



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 31, 2026 – 12:11 PM UTC

PDB ID : 6SJJ / pdb_00006sjj
Title : A new modulated crystal structure of ANS complex of St John's wort Hyp-1 protein with 36 protein molecules in the asymmetric unit of the supercell
Authors : Smietanska, J.; Sliwiak, J.; Gilski, M.; Dauter, Z.; Strzalka, R.; Wolny, J.; Jaskolski, M.
Deposited on : 2019-08-13
Resolution : 2.30 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

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

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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

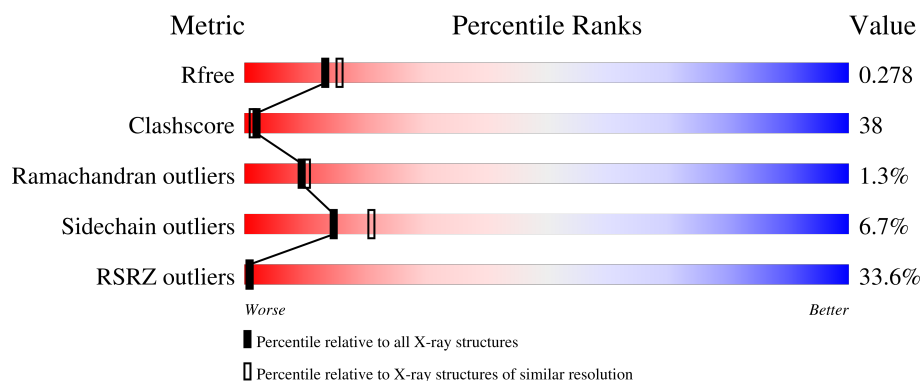
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	163	
1	B	163	
1	C	163	
1	D	163	

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Mol	Chain	Length	Quality of chain
1	E	163	
1	F	163	
1	G	163	
1	H	163	
1	I	163	
1	J	163	
1	K	163	
1	L	163	
1	M	163	
1	N	163	
1	O	163	
1	P	163	
1	Q	163	
1	R	163	
1	S	163	
1	T	163	
1	U	163	
1	V	163	
1	W	163	
1	X	163	
1	Y	163	
1	Z	163	
1	a	163	
1	b	163	
1	c	163	

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	2AN	A	202	-	-	X	-
2	2AN	A	204	-	-	-	X
2	2AN	B	201	-	-	X	-
2	2AN	B	202	-	-	X	-
2	2AN	B	203	-	-	X	-
2	2AN	B	204	-	-	X	-
2	2AN	C	202	-	-	X	-
2	2AN	D	201	-	-	X	-
2	2AN	D	203	-	-	X	-
2	2AN	F	201	-	-	X	-
2	2AN	F	202	-	-	X	-
2	2AN	F	203	-	-	X	-
2	2AN	F	204	-	-	X	-
2	2AN	F	206	-	-	X	-
2	2AN	G	203	-	-	X	-
2	2AN	H	204	-	-	X	-
2	2AN	I	203	-	-	X	-
2	2AN	I	204	-	-	X	-
2	2AN	I	205	-	-	X	-
2	2AN	J	202	-	-	X	-
2	2AN	K	202	-	-	X	-
2	2AN	L	201	-	-	X	-
2	2AN	L	204	-	-	X	-
2	2AN	N	201	-	-	X	-
2	2AN	N	203	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	2AN	N	205	-	-	X	-
2	2AN	O	201	-	-	X	-
2	2AN	P	203	-	-	X	-
2	2AN	R	201	-	-	X	-
2	2AN	R	203	-	-	X	-
2	2AN	R	204	-	-	X	-
2	2AN	R	205	-	-	X	-
2	2AN	S	204	-	-	X	X
2	2AN	T	201	-	-	X	-
2	2AN	T	203	-	-	X	-
2	2AN	U	201	-	-	X	-
2	2AN	V	201	-	-	X	-
2	2AN	V	203	-	-	X	-
2	2AN	V	204	-	-	X	-
2	2AN	V	205	-	-	X	-
2	2AN	V	208	-	-	X	-
2	2AN	X	202	-	-	X	-
2	2AN	X	203	-	-	X	-
2	2AN	X	206	-	-	X	-
2	2AN	Y	201	-	-	X	-
2	2AN	Y	204	-	-	X	-
2	2AN	Z	203	-	-	X	-
2	2AN	Z	206	-	-	X	-
2	2AN	a	203	-	-	X	-
2	2AN	a	204	-	-	X	-
2	2AN	b	201	-	-	X	-
2	2AN	b	202	-	-	X	-
2	2AN	b	203	-	-	X	-
2	2AN	b	204	-	-	X	-
2	2AN	b	205	-	-	X	-
2	2AN	c	201	-	-	X	-
2	2AN	c	202	-	-	X	-
2	2AN	c	206	-	-	X	-
2	2AN	d	201	-	-	X	-
2	2AN	d	202	-	-	X	-
2	2AN	d	204	-	-	X	-
2	2AN	f	202	-	-	X	-
2	2AN	f	204	-	-	X	-
2	2AN	f	205	-	-	X	-
2	2AN	f	206	-	-	X	-
2	2AN	g	202	-	-	X	-
2	2AN	h	202	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	2AN	h	204	-	-	X	-
2	2AN	j	201	-	-	X	-
2	2AN	j	203	-	-	X	-
2	2AN	j	204	-	-	X	-
2	2AN	j	205	-	-	X	-
3	SO4	A	205	-	-	X	-
3	SO4	Y	205	-	-	X	-
5	DMS	X	207	-	-	-	X
6	FLC	G	206	-	X	-	-
6	FLC	j	208	-	-	X	-

2 Entry composition

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

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called PR-10 protein.

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

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

There are 144 discrepancies between the modelled and reference sequences:

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

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

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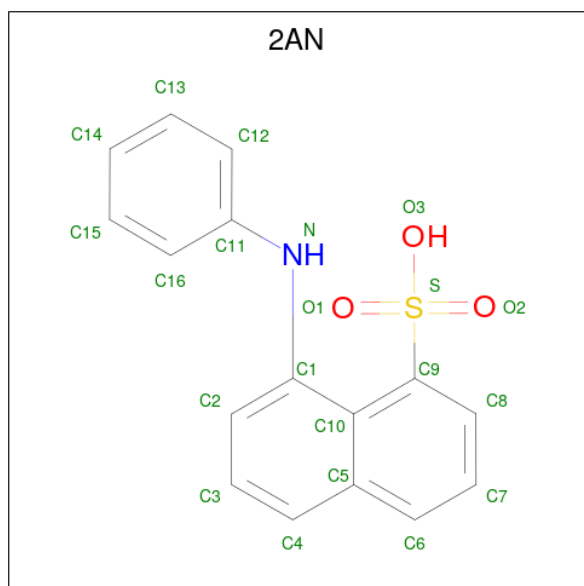
Chain	Residue	Modelled	Actual	Comment	Reference
c	-2	PRO	-	expression tag	UNP A0A160HRF0
c	-1	PHE	-	expression tag	UNP A0A160HRF0
c	0	THR	-	expression tag	UNP A0A160HRF0
b	-3	ASP	-	expression tag	UNP A0A160HRF0
b	-2	PRO	-	expression tag	UNP A0A160HRF0
b	-1	PHE	-	expression tag	UNP A0A160HRF0
b	0	THR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

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

- Molecule 2 is 8-ANILINO-1-NAPHTHALENE SULFONATE (CCD ID: 2AN) (formula: $C_{16}H_{13}NO_3S$) (labeled as "Ligand of Interest" by depositor).



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

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

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

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

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

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

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

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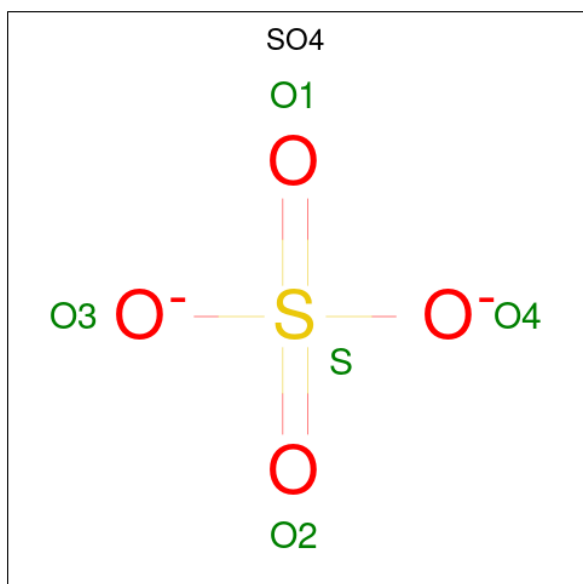
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	V	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	U	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	U	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	T	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	T	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	T	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	T	1	Total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

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

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



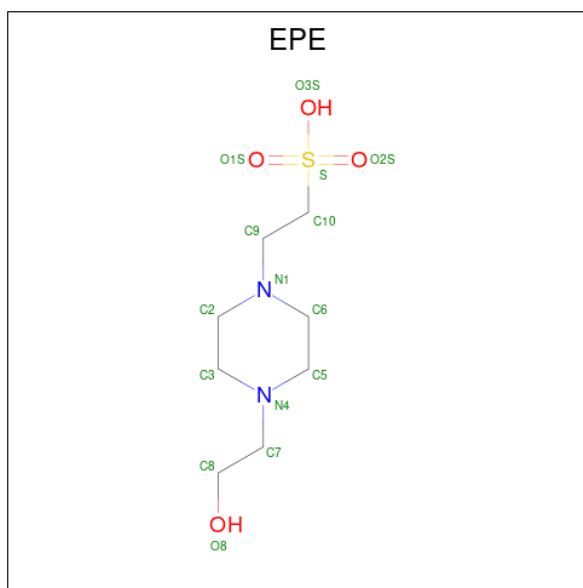
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	Q	1	Total	O	S	0	0
			5	4	1		
3	I	1	Total	O	S	0	0
			5	4	1		

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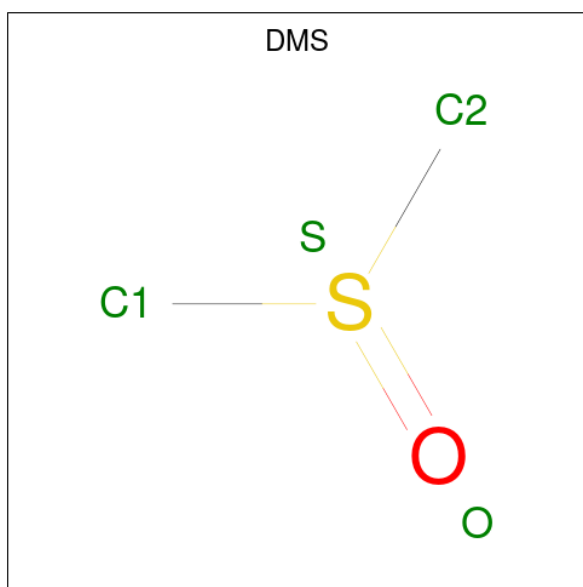
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	G	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	c	1	Total	O	S	0	0
			5	4	1		
3	c	1	Total	O	S	0	0
			5	4	1		
3	c	1	Total	O	S	0	0
			5	4	1		
3	Y	1	Total	O	S	0	0
			5	4	1		
3	g	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (CCD ID: EPE) (formula: $C_8H_{18}N_2O_4S$).



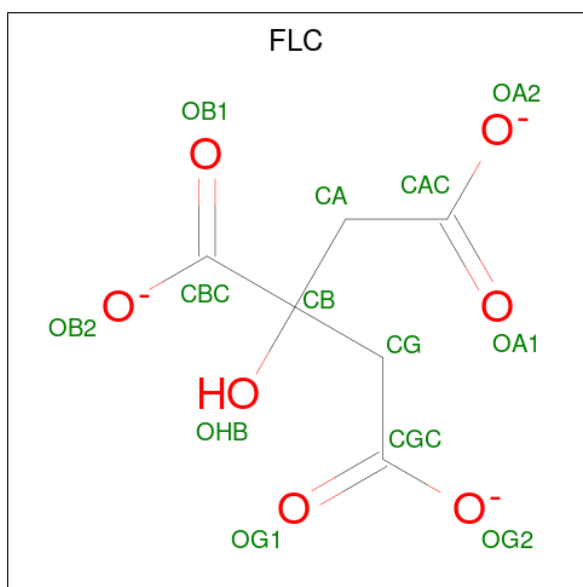
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	P	1	Total	C	N	O	S	0
			15	8	2	4	1	0

- Molecule 5 is DIMETHYL SULFOXIDE (CCD ID: DMS) (formula: C_2H_6OS).



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

- Molecule 6 is CITRATE ANION (CCD ID: FLC) (formula: $C_6H_5O_7$).



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

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

- Molecule 7 is water.

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

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

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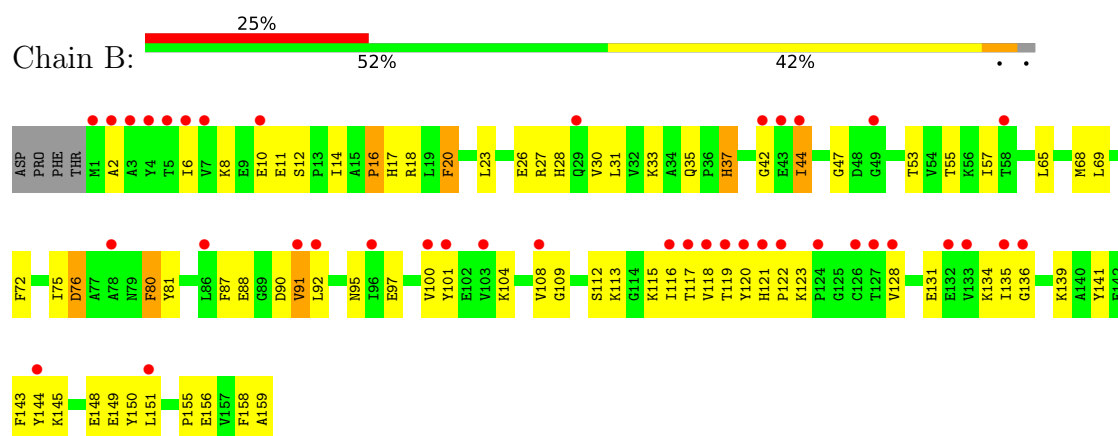
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	g	4	Total	O	0	0
			4	4		

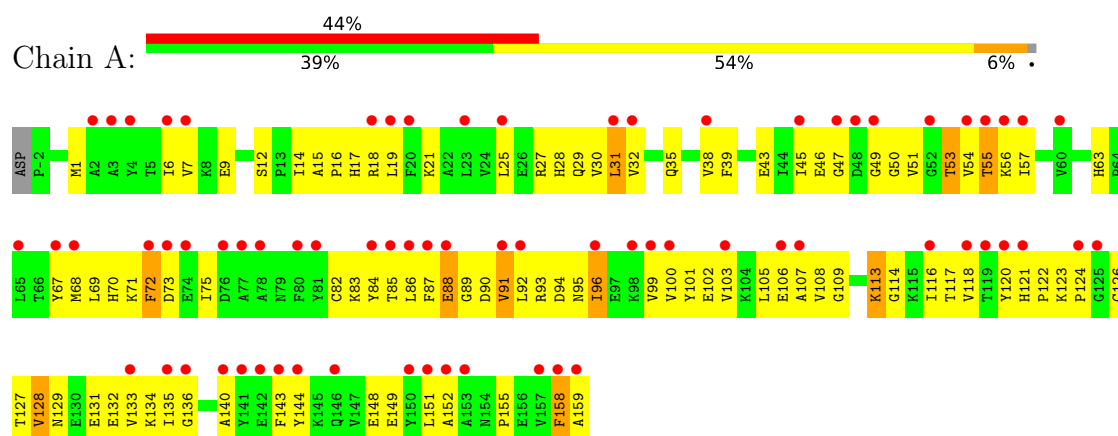
3 Residue-property plots [i](#)

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

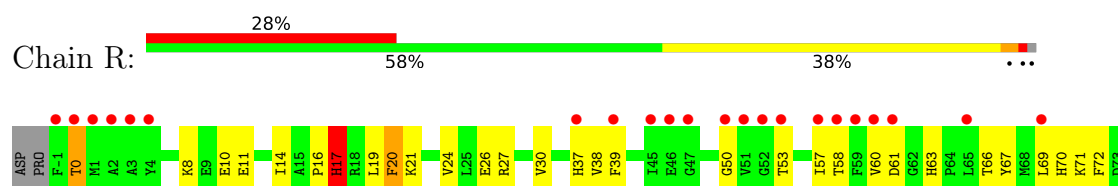
• Molecule 1: PR-10 protein

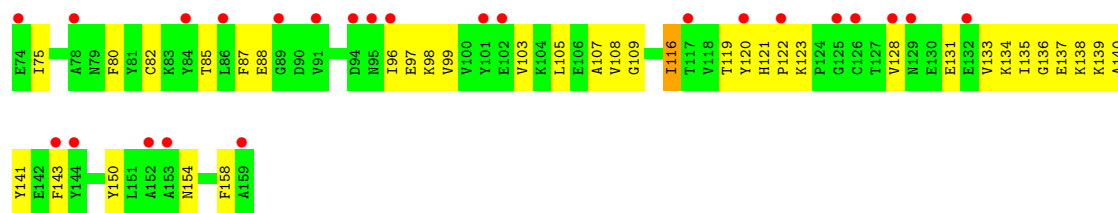


• Molecule 1: PR-10 protein

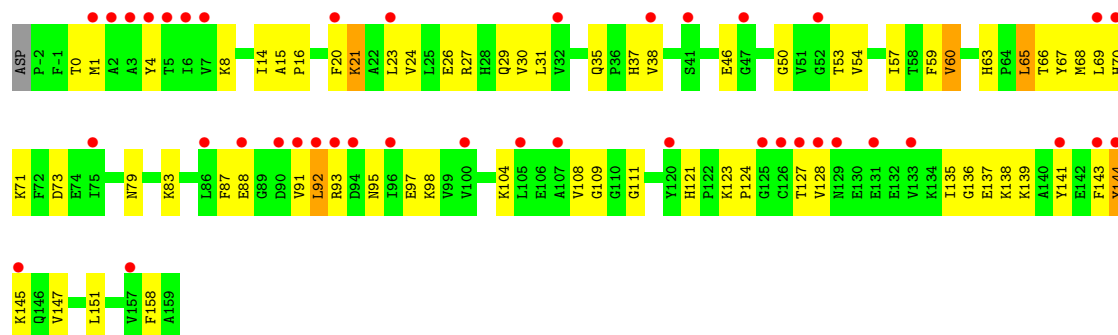


• Molecule 1: PR-10 protein

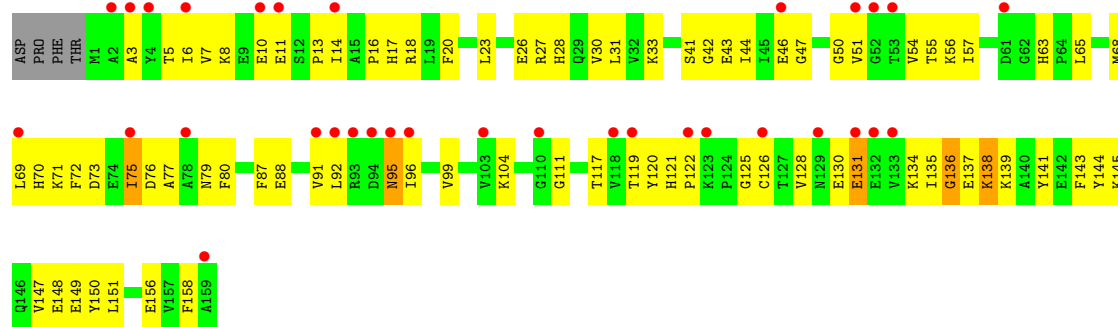




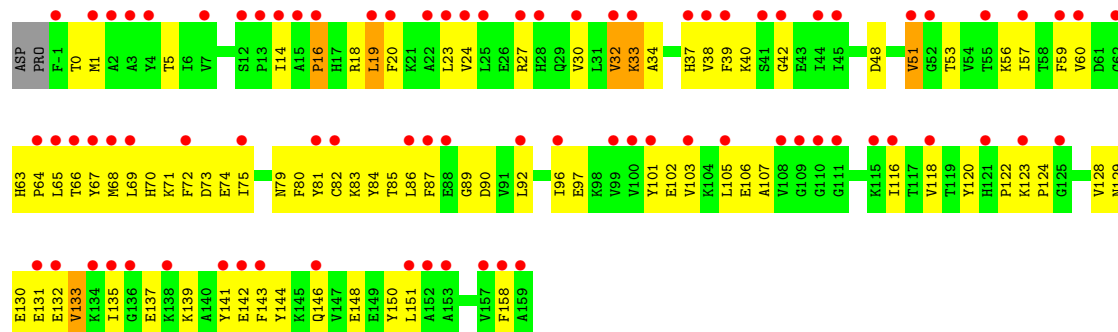
• Molecule 1: PR-10 protein



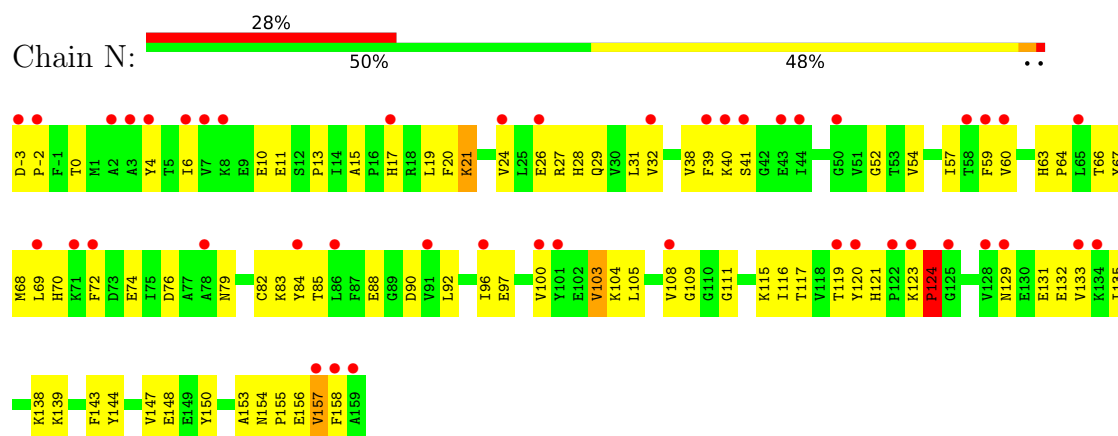
• Molecule 1: PR-10 protein



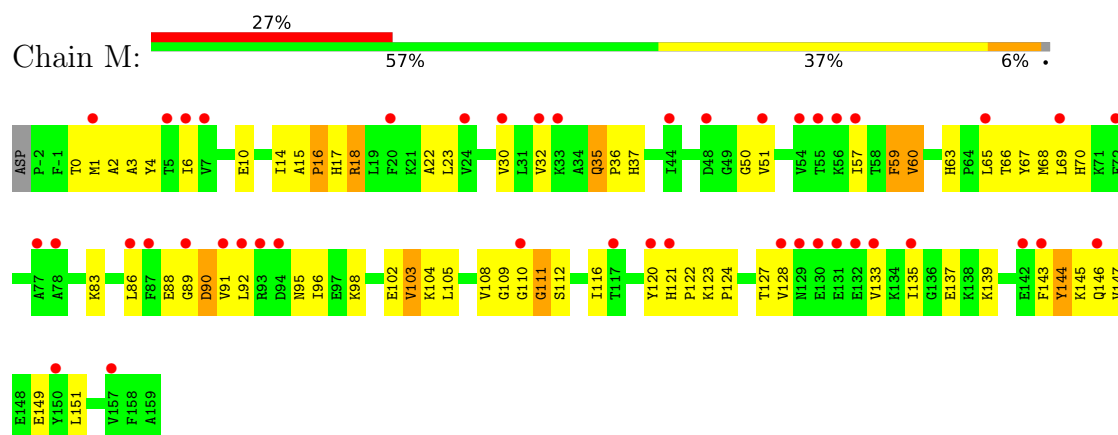
• Molecule 1: PR-10 protein



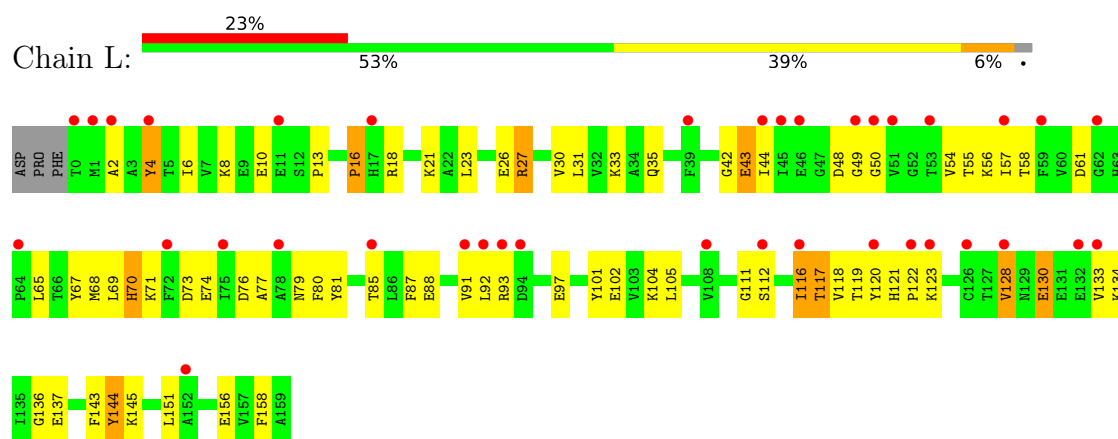
- Molecule 1: PR-10 protein



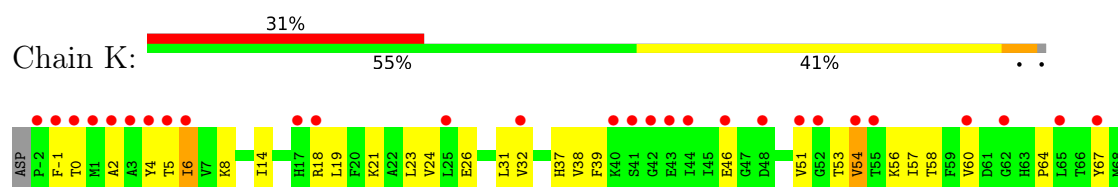
- Molecule 1: PR-10 protein

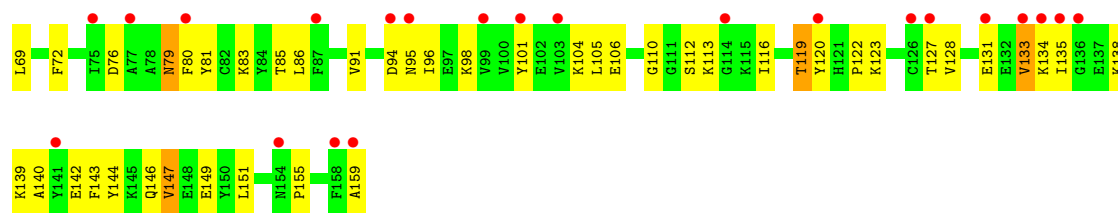


- Molecule 1: PR-10 protein

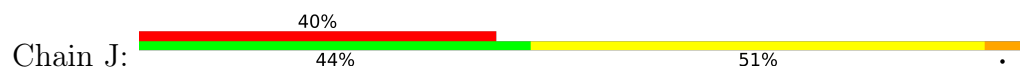


- Molecule 1: PR-10 protein

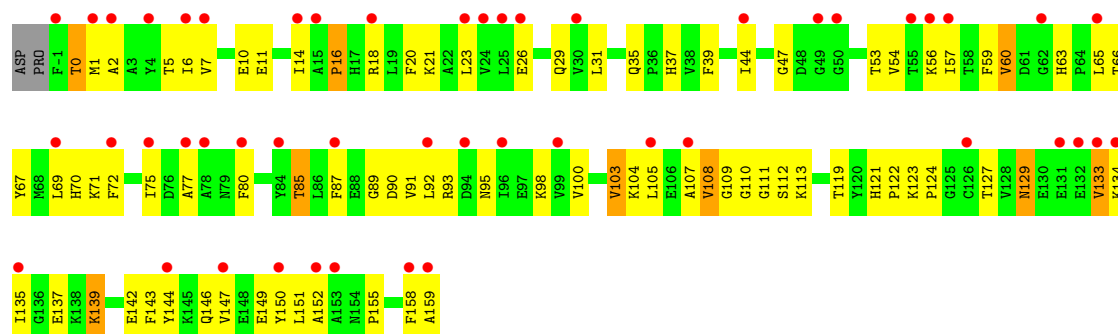




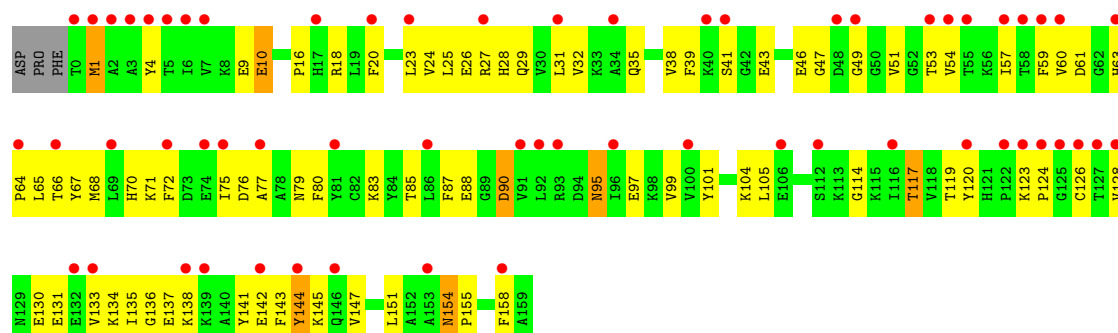
● Molecule 1: PR-10 protein



● Molecule 1: PR-10 protein

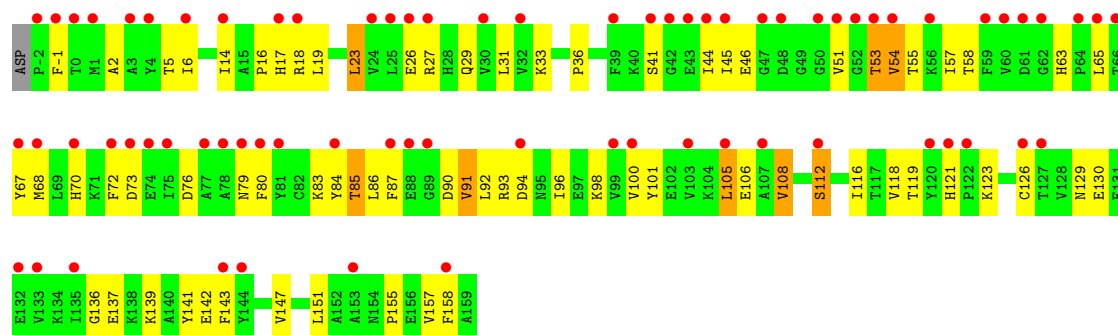


● Molecule 1: PR-10 protein



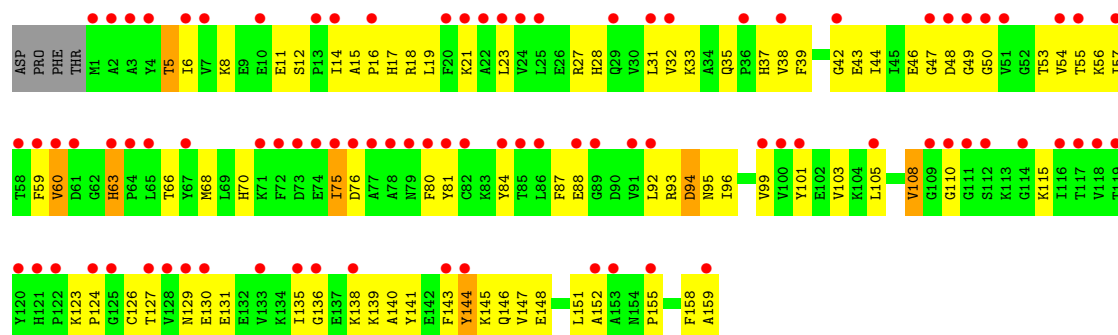
- Molecule 1: PR-10 protein

Chain G: 



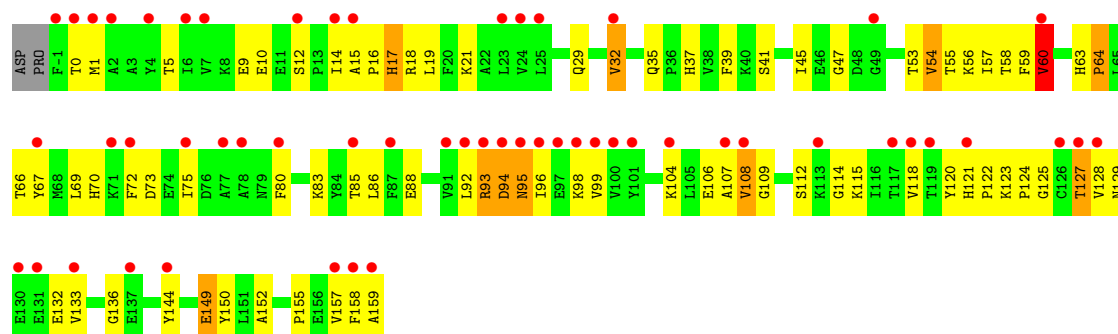
- Molecule 1: PR-10 protein

Chain F: 



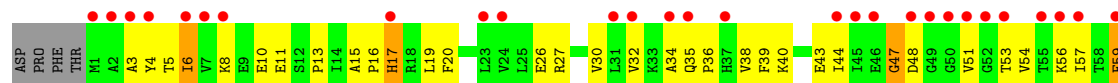
- Molecule 1: PR-10 protein

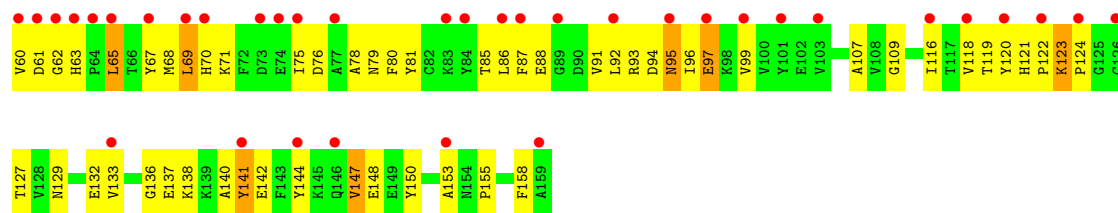
Chain E: 



- Molecule 1: PR-10 protein

Chain D: 

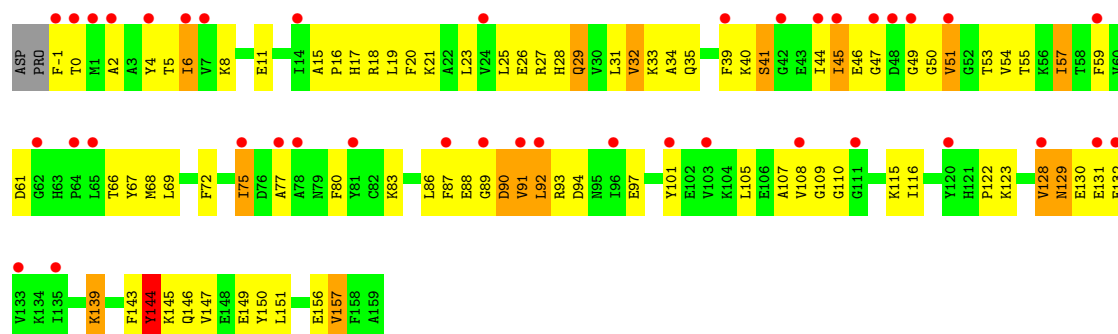
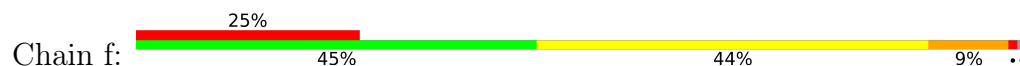




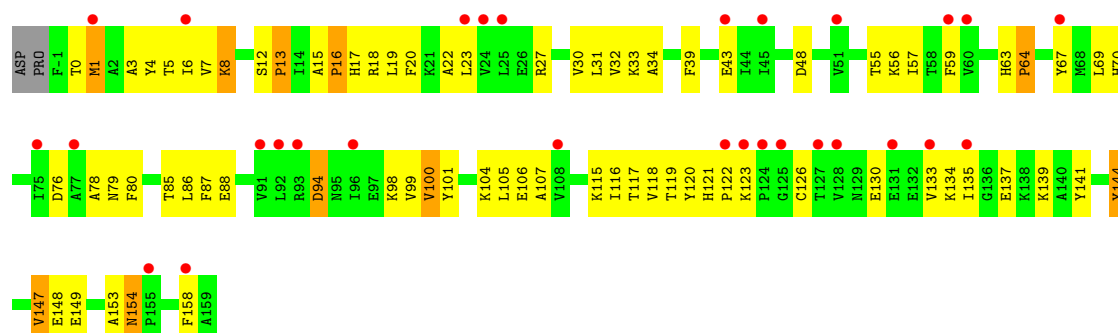
● Molecule 1: PR-10 protein



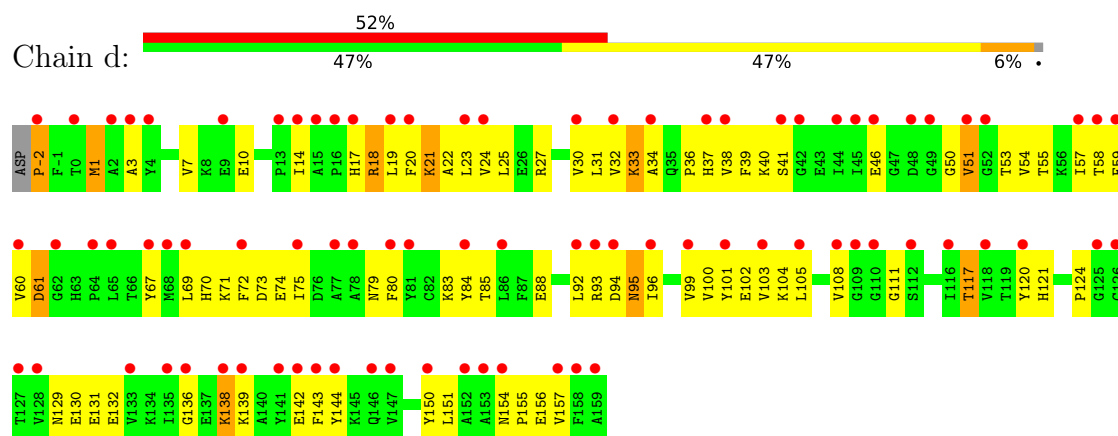
● Molecule 1: PR-10 protein



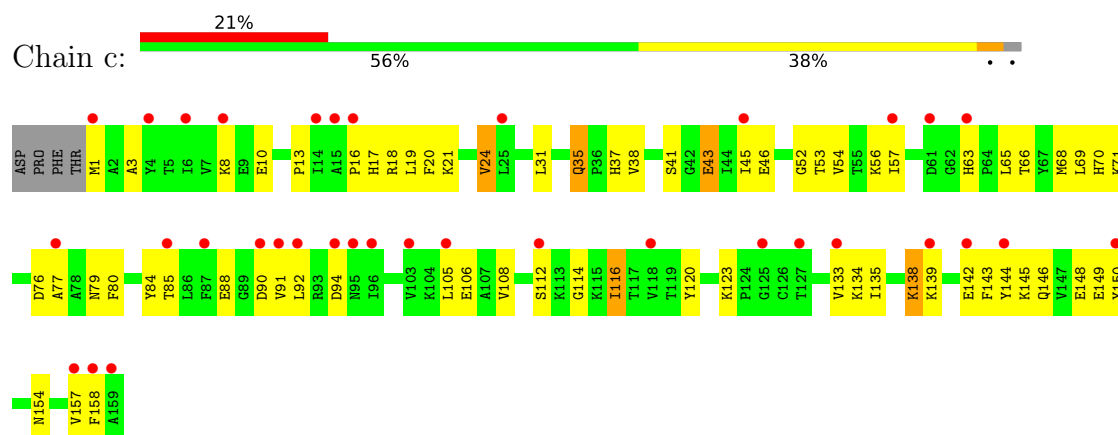
● Molecule 1: PR-10 protein



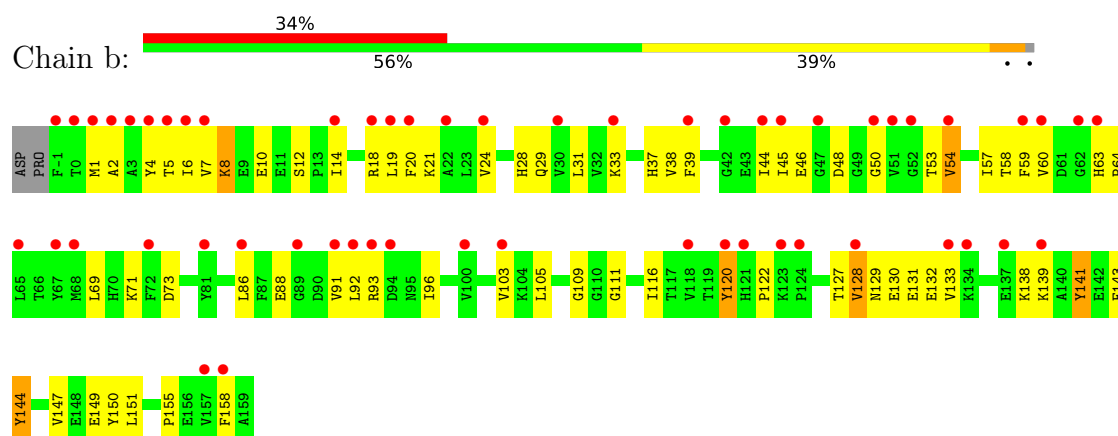
- Molecule 1: PR-10 protein



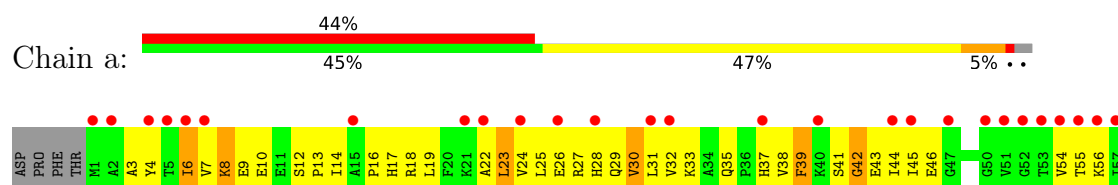
- Molecule 1: PR-10 protein



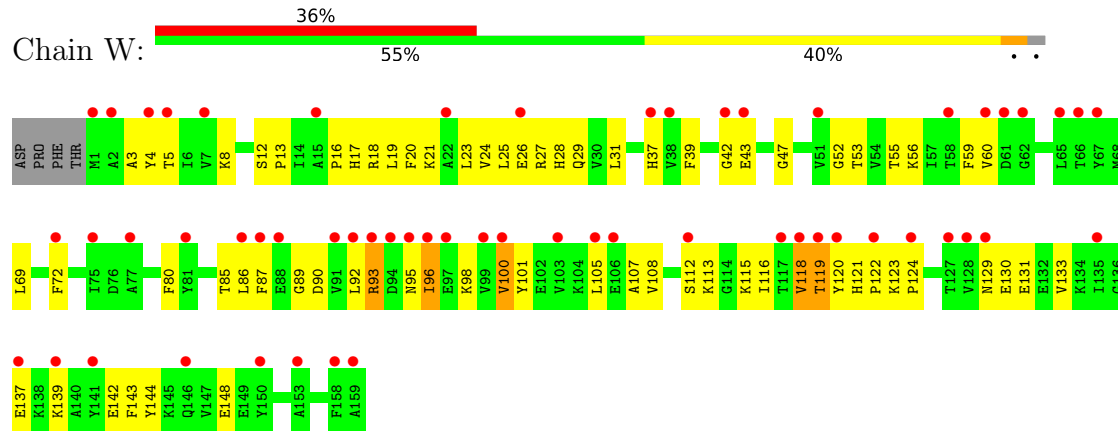
- Molecule 1: PR-10 protein



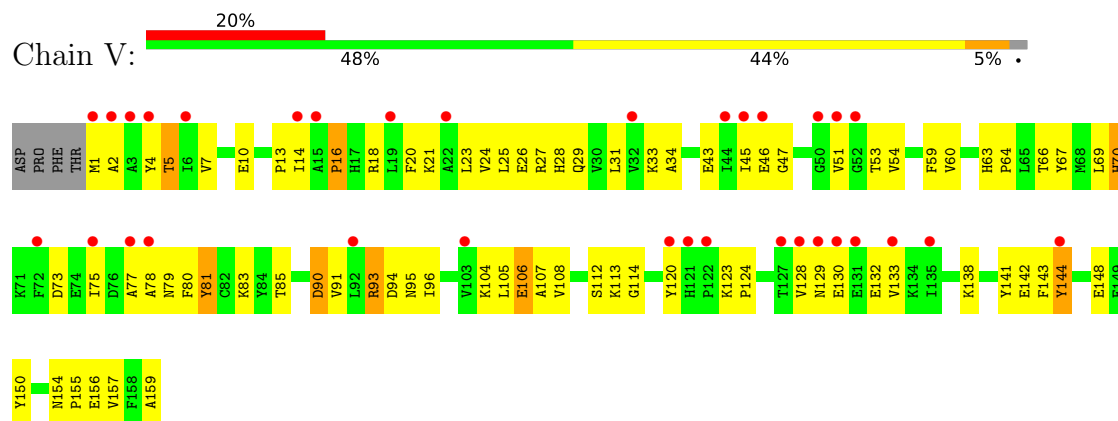
- Molecule 1: PR-10 protein



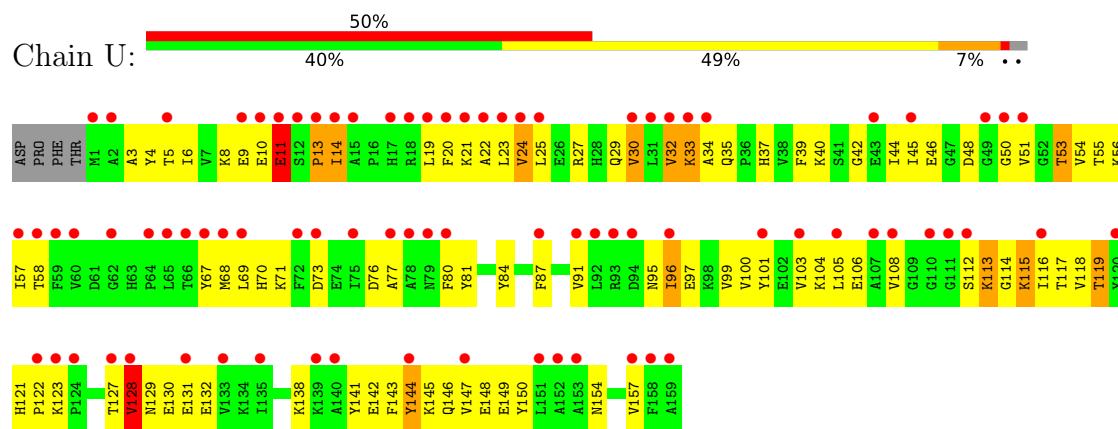
- Molecule 1: PR-10 protein



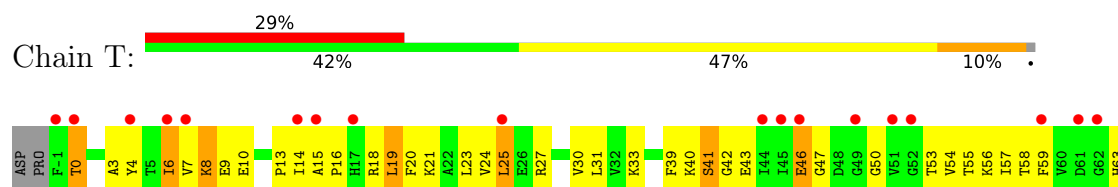
- Molecule 1: PR-10 protein

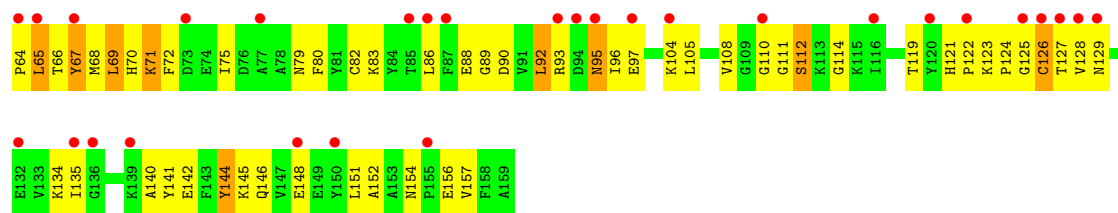


- Molecule 1: PR-10 protein

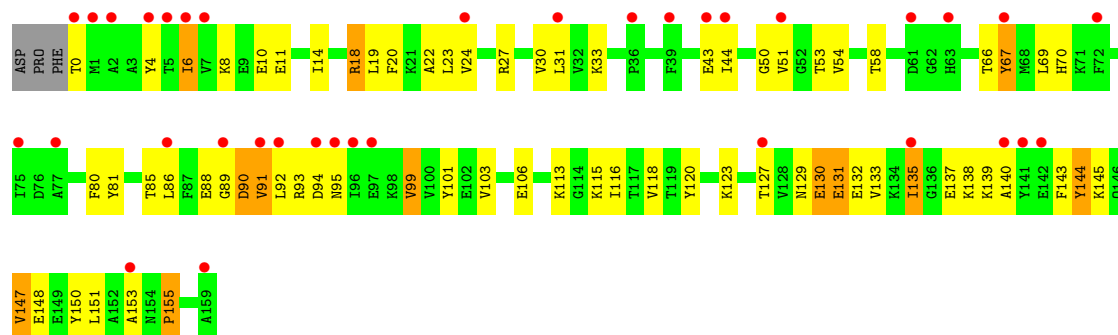


- Molecule 1: PR-10 protein

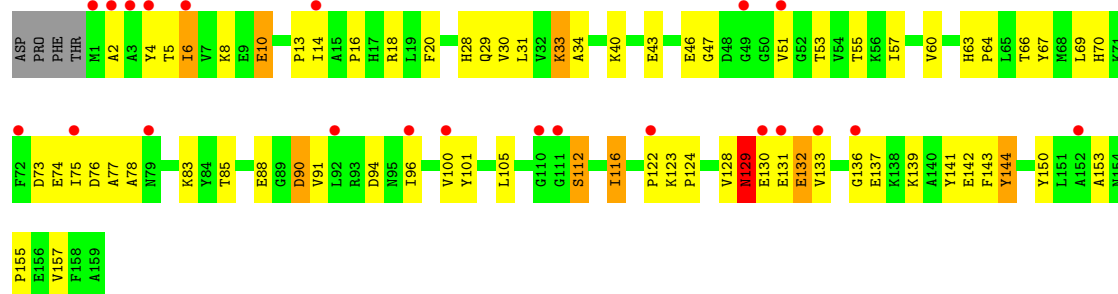




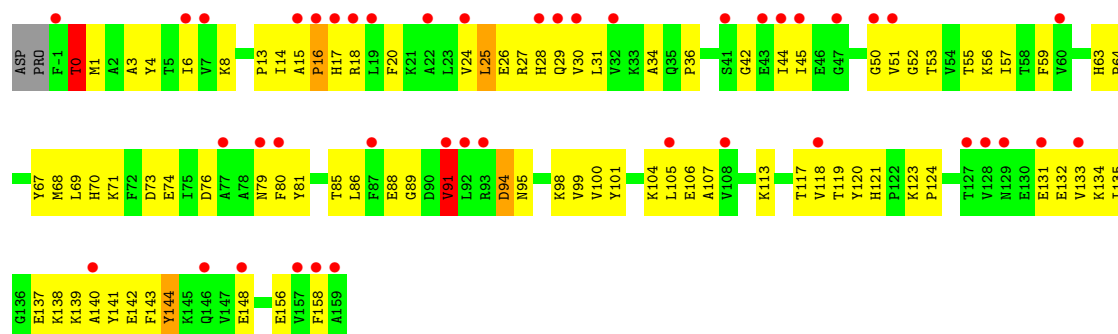
● Molecule 1: PR-10 protein



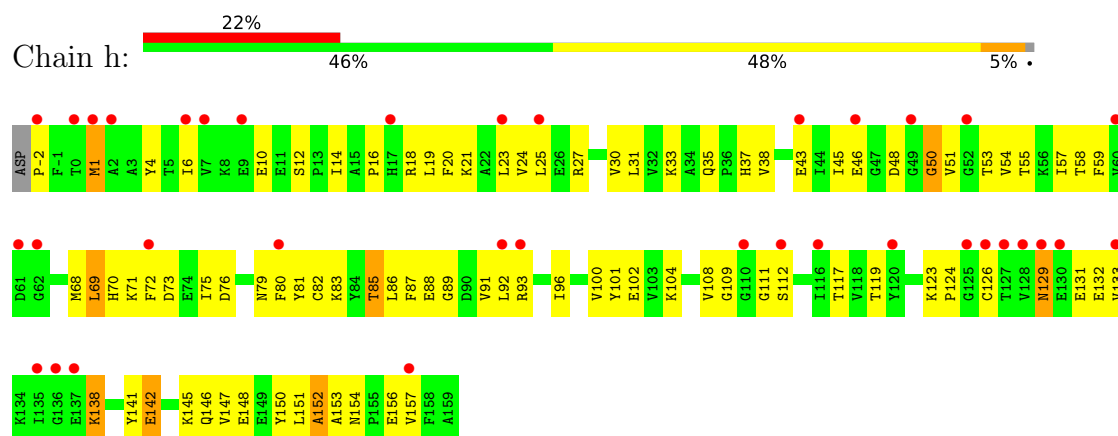
● Molecule 1: PR-10 protein



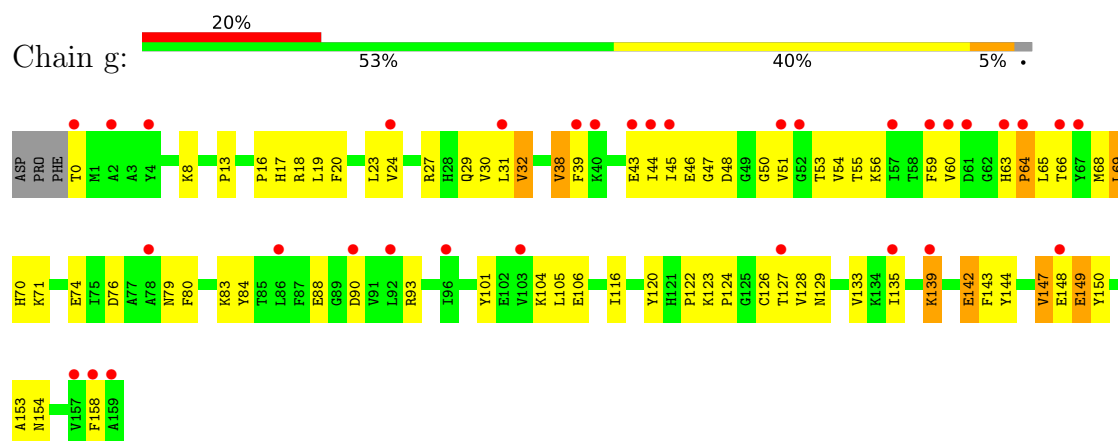
● Molecule 1: PR-10 protein



- Molecule 1: PR-10 protein



- Molecule 1: PR-10 protein



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	145.85Å 145.85Å 385.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	31.58 – 2.30 31.58 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.3 (31.58-2.30) 99.4 (31.58-2.30)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.23 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.8.0222	Depositor
R, R_{free}	0.226 , 0.255 0.270 , 0.278	Depositor DCC
R_{free} test set	3979 reflections (1.11%)	wwPDB-VP
Wilson B-factor (Å ²)	57.8	Xtriage
Anisotropy	0.131	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 63.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.064 for k,h,-l 0.054 for -k,-h,-l 0.084 for -h,-k,l	Xtriage
Reported twinning fraction	0.241 for H, K, L 0.242 for K, H, -L 0.233 for -K, -H, -L 0.284 for h,-k,-l	Depositor
Outliers	18 of 357481 reflections (0.005%)	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	48343	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

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

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.83	0/1233	1.26	5/1682 (0.3%)
1	B	0.89	3/1273 (0.2%)	1.27	5/1722 (0.3%)
1	C	0.75	0/1263	1.14	0/1709
1	D	0.80	0/1252	1.29	8/1697 (0.5%)
1	E	0.97	2/1279 (0.2%)	1.29	1/1731 (0.1%)
1	F	0.84	1/1215 (0.1%)	1.23	1/1649 (0.1%)
1	G	0.90	0/1262	1.20	3/1712 (0.2%)
1	H	0.89	1/1261 (0.1%)	1.29	6/1709 (0.4%)
1	I	0.99	5/1282 (0.4%)	1.25	4/1734 (0.2%)
1	J	0.82	0/1287	1.33	7/1746 (0.4%)
1	K	0.95	1/1297 (0.1%)	1.27	5/1755 (0.3%)
1	L	0.90	0/1285	1.25	2/1738 (0.1%)
1	M	0.93	3/1301 (0.2%)	1.23	2/1760 (0.1%)
1	N	0.92	0/1295	1.40	7/1757 (0.4%)
1	O	0.87	0/1242	1.27	6/1684 (0.4%)
1	P	1.03	2/1278 (0.2%)	1.39	8/1729 (0.5%)
1	Q	0.84	0/1296	1.24	3/1753 (0.2%)
1	R	0.93	3/1280 (0.2%)	1.28	1/1732 (0.1%)
1	S	0.93	2/1282 (0.2%)	1.26	2/1733 (0.1%)
1	T	0.91	0/1291	1.34	8/1747 (0.5%)
1	U	0.80	0/1246	1.22	3/1690 (0.2%)
1	V	0.97	3/1275 (0.2%)	1.29	2/1726 (0.1%)
1	W	0.85	0/1249	1.16	0/1689
1	X	0.83	0/1254	1.31	3/1697 (0.2%)
1	Y	0.83	0/1256	1.21	4/1699 (0.2%)
1	Z	0.86	1/1246 (0.1%)	1.20	0/1687
1	a	0.91	0/1253	1.32	3/1695 (0.2%)
1	b	0.79	0/1274	1.24	1/1727 (0.1%)
1	c	0.95	2/1277 (0.2%)	1.30	1/1725 (0.1%)
1	d	0.80	0/1284	1.26	1/1735 (0.1%)
1	e	0.94	3/1282 (0.2%)	1.29	3/1734 (0.2%)
1	f	0.96	2/1292 (0.2%)	1.29	6/1748 (0.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	g	0.84	2/1286 (0.2%)	1.27	4/1738 (0.2%)
1	h	0.92	0/1294	1.29	2/1749 (0.1%)
1	i	0.92	2/1279 (0.2%)	1.29	7/1730 (0.4%)
1	j	1.04	1/1272 (0.1%)	1.38	5/1722 (0.3%)
All	All	0.90	39/45773 (0.1%)	1.27	129/61970 (0.2%)

The worst 5 of 39 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	63	HIS	N-CA	7.87	1.54	1.45
1	g	56	LYS	C-O	-7.59	1.15	1.24
1	P	20	PHE	N-CA	-7.01	1.37	1.46
1	S	147	VAL	C-O	-6.67	1.16	1.24
1	E	37	HIS	N-CA	-6.43	1.37	1.46

The worst 5 of 129 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	41	SER	CA-C-N	8.89	127.70	121.65
1	H	41	SER	C-N-CA	8.89	127.70	121.65
1	i	0	THR	CB-CA-C	8.37	123.34	109.53
1	A	90	ASP	CA-CB-CG	6.98	119.58	112.60
1	Q	92	LEU	N-CA-C	-6.81	99.96	110.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1204	0	1098	133	0
1	B	1244	0	1232	74	0
1	C	1235	0	1201	83	0
1	D	1223	0	1185	116	0
1	E	1250	0	1224	78	0
1	F	1188	0	1101	97	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	1232	0	1183	93	0
1	H	1232	0	1183	90	0
1	I	1253	0	1234	85	0
1	J	1257	0	1204	92	0
1	K	1266	0	1247	63	0
1	L	1256	0	1245	66	0
1	M	1271	0	1256	72	0
1	N	1265	0	1222	77	0
1	O	1215	0	1153	78	0
1	P	1249	0	1233	80	0
1	Q	1266	0	1252	65	0
1	R	1252	0	1233	75	0
1	S	1253	0	1250	81	0
1	T	1261	0	1230	91	0
1	U	1218	0	1178	124	0
1	V	1246	0	1222	94	0
1	W	1220	0	1178	68	0
1	X	1226	0	1190	125	0
1	Y	1227	0	1176	78	0
1	Z	1218	0	1159	79	0
1	a	1224	0	1175	94	0
1	b	1244	0	1200	79	0
1	c	1248	0	1233	65	0
1	d	1254	0	1223	112	0
1	e	1253	0	1227	77	0
1	f	1262	0	1238	95	0
1	g	1257	0	1252	59	0
1	h	1264	0	1237	92	0
1	i	1250	0	1225	85	0
1	j	1243	0	1222	83	0
2	A	84	0	48	15	0
2	B	126	0	73	44	0
2	C	63	0	37	18	0
2	D	84	0	49	31	0
2	E	84	0	48	16	0
2	F	126	0	74	66	0
2	G	126	0	74	28	0
2	H	84	0	50	24	0
2	I	147	0	85	46	0
2	J	63	0	37	19	0
2	K	63	0	38	22	0
2	L	84	0	49	27	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	M	63	0	37	10	0
2	N	105	0	64	30	0
2	O	63	0	36	22	0
2	P	84	0	51	23	0
2	Q	63	0	36	12	0
2	R	105	0	63	41	0
2	S	84	0	48	27	0
2	T	105	0	62	38	0
2	U	42	0	25	12	0
2	V	168	0	99	77	0
2	W	21	0	12	6	0
2	X	126	0	72	83	0
2	Y	84	0	49	30	0
2	Z	126	0	74	38	0
2	a	84	0	48	33	0
2	b	126	0	74	51	0
2	c	126	0	74	30	0
2	d	84	0	49	45	0
2	e	21	0	13	4	0
2	f	126	0	73	44	0
2	g	63	0	37	16	0
2	h	126	0	74	39	0
2	i	21	0	13	3	0
2	j	147	0	84	44	0
3	A	5	0	0	6	0
3	E	5	0	0	0	0
3	G	5	0	0	0	0
3	I	5	0	0	0	0
3	Q	5	0	0	0	0
3	Y	5	0	0	2	0
3	c	15	0	0	1	0
3	g	5	0	0	1	0
4	P	15	0	18	6	0
5	G	4	0	6	1	0
5	N	4	0	6	2	0
5	X	4	0	6	0	0
6	G	13	0	5	2	0
6	a	26	0	10	1	0
6	e	13	0	5	1	0
6	i	26	0	10	3	0
6	j	13	0	5	9	0
7	A	6	0	0	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	B	5	0	0	0	0
7	C	4	0	0	6	0
7	D	3	0	0	0	0
7	E	5	0	0	3	0
7	F	1	0	0	1	0
7	G	5	0	0	3	0
7	H	3	0	0	0	0
7	I	5	0	0	1	0
7	J	2	0	0	2	0
7	K	6	0	0	1	0
7	L	3	0	0	0	0
7	M	1	0	0	1	0
7	N	3	0	0	0	0
7	O	4	0	0	1	0
7	P	5	0	0	1	0
7	Q	1	0	0	0	0
7	R	3	0	0	1	0
7	S	1	0	0	0	0
7	T	5	0	0	1	0
7	V	9	0	0	2	0
7	W	2	0	0	0	0
7	X	3	0	0	6	0
7	Y	4	0	0	0	0
7	Z	4	0	0	5	0
7	a	8	0	0	1	0
7	b	6	0	0	1	0
7	c	3	0	0	0	0
7	d	2	0	0	1	0
7	e	9	0	0	2	0
7	f	8	0	0	1	0
7	g	4	0	0	0	0
7	h	8	0	0	2	0
7	i	6	0	0	2	0
7	j	5	0	0	0	0
All	All	48343	0	45501	3588	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 38.

The worst 5 of 3588 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:27:ARG:NH1	2:S:204:2AN:H8	1.39	1.34
1:Y:94:ASP:O	1:Y:123:LYS:HD3	1.30	1.28
1:H:138:LYS:HE2	1:G:-1:PHE:CE1	1.69	1.26
1:a:84:TYR:OH	2:a:204:2AN:H6	1.36	1.25
1:X:10:GLU:CG	2:X:206:2AN:H13	1.65	1.24

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	160/163 (98%)	137 (86%)	20 (12%)	3 (2%)	6	5
1	B	157/163 (96%)	134 (85%)	21 (13%)	2 (1%)	9	10
1	C	159/163 (98%)	141 (89%)	16 (10%)	2 (1%)	9	10
1	D	157/163 (96%)	122 (78%)	30 (19%)	5 (3%)	3	2
1	E	159/163 (98%)	134 (84%)	21 (13%)	4 (2%)	4	3
1	F	157/163 (96%)	142 (90%)	12 (8%)	3 (2%)	6	5
1	G	160/163 (98%)	137 (86%)	22 (14%)	1 (1%)	21	27
1	H	158/163 (97%)	145 (92%)	13 (8%)	0	100	100
1	I	159/163 (98%)	143 (90%)	13 (8%)	3 (2%)	6	5
1	J	161/163 (99%)	138 (86%)	22 (14%)	1 (1%)	21	27
1	K	160/163 (98%)	148 (92%)	10 (6%)	2 (1%)	9	10
1	L	158/163 (97%)	142 (90%)	13 (8%)	3 (2%)	6	5
1	M	160/163 (98%)	145 (91%)	13 (8%)	2 (1%)	9	10
1	N	161/163 (99%)	144 (89%)	16 (10%)	1 (1%)	21	27
1	O	159/163 (98%)	140 (88%)	15 (9%)	4 (2%)	4	3
1	P	157/163 (96%)	137 (87%)	19 (12%)	1 (1%)	21	27

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Q	160/163 (98%)	148 (92%)	11 (7%)	1 (1%)	21	27
1	R	159/163 (98%)	146 (92%)	13 (8%)	0	100	100
1	S	158/163 (97%)	146 (92%)	11 (7%)	1 (1%)	21	27
1	T	159/163 (98%)	141 (89%)	16 (10%)	2 (1%)	9	10
1	U	157/163 (96%)	136 (87%)	17 (11%)	4 (2%)	4	3
1	V	157/163 (96%)	146 (93%)	9 (6%)	2 (1%)	9	10
1	W	157/163 (96%)	134 (85%)	19 (12%)	4 (2%)	4	3
1	X	157/163 (96%)	139 (88%)	16 (10%)	2 (1%)	9	10
1	Y	157/163 (96%)	143 (91%)	12 (8%)	2 (1%)	9	10
1	Z	157/163 (96%)	134 (85%)	20 (13%)	3 (2%)	6	5
1	a	157/163 (96%)	140 (89%)	16 (10%)	1 (1%)	21	27
1	b	159/163 (98%)	142 (89%)	16 (10%)	1 (1%)	21	27
1	c	157/163 (96%)	145 (92%)	12 (8%)	0	100	100
1	d	160/163 (98%)	139 (87%)	17 (11%)	4 (2%)	4	3
1	e	159/163 (98%)	137 (86%)	20 (13%)	2 (1%)	9	10
1	f	159/163 (98%)	141 (89%)	15 (9%)	3 (2%)	6	5
1	g	158/163 (97%)	140 (89%)	18 (11%)	0	100	100
1	h	160/163 (98%)	144 (90%)	13 (8%)	3 (2%)	6	5
1	i	159/163 (98%)	145 (91%)	12 (8%)	2 (1%)	9	10
1	j	157/163 (96%)	144 (92%)	12 (8%)	1 (1%)	21	27
All	All	5705/5868 (97%)	5059 (89%)	571 (10%)	75 (1%)	9	10

5 of 75 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	76	ASP
1	O	51	VAL
1	F	94	ASP
1	X	123	LYS
1	O	24	VAL

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar

resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	114/138 (83%)	108 (95%)	6 (5%)	20	30
1	B	130/138 (94%)	128 (98%)	2 (2%)	57	75
1	C	124/138 (90%)	121 (98%)	3 (2%)	43	62
1	D	123/138 (89%)	115 (94%)	8 (6%)	15	22
1	E	128/138 (93%)	118 (92%)	10 (8%)	11	16
1	F	114/138 (83%)	102 (90%)	12 (10%)	6	8
1	G	122/138 (88%)	112 (92%)	10 (8%)	10	14
1	H	125/138 (91%)	113 (90%)	12 (10%)	8	10
1	I	130/138 (94%)	121 (93%)	9 (7%)	14	20
1	J	128/138 (93%)	117 (91%)	11 (9%)	10	13
1	K	132/138 (96%)	125 (95%)	7 (5%)	20	30
1	L	132/138 (96%)	121 (92%)	11 (8%)	10	14
1	M	134/138 (97%)	129 (96%)	5 (4%)	30	45
1	N	131/138 (95%)	127 (97%)	4 (3%)	35	52
1	O	120/138 (87%)	116 (97%)	4 (3%)	33	50
1	P	131/138 (95%)	127 (97%)	4 (3%)	35	52
1	Q	132/138 (96%)	127 (96%)	5 (4%)	29	44
1	R	130/138 (94%)	125 (96%)	5 (4%)	29	44
1	S	131/138 (95%)	119 (91%)	12 (9%)	8	11
1	T	131/138 (95%)	117 (89%)	14 (11%)	6	8
1	U	123/138 (89%)	112 (91%)	11 (9%)	9	12
1	V	131/138 (95%)	125 (95%)	6 (5%)	24	36
1	W	121/138 (88%)	116 (96%)	5 (4%)	27	41
1	X	124/138 (90%)	113 (91%)	11 (9%)	9	12
1	Y	123/138 (89%)	113 (92%)	10 (8%)	11	14
1	Z	122/138 (88%)	111 (91%)	11 (9%)	9	12
1	a	123/138 (89%)	110 (89%)	13 (11%)	6	8
1	b	127/138 (92%)	115 (91%)	12 (9%)	8	11
1	c	130/138 (94%)	124 (95%)	6 (5%)	24	36

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	d	127/138 (92%)	117 (92%)	10 (8%)	11	15
1	e	129/138 (94%)	119 (92%)	10 (8%)	11	16
1	f	132/138 (96%)	116 (88%)	16 (12%)	5	5
1	g	132/138 (96%)	122 (92%)	10 (8%)	12	16
1	h	131/138 (95%)	125 (95%)	6 (5%)	24	36
1	i	129/138 (94%)	122 (95%)	7 (5%)	20	29
1	j	130/138 (94%)	120 (92%)	10 (8%)	12	16
All	All	4576/4968 (92%)	4268 (93%)	308 (7%)	15	21

5 of 308 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	W	144	TYR
1	i	8	LYS
1	U	11	GLU
1	T	95	ASN
1	g	43	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 66 such sidechains are listed below:

Mol	Chain	Res	Type
1	i	79	ASN
1	i	146	GLN
1	g	121	HIS
1	H	154	ASN
1	H	70	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

178 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	2AN	e	201	-	22,23,23	2.01	6 (27%)	29,33,33	1.59	6 (20%)
2	2AN	T	202	-	22,23,23	2.00	4 (18%)	29,33,33	1.58	3 (10%)
2	2AN	a	202	-	22,23,23	1.96	4 (18%)	29,33,33	1.54	6 (20%)
3	SO4	A	205	-	4,4,4	0.41	0	6,6,6	0.78	0
2	2AN	J	203	-	22,23,23	1.76	4 (18%)	29,33,33	1.63	6 (20%)
2	2AN	T	205	-	22,23,23	2.27	6 (27%)	29,33,33	2.23	10 (34%)
2	2AN	Z	204	-	22,23,23	1.78	4 (18%)	29,33,33	1.42	3 (10%)
2	2AN	a	204	-	22,23,23	1.90	5 (22%)	29,33,33	1.21	2 (6%)
4	EPE	P	205	-	15,15,15	2.10	1 (6%)	19,20,20	1.74	7 (36%)
2	2AN	E	203	-	22,23,23	1.91	4 (18%)	29,33,33	1.87	8 (27%)
2	2AN	Q	201	-	22,23,23	1.94	5 (22%)	29,33,33	1.73	6 (20%)
2	2AN	V	208	-	22,23,23	2.11	6 (27%)	29,33,33	3.43	10 (34%)
2	2AN	d	201	-	22,23,23	1.58	3 (13%)	29,33,33	1.59	5 (17%)
2	2AN	a	203	-	22,23,23	2.19	7 (31%)	29,33,33	1.51	3 (10%)
2	2AN	d	202	-	22,23,23	1.96	5 (22%)	29,33,33	1.41	2 (6%)
3	SO4	c	208	-	4,4,4	0.45	0	6,6,6	0.38	0
2	2AN	j	201	-	22,23,23	1.66	4 (18%)	29,33,33	1.60	5 (17%)
2	2AN	d	204	-	22,23,23	1.64	4 (18%)	29,33,33	2.01	5 (17%)
5	DMS	N	206	-	3,3,3	0.50	0	3,3,3	0.85	0
2	2AN	f	204	-	22,23,23	1.67	7 (31%)	29,33,33	1.35	2 (6%)
2	2AN	W	201	-	22,23,23	2.06	5 (22%)	29,33,33	1.63	5 (17%)
2	2AN	h	206	-	22,23,23	2.03	4 (18%)	29,33,33	1.63	6 (20%)
2	2AN	N	205	-	22,23,23	2.42	7 (31%)	29,33,33	1.65	5 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	2AN	F	203	-	22,23,23	1.45	4 (18%)	29,33,33	1.36	4 (13%)
3	SO4	c	209	-	4,4,4	0.49	0	6,6,6	0.62	0
2	2AN	I	202	-	22,23,23	1.78	5 (22%)	29,33,33	1.36	4 (13%)
2	2AN	I	207	-	22,23,23	2.37	4 (18%)	29,33,33	1.69	10 (34%)
3	SO4	E	205	-	4,4,4	0.19	0	6,6,6	0.13	0
2	2AN	E	202	-	22,23,23	1.44	3 (13%)	29,33,33	1.68	7 (24%)
2	2AN	f	205	-	22,23,23	1.68	4 (18%)	29,33,33	1.29	5 (17%)
2	2AN	M	202	-	22,23,23	1.58	5 (22%)	29,33,33	2.09	9 (31%)
2	2AN	c	205	-	22,23,23	1.66	5 (22%)	29,33,33	1.09	2 (6%)
2	2AN	c	206	-	22,23,23	1.35	3 (13%)	29,33,33	1.25	3 (10%)
2	2AN	Y	203	-	22,23,23	1.71	5 (22%)	29,33,33	1.54	6 (20%)
2	2AN	D	203	-	22,23,23	1.87	6 (27%)	29,33,33	1.62	5 (17%)
2	2AN	j	203	-	22,23,23	1.71	6 (27%)	29,33,33	1.73	8 (27%)
2	2AN	A	202	-	22,23,23	2.07	7 (31%)	29,33,33	1.79	8 (27%)
2	2AN	h	204	-	22,23,23	1.51	4 (18%)	29,33,33	1.58	2 (6%)
6	FLC	G	206	-	12,12,12	1.04	0	17,17,17	1.93	5 (29%)
2	2AN	F	202	-	22,23,23	2.04	4 (18%)	29,33,33	2.07	13 (44%)
2	2AN	Z	206	-	22,23,23	2.02	5 (22%)	29,33,33	1.73	6 (20%)
2	2AN	I	201	-	22,23,23	1.32	3 (13%)	29,33,33	1.89	7 (24%)
2	2AN	X	206	-	22,23,23	1.81	5 (22%)	29,33,33	0.90	2 (6%)
2	2AN	D	201	-	22,23,23	1.77	6 (27%)	29,33,33	1.56	5 (17%)
2	2AN	V	201	-	22,23,23	1.83	5 (22%)	29,33,33	1.58	6 (20%)
2	2AN	P	201	-	22,23,23	1.68	3 (13%)	29,33,33	1.16	3 (10%)
2	2AN	K	201	-	22,23,23	1.70	5 (22%)	29,33,33	1.79	7 (24%)
2	2AN	J	201	-	22,23,23	1.48	3 (13%)	29,33,33	1.01	1 (3%)
2	2AN	F	206	-	22,23,23	1.88	5 (22%)	29,33,33	1.61	7 (24%)
2	2AN	X	205	-	22,23,23	2.06	5 (22%)	29,33,33	1.30	3 (10%)
2	2AN	f	203	-	22,23,23	1.81	5 (22%)	29,33,33	0.91	2 (6%)
2	2AN	c	202	-	22,23,23	2.14	5 (22%)	29,33,33	1.80	10 (34%)
2	2AN	R	201	-	22,23,23	1.84	5 (22%)	29,33,33	1.00	1 (3%)
2	2AN	A	204	-	22,23,23	1.81	5 (22%)	29,33,33	0.88	2 (6%)
2	2AN	c	203	-	22,23,23	1.69	3 (13%)	29,33,33	1.19	2 (6%)
2	2AN	Y	204	-	22,23,23	1.68	4 (18%)	29,33,33	0.90	2 (6%)
2	2AN	f	202	-	22,23,23	1.36	2 (9%)	29,33,33	1.52	4 (13%)
2	2AN	F	204	-	22,23,23	1.77	4 (18%)	29,33,33	1.29	4 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	2AN	Z	201	-	22,23,23	2.32	6 (27%)	29,33,33	1.60	8 (27%)
2	2AN	A	203	-	22,23,23	2.11	4 (18%)	29,33,33	1.39	4 (13%)
2	2AN	C	202	-	22,23,23	1.75	5 (22%)	29,33,33	1.02	1 (3%)
2	2AN	h	202	-	22,23,23	1.63	5 (22%)	29,33,33	1.68	6 (20%)
2	2AN	O	203	-	22,23,23	2.08	4 (18%)	29,33,33	1.52	3 (10%)
2	2AN	T	204	-	22,23,23	2.27	5 (22%)	29,33,33	1.64	9 (31%)
2	2AN	b	201	-	22,23,23	1.78	4 (18%)	29,33,33	1.01	1 (3%)
2	2AN	I	204	-	22,23,23	2.03	5 (22%)	29,33,33	1.43	4 (13%)
2	2AN	S	202	-	22,23,23	1.85	4 (18%)	29,33,33	1.85	9 (31%)
2	2AN	P	204	-	22,23,23	1.81	5 (22%)	29,33,33	1.51	3 (10%)
2	2AN	O	201	-	22,23,23	1.44	2 (9%)	29,33,33	1.42	3 (10%)
2	2AN	g	201	-	22,23,23	1.96	6 (27%)	29,33,33	1.75	8 (27%)
2	2AN	P	203	-	22,23,23	1.65	6 (27%)	29,33,33	1.57	4 (13%)
3	SO4	g	204	-	4,4,4	0.60	0	6,6,6	0.47	0
2	2AN	E	204	-	22,23,23	2.09	6 (27%)	29,33,33	1.89	5 (17%)
2	2AN	M	201	-	22,23,23	2.11	4 (18%)	29,33,33	2.09	9 (31%)
6	FLC	j	208	-	12,12,12	2.27	1 (8%)	17,17,17	2.39	6 (35%)
2	2AN	h	205	-	22,23,23	2.11	5 (22%)	29,33,33	1.30	2 (6%)
2	2AN	G	202	-	22,23,23	1.51	4 (18%)	29,33,33	1.62	5 (17%)
2	2AN	B	201	-	22,23,23	1.80	5 (22%)	29,33,33	2.02	12 (41%)
2	2AN	R	203	-	22,23,23	1.84	6 (27%)	29,33,33	1.36	3 (10%)
2	2AN	X	202	-	22,23,23	1.82	6 (27%)	29,33,33	1.33	2 (6%)
2	2AN	Y	202	-	22,23,23	1.85	6 (27%)	29,33,33	1.42	6 (20%)
6	FLC	a	206	-	12,12,12	1.15	0	17,17,17	1.43	3 (17%)
2	2AN	L	202	-	22,23,23	1.76	4 (18%)	29,33,33	1.29	3 (10%)
2	2AN	D	202	-	22,23,23	1.81	6 (27%)	29,33,33	1.21	2 (6%)
2	2AN	V	202	-	22,23,23	1.48	5 (22%)	29,33,33	1.71	7 (24%)
2	2AN	j	205	-	22,23,23	1.80	4 (18%)	29,33,33	1.87	10 (34%)
2	2AN	b	206	-	22,23,23	2.33	5 (22%)	29,33,33	1.60	4 (13%)
6	FLC	i	202	-	12,12,12	1.34	2 (16%)	17,17,17	1.21	1 (5%)
2	2AN	K	203	-	22,23,23	1.74	4 (18%)	29,33,33	1.26	1 (3%)
2	2AN	G	205	-	22,23,23	1.88	4 (18%)	29,33,33	1.19	3 (10%)
2	2AN	Q	202	-	22,23,23	1.80	4 (18%)	29,33,33	1.24	2 (6%)
2	2AN	B	204	-	22,23,23	1.60	4 (18%)	29,33,33	1.49	4 (13%)
2	2AN	S	203	-	22,23,23	1.72	4 (18%)	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	R	204	-	22,23,23	2.16	4 (18%)	29,33,33	1.56	6 (20%)
2	2AN	H	203	-	22,23,23	1.69	5 (22%)	29,33,33	1.29	2 (6%)
2	2AN	K	202	-	22,23,23	1.63	4 (18%)	29,33,33	1.10	4 (13%)
2	2AN	J	202	-	22,23,23	1.49	4 (18%)	29,33,33	0.99	2 (6%)
2	2AN	f	206	-	22,23,23	1.87	4 (18%)	29,33,33	1.28	2 (6%)
2	2AN	E	201	-	22,23,23	1.71	4 (18%)	29,33,33	1.14	2 (6%)
2	2AN	a	201	-	22,23,23	1.98	5 (22%)	29,33,33	2.21	8 (27%)
2	2AN	M	203	-	22,23,23	1.87	7 (31%)	29,33,33	1.84	6 (20%)
2	2AN	G	207	-	22,23,23	2.04	5 (22%)	29,33,33	1.05	1 (3%)
2	2AN	R	202	-	22,23,23	2.09	8 (36%)	29,33,33	1.30	5 (17%)
2	2AN	j	207	-	22,23,23	2.30	5 (22%)	29,33,33	1.13	2 (6%)
3	SO4	c	207	-	4,4,4	0.43	0	6,6,6	0.45	0
2	2AN	g	203	-	22,23,23	1.79	6 (27%)	29,33,33	1.55	4 (13%)
2	2AN	V	205	-	22,23,23	1.58	7 (31%)	29,33,33	1.65	6 (20%)
5	DMS	X	207	-	3,3,3	0.56	0	3,3,3	0.62	0
2	2AN	b	205	-	22,23,23	2.00	5 (22%)	29,33,33	1.57	5 (17%)
2	2AN	N	201	-	22,23,23	1.39	4 (18%)	29,33,33	1.22	2 (6%)
2	2AN	B	202	-	22,23,23	1.65	3 (13%)	29,33,33	0.95	1 (3%)
2	2AN	H	201	-	22,23,23	1.60	5 (22%)	29,33,33	1.38	3 (10%)
2	2AN	g	202	-	22,23,23	1.63	4 (18%)	29,33,33	1.86	7 (24%)
3	SO4	G	209	-	4,4,4	0.52	0	6,6,6	0.20	0
2	2AN	U	201	-	22,23,23	1.94	5 (22%)	29,33,33	1.26	1 (3%)
2	2AN	S	204	-	22,23,23	1.69	6 (27%)	29,33,33	2.56	4 (13%)
5	DMS	G	208	-	3,3,3	0.52	0	3,3,3	1.10	0
2	2AN	c	204	-	22,23,23	1.44	4 (18%)	29,33,33	1.52	4 (13%)
2	2AN	f	201	-	22,23,23	2.07	6 (27%)	29,33,33	1.92	9 (31%)
2	2AN	Q	203	-	22,23,23	2.14	5 (22%)	29,33,33	1.75	5 (17%)
2	2AN	T	201	-	22,23,23	1.77	7 (31%)	29,33,33	1.31	2 (6%)
2	2AN	h	201	-	22,23,23	2.23	4 (18%)	29,33,33	1.35	6 (20%)
6	FLC	i	203	-	12,12,12	1.39	1 (8%)	17,17,17	2.32	5 (29%)
2	2AN	B	206	-	22,23,23	1.81	4 (18%)	29,33,33	0.96	1 (3%)
2	2AN	Y	201	-	22,23,23	2.49	6 (27%)	29,33,33	2.18	12 (41%)
2	2AN	j	202	-	22,23,23	1.39	3 (13%)	29,33,33	1.99	8 (27%)
2	2AN	b	202	-	22,23,23	1.86	5 (22%)	29,33,33	1.24	3 (10%)
2	2AN	Z	205	-	22,23,23	1.63	4 (18%)	29,33,33	1.61	5 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	2AN	X	203	-	22,23,23	1.79	5 (22%)	29,33,33	0.90	1 (3%)
2	2AN	V	204	-	22,23,23	1.74	5 (22%)	29,33,33	1.37	3 (10%)
6	FLC	e	202	-	12,12,12	1.54	1 (8%)	17,17,17	1.85	3 (17%)
2	2AN	I	203	-	22,23,23	1.92	5 (22%)	29,33,33	1.26	3 (10%)
2	2AN	V	207	-	22,23,23	1.74	5 (22%)	29,33,33	0.90	1 (3%)
2	2AN	A	201	-	22,23,23	1.67	6 (27%)	29,33,33	1.40	6 (20%)
2	2AN	D	204	-	22,23,23	2.40	5 (22%)	29,33,33	2.15	10 (34%)
2	2AN	V	203	-	22,23,23	1.97	6 (27%)	29,33,33	1.59	6 (20%)
2	2AN	h	203	-	22,23,23	2.21	6 (27%)	29,33,33	1.84	8 (27%)
2	2AN	O	202	-	22,23,23	2.12	4 (18%)	29,33,33	1.29	4 (13%)
2	2AN	G	203	-	22,23,23	1.39	4 (18%)	29,33,33	1.23	3 (10%)
2	2AN	Z	202	-	22,23,23	2.01	5 (22%)	29,33,33	1.55	5 (17%)
2	2AN	c	201	-	22,23,23	1.69	6 (27%)	29,33,33	1.52	4 (13%)
2	2AN	N	202	-	22,23,23	1.73	6 (27%)	29,33,33	1.59	6 (20%)
2	2AN	H	202	-	22,23,23	1.82	4 (18%)	29,33,33	1.55	5 (17%)
2	2AN	G	201	-	22,23,23	1.71	4 (18%)	29,33,33	1.38	5 (17%)
2	2AN	j	206	-	22,23,23	1.94	6 (27%)	29,33,33	1.36	3 (10%)
2	2AN	P	202	-	22,23,23	1.84	7 (31%)	29,33,33	1.96	10 (34%)
2	2AN	C	201	-	22,23,23	1.64	5 (22%)	29,33,33	1.39	4 (13%)
2	2AN	B	205	-	22,23,23	1.71	4 (18%)	29,33,33	1.31	4 (13%)
2	2AN	X	201	-	22,23,23	2.00	5 (22%)	29,33,33	1.63	4 (13%)
2	2AN	N	204	-	22,23,23	1.56	5 (22%)	29,33,33	1.90	5 (17%)
2	2AN	I	205	-	22,23,23	2.69	5 (22%)	29,33,33	1.61	7 (24%)
2	2AN	L	204	-	22,23,23	1.98	5 (22%)	29,33,33	1.55	6 (20%)
2	2AN	b	204	-	22,23,23	1.73	3 (13%)	29,33,33	1.11	2 (6%)
6	FLC	a	205	-	12,12,12	1.33	1 (8%)	17,17,17	1.47	5 (29%)
2	2AN	d	203	-	22,23,23	1.74	5 (22%)	29,33,33	0.92	1 (3%)
2	2AN	F	201	-	22,23,23	1.55	4 (18%)	29,33,33	1.45	6 (20%)
2	2AN	Z	203	-	22,23,23	1.90	5 (22%)	29,33,33	1.64	7 (24%)
3	SO4	Q	204	-	4,4,4	0.53	0	6,6,6	0.58	0
2	2AN	G	204	-	22,23,23	2.05	5 (22%)	29,33,33	1.39	5 (17%)
2	2AN	j	204	-	22,23,23	1.68	5 (22%)	29,33,33	1.50	4 (13%)
2	2AN	N	203	-	22,23,23	1.97	5 (22%)	29,33,33	2.66	9 (31%)
2	2AN	X	204	-	22,23,23	1.91	4 (18%)	29,33,33	1.41	5 (17%)
2	2AN	R	205	-	22,23,23	1.83	5 (22%)	29,33,33	1.36	2 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	2AN	S	201	-	22,23,23	2.06	4 (18%)	29,33,33	1.84	4 (13%)
2	2AN	U	202	-	22,23,23	1.79	5 (22%)	29,33,33	1.30	2 (6%)
3	SO4	I	208	-	4,4,4	0.32	0	6,6,6	0.90	0
2	2AN	C	203[A]	-	22,23,23	0.61	0	29,33,33	1.44	5 (17%)
2	2AN	H	204	-	22,23,23	2.01	5 (22%)	29,33,33	1.41	2 (6%)
2	2AN	L	203	-	22,23,23	1.60	4 (18%)	29,33,33	1.92	8 (27%)
2	2AN	b	203	-	22,23,23	1.75	5 (22%)	29,33,33	1.06	2 (6%)
2	2AN	F	205	-	22,23,23	1.71	4 (18%)	29,33,33	1.27	3 (10%)
2	2AN	T	203	-	22,23,23	1.60	5 (22%)	29,33,33	1.92	7 (24%)
3	SO4	Y	205	-	4,4,4	0.31	0	6,6,6	0.63	0
2	2AN	B	203	-	22,23,23	1.71	5 (22%)	29,33,33	1.53	4 (13%)
2	2AN	L	201	-	22,23,23	1.62	5 (22%)	29,33,33	1.25	2 (6%)
2	2AN	I	206	-	22,23,23	2.36	6 (27%)	29,33,33	1.81	7 (24%)
2	2AN	V	206	-	22,23,23	1.71	4 (18%)	29,33,33	1.87	8 (27%)
2	2AN	i	201	-	22,23,23	1.75	4 (18%)	29,33,33	1.72	6 (20%)

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	e	201	-	-	4/10/10/10	0/3/3/3
2	2AN	T	202	-	-	1/10/10/10	0/3/3/3
2	2AN	a	202	-	-	0/10/10/10	0/3/3/3
2	2AN	J	203	-	-	2/10/10/10	0/3/3/3
2	2AN	T	205	-	-	5/10/10/10	0/3/3/3
2	2AN	Z	204	-	-	0/10/10/10	0/3/3/3
2	2AN	a	204	-	-	0/10/10/10	0/3/3/3
4	EPE	P	205	-	-	2/9/19/19	0/1/1/1
2	2AN	E	203	-	-	3/10/10/10	0/3/3/3
2	2AN	Q	201	-	-	1/10/10/10	0/3/3/3
2	2AN	V	208	-	-	4/10/10/10	0/3/3/3
2	2AN	d	201	-	-	0/10/10/10	0/3/3/3
2	2AN	a	203	-	-	0/10/10/10	0/3/3/3
2	2AN	d	202	-	-	6/10/10/10	0/3/3/3
2	2AN	j	201	-	-	6/10/10/10	0/3/3/3
2	2AN	d	204	-	-	0/10/10/10	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	2AN	f	204	-	-	0/10/10/10	0/3/3/3
2	2AN	W	201	-	-	6/10/10/10	0/3/3/3
2	2AN	h	206	-	-	0/10/10/10	0/3/3/3
2	2AN	N	205	-	-	0/10/10/10	0/3/3/3
2	2AN	F	203	-	-	0/10/10/10	0/3/3/3
2	2AN	I	202	-	-	0/10/10/10	0/3/3/3
2	2AN	I	207	-	-	5/10/10/10	0/3/3/3
2	2AN	E	202	-	-	1/10/10/10	0/3/3/3
2	2AN	f	205	-	-	0/10/10/10	0/3/3/3
2	2AN	M	202	-	-	3/10/10/10	0/3/3/3
2	2AN	c	205	-	-	0/10/10/10	0/3/3/3
2	2AN	c	206	-	-	0/10/10/10	0/3/3/3
2	2AN	Y	203	-	-	0/10/10/10	0/3/3/3
2	2AN	D	203	-	-	6/10/10/10	0/3/3/3
2	2AN	j	203	-	-	0/10/10/10	0/3/3/3
2	2AN	A	202	-	-	2/10/10/10	0/3/3/3
2	2AN	h	204	-	-	0/10/10/10	0/3/3/3
6	FLC	G	206	-	-	14/16/16/16	-
2	2AN	F	202	-	-	8/10/10/10	0/3/3/3
2	2AN	Z	206	-	-	6/10/10/10	0/3/3/3
2	2AN	I	201	-	-	2/10/10/10	0/3/3/3
2	2AN	X	206	-	-	2/10/10/10	0/3/3/3
2	2AN	D	201	-	-	0/10/10/10	0/3/3/3
2	2AN	V	201	-	-	2/10/10/10	0/3/3/3
2	2AN	P	201	-	-	0/10/10/10	0/3/3/3
2	2AN	K	201	-	-	4/10/10/10	0/3/3/3
2	2AN	J	201	-	-	0/10/10/10	0/3/3/3
2	2AN	F	206	-	-	2/10/10/10	0/3/3/3
2	2AN	X	205	-	-	0/10/10/10	0/3/3/3
2	2AN	f	203	-	-	2/10/10/10	0/3/3/3
2	2AN	c	202	-	-	0/10/10/10	0/3/3/3
2	2AN	R	201	-	-	0/10/10/10	0/3/3/3
2	2AN	A	204	-	-	4/10/10/10	0/3/3/3
2	2AN	c	203	-	-	3/10/10/10	0/3/3/3
2	2AN	Y	204	-	-	7/10/10/10	0/3/3/3
2	2AN	f	202	-	-	1/10/10/10	0/3/3/3
2	2AN	F	204	-	-	2/10/10/10	0/3/3/3
2	2AN	Z	201	-	-	2/10/10/10	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	2AN	A	203	-	-	6/10/10/10	0/3/3/3
2	2AN	C	202	-	-	0/10/10/10	0/3/3/3
2	2AN	h	202	-	-	0/10/10/10	0/3/3/3
2	2AN	O	203	-	-	6/10/10/10	0/3/3/3
2	2AN	T	204	-	-	6/10/10/10	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	S	202	-	-	6/10/10/10	0/3/3/3
2	2AN	P	204	-	-	1/10/10/10	0/3/3/3
2	2AN	O	201	-	-	5/10/10/10	0/3/3/3
2	2AN	g	201	-	-	0/10/10/10	0/3/3/3
2	2AN	P	203	-	-	6/10/10/10	0/3/3/3
6	FLC	j	208	-	-	7/16/16/16	-
2	2AN	E	204	-	-	8/10/10/10	0/3/3/3
2	2AN	M	201	-	-	0/10/10/10	0/3/3/3
2	2AN	h	205	-	-	0/10/10/10	0/3/3/3
2	2AN	G	202	-	-	2/10/10/10	0/3/3/3
2	2AN	B	201	-	-	2/10/10/10	0/3/3/3
2	2AN	R	203	-	-	6/10/10/10	0/3/3/3
2	2AN	X	202	-	-	0/10/10/10	0/3/3/3
2	2AN	Y	202	-	-	6/10/10/10	0/3/3/3
6	FLC	a	206	-	-	7/16/16/16	-
2	2AN	L	202	-	-	0/10/10/10	0/3/3/3
2	2AN	D	202	-	-	1/10/10/10	0/3/3/3
2	2AN	V	202	-	-	1/10/10/10	0/3/3/3
2	2AN	j	205	-	-	1/10/10/10	0/3/3/3
2	2AN	b	206	-	-	7/10/10/10	0/3/3/3
6	FLC	i	202	-	-	8/16/16/16	-
2	2AN	K	203	-	-	0/10/10/10	0/3/3/3
2	2AN	G	205	-	-	6/10/10/10	0/3/3/3
2	2AN	Q	202	-	-	0/10/10/10	0/3/3/3
2	2AN	B	204	-	-	0/10/10/10	0/3/3/3
2	2AN	S	203	-	-	0/10/10/10	0/3/3/3
2	2AN	R	204	-	-	6/10/10/10	0/3/3/3
2	2AN	H	203	-	-	6/10/10/10	0/3/3/3
2	2AN	K	202	-	-	0/10/10/10	0/3/3/3
2	2AN	J	202	-	-	0/10/10/10	0/3/3/3
2	2AN	f	206	-	-	1/10/10/10	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	2AN	E	201	-	-	0/10/10/10	0/3/3/3
2	2AN	a	201	-	-	2/10/10/10	0/3/3/3
2	2AN	M	203	-	-	8/10/10/10	0/3/3/3
2	2AN	G	207	-	-	0/10/10/10	0/3/3/3
2	2AN	R	202	-	-	2/10/10/10	0/3/3/3
2	2AN	j	207	-	-	0/10/10/10	0/3/3/3
2	2AN	g	203	-	-	2/10/10/10	0/3/3/3
2	2AN	V	205	-	-	2/10/10/10	0/3/3/3
2	2AN	b	205	-	-	0/10/10/10	0/3/3/3
2	2AN	N	201	-	-	0/10/10/10	0/3/3/3
2	2AN	B	202	-	-	0/10/10/10	0/3/3/3
2	2AN	H	201	-	-	0/10/10/10	0/3/3/3
2	2AN	g	202	-	-	4/10/10/10	0/3/3/3
2	2AN	U	201	-	-	6/10/10/10	0/3/3/3
2	2AN	S	204	-	-	8/10/10/10	0/3/3/3
2	2AN	c	204	-	-	2/10/10/10	0/3/3/3
2	2AN	f	201	-	-	0/10/10/10	0/3/3/3
2	2AN	Q	203	-	-	5/10/10/10	0/3/3/3
2	2AN	T	201	-	-	0/10/10/10	0/3/3/3
2	2AN	h	201	-	-	0/10/10/10	0/3/3/3
6	FLC	i	203	-	-	9/16/16/16	-
2	2AN	B	206	-	-	1/10/10/10	0/3/3/3
2	2AN	Y	201	-	-	0/10/10/10	0/3/3/3
2	2AN	j	202	-	-	1/10/10/10	0/3/3/3
2	2AN	b	202	-	-	0/10/10/10	0/3/3/3
2	2AN	Z	205	-	-	0/10/10/10	0/3/3/3
2	2AN	X	203	-	-	2/10/10/10	0/3/3/3
2	2AN	V	204	-	-	0/10/10/10	0/3/3/3
6	FLC	e	202	-	-	11/16/16/16	-
2	2AN	I	203	-	-	0/10/10/10	0/3/3/3
2	2AN	V	207	-	-	0/10/10/10	0/3/3/3
2	2AN	A	201	-	-	0/10/10/10	0/3/3/3
2	2AN	D	204	-	-	8/10/10/10	0/3/3/3
2	2AN	V	203	-	-	1/10/10/10	0/3/3/3
2	2AN	h	203	-	-	3/10/10/10	0/3/3/3
2	2AN	O	202	-	-	0/10/10/10	0/3/3/3
2	2AN	G	203	-	-	0/10/10/10	0/3/3/3
2	2AN	Z	202	-	-	0/10/10/10	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	2AN	c	201	-	-	2/10/10/10	0/3/3/3
2	2AN	N	202	-	-	1/10/10/10	0/3/3/3
2	2AN	H	202	-	-	2/10/10/10	0/3/3/3
2	2AN	G	201	-	-	1/10/10/10	0/3/3/3
2	2AN	j	206	-	-	0/10/10/10	0/3/3/3
2	2AN	P	202	-	-	2/10/10/10	0/3/3/3
2	2AN	C	201	-	-	1/10/10/10	0/3/3/3
2	2AN	B	205	-	-	7/10/10/10	0/3/3/3
2	2AN	X	201	-	-	0/10/10/10	0/3/3/3
2	2AN	N	204	-	-	0/10/10/10	0/3/3/3
2	2AN	I	205	-	-	6/10/10/10	0/3/3/3
2	2AN	L	204	-	-	5/10/10/10	0/3/3/3
2	2AN	b	204	-	-	0/10/10/10	0/3/3/3
6	FLC	a	205	-	-	9/16/16/16	-
2	2AN	d	203	-	-	2/10/10/10	0/3/3/3
2	2AN	F	201	-	-	6/10/10/10	0/3/3/3
2	2AN	Z	203	-	-	0/10/10/10	0/3/3/3
2	2AN	G	204	-	-	0/10/10/10	0/3/3/3
2	2AN	j	204	-	-	5/10/10/10	0/3/3/3
2	2AN	N	203	-	-	8/10/10/10	0/3/3/3
2	2AN	X	204	-	-	3/10/10/10	0/3/3/3
2	2AN	R	205	-	-	0/10/10/10	0/3/3/3
2	2AN	S	201	-	-	8/10/10/10	0/3/3/3
2	2AN	U	202	-	-	5/10/10/10	0/3/3/3
2	2AN	C	203[A]	-	-	7/10/10/10	0/3/3/3
2	2AN	H	204	-	-	2/10/10/10	0/3/3/3
2	2AN	L	203	-	-	2/10/10/10	0/3/3/3
2	2AN	b	203	-	-	6/10/10/10	0/3/3/3
2	2AN	F	205	-	-	3/10/10/10	0/3/3/3
2	2AN	T	203	-	-	0/10/10/10	0/3/3/3
2	2AN	B	203	-	-	0/10/10/10	0/3/3/3
2	2AN	L	201	-	-	0/10/10/10	0/3/3/3
2	2AN	I	206	-	-	2/10/10/10	0/3/3/3
2	2AN	V	206	-	-	0/10/10/10	0/3/3/3
2	2AN	i	201	-	-	3/10/10/10	0/3/3/3

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

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

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

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

There are no chirality outliers.

5 of 404 torsion outliers are listed below:

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

There are no ring outliers.

167 monomers are involved in 1144 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	e	201	2AN	4	0
2	T	202	2AN	5	0
2	a	202	2AN	3	0
3	A	205	SO4	6	0
2	J	203	2AN	5	0
2	T	205	2AN	5	0
2	Z	204	2AN	3	0
2	a	204	2AN	19	0
4	P	205	EPE	6	0
2	E	203	2AN	5	0
2	Q	201	2AN	3	0
2	V	208	2AN	21	0
2	d	201	2AN	19	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	a	203	2AN	8	0
2	d	202	2AN	7	0
2	j	201	2AN	8	0
2	d	204	2AN	13	0
5	N	206	DMS	2	0
2	f	204	2AN	8	0
2	W	201	2AN	6	0
2	h	206	2AN	6	0
2	N	205	2AN	8	0
2	F	203	2AN	9	0
2	I	202	2AN	6	0
2	I	207	2AN	5	0
2	E	202	2AN	3	0
2	f	205	2AN	10	0
2	M	202	2AN	2	0
2	c	205	2AN	1	0
2	c	206	2AN	7	0
2	Y	203	2AN	6	0
2	D	203	2AN	12	0
2	j	203	2AN	7	0
2	A	202	2AN	7	0
2	h	204	2AN	17	0
6	G	206	FLC	2	0
2	F	202	2AN	20	0
2	Z	206	2AN	14	0
2	I	201	2AN	3	0
2	X	206	2AN	56	0
2	D	201	2AN	8	0
2	V	201	2AN	15	0
2	P	201	2AN	6	0
2	K	201	2AN	4	0
2	J	201	2AN	6	0
2	F	206	2AN	14	0
2	X	205	2AN	4	0
2	f	203	2AN	5	0
2	c	202	2AN	7	0
2	R	201	2AN	8	0
2	c	203	2AN	5	0
2	Y	204	2AN	10	0
2	f	202	2AN	8	0
2	F	204	2AN	8	0
2	Z	201	2AN	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	203	2AN	4	0
2	C	202	2AN	11	0
2	h	202	2AN	7	0
2	O	203	2AN	5	0
2	T	204	2AN	3	0
2	b	201	2AN	11	0
2	I	204	2AN	8	0
2	S	202	2AN	4	0
2	P	204	2AN	4	0
2	O	201	2AN	12	0
2	g	201	2AN	4	0
2	P	203	2AN	9	0
3	g	204	SO4	1	0
2	E	204	2AN	3	0
2	M	201	2AN	6	0
6	j	208	FLC	9	0
2	h	205	2AN	3	0
2	G	202	2AN	4	0
2	B	201	2AN	7	0
2	R	203	2AN	10	0
2	X	202	2AN	9	0
2	Y	202	2AN	5	0
2	L	202	2AN	6	0
2	D	202	2AN	5	0
2	V	202	2AN	3	0
2	j	205	2AN	9	0
2	b	206	2AN	5	0
2	K	203	2AN	6	0
2	Q	202	2AN	6	0
2	B	204	2AN	8	0
2	S	203	2AN	2	0
2	R	204	2AN	10	0
2	H	203	2AN	5	0
2	K	202	2AN	12	0
2	J	202	2AN	8	0
2	f	206	2AN	9	0
2	E	201	2AN	5	0
2	a	201	2AN	3	0
2	M	203	2AN	2	0
2	G	207	2AN	6	0
2	R	202	2AN	4	0
2	j	207	2AN	4	0

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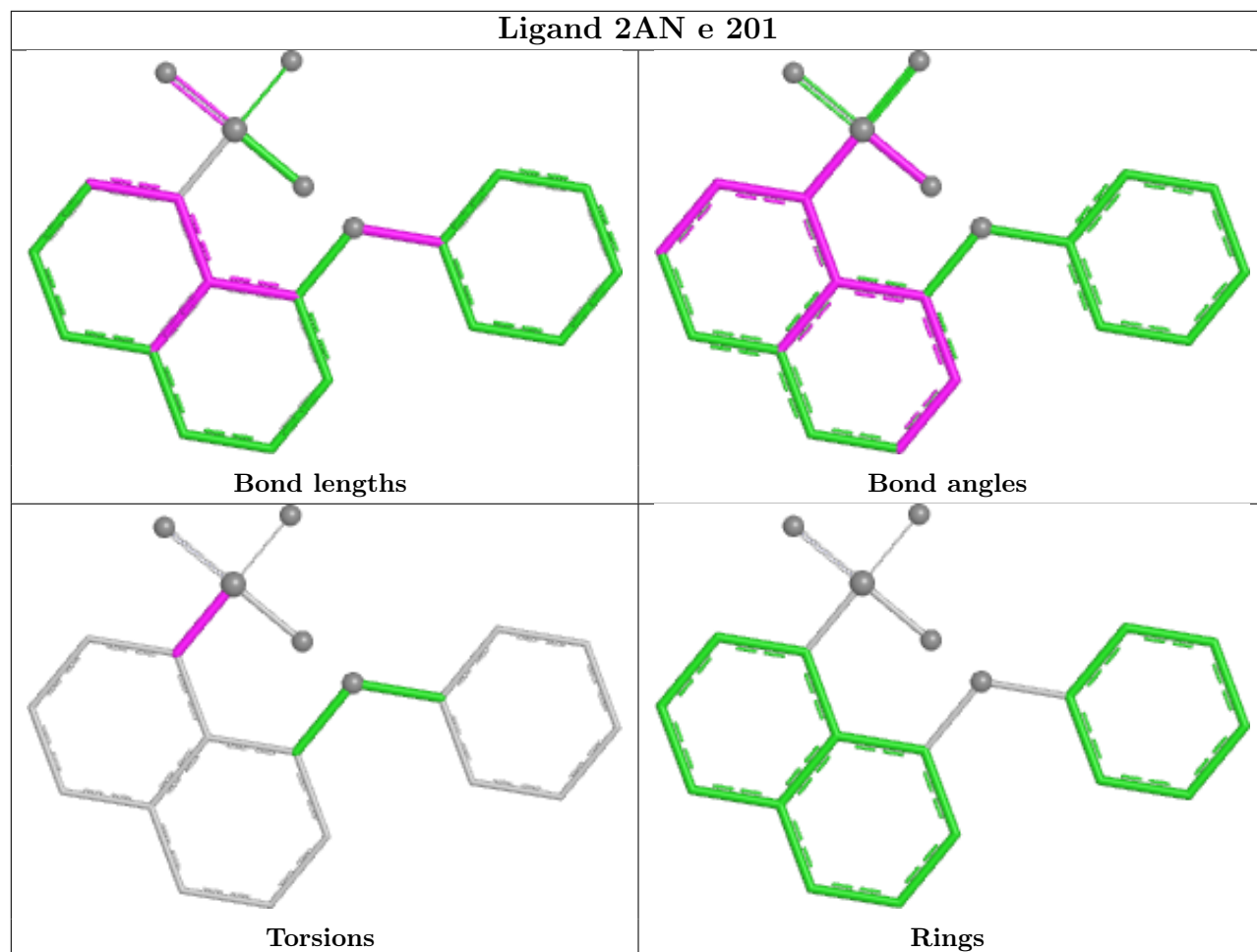
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	c	207	SO4	1	0
2	g	203	2AN	4	0
2	V	205	2AN	12	0
2	b	205	2AN	8	0
2	N	201	2AN	10	0
2	B	202	2AN	8	0
2	H	201	2AN	5	0
2	g	202	2AN	10	0
2	U	201	2AN	7	0
2	S	204	2AN	17	0
5	G	208	DMS	1	0
2	c	204	2AN	4	0
2	f	201	2AN	4	0
2	Q	203	2AN	3	0
2	T	201	2AN	13	0
2	h	201	2AN	3	0
6	i	203	FLC	3	0
2	B	206	2AN	6	0
2	Y	201	2AN	9	0
2	j	202	2AN	4	0
2	b	202	2AN	11	0
2	Z	205	2AN	5	0
2	X	203	2AN	7	0
2	V	204	2AN	11	0
6	e	202	FLC	1	0
2	I	203	2AN	7	0
2	V	207	2AN	5	0
2	A	201	2AN	4	0
2	D	204	2AN	6	0
2	V	203	2AN	11	0
2	h	203	2AN	3	0
2	O	202	2AN	5	0
2	G	203	2AN	9	0
2	Z	202	2AN	4	0
2	c	201	2AN	7	0
2	N	202	2AN	4	0
2	H	202	2AN	4	0
2	G	201	2AN	3	0
2	j	206	2AN	5	0
2	P	202	2AN	4	0
2	C	201	2AN	4	0
2	B	205	2AN	6	0

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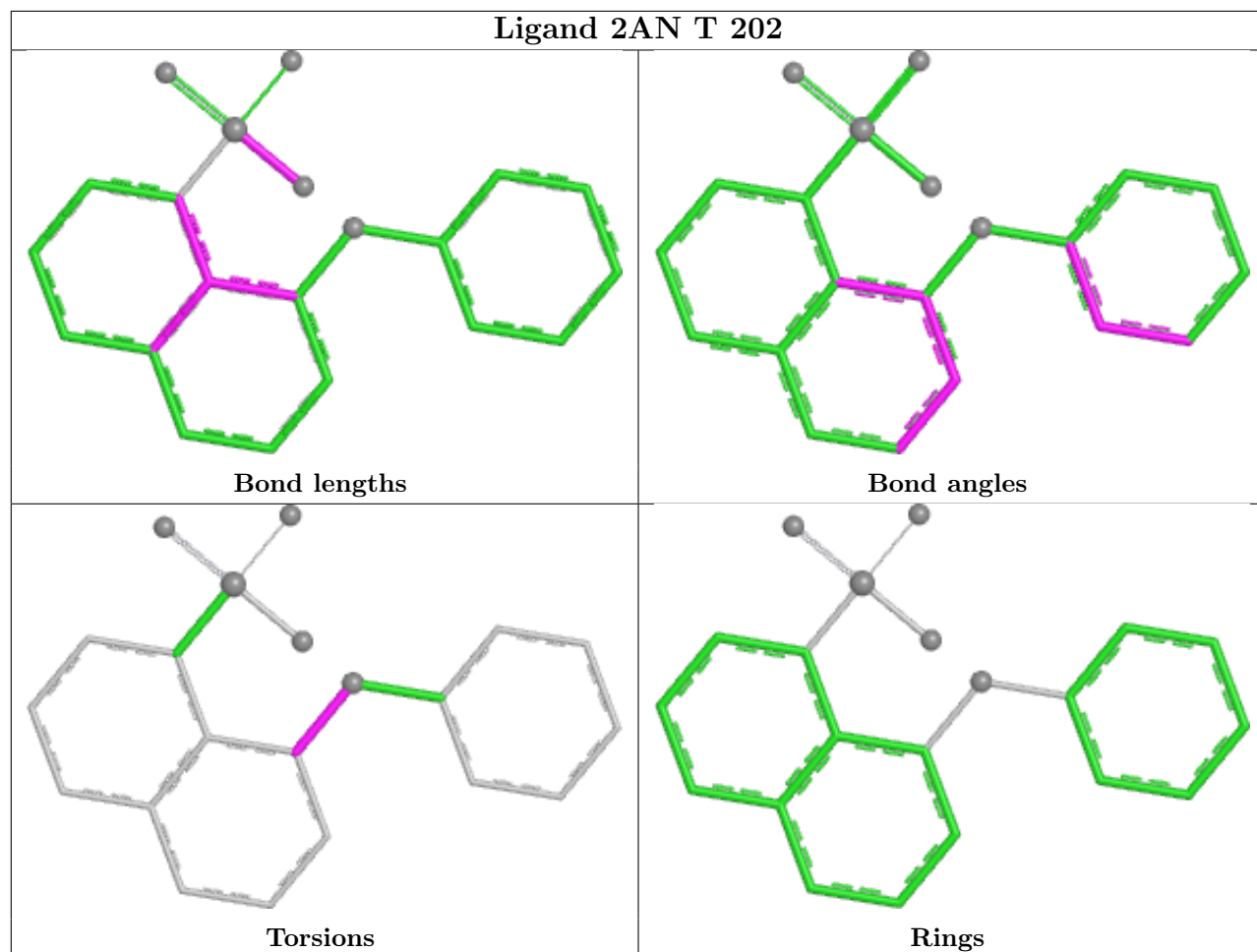
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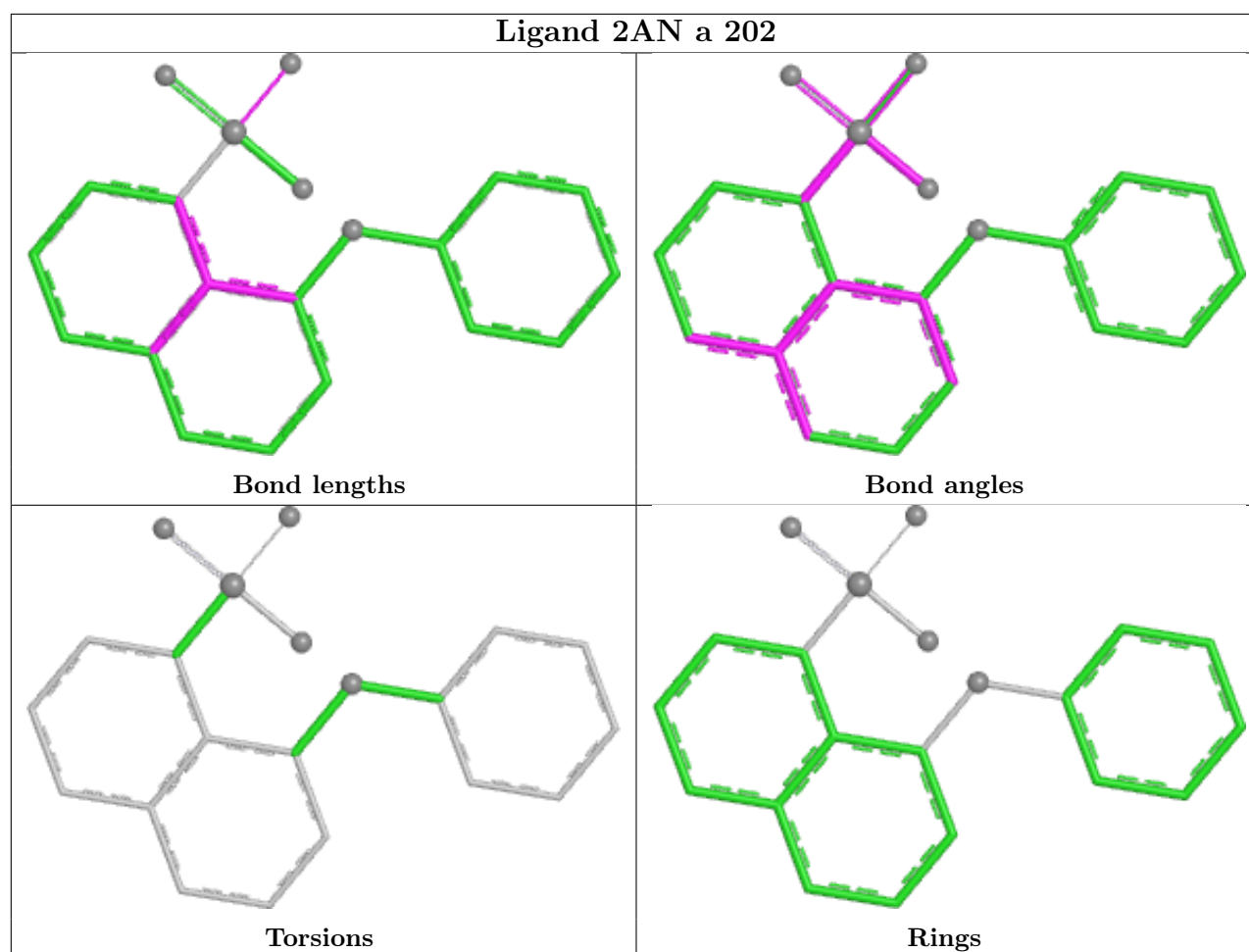
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	X	201	2AN	3	0
2	N	204	2AN	5	0
2	I	205	2AN	13	0
2	L	204	2AN	10	0
2	b	204	2AN	9	0
6	a	205	FLC	1	0
2	d	203	2AN	6	0
2	F	201	2AN	11	0
2	Z	203	2AN	10	0
2	G	204	2AN	6	0
2	j	204	2AN	7	0
2	N	203	2AN	3	0
2	X	204	2AN	4	0
2	R	205	2AN	9	0
2	S	201	2AN	4	0
2	U	202	2AN	5	0
2	C	203[A]	2AN	3	0
2	H	204	2AN	10	0
2	L	203	2AN	4	0
2	b	203	2AN	9	0
2	F	205	2AN	4	0
2	T	203	2AN	12	0
3	Y	205	SO4	2	0
2	B	203	2AN	9	0
2	L	201	2AN	7	0
2	I	206	2AN	4	0
2	V	206	2AN	4	0
2	i	201	2AN	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

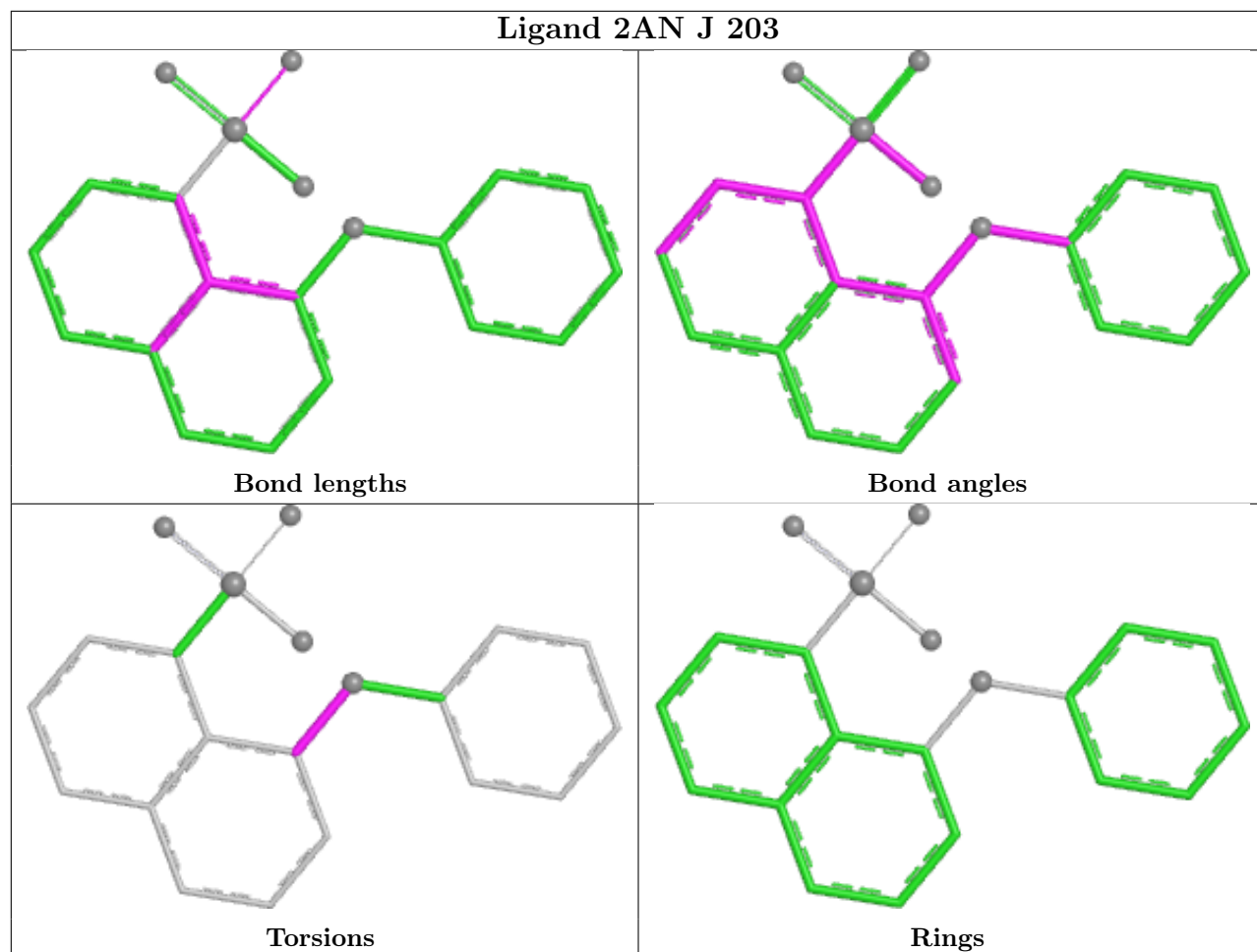


Ligand 2AN T 202

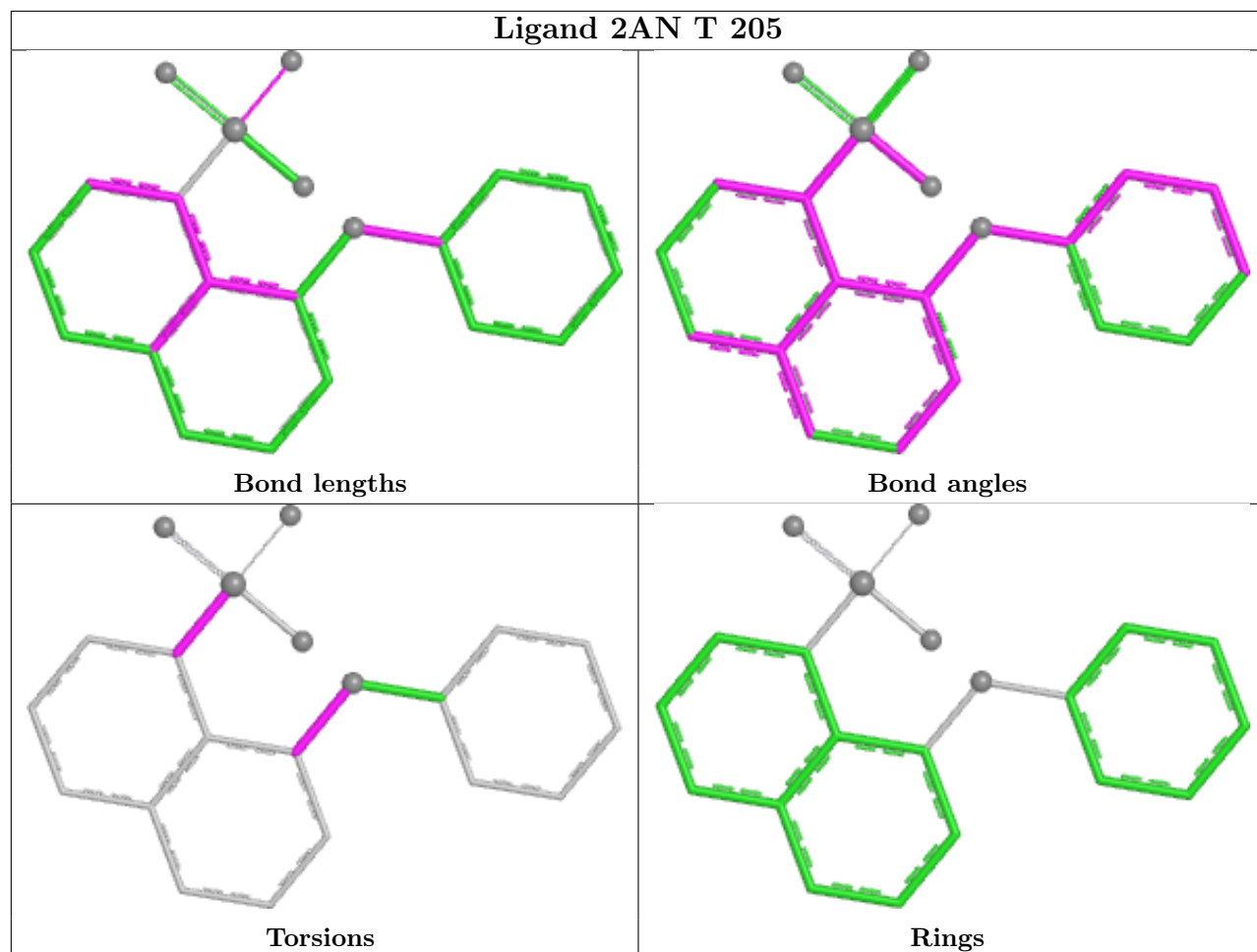


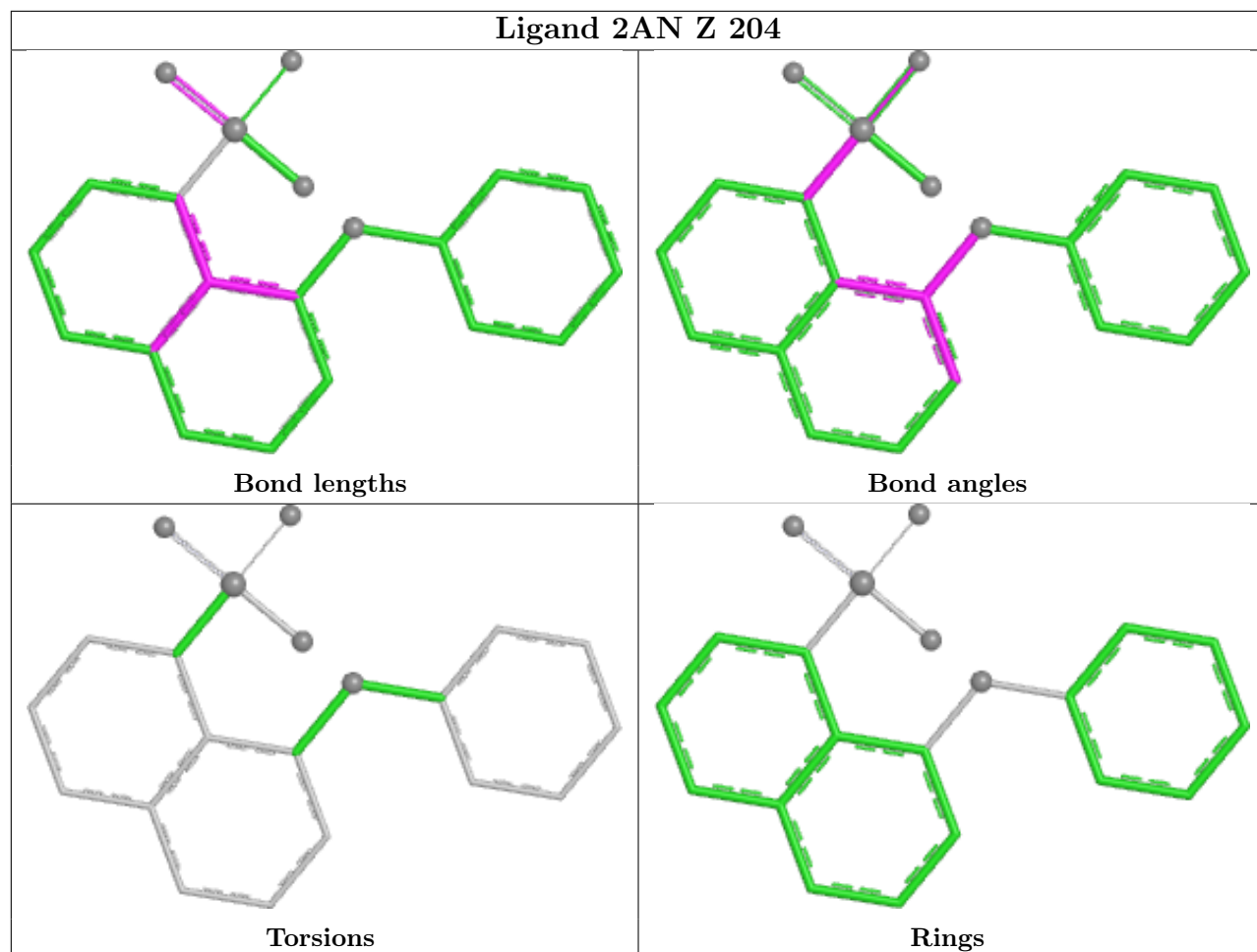


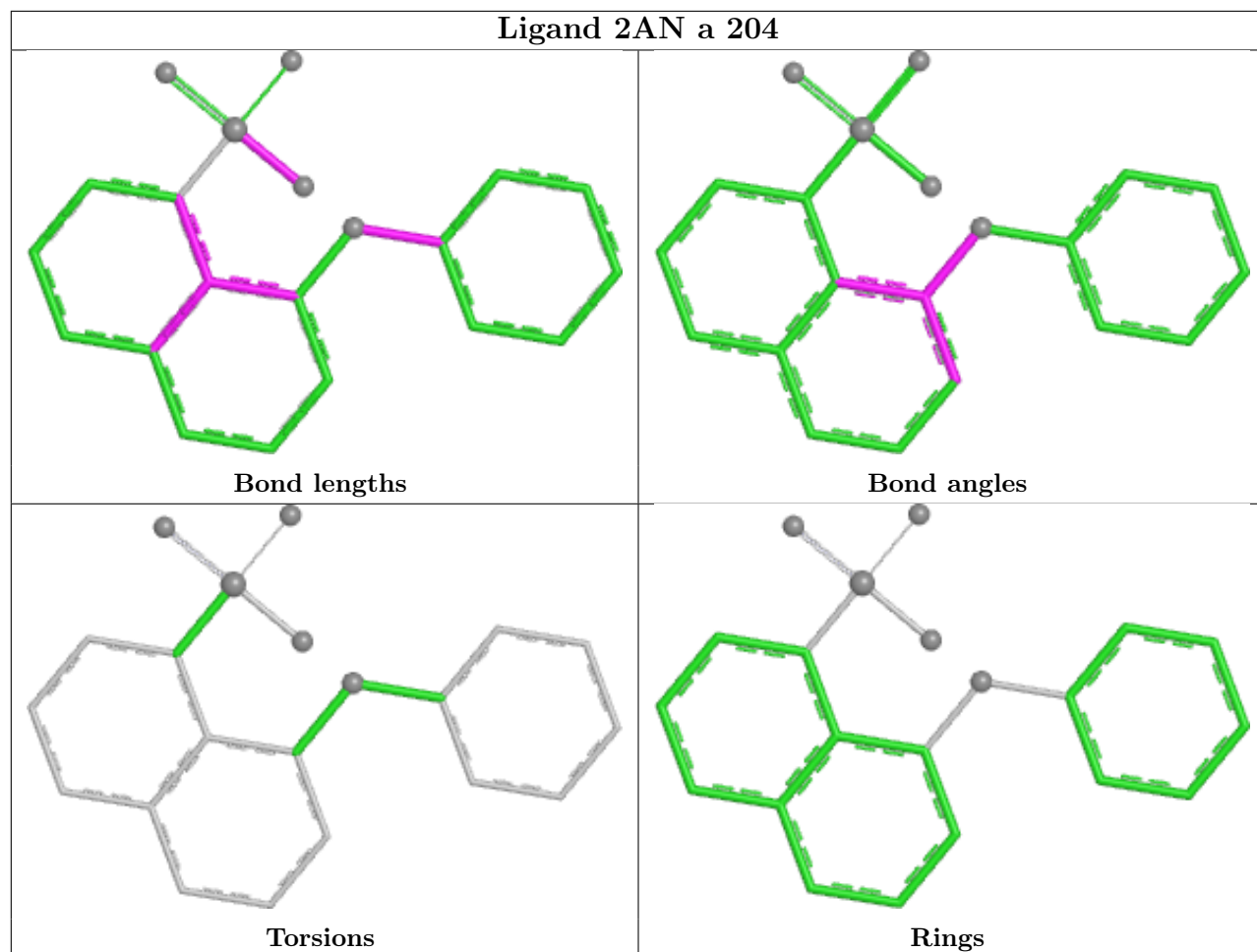
Ligand 2AN J 203

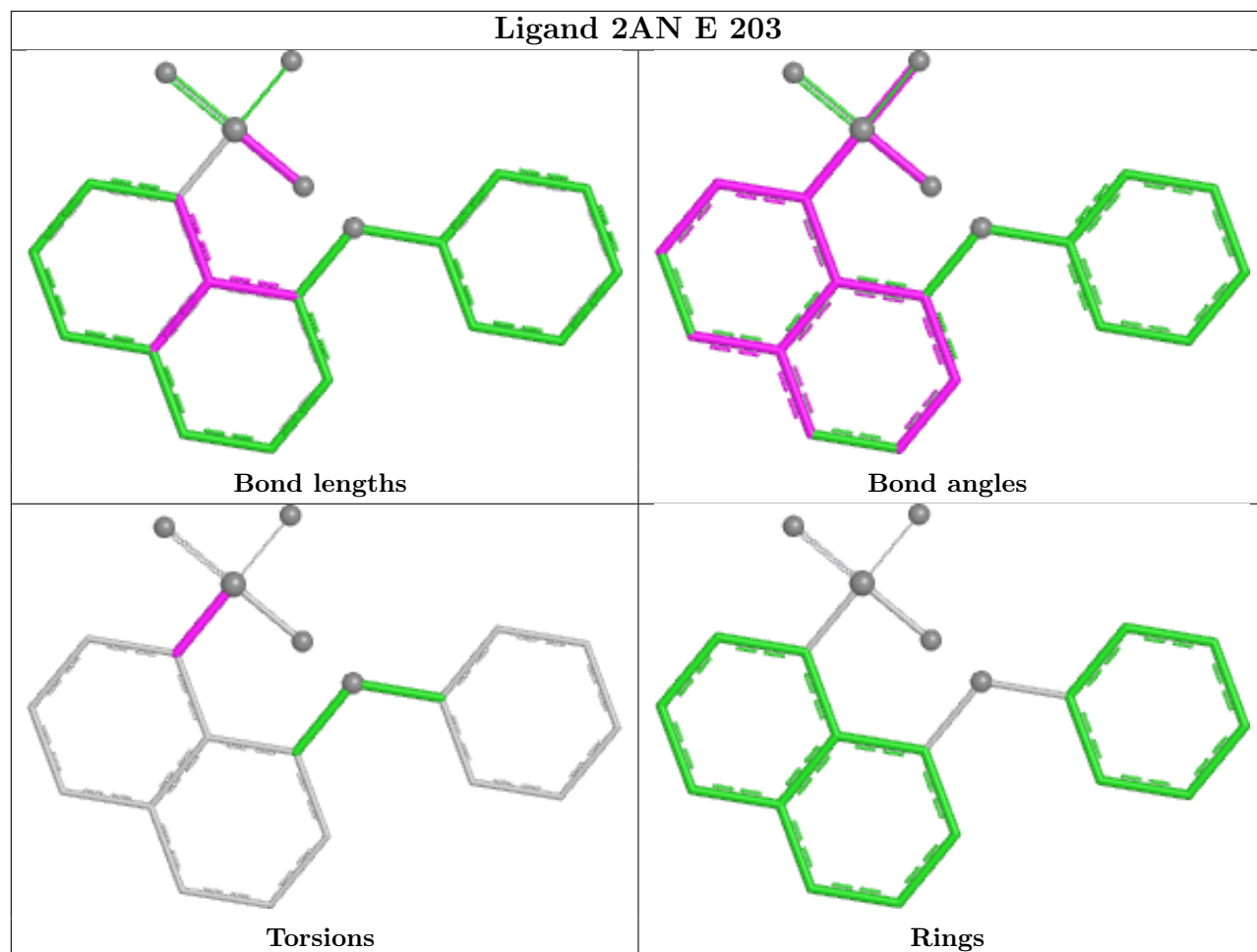


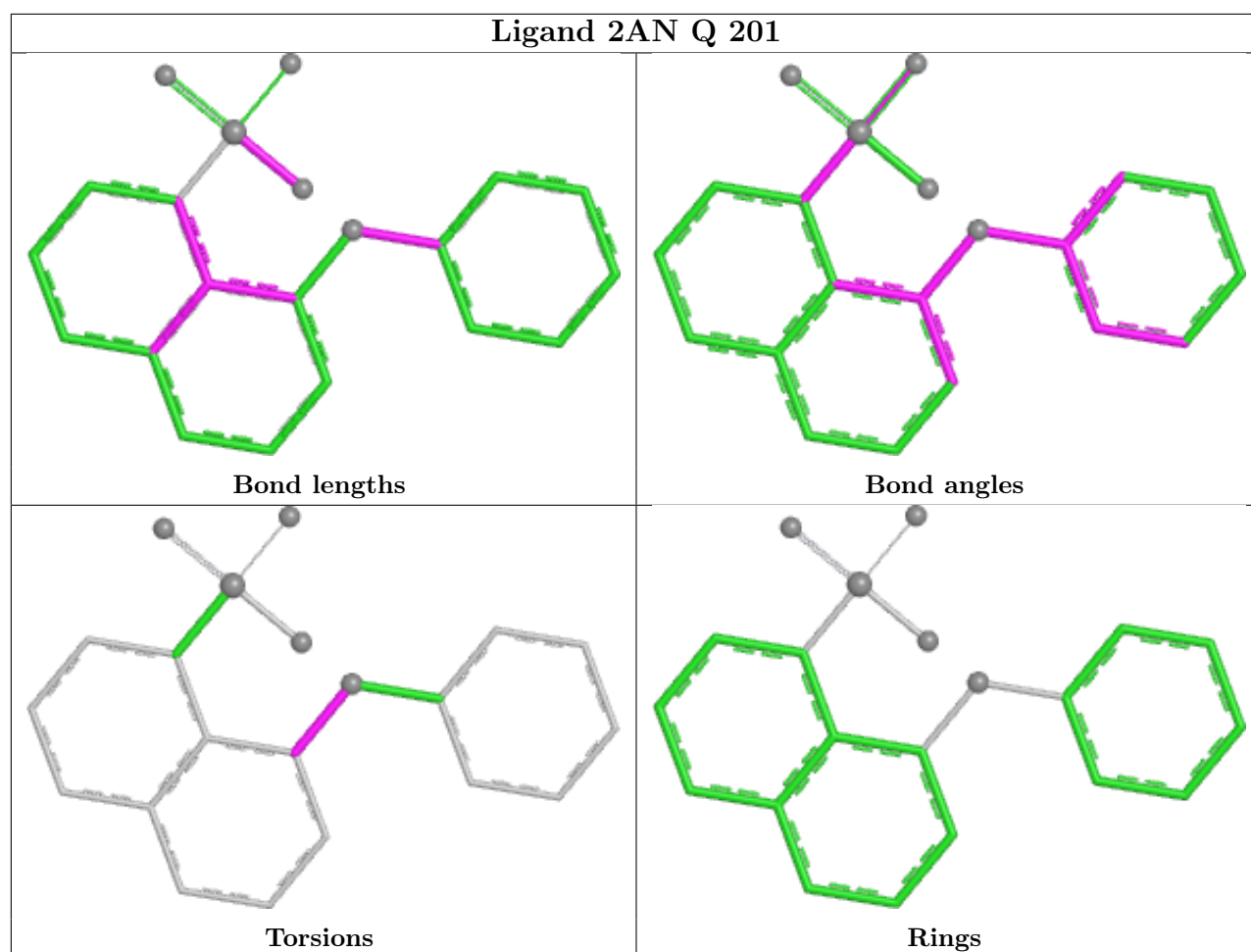
Ligand 2AN T 205



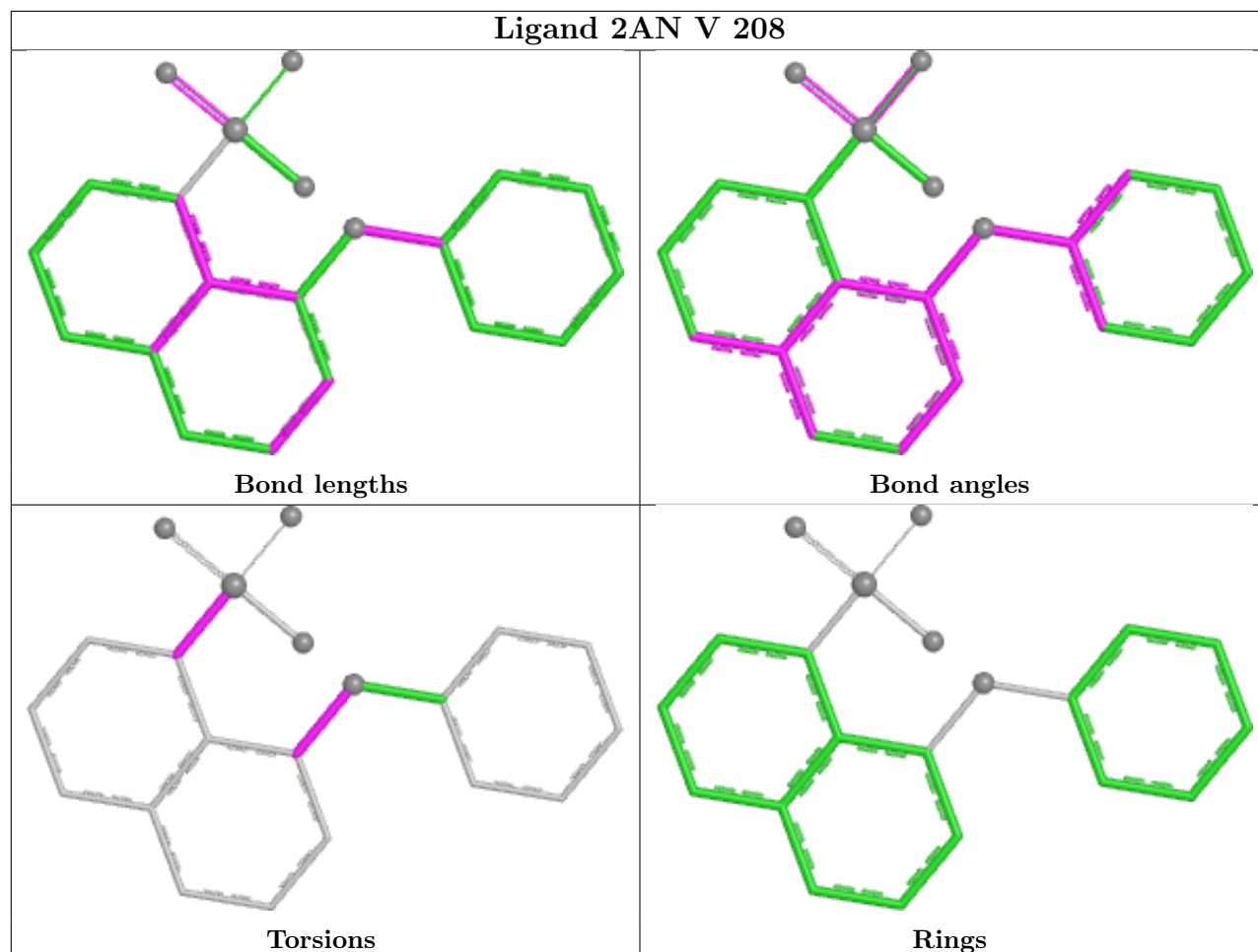




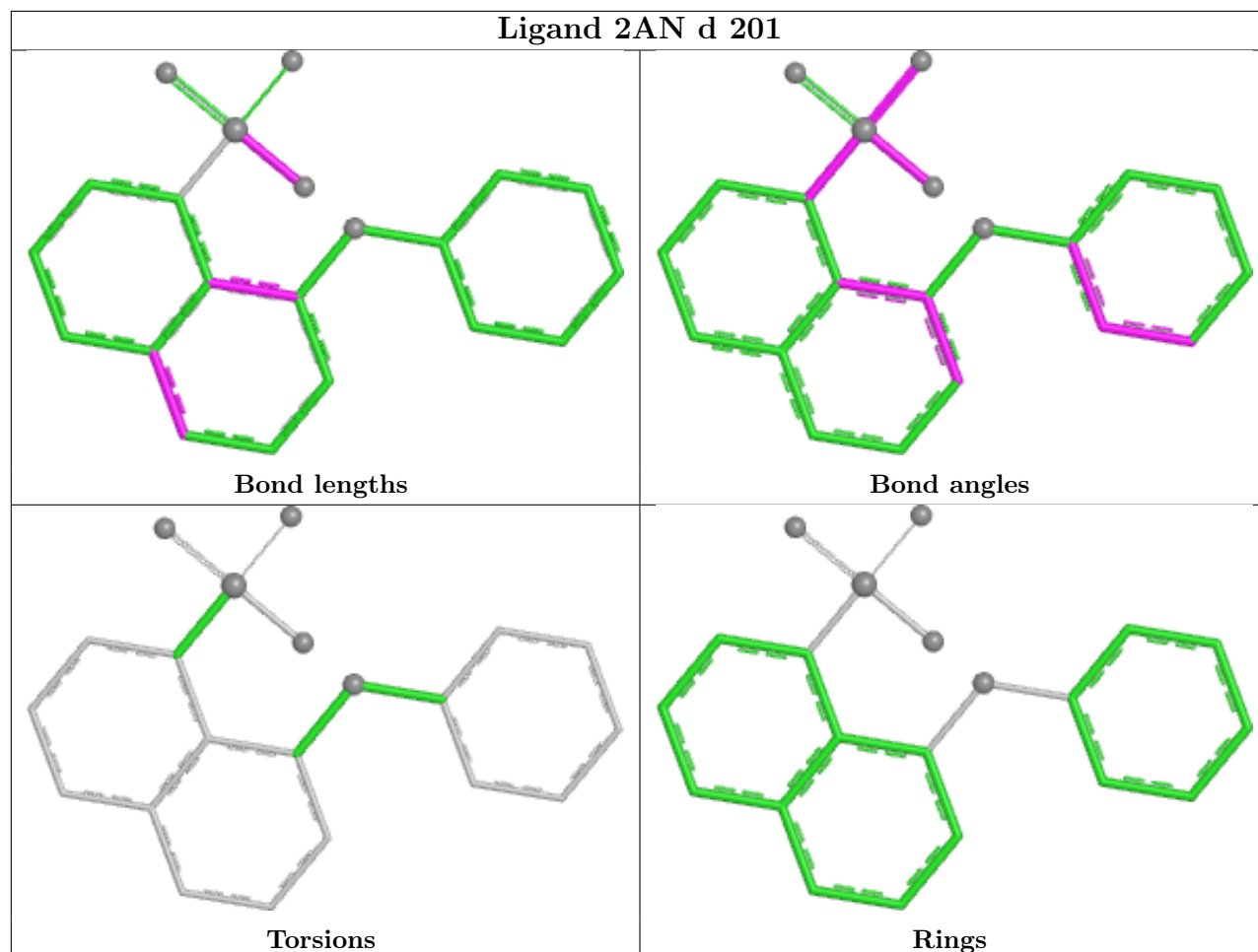


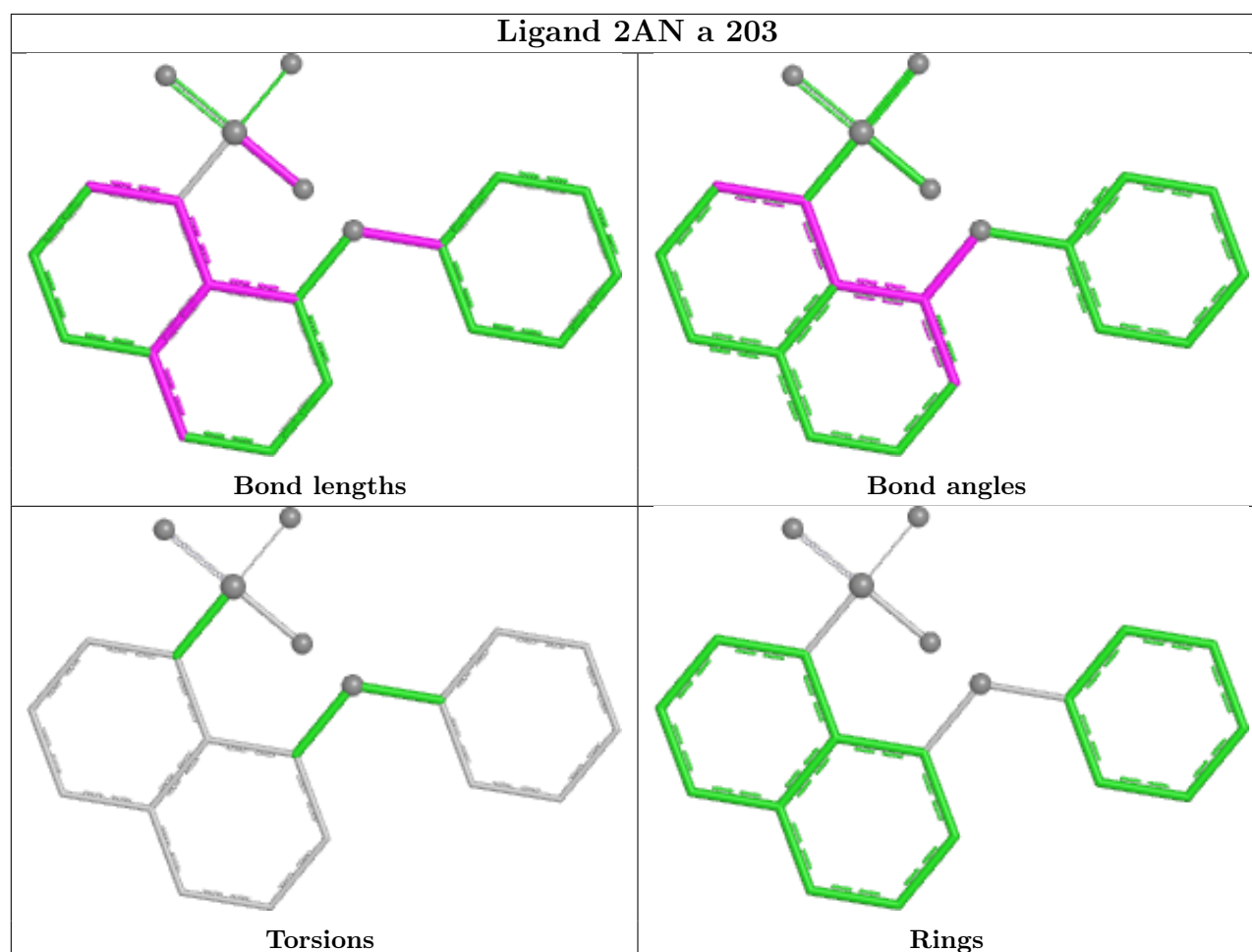


Ligand 2AN V 208

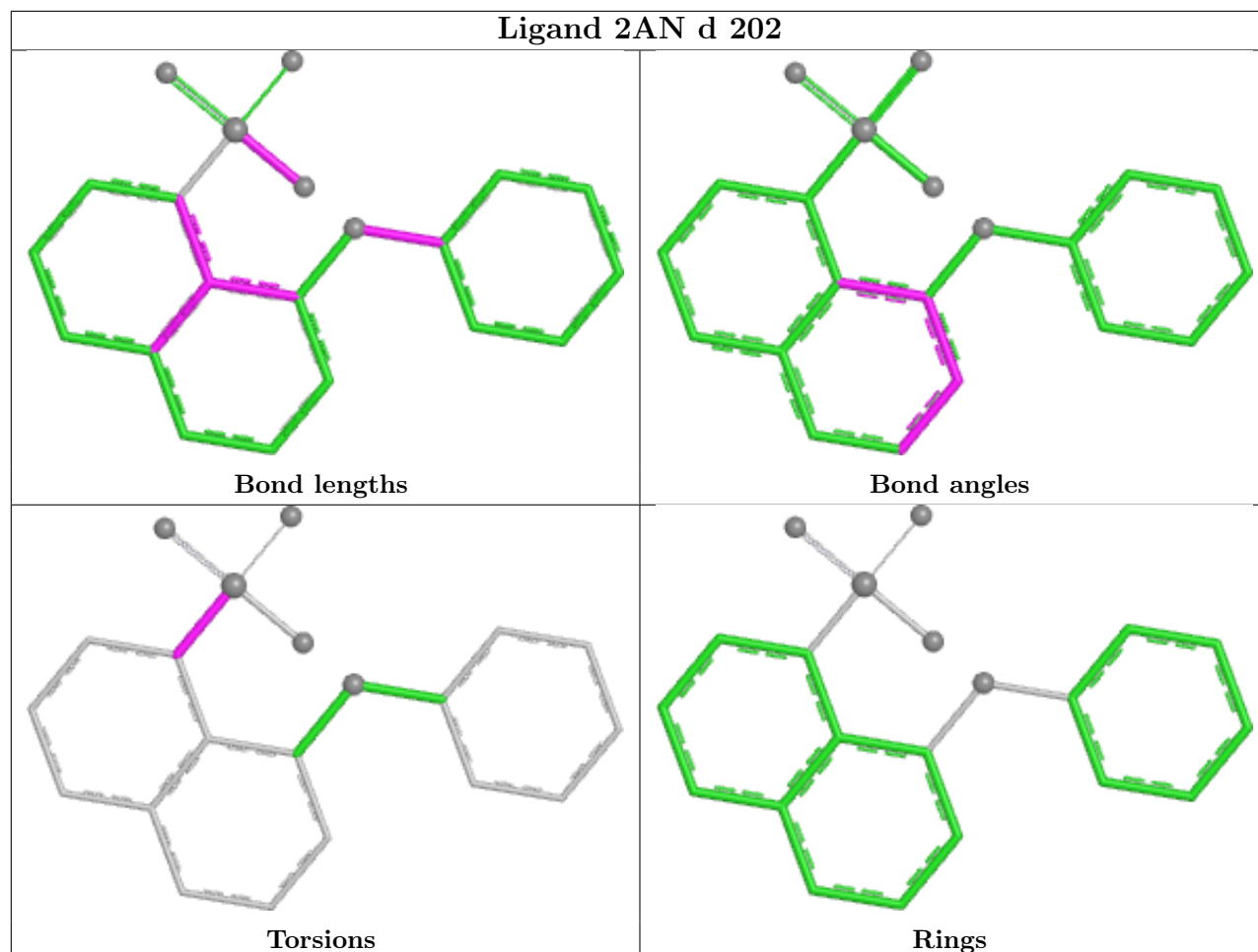


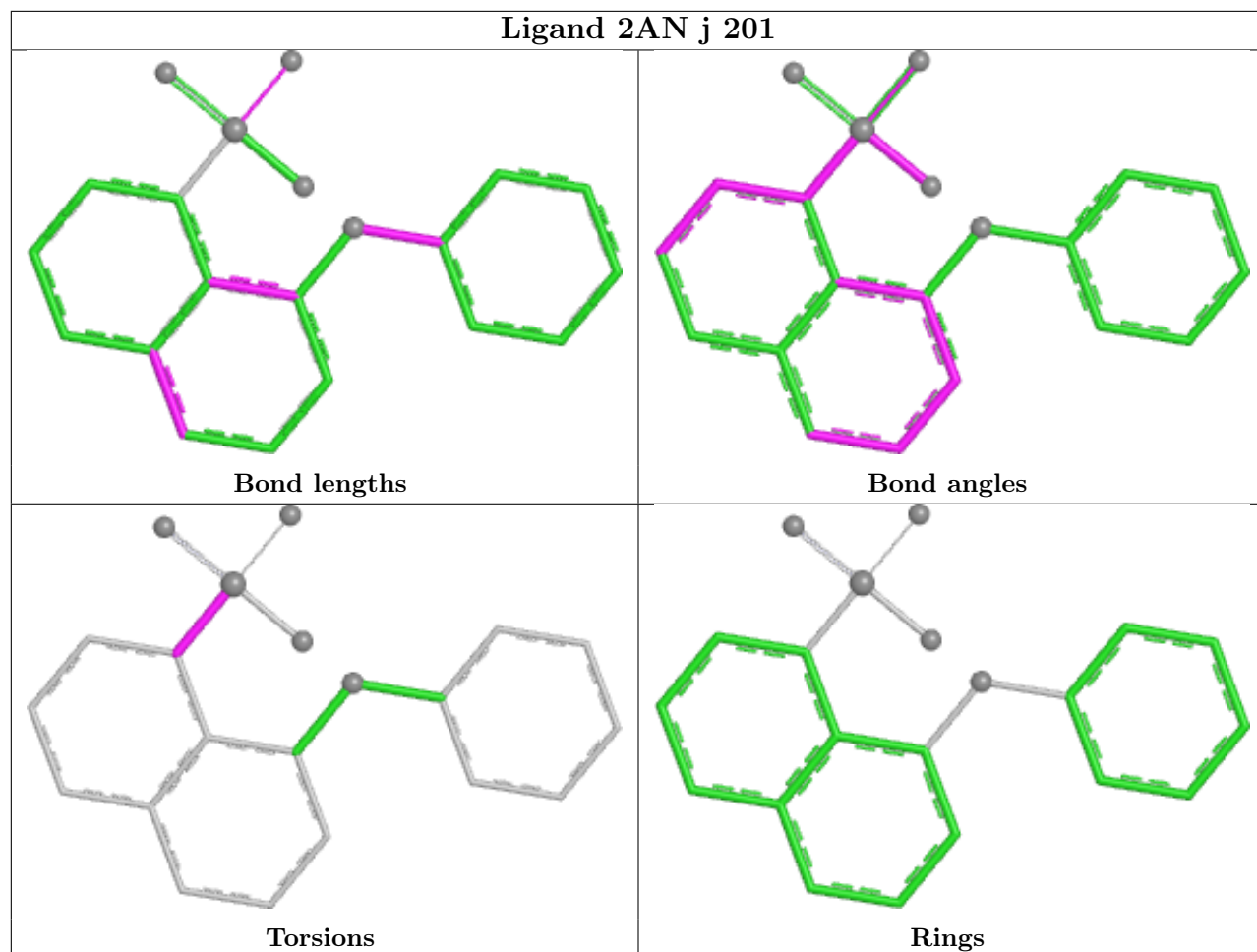
Ligand 2AN d 201



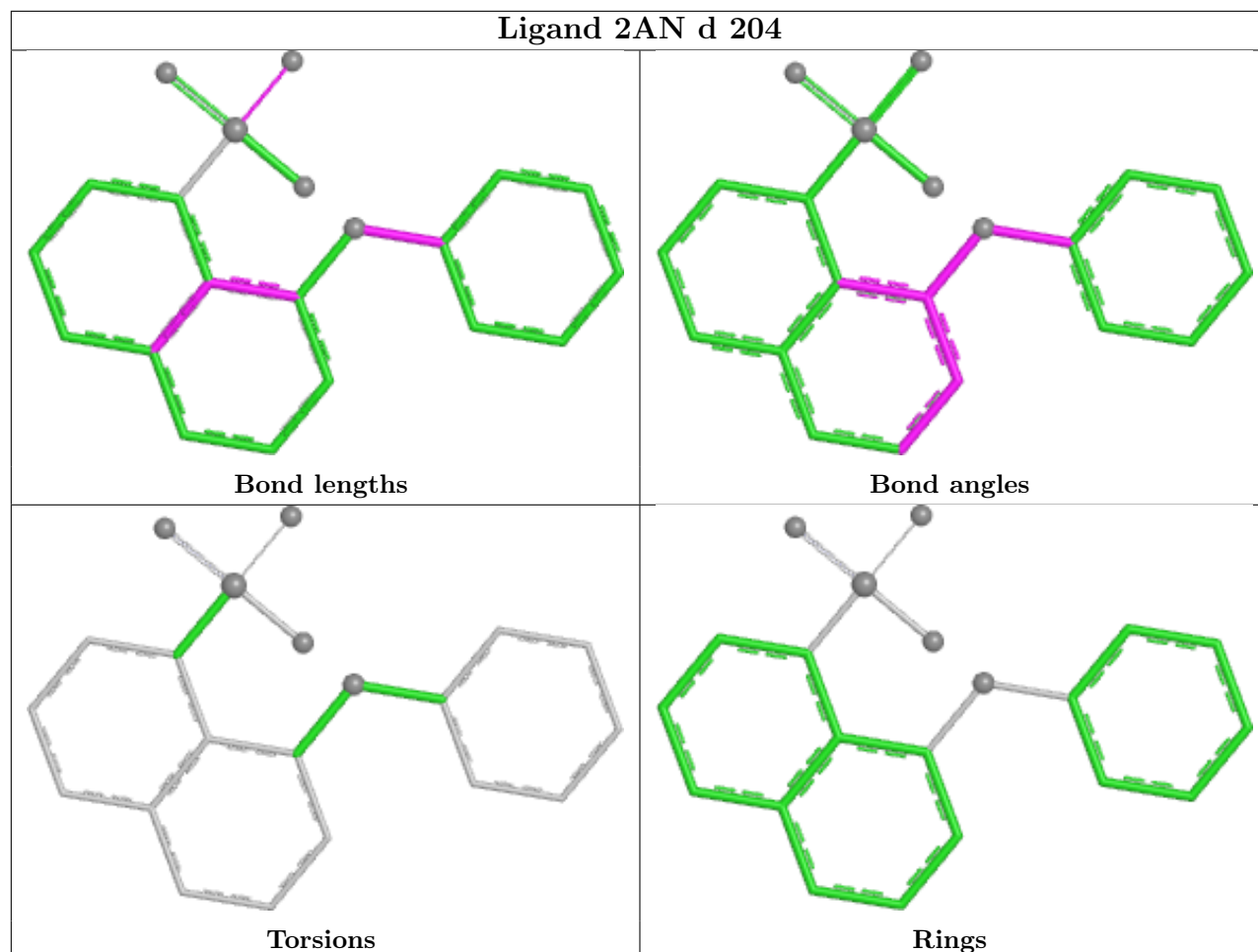


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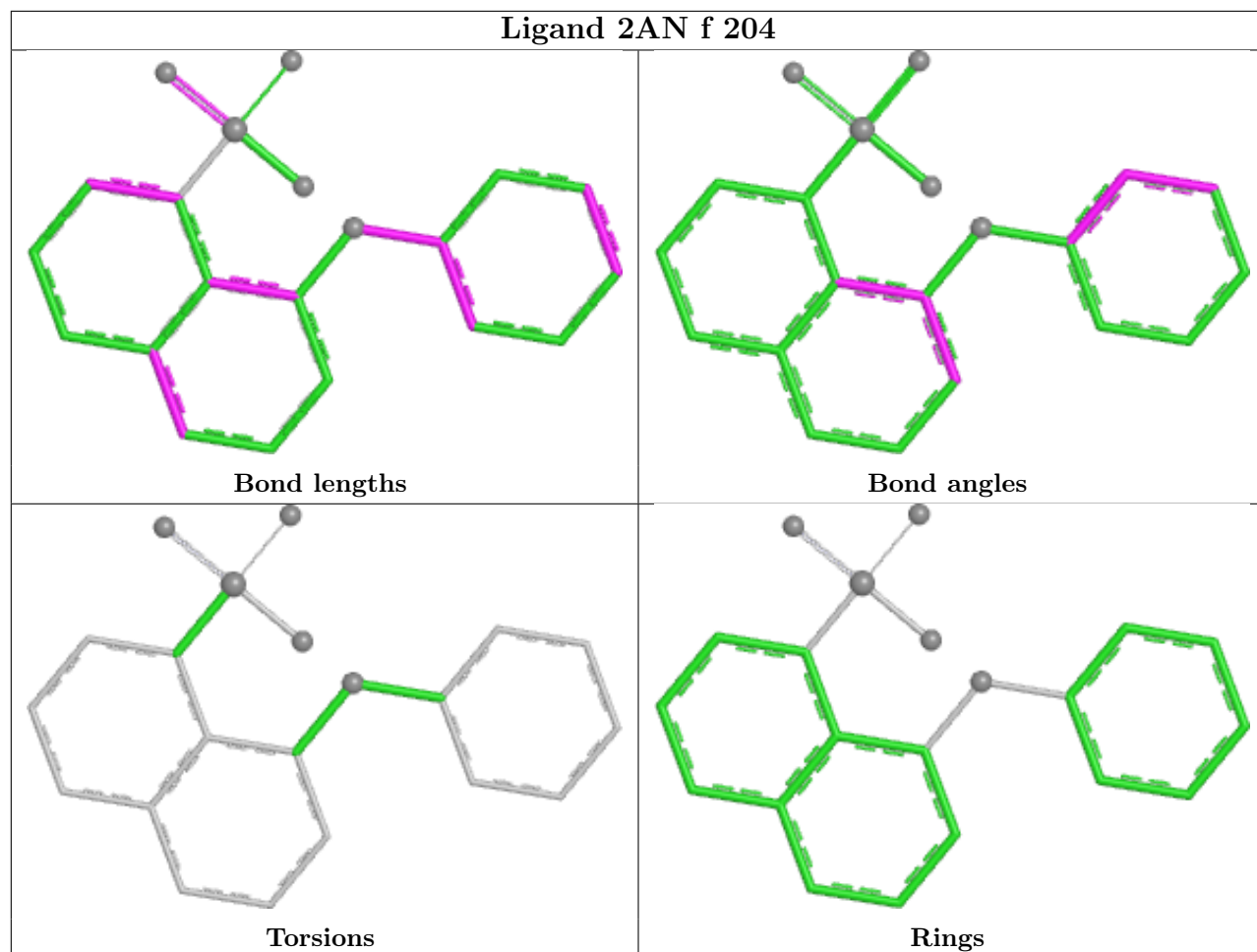


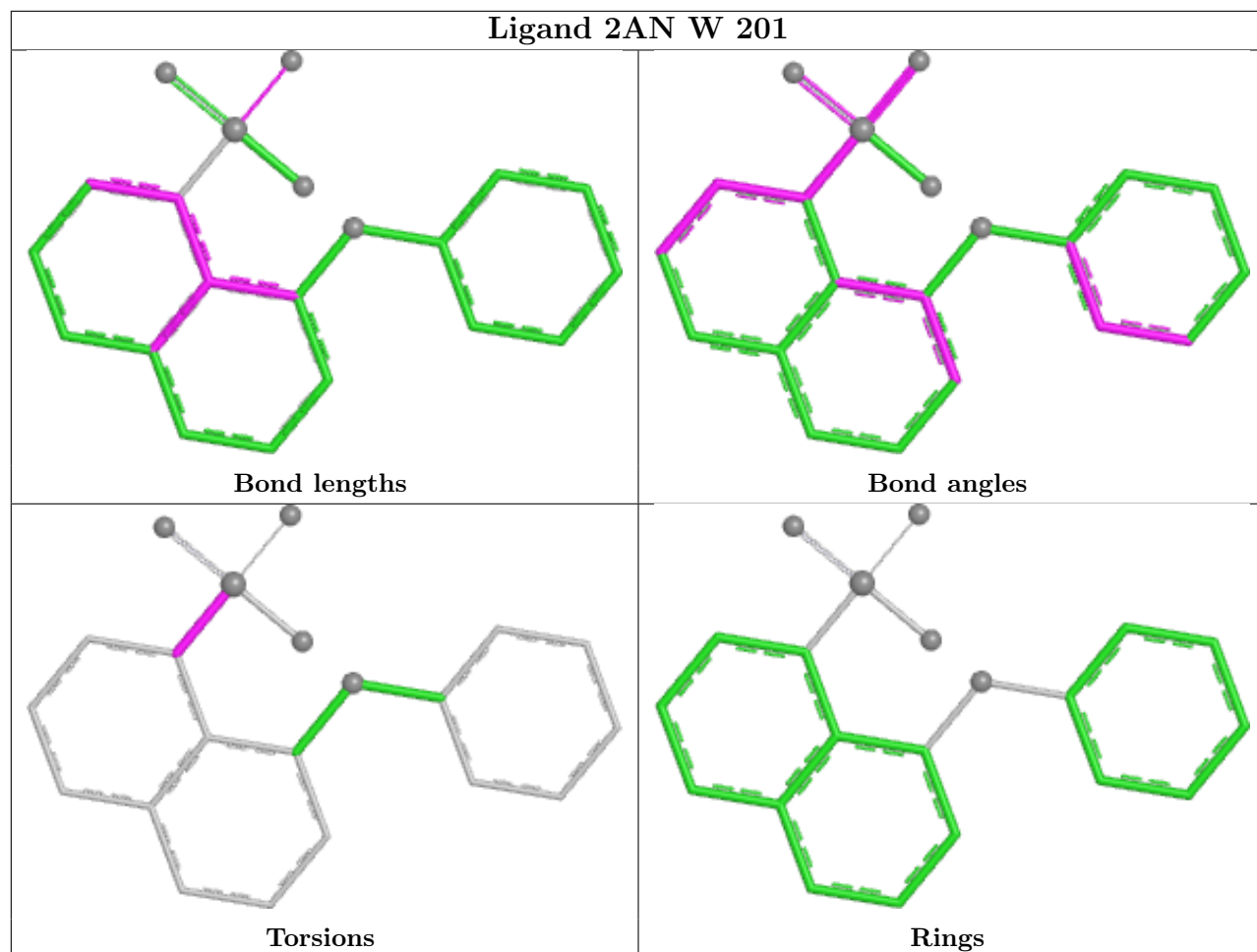


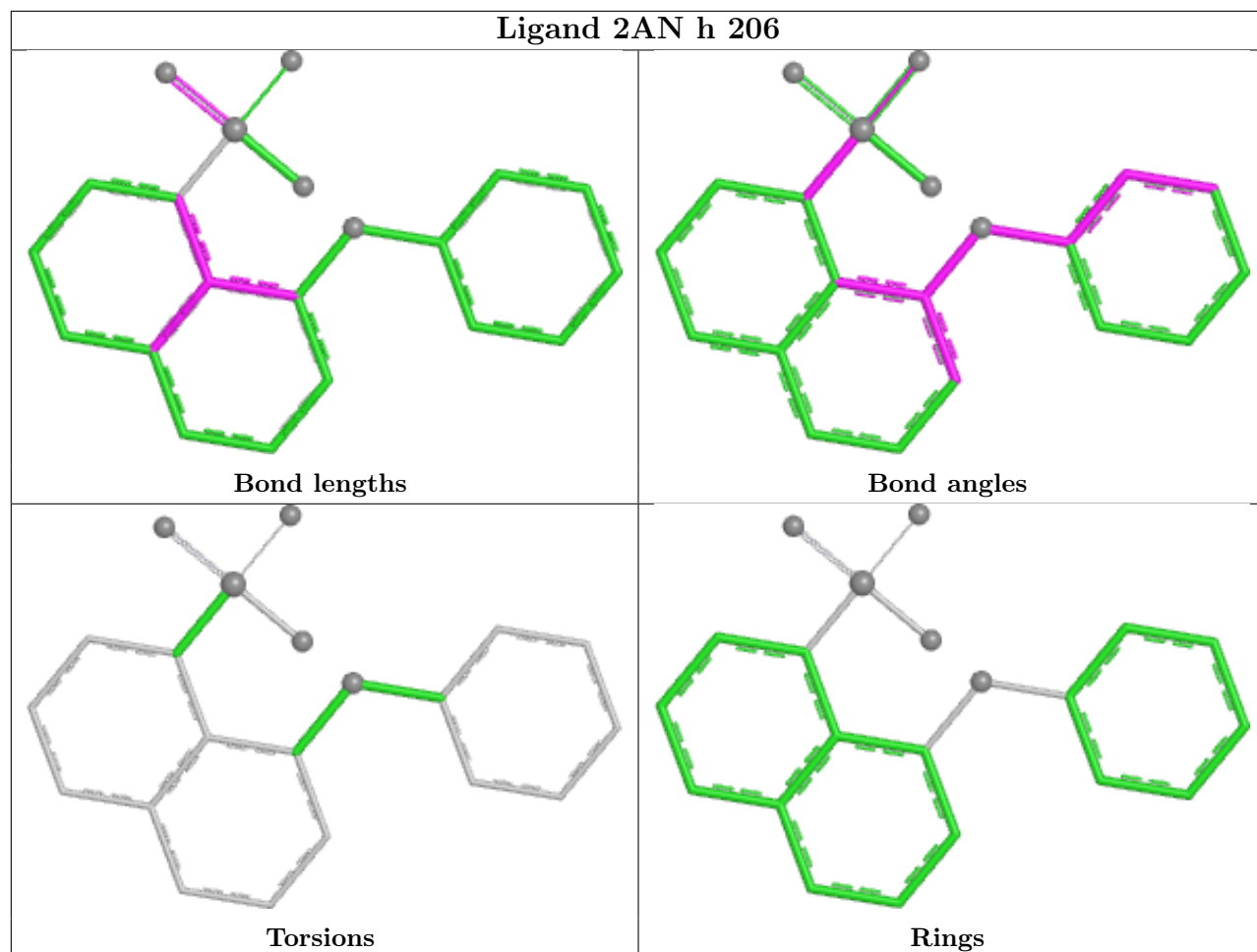
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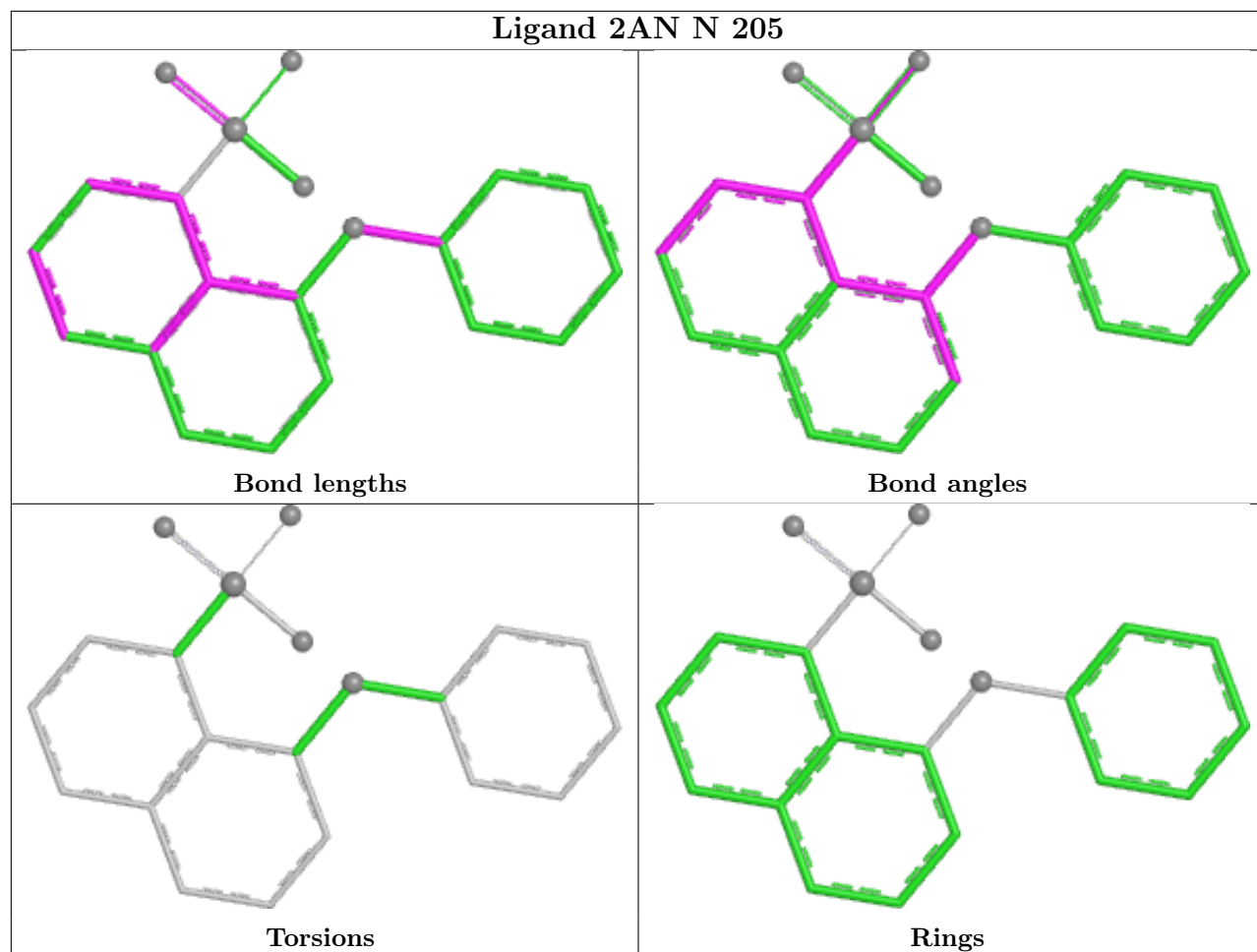


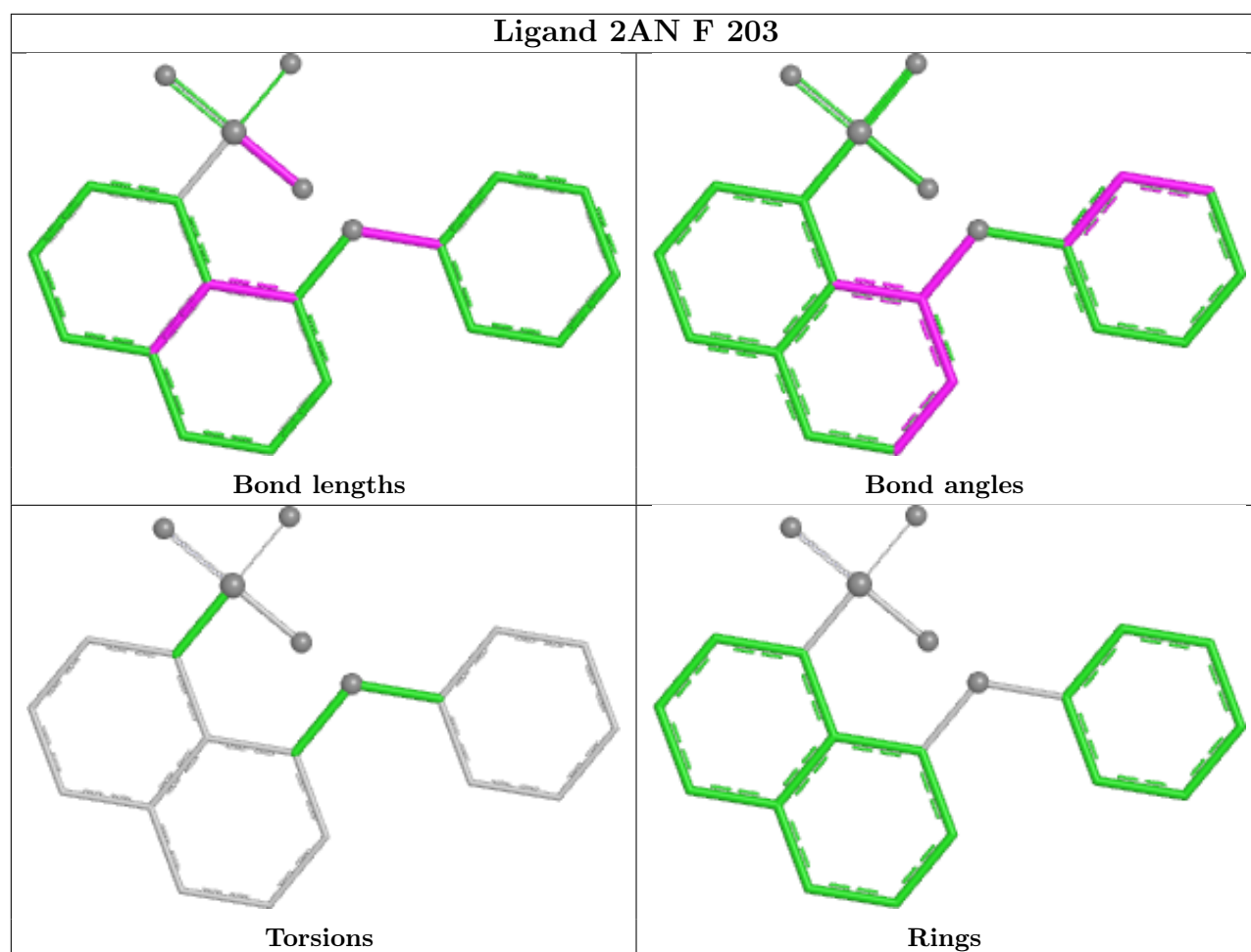
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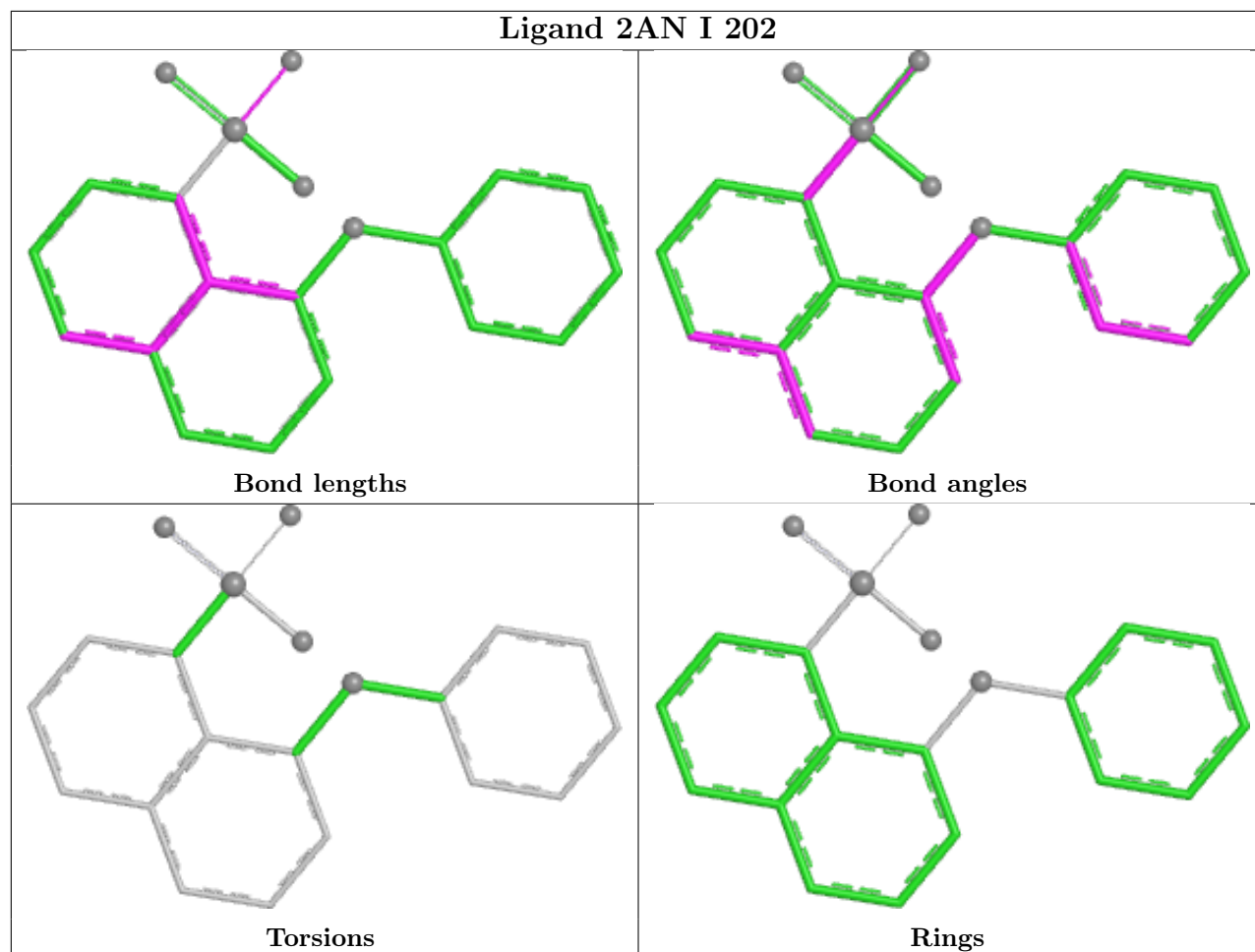




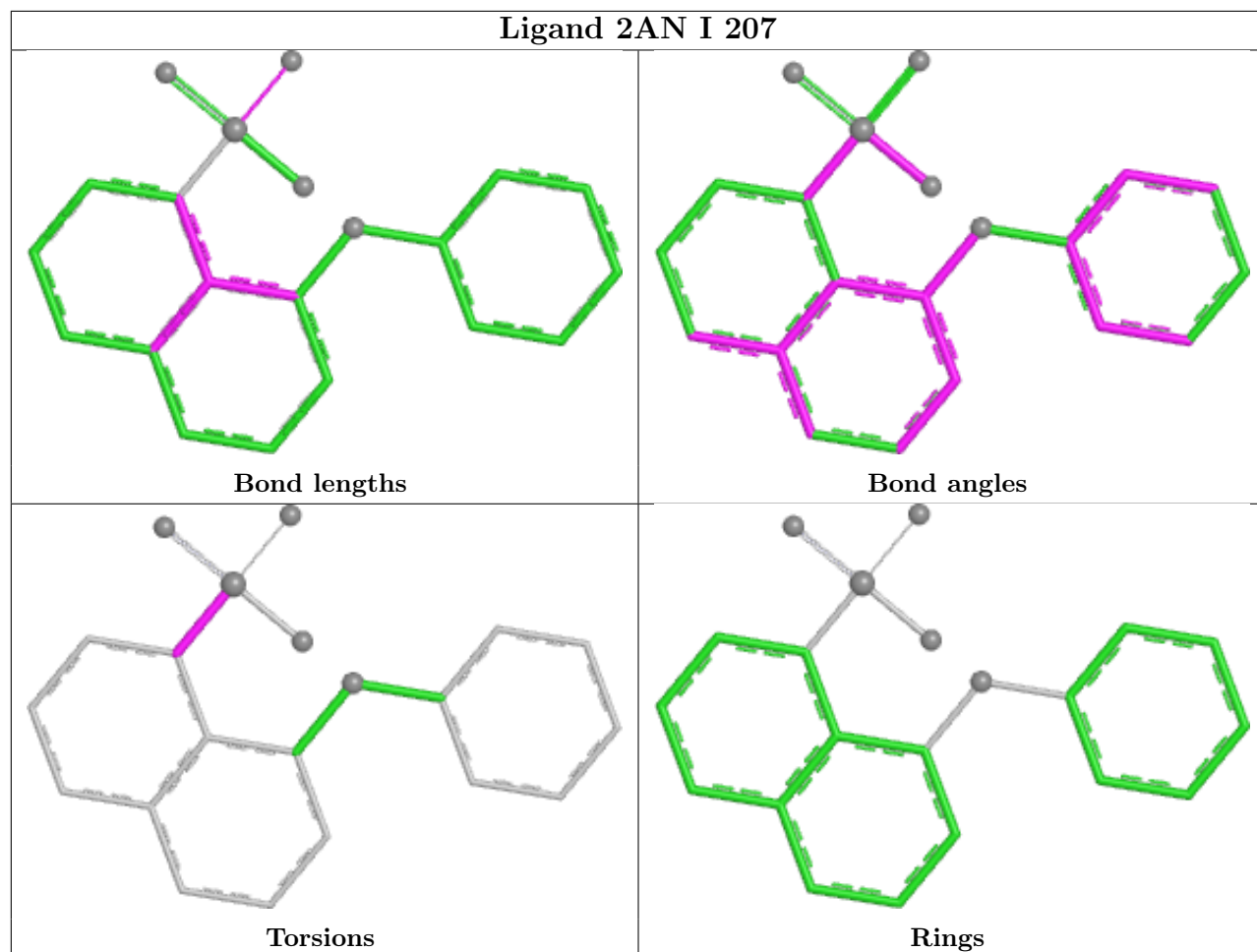




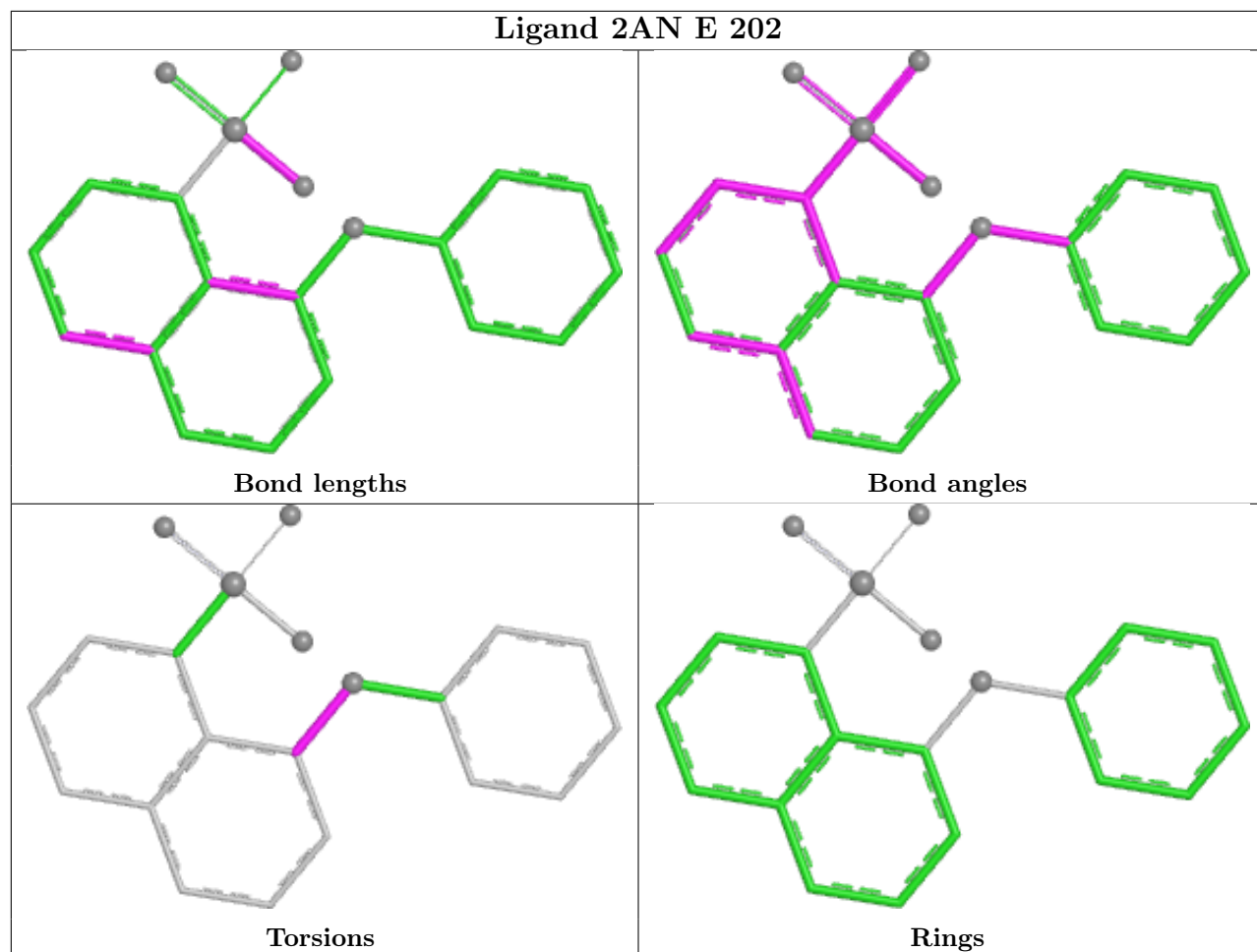
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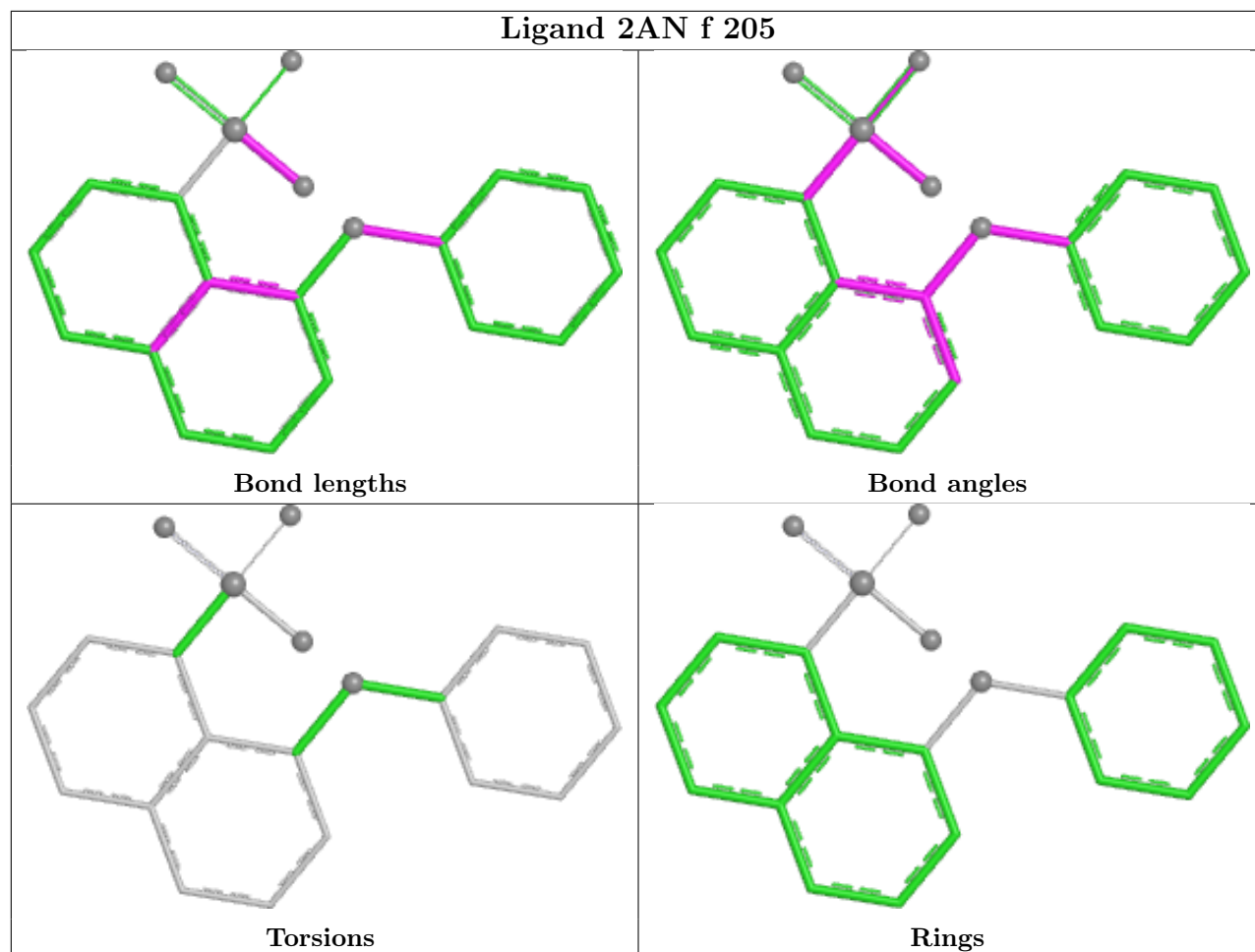


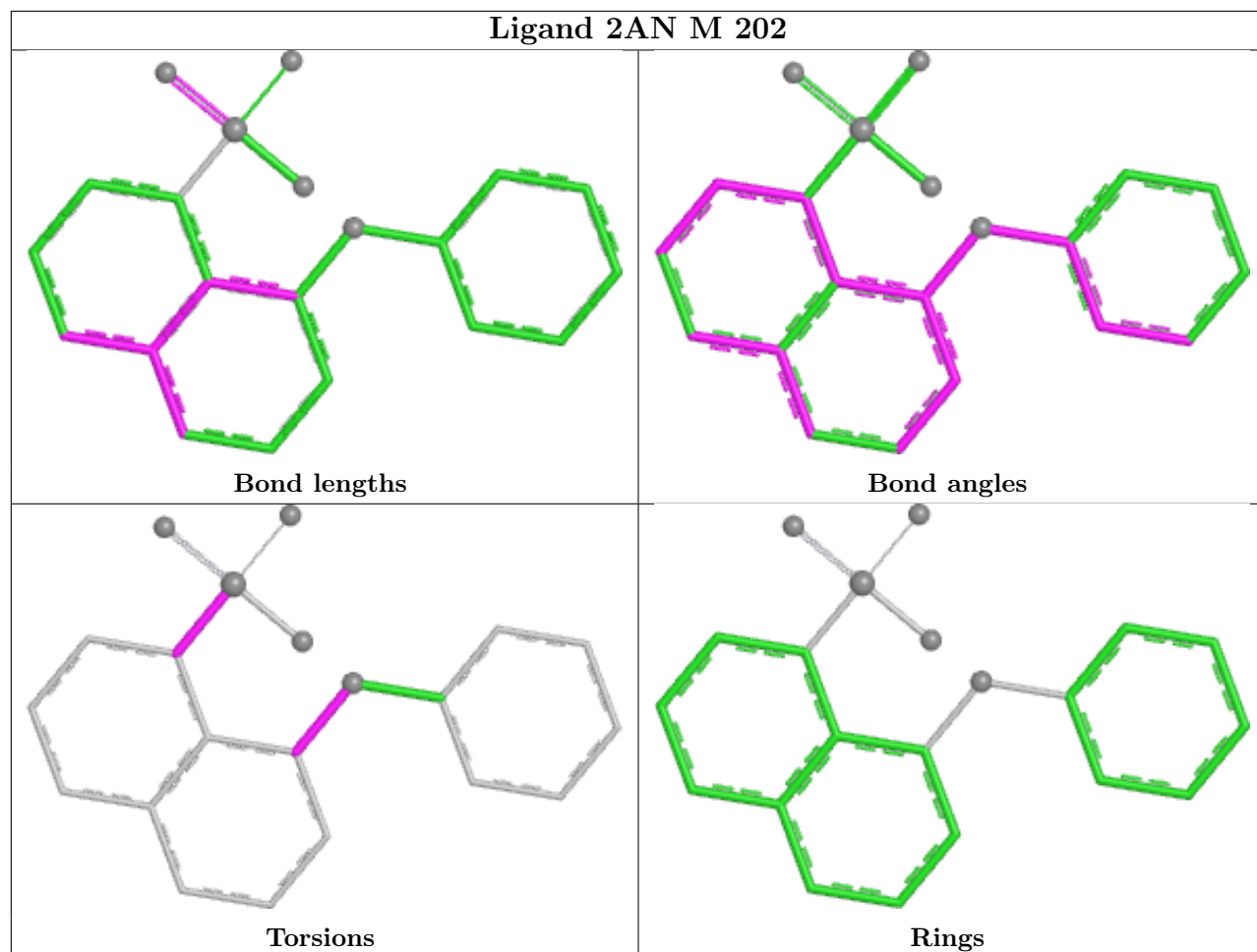
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