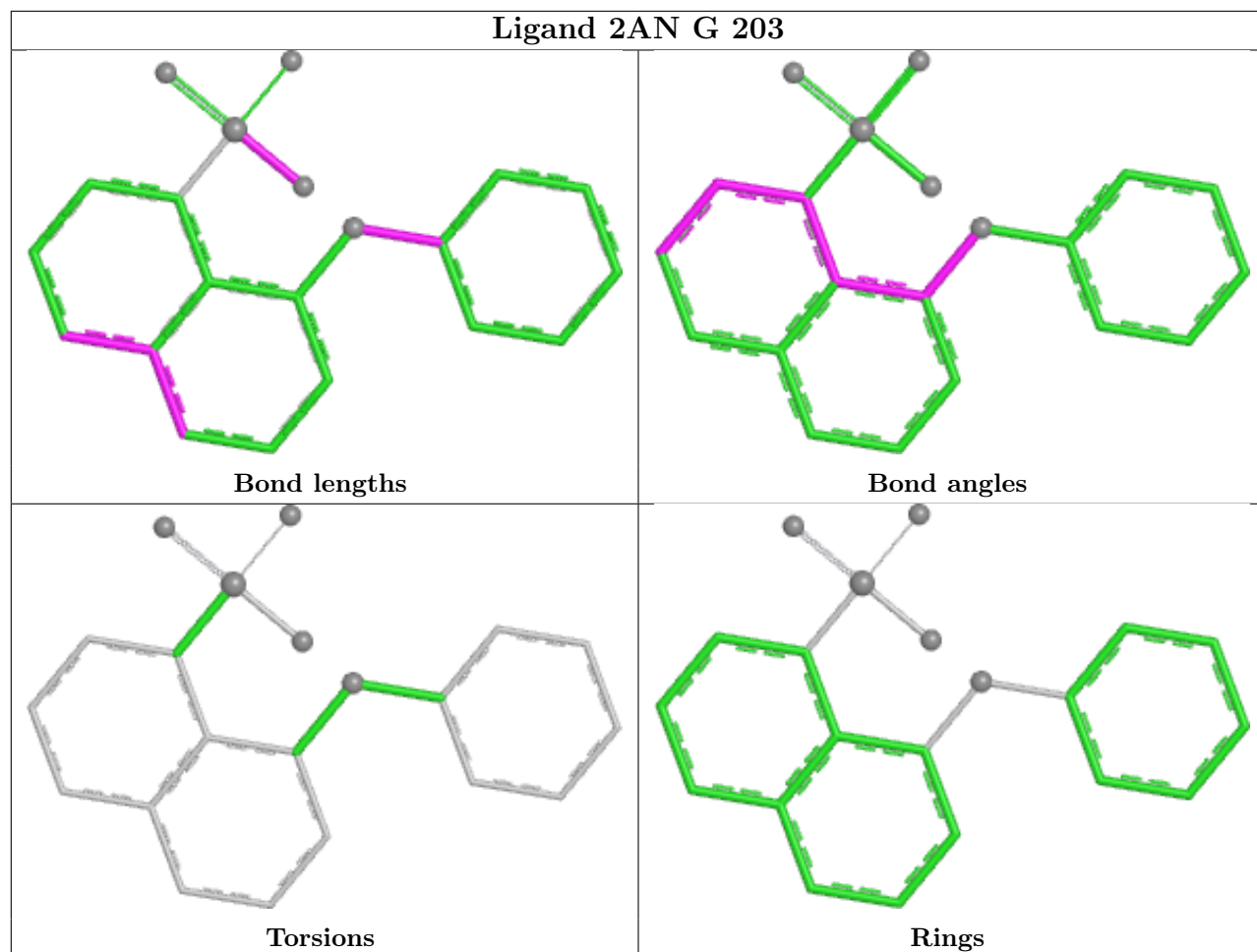




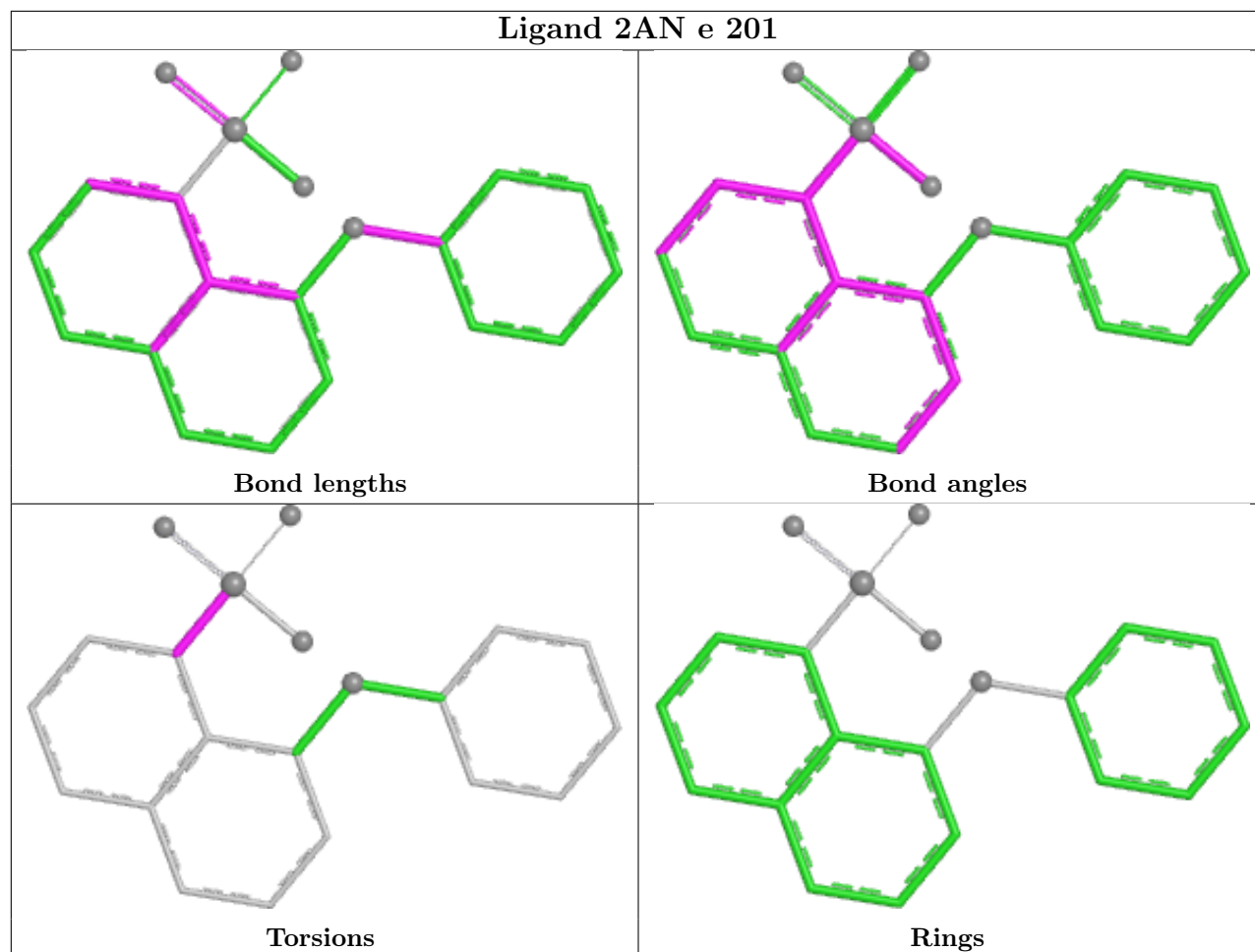


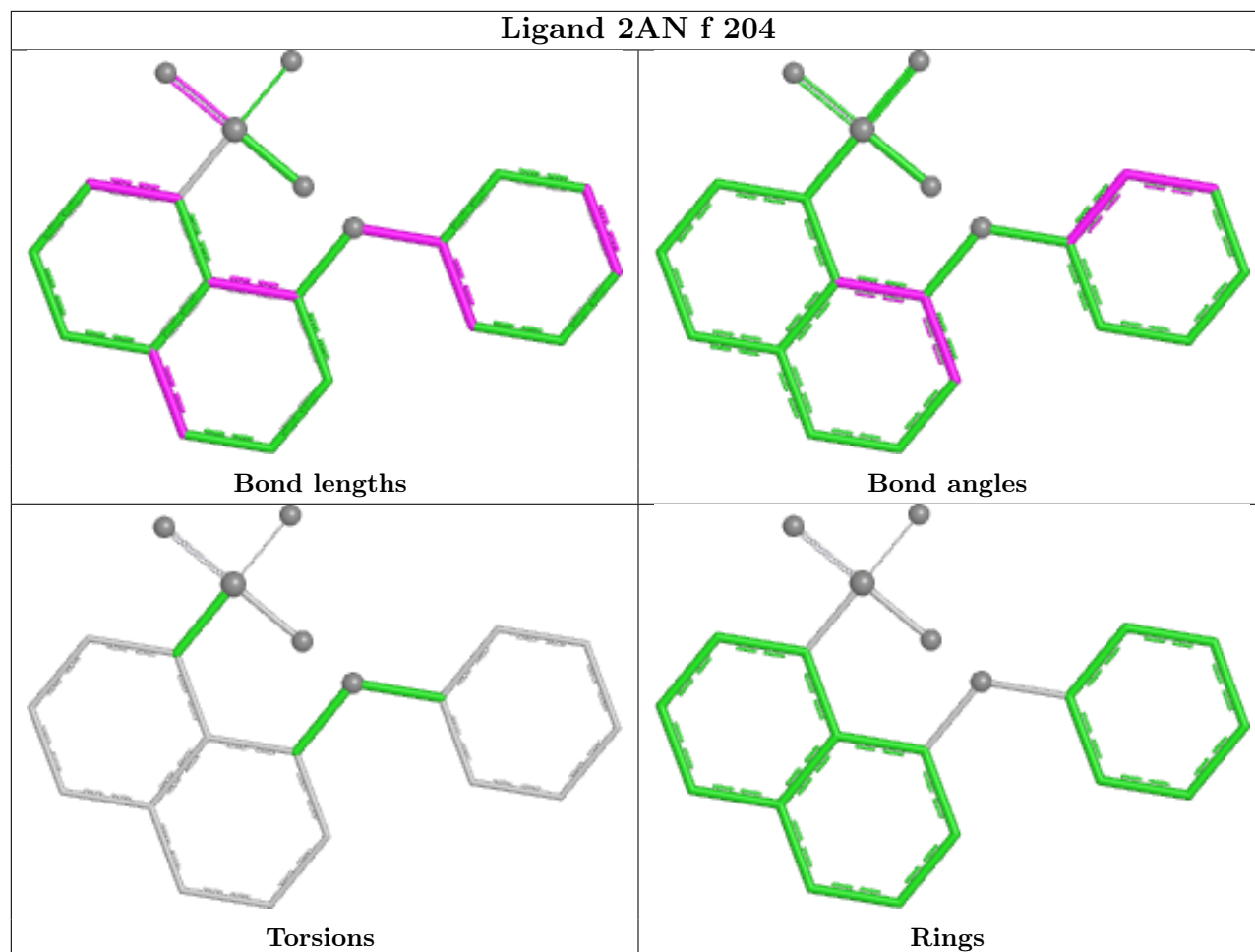


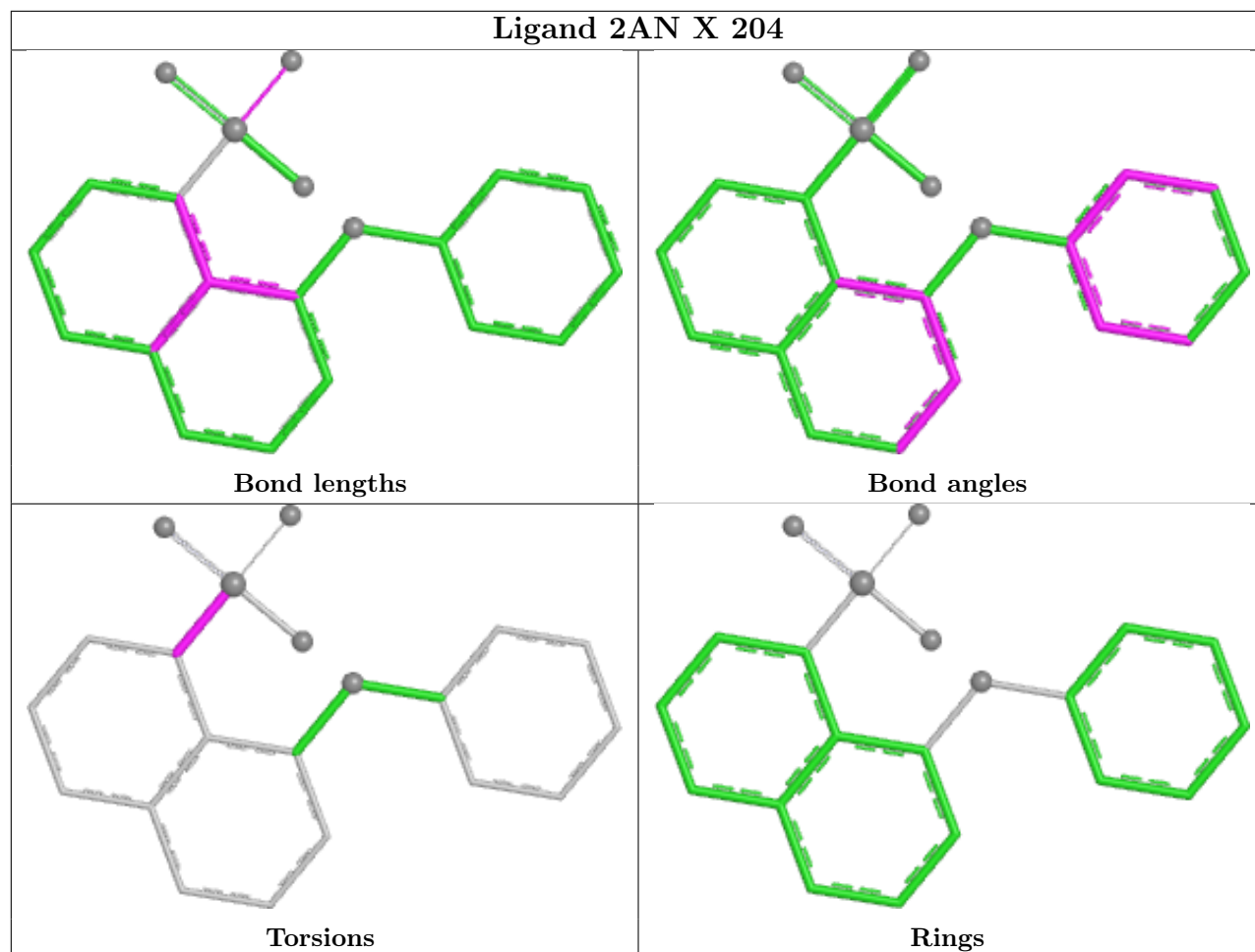


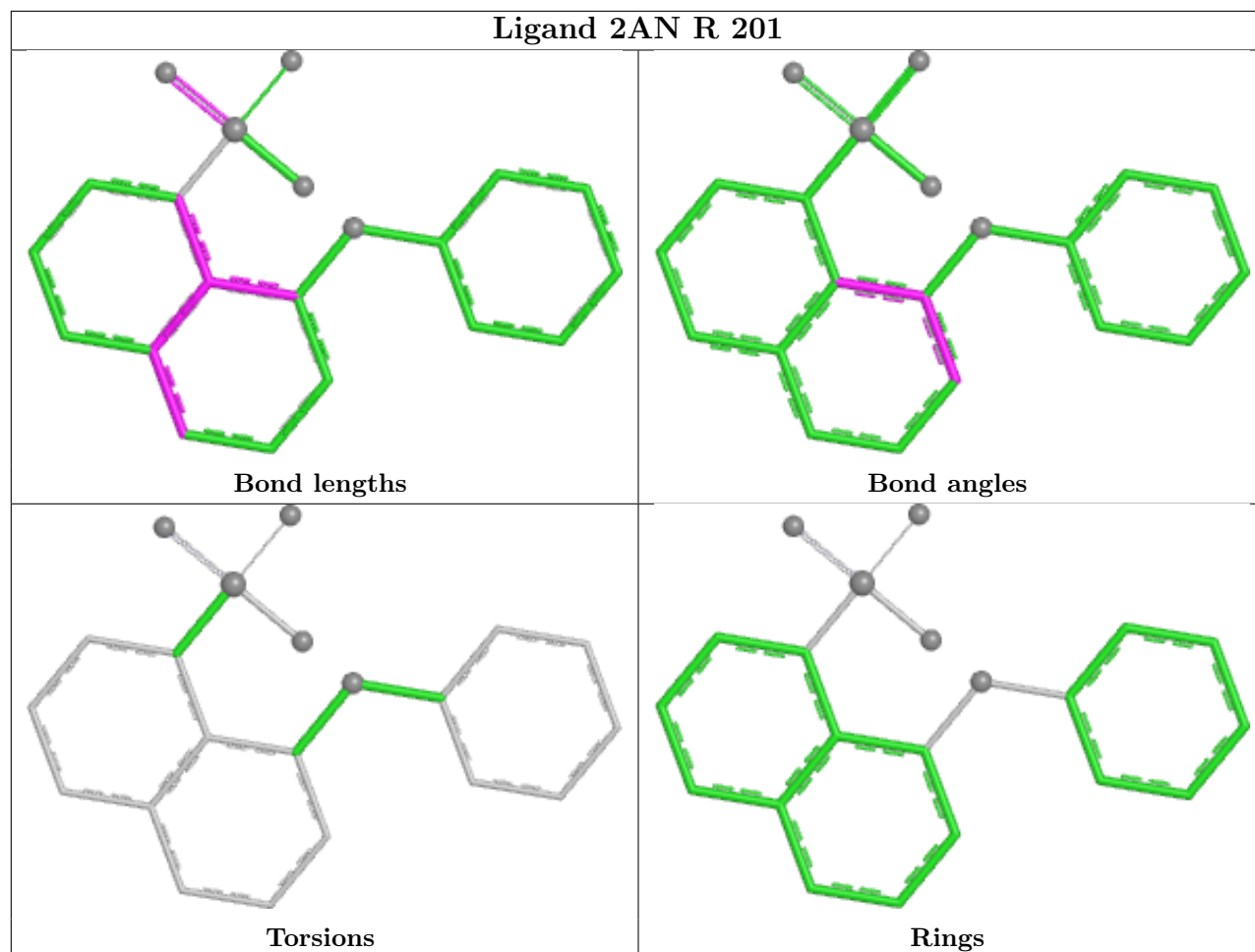


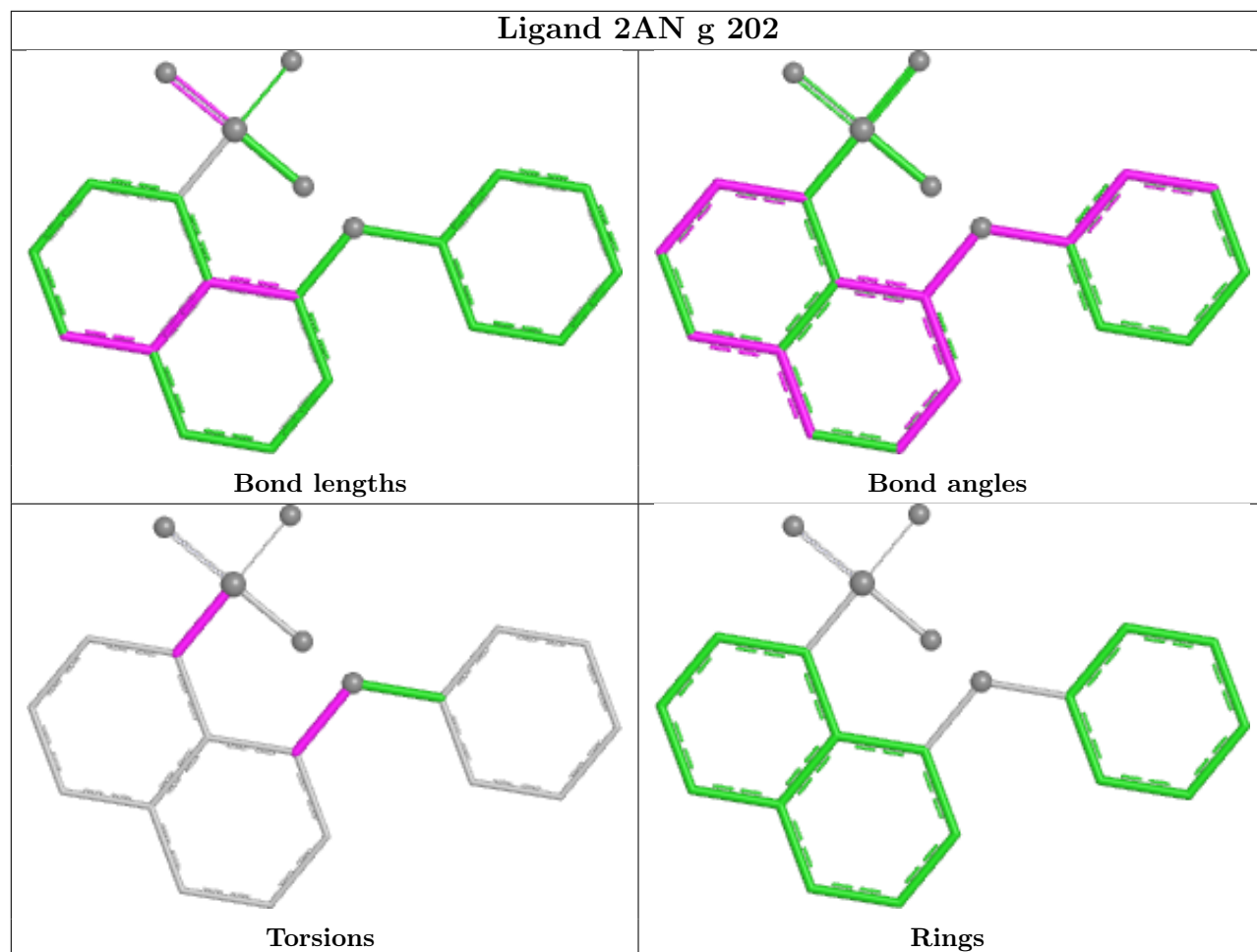


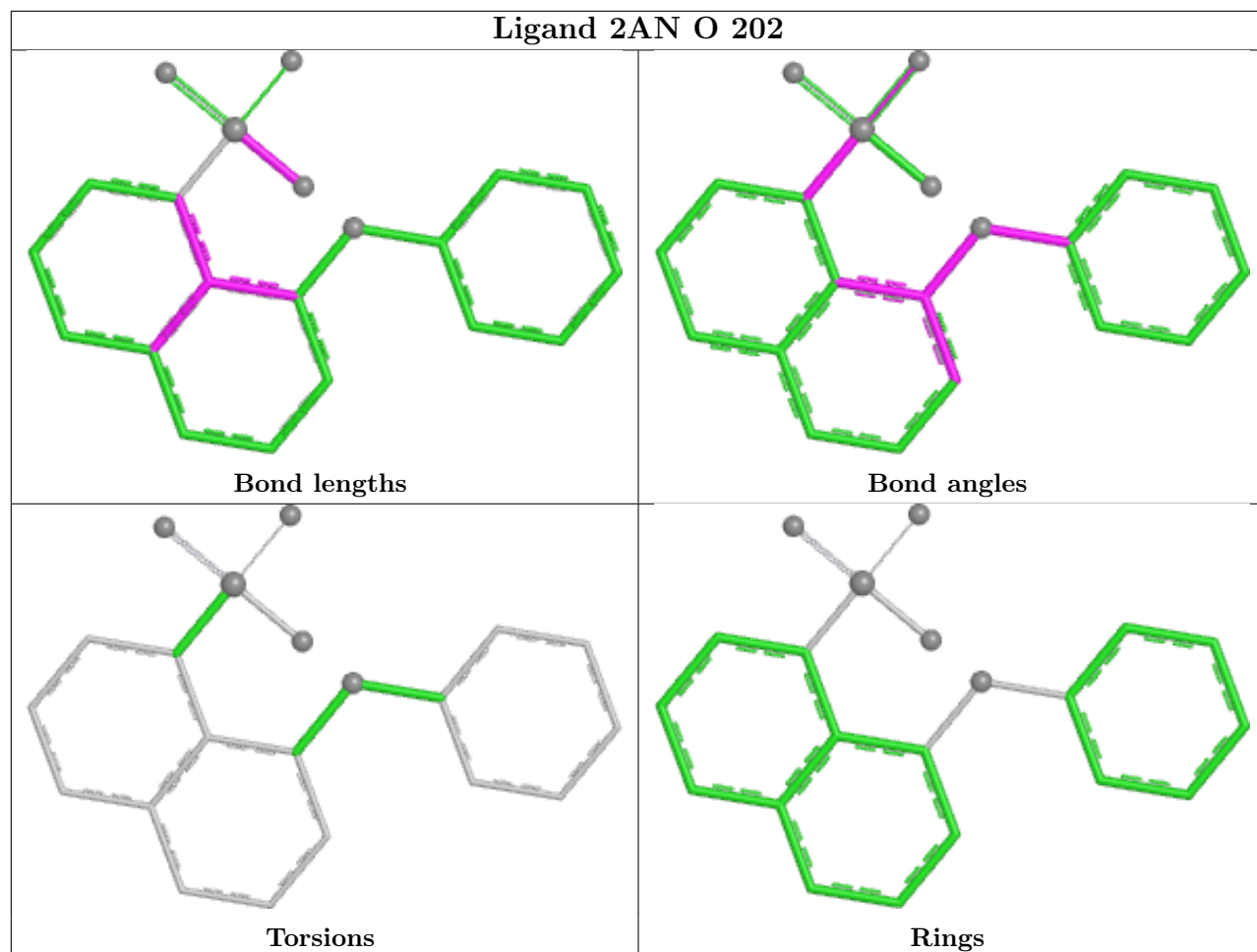


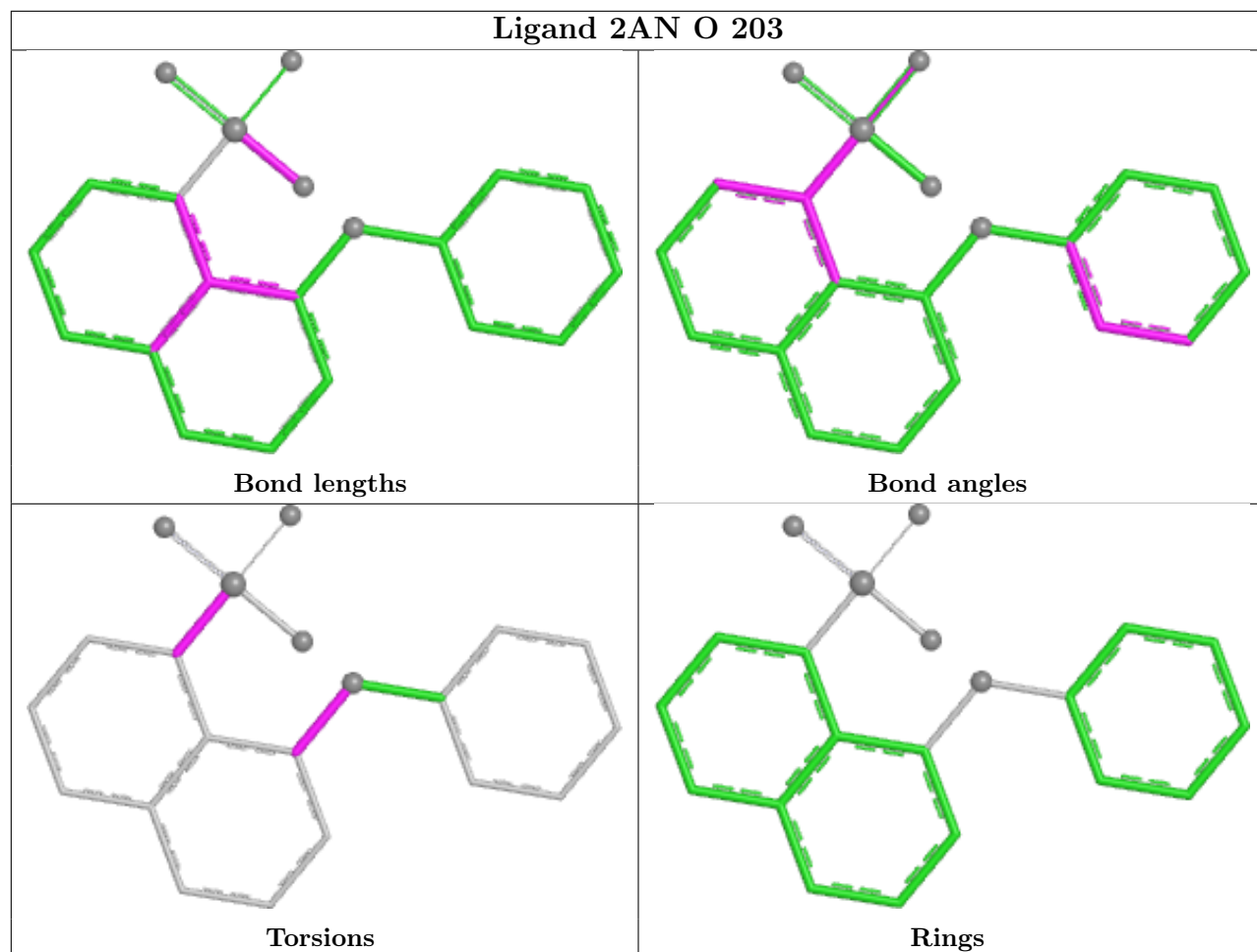


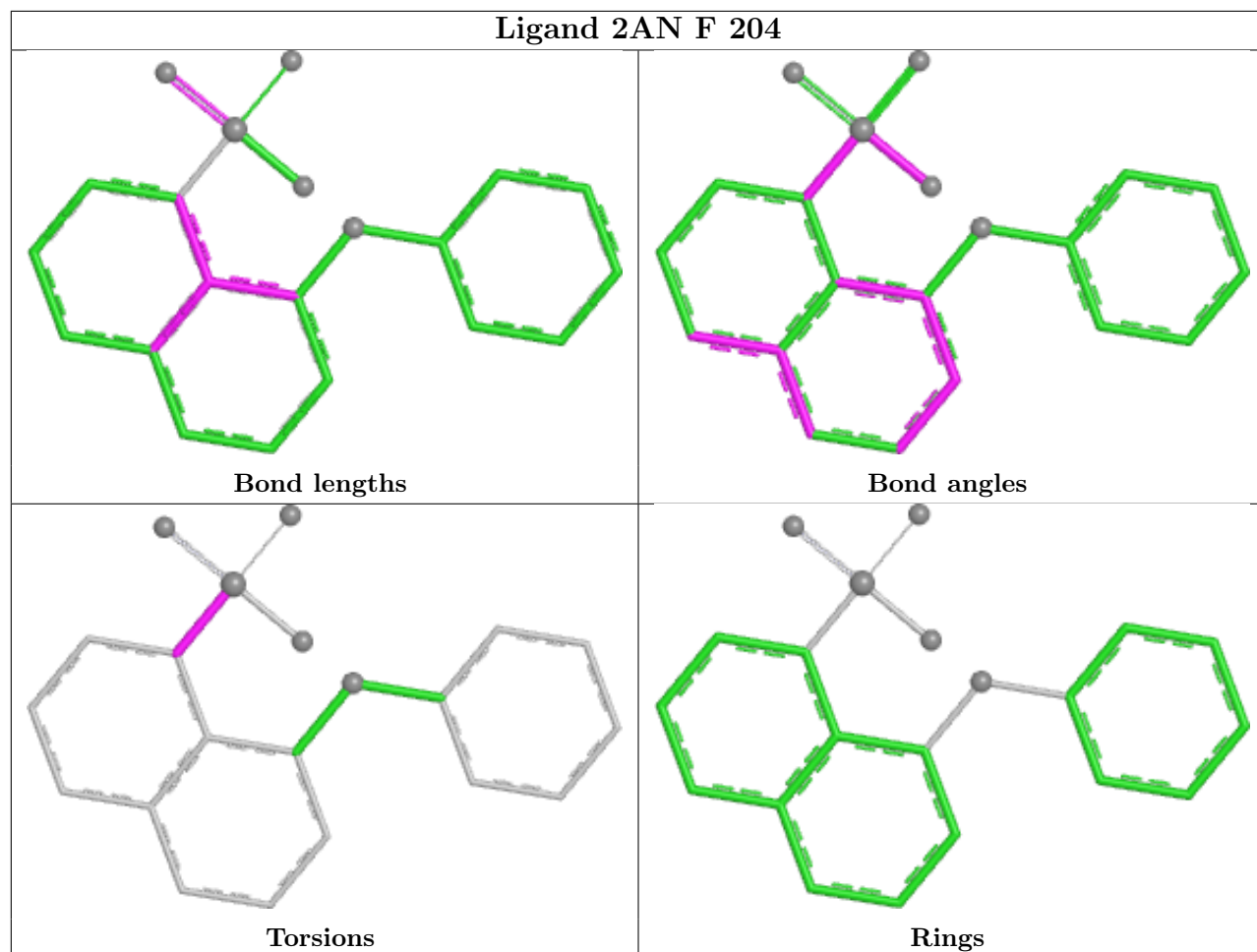




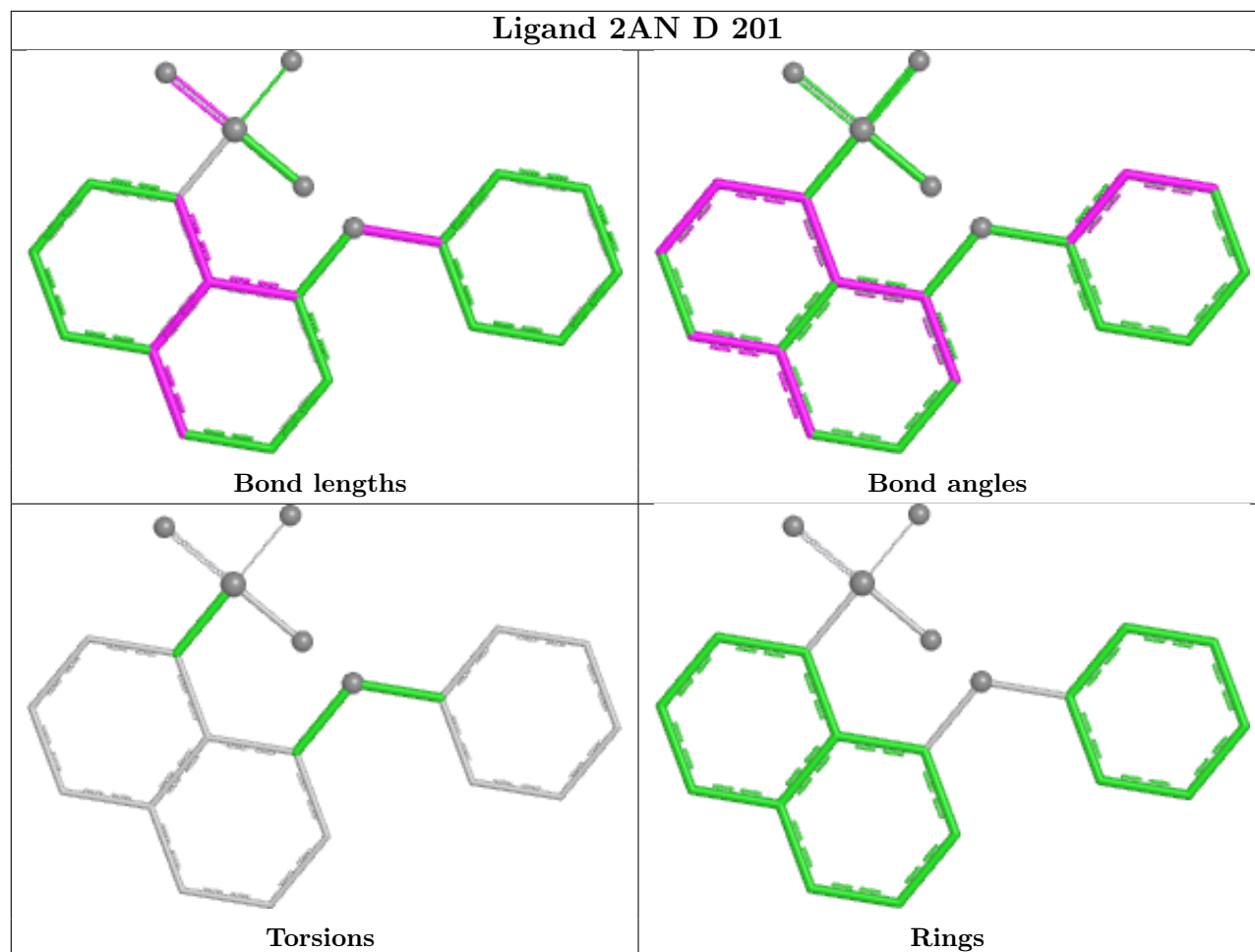


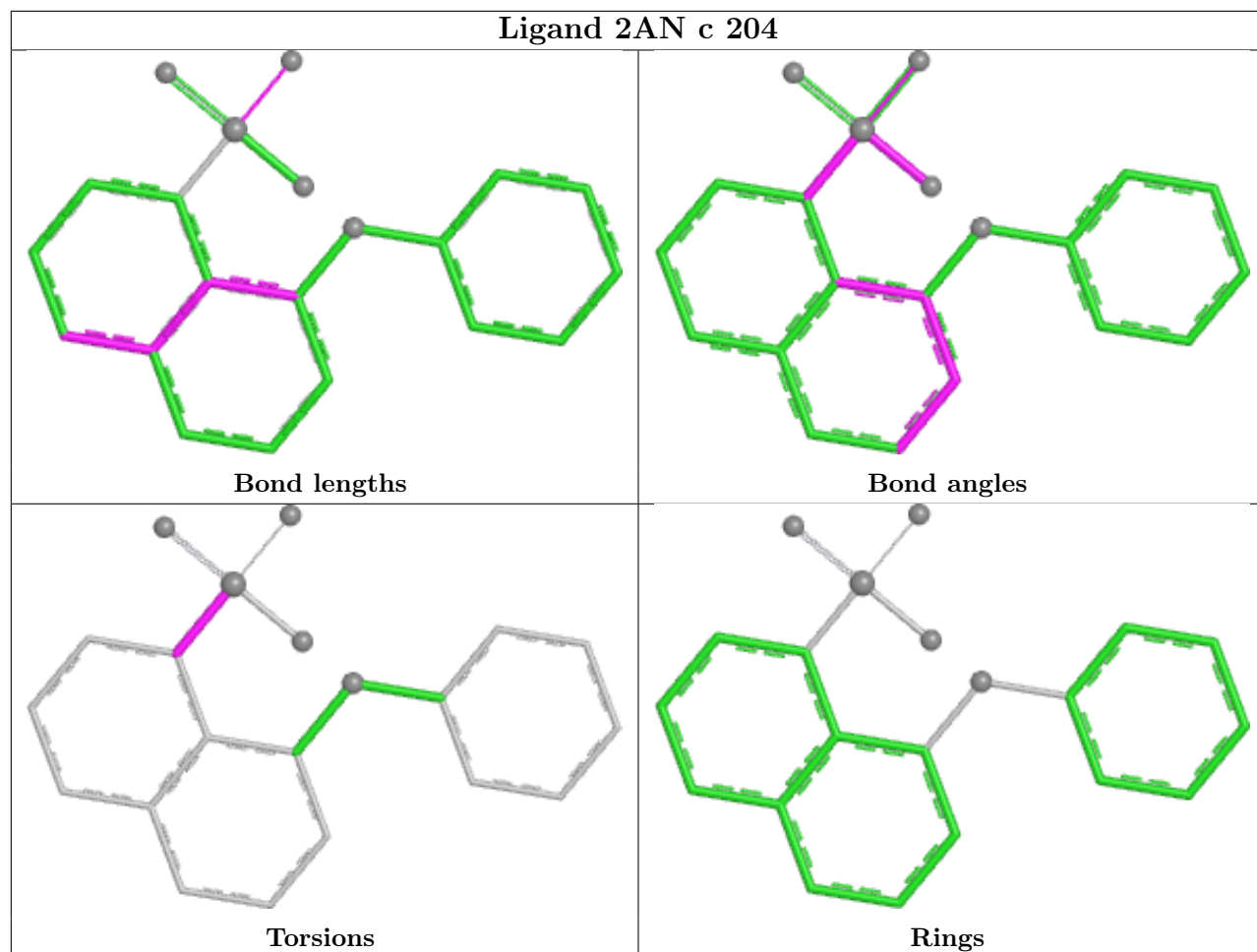


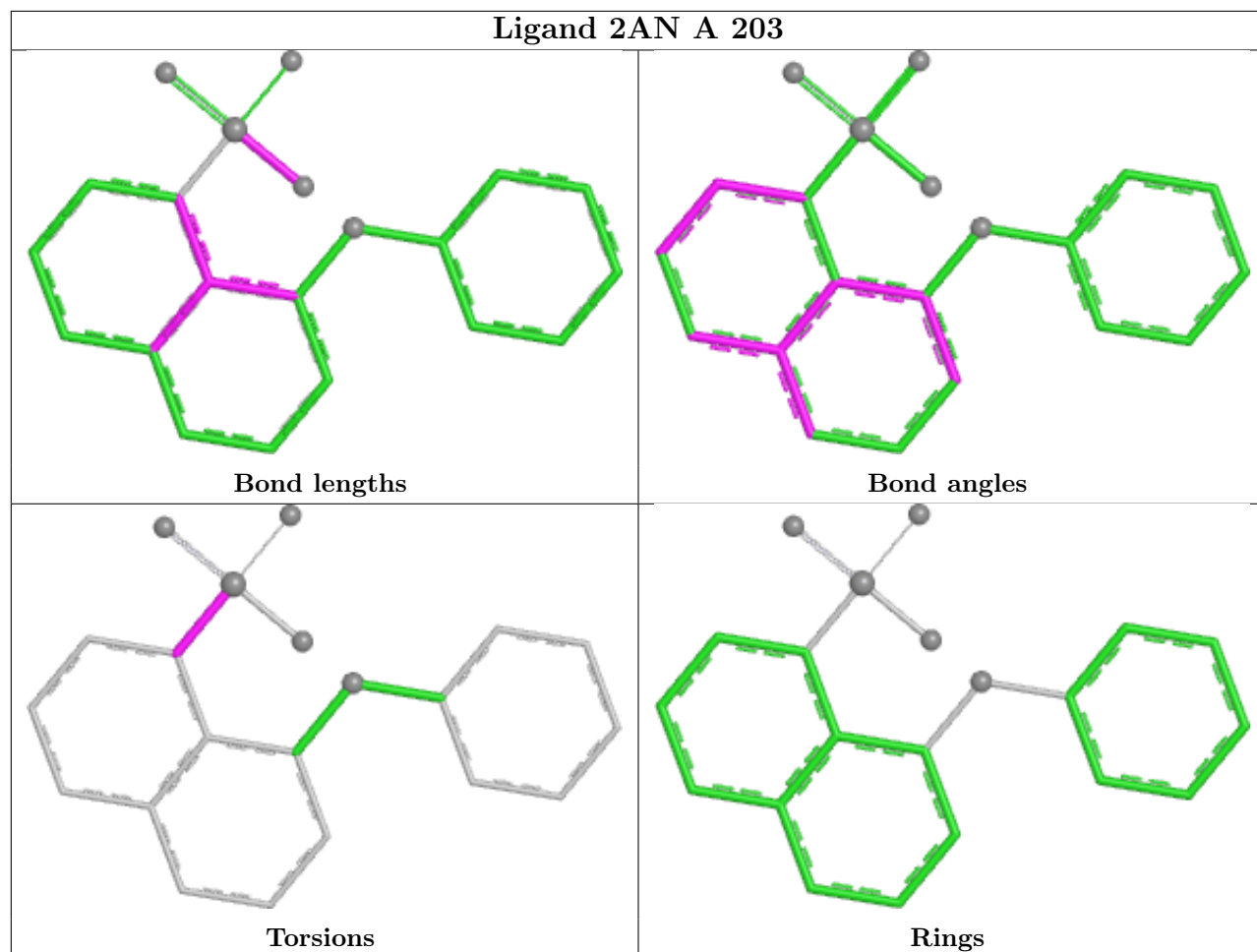


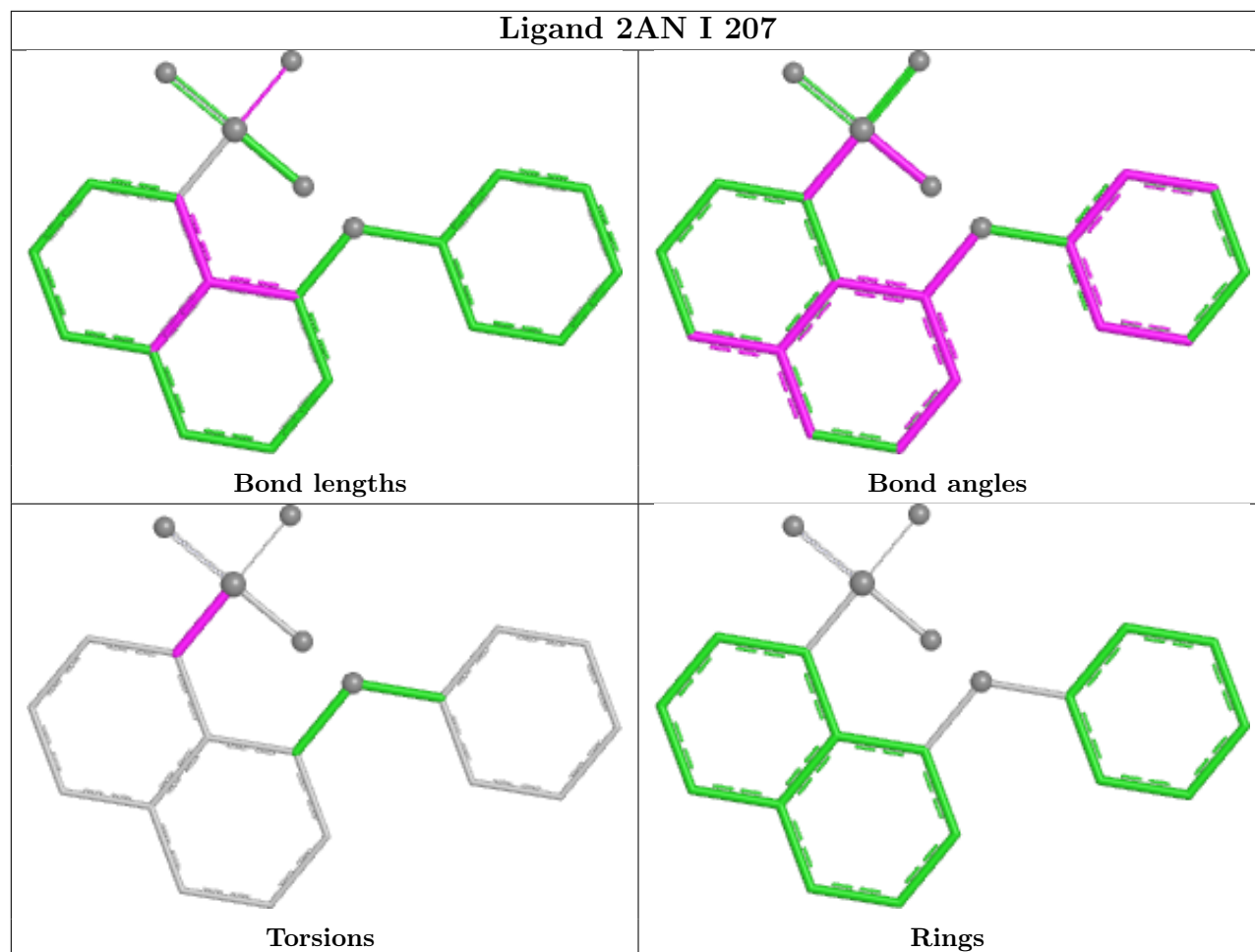


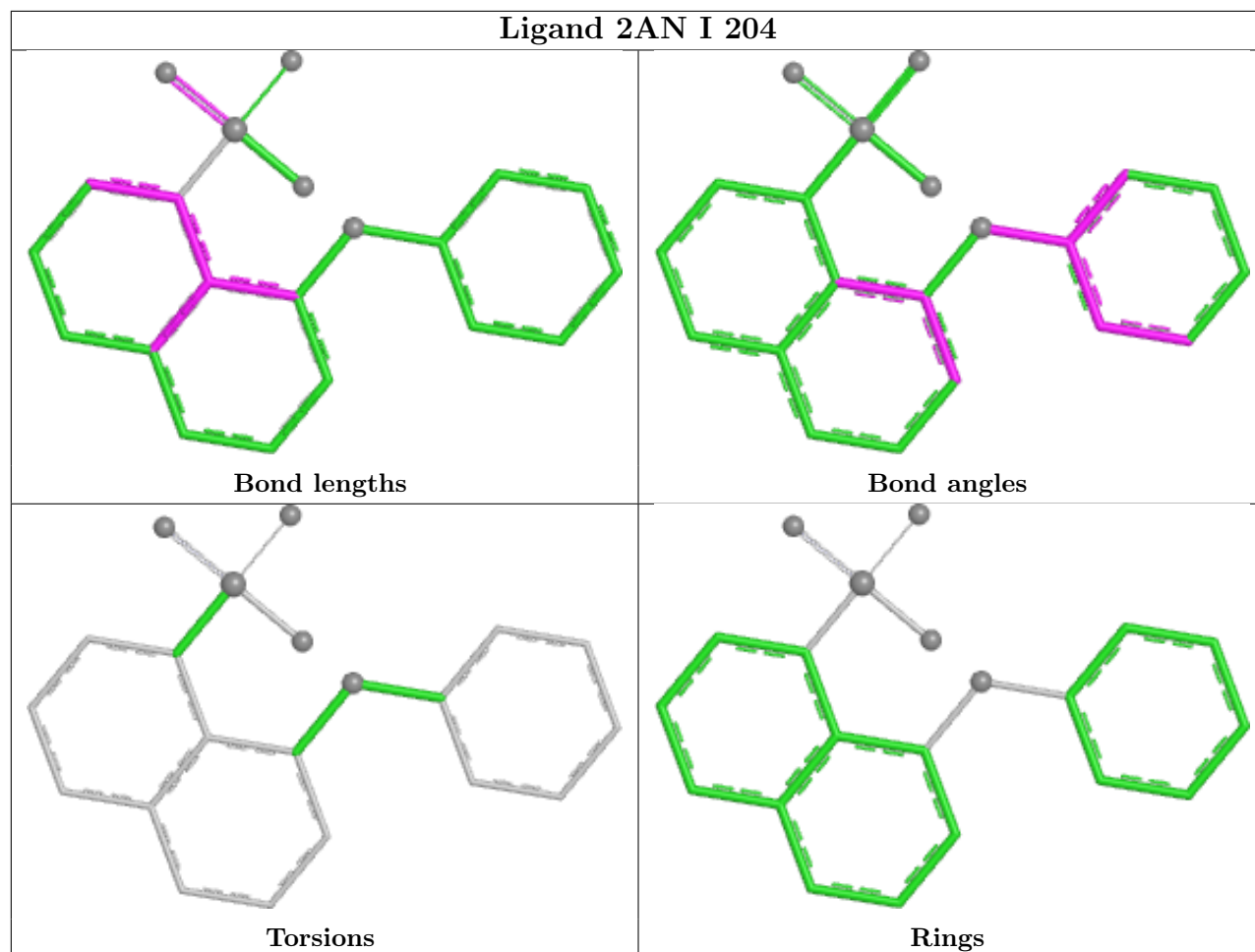


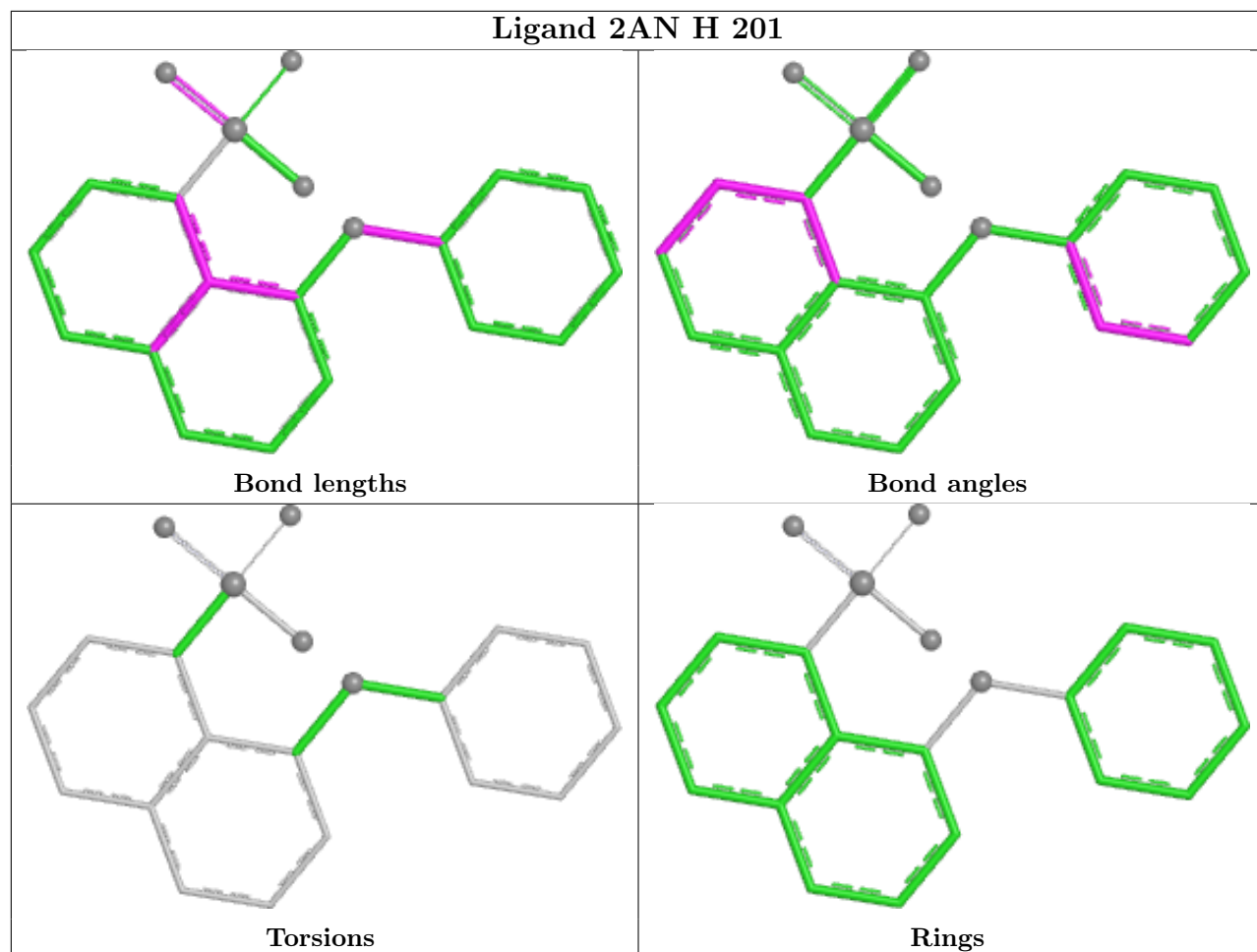


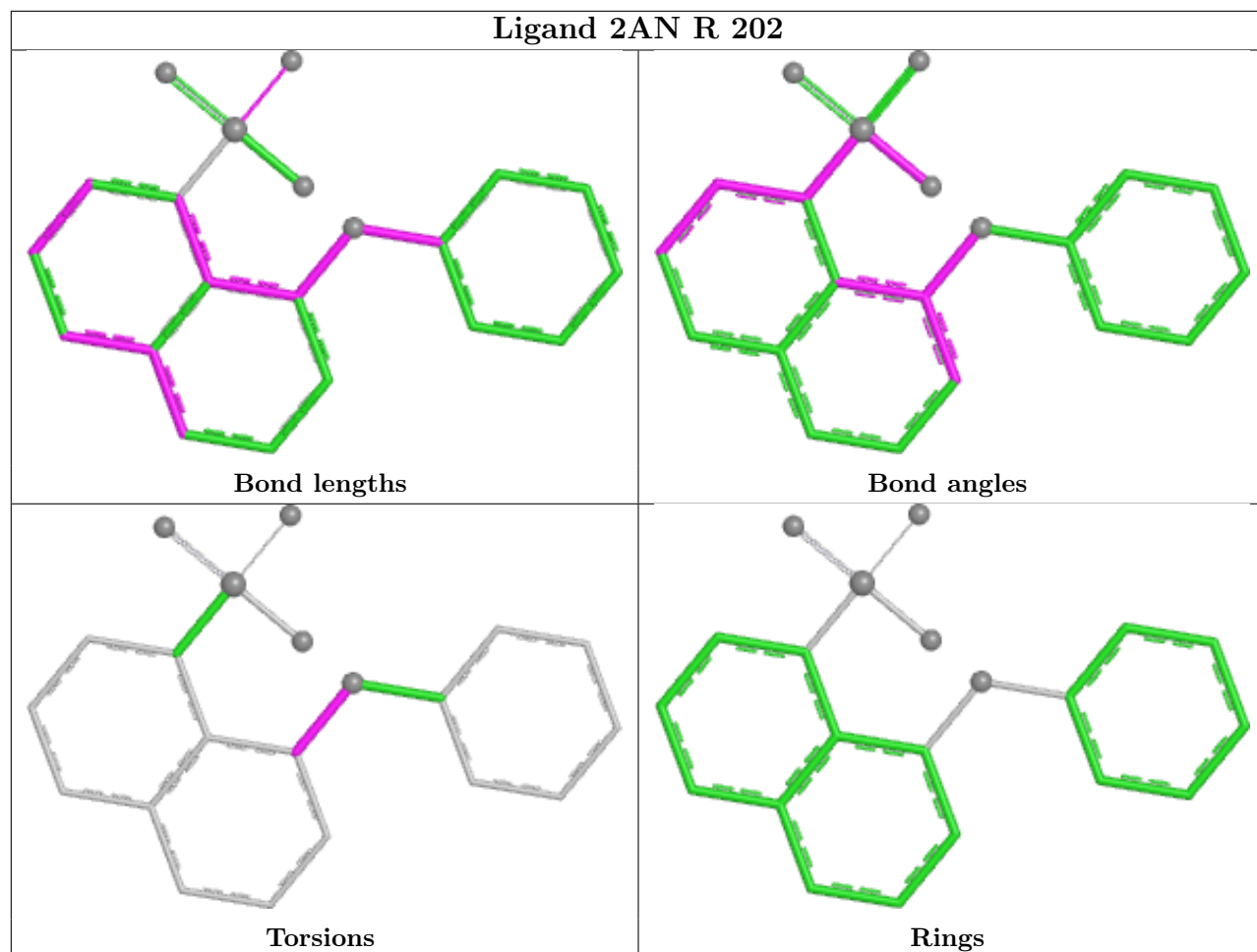


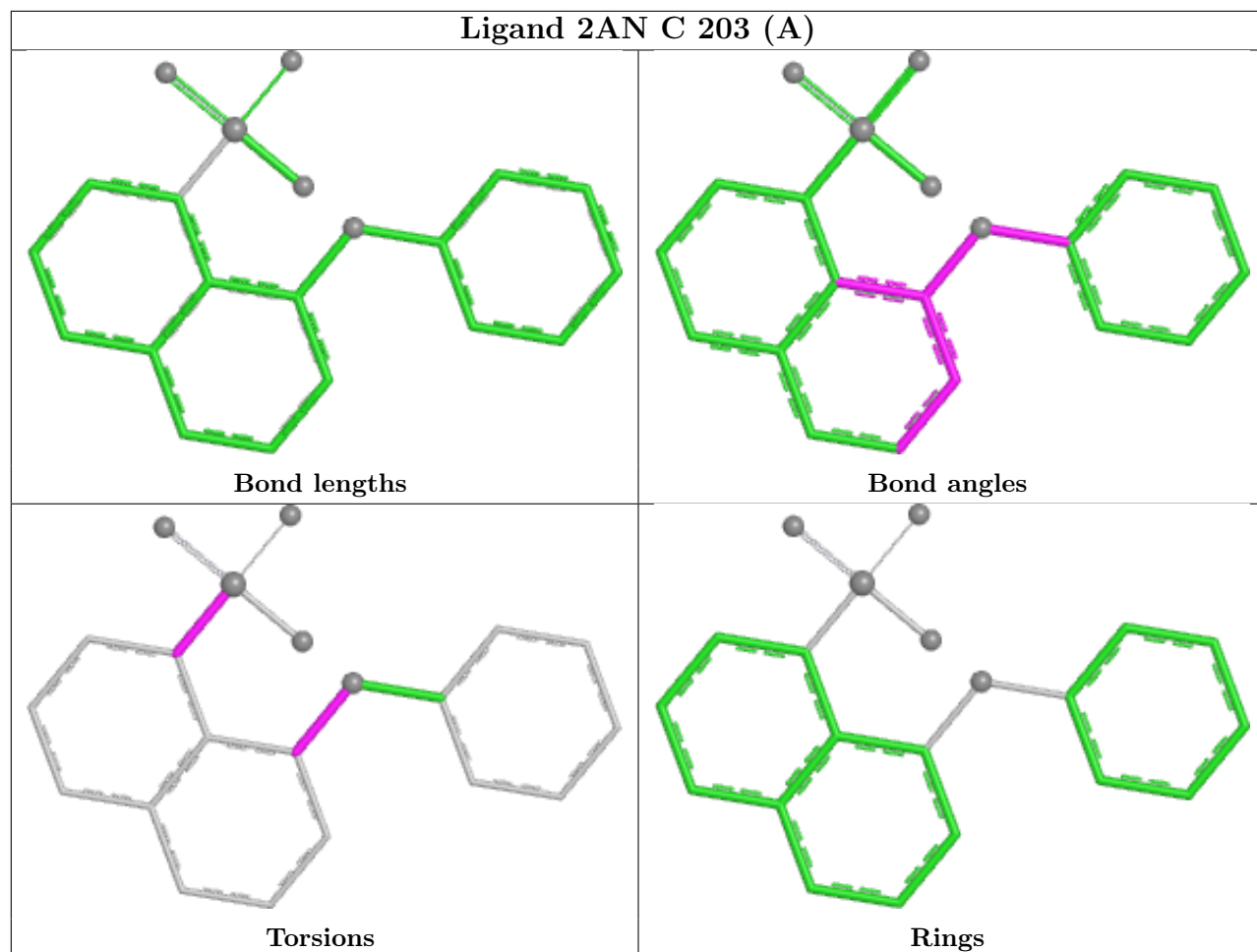




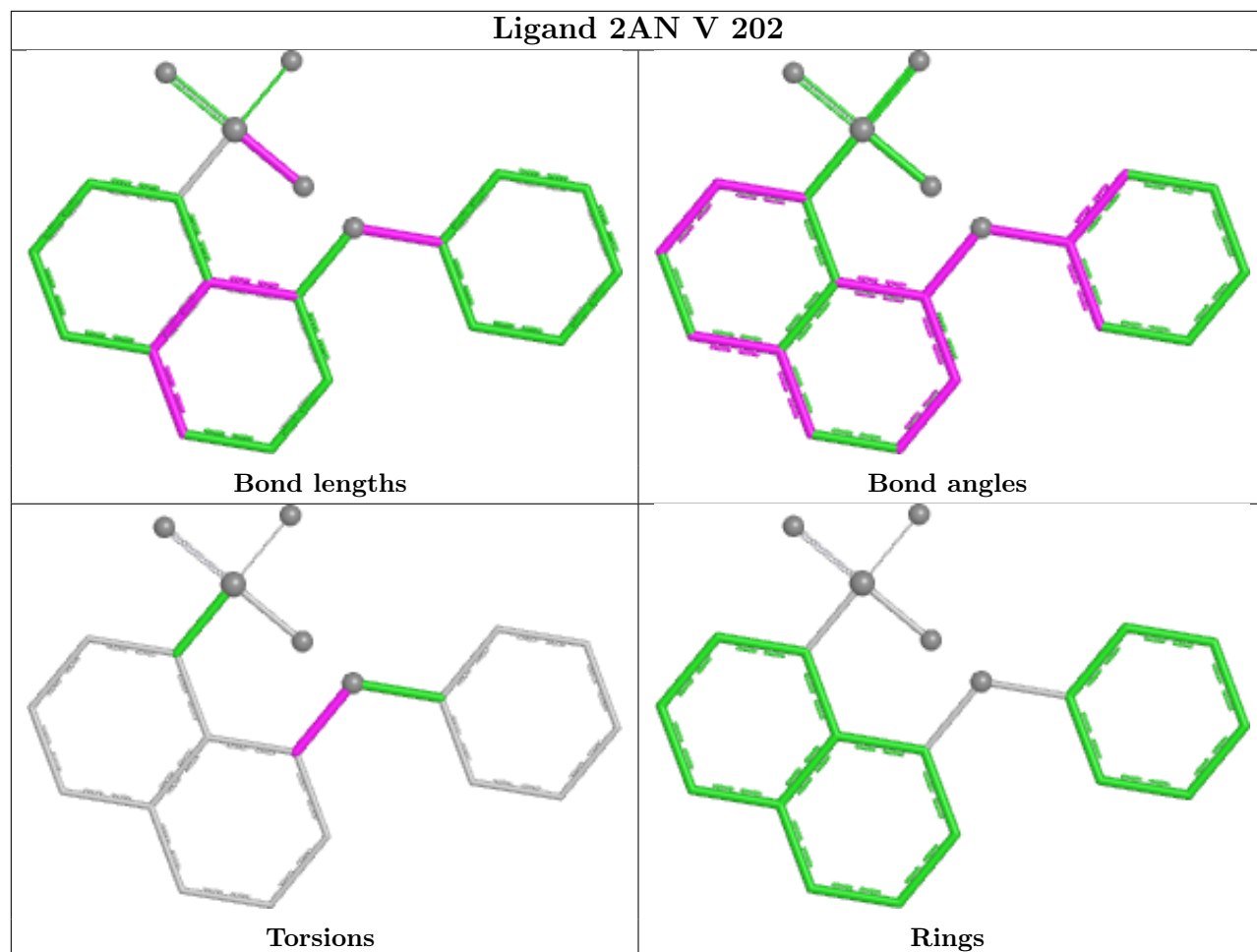


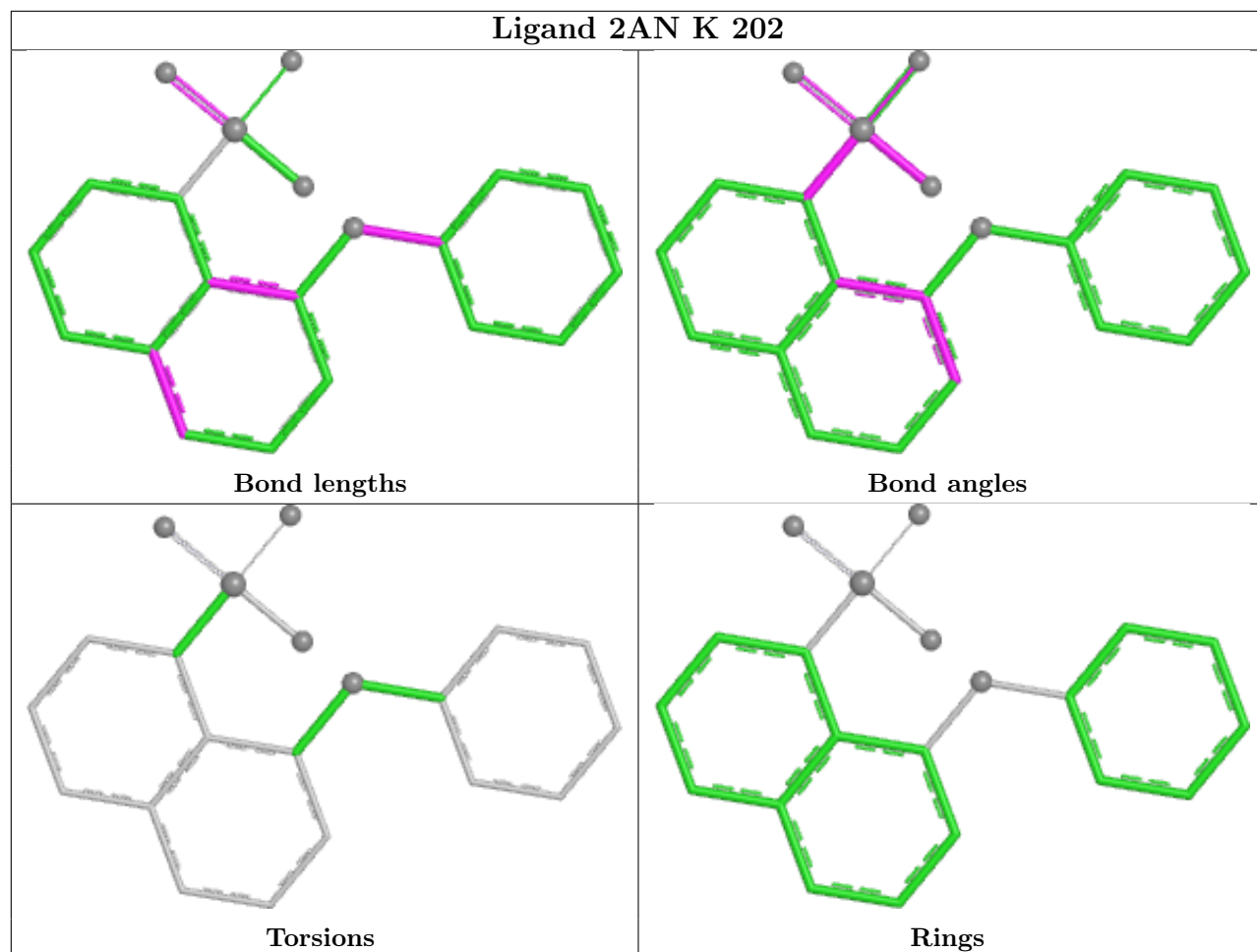


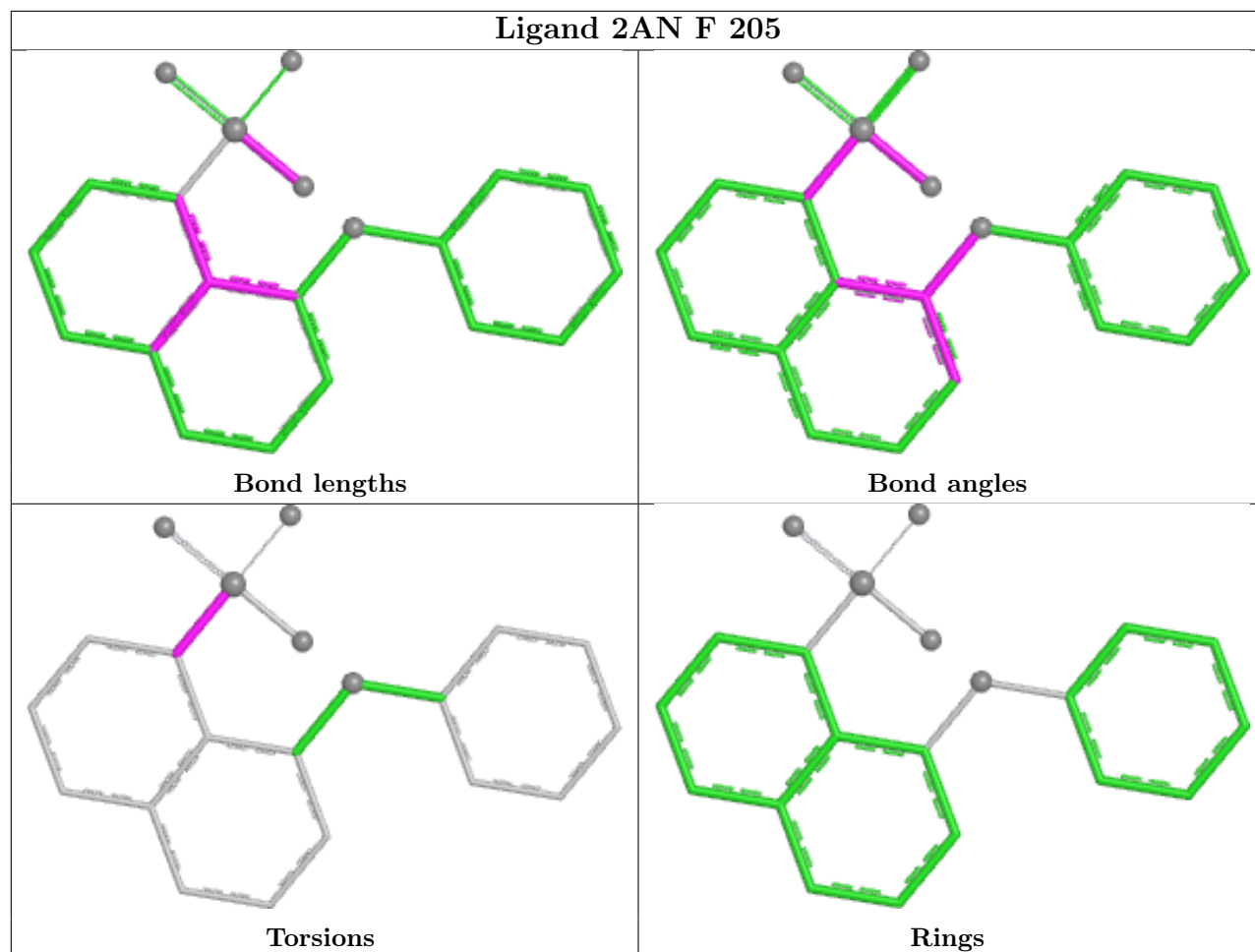


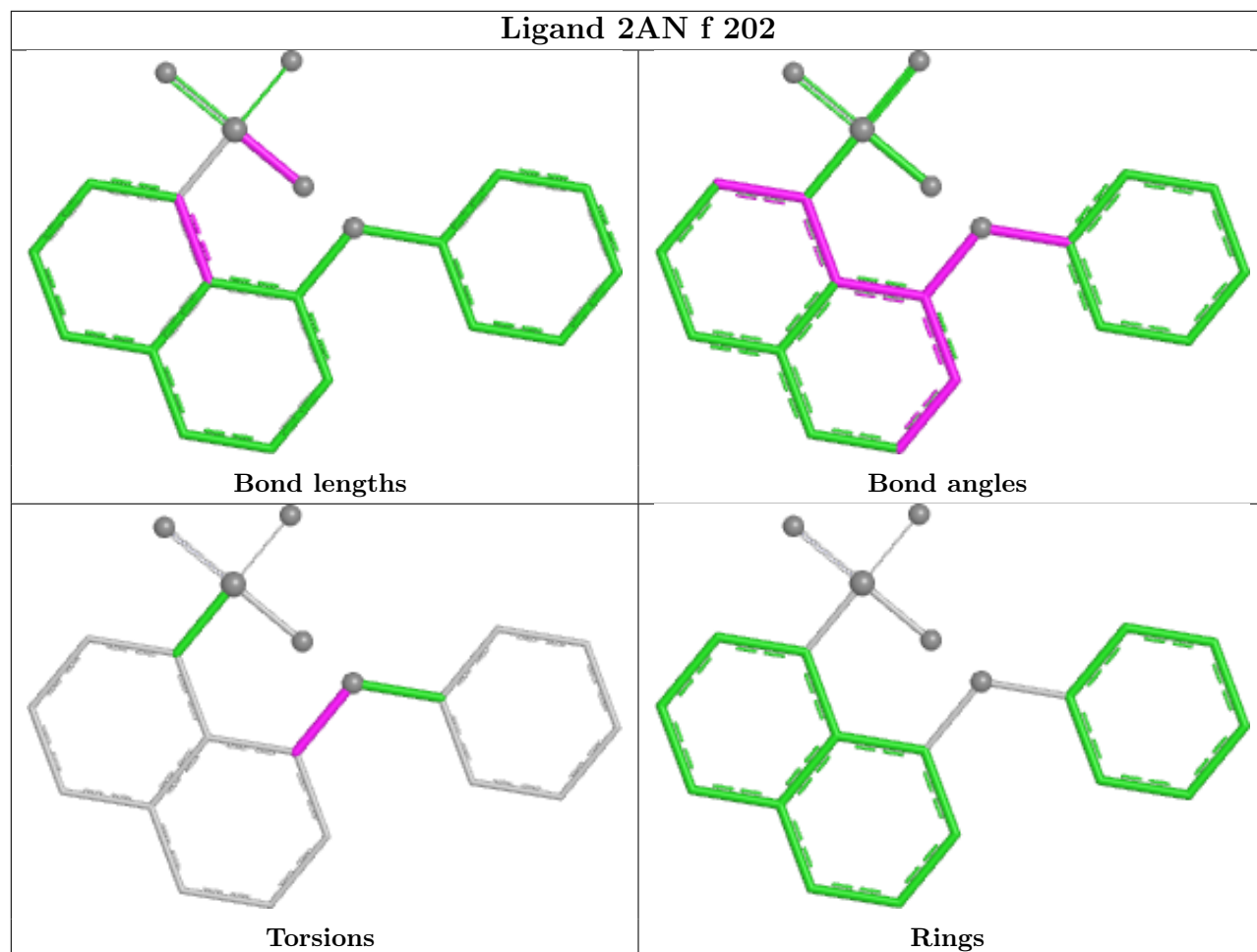


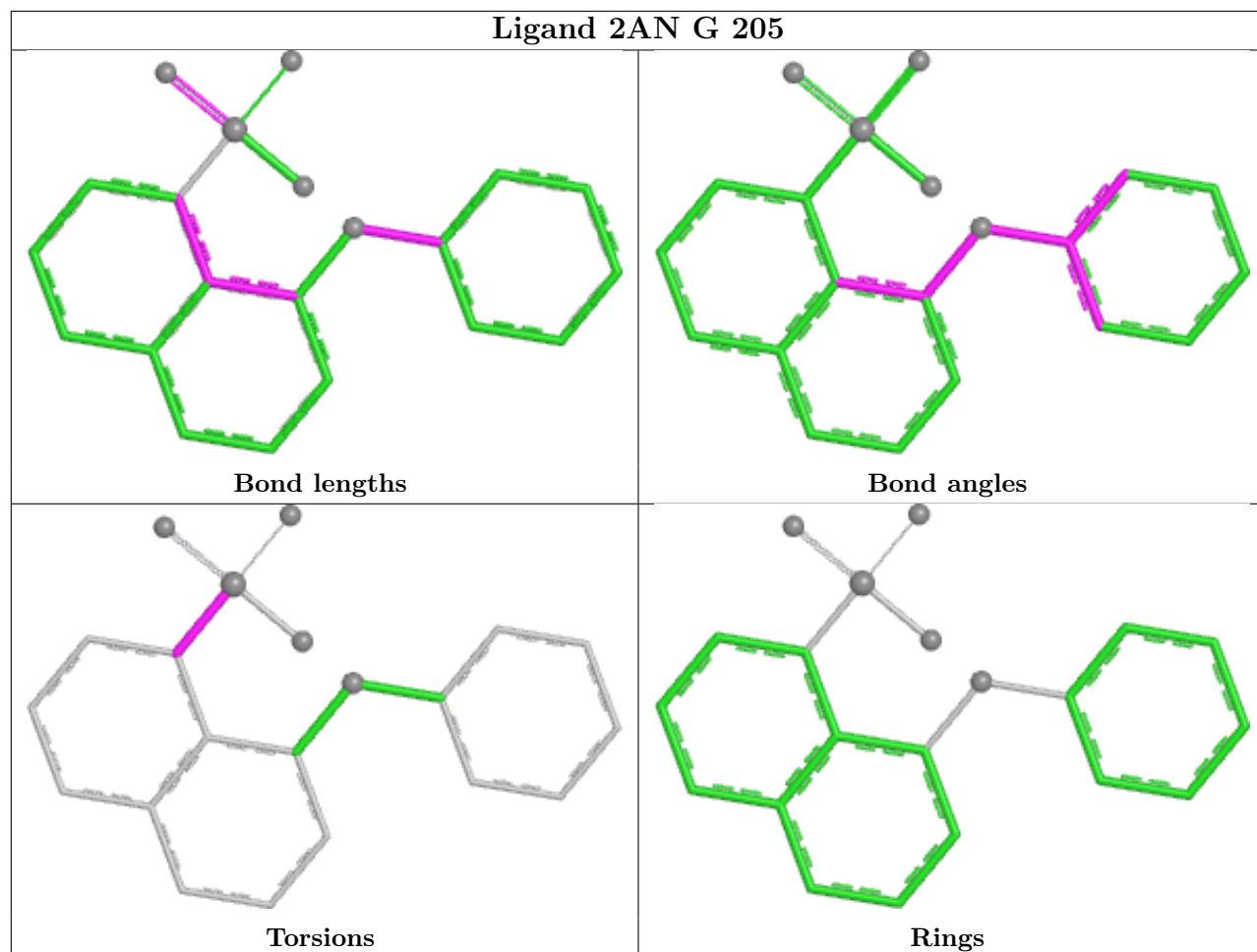


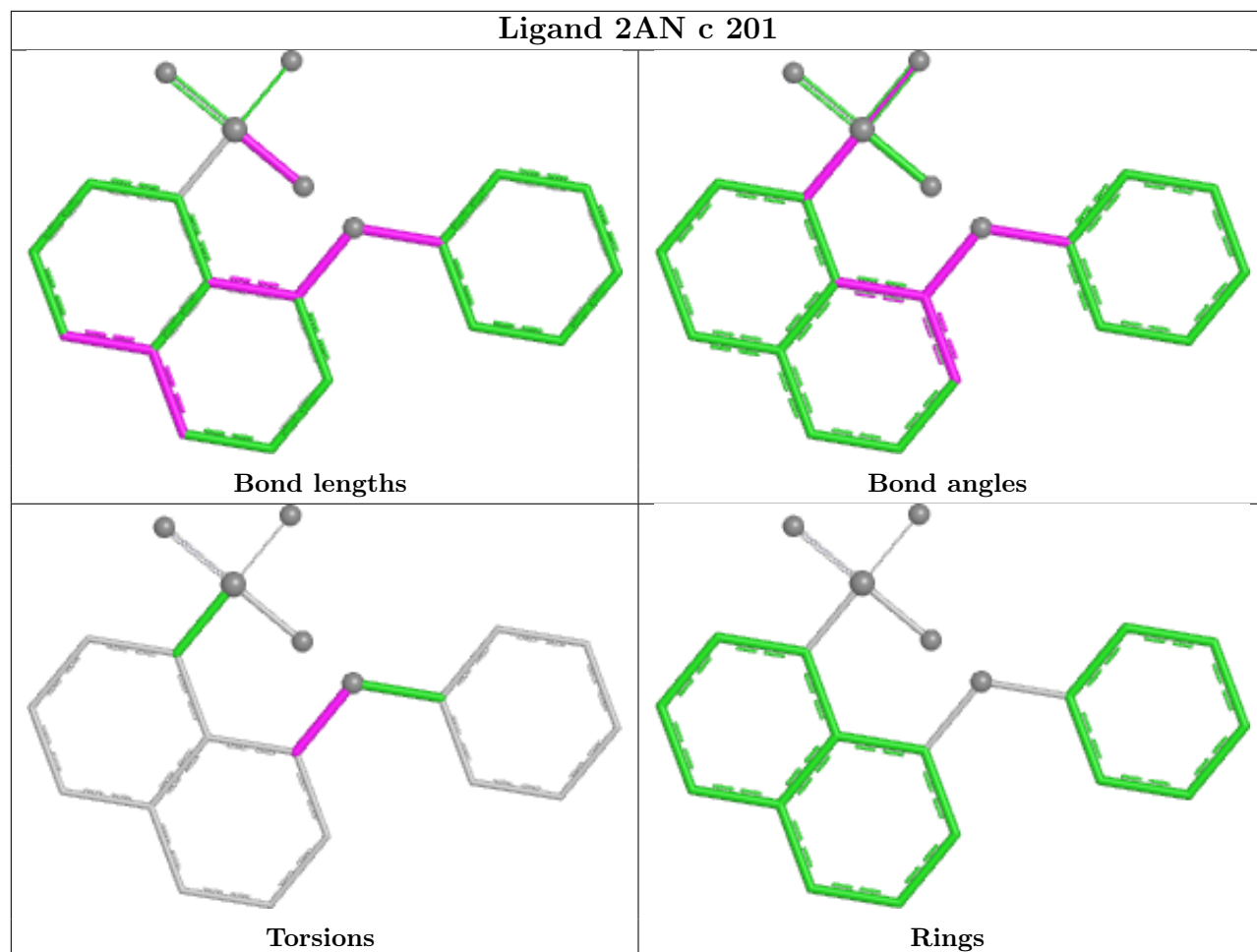


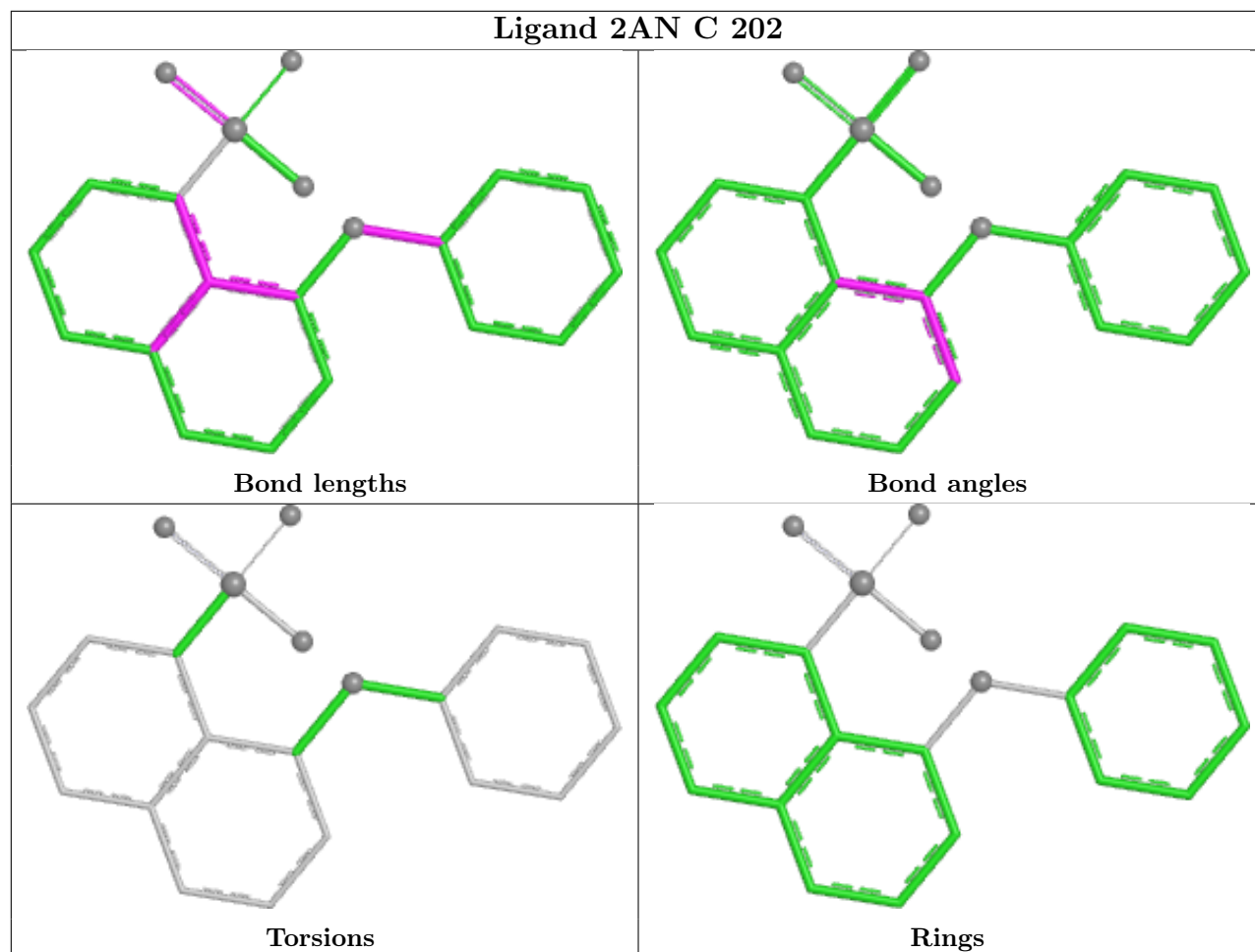


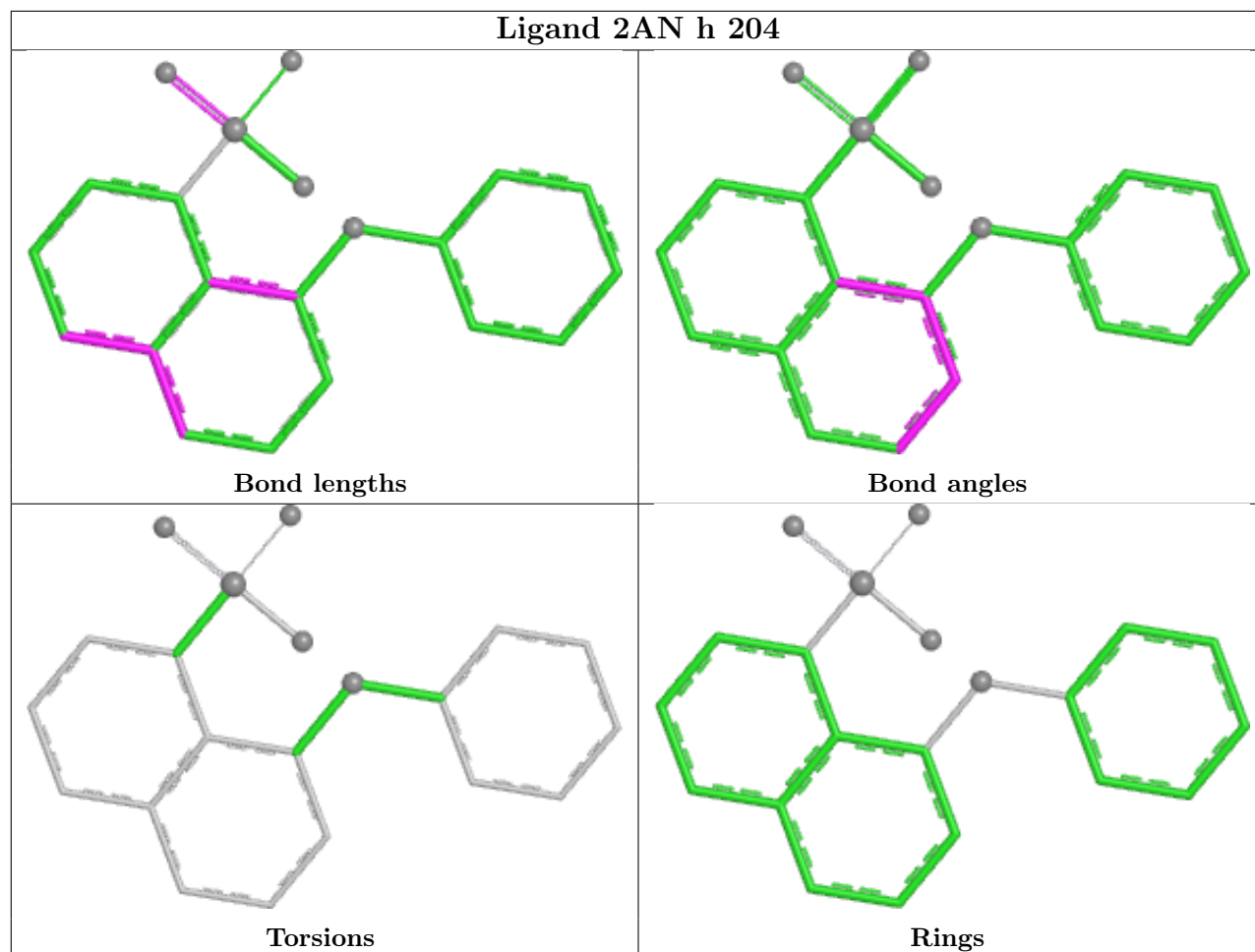




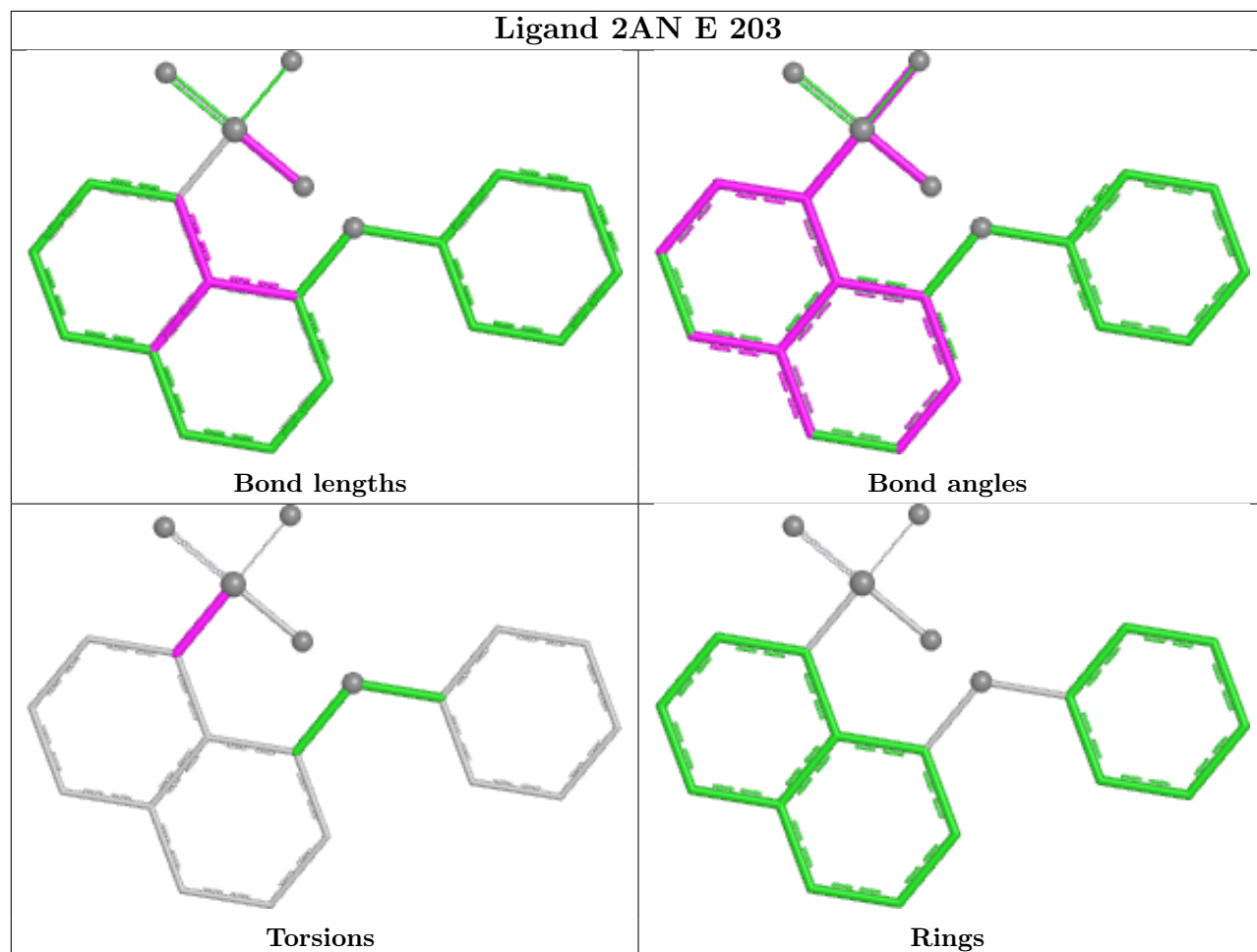


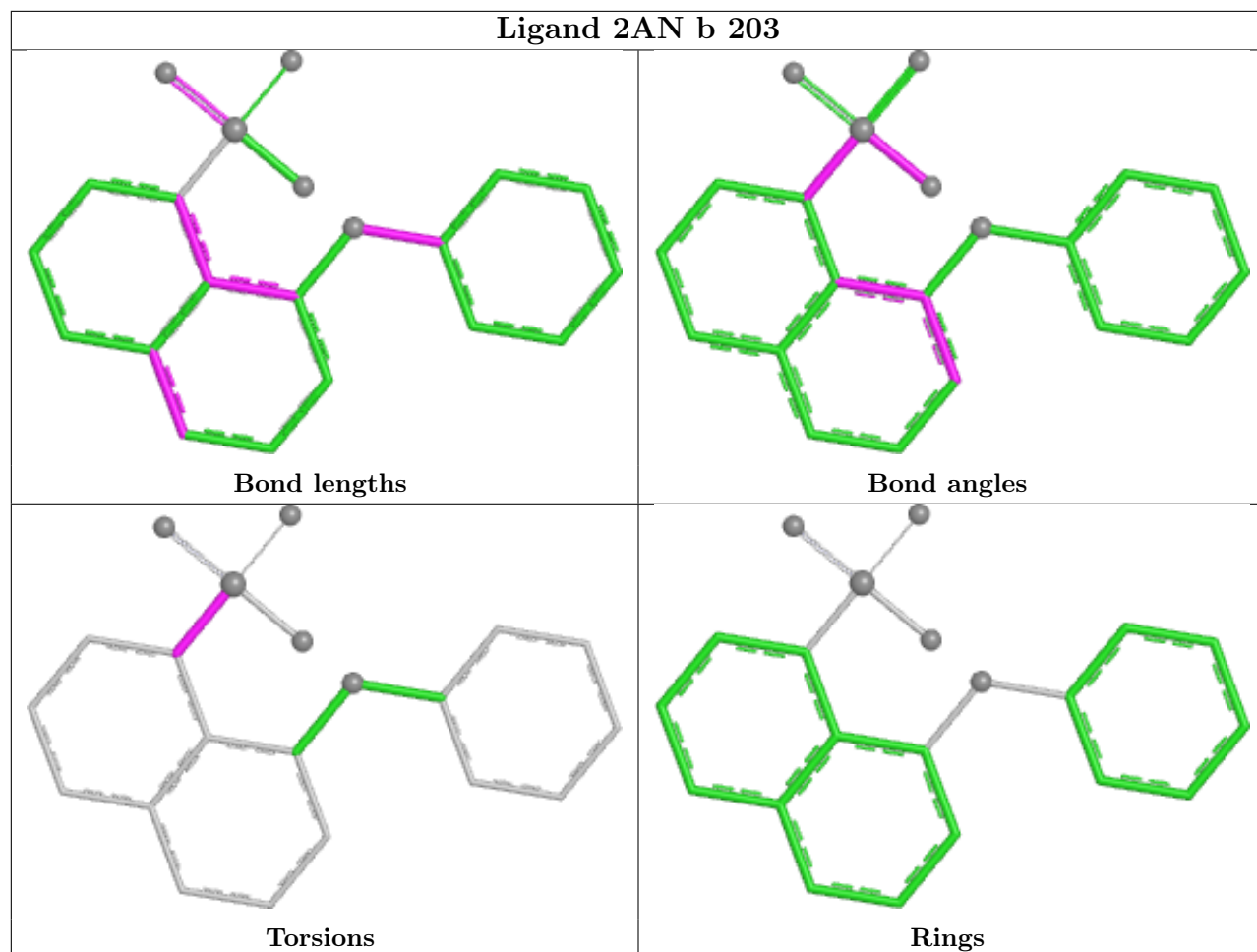


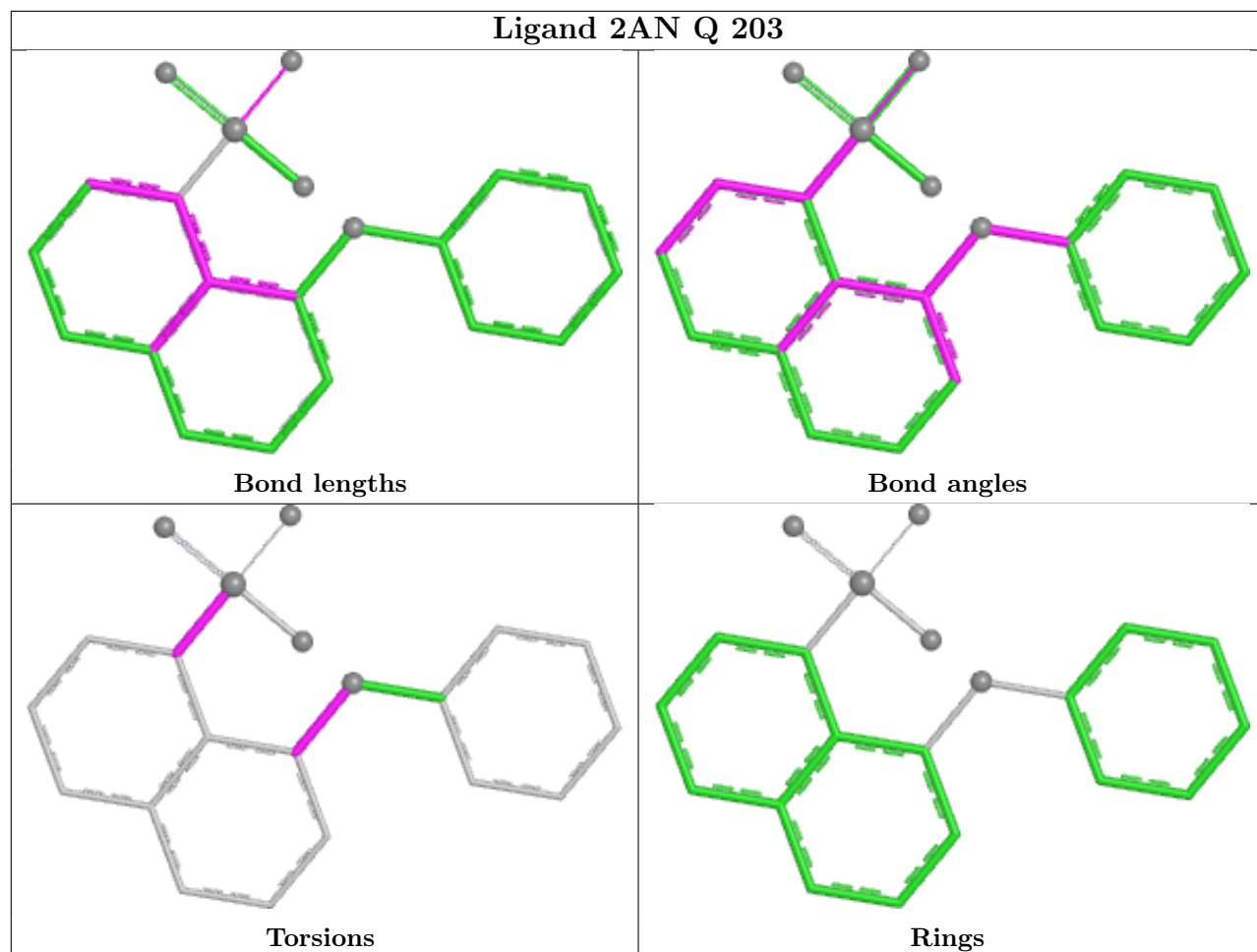


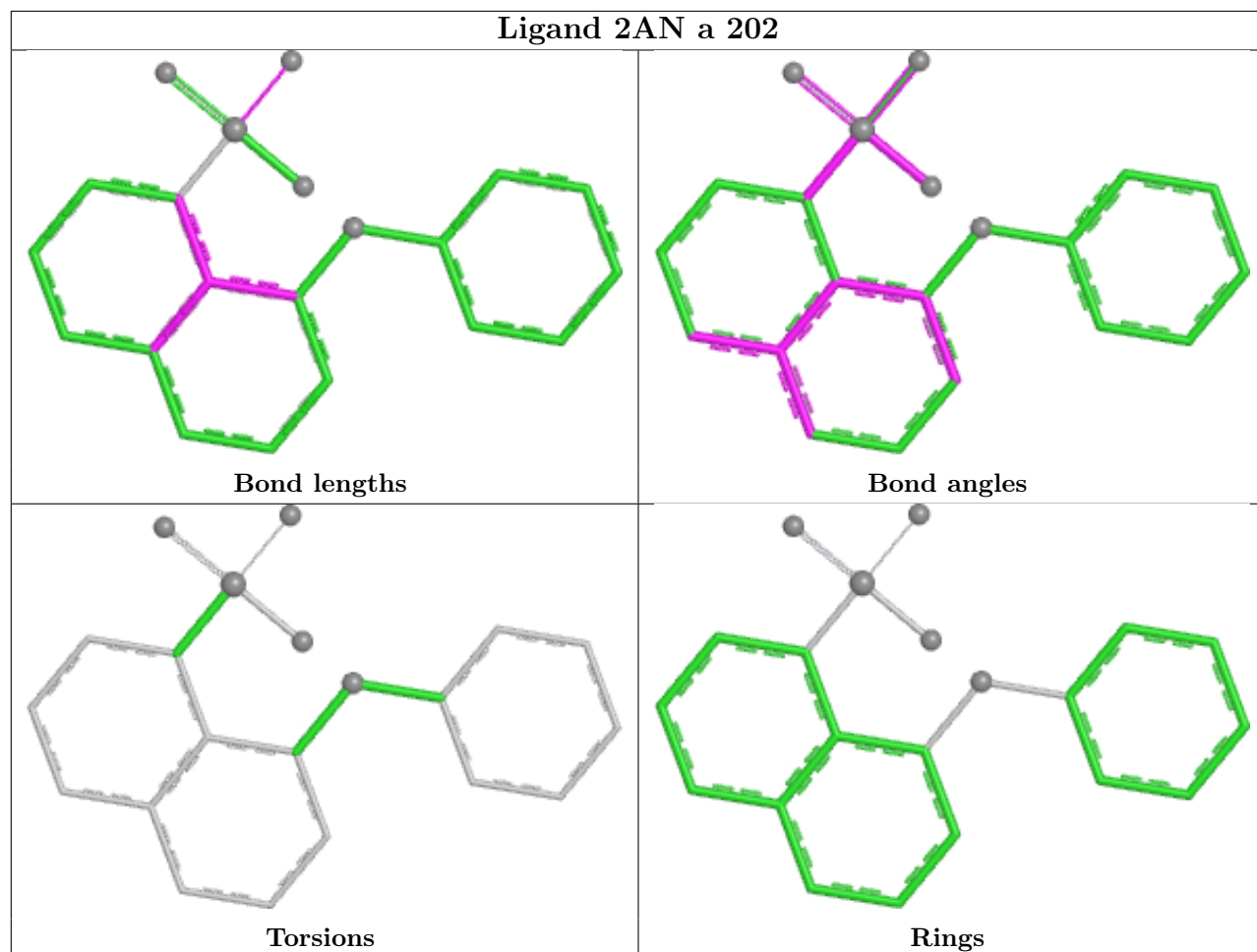


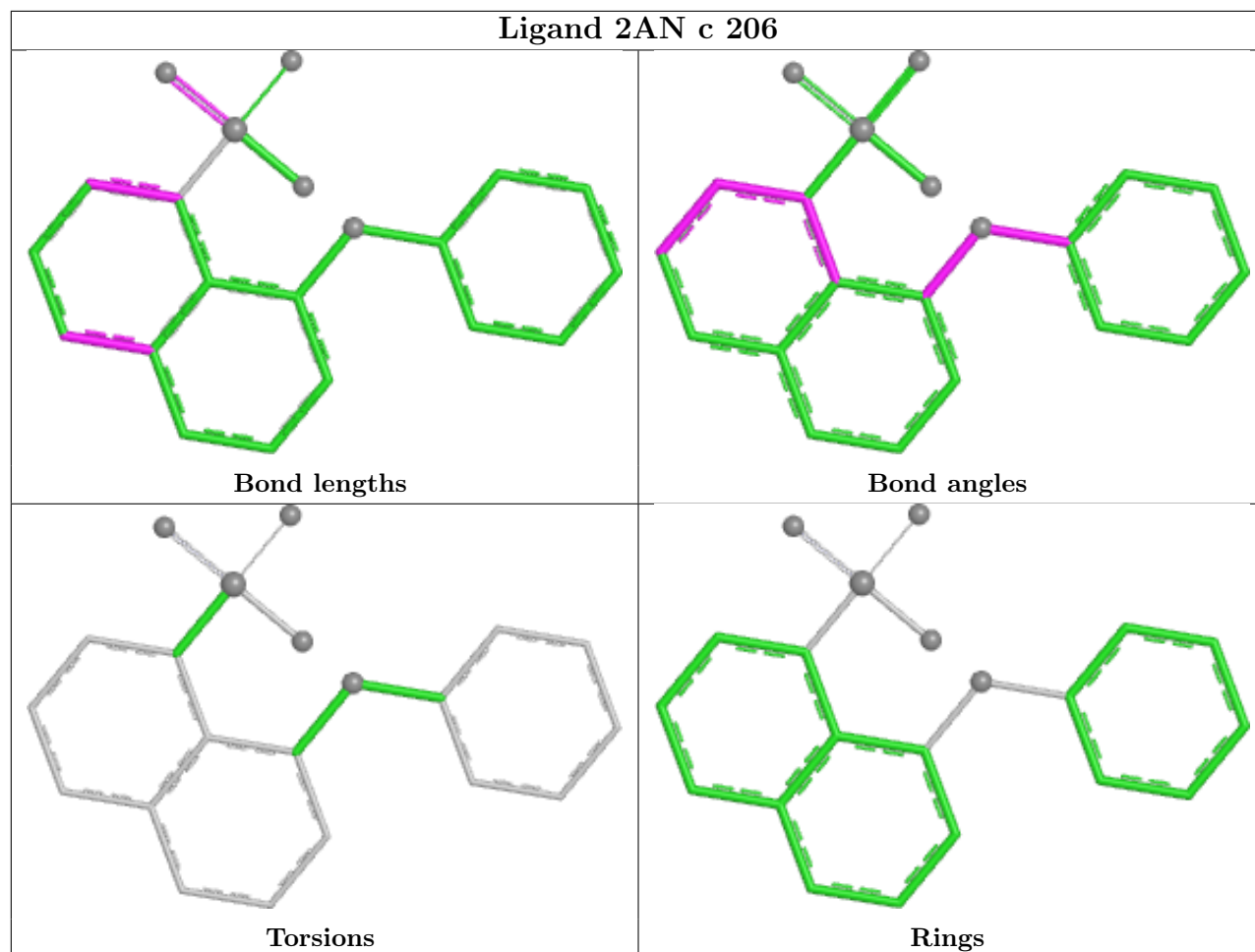


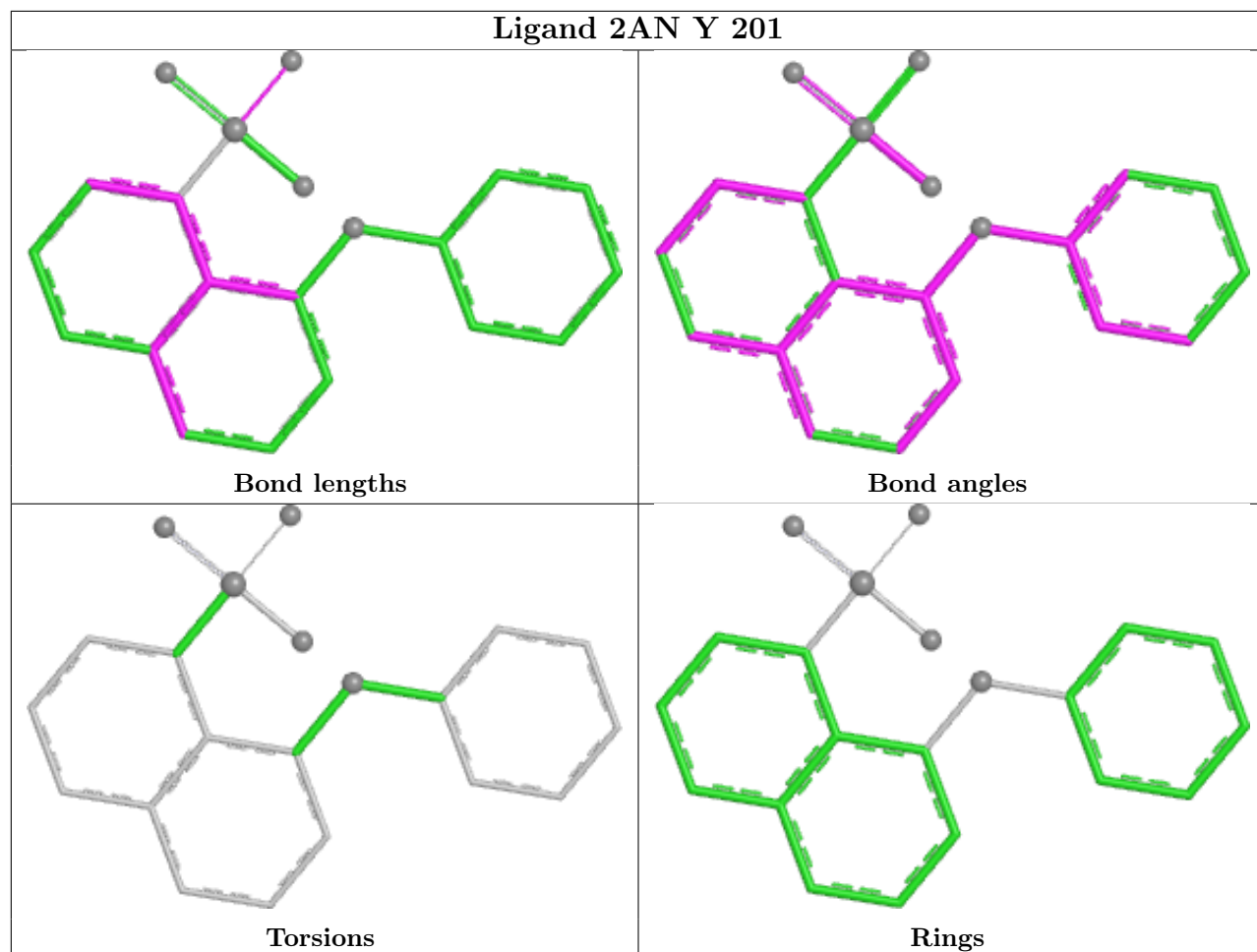


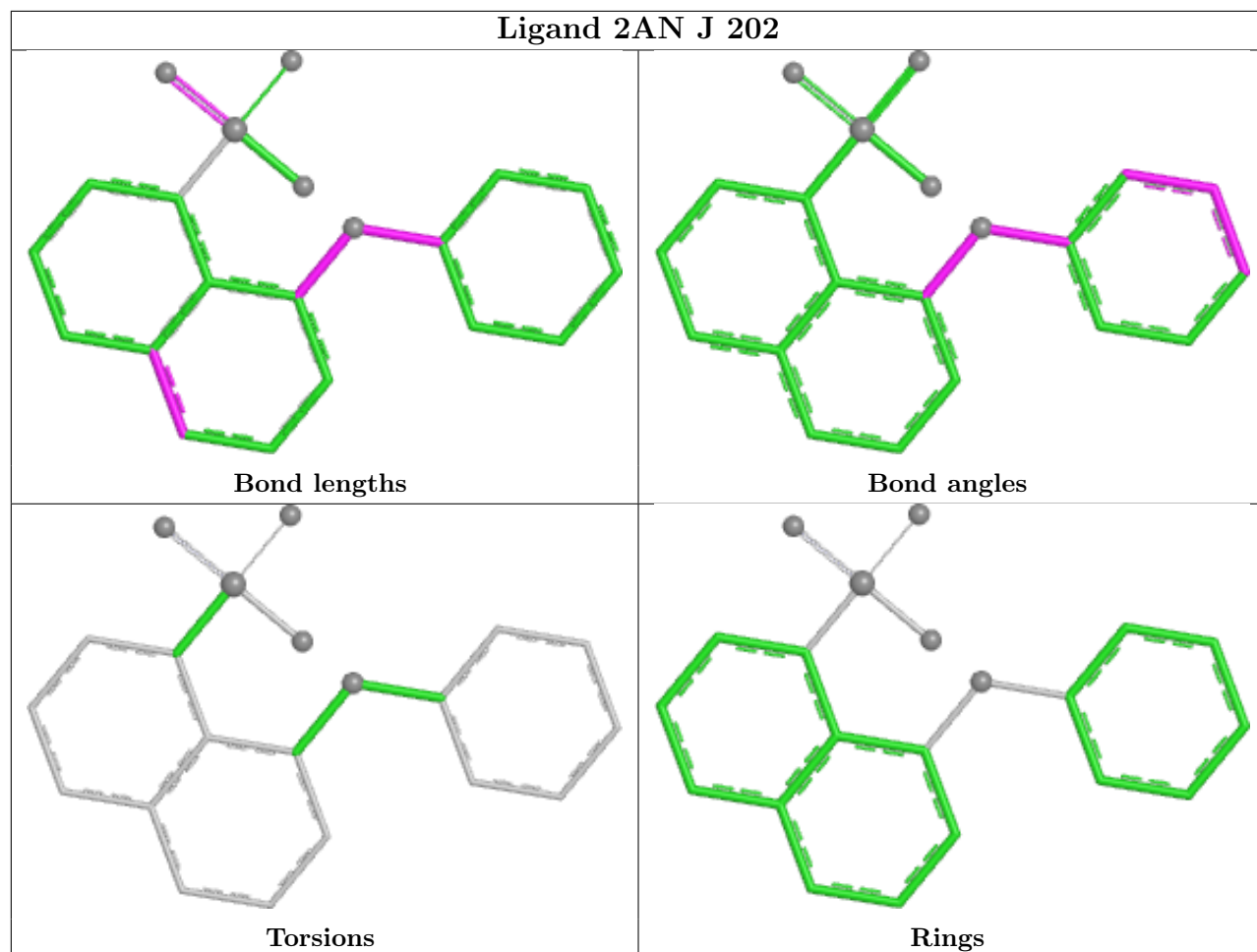


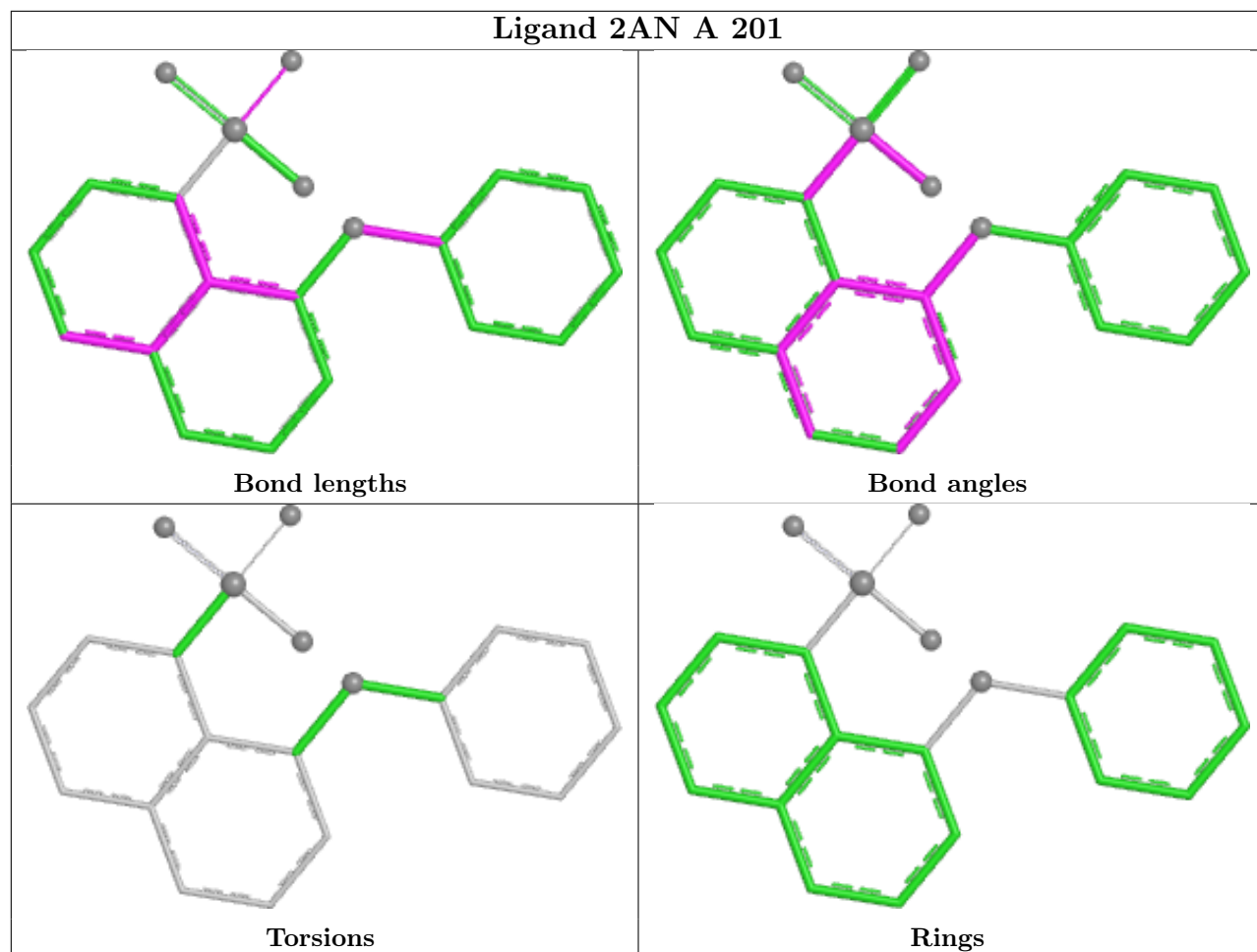




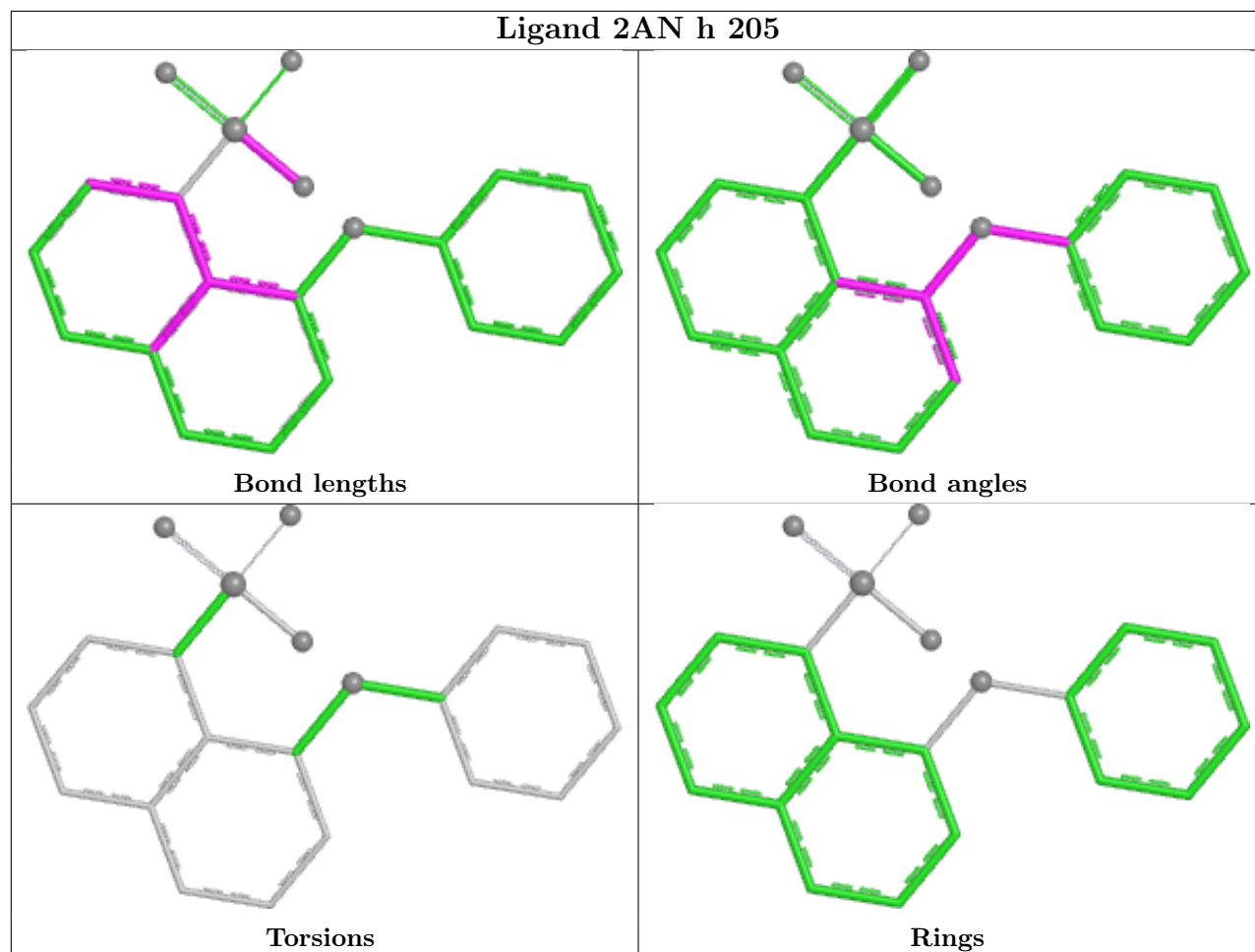


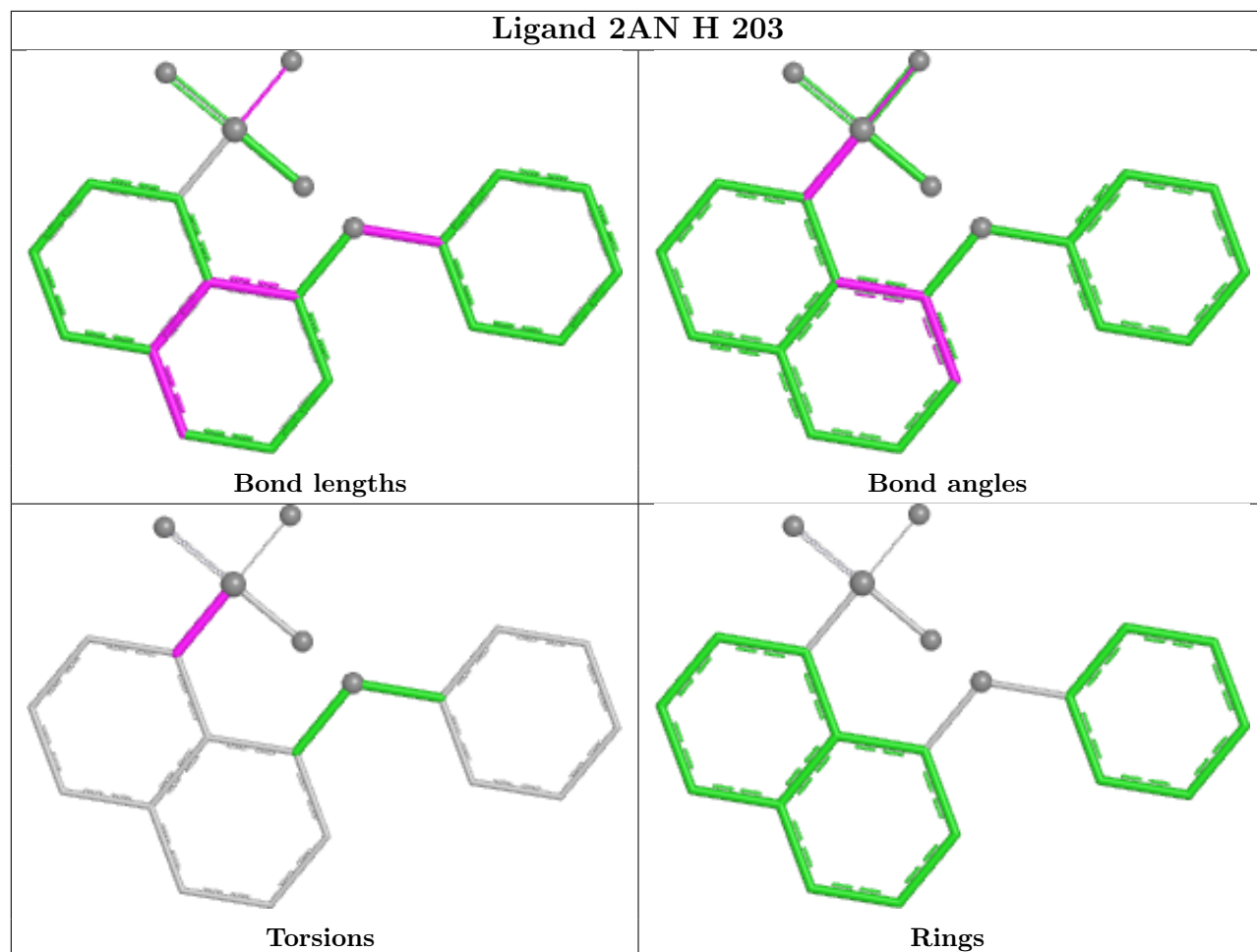


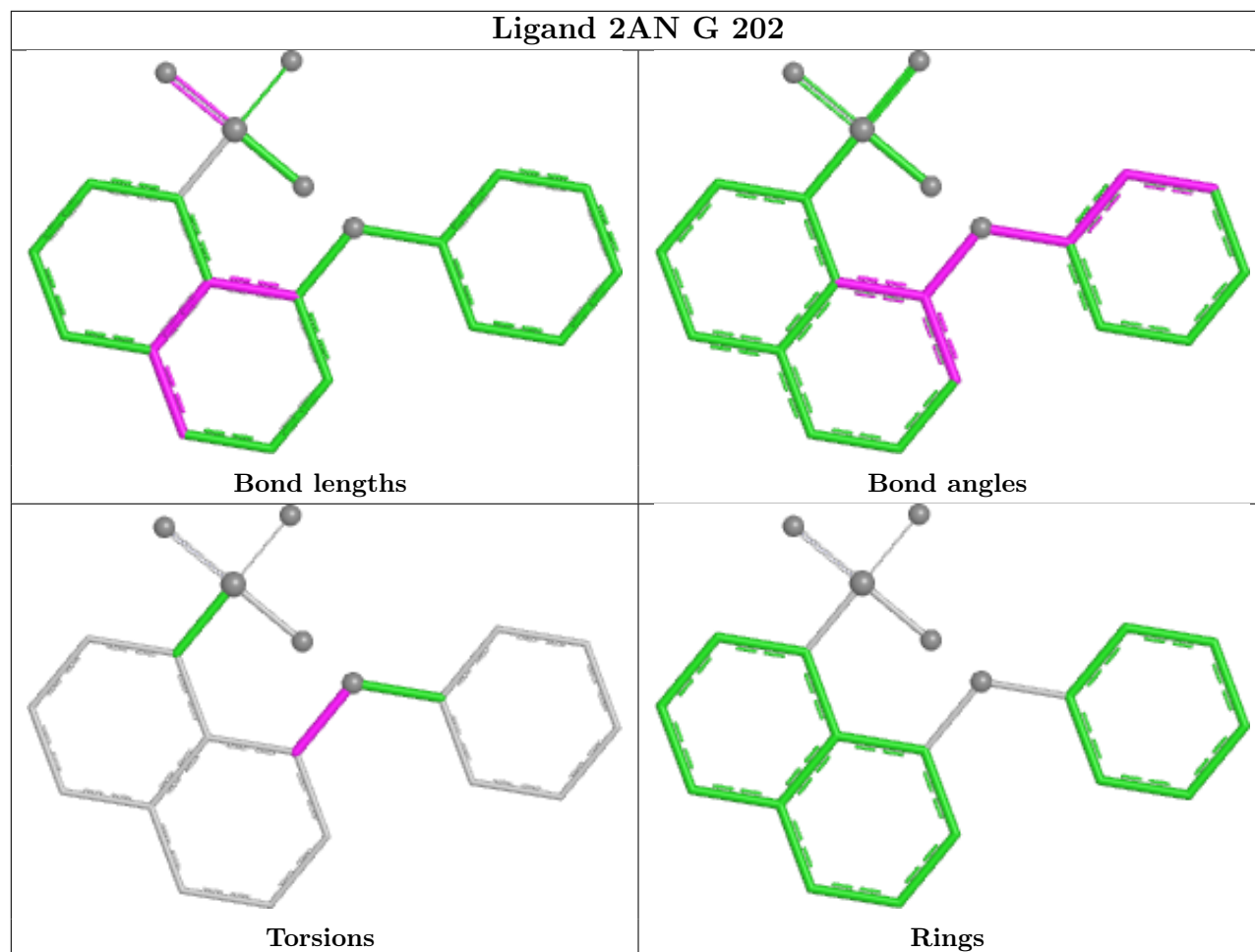


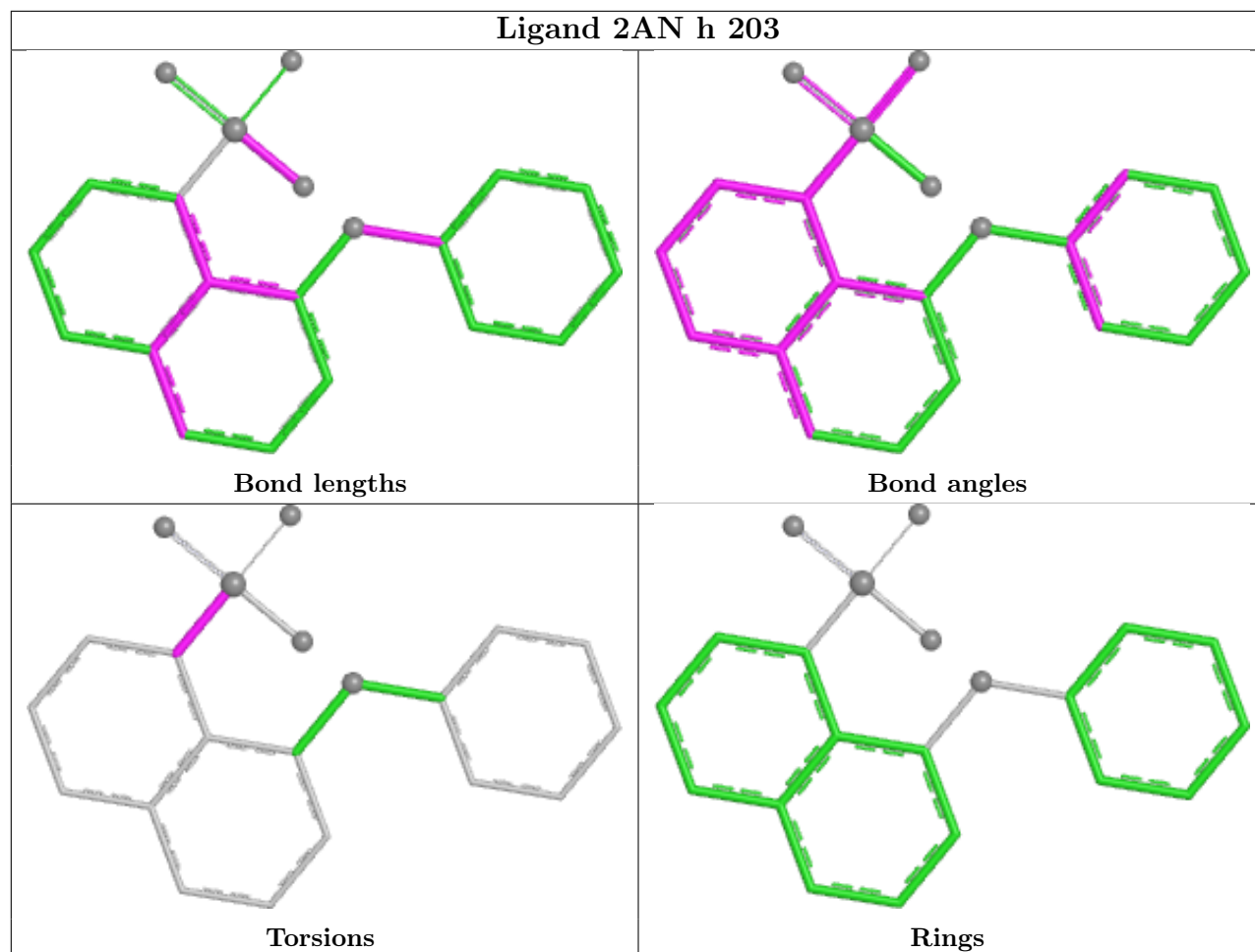


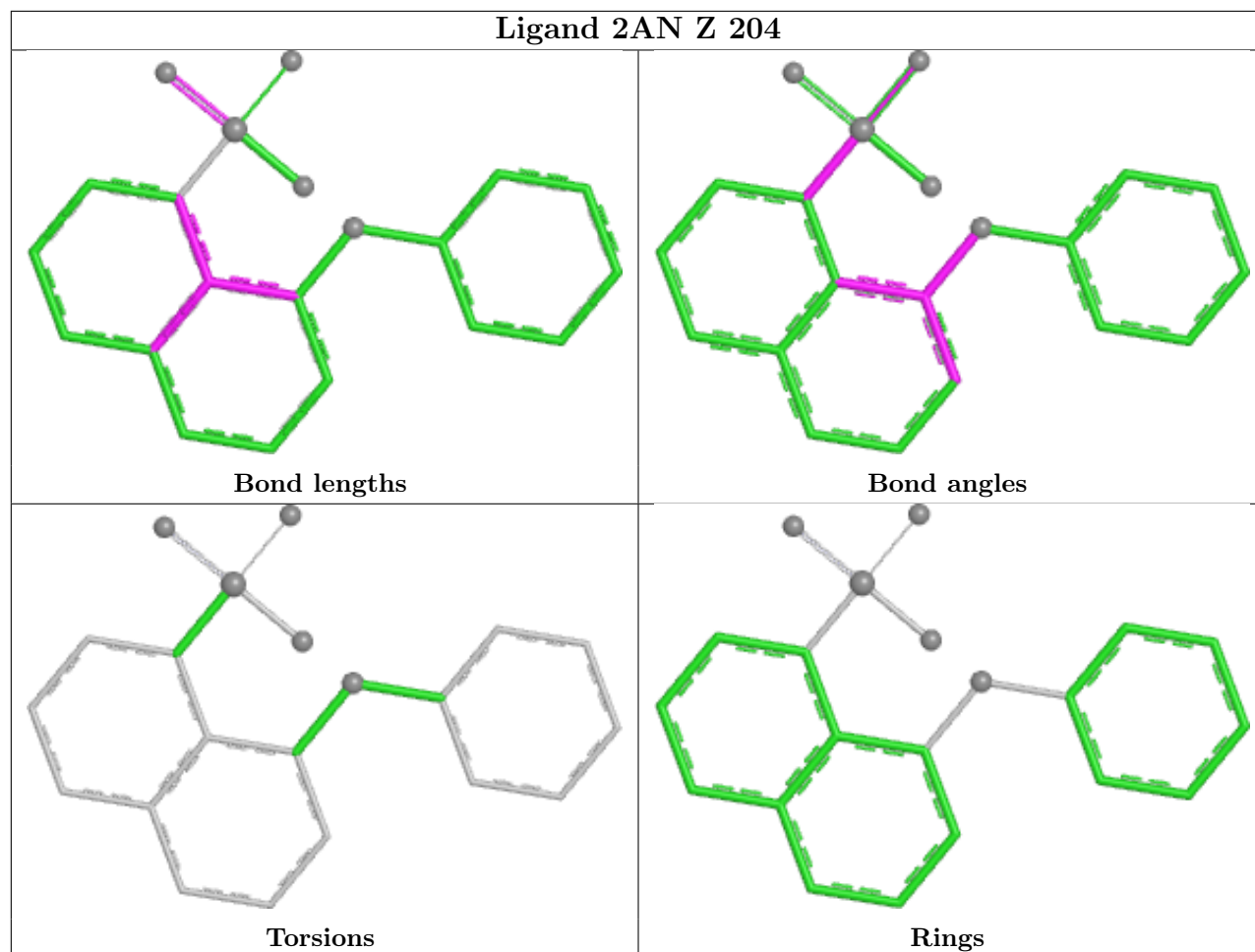


