



# wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 12, 2023 – 05:28 PM EDT

PDB ID : 4N3E  
Title : Crystal structure of Hyp-1, a St John's wort PR-10 protein, in complex with 8-anilino-1-naphthalene sulfonate (ANS)  
Authors : Sliwiak, J.; Dauter, Z.; Mccoy, A.J.; Read, R.J.; Jaskolski, M.  
Deposited on : 2013-10-07  
Resolution : 2.43 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>.

---

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.35.1  
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) : 2.35.1

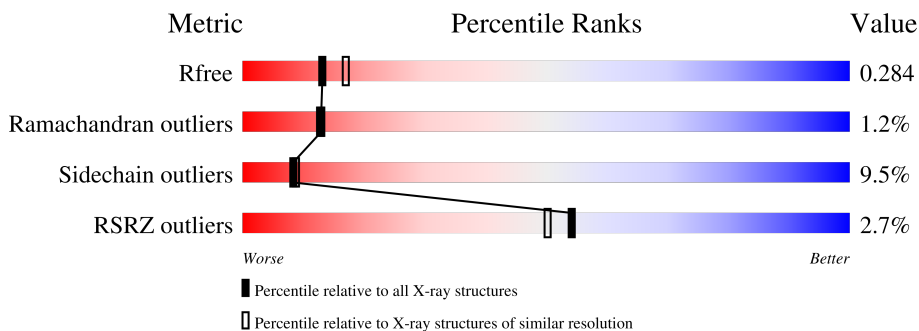
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*



The reported resolution of this entry is 2.43 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	1564 (2.46-2.42)
Ramachandran outliers	138981	1617 (2.46-2.42)
Sidechain outliers	138945	1617 (2.46-2.42)
RSRZ outliers	127900	1547 (2.46-2.42)

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	165	
1	B	165	
1	C	165	
1	D	165	
1	E	165	
1	F	165	

*Continued on next page...*

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	G	165	<p>2% 82% 12% . .</p>
1	H	165	<p>% 90% 6% .</p>
1	I	165	<p>% 87% 10% .</p>
1	J	165	<p>86% 10% . .</p>
1	K	165	<p>2% 88% 8% . .</p>
1	L	165	<p>% 87% 9% . .</p>
1	M	165	<p>4% 88% 8% .</p>
1	N	165	<p>4% 88% 8% .</p>
1	O	165	<p>4% 89% 7% . .</p>
1	P	165	<p>2% 87% 9% . .</p>
1	Q	165	<p>3% 89% 7% .</p>
1	R	165	<p>2% 88% 8% .</p>
1	S	165	<p>4% 90% 7% .</p>
1	T	165	<p>8% 85% 11% . .</p>
1	U	165	<p>% 85% 12% .</p>
1	V	165	<p>5% 86% 10% .</p>
1	W	165	<p>2% 89% 7% .</p>
1	X	165	<p>% 87% 10% .</p>
1	Y	165	<p>% 85% 12% .</p>
1	Z	165	<p>% 85% 10% . .</p>
1	a	165	<p>% 90% 6% .</p>
1	b	165	<p>% 90% 6% .</p>

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 37252 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 Phenolic oxidative coupling protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	159	1269	820	204	241	4	0	1	0
1	B	159	1256	813	203	236	4	1	0	0
1	C	159	1256	813	203	236	4	0	0	0
1	D	159	1257	814	203	236	4	0	0	0
1	E	159	1260	815	203	238	4	1	0	0
1	F	159	1257	814	202	237	4	0	0	0
1	G	159	1259	815	202	238	4	0	0	0
1	H	159	1260	815	203	238	4	0	0	0
1	I	159	1255	813	202	236	4	0	0	0
1	J	159	1255	812	203	236	4	0	0	0
1	K	159	1260	815	203	238	4	0	0	0
1	L	159	1260	815	203	238	4	1	0	0
1	M	159	1256	813	203	236	4	0	0	0
1	N	159	1269	820	204	241	4	0	1	0
1	O	159	1258	814	203	237	4	0	0	0
1	P	159	1260	815	203	238	4	0	0	0

*Continued on next page...*



Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	Q	159	1257	812	203	238	4	0	0	0
1	R	159	1260	815	203	238	4	1	0	0
1	S	159	1257	812	203	238	4	0	0	0
1	T	159	1307	844	210	249	4	0	6	0
1	U	159	1260	815	203	238	4	1	0	0
1	V	159	1257	814	203	236	4	0	0	0
1	W	159	1258	814	203	237	4	0	0	0
1	X	159	1260	815	203	238	4	0	0	0
1	Y	159	1260	815	203	238	4	1	0	0
1	Z	159	1256	813	203	236	4	0	0	0
1	a	159	1270	821	206	239	4	0	1	0
1	b	159	1254	813	202	235	4	1	0	0

There are 252 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	GLY	-	expression tag	UNP Q8H1L1
A	-4	ILE	-	expression tag	UNP Q8H1L1
A	-3	ASP	-	expression tag	UNP Q8H1L1
A	-2	PRO	-	expression tag	UNP Q8H1L1
A	-1	PHE	-	expression tag	UNP Q8H1L1
A	0	THR	-	expression tag	UNP Q8H1L1
A	14	ILE	THR	SEE REMARK 999	UNP Q8H1L1
A	86	LEU	ILE	SEE REMARK 999	UNP Q8H1L1
A	119	THR	SER	SEE REMARK 999	UNP Q8H1L1
B	-5	GLY	-	expression tag	UNP Q8H1L1
B	-4	ILE	-	expression tag	UNP Q8H1L1
B	-3	ASP	-	expression tag	UNP Q8H1L1
B	-2	PRO	-	expression tag	UNP Q8H1L1
B	-1	PHE	-	expression tag	UNP Q8H1L1
B	0	THR	-	expression tag	UNP Q8H1L1

Continued on next page...

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
B	14	ILE	THR	SEE REMARK 999	UNP Q8H1L1
B	86	LEU	ILE	SEE REMARK 999	UNP Q8H1L1
B	119	THR	SER	SEE REMARK 999	UNP Q8H1L1
C	-5	GLY	-	expression tag	UNP Q8H1L1
C	-4	ILE	-	expression tag	UNP Q8H1L1
C	-3	ASP	-	expression tag	UNP Q8H1L1
C	-2	PRO	-	expression tag	UNP Q8H1L1
C	-1	PHE	-	expression tag	UNP Q8H1L1
C	0	THR	-	expression tag	UNP Q8H1L1
C	14	ILE	THR	SEE REMARK 999	UNP Q8H1L1
C	86	LEU	ILE	SEE REMARK 999	UNP Q8H1L1
C	119	THR	SER	SEE REMARK 999	UNP Q8H1L1
D	-5	GLY	-	expression tag	UNP Q8H1L1
D	-4	ILE	-	expression tag	UNP Q8H1L1
D	-3	ASP	-	expression tag	UNP Q8H1L1
D	-2	PRO	-	expression tag	UNP Q8H1L1
D	-1	PHE	-	expression tag	UNP Q8H1L1
D	0	THR	-	expression tag	UNP Q8H1L1
D	14	ILE	THR	SEE REMARK 999	UNP Q8H1L1
D	86	LEU	ILE	SEE REMARK 999	UNP Q8H1L1
D	119	THR	SER	SEE REMARK 999	UNP Q8H1L1
E	-5	GLY	-	expression tag	UNP Q8H1L1
E	-4	ILE	-	expression tag	UNP Q8H1L1
E	-3	ASP	-	expression tag	UNP Q8H1L1
E	-2	PRO	-	expression tag	UNP Q8H1L1
E	-1	PHE	-	expression tag	UNP Q8H1L1
E	0	THR	-	expression tag	UNP Q8H1L1
E	14	ILE	THR	SEE REMARK 999	UNP Q8H1L1
E	86	LEU	ILE	SEE REMARK 999	UNP Q8H1L1
E	119	THR	SER	SEE REMARK 999	UNP Q8H1L1
F	-5	GLY	-	expression tag	UNP Q8H1L1
F	-4	ILE	-	expression tag	UNP Q8H1L1
F	-3	ASP	-	expression tag	UNP Q8H1L1
F	-2	PRO	-	expression tag	UNP Q8H1L1
F	-1	PHE	-	expression tag	UNP Q8H1L1
F	0	THR	-	expression tag	UNP Q8H1L1
F	14	ILE	THR	SEE REMARK 999	UNP Q8H1L1
F	86	LEU	ILE	SEE REMARK 999	UNP Q8H1L1
F	119	THR	SER	SEE REMARK 999	UNP Q8H1L1
G	-5	GLY	-	expression tag	UNP Q8H1L1
G	-4	ILE	-	expression tag	UNP Q8H1L1
G	-3	ASP	-	expression tag	UNP Q8H1L1

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
G	-2	PRO	-	expression tag	UNP Q8H1L1
G	-1	PHE	-	expression tag	UNP Q8H1L1
G	0	THR	-	expression tag	UNP Q8H1L1
G	14	ILE	THR	SEE REMARK 999	UNP Q8H1L1
G	86	LEU	ILE	SEE REMARK 999	UNP Q8H1L1
G	119	THR	SER	SEE REMARK 999	UNP Q8H1L1
H	-5	GLY	-	expression tag	UNP Q8H1L1
H	-4	ILE	-	expression tag	UNP Q8H1L1
H	-3	ASP	-	expression tag	UNP Q8H1L1
H	-2	PRO	-	expression tag	UNP Q8H1L1
H	-1	PHE	-	expression tag	UNP Q8H1L1
H	0	THR	-	expression tag	UNP Q8H1L1
H	14	ILE	THR	SEE REMARK 999	UNP Q8H1L1
H	86	LEU	ILE	SEE REMARK 999	UNP Q8H1L1
H	119	THR	SER	SEE REMARK 999	UNP Q8H1L1
I	-5	GLY	-	expression tag	UNP Q8H1L1
I	-4	ILE	-	expression tag	UNP Q8H1L1
I	-3	ASP	-	expression tag	UNP Q8H1L1
I	-2	PRO	-	expression tag	UNP Q8H1L1
I	-1	PHE	-	expression tag	UNP Q8H1L1
I	0	THR	-	expression tag	UNP Q8H1L1
I	14	ILE	THR	SEE REMARK 999	UNP Q8H1L1
I	86	LEU	ILE	SEE REMARK 999	UNP Q8H1L1
I	119	THR	SER	SEE REMARK 999	UNP Q8H1L1
J	-5	GLY	-	expression tag	UNP Q8H1L1
J	-4	ILE	-	expression tag	UNP Q8H1L1
J	-3	ASP	-	expression tag	UNP Q8H1L1
J	-2	PRO	-	expression tag	UNP Q8H1L1
J	-1	PHE	-	expression tag	UNP Q8H1L1
J	0	THR	-	expression tag	UNP Q8H1L1
J	14	ILE	THR	SEE REMARK 999	UNP Q8H1L1
J	86	LEU	ILE	SEE REMARK 999	UNP Q8H1L1
J	119	THR	SER	SEE REMARK 999	UNP Q8H1L1
K	-5	GLY	-	expression tag	UNP Q8H1L1
K	-4	ILE	-	expression tag	UNP Q8H1L1
K	-3	ASP	-	expression tag	UNP Q8H1L1
K	-2	PRO	-	expression tag	UNP Q8H1L1
K	-1	PHE	-	expression tag	UNP Q8H1L1
K	0	THR	-	expression tag	UNP Q8H1L1
K	14	ILE	THR	SEE REMARK 999	UNP Q8H1L1
K	86	LEU	ILE	SEE REMARK 999	UNP Q8H1L1
K	119	THR	SER	SEE REMARK 999	UNP Q8H1L1

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
L	-5	GLY	-	expression tag	UNP Q8H1L1
L	-4	ILE	-	expression tag	UNP Q8H1L1
L	-3	ASP	-	expression tag	UNP Q8H1L1
L	-2	PRO	-	expression tag	UNP Q8H1L1
L	-1	PHE	-	expression tag	UNP Q8H1L1
L	0	THR	-	expression tag	UNP Q8H1L1
L	14	ILE	THR	SEE REMARK 999	UNP Q8H1L1
L	86	LEU	ILE	SEE REMARK 999	UNP Q8H1L1
L	119	THR	SER	SEE REMARK 999	UNP Q8H1L1
M	-5	GLY	-	expression tag	UNP Q8H1L1
M	-4	ILE	-	expression tag	UNP Q8H1L1
M	-3	ASP	-	expression tag	UNP Q8H1L1
M	-2	PRO	-	expression tag	UNP Q8H1L1
M	-1	PHE	-	expression tag	UNP Q8H1L1
M	0	THR	-	expression tag	UNP Q8H1L1
M	14	ILE	THR	SEE REMARK 999	UNP Q8H1L1
M	86	LEU	ILE	SEE REMARK 999	UNP Q8H1L1
M	119	THR	SER	SEE REMARK 999	UNP Q8H1L1
N	-5	GLY	-	expression tag	UNP Q8H1L1
N	-4	ILE	-	expression tag	UNP Q8H1L1
N	-3	ASP	-	expression tag	UNP Q8H1L1
N	-2	PRO	-	expression tag	UNP Q8H1L1
N	-1	PHE	-	expression tag	UNP Q8H1L1
N	0	THR	-	expression tag	UNP Q8H1L1
N	14	ILE	THR	SEE REMARK 999	UNP Q8H1L1
N	86	LEU	ILE	SEE REMARK 999	UNP Q8H1L1
N	119	THR	SER	SEE REMARK 999	UNP Q8H1L1
O	-5	GLY	-	expression tag	UNP Q8H1L1
O	-4	ILE	-	expression tag	UNP Q8H1L1
O	-3	ASP	-	expression tag	UNP Q8H1L1
O	-2	PRO	-	expression tag	UNP Q8H1L1
O	-1	PHE	-	expression tag	UNP Q8H1L1
O	0	THR	-	expression tag	UNP Q8H1L1
O	14	ILE	THR	SEE REMARK 999	UNP Q8H1L1
O	86	LEU	ILE	SEE REMARK 999	UNP Q8H1L1
O	119	THR	SER	SEE REMARK 999	UNP Q8H1L1
P	-5	GLY	-	expression tag	UNP Q8H1L1
P	-4	ILE	-	expression tag	UNP Q8H1L1
P	-3	ASP	-	expression tag	UNP Q8H1L1
P	-2	PRO	-	expression tag	UNP Q8H1L1
P	-1	PHE	-	expression tag	UNP Q8H1L1
P	0	THR	-	expression tag	UNP Q8H1L1

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
P	14	ILE	THR	SEE REMARK 999	UNP Q8H1L1
P	86	LEU	ILE	SEE REMARK 999	UNP Q8H1L1
P	119	THR	SER	SEE REMARK 999	UNP Q8H1L1
Q	-5	GLY	-	expression tag	UNP Q8H1L1
Q	-4	ILE	-	expression tag	UNP Q8H1L1
Q	-3	ASP	-	expression tag	UNP Q8H1L1
Q	-2	PRO	-	expression tag	UNP Q8H1L1
Q	-1	PHE	-	expression tag	UNP Q8H1L1
Q	0	THR	-	expression tag	UNP Q8H1L1
Q	14	ILE	THR	SEE REMARK 999	UNP Q8H1L1
Q	86	LEU	ILE	SEE REMARK 999	UNP Q8H1L1
Q	119	THR	SER	SEE REMARK 999	UNP Q8H1L1
R	-5	GLY	-	expression tag	UNP Q8H1L1
R	-4	ILE	-	expression tag	UNP Q8H1L1
R	-3	ASP	-	expression tag	UNP Q8H1L1
R	-2	PRO	-	expression tag	UNP Q8H1L1
R	-1	PHE	-	expression tag	UNP Q8H1L1
R	0	THR	-	expression tag	UNP Q8H1L1
R	14	ILE	THR	SEE REMARK 999	UNP Q8H1L1
R	86	LEU	ILE	SEE REMARK 999	UNP Q8H1L1
R	119	THR	SER	SEE REMARK 999	UNP Q8H1L1
S	-5	GLY	-	expression tag	UNP Q8H1L1
S	-4	ILE	-	expression tag	UNP Q8H1L1
S	-3	ASP	-	expression tag	UNP Q8H1L1
S	-2	PRO	-	expression tag	UNP Q8H1L1
S	-1	PHE	-	expression tag	UNP Q8H1L1
S	0	THR	-	expression tag	UNP Q8H1L1
S	14	ILE	THR	SEE REMARK 999	UNP Q8H1L1
S	86	LEU	ILE	SEE REMARK 999	UNP Q8H1L1
S	119	THR	SER	SEE REMARK 999	UNP Q8H1L1
T	-5	GLY	-	expression tag	UNP Q8H1L1
T	-4	ILE	-	expression tag	UNP Q8H1L1
T	-3	ASP	-	expression tag	UNP Q8H1L1
T	-2	PRO	-	expression tag	UNP Q8H1L1
T	-1	PHE	-	expression tag	UNP Q8H1L1
T	0	THR	-	expression tag	UNP Q8H1L1
T	14	ILE	THR	SEE REMARK 999	UNP Q8H1L1
T	86	LEU	ILE	SEE REMARK 999	UNP Q8H1L1
T	119	THR	SER	SEE REMARK 999	UNP Q8H1L1
U	-5	GLY	-	expression tag	UNP Q8H1L1
U	-4	ILE	-	expression tag	UNP Q8H1L1
U	-3	ASP	-	expression tag	UNP Q8H1L1

*Continued on next page...*

*Continued from previous page...*

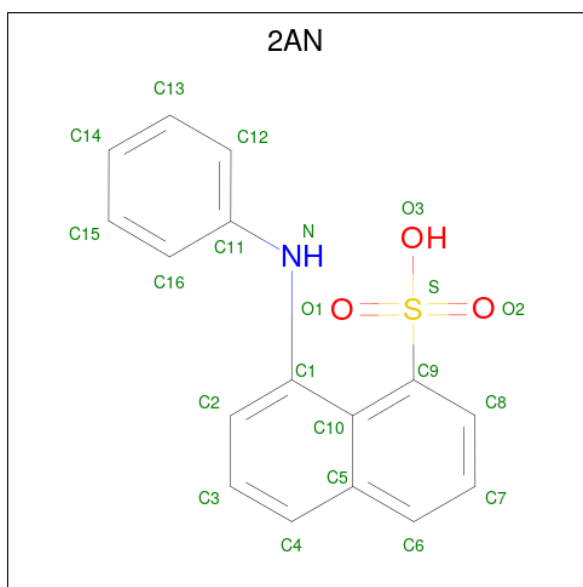
Chain	Residue	Modelled	Actual	Comment	Reference
U	-2	PRO	-	expression tag	UNP Q8H1L1
U	-1	PHE	-	expression tag	UNP Q8H1L1
U	0	THR	-	expression tag	UNP Q8H1L1
U	14	ILE	THR	SEE REMARK 999	UNP Q8H1L1
U	86	LEU	ILE	SEE REMARK 999	UNP Q8H1L1
U	119	THR	SER	SEE REMARK 999	UNP Q8H1L1
V	-5	GLY	-	expression tag	UNP Q8H1L1
V	-4	ILE	-	expression tag	UNP Q8H1L1
V	-3	ASP	-	expression tag	UNP Q8H1L1
V	-2	PRO	-	expression tag	UNP Q8H1L1
V	-1	PHE	-	expression tag	UNP Q8H1L1
V	0	THR	-	expression tag	UNP Q8H1L1
V	14	ILE	THR	SEE REMARK 999	UNP Q8H1L1
V	86	LEU	ILE	SEE REMARK 999	UNP Q8H1L1
V	119	THR	SER	SEE REMARK 999	UNP Q8H1L1
W	-5	GLY	-	expression tag	UNP Q8H1L1
W	-4	ILE	-	expression tag	UNP Q8H1L1
W	-3	ASP	-	expression tag	UNP Q8H1L1
W	-2	PRO	-	expression tag	UNP Q8H1L1
W	-1	PHE	-	expression tag	UNP Q8H1L1
W	0	THR	-	expression tag	UNP Q8H1L1
W	14	ILE	THR	SEE REMARK 999	UNP Q8H1L1
W	86	LEU	ILE	SEE REMARK 999	UNP Q8H1L1
W	119	THR	SER	SEE REMARK 999	UNP Q8H1L1
X	-5	GLY	-	expression tag	UNP Q8H1L1
X	-4	ILE	-	expression tag	UNP Q8H1L1
X	-3	ASP	-	expression tag	UNP Q8H1L1
X	-2	PRO	-	expression tag	UNP Q8H1L1
X	-1	PHE	-	expression tag	UNP Q8H1L1
X	0	THR	-	expression tag	UNP Q8H1L1
X	14	ILE	THR	SEE REMARK 999	UNP Q8H1L1
X	86	LEU	ILE	SEE REMARK 999	UNP Q8H1L1
X	119	THR	SER	SEE REMARK 999	UNP Q8H1L1
Y	-5	GLY	-	expression tag	UNP Q8H1L1
Y	-4	ILE	-	expression tag	UNP Q8H1L1
Y	-3	ASP	-	expression tag	UNP Q8H1L1
Y	-2	PRO	-	expression tag	UNP Q8H1L1
Y	-1	PHE	-	expression tag	UNP Q8H1L1
Y	0	THR	-	expression tag	UNP Q8H1L1
Y	14	ILE	THR	SEE REMARK 999	UNP Q8H1L1
Y	86	LEU	ILE	SEE REMARK 999	UNP Q8H1L1
Y	119	THR	SER	SEE REMARK 999	UNP Q8H1L1

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
Z	-5	GLY	-	expression tag	UNP Q8H1L1
Z	-4	ILE	-	expression tag	UNP Q8H1L1
Z	-3	ASP	-	expression tag	UNP Q8H1L1
Z	-2	PRO	-	expression tag	UNP Q8H1L1
Z	-1	PHE	-	expression tag	UNP Q8H1L1
Z	0	THR	-	expression tag	UNP Q8H1L1
Z	14	ILE	THR	SEE REMARK 999	UNP Q8H1L1
Z	86	LEU	ILE	SEE REMARK 999	UNP Q8H1L1
Z	119	THR	SER	SEE REMARK 999	UNP Q8H1L1
a	-5	GLY	-	expression tag	UNP Q8H1L1
a	-4	ILE	-	expression tag	UNP Q8H1L1
a	-3	ASP	-	expression tag	UNP Q8H1L1
a	-2	PRO	-	expression tag	UNP Q8H1L1
a	-1	PHE	-	expression tag	UNP Q8H1L1
a	0	THR	-	expression tag	UNP Q8H1L1
a	14	ILE	THR	SEE REMARK 999	UNP Q8H1L1
a	86	LEU	ILE	SEE REMARK 999	UNP Q8H1L1
a	119	THR	SER	SEE REMARK 999	UNP Q8H1L1
b	-5	GLY	-	expression tag	UNP Q8H1L1
b	-4	ILE	-	expression tag	UNP Q8H1L1
b	-3	ASP	-	expression tag	UNP Q8H1L1
b	-2	PRO	-	expression tag	UNP Q8H1L1
b	-1	PHE	-	expression tag	UNP Q8H1L1
b	0	THR	-	expression tag	UNP Q8H1L1
b	14	ILE	THR	SEE REMARK 999	UNP Q8H1L1
b	86	LEU	ILE	SEE REMARK 999	UNP Q8H1L1
b	119	THR	SER	SEE REMARK 999	UNP Q8H1L1

- 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).



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

*Continued on next page...*



*Continued from previous page...*

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	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	F	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	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	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		

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
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	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	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	L	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	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	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	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		

*Continued on next page...*

*Continued from previous page...*

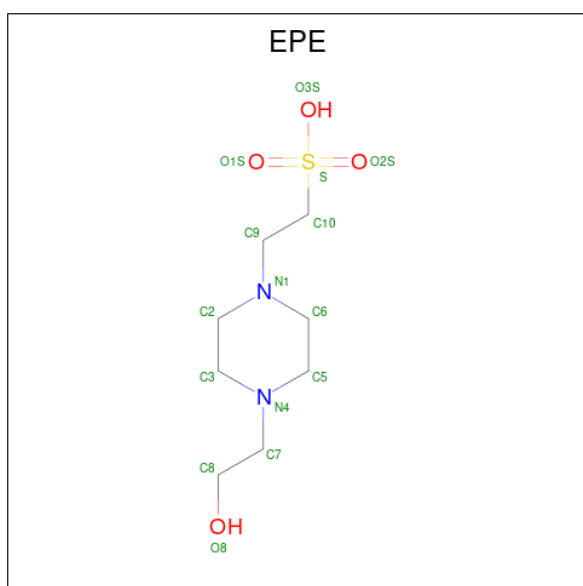
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	Q	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	Q	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	Q	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	R	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	R	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	R	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	R	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	S	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	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	U	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	W	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	W	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	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		

*Continued on next page...*

Continued from previous page...

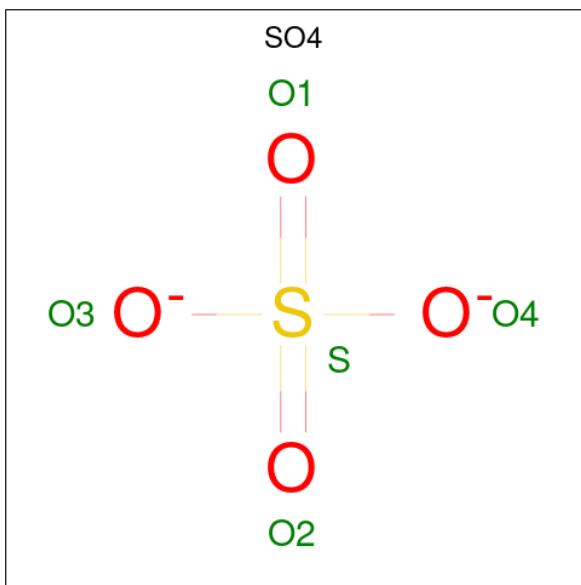
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	X	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	Y	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	Y	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	Y	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	Y	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	Z	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	Z	1	Total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

- Molecule 3 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
3	C	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
3	Z	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	V	1	Total	O	S	0	0
			5	4	1		
4	X	1	Total	O	S	0	0
			5	4	1		
4	b	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	5	Total	O	0	0
			5	5		
5	C	2	Total	O	0	0
			2	2		
5	D	1	Total	O	0	0
			1	1		
5	E	2	Total	O	0	0
			2	2		
5	F	2	Total	O	0	0
			2	2		

*Continued on next page...*

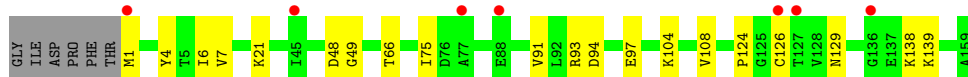
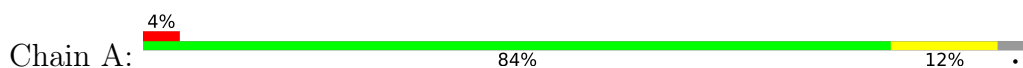
*Continued from previous page...*

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	G	1	Total O 1 1	0	0
5	H	4	Total O 4 4	0	0
5	I	2	Total O 2 2	0	0
5	L	2	Total O 2 2	0	0
5	R	2	Total O 2 2	0	0
5	T	1	Total O 1 1	0	0
5	U	1	Total O 1 1	0	0
5	W	2	Total O 2 2	0	0
5	Y	2	Total O 2 2	0	0
5	Z	3	Total O 3 3	0	0
5	a	2	Total O 2 2	0	0
5	b	1	Total O 1 1	0	0

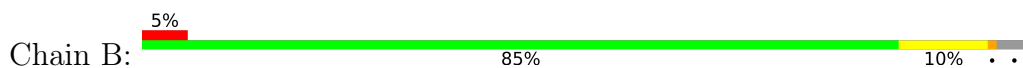
### 3 Residue-property plots [i](#)

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.

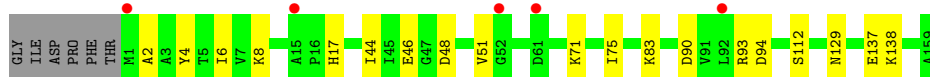
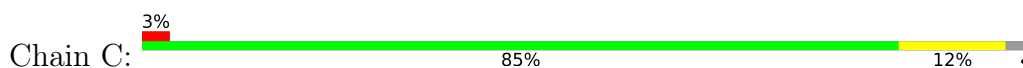
- Molecule 1: Phenolic oxidative coupling protein



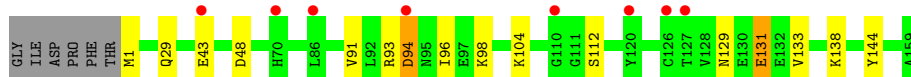
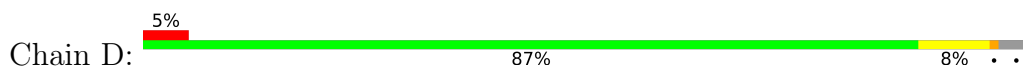
- Molecule 1: Phenolic oxidative coupling protein



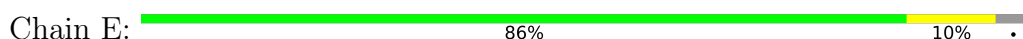
- Molecule 1: Phenolic oxidative coupling protein



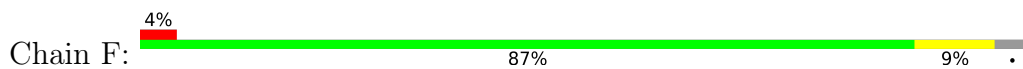
- Molecule 1: Phenolic oxidative coupling protein



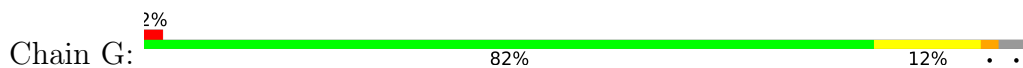
- Molecule 1: Phenolic oxidative coupling protein



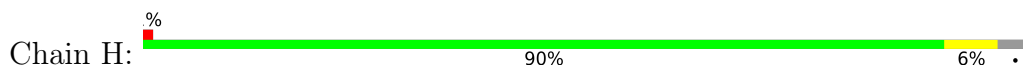
- Molecule 1: Phenolic oxidative coupling protein



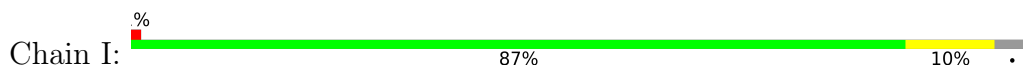
- Molecule 1: Phenolic oxidative coupling protein



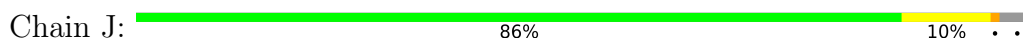
- Molecule 1: Phenolic oxidative coupling protein



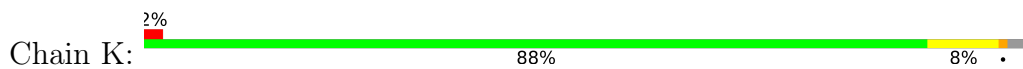
- Molecule 1: Phenolic oxidative coupling protein



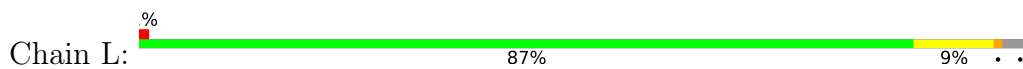
- Molecule 1: Phenolic oxidative coupling protein



- Molecule 1: Phenolic oxidative coupling protein

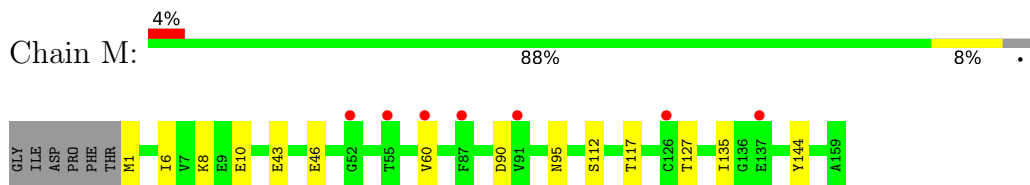


- Molecule 1: Phenolic oxidative coupling protein

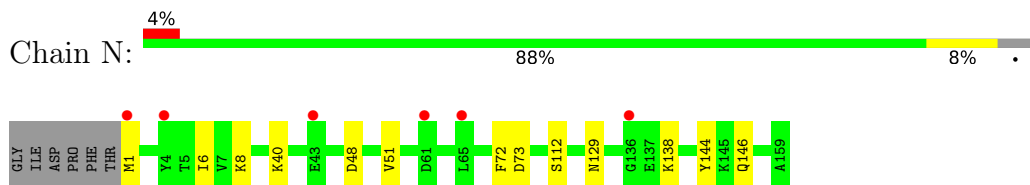




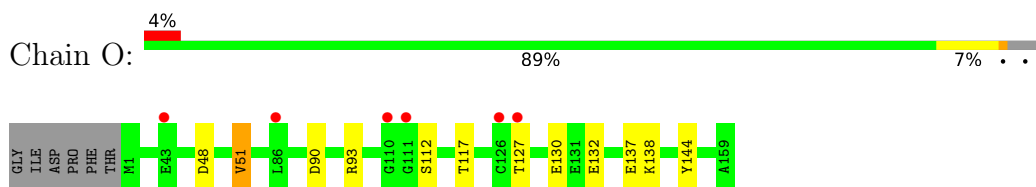
- Molecule 1: Phenolic oxidative coupling protein



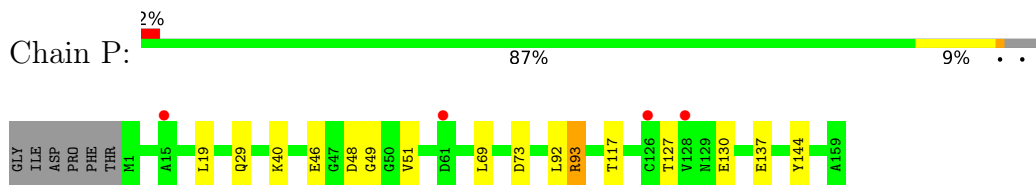
- Molecule 1: Phenolic oxidative coupling protein



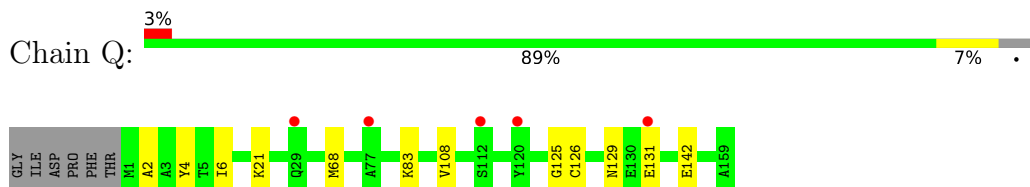
- Molecule 1: Phenolic oxidative coupling protein



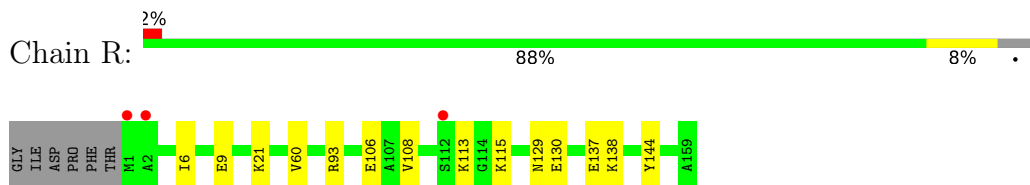
- Molecule 1: Phenolic oxidative coupling protein



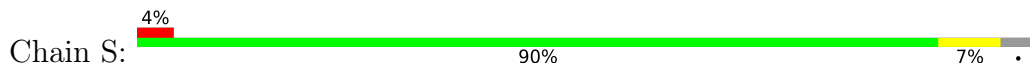
- Molecule 1: Phenolic oxidative coupling protein



- Molecule 1: Phenolic oxidative coupling protein

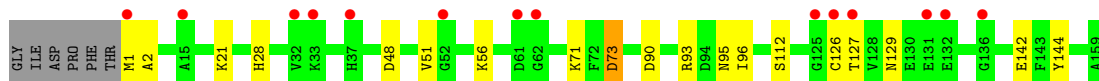
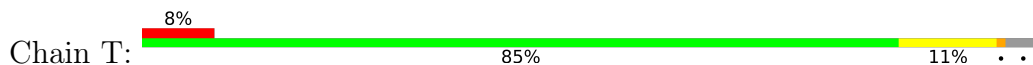


- Molecule 1: Phenolic oxidative coupling protein

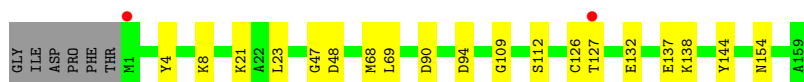
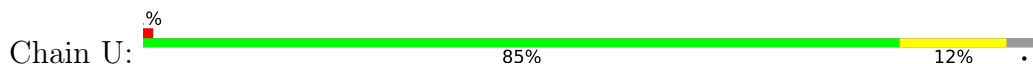




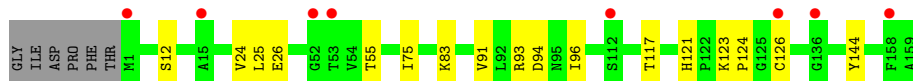
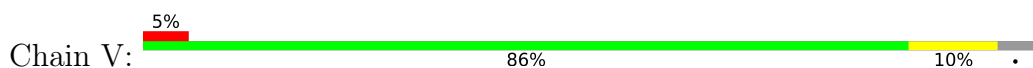
- Molecule 1: Phenolic oxidative coupling protein



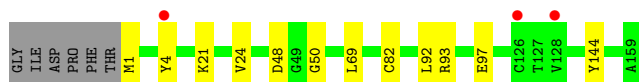
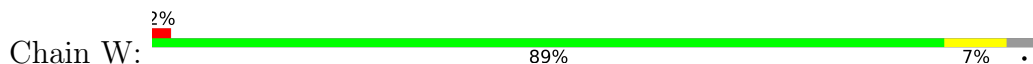
- Molecule 1: Phenolic oxidative coupling protein



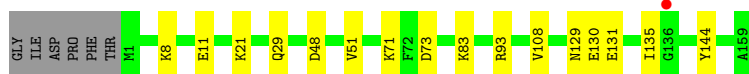
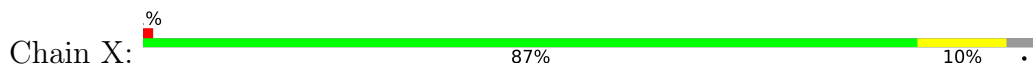
- Molecule 1: Phenolic oxidative coupling protein



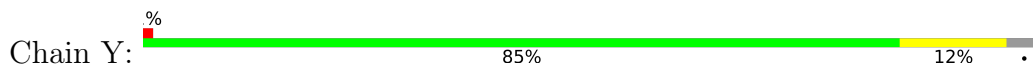
- Molecule 1: Phenolic oxidative coupling protein



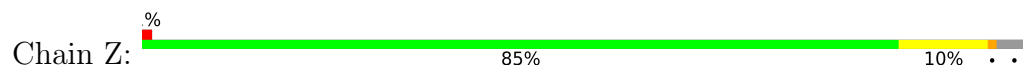
- Molecule 1: Phenolic oxidative coupling protein



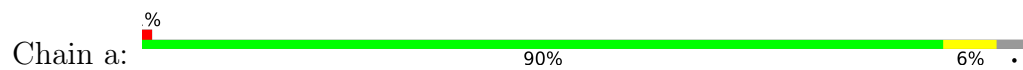
- Molecule 1: Phenolic oxidative coupling protein



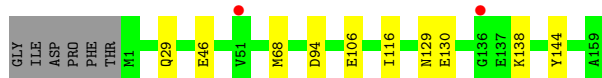
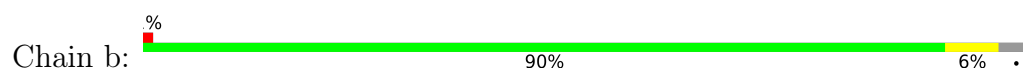
- Molecule 1: Phenolic oxidative coupling protein



- Molecule 1: Phenolic oxidative coupling protein



- Molecule 1: Phenolic oxidative coupling protein



## 4 Data and refinement statistics i

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	146.29Å 146.29Å 298.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.87 – 2.43 48.87 – 2.43	Depositor EDS
% Data completeness (in resolution range)	99.7 (48.87-2.43) 99.7 (48.87-2.43)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.69 (at 2.42Å)	Xtrriage
Refinement program	REFMAC 5.7.0029	Depositor
R, $R_{free}$	0.223 , 0.278 0.229 , 0.284	Depositor DCC
$R_{free}$ test set	3078 reflections (1.31%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	49.9	Xtrriage
Anisotropy	0.143	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 22.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	0.489 for k,h,-l 0.489 for -k,-h,-l 0.489 for -h,-k,l	Xtrriage
Reported twinning fraction	0.251 for H, K, L 0.292 for -K, -H, -L 0.249 for -h,-k,l 0.209 for K, H, -L	Depositor
Outliers	2 of 235350 reflections (0.001%)	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	37252	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	46.0	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 67.36 % 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 5.2079e-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 i

### 5.1 Standard geometry i

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

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	0.74	0/1298	1.03	0/1753
1	B	0.81	0/1285	1.08	2/1736 (0.1%)
1	C	0.72	0/1285	1.04	1/1736 (0.1%)
1	D	0.69	0/1286	0.97	0/1737
1	E	0.93	0/1289	1.17	4/1741 (0.2%)
1	F	0.61	0/1286	0.93	2/1737 (0.1%)
1	G	0.97	1/1288 (0.1%)	1.17	4/1740 (0.2%)
1	H	0.77	0/1289	1.06	2/1741 (0.1%)
1	I	0.82	0/1284	1.09	2/1735 (0.1%)
1	J	0.93	0/1284	1.18	4/1734 (0.2%)
1	K	0.68	0/1289	1.01	0/1741
1	L	0.89	0/1289	1.17	2/1741 (0.1%)
1	M	0.75	0/1285	1.08	1/1736 (0.1%)
1	N	0.76	0/1298	1.05	0/1753
1	O	0.72	0/1287	1.04	1/1738 (0.1%)
1	P	0.70	0/1289	1.07	2/1741 (0.1%)
1	Q	0.70	0/1286	1.04	1/1737 (0.1%)
1	R	0.81	0/1289	1.11	0/1741
1	S	0.64	0/1286	0.99	0/1737
1	T	0.61	0/1337	0.96	2/1806 (0.1%)
1	U	0.91	0/1289	1.19	3/1741 (0.2%)
1	V	0.59	0/1286	0.94	0/1737
1	W	0.86	0/1287	1.14	2/1738 (0.1%)
1	X	0.78	0/1289	1.07	1/1741 (0.1%)
1	Y	0.81	0/1289	1.15	3/1741 (0.2%)
1	Z	0.82	0/1285	1.08	3/1736 (0.2%)
1	a	0.75	0/1300	1.06	0/1756
1	b	0.89	0/1283	1.18	1/1733 (0.1%)
All	All	0.78	1/36117 (0.0%)	1.08	43/48784 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	148	GLU	CG-CD	-5.36	1.44	1.51

The worst 5 of 43 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	U	109	GLY	N-CA-C	-5.90	98.36	113.10
1	E	6	ILE	CB-CA-C	-5.87	99.87	111.60
1	G	51	VAL	CB-CA-C	-5.78	100.41	111.40
1	I	6	ILE	CB-CA-C	-5.76	100.08	111.60
1	W	50	GLY	N-CA-C	-5.75	98.74	113.10

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	158/165 (96%)	148 (94%)	7 (4%)	3 (2%)	8	6
1	B	157/165 (95%)	143 (91%)	12 (8%)	2 (1%)	12	11
1	C	157/165 (95%)	139 (88%)	16 (10%)	2 (1%)	12	11
1	D	157/165 (95%)	140 (89%)	14 (9%)	3 (2%)	8	6
1	E	157/165 (95%)	142 (90%)	12 (8%)	3 (2%)	8	6
1	F	157/165 (95%)	145 (92%)	11 (7%)	1 (1%)	25	29
1	G	157/165 (95%)	145 (92%)	9 (6%)	3 (2%)	8	6
1	H	157/165 (95%)	150 (96%)	7 (4%)	0	100	100

*Continued on next page...*

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	I	157/165 (95%)	145 (92%)	10 (6%)	2 (1%)	12	11
1	J	157/165 (95%)	143 (91%)	12 (8%)	2 (1%)	12	11
1	K	157/165 (95%)	143 (91%)	10 (6%)	4 (2%)	5	3
1	L	157/165 (95%)	149 (95%)	6 (4%)	2 (1%)	12	11
1	M	157/165 (95%)	147 (94%)	10 (6%)	0	100	100
1	N	158/165 (96%)	145 (92%)	13 (8%)	0	100	100
1	O	157/165 (95%)	147 (94%)	10 (6%)	0	100	100
1	P	157/165 (95%)	139 (88%)	14 (9%)	4 (2%)	5	3
1	Q	157/165 (95%)	142 (90%)	13 (8%)	2 (1%)	12	11
1	R	157/165 (95%)	146 (93%)	9 (6%)	2 (1%)	12	11
1	S	157/165 (95%)	141 (90%)	15 (10%)	1 (1%)	25	29
1	T	163/165 (99%)	151 (93%)	11 (7%)	1 (1%)	25	29
1	U	157/165 (95%)	145 (92%)	11 (7%)	1 (1%)	25	29
1	V	157/165 (95%)	139 (88%)	16 (10%)	2 (1%)	12	11
1	W	157/165 (95%)	151 (96%)	4 (2%)	2 (1%)	12	11
1	X	157/165 (95%)	148 (94%)	7 (4%)	2 (1%)	12	11
1	Y	157/165 (95%)	145 (92%)	11 (7%)	1 (1%)	25	29
1	Z	157/165 (95%)	142 (90%)	12 (8%)	3 (2%)	8	6
1	a	158/165 (96%)	143 (90%)	13 (8%)	2 (1%)	12	11
1	b	157/165 (95%)	141 (90%)	15 (10%)	1 (1%)	25	29
All	All	4405/4620 (95%)	4044 (92%)	310 (7%)	51 (1%)	13	13

5 of 51 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	94	ASP
1	D	131	GLU
1	E	126	CYS
1	I	2	ALA
1	J	3	ALA

### 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	135/139 (97%)	118 (87%)	17 (13%)	4	3
1	B	133/139 (96%)	118 (89%)	15 (11%)	6	5
1	C	133/139 (96%)	117 (88%)	16 (12%)	5	4
1	D	133/139 (96%)	118 (89%)	15 (11%)	6	5
1	E	134/139 (96%)	124 (92%)	10 (8%)	13	16
1	F	133/139 (96%)	121 (91%)	12 (9%)	9	10
1	G	133/139 (96%)	114 (86%)	19 (14%)	3	2
1	H	134/139 (96%)	126 (94%)	8 (6%)	19	25
1	I	132/139 (95%)	120 (91%)	12 (9%)	9	10
1	J	133/139 (96%)	121 (91%)	12 (9%)	9	10
1	K	134/139 (96%)	123 (92%)	11 (8%)	11	13
1	L	134/139 (96%)	121 (90%)	13 (10%)	8	8
1	M	133/139 (96%)	120 (90%)	13 (10%)	8	8
1	N	135/139 (97%)	122 (90%)	13 (10%)	8	8
1	O	133/139 (96%)	121 (91%)	12 (9%)	9	10
1	P	134/139 (96%)	123 (92%)	11 (8%)	11	13
1	Q	133/139 (96%)	124 (93%)	9 (7%)	16	19
1	R	134/139 (96%)	122 (91%)	12 (9%)	9	10
1	S	133/139 (96%)	123 (92%)	10 (8%)	13	16
1	T	139/139 (100%)	121 (87%)	18 (13%)	4	3
1	U	134/139 (96%)	119 (89%)	15 (11%)	6	5
1	V	133/139 (96%)	118 (89%)	15 (11%)	6	5
1	W	133/139 (96%)	125 (94%)	8 (6%)	19	25
1	X	134/139 (96%)	121 (90%)	13 (10%)	8	8
1	Y	134/139 (96%)	118 (88%)	16 (12%)	5	4
1	Z	133/139 (96%)	120 (90%)	13 (10%)	8	8
1	a	135/139 (97%)	127 (94%)	8 (6%)	19	25
1	b	132/139 (95%)	124 (94%)	8 (6%)	18	24
All	All	3743/3892 (96%)	3389 (90%)	354 (10%)	8	9



5 of 354 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	S	10	GLU
1	V	126	CYS
1	S	129	ASN
1	U	21	LYS
1	X	51	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 44 such sidechains are listed below:

Mol	Chain	Res	Type
1	P	28	HIS
1	T	154	ASN
1	R	129	ASN
1	S	129	ASN
1	V	129	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

94 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	Y	204	-	22,23,23	0.56	0	29,33,33	0.84	1 (3%)
2	2AN	E	202	-	22,23,23	0.62	0	29,33,33	1.04	2 (6%)
2	2AN	P	202	-	22,23,23	0.64	0	29,33,33	1.07	3 (10%)
2	2AN	V	202	-	22,23,23	0.65	0	29,33,33	1.09	2 (6%)
2	2AN	N	204	-	22,23,23	1.10	2 (9%)	29,33,33	1.03	3 (10%)
2	2AN	I	201	-	22,23,23	0.71	0	29,33,33	0.91	2 (6%)
2	2AN	b	202	-	22,23,23	0.87	0	29,33,33	0.96	1 (3%)
2	2AN	a	201	-	22,23,23	0.52	0	29,33,33	0.73	1 (3%)
2	2AN	U	201	-	22,23,23	0.72	1 (4%)	29,33,33	0.84	1 (3%)
2	2AN	b	201	-	22,23,23	0.58	0	29,33,33	1.05	1 (3%)
2	2AN	X	202	-	22,23,23	0.54	0	29,33,33	0.98	2 (6%)
2	2AN	Y	201	-	22,23,23	0.87	2 (9%)	29,33,33	0.88	1 (3%)
3	EPE	C	205	-	15,15,15	1.85	2 (13%)	18,20,20	3.65	13 (72%)
2	2AN	H	202	-	22,23,23	0.67	0	29,33,33	0.79	1 (3%)
2	2AN	E	203	-	22,23,23	0.74	1 (4%)	29,33,33	1.08	2 (6%)
2	2AN	K	201	-	22,23,23	0.82	0	29,33,33	0.94	1 (3%)
2	2AN	X	203	-	22,23,23	0.58	0	29,33,33	0.93	2 (6%)
2	2AN	F	201	-	22,23,23	0.69	0	29,33,33	0.90	1 (3%)
2	2AN	E	201	-	22,23,23	1.17	2 (9%)	29,33,33	1.24	3 (10%)
2	2AN	N	202	-	22,23,23	0.76	0	29,33,33	0.86	0
2	2AN	b	203	-	22,23,23	0.67	0	29,33,33	0.90	2 (6%)
2	2AN	G	204	-	22,23,23	1.02	1 (4%)	29,33,33	1.09	2 (6%)
2	2AN	U	204	-	22,23,23	0.70	0	29,33,33	0.81	1 (3%)
2	2AN	R	203	-	22,23,23	0.59	0	29,33,33	0.98	2 (6%)
2	2AN	R	204	-	22,23,23	0.73	0	29,33,33	0.85	0
2	2AN	I	202	-	22,23,23	0.90	0	29,33,33	0.85	1 (3%)
2	2AN	P	201	-	22,23,23	0.72	0	29,33,33	0.87	2 (6%)
2	2AN	K	202	-	22,23,23	0.49	0	29,33,33	0.89	1 (3%)
2	2AN	A	203	-	22,23,23	0.72	0	29,33,33	0.85	1 (3%)
2	2AN	K	203	-	22,23,23	0.47	0	29,33,33	0.90	2 (6%)
2	2AN	V	201	-	22,23,23	0.67	0	29,33,33	0.89	0
2	2AN	L	203	-	22,23,23	0.81	0	29,33,33	1.09	2 (6%)
2	2AN	G	202	-	22,23,23	0.80	0	29,33,33	0.96	2 (6%)
2	2AN	B	202	-	22,23,23	0.57	0	29,33,33	0.97	3 (10%)
2	2AN	G	201	-	22,23,23	1.34	2 (9%)	29,33,33	1.08	2 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	2AN	W	202	-	22,23,23	0.70	1 (4%)	29,33,33	0.86	1 (3%)
4	SO4	b	204	-	4,4,4	0.34	0	6,6,6	1.32	0
2	2AN	L	202	-	22,23,23	0.81	0	29,33,33	0.85	1 (3%)
2	2AN	A	204	-	22,23,23	0.89	0	29,33,33	1.03	2 (6%)
4	SO4	V	203	-	4,4,4	0.46	0	6,6,6	1.23	0
2	2AN	G	203	-	22,23,23	0.69	0	29,33,33	0.79	0
2	2AN	B	205	-	22,23,23	0.54	0	29,33,33	0.91	2 (6%)
2	2AN	R	201	-	22,23,23	0.66	0	29,33,33	1.06	3 (10%)
2	2AN	D	201	-	22,23,23	0.67	0	29,33,33	0.74	0
2	2AN	U	205	-	22,23,23	0.53	0	29,33,33	0.75	0
4	SO4	X	204	-	4,4,4	0.51	0	6,6,6	0.66	0
2	2AN	G	205	-	22,23,23	0.52	0	29,33,33	0.92	2 (6%)
2	2AN	C	203	-	22,23,23	0.64	0	29,33,33	0.99	1 (3%)
2	2AN	J	201	-	22,23,23	0.84	1 (4%)	29,33,33	0.78	2 (6%)
2	2AN	Z	201	-	22,23,23	0.75	0	29,33,33	0.92	2 (6%)
2	2AN	L	205	-	22,23,23	0.63	0	29,33,33	0.84	1 (3%)
2	2AN	A	201	-	22,23,23	0.77	0	29,33,33	1.08	2 (6%)
2	2AN	M	202	-	22,23,23	0.80	1 (4%)	29,33,33	0.85	1 (3%)
2	2AN	R	202	-	22,23,23	0.71	0	29,33,33	0.97	1 (3%)
2	2AN	Y	202	-	22,23,23	0.71	0	29,33,33	0.84	1 (3%)
2	2AN	D	202	-	22,23,23	0.59	0	29,33,33	0.89	2 (6%)
2	2AN	Z	202	-	22,23,23	0.82	0	29,33,33	1.04	3 (10%)
2	2AN	N	201	-	22,23,23	0.73	0	29,33,33	0.96	2 (6%)
2	2AN	L	201	-	22,23,23	0.60	0	29,33,33	0.90	1 (3%)
2	2AN	B	203	-	22,23,23	0.58	0	29,33,33	0.84	1 (3%)
2	2AN	B	201	-	22,23,23	0.58	0	29,33,33	0.82	1 (3%)
2	2AN	I	204	-	22,23,23	0.71	0	29,33,33	1.32	4 (13%)
2	2AN	W	203	-	22,23,23	0.93	1 (4%)	29,33,33	0.92	2 (6%)
2	2AN	C	201	-	22,23,23	0.92	1 (4%)	29,33,33	0.88	1 (3%)
2	2AN	Q	202	-	22,23,23	0.60	0	29,33,33	0.96	1 (3%)
2	2AN	M	203	-	22,23,23	0.51	0	29,33,33	0.91	2 (6%)
2	2AN	C	204	-	22,23,23	0.83	1 (4%)	29,33,33	0.91	3 (10%)
2	2AN	Q	201	-	22,23,23	0.62	0	29,33,33	0.91	1 (3%)
2	2AN	O	202	-	22,23,23	0.83	1 (4%)	29,33,33	0.89	1 (3%)
2	2AN	B	204	-	22,23,23	0.78	0	29,33,33	0.91	1 (3%)
2	2AN	M	201	-	22,23,23	0.82	1 (4%)	29,33,33	0.83	1 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	2AN	X	201	-	22,23,23	0.65	0	29,33,33	0.80	2 (6%)
2	2AN	W	204	-	22,23,23	0.81	0	29,33,33	1.06	3 (10%)
2	2AN	E	204	-	22,23,23	0.83	1 (4%)	29,33,33	0.97	1 (3%)
2	2AN	H	203	-	22,23,23	0.83	1 (4%)	29,33,33	1.01	2 (6%)
2	2AN	S	201	-	22,23,23	0.81	1 (4%)	29,33,33	0.82	1 (3%)
2	2AN	U	202	-	22,23,23	0.84	0	29,33,33	0.94	2 (6%)
2	2AN	Y	203	-	22,23,23	0.54	0	29,33,33	0.86	0
2	2AN	D	203	-	22,23,23	0.64	0	29,33,33	0.85	1 (3%)
2	2AN	L	204	-	22,23,23	0.58	0	29,33,33	1.02	2 (6%)
2	2AN	Z	203	-	22,23,23	0.47	0	29,33,33	0.94	2 (6%)
2	2AN	O	201	-	22,23,23	0.84	1 (4%)	29,33,33	0.89	1 (3%)
2	2AN	E	205	-	22,23,23	0.77	0	29,33,33	0.99	3 (10%)
2	2AN	C	202	-	22,23,23	0.71	0	29,33,33	0.93	3 (10%)
2	2AN	I	203	-	22,23,23	0.57	0	29,33,33	0.96	2 (6%)
2	2AN	Q	203	-	22,23,23	0.62	0	29,33,33	0.82	1 (3%)
2	2AN	W	201	-	22,23,23	0.88	1 (4%)	29,33,33	1.11	4 (13%)
2	2AN	U	203	-	22,23,23	0.74	0	29,33,33	0.97	2 (6%)
3	EPE	Z	204	-	15,15,15	2.20	1 (6%)	18,20,20	4.18	11 (61%)
2	2AN	H	201	-	22,23,23	0.82	0	29,33,33	1.04	3 (10%)
2	2AN	I	205	-	22,23,23	0.56	0	29,33,33	0.92	2 (6%)
2	2AN	J	202	-	22,23,23	0.75	0	29,33,33	0.96	2 (6%)
2	2AN	A	202	-	22,23,23	0.82	0	29,33,33	0.87	1 (3%)
2	2AN	N	203	-	22,23,23	0.80	0	29,33,33	1.03	2 (6%)

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	Y	204	-	-	0/10/10/10	0/3/3/3
2	2AN	E	202	-	-	0/10/10/10	0/3/3/3
2	2AN	P	202	-	-	1/10/10/10	0/3/3/3
2	2AN	V	202	-	-	2/10/10/10	0/3/3/3
2	2AN	N	204	-	-	0/10/10/10	0/3/3/3
2	2AN	I	201	-	-	1/10/10/10	0/3/3/3
2	2AN	b	202	-	-	0/10/10/10	0/3/3/3

Continued on next page...

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	2AN	a	201	-	-	0/10/10/10	0/3/3/3
2	2AN	U	201	-	-	0/10/10/10	0/3/3/3
2	2AN	b	201	-	-	0/10/10/10	0/3/3/3
2	2AN	X	202	-	-	1/10/10/10	0/3/3/3
2	2AN	Y	201	-	-	0/10/10/10	0/3/3/3
3	EPE	C	205	-	-	3/9/19/19	0/1/1/1
2	2AN	H	202	-	-	0/10/10/10	0/3/3/3
2	2AN	E	203	-	-	0/10/10/10	0/3/3/3
2	2AN	K	201	-	-	0/10/10/10	0/3/3/3
2	2AN	X	203	-	-	0/10/10/10	0/3/3/3
2	2AN	F	201	-	-	0/10/10/10	0/3/3/3
2	2AN	E	201	-	-	0/10/10/10	0/3/3/3
2	2AN	N	202	-	-	0/10/10/10	0/3/3/3
2	2AN	b	203	-	-	0/10/10/10	0/3/3/3
2	2AN	G	204	-	-	0/10/10/10	0/3/3/3
2	2AN	U	204	-	-	0/10/10/10	0/3/3/3
2	2AN	R	203	-	-	0/10/10/10	0/3/3/3
2	2AN	R	204	-	-	2/10/10/10	0/3/3/3
2	2AN	I	202	-	-	2/10/10/10	0/3/3/3
2	2AN	P	201	-	-	0/10/10/10	0/3/3/3
2	2AN	K	202	-	-	0/10/10/10	0/3/3/3
2	2AN	A	203	-	-	0/10/10/10	0/3/3/3
2	2AN	K	203	-	-	0/10/10/10	0/3/3/3
2	2AN	V	201	-	-	2/10/10/10	0/3/3/3
2	2AN	L	203	-	-	0/10/10/10	0/3/3/3
2	2AN	G	202	-	-	0/10/10/10	0/3/3/3
2	2AN	B	202	-	-	0/10/10/10	0/3/3/3
2	2AN	G	201	-	-	0/10/10/10	0/3/3/3
2	2AN	W	202	-	-	0/10/10/10	0/3/3/3
2	2AN	L	202	-	-	0/10/10/10	0/3/3/3
2	2AN	A	204	-	-	0/10/10/10	0/3/3/3
2	2AN	G	203	-	-	0/10/10/10	0/3/3/3
2	2AN	B	205	-	-	0/10/10/10	0/3/3/3
2	2AN	R	201	-	-	1/10/10/10	0/3/3/3
2	2AN	D	201	-	-	0/10/10/10	0/3/3/3
2	2AN	U	205	-	-	2/10/10/10	0/3/3/3
2	2AN	G	205	-	-	0/10/10/10	0/3/3/3
2	2AN	C	203	-	-	2/10/10/10	0/3/3/3
2	2AN	J	201	-	-	0/10/10/10	0/3/3/3
2	2AN	Z	201	-	-	0/10/10/10	0/3/3/3
2	2AN	L	205	-	-	0/10/10/10	0/3/3/3

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	2AN	A	201	-	-	0/10/10/10	0/3/3/3
2	2AN	M	202	-	-	1/10/10/10	0/3/3/3
2	2AN	R	202	-	-	0/10/10/10	0/3/3/3
2	2AN	Y	202	-	-	0/10/10/10	0/3/3/3
2	2AN	D	202	-	-	0/10/10/10	0/3/3/3
2	2AN	Z	202	-	-	0/10/10/10	0/3/3/3
2	2AN	N	201	-	-	0/10/10/10	0/3/3/3
2	2AN	L	201	-	-	0/10/10/10	0/3/3/3
2	2AN	B	203	-	-	0/10/10/10	0/3/3/3
2	2AN	B	201	-	-	0/10/10/10	0/3/3/3
2	2AN	I	204	-	-	0/10/10/10	0/3/3/3
2	2AN	W	203	-	-	2/10/10/10	0/3/3/3
2	2AN	C	201	-	-	0/10/10/10	0/3/3/3
2	2AN	Q	202	-	-	1/10/10/10	0/3/3/3
2	2AN	M	203	-	-	0/10/10/10	0/3/3/3
2	2AN	C	204	-	-	0/10/10/10	0/3/3/3
2	2AN	Q	201	-	-	0/10/10/10	0/3/3/3
2	2AN	O	202	-	-	0/10/10/10	0/3/3/3
2	2AN	B	204	-	-	0/10/10/10	0/3/3/3
2	2AN	M	201	-	-	0/10/10/10	0/3/3/3
2	2AN	X	201	-	-	0/10/10/10	0/3/3/3
2	2AN	W	204	-	-	1/10/10/10	0/3/3/3
2	2AN	E	204	-	-	0/10/10/10	0/3/3/3
2	2AN	H	203	-	-	0/10/10/10	0/3/3/3
2	2AN	S	201	-	-	0/10/10/10	0/3/3/3
2	2AN	U	202	-	-	0/10/10/10	0/3/3/3
2	2AN	Y	203	-	-	0/10/10/10	0/3/3/3
2	2AN	D	203	-	-	0/10/10/10	0/3/3/3
2	2AN	L	204	-	-	0/10/10/10	0/3/3/3
2	2AN	Z	203	-	-	0/10/10/10	0/3/3/3
2	2AN	O	201	-	-	0/10/10/10	0/3/3/3
2	2AN	E	205	-	-	0/10/10/10	0/3/3/3
2	2AN	C	202	-	-	0/10/10/10	0/3/3/3
2	2AN	I	203	-	-	0/10/10/10	0/3/3/3
2	2AN	Q	203	-	-	0/10/10/10	0/3/3/3
2	2AN	W	201	-	-	1/10/10/10	0/3/3/3
2	2AN	U	203	-	-	0/10/10/10	0/3/3/3
3	EPE	Z	204	-	-	6/9/19/19	0/1/1/1
2	2AN	H	201	-	-	0/10/10/10	0/3/3/3
2	2AN	I	205	-	-	0/10/10/10	0/3/3/3
2	2AN	J	202	-	-	0/10/10/10	0/3/3/3
2	2AN	A	202	-	-	0/10/10/10	0/3/3/3

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	2AN	N	203	-	-	0/10/10/10	0/3/3/3

The worst 5 of 27 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	Z	204	EPE	C10-S	-7.89	1.66	1.77
3	C	205	EPE	C10-S	-5.95	1.69	1.77
2	G	201	2AN	C9-C10	3.60	1.48	1.43
2	N	204	2AN	C16-C11	-3.22	1.33	1.39
2	G	204	2AN	C13-C12	-3.17	1.32	1.38

The worst 5 of 168 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	Z	204	EPE	O3S-S-C10	9.81	121.63	105.77
3	Z	204	EPE	O2S-S-C10	-7.63	97.72	106.92
3	C	205	EPE	C7-N4-C3	7.41	130.19	111.23
3	Z	204	EPE	C6-N1-C2	6.78	124.09	108.83
3	C	205	EPE	O1S-S-C10	5.64	113.71	106.92

There are no chirality outliers.

5 of 31 torsion outliers are listed below:

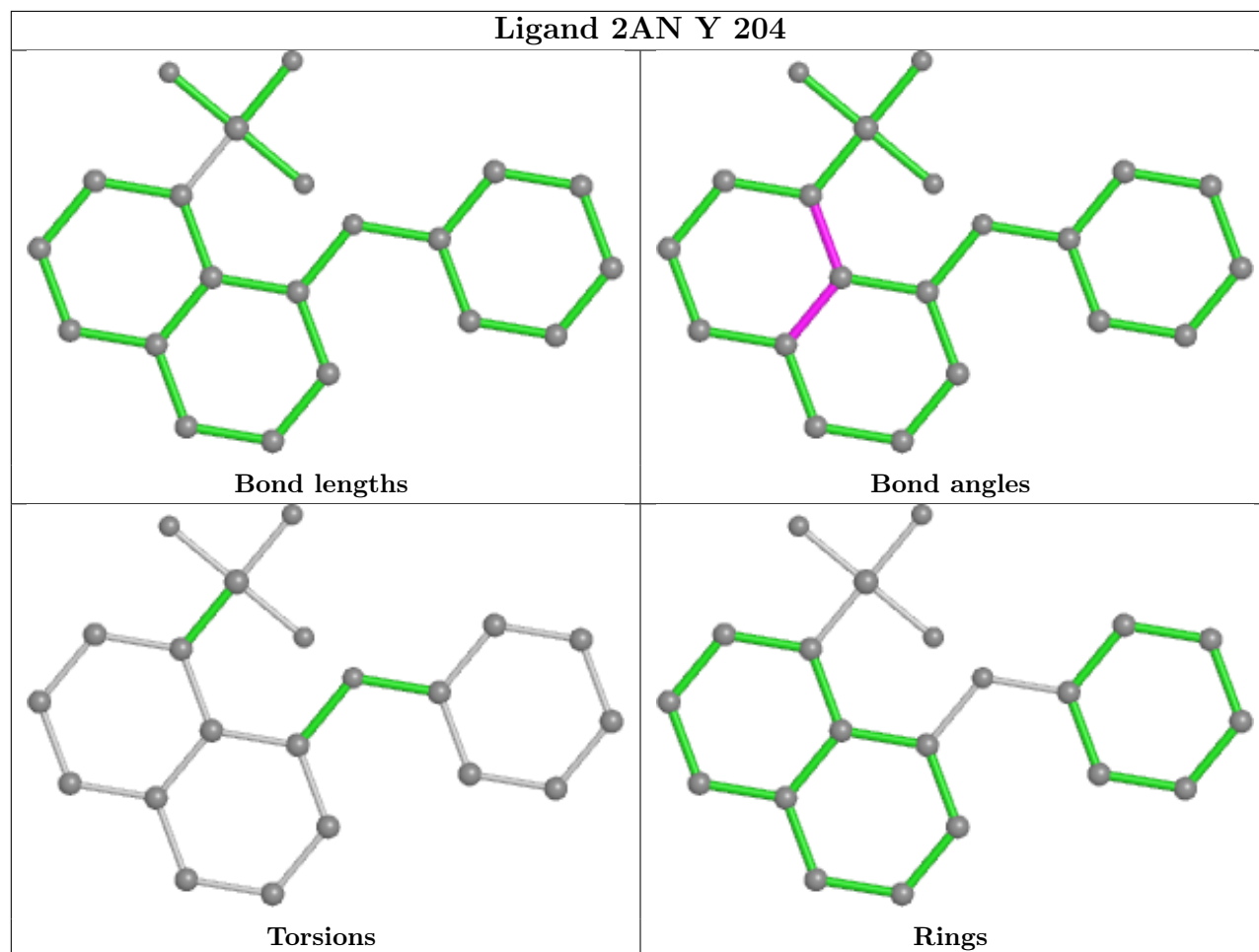
Mol	Chain	Res	Type	Atoms
3	C	205	EPE	C8-C7-N4-C3
3	C	205	EPE	S-C10-C9-N1
3	Z	204	EPE	C10-C9-N1-C6
3	Z	204	EPE	N4-C7-C8-O8
3	Z	204	EPE	S-C10-C9-N1

There are no ring outliers.

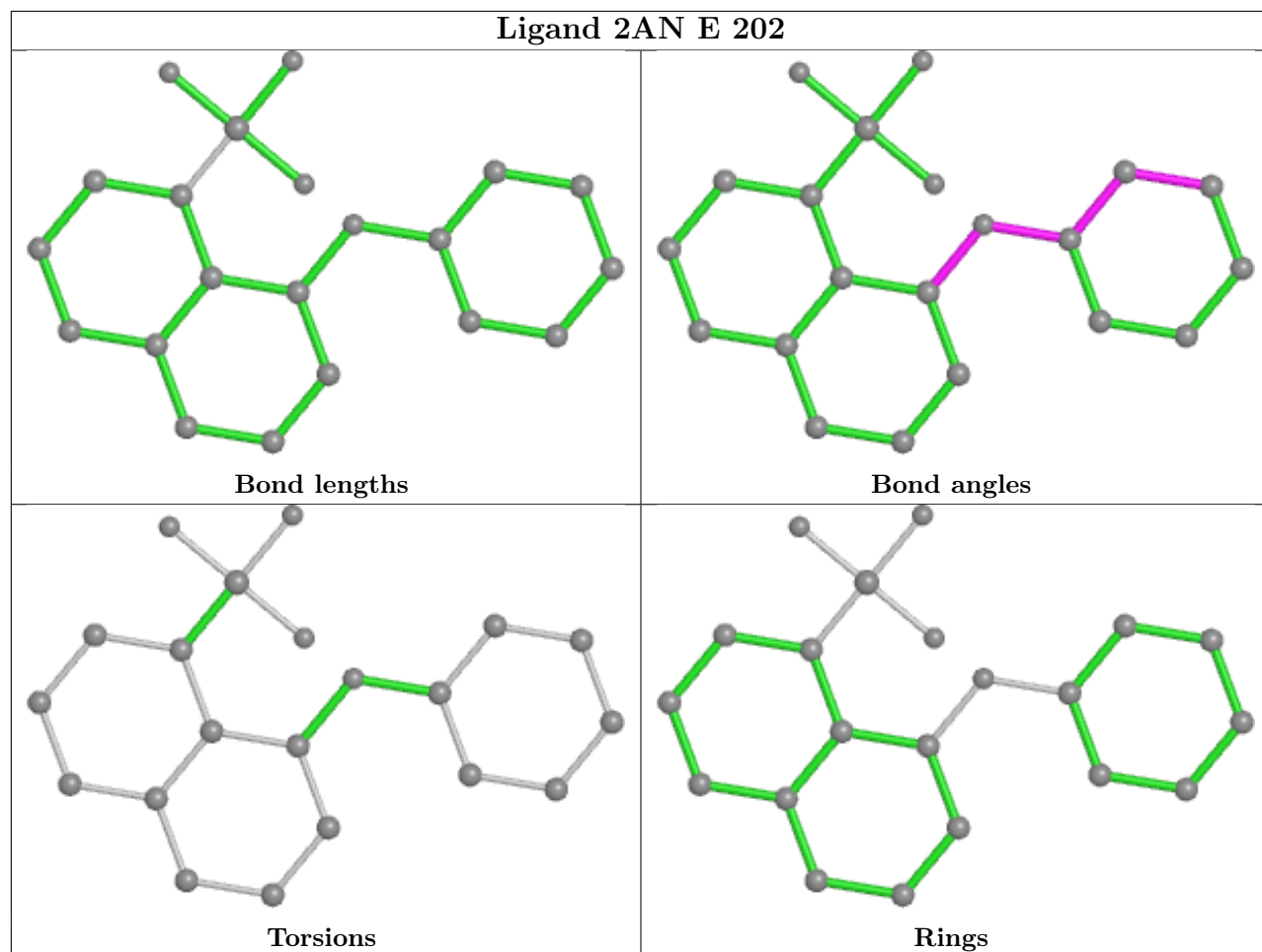
No monomer is involved in short contacts.

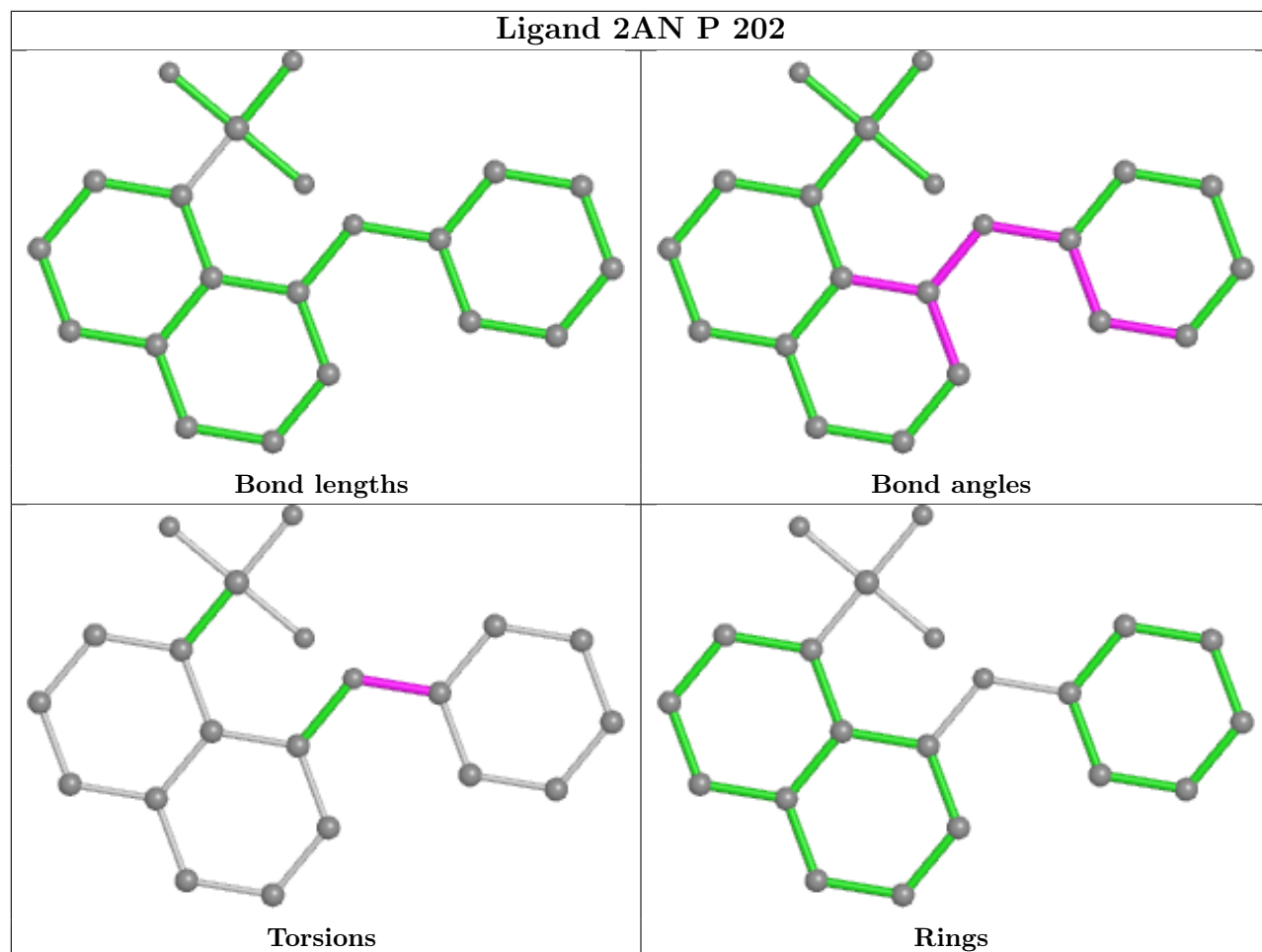
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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

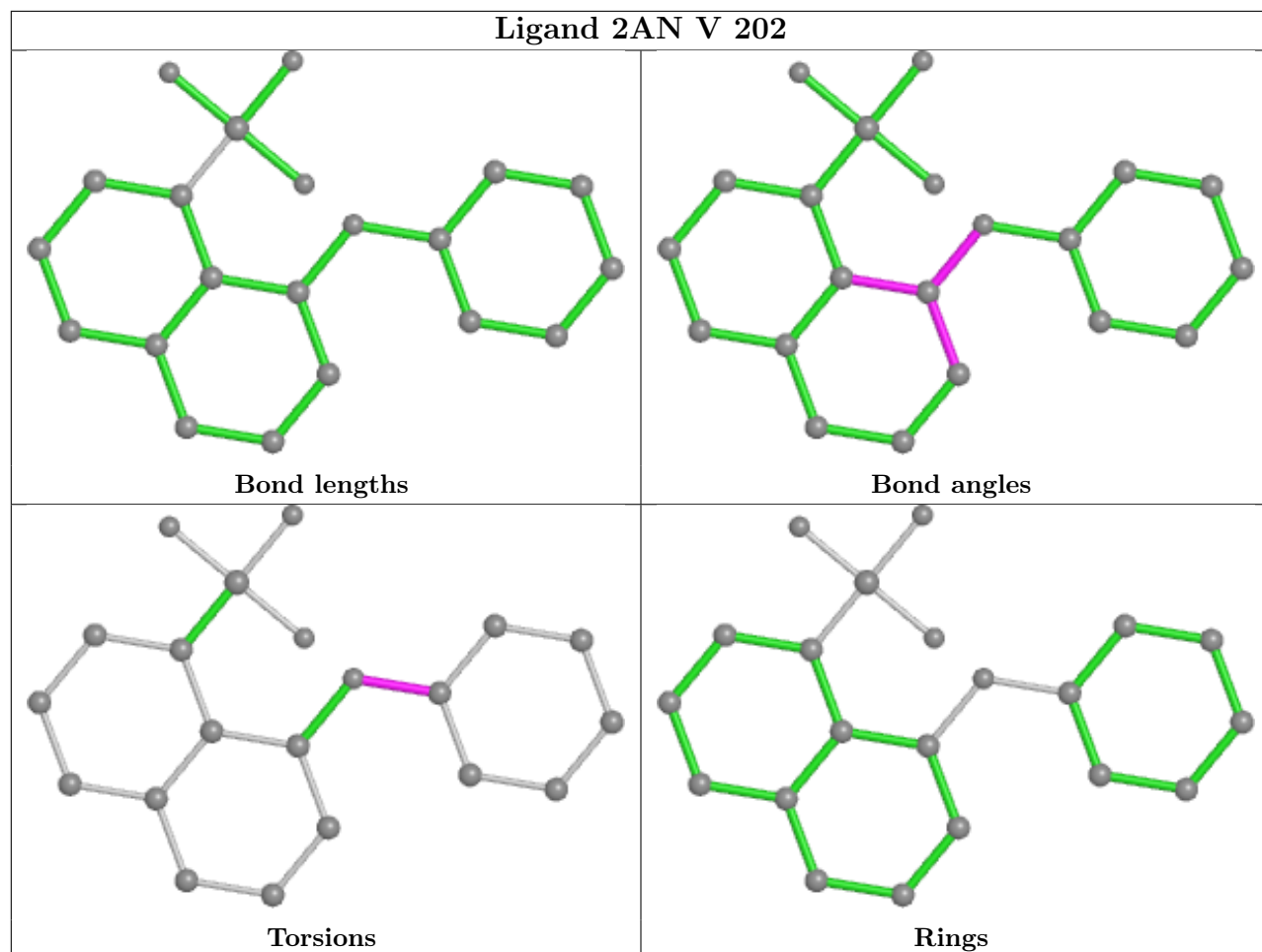
any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

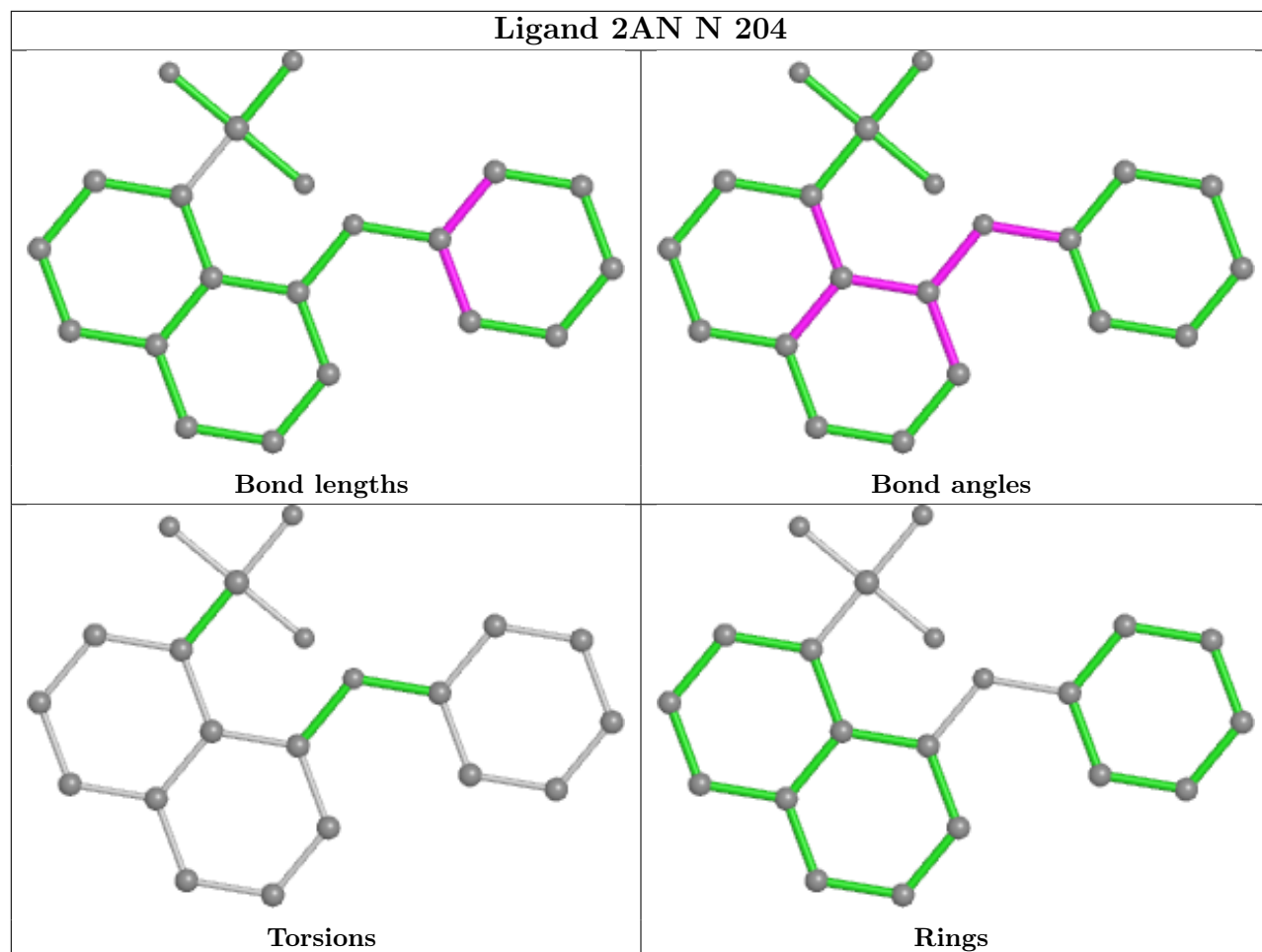


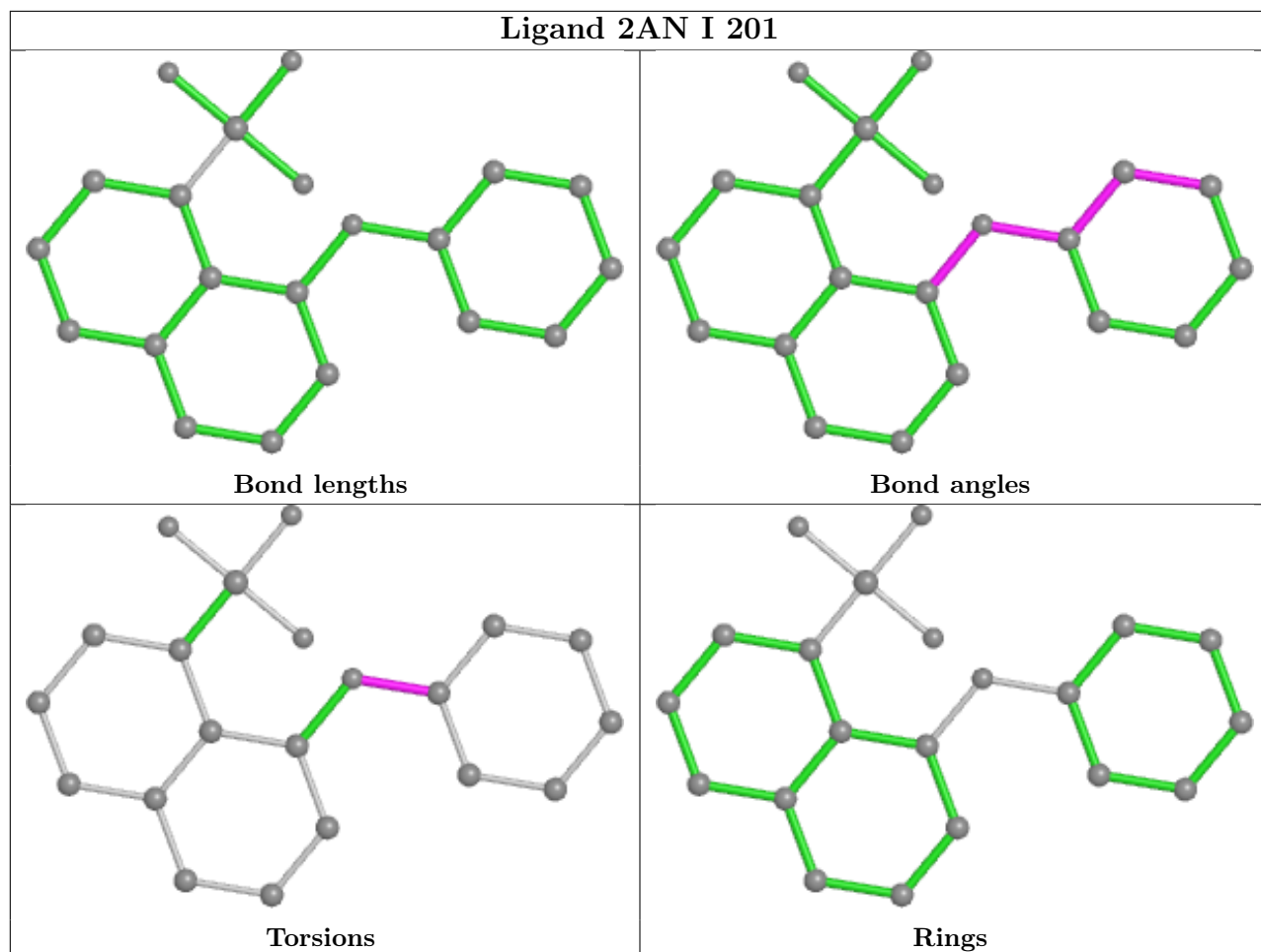


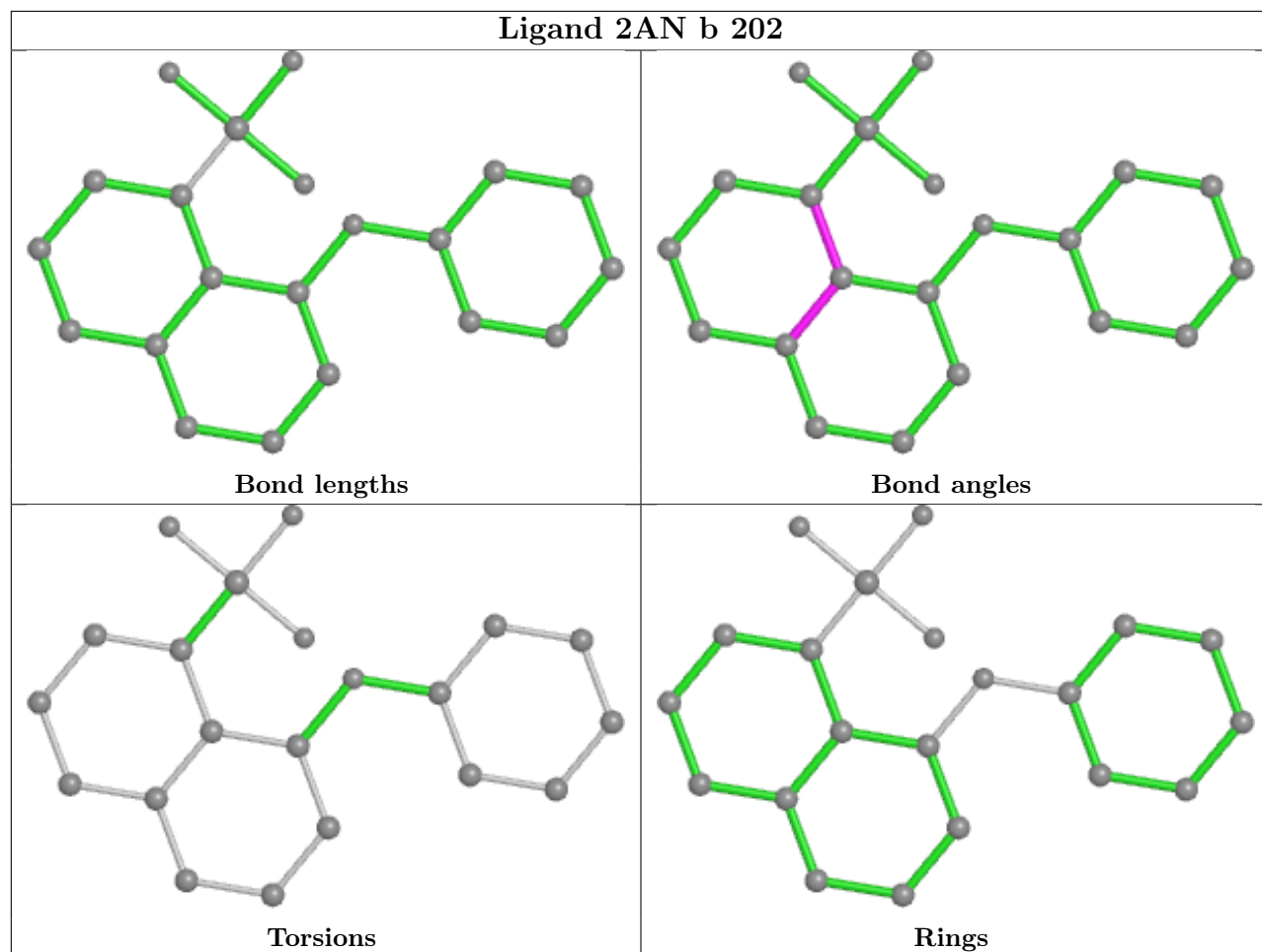


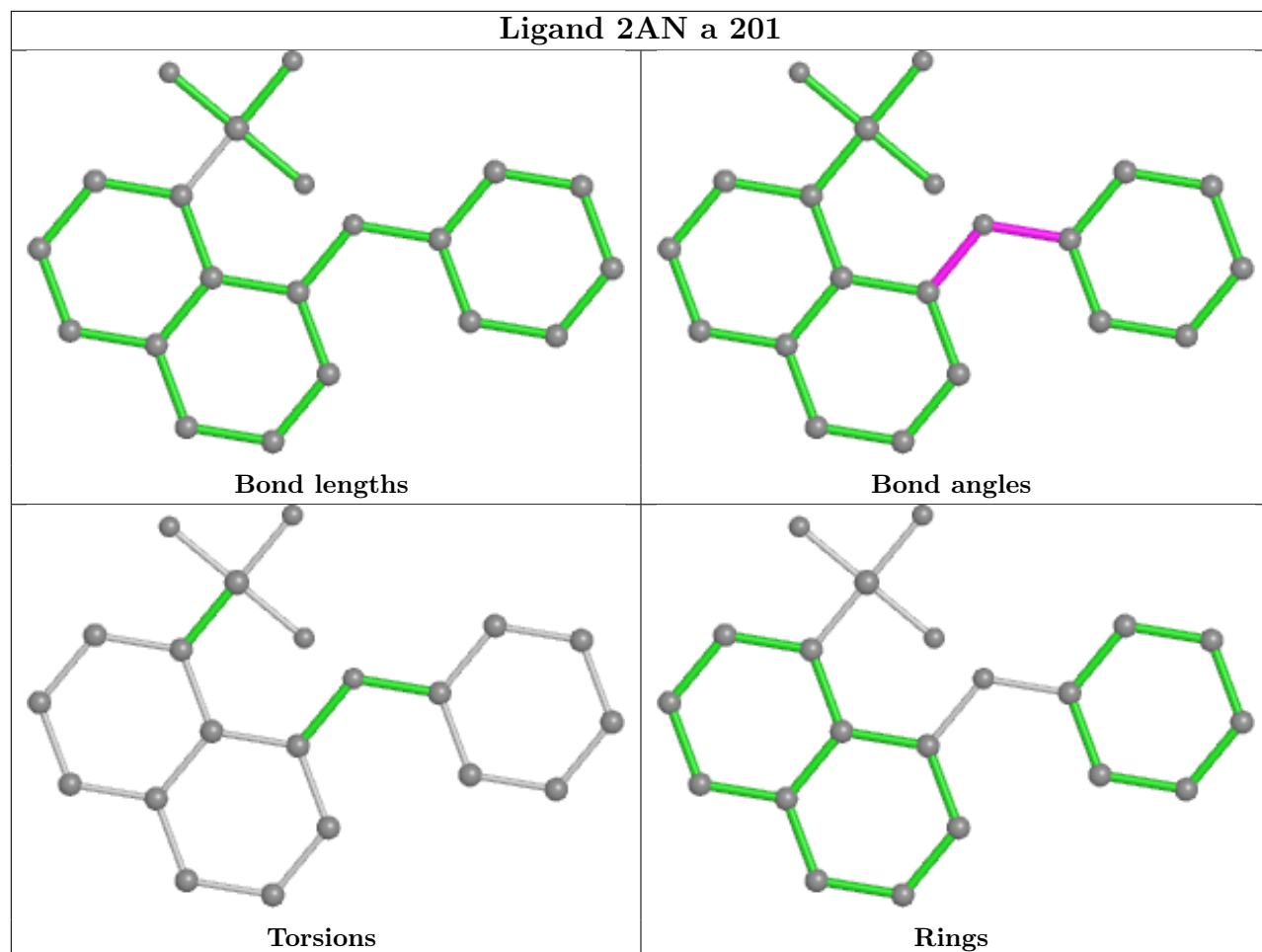


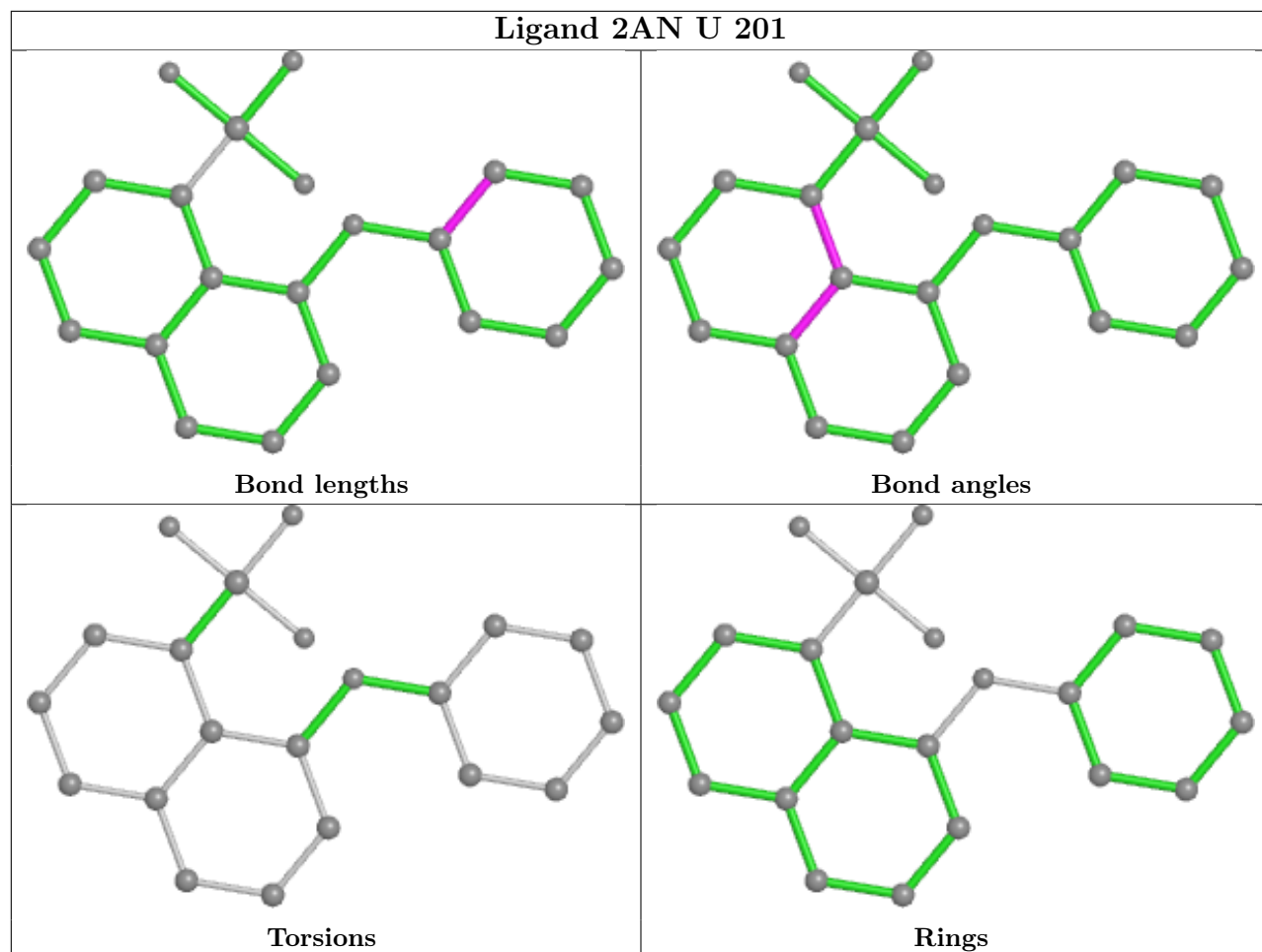




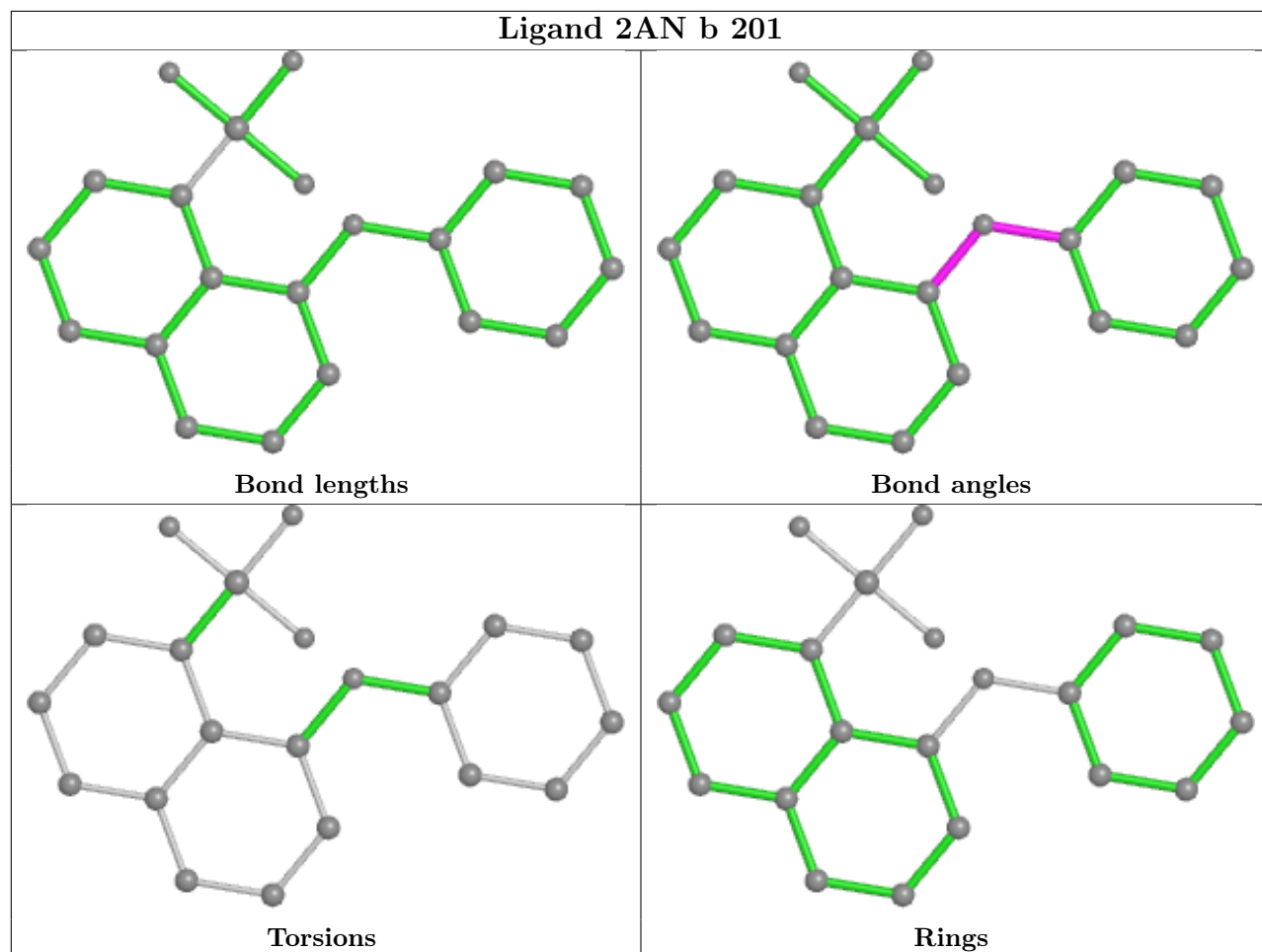


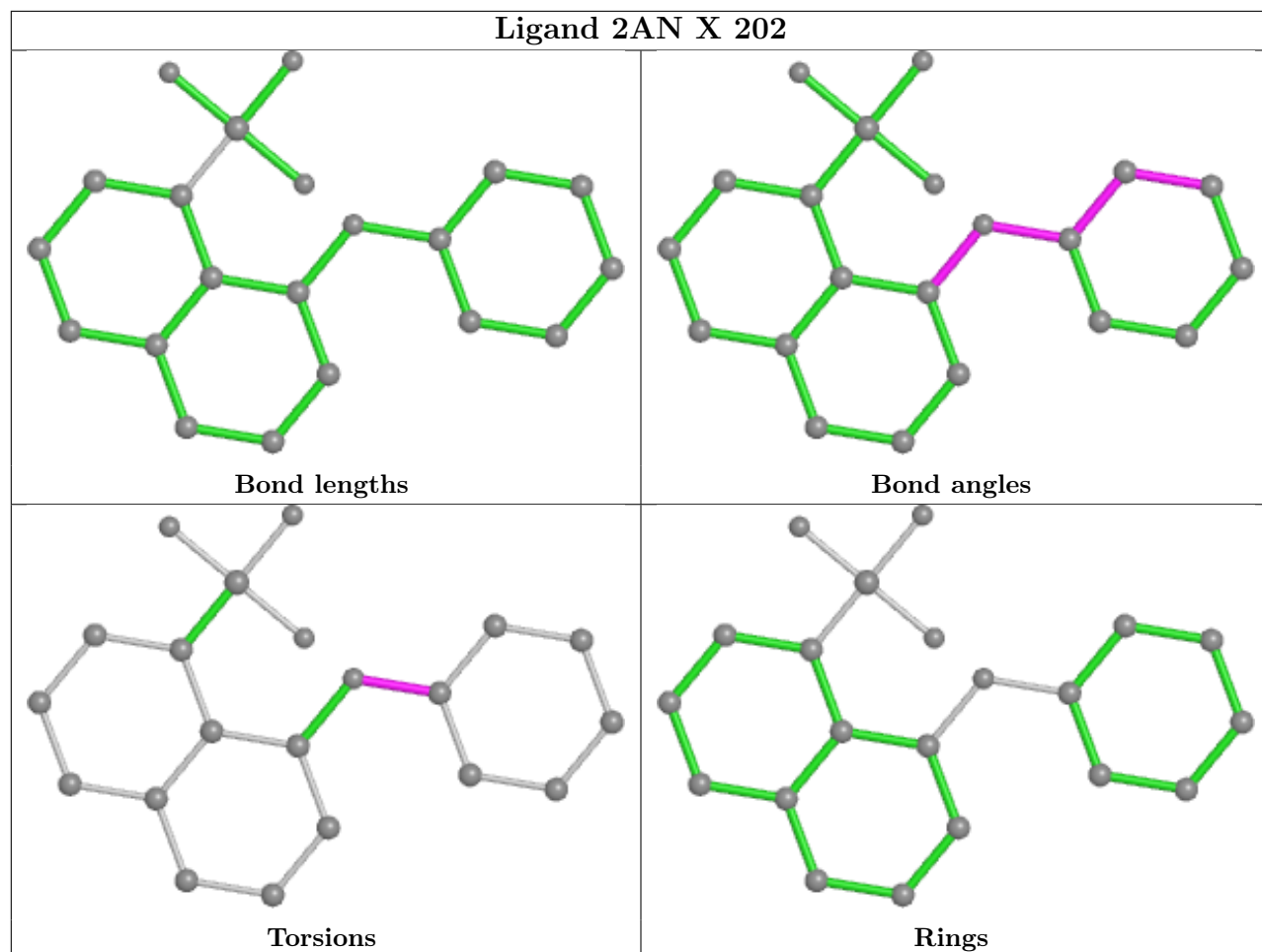


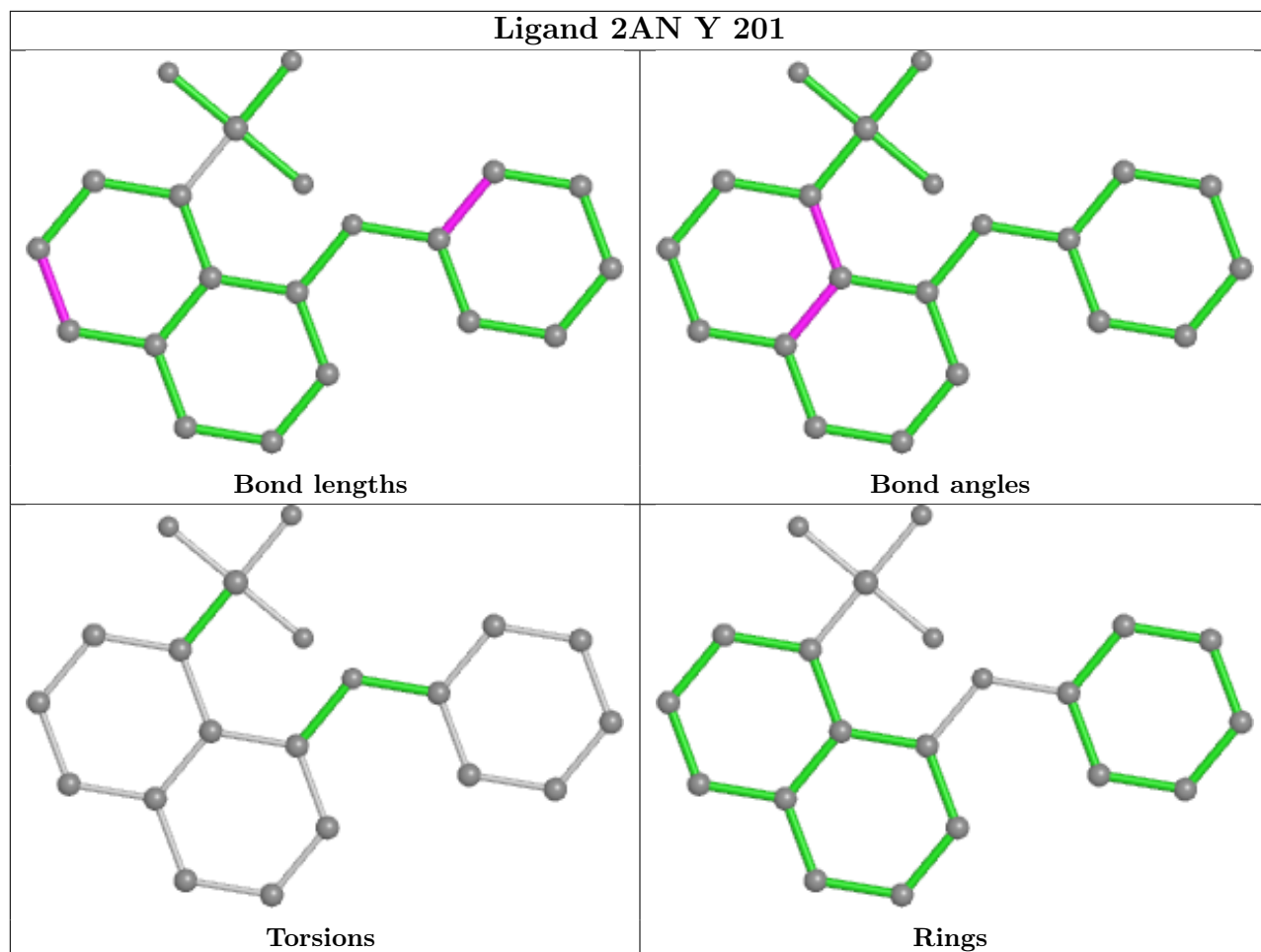


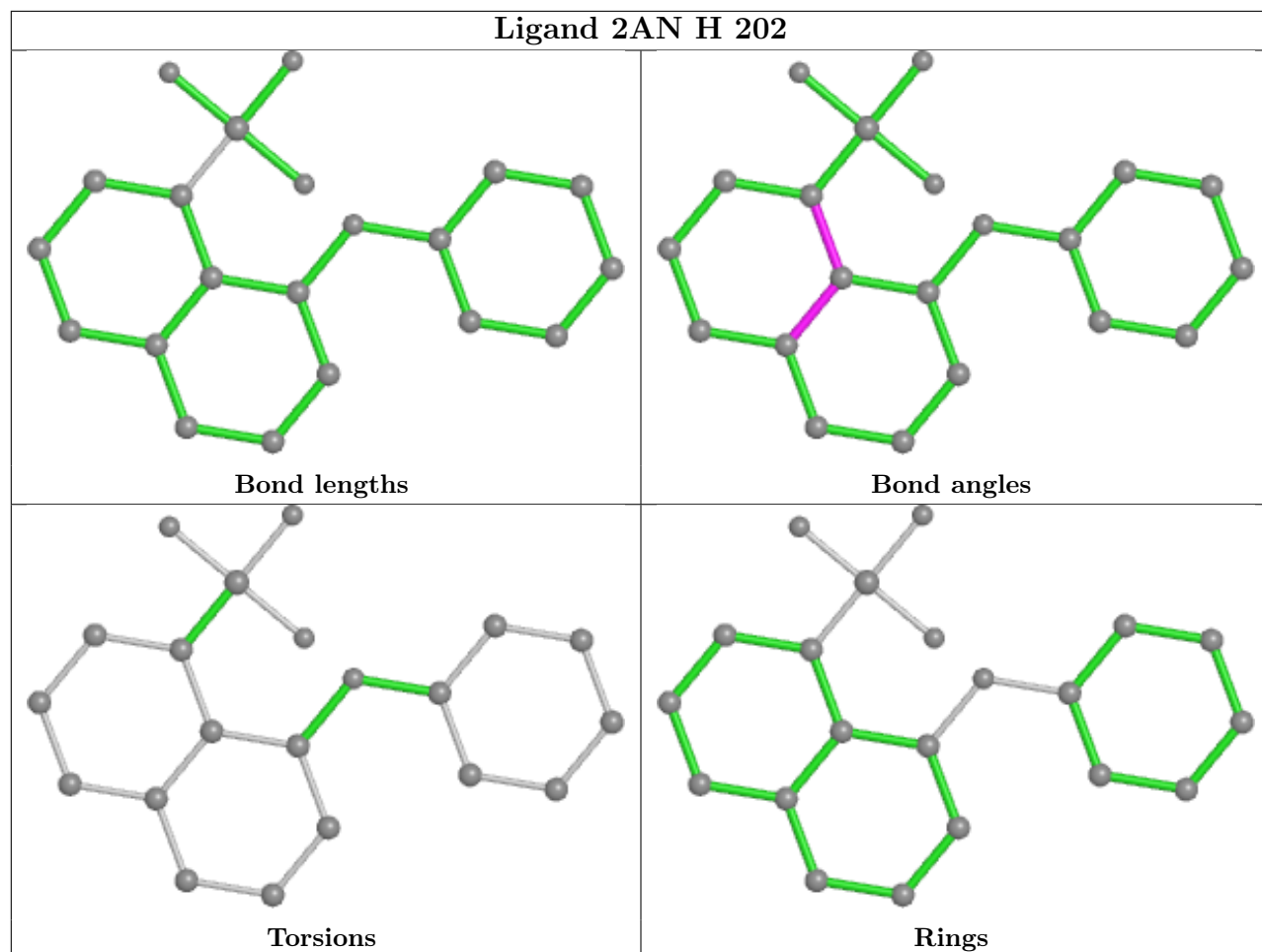


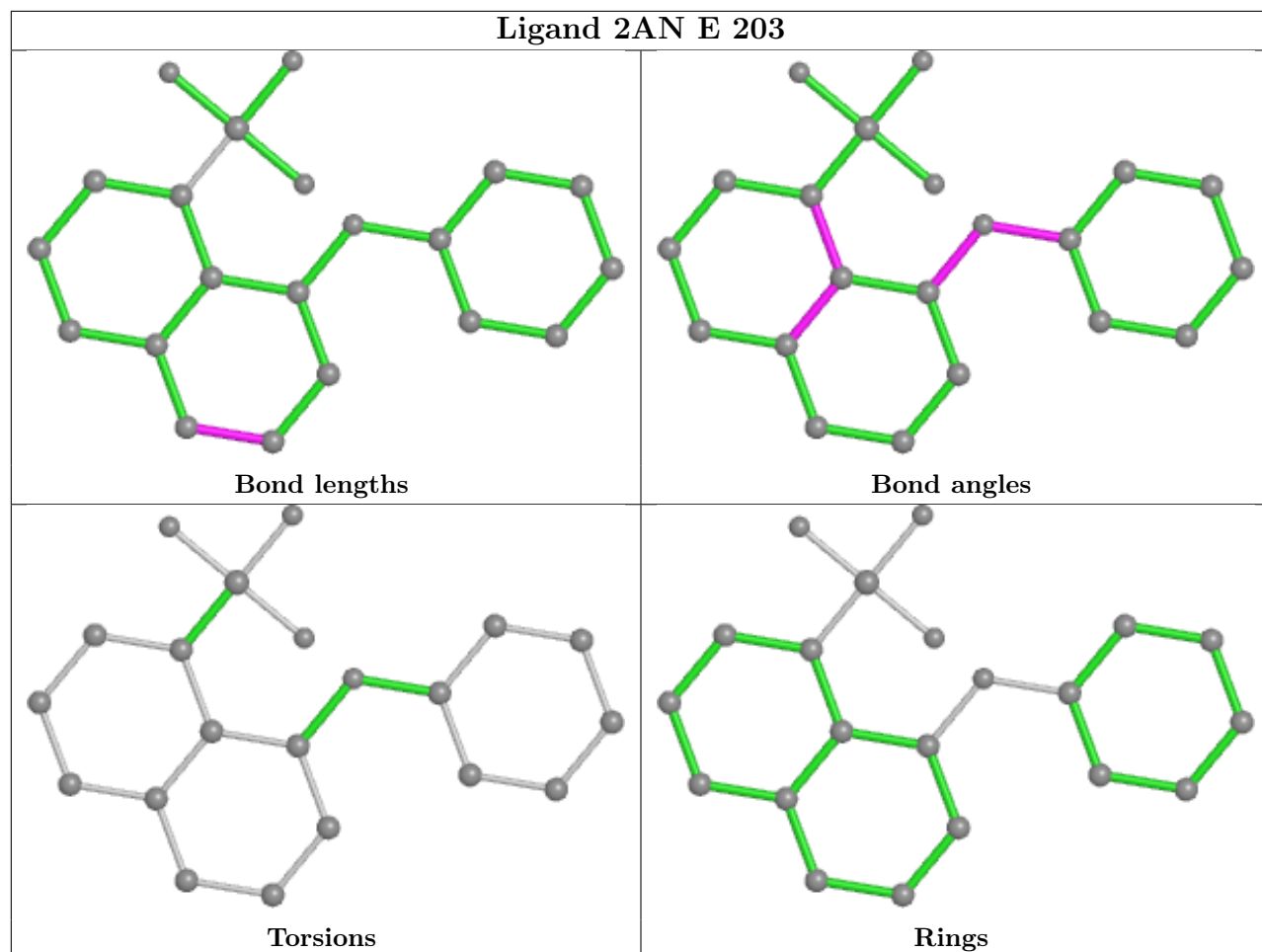


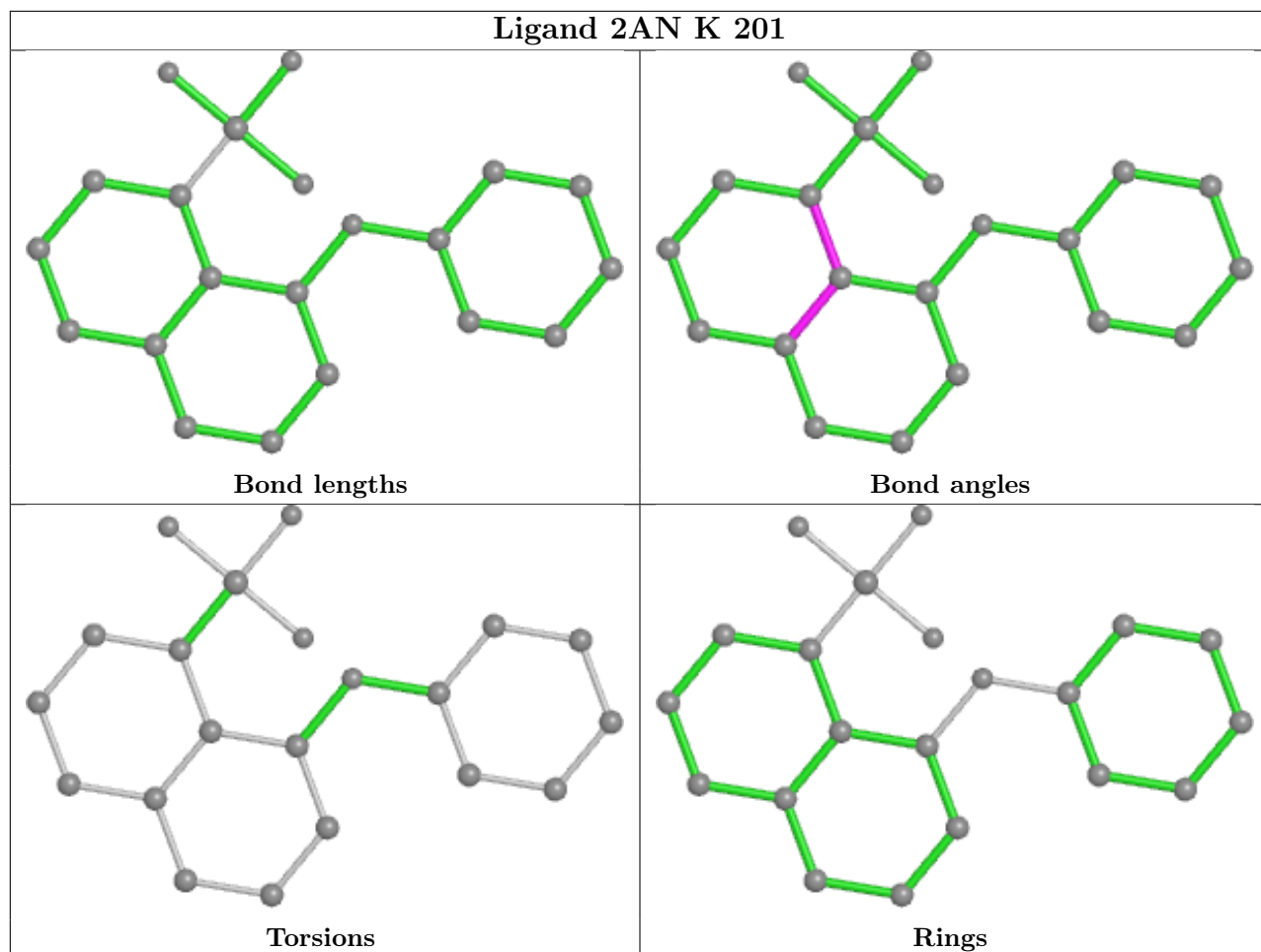


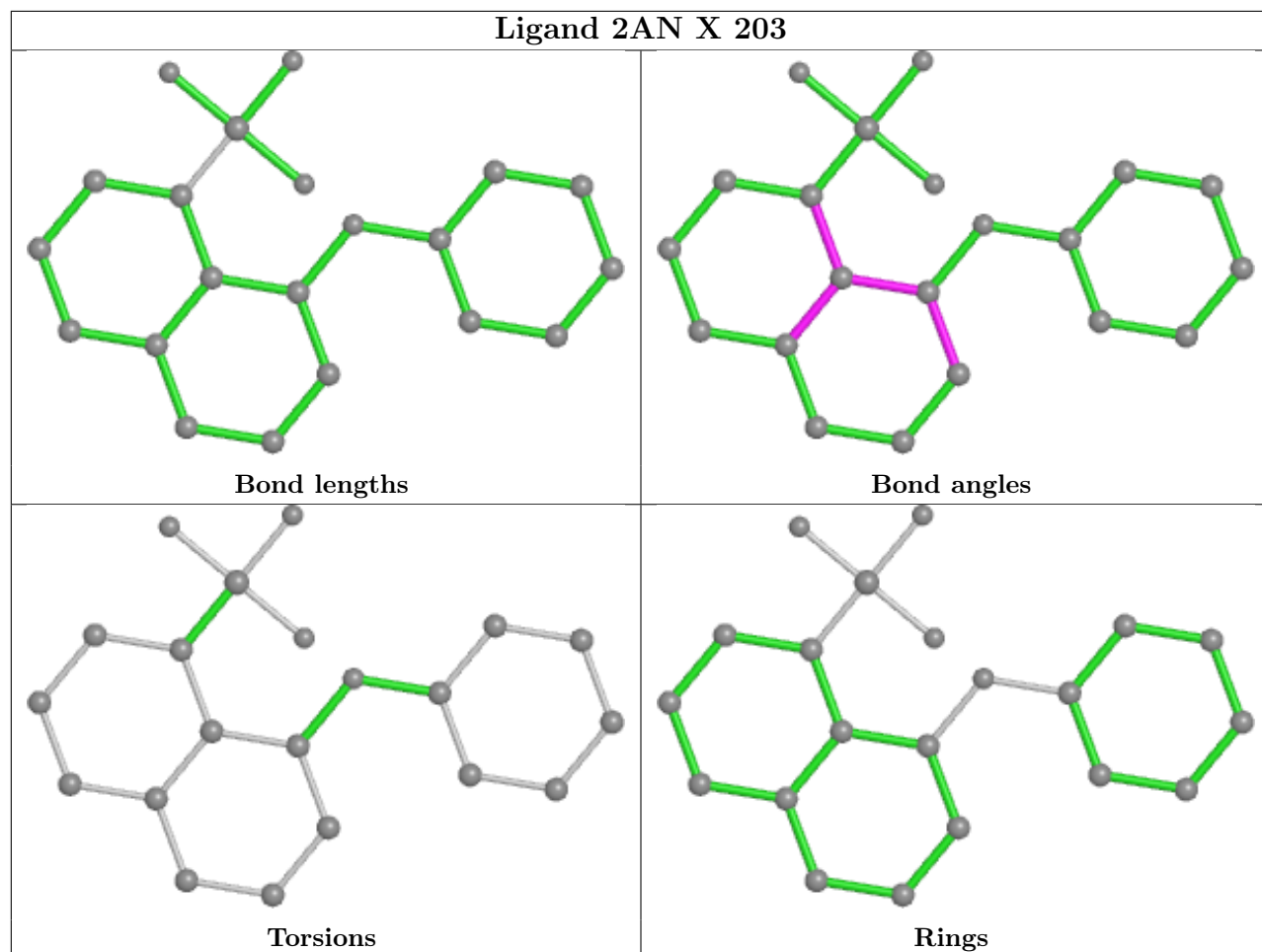


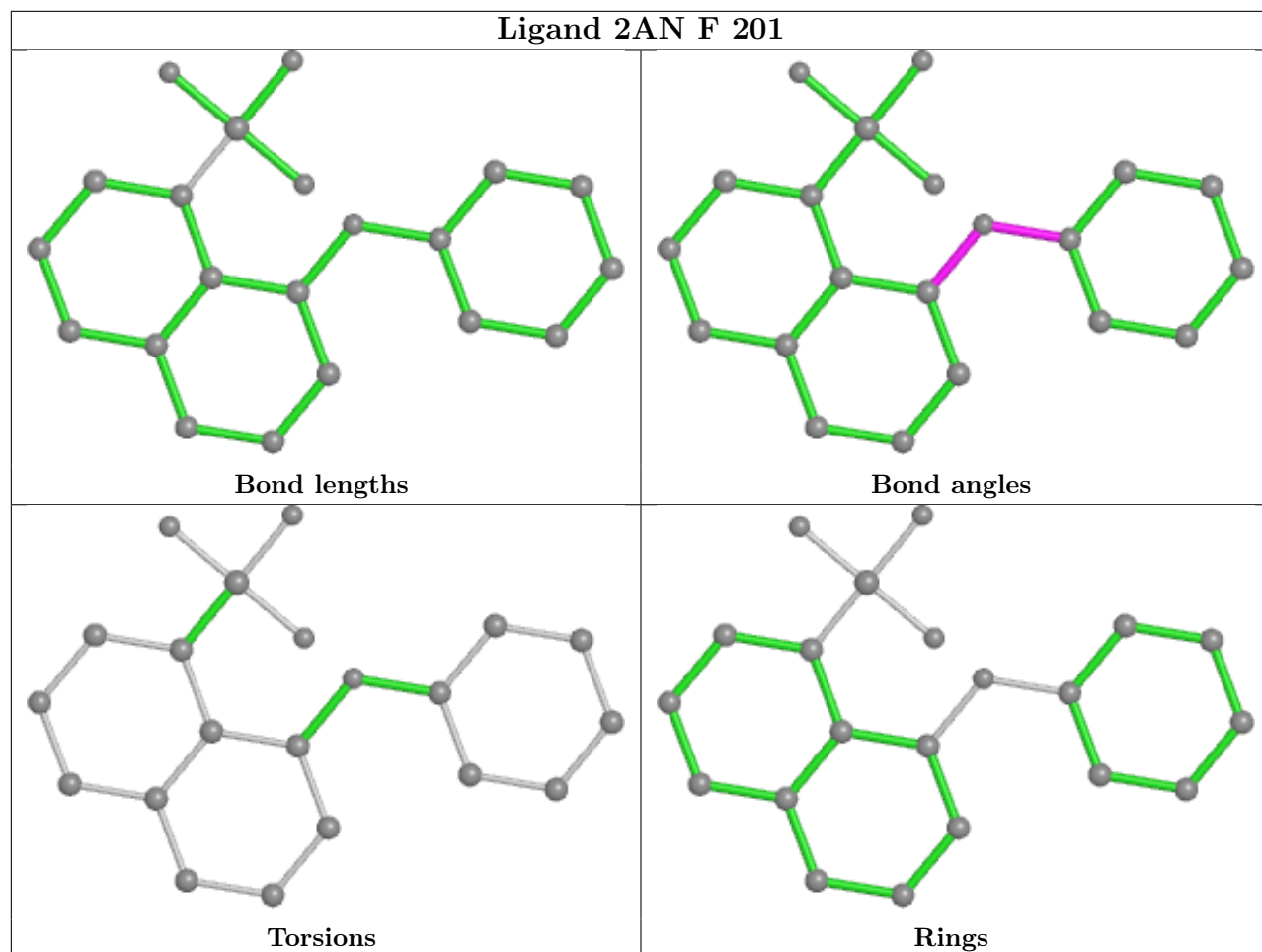




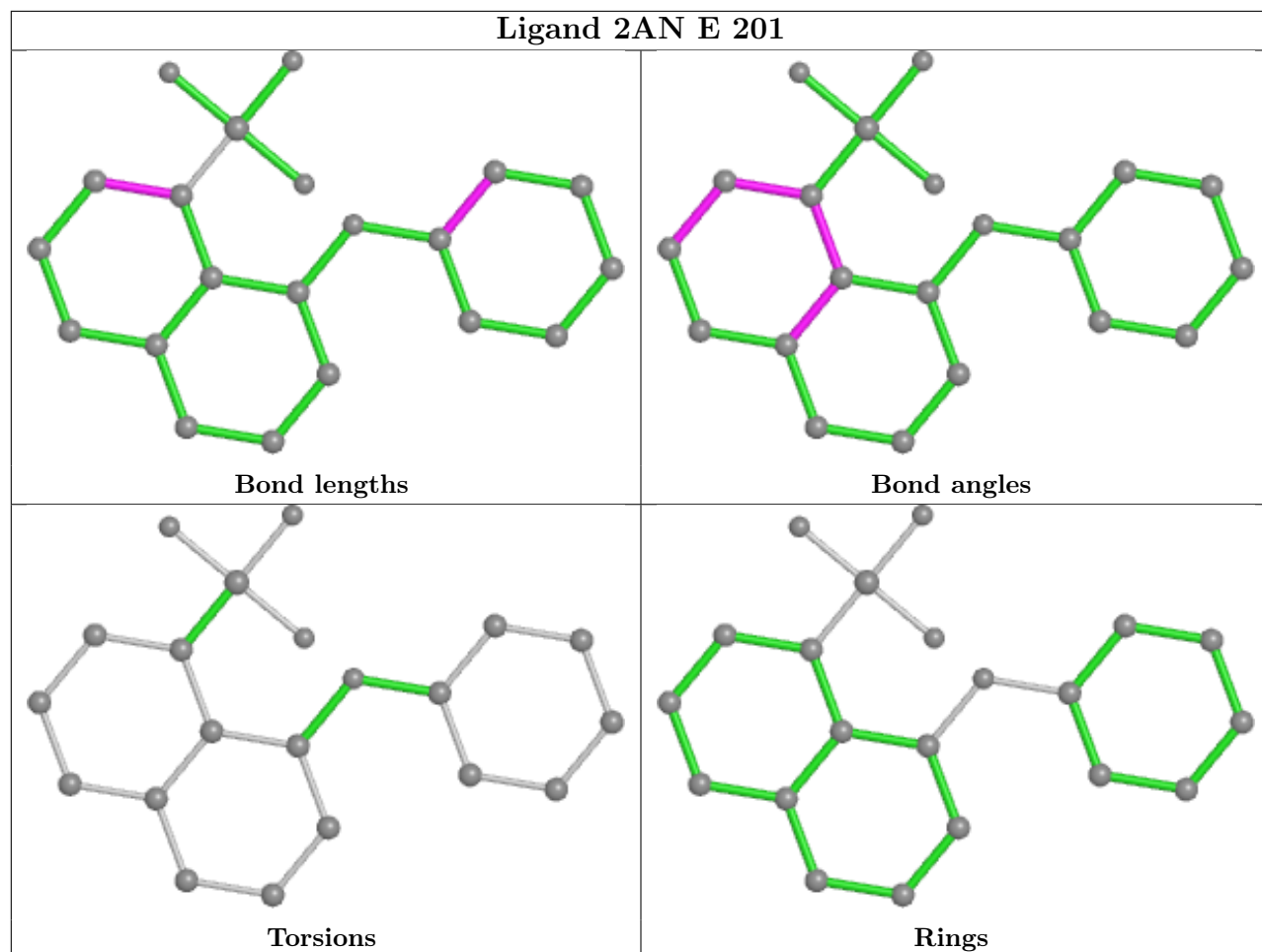


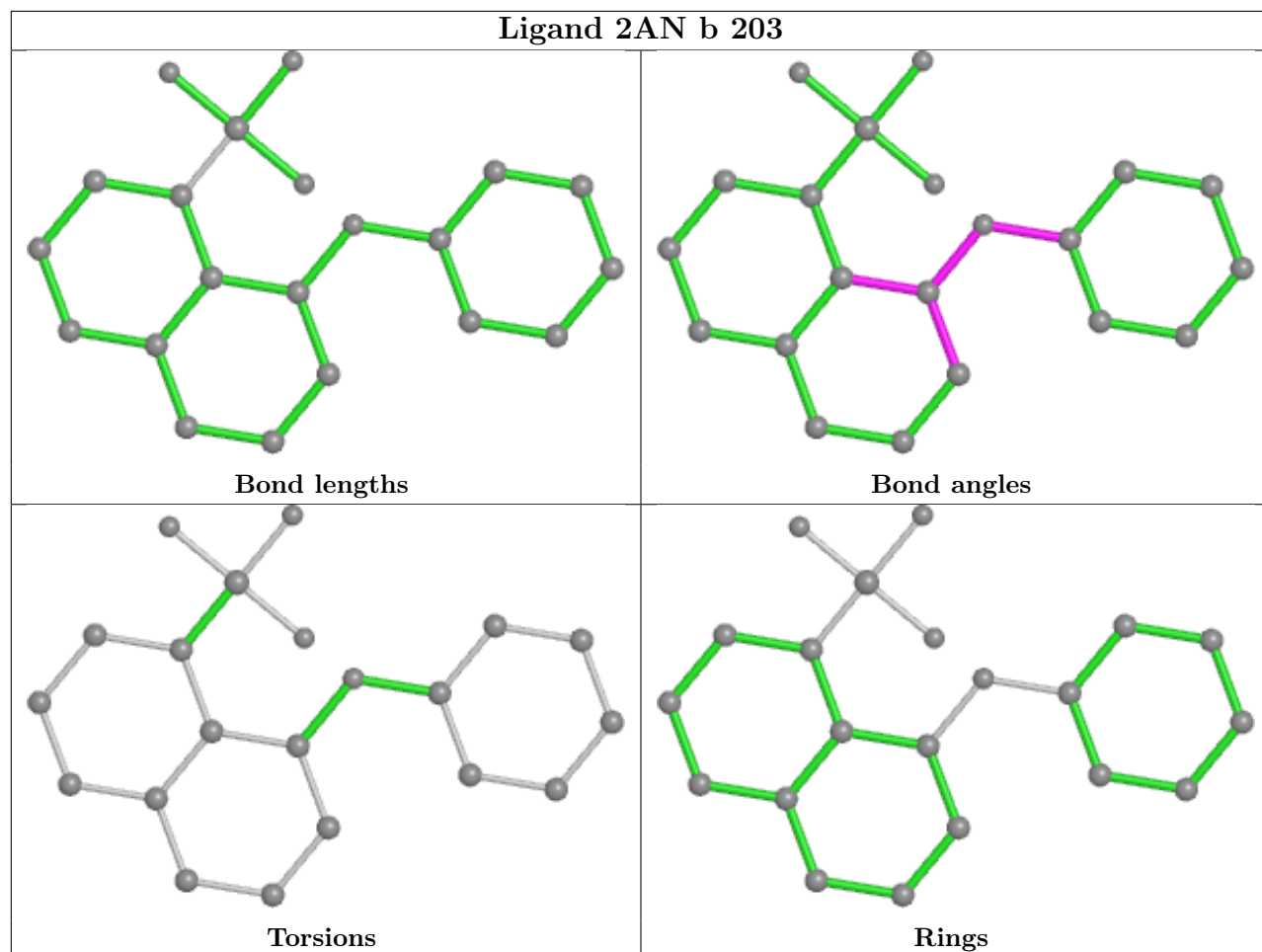


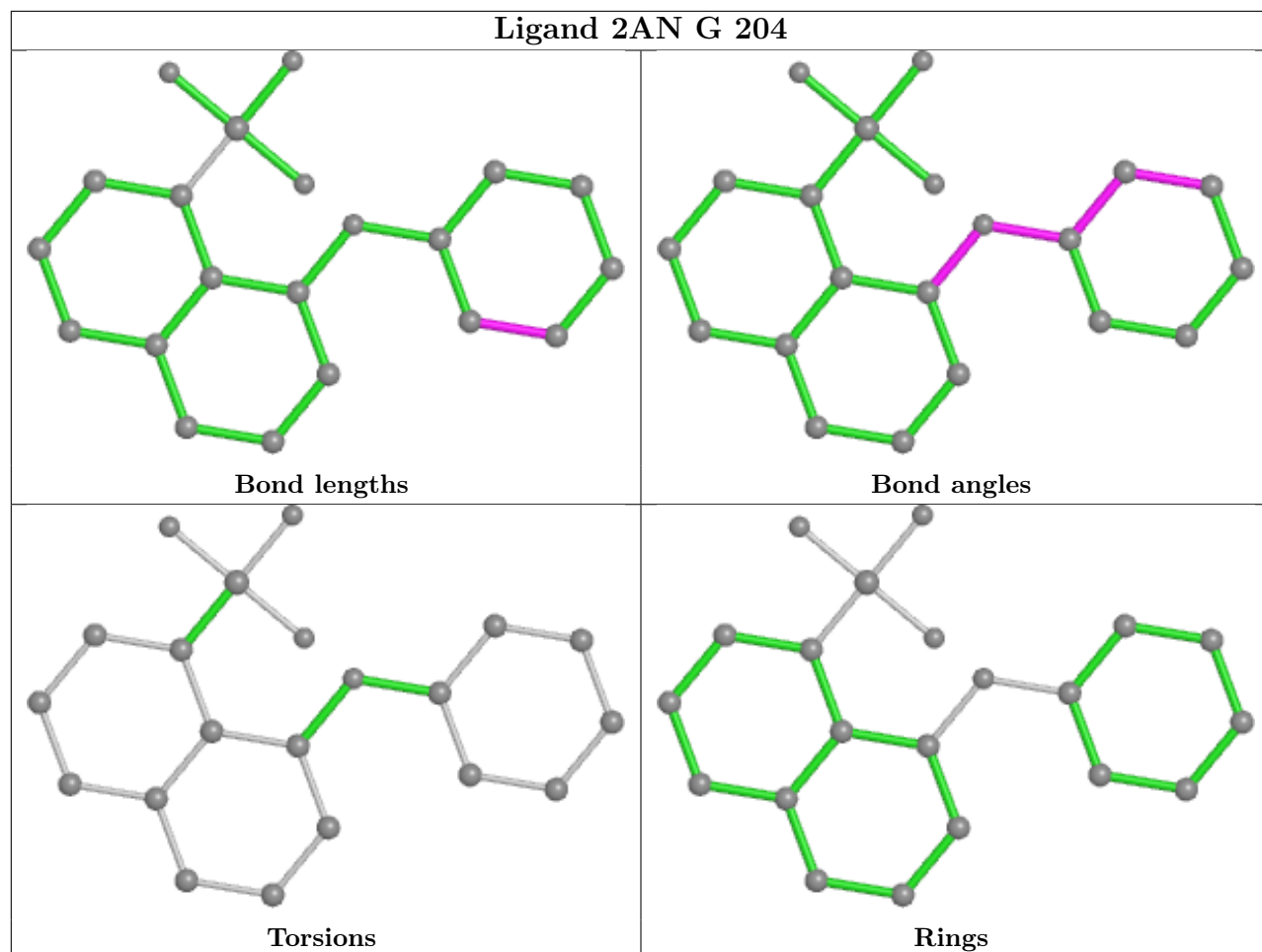


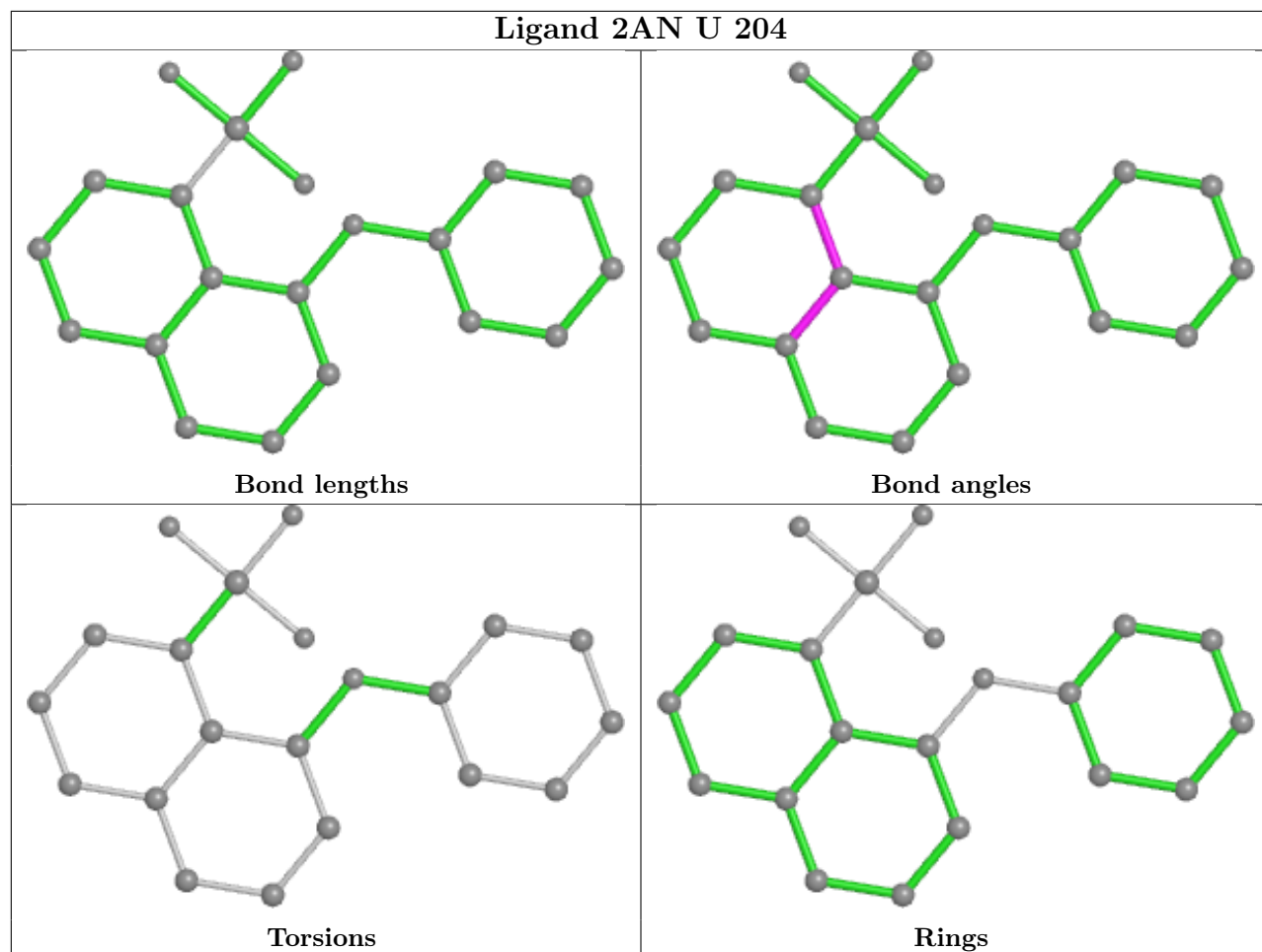


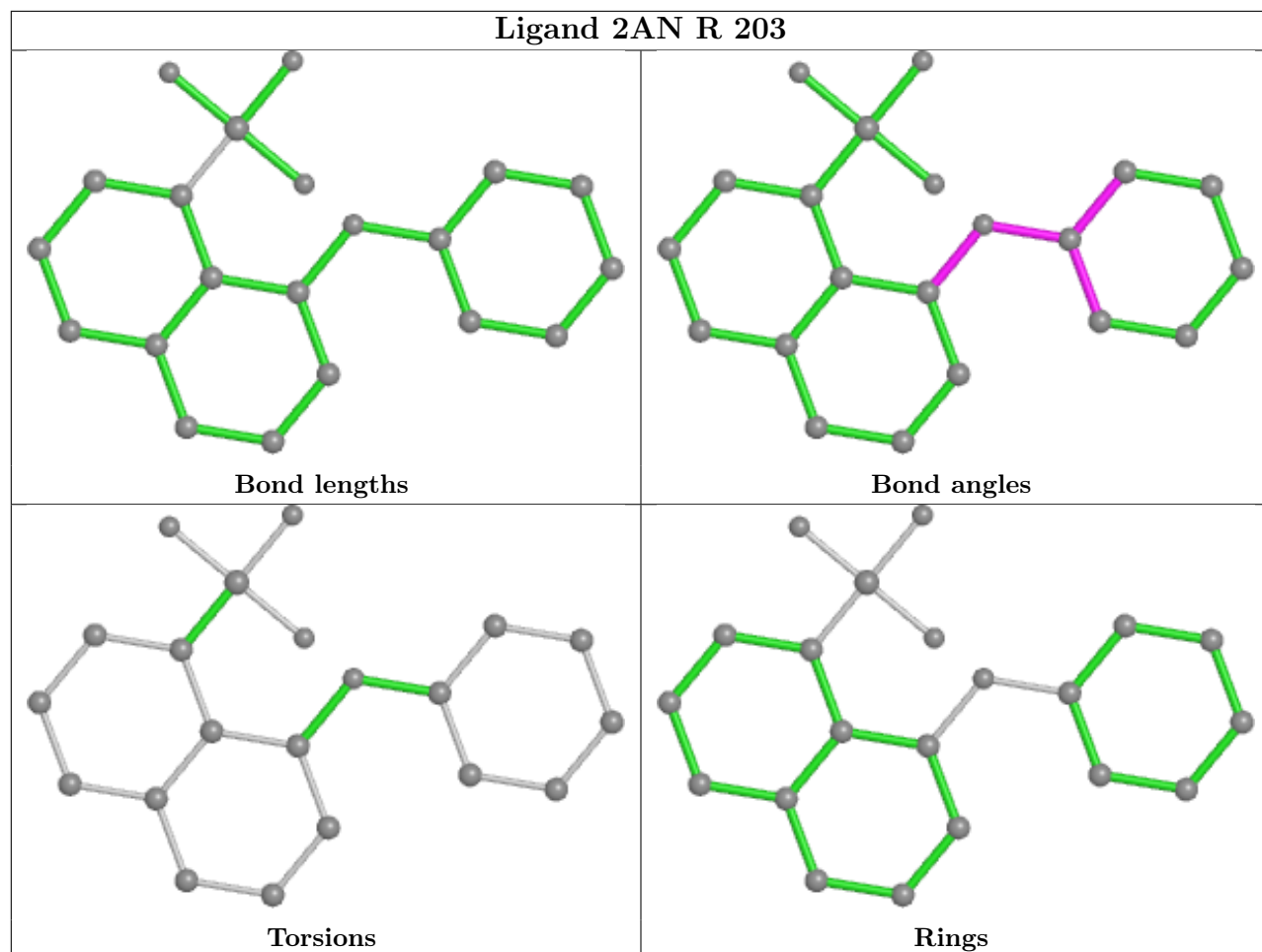


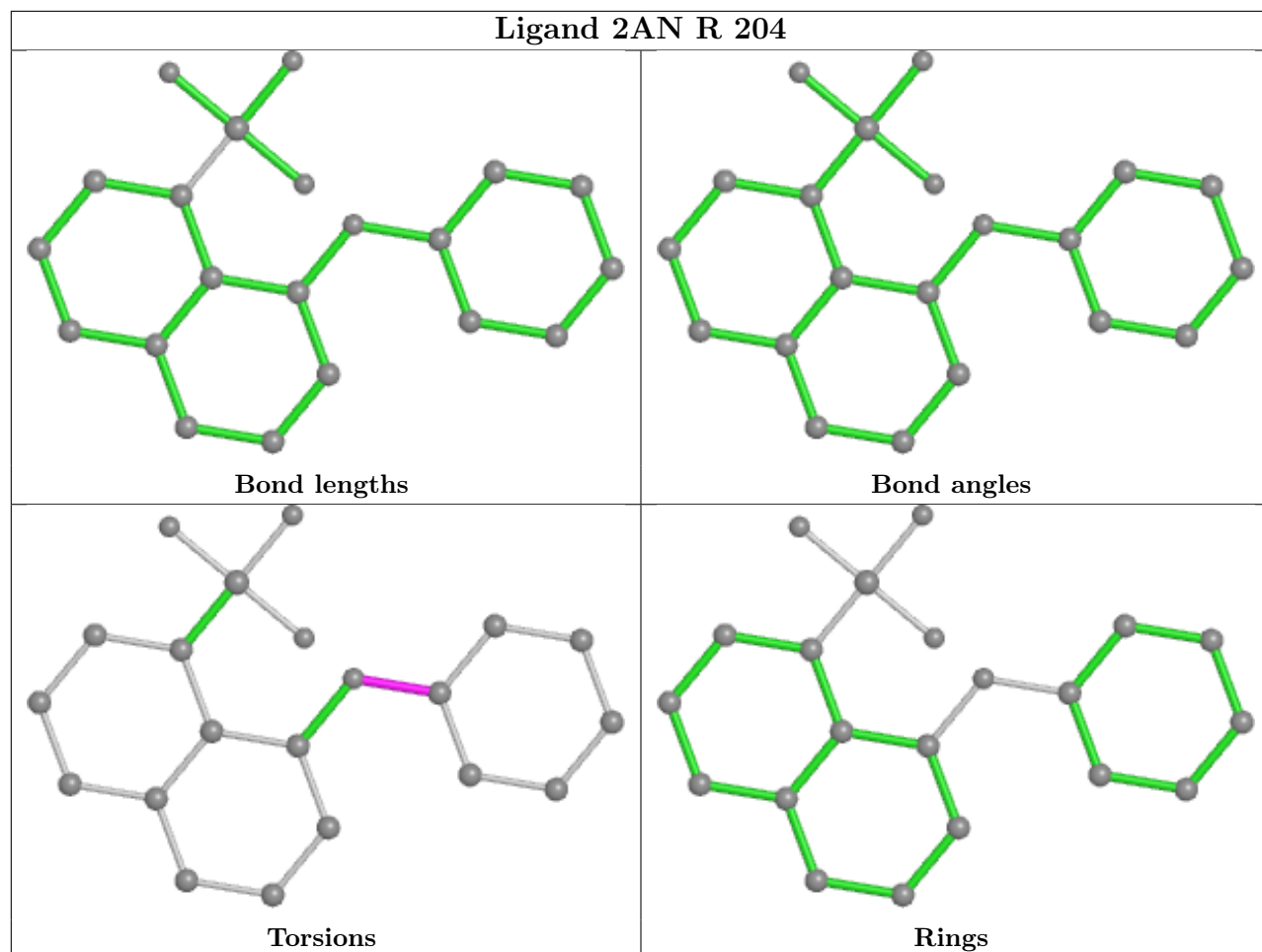


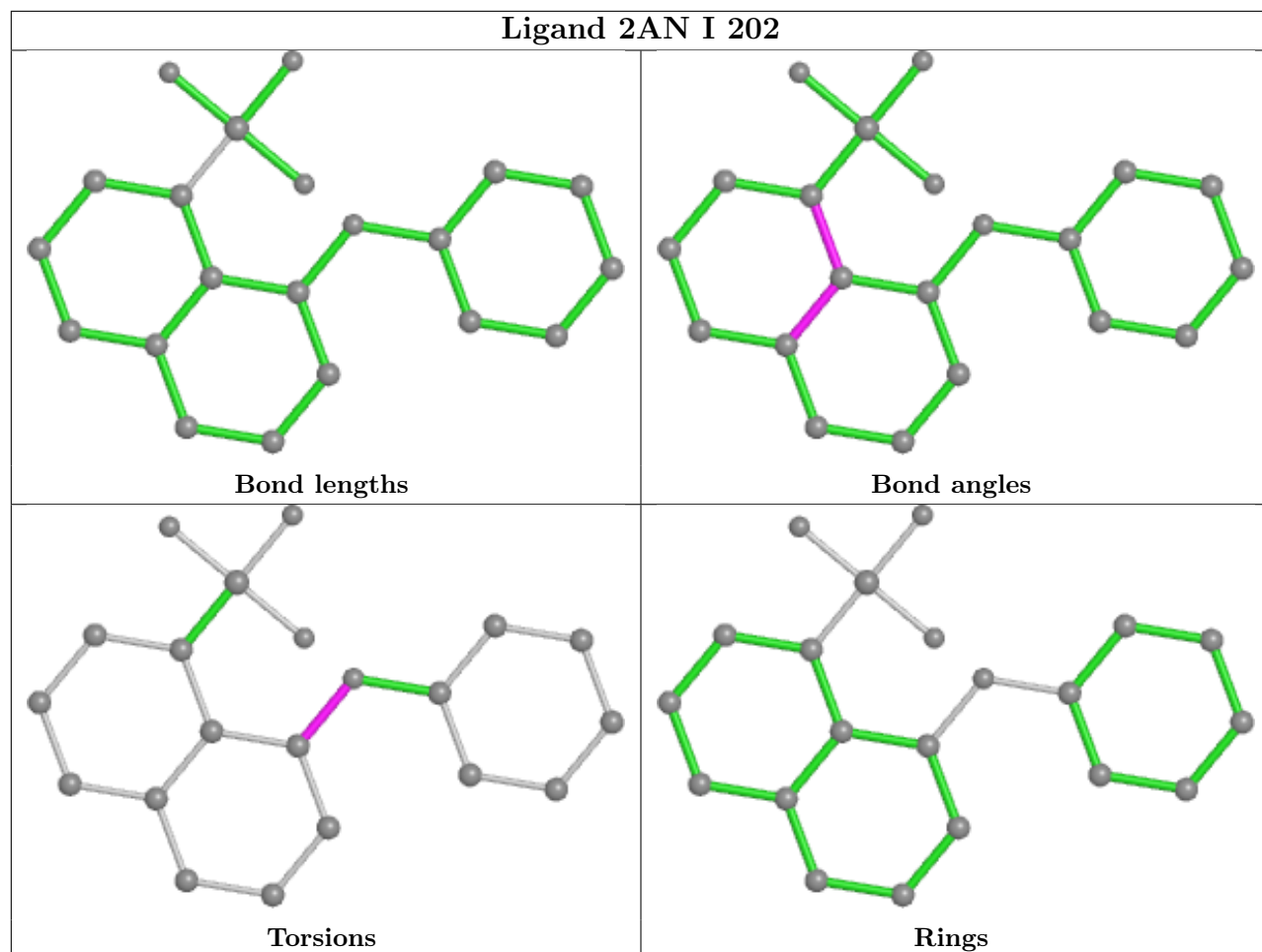


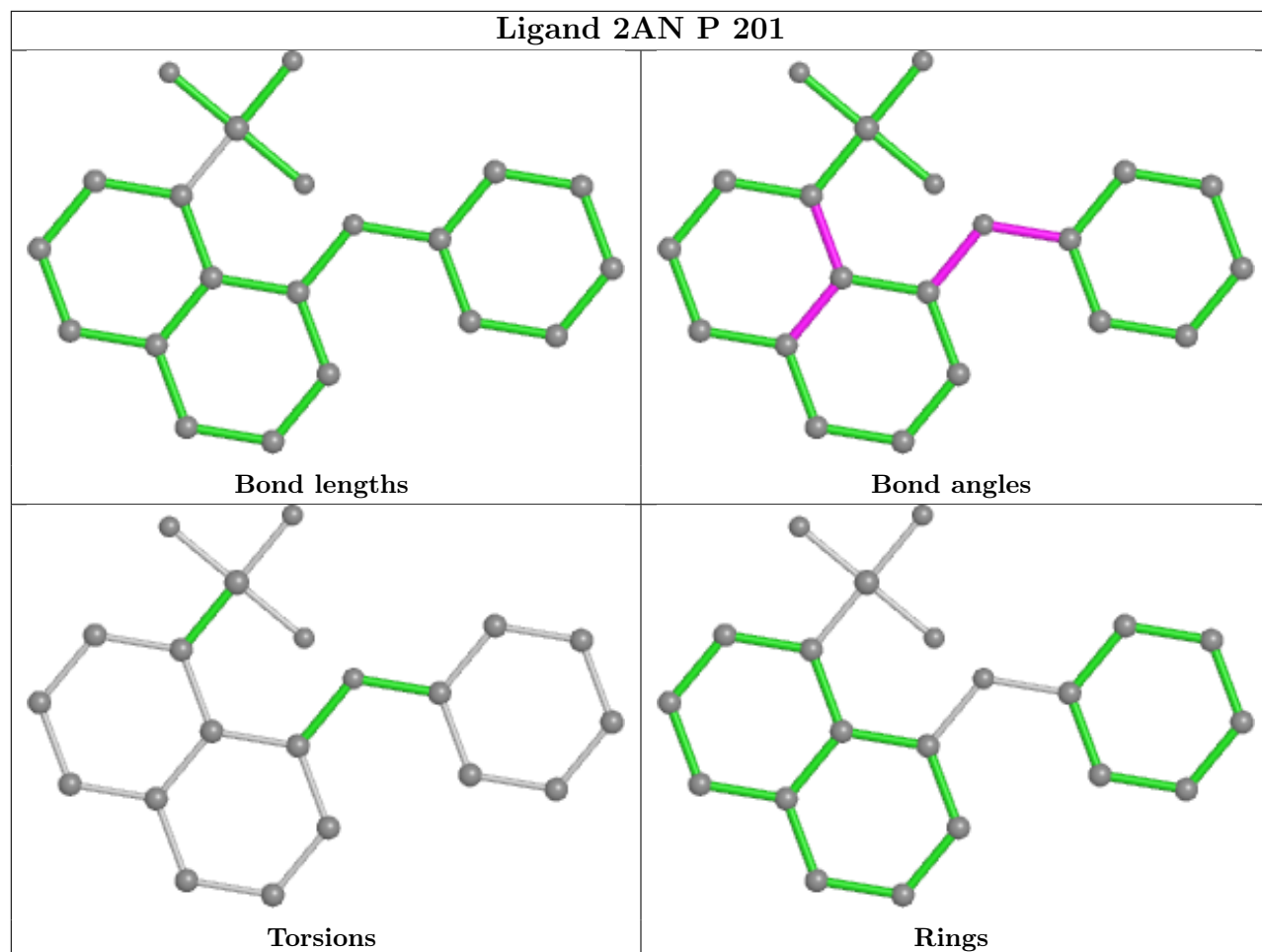




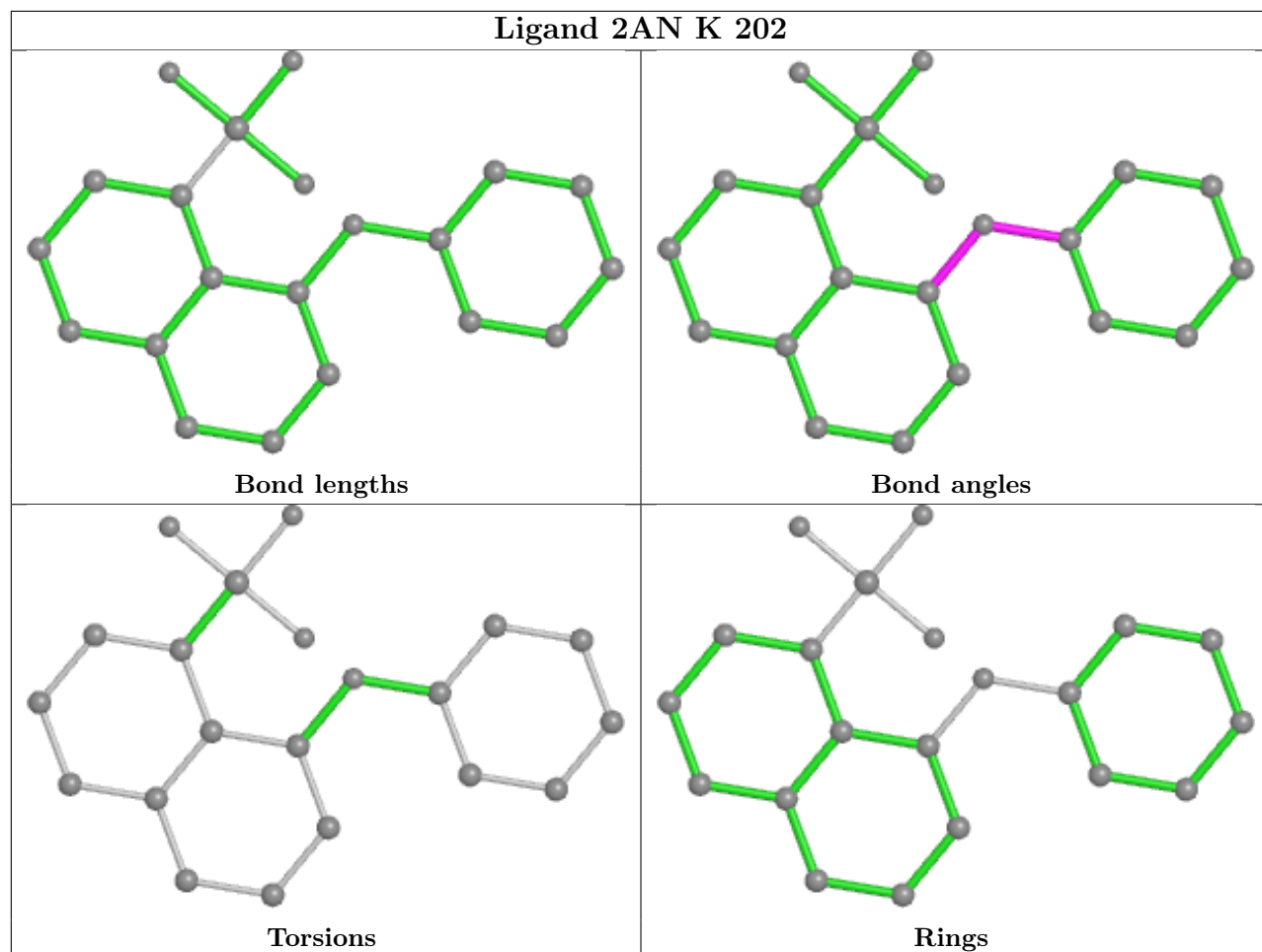


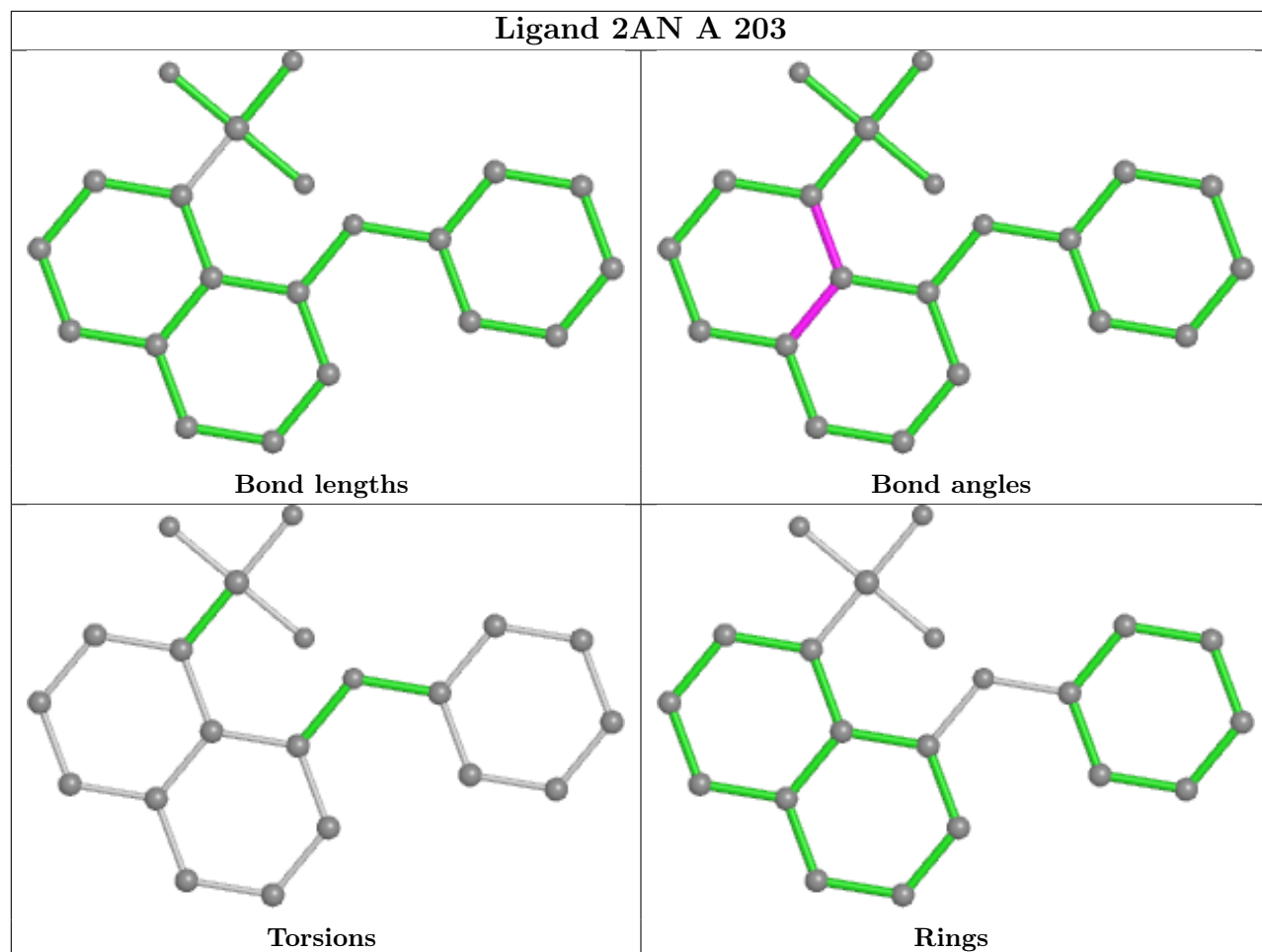


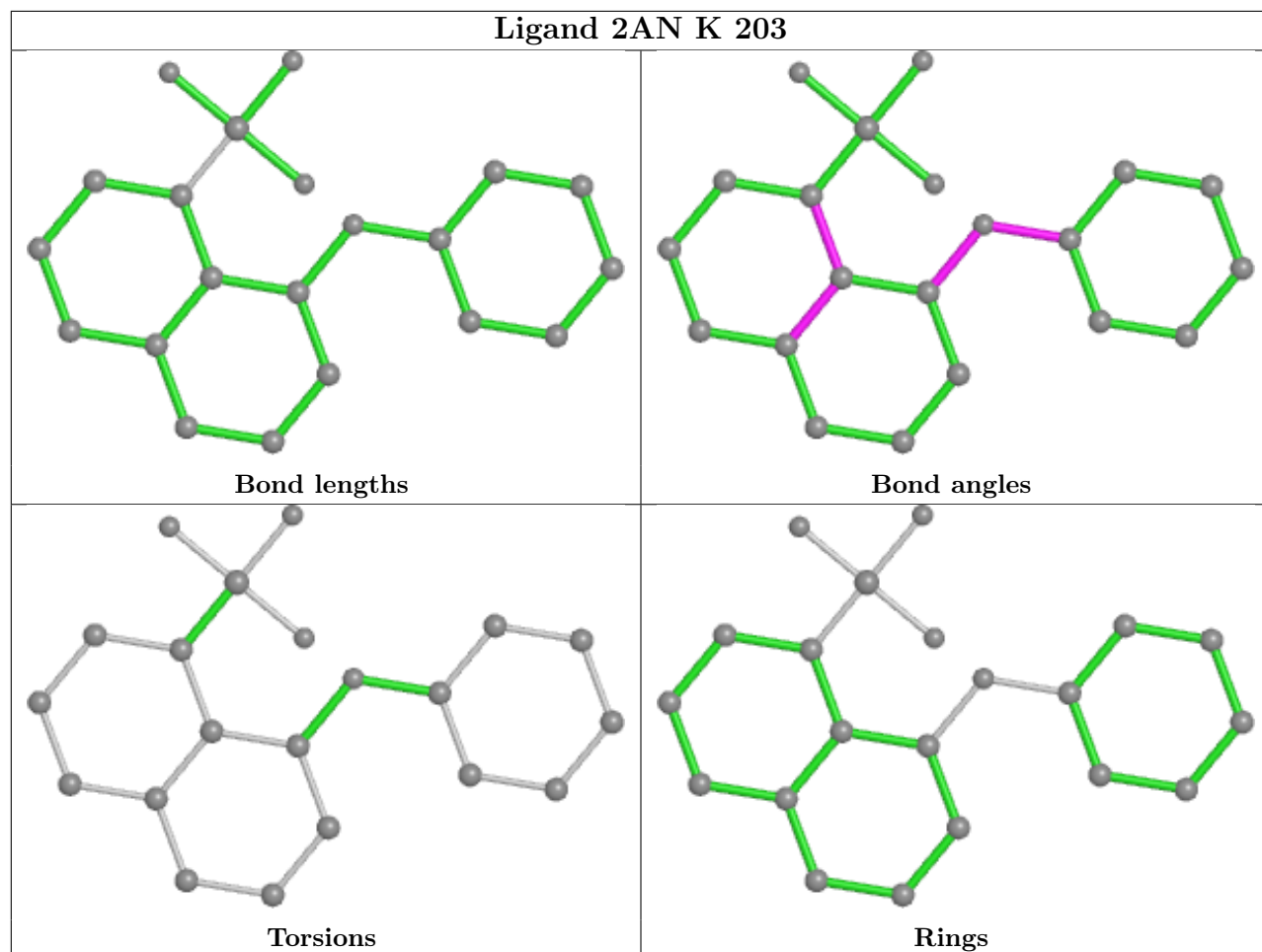


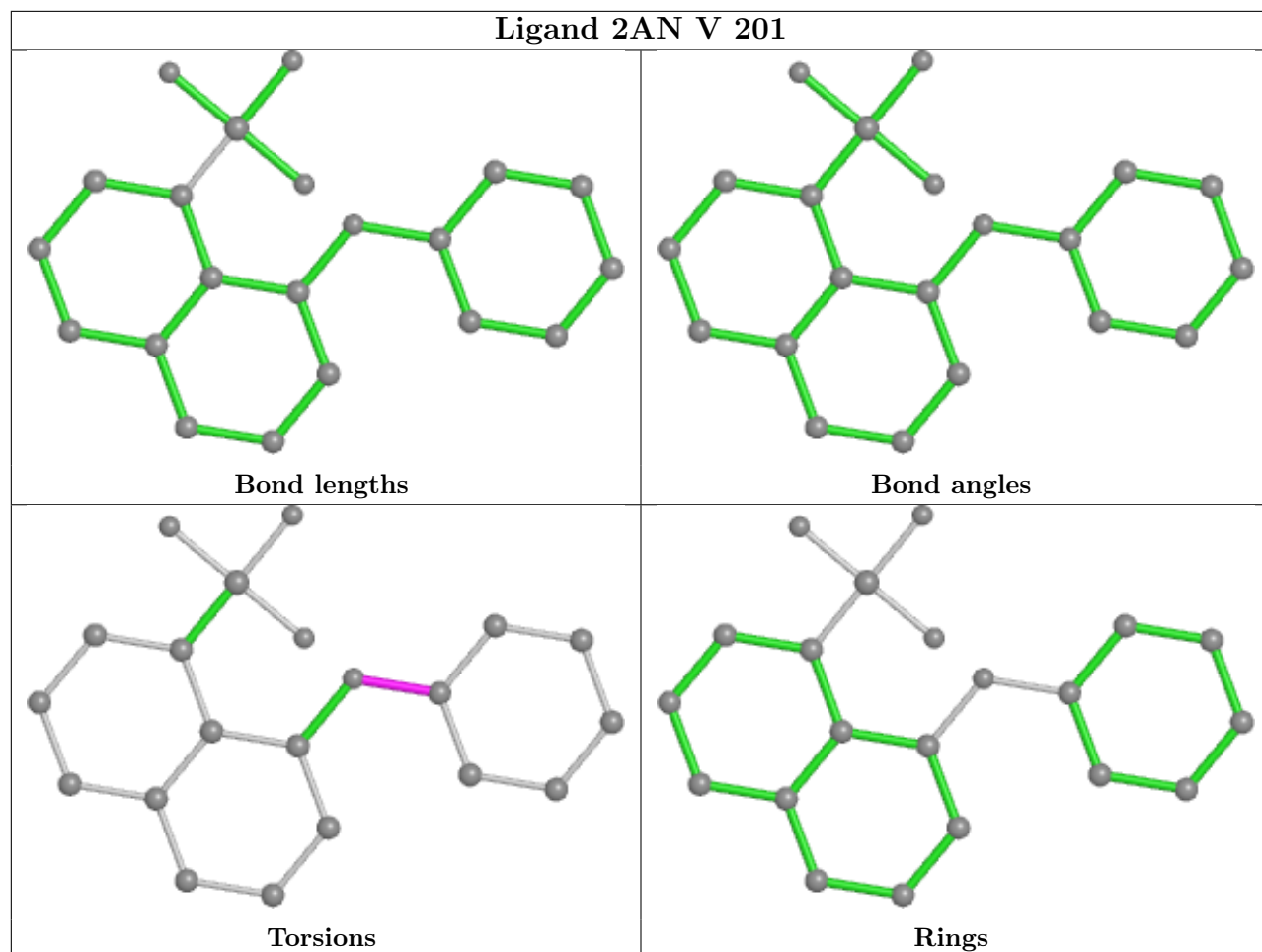


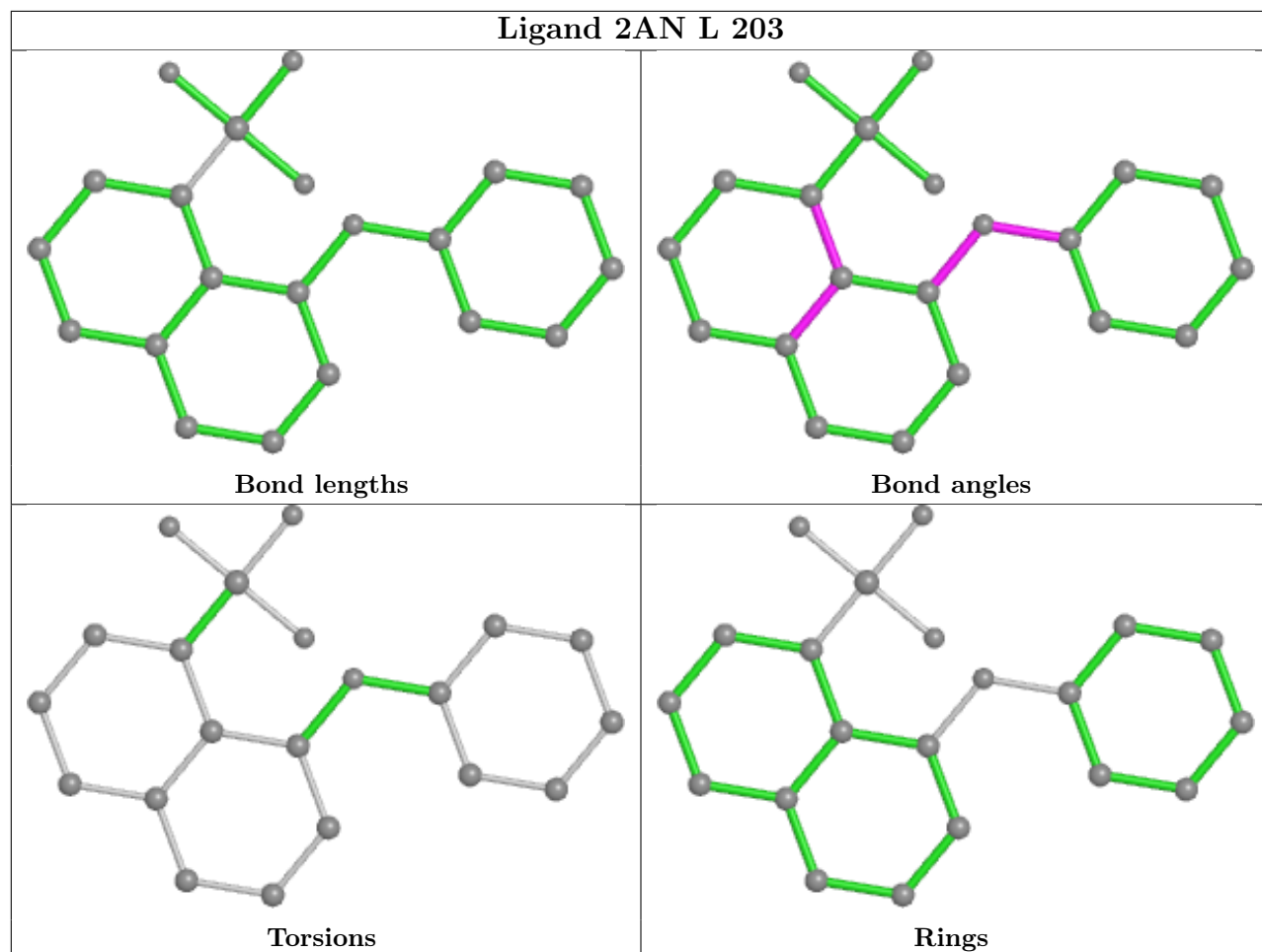


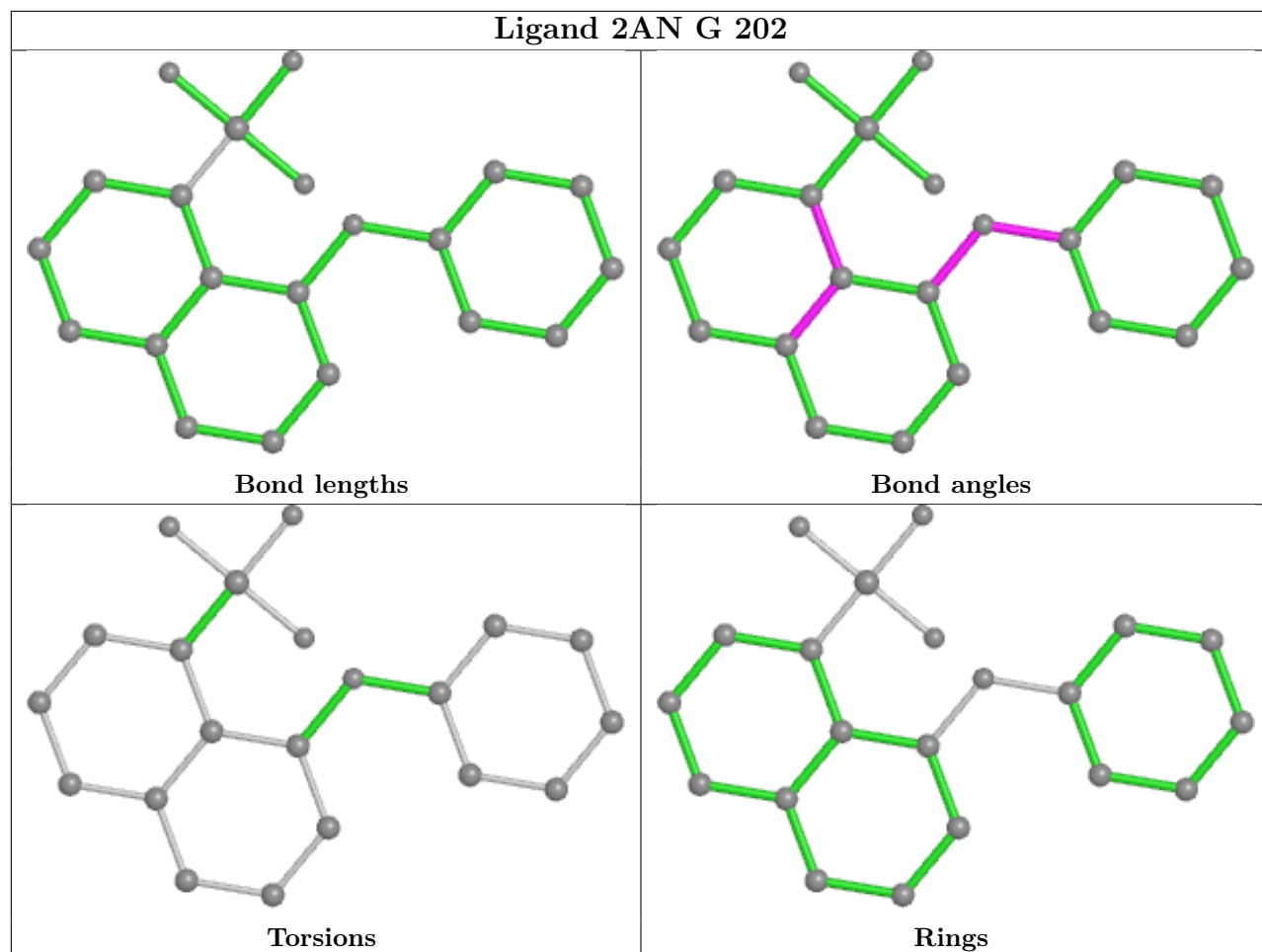


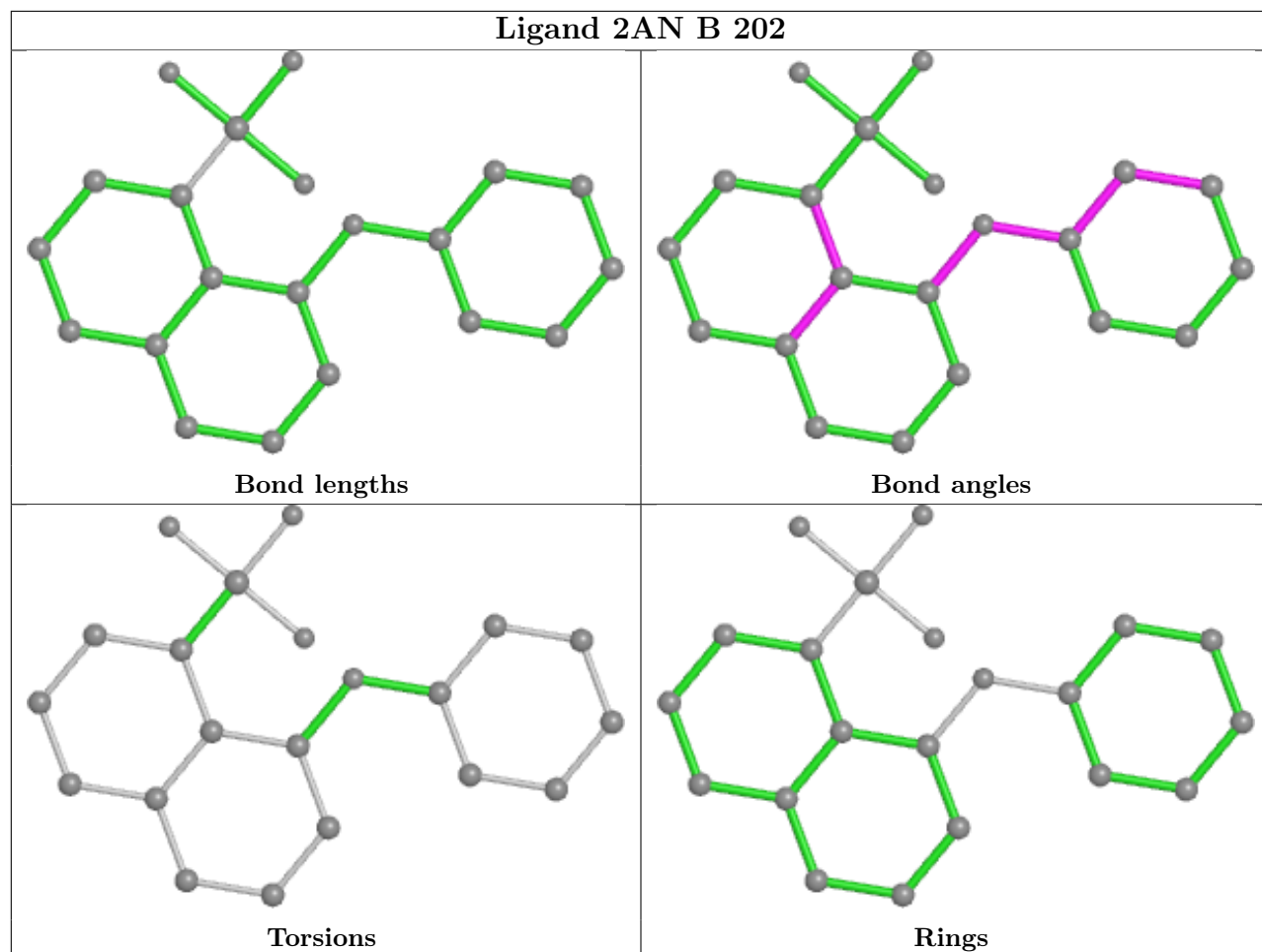


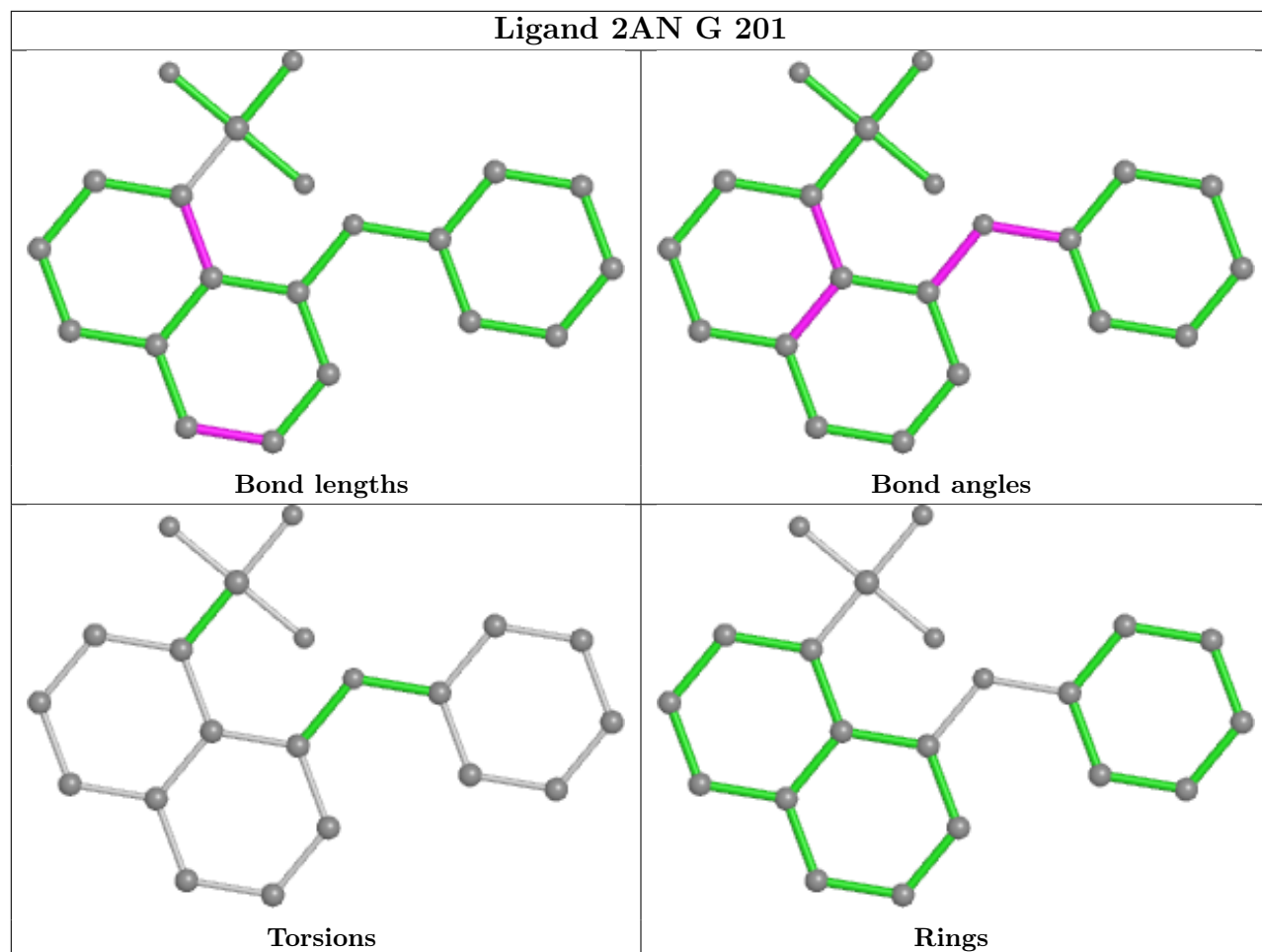




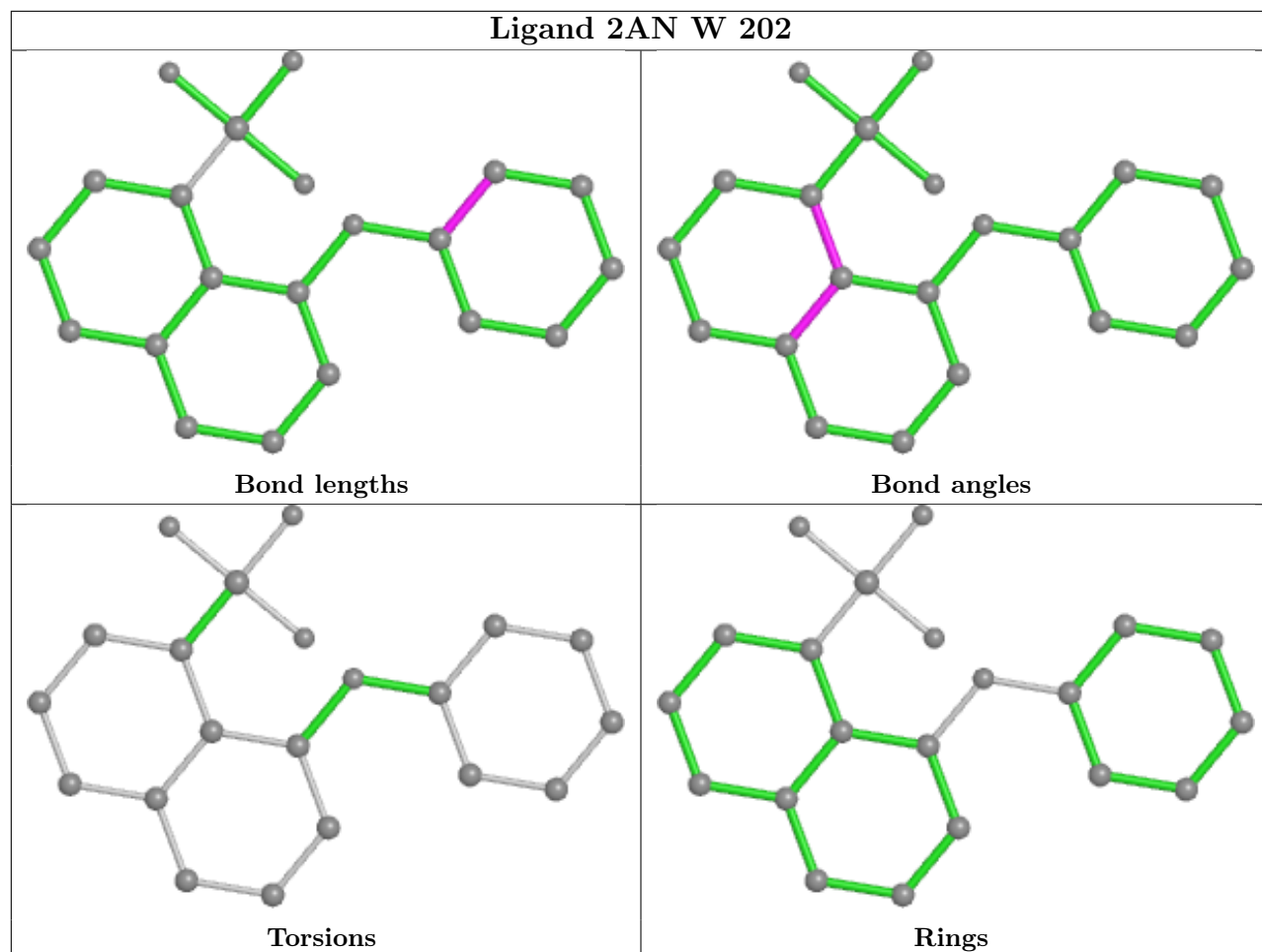


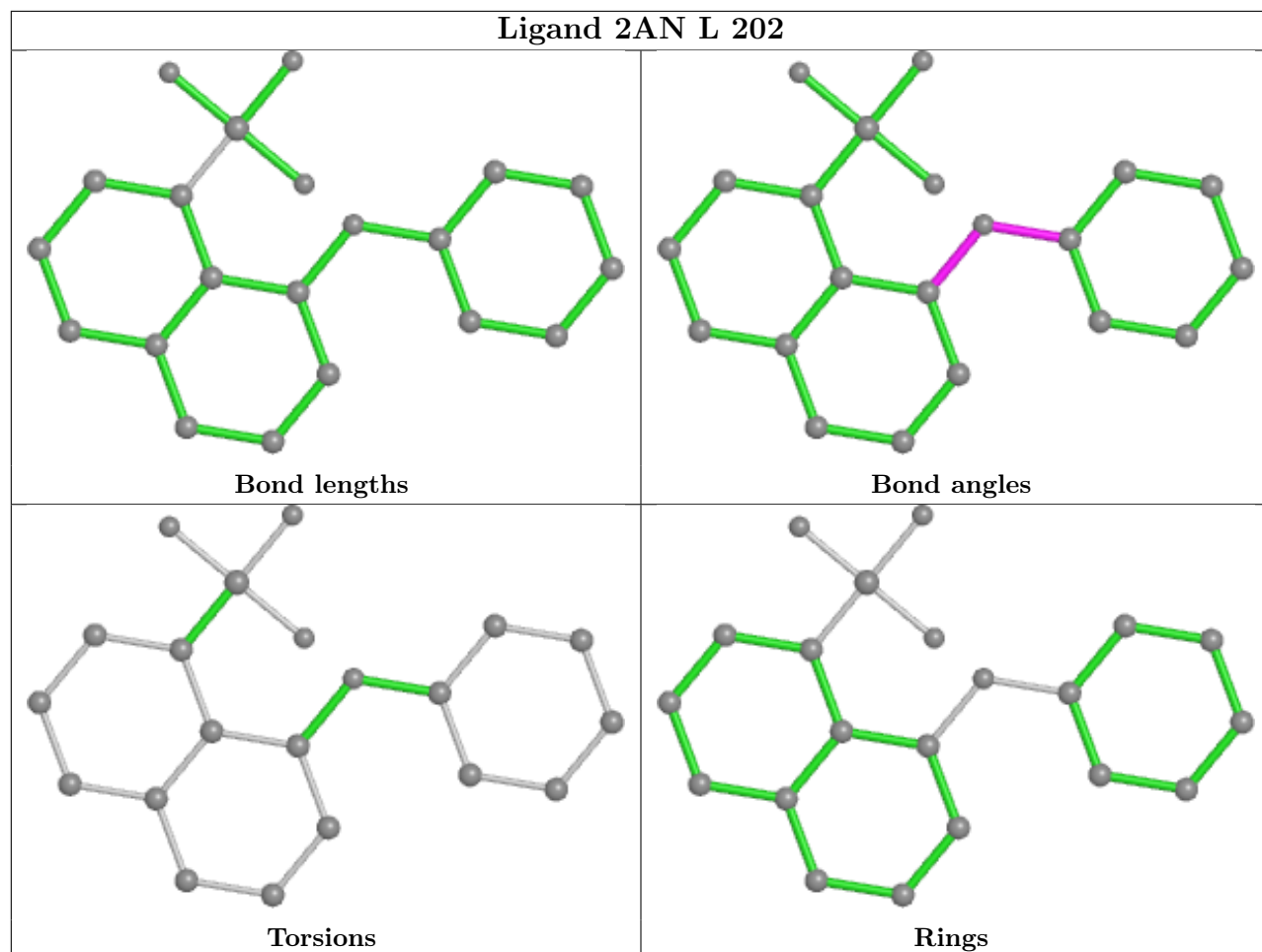


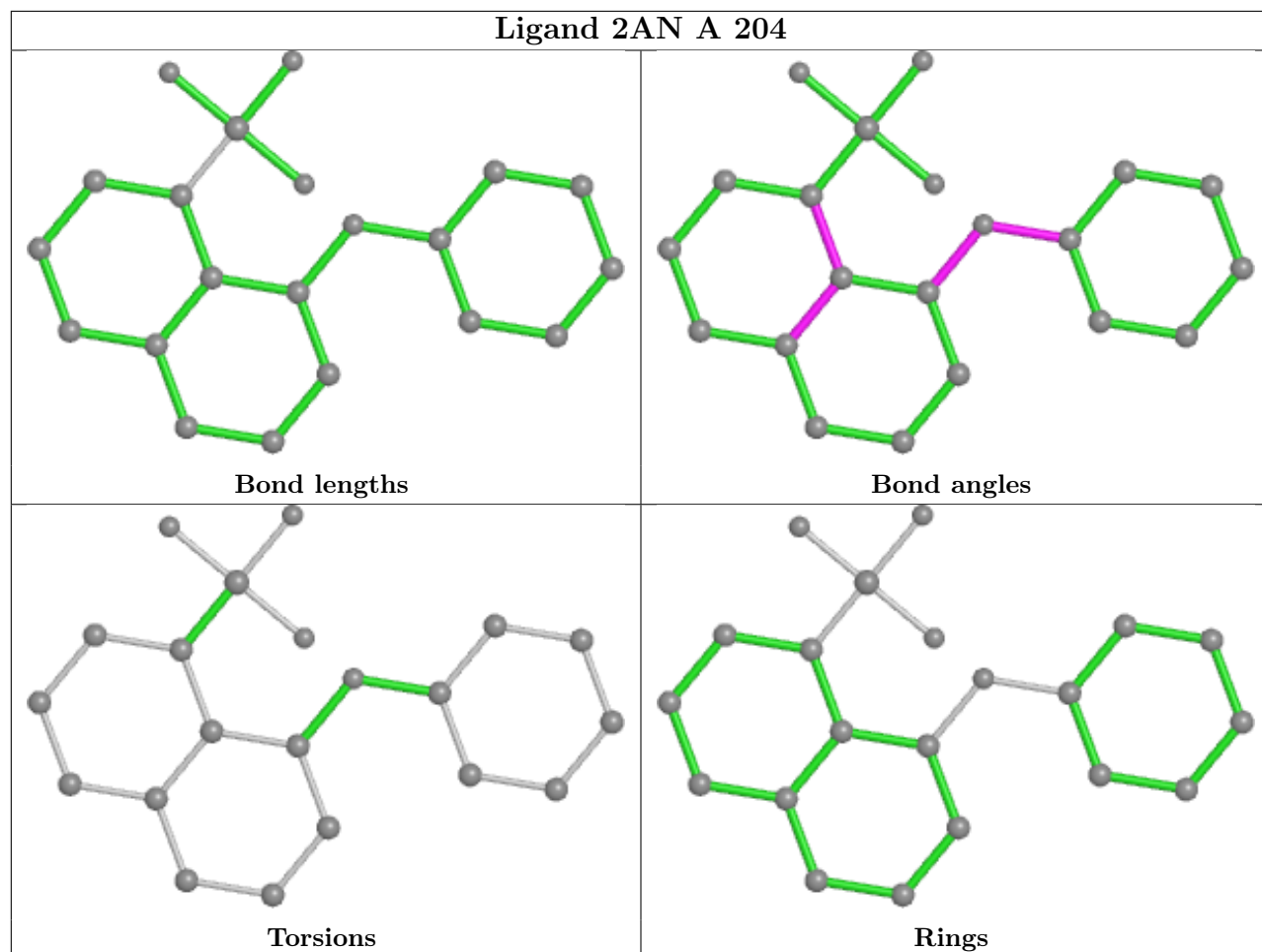


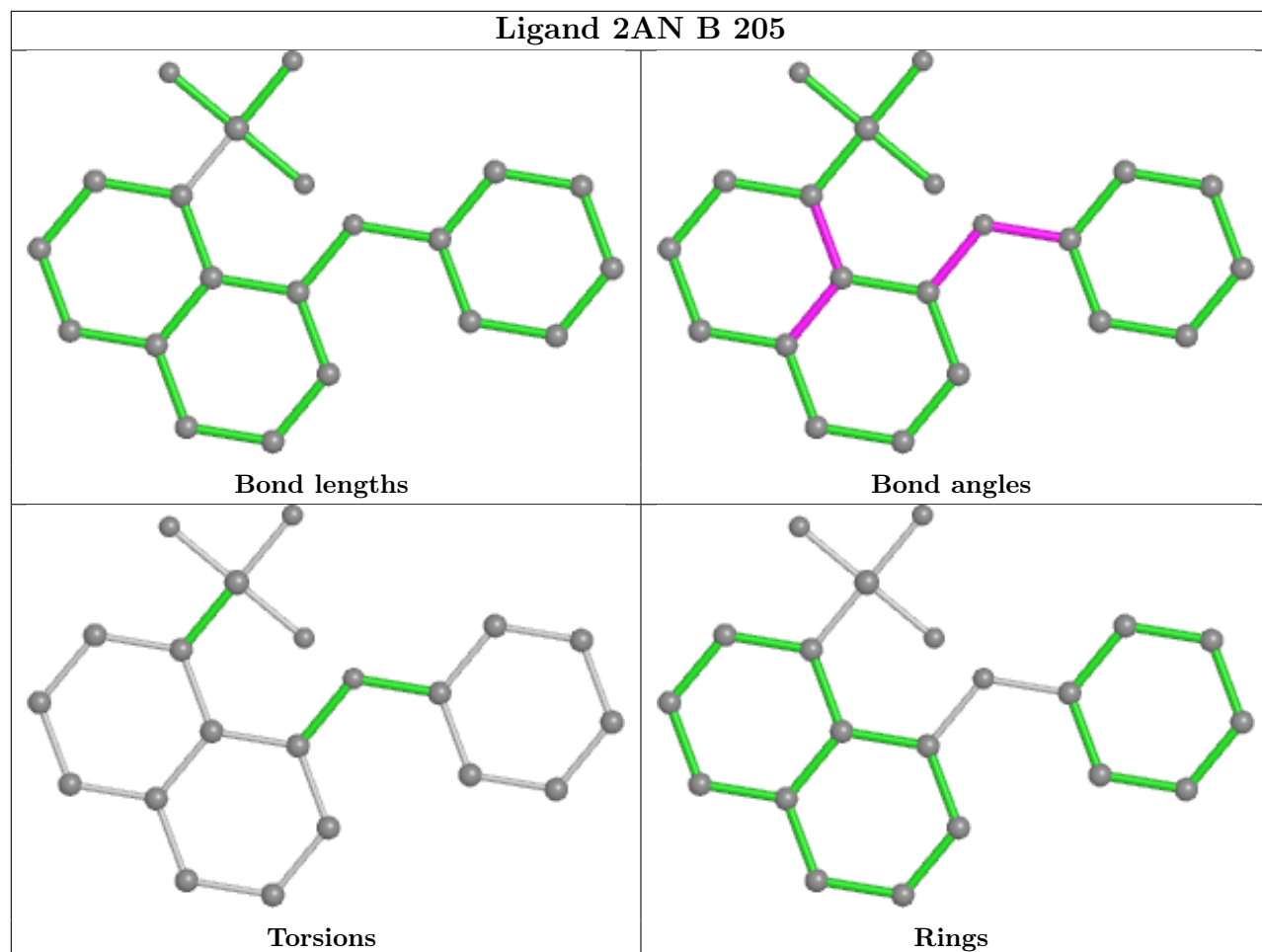


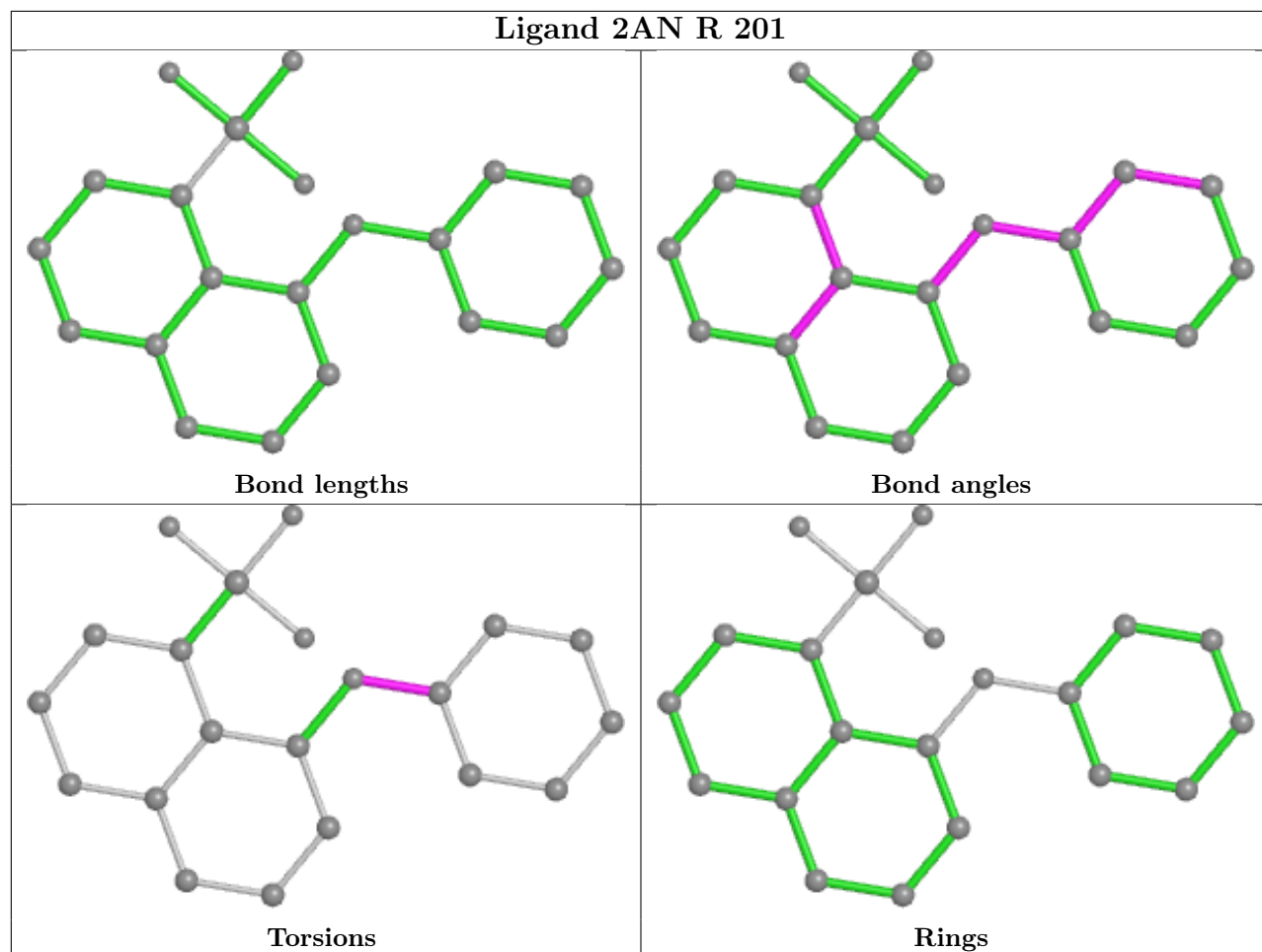


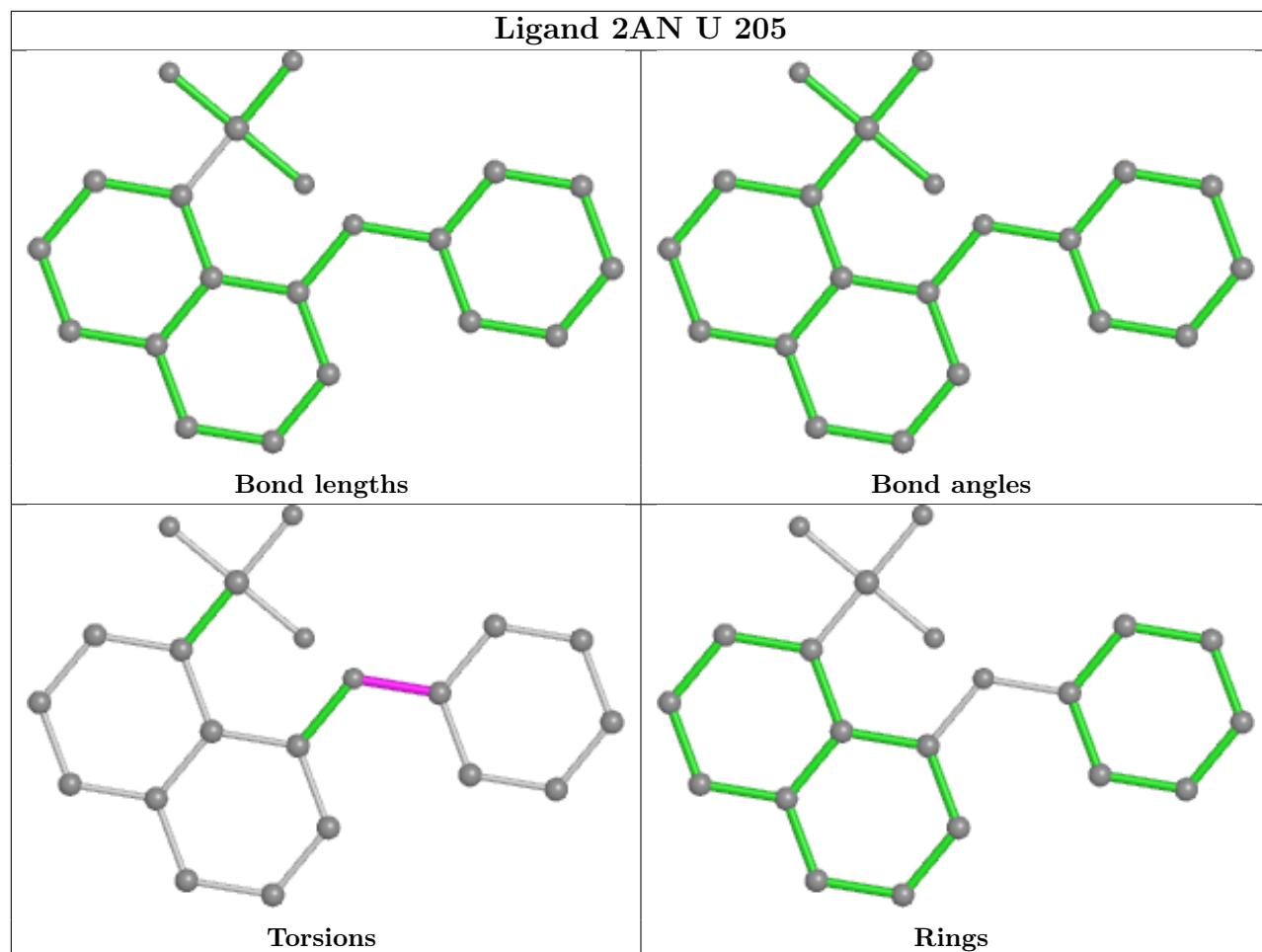


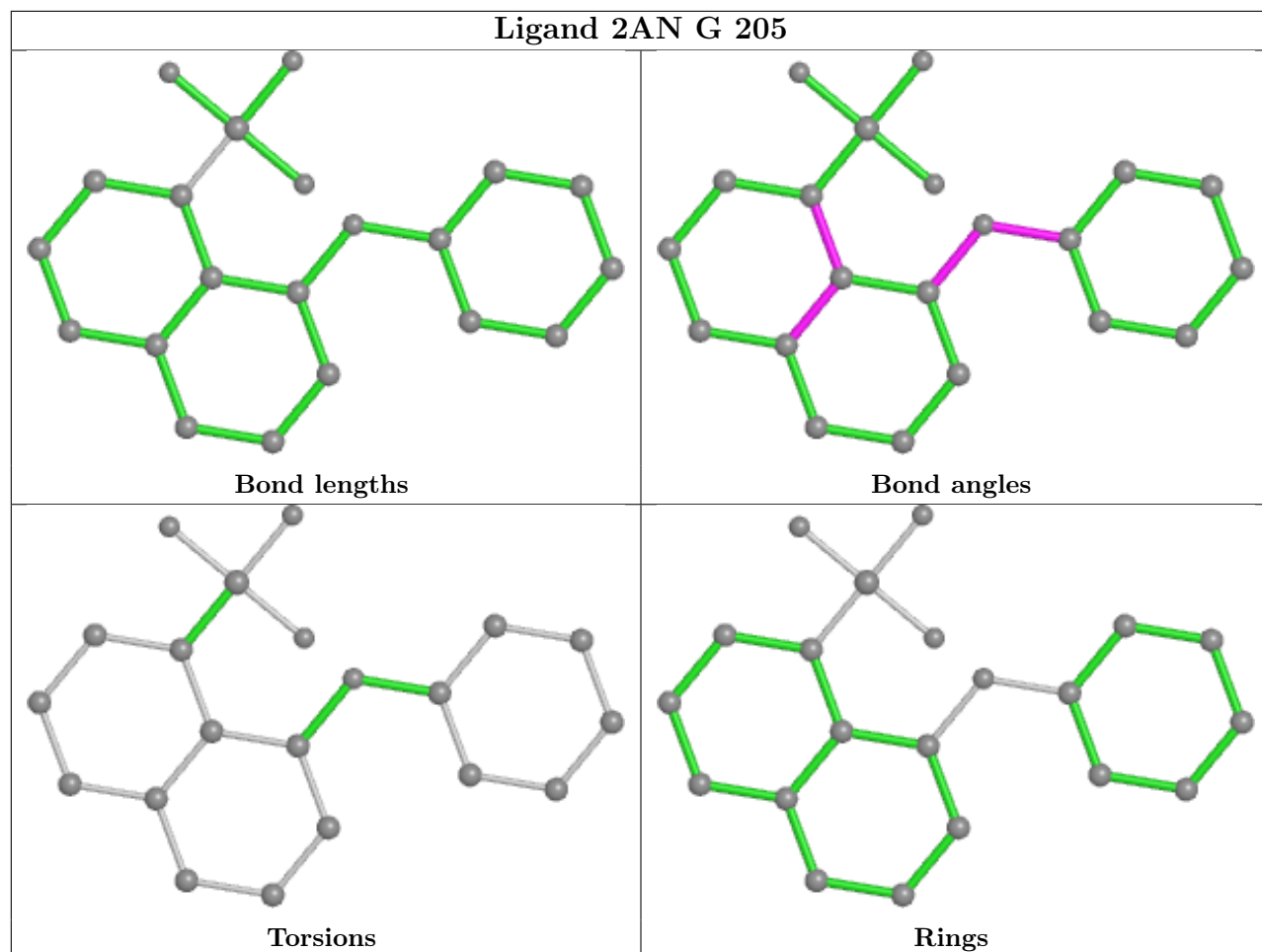


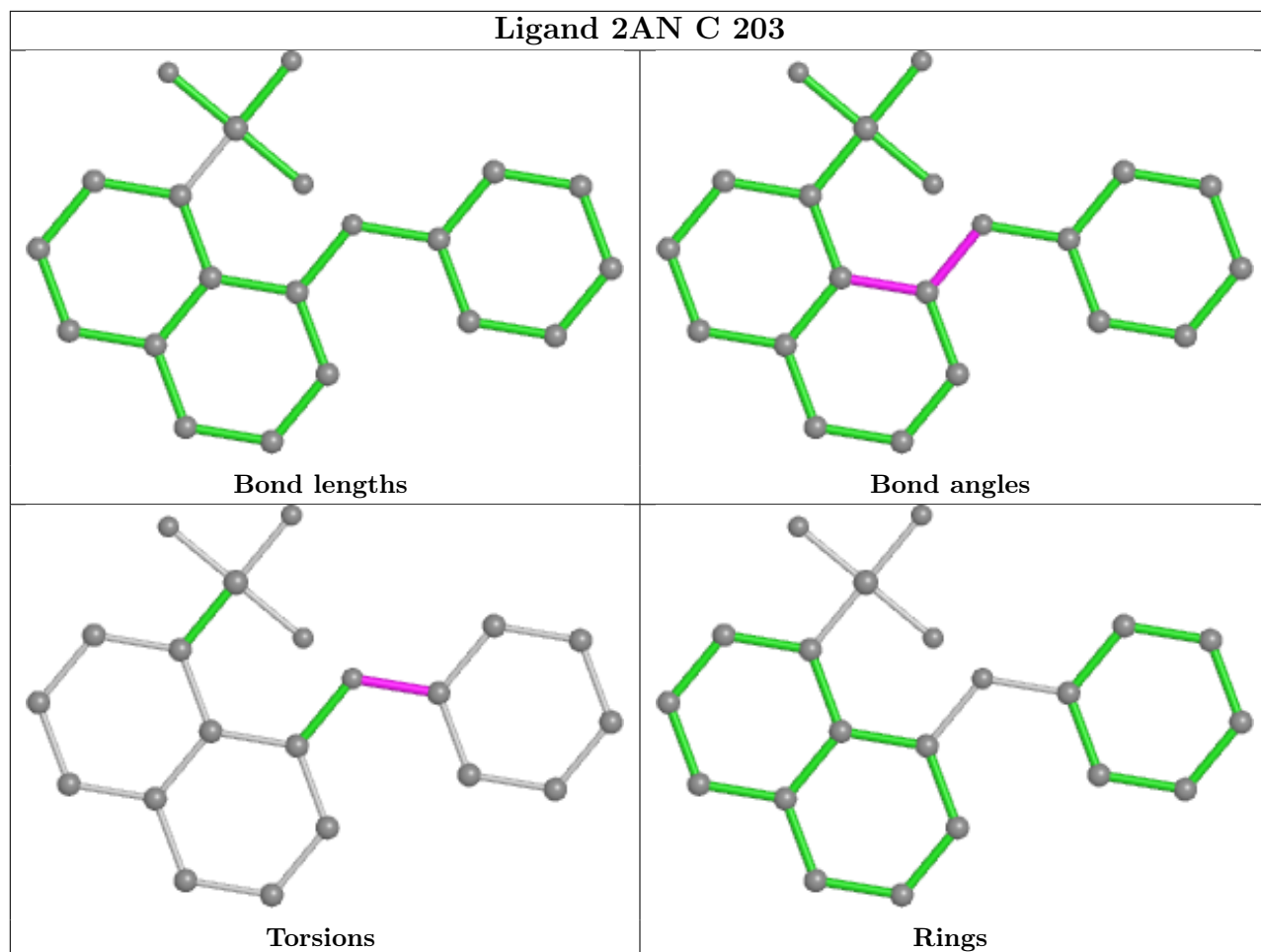




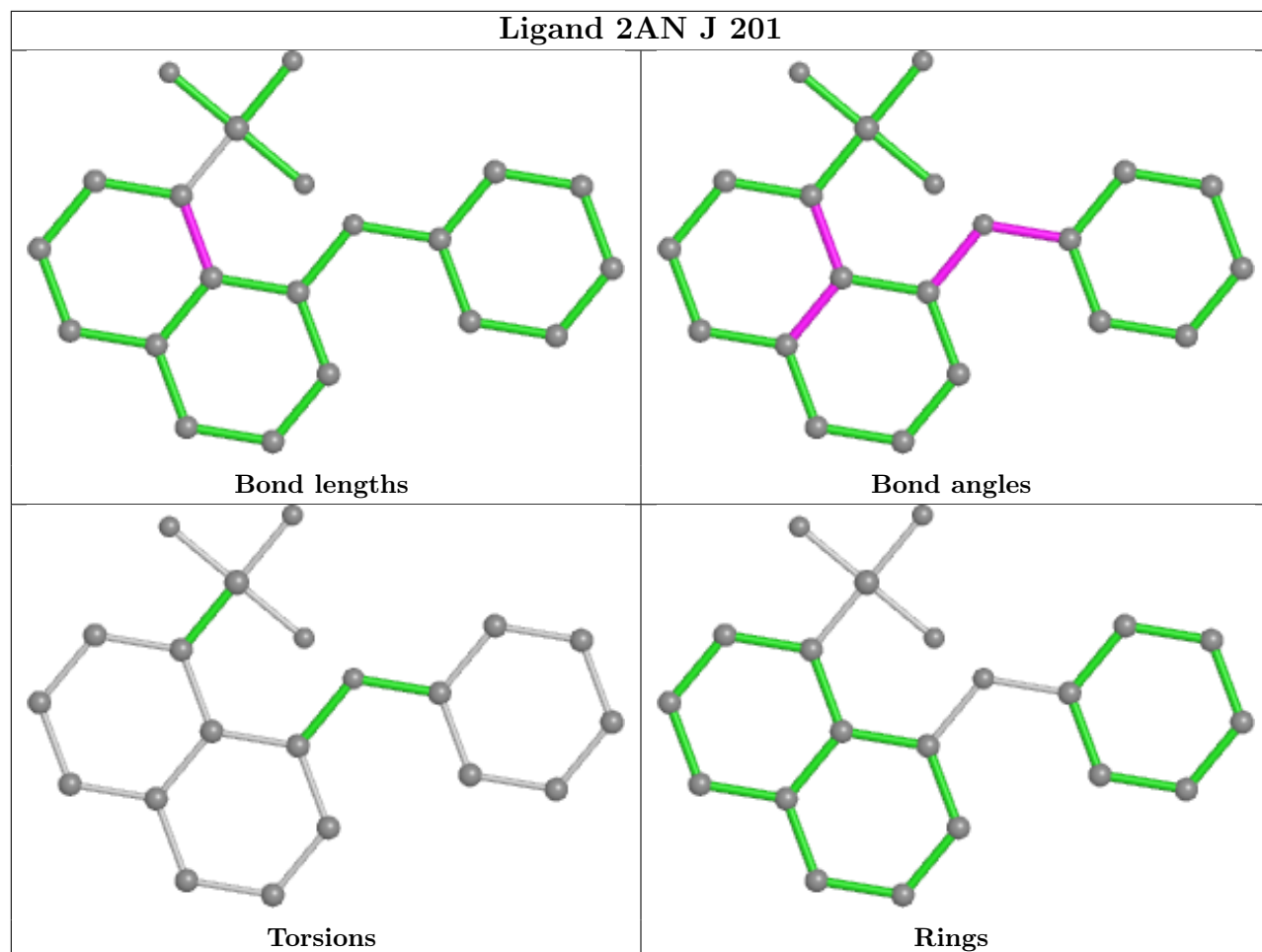


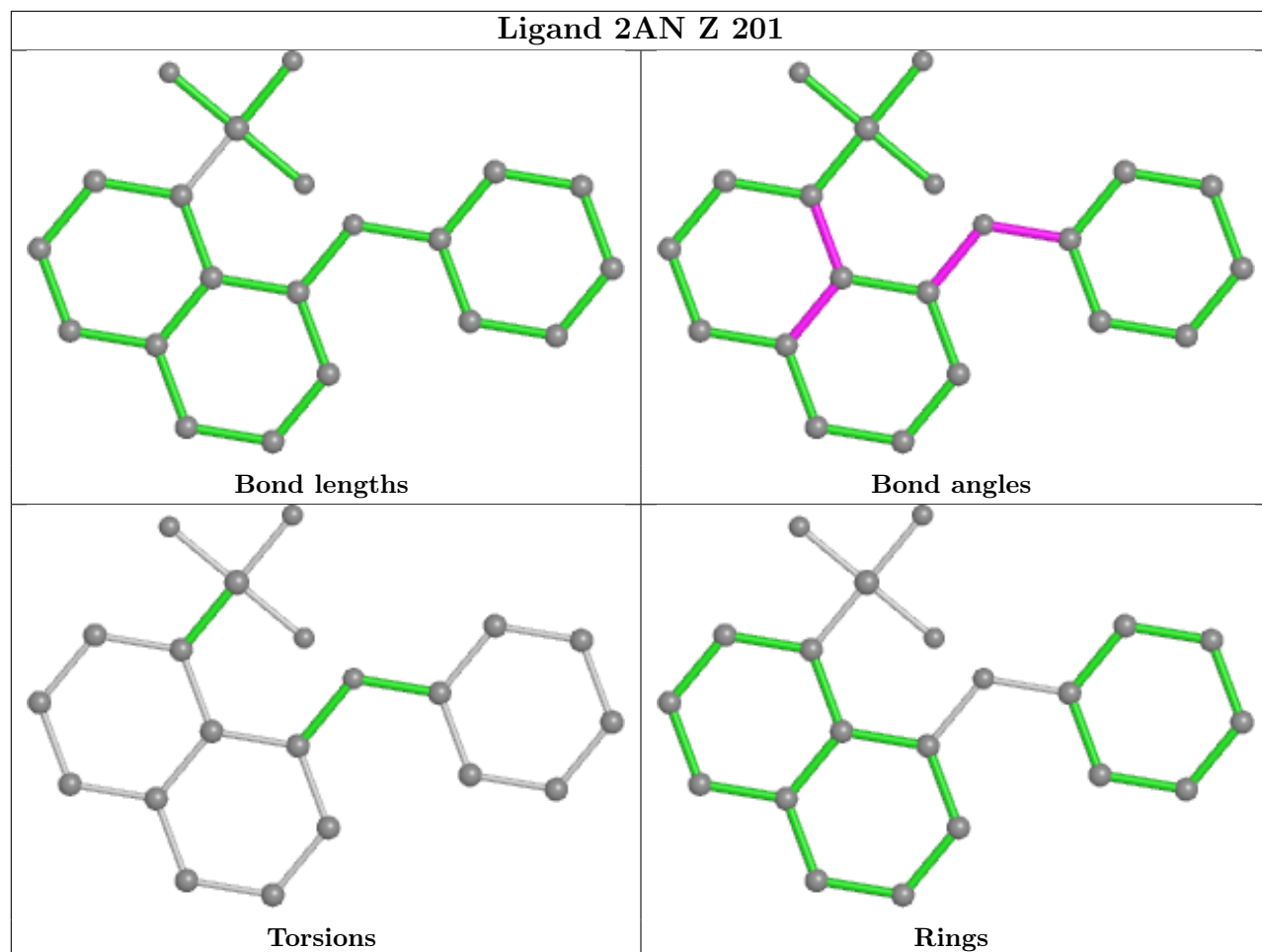


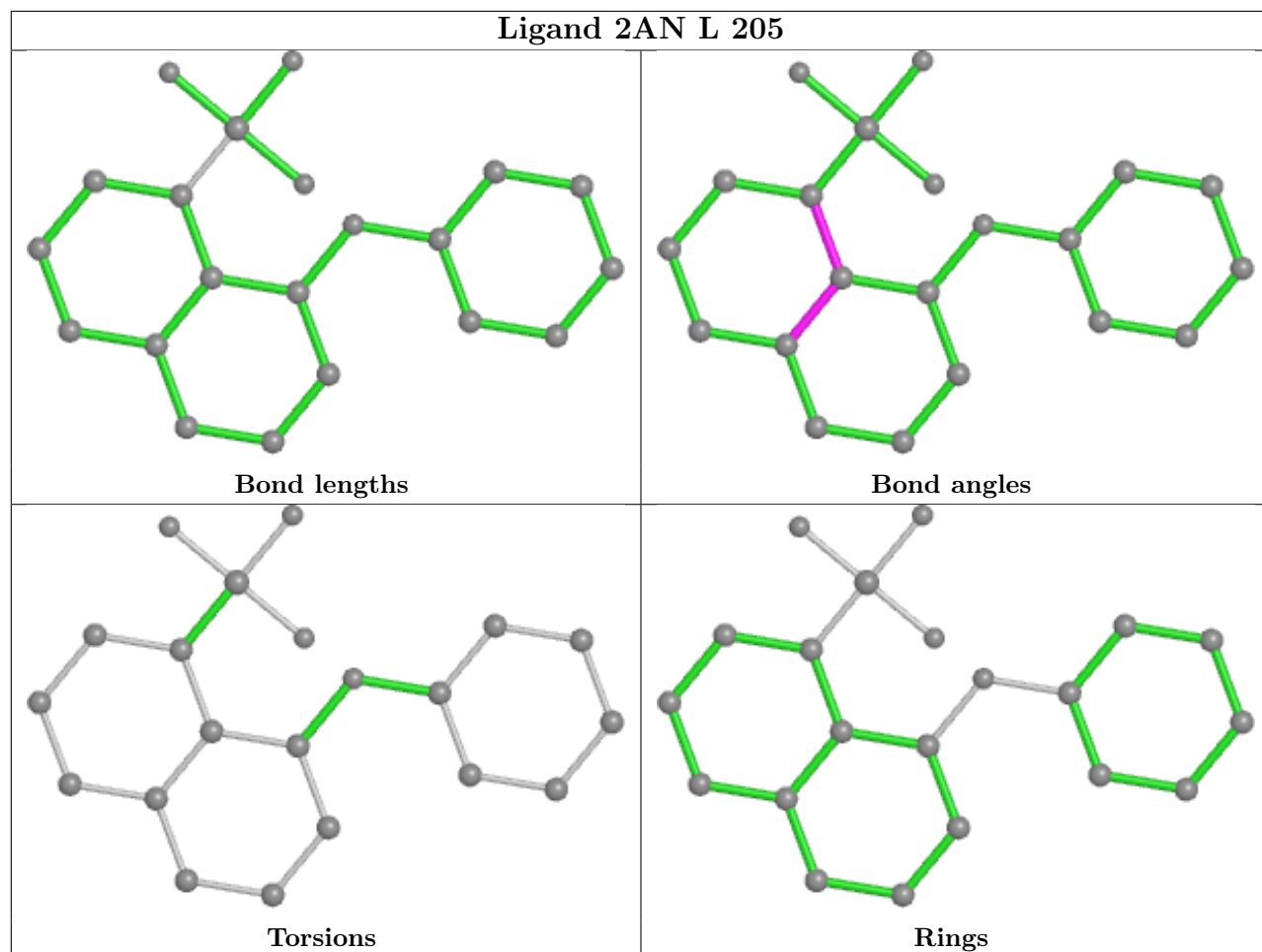


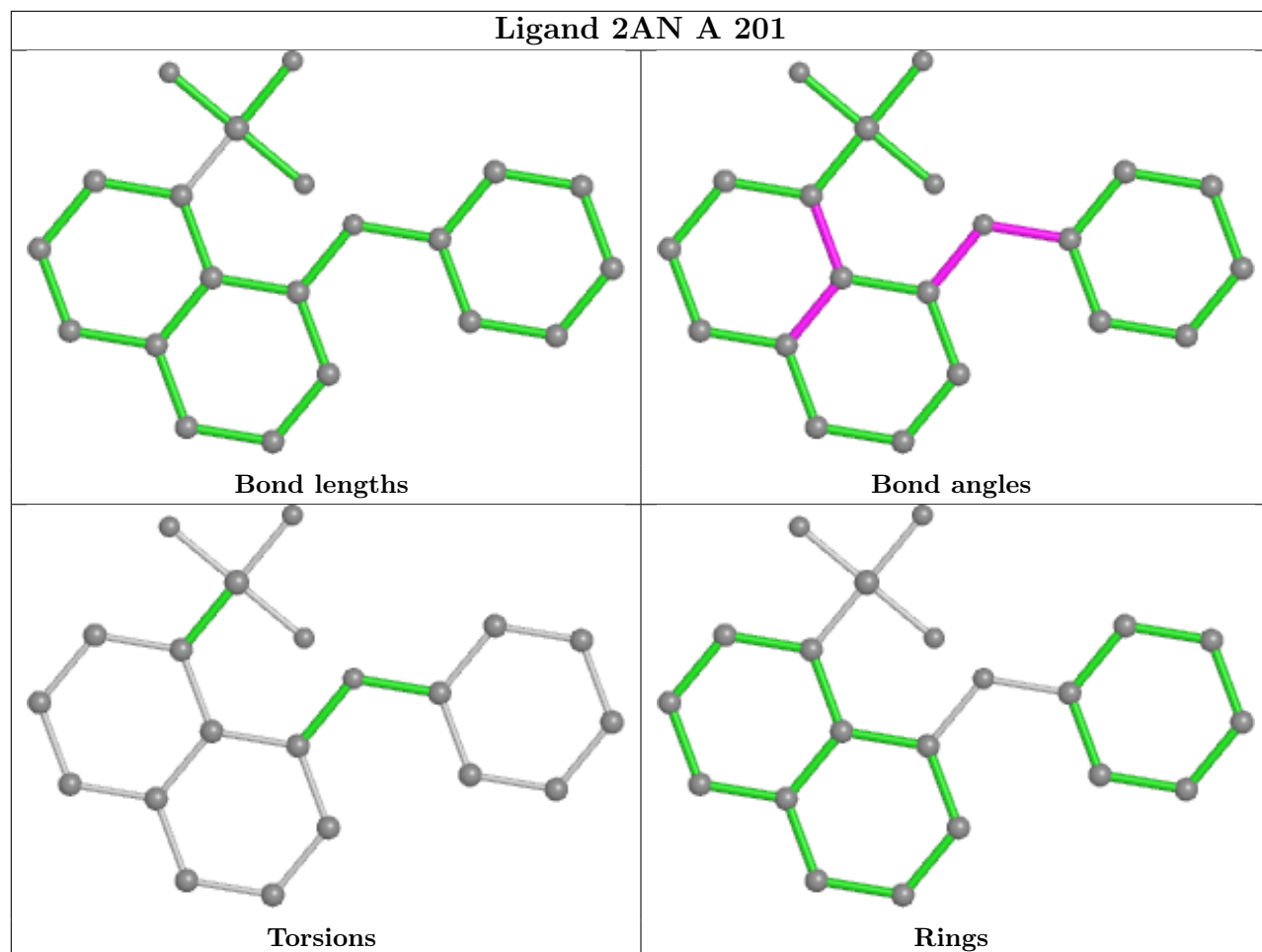


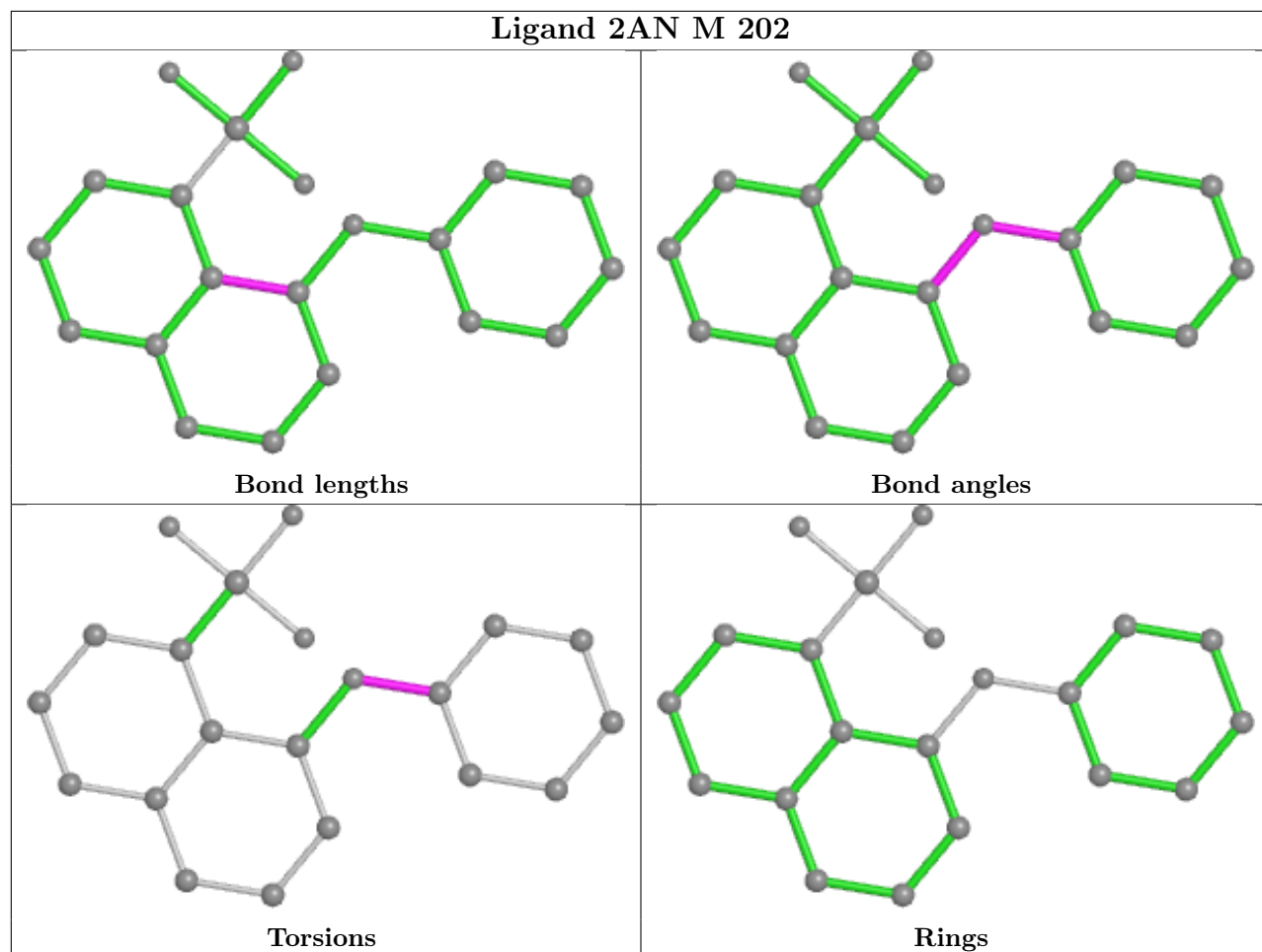


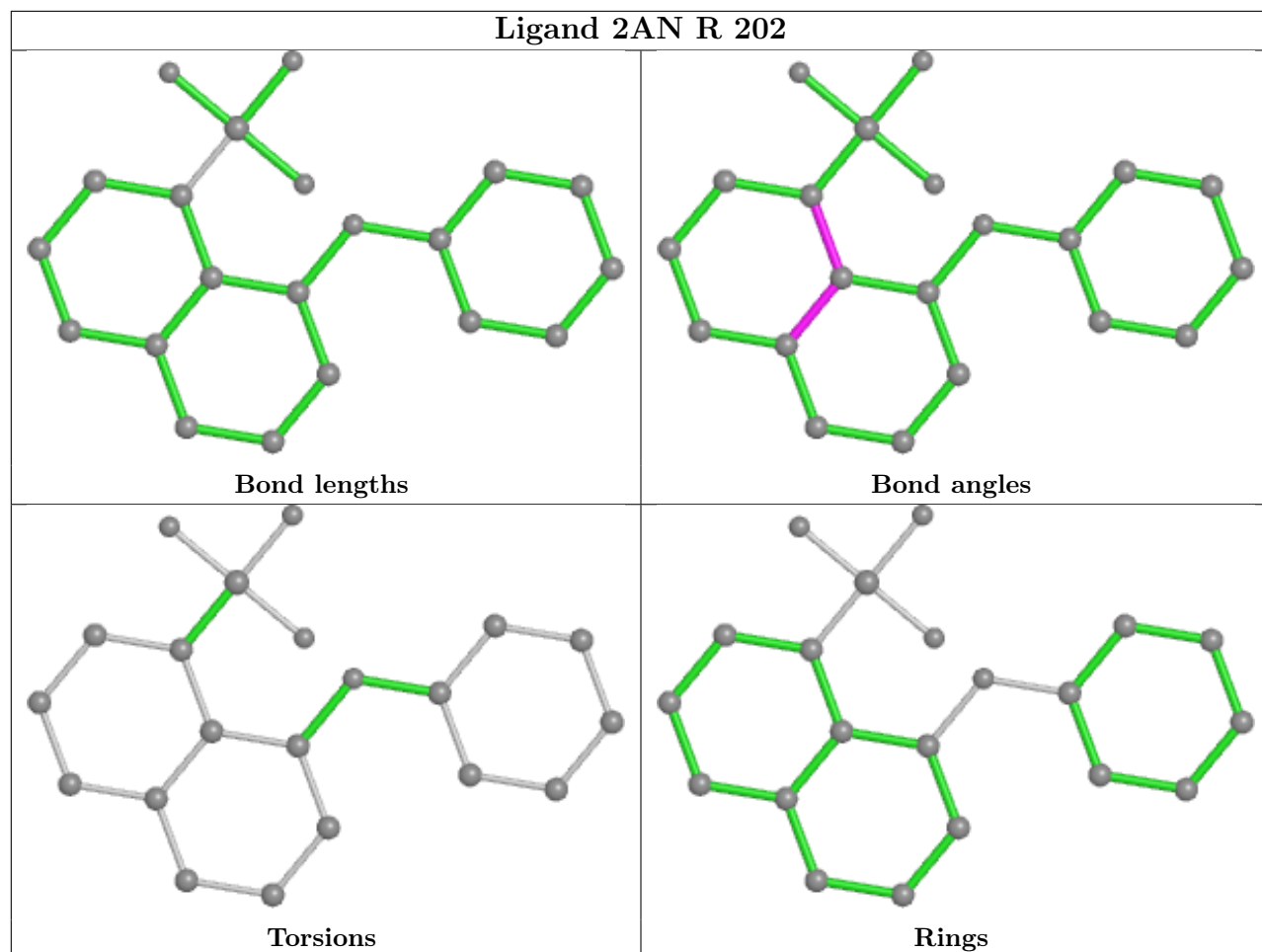


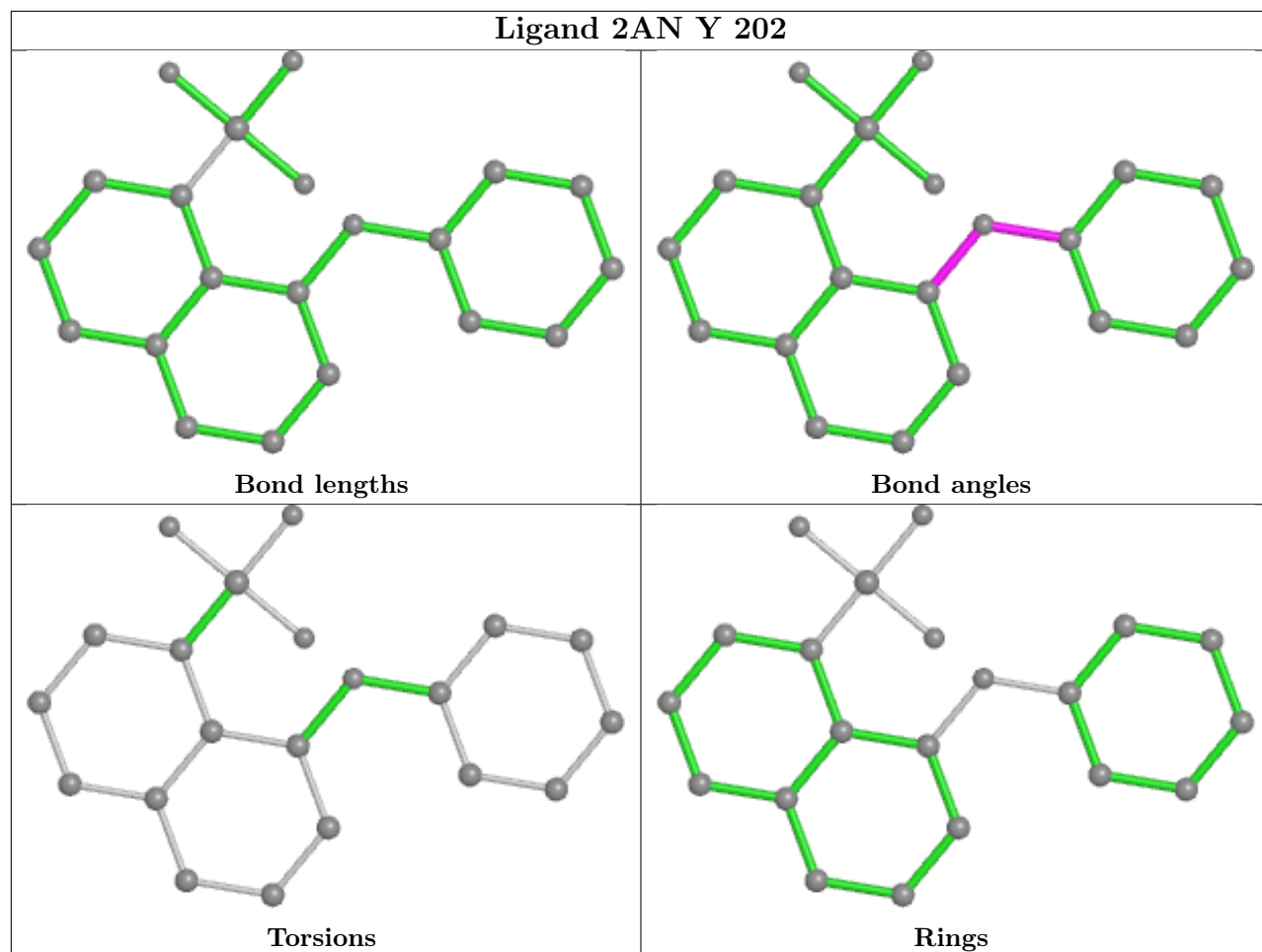


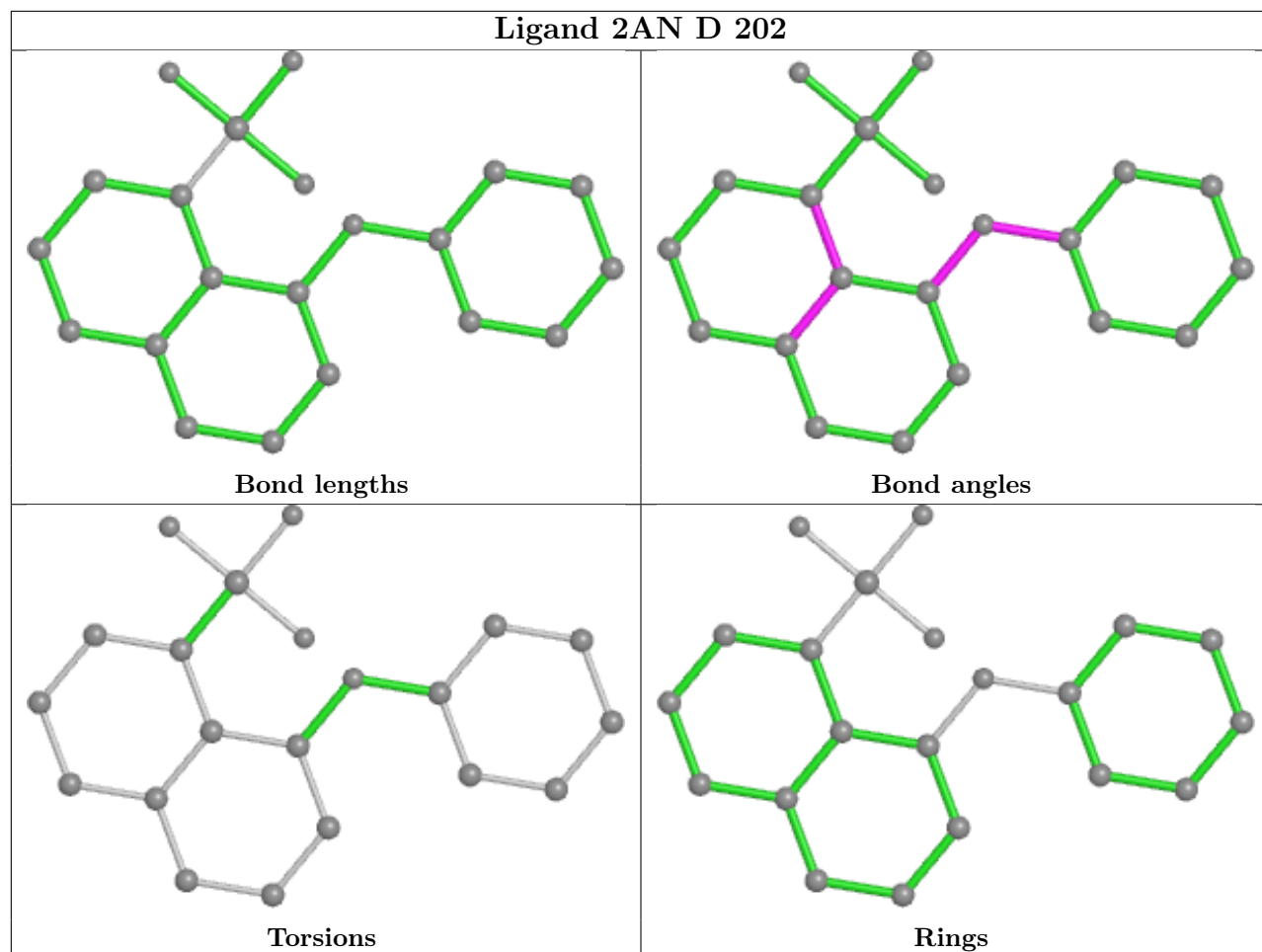




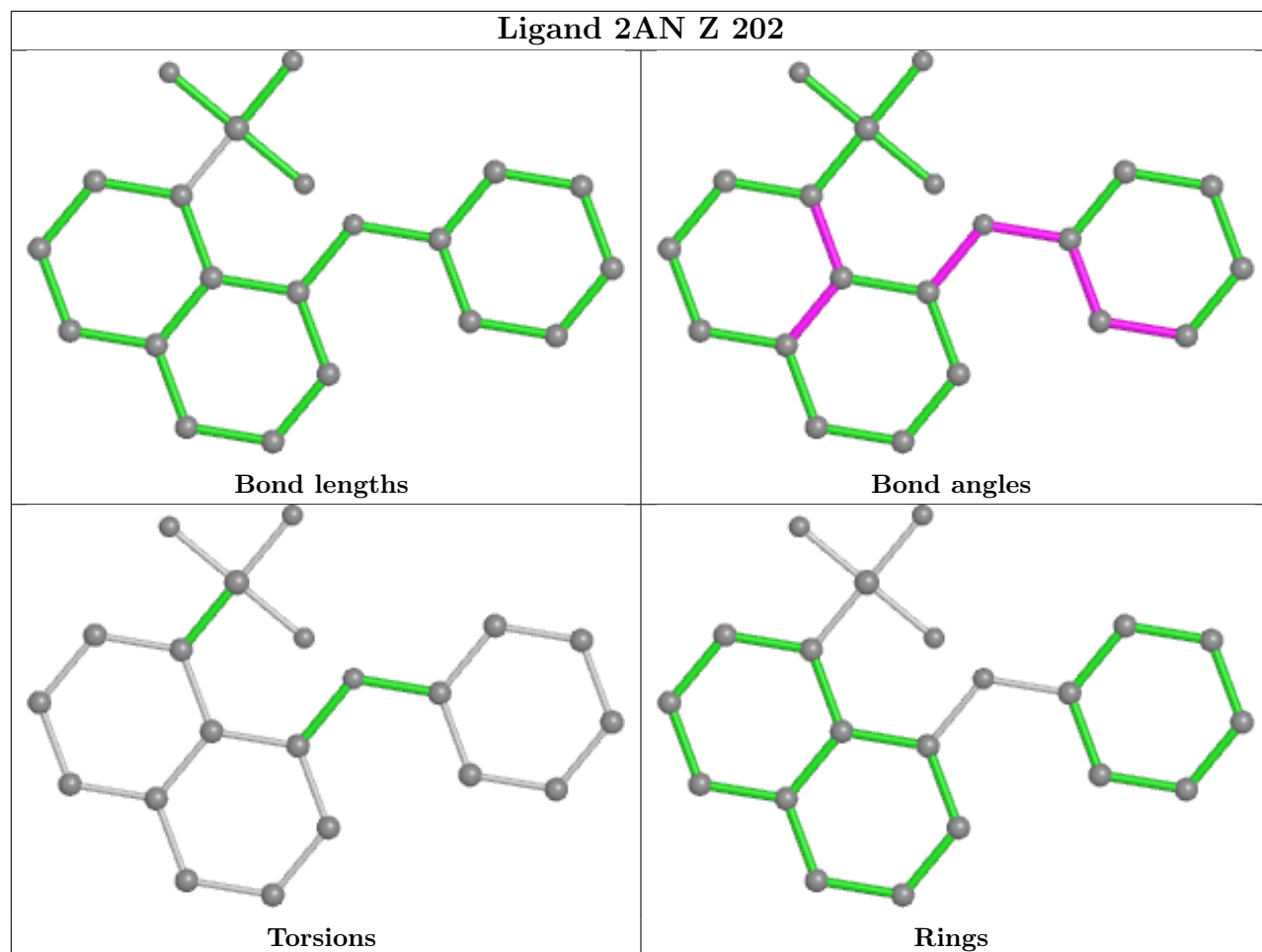


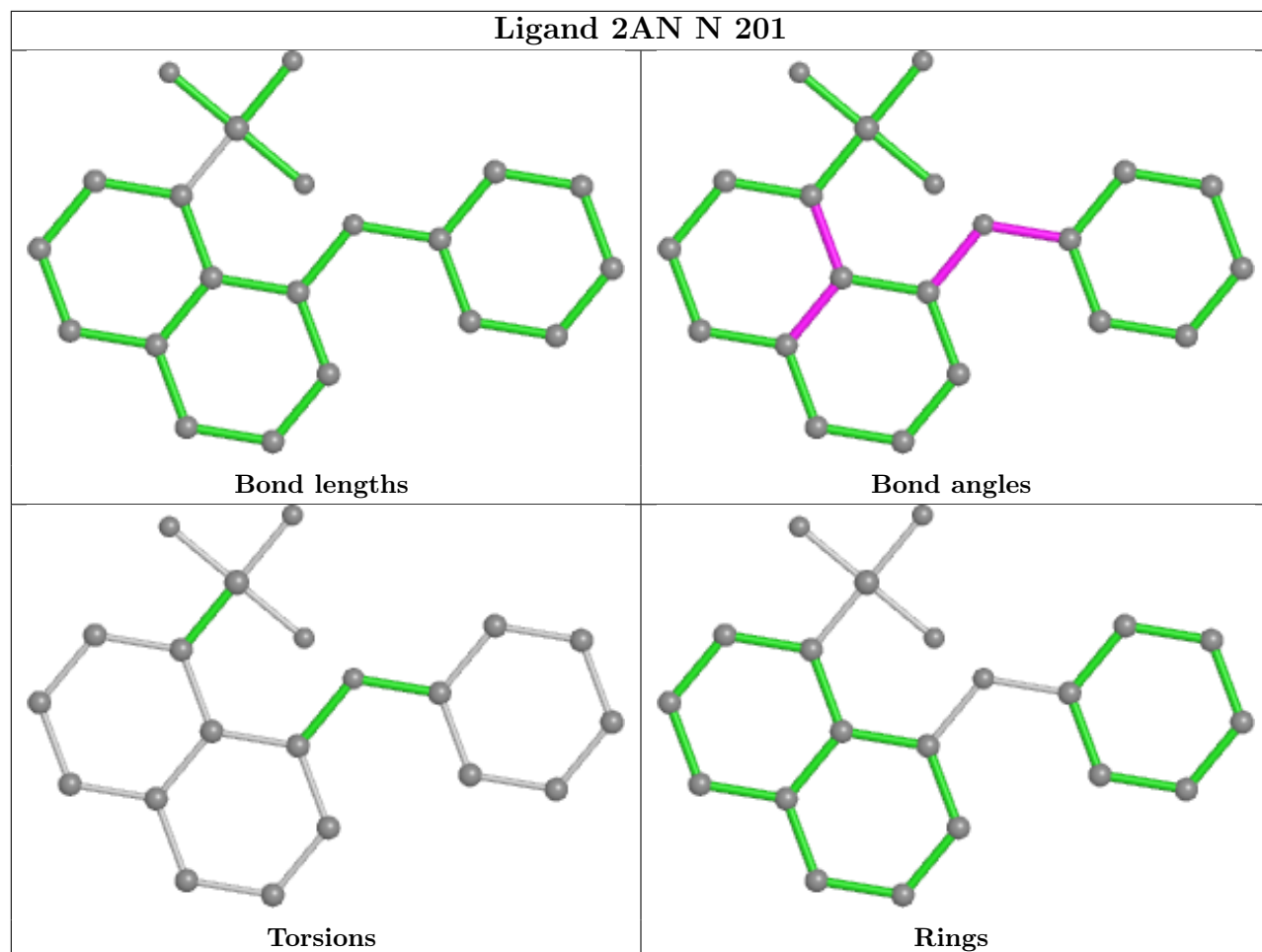


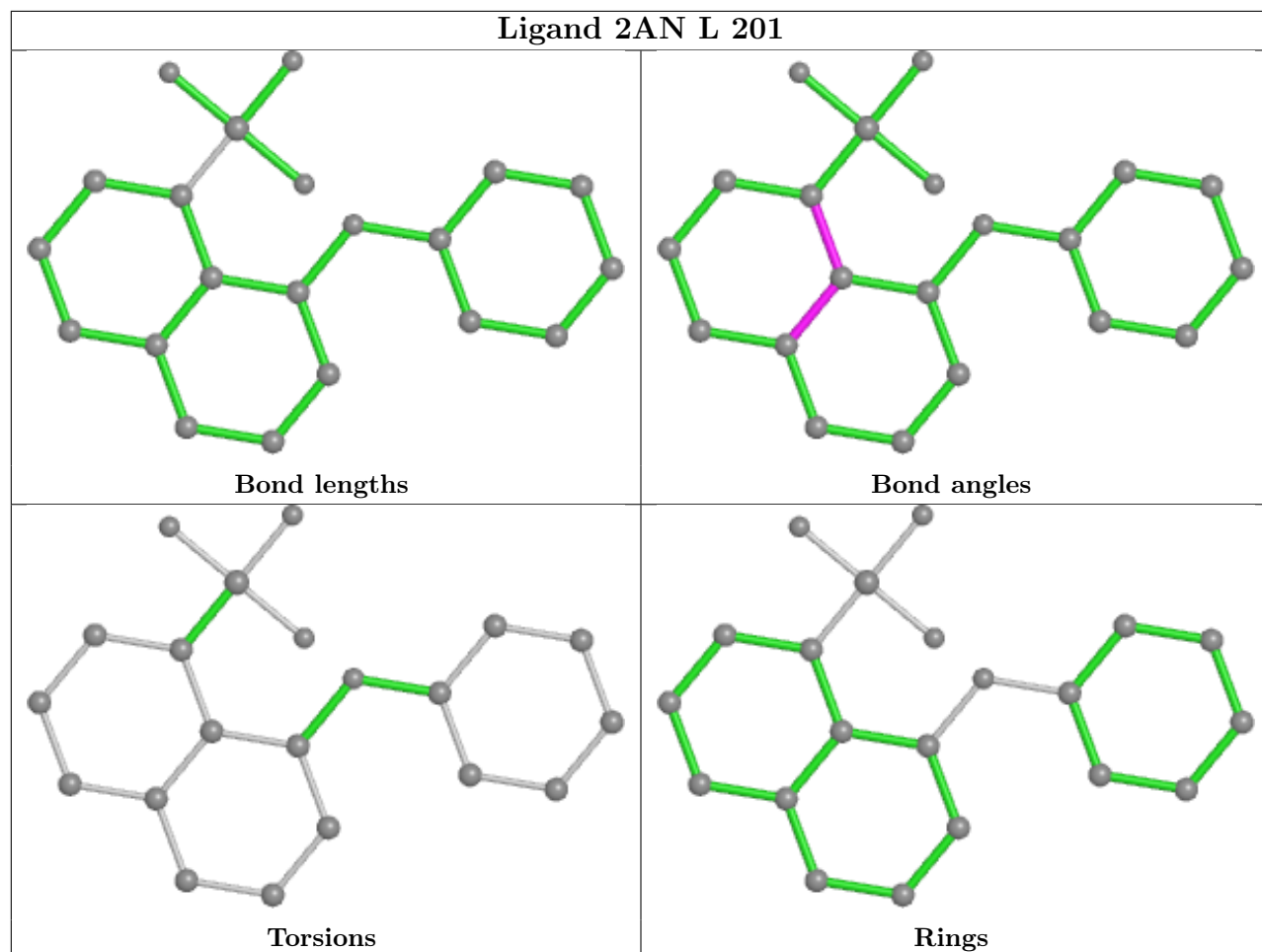


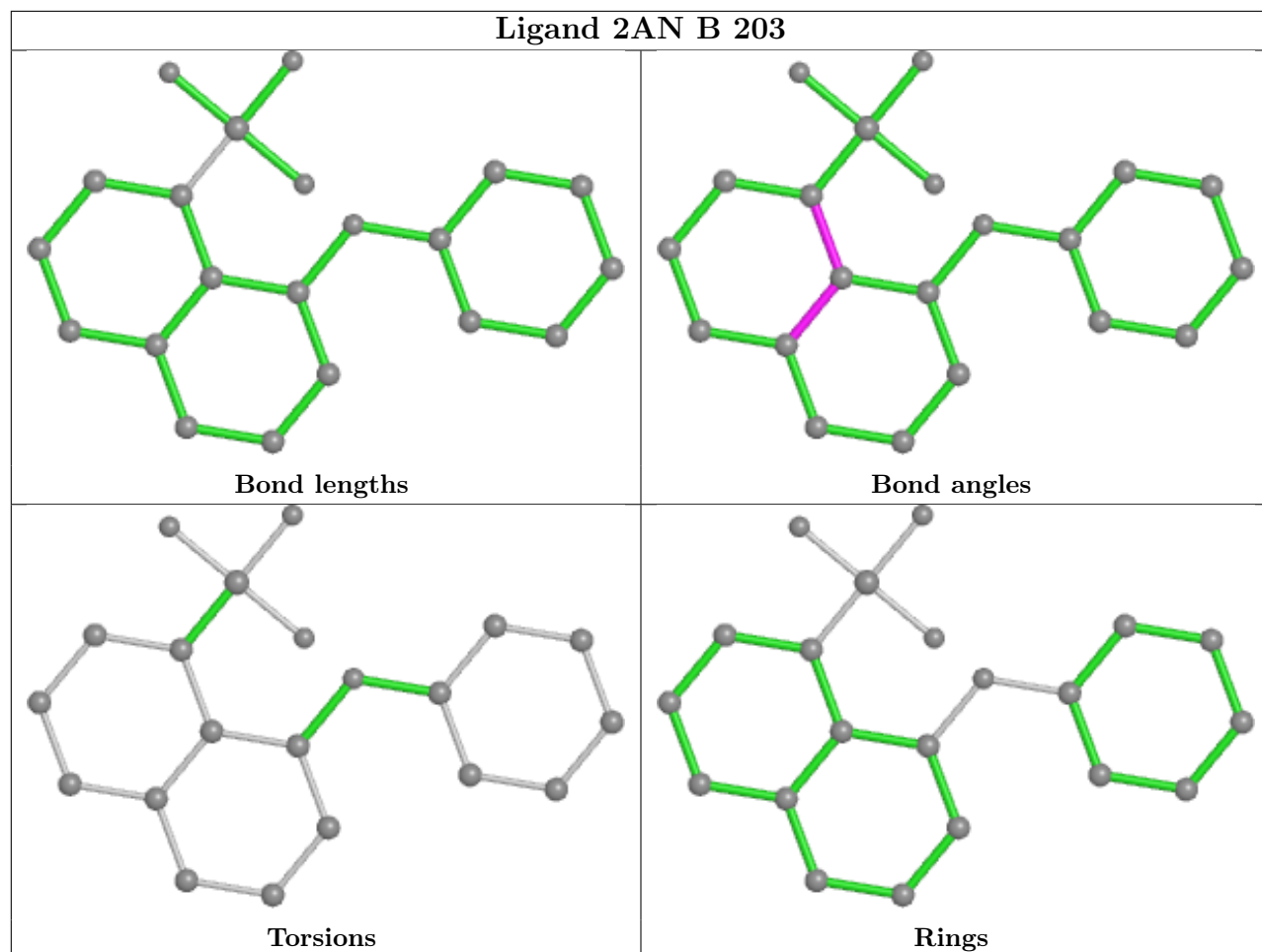


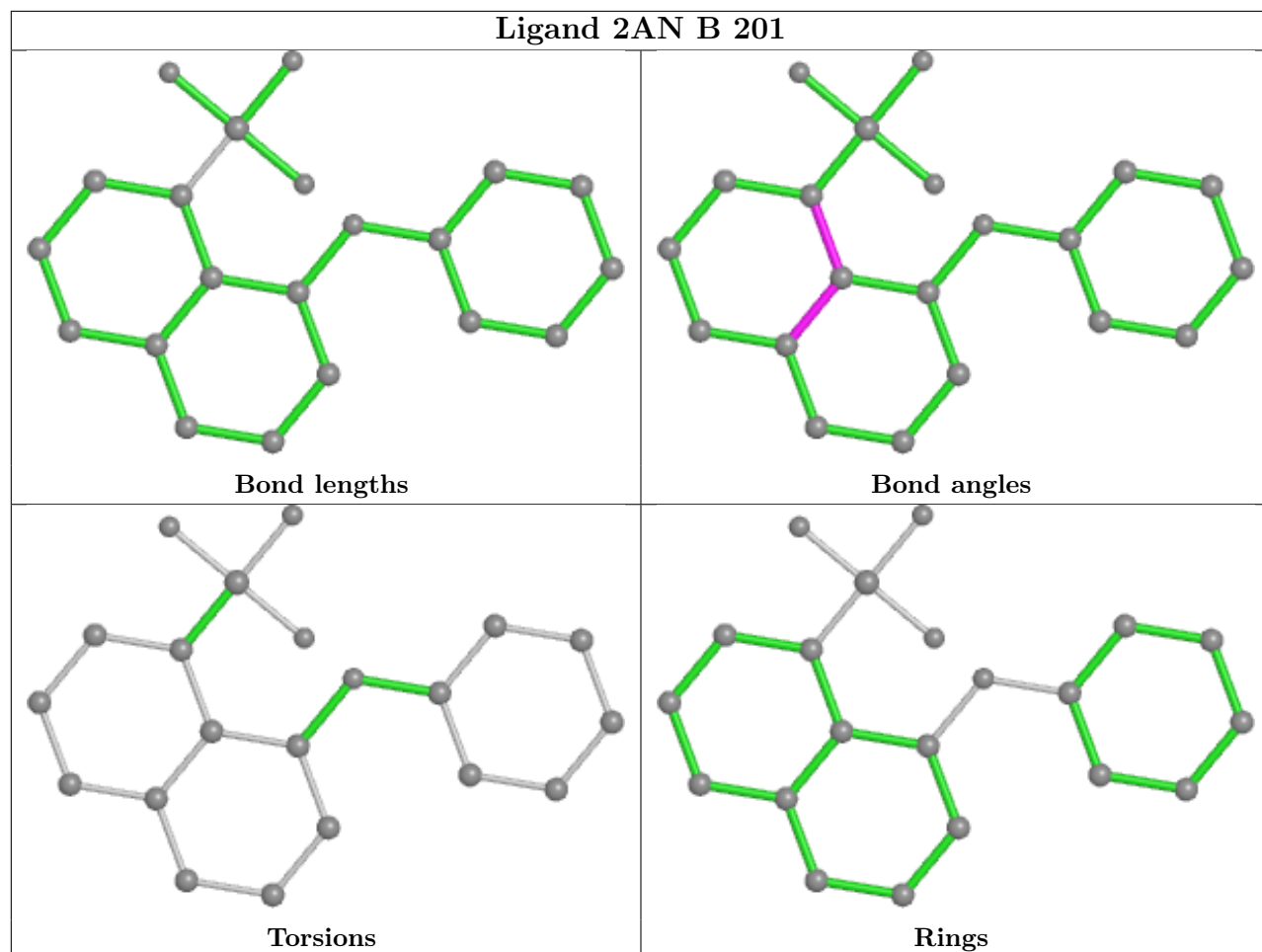


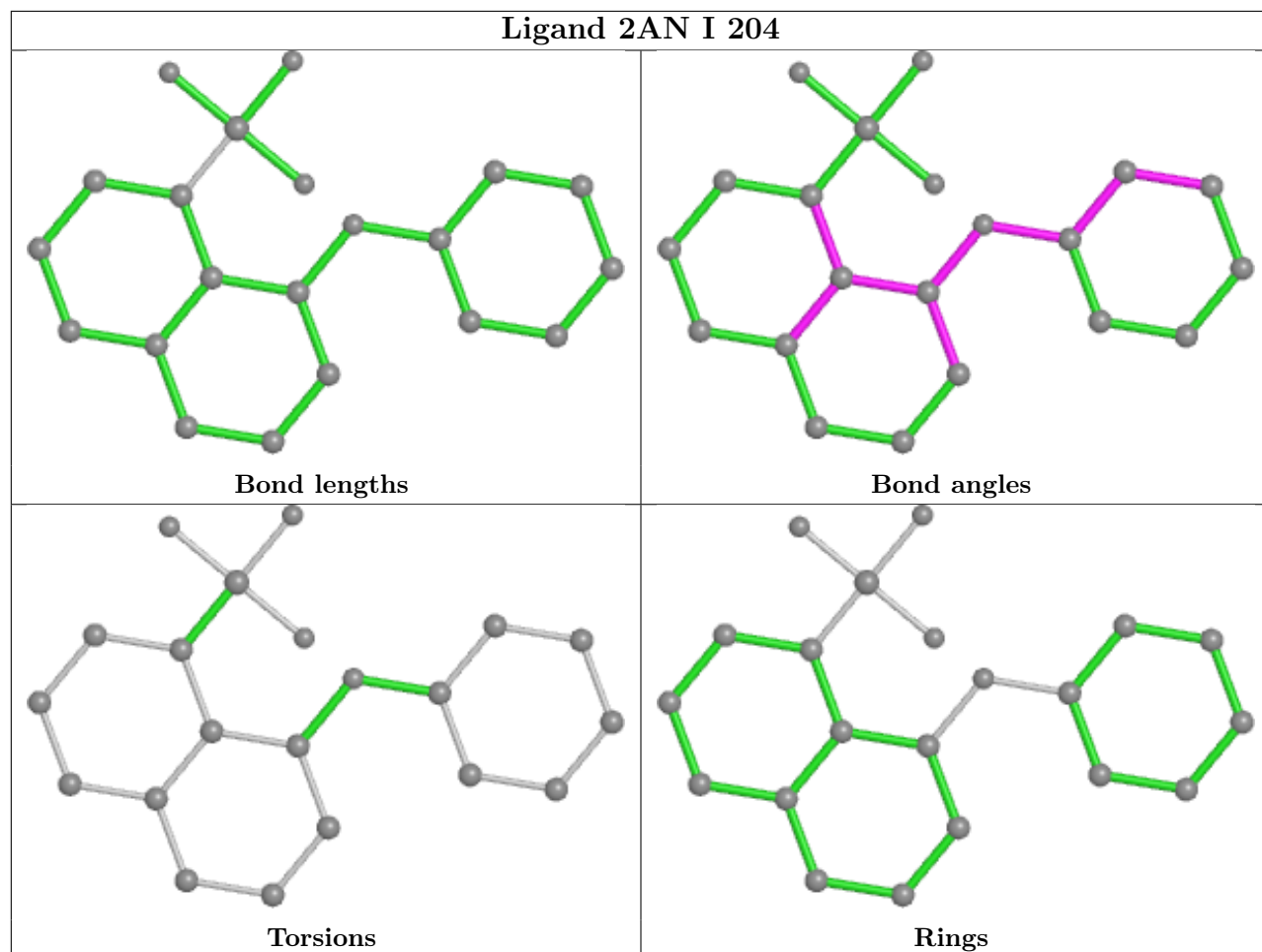


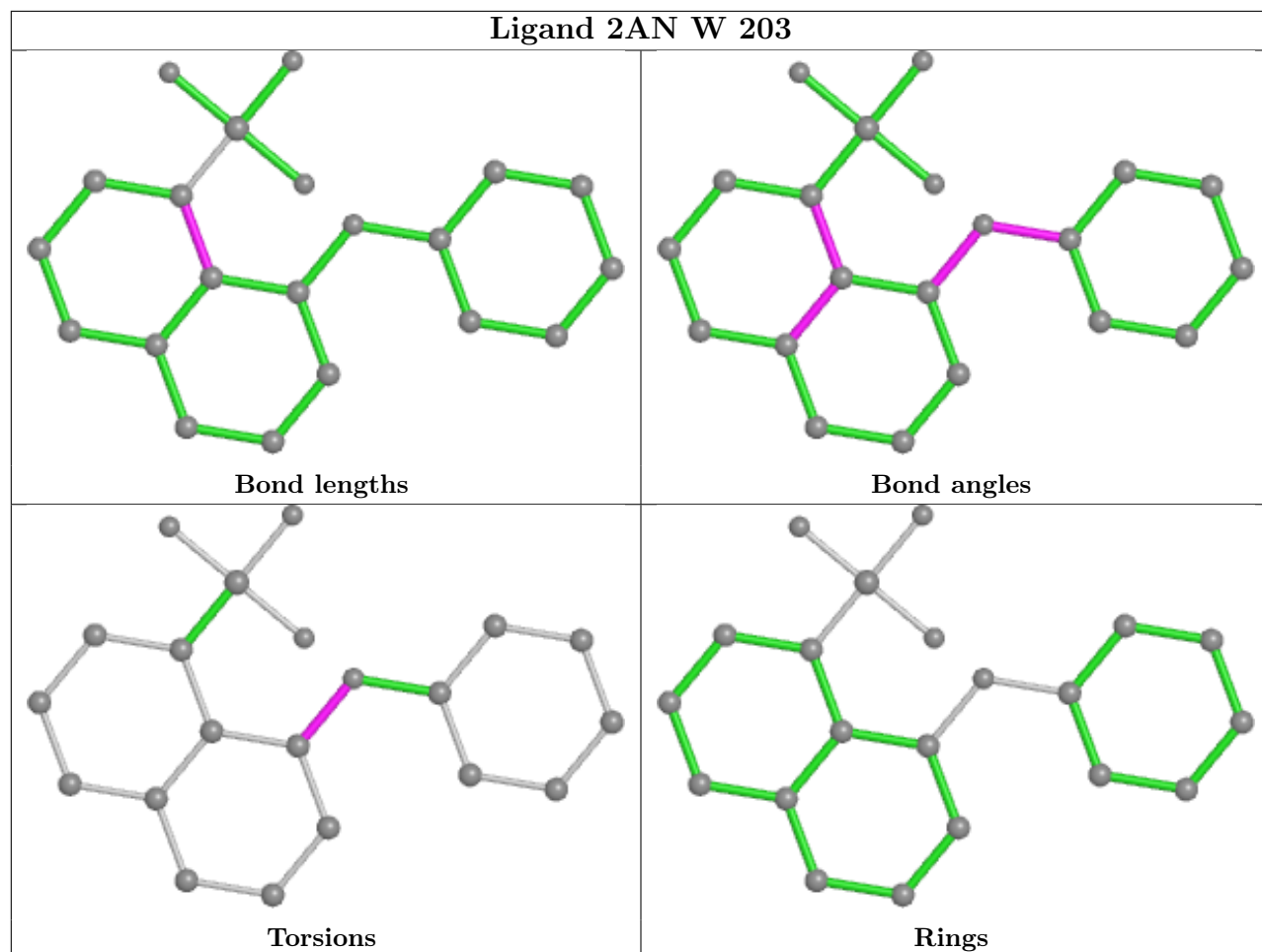


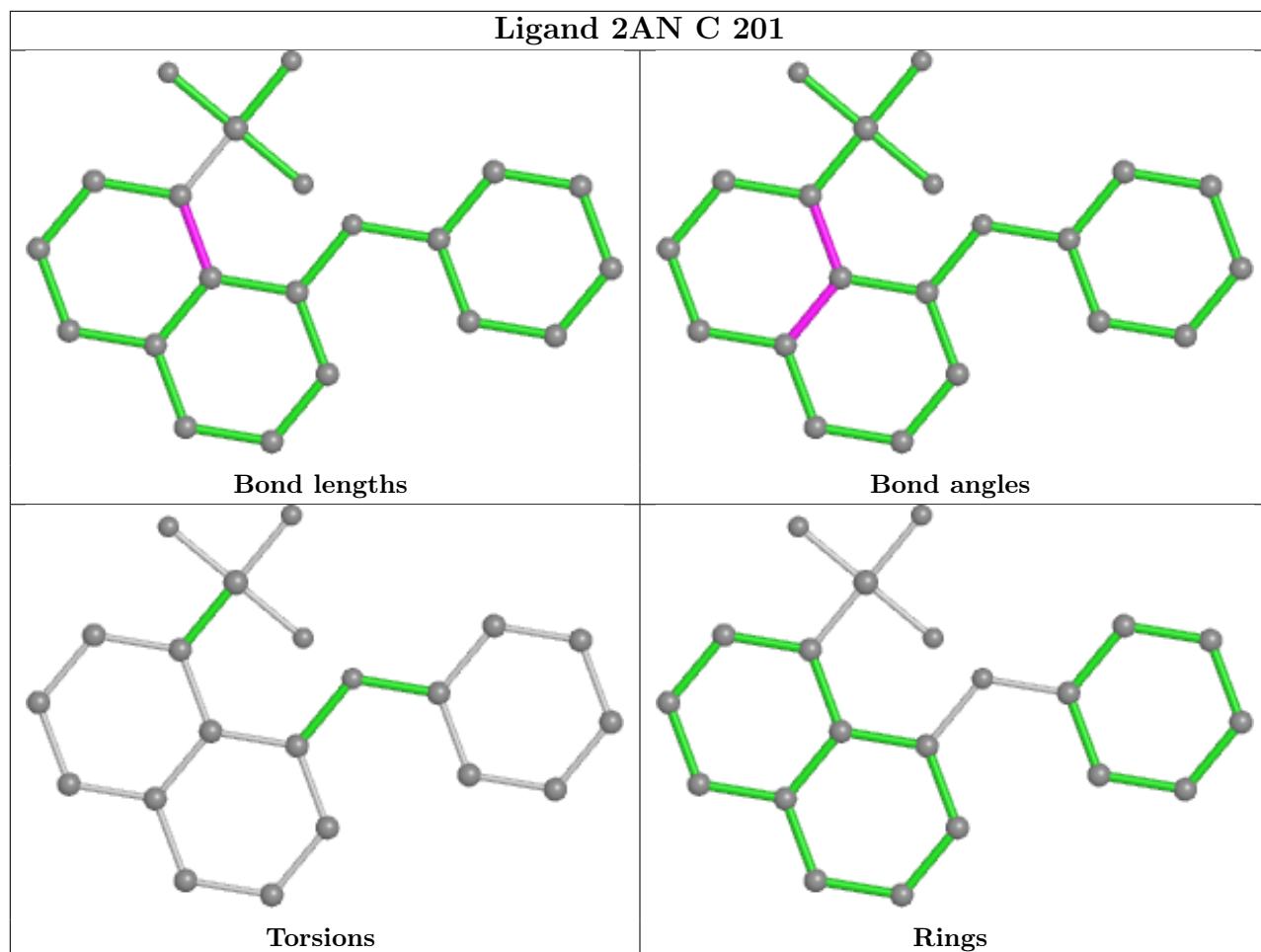




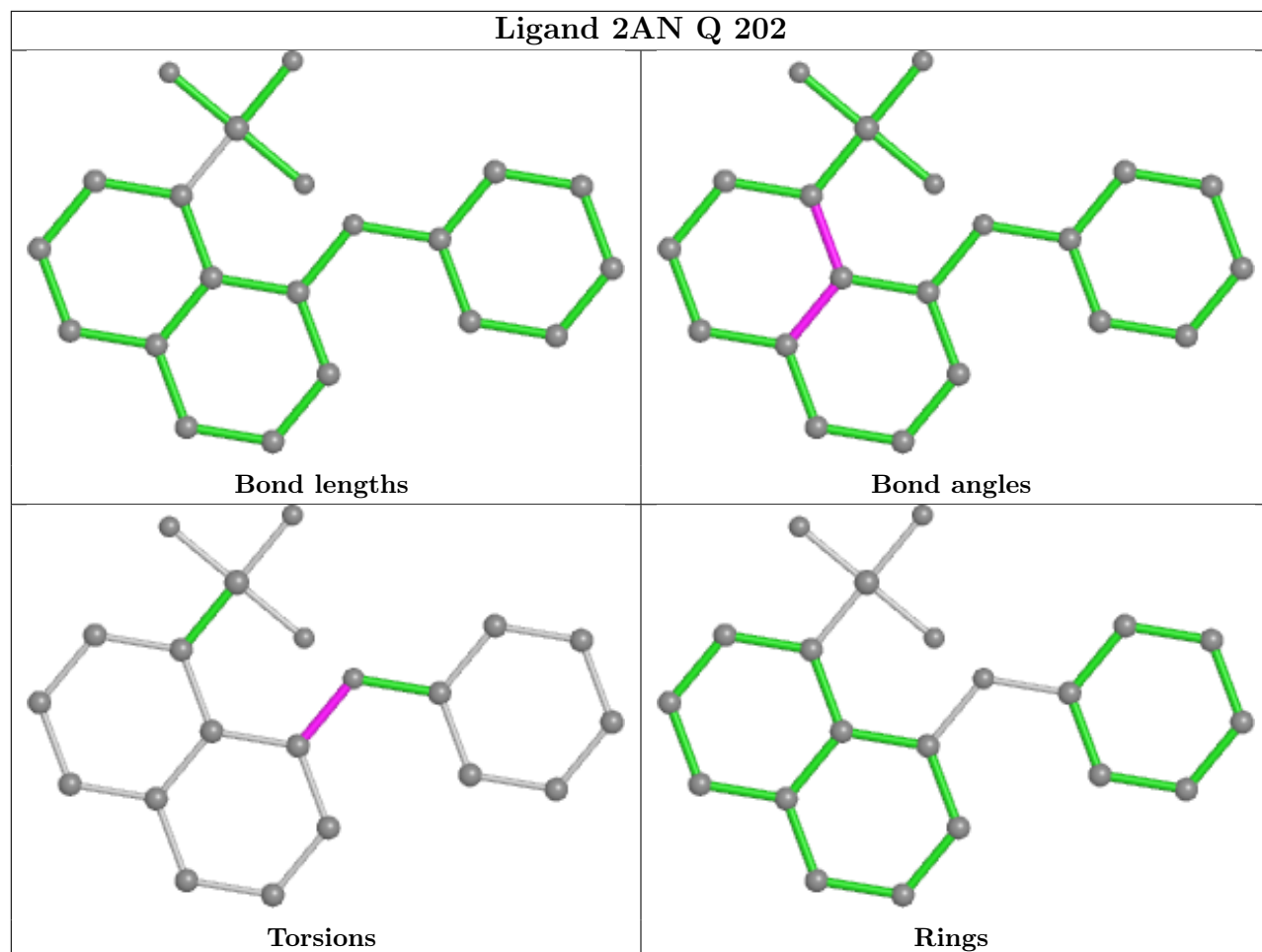


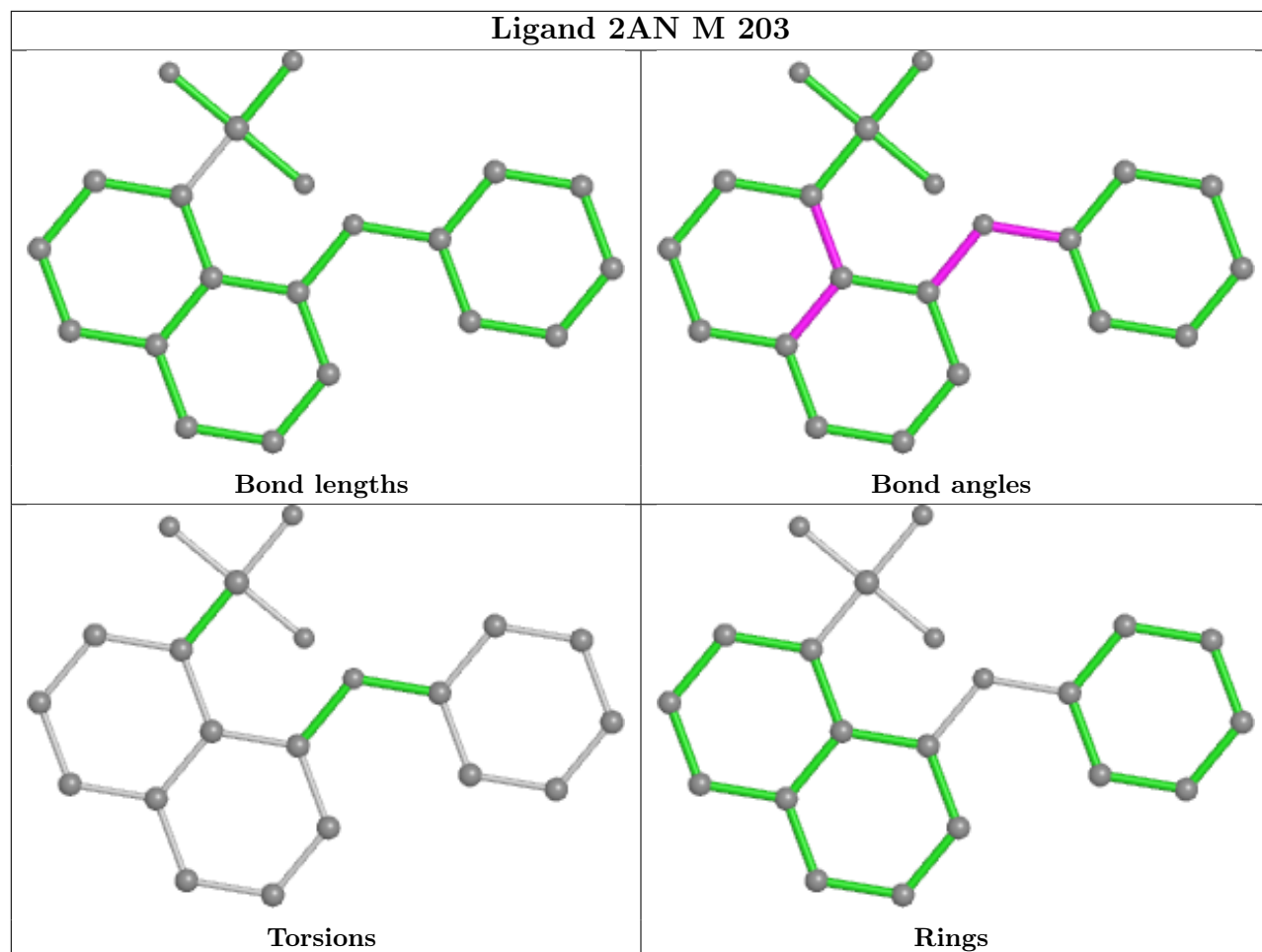


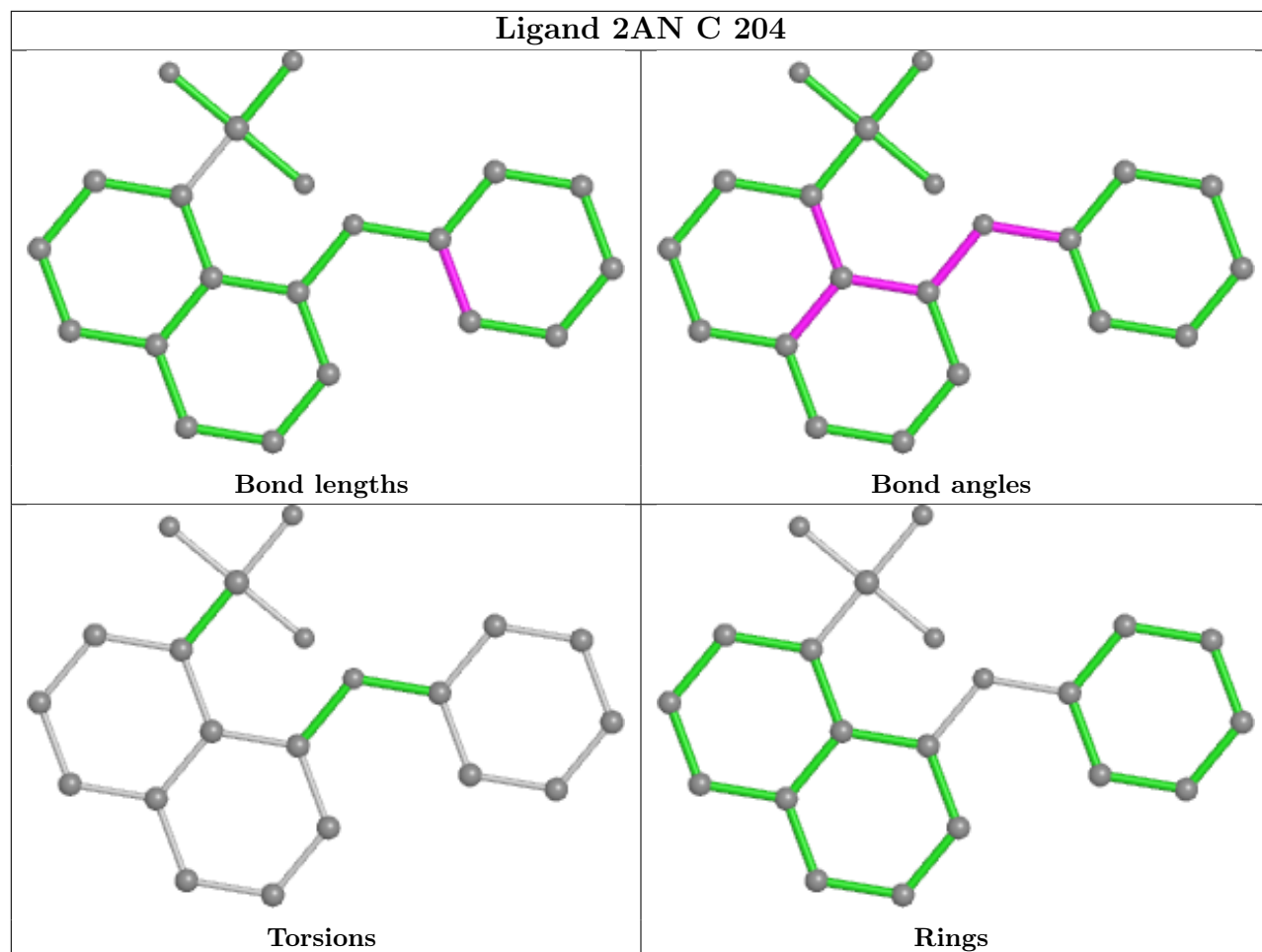


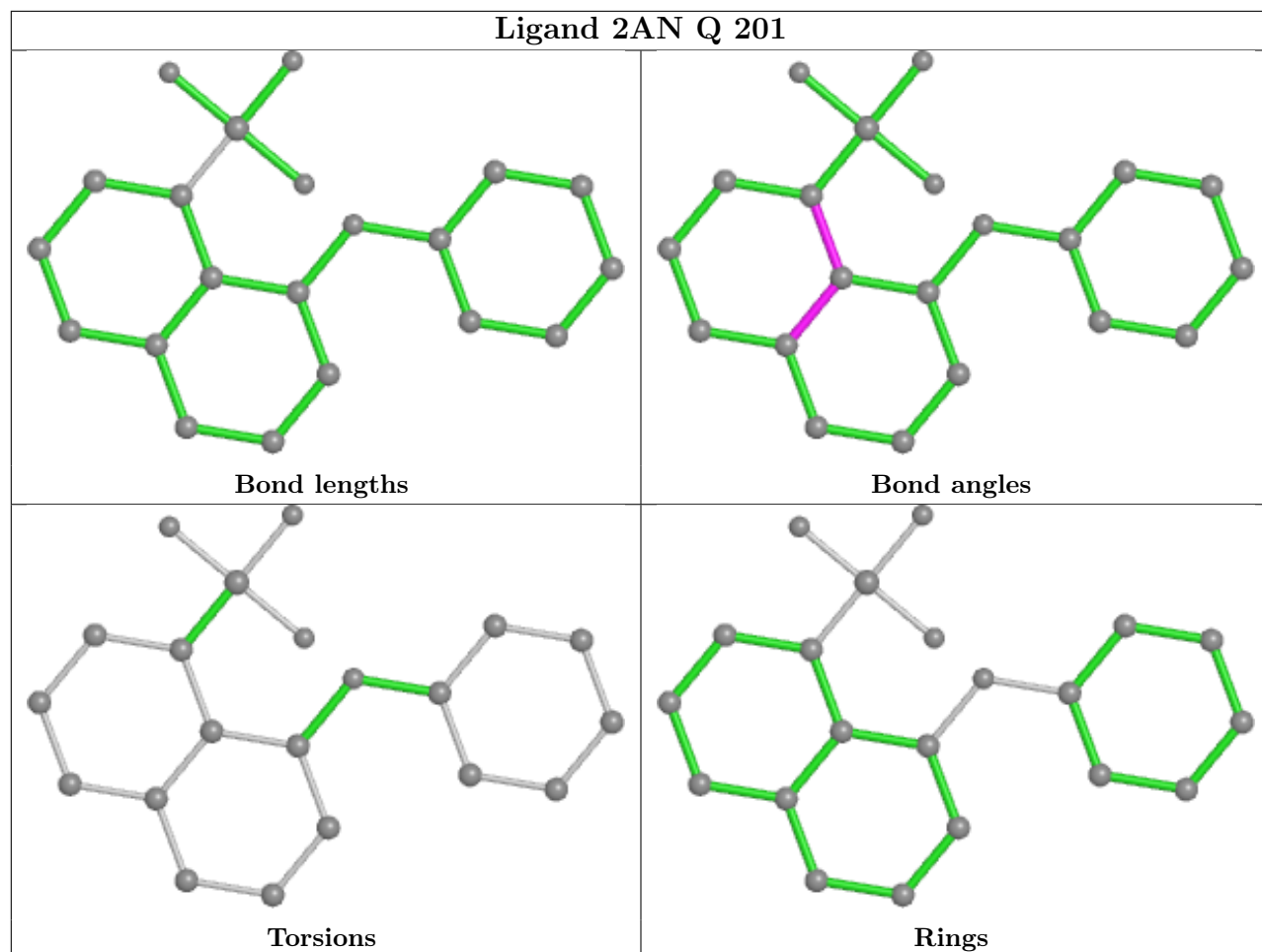


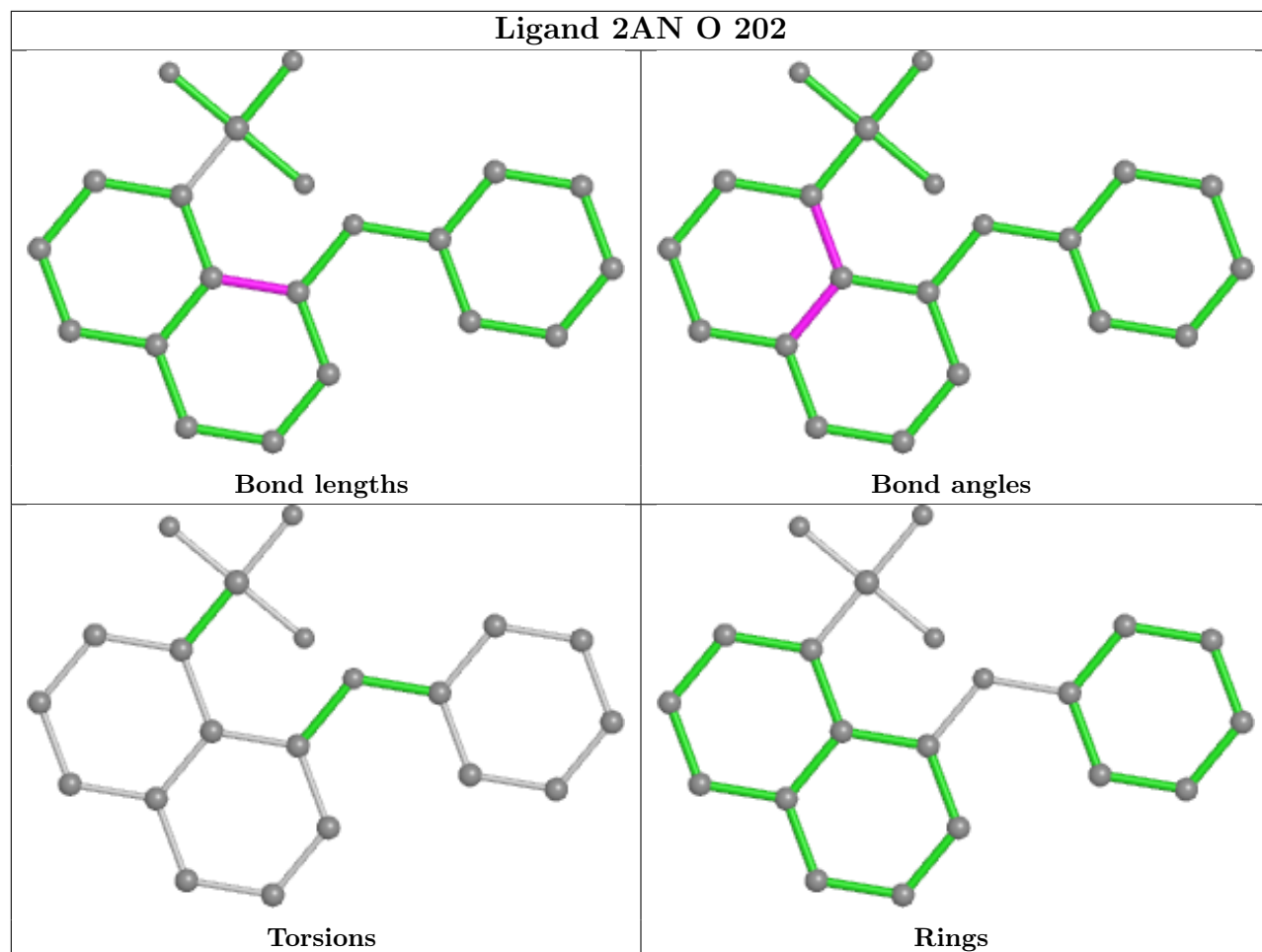


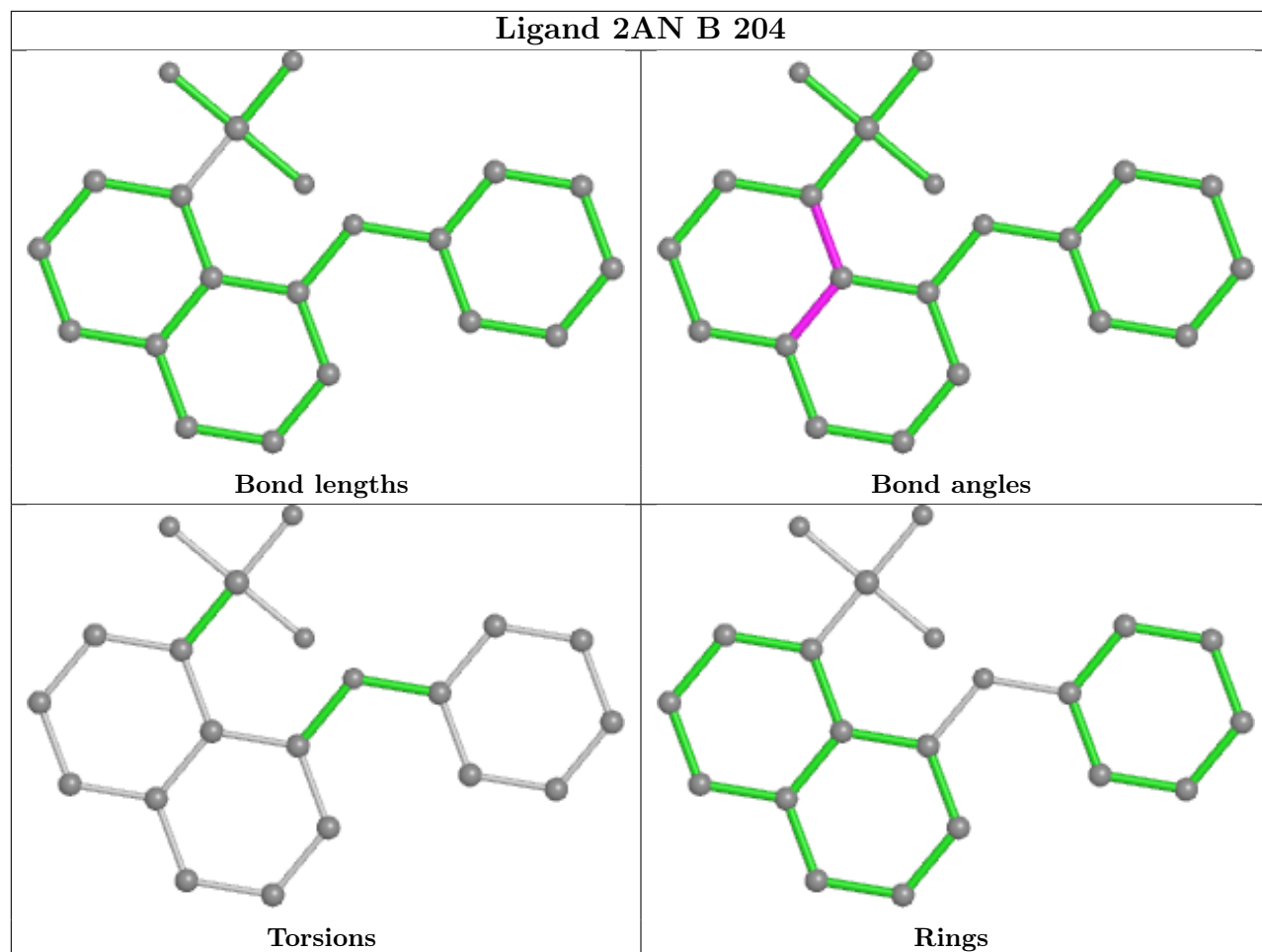


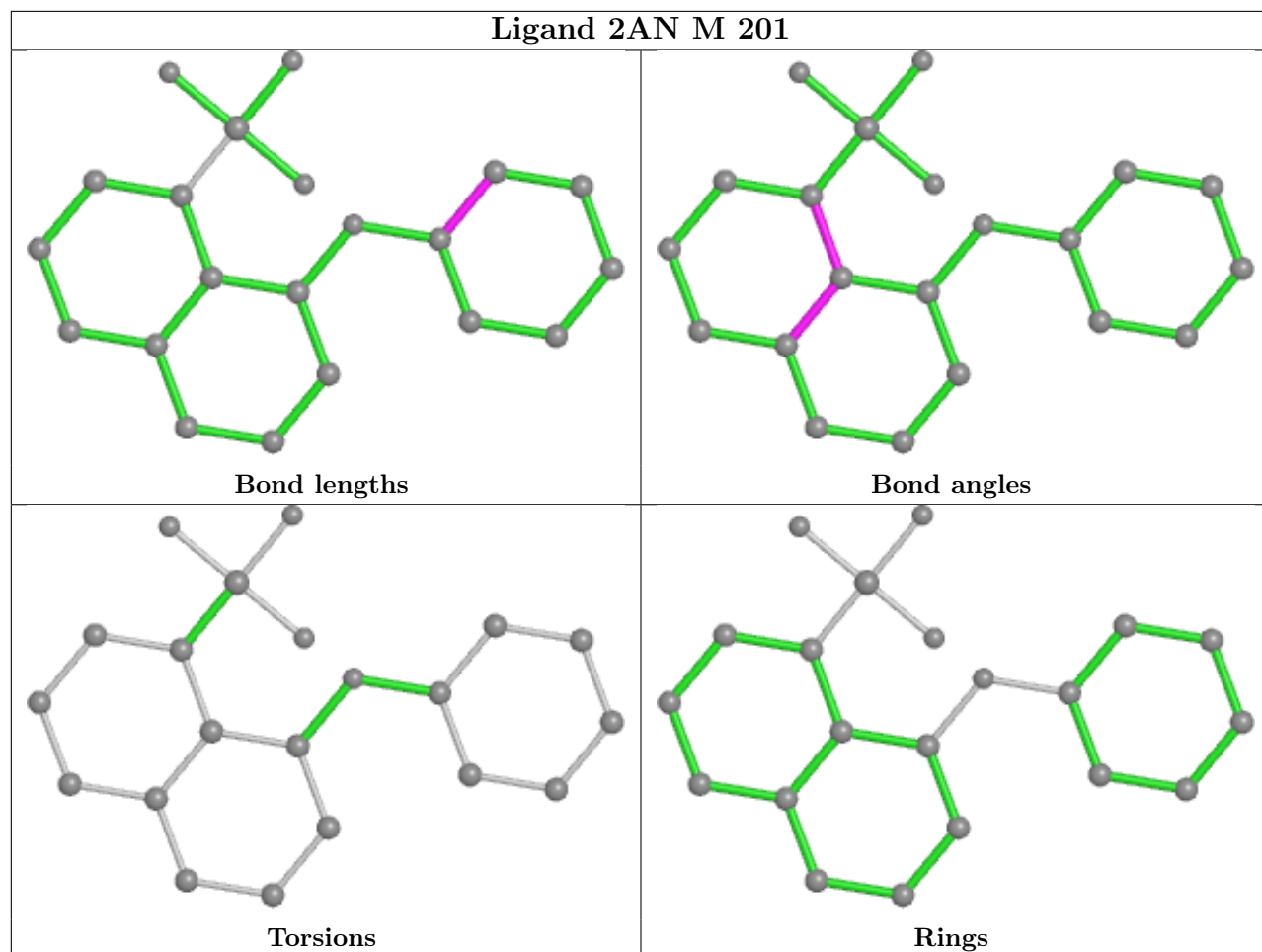


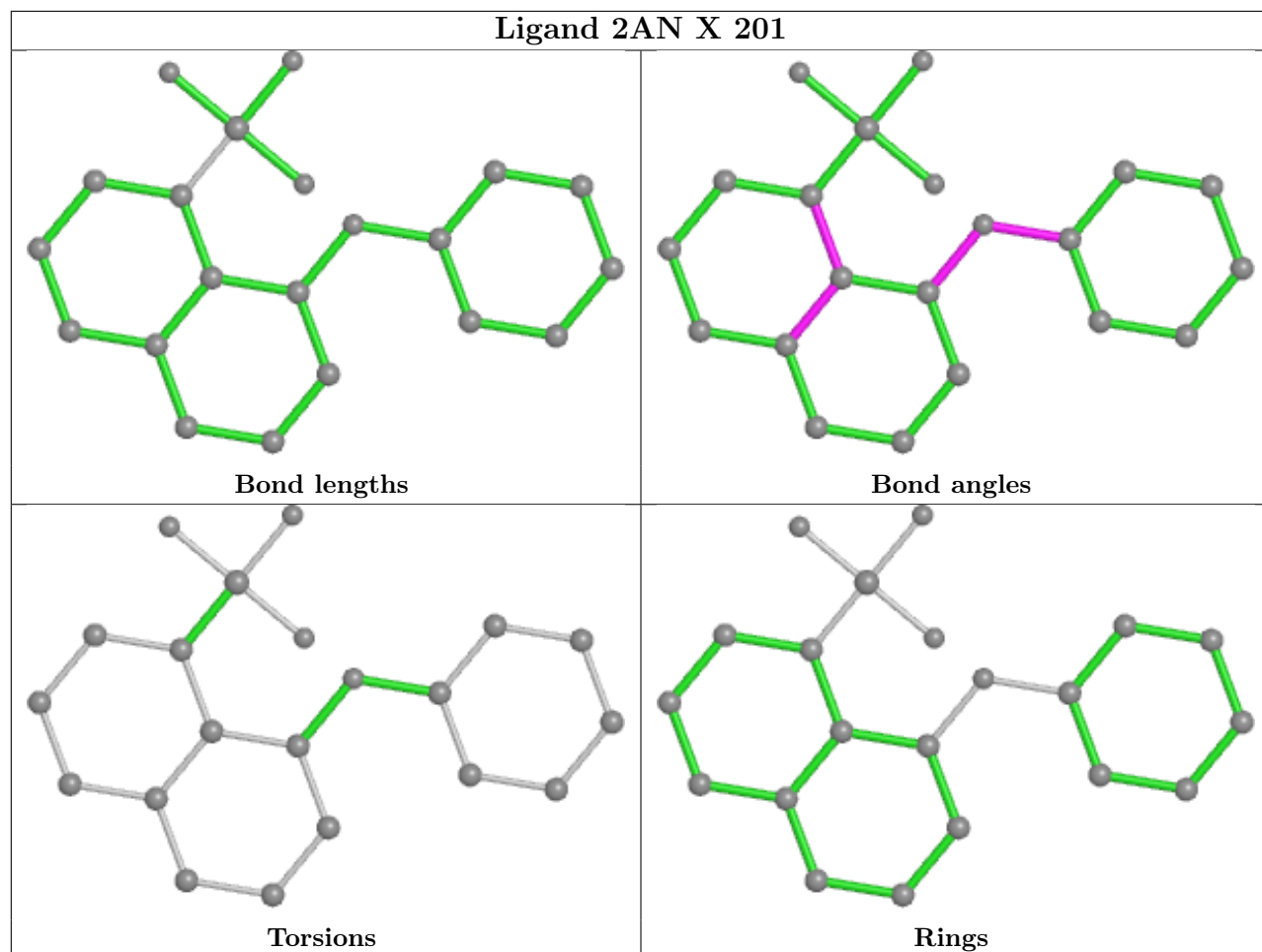




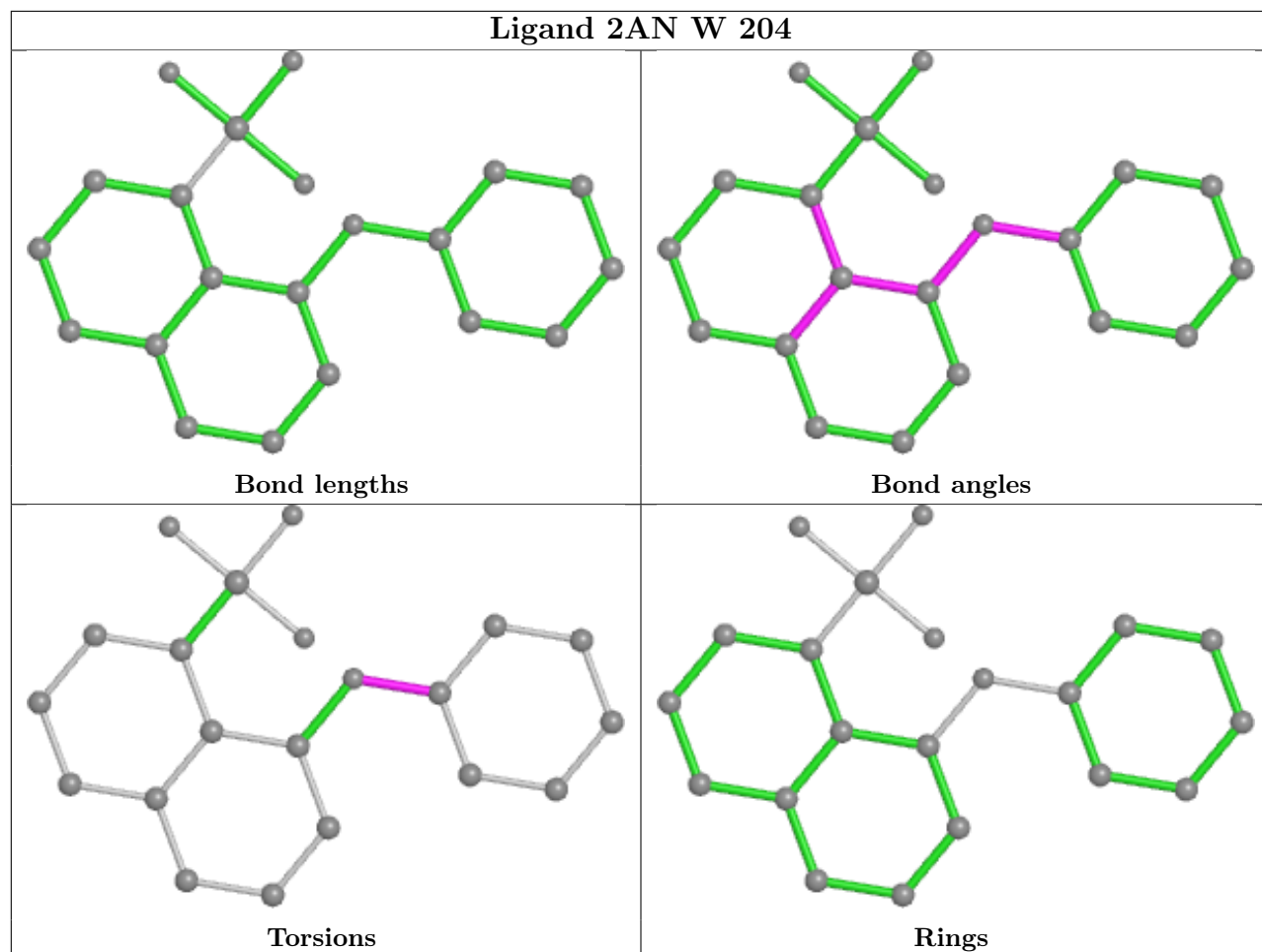


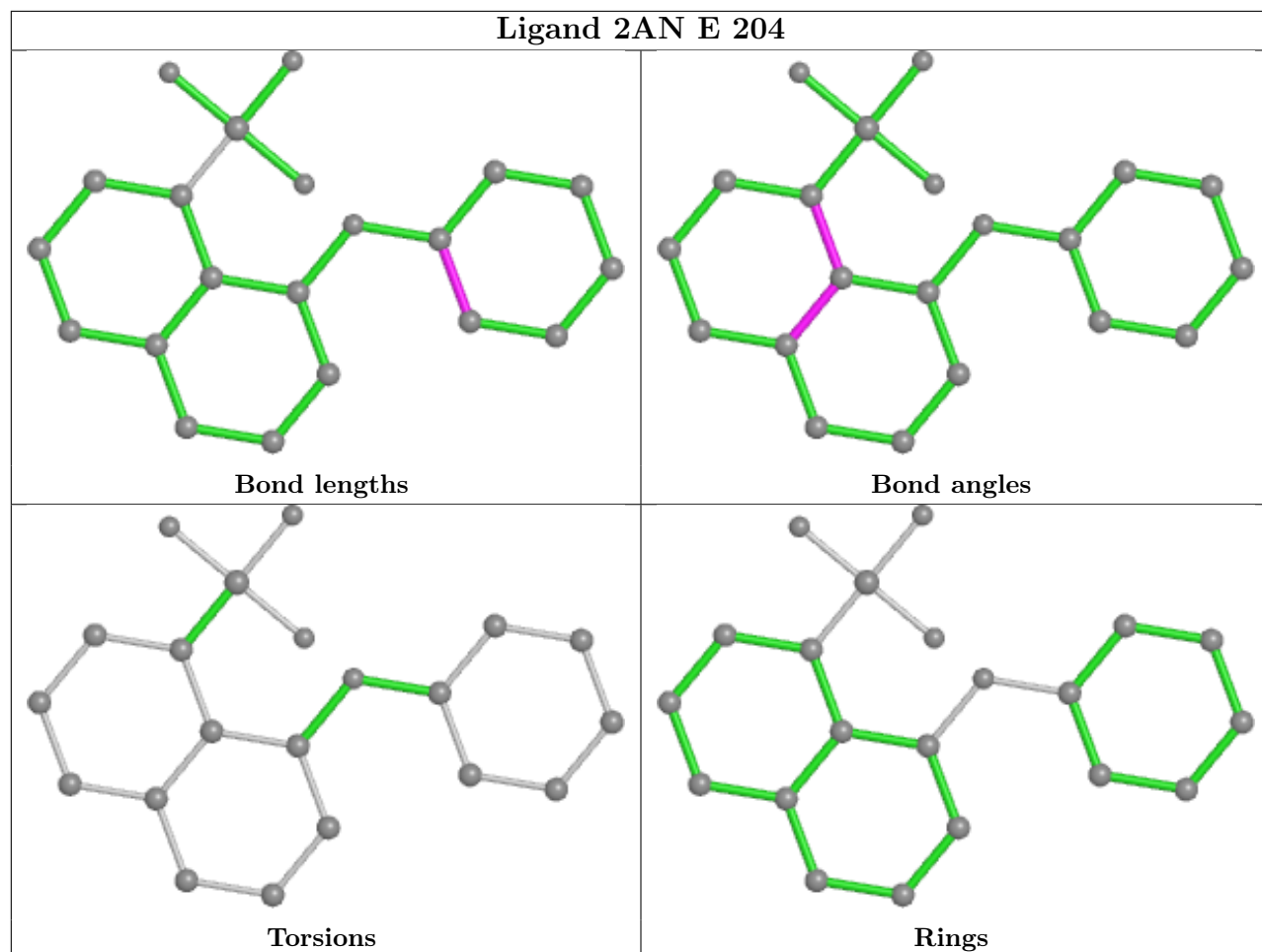


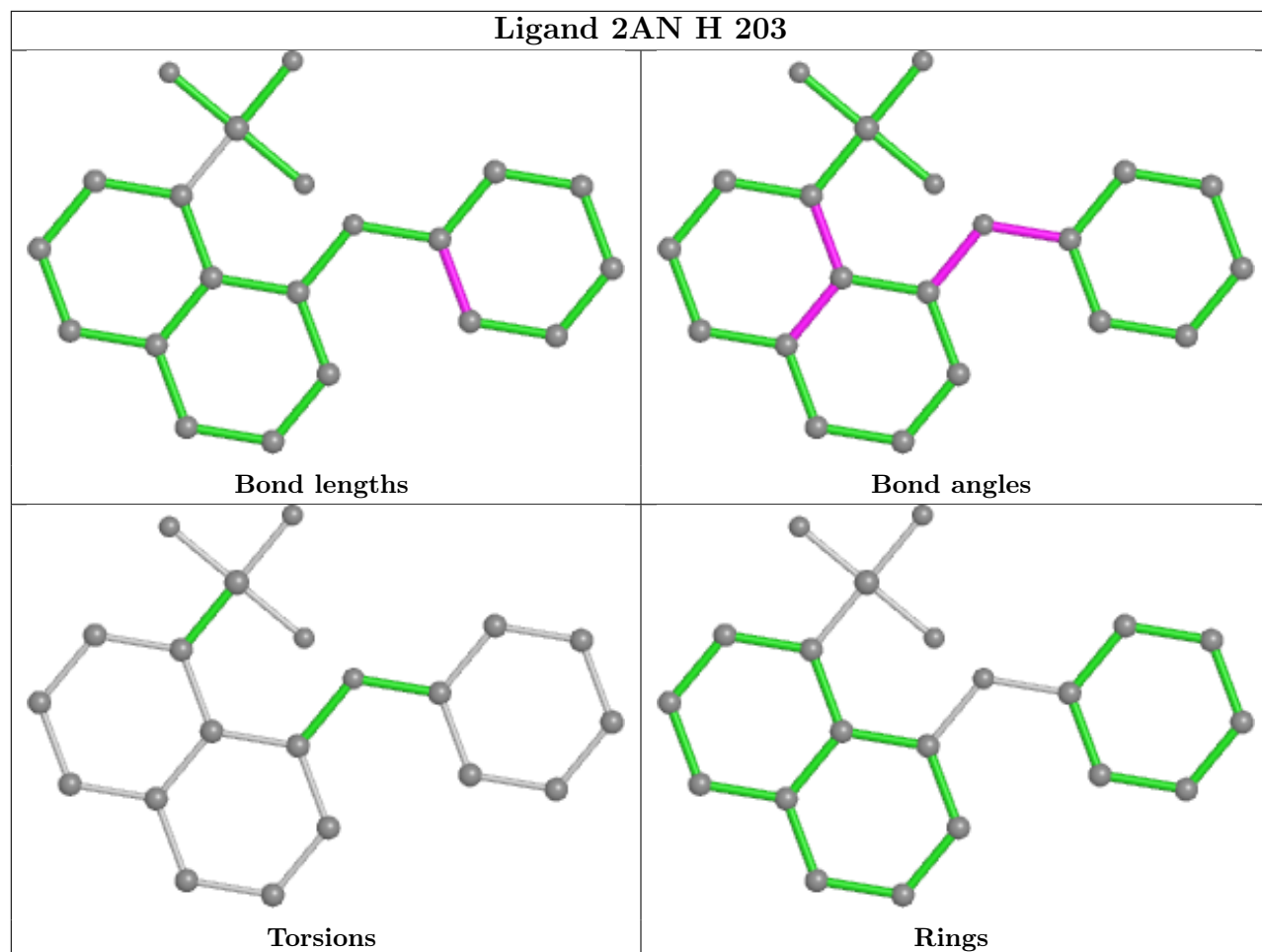


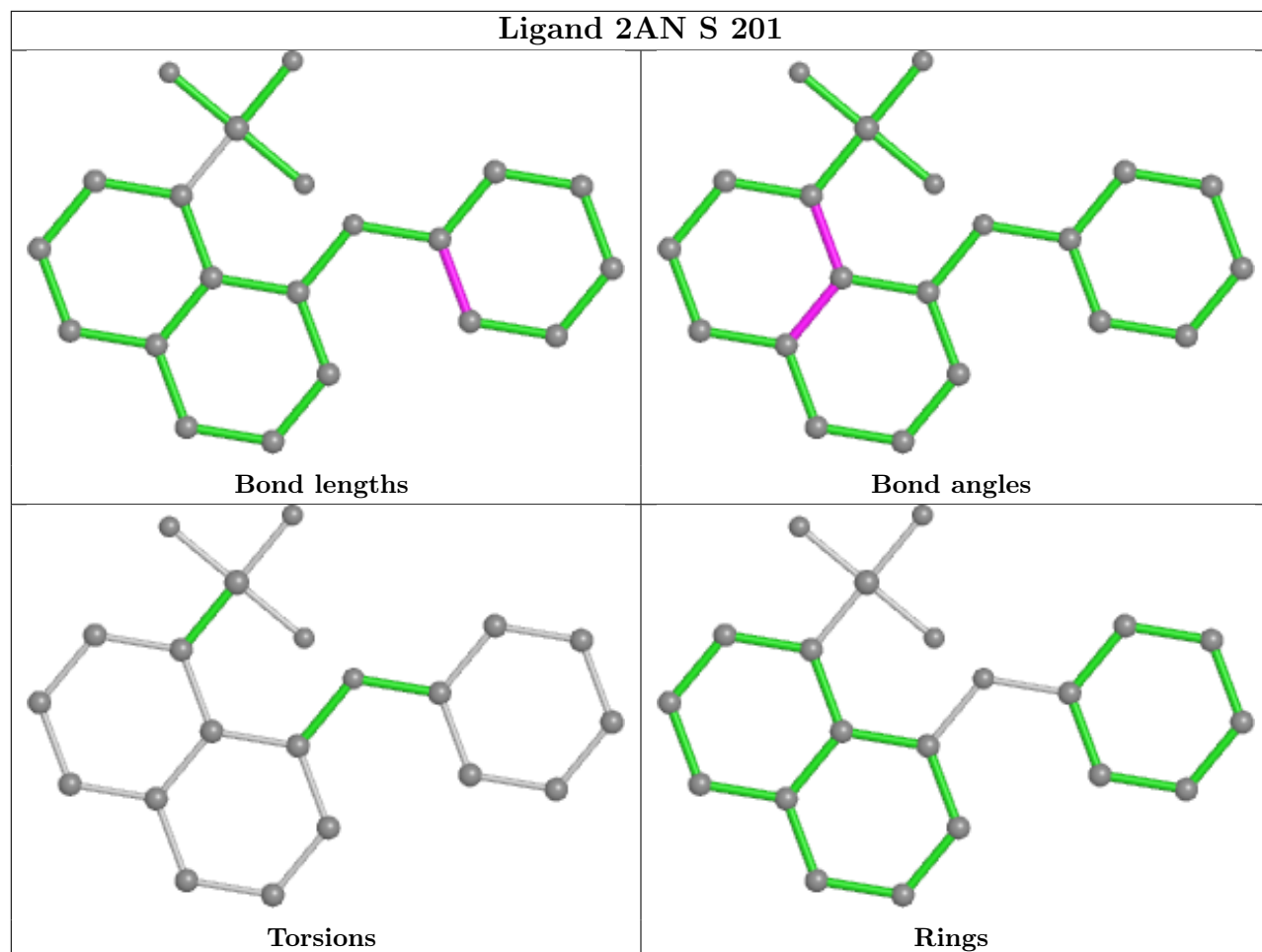


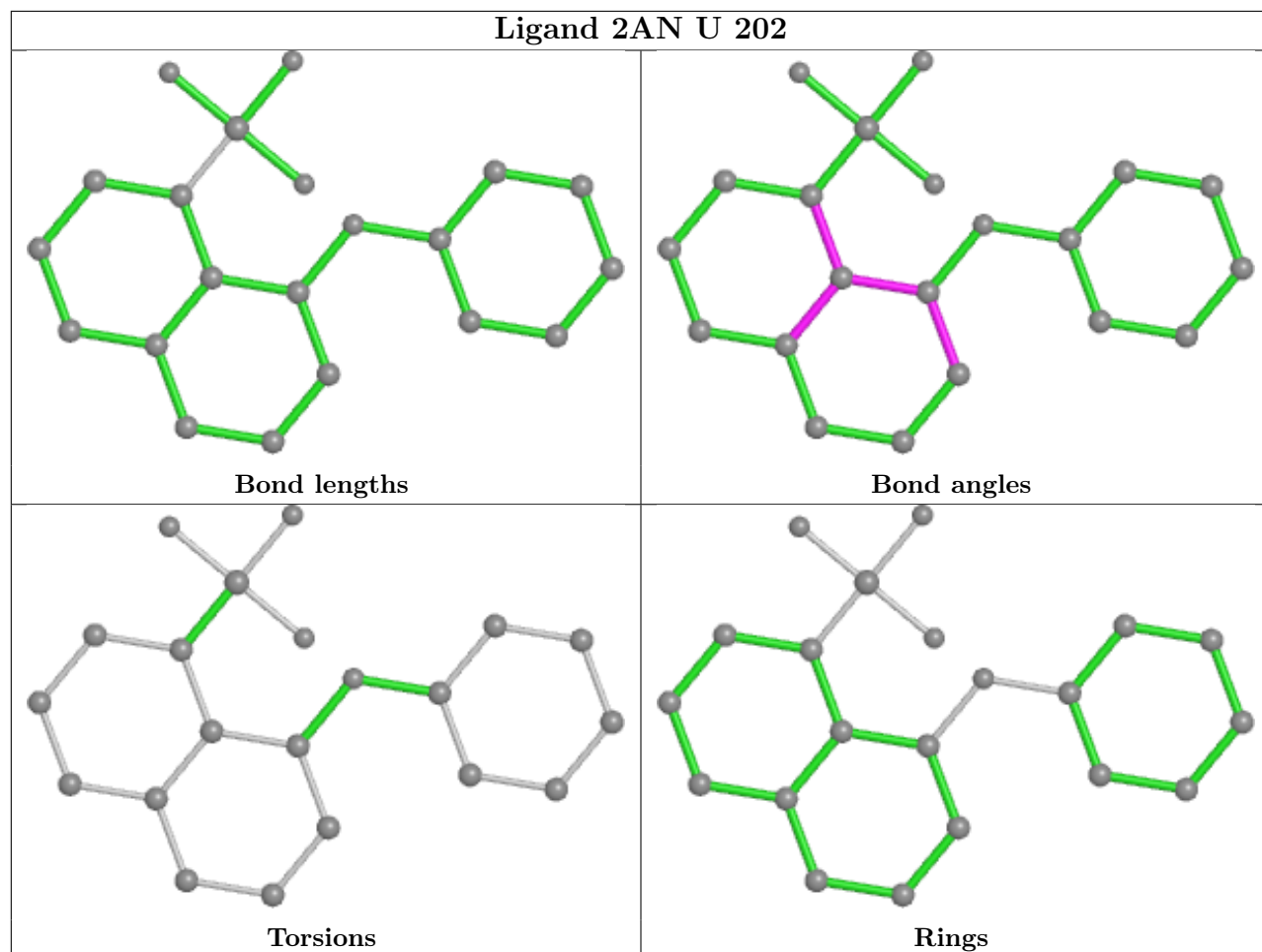


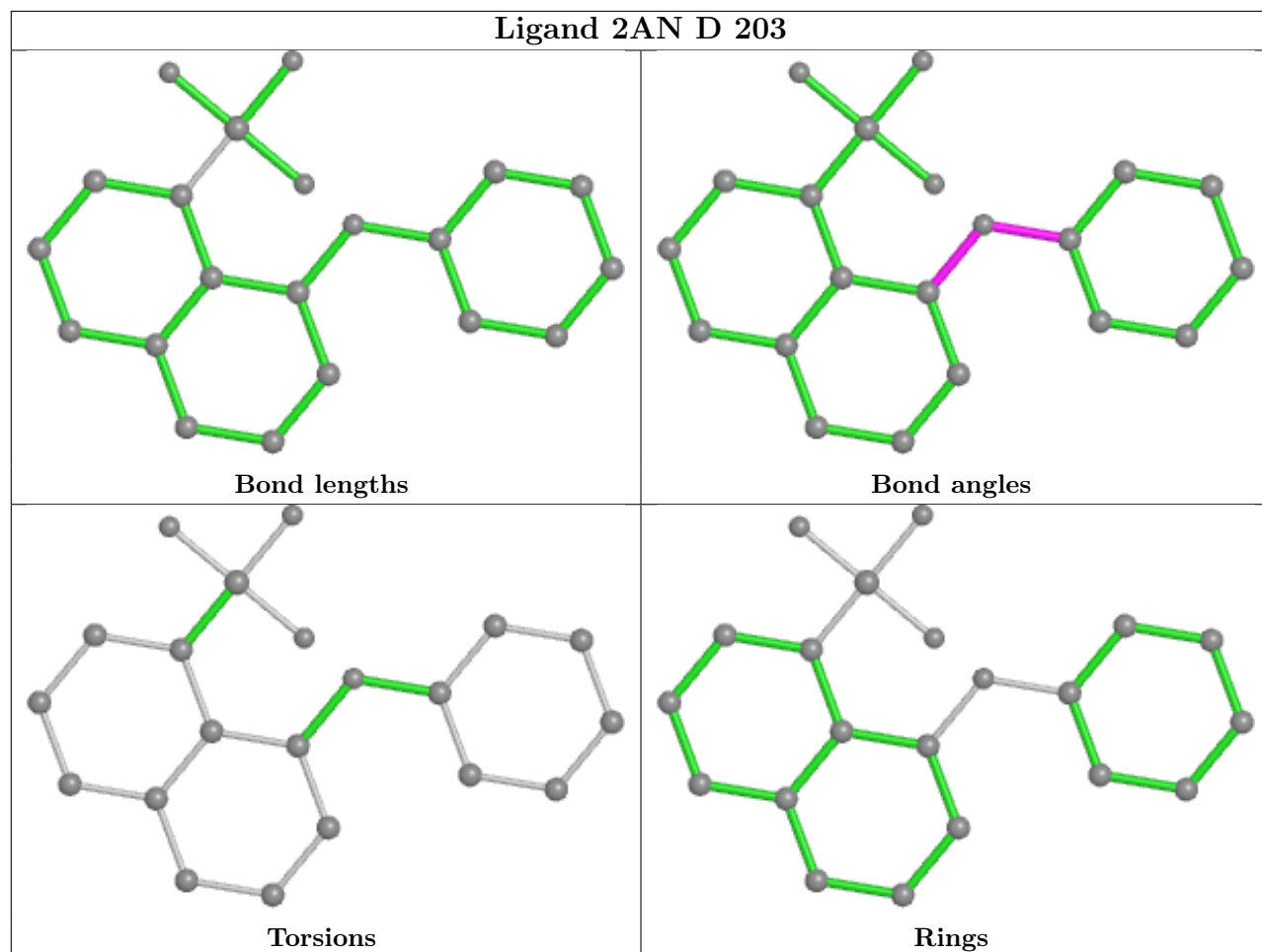


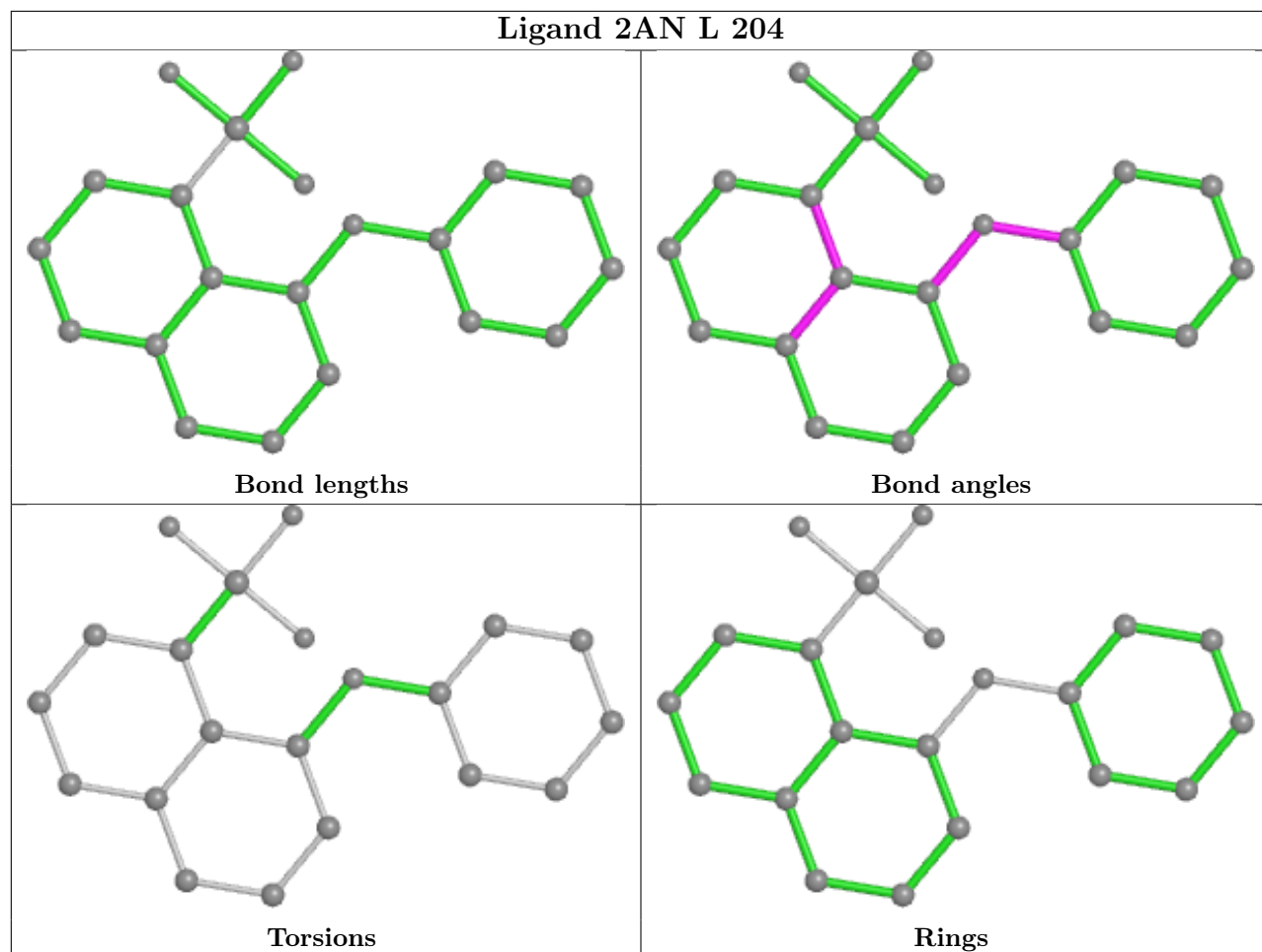


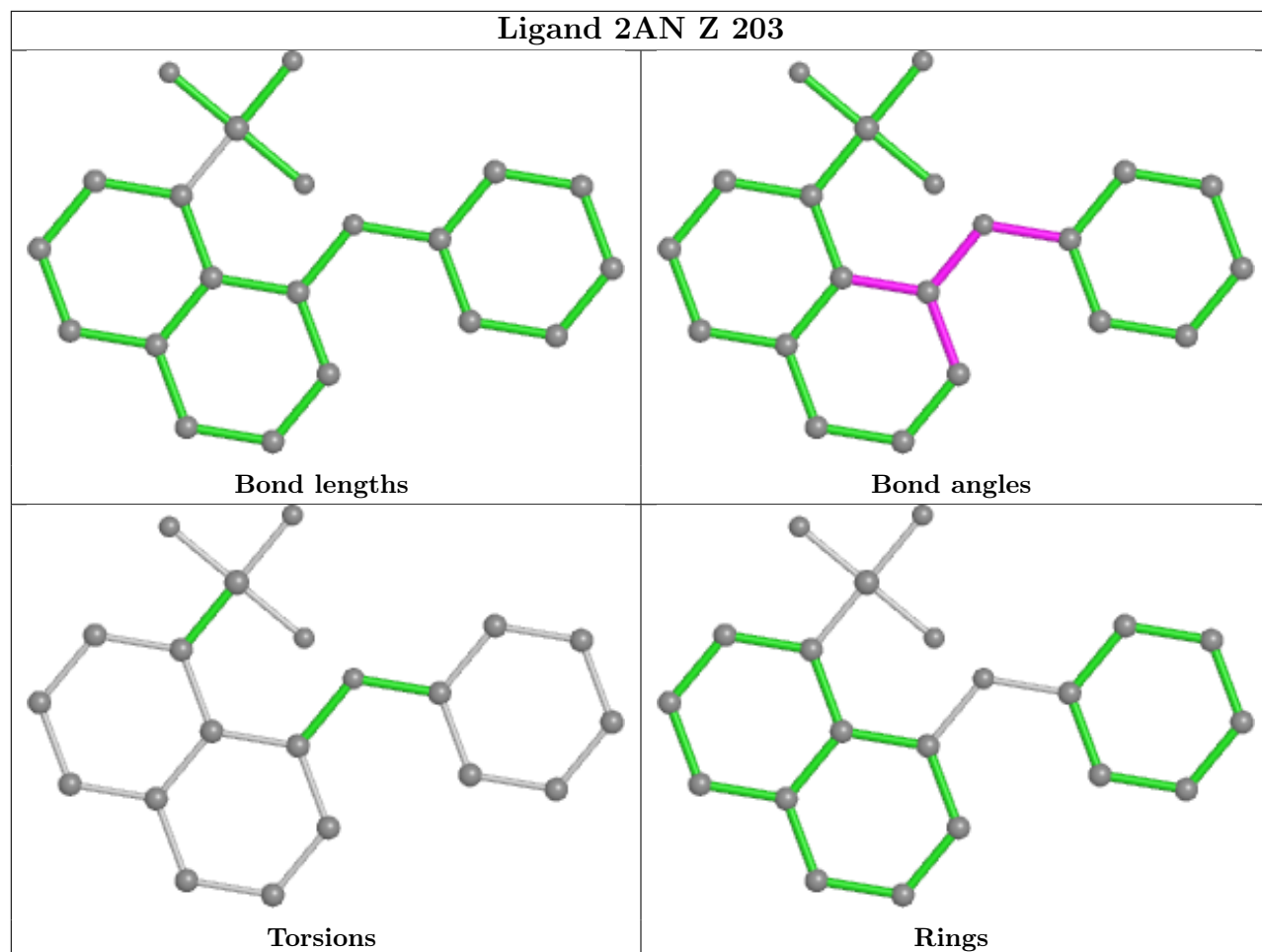




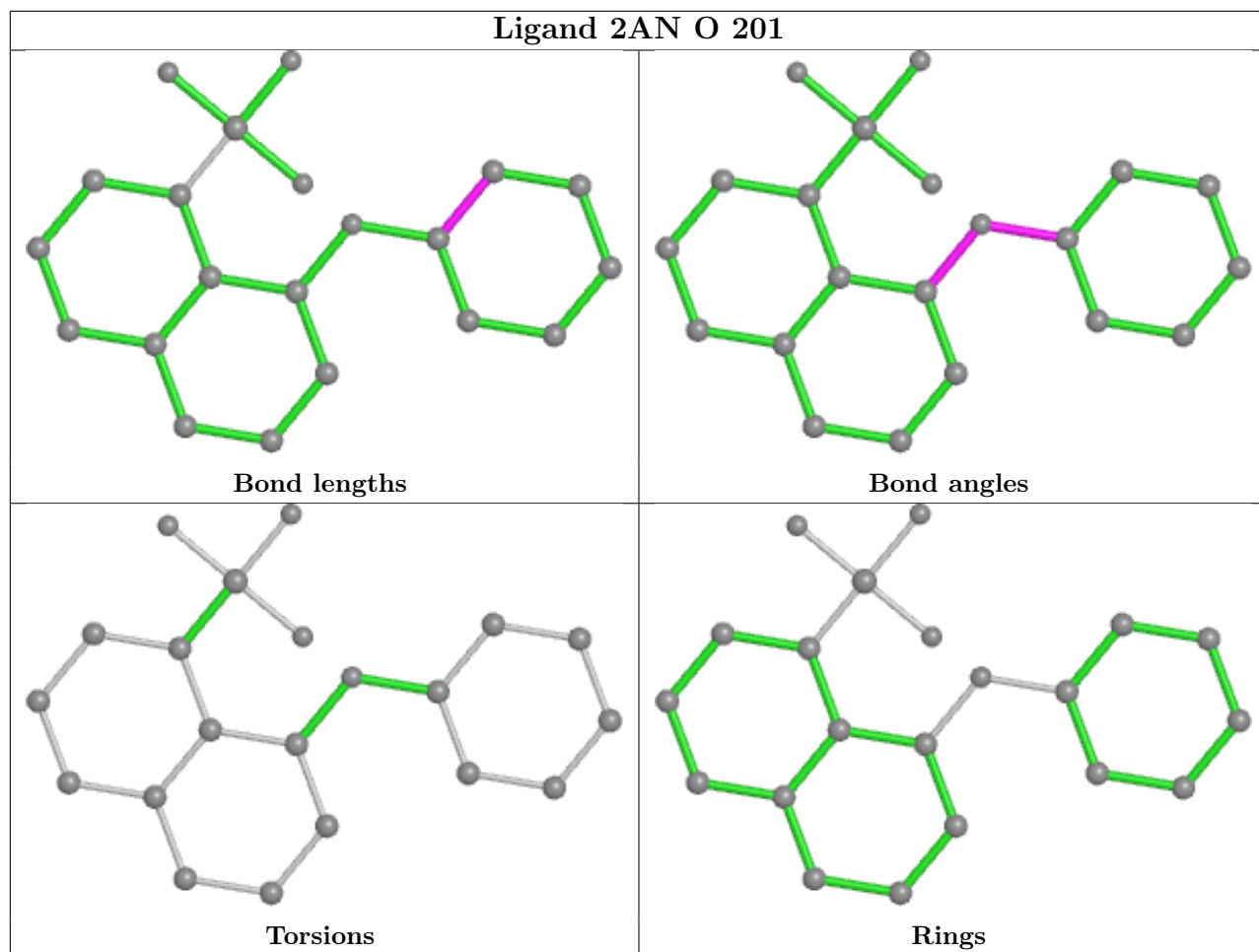


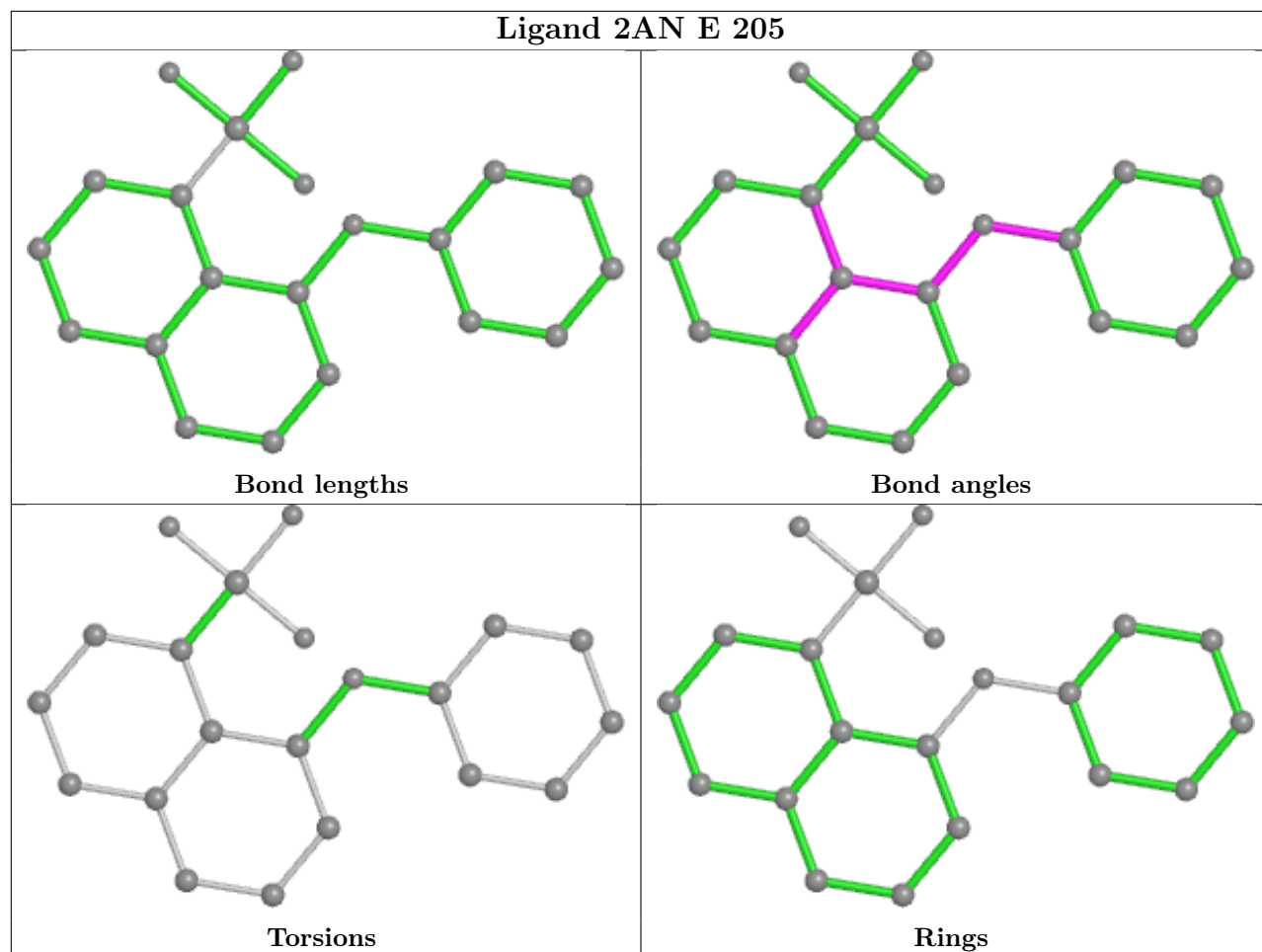


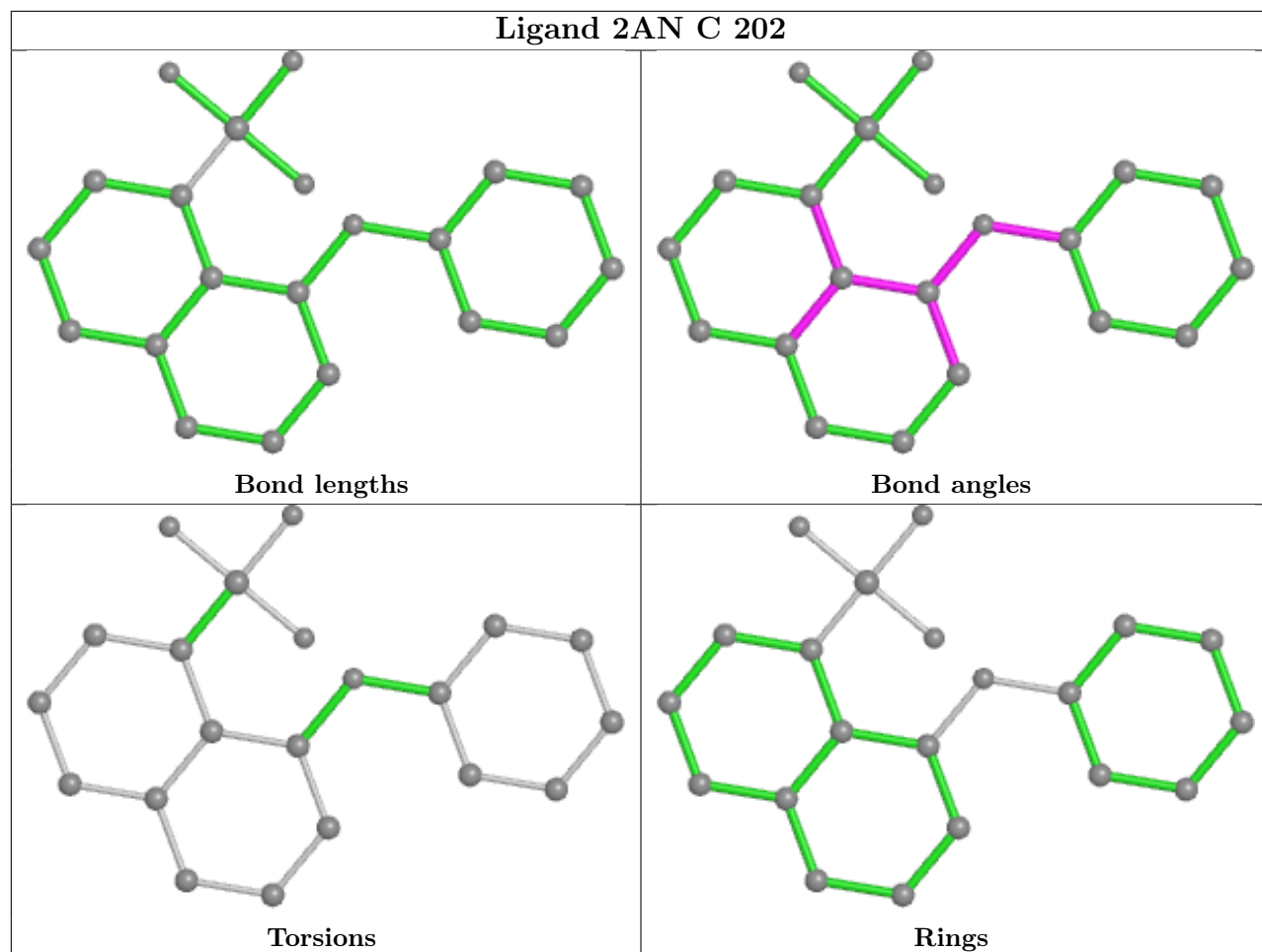


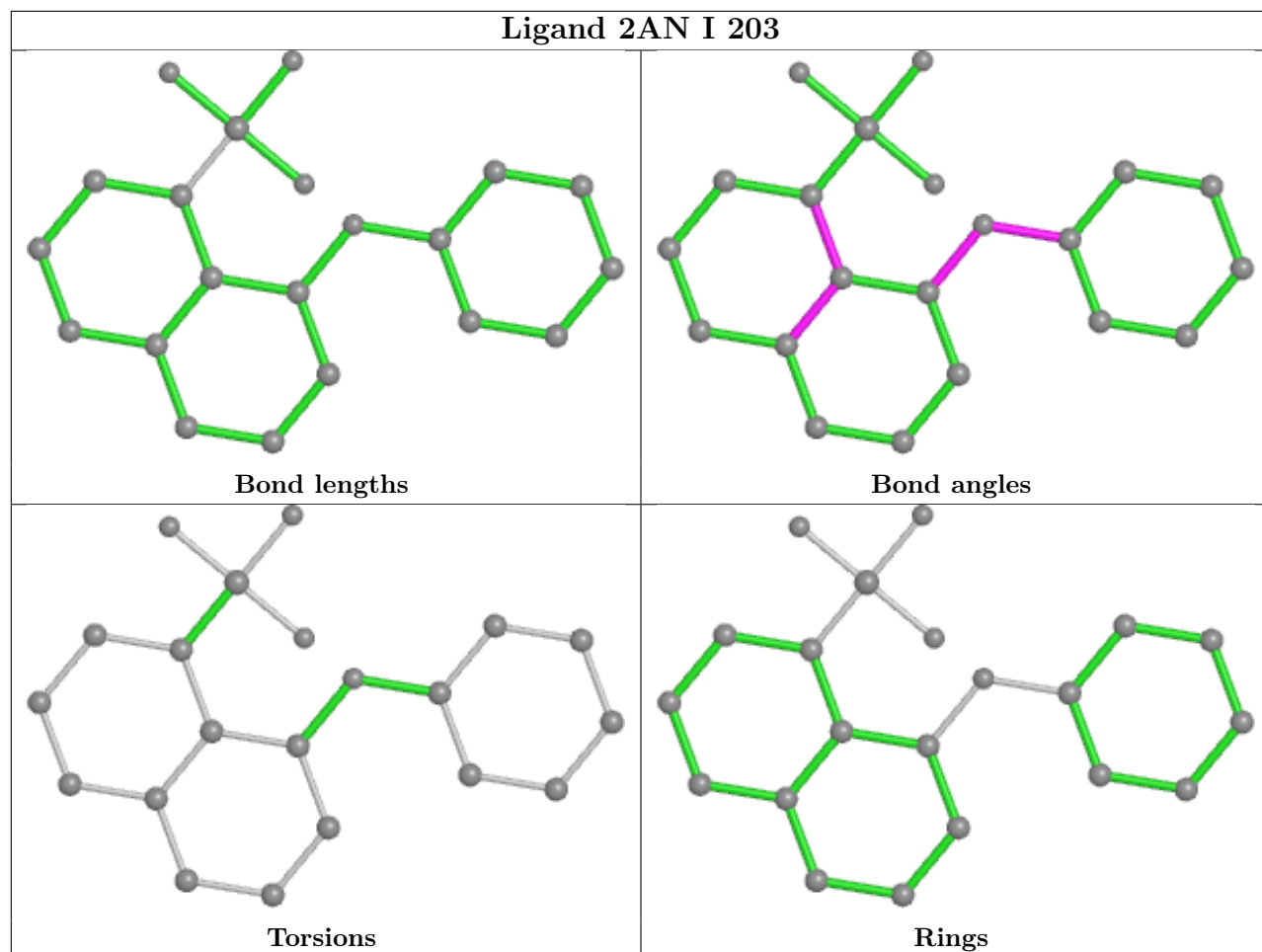


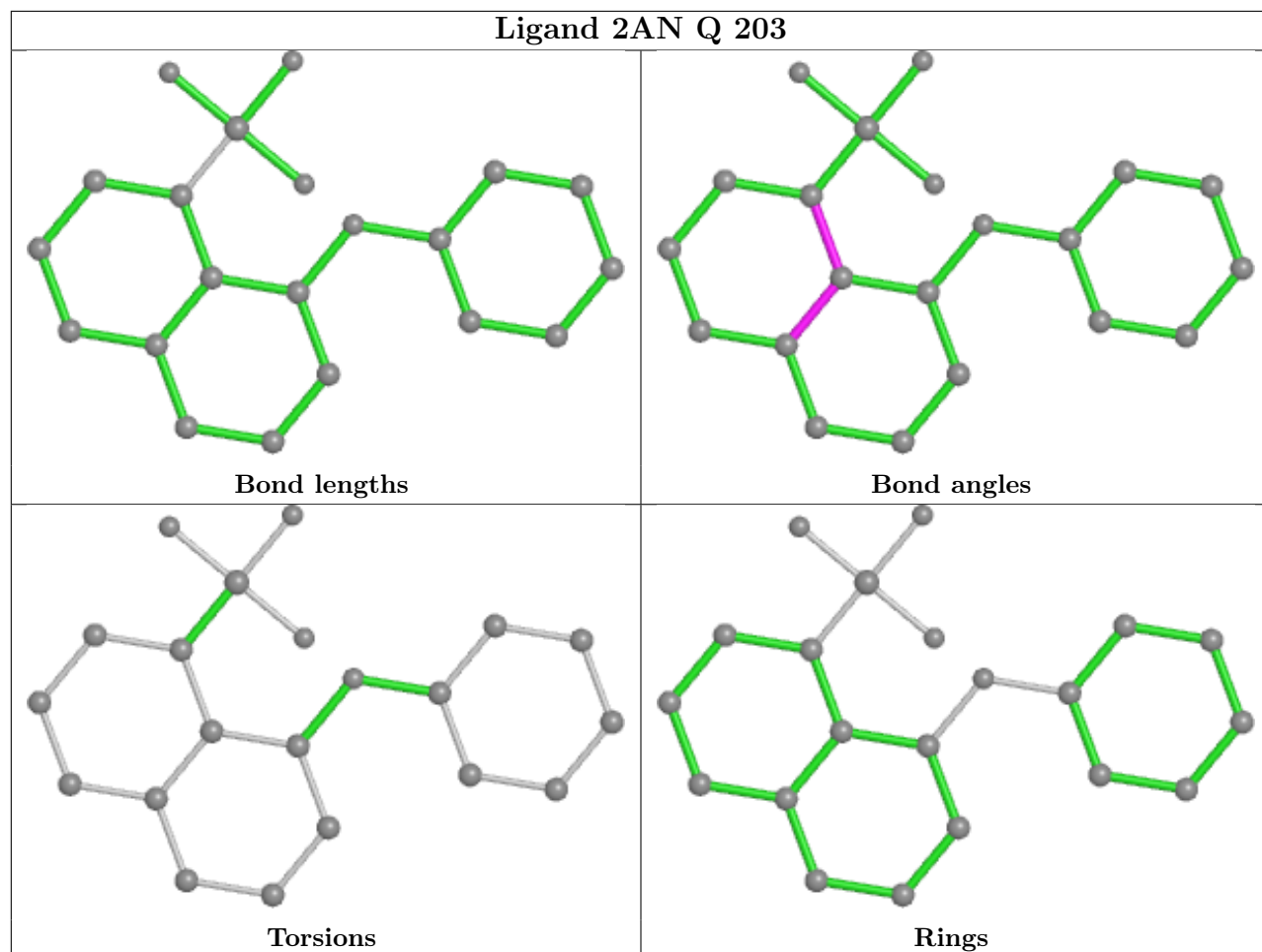


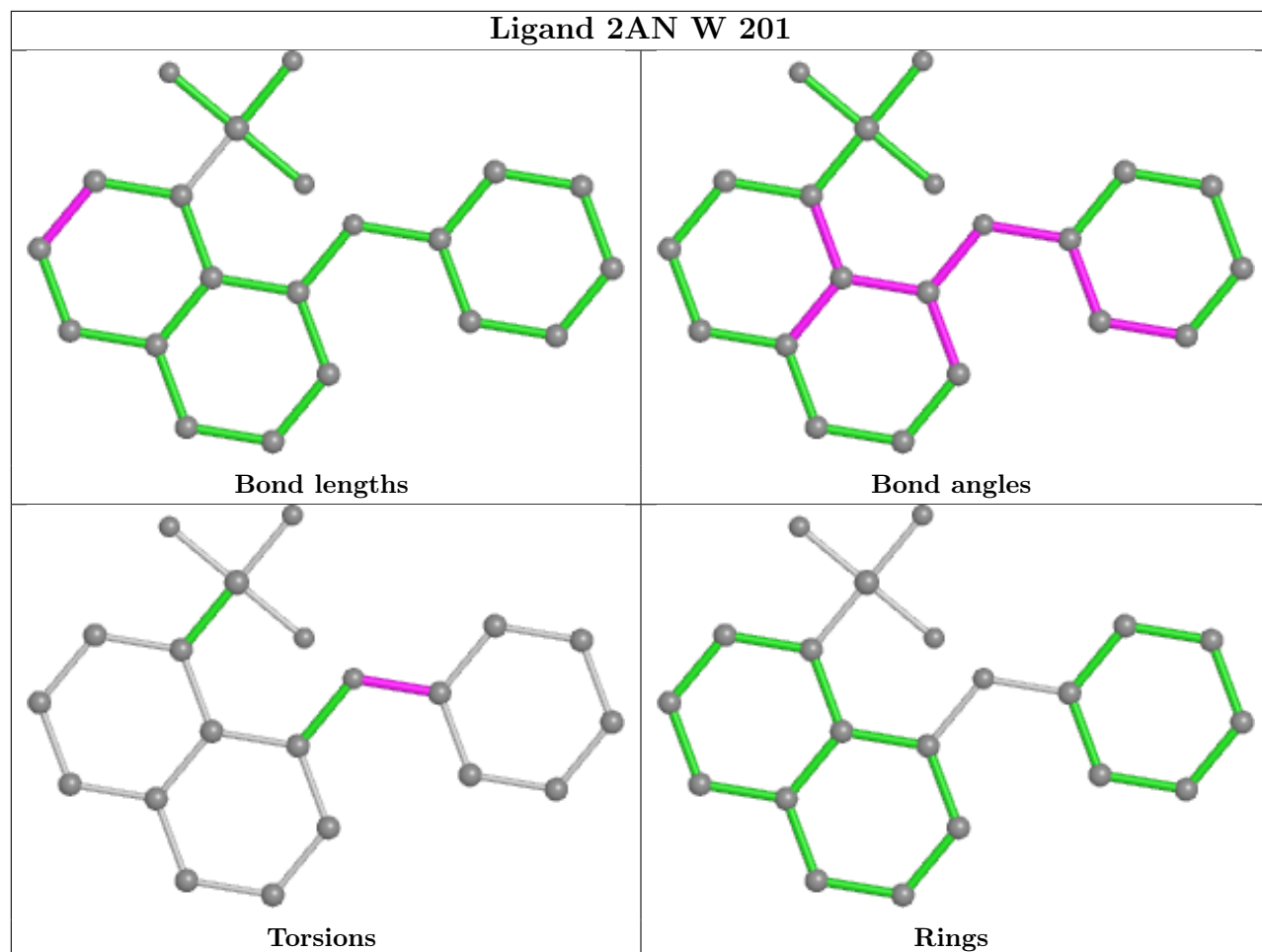


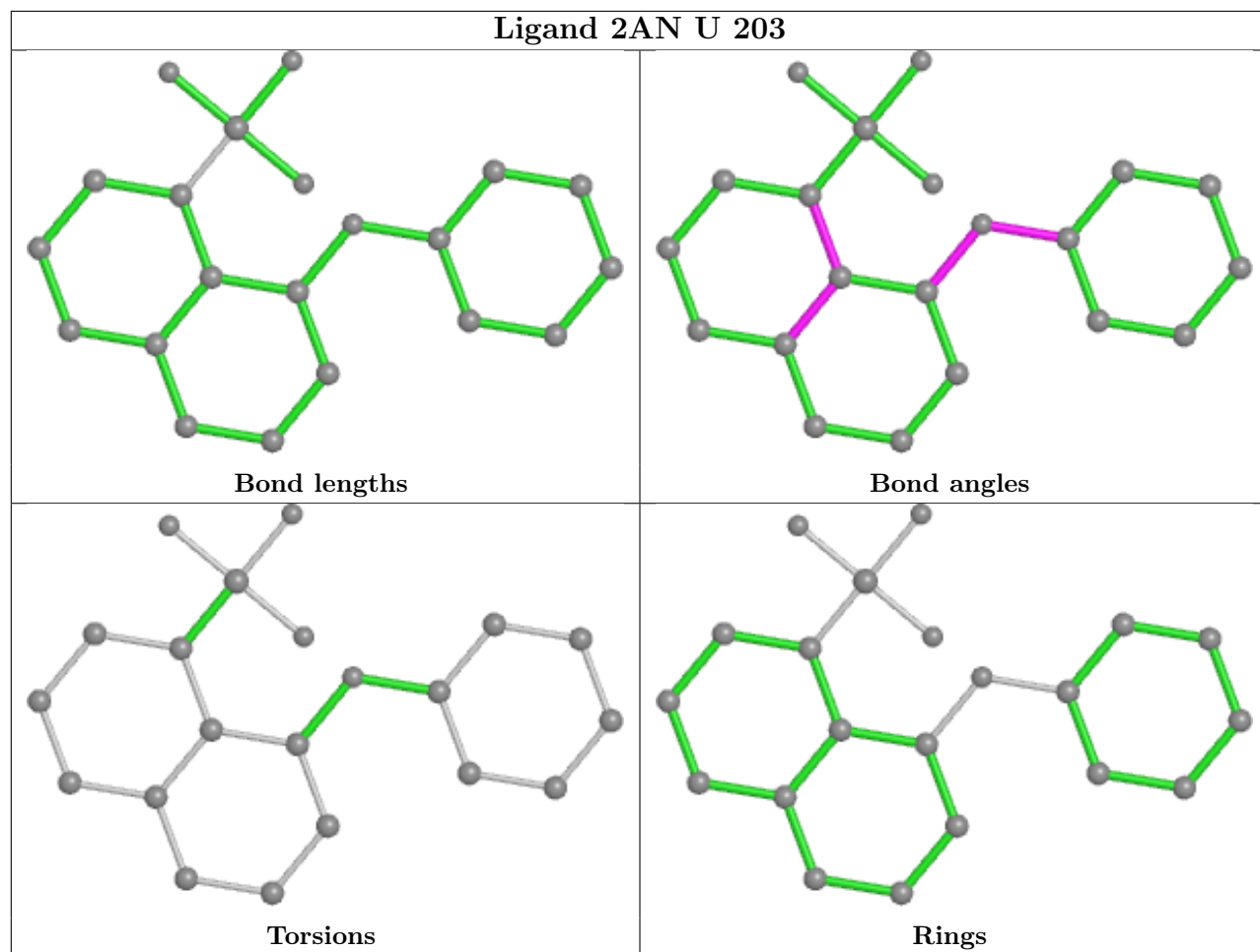


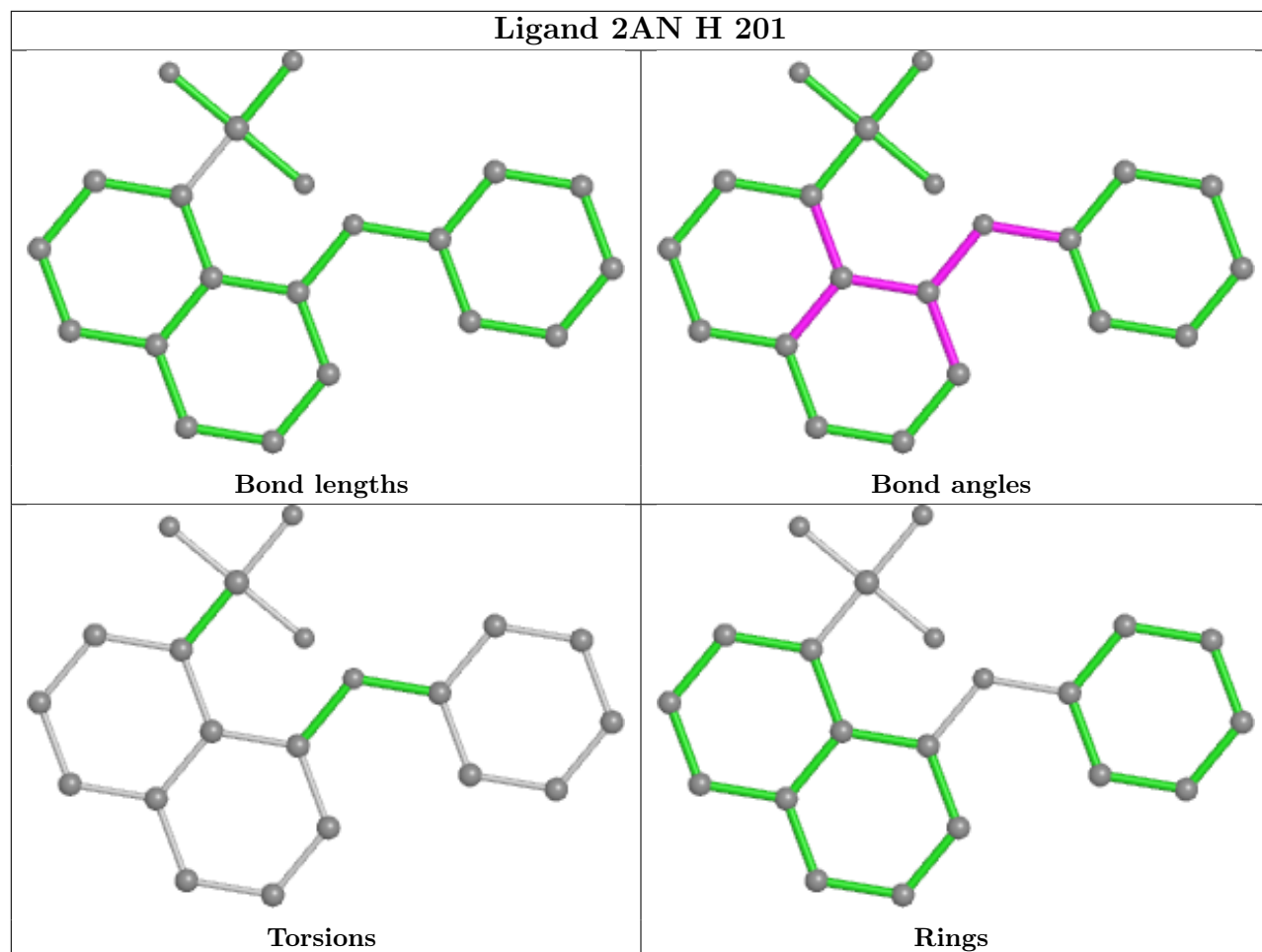




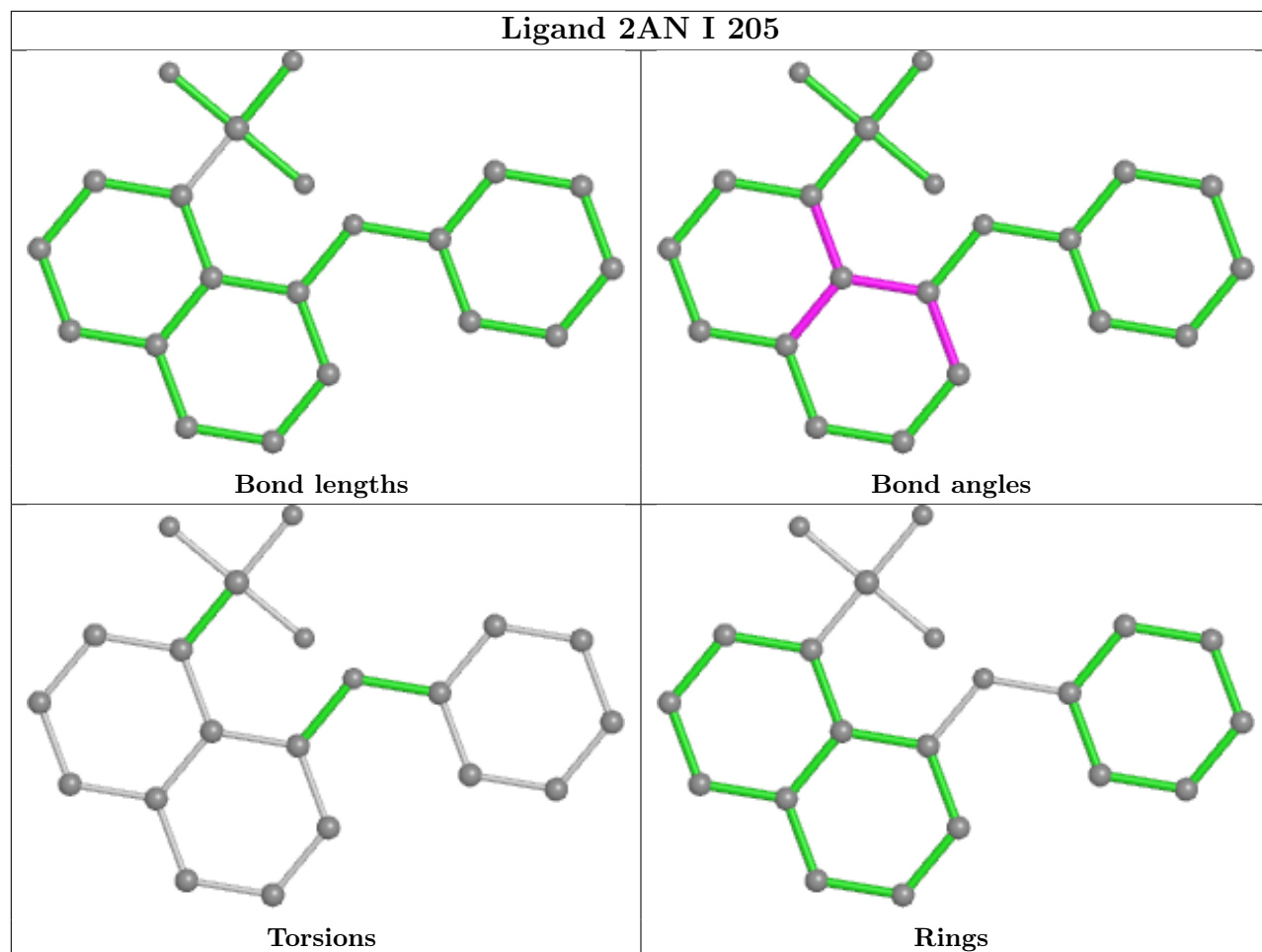


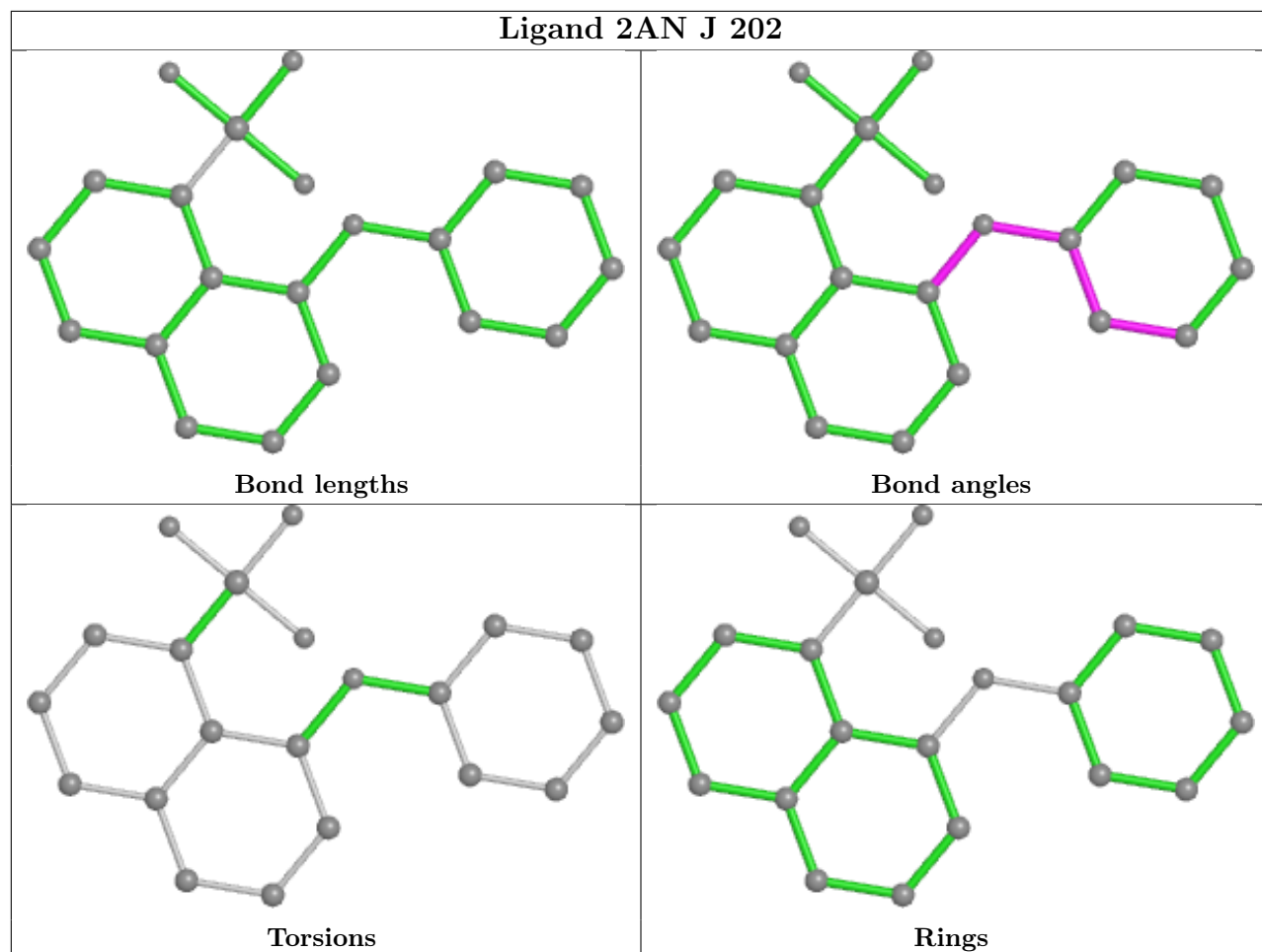


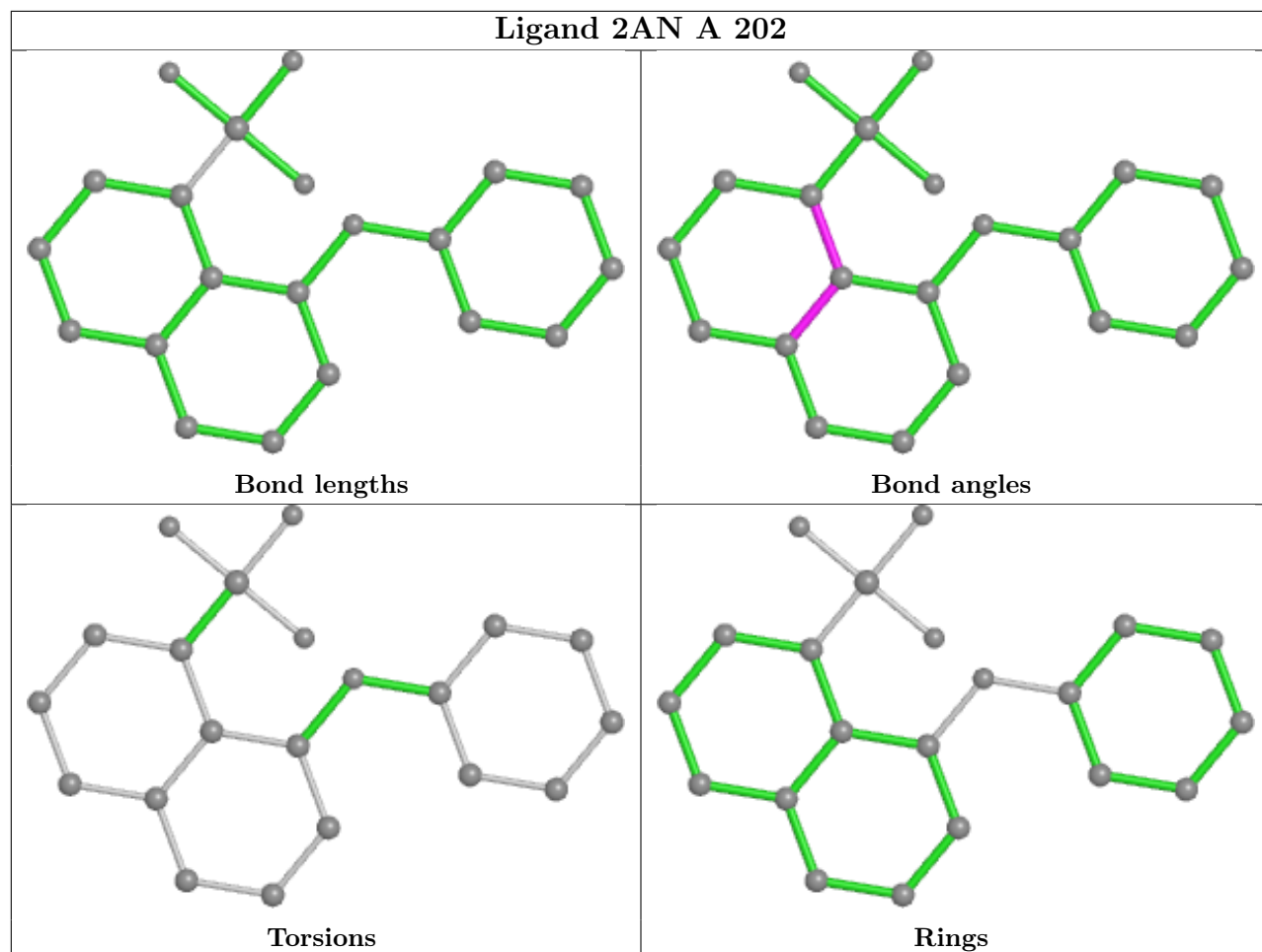


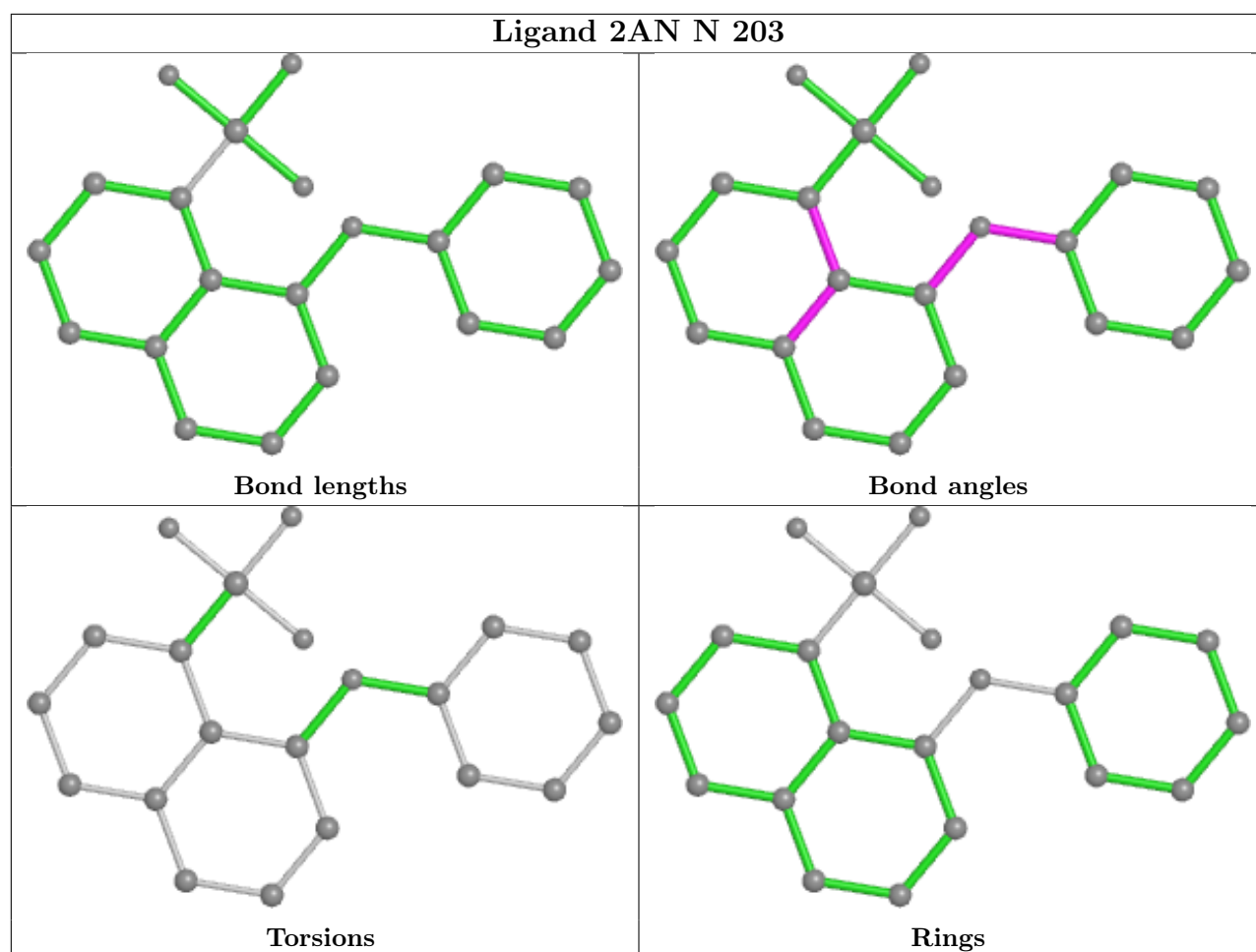












## 5.7 Other polymers [i](#)

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	159/165 (96%)	0.13	7 (4%) 34 32	27, 48, 69, 87	1 (0%)
1	B	159/165 (96%)	0.12	8 (5%) 28 26	25, 46, 77, 108	1 (0%)
1	C	159/165 (96%)	0.19	5 (3%) 49 45	29, 50, 73, 84	0
1	D	159/165 (96%)	0.17	8 (5%) 28 26	29, 50, 83, 123	0
1	E	159/165 (96%)	-0.21	0 100 100	20, 35, 57, 76	2 (1%)
1	F	159/165 (96%)	0.26	6 (3%) 40 37	34, 56, 82, 98	2 (1%)
1	G	159/165 (96%)	-0.03	3 (1%) 66 63	20, 39, 64, 83	3 (1%)
1	H	159/165 (96%)	-0.01	1 (0%) 89 89	24, 45, 65, 77	2 (1%)
1	I	159/165 (96%)	-0.07	1 (0%) 89 89	21, 40, 66, 83	4 (2%)
1	J	159/165 (96%)	-0.06	0 100 100	17, 40, 63, 72	1 (0%)
1	K	159/165 (96%)	0.10	4 (2%) 57 53	34, 48, 71, 77	3 (1%)
1	L	159/165 (96%)	-0.13	2 (1%) 77 75	19, 37, 62, 83	3 (1%)
1	M	159/165 (96%)	0.07	7 (4%) 34 32	25, 46, 79, 91	1 (0%)
1	N	159/165 (96%)	0.17	6 (3%) 40 37	23, 47, 72, 96	3 (1%)
1	O	159/165 (96%)	0.04	6 (3%) 40 37	28, 47, 77, 92	2 (1%)
1	P	159/165 (96%)	0.08	4 (2%) 57 53	29, 46, 70, 83	2 (1%)
1	Q	159/165 (96%)	0.18	5 (3%) 49 45	26, 50, 75, 86	2 (1%)
1	R	159/165 (96%)	-0.02	3 (1%) 66 63	23, 44, 66, 107	2 (1%)
1	S	159/165 (96%)	0.33	7 (4%) 34 32	31, 57, 86, 99	2 (1%)
1	T	159/165 (96%)	0.37	14 (8%) 10 7	36, 54, 88, 115	1 (0%)
1	U	159/165 (96%)	-0.17	2 (1%) 77 75	17, 37, 55, 103	3 (1%)
1	V	159/165 (96%)	0.46	8 (5%) 28 26	35, 61, 86, 102	0
1	W	159/165 (96%)	0.04	3 (1%) 66 63	23, 40, 67, 74	2 (1%)
1	X	159/165 (96%)	-0.02	1 (0%) 89 89	25, 44, 67, 80	2 (1%)

*Continued on next page...*

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	Y	159/165 (96%)	-0.18	1 (0%) 89 89	20, 39, 58, 78	3 (1%)
1	Z	159/165 (96%)	-0.03	2 (1%) 77 75	27, 44, 63, 77	2 (1%)
1	a	159/165 (96%)	-0.08	2 (1%) 77 75	28, 43, 65, 76	3 (1%)
1	b	159/165 (96%)	-0.16	2 (1%) 77 75	20, 38, 59, 69	2 (1%)
All	All	4452/4620 (96%)	0.05	118 (2%) 54 50	17, 45, 74, 123	54 (1%)

The worst 5 of 118 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	127	THR	6.7
1	T	126	CYS	6.5
1	V	112	SER	6.3
1	A	127	THR	6.2
1	S	62	GLY	6.2

## 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	Z	202	21/21	0.82	0.29	21,29,35,38	21
2	2AN	W	204	21/21	0.84	0.21	41,53,68,75	0
2	2AN	G	205	21/21	0.85	0.23	52,66,74,85	0
2	2AN	N	203	21/21	0.86	0.20	41,48,58,62	0
2	2AN	R	203	21/21	0.86	0.30	21,26,39,41	21
2	2AN	R	201	21/21	0.87	0.22	35,45,68,70	0
2	2AN	G	204	21/21	0.87	0.24	22,32,42,45	0

Continued on next page...

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	2AN	W	203	21/21	0.88	0.32	16,21,29,33	21
2	2AN	E	204	21/21	0.88	0.19	35,46,58,73	0
2	2AN	Q	203	21/21	0.88	0.21	70,81,96,100	0
2	2AN	I	201	21/21	0.89	0.18	21,28,35,42	0
2	2AN	I	204	21/21	0.89	0.19	42,57,68,81	0
2	2AN	X	202	21/21	0.89	0.23	27,32,37,44	21
2	2AN	E	202	21/21	0.89	0.16	23,31,39,53	0
2	2AN	D	203	21/21	0.90	0.21	40,48,58,62	0
2	2AN	Y	203	21/21	0.90	0.16	32,38,47,48	0
2	2AN	I	205	21/21	0.90	0.18	46,60,65,70	0
2	2AN	b	201	21/21	0.90	0.20	34,44,49,52	0
2	2AN	F	201	21/21	0.91	0.17	31,37,47,56	0
2	2AN	C	201	21/21	0.91	0.20	28,39,47,61	0
2	2AN	L	204	21/21	0.91	0.18	31,40,46,52	0
2	2AN	N	201	21/21	0.91	0.22	24,29,34,37	0
2	2AN	U	202	21/21	0.91	0.25	24,31,42,48	0
2	2AN	W	201	21/21	0.91	0.24	35,44,54,63	0
2	2AN	b	203	21/21	0.91	0.19	29,43,52,55	0
2	2AN	K	203	21/21	0.92	0.16	33,42,66,74	0
2	2AN	N	204	21/21	0.92	0.20	25,32,44,52	0
2	2AN	P	202	21/21	0.92	0.15	40,51,66,71	0
2	2AN	C	203	21/21	0.92	0.19	41,51,70,81	0
2	2AN	M	202	21/21	0.92	0.18	26,30,37,43	0
2	2AN	M	203	21/21	0.92	0.20	42,53,70,74	0
2	2AN	a	201	21/21	0.92	0.17	25,36,46,49	0
2	2AN	S	201	21/21	0.92	0.22	27,33,38,52	0
2	2AN	J	201	21/21	0.92	0.23	20,23,29,33	21
2	2AN	O	201	21/21	0.93	0.17	28,35,40,43	0
2	2AN	L	205	21/21	0.93	0.20	37,44,50,54	0
2	2AN	A	203	21/21	0.93	0.18	31,43,46,54	0
2	2AN	E	203	21/21	0.93	0.21	23,32,48,61	0
2	2AN	Y	202	21/21	0.93	0.17	27,32,35,38	0
2	2AN	K	202	21/21	0.93	0.14	43,46,53,59	0
2	2AN	Y	204	21/21	0.93	0.16	30,47,51,57	0
2	2AN	R	204	21/21	0.93	0.21	30,39,58,61	0
2	2AN	B	204	21/21	0.93	0.16	29,40,59,67	0
2	2AN	B	205	21/21	0.93	0.16	39,54,64,68	0
2	2AN	U	205	21/21	0.93	0.15	37,47,60,78	0
3	EPE	C	205	15/15	0.93	0.18	29,34,52,57	0
2	2AN	B	202	21/21	0.94	0.13	28,34,53,63	0
2	2AN	X	201	21/21	0.94	0.30	37,41,48,50	0
2	2AN	E	201	21/21	0.94	0.18	15,21,28,38	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	2AN	X	203	21/21	0.94	0.22	22,31,53,61	0
2	2AN	H	201	21/21	0.94	0.19	26,31,43,45	0
2	2AN	Q	202	21/21	0.94	0.15	35,50,64,68	0
2	2AN	U	203	21/21	0.94	0.14	24,38,46,50	0
2	2AN	C	204	21/21	0.94	0.17	33,39,48,56	0
2	2AN	Z	203	21/21	0.94	0.17	35,43,56,64	0
2	2AN	V	201	21/21	0.94	0.13	44,51,56,61	0
2	2AN	V	202	21/21	0.94	0.17	34,46,79,82	0
2	2AN	b	202	21/21	0.94	0.20	19,23,34,40	0
2	2AN	G	203	21/21	0.94	0.22	25,34,56,60	0
2	2AN	R	202	21/21	0.94	0.19	21,29,48,53	0
3	EPE	Z	204	15/15	0.94	0.19	36,44,54,54	0
2	2AN	U	201	21/21	0.95	0.14	28,34,43,47	0
2	2AN	Y	201	21/21	0.95	0.17	22,24,30,36	0
2	2AN	A	201	21/21	0.95	0.18	25,34,46,71	0
2	2AN	P	201	21/21	0.95	0.19	25,30,38,41	21
2	2AN	U	204	21/21	0.95	0.15	24,26,34,45	0
2	2AN	Z	201	21/21	0.95	0.20	26,36,46,48	0
2	2AN	L	202	21/21	0.95	0.14	23,28,32,33	0
2	2AN	I	202	21/21	0.95	0.16	19,23,30,38	0
2	2AN	A	202	21/21	0.95	0.17	23,35,40,41	0
2	2AN	D	202	21/21	0.95	0.16	32,39,44,48	0
2	2AN	B	203	21/21	0.95	0.15	38,44,50,56	0
2	2AN	J	202	21/21	0.95	0.19	22,27,39,44	0
2	2AN	K	201	21/21	0.95	0.17	28,33,36,42	0
2	2AN	E	205	21/21	0.95	0.20	31,42,54,63	0
2	2AN	B	201	21/21	0.96	0.15	27,34,44,47	0
2	2AN	I	203	21/21	0.96	0.17	23,32,55,59	0
2	2AN	L	201	21/21	0.96	0.15	19,26,30,37	0
2	2AN	W	202	21/21	0.96	0.13	24,30,35,40	0
2	2AN	A	204	21/21	0.96	0.15	35,43,51,54	0
2	2AN	O	202	21/21	0.96	0.18	23,28,33,37	0
2	2AN	G	201	21/21	0.96	0.16	15,23,26,34	0
2	2AN	H	202	21/21	0.96	0.17	25,36,40,43	0
2	2AN	Q	201	21/21	0.96	0.16	30,37,45,51	0
2	2AN	H	203	21/21	0.96	0.16	22,28,34,38	0
2	2AN	D	201	21/21	0.96	0.18	37,45,53,56	0
4	SO4	X	204	5/5	0.96	0.10	39,42,44,49	0
2	2AN	M	201	21/21	0.97	0.17	30,35,38,45	0
2	2AN	N	202	21/21	0.97	0.13	25,30,46,54	0
2	2AN	G	202	21/21	0.97	0.15	18,27,34,41	0
4	SO4	V	203	5/5	0.97	0.14	35,48,55,57	0

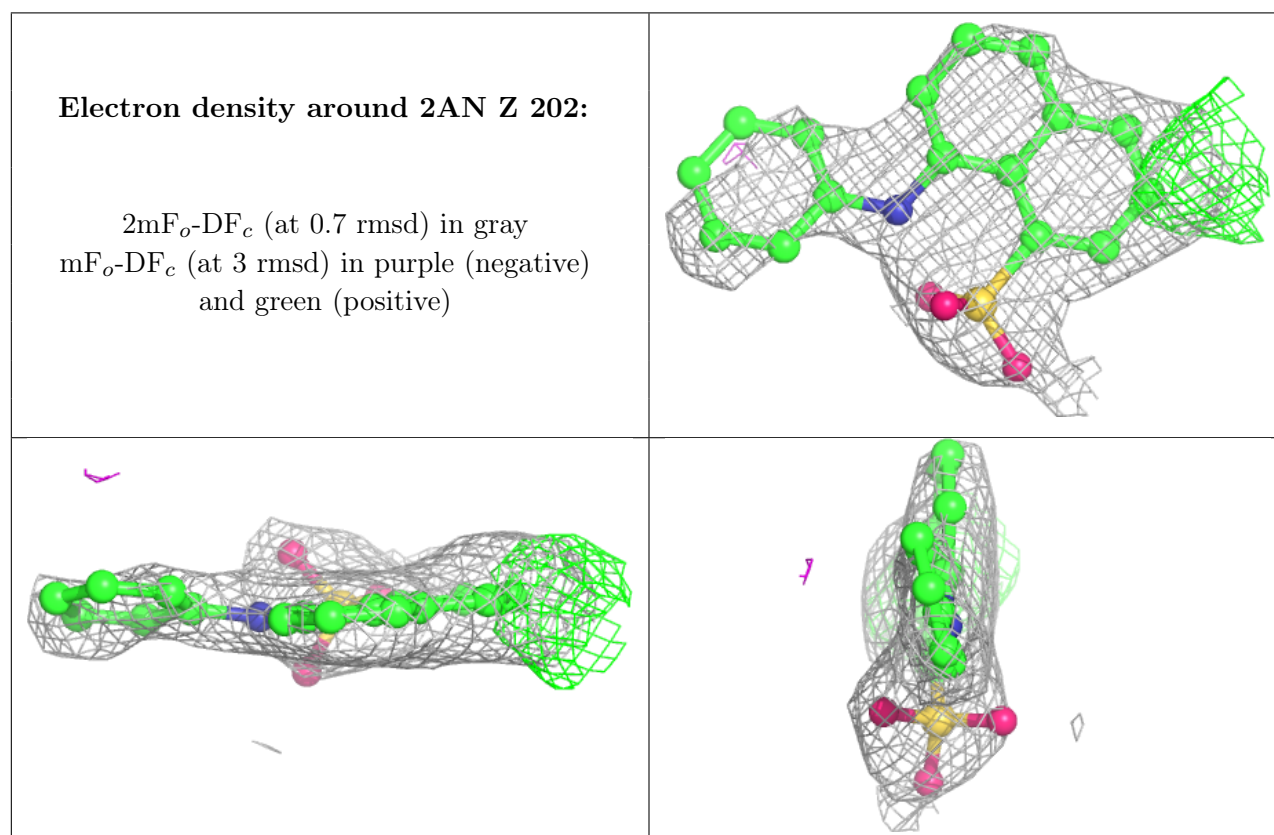
*Continued on next page...*



Continued from previous page...

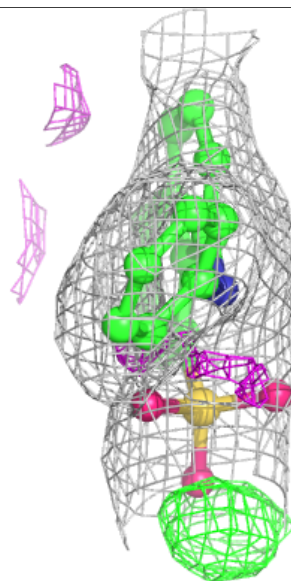
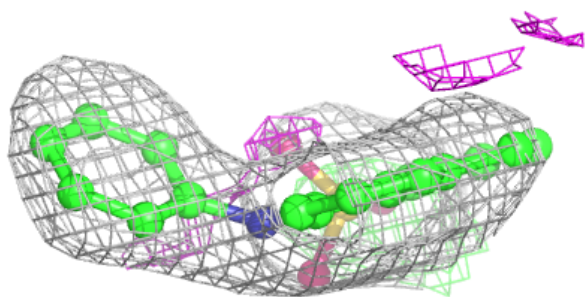
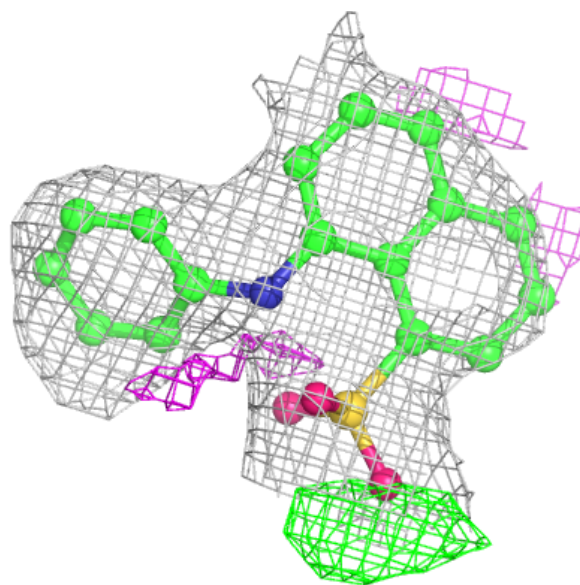
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	2AN	L	203	21/21	0.97	0.14	18,31,40,48	0
4	SO4	b	204	5/5	0.97	0.10	32,36,40,41	0
2	2AN	C	202	21/21	0.98	0.15	24,39,49,53	0

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.



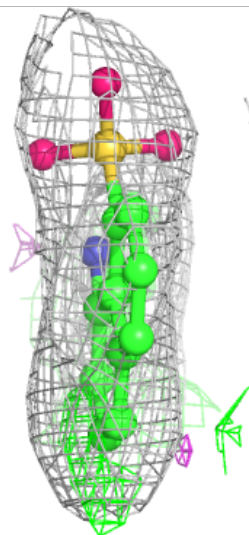
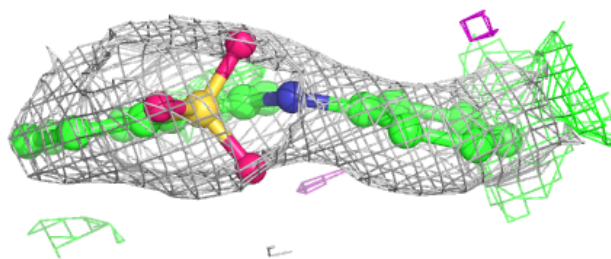
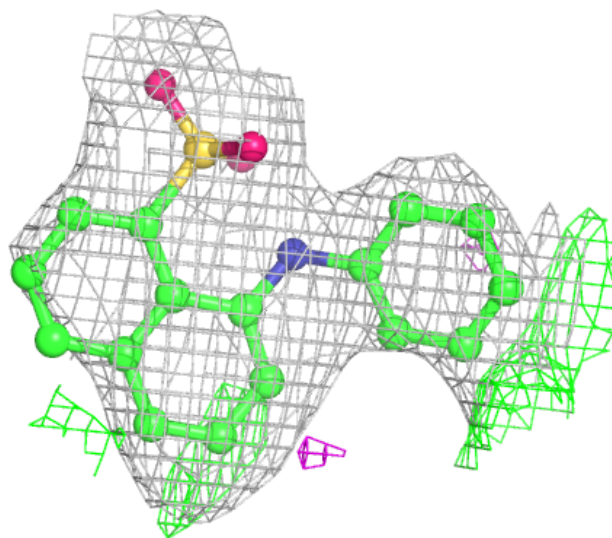
**Electron density around 2AN W 204:**

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



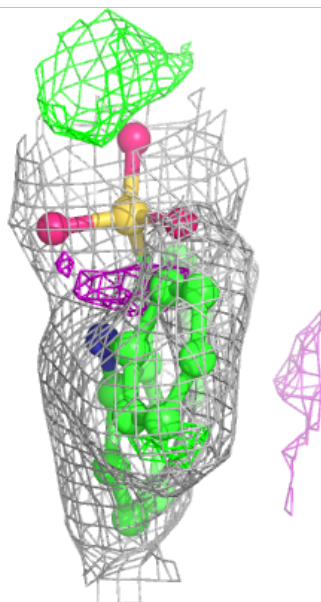
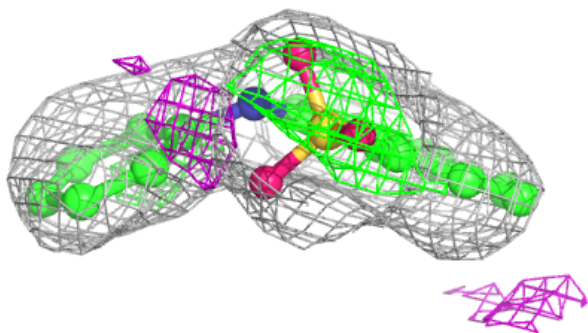
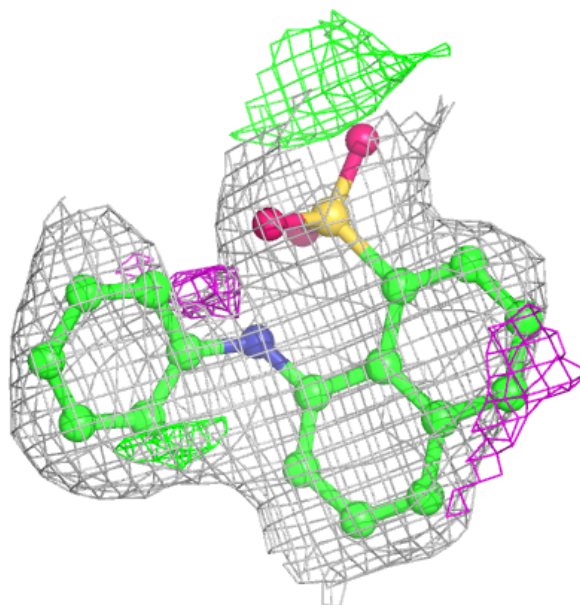
**Electron density around 2AN G 205:**

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



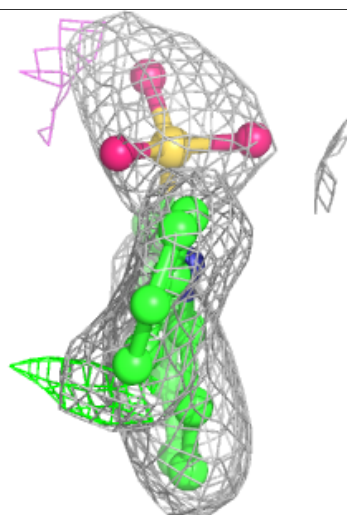
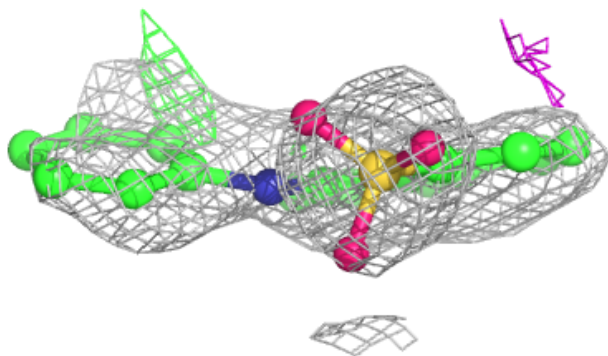
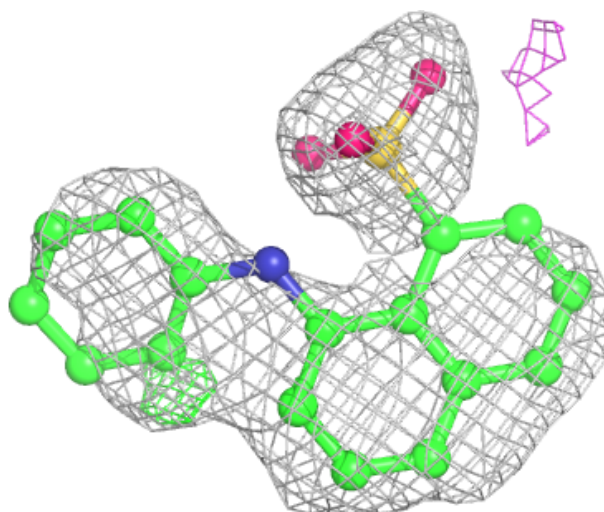
**Electron density around 2AN N 203:**

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



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

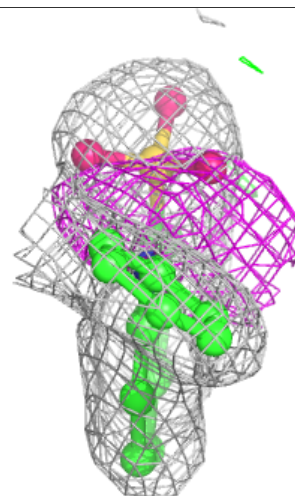
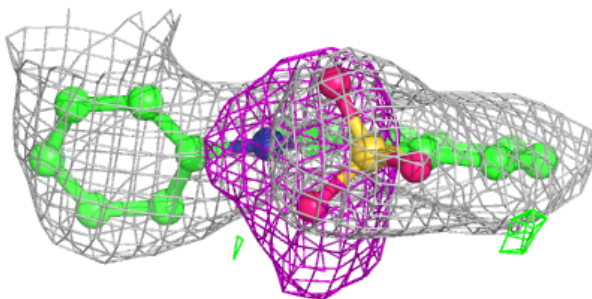
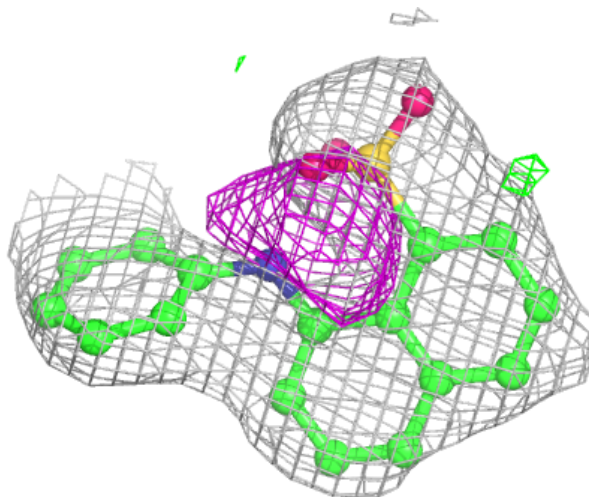
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





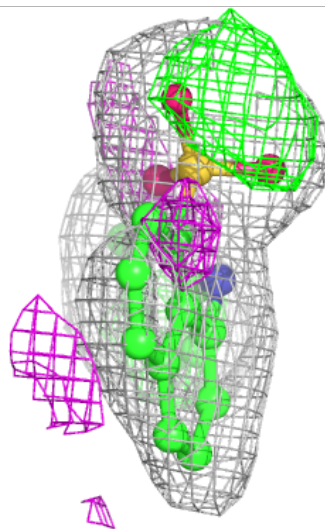
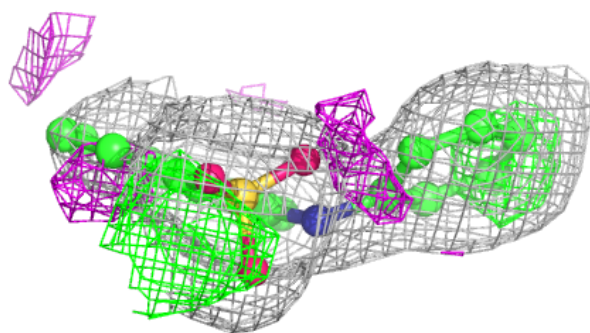
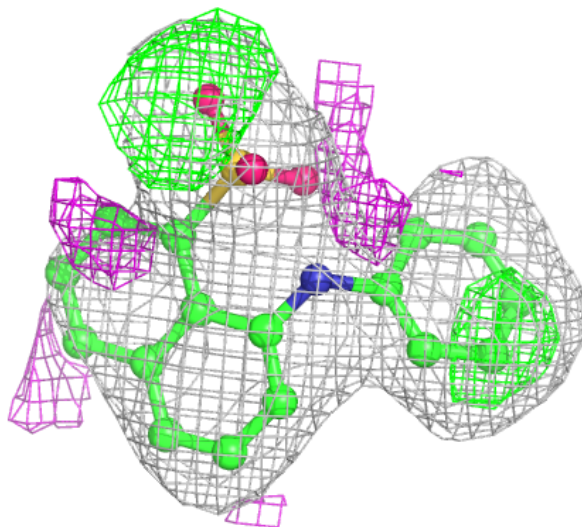
**Electron density around 2AN R 201:**

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



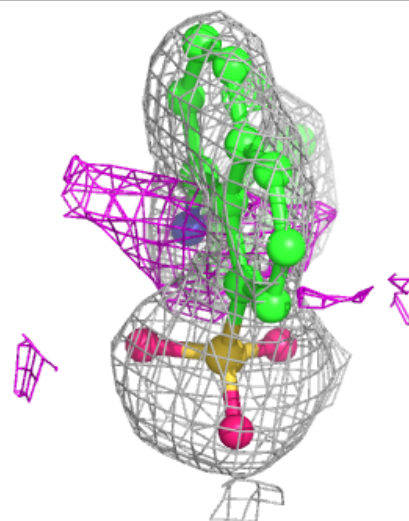
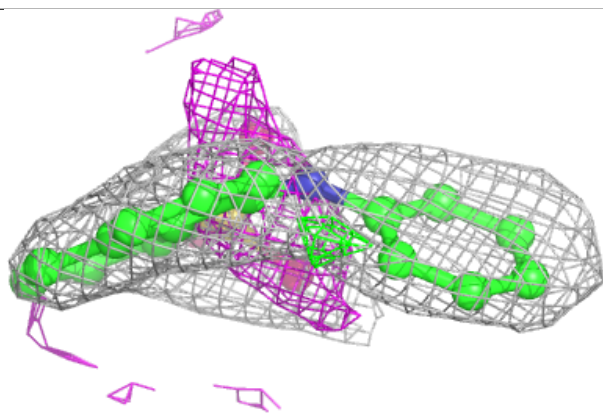
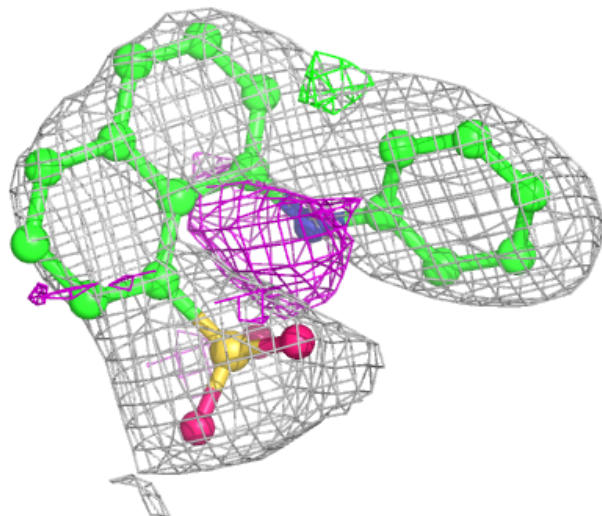
**Electron density around 2AN G 204:**

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



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

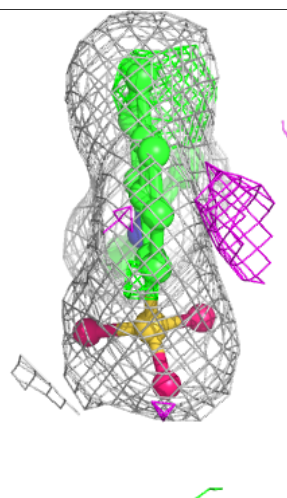
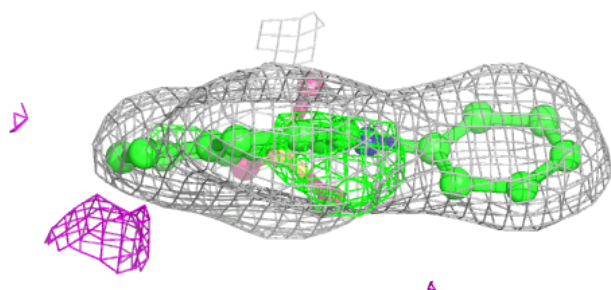
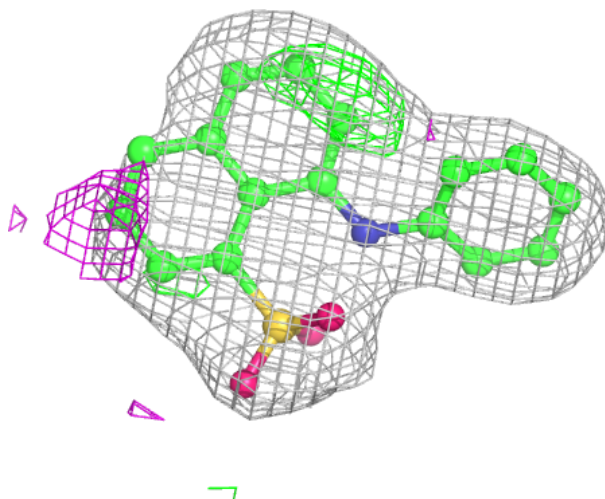
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





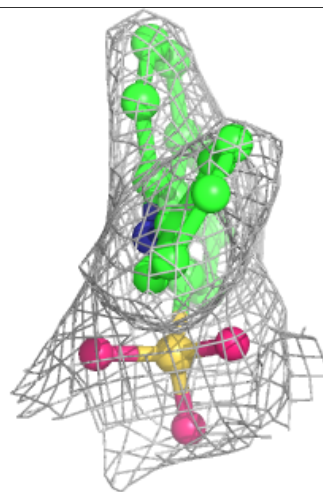
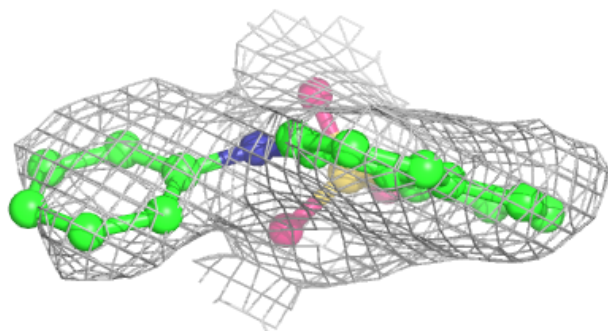
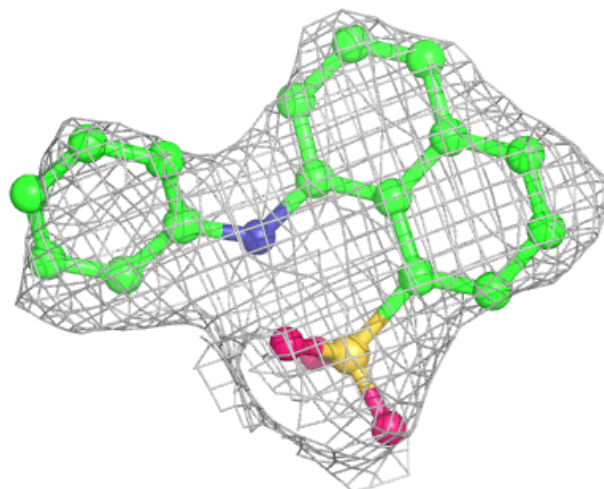
**Electron density around 2AN E 204:**

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



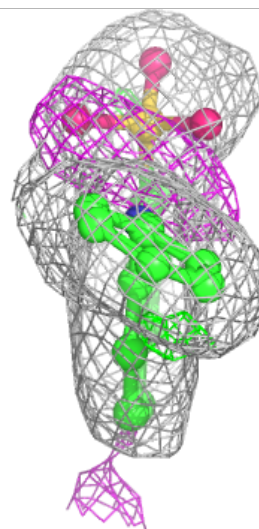
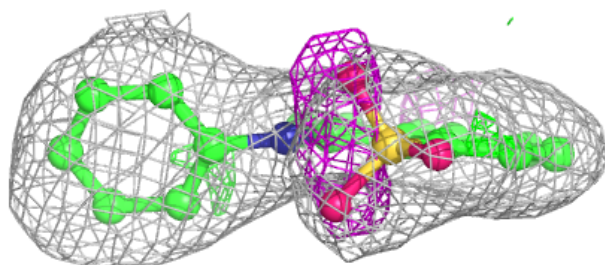
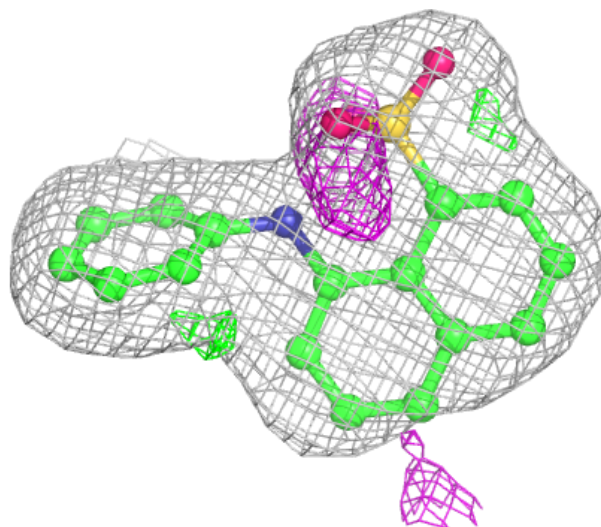
**Electron density around 2AN Q 203:**

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



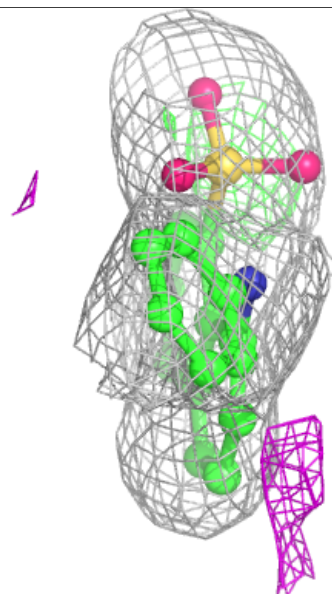
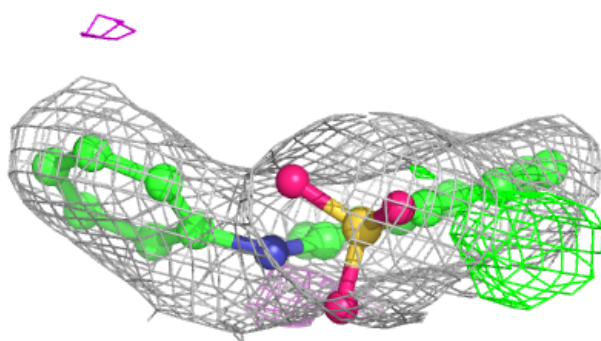
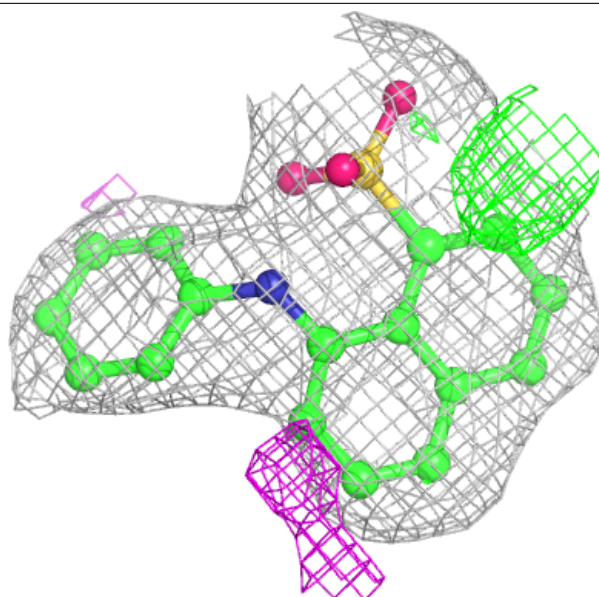
**Electron density around 2AN I 201:**

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



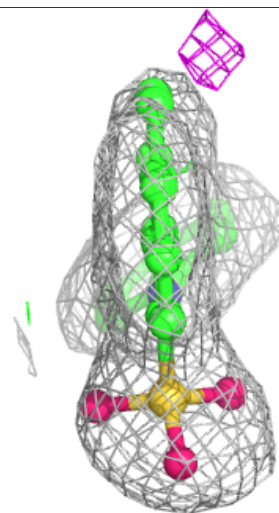
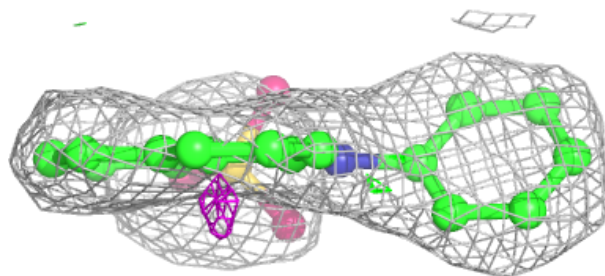
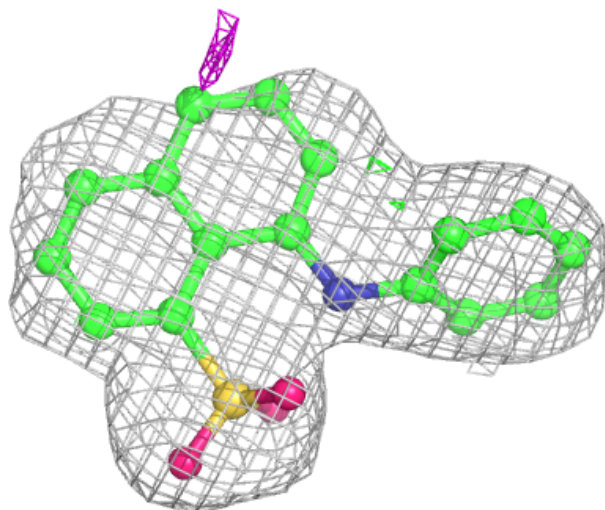
**Electron density around 2AN I 204:**

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



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

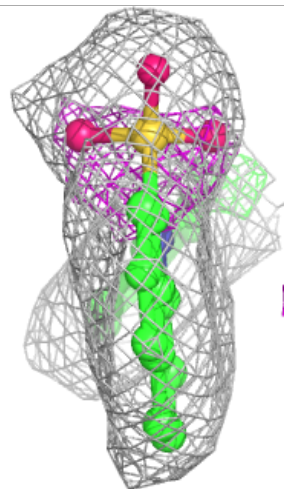
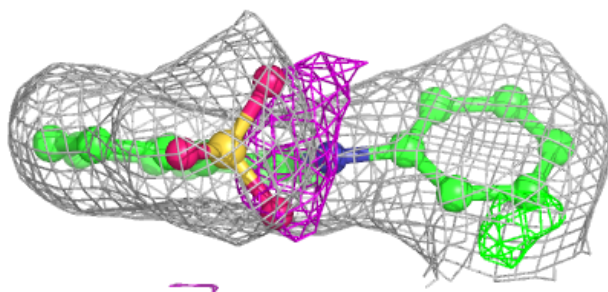
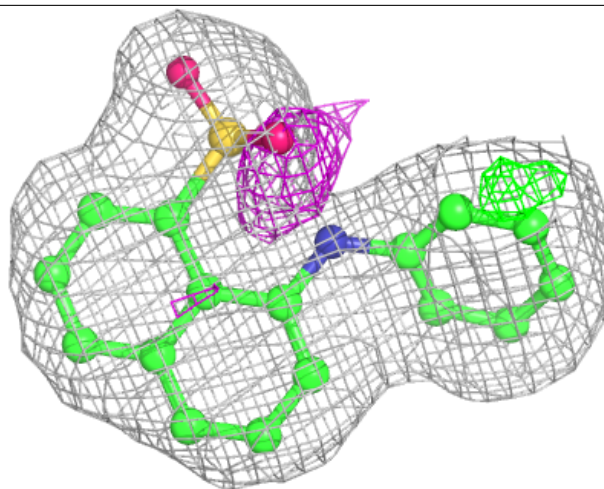
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





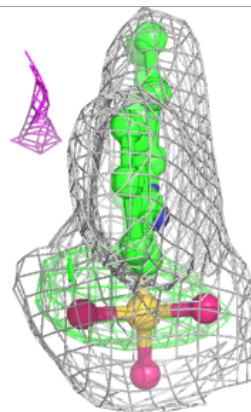
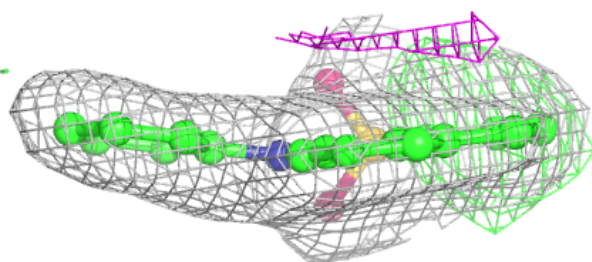
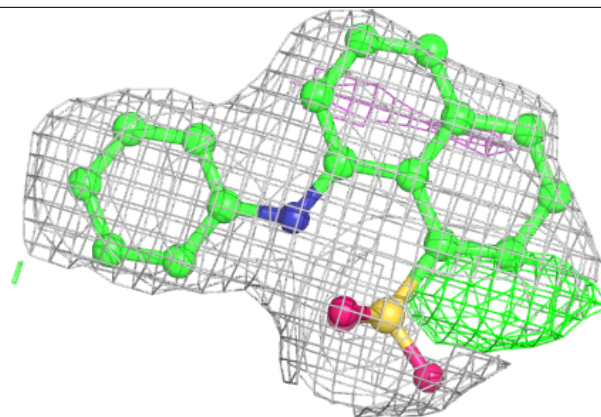
**Electron density around 2AN E 202:**

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

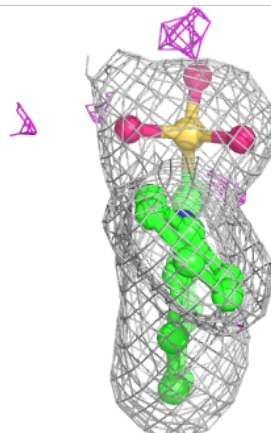
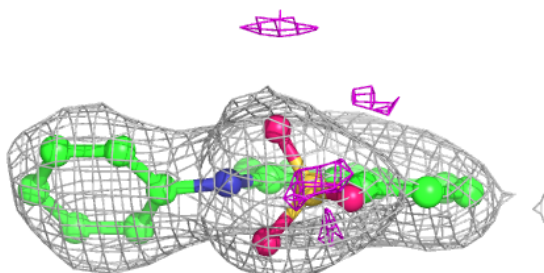
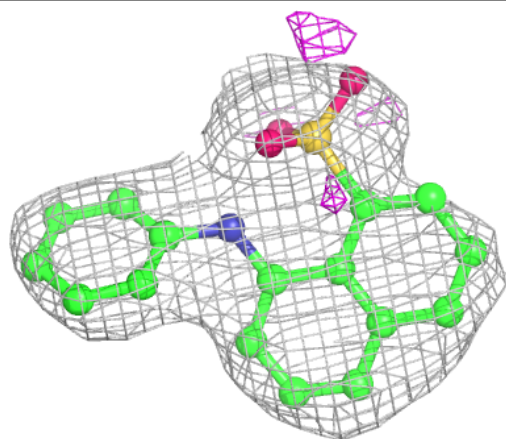


**Electron density around 2AN D 203:**

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

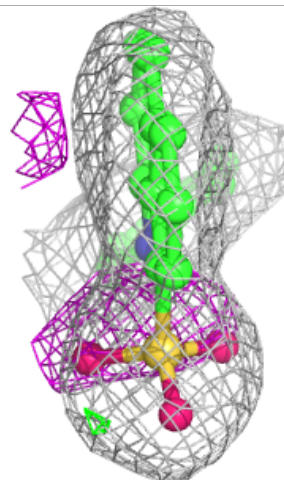
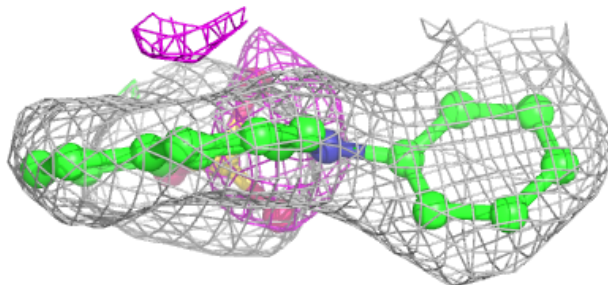
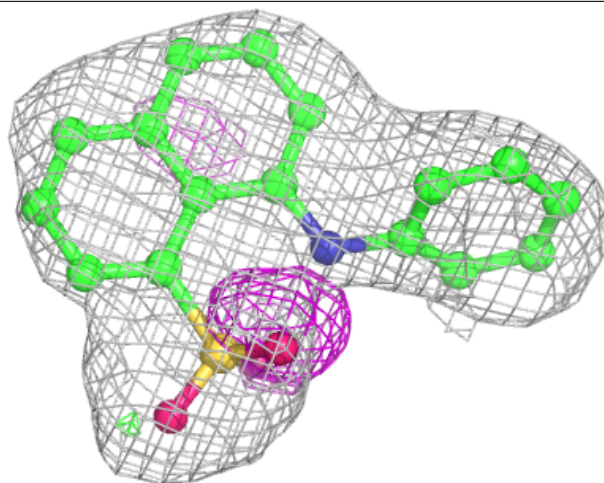
**Electron density around 2AN I 205:**

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



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

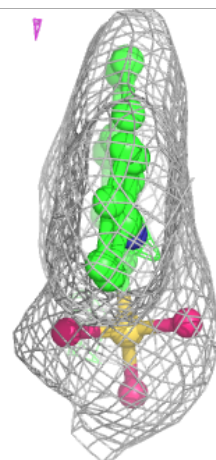
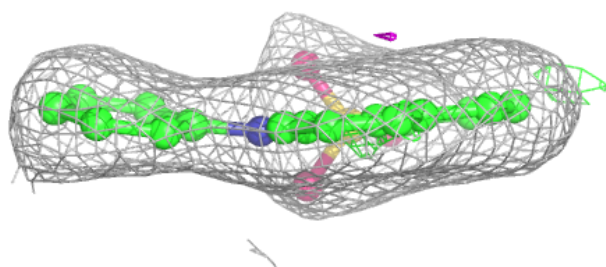
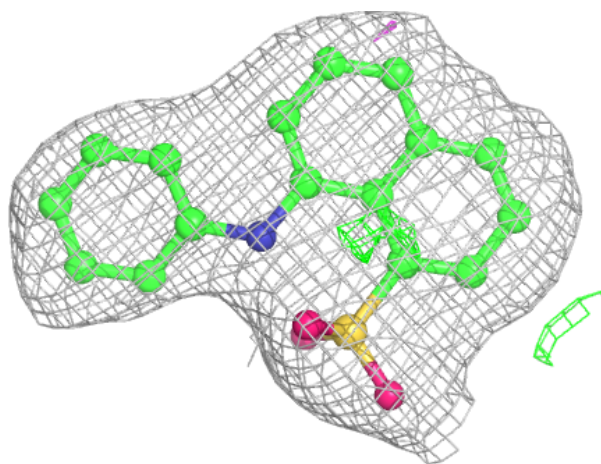
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





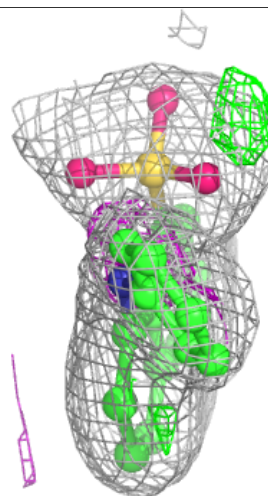
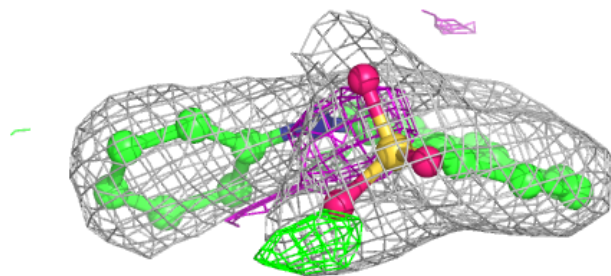
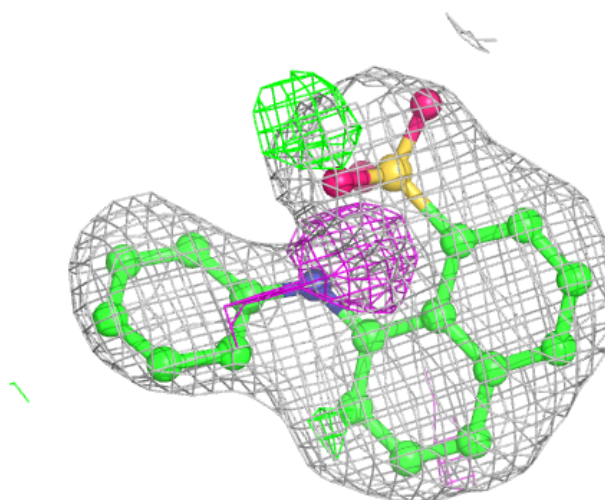
**Electron density around 2AN F 201:**

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



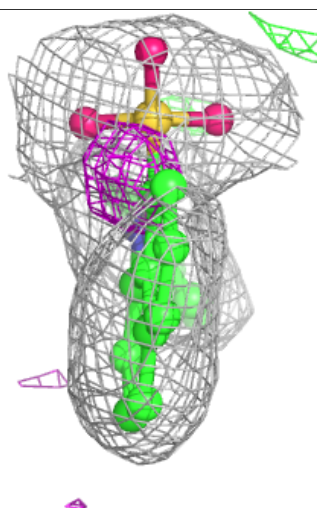
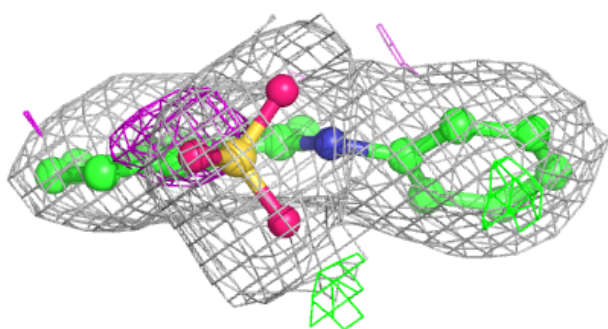
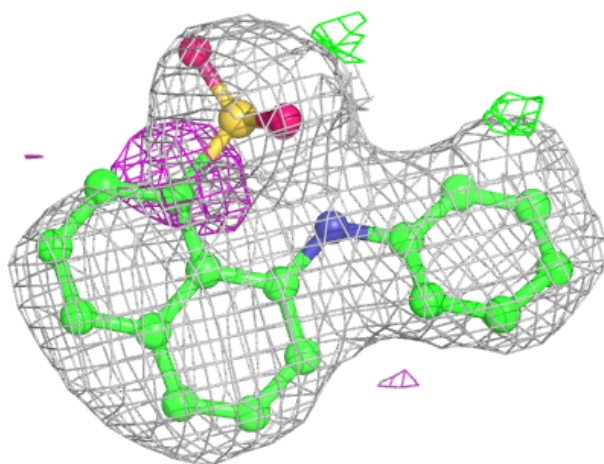
**Electron density around 2AN C 201:**

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



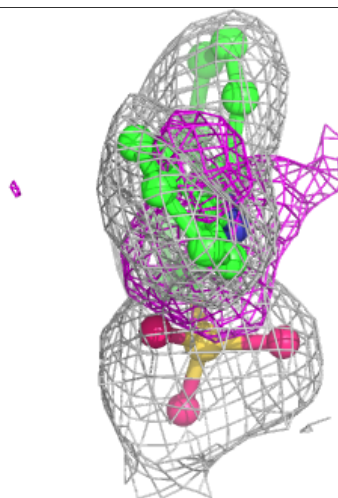
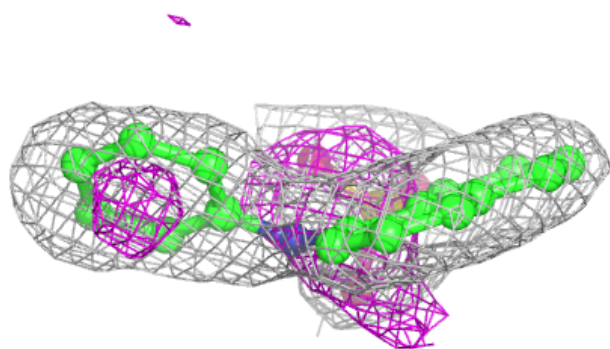
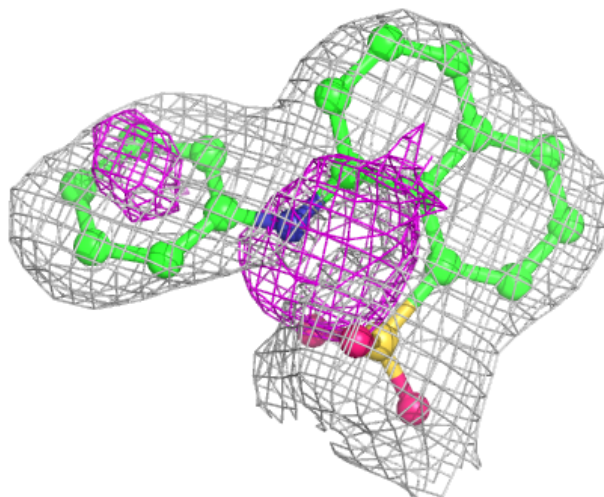
**Electron density around 2AN L 204:**

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



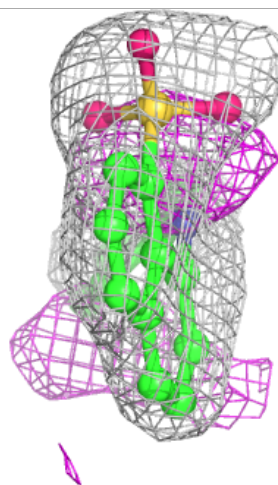
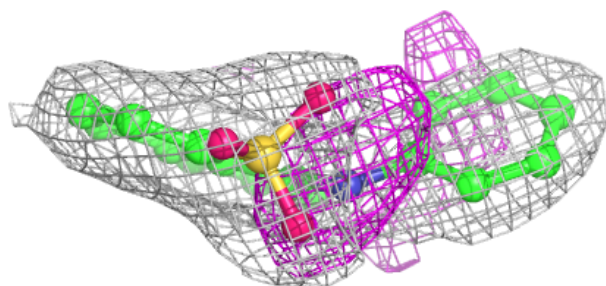
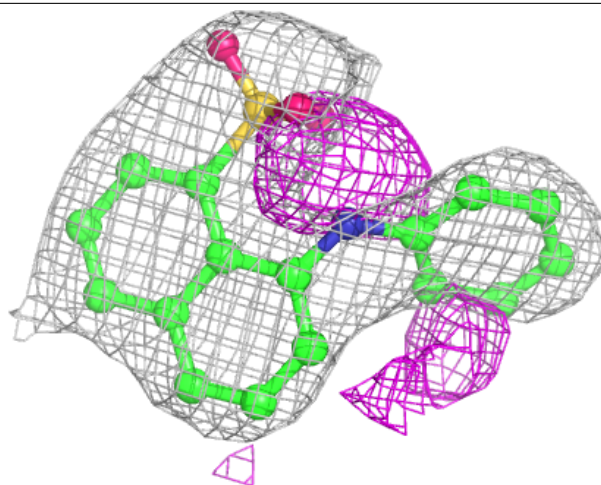
**Electron density around 2AN N 201:**

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



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

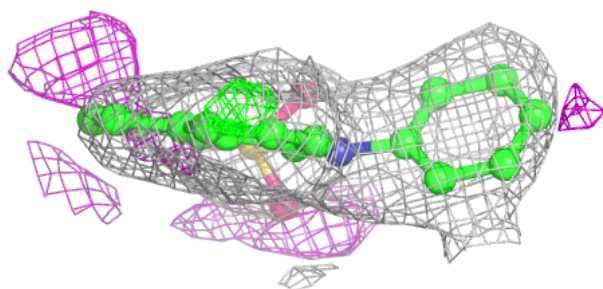
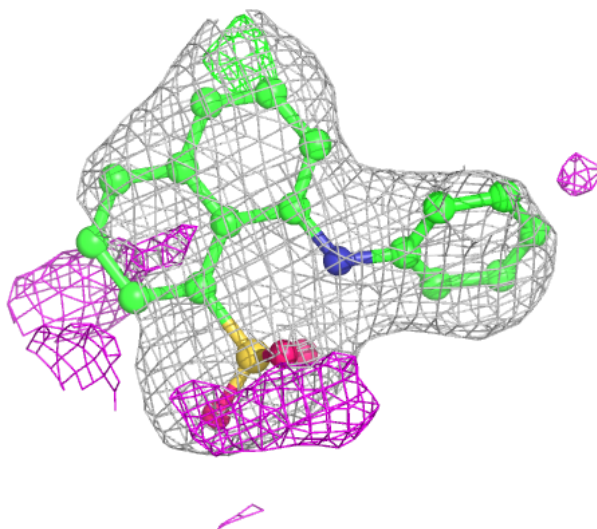
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





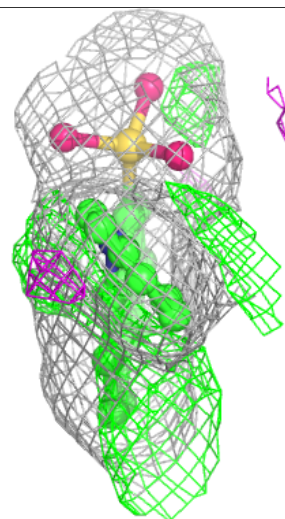
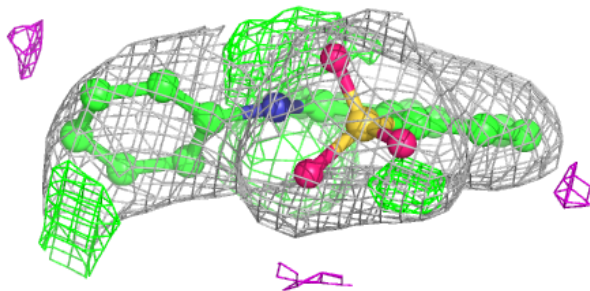
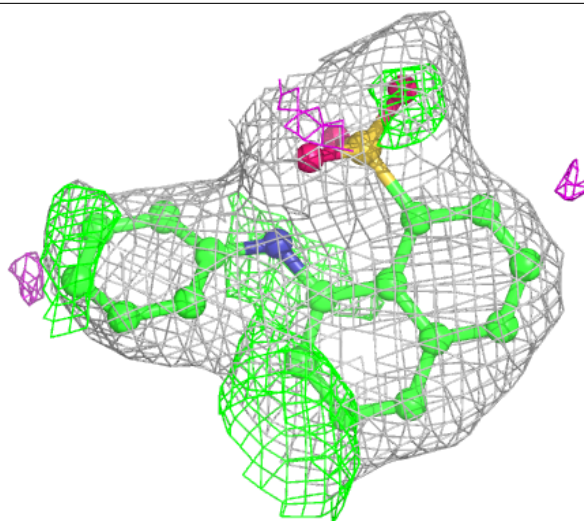
**Electron density around 2AN W 201:**

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



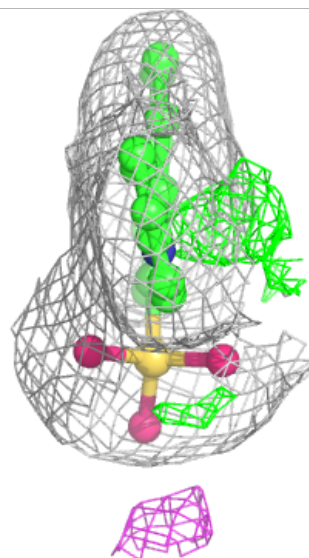
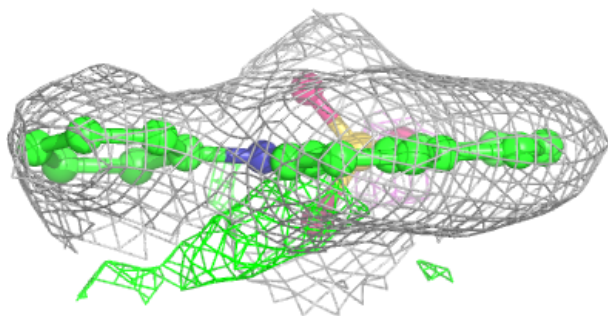
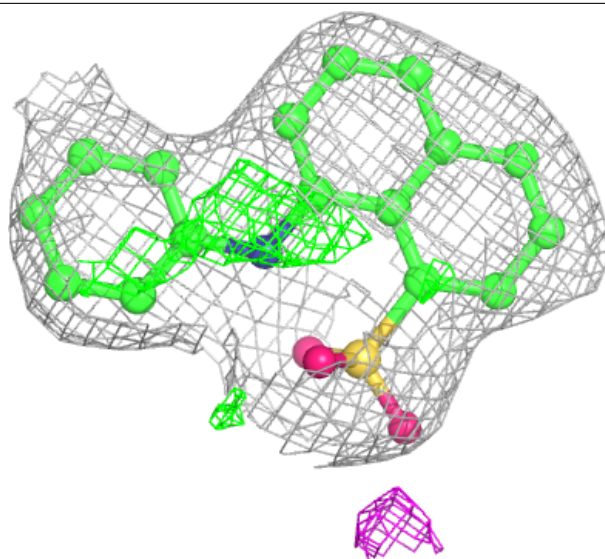
**Electron density around 2AN b 203:**

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



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

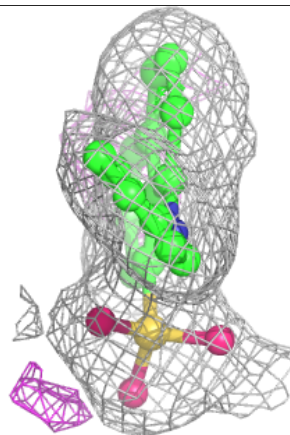
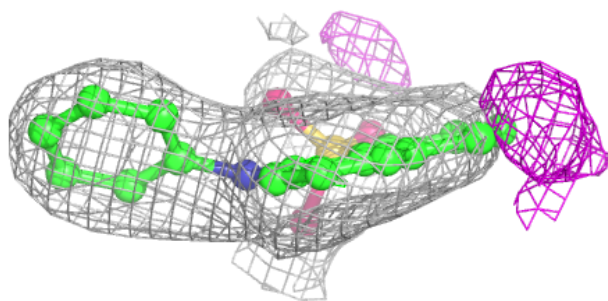
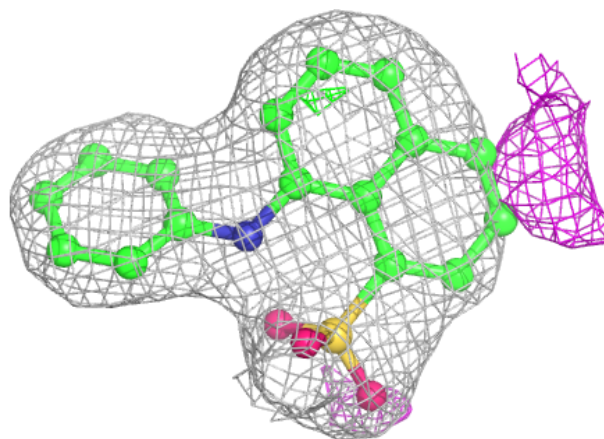
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





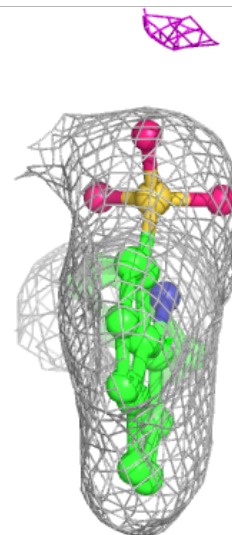
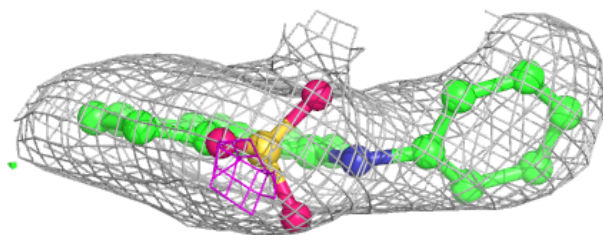
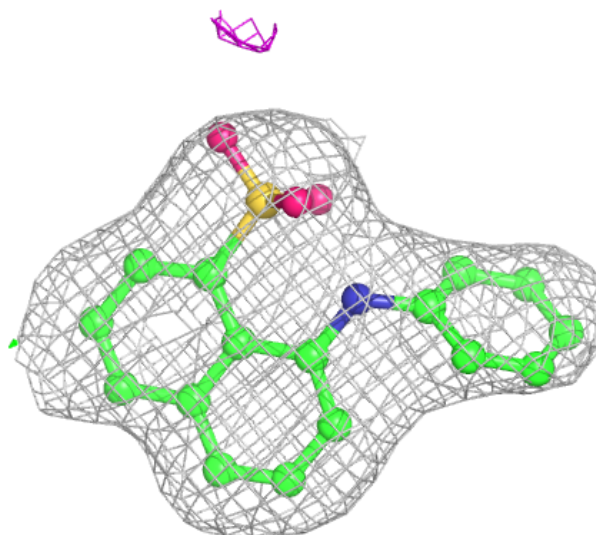
**Electron density around 2AN N 204:**

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



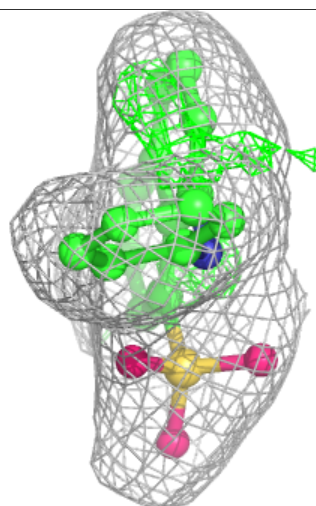
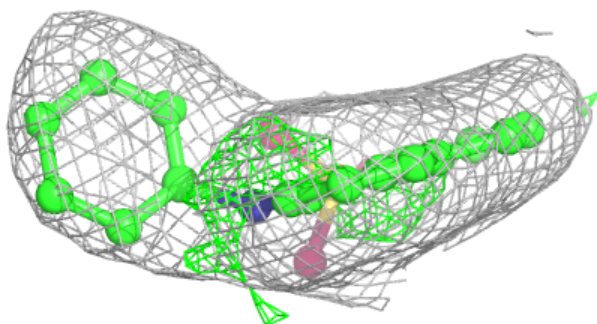
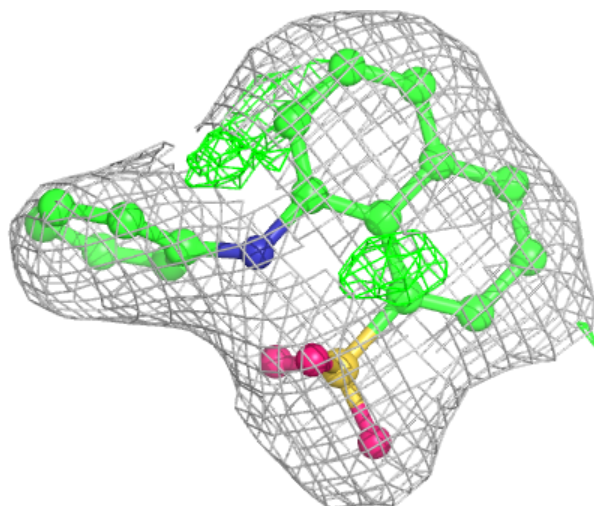
**Electron density around 2AN P 202:**

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



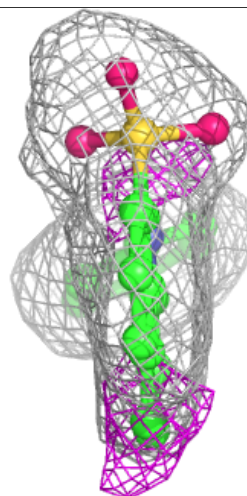
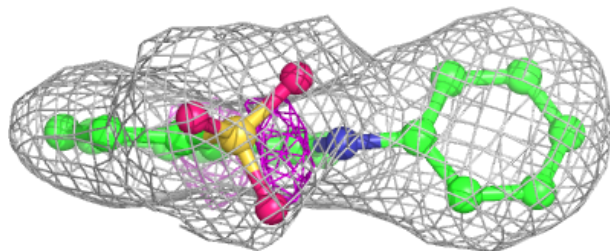
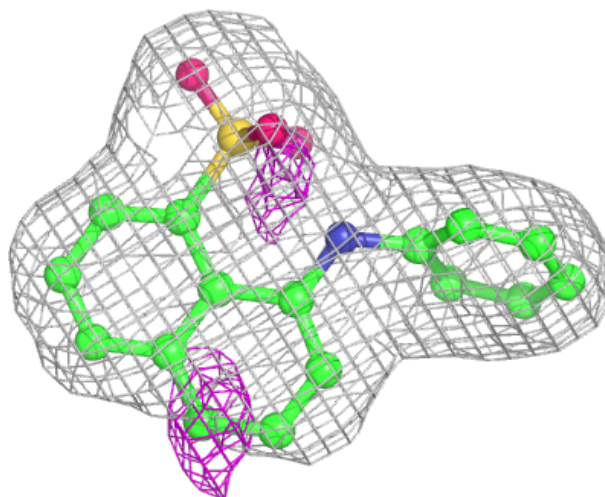
**Electron density around 2AN C 203:**

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



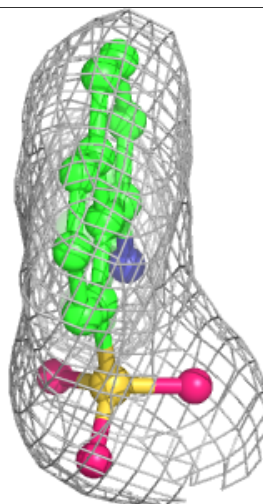
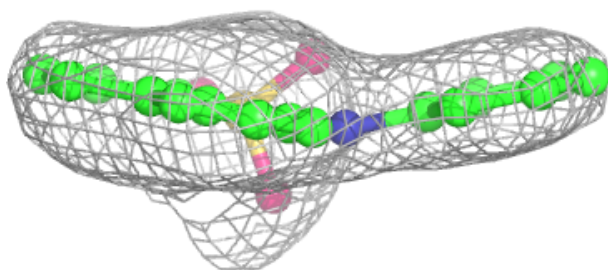
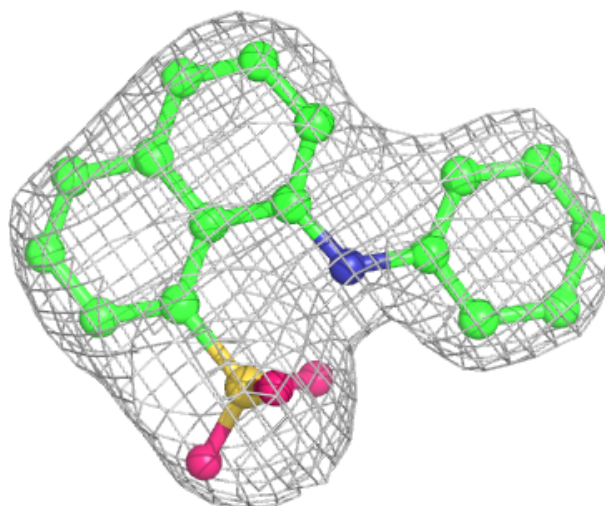
**Electron density around 2AN M 202:**

$2mF_o-DF_c$  (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:**

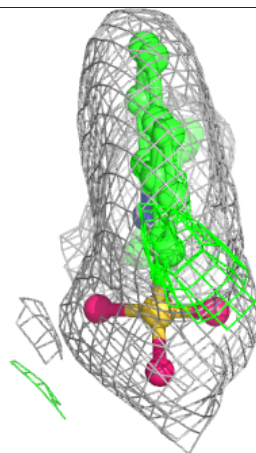
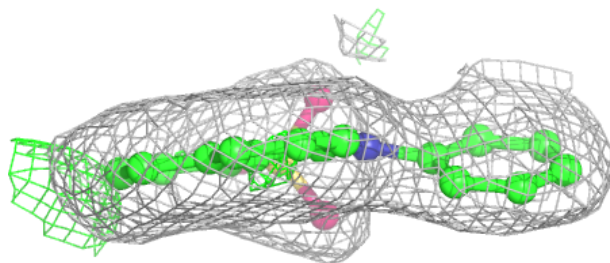
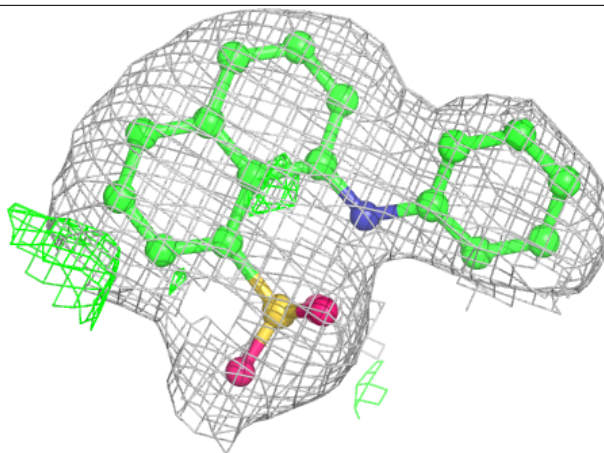
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





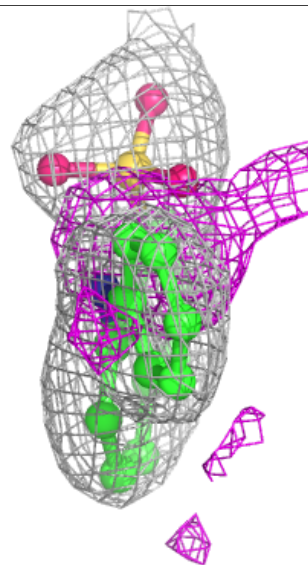
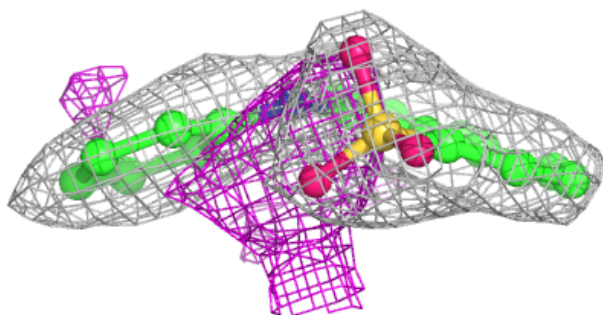
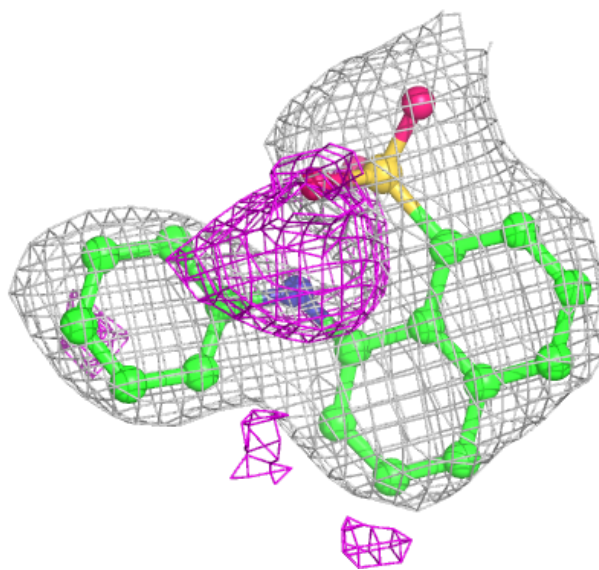
**Electron density around 2AN a 201:**

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



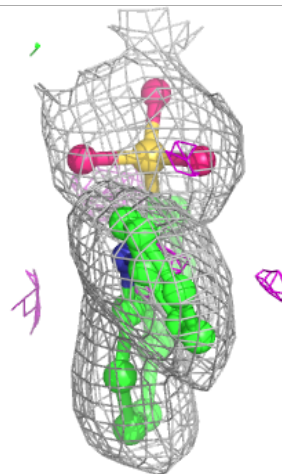
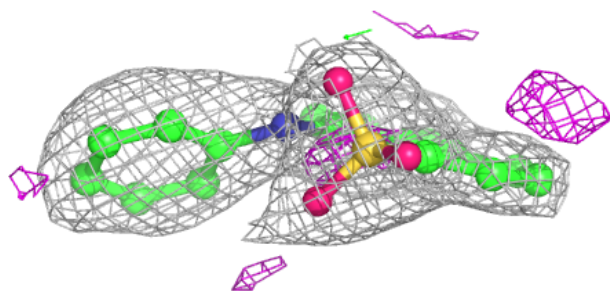
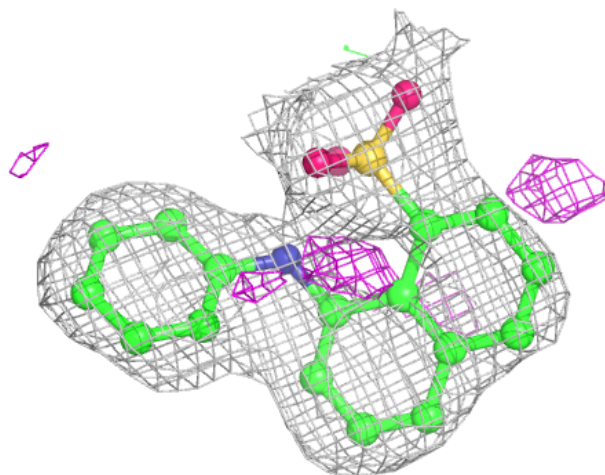
**Electron density around 2AN S 201:**

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



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

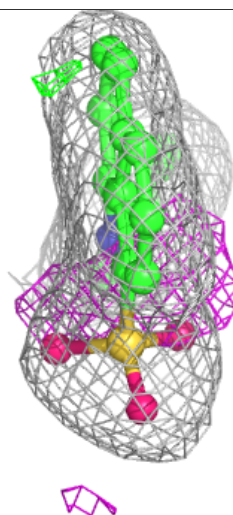
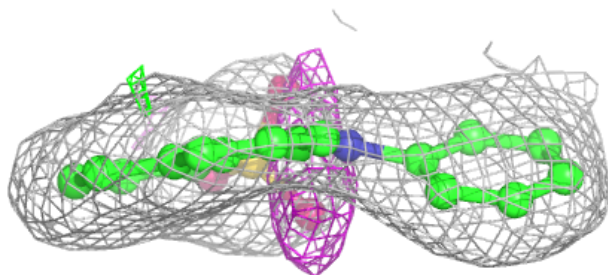
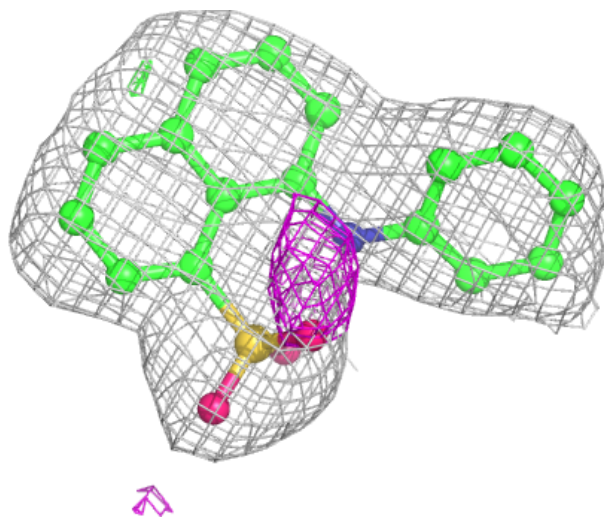
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





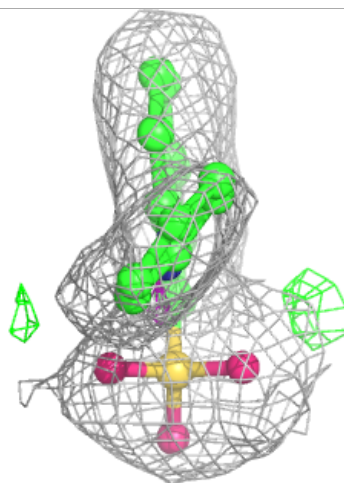
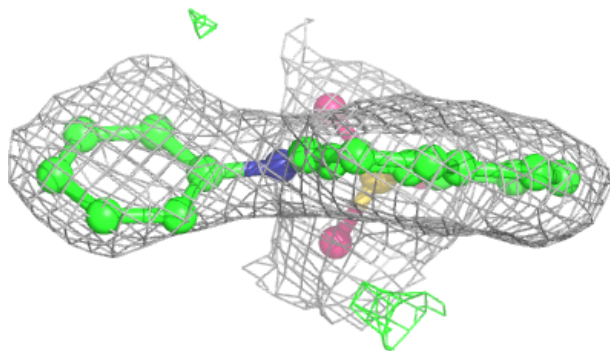
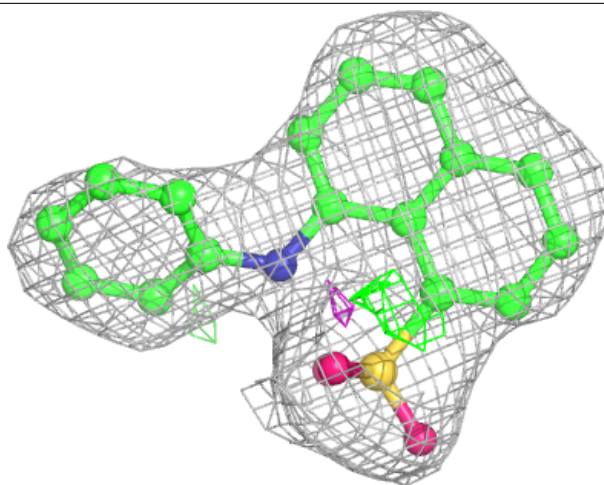
**Electron density around 2AN O 201:**

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



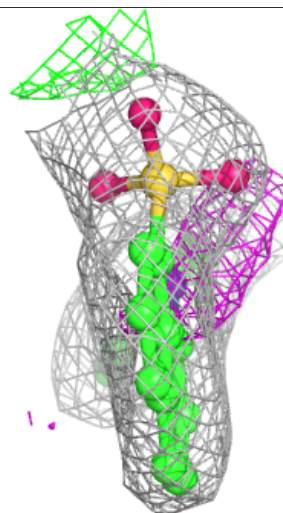
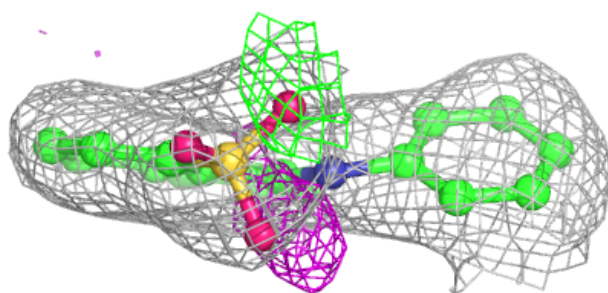
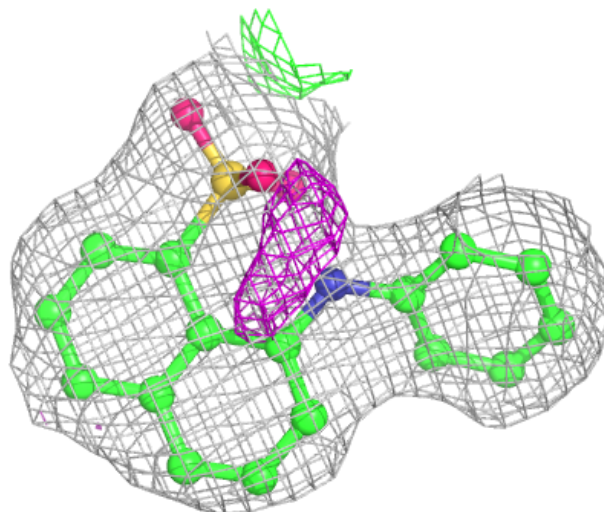
**Electron density around 2AN L 205:**

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



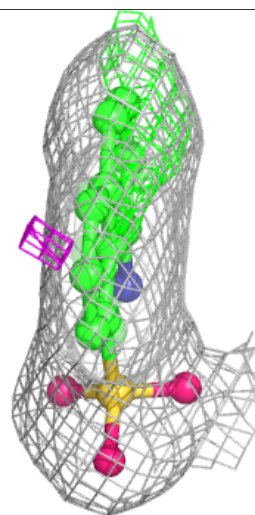
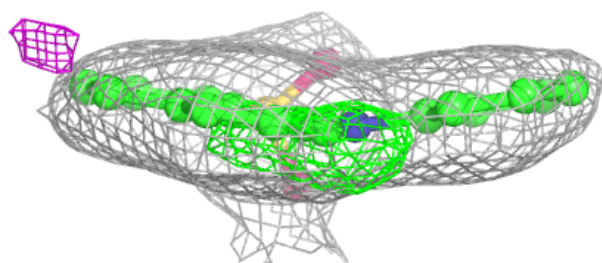
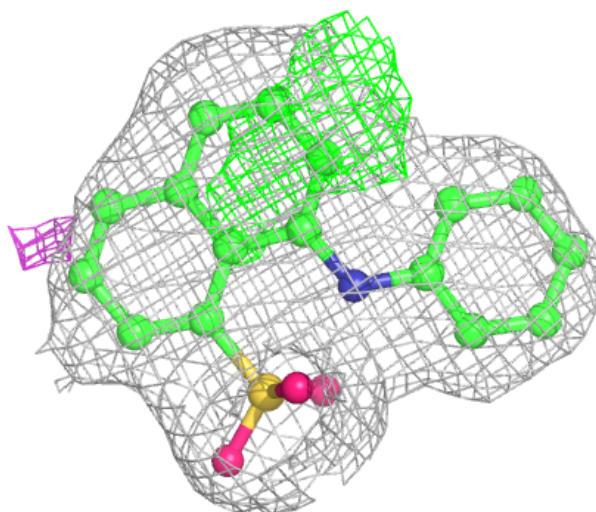
**Electron density around 2AN A 203:**

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



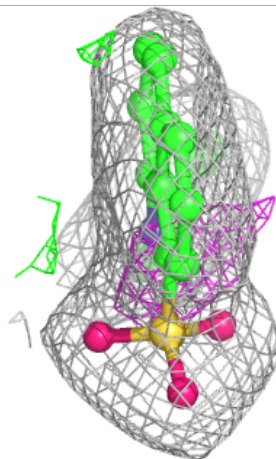
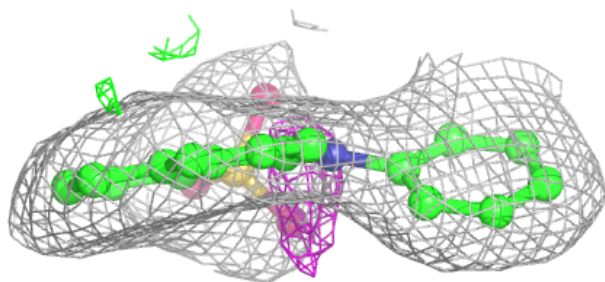
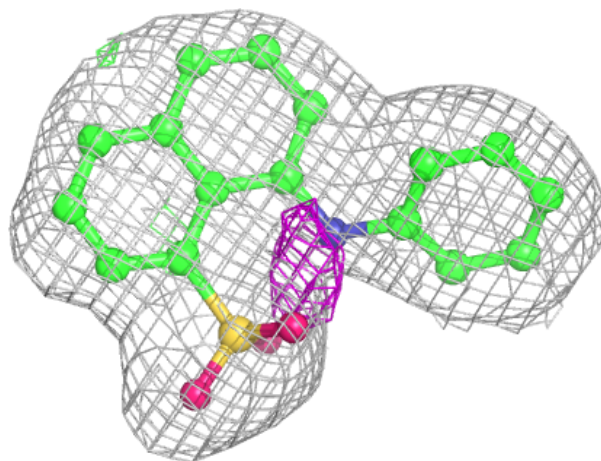
**Electron density around 2AN E 203:**

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



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

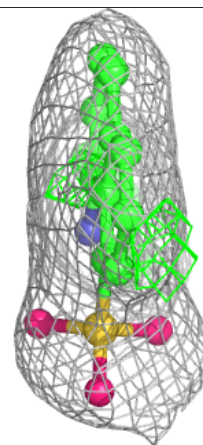
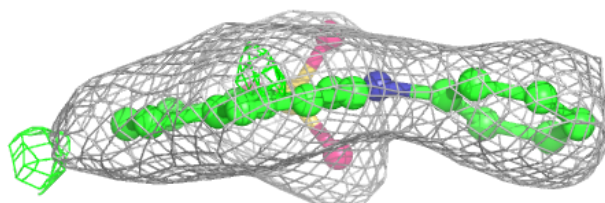
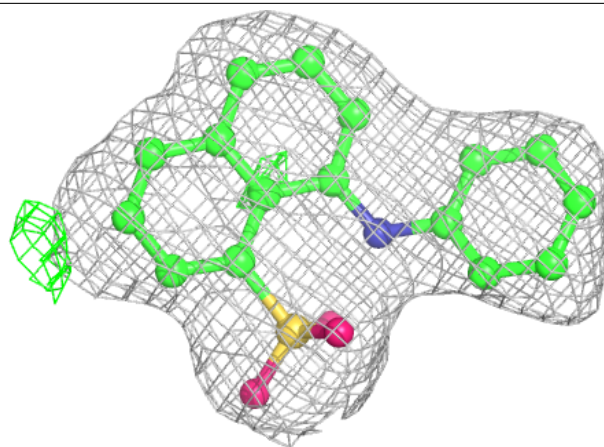
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





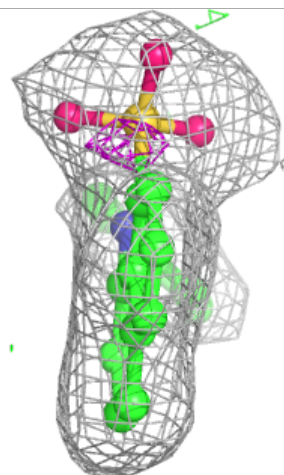
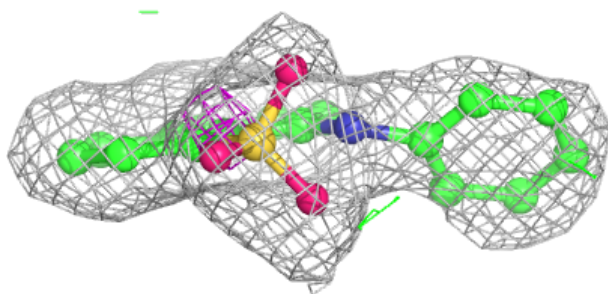
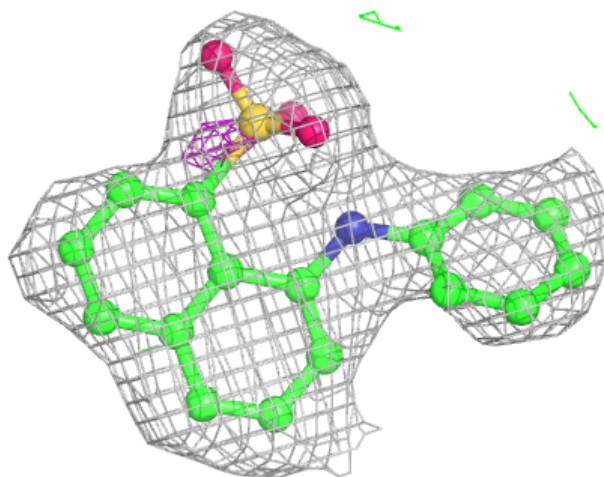
**Electron density around 2AN K 202:**

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



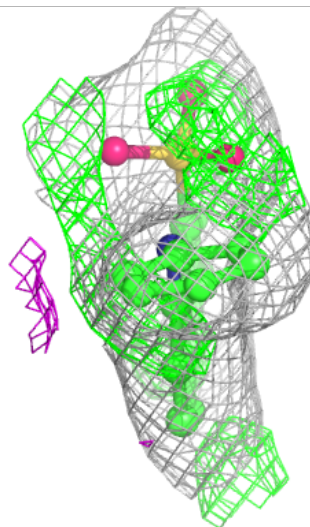
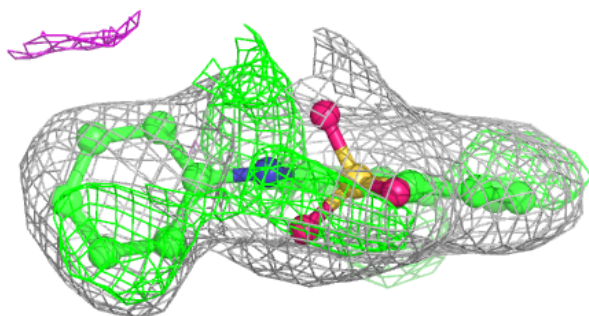
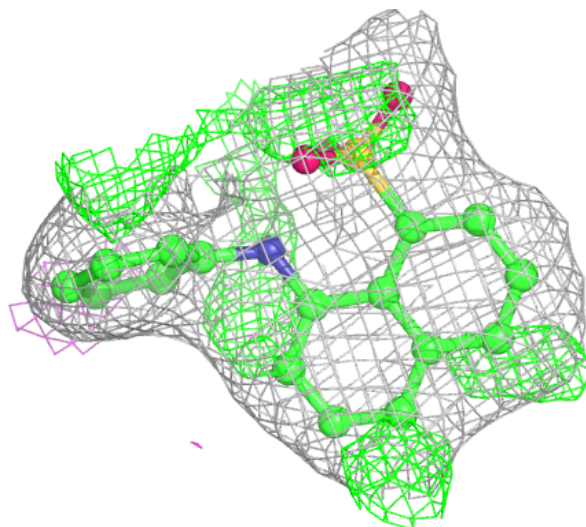
**Electron density around 2AN Y 204:**

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



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

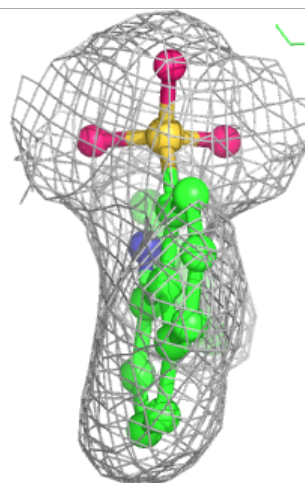
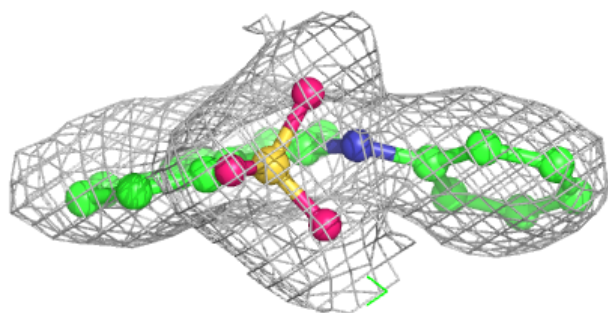
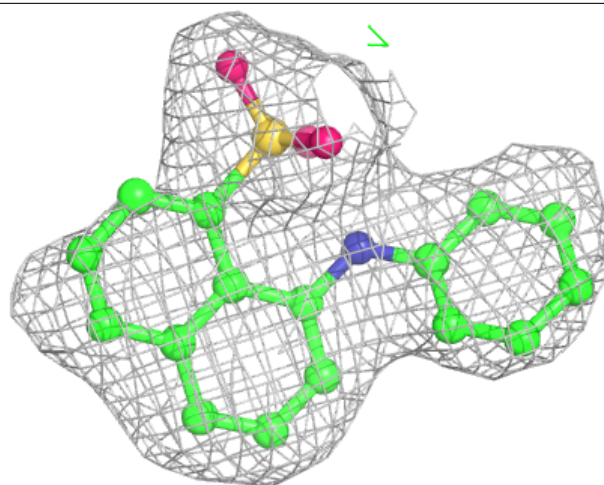
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





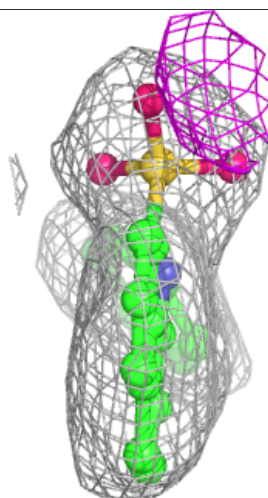
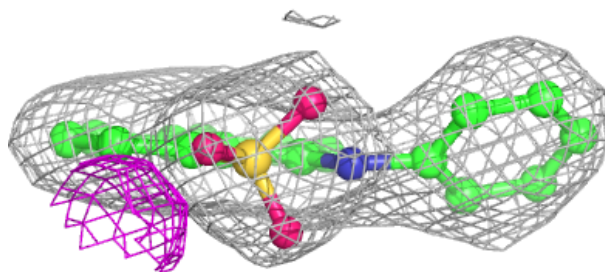
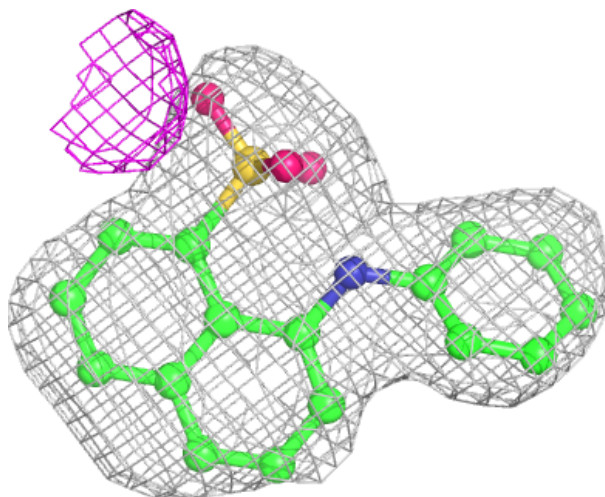
**Electron density around 2AN B 204:**

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



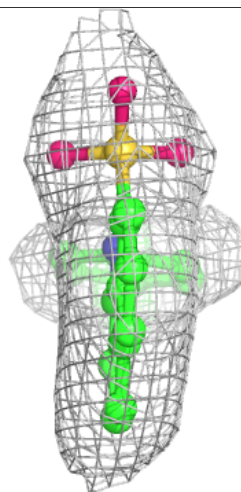
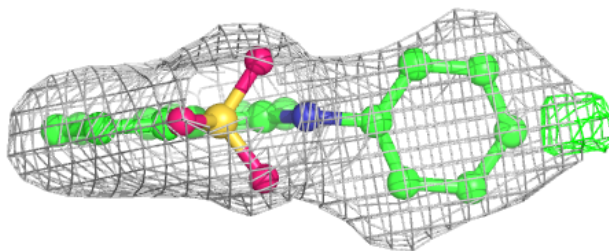
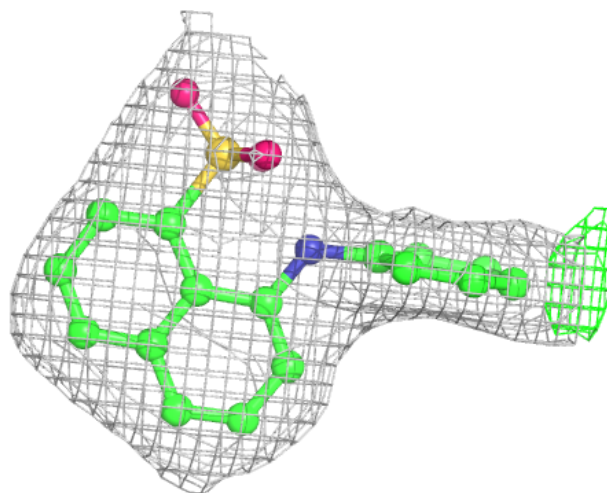
**Electron density around 2AN B 205:**

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



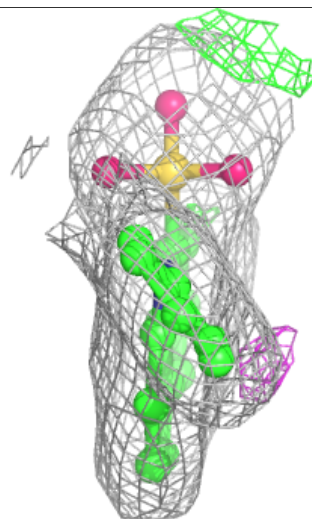
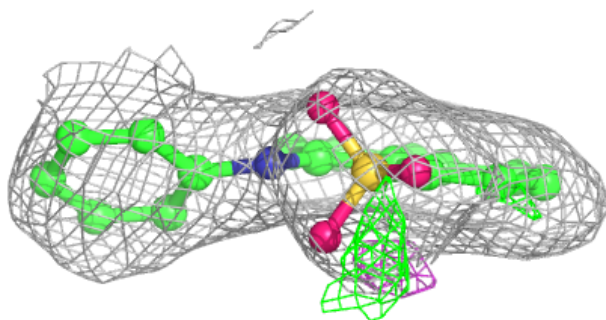
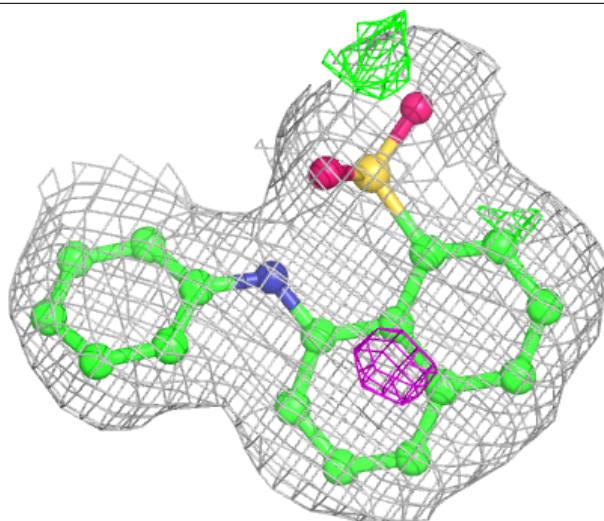
**Electron density around 2AN U 205:**

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



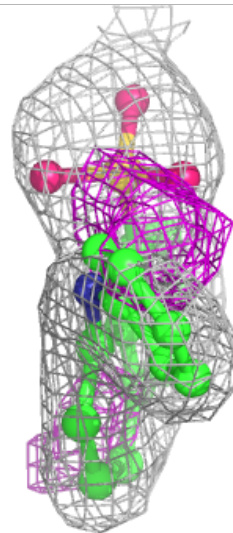
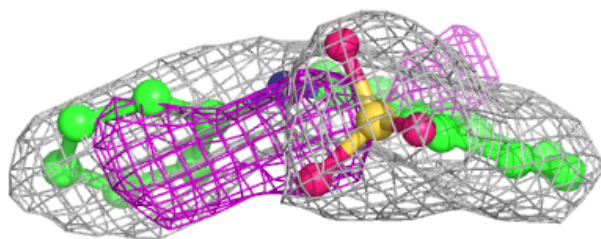
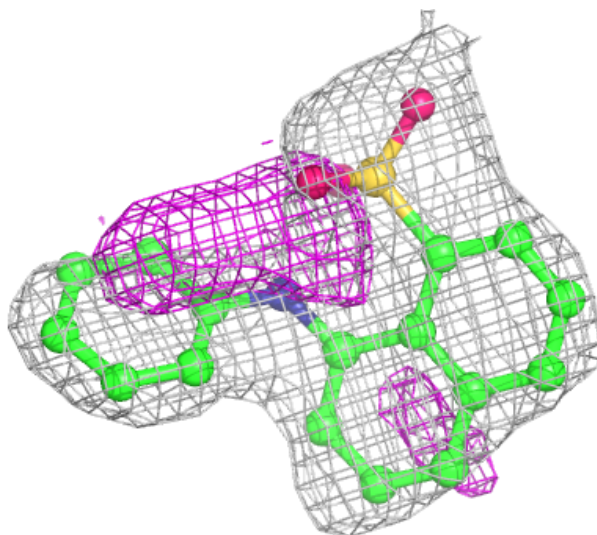
**Electron density around 2AN B 202:**

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



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

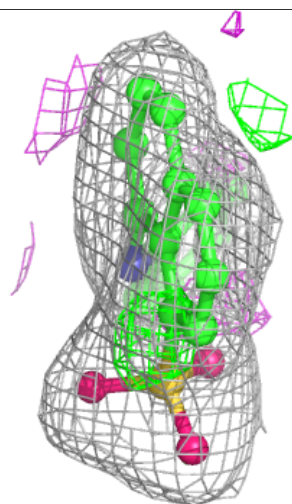
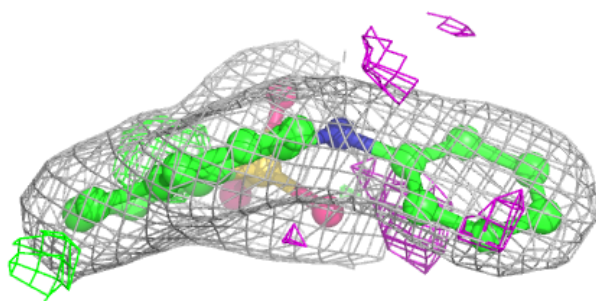
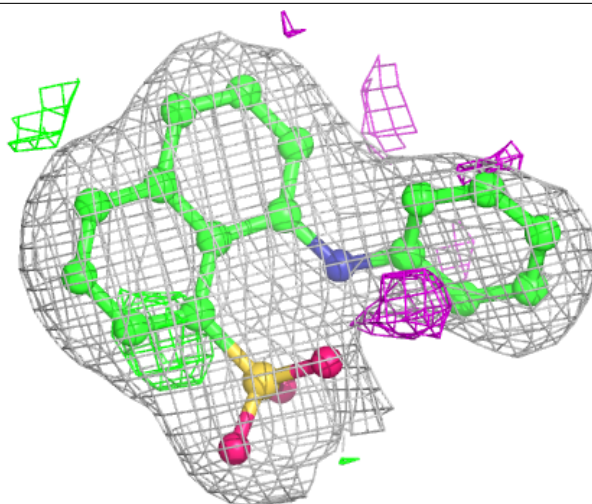
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





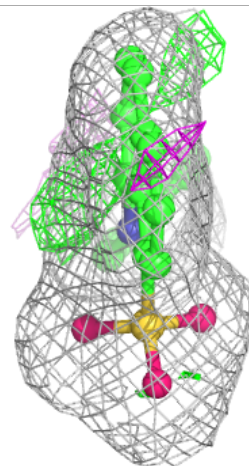
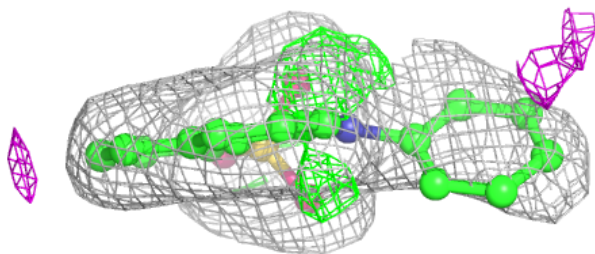
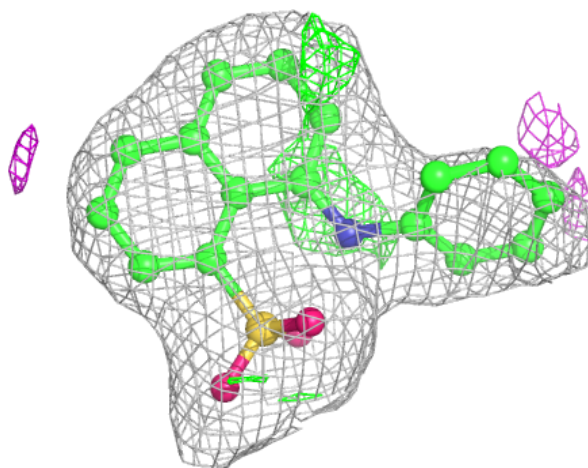
**Electron density around 2AN E 201:**

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



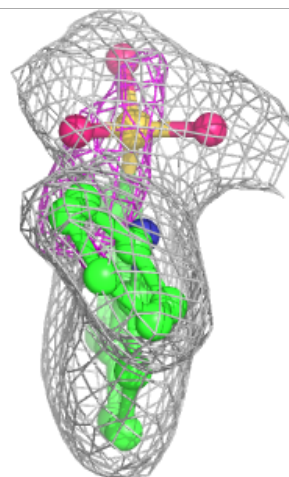
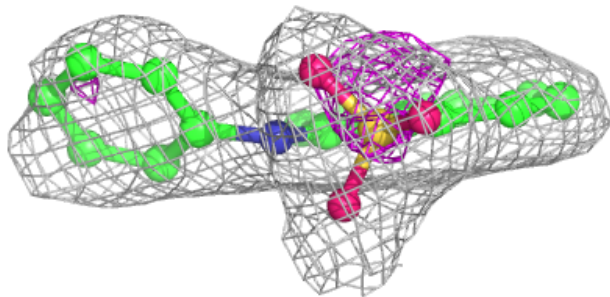
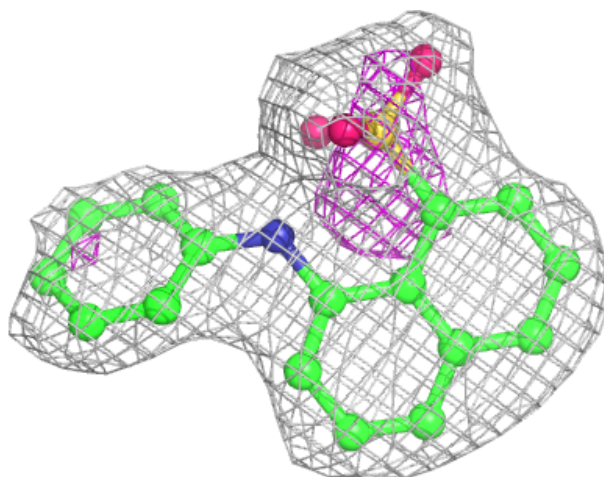
**Electron density around 2AN X 203:**

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



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

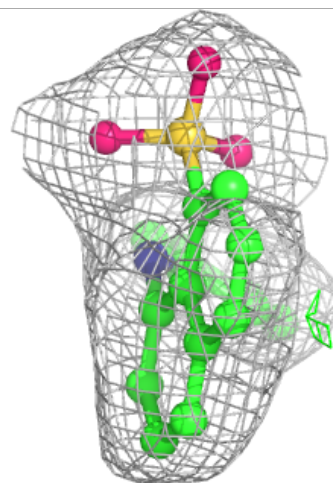
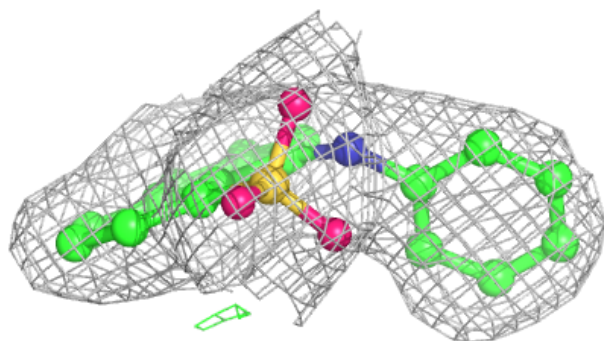
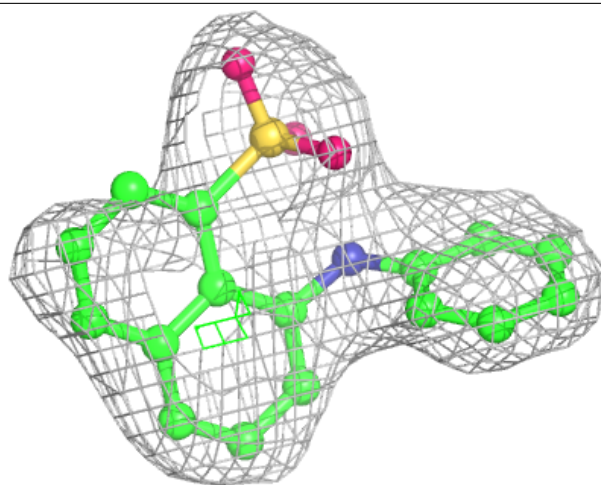
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





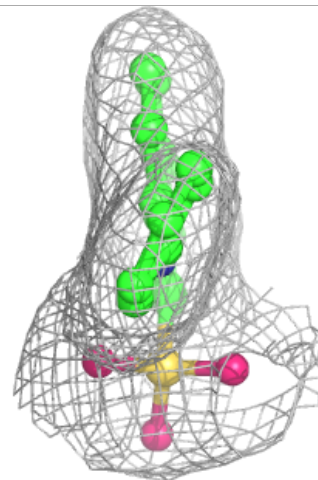
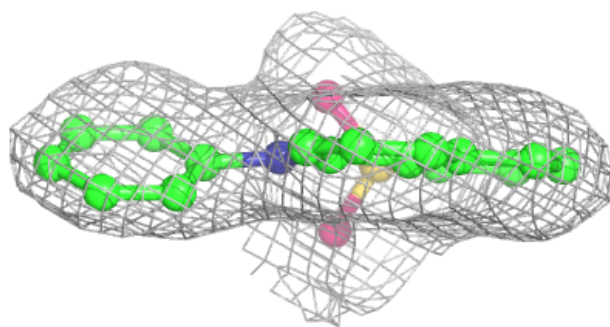
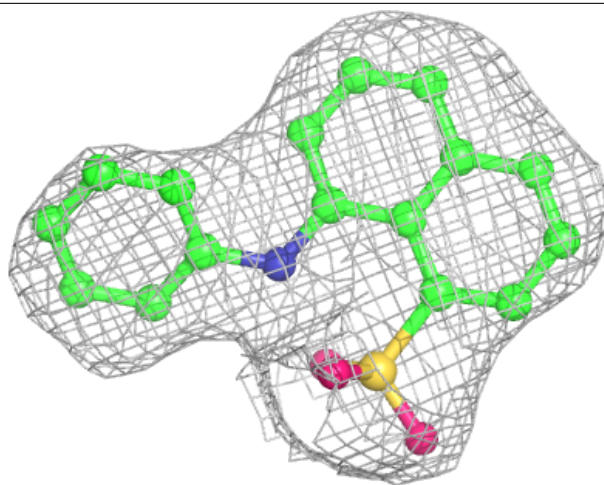
**Electron density around 2AN Q 202:**

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



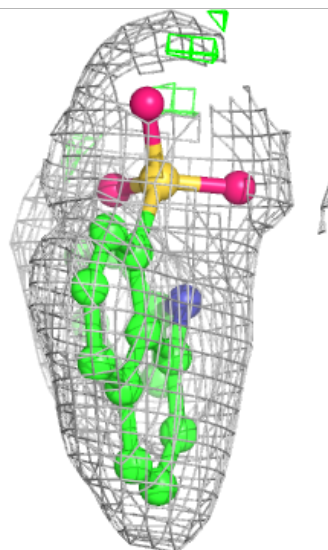
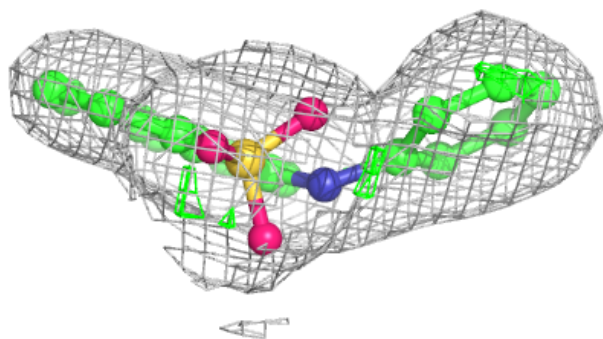
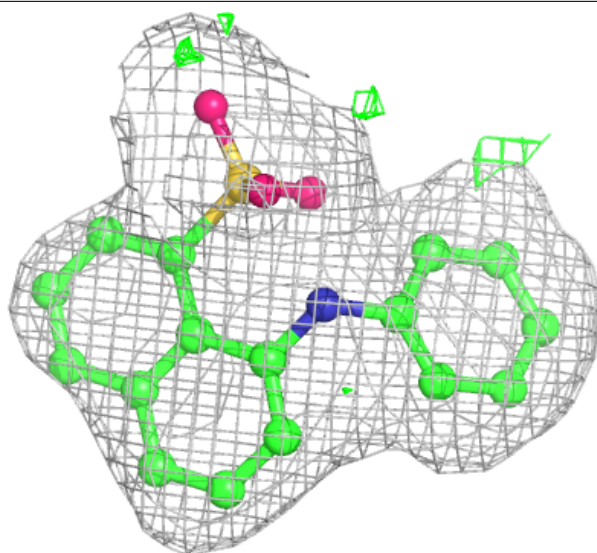
**Electron density around 2AN U 203:**

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



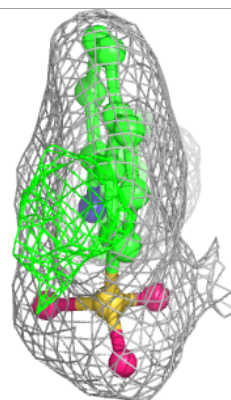
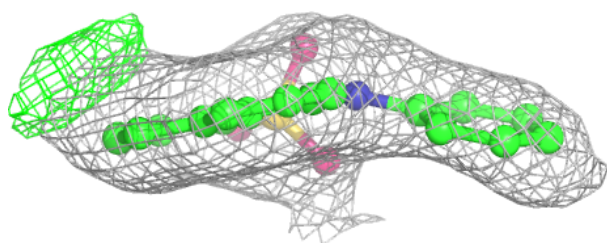
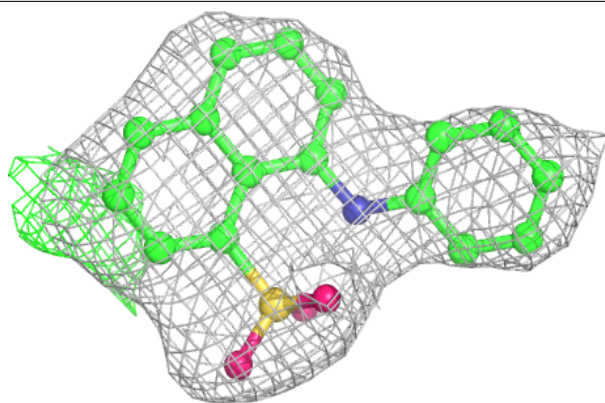
**Electron density around 2AN C 204:**

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



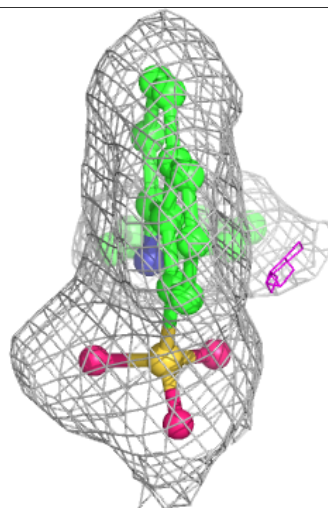
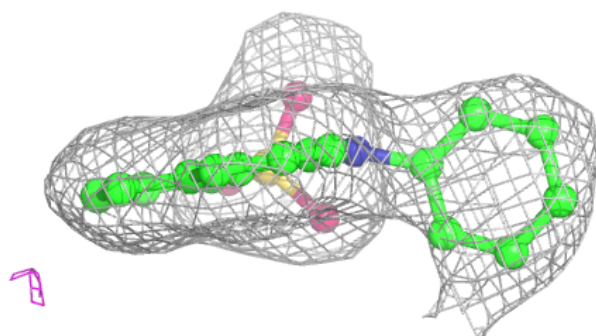
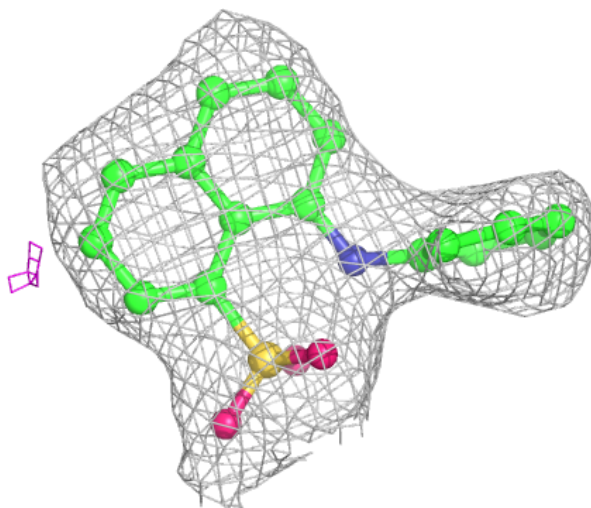
**Electron density around 2AN Z 203:**

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



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

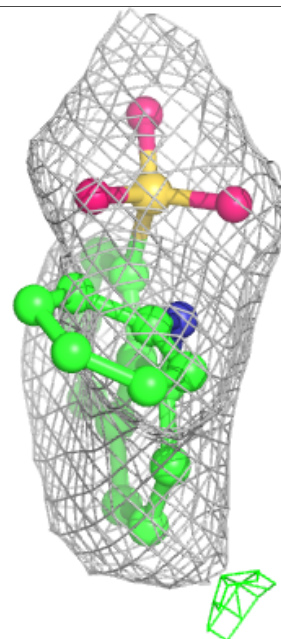
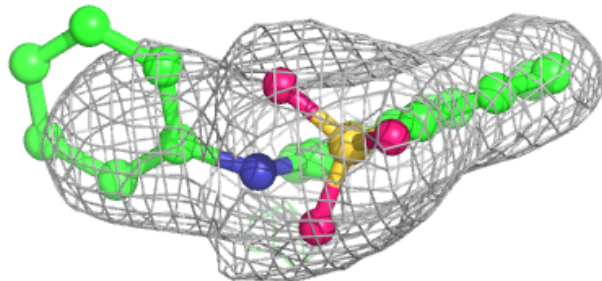
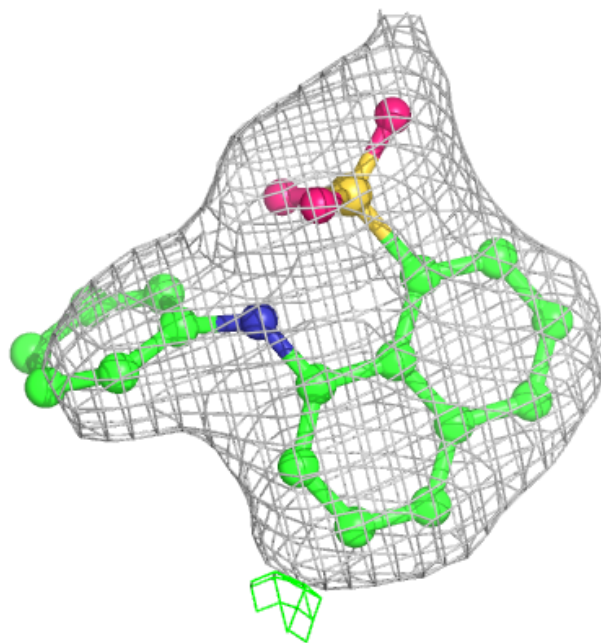
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





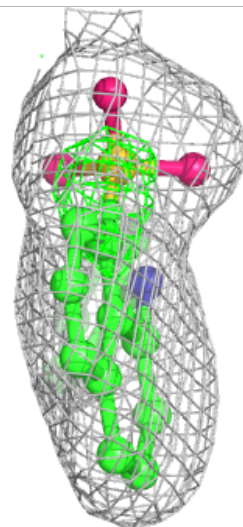
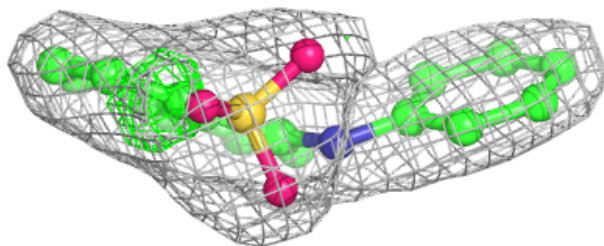
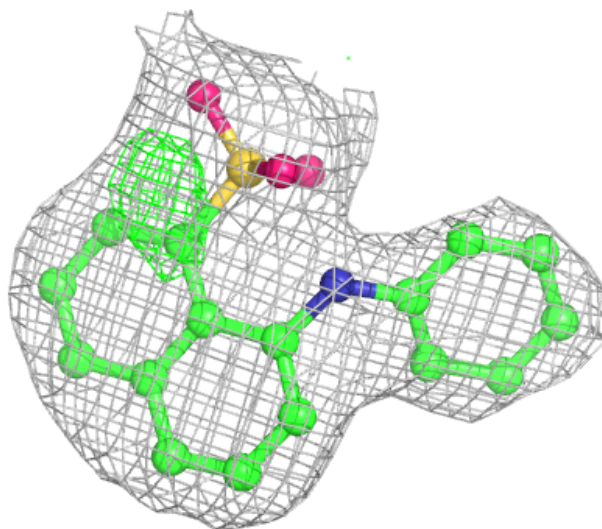
**Electron density around 2AN V 202:**

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



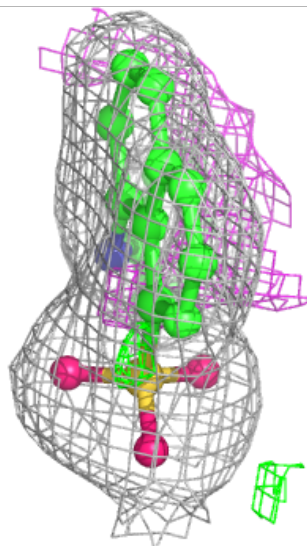
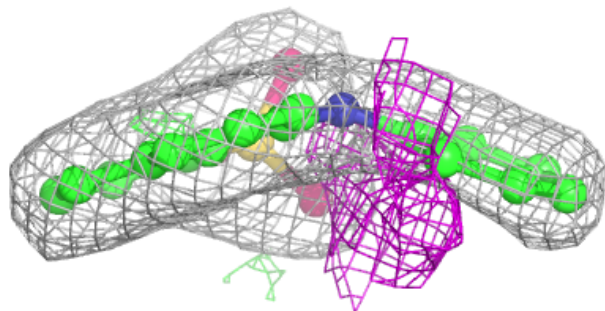
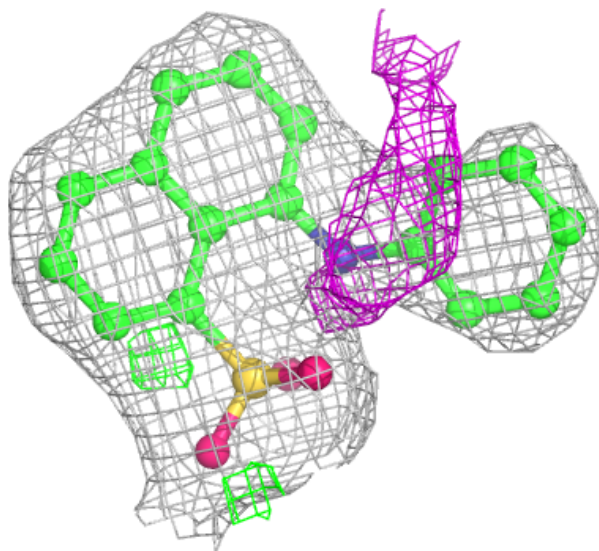
**Electron density around 2AN b 202:**

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



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

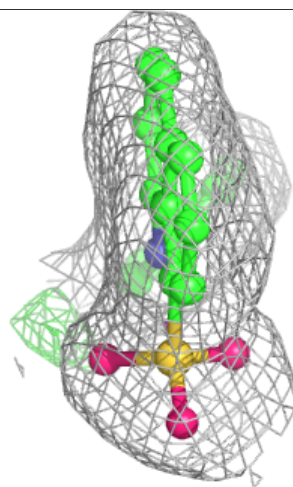
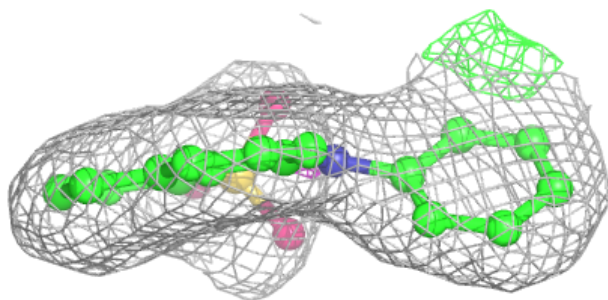
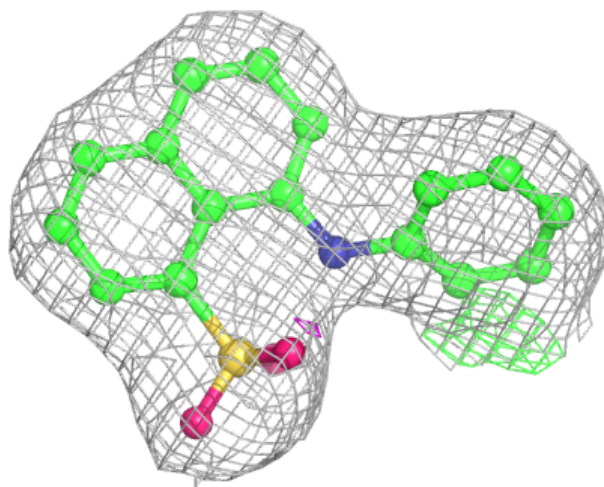
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





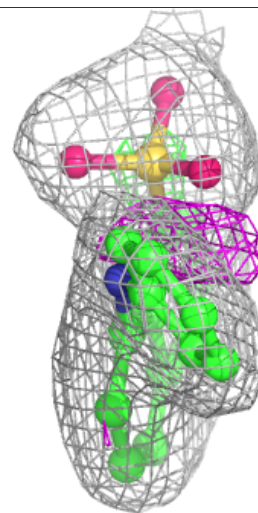
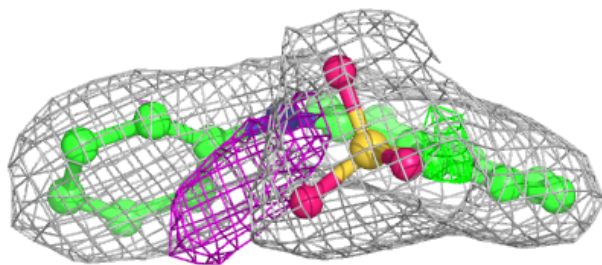
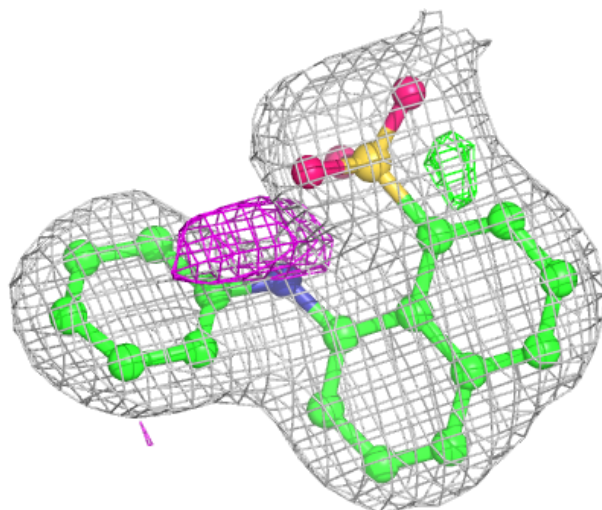
**Electron density around 2AN U 201:**

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



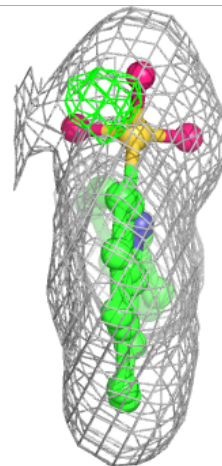
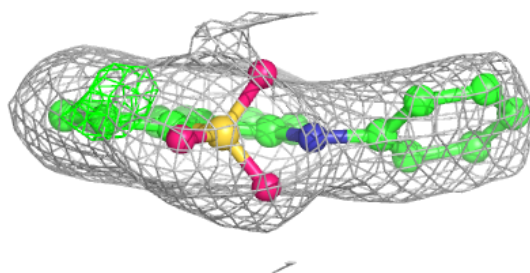
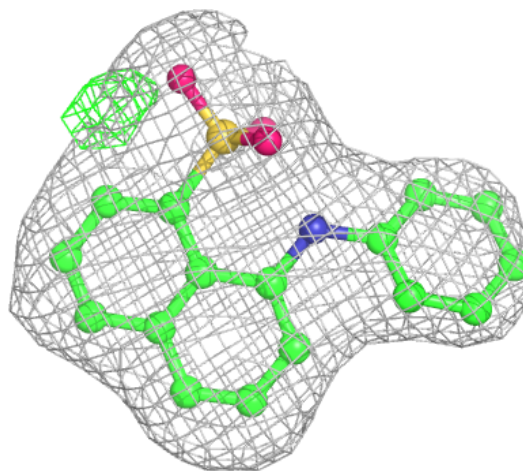
**Electron density around 2AN Y 201:**

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



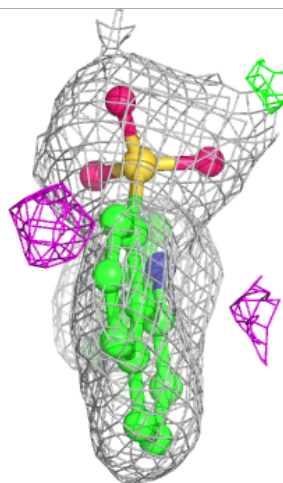
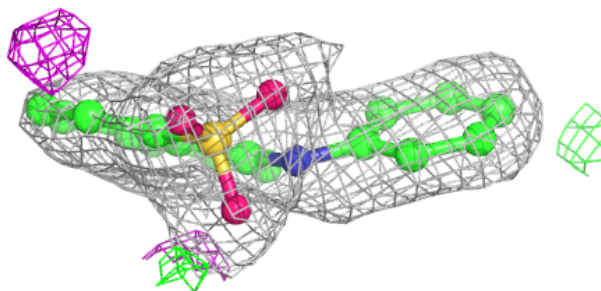
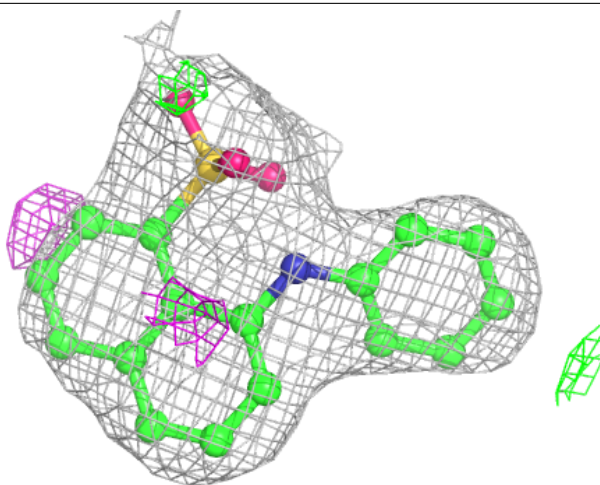
**Electron density around 2AN A 201:**

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



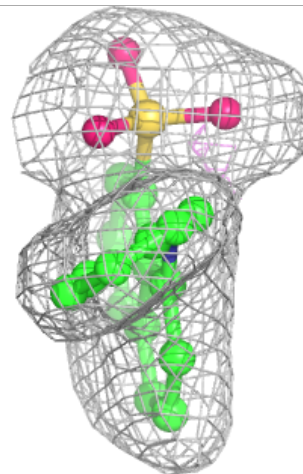
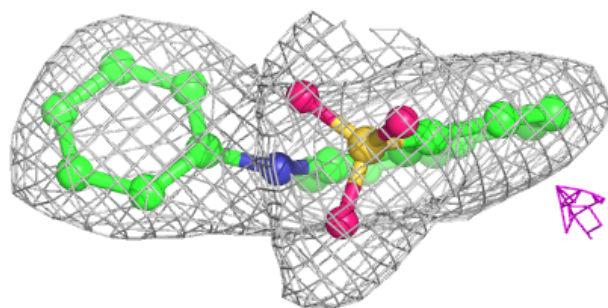
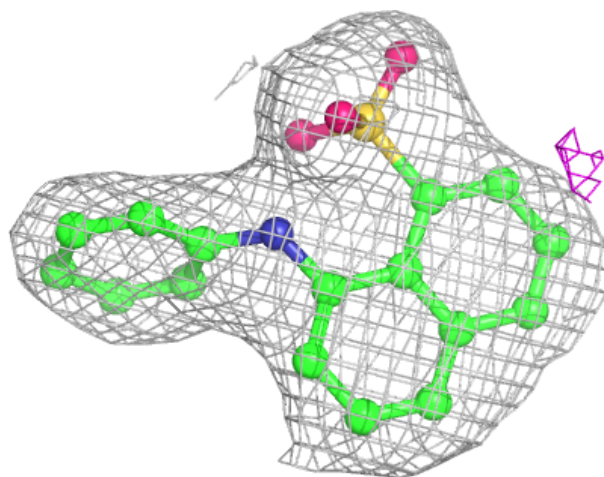
**Electron density around 2AN P 201:**

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



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

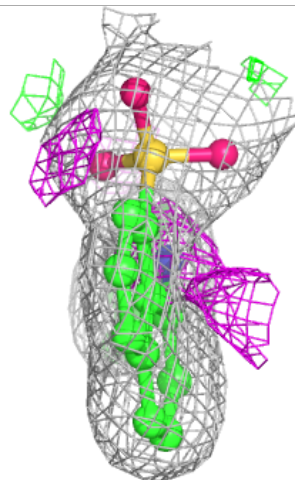
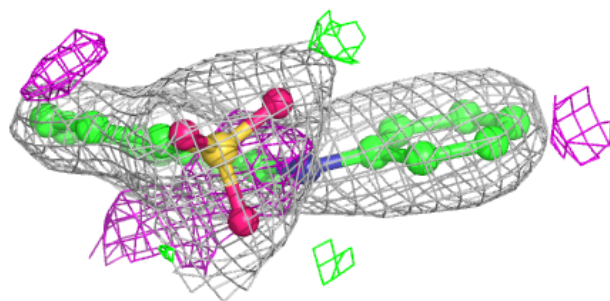
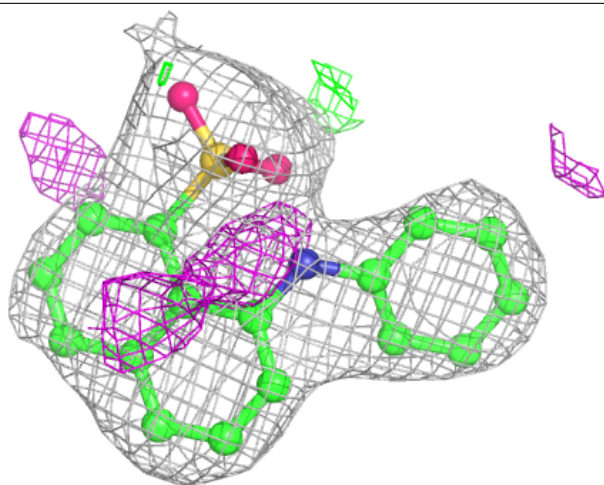
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





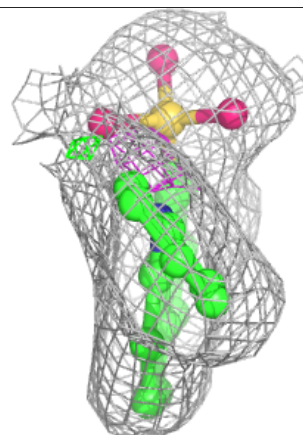
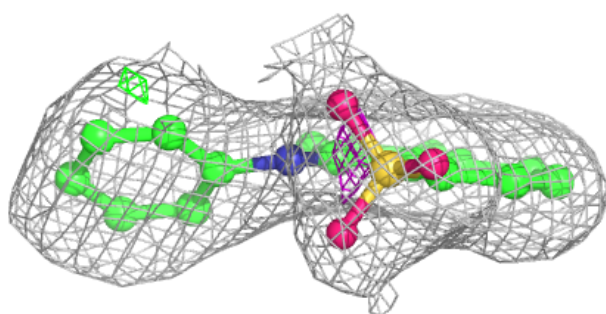
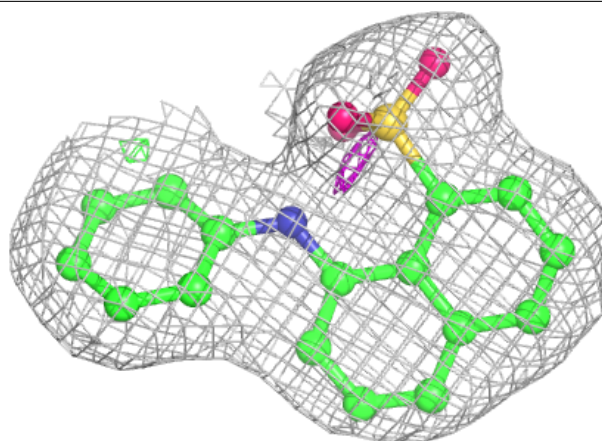
**Electron density around 2AN Z 201:**

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



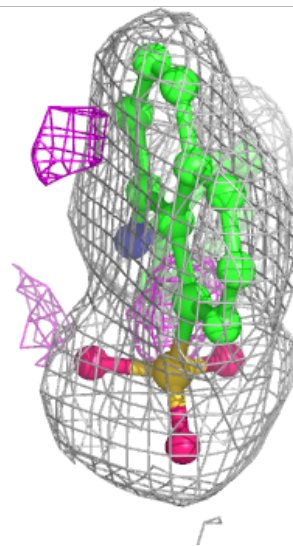
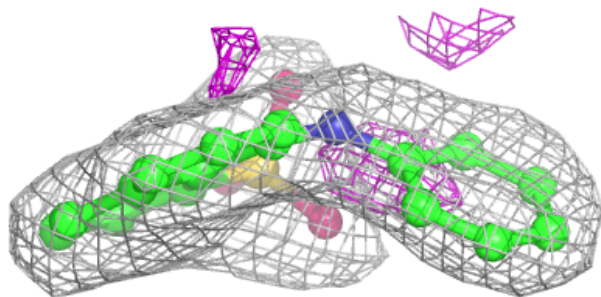
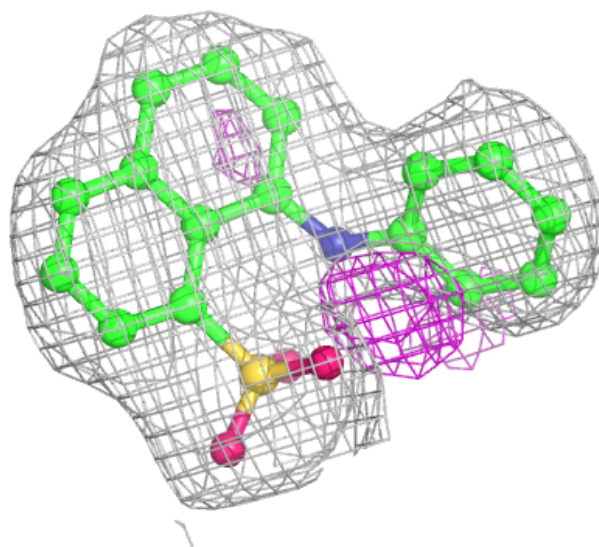
**Electron density around 2AN L 202:**

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



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

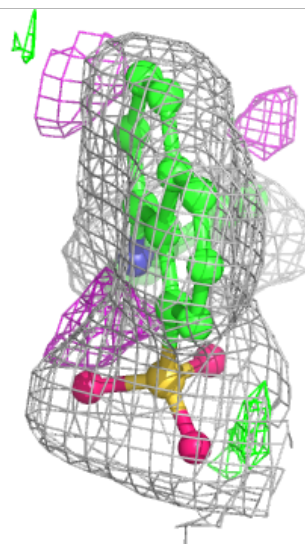
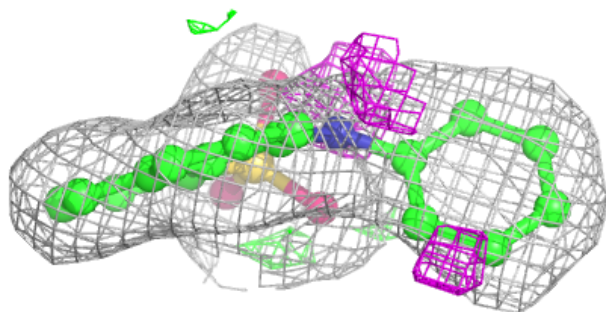
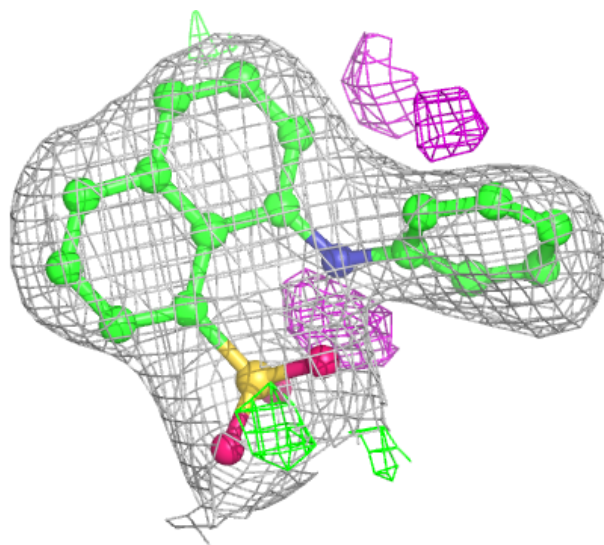
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





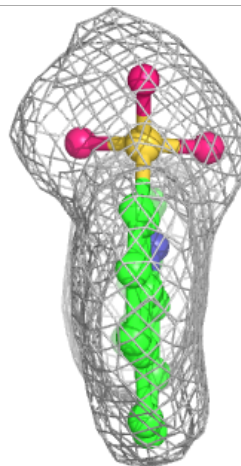
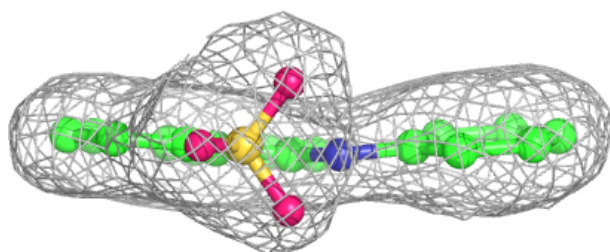
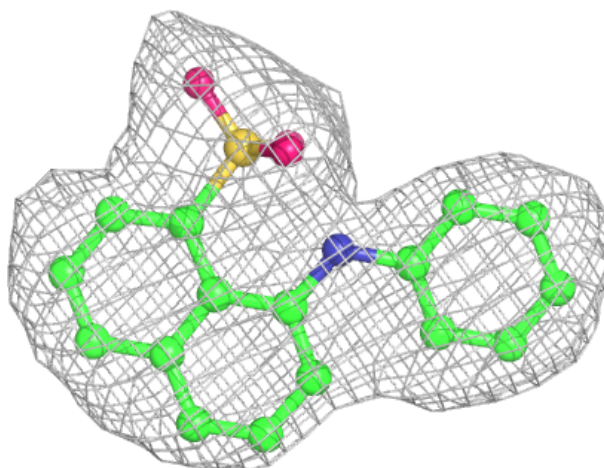
**Electron density around 2AN A 202:**

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



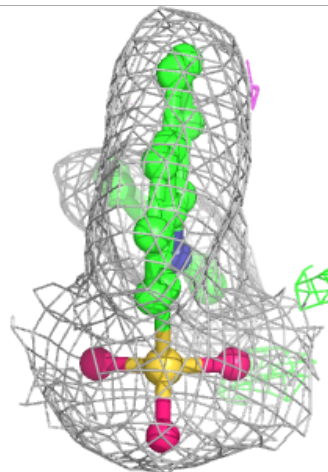
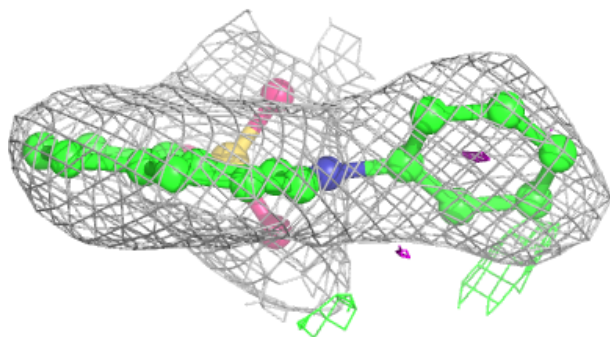
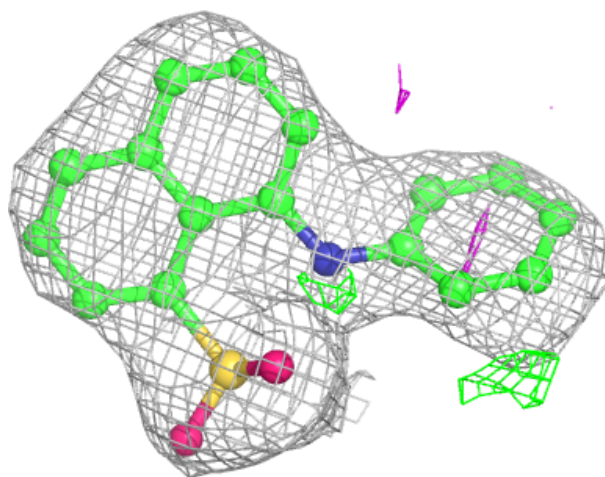
**Electron density around 2AN D 202:**

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



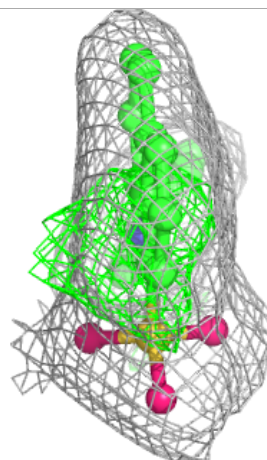
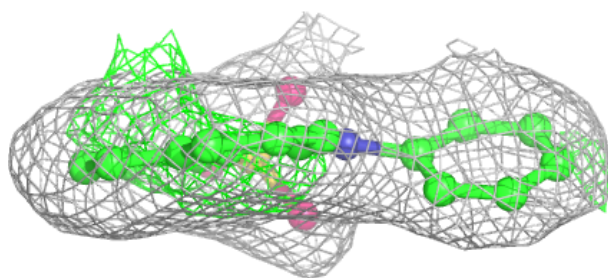
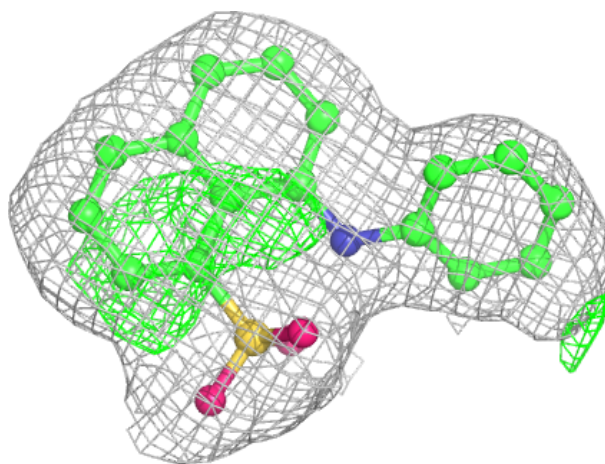
**Electron density around 2AN B 203:**

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



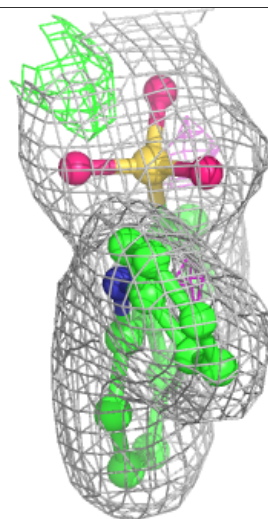
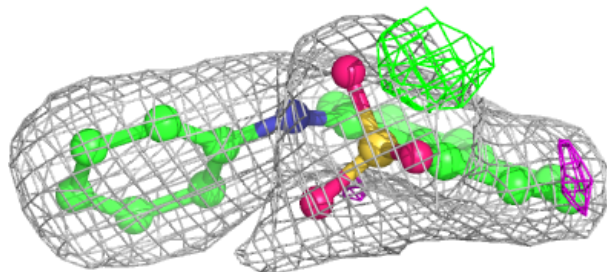
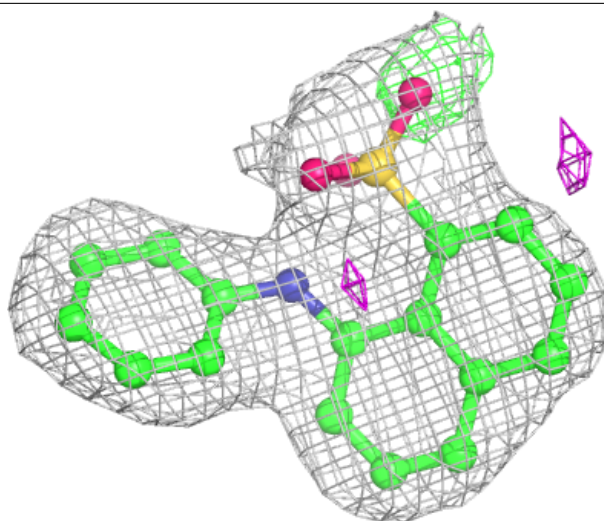
**Electron density around 2AN J 202:**

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



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

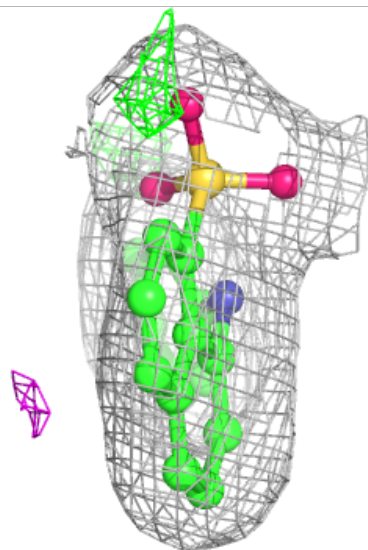
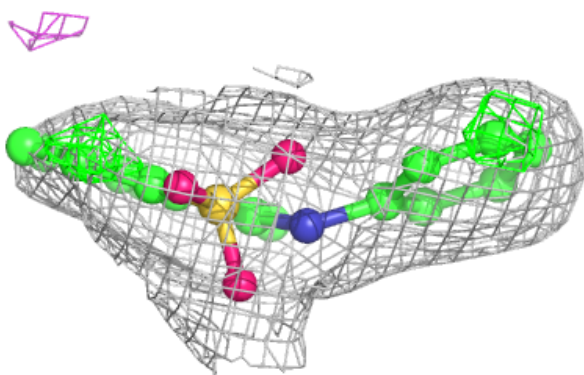
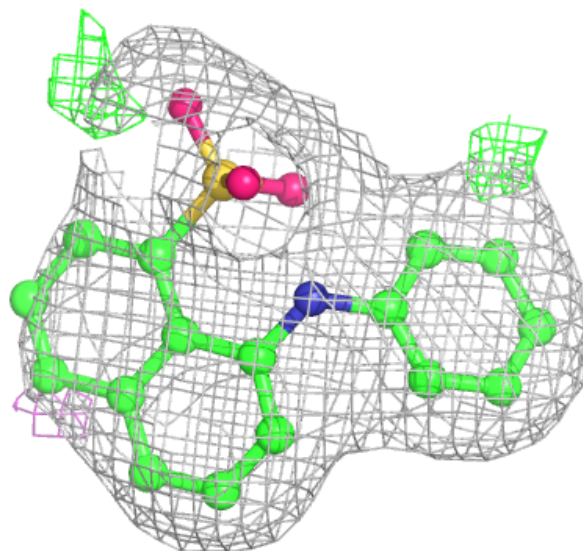
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





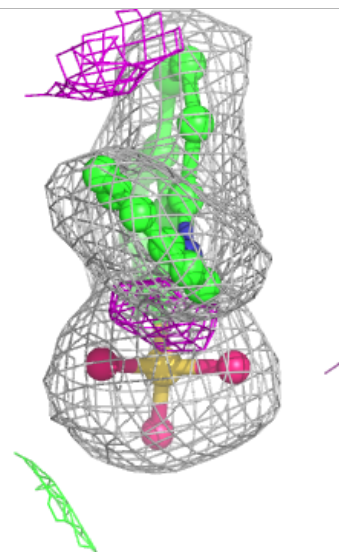
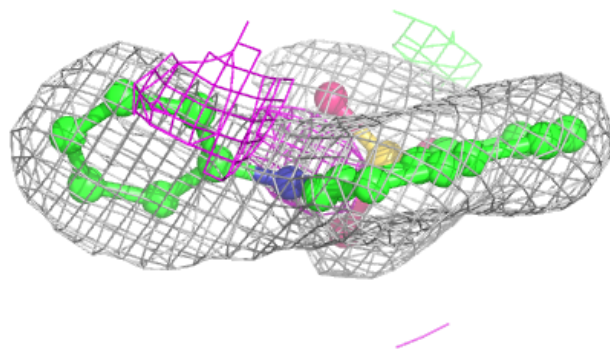
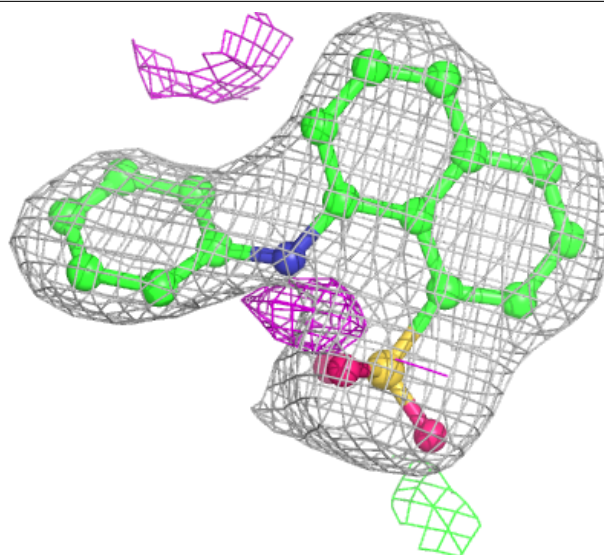
**Electron density around 2AN E 205:**

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



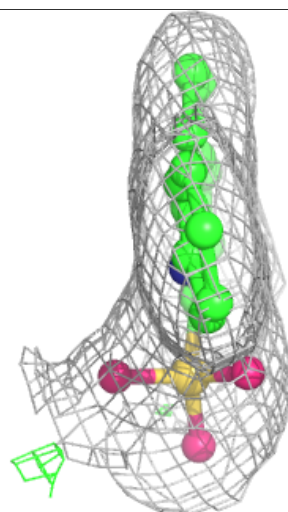
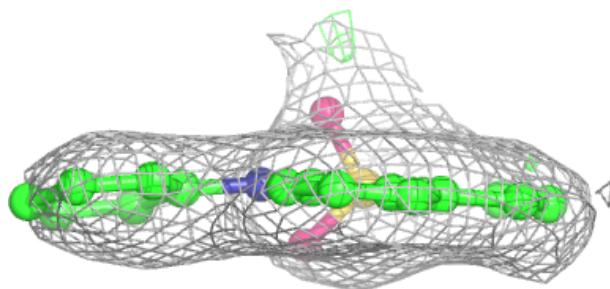
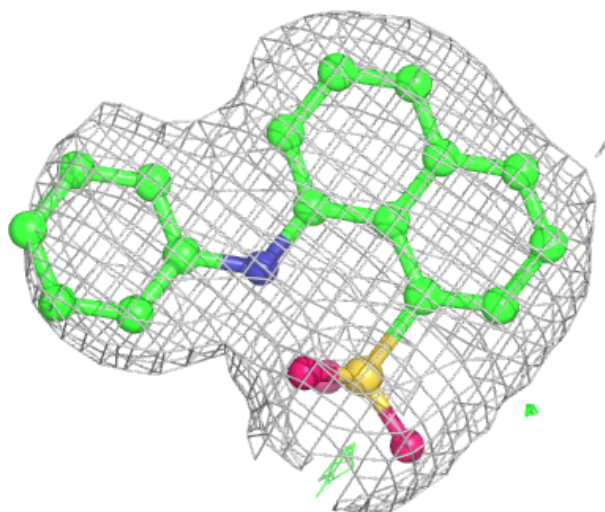
**Electron density around 2AN B 201:**

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



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

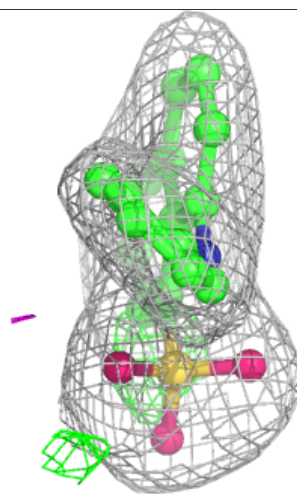
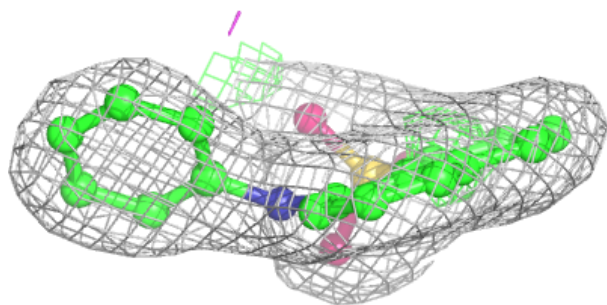
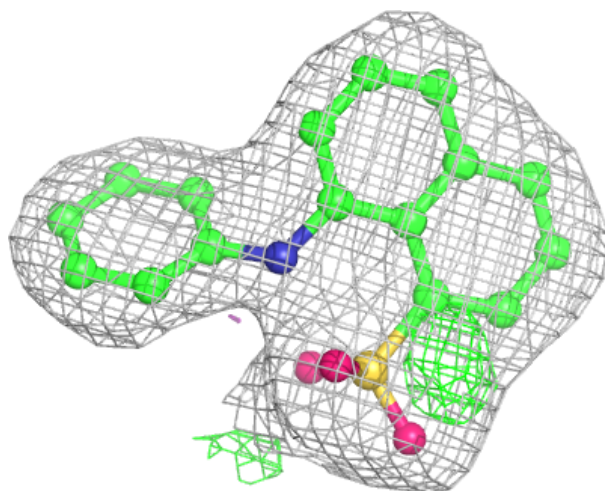
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





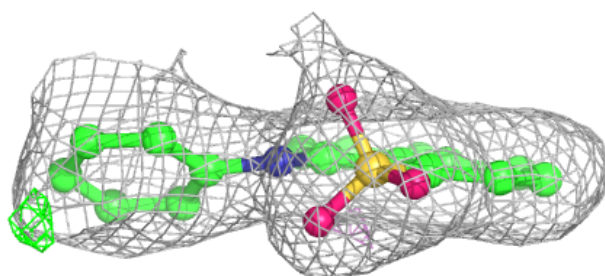
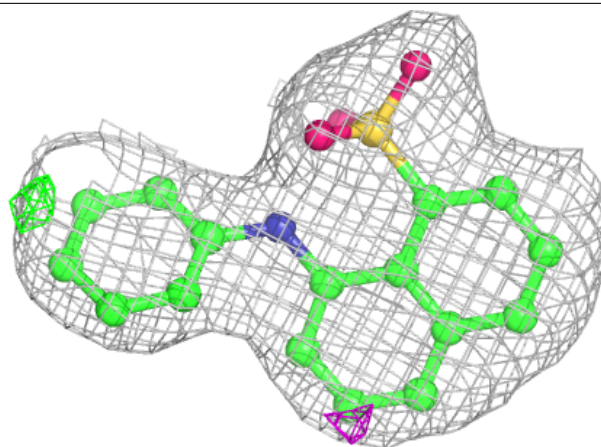
**Electron density around 2AN L 201:**

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



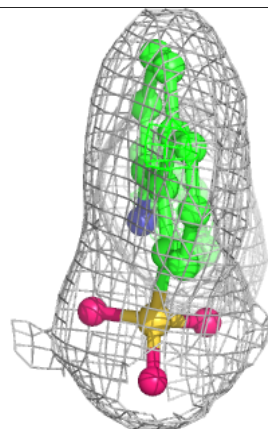
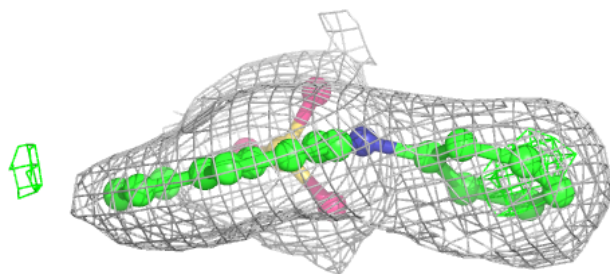
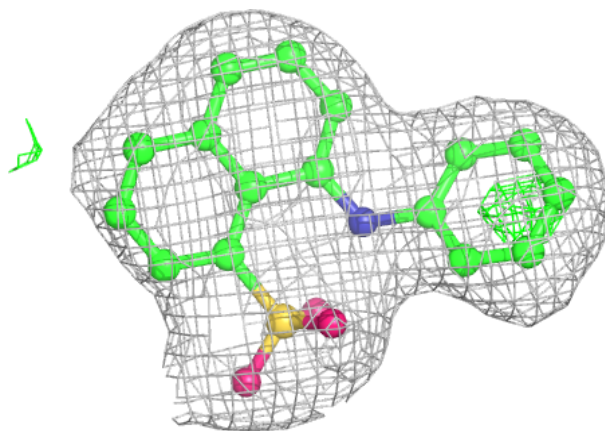
**Electron density around 2AN W 202:**

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



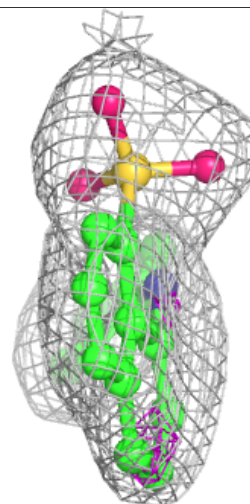
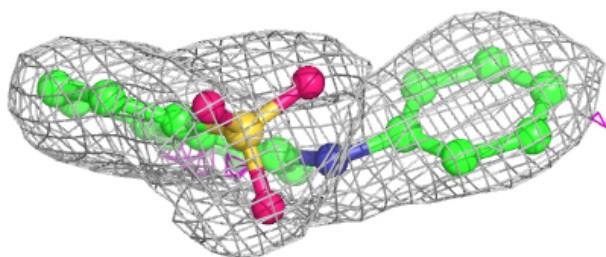
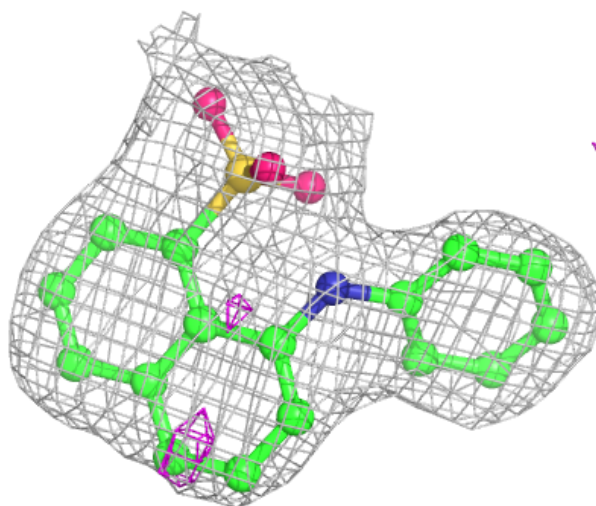
**Electron density around 2AN A 204:**

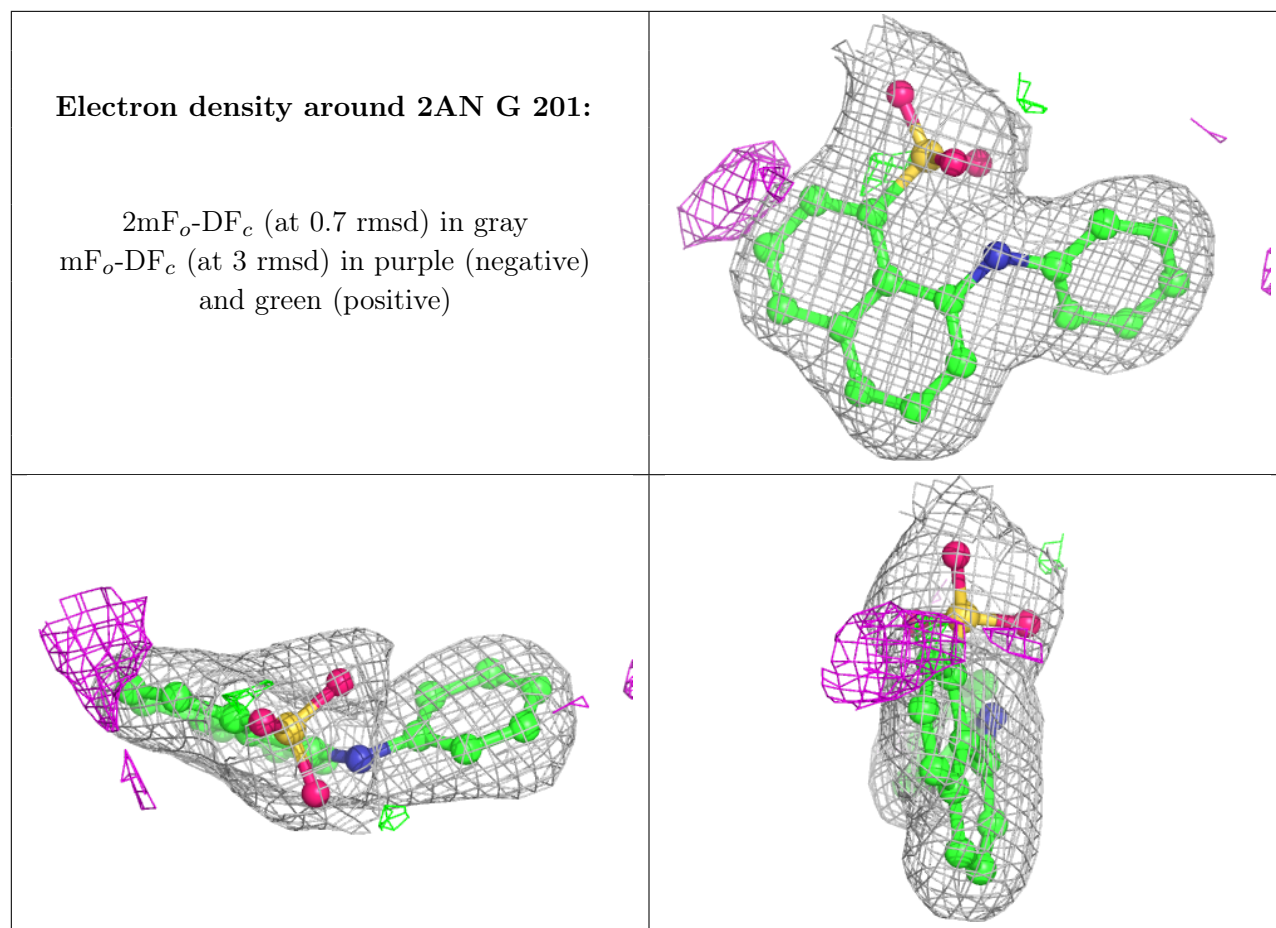
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around 2AN 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)

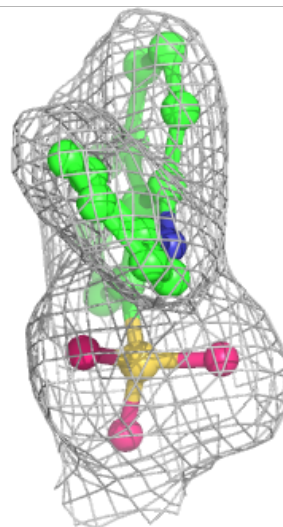
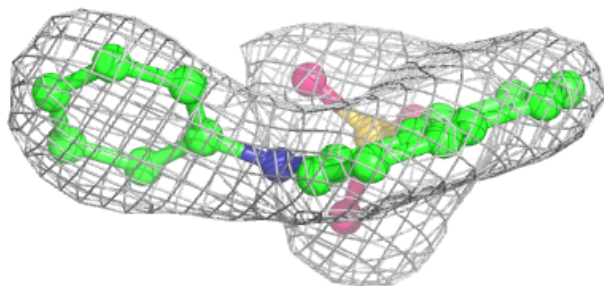
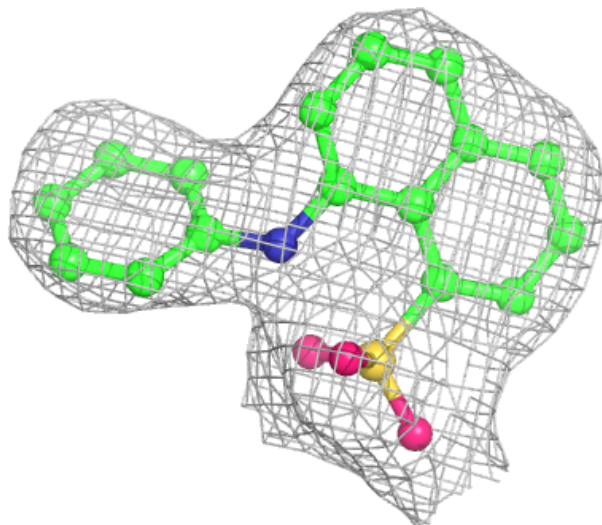






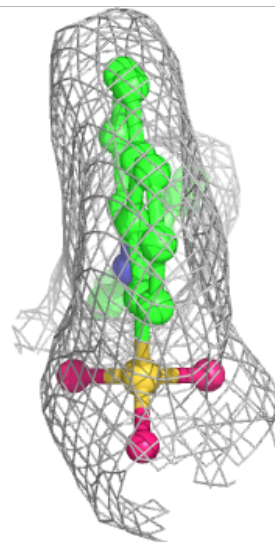
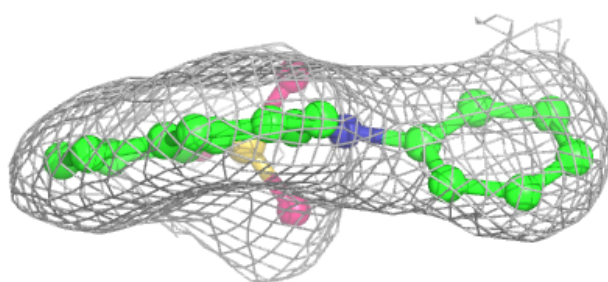
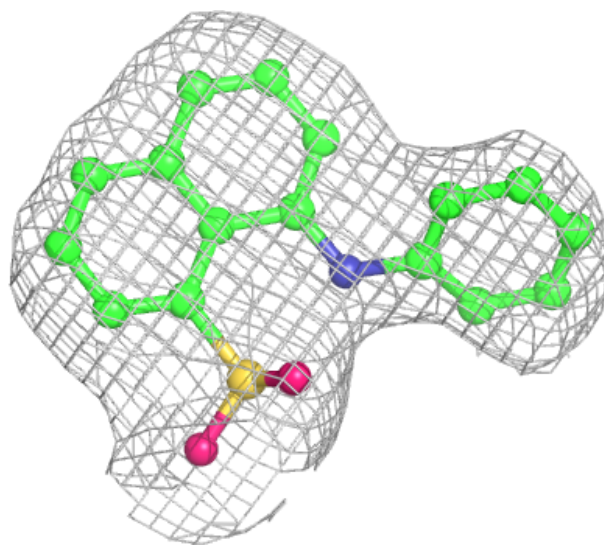
**Electron density around 2AN H 202:**

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



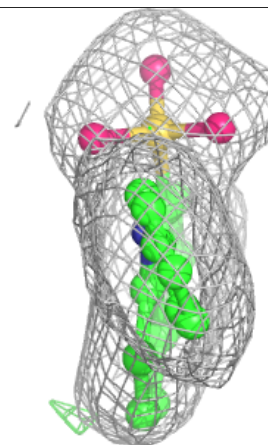
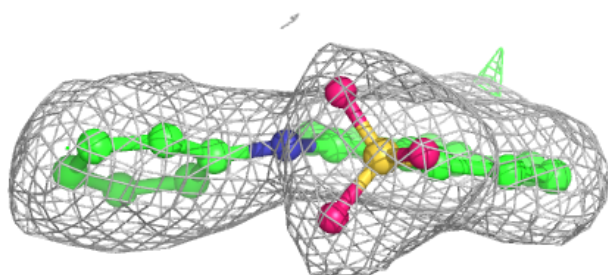
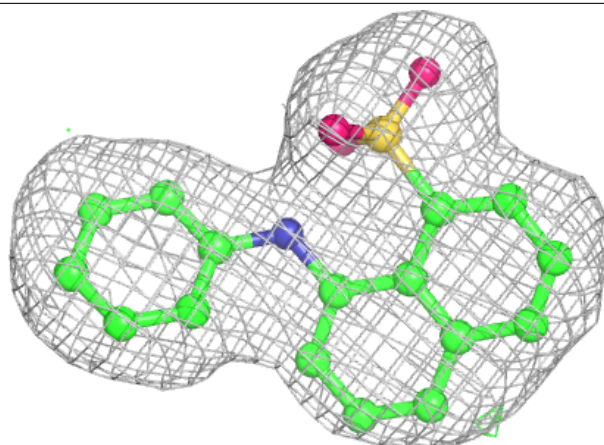
**Electron density around 2AN Q 201:**

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



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

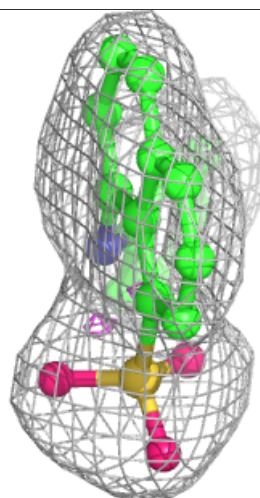
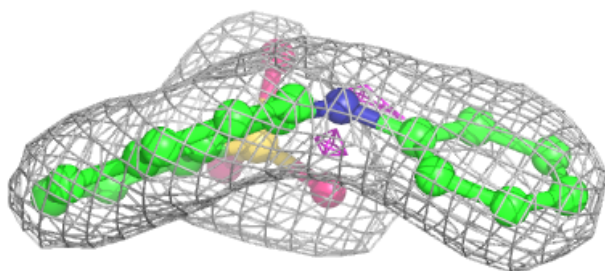
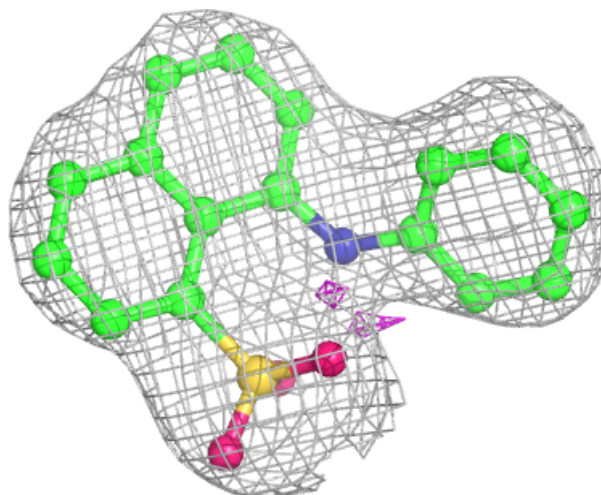
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





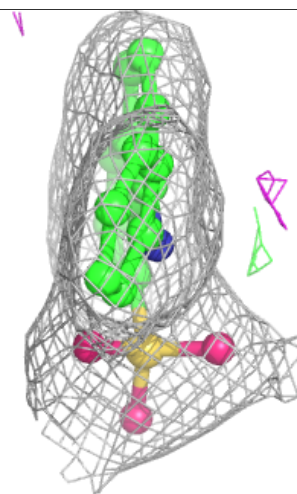
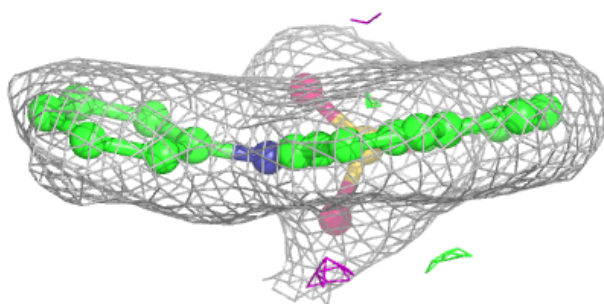
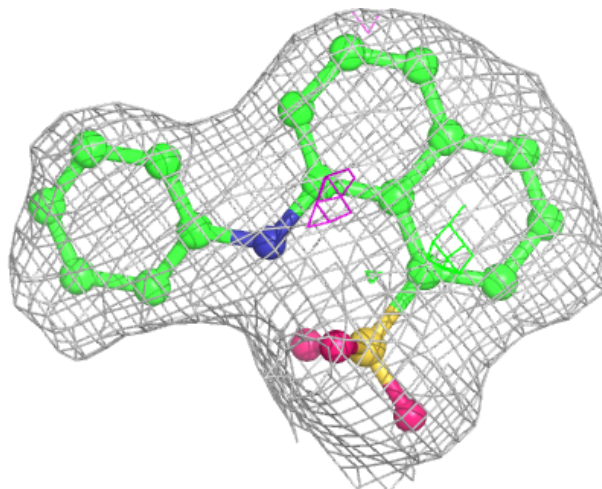
**Electron density around 2AN M 201:**

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



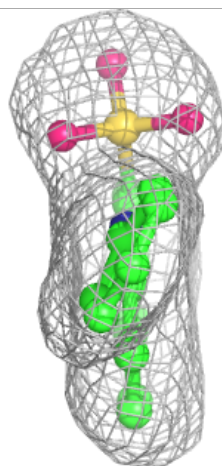
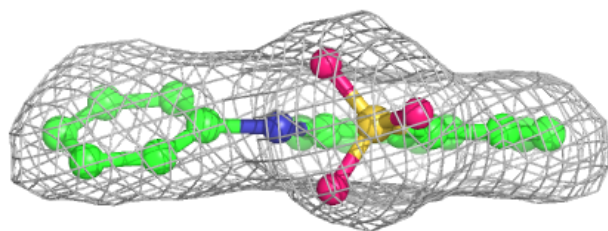
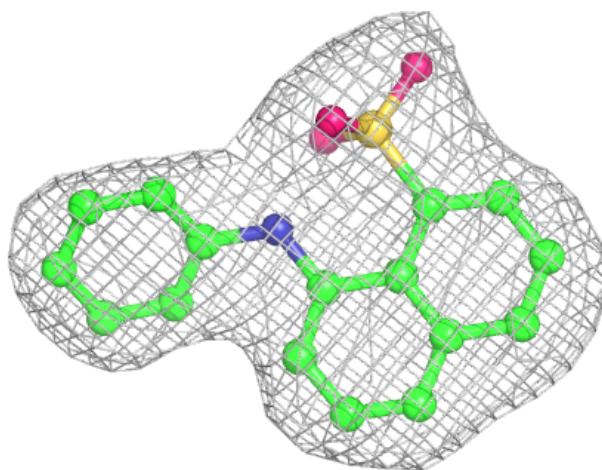
**Electron density around 2AN G 202:**

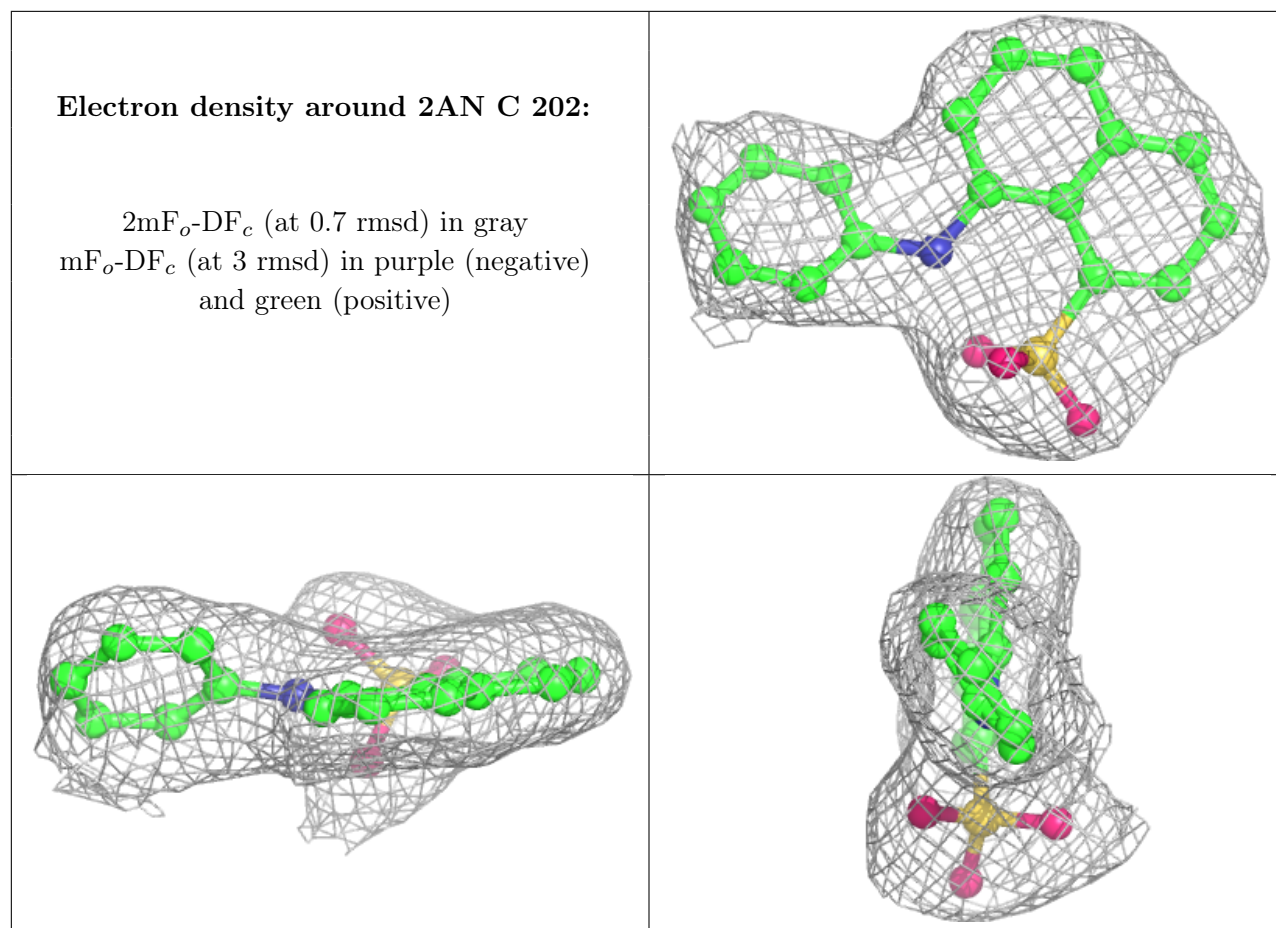
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around 2AN 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)





## 6.5 Other polymers [i](#)

There are no such residues in this entry.