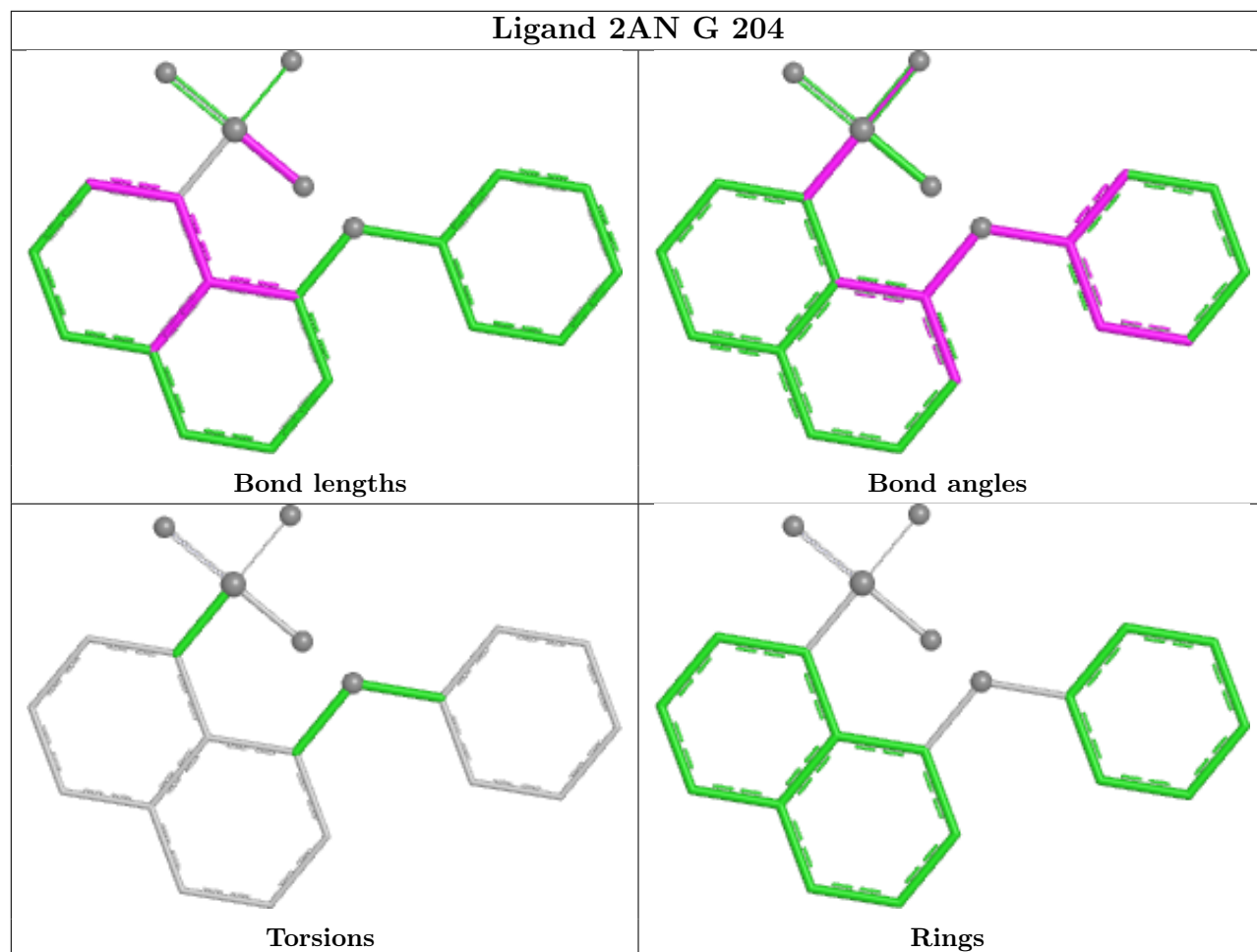


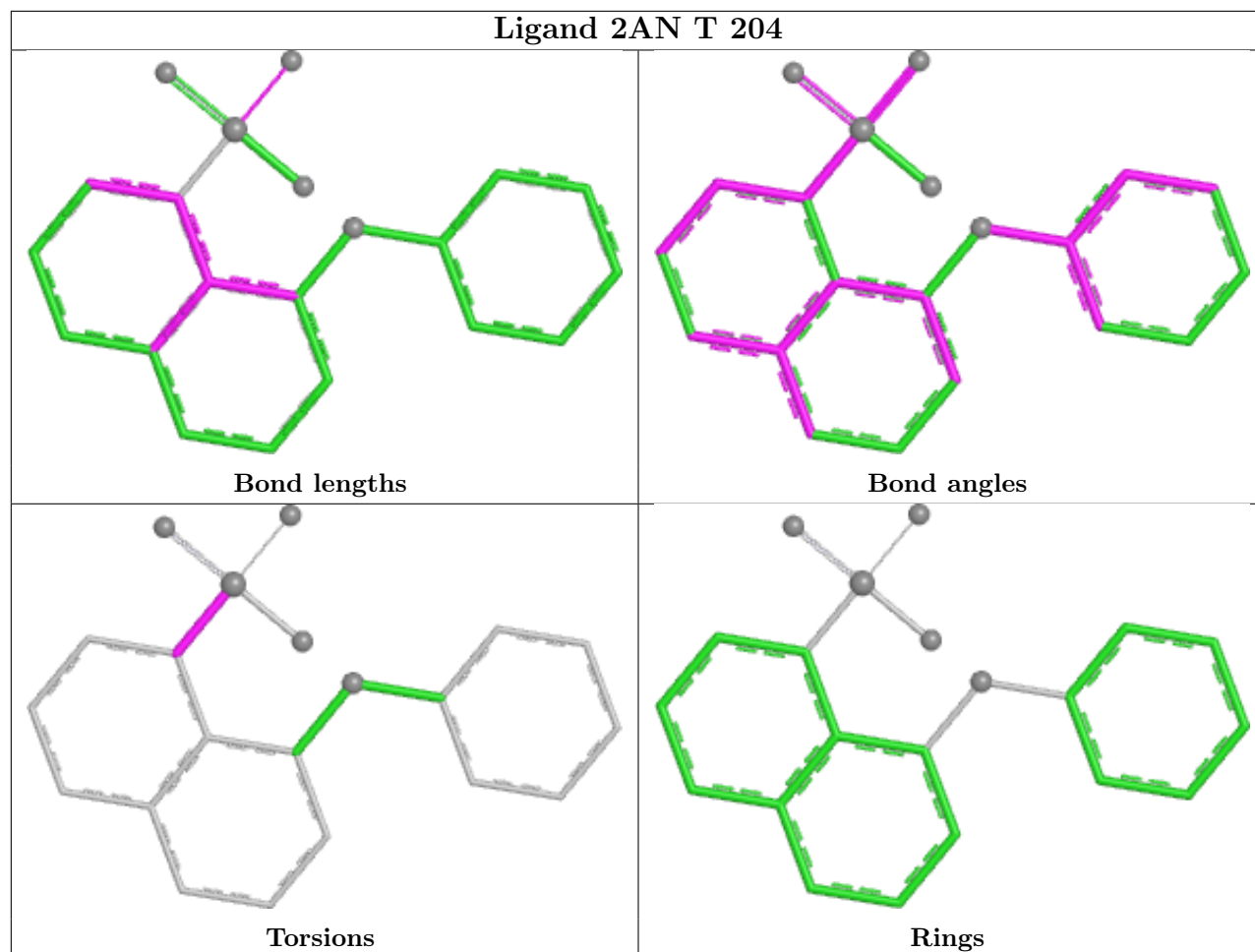


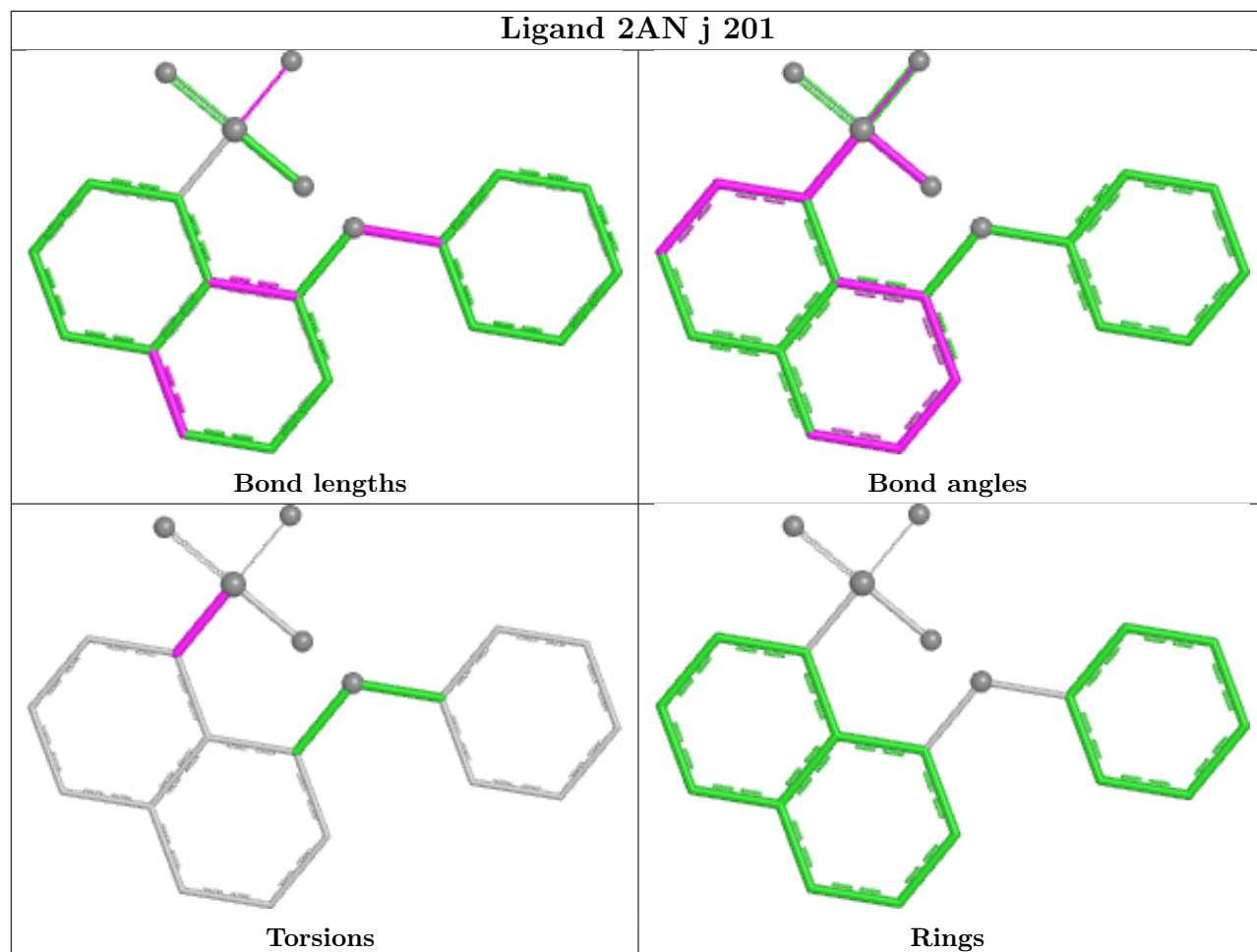




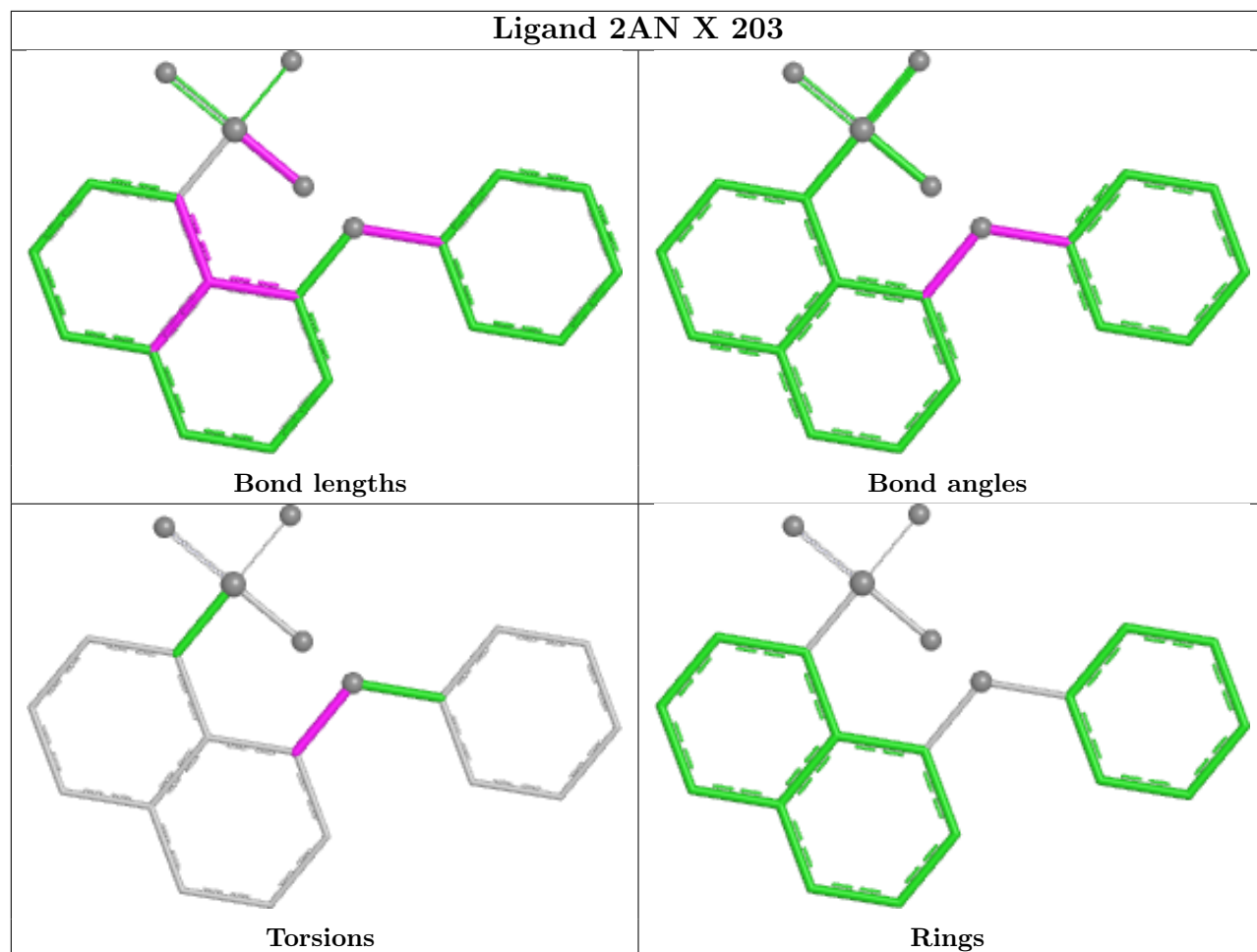


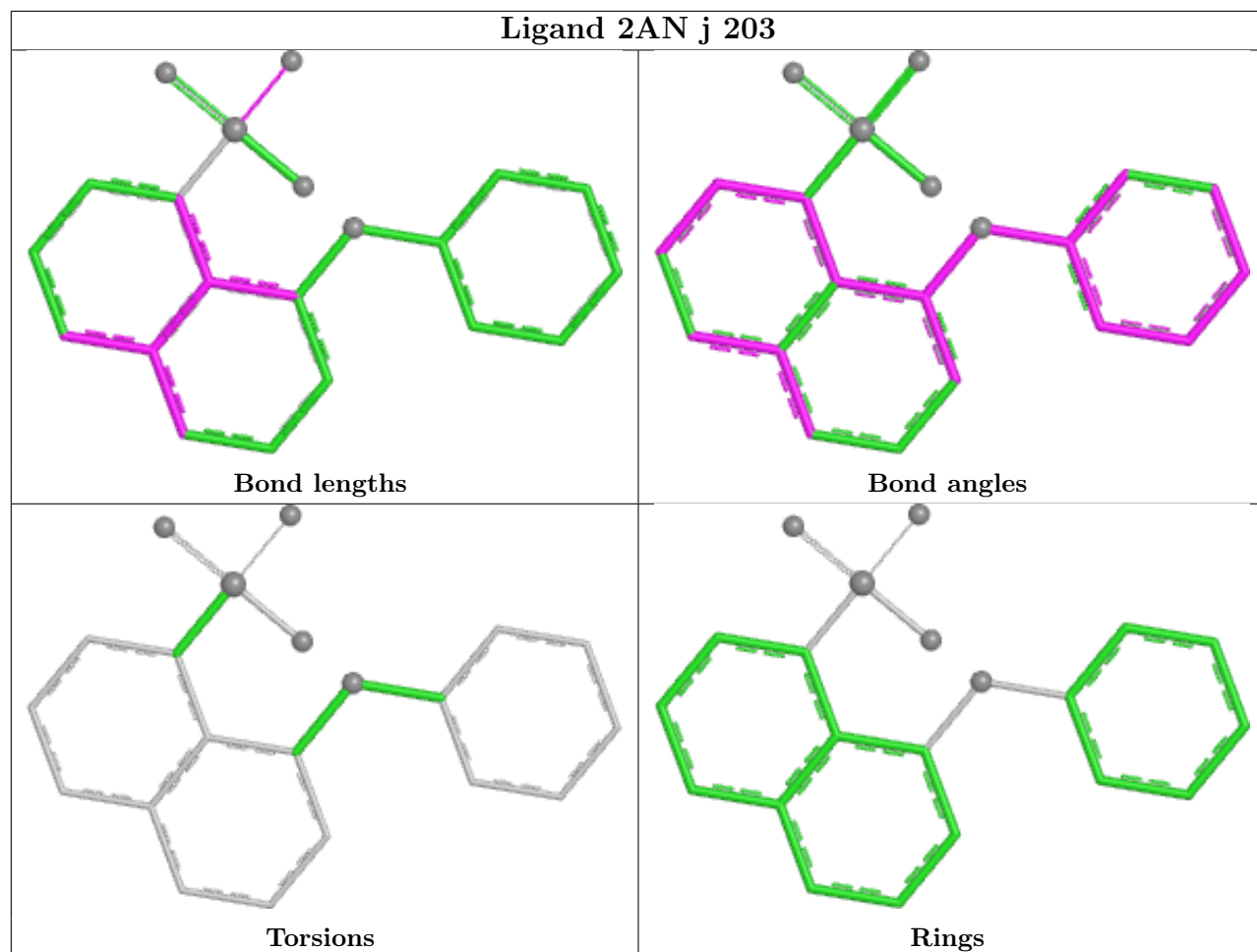


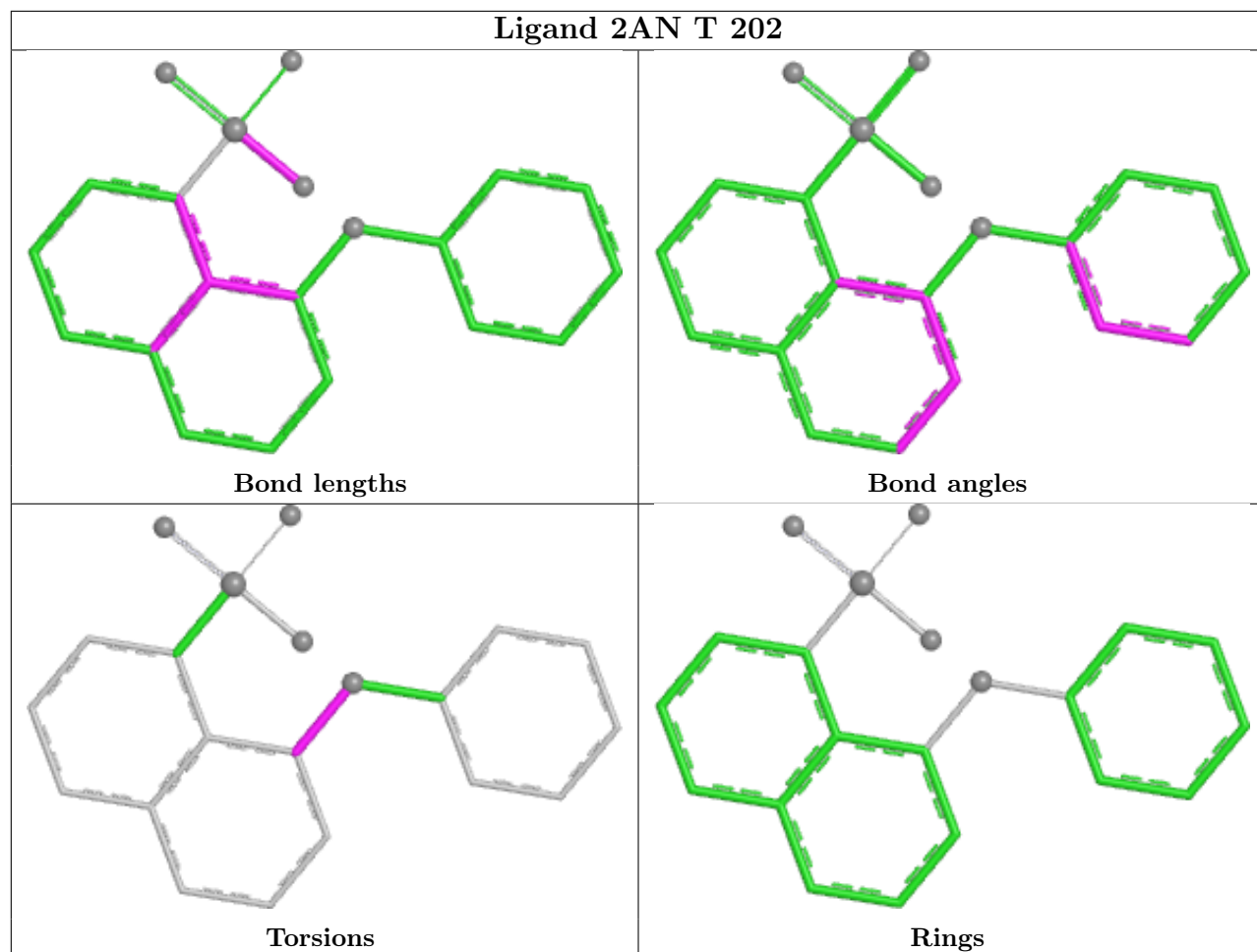


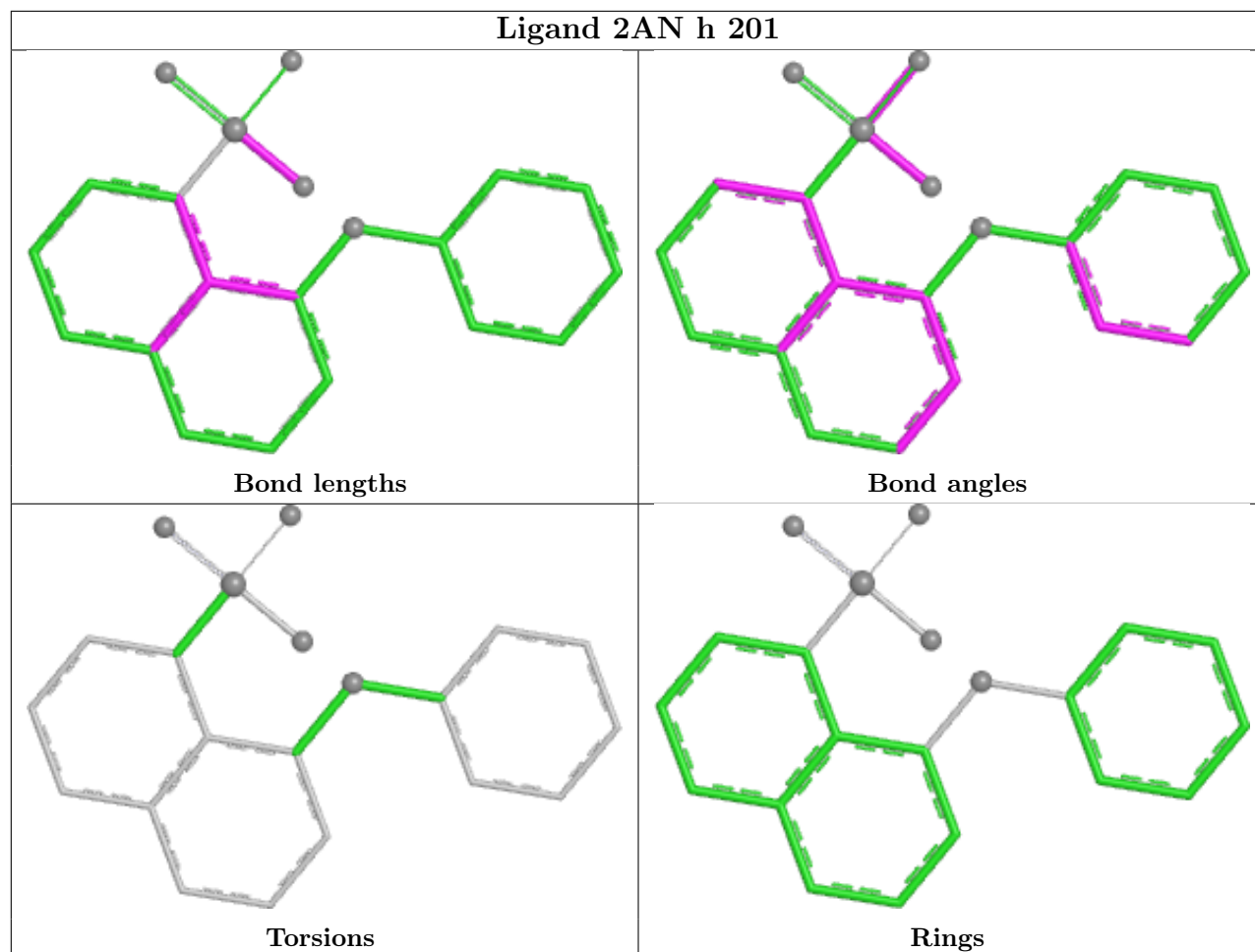


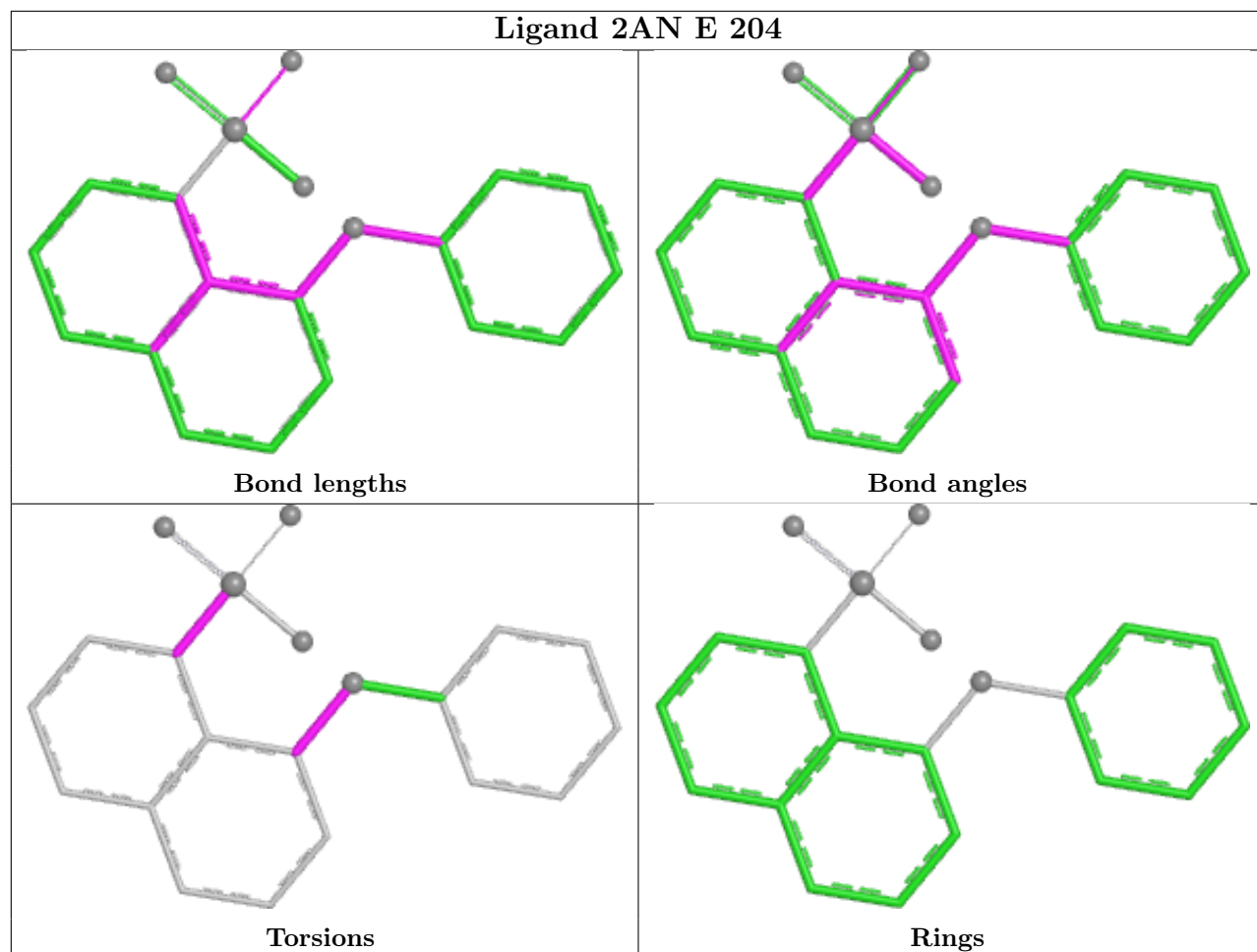


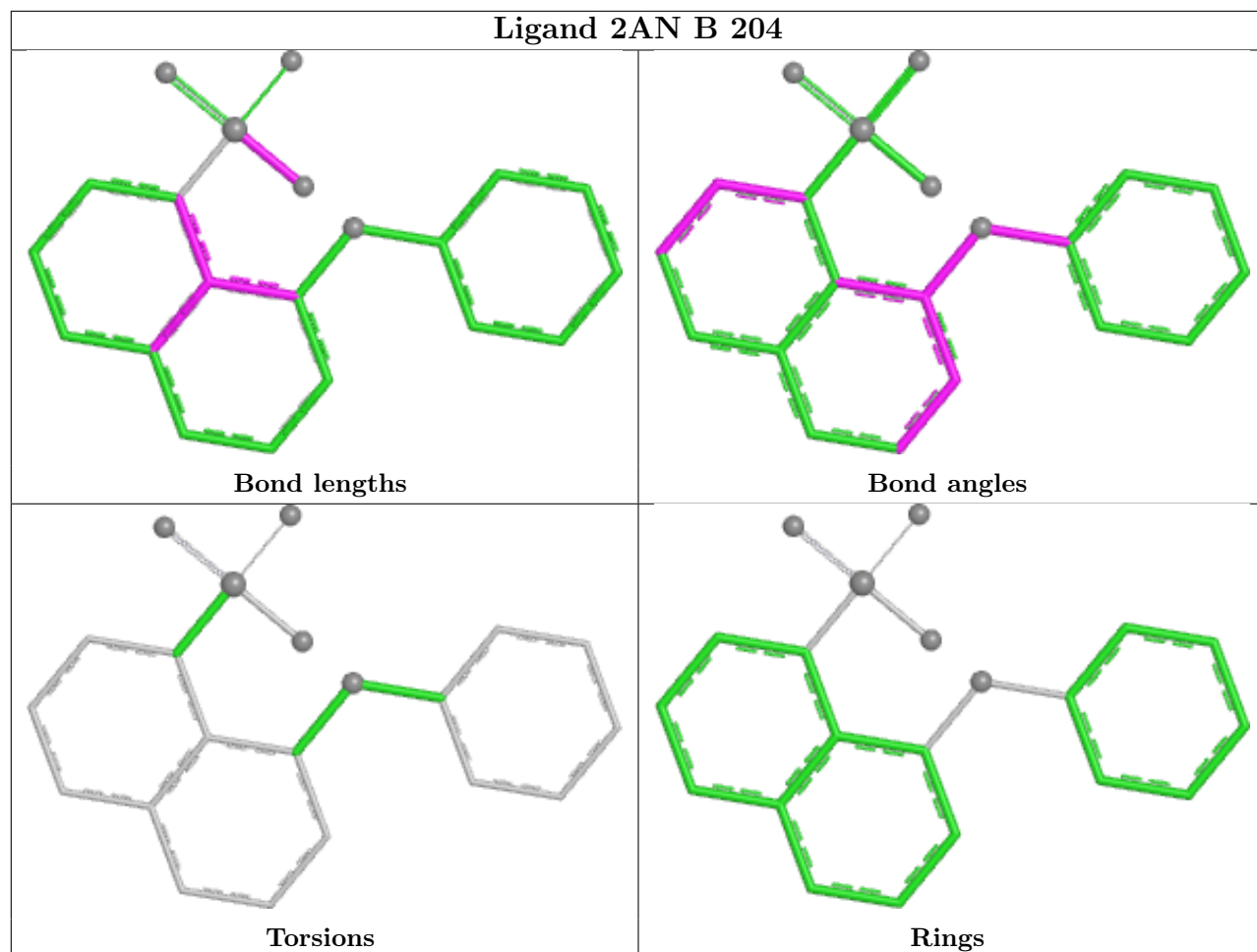


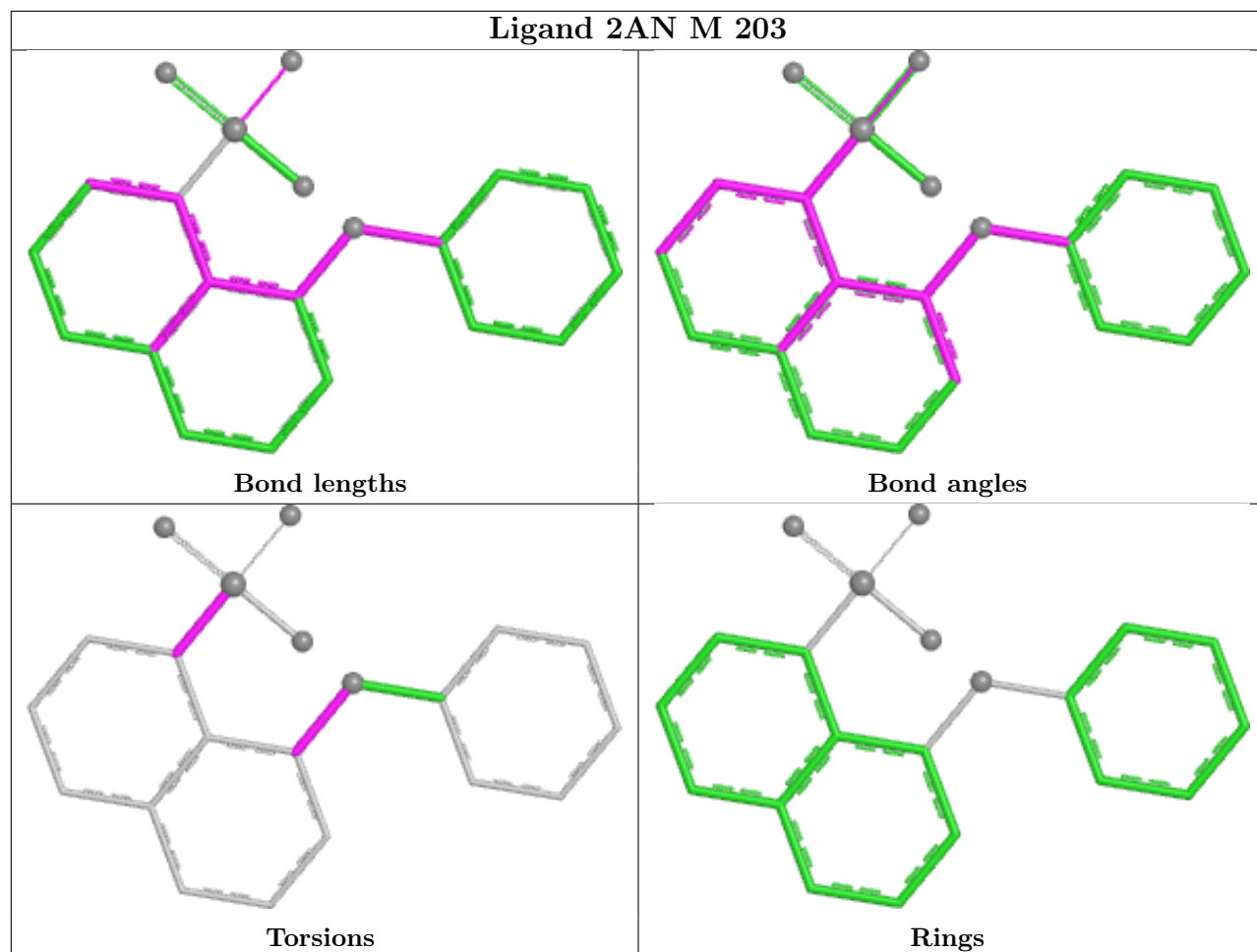


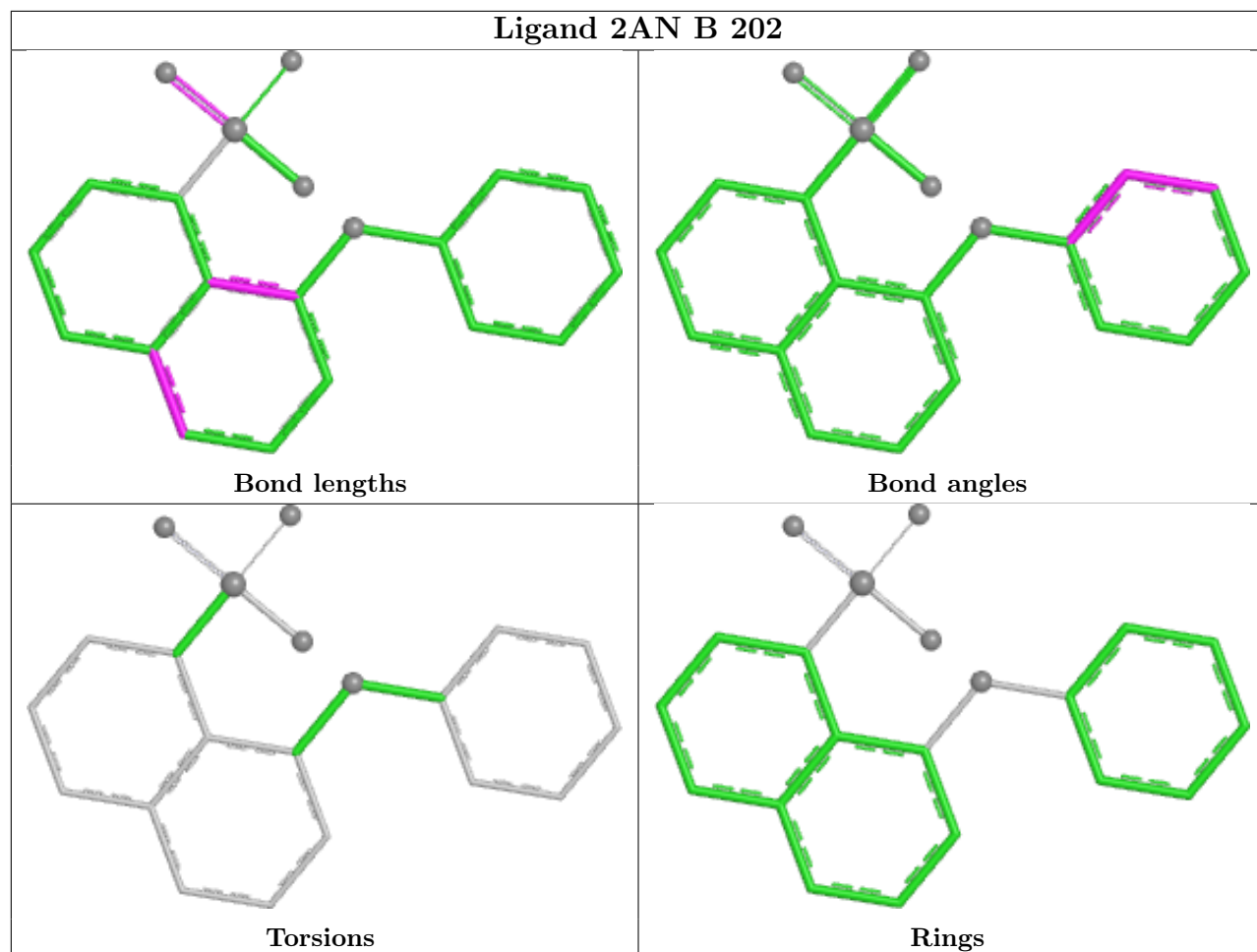




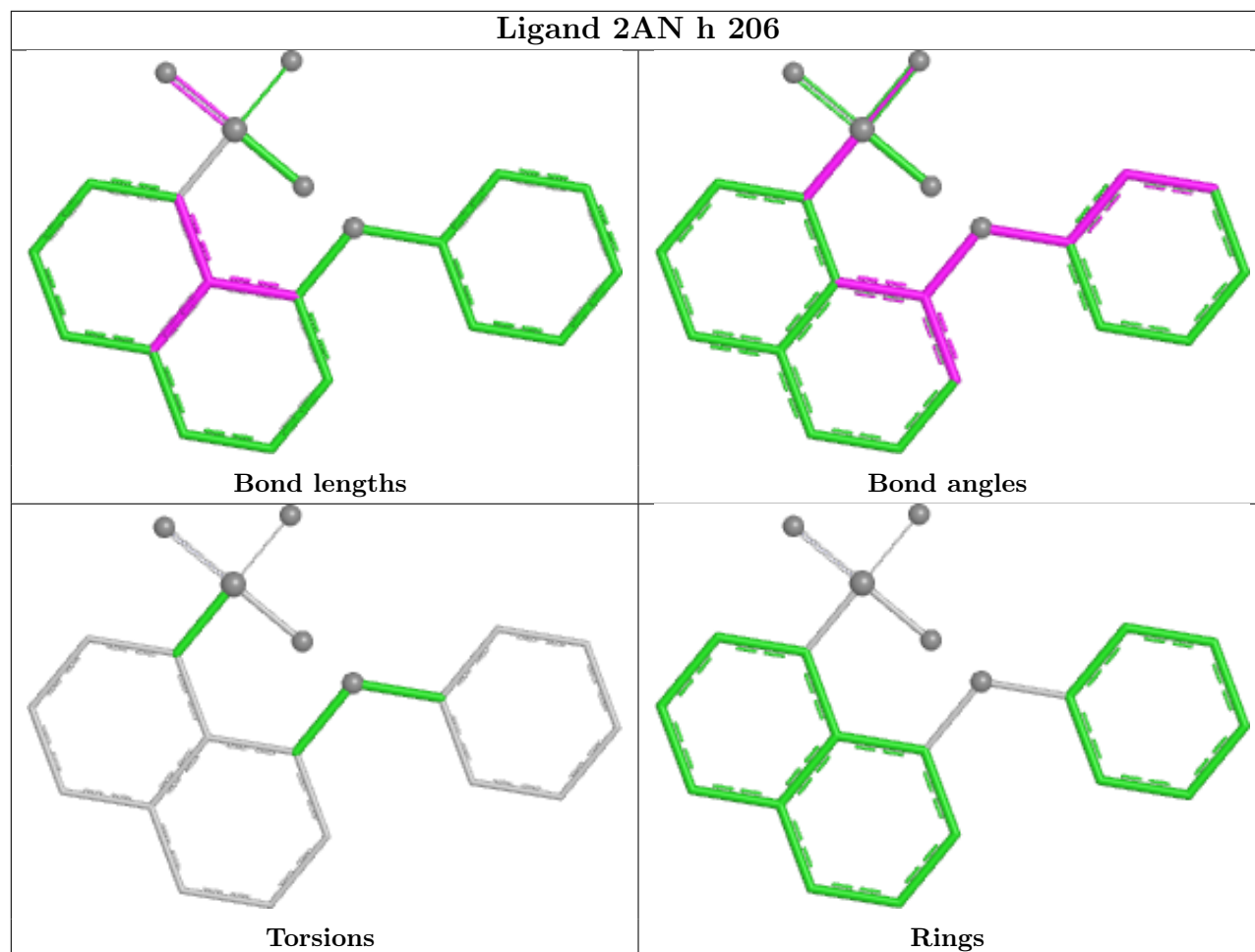


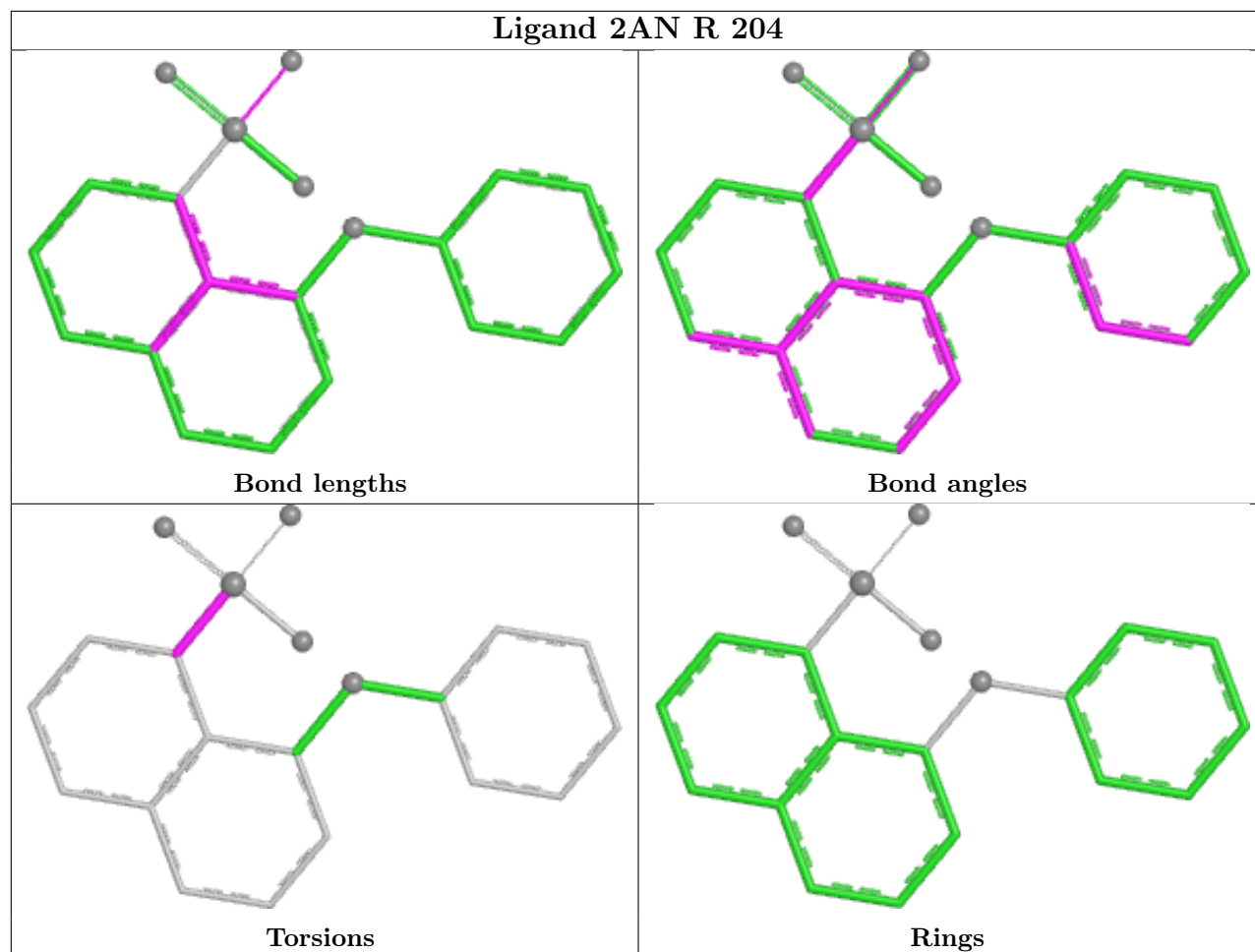


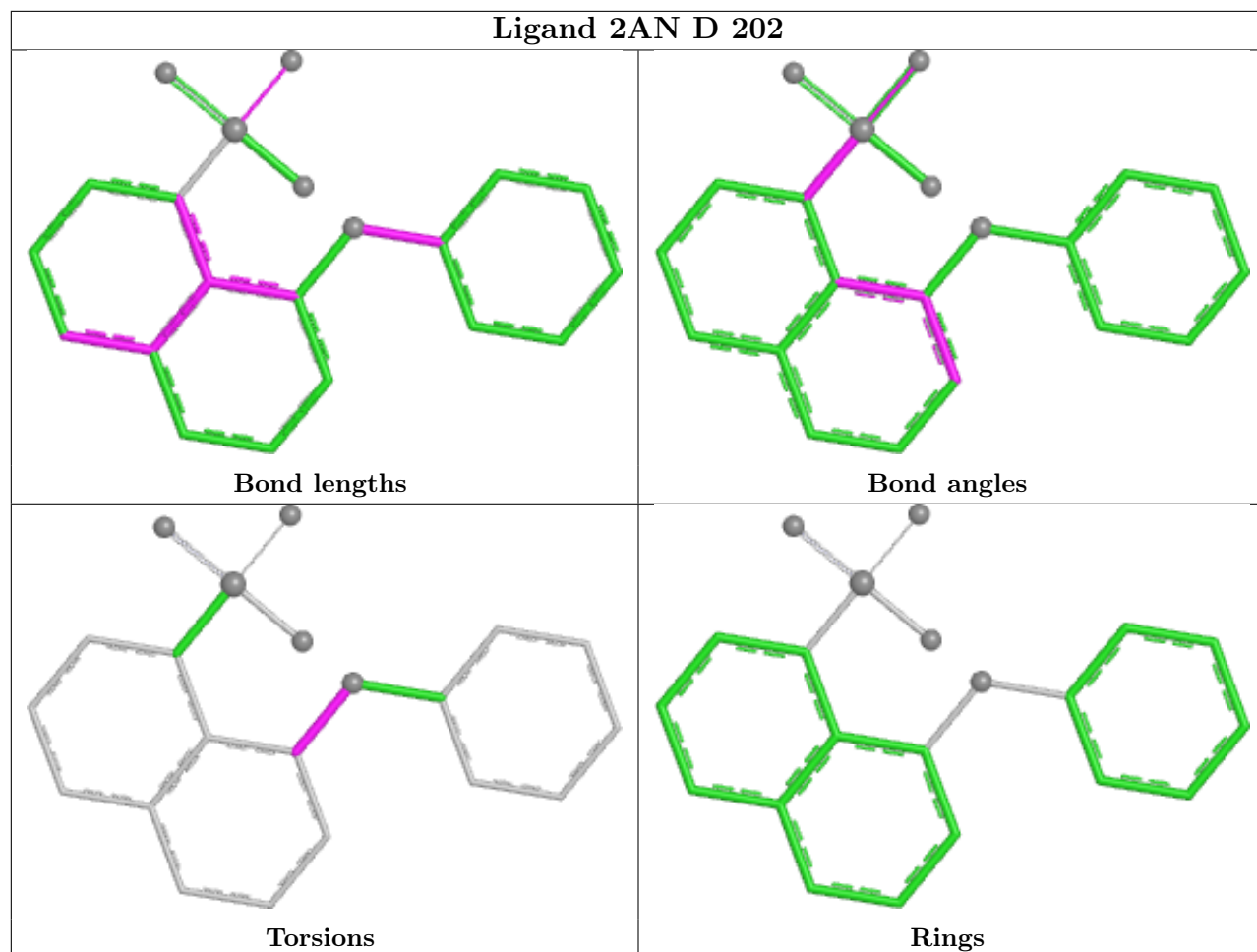


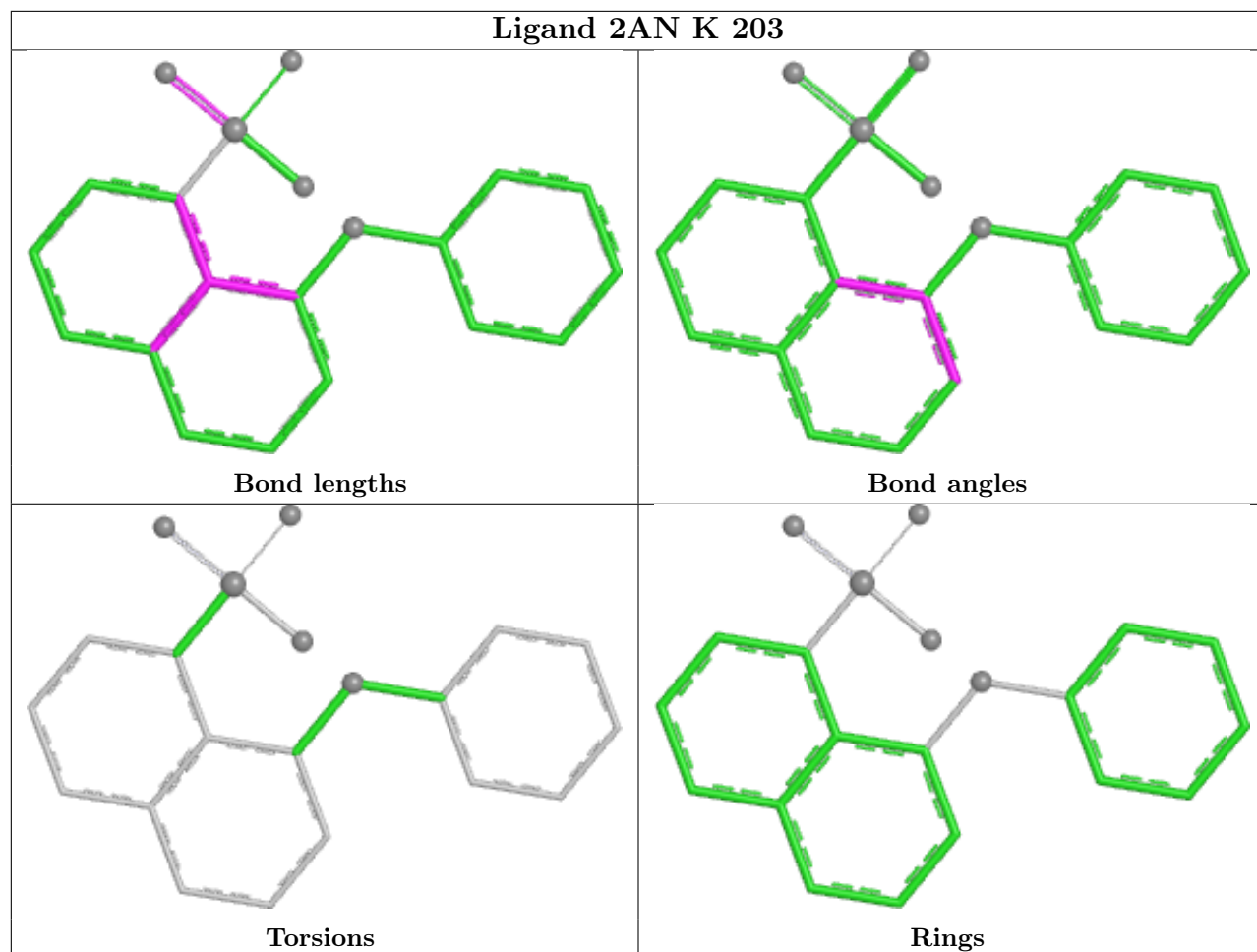


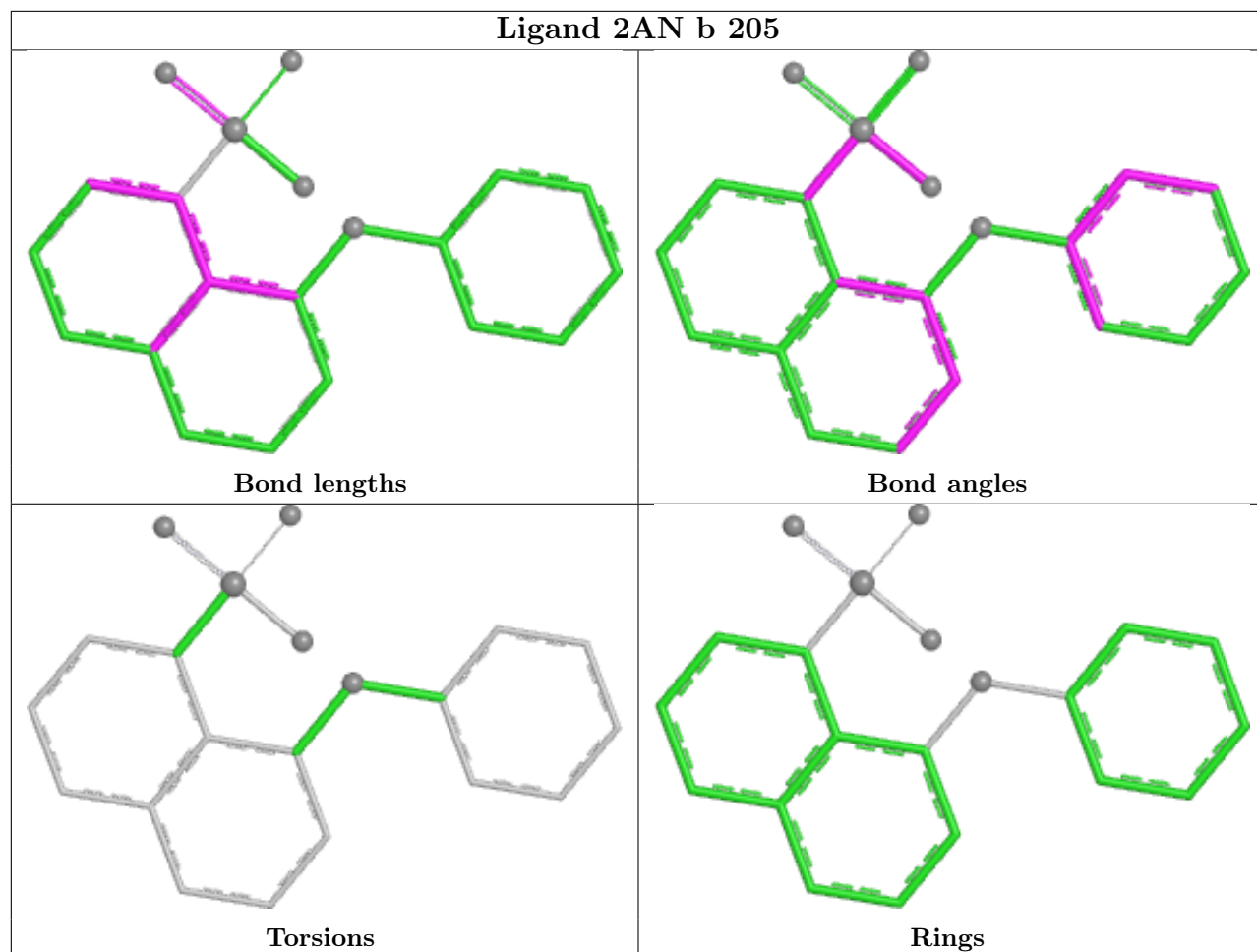


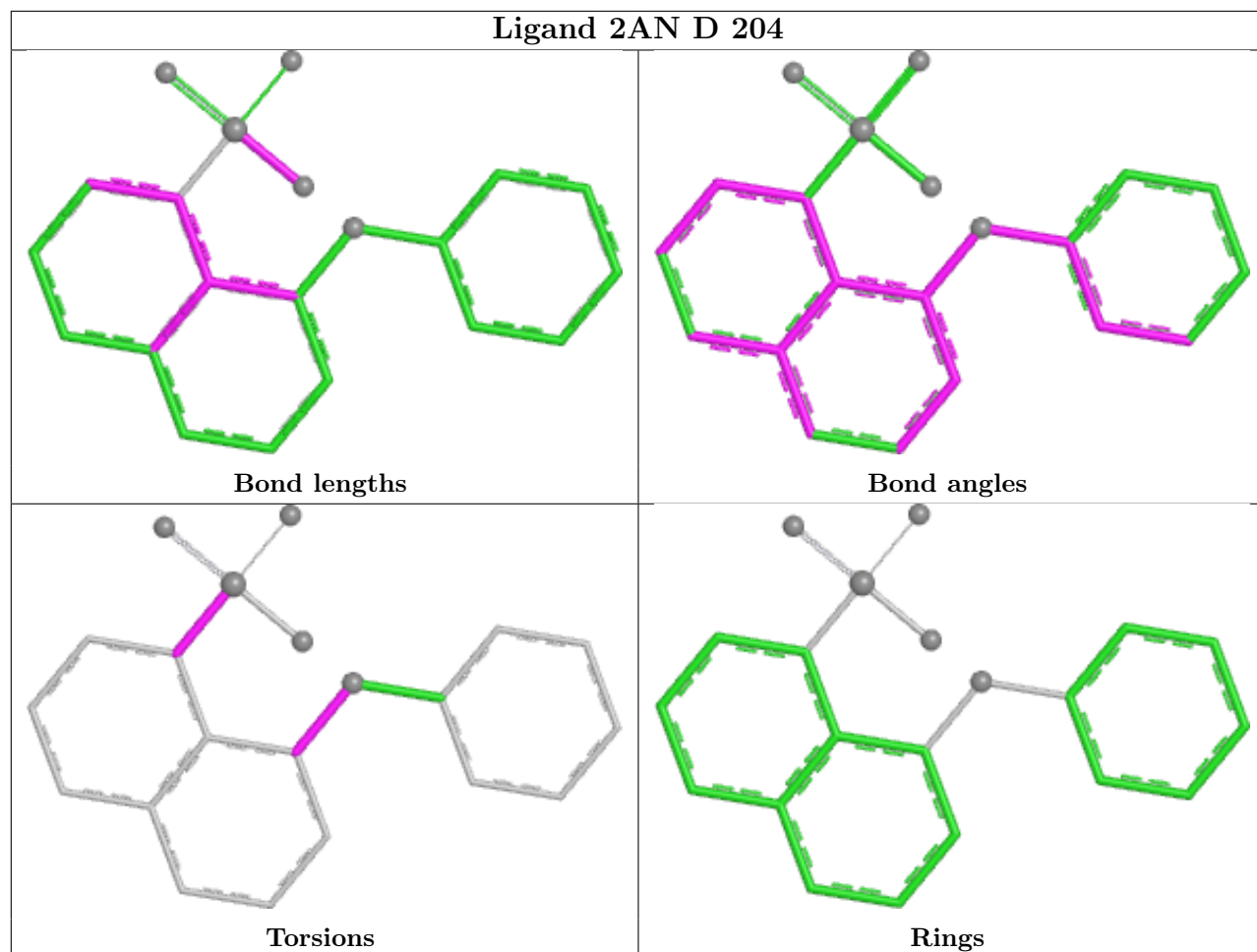


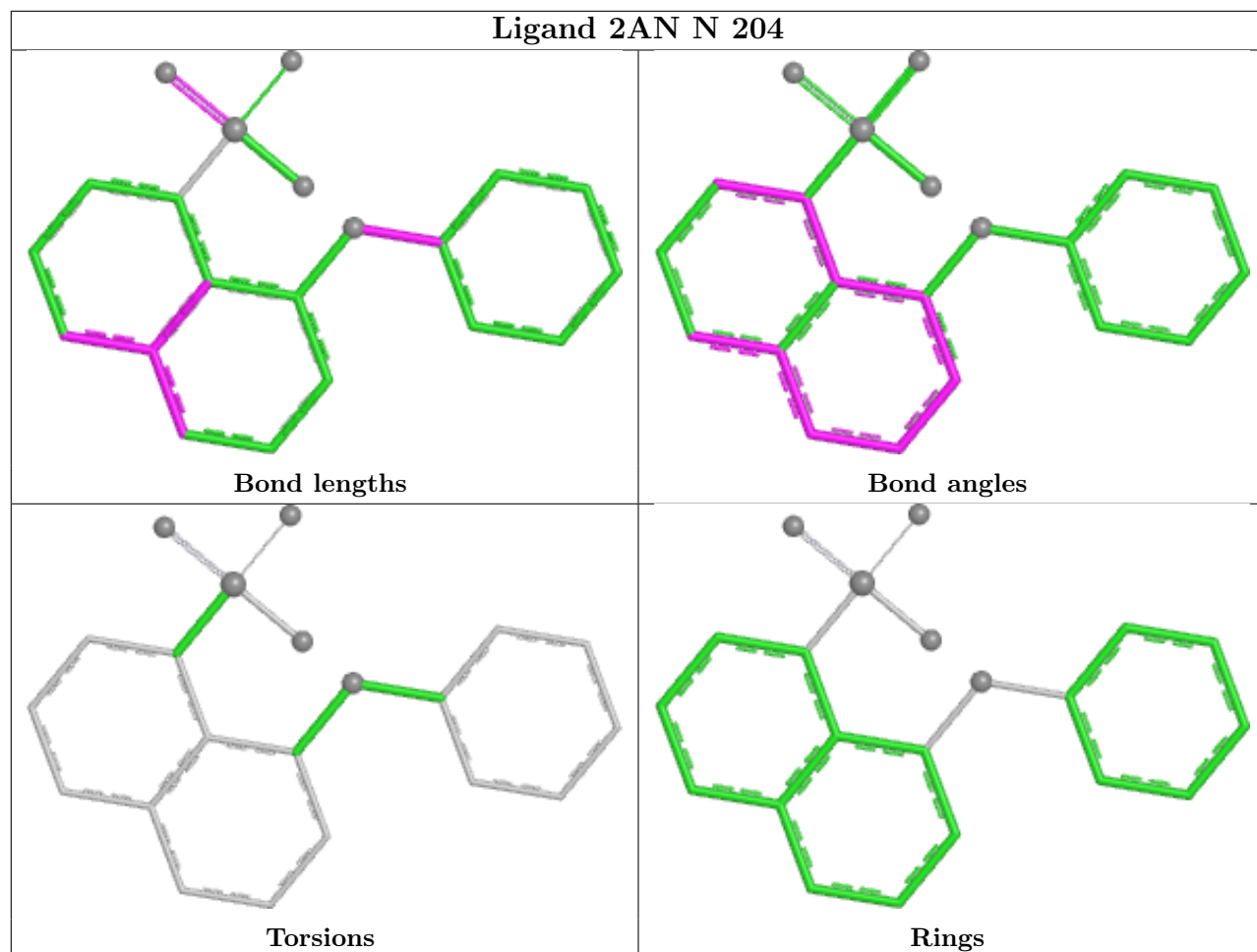


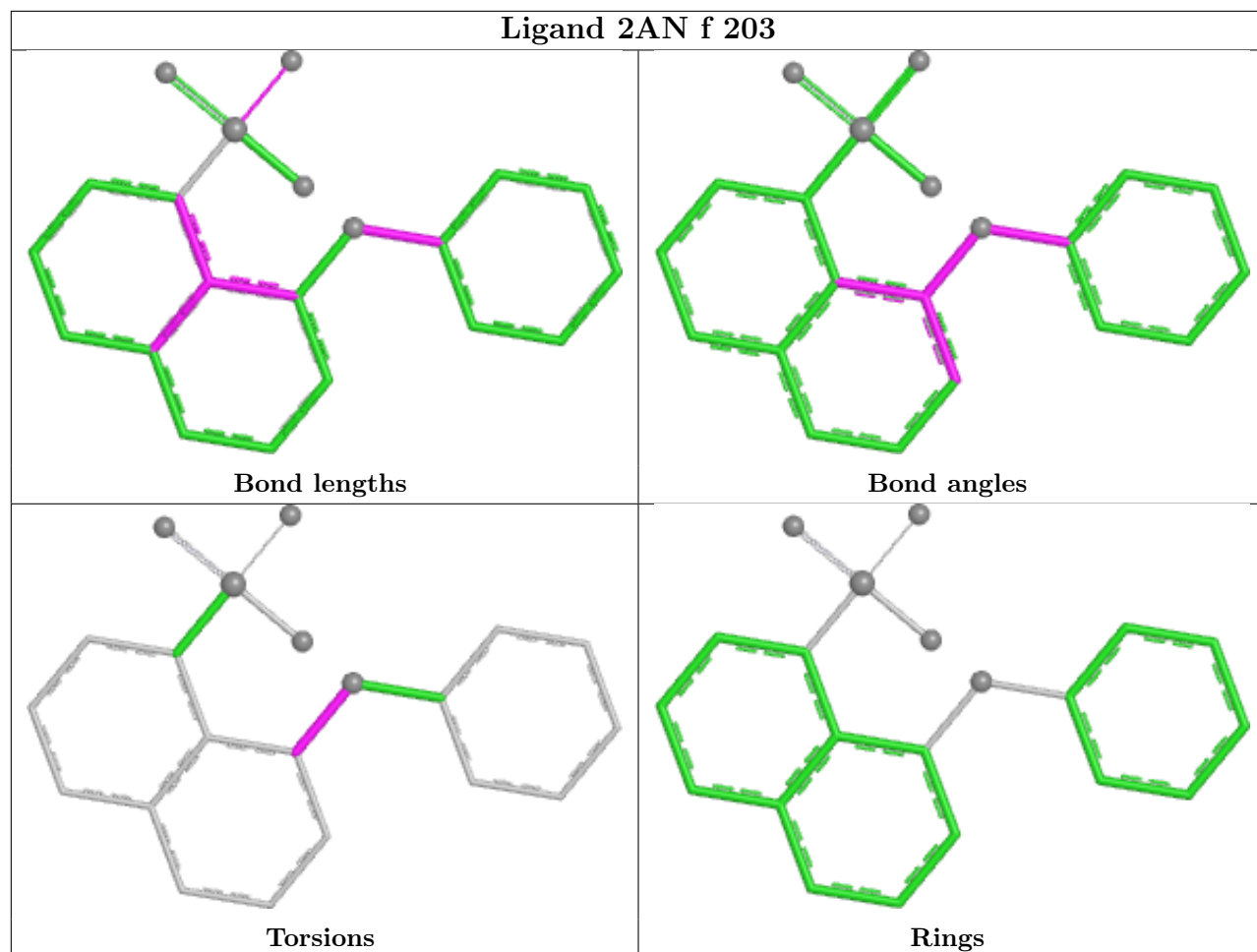




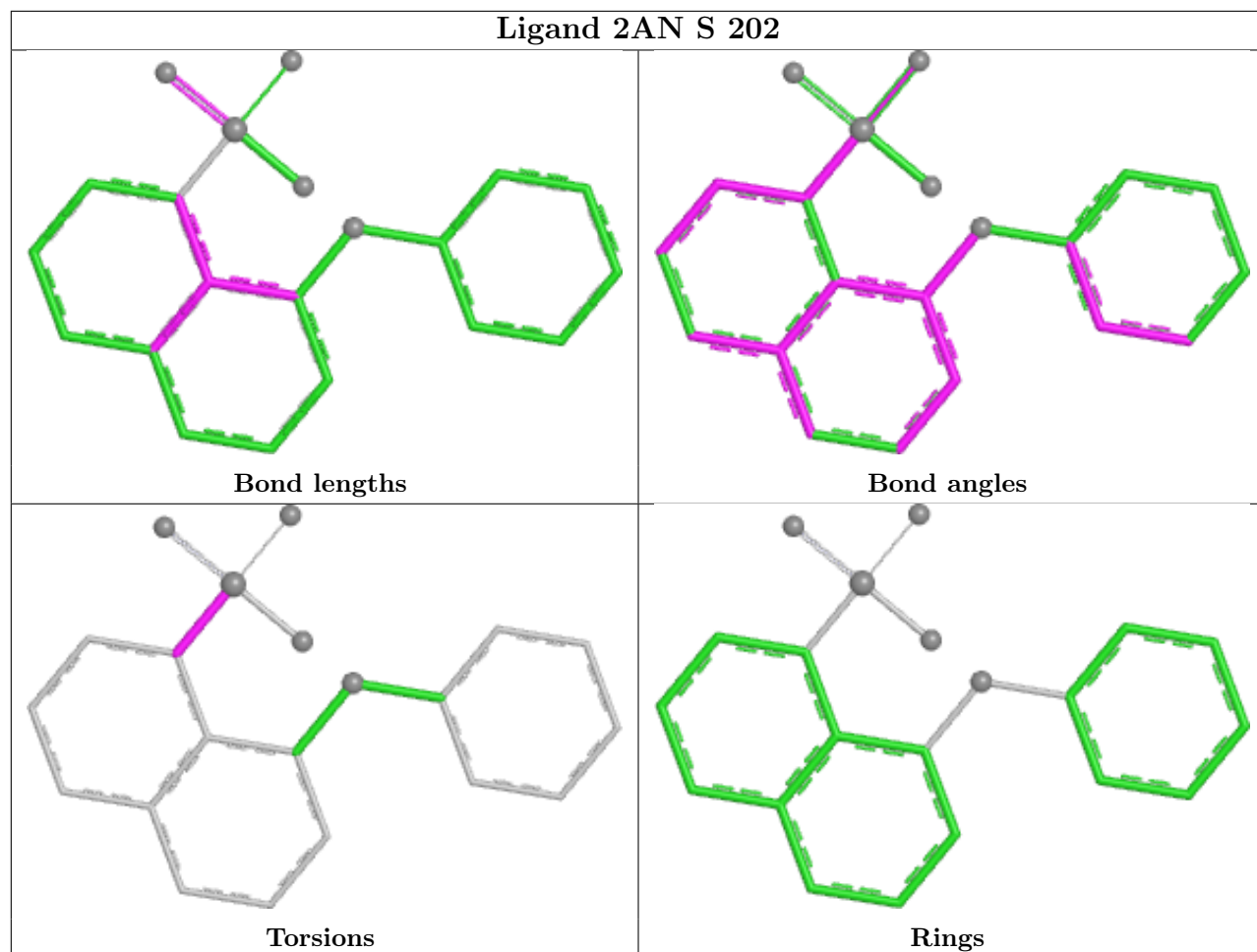


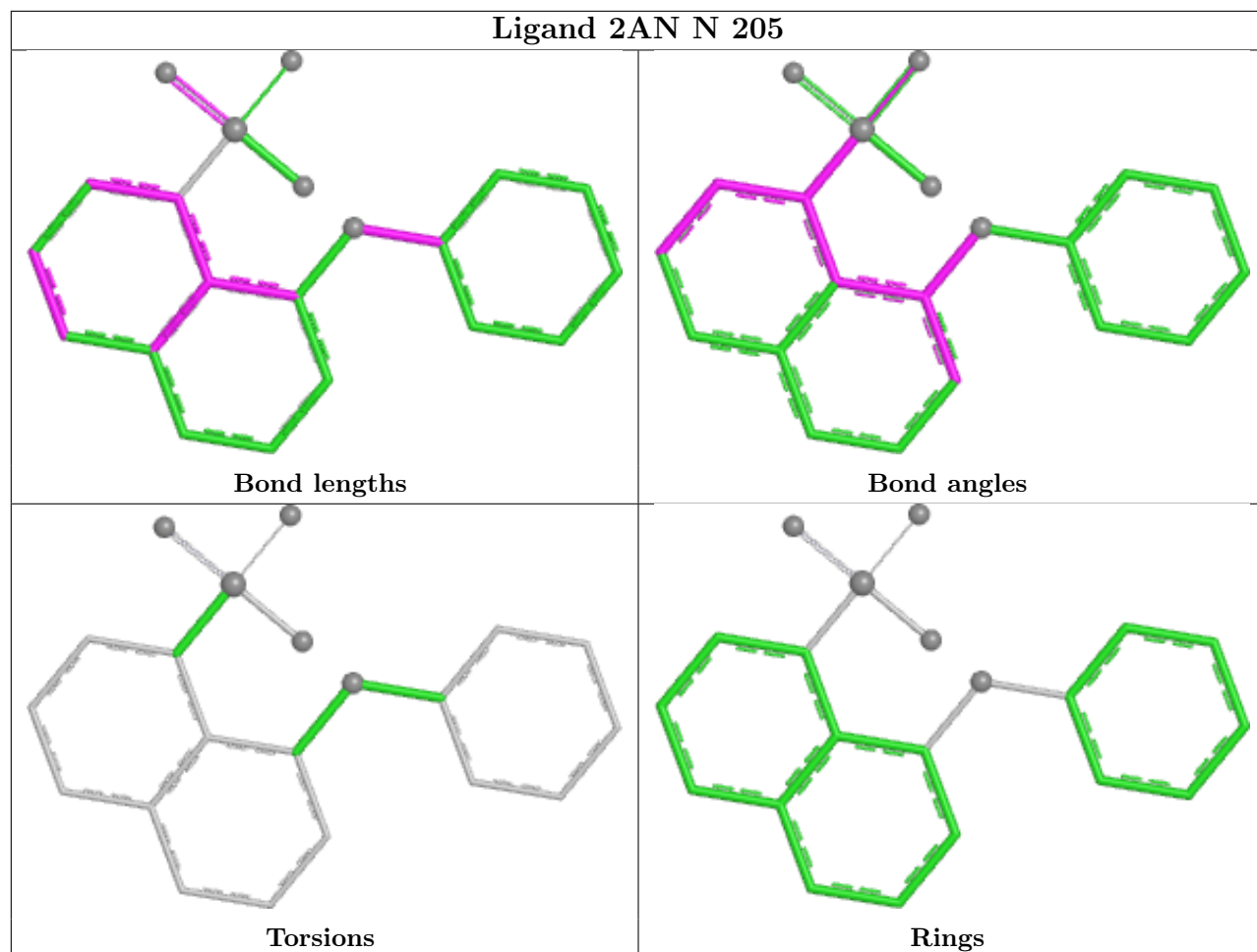


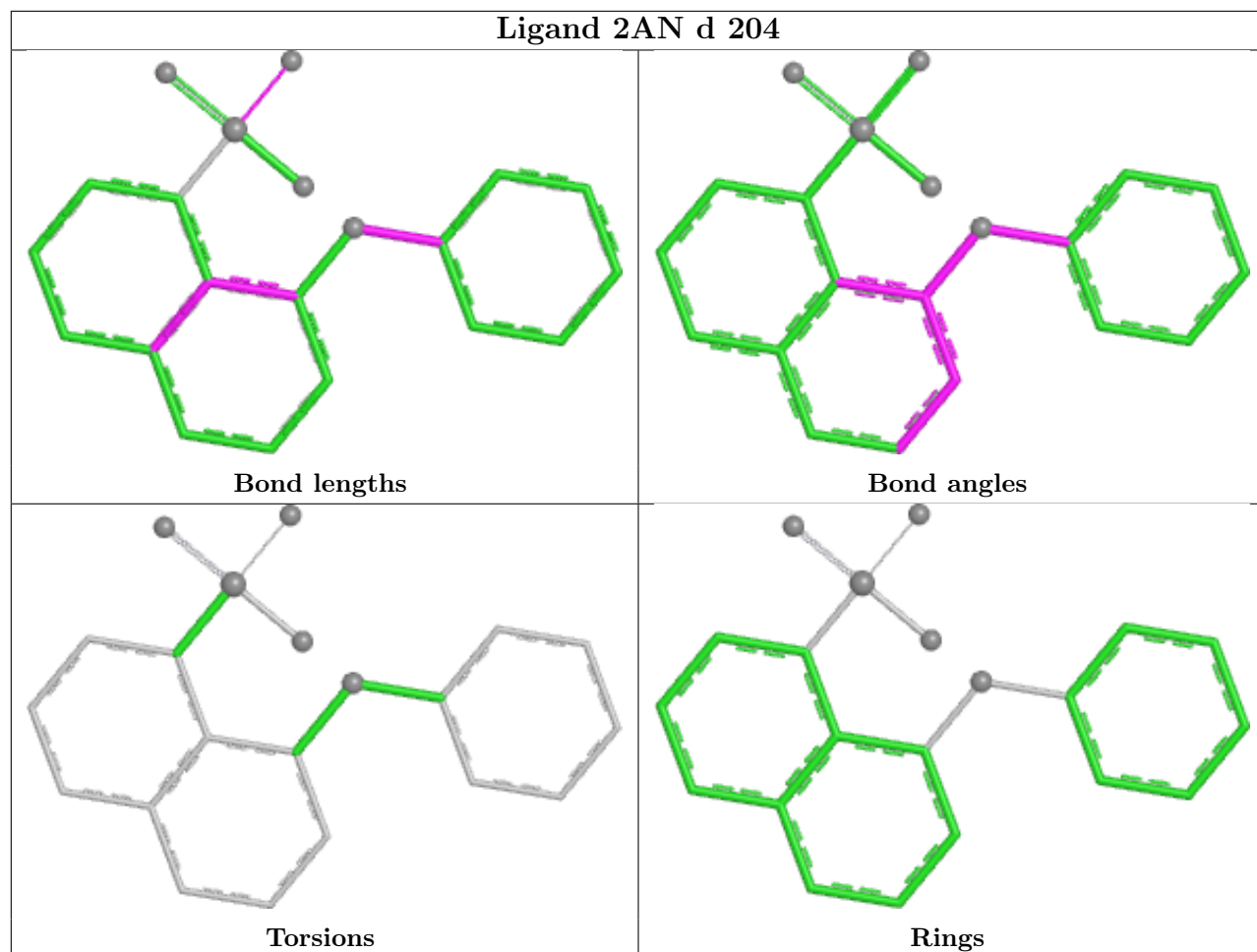


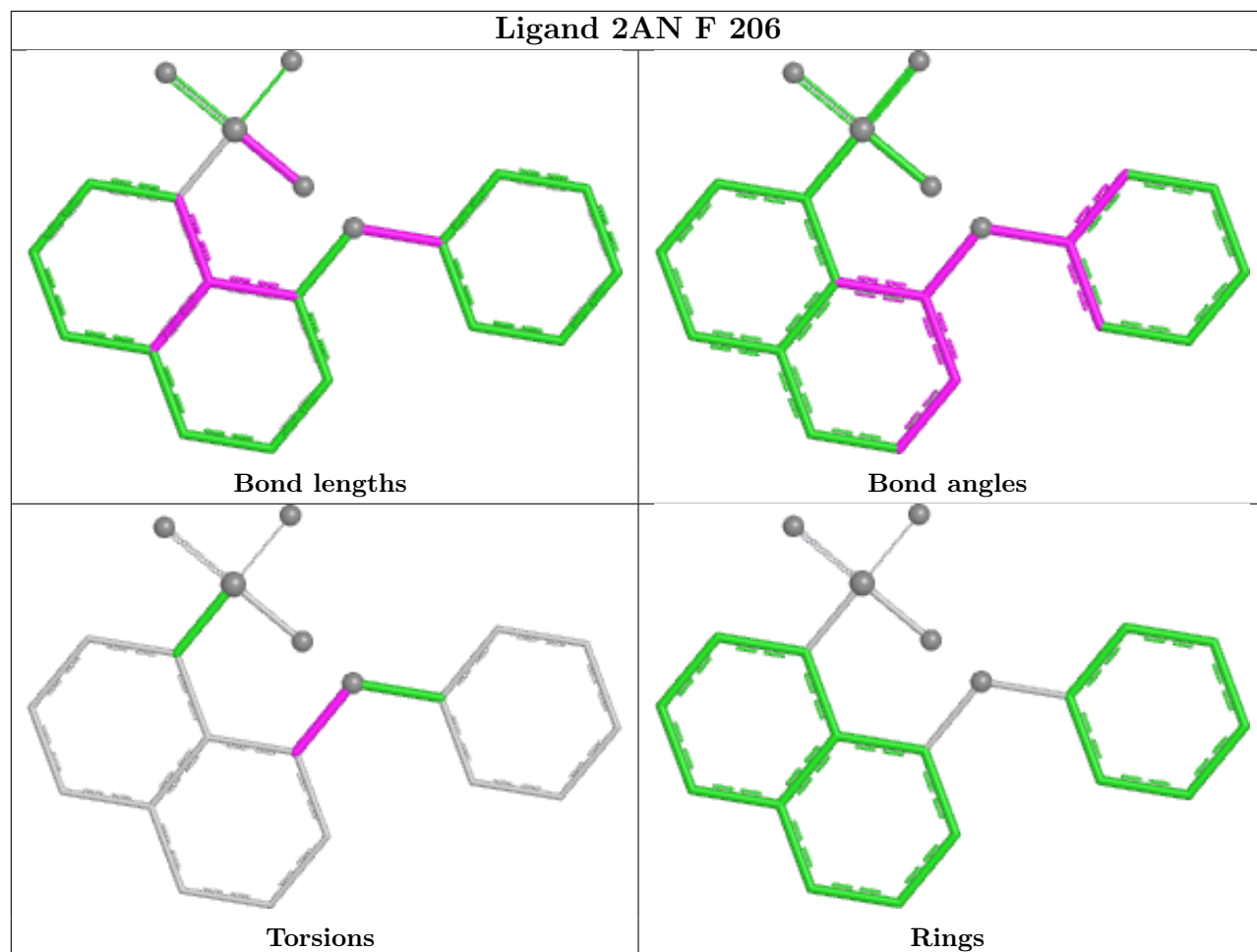


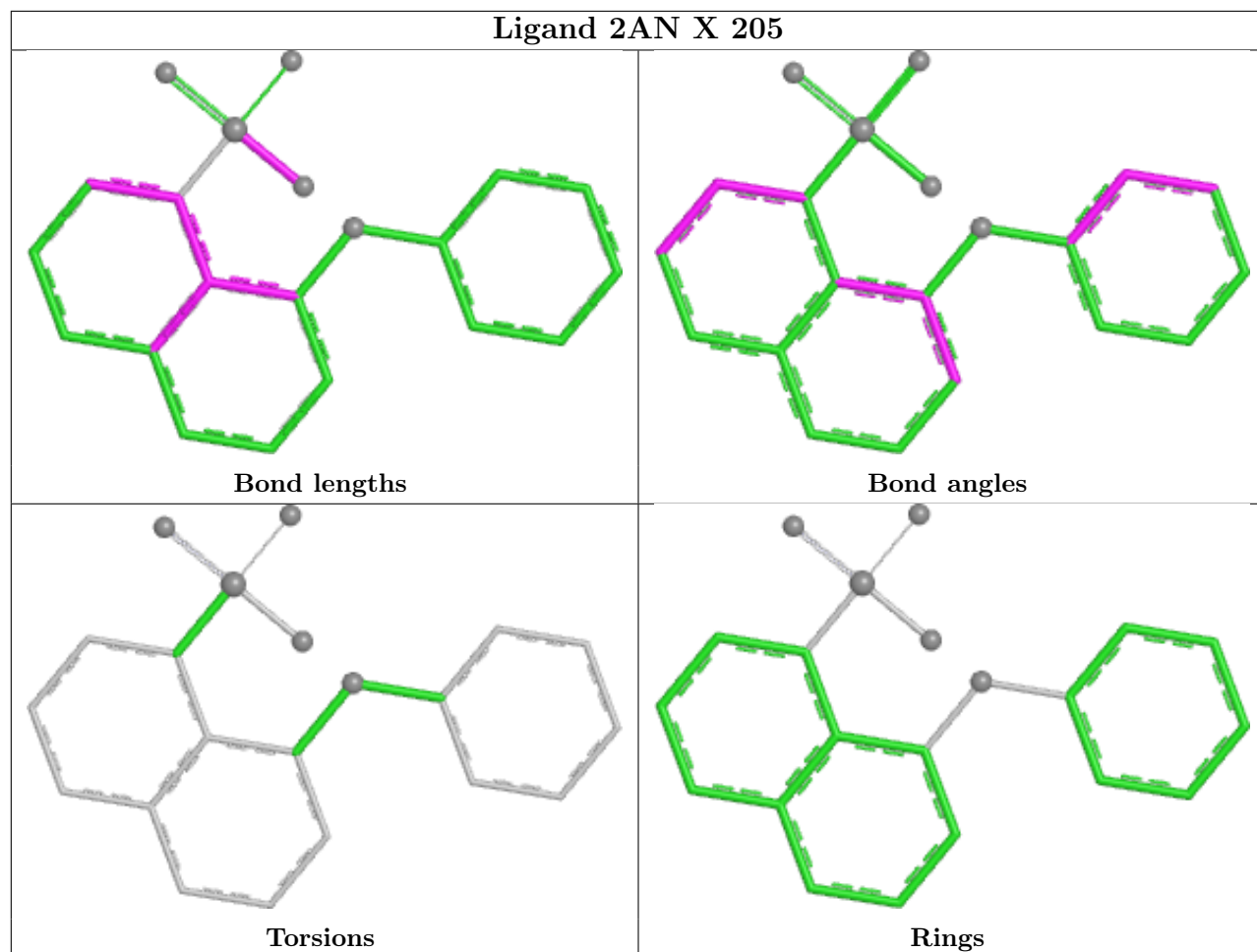


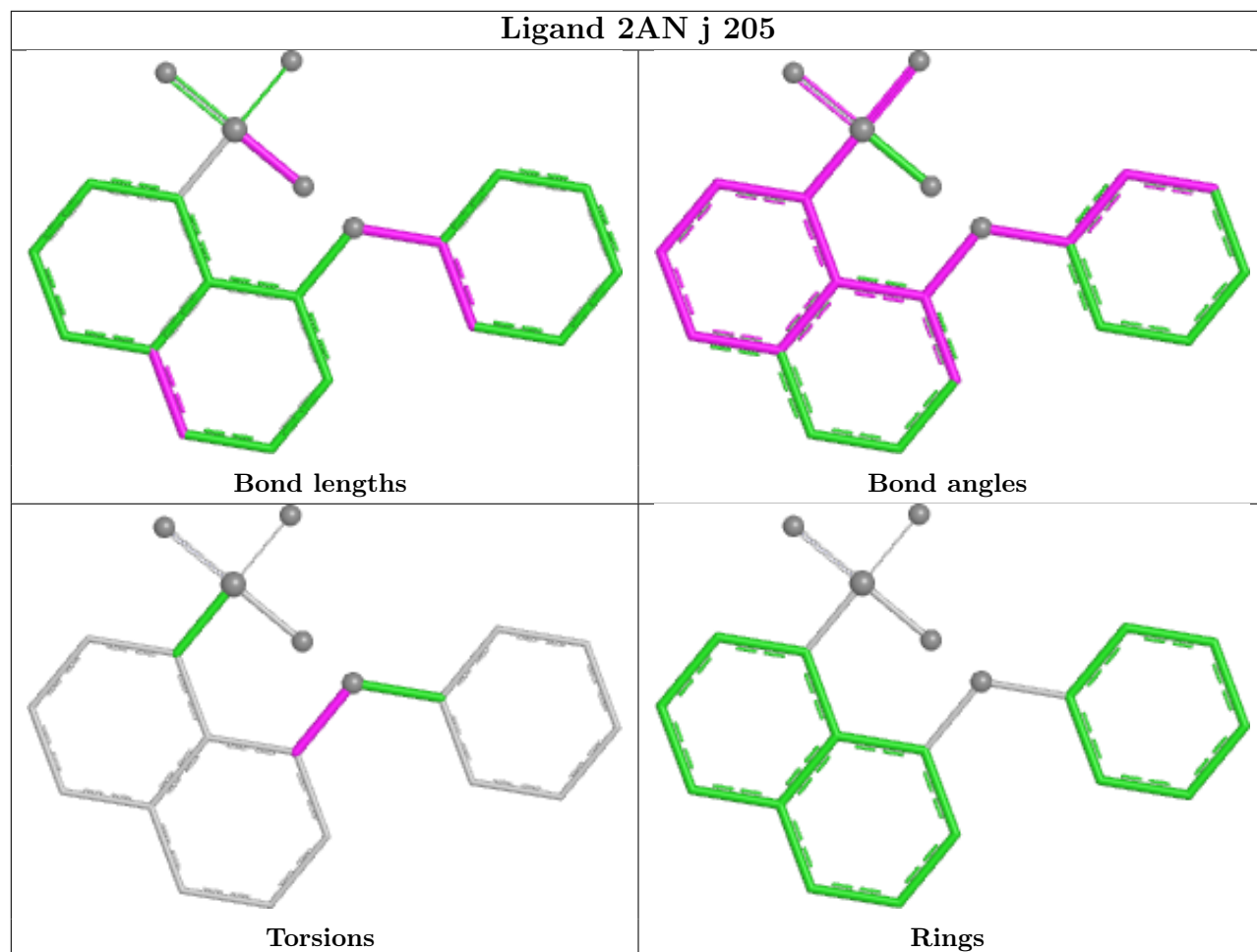


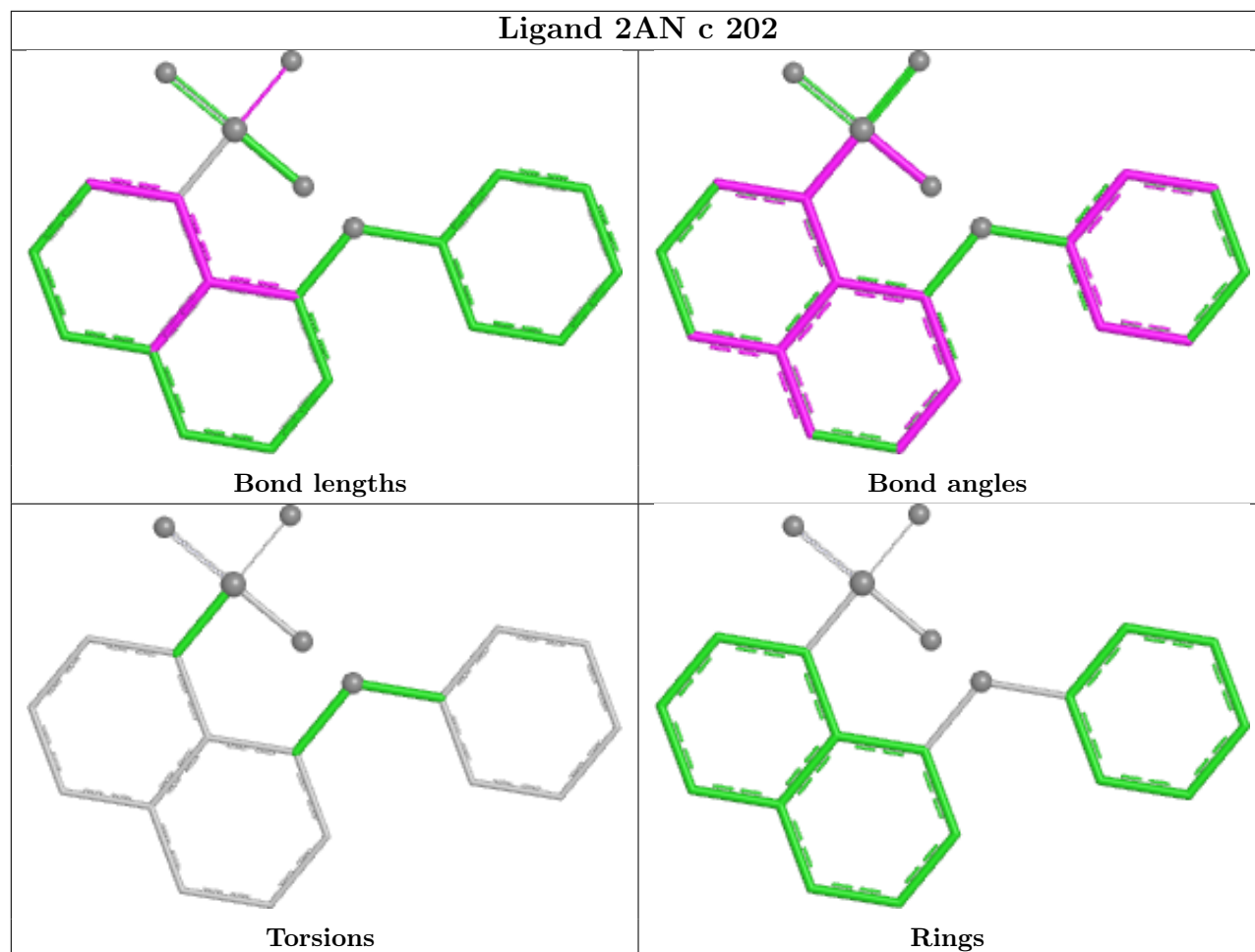


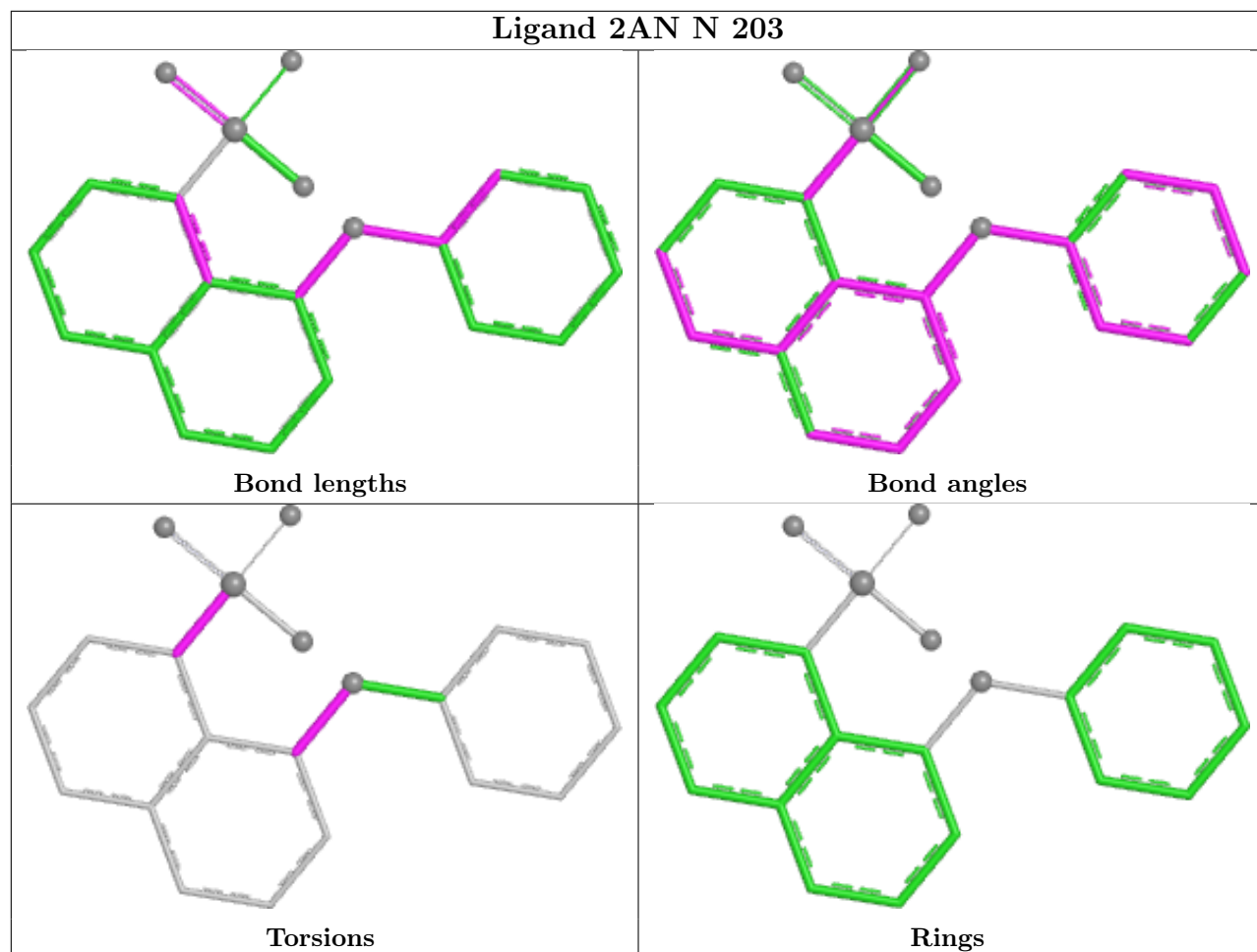




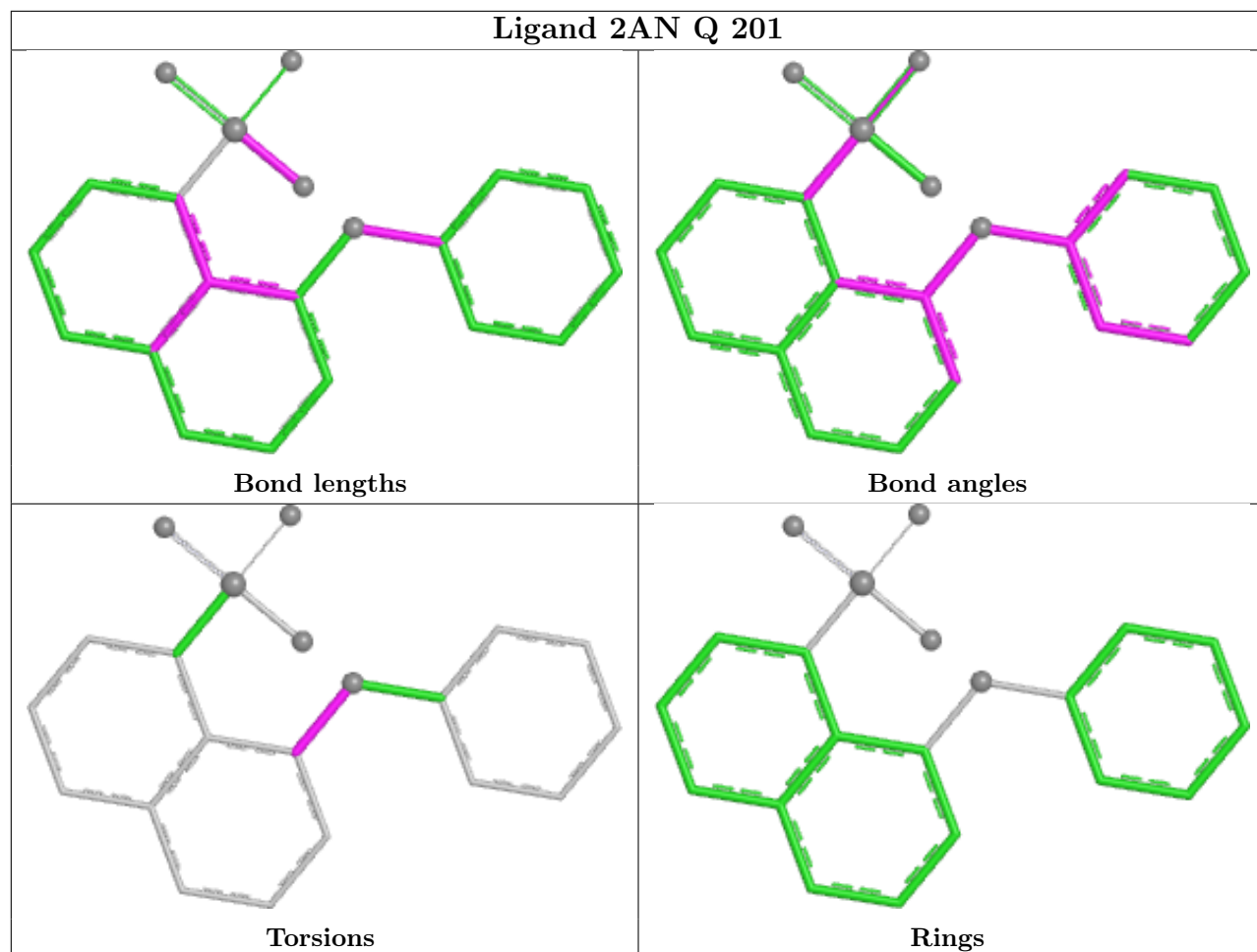


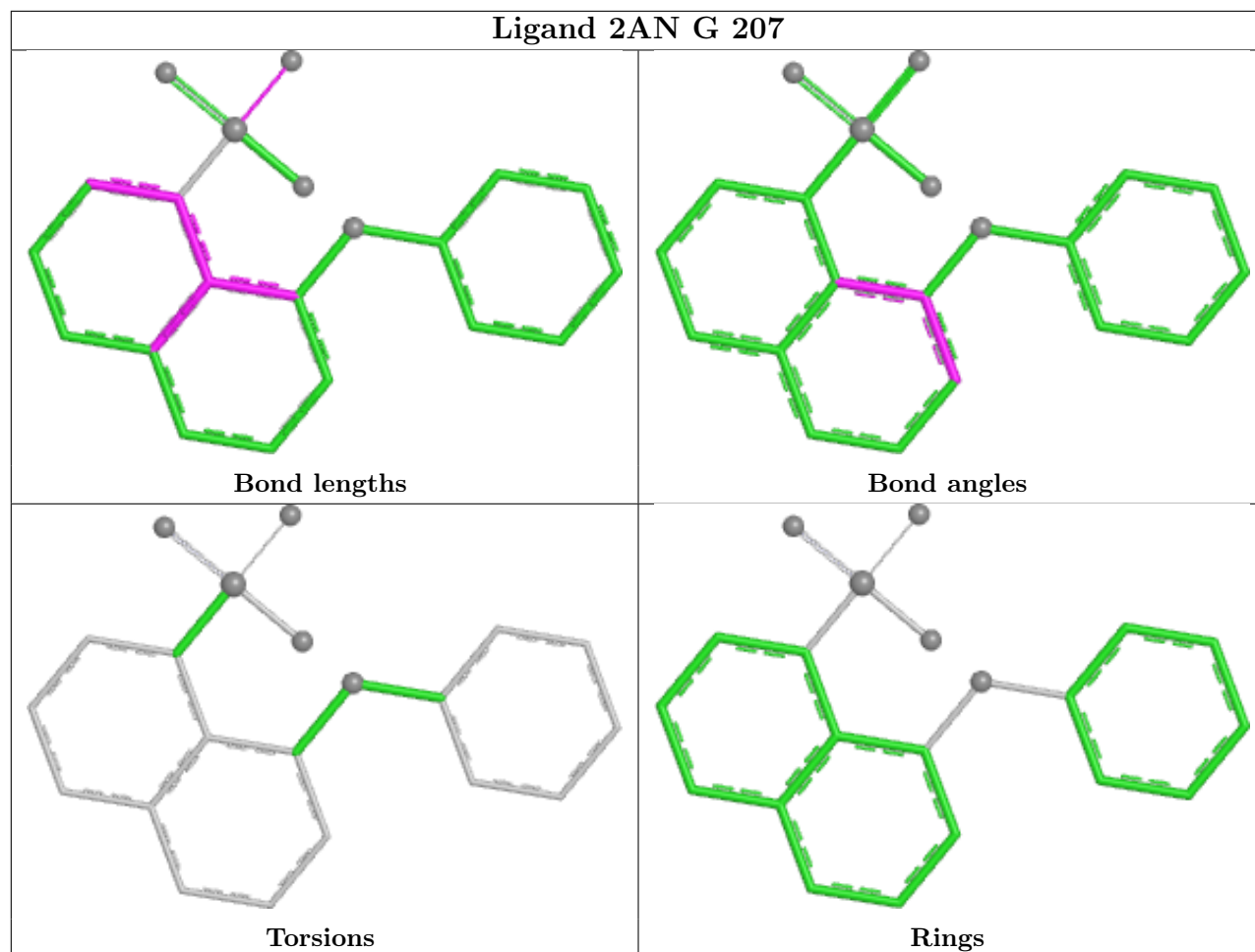


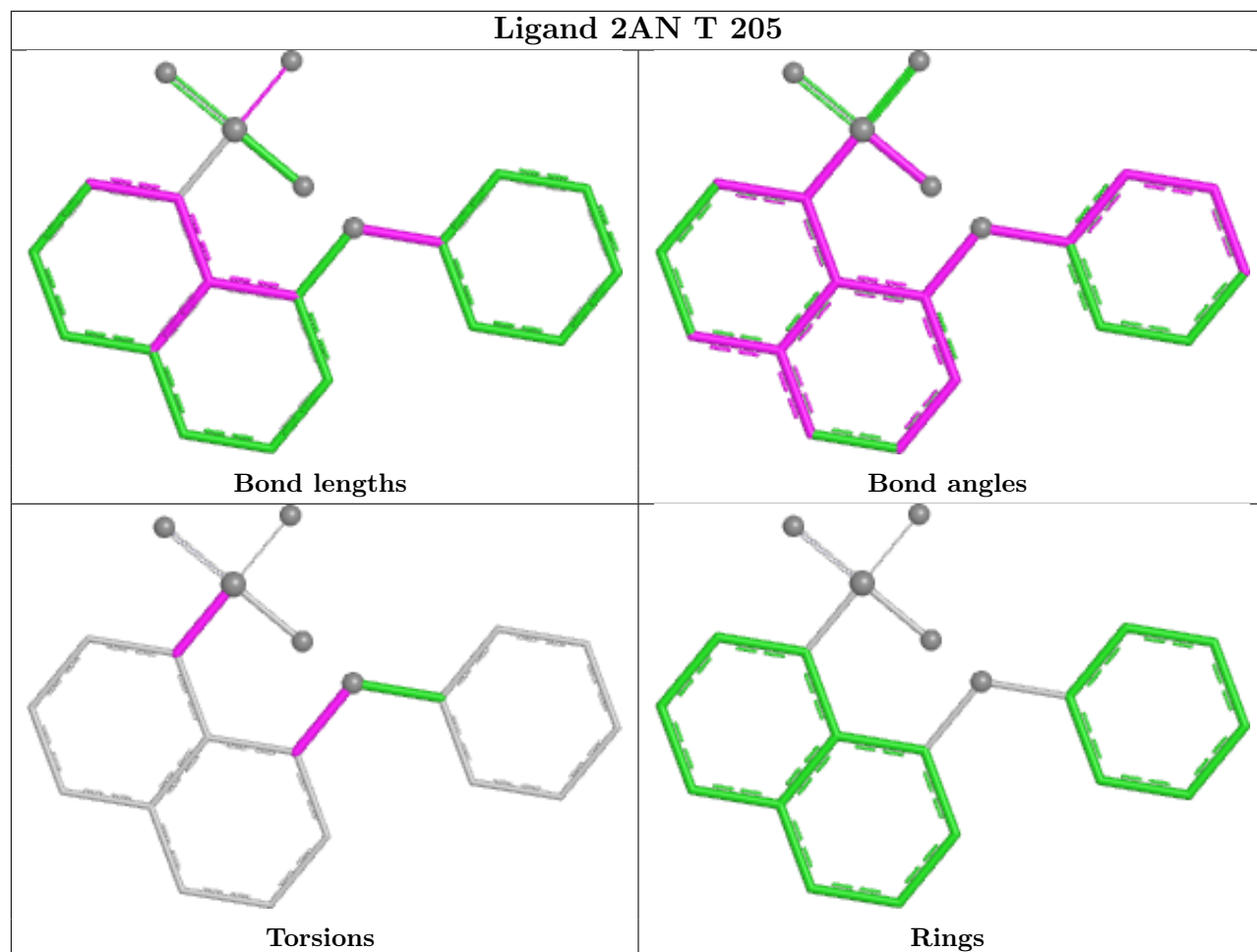


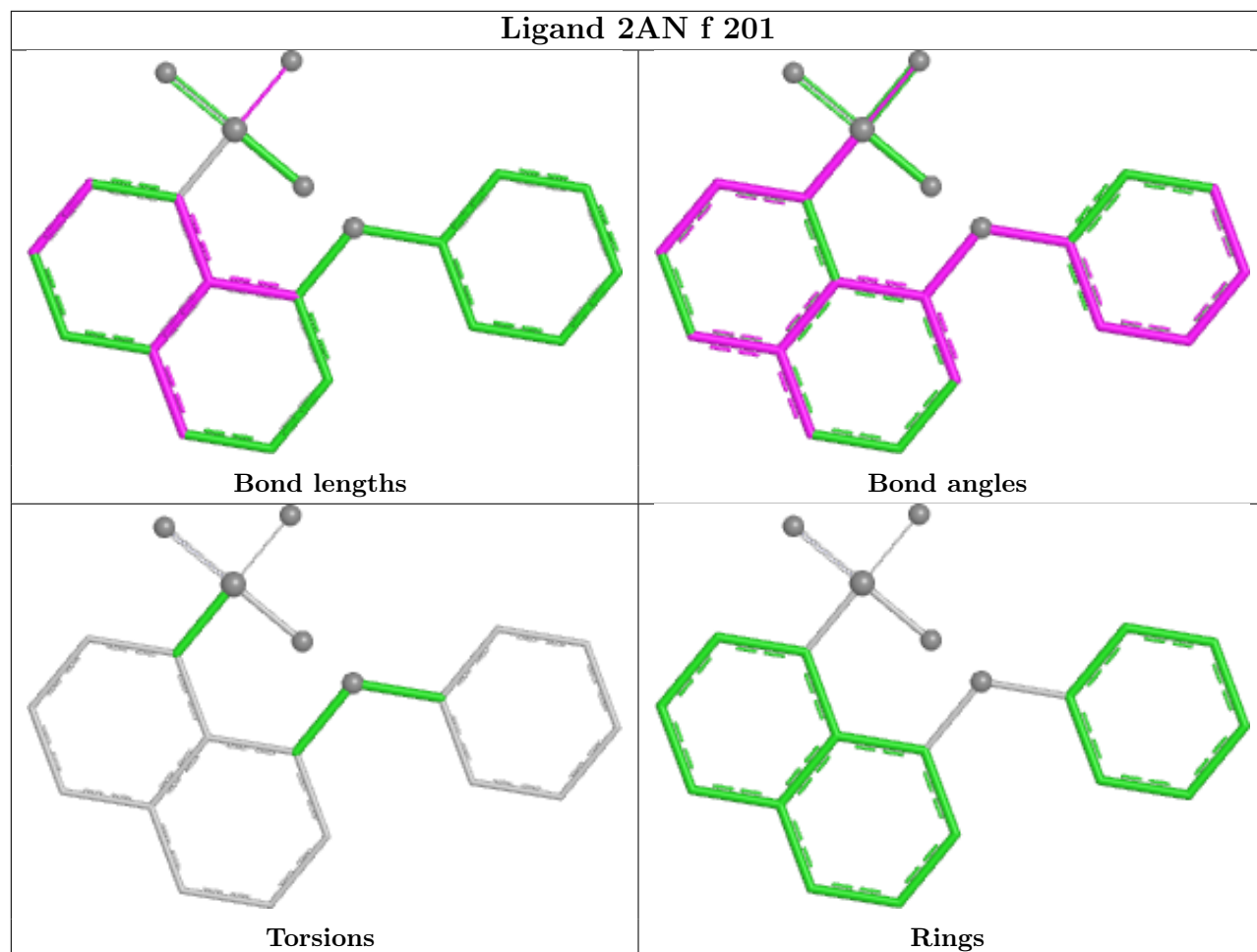


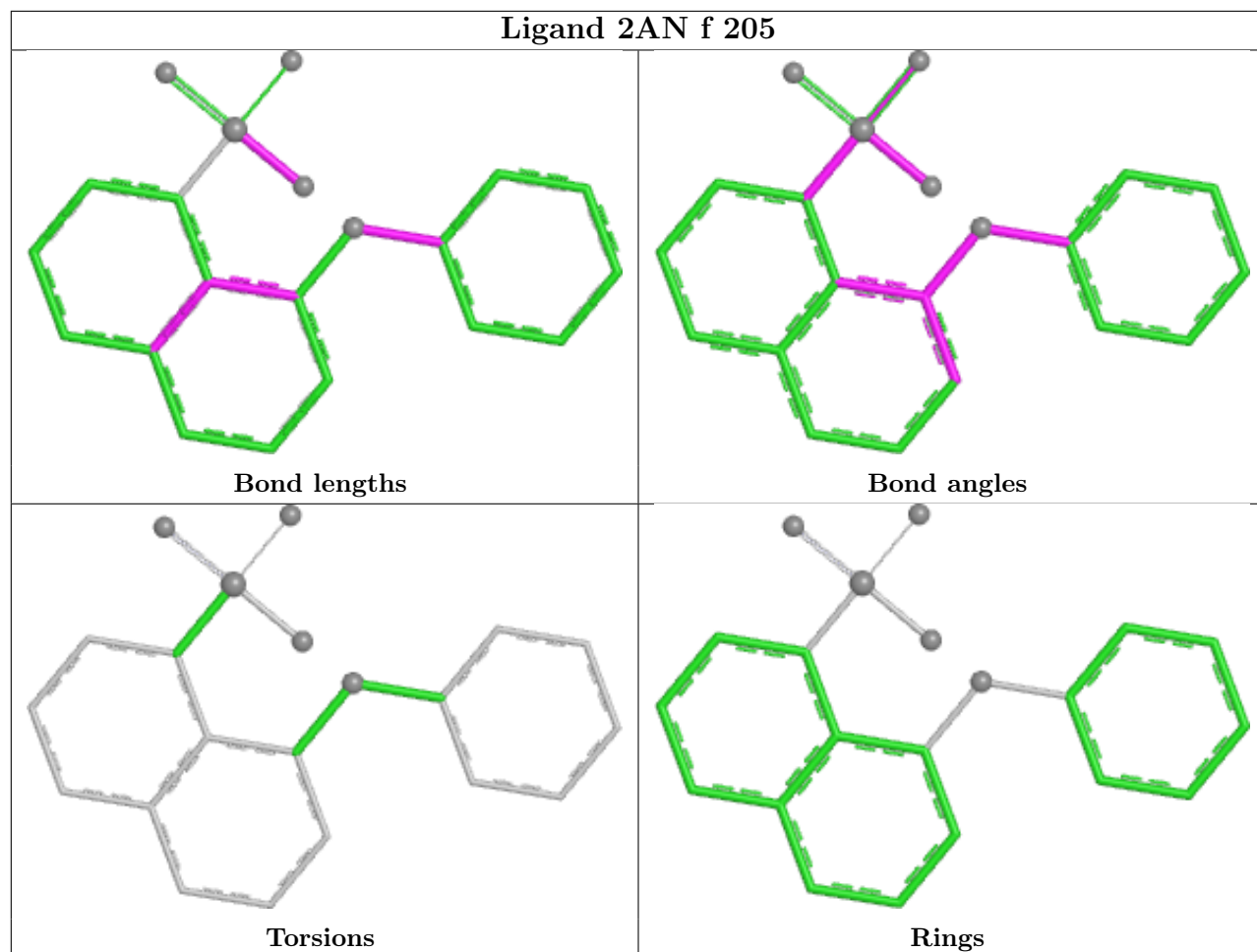


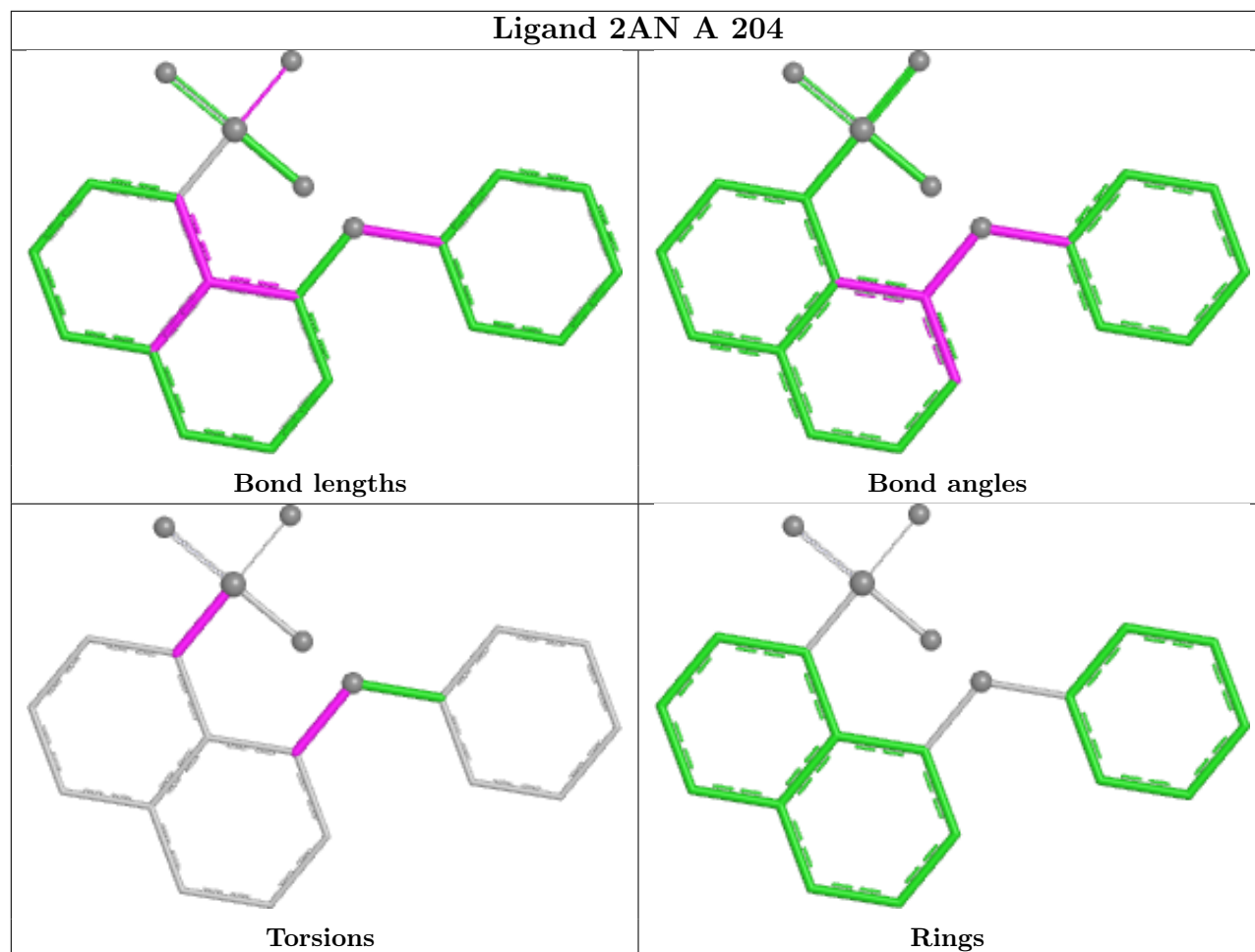


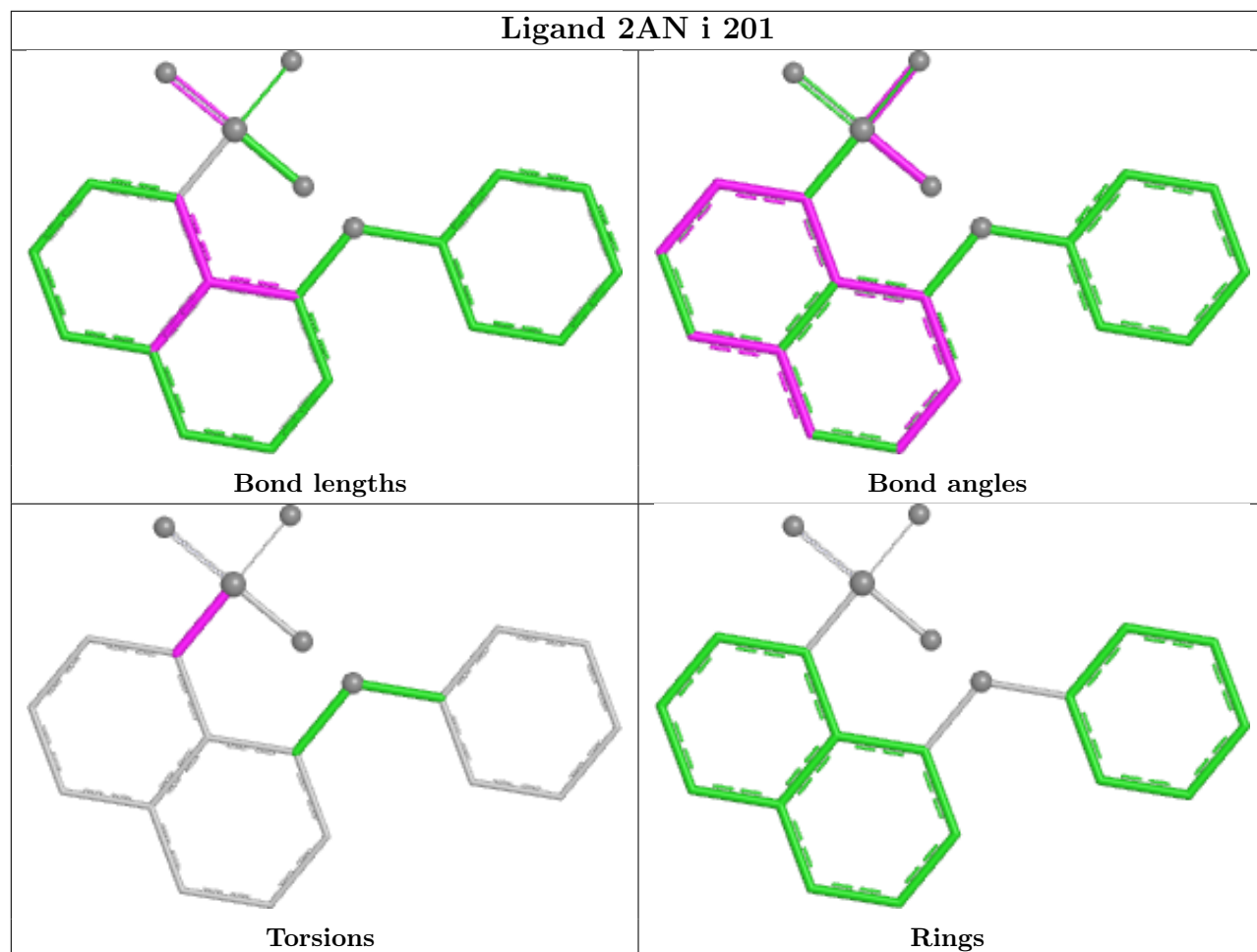


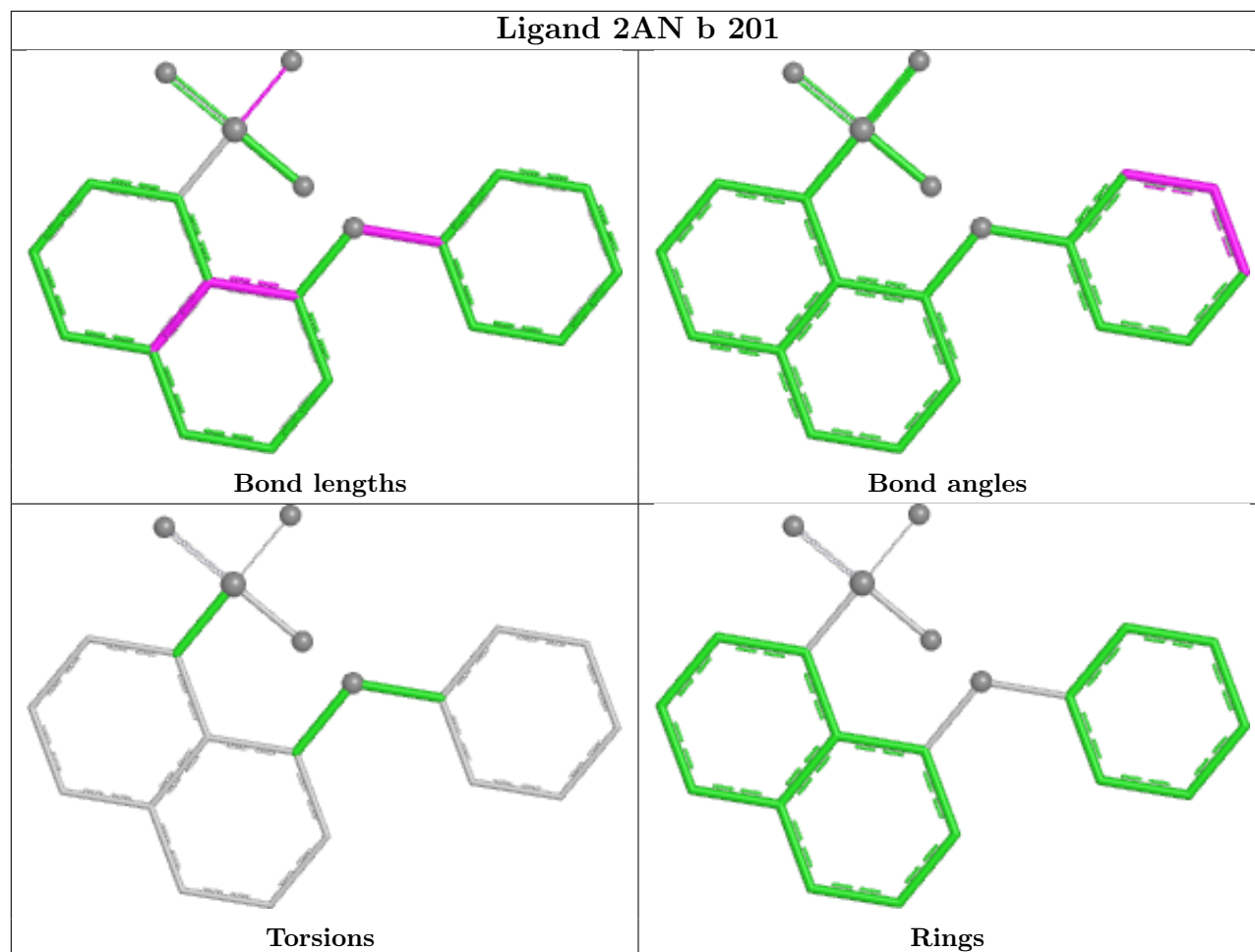




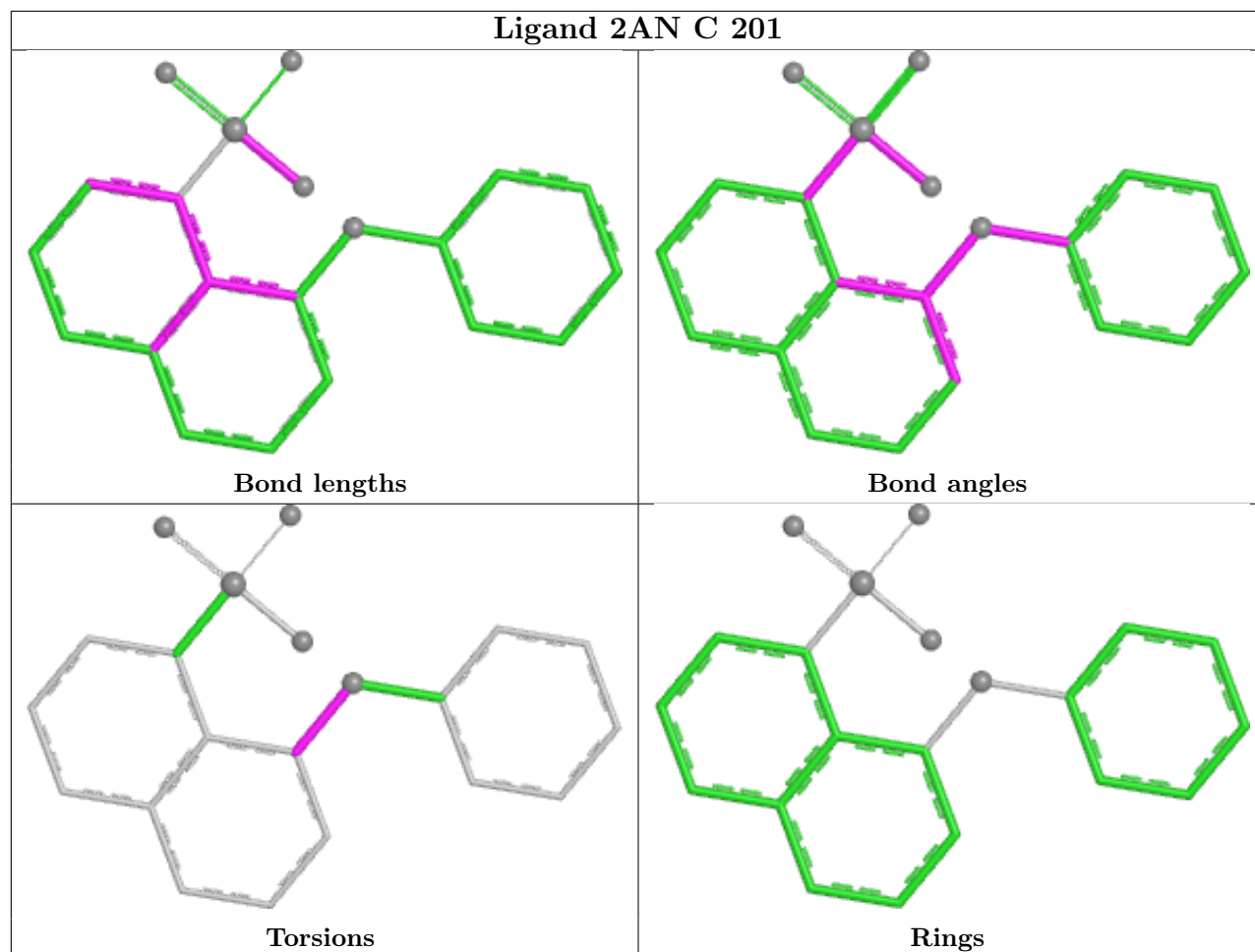


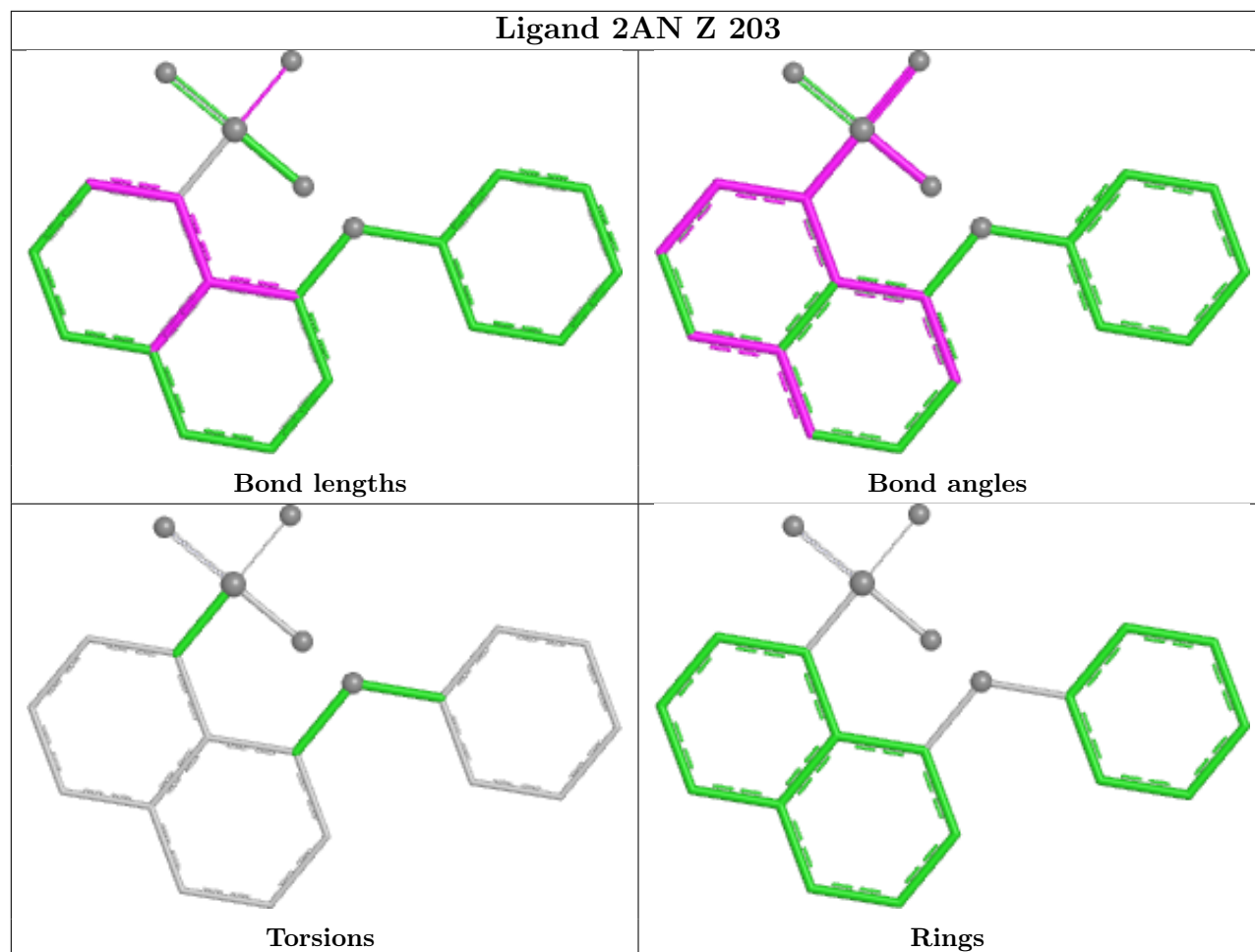


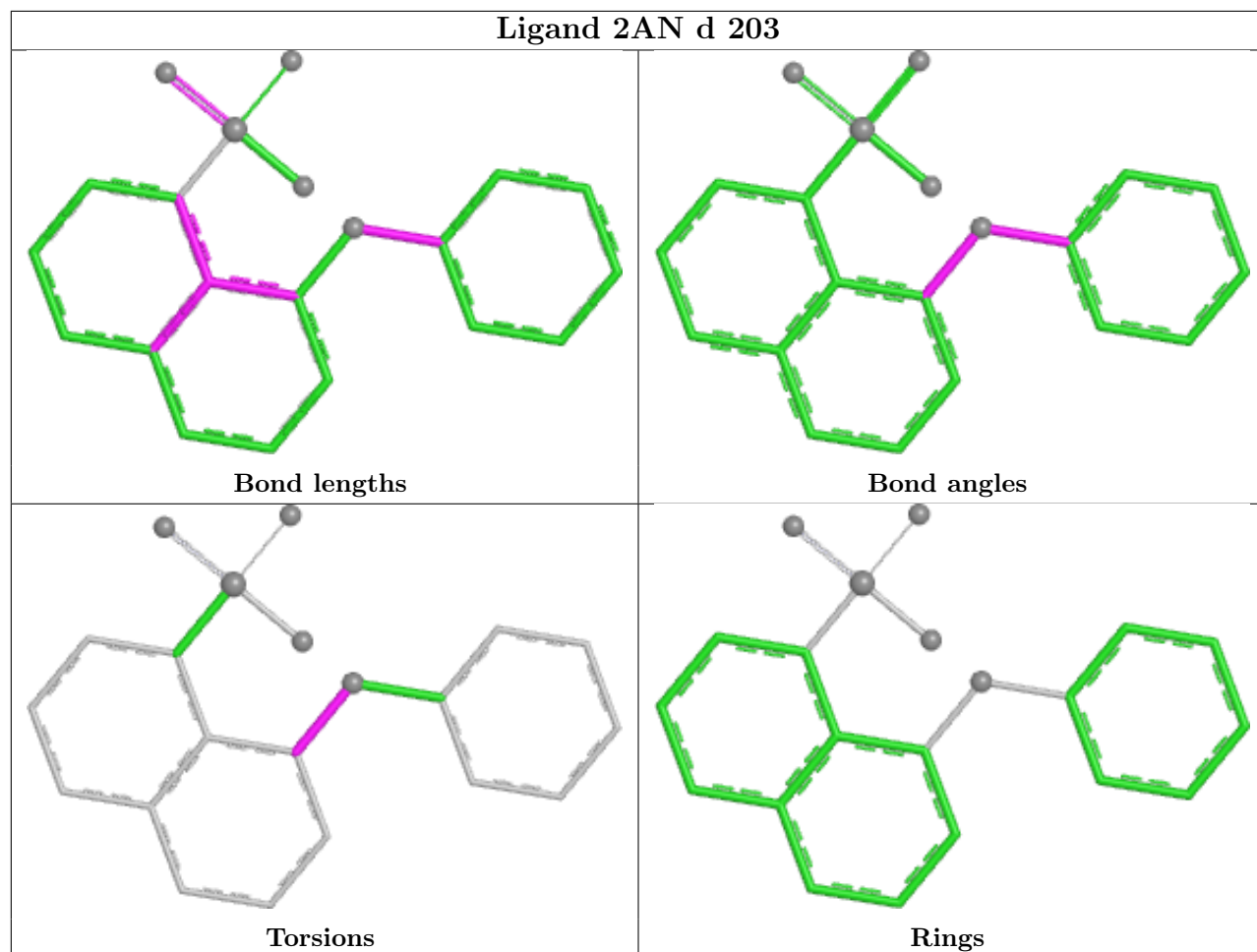


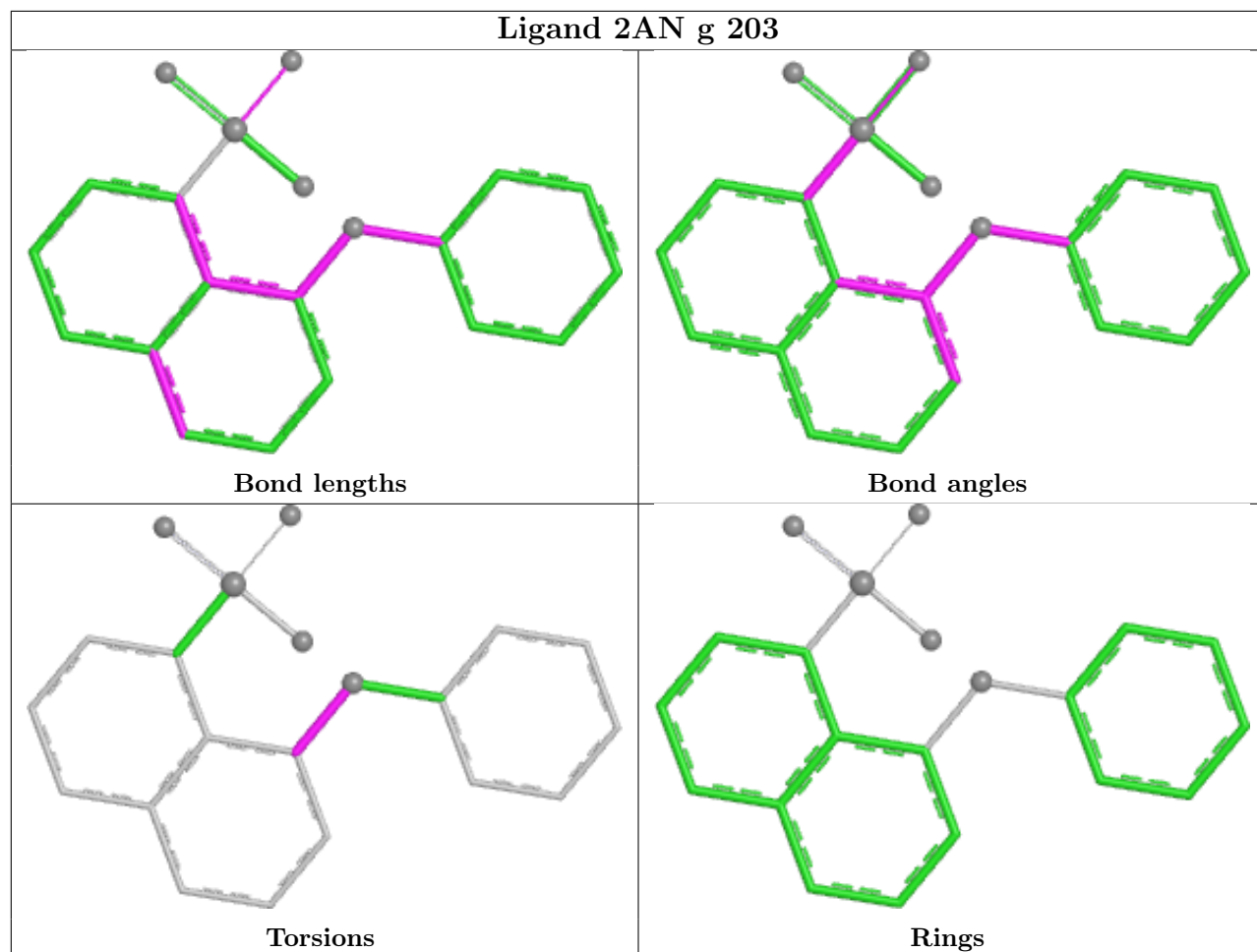


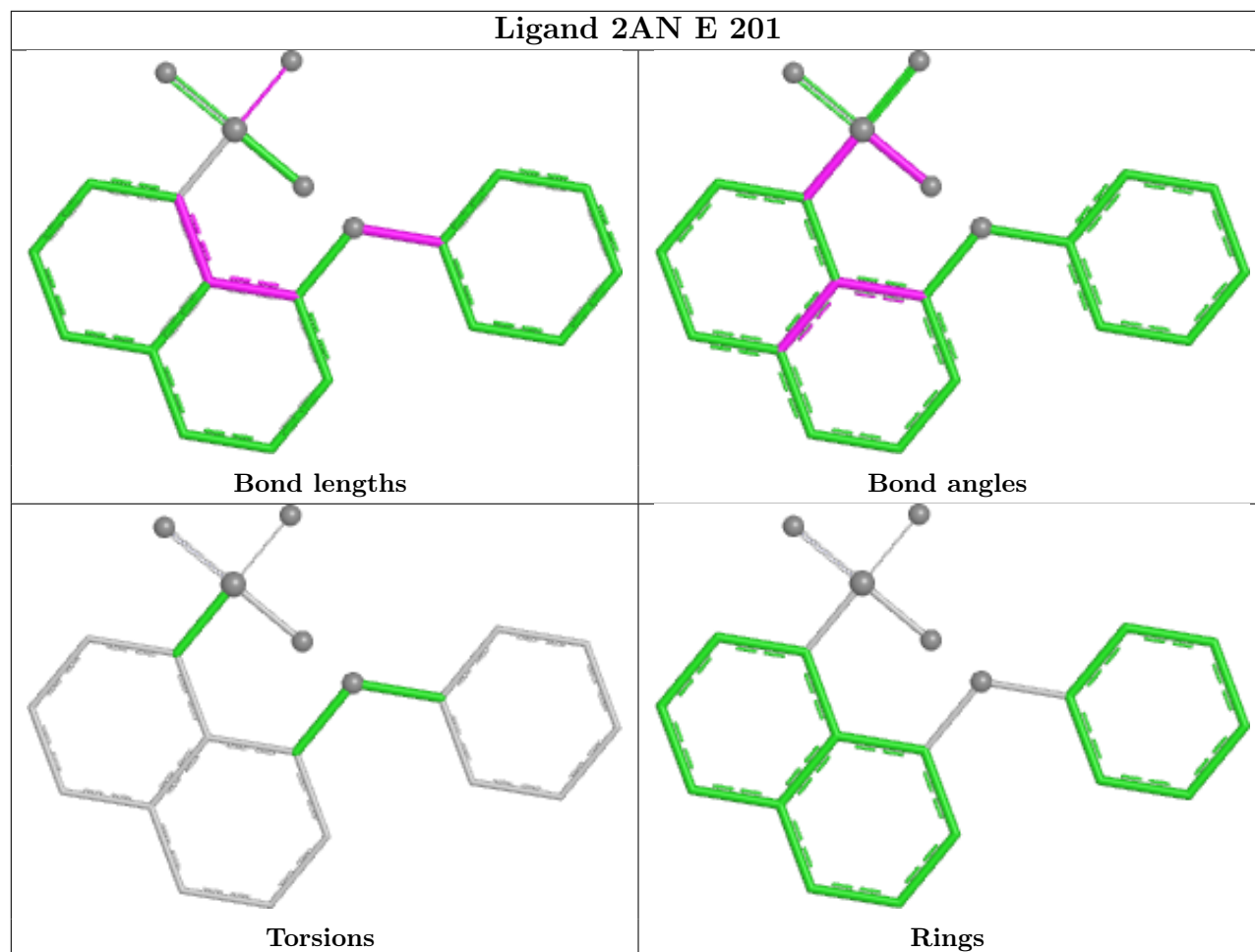


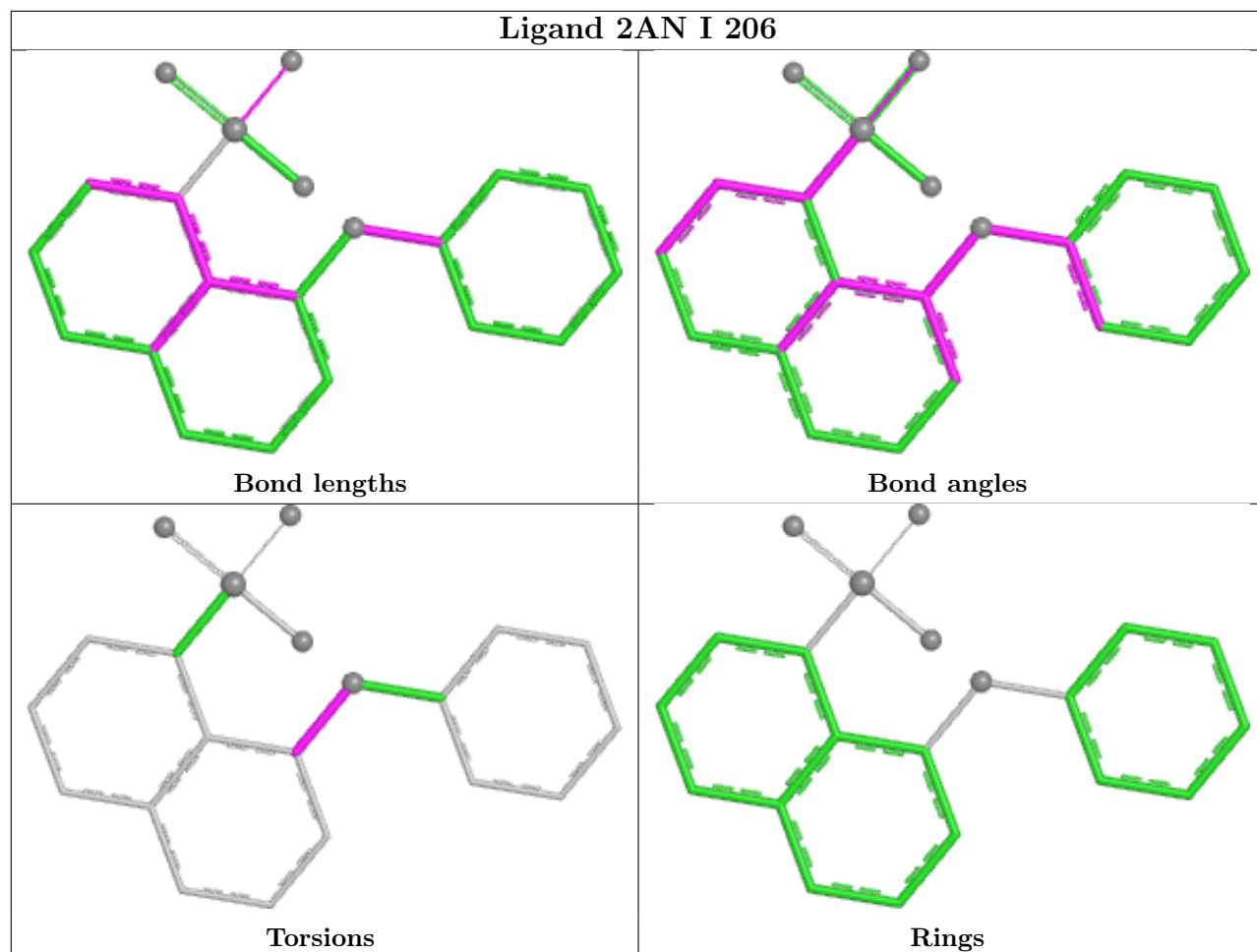


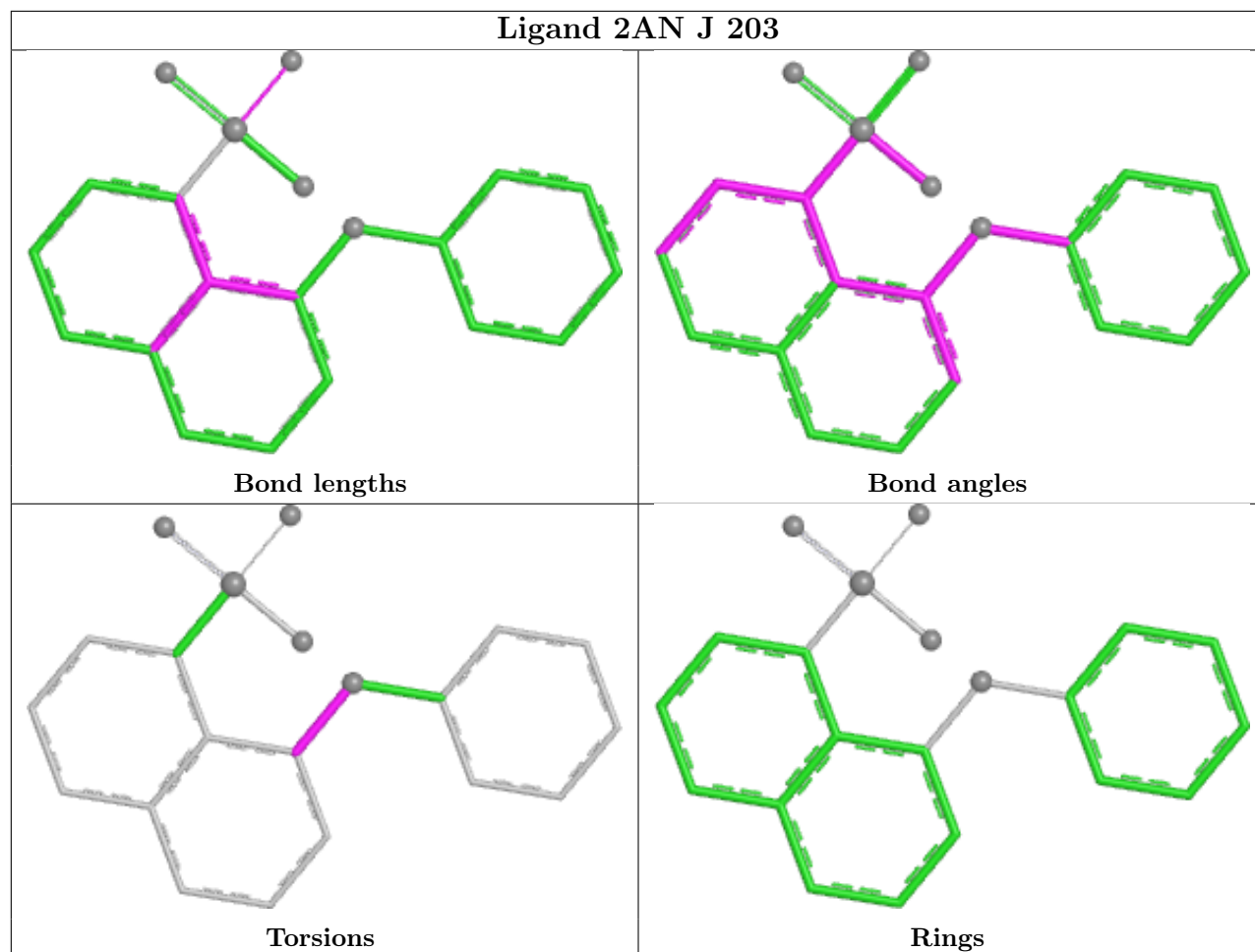


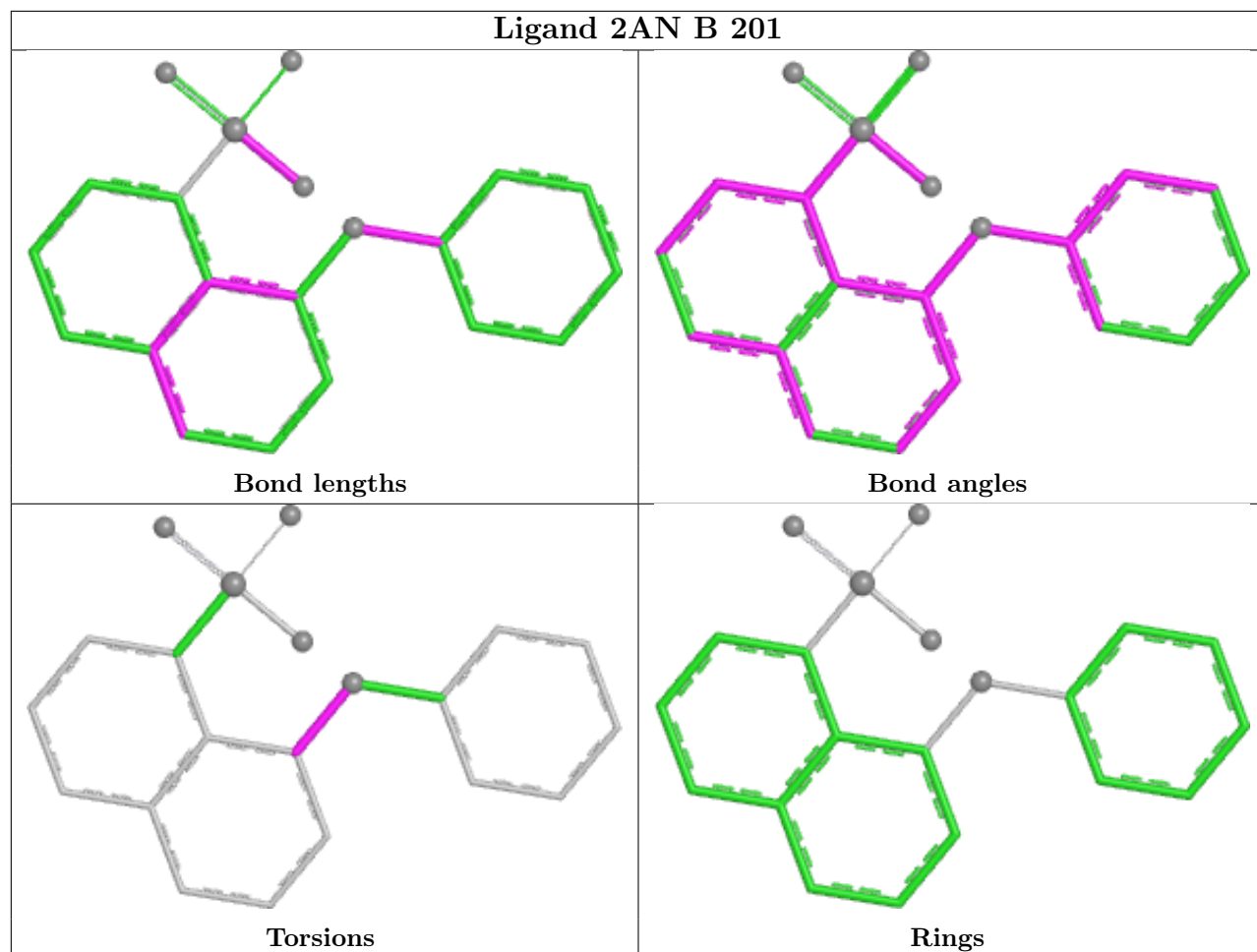




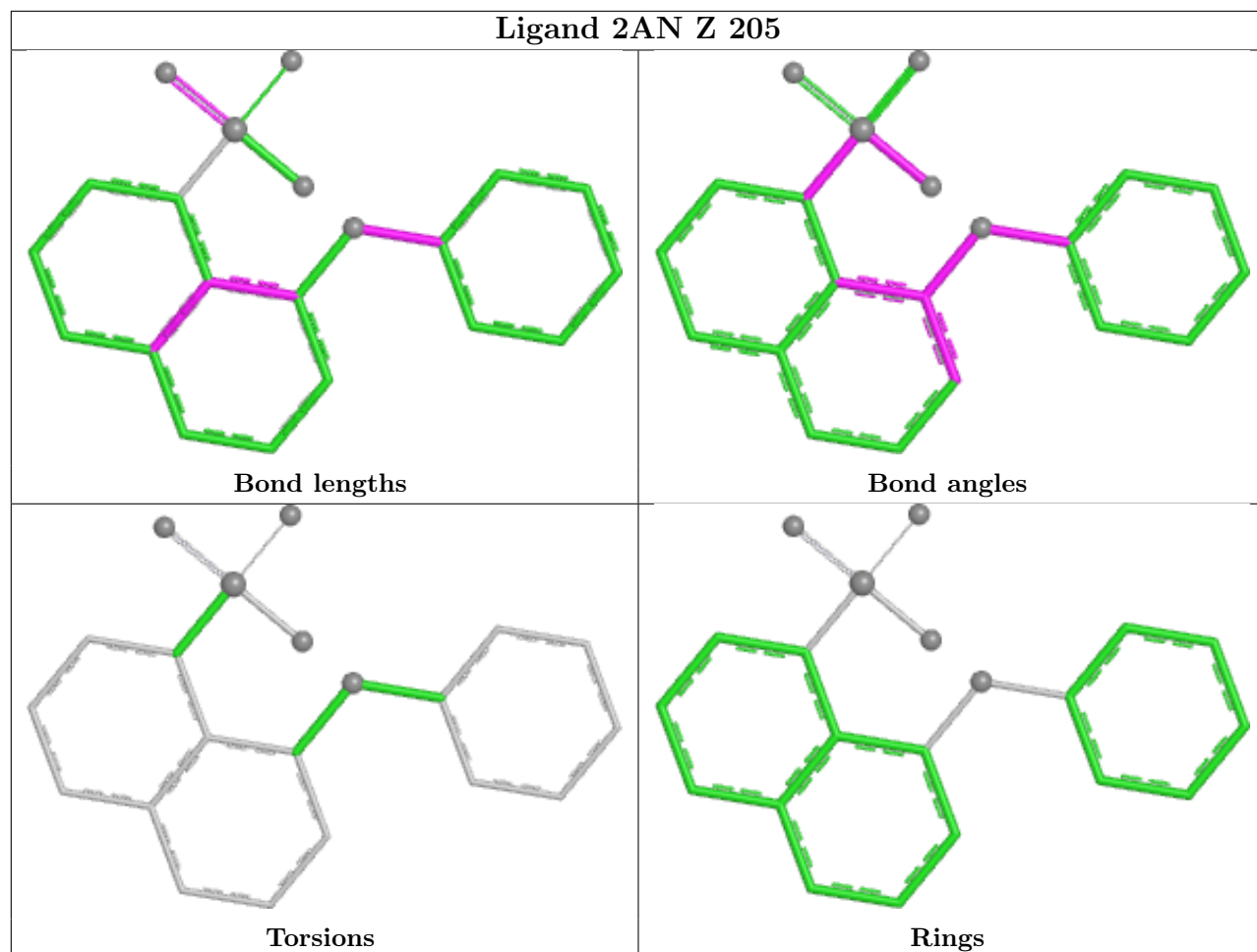


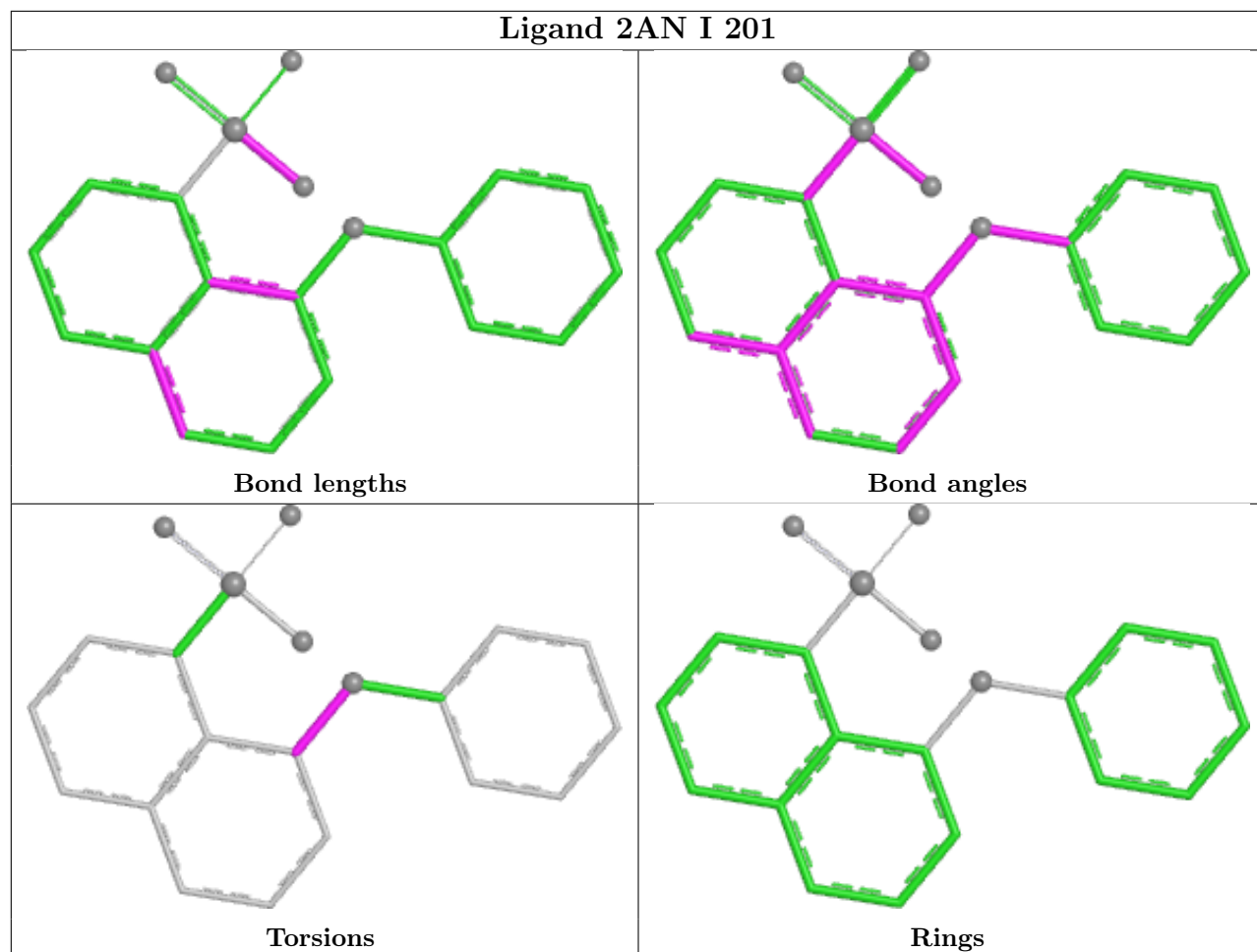


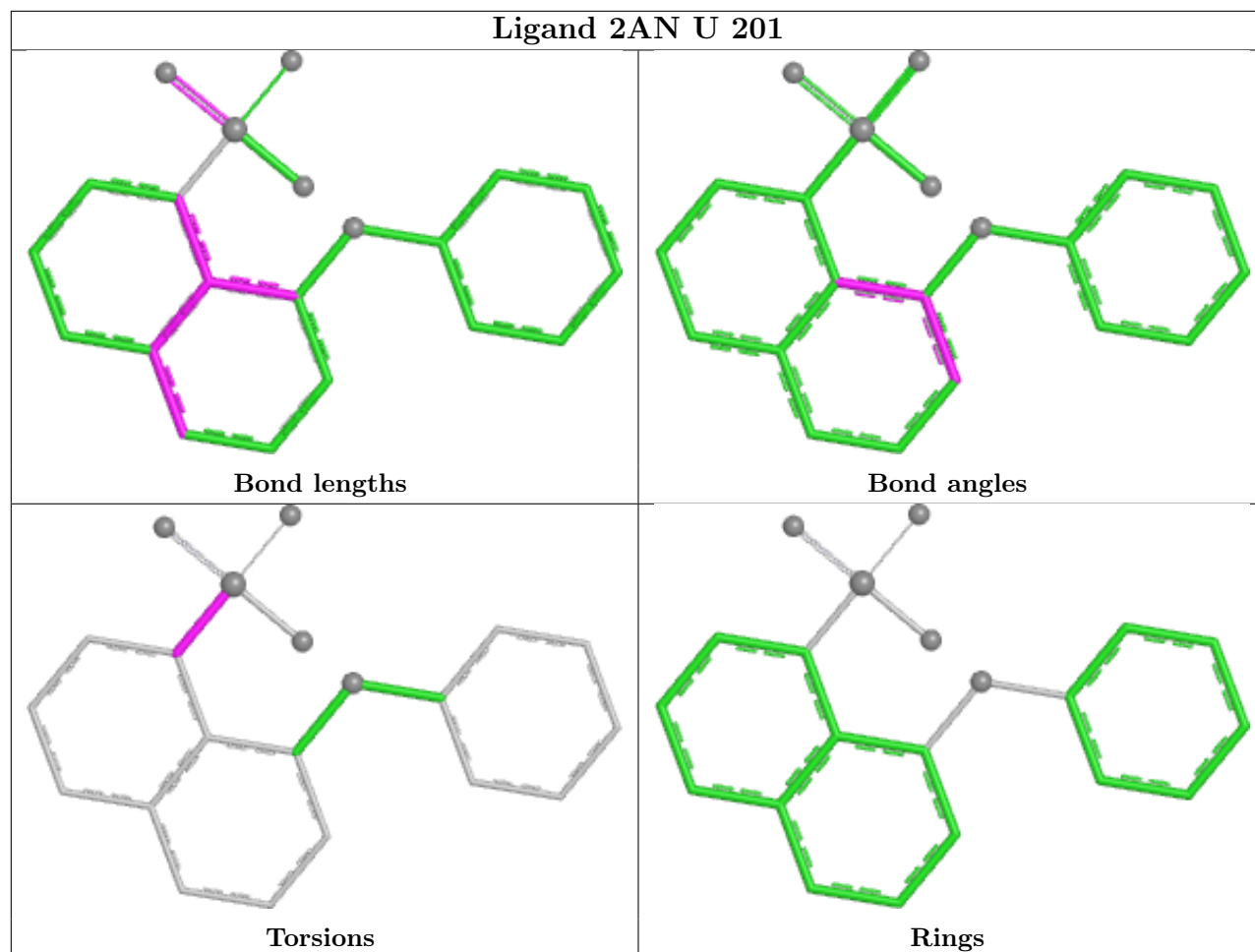


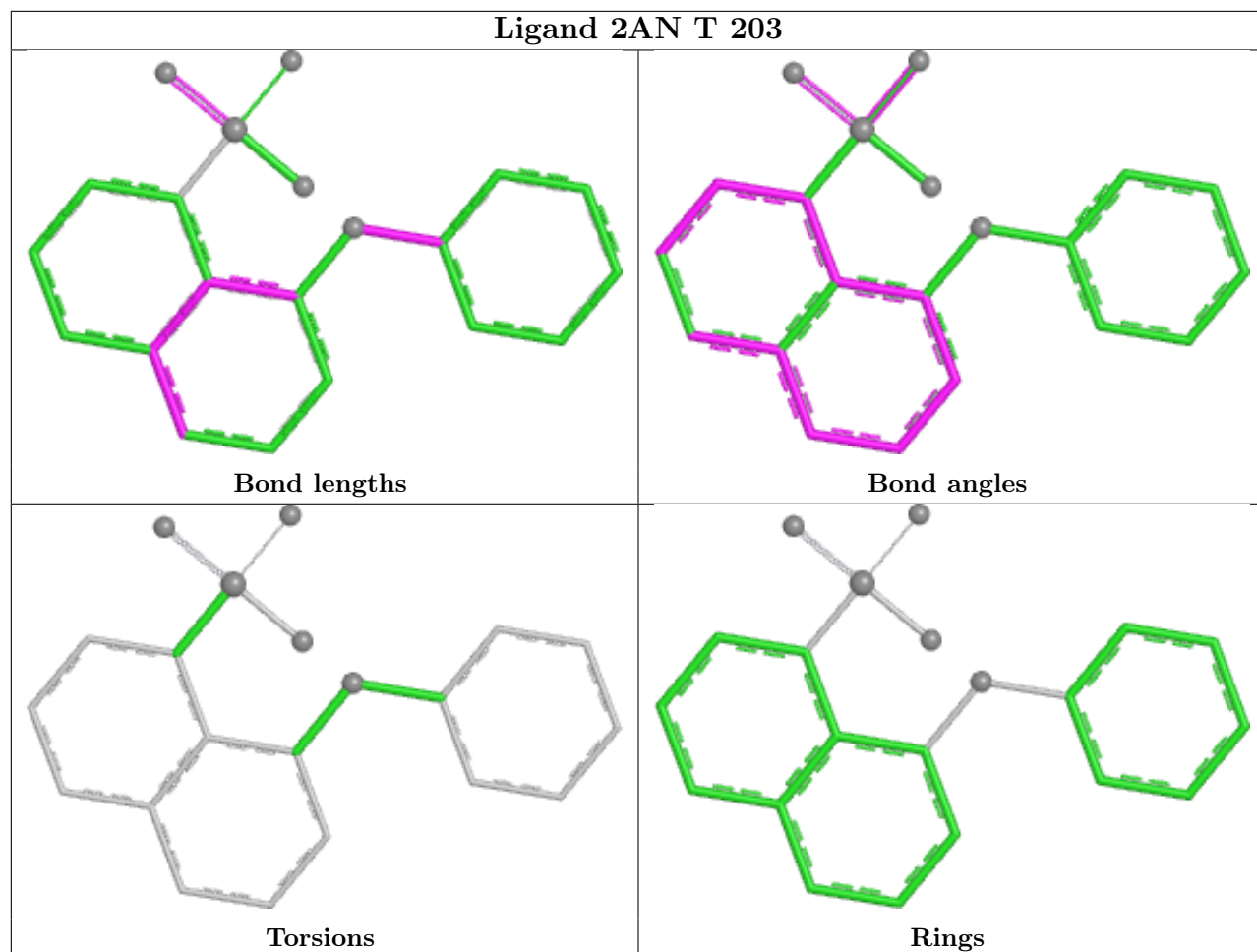


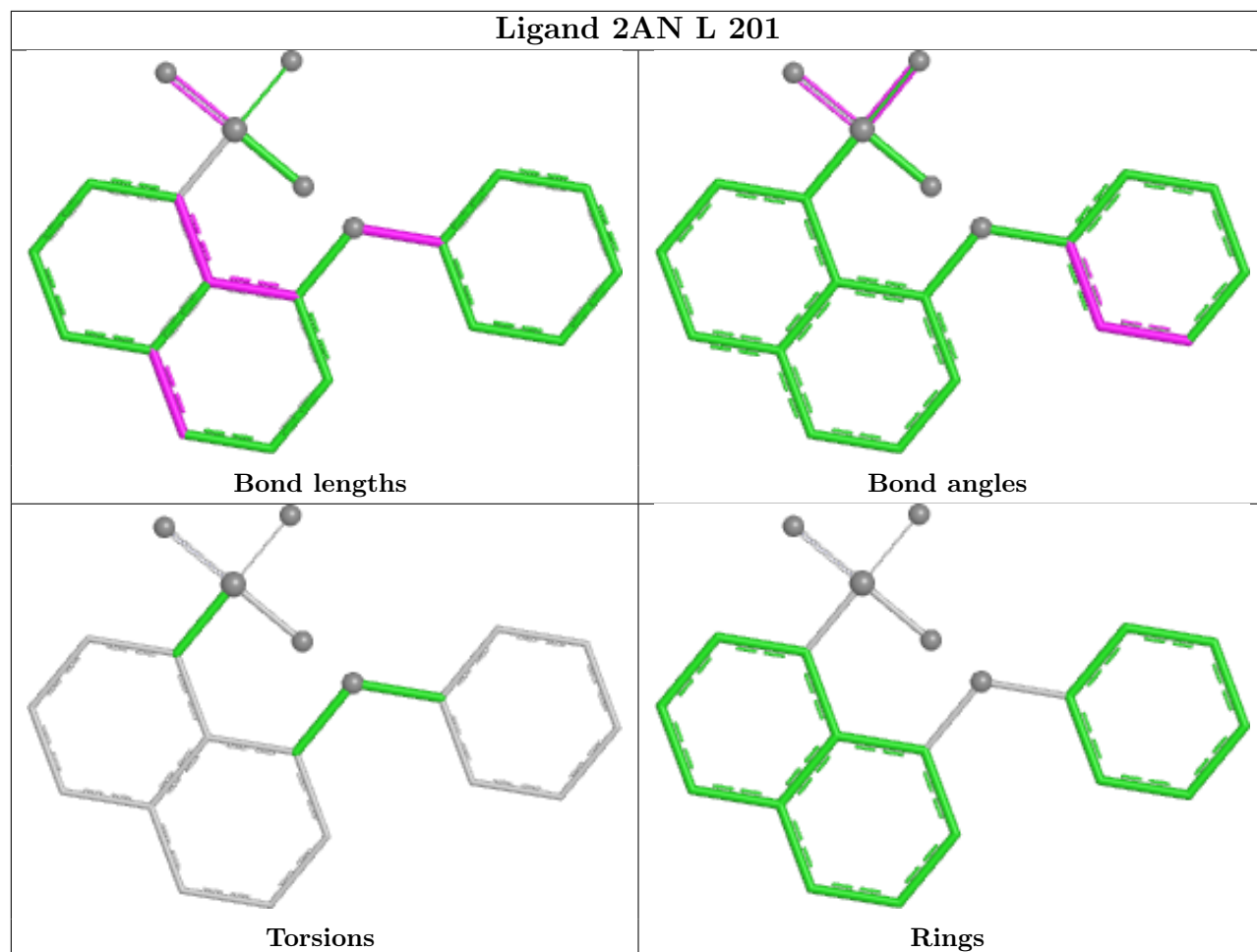


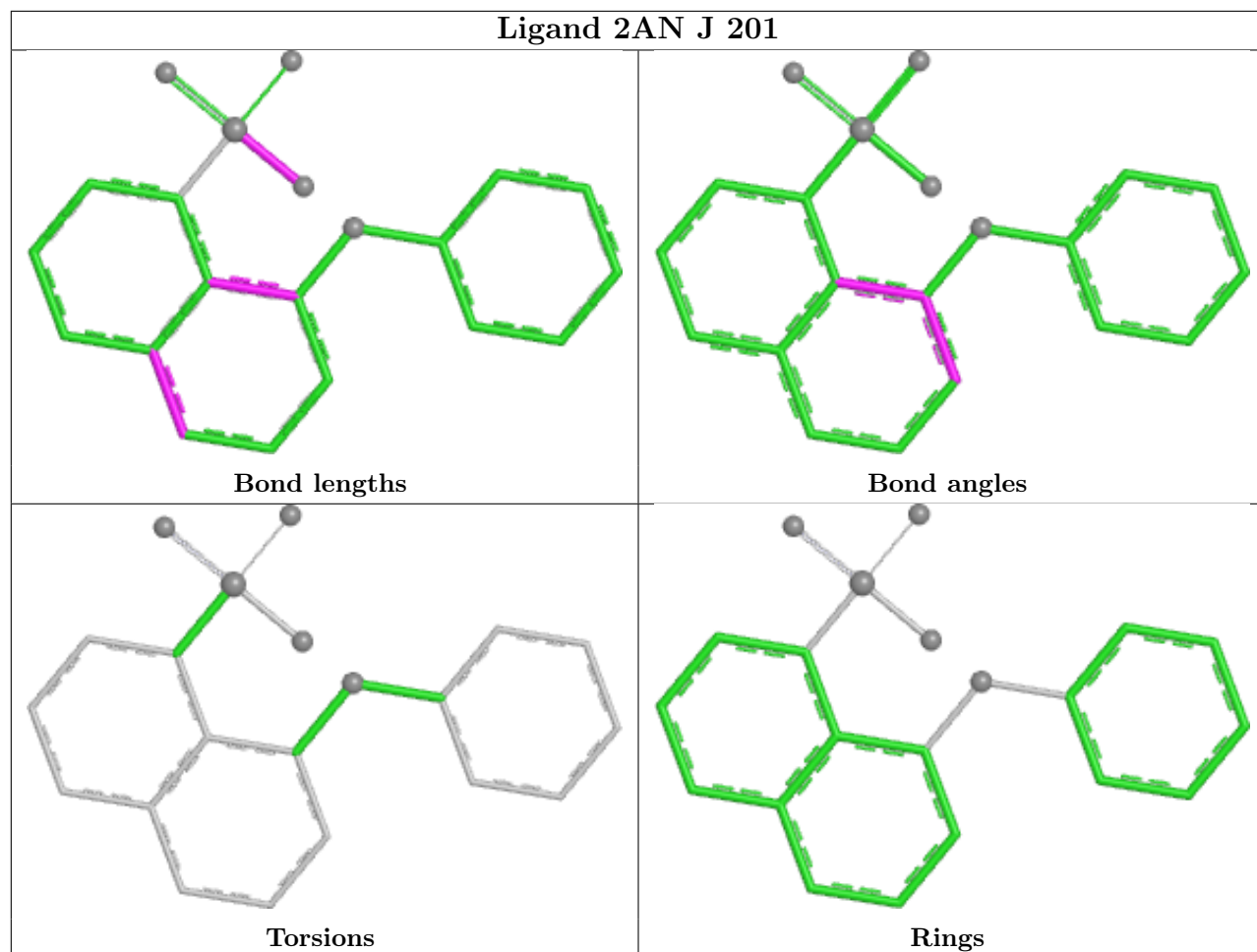


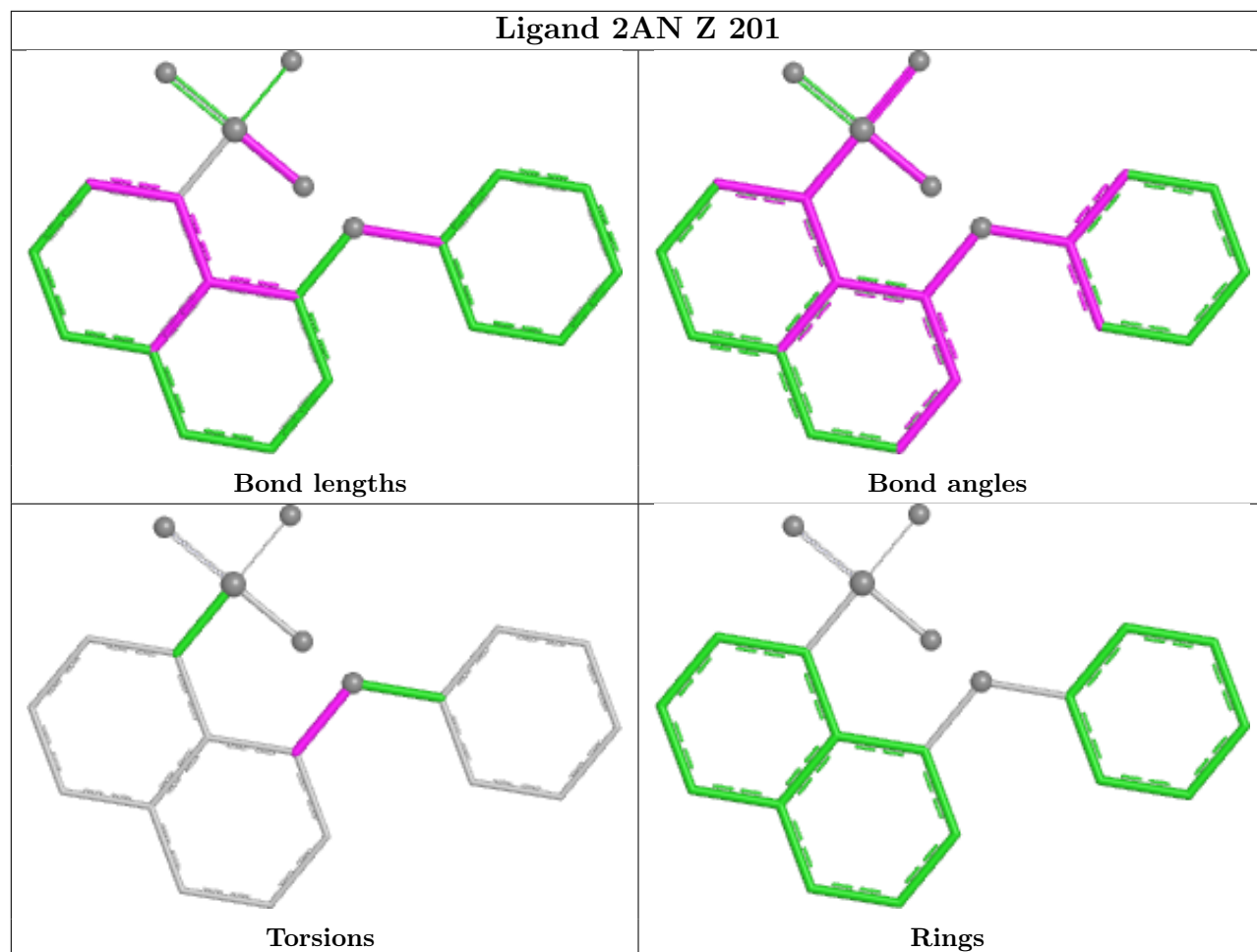


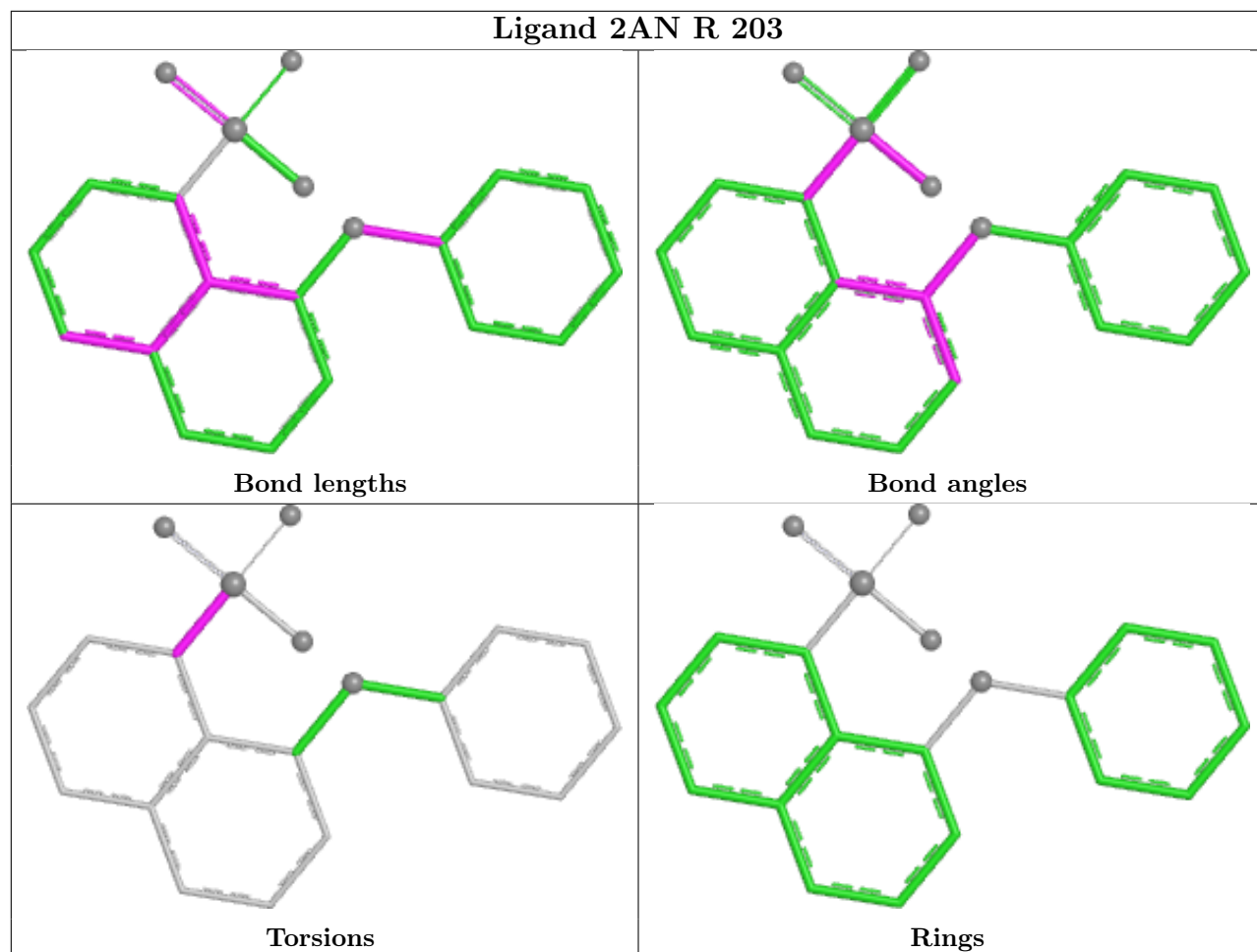




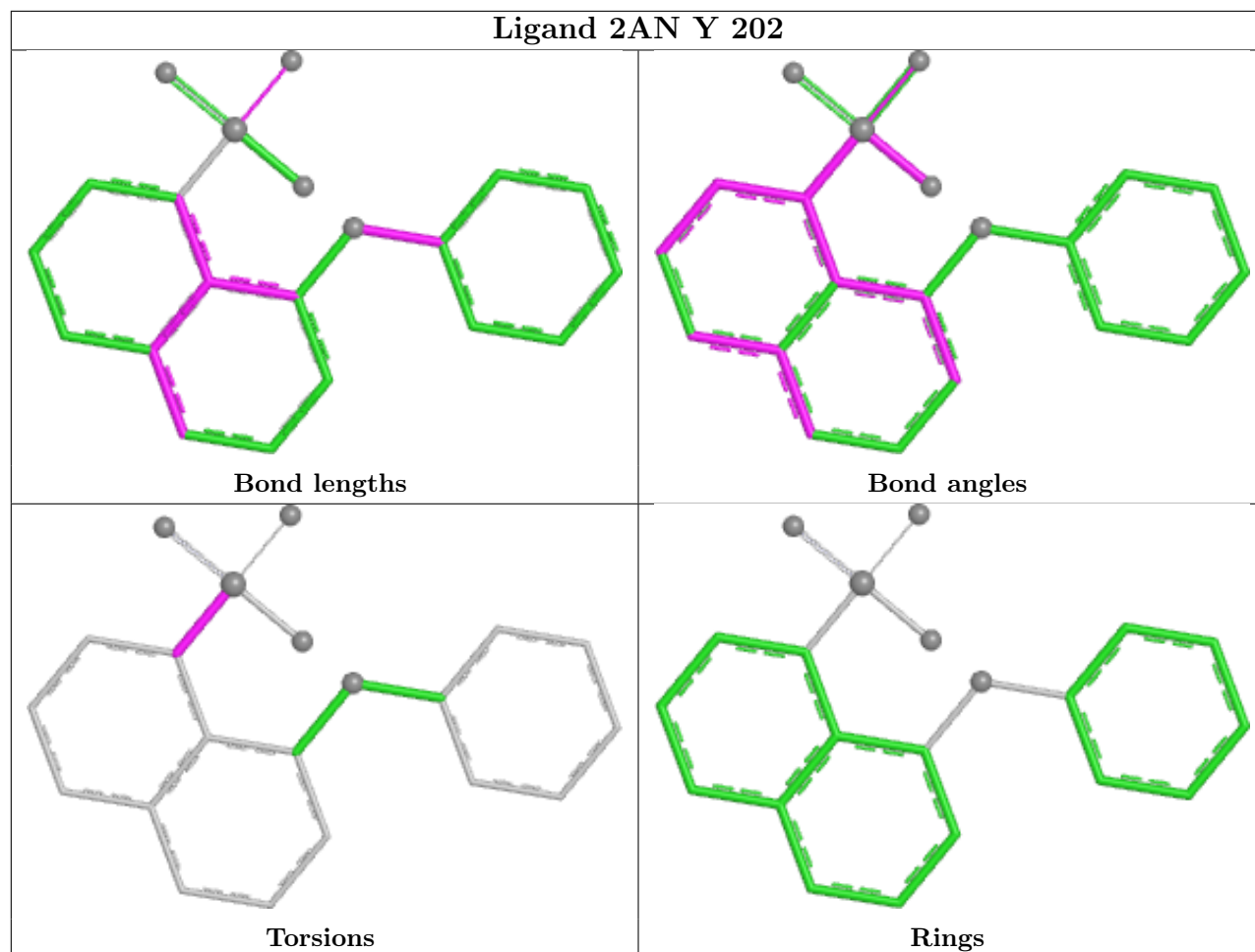


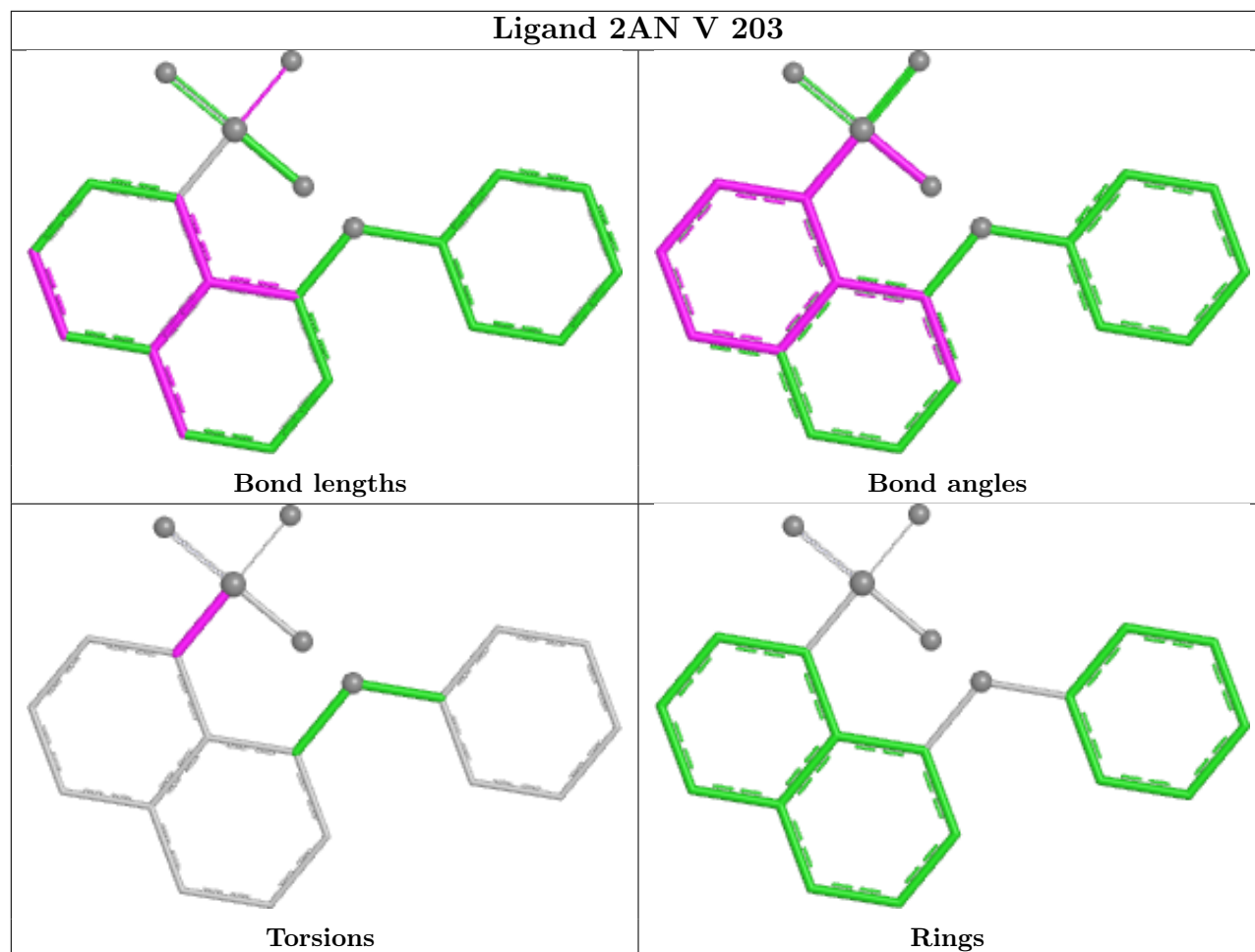


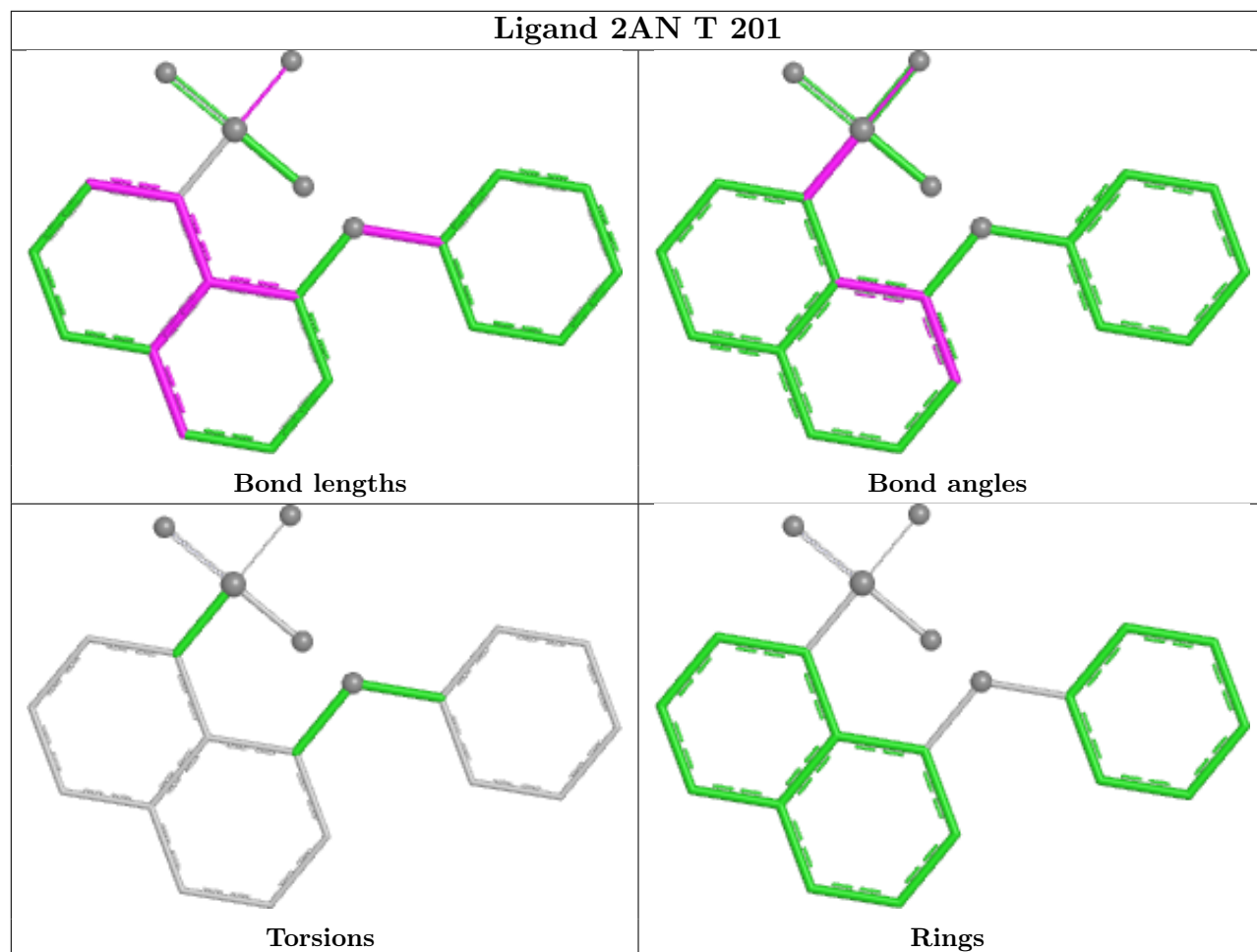


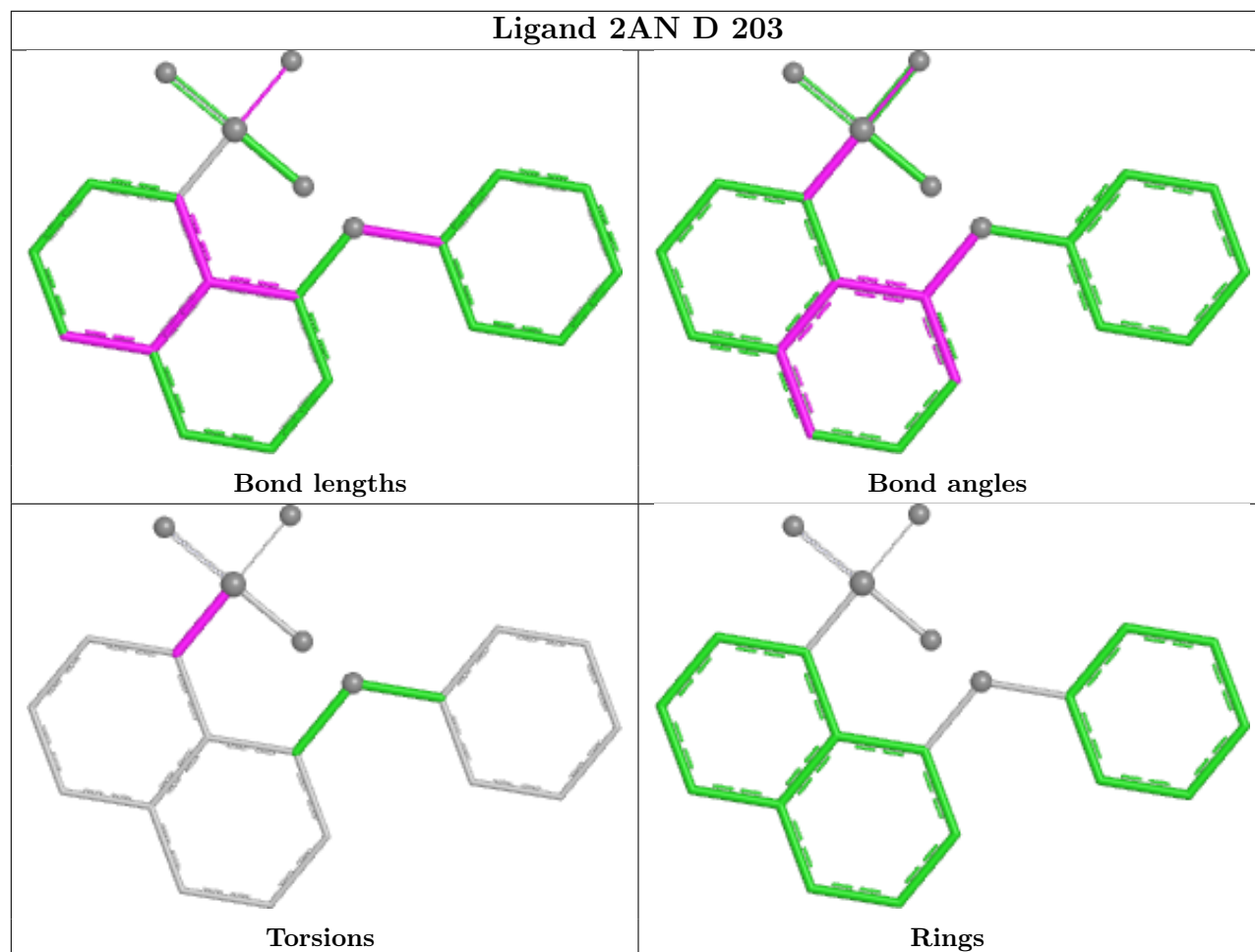


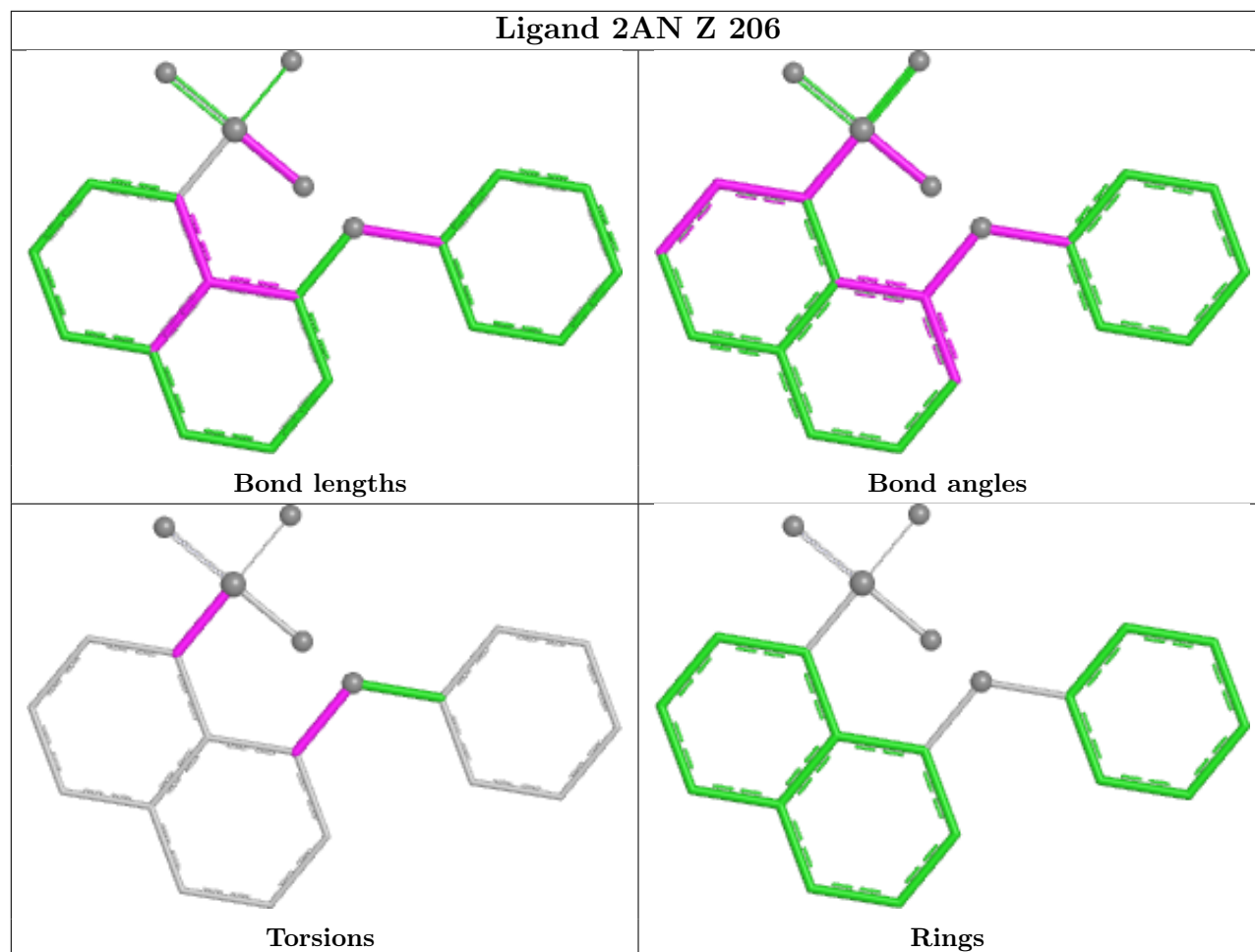


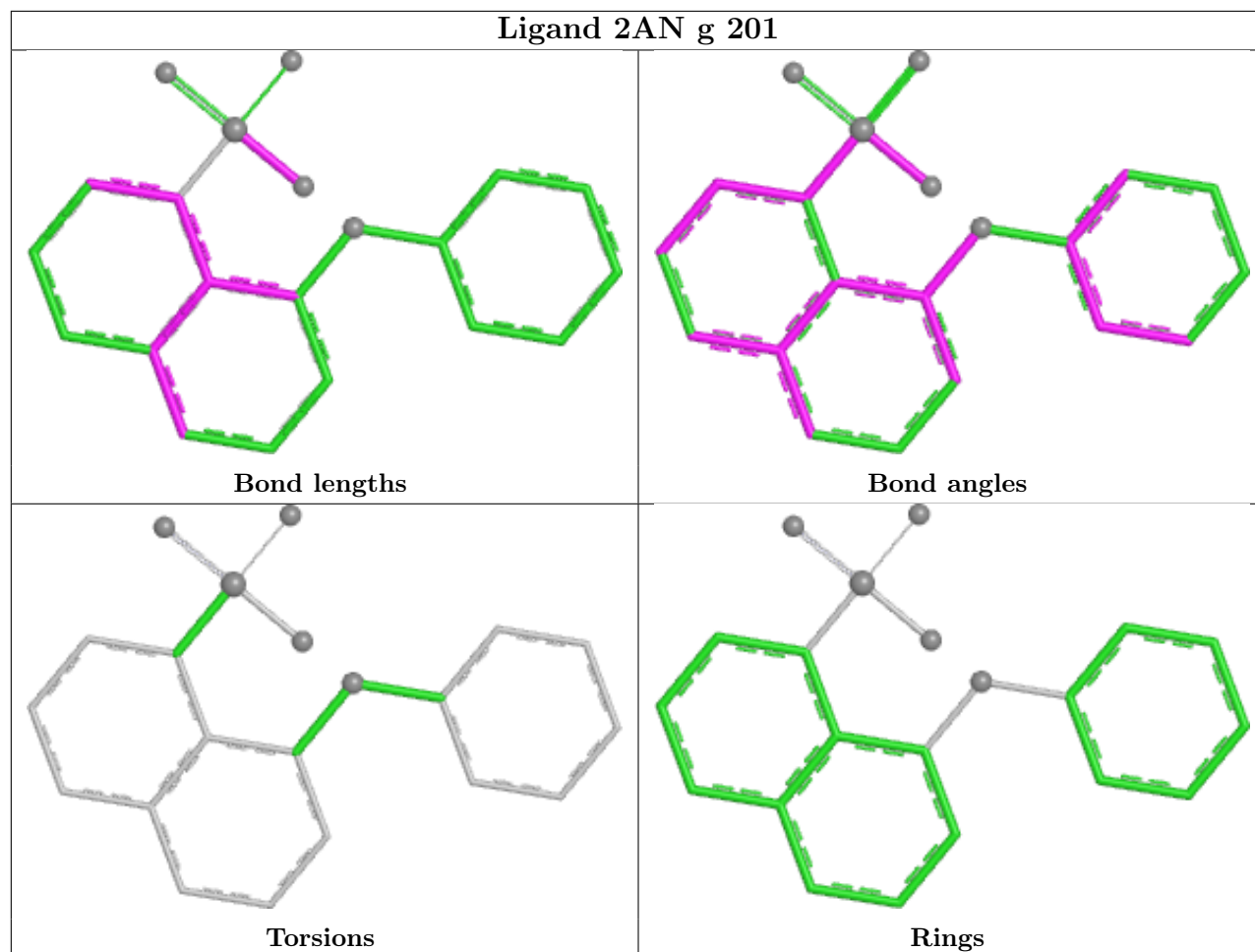


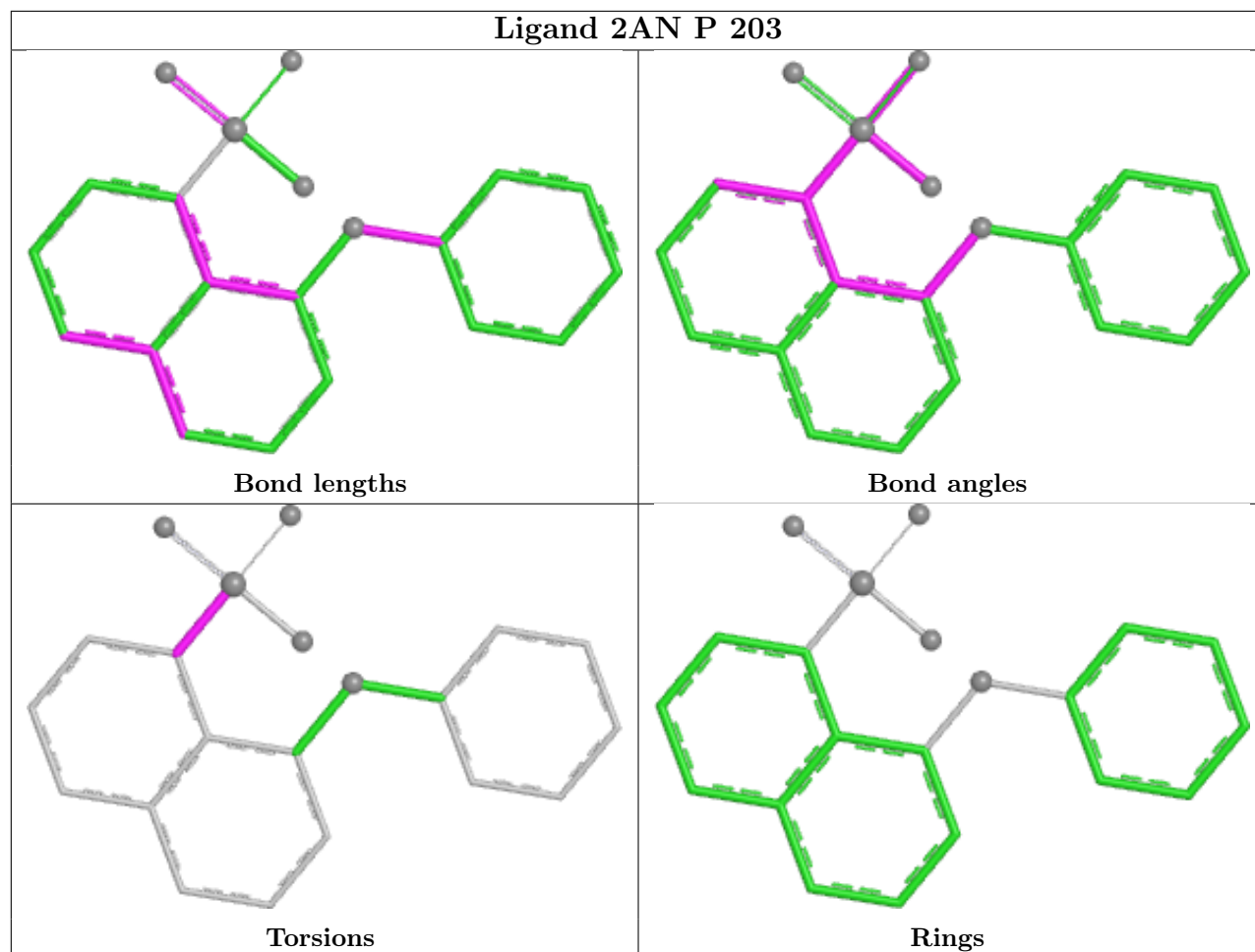


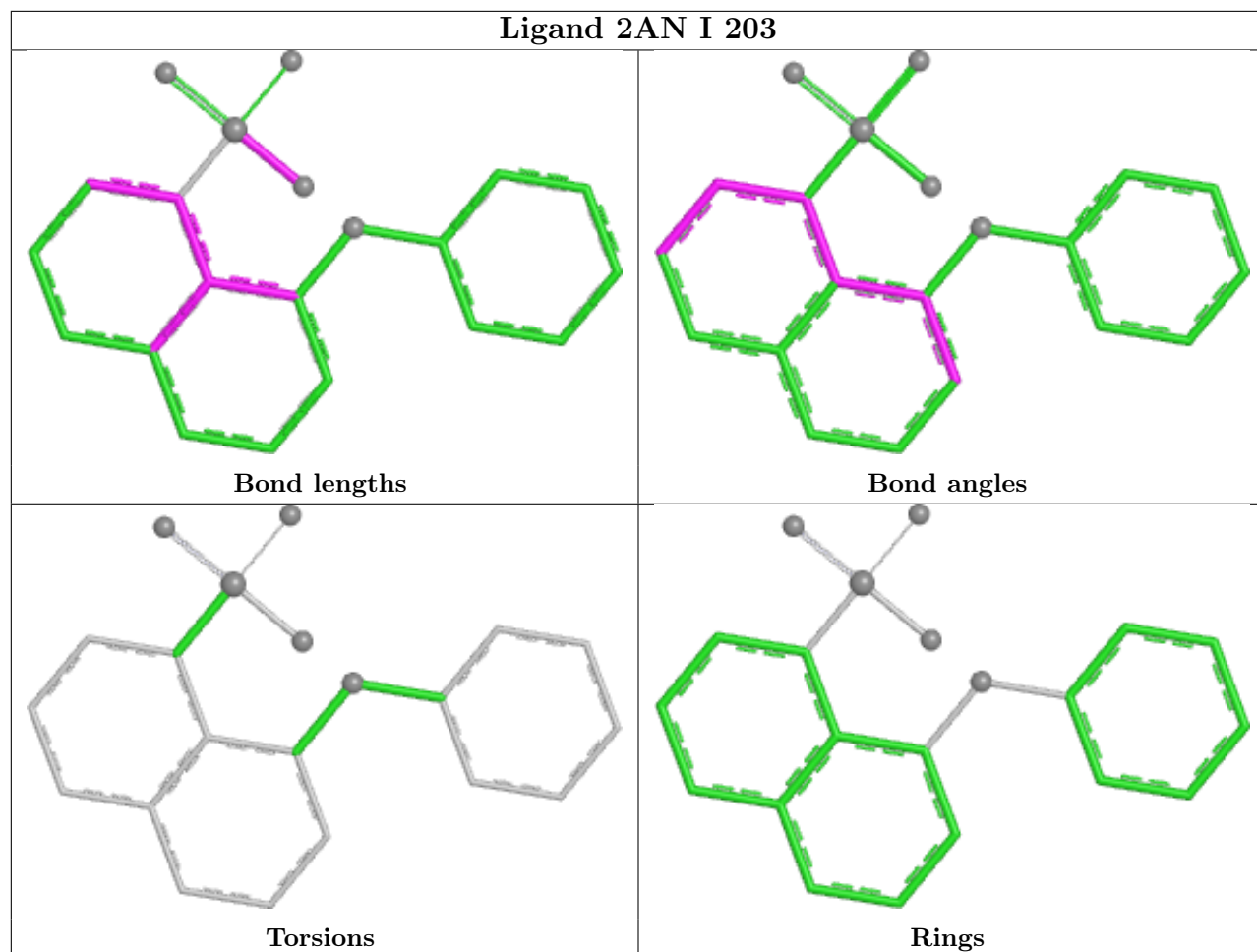




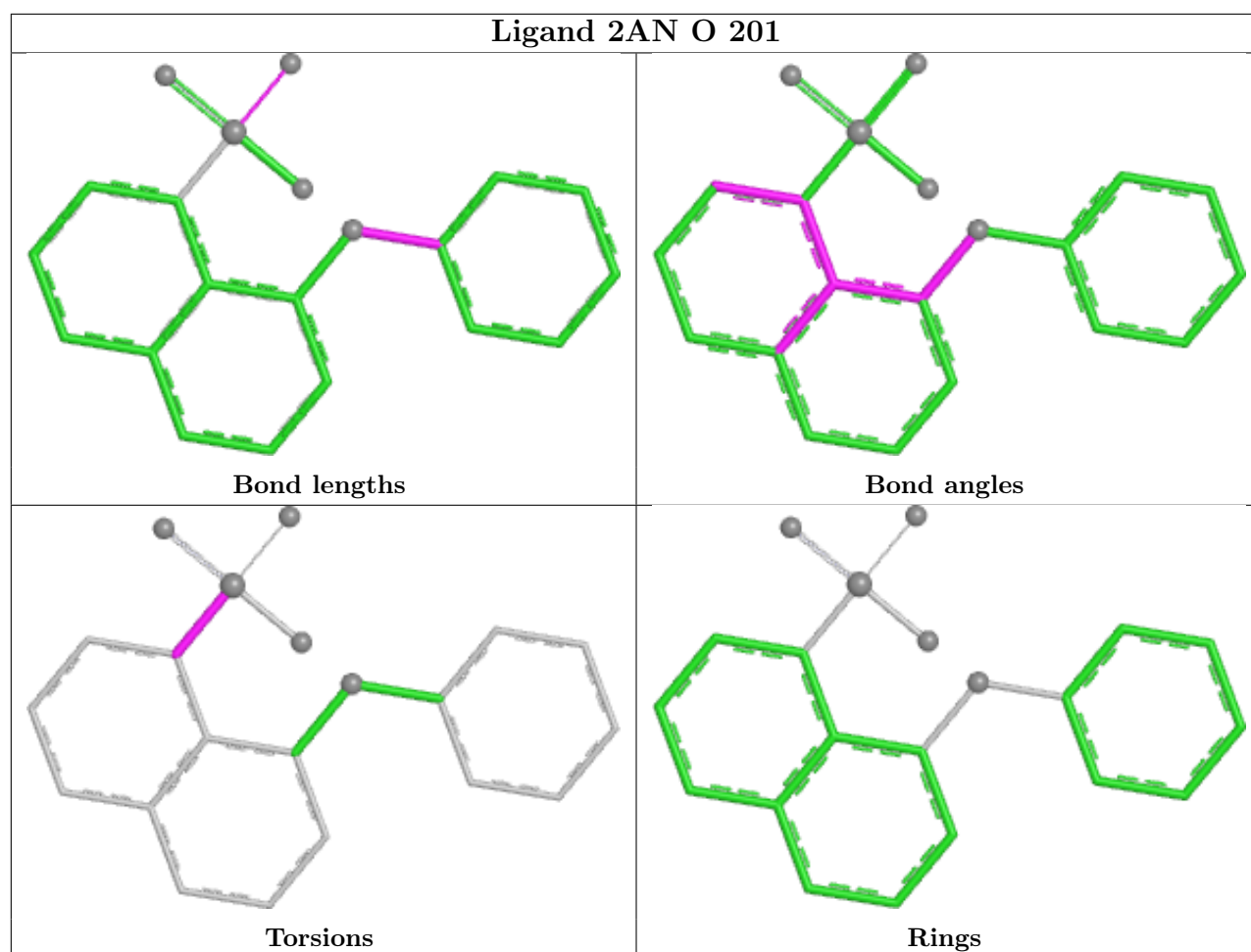












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	162/163 (99%)	1.04	30 (18%) 1 1	56, 78, 120, 132	0
1	B	159/163 (97%)	0.34	10 (6%) 20 25	39, 62, 107, 131	2 (1%)
1	C	161/163 (98%)	0.70	15 (9%) 8 11	58, 83, 115, 139	0
1	D	159/163 (97%)	0.71	21 (13%) 3 4	46, 76, 120, 146	0
1	E	161/163 (98%)	0.35	8 (4%) 28 35	42, 63, 96, 114	0
1	F	159/163 (97%)	0.93	29 (18%) 1 1	53, 80, 115, 147	2 (1%)
1	G	162/163 (99%)	0.57	14 (8%) 10 14	43, 72, 105, 119	4 (2%)
1	H	160/163 (98%)	0.54	17 (10%) 6 8	45, 70, 112, 153	1 (0%)
1	I	161/163 (98%)	0.32	5 (3%) 49 56	39, 62, 90, 108	1 (0%)
1	J	163/163 (100%)	0.60	11 (6%) 17 23	47, 73, 98, 259	1 (0%)
1	K	162/163 (99%)	0.33	3 (1%) 66 73	42, 63, 88, 111	2 (1%)
1	L	160/163 (98%)	0.26	8 (5%) 28 35	39, 61, 97, 124	4 (2%)
1	M	162/163 (99%)	0.25	6 (3%) 41 48	41, 65, 89, 131	1 (0%)
1	N	163/163 (100%)	0.31	10 (6%) 21 27	38, 62, 91, 131	0
1	O	161/163 (98%)	0.98	25 (15%) 2 3	58, 81, 105, 123	1 (0%)
1	P	159/163 (97%)	0.28	8 (5%) 28 35	22, 57, 89, 106	0
1	Q	162/163 (99%)	0.19	6 (3%) 41 48	40, 69, 102, 140	0
1	R	161/163 (98%)	0.39	14 (8%) 10 14	43, 66, 99, 120	0
1	S	160/163 (98%)	0.29	8 (5%) 28 35	35, 62, 96, 120	1 (0%)
1	T	161/163 (98%)	0.35	6 (3%) 41 48	37, 61, 93, 146	3 (1%)
1	U	159/163 (97%)	1.09	29 (18%) 1 1	50, 86, 123, 163	0
1	V	159/163 (97%)	0.24	9 (5%) 23 30	34, 59, 88, 121	0
1	W	159/163 (97%)	0.63	23 (14%) 2 3	45, 73, 118, 148	7 (4%)
1	X	159/163 (97%)	0.66	17 (10%) 6 8	52, 79, 113, 135	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	Y	159/163 (97%)	0.58	17 (10%) 6 8	46, 72, 102, 124	1 (0%)
1	Z	159/163 (97%)	0.96	24 (15%) 2 3	50, 78, 104, 126	2 (1%)
1	a	159/163 (97%)	0.56	14 (8%) 10 13	40, 71, 104, 180	2 (1%)
1	b	161/163 (98%)	0.58	14 (8%) 10 14	49, 74, 102, 122	1 (0%)
1	c	159/163 (97%)	0.10	4 (2%) 57 64	36, 59, 89, 122	1 (0%)
1	d	162/163 (99%)	0.89	25 (15%) 2 3	53, 76, 108, 161	4 (2%)
1	e	161/163 (98%)	0.08	4 (2%) 57 64	32, 58, 86, 104	1 (0%)
1	f	161/163 (98%)	0.29	7 (4%) 35 42	33, 61, 91, 118	0
1	g	160/163 (98%)	0.19	8 (5%) 28 35	38, 61, 86, 115	0
1	h	162/163 (99%)	0.23	8 (4%) 29 36	39, 59, 86, 126	4 (2%)
1	i	161/163 (98%)	0.37	9 (5%) 24 30	40, 65, 93, 134	1 (0%)
1	j	159/163 (97%)	-0.03	3 (1%) 66 73	30, 54, 78, 129	1 (0%)
All	All	5777/5868 (98%)	0.48	469 (8%) 12 16	22, 68, 105, 259	48 (0%)

The worst 5 of 469 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	a	125	GLY	12.7
1	J	-3	ASP	11.4
1	T	128	VAL	10.6
1	H	59	PHE	9.0
1	H	124	PRO	8.0

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

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	2AN	h	205	21/21	0.21	0.80	127,179,191,208	0
2	2AN	N	203	21/21	0.28	0.56	56,74,126,131	0
2	2AN	U	202	21/21	0.45	0.90	76,90,110,117	21
2	2AN	A	204	21/21	0.48	0.80	58,79,92,95	21
2	2AN	j	207	21/21	0.52	0.58	87,134,147,162	0
2	2AN	f	203	21/21	0.55	0.42	60,68,80,86	0
2	2AN	b	206	21/21	0.58	0.38	57,86,103,108	21
2	2AN	S	204	21/21	0.58	0.59	50,62,75,79	21
2	2AN	F	206	21/21	0.61	0.44	49,63,97,104	21
2	2AN	d	203	21/21	0.66	0.24	66,79,115,120	0
2	2AN	Y	204	21/21	0.66	0.36	47,58,66,70	21
2	2AN	G	207	21/21	0.67	0.34	62,68,79,90	21
2	2AN	D	204	21/21	0.68	0.39	68,98,111,114	0
2	2AN	S	203	21/21	0.69	0.33	46,51,80,83	21
2	2AN	I	207	21/21	0.70	0.39	68,96,114,116	21
6	FLC	e	202	13/13	0.70	0.24	62,69,75,77	0
2	2AN	I	204	21/21	0.72	0.39	57,71,83,89	21
2	2AN	I	205	21/21	0.73	0.41	57,74,84,86	21
2	2AN	X	203	21/21	0.73	0.34	53,62,71,76	0
2	2AN	d	204	21/21	0.73	0.74	50,68,80,82	21
2	2AN	O	202	21/21	0.73	0.33	74,83,90,94	21
3	SO4	A	205	5/5	0.74	0.96	23,24,27,29	5
2	2AN	X	206	21/21	0.74	0.29	48,61,70,74	0
2	2AN	c	202	21/21	0.76	0.24	56,68,103,110	0
5	DMS	G	208	4/4	0.76	0.36	61,61,63,75	4
2	2AN	G	204	21/21	0.76	0.32	47,66,102,109	21
2	2AN	j	205	21/21	0.77	0.26	31,43,51,57	0
2	2AN	b	205	21/21	0.77	0.27	114,123,138,168	0
2	2AN	Z	206	21/21	0.77	0.17	55,78,100,109	0
2	2AN	T	203	21/21	0.78	0.24	45,60,101,108	0
6	FLC	a	206	13/13	0.78	0.15	60,76,89,90	13
2	2AN	R	204	21/21	0.79	0.26	61,75,82,83	0
2	2AN	c	205	21/21	0.79	0.30	38,48,57,61	21
2	2AN	T	204	21/21	0.79	0.24	50,64,70,85	0
2	2AN	I	203	21/21	0.79	0.34	63,75,83,91	21
2	2AN	G	205	21/21	0.79	0.33	32,40,50,55	21
2	2AN	V	207	21/21	0.79	0.23	48,62,88,96	0
4	EPE	P	205	15/15	0.80	0.27	57,75,92,109	0
2	2AN	R	205	21/21	0.80	0.26	77,99,112,117	0
6	FLC	j	208	13/13	0.80	0.46	30,38,45,59	13

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	2AN	U	201	21/21	0.81	0.24	89,112,138,139	0
5	DMS	X	207	4/4	0.82	0.43	68,68,69,71	4
6	FLC	G	206	13/13	0.82	0.23	45,60,64,69	13
2	2AN	a	204	21/21	0.82	0.46	54,112,142,163	21
2	2AN	H	204	21/21	0.82	0.24	71,79,107,109	21
2	2AN	E	204	21/21	0.82	0.36	48,69,105,112	21
2	2AN	F	204	21/21	0.83	0.29	74,96,127,138	0
6	FLC	i	202	13/13	0.83	0.16	47,60,64,70	13
2	2AN	C	203[A]	21/21	0.84	0.37	51,60,72,76	21
2	2AN	T	205	21/21	0.84	0.16	54,60,75,78	0
2	2AN	W	201	21/21	0.85	0.30	45,60,69,73	21
2	2AN	Y	201	21/21	0.85	0.19	63,72,89,91	0
2	2AN	N	205	21/21	0.85	0.21	53,68,76,88	0
2	2AN	j	206	21/21	0.86	0.18	52,69,105,107	0
2	2AN	A	203	21/21	0.86	0.22	61,67,94,98	21
6	FLC	i	203	13/13	0.86	0.19	45,52,60,62	0
2	2AN	S	201	21/21	0.87	0.18	81,103,116,120	0
2	2AN	c	203	21/21	0.87	0.18	58,78,115,123	0
2	2AN	g	203	21/21	0.87	0.15	48,76,86,88	0
2	2AN	f	206	21/21	0.87	0.28	62,76,97,101	21
3	SO4	Q	204	5/5	0.87	0.23	47,67,73,75	5
2	2AN	X	202	21/21	0.87	0.17	70,81,106,111	0
2	2AN	B	206	21/21	0.87	0.22	65,80,111,114	0
2	2AN	F	202	21/21	0.88	0.19	50,81,108,112	0
2	2AN	I	206	21/21	0.88	0.19	54,78,87,90	0
2	2AN	K	203	21/21	0.88	0.20	45,61,72,73	21
2	2AN	a	201	21/21	0.88	0.20	58,96,117,123	0
2	2AN	X	201	21/21	0.88	0.21	40,49,81,90	0
2	2AN	V	208	21/21	0.88	0.32	54,67,114,129	21
2	2AN	h	201	21/21	0.89	0.29	34,48,53,62	21
2	2AN	a	203	21/21	0.89	0.18	58,67,76,81	0
2	2AN	h	206	21/21	0.89	0.17	39,57,75,82	0
2	2AN	d	201	21/21	0.89	0.22	46,61,68,72	0
2	2AN	Z	205	21/21	0.89	0.16	68,75,126,139	0
2	2AN	O	203	21/21	0.90	0.15	53,63,74,92	0
2	2AN	Y	202	21/21	0.90	0.22	45,53,56,59	21
2	2AN	j	201	21/21	0.90	0.13	34,48,58,61	0
2	2AN	E	203	21/21	0.90	0.23	44,52,76,79	21
2	2AN	V	206	21/21	0.90	0.16	50,64,84,93	0
2	2AN	Q	203	21/21	0.90	0.20	81,100,118,121	0
2	2AN	A	201	21/21	0.90	0.25	46,57,80,91	0
2	2AN	D	203	21/21	0.91	0.13	72,78,87,91	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	DMS	N	206	4/4	0.91	0.23	36,47,47,48	4
2	2AN	Z	202	21/21	0.91	0.19	88,99,106,119	0
2	2AN	F	201	21/21	0.91	0.20	61,70,79,84	0
2	2AN	G	201	21/21	0.91	0.17	48,55,82,93	0
2	2AN	g	201	21/21	0.91	0.19	46,57,79,83	21
6	FLC	a	205	13/13	0.91	0.15	55,64,75,77	13
2	2AN	X	205	21/21	0.91	0.12	55,66,81,86	0
2	2AN	B	204	21/21	0.91	0.15	43,52,59,59	21
2	2AN	D	202	21/21	0.91	0.17	50,59,76,79	0
3	SO4	Y	205	5/5	0.91	0.51	29,31,38,41	5
2	2AN	d	202	21/21	0.92	0.14	50,61,76,81	0
2	2AN	Z	203	21/21	0.92	0.17	60,69,82,90	0
2	2AN	R	202	21/21	0.92	0.17	36,49,57,62	0
2	2AN	L	204	21/21	0.92	0.18	65,75,91,95	0
2	2AN	i	201	21/21	0.92	0.30	40,48,51,52	21
3	SO4	c	208	5/5	0.92	0.24	32,36,36,41	5
2	2AN	b	202	21/21	0.92	0.18	54,68,80,85	0
2	2AN	h	204	21/21	0.92	0.18	48,67,91,97	0
2	2AN	b	204	21/21	0.92	0.14	65,72,87,92	0
2	2AN	P	203	21/21	0.93	0.16	44,55,68,85	0
2	2AN	R	203	21/21	0.93	0.14	54,73,82,84	0
3	SO4	G	209	5/5	0.93	0.16	52,59,68,70	5
3	SO4	c	207	5/5	0.93	0.40	27,27,32,36	5
2	2AN	b	201	21/21	0.93	0.19	44,52,58,60	0
3	SO4	c	209	5/5	0.93	0.20	47,52,58,61	5
2	2AN	j	204	21/21	0.93	0.15	44,54,66,71	0
2	2AN	F	205	21/21	0.93	0.15	67,91,99,104	0
2	2AN	J	201	21/21	0.93	0.17	53,69,97,103	0
2	2AN	E	201	21/21	0.93	0.20	40,49,68,76	0
2	2AN	B	202	21/21	0.93	0.18	45,59,67,68	0
2	2AN	T	202	21/21	0.93	0.28	31,39,49,52	21
2	2AN	h	203	21/21	0.93	0.17	36,44,58,66	0
2	2AN	B	205	21/21	0.93	0.17	48,62,80,82	0
2	2AN	A	202	21/21	0.93	0.16	54,71,83,94	0
2	2AN	M	203	21/21	0.93	0.16	57,73,80,81	0
2	2AN	Z	201	21/21	0.93	0.16	54,62,71,78	0
2	2AN	S	202	21/21	0.93	0.26	46,56,69,70	21
2	2AN	X	204	21/21	0.94	0.13	63,74,85,91	0
2	2AN	H	202	21/21	0.94	0.21	48,67,79,83	0
2	2AN	C	201	21/21	0.94	0.15	46,57,67,84	0
2	2AN	Y	203	21/21	0.94	0.14	52,68,87,92	0
2	2AN	V	201	21/21	0.94	0.13	46,58,79,93	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	2AN	V	203	21/21	0.94	0.18	44,52,61,62	0
2	2AN	I	202	21/21	0.94	0.20	37,47,59,69	0
2	2AN	Z	204	21/21	0.94	0.10	69,80,92,97	0
2	2AN	O	201	21/21	0.94	0.20	42,62,79,92	0
2	2AN	N	201	21/21	0.94	0.20	36,44,54,58	0
2	2AN	e	201	21/21	0.95	0.17	39,50,52,57	0
2	2AN	J	203	21/21	0.95	0.19	43,69,75,80	0
2	2AN	M	201	21/21	0.95	0.21	40,49,59,60	0
2	2AN	g	202	21/21	0.95	0.17	37,51,60,64	0
2	2AN	E	202	21/21	0.95	0.17	34,41,50,65	0
2	2AN	T	201	21/21	0.95	0.20	38,49,58,65	0
2	2AN	G	202	21/21	0.95	0.17	56,64,68,75	0
2	2AN	G	203	21/21	0.95	0.21	42,52,92,100	0
2	2AN	B	203	21/21	0.95	0.15	38,49,74,80	0
2	2AN	c	204	21/21	0.95	0.17	39,46,53,55	21
2	2AN	Q	202	21/21	0.95	0.20	46,64,70,74	0
2	2AN	K	201	21/21	0.95	0.17	38,44,66,82	0
2	2AN	N	204	21/21	0.95	0.16	53,64,92,95	0
2	2AN	C	202	21/21	0.95	0.19	66,99,110,116	0
2	2AN	P	204	21/21	0.95	0.19	36,52,60,62	0
2	2AN	f	202	21/21	0.95	0.22	33,49,57,62	0
2	2AN	H	201	21/21	0.95	0.18	44,58,62,65	0
2	2AN	a	202	21/21	0.95	0.17	46,52,60,66	0
2	2AN	f	204	21/21	0.95	0.12	38,50,60,72	0
2	2AN	f	205	21/21	0.95	0.12	41,54,66,68	0
2	2AN	V	204	21/21	0.95	0.14	50,63,75,86	0
2	2AN	V	205	21/21	0.95	0.11	42,59,68,72	0
2	2AN	J	202	21/21	0.95	0.22	44,52,71,73	0
2	2AN	P	201	21/21	0.96	0.18	38,50,59,61	0
2	2AN	H	203	21/21	0.96	0.12	53,66,79,84	0
2	2AN	c	206	21/21	0.96	0.18	30,44,58,62	0
2	2AN	h	202	21/21	0.96	0.21	37,52,59,61	0
2	2AN	D	201	21/21	0.96	0.16	38,69,79,84	0
2	2AN	Q	201	21/21	0.96	0.18	40,50,60,67	0
2	2AN	b	203	21/21	0.96	0.09	47,55,66,72	0
2	2AN	F	203	21/21	0.96	0.16	51,61,81,84	0
2	2AN	K	202	21/21	0.96	0.24	45,54,83,89	0
2	2AN	B	201	21/21	0.96	0.19	35,51,62,63	0
2	2AN	R	201	21/21	0.96	0.18	29,52,60,61	0
2	2AN	L	202	21/21	0.96	0.11	46,54,67,71	0
2	2AN	f	201	21/21	0.96	0.20	34,40,48,49	0
3	SO4	I	208	5/5	0.96	0.14	35,36,41,46	5

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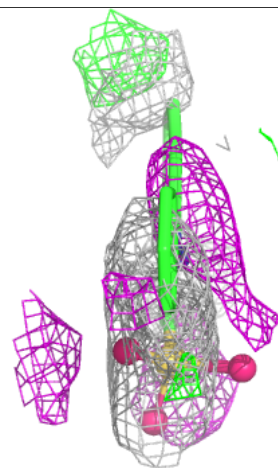
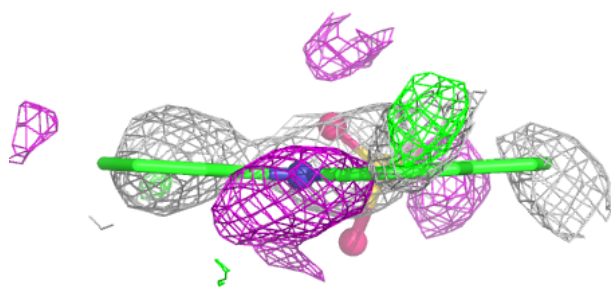
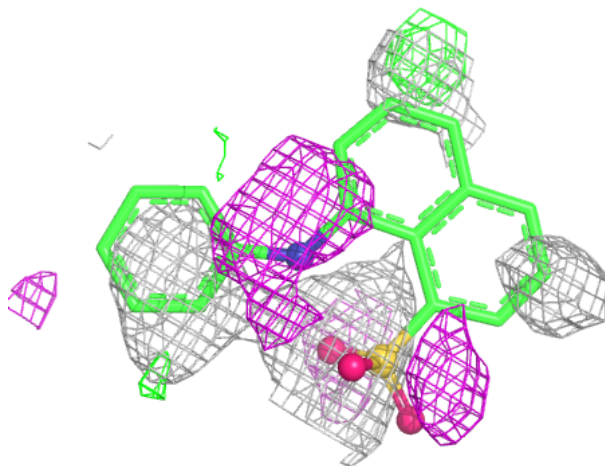
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	2AN	L	203	21/21	0.96	0.18	33,53,64,65	0
2	2AN	c	201	21/21	0.97	0.15	35,45,58,59	0
2	2AN	N	202	21/21	0.97	0.19	37,52,61,64	0
2	2AN	P	202	21/21	0.97	0.21	29,43,52,57	0
2	2AN	L	201	21/21	0.97	0.19	37,47,56,57	0
2	2AN	V	202	21/21	0.97	0.21	26,40,56,62	0
2	2AN	j	202	21/21	0.97	0.22	26,40,57,58	0
2	2AN	j	203	21/21	0.97	0.18	32,40,49,58	0
2	2AN	I	201	21/21	0.97	0.19	28,39,57,62	0
3	SO4	g	204	5/5	0.98	0.20	24,30,34,38	5
2	2AN	M	202	21/21	0.98	0.17	38,48,54,56	0
3	SO4	E	205	5/5	0.98	0.13	34,41,51,56	5

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



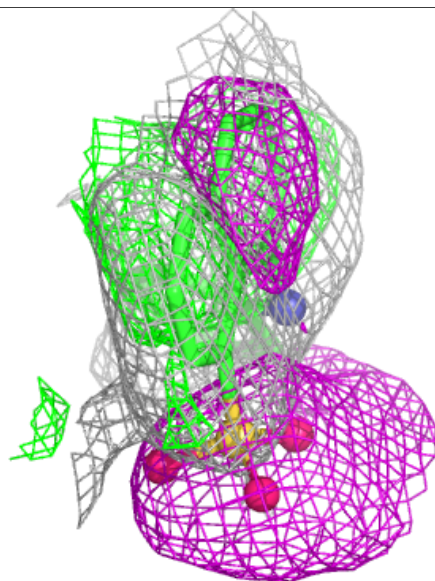
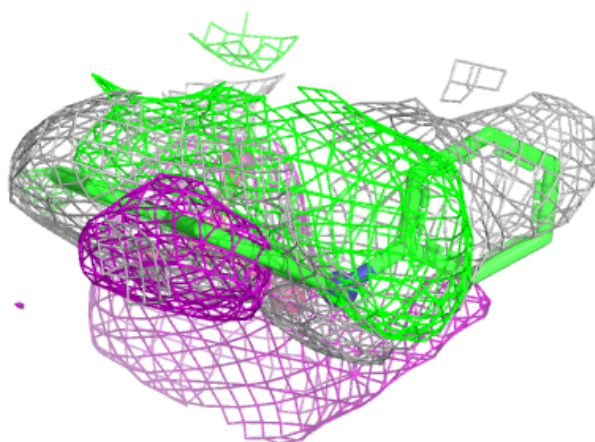
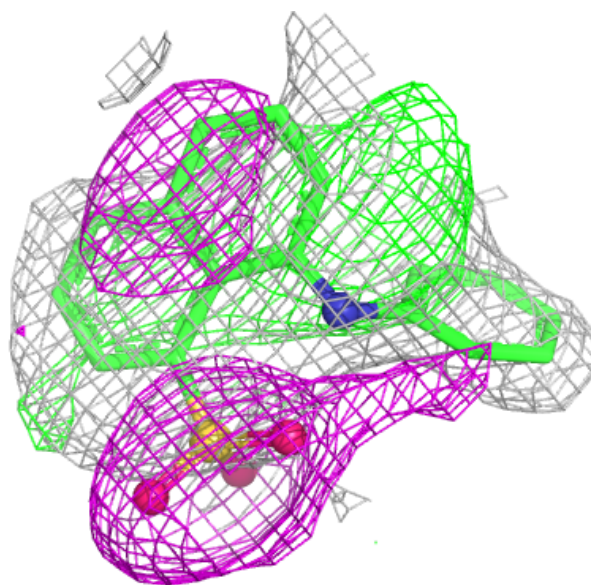
**Electron density around 2AN h 205:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



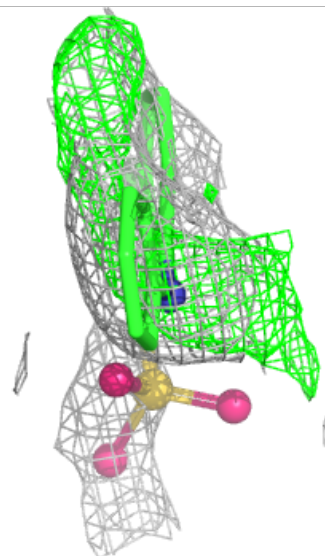
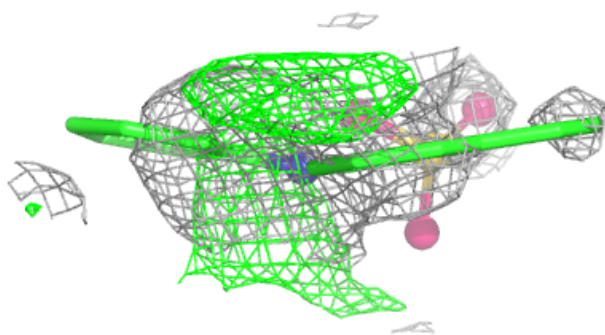
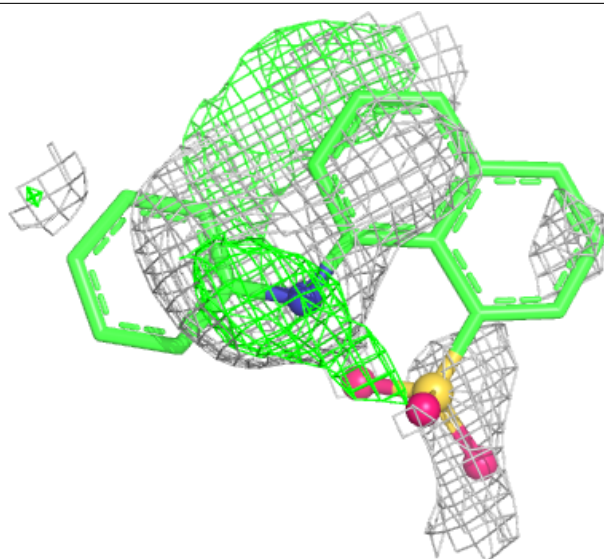
**Electron density around 2AN N 203:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



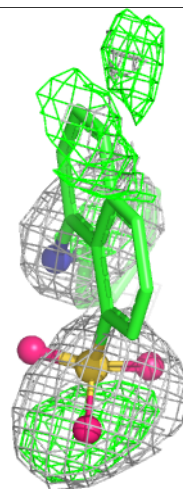
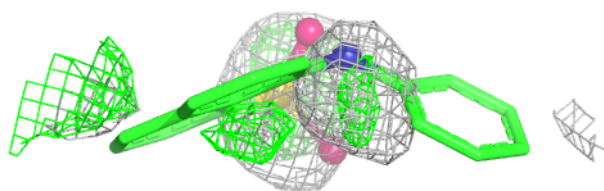
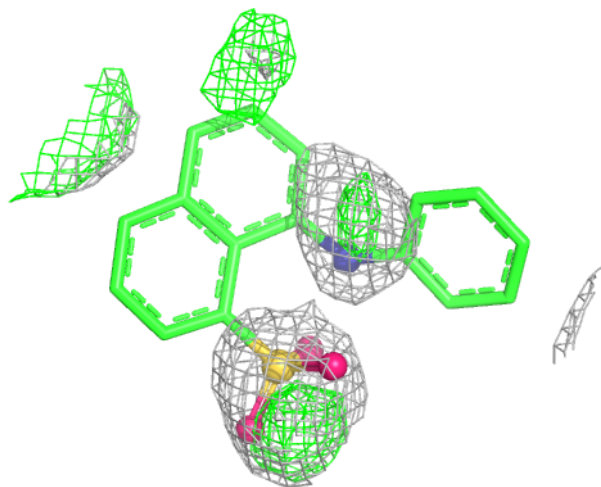
**Electron density around 2AN U 202:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



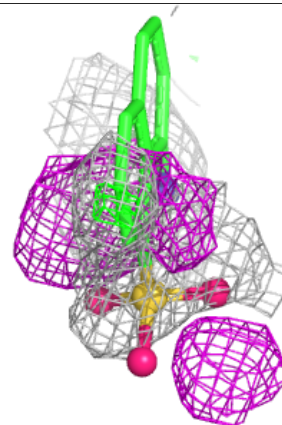
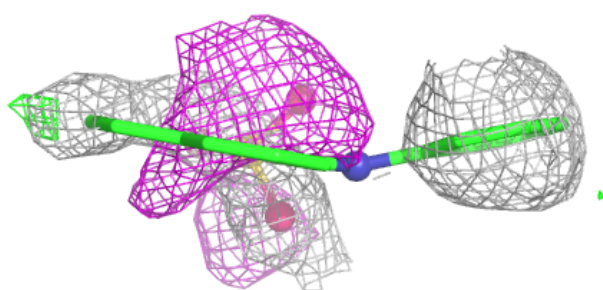
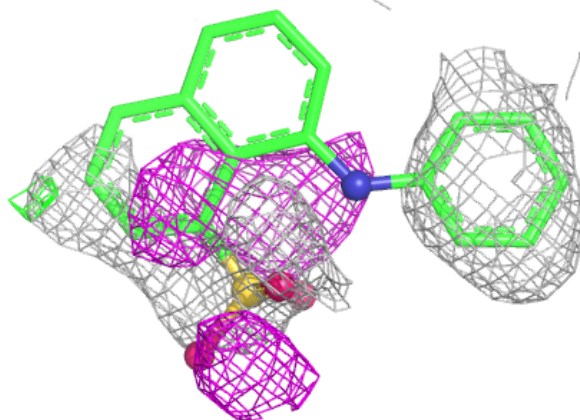
**Electron density around 2AN A 204:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around 2AN j 207:**

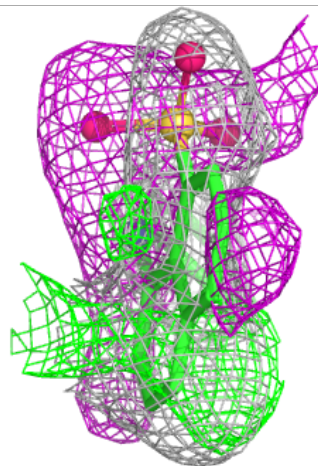
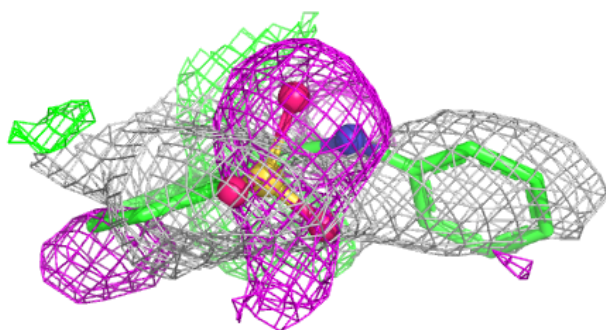
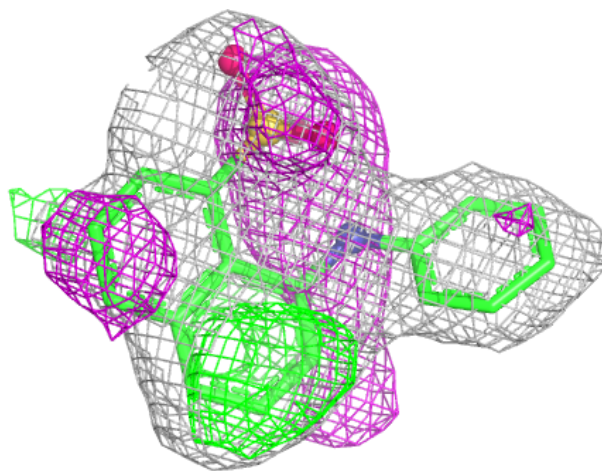
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





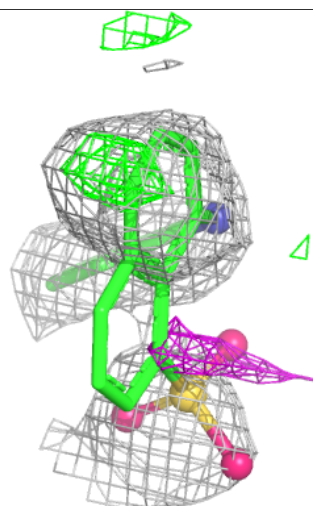
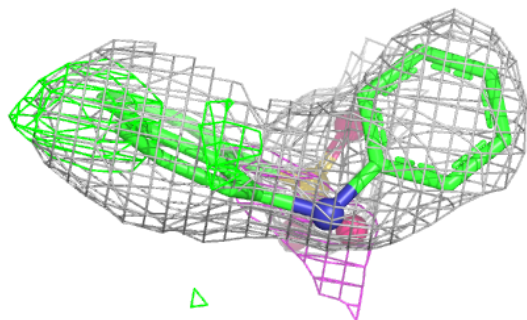
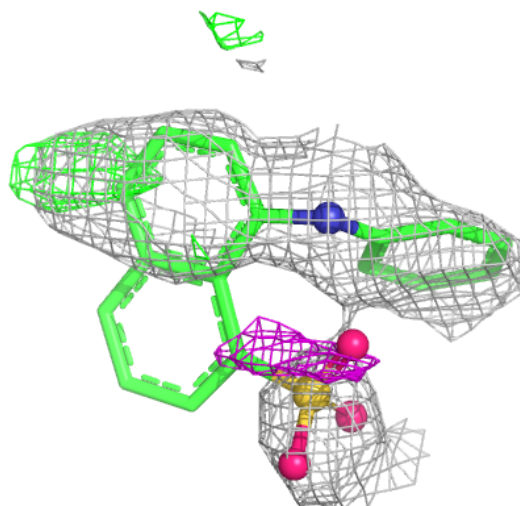
**Electron density around 2AN f 203:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



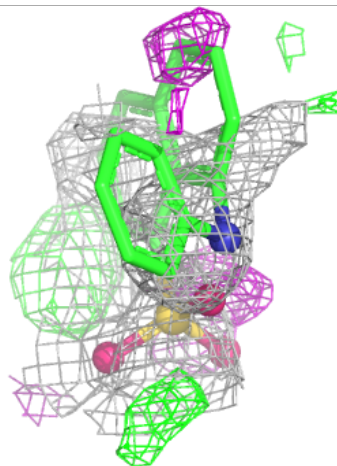
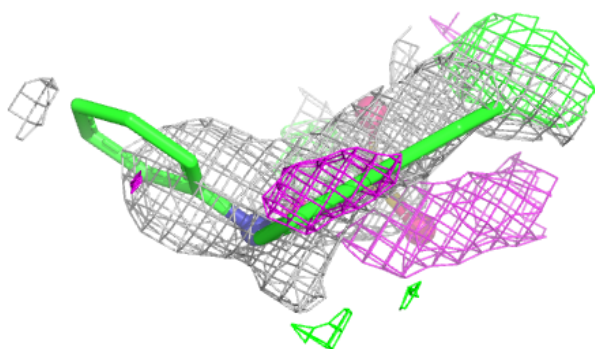
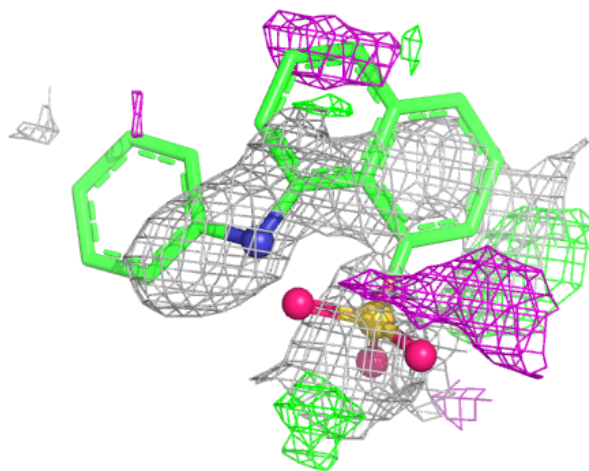
**Electron density around 2AN b 206:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around 2AN S 204:**

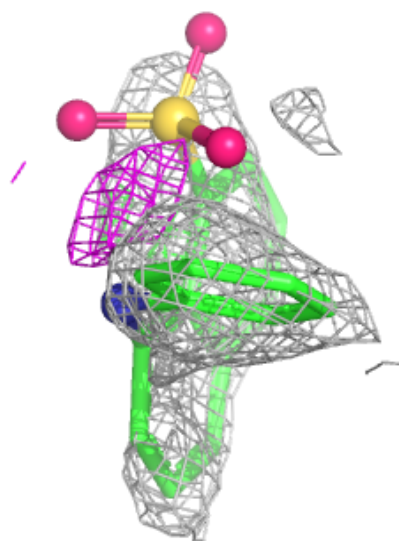
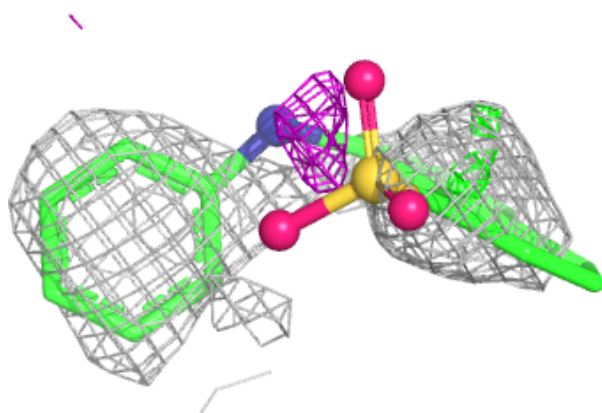
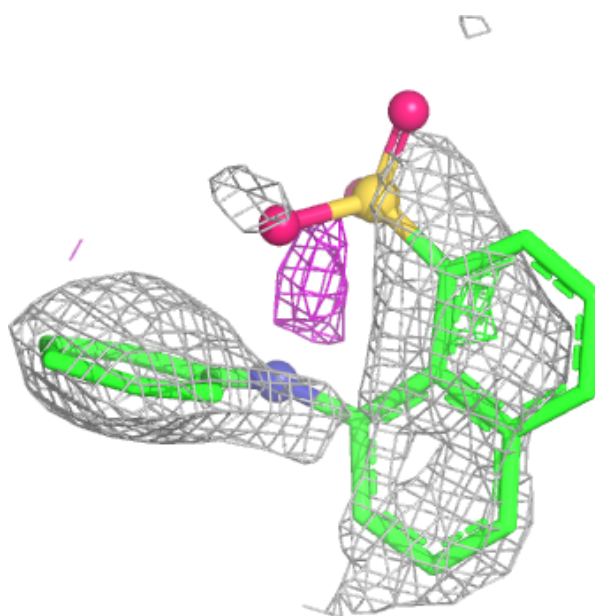
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





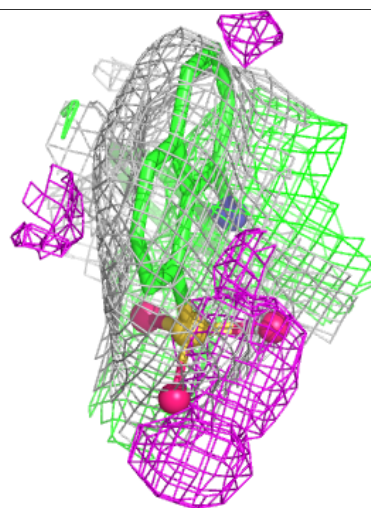
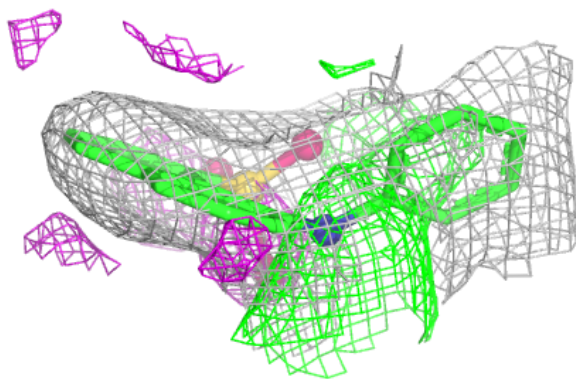
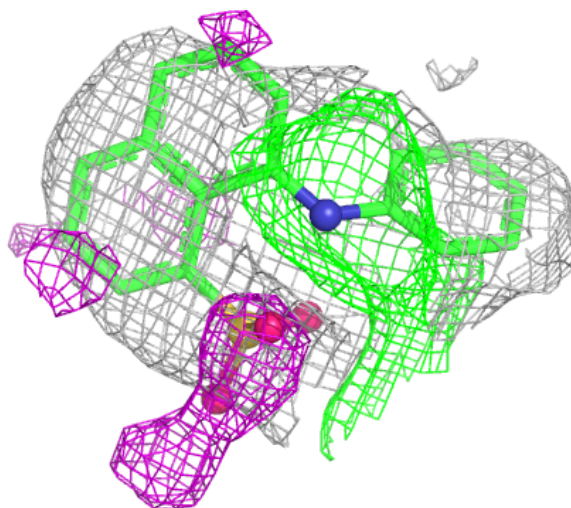
**Electron density around 2AN F 206:**

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 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



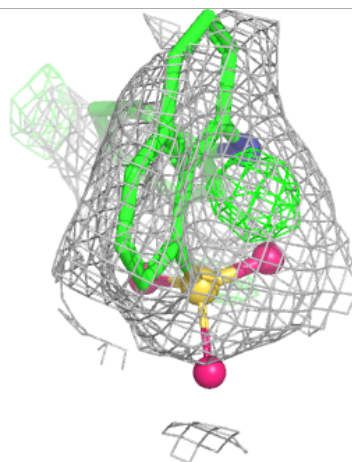
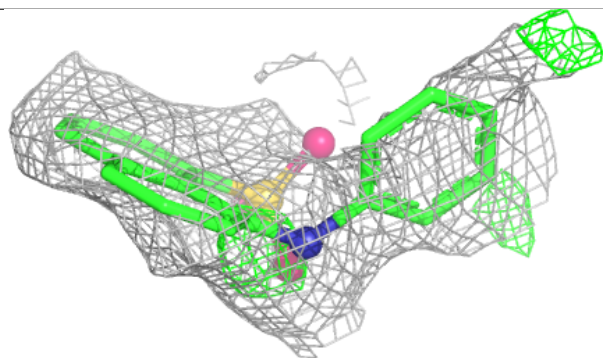
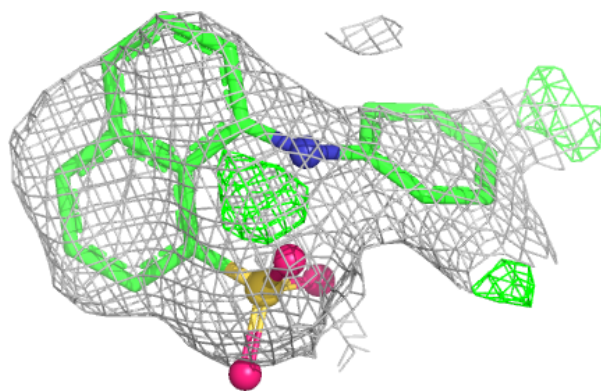
**Electron density around 2AN d 203:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



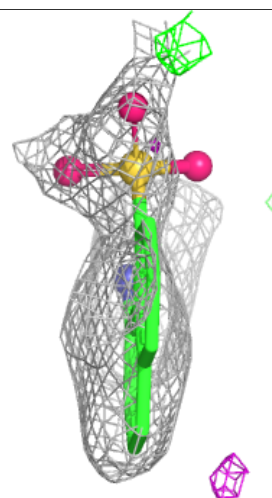
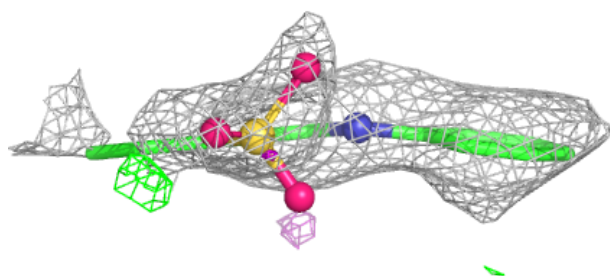
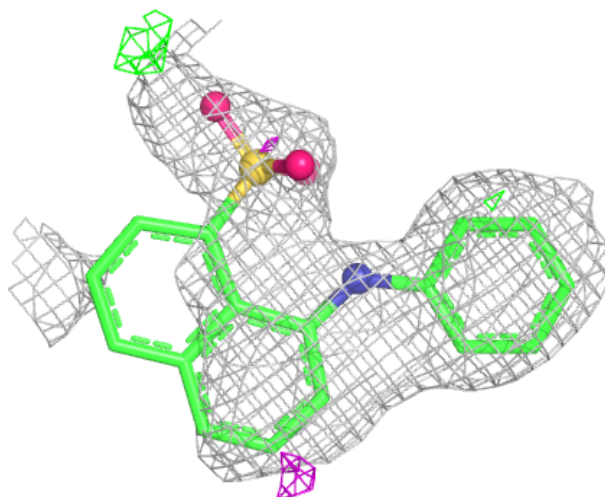
**Electron density around 2AN Y 204:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
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and green (positive)



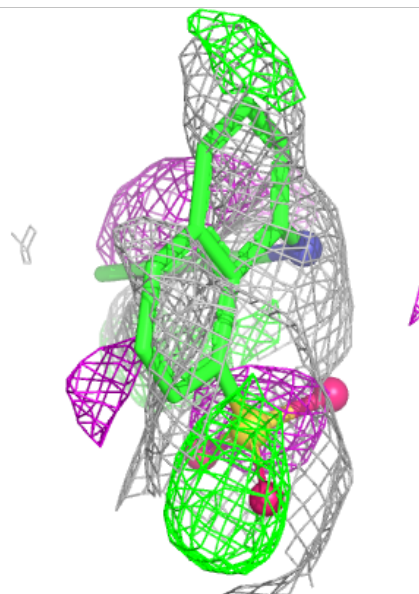
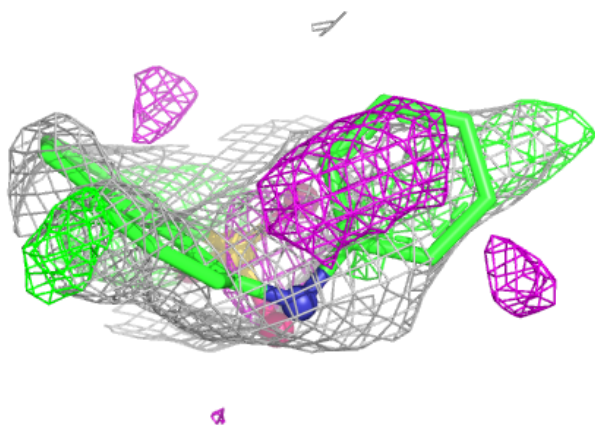
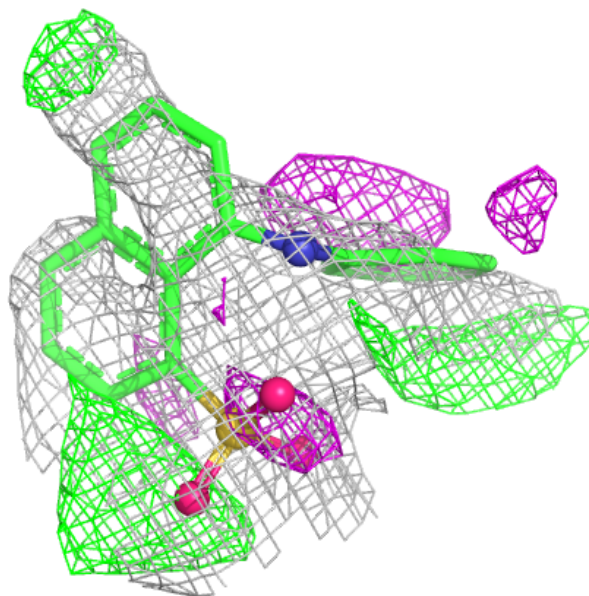
**Electron density around 2AN G 207:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around 2AN D 204:**

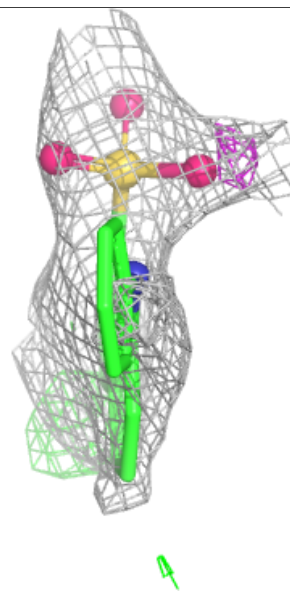
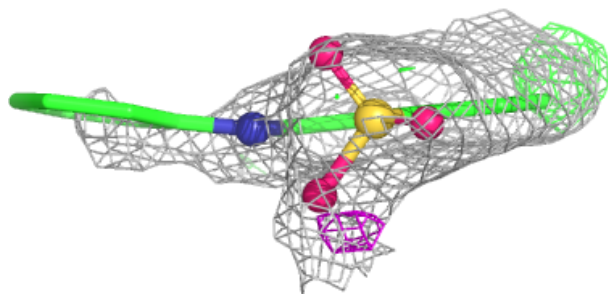
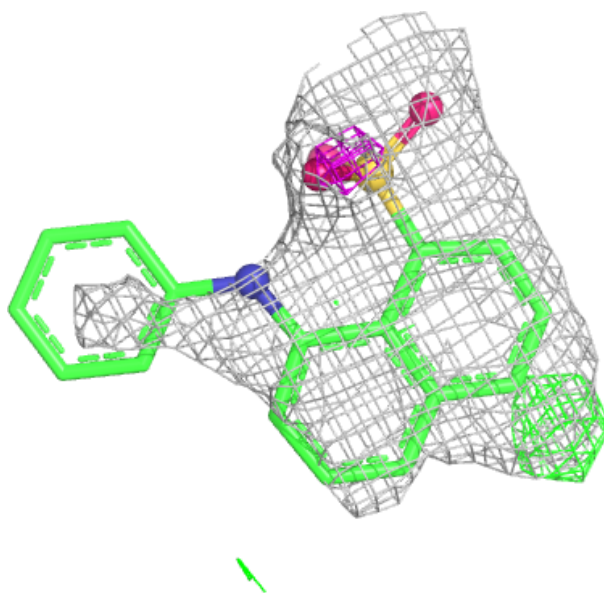
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





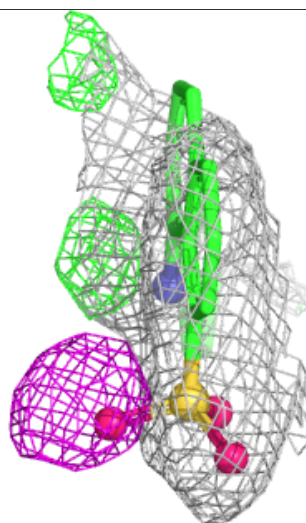
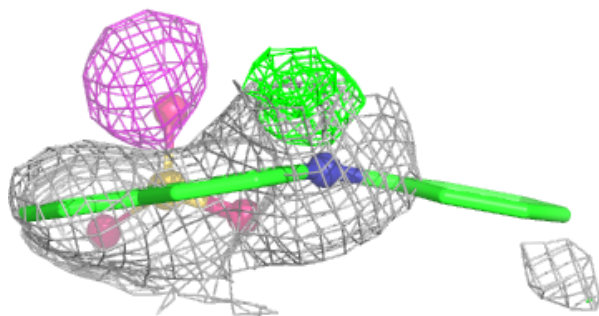
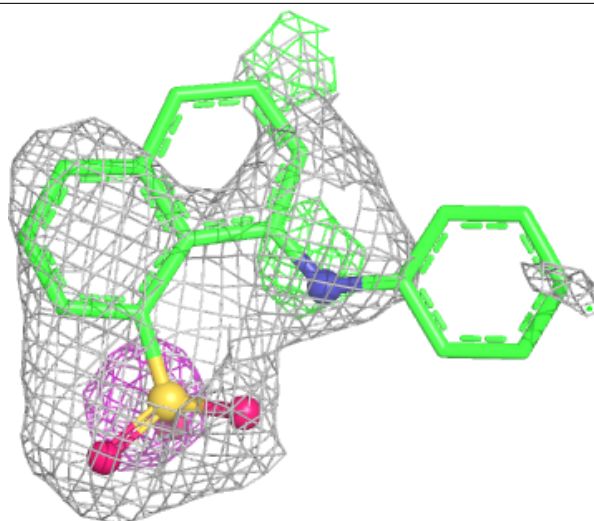
**Electron density around 2AN S 203:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



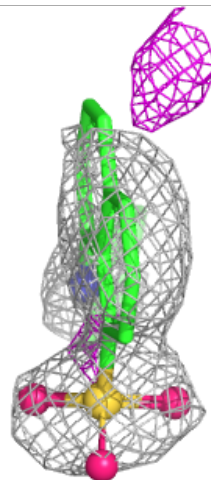
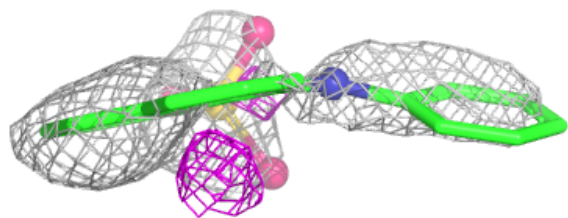
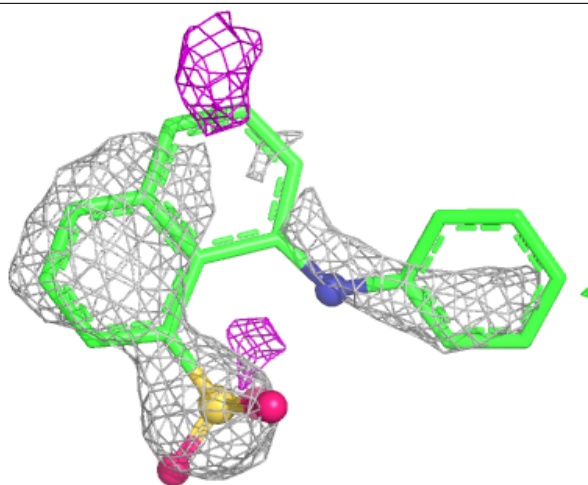
**Electron density around 2AN I 207:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around 2AN I 204:**

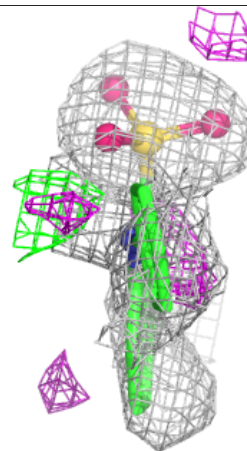
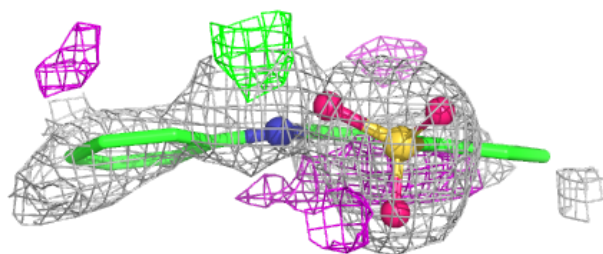
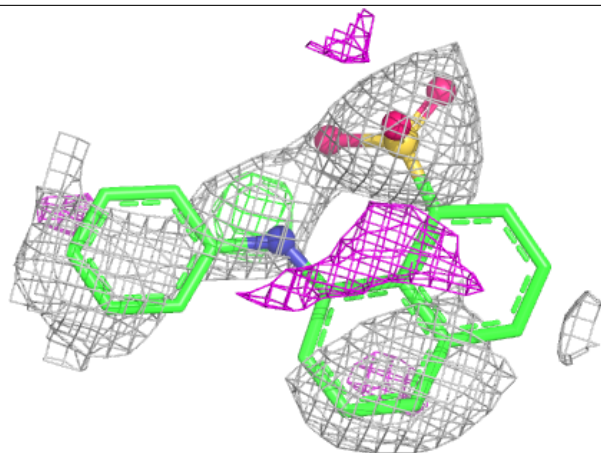
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
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and green (positive)





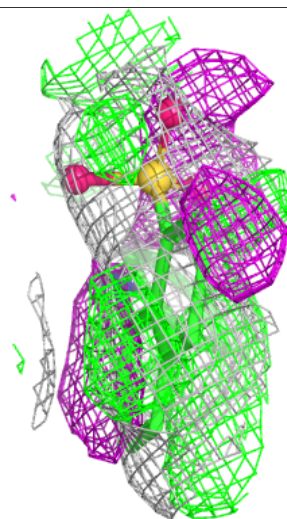
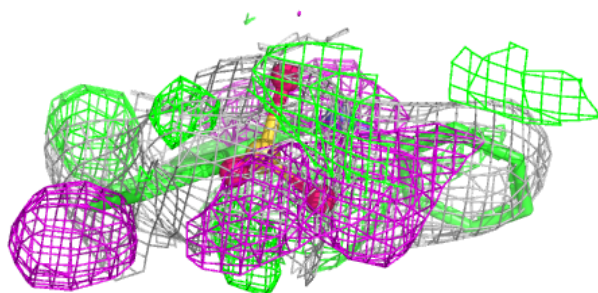
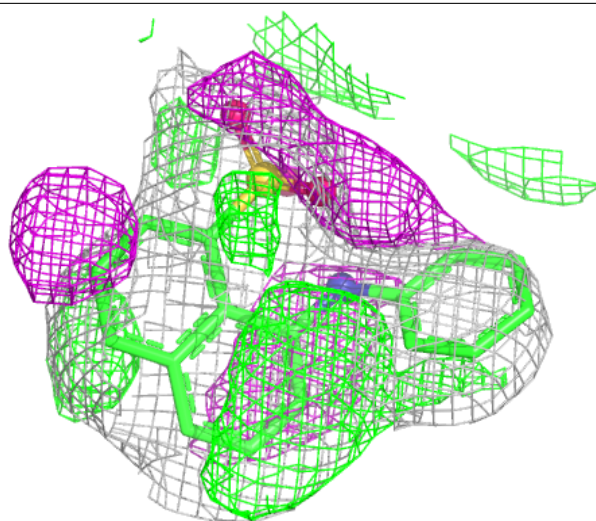
**Electron density around 2AN I 205:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



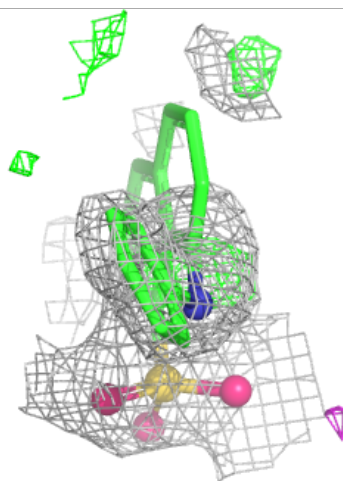
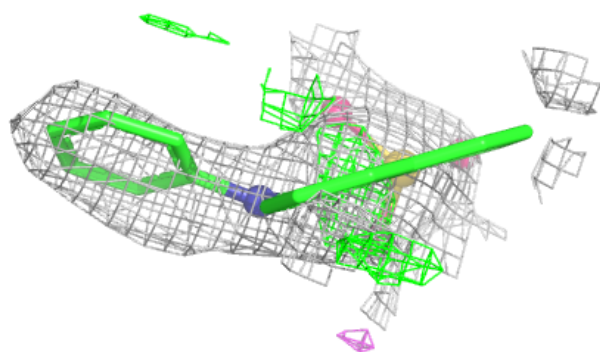
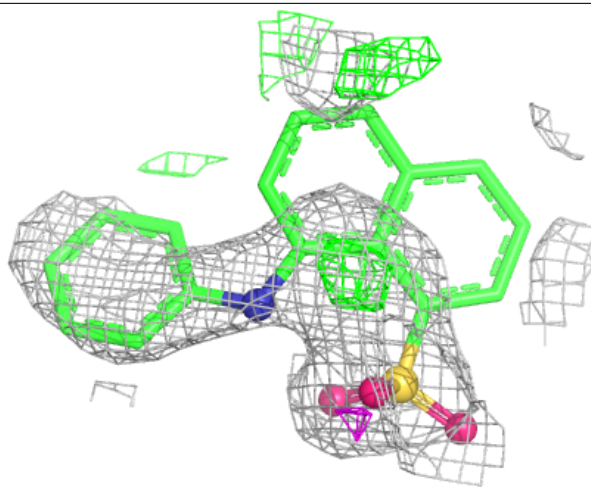
**Electron density around 2AN X 203:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



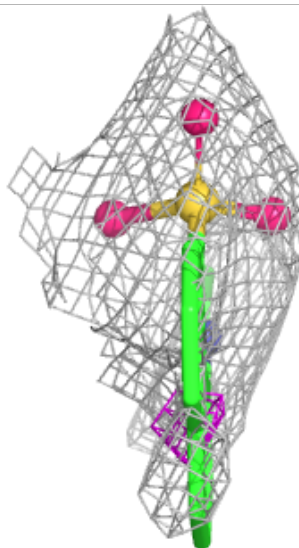
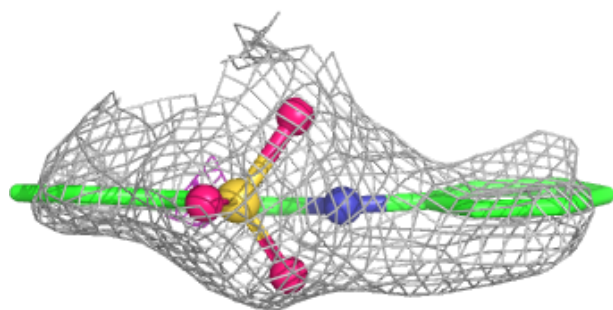
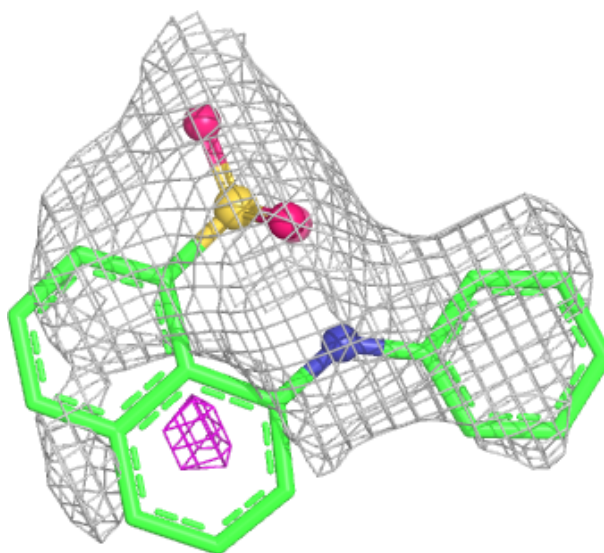
**Electron density around 2AN d 204:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



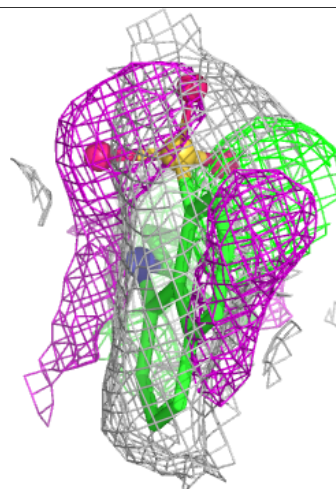
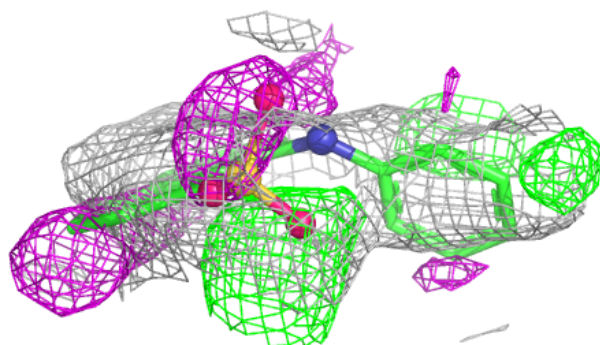
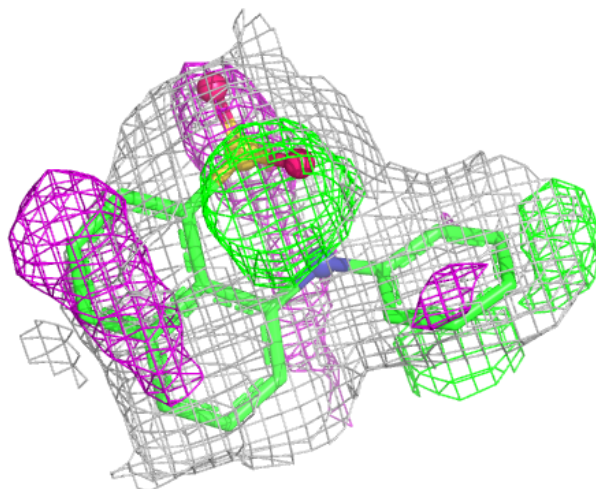
**Electron density around 2AN O 202:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around 2AN X 206:**

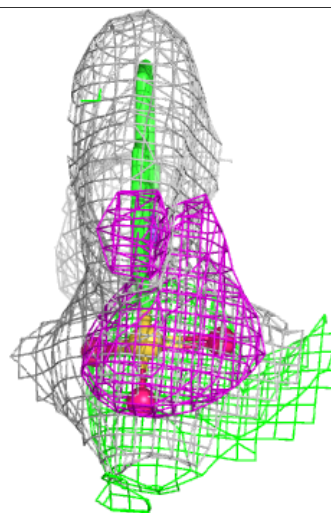
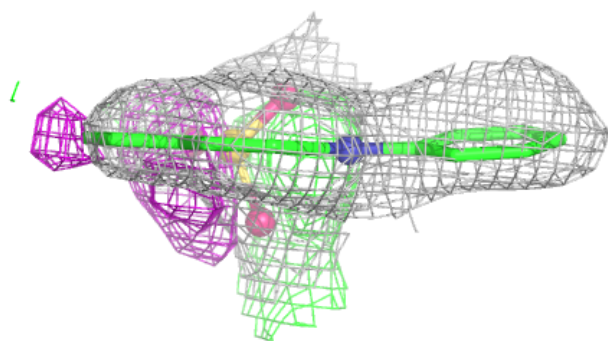
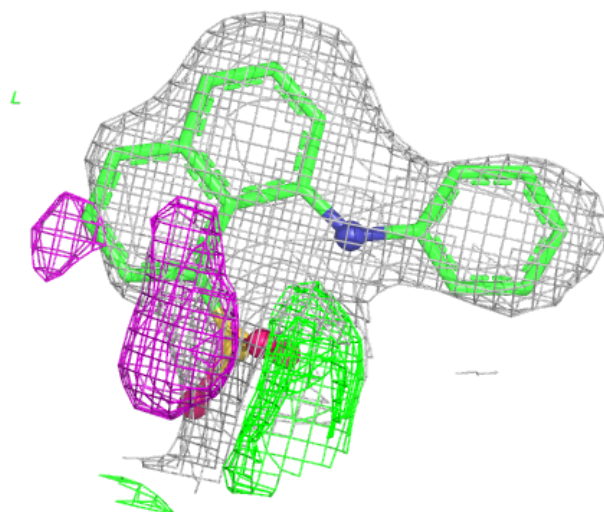
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





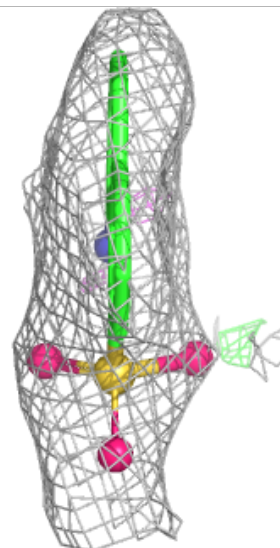
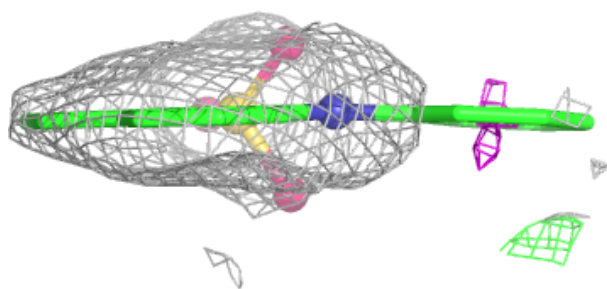
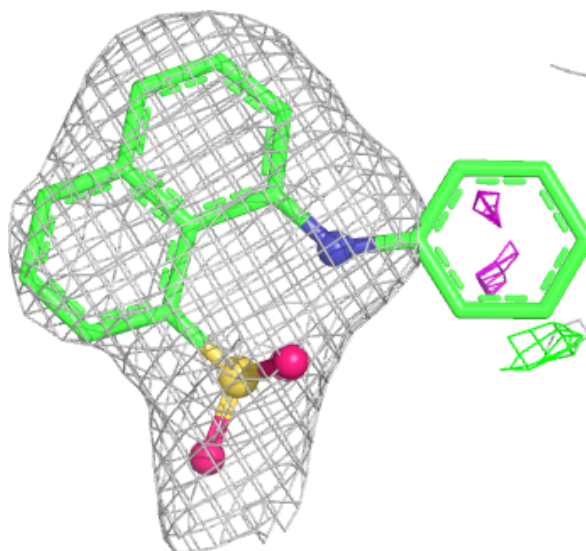
**Electron density around 2AN c 202:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



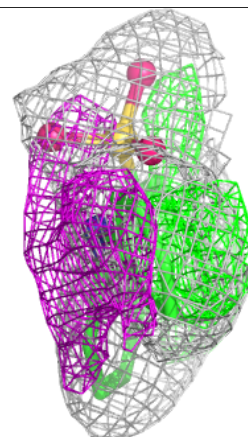
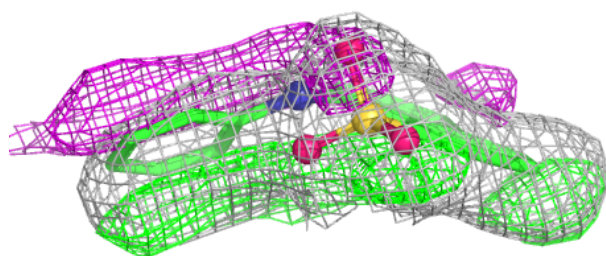
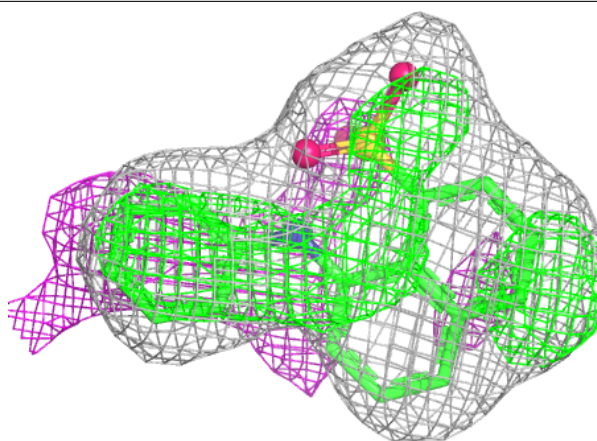
**Electron density around 2AN G 204:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

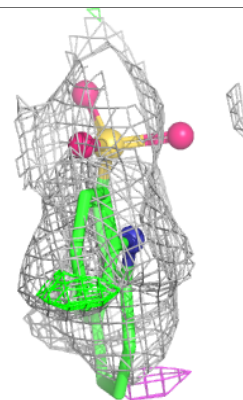
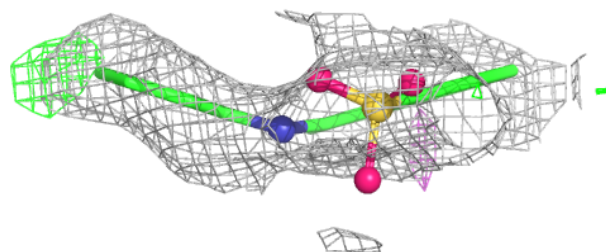
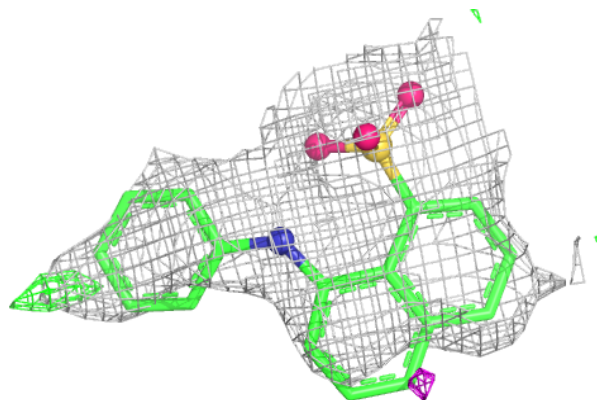


**Electron density around 2AN j 205:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around 2AN b 205:**

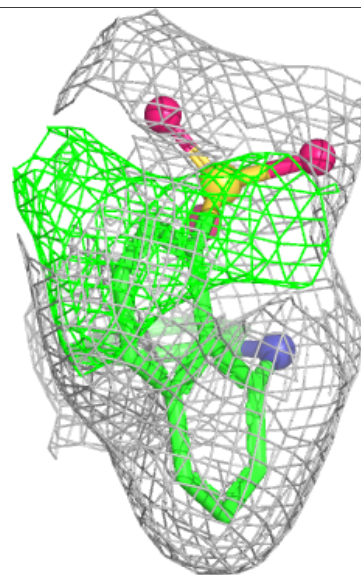
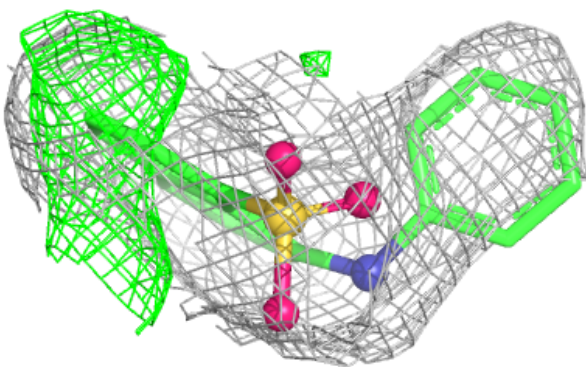
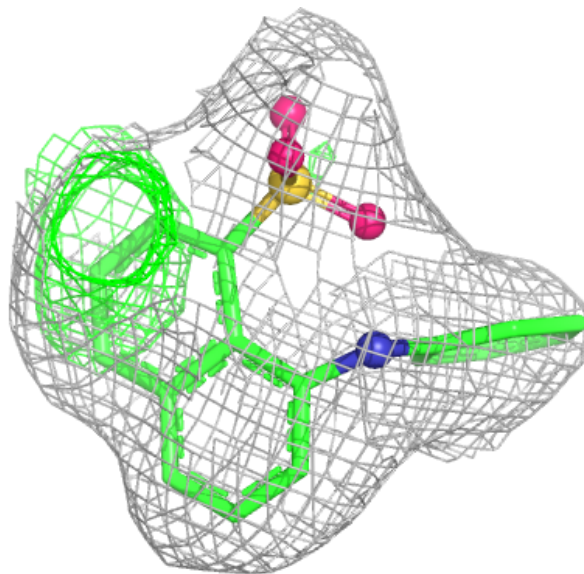
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





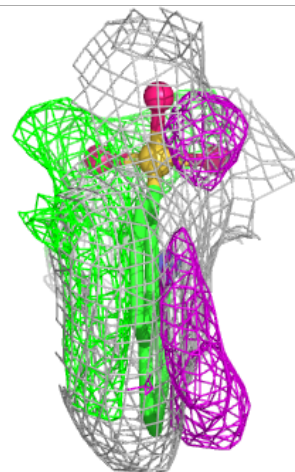
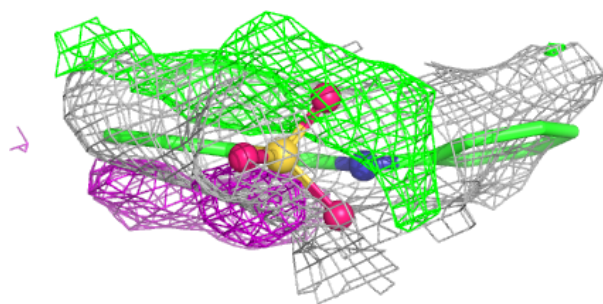
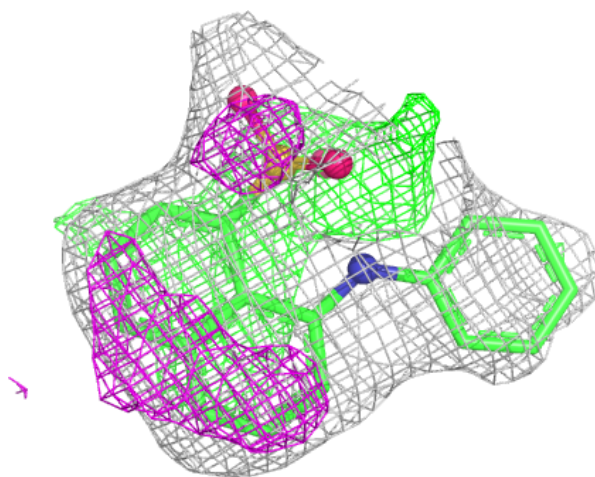
**Electron density around 2AN Z 206:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



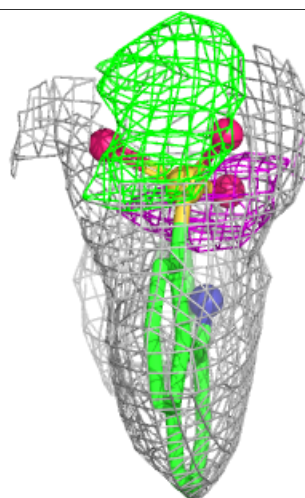
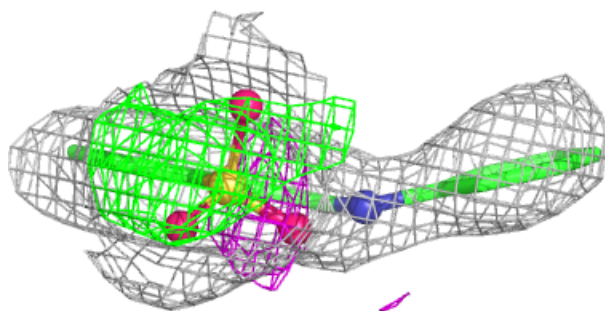
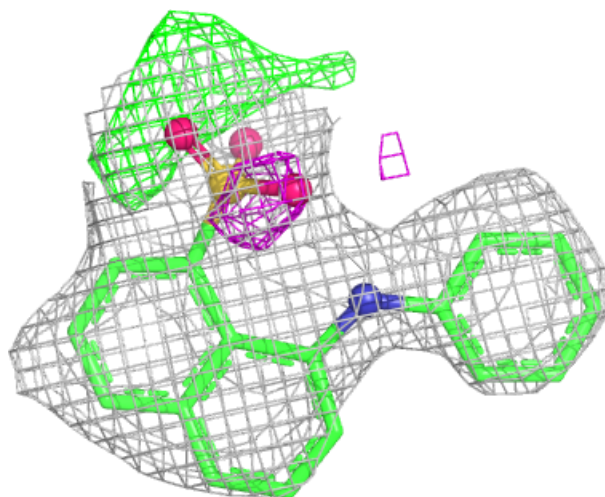
**Electron density around 2AN T 203:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



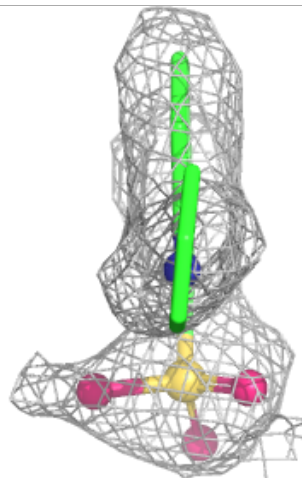
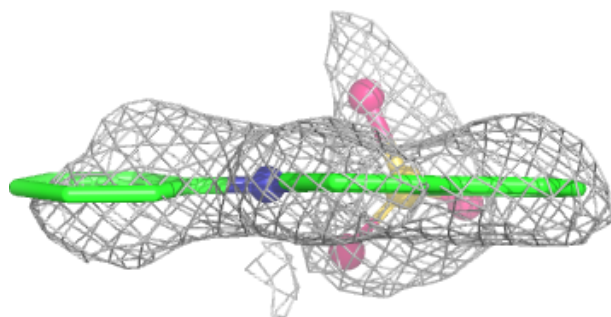
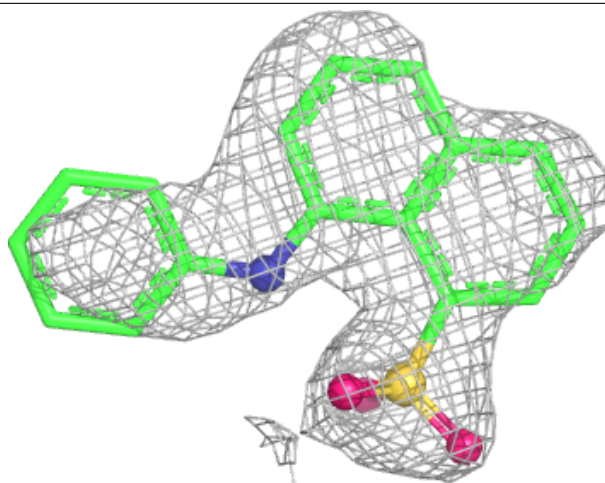
**Electron density around 2AN R 204:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



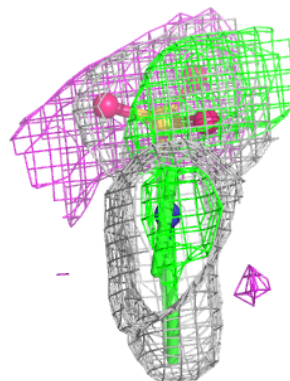
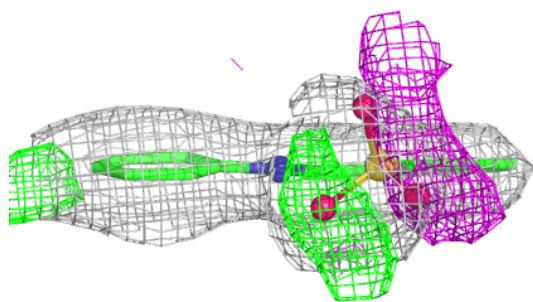
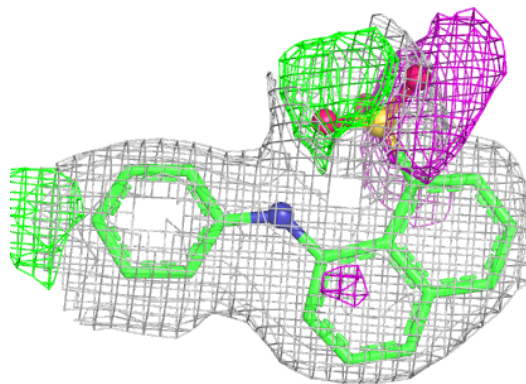
**Electron density around 2AN c 205:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around 2AN T 204:**

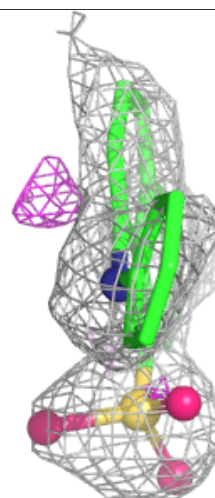
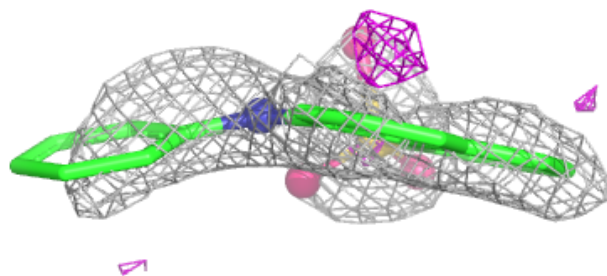
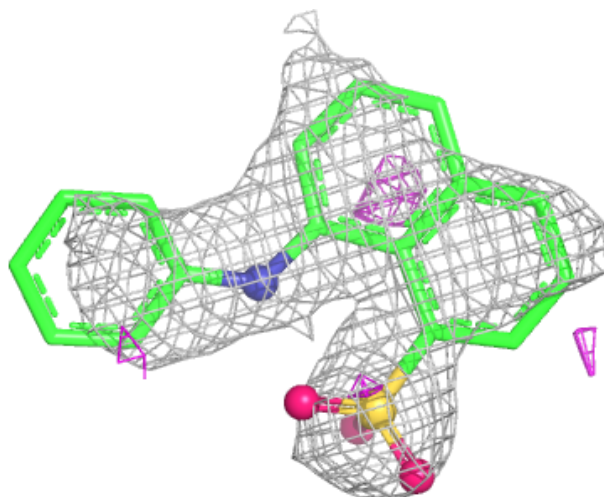
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

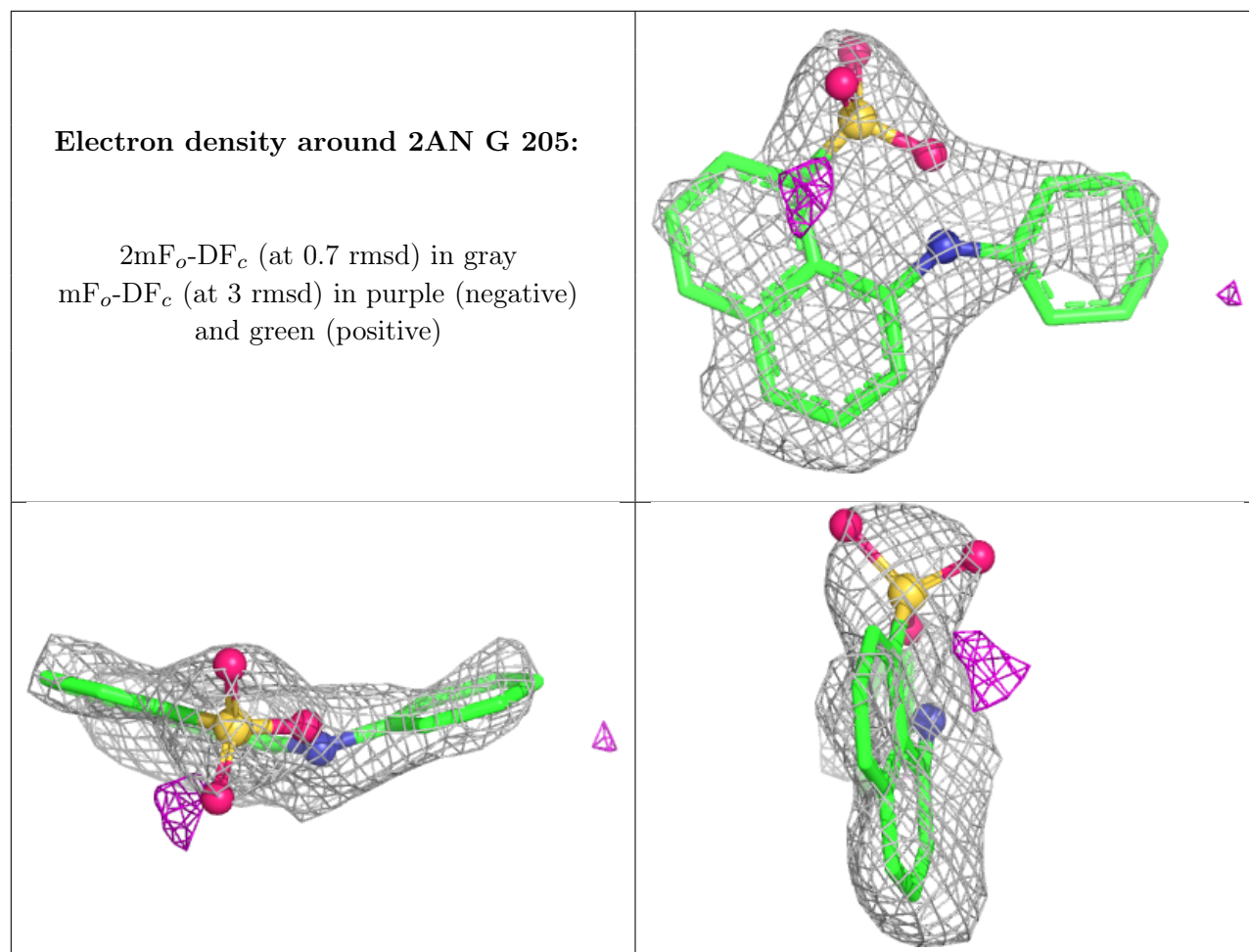




**Electron density around 2AN I 203:**

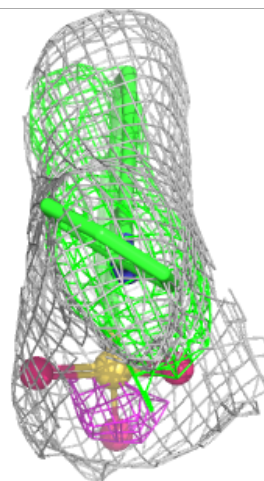
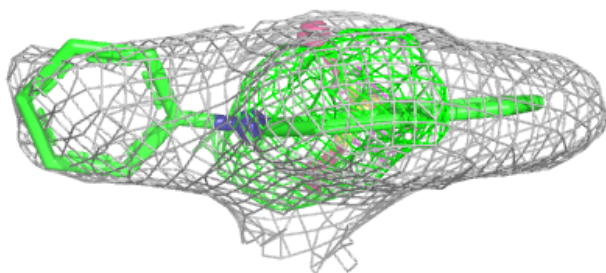
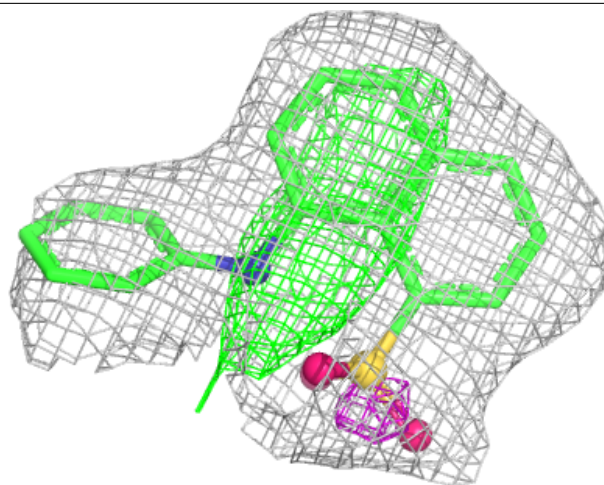
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around 2AN V 207:**

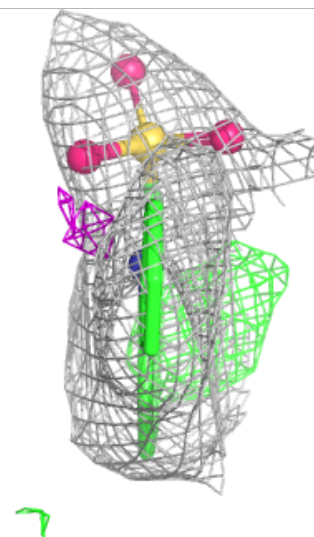
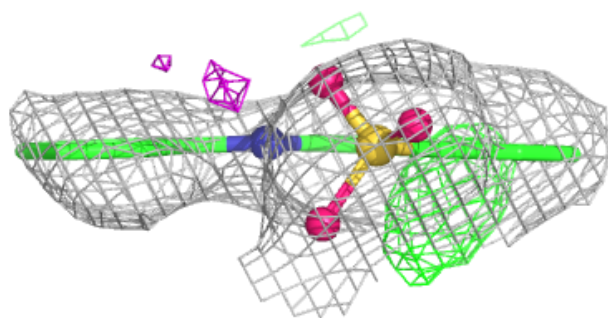
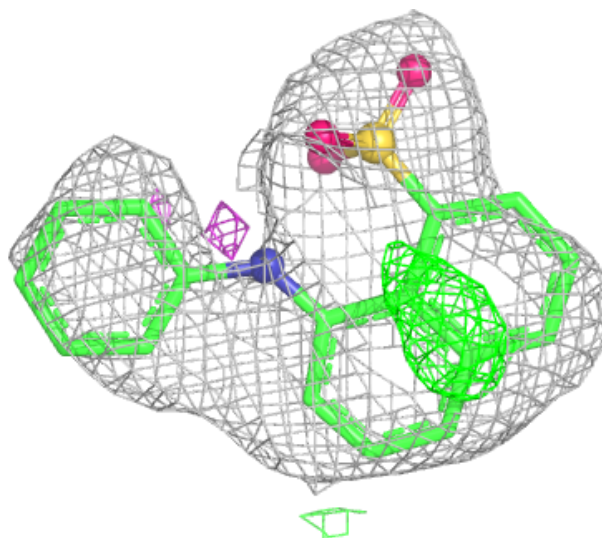
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





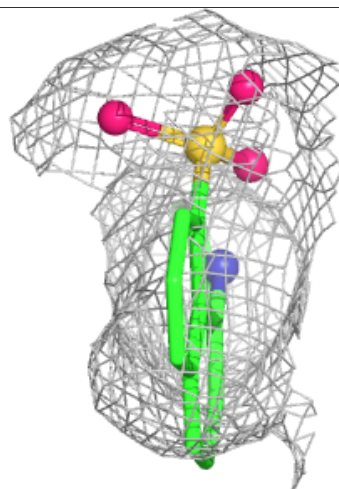
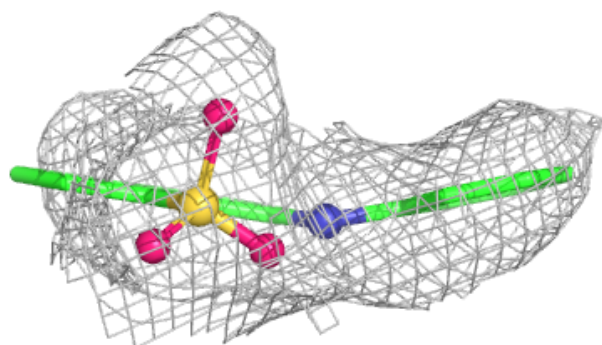
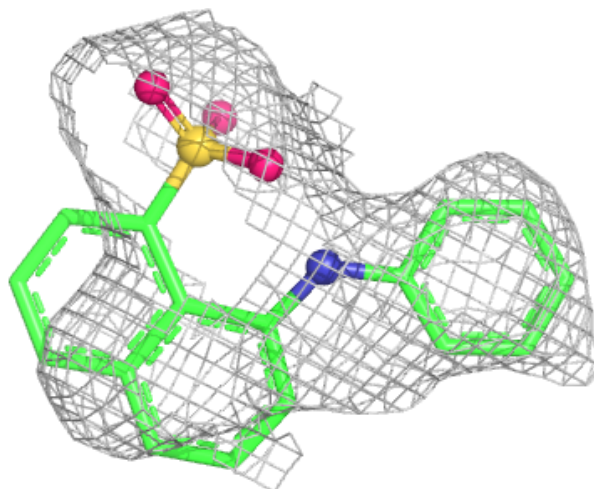
**Electron density around 2AN R 205:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



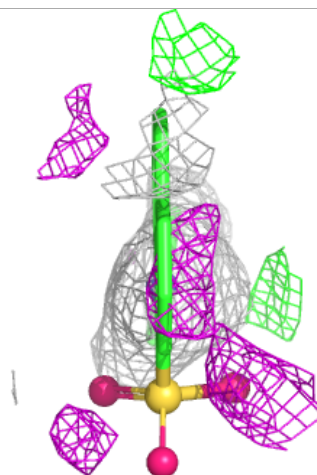
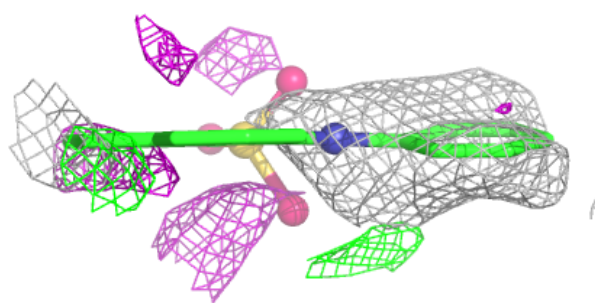
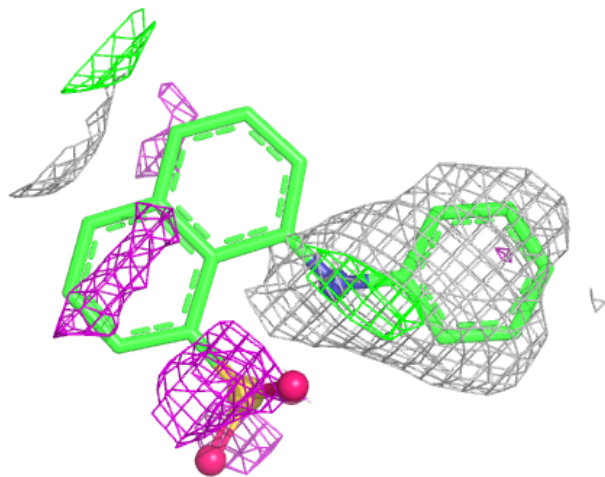
**Electron density around 2AN U 201:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



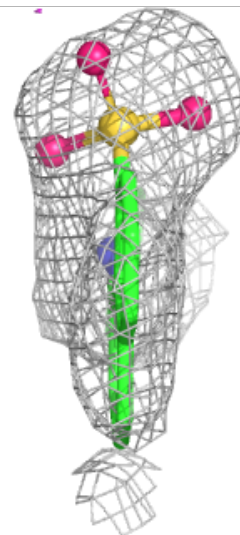
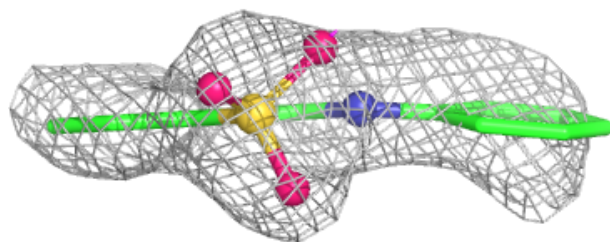
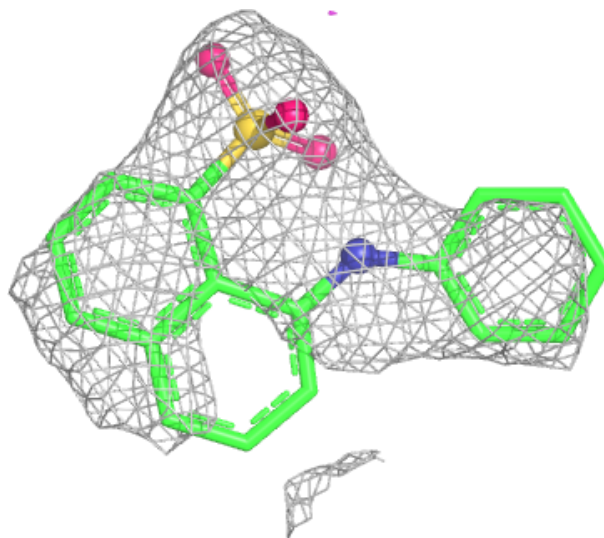
**Electron density around 2AN a 204:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



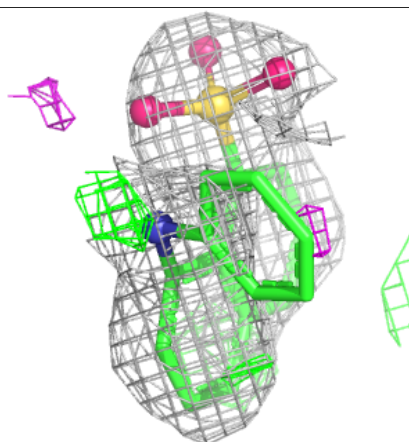
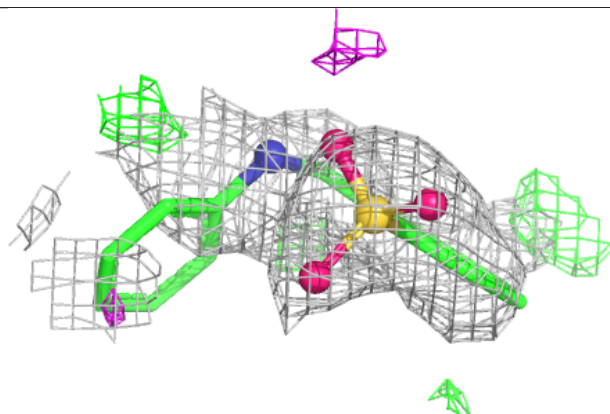
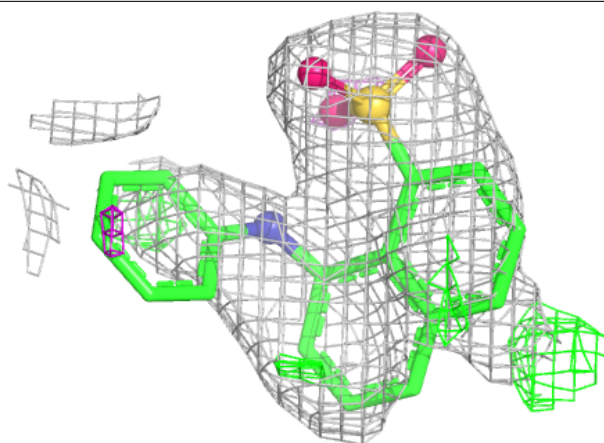
**Electron density around 2AN H 204:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



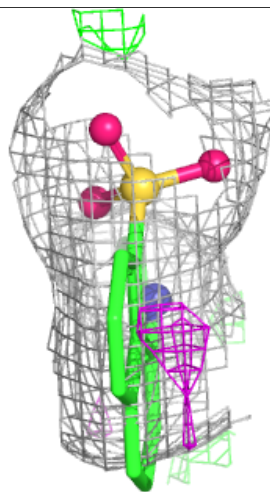
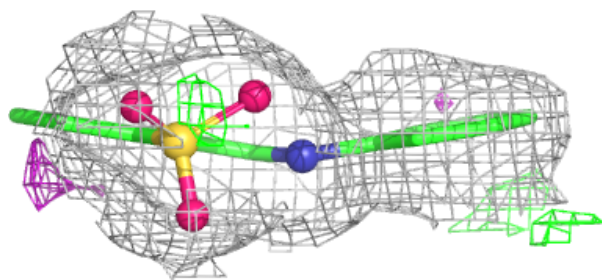
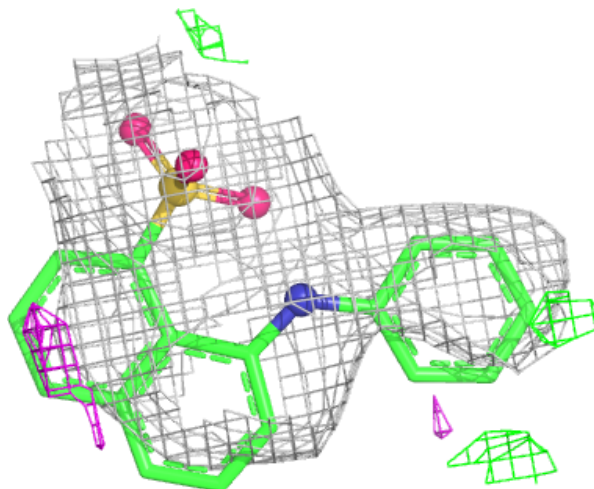
**Electron density around 2AN E 204:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around 2AN F 204:**

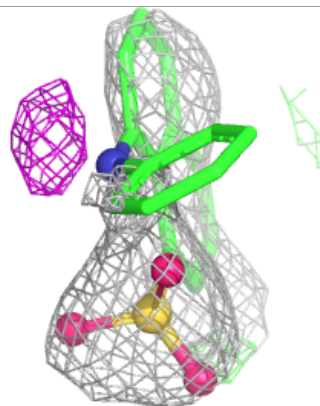
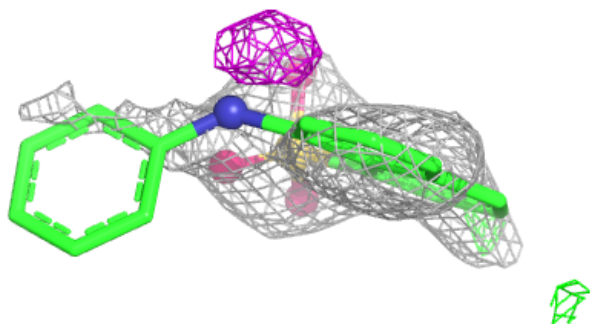
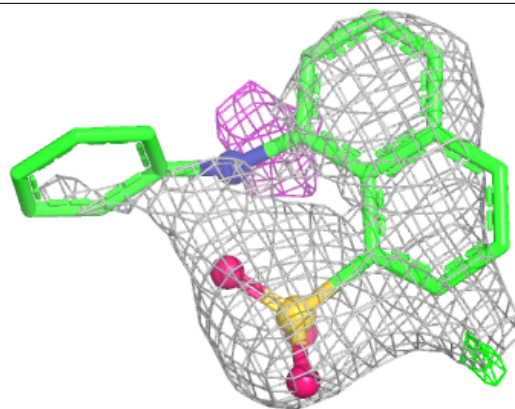
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





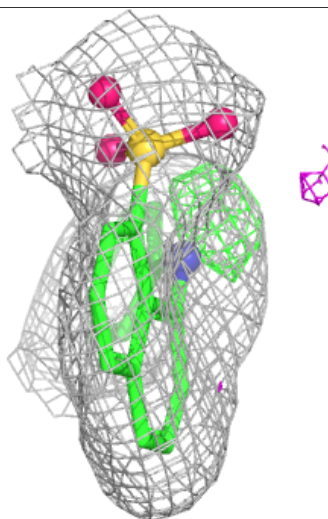
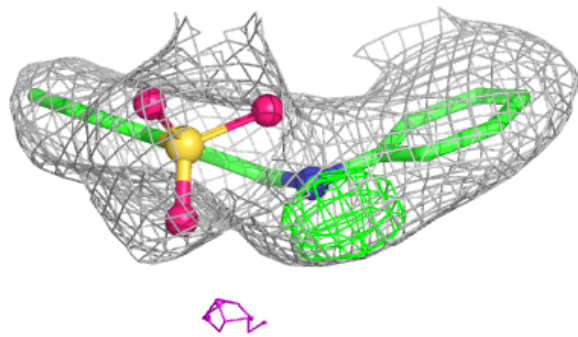
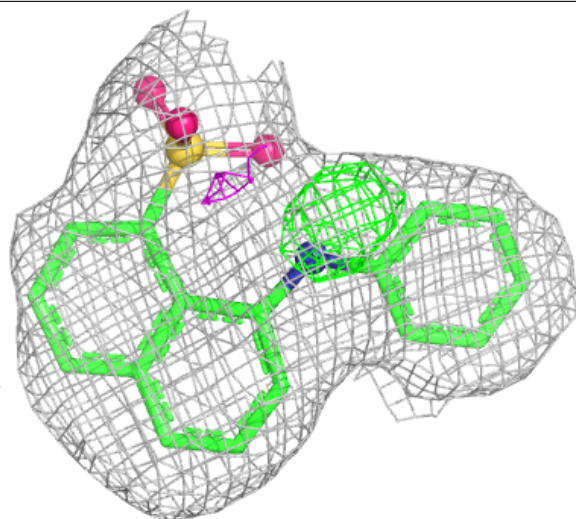
**Electron density around 2AN C 203 (A):**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around 2AN T 205:**

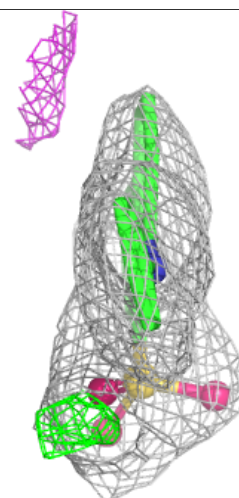
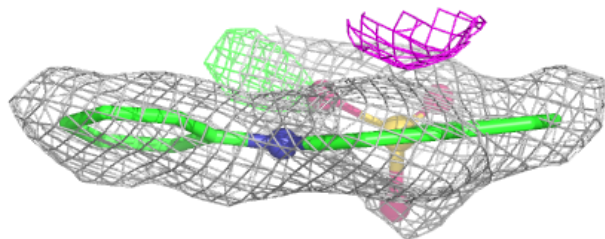
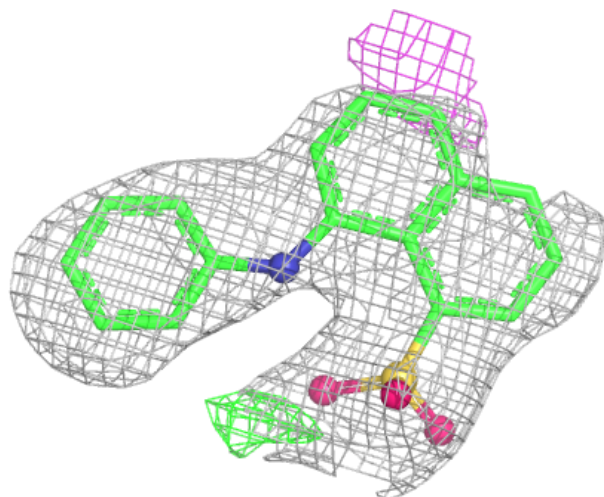
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





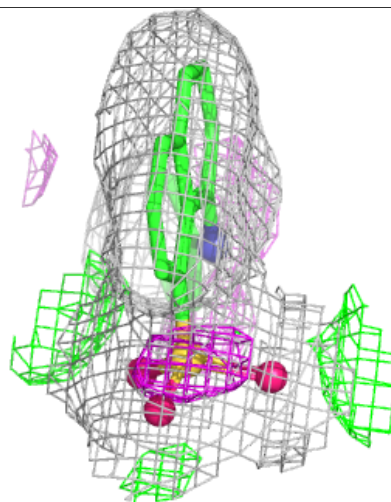
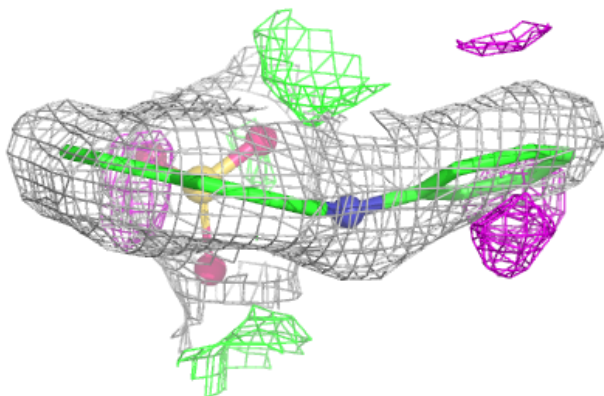
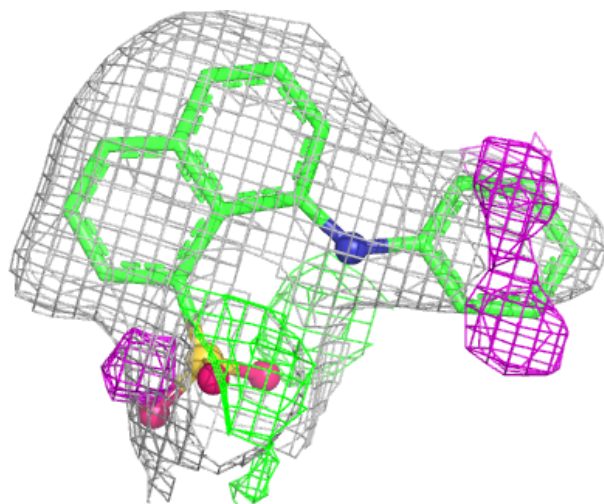
**Electron density around 2AN W 201:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



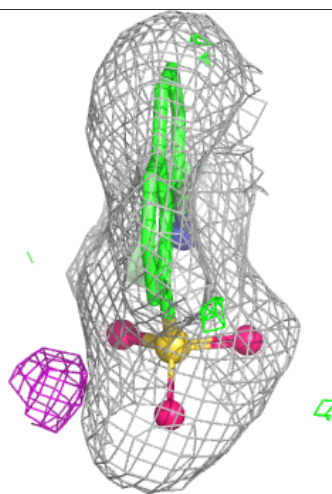
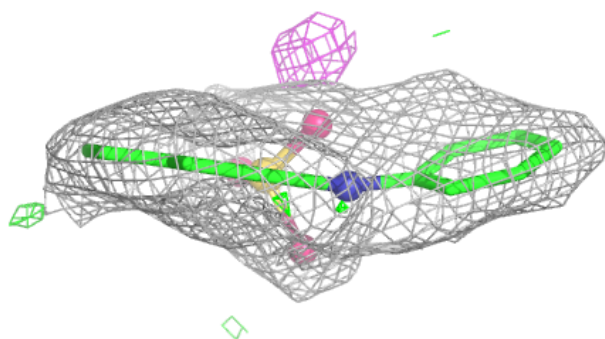
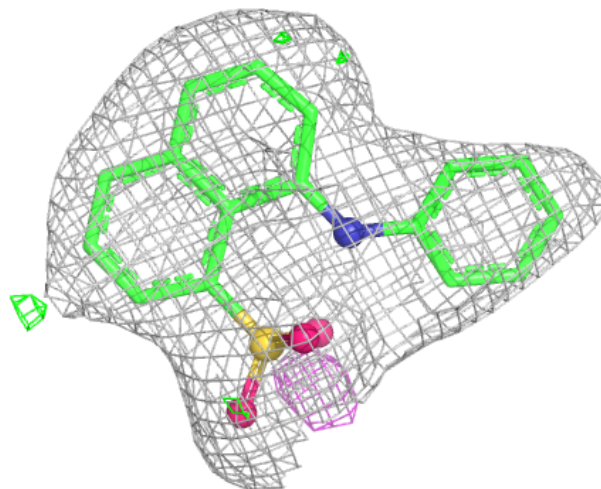
**Electron density around 2AN Y 201:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



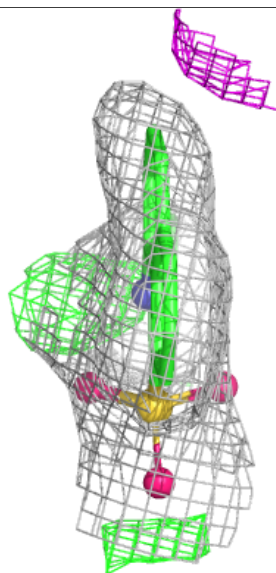
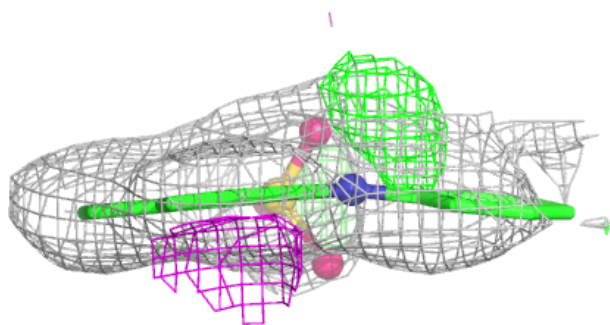
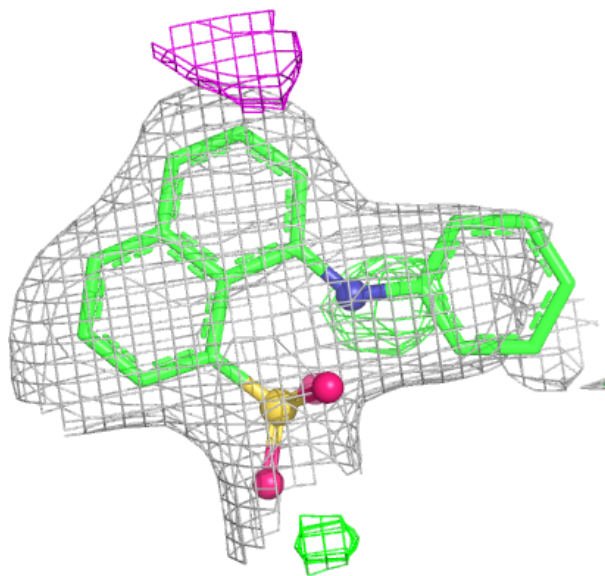
**Electron density around 2AN N 205:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



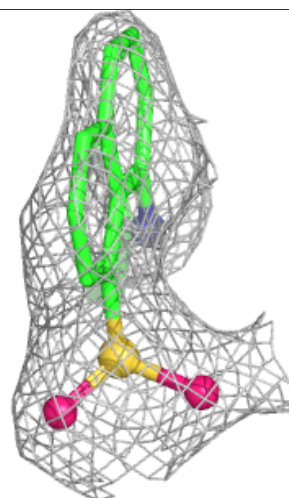
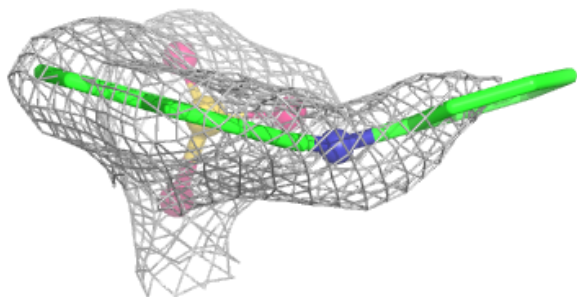
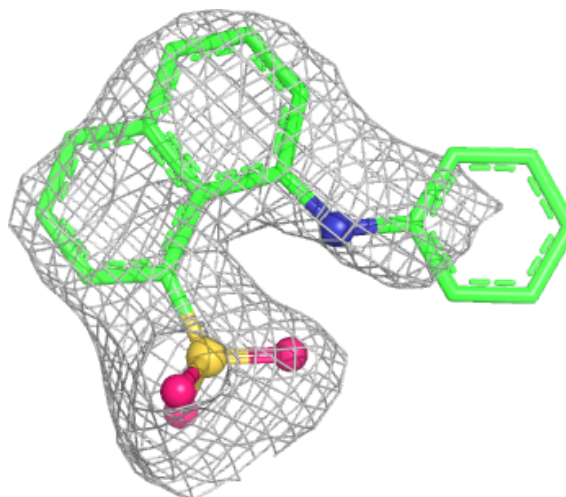
**Electron density around 2AN j 206:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



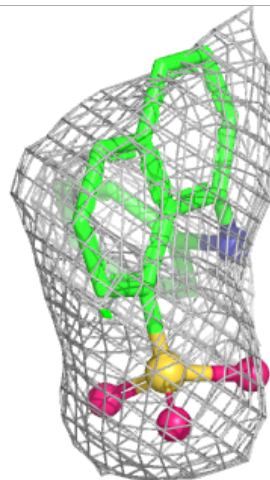
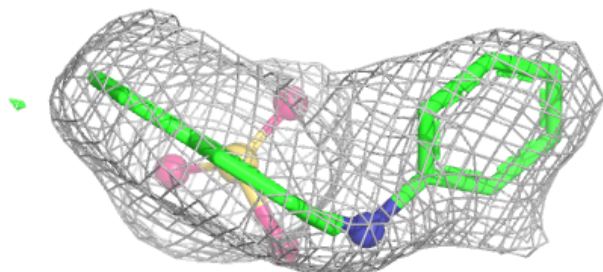
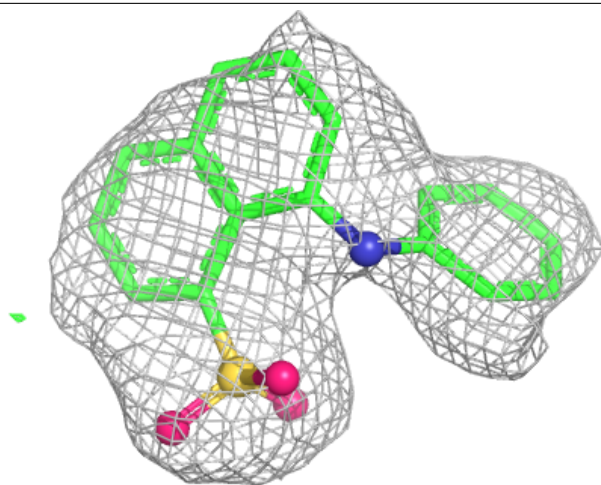
**Electron density around 2AN A 203:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around 2AN S 201:**

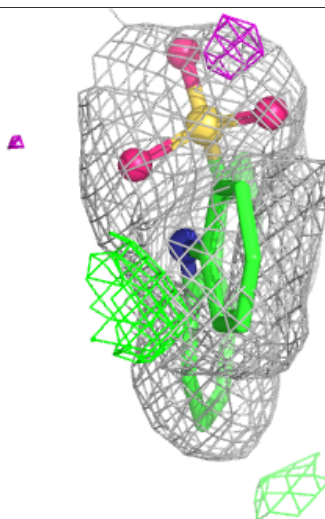
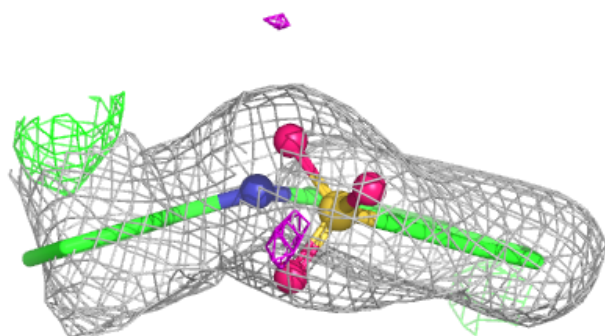
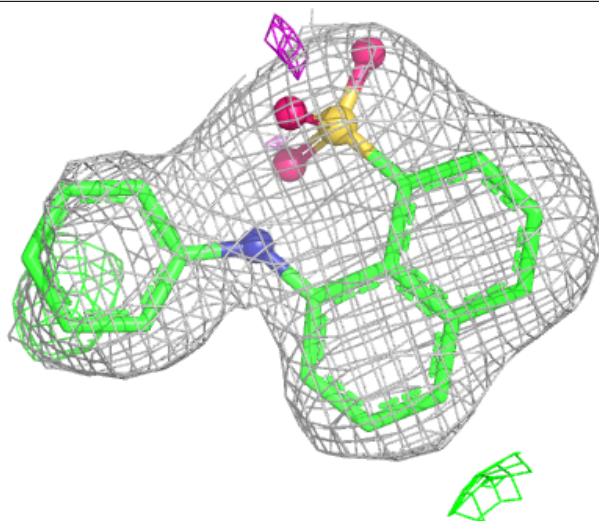
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





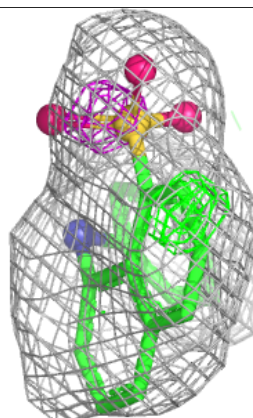
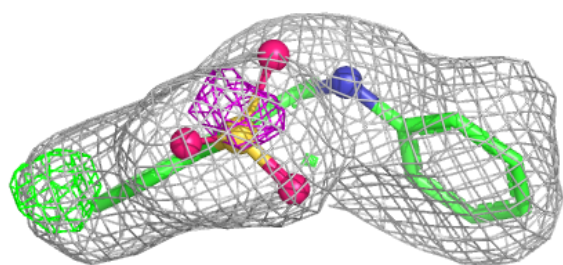
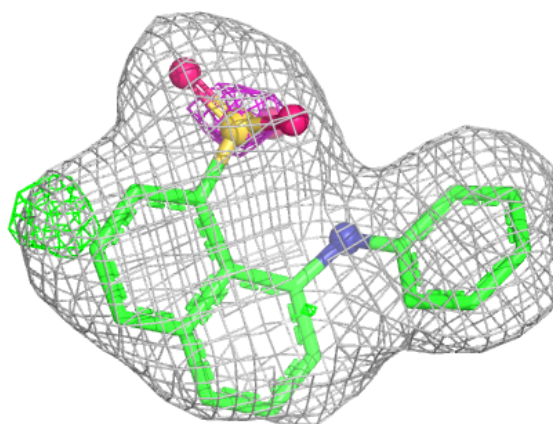
**Electron density around 2AN c 203:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around 2AN g 203:**

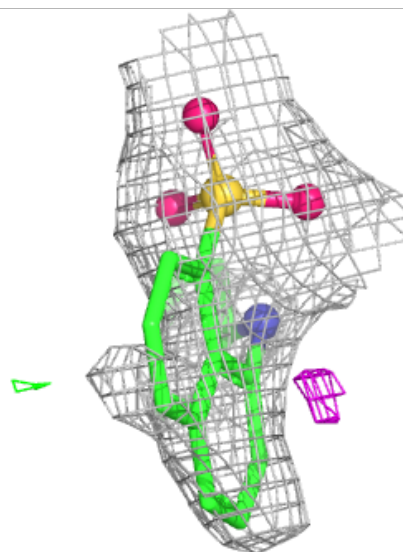
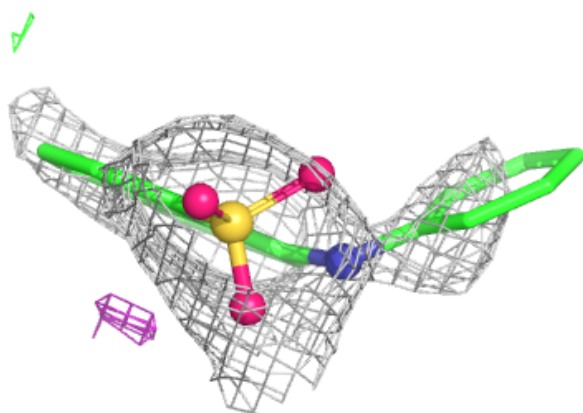
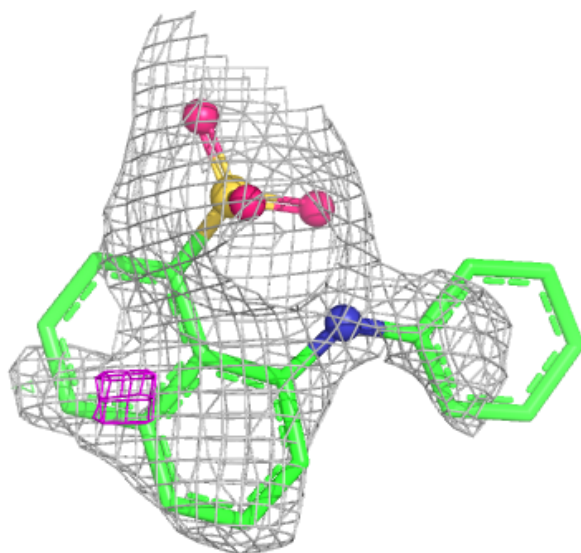
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





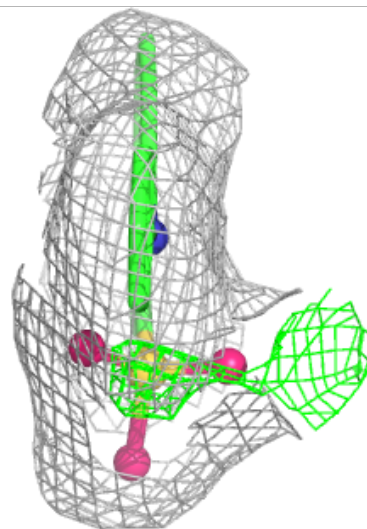
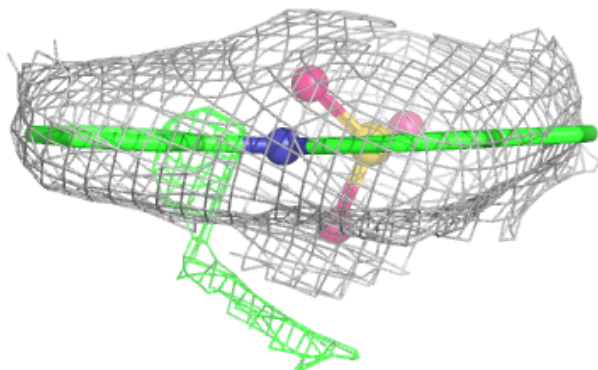
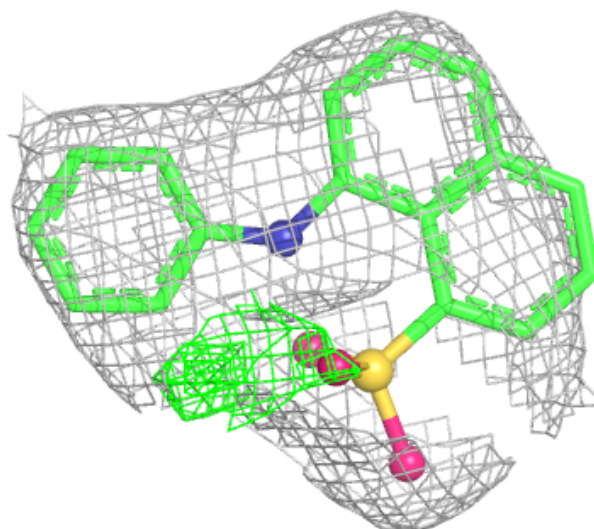
**Electron density around 2AN f 206:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



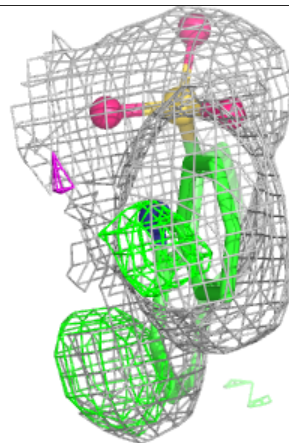
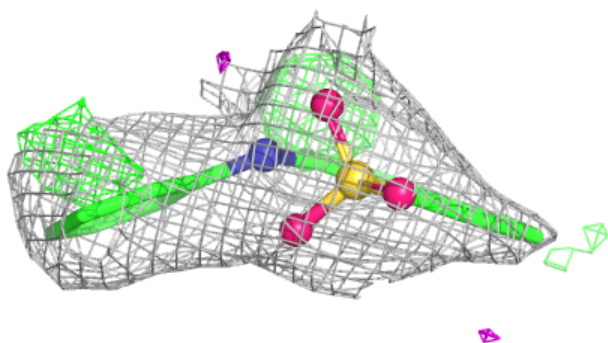
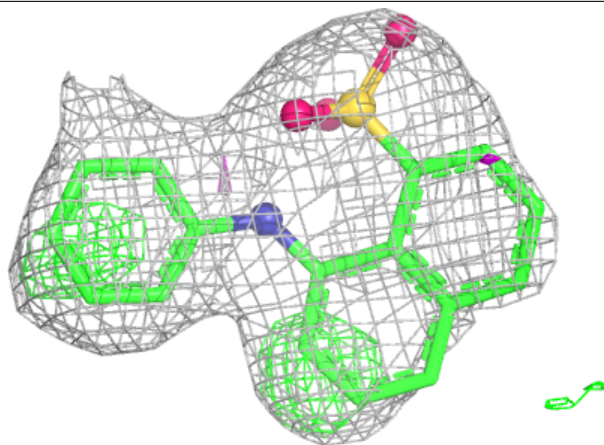
**Electron density around 2AN X 202:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



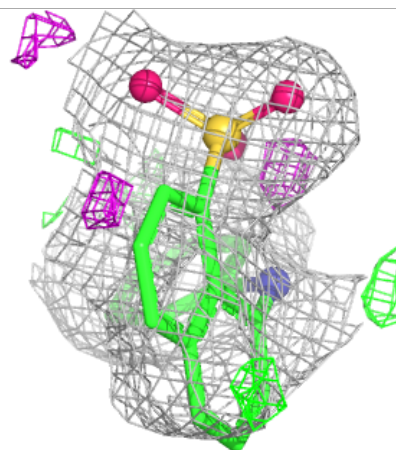
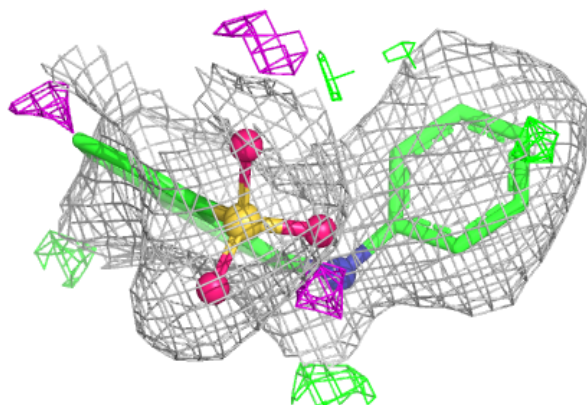
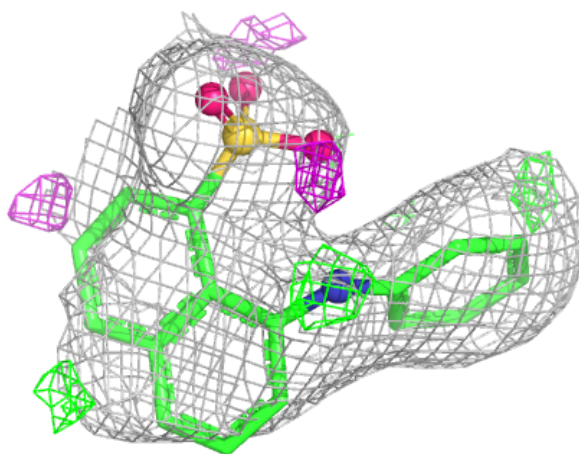
**Electron density around 2AN B 206:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



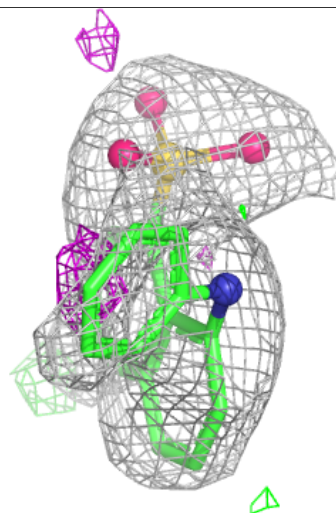
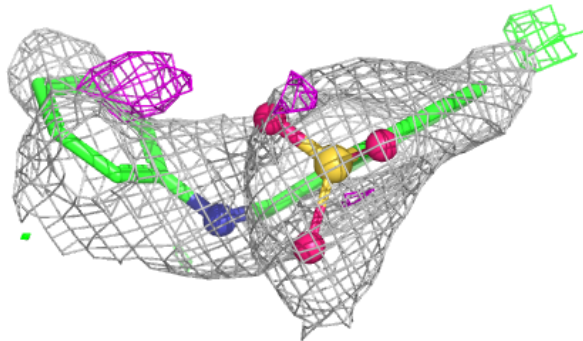
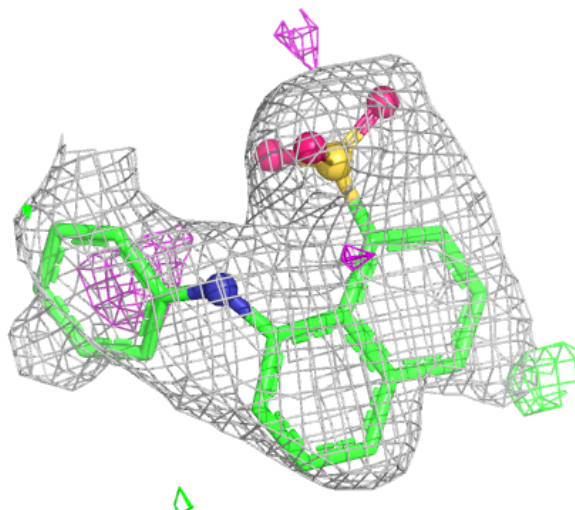
**Electron density around 2AN F 202:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

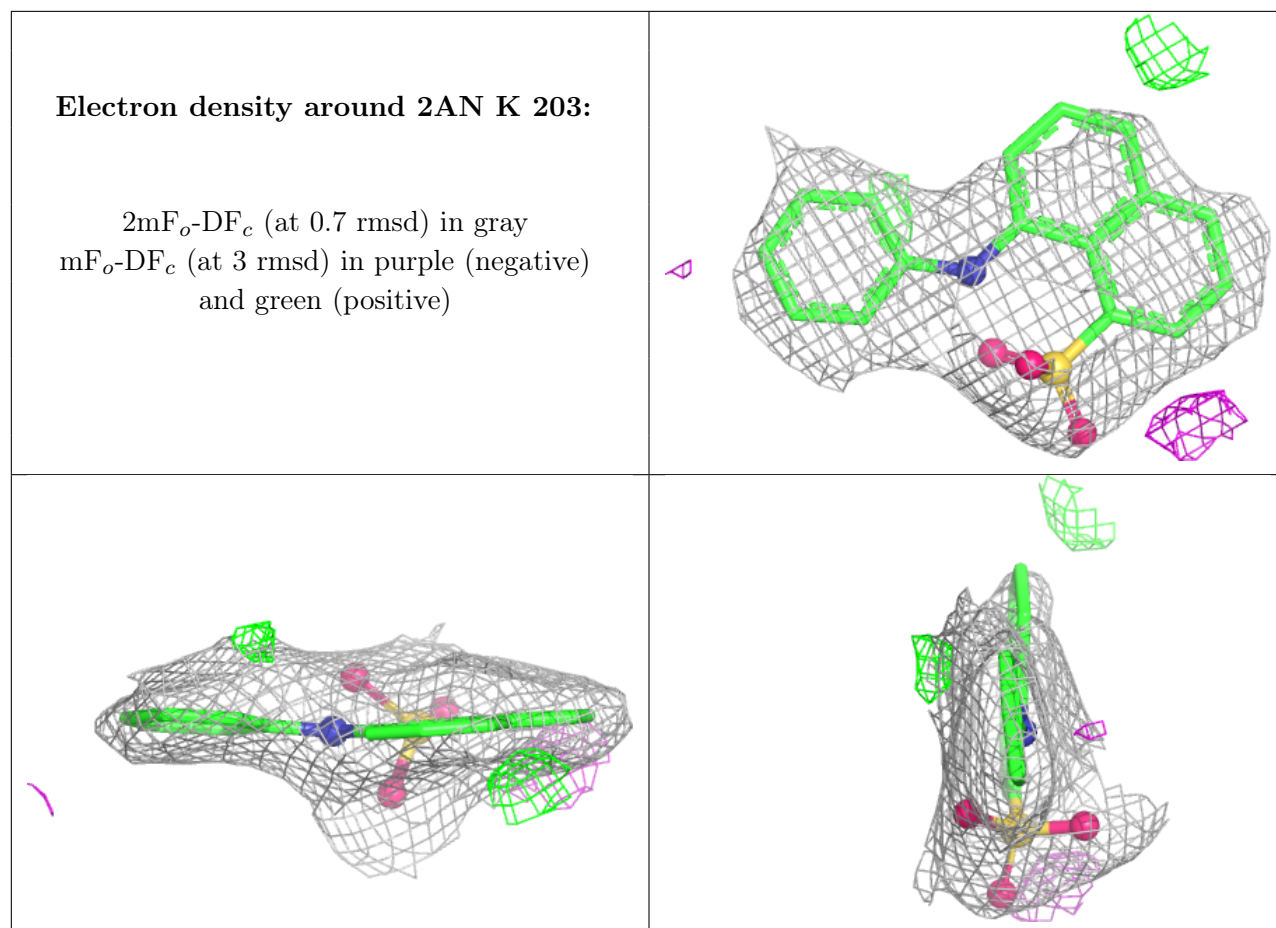


**Electron density around 2AN I 206:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

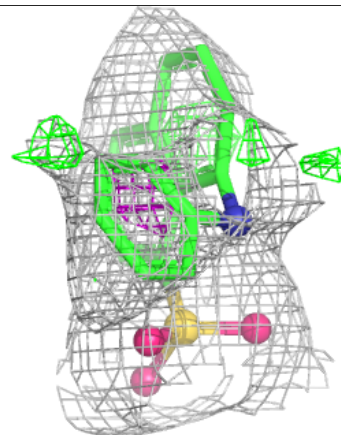
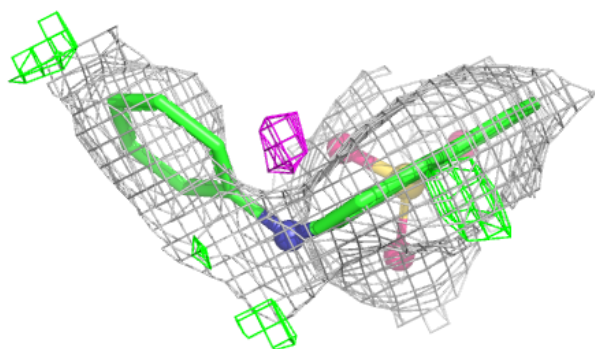
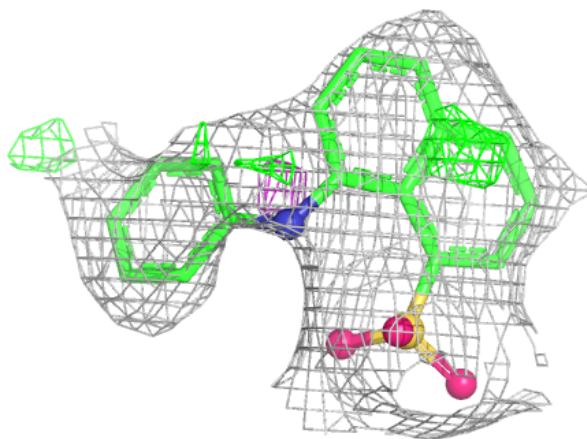






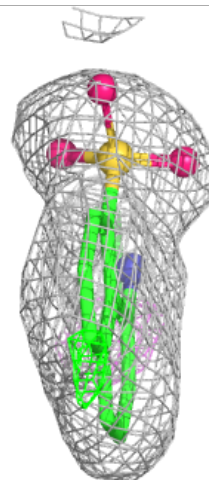
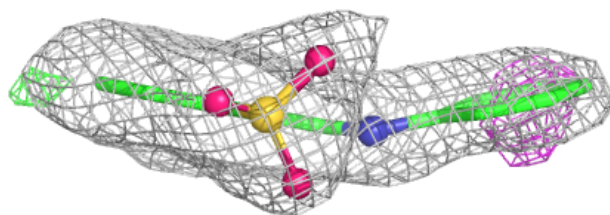
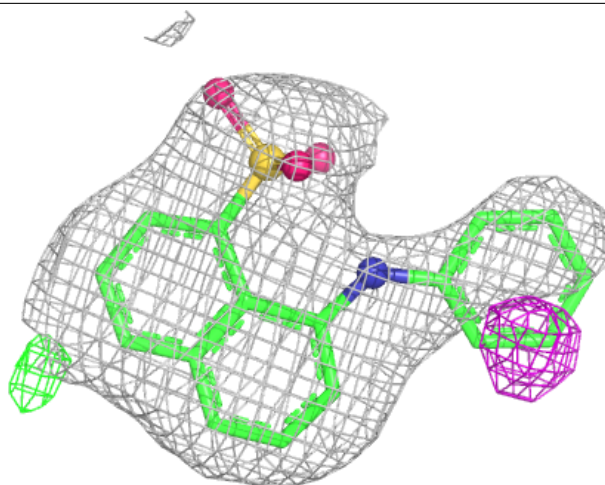
**Electron density around 2AN a 201:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around 2AN X 201:**

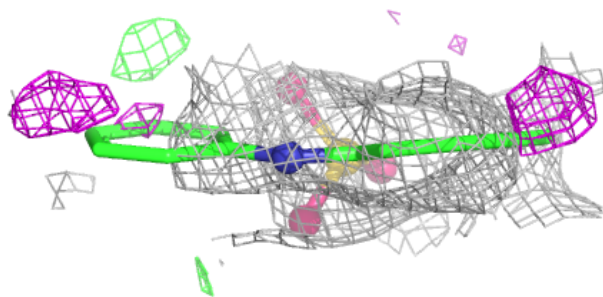
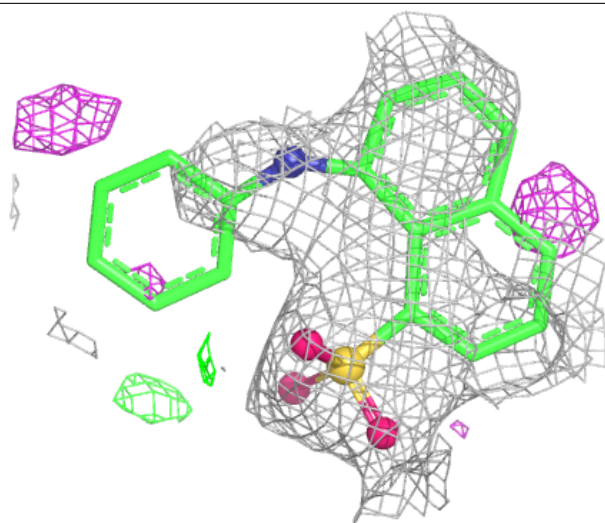
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





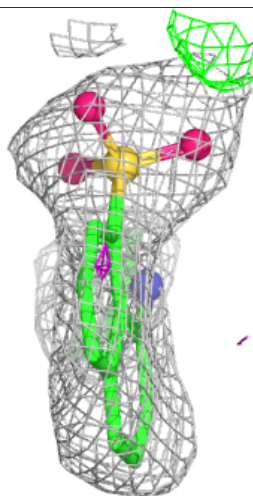
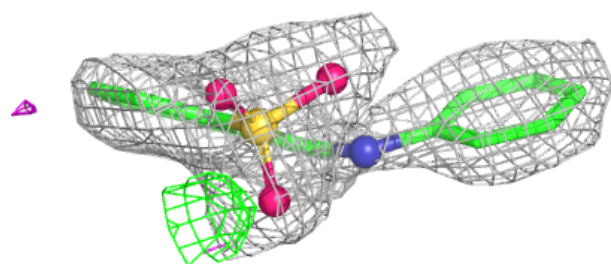
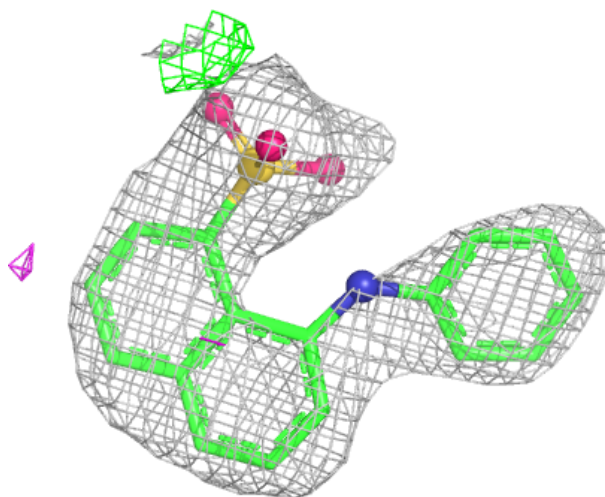
**Electron density around 2AN V 208:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



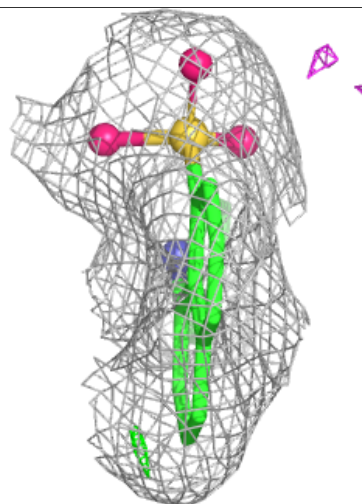
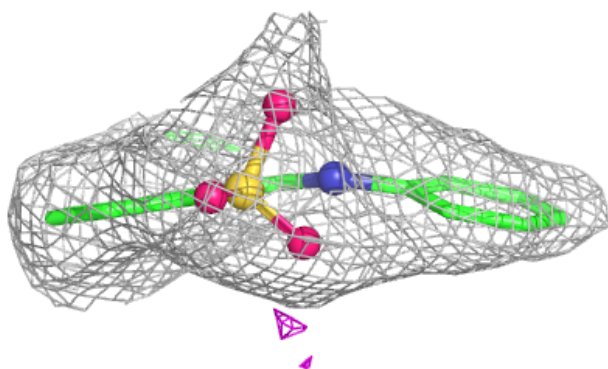
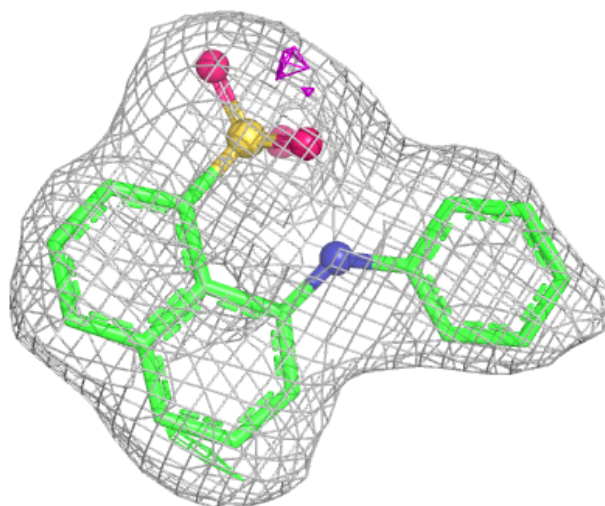
**Electron density around 2AN h 201:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



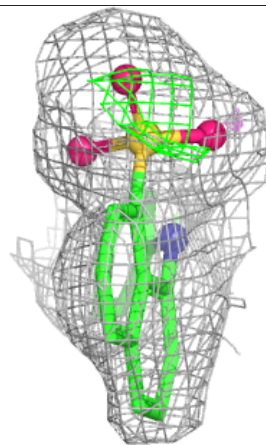
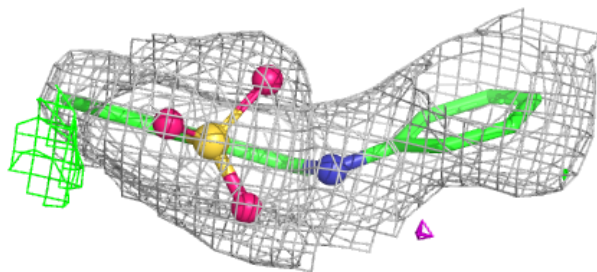
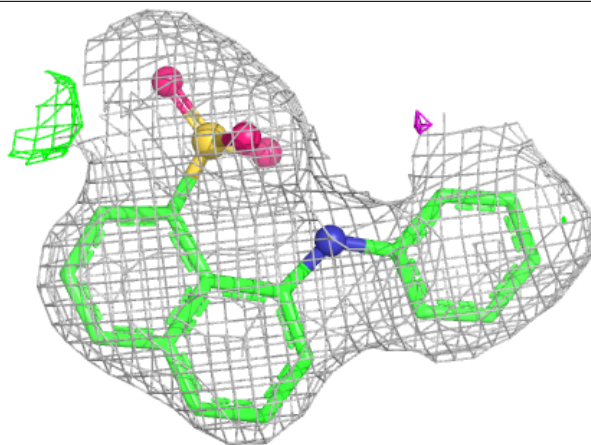
**Electron density around 2AN a 203:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



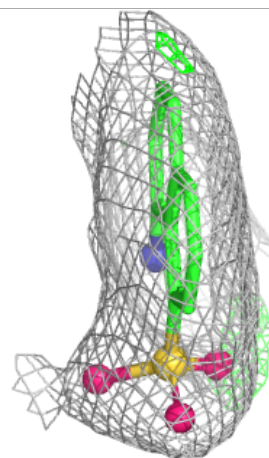
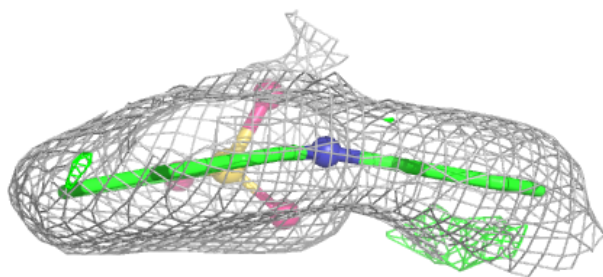
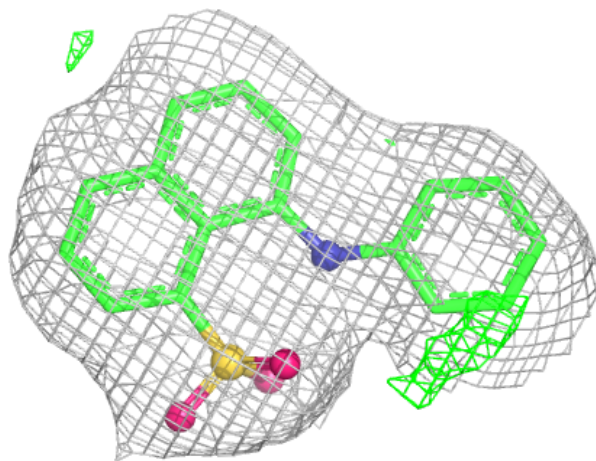
**Electron density around 2AN h 206:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



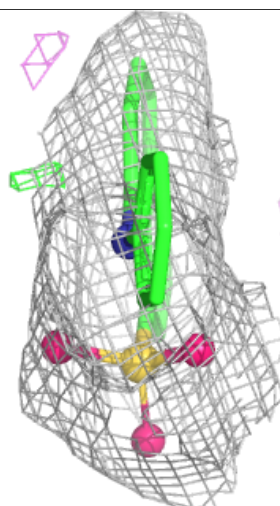
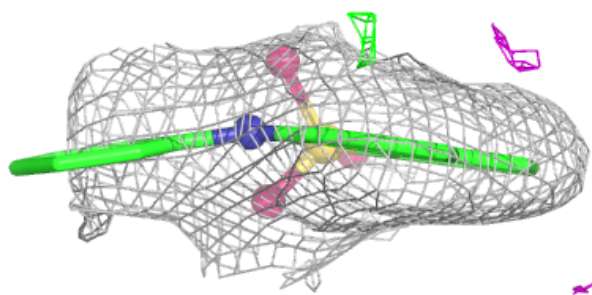
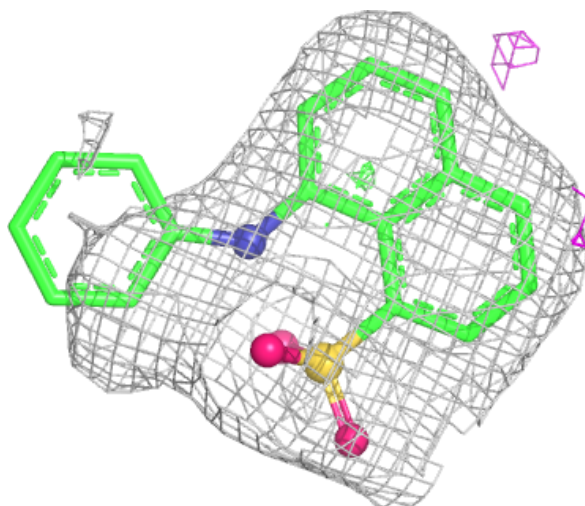
**Electron density around 2AN d 201:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around 2AN Z 205:**

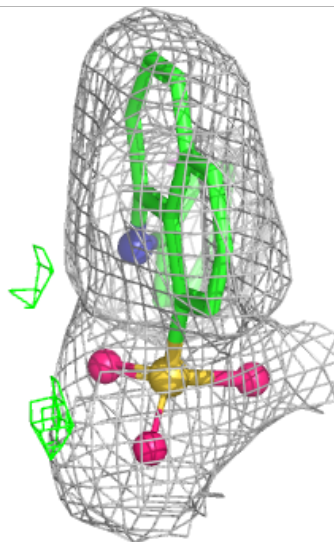
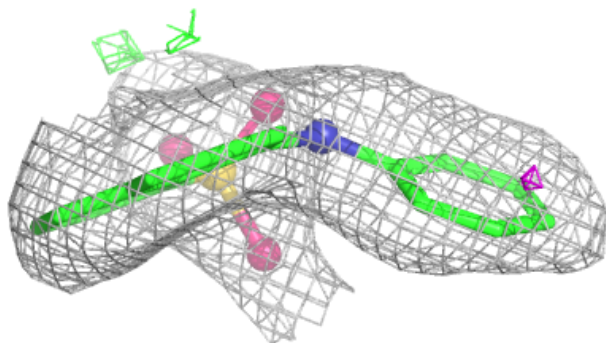
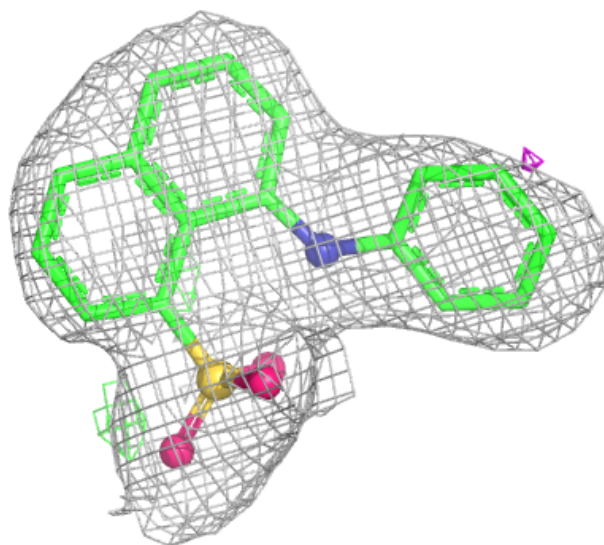
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

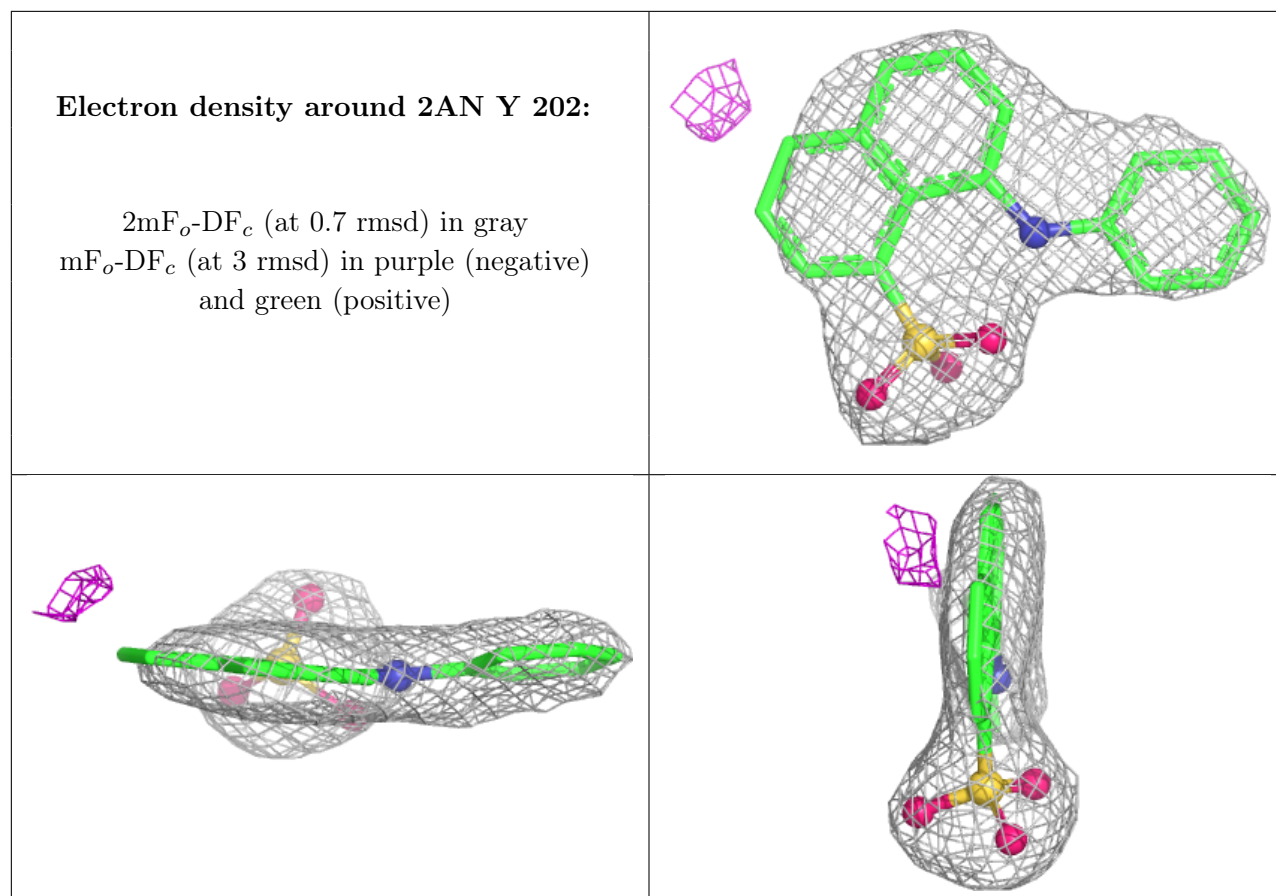




**Electron density around 2AN O 203:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

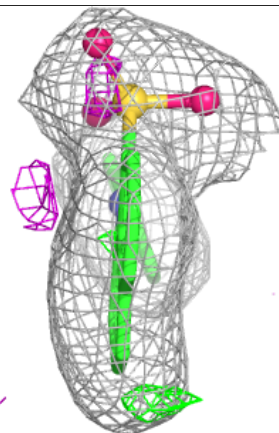
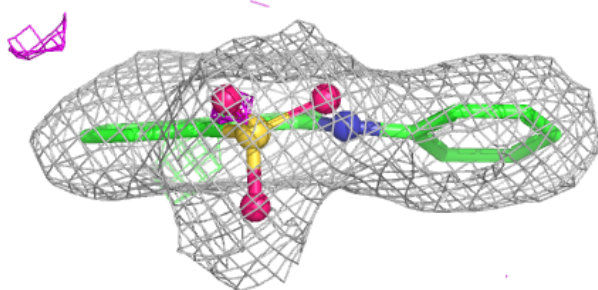
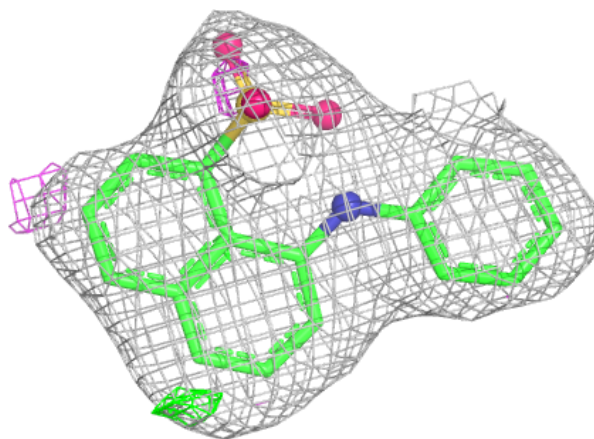






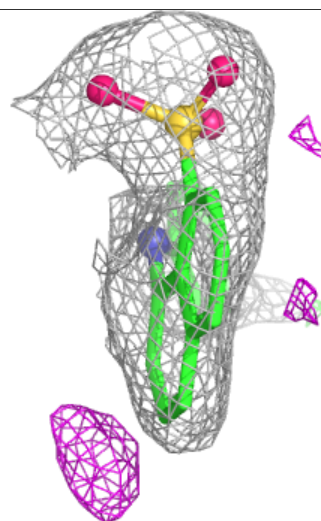
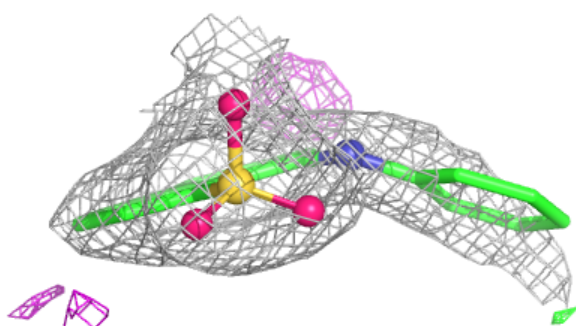
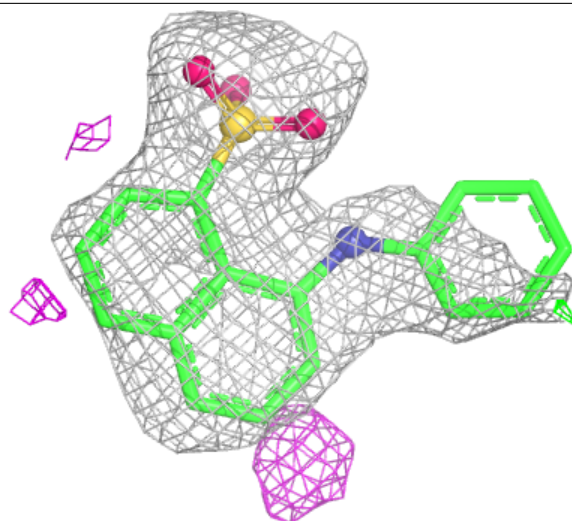
**Electron density around 2AN j 201:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



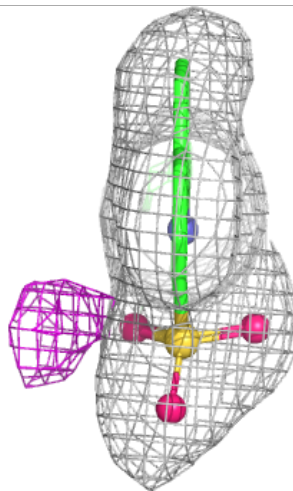
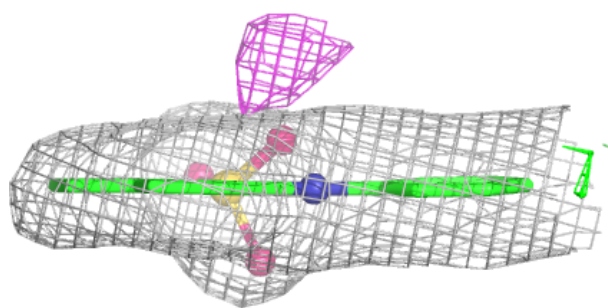
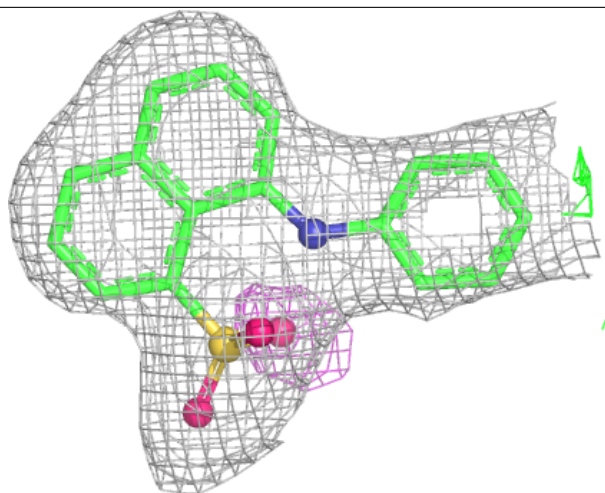
**Electron density around 2AN E 203:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



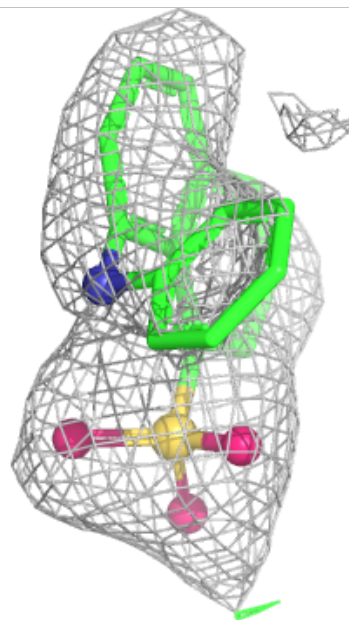
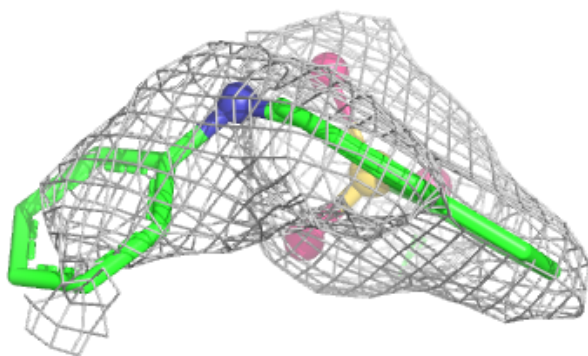
**Electron density around 2AN V 206:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



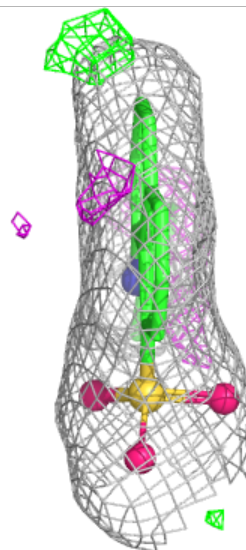
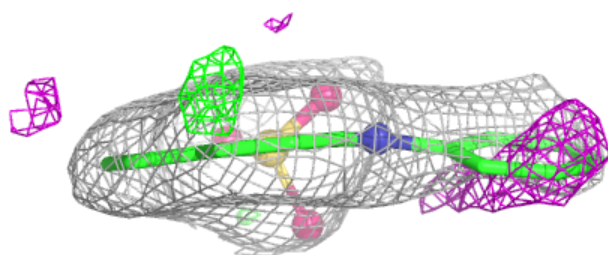
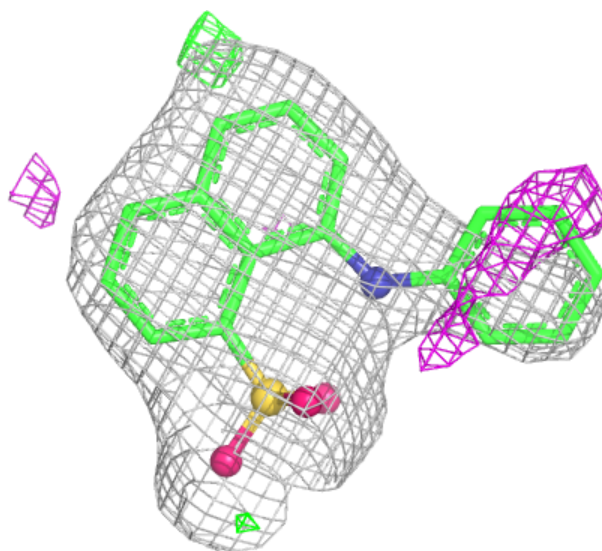
**Electron density around 2AN Q 203:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around 2AN A 201:**

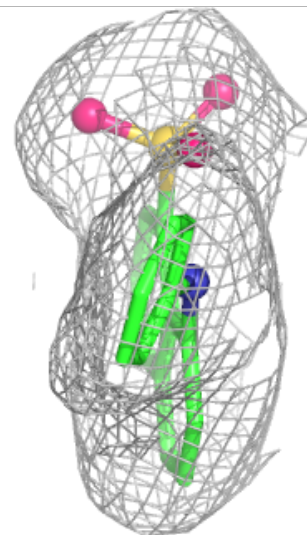
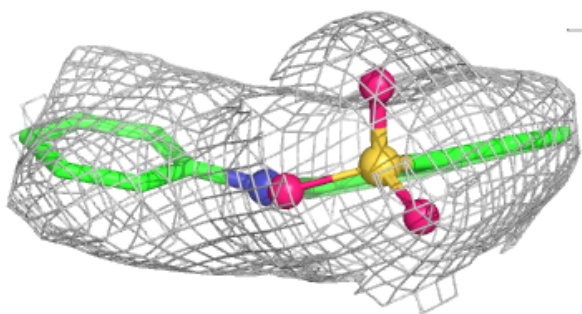
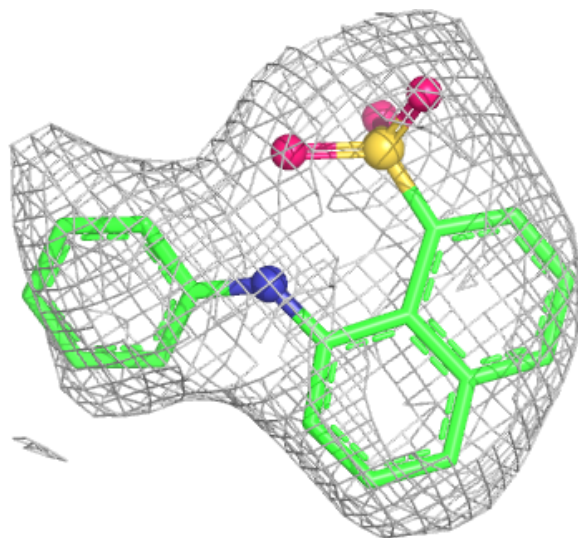
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





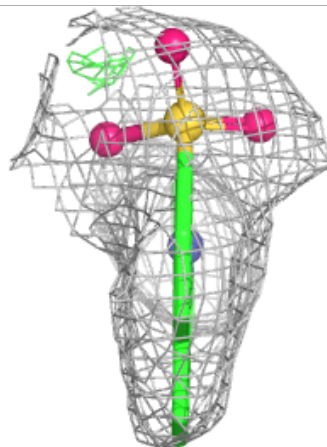
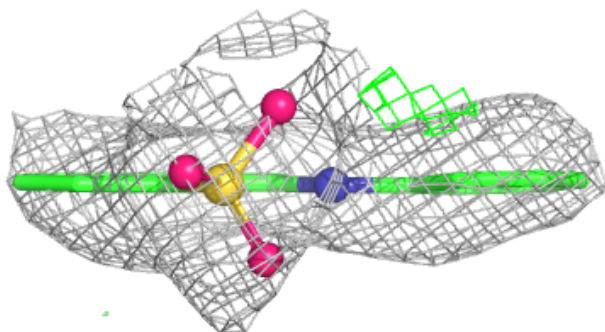
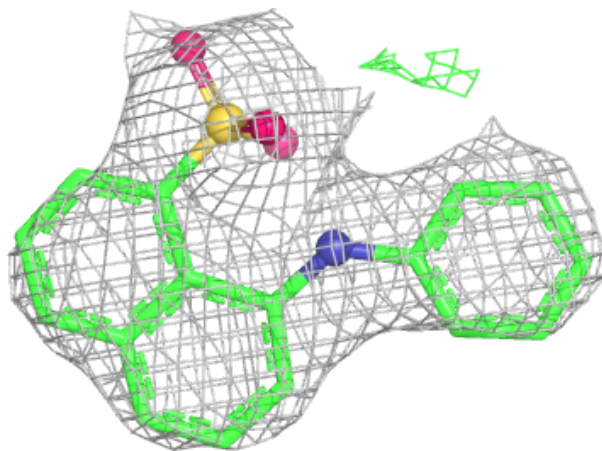
**Electron density around 2AN D 203:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



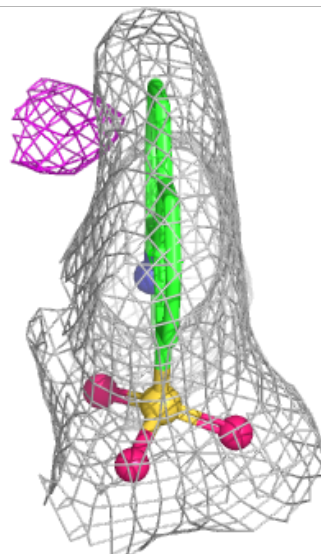
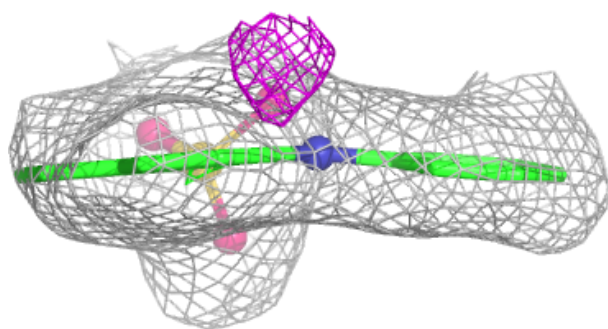
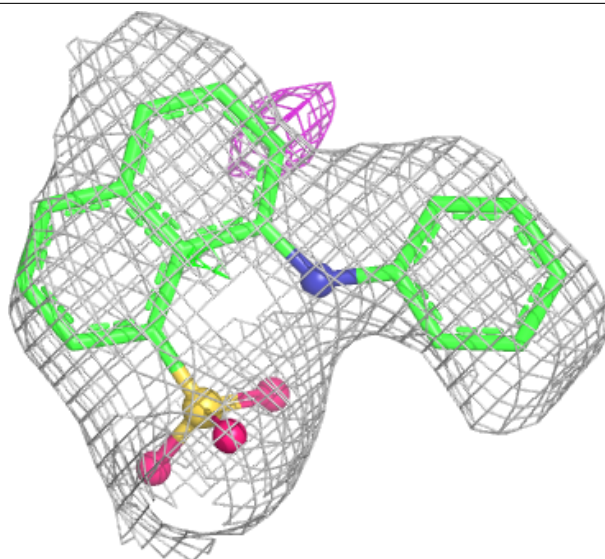
**Electron density around 2AN Z 202:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

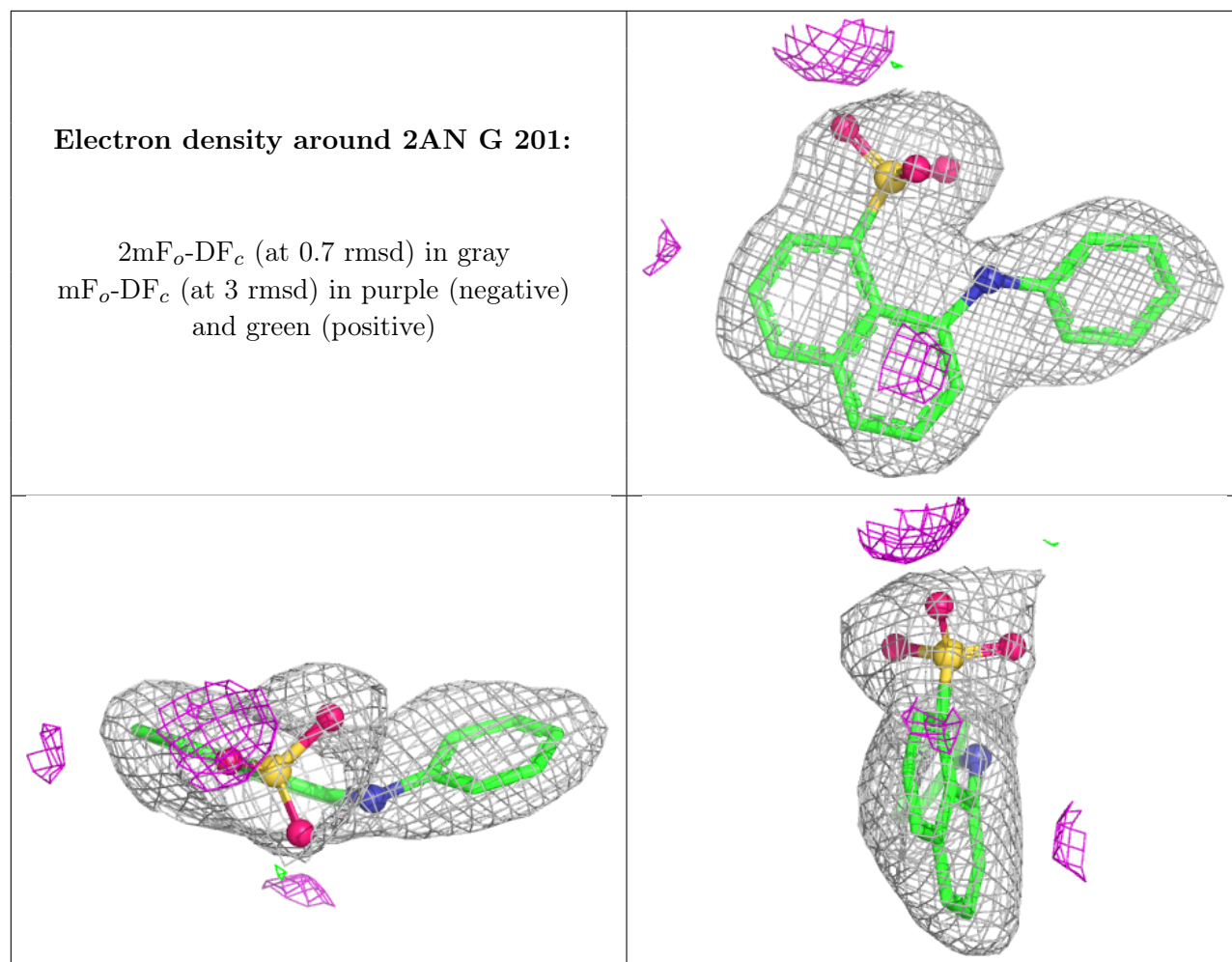


**Electron density around 2AN F 201:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

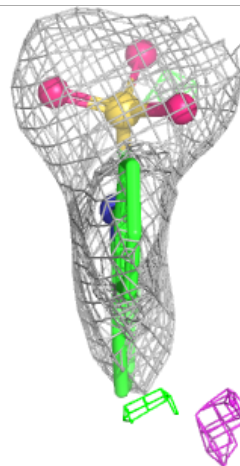
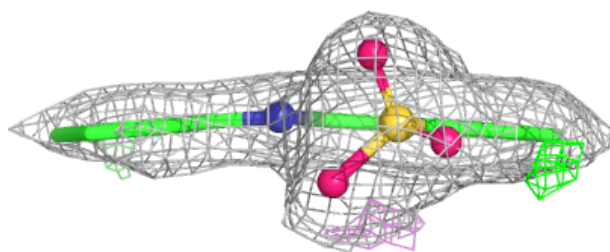
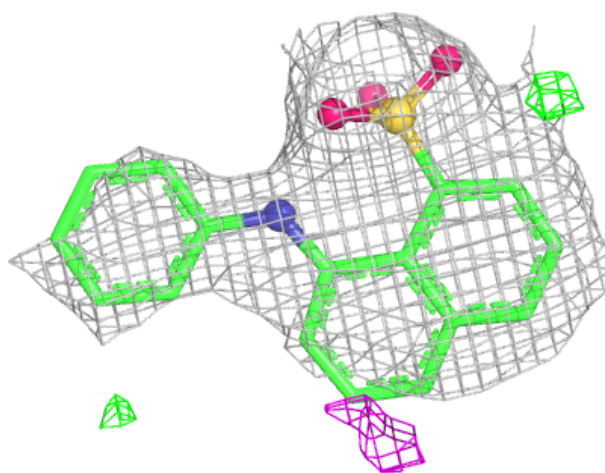






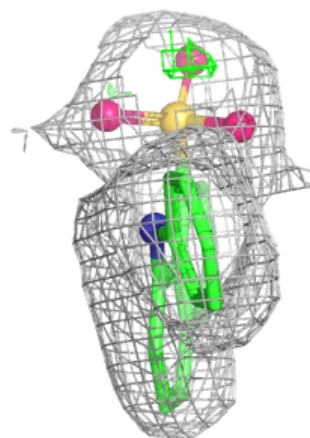
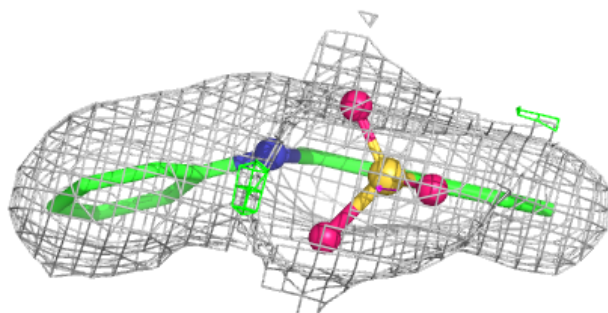
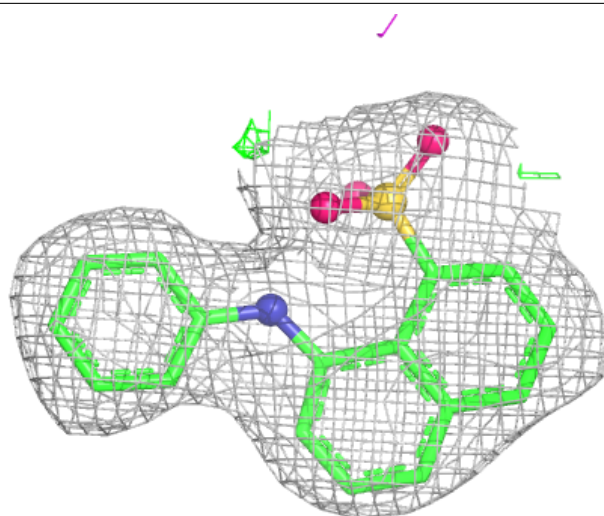
**Electron density around 2AN g 201:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



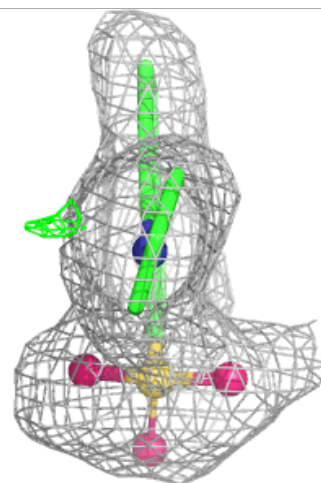
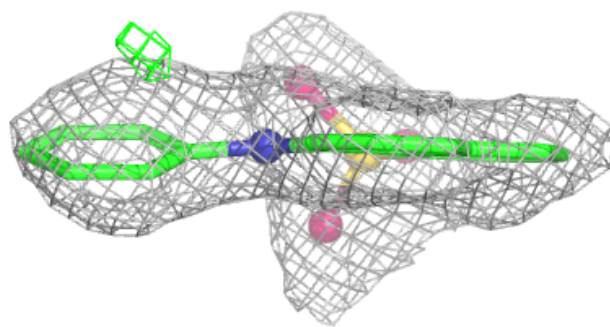
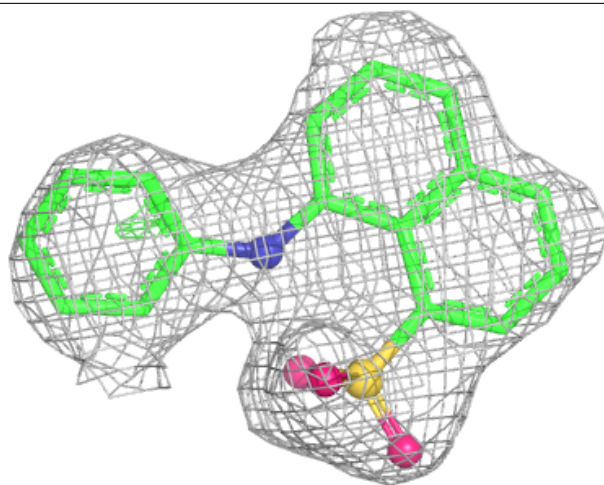
**Electron density around 2AN X 205:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



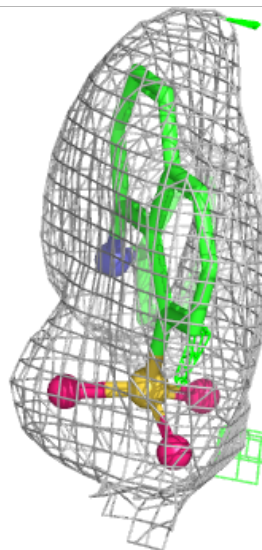
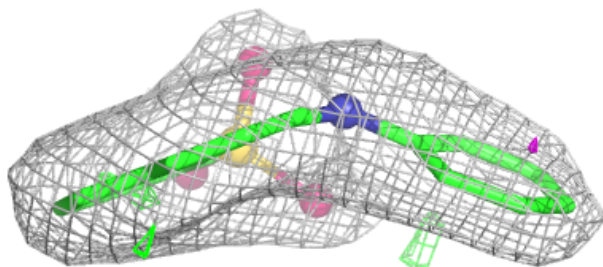
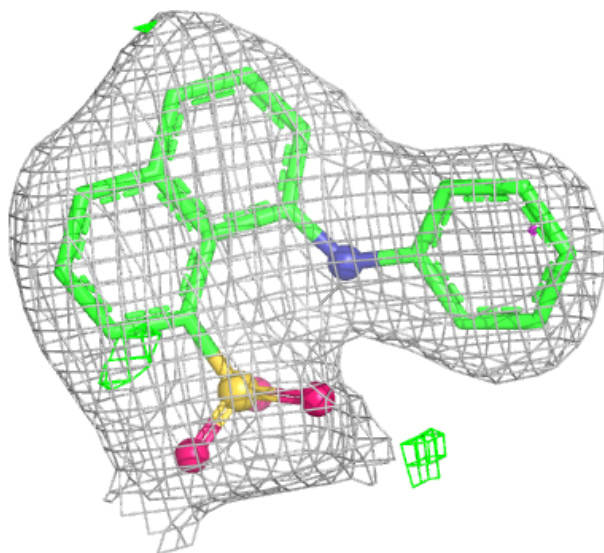
**Electron density around 2AN B 204:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



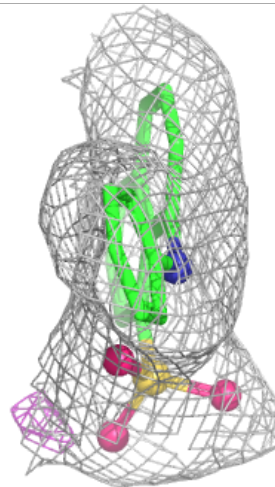
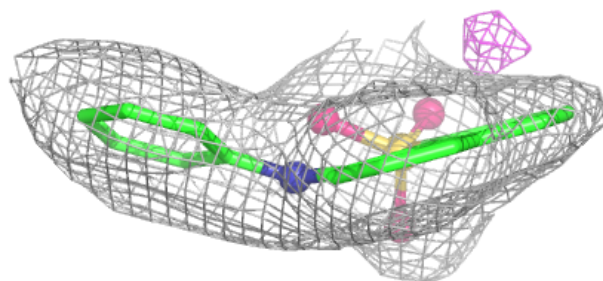
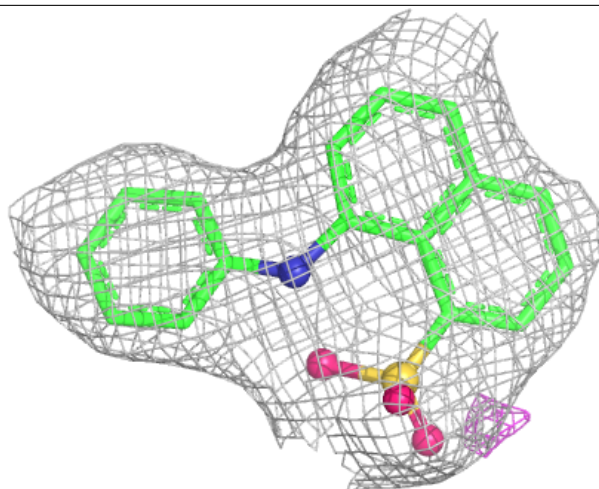
**Electron density around 2AN D 202:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around 2AN d 202:**

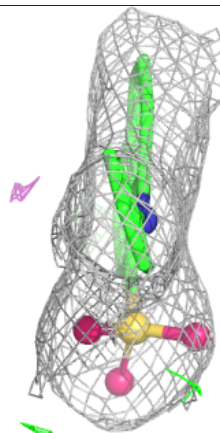
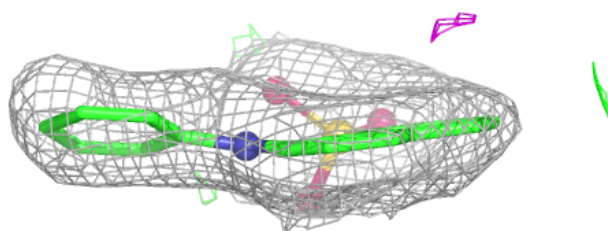
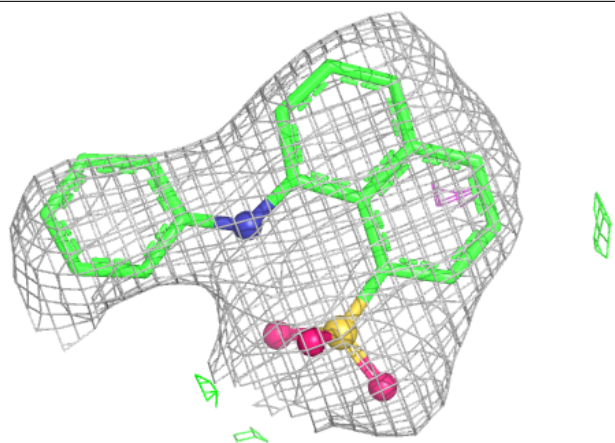
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





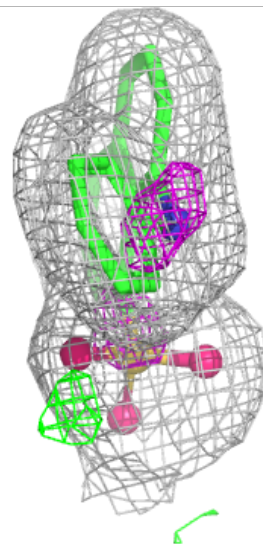
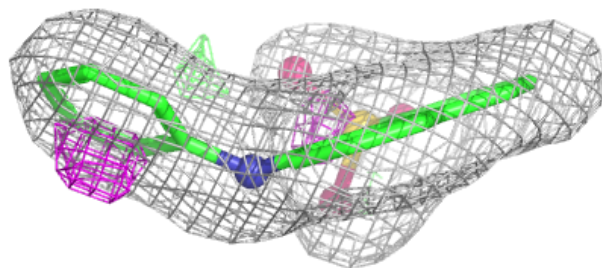
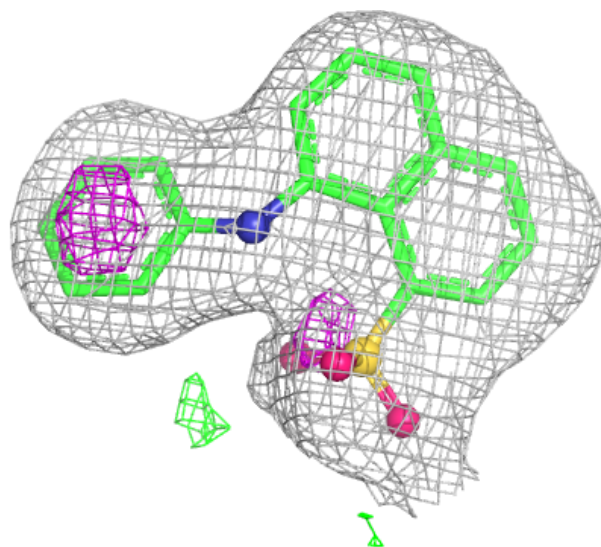
**Electron density around 2AN Z 203:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around 2AN R 202:**

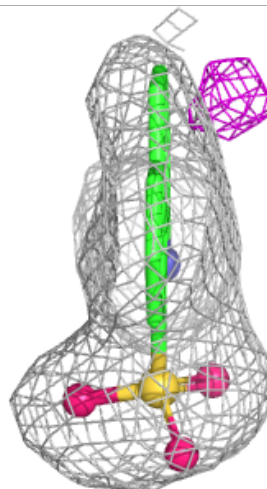
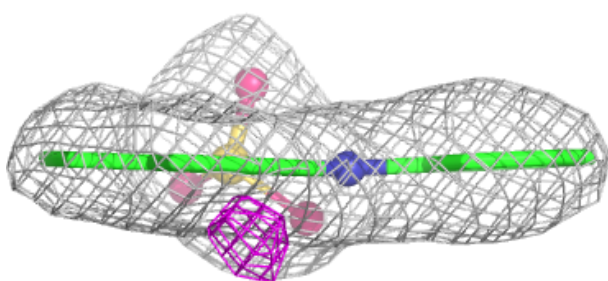
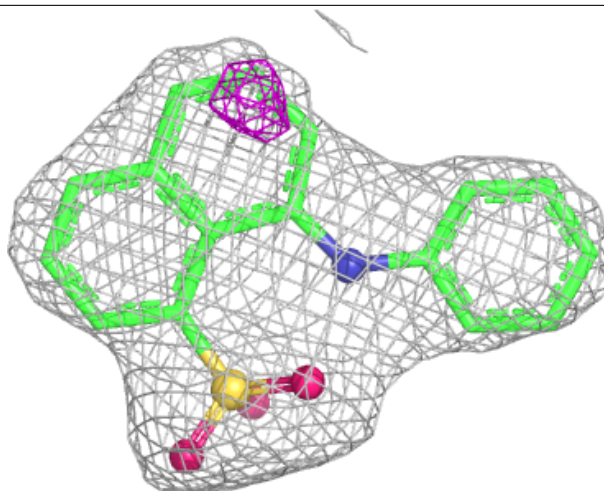
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





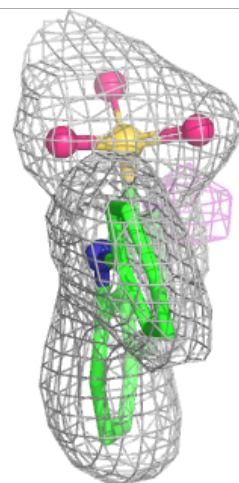
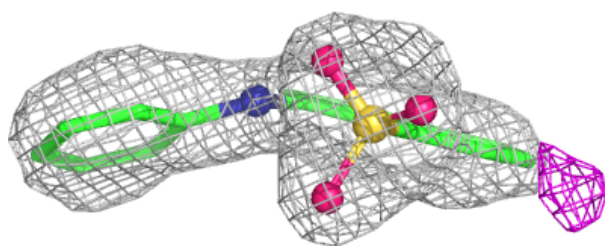
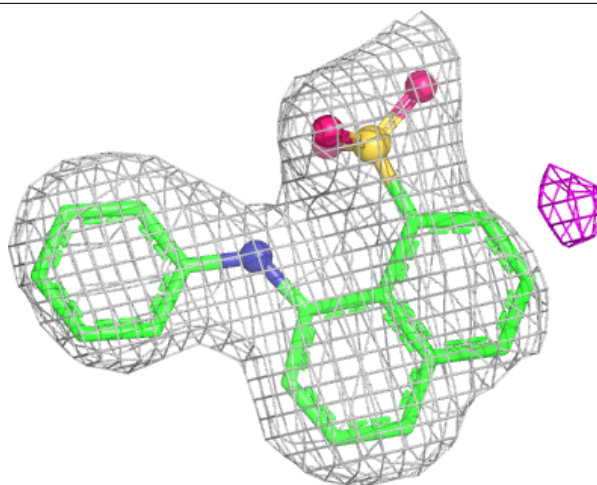
**Electron density around 2AN L 204:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



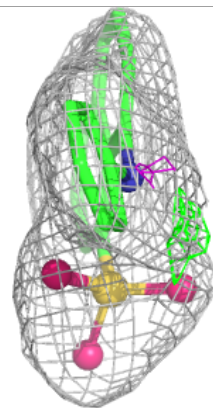
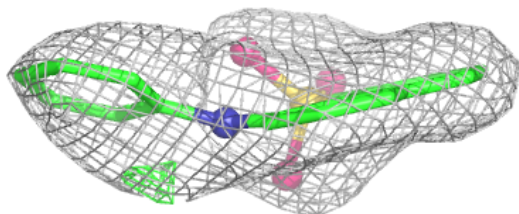
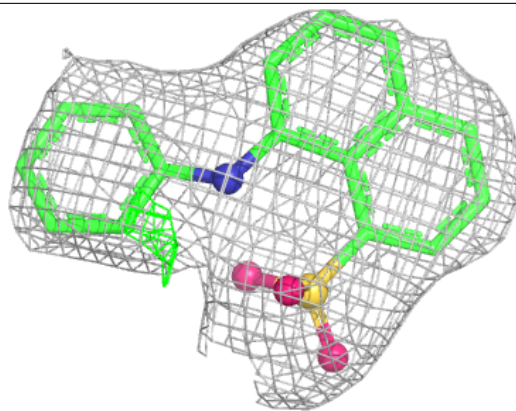
**Electron density around 2AN i 201:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



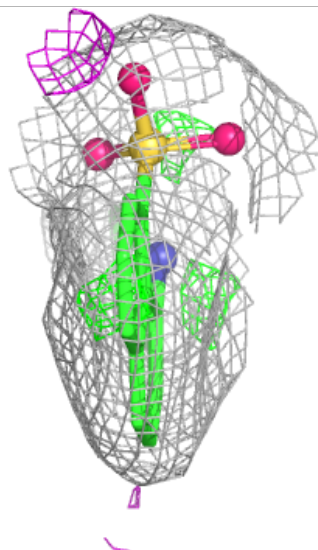
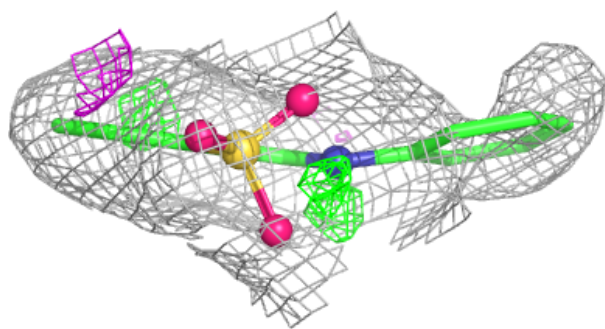
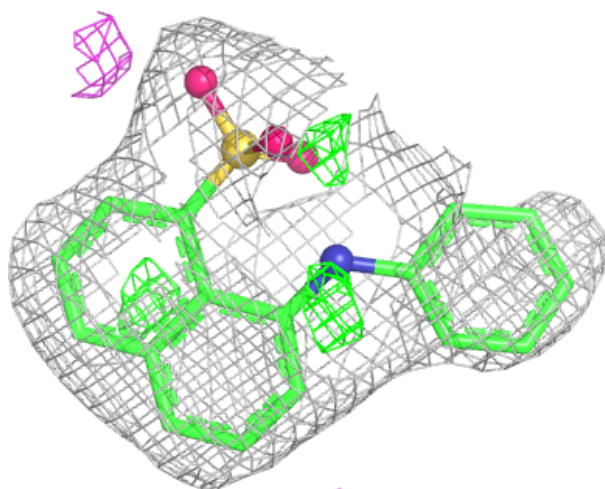
**Electron density around 2AN b 202:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



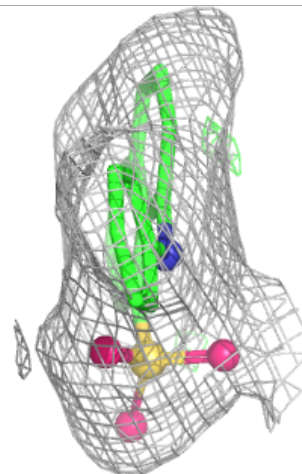
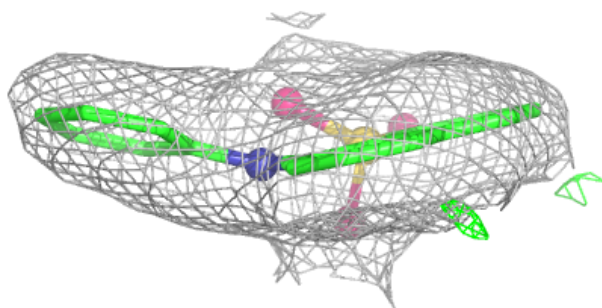
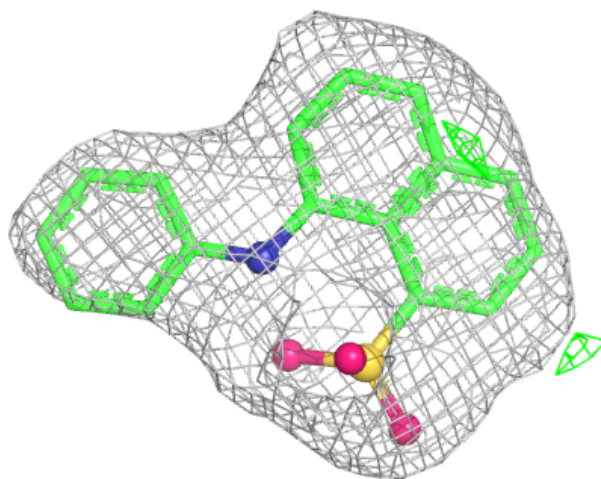
**Electron density around 2AN h 204:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



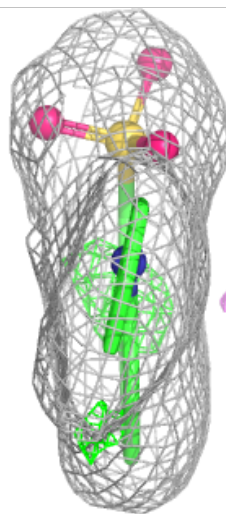
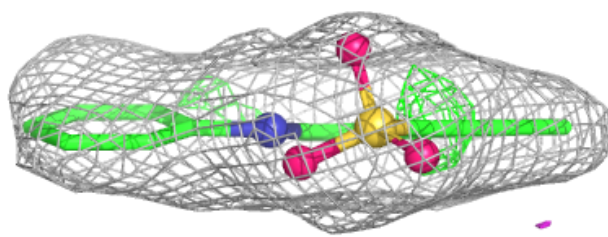
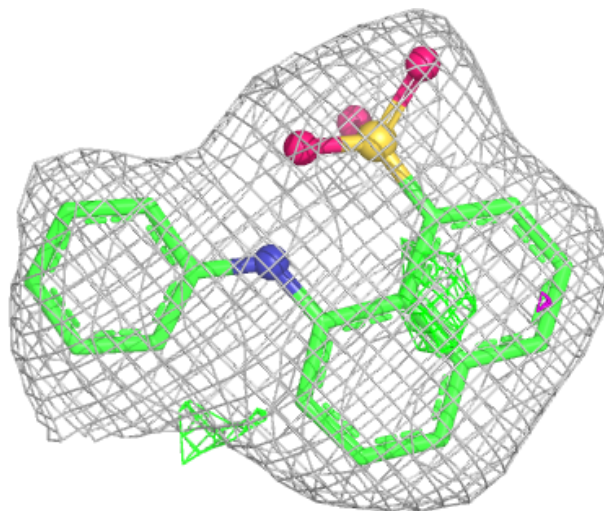
**Electron density around 2AN b 204:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around 2AN P 203:**

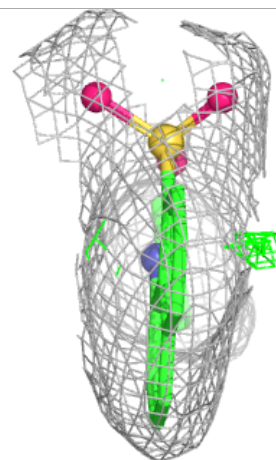
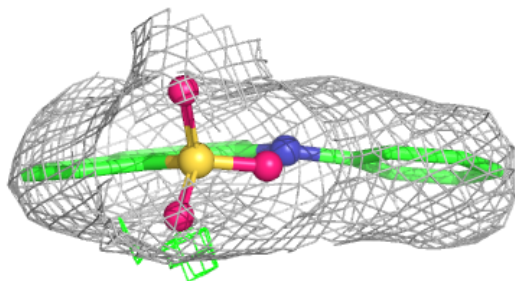
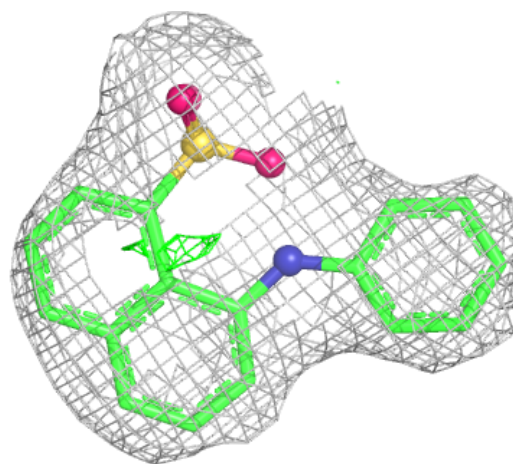
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





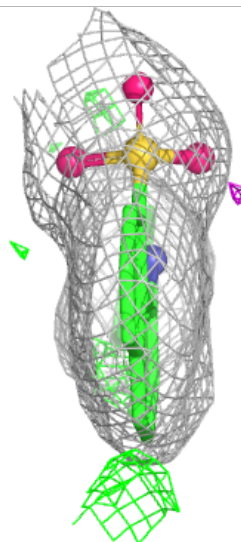
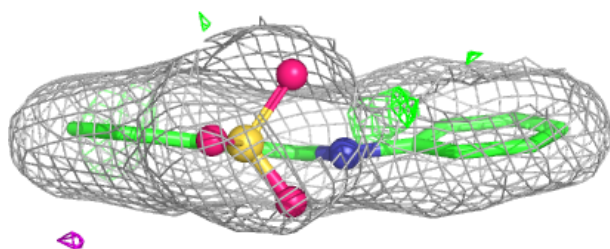
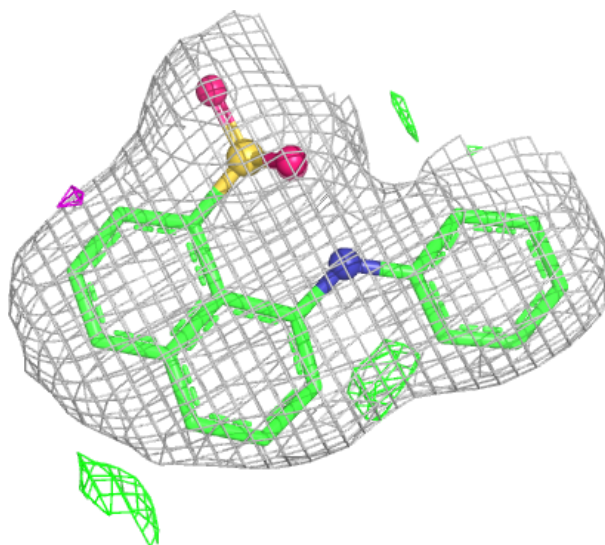
**Electron density around 2AN R 203:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around 2AN b 201:**

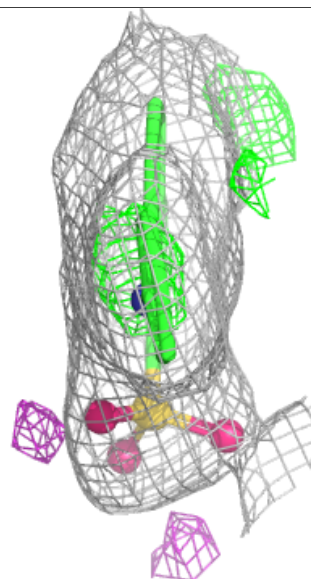
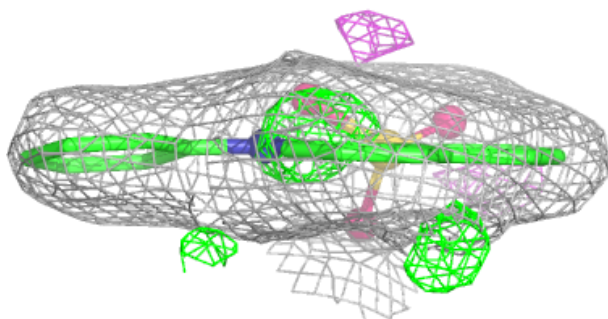
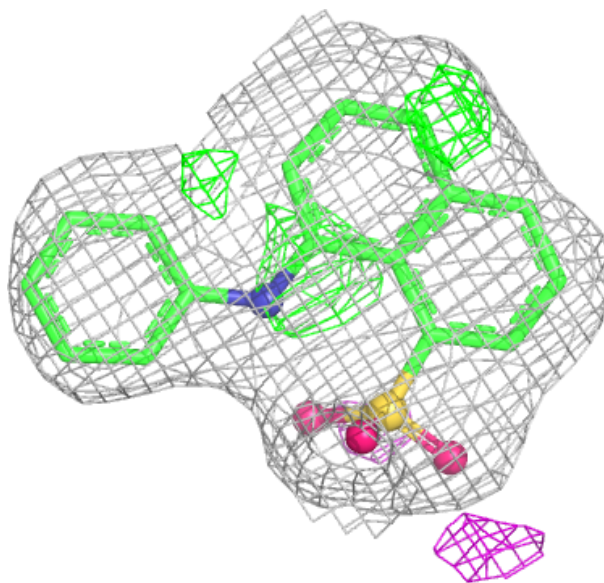
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





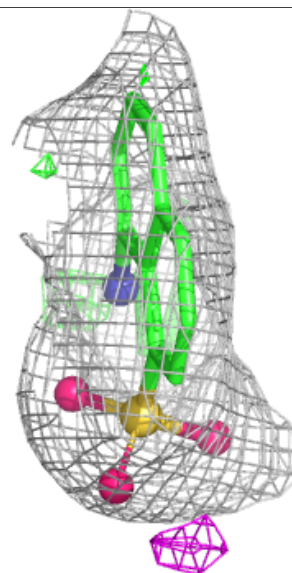
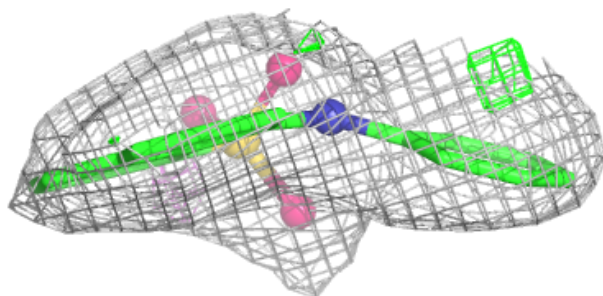
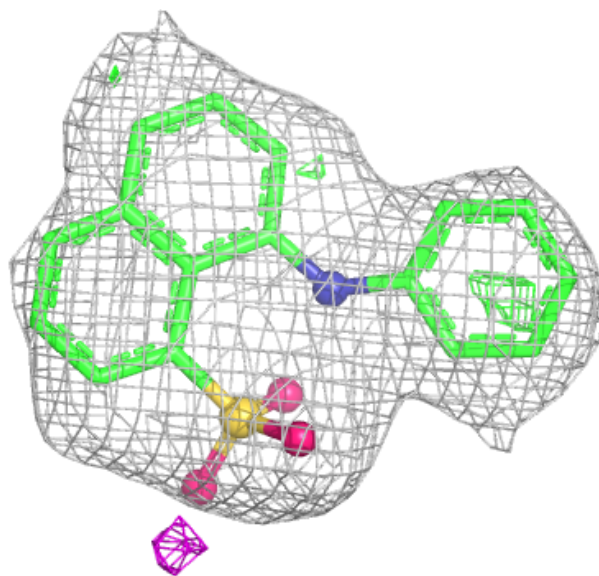
**Electron density around 2AN j 204:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



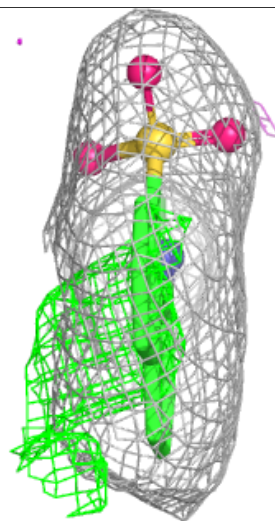
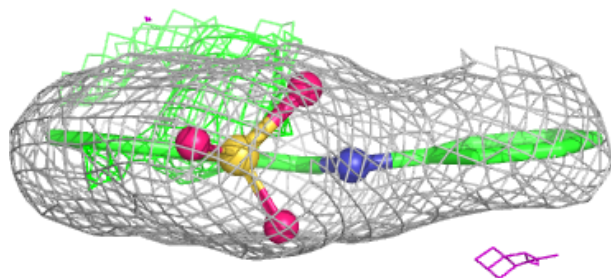
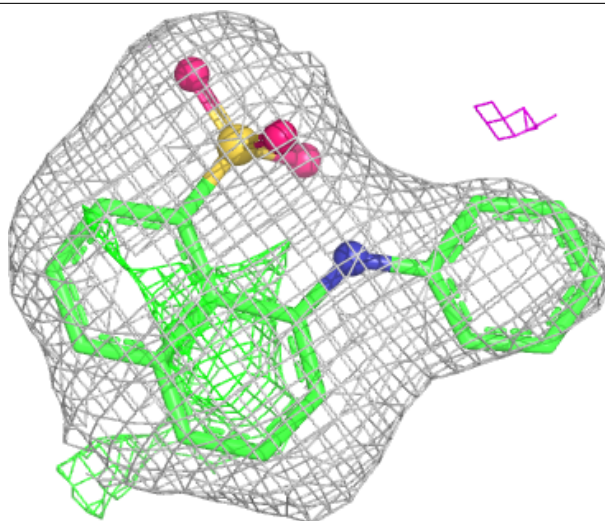
**Electron density around 2AN F 205:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



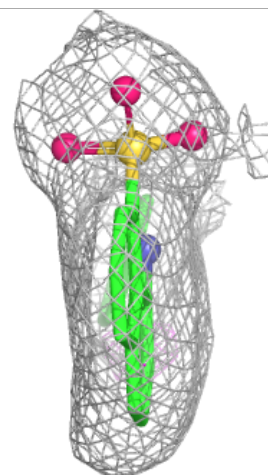
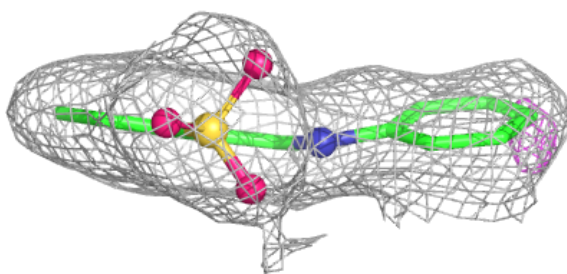
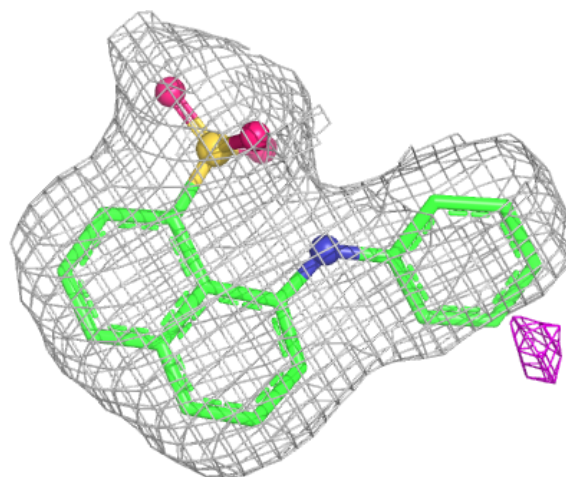
**Electron density around 2AN J 201:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



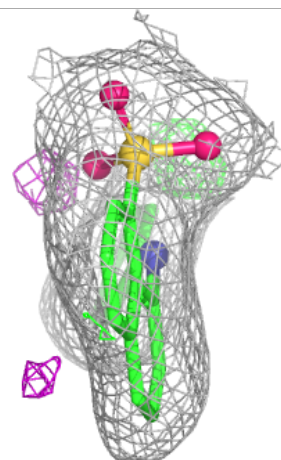
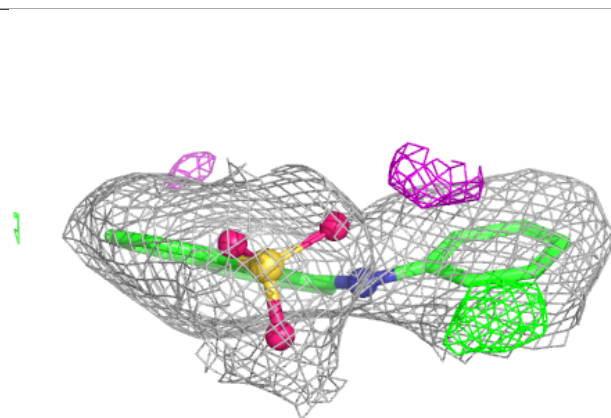
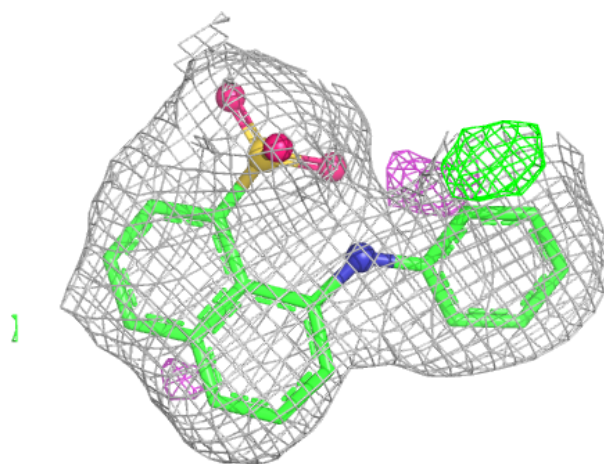
**Electron density around 2AN E 201:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around 2AN B 202:**

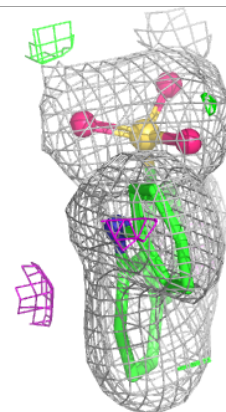
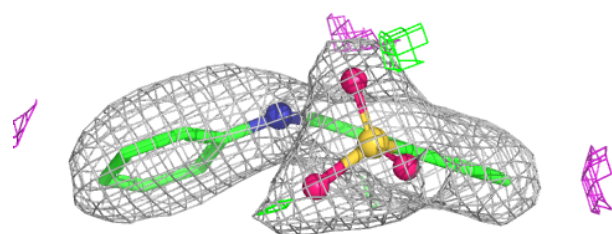
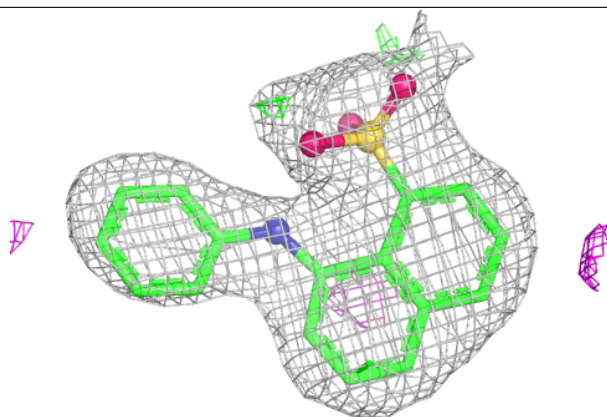
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





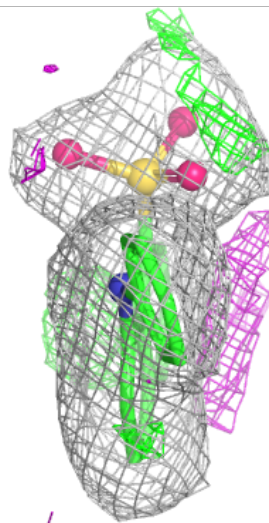
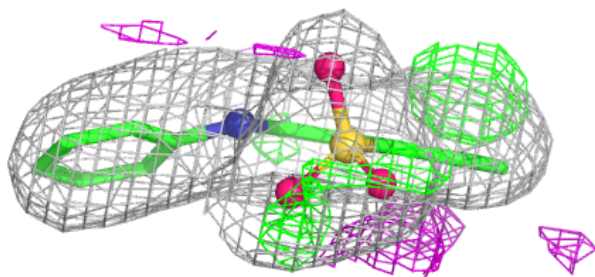
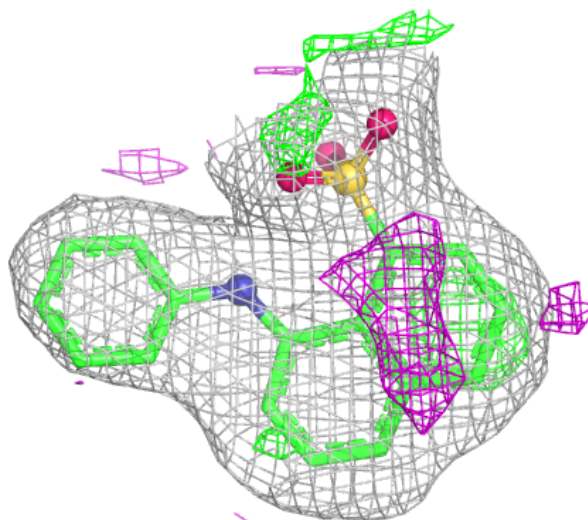
**Electron density around 2AN T 202:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



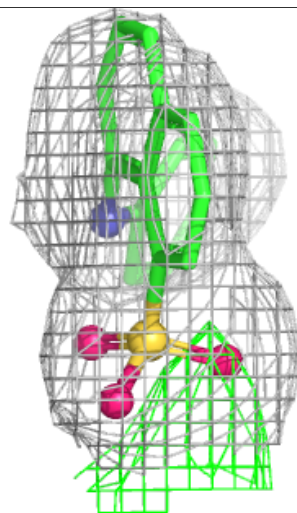
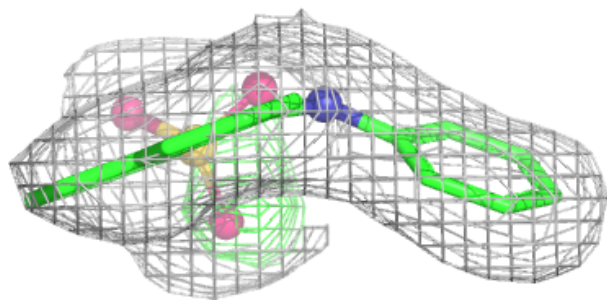
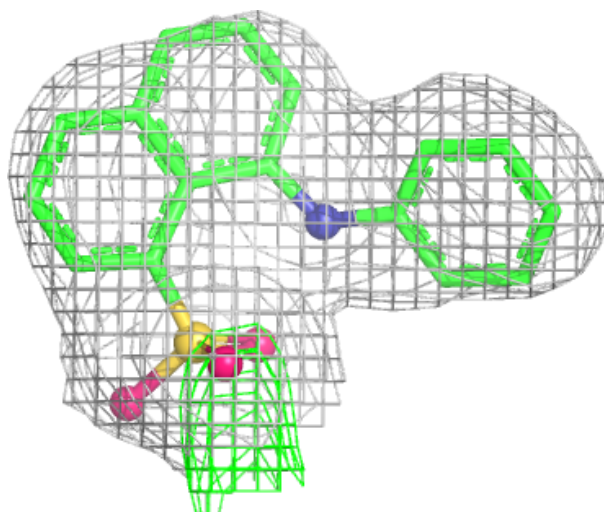
**Electron density around 2AN h 203:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around 2AN B 205:**

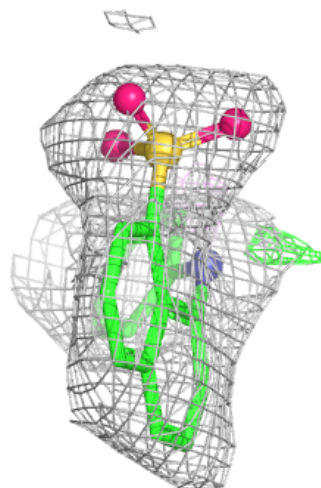
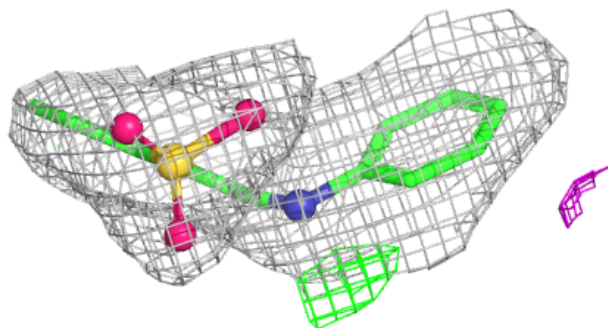
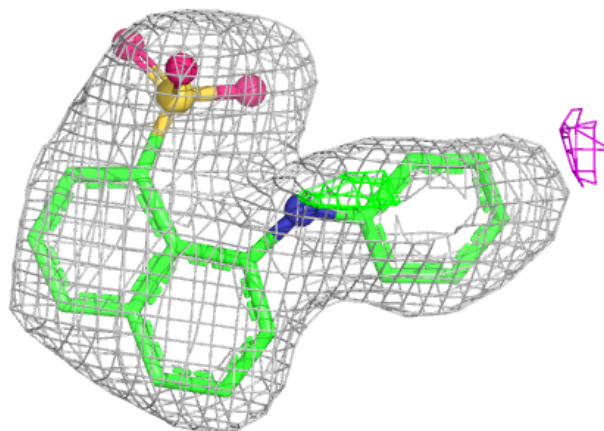
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





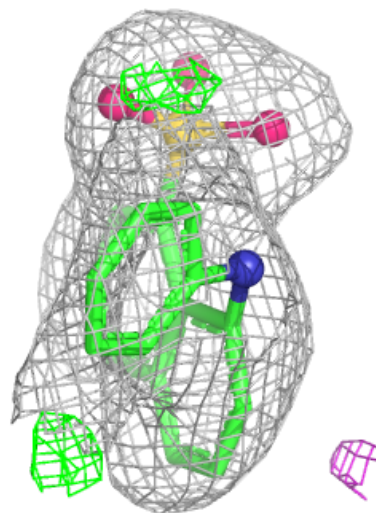
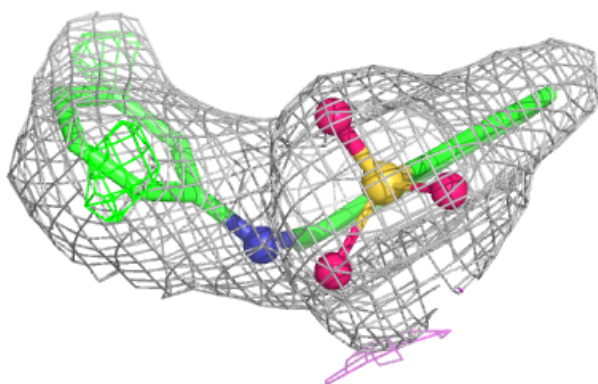
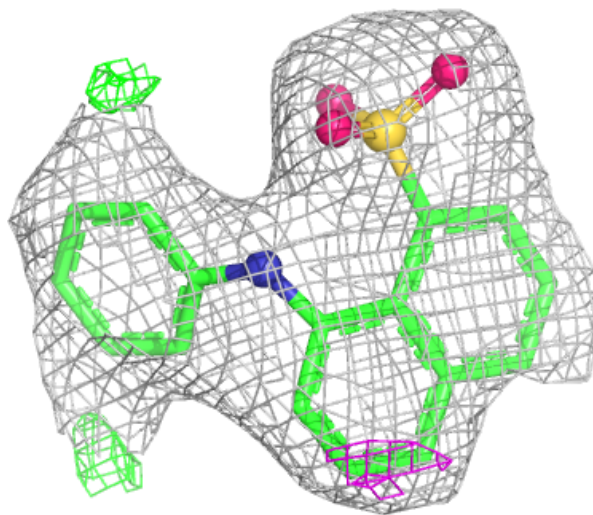
**Electron density around 2AN A 202:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



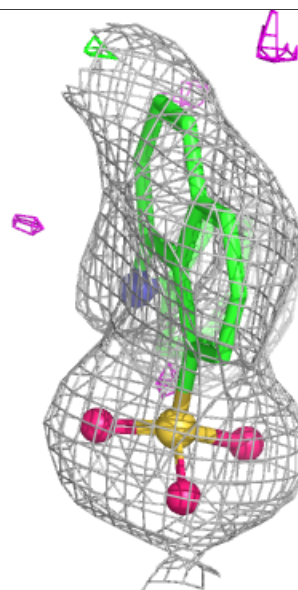
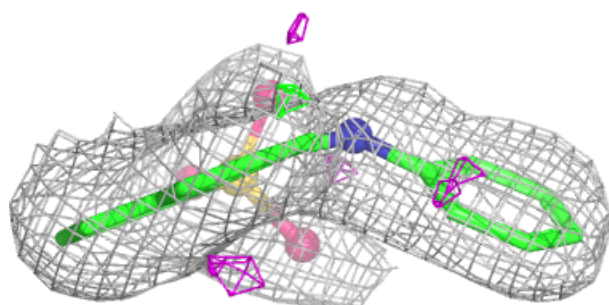
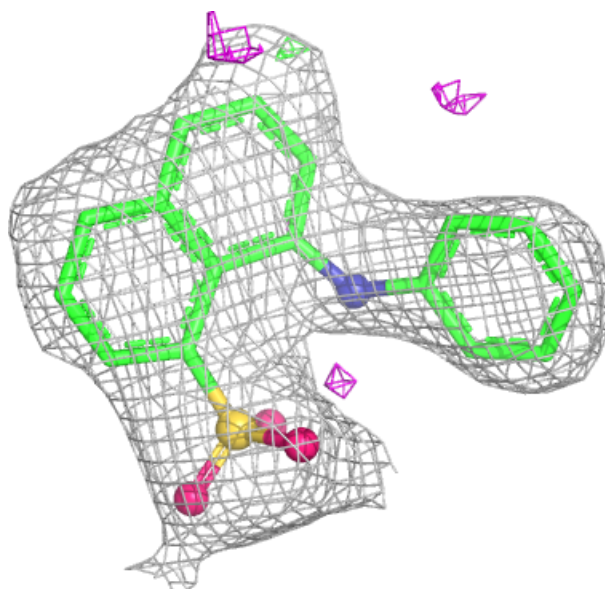
**Electron density around 2AN M 203:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



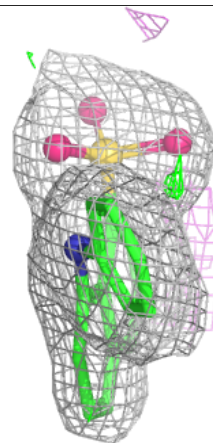
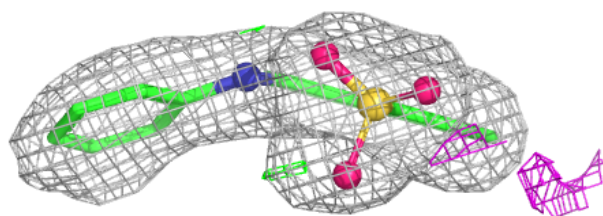
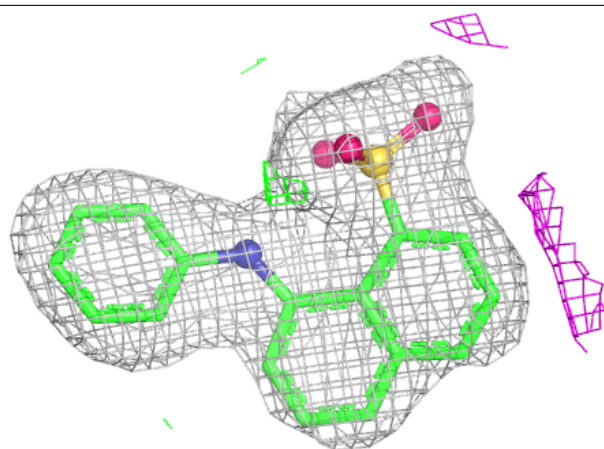
**Electron density around 2AN Z 201:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



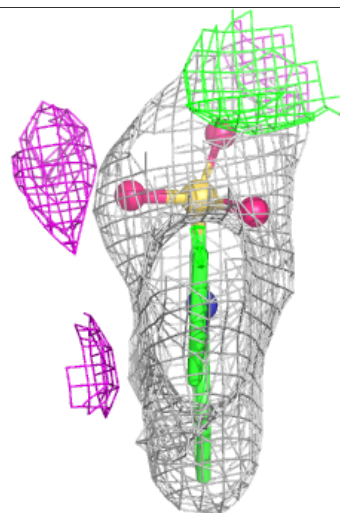
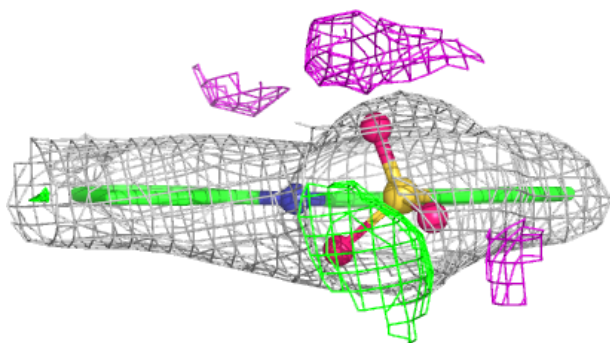
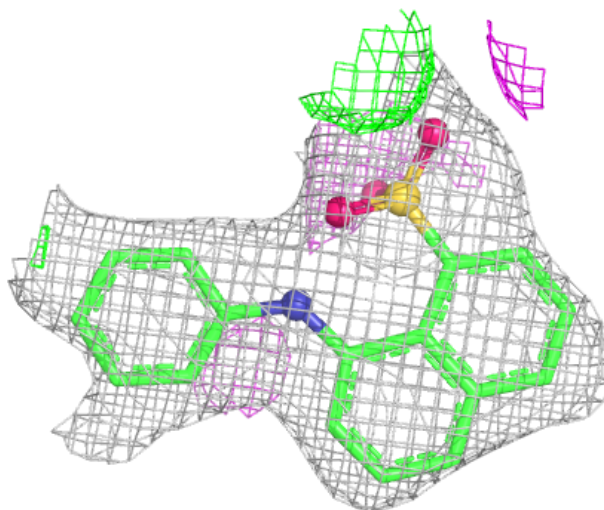
**Electron density around 2AN S 202:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around 2AN X 204:**

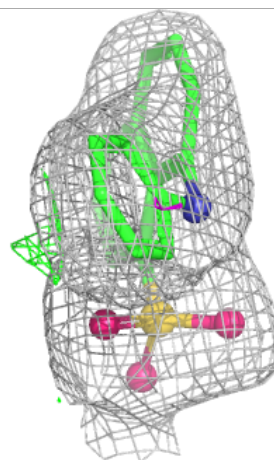
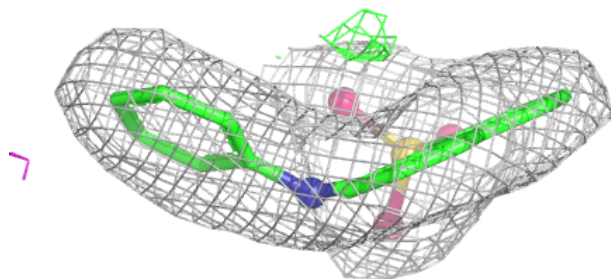
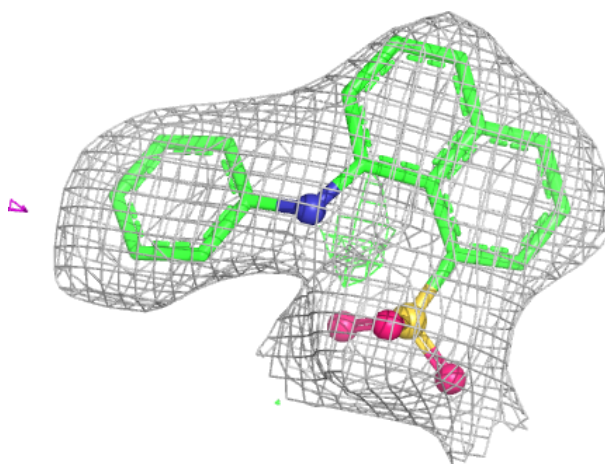
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





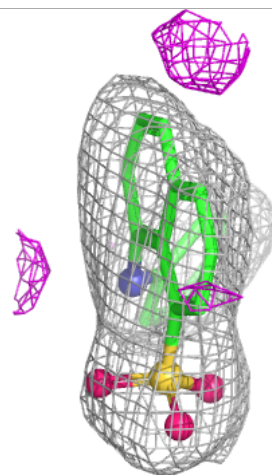
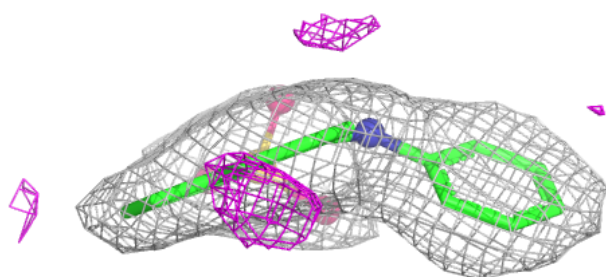
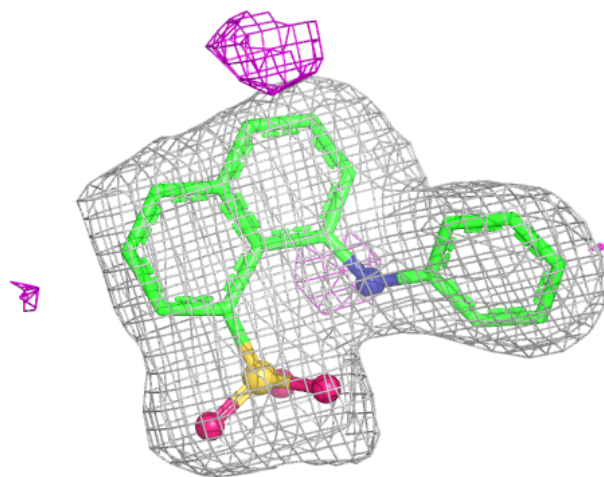
**Electron density around 2AN H 202:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



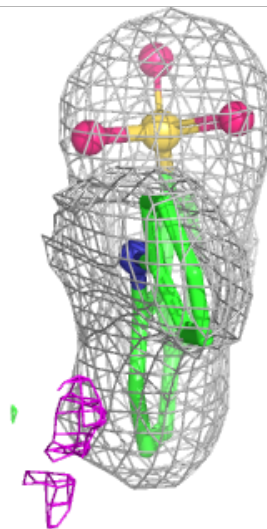
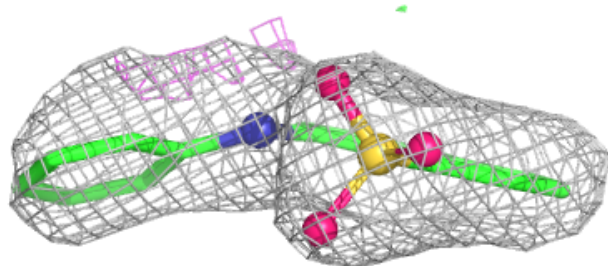
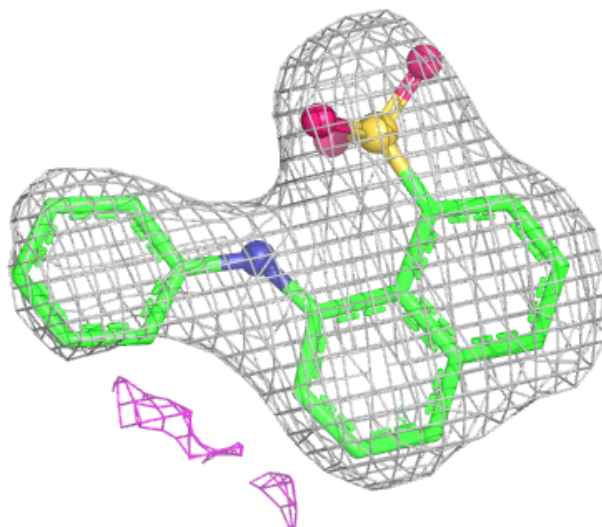
**Electron density around 2AN C 201:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around 2AN Y 203:**

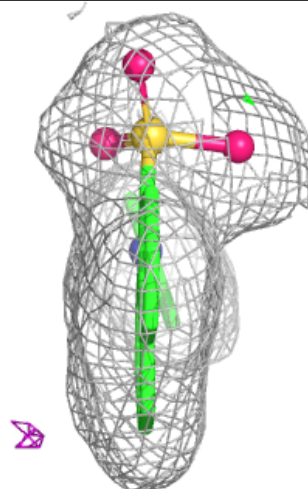
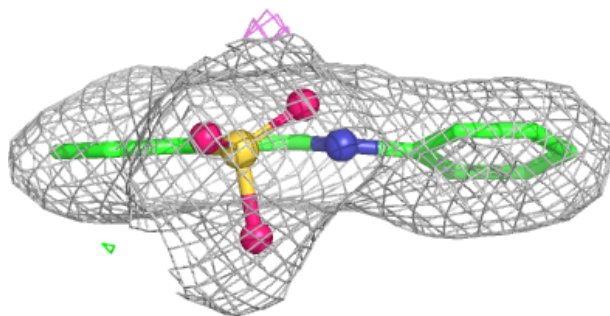
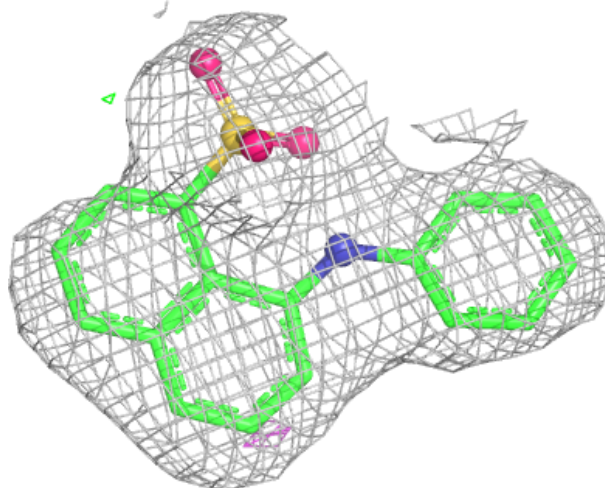
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





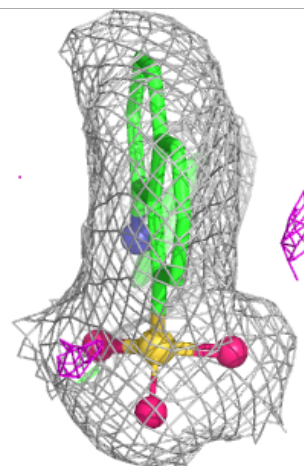
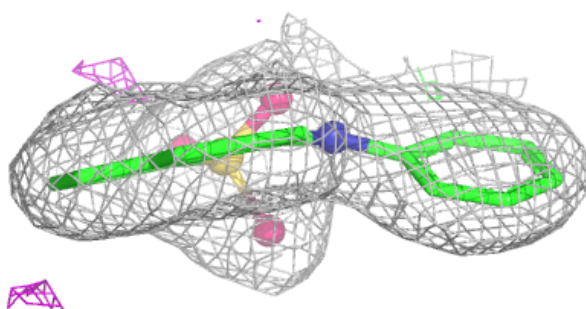
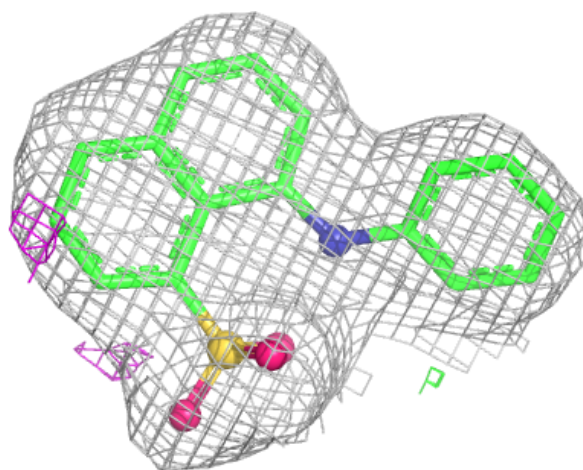
**Electron density around 2AN V 201:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



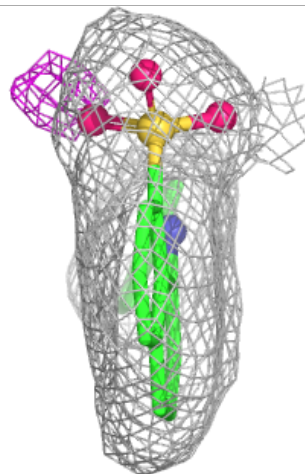
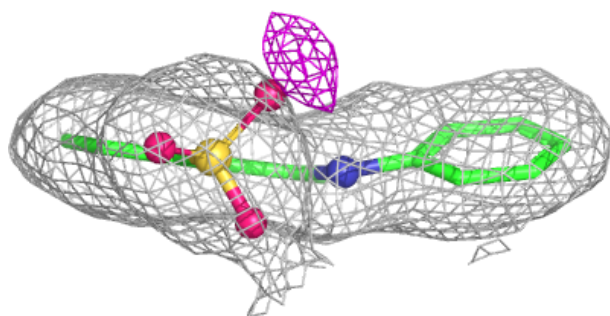
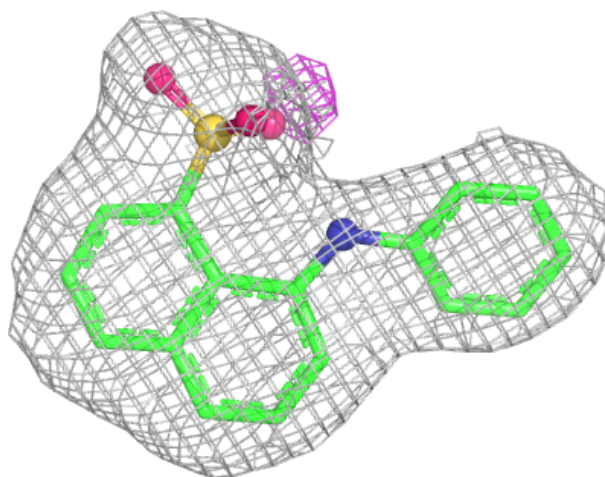
**Electron density around 2AN V 203:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



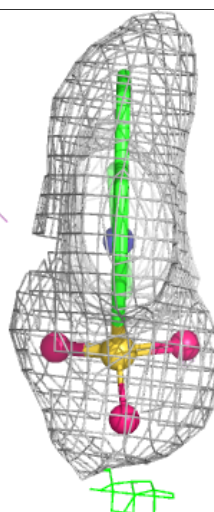
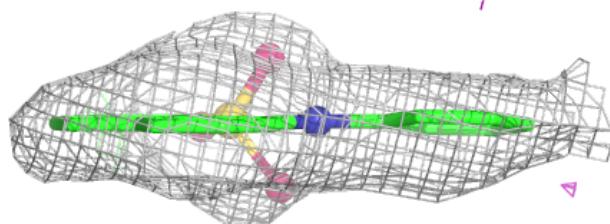
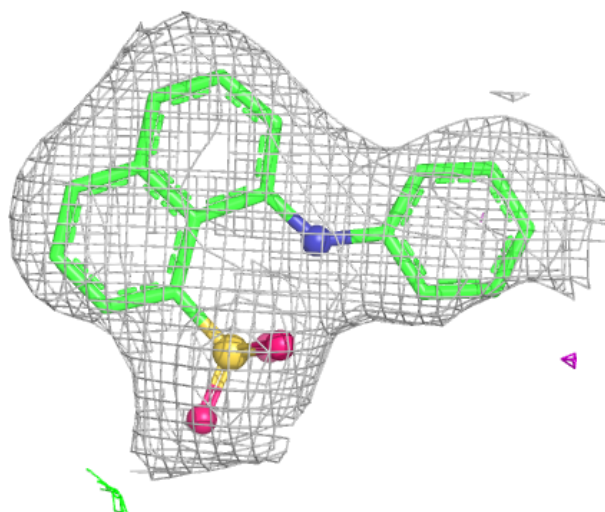
**Electron density around 2AN I 202:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



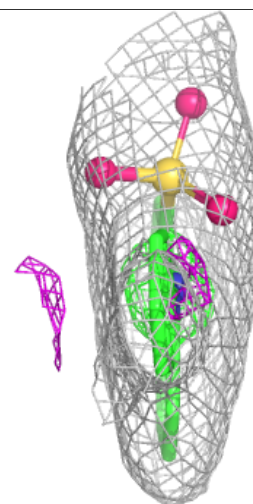
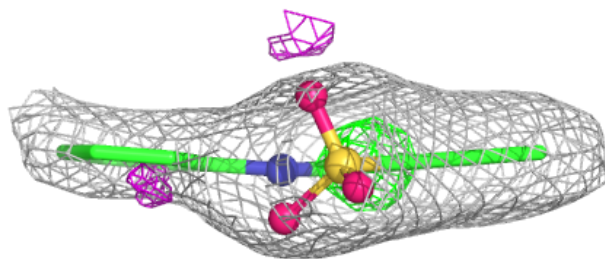
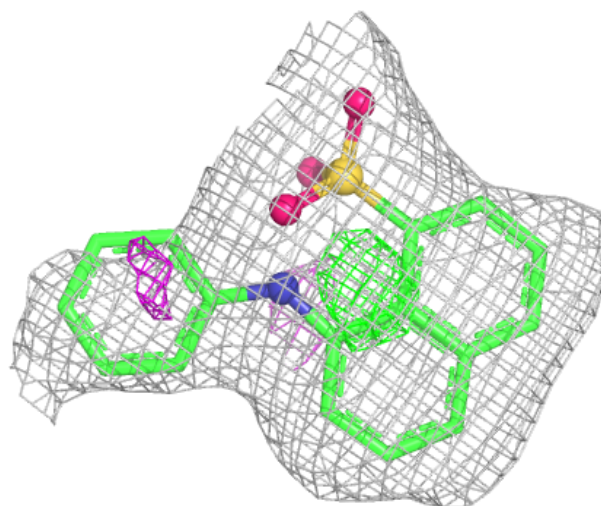
**Electron density around 2AN Z 204:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



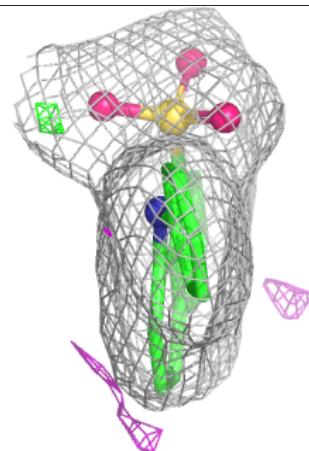
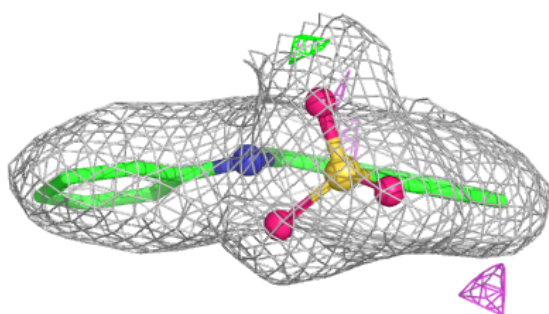
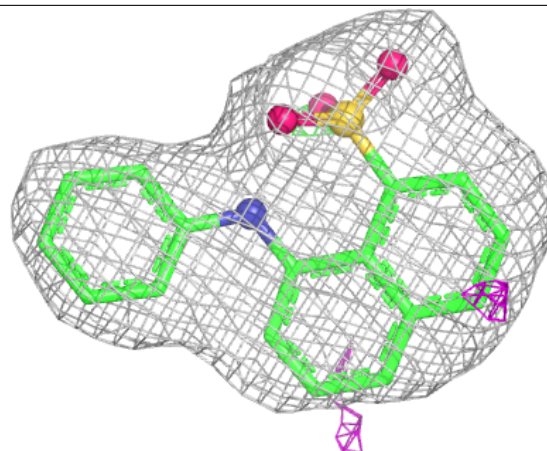
**Electron density around 2AN O 201:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around 2AN N 201:**

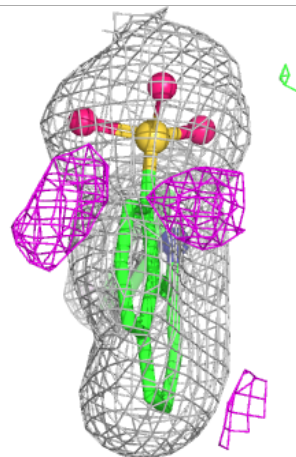
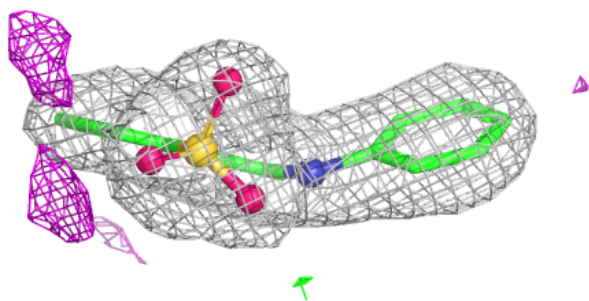
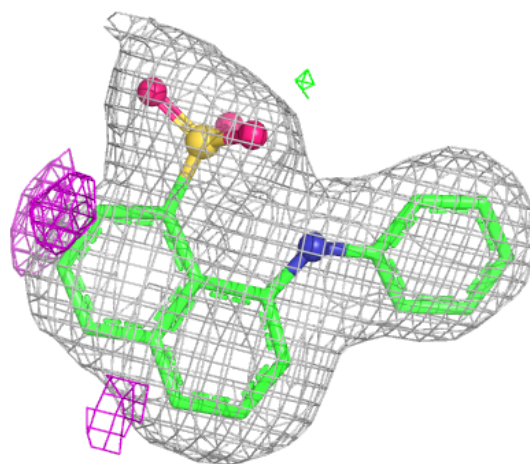
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





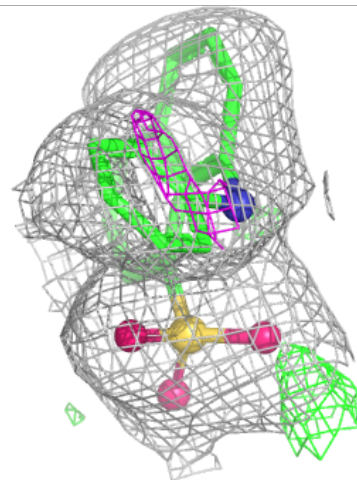
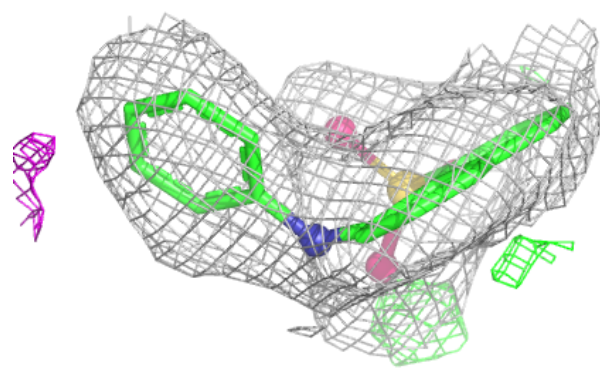
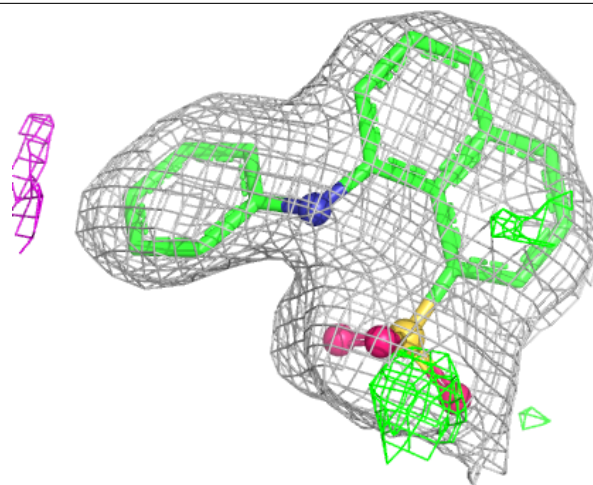
**Electron density around 2AN e 201:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

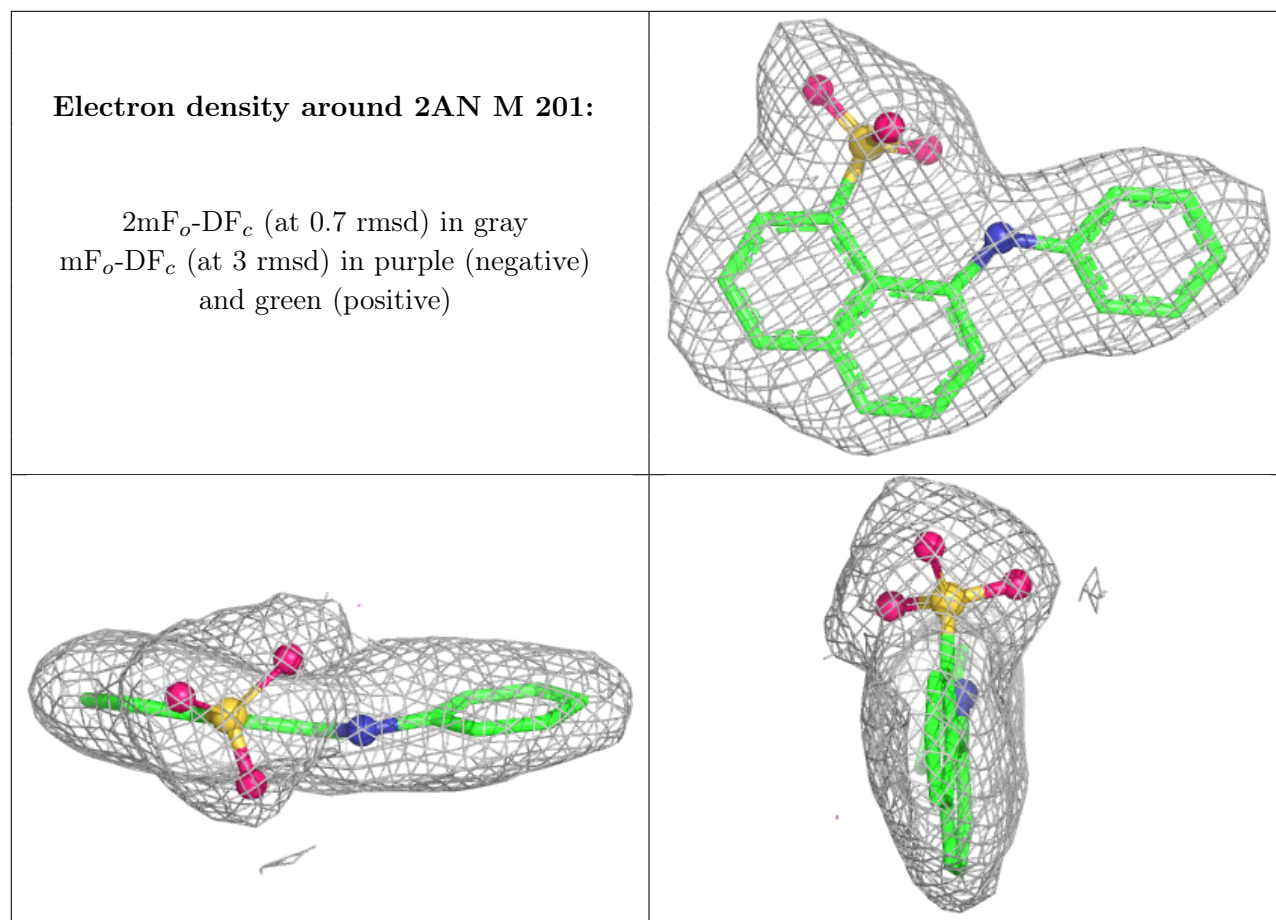


**Electron density around 2AN J 203:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

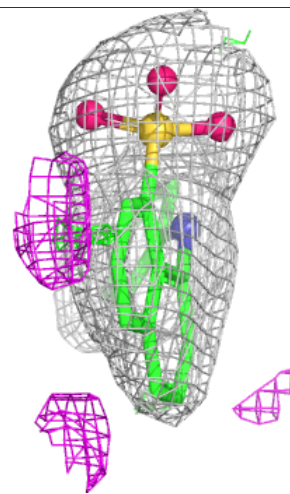
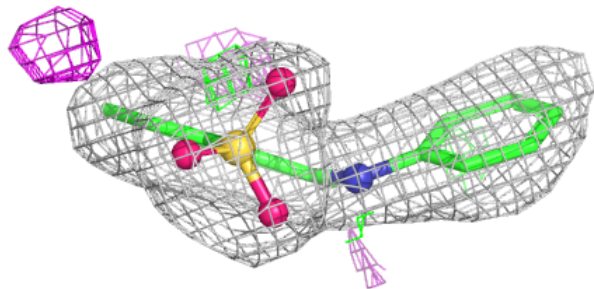
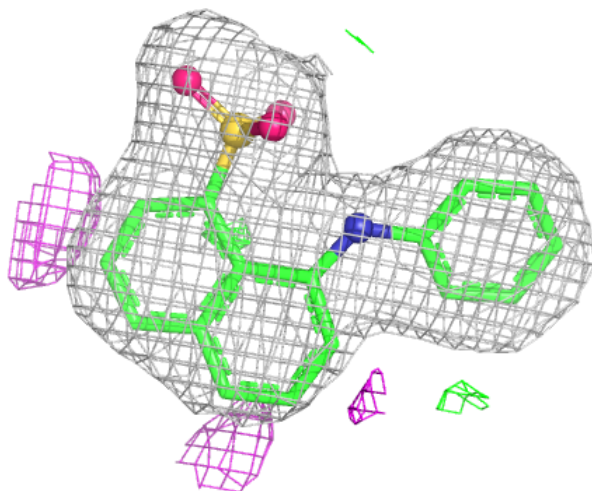






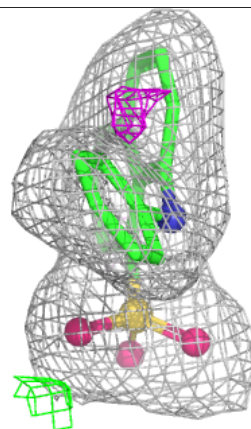
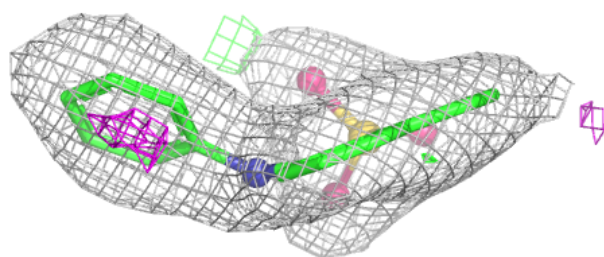
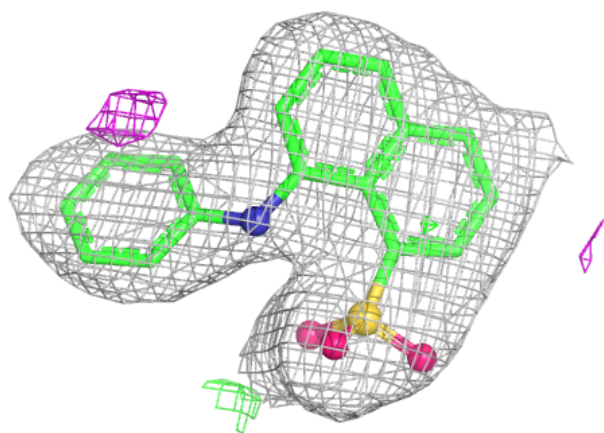
**Electron density around 2AN g 202:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



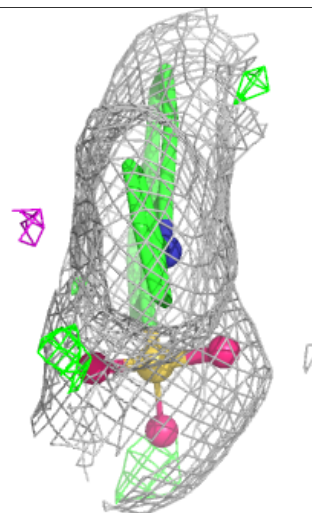
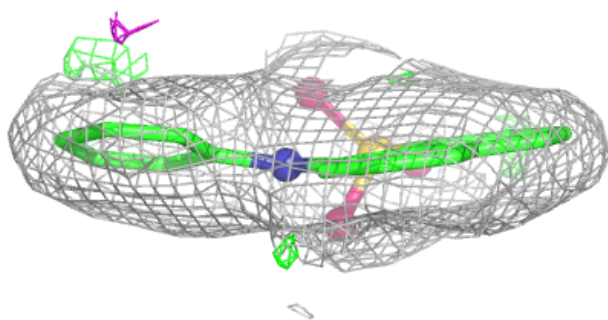
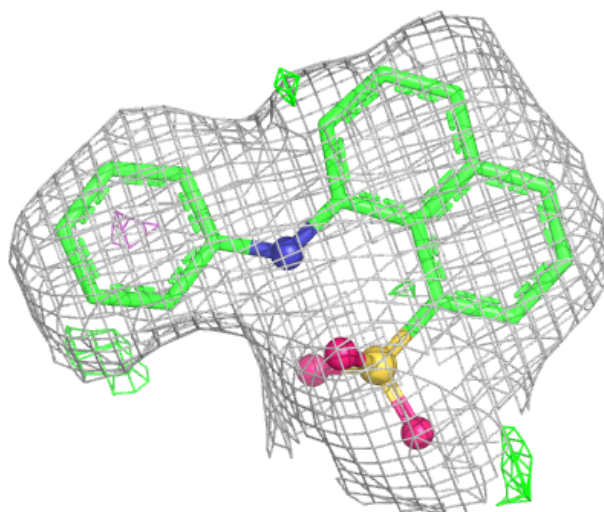
**Electron density around 2AN E 202:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



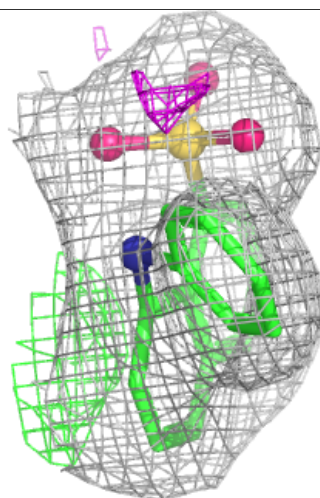
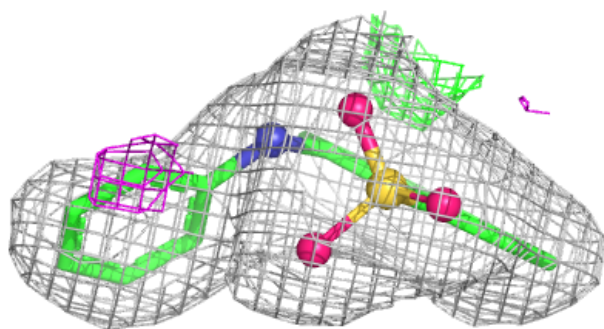
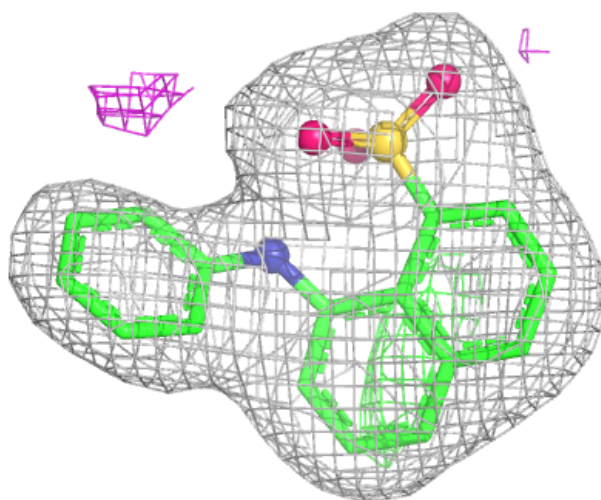
**Electron density around 2AN T 201:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around 2AN G 202:**

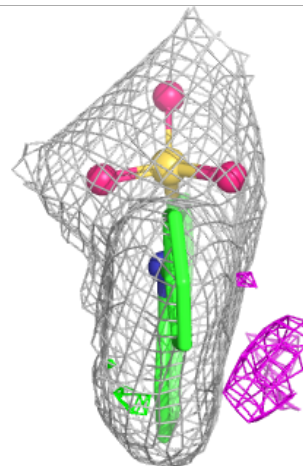
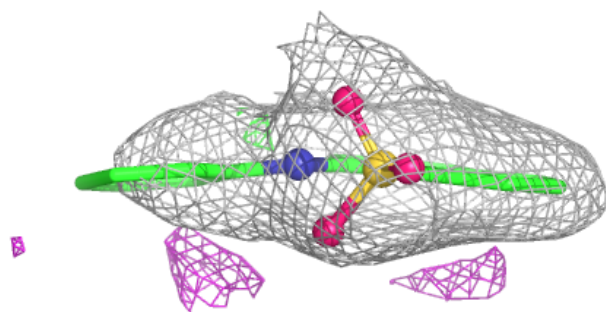
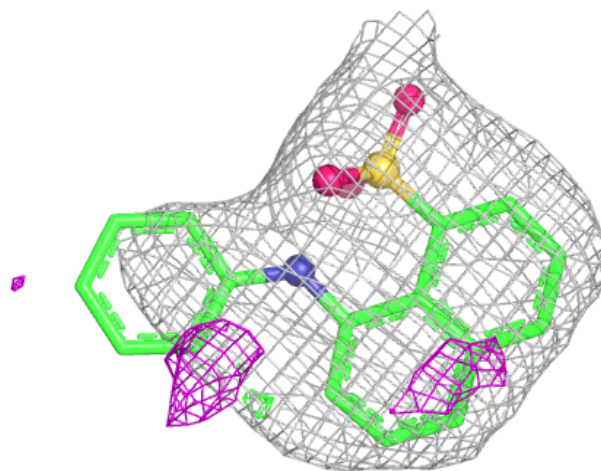
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





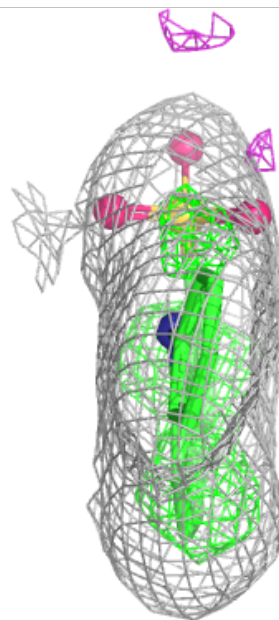
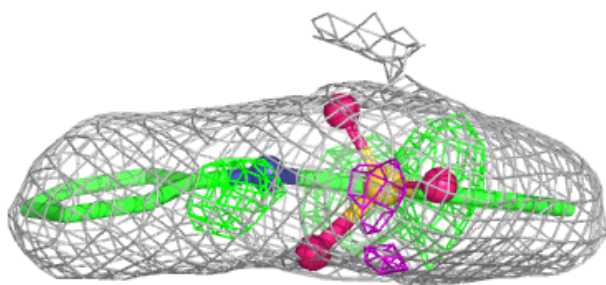
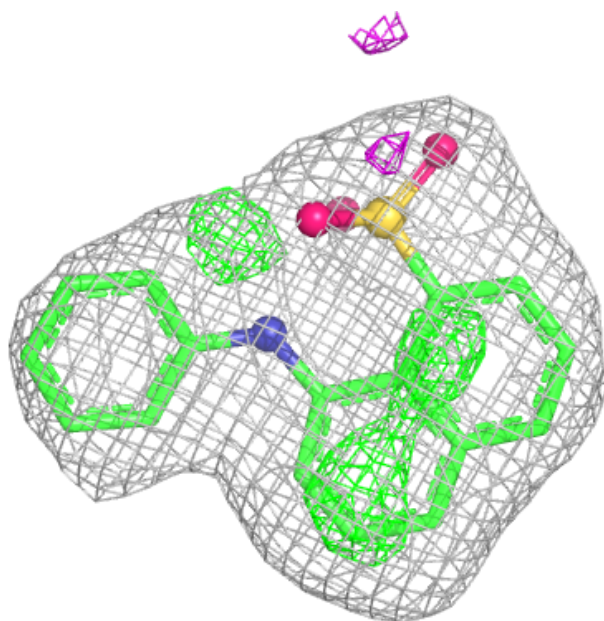
**Electron density around 2AN G 203:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



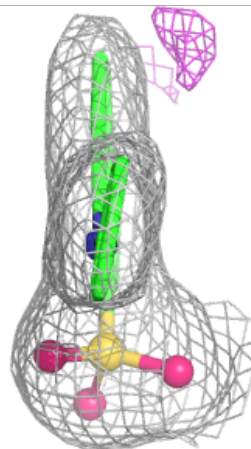
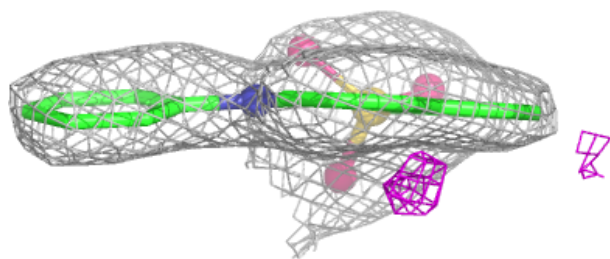
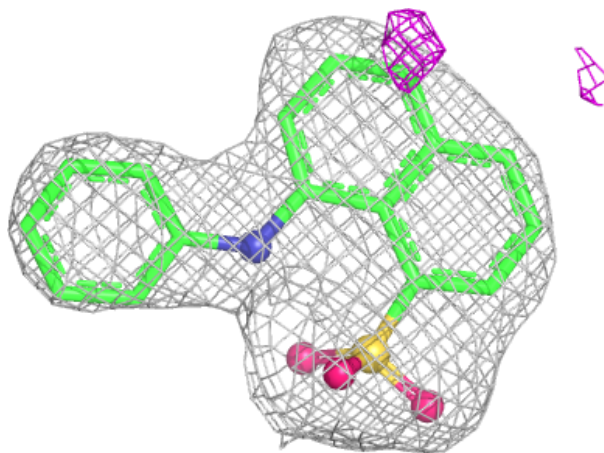
**Electron density around 2AN B 203:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around 2AN c 204:**

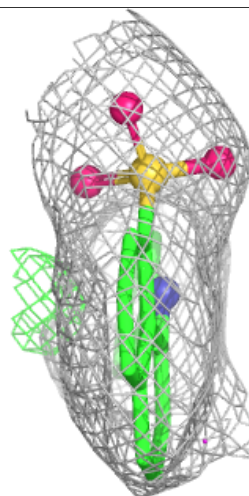
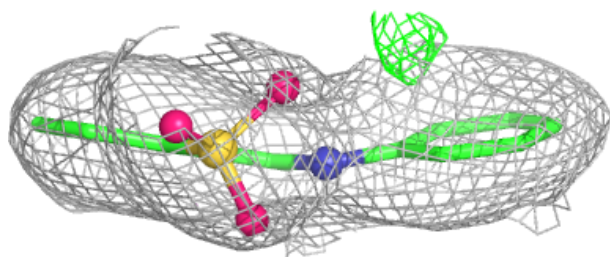
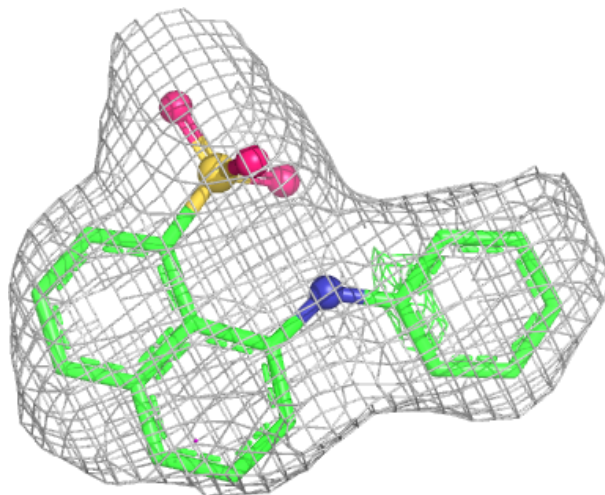
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





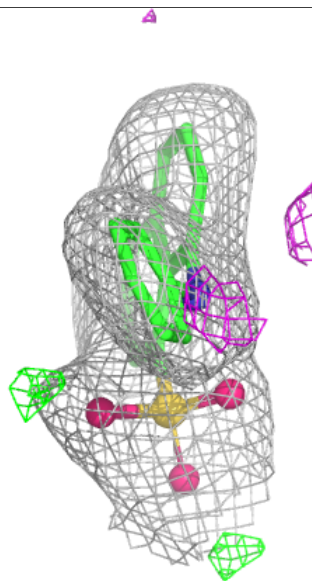
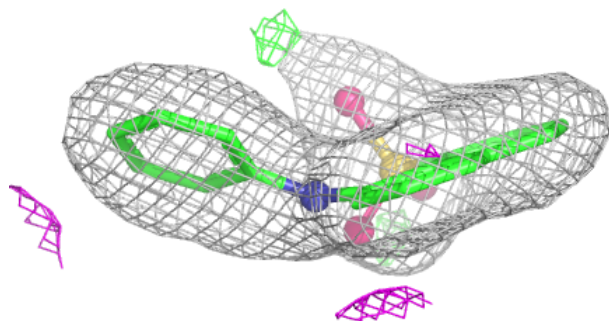
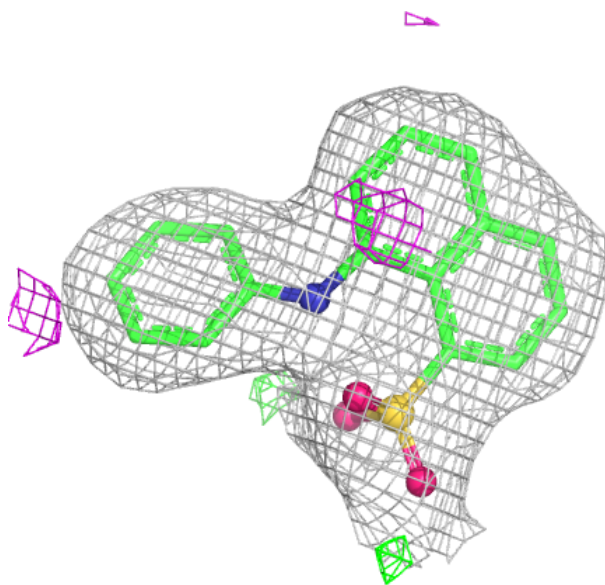
**Electron density around 2AN Q 202:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



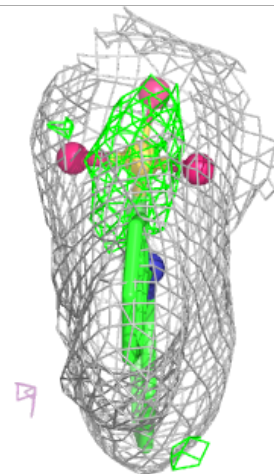
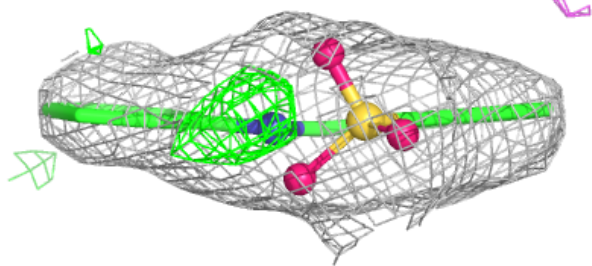
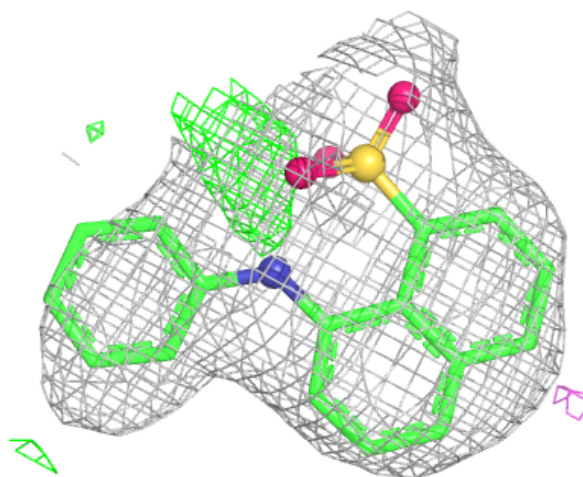
**Electron density around 2AN K 201:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



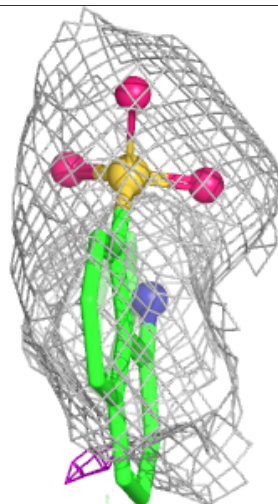
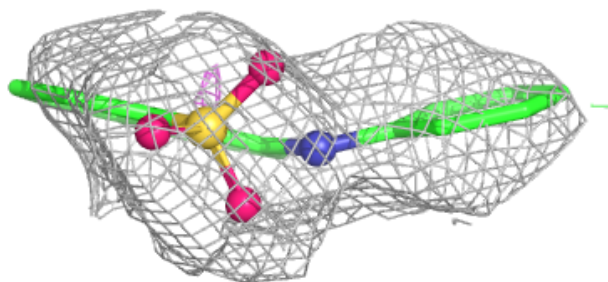
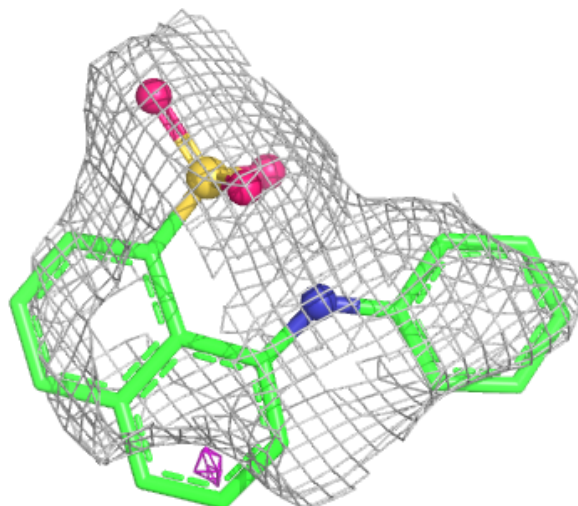
**Electron density around 2AN N 204:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



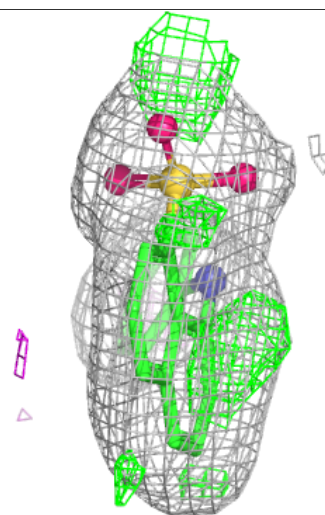
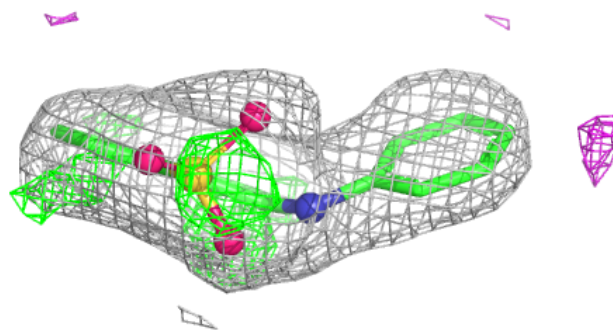
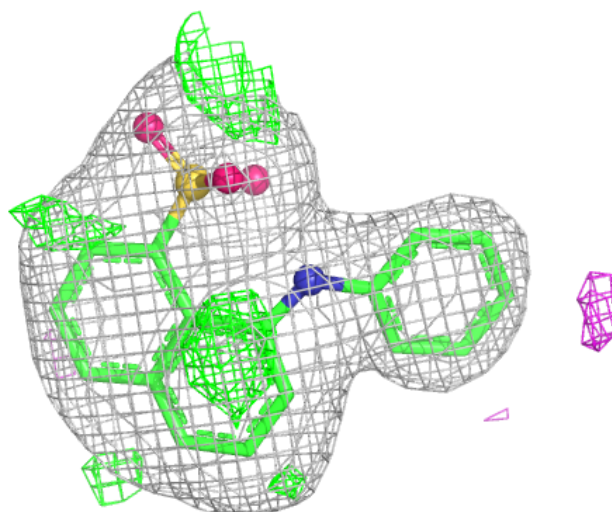
**Electron density around 2AN C 202:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around 2AN P 204:**

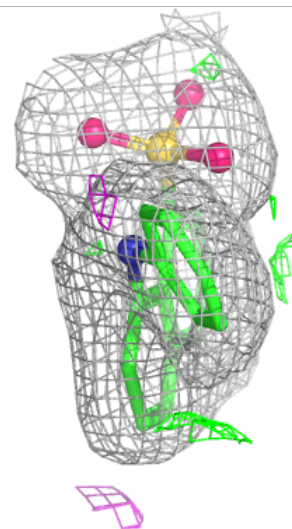
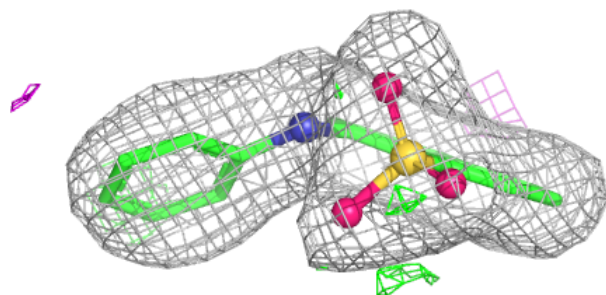
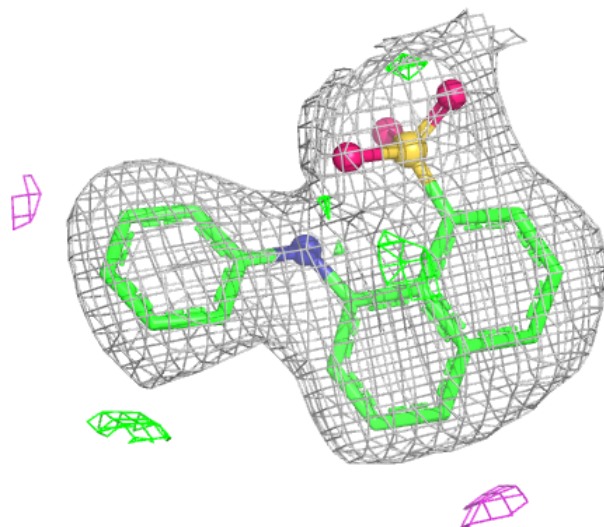
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





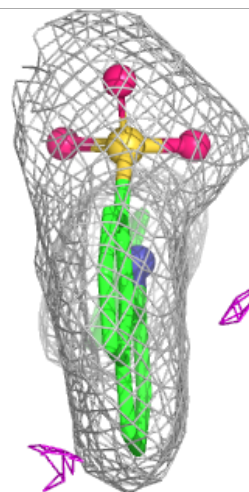
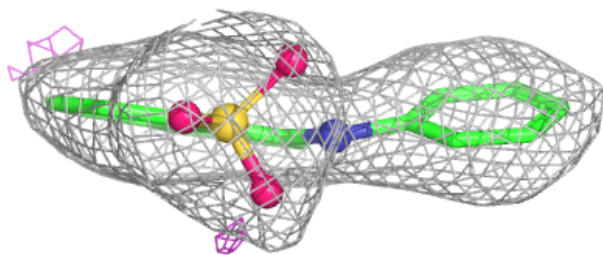
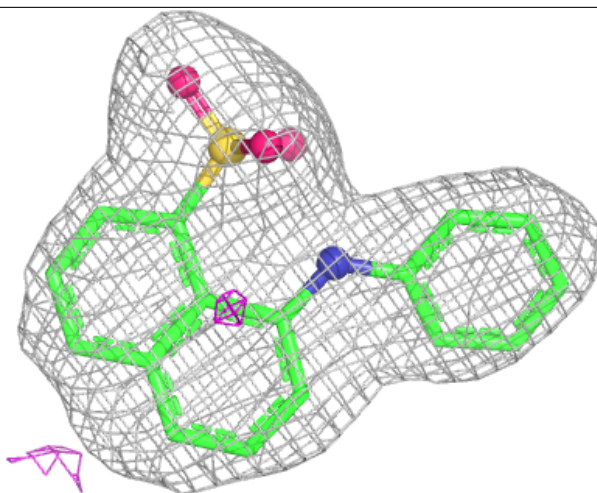
**Electron density around 2AN f 202:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



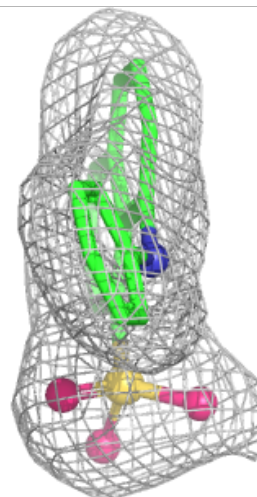
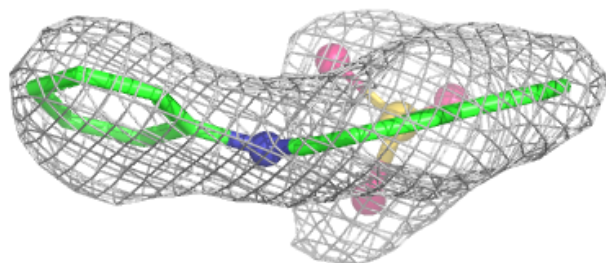
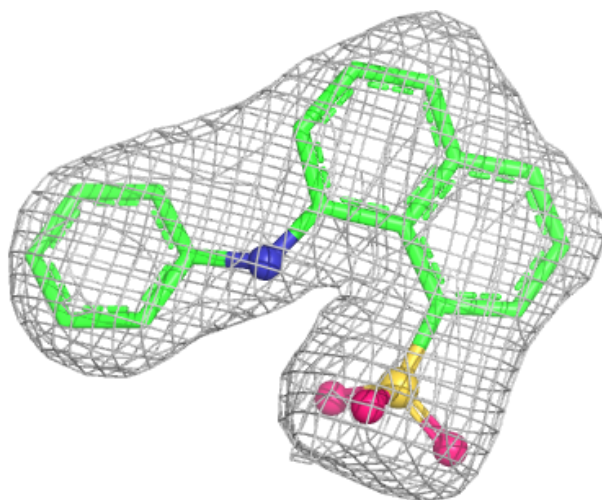
**Electron density around 2AN H 201:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around 2AN a 202:**

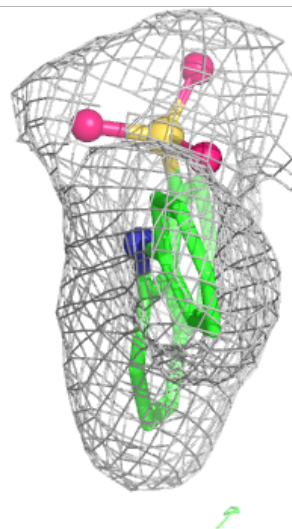
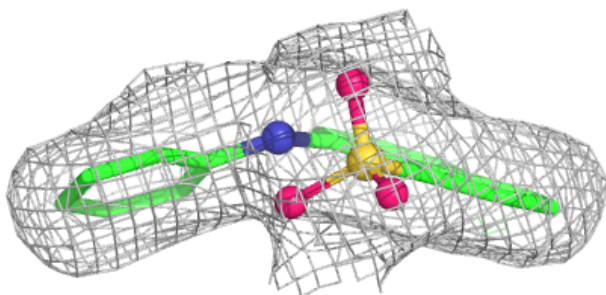
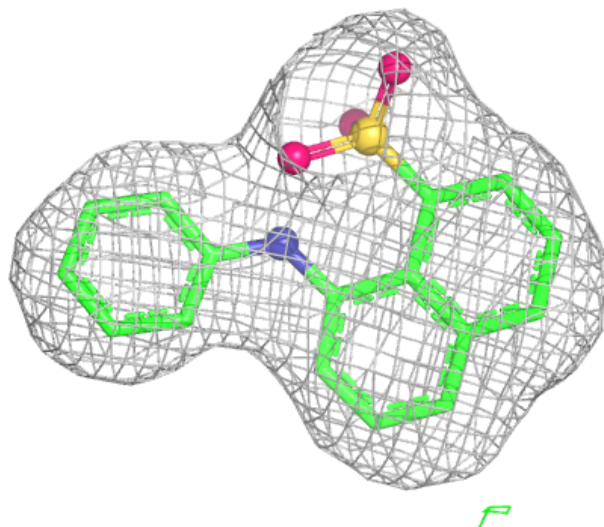
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





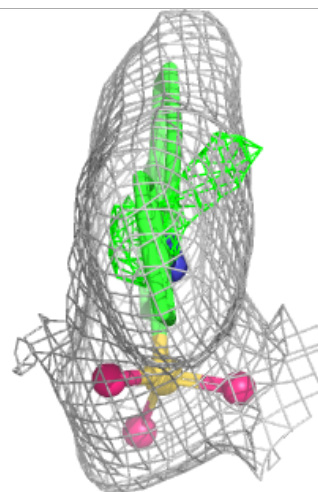
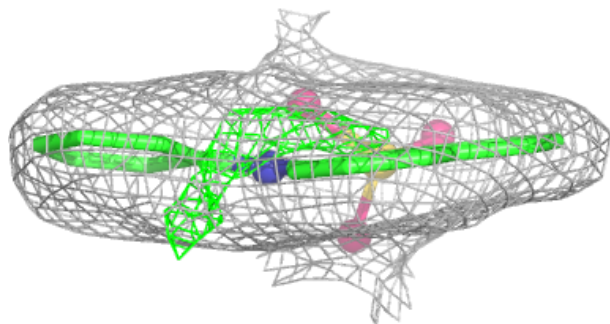
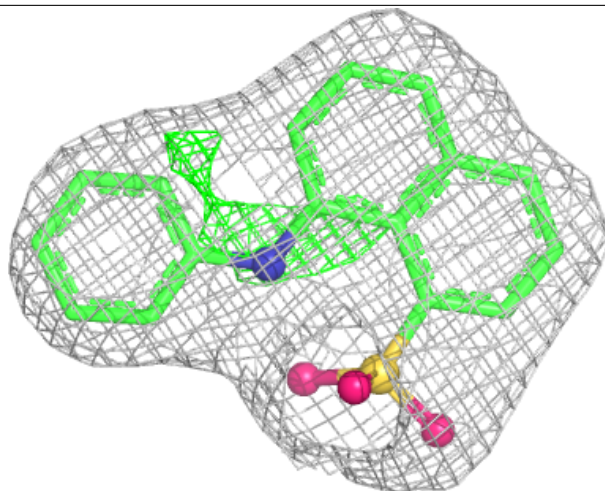
**Electron density around 2AN f 204:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



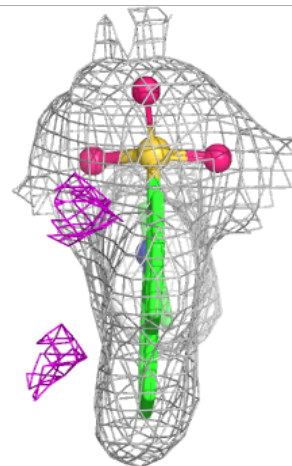
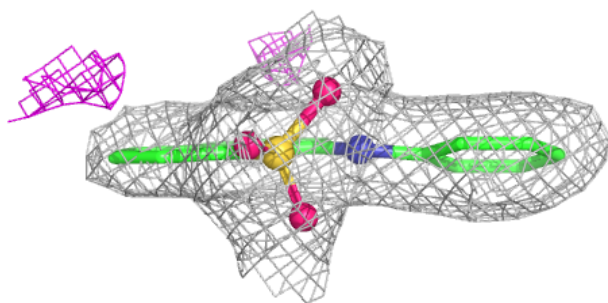
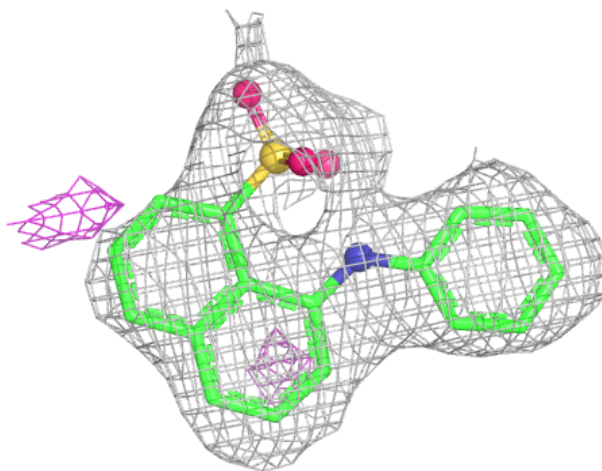
**Electron density around 2AN f 205:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



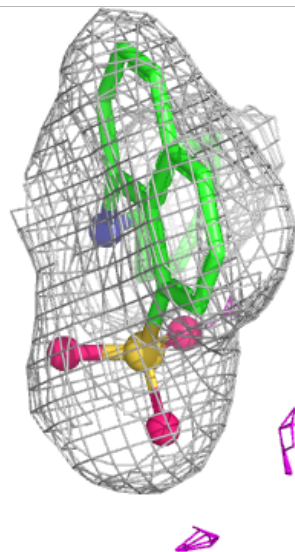
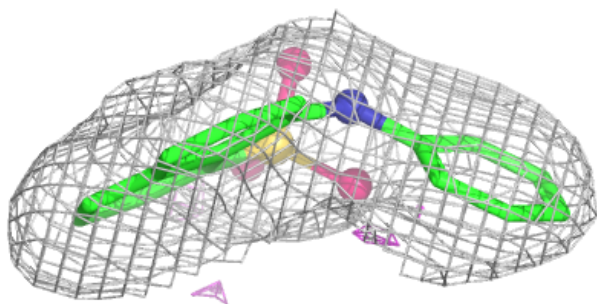
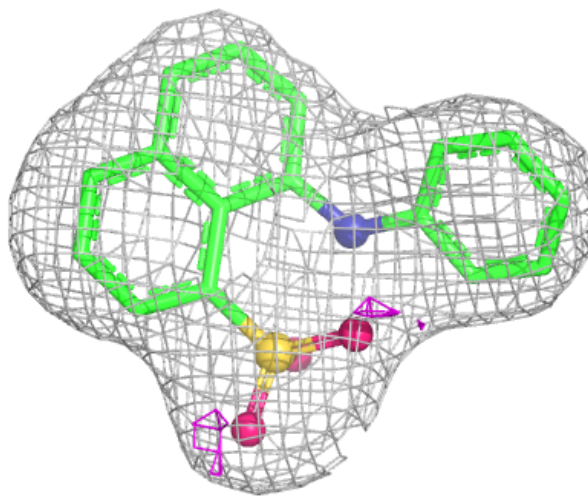
**Electron density around 2AN V 204:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



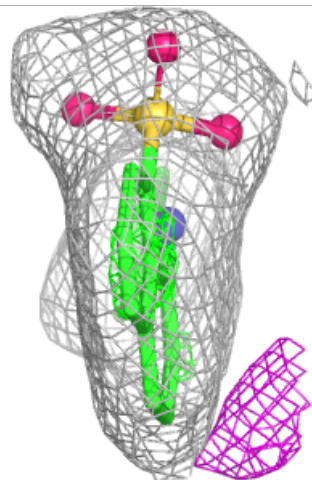
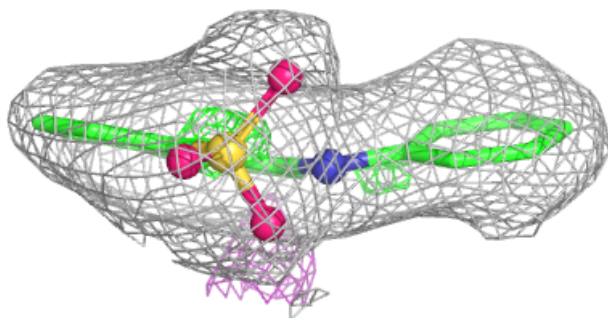
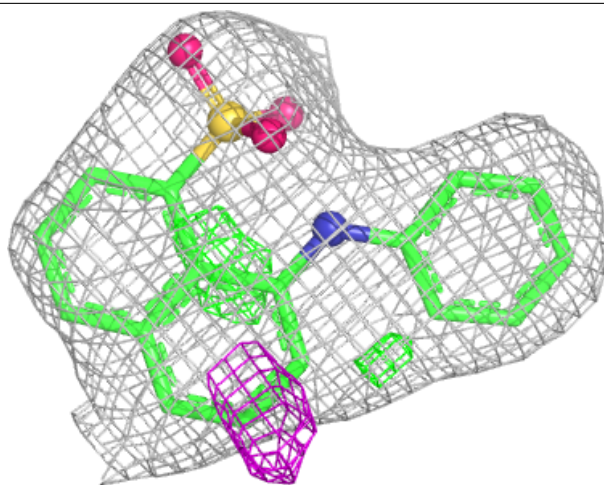
**Electron density around 2AN V 205:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around 2AN J 202:**

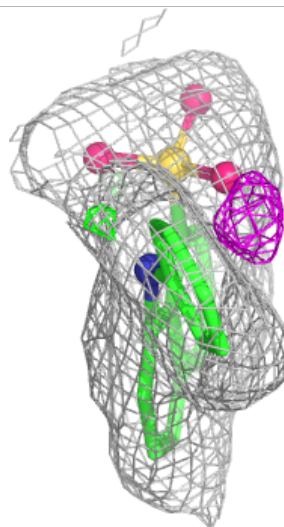
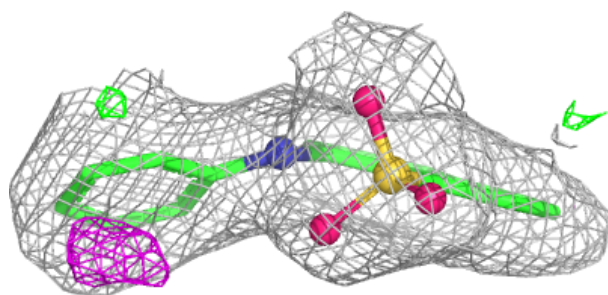
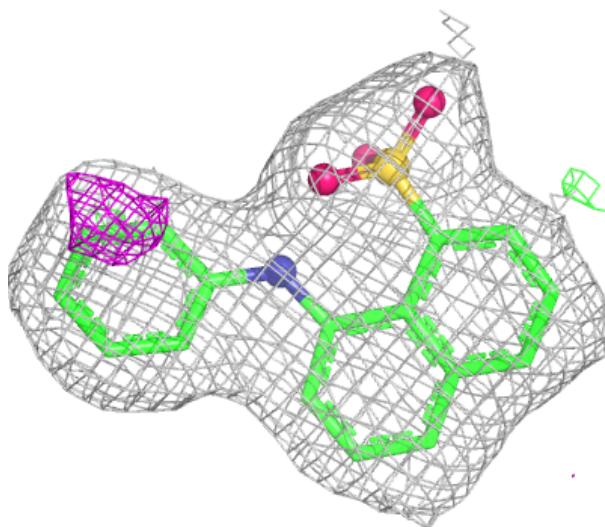
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





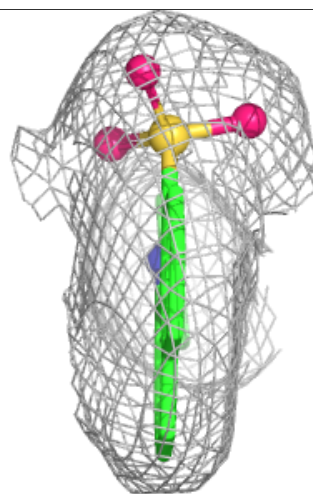
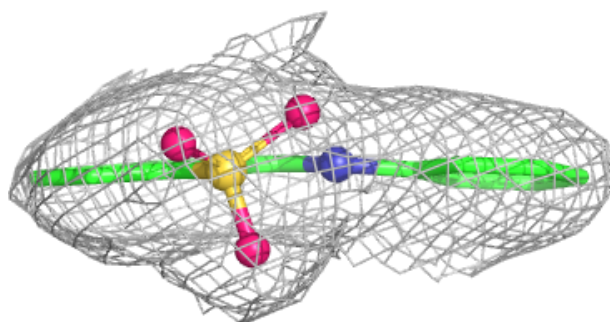
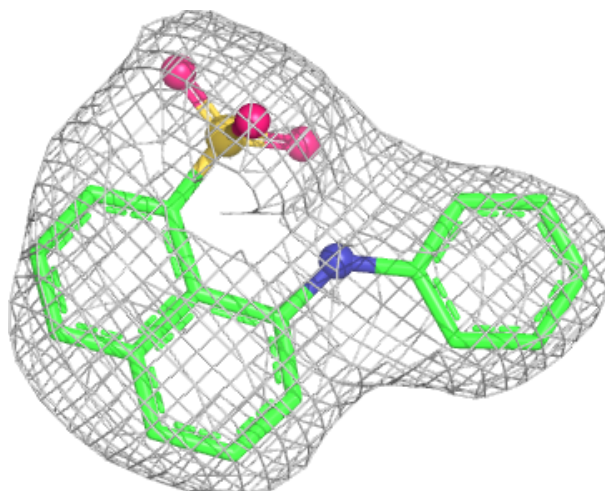
**Electron density around 2AN P 201:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



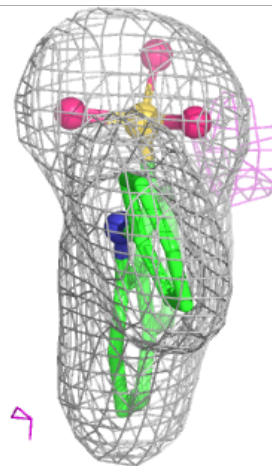
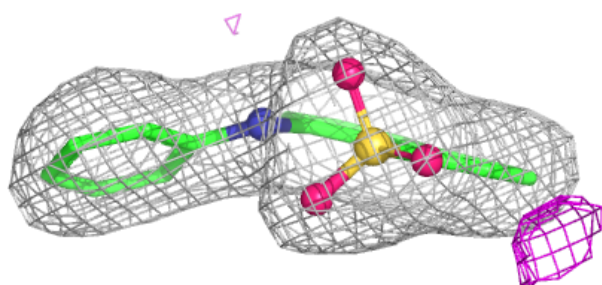
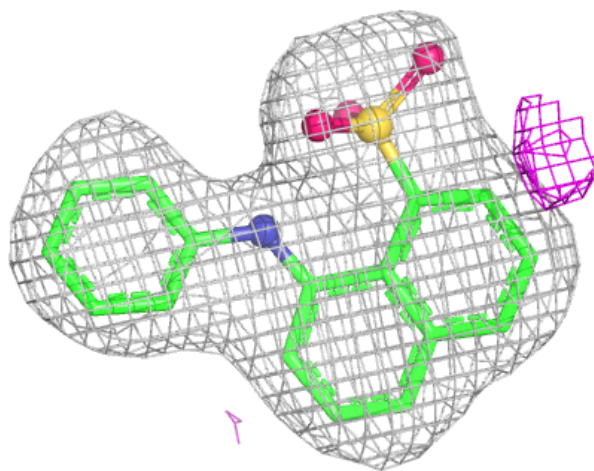
**Electron density around 2AN H 203:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around 2AN c 206:**

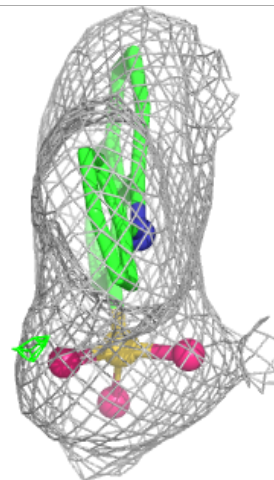
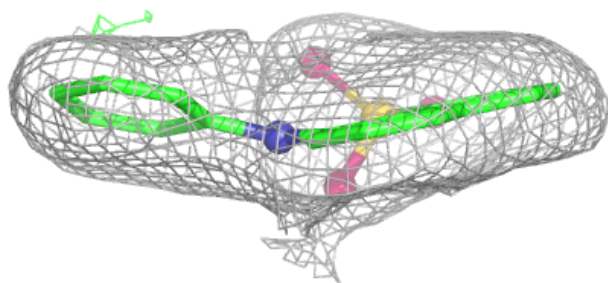
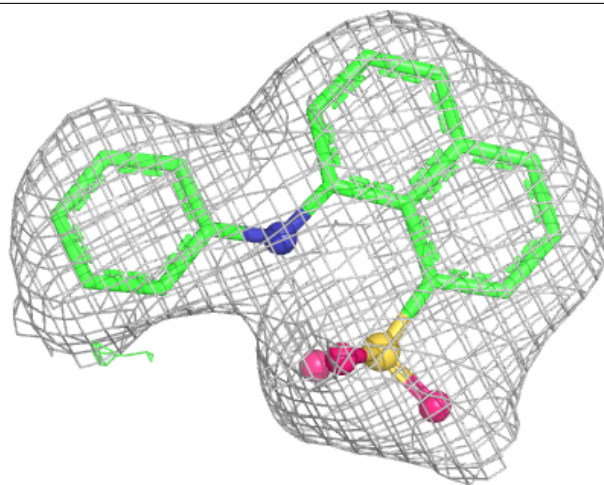
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





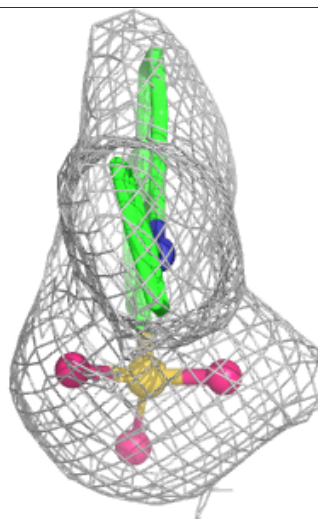
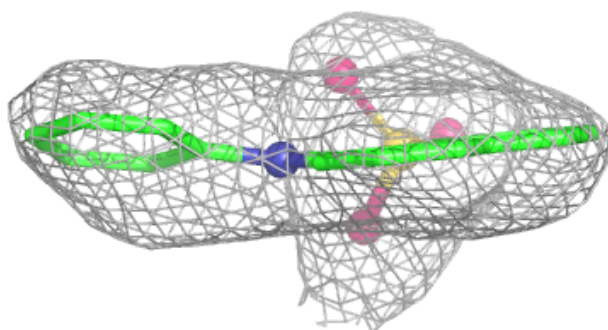
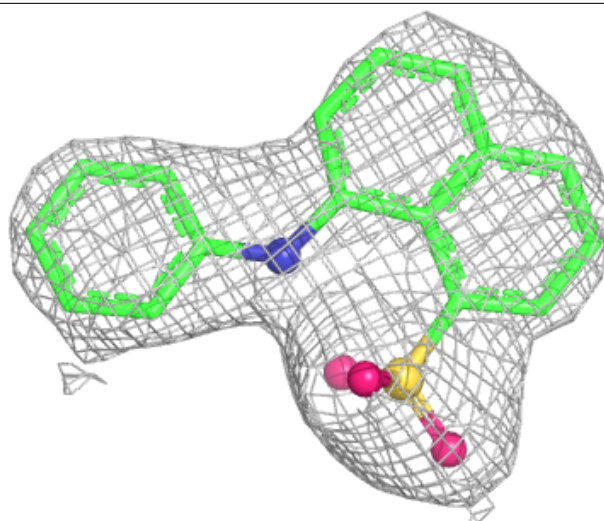
**Electron density around 2AN h 202:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



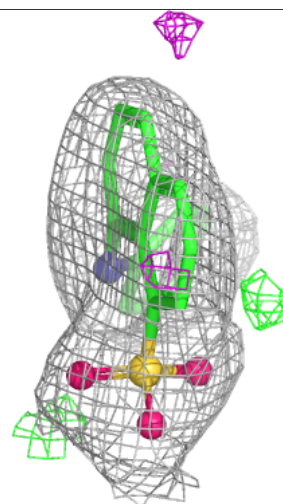
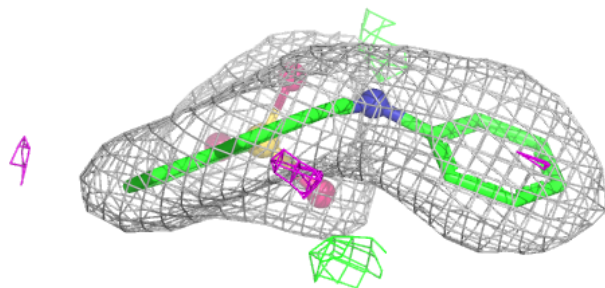
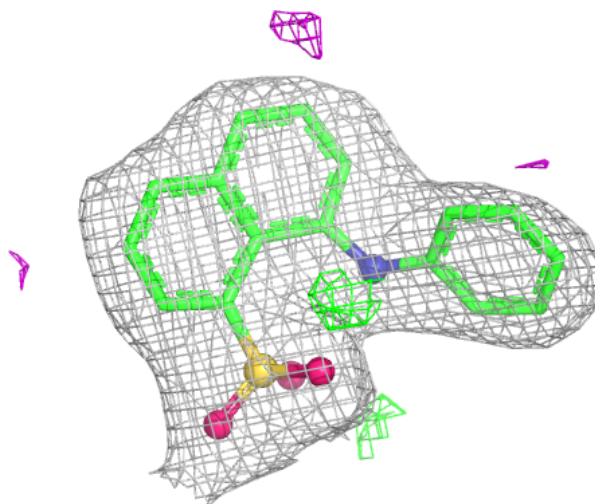
**Electron density around 2AN D 201:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



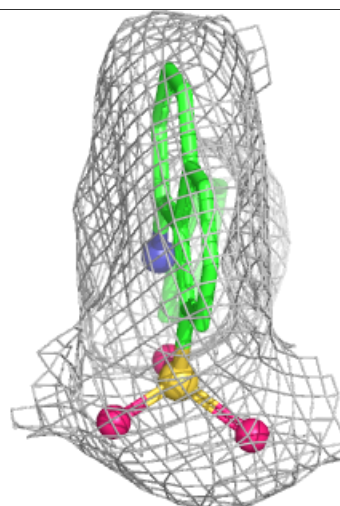
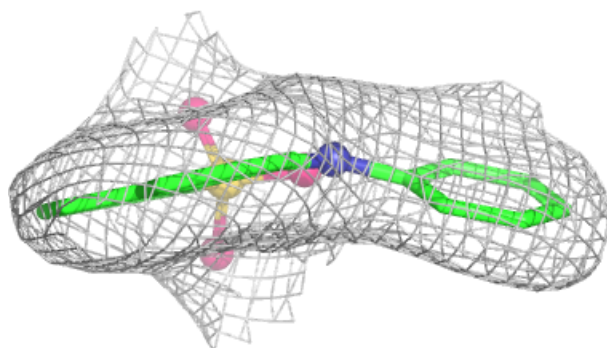
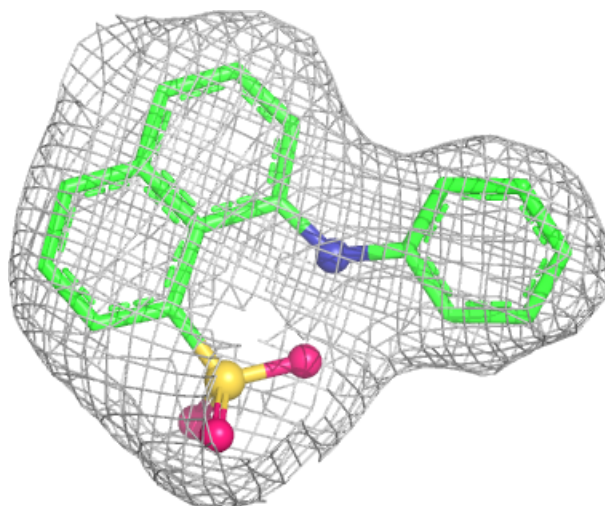
**Electron density around 2AN Q 201:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



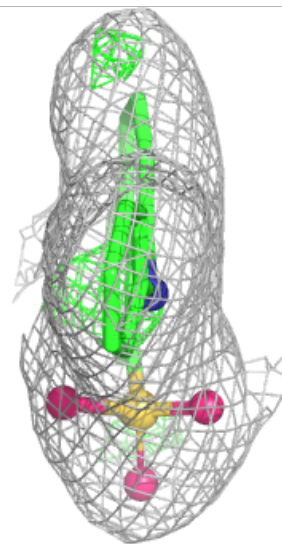
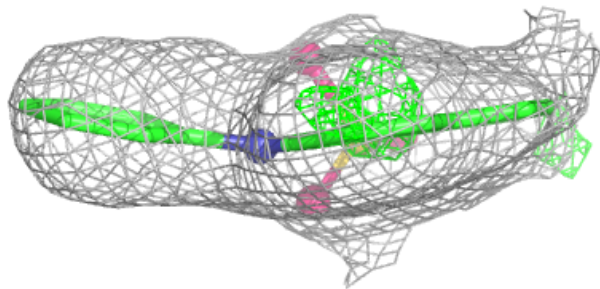
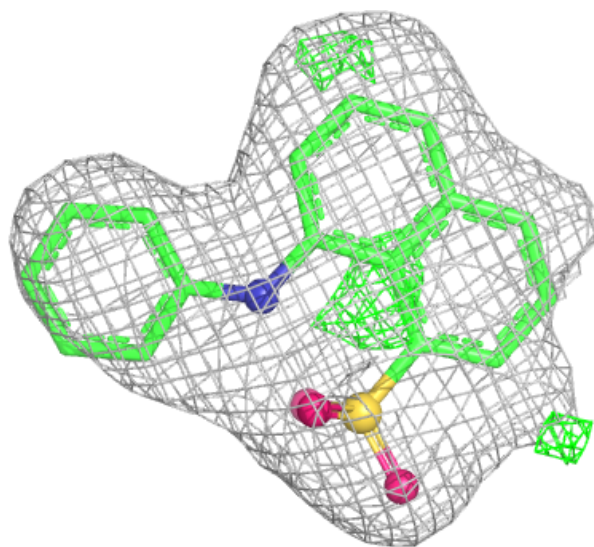
**Electron density around 2AN b 203:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around 2AN F 203:**

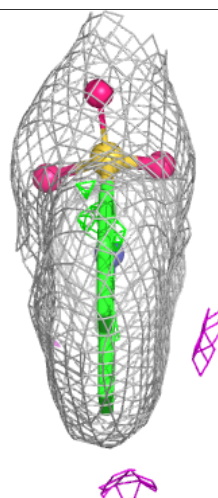
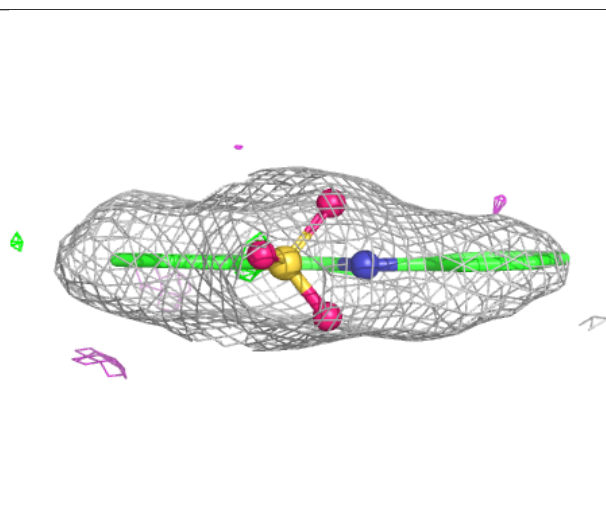
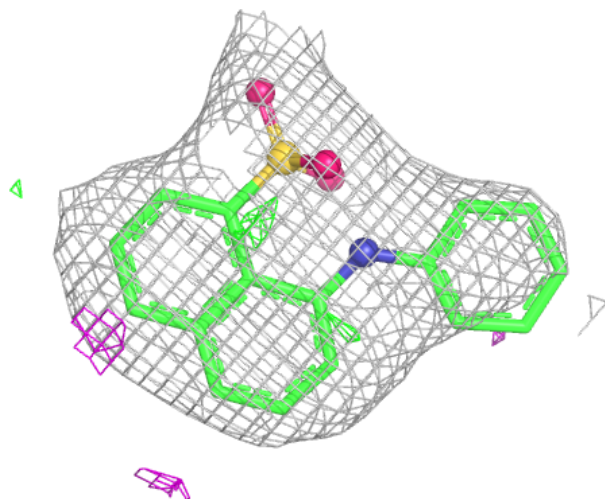
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





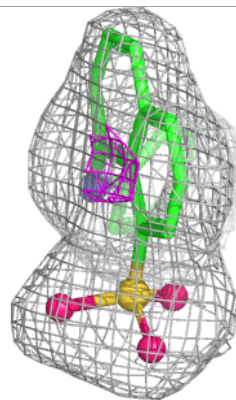
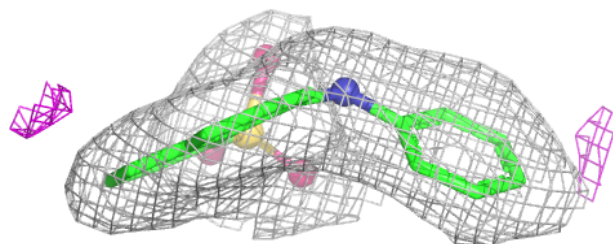
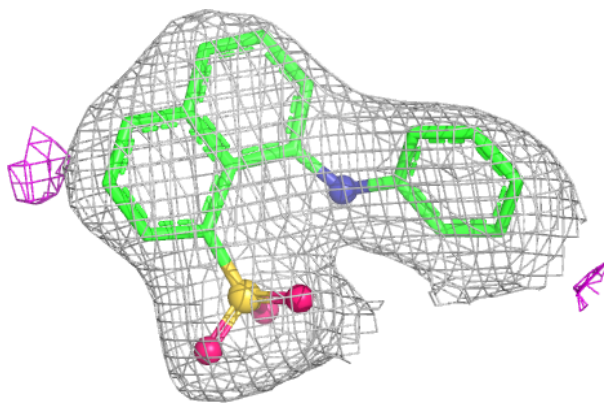
**Electron density around 2AN K 202:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



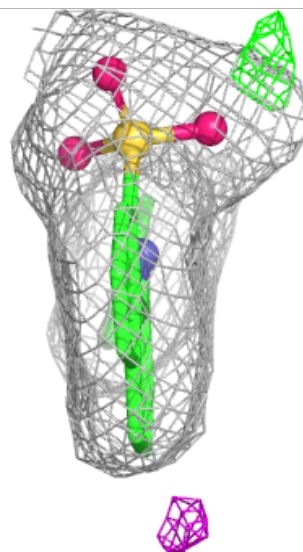
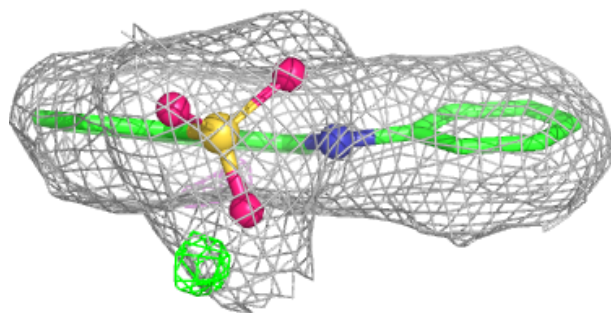
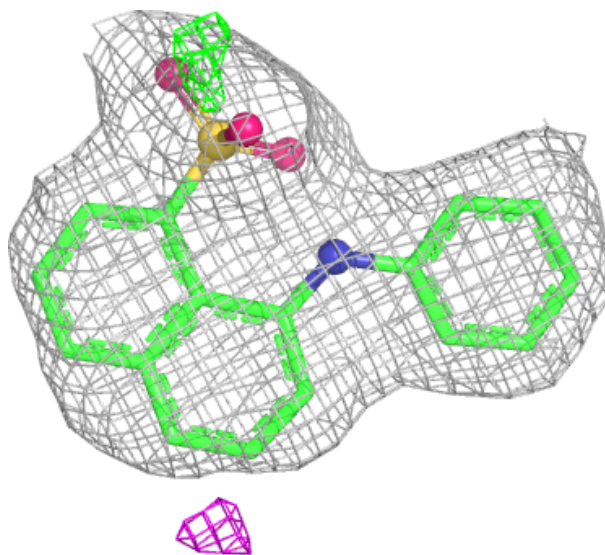
**Electron density around 2AN B 201:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around 2AN R 201:**

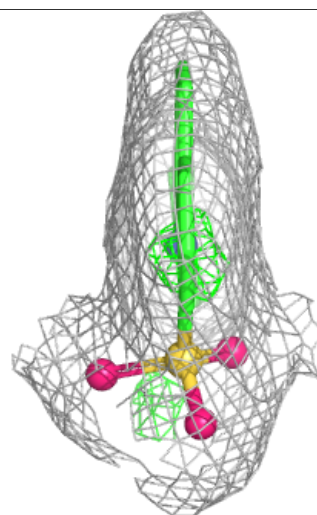
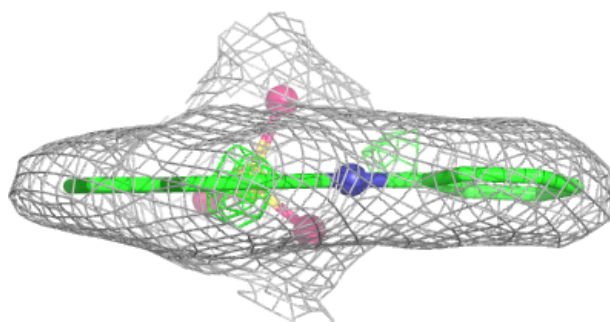
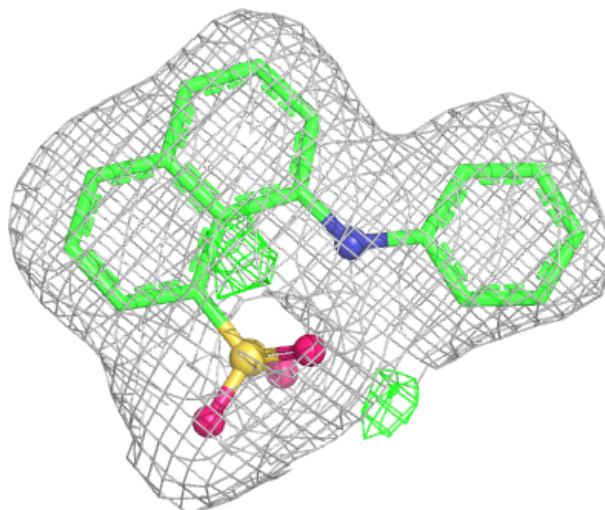
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





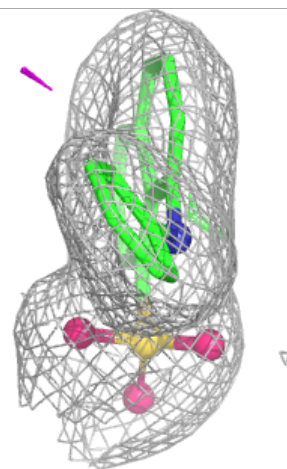
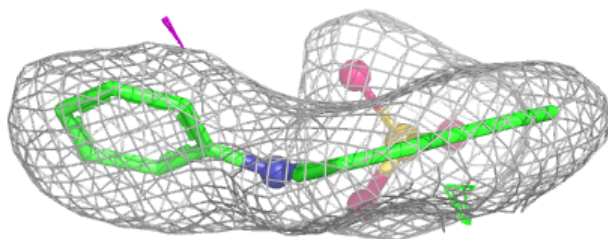
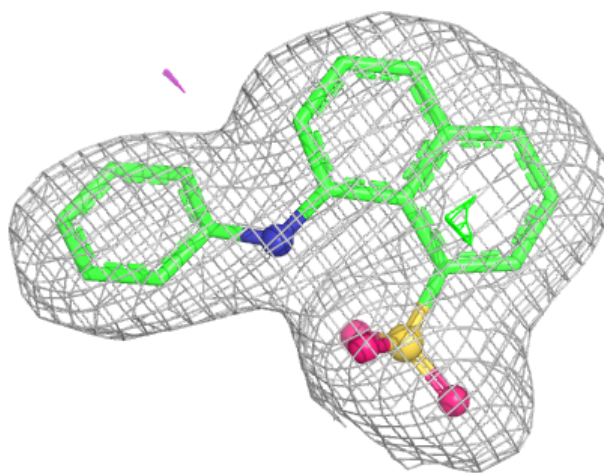
**Electron density around 2AN L 202:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



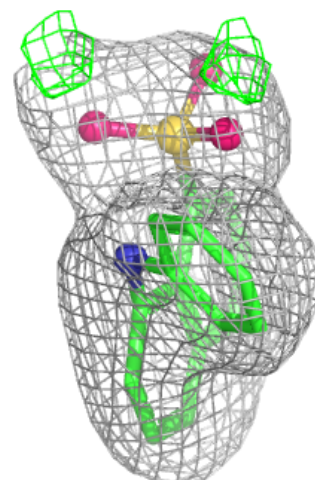
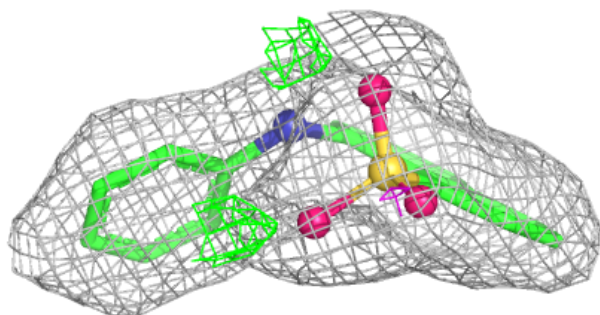
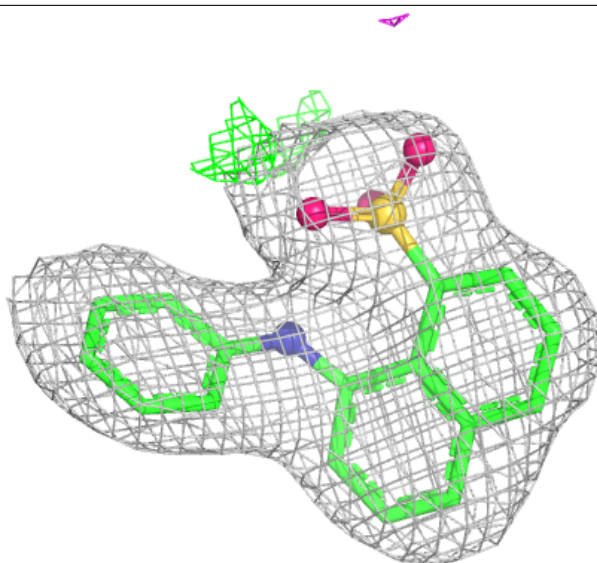
**Electron density around 2AN f 201:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



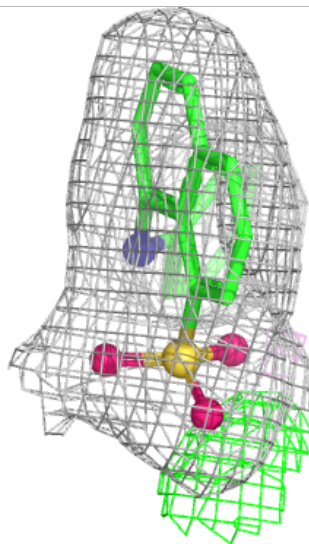
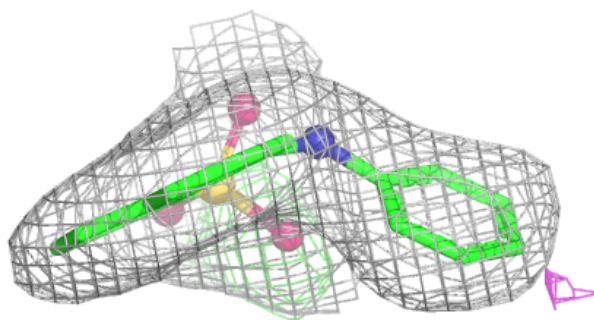
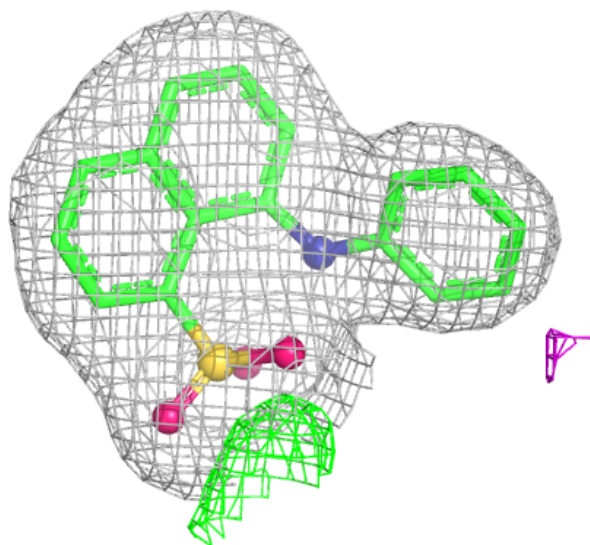
**Electron density around 2AN L 203:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



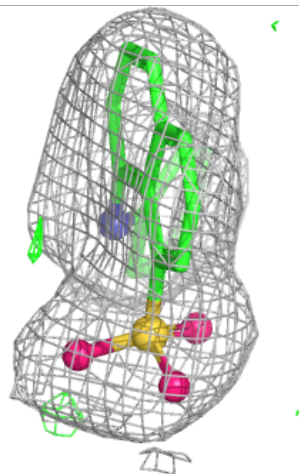
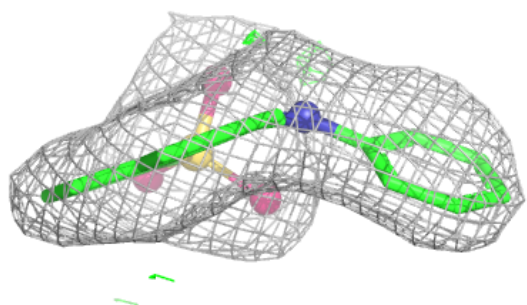
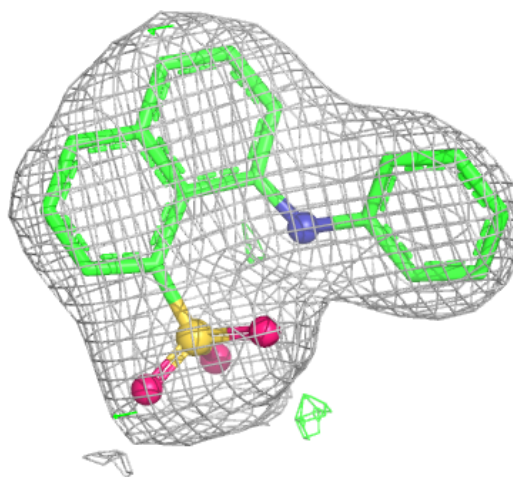
**Electron density around 2AN c 201:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around 2AN N 202:**

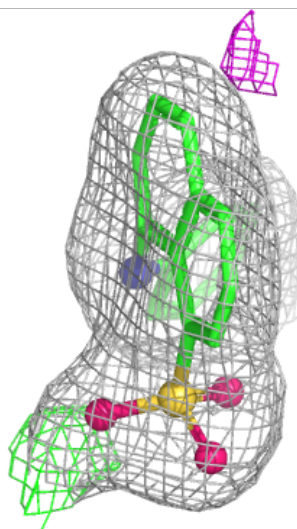
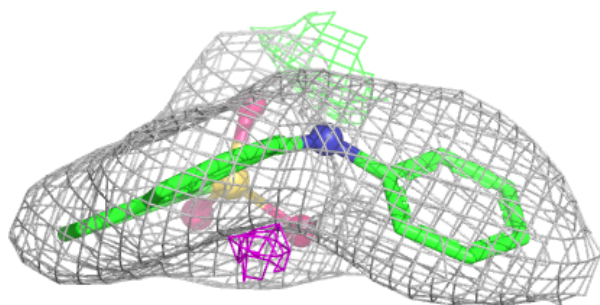
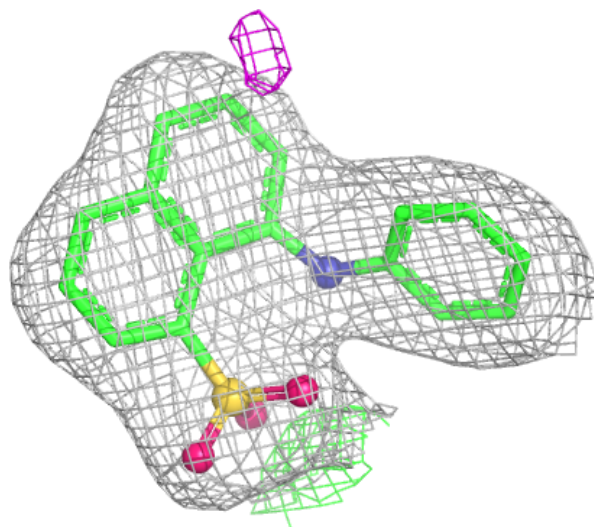
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





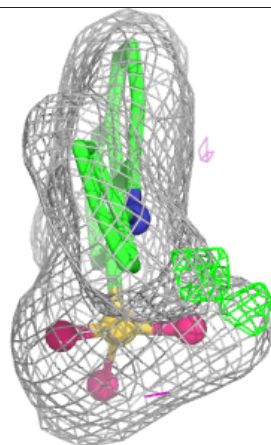
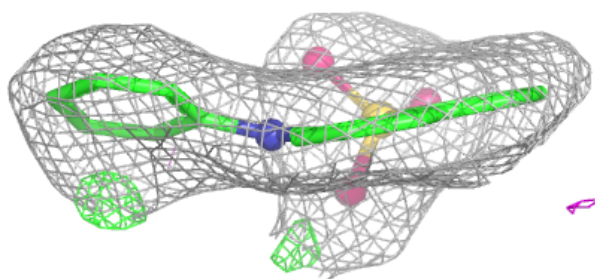
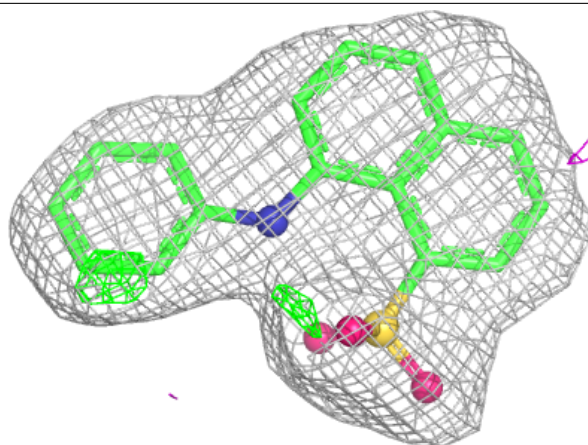
**Electron density around 2AN P 202:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



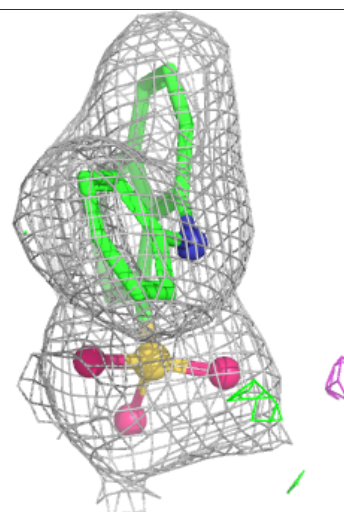
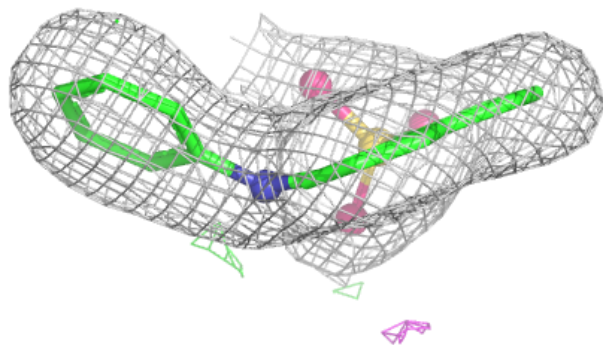
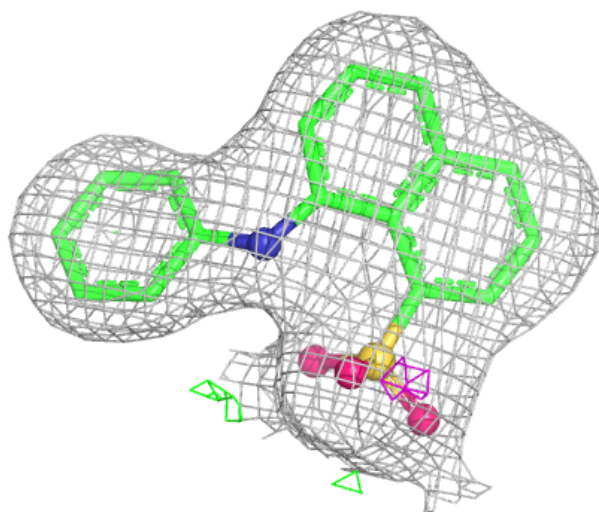
**Electron density around 2AN L 201:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around 2AN V 202:**

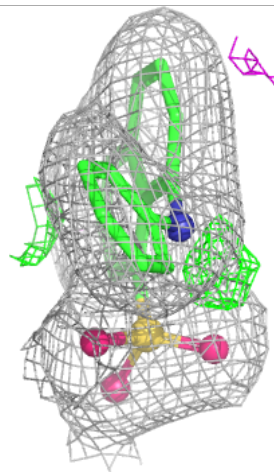
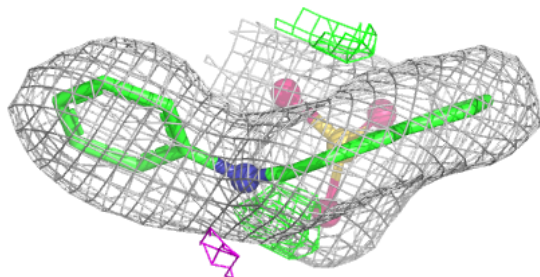
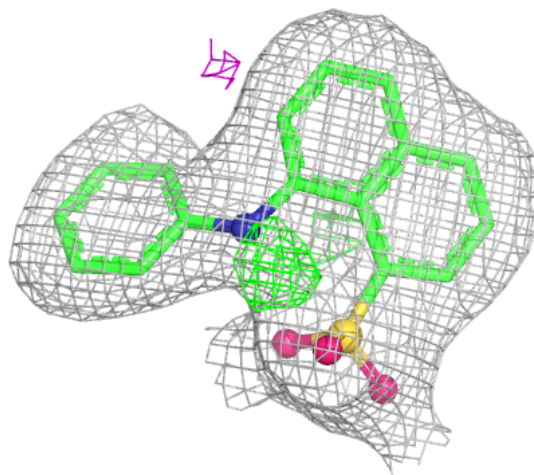
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





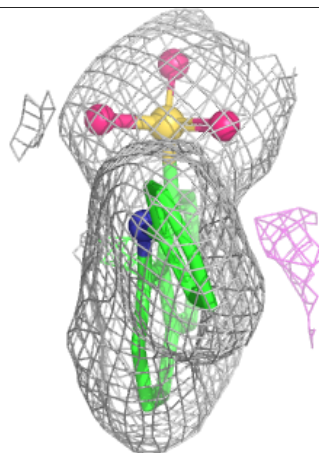
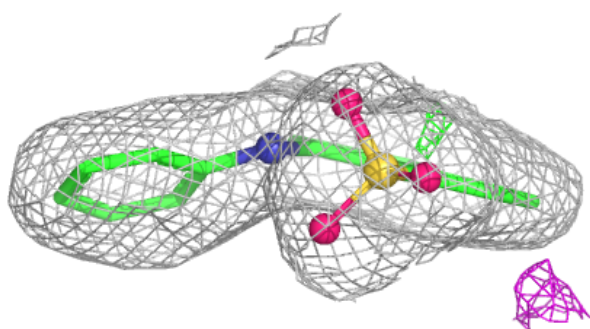
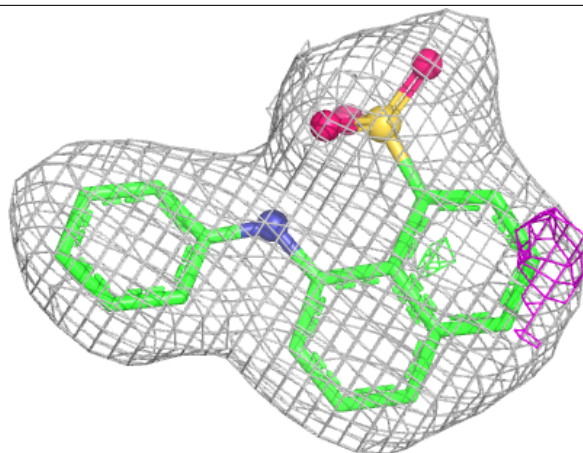
**Electron density around 2AN j 202:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



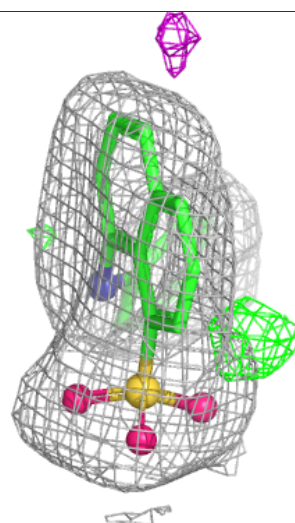
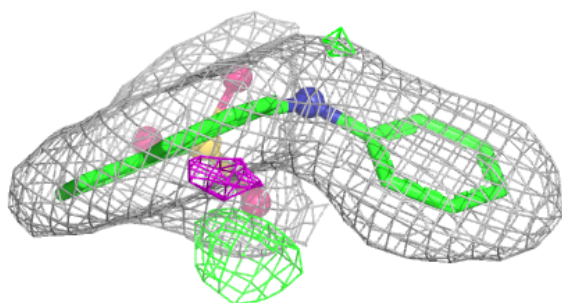
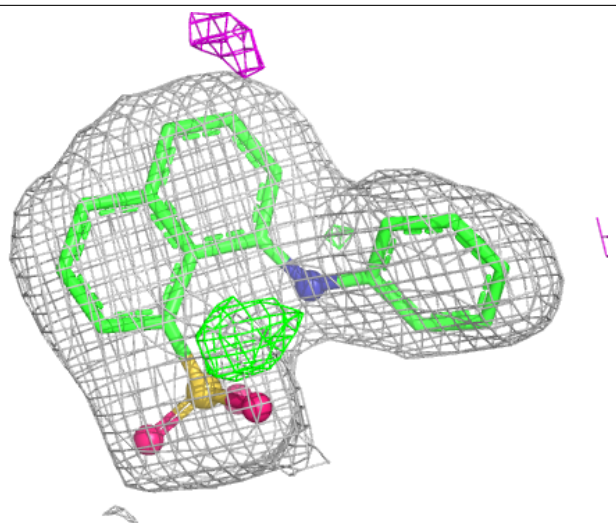
**Electron density around 2AN j 203:**

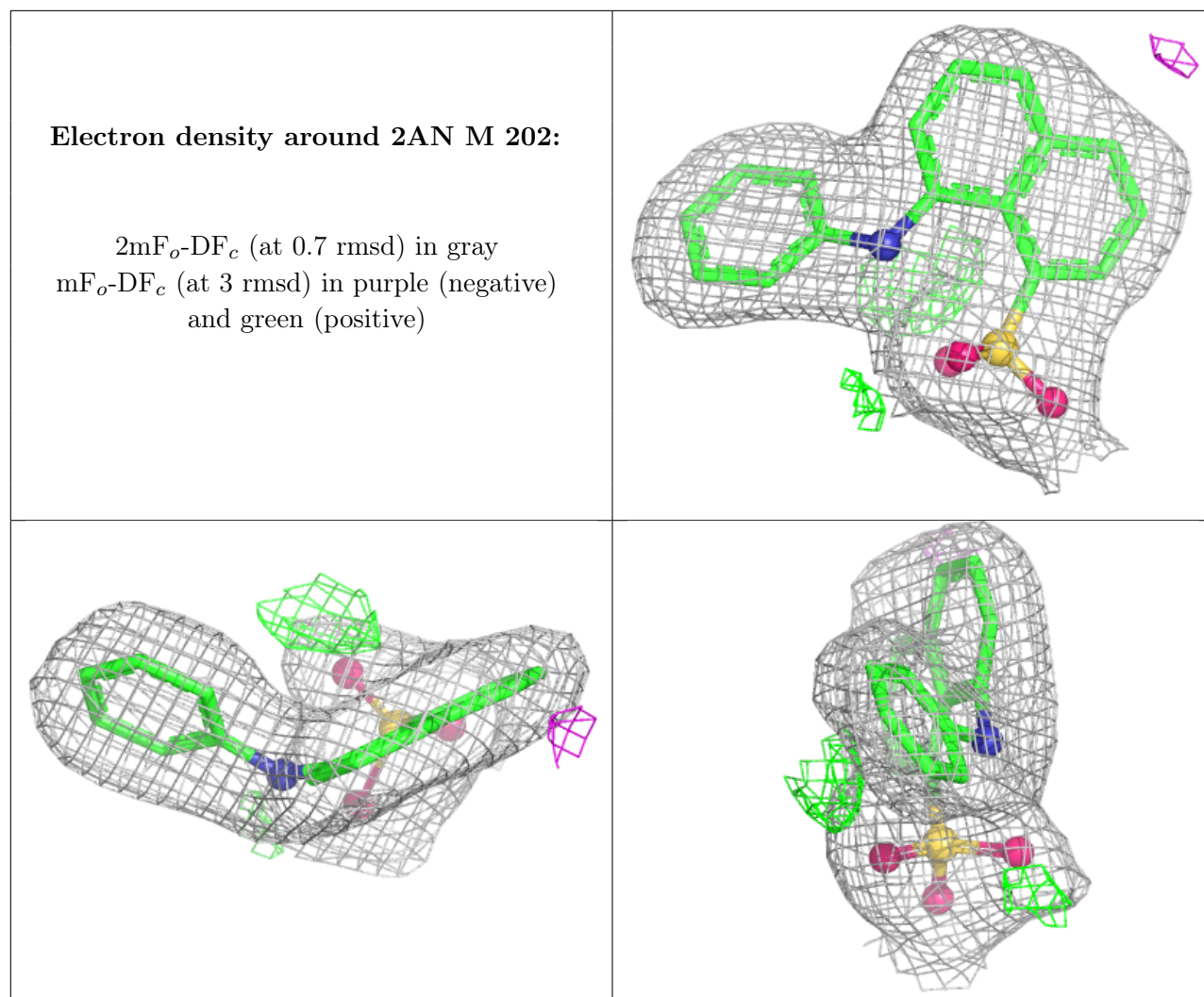
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around 2AN I 201:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





## 6.5 Other polymers [i](#)

There are no such residues in this entry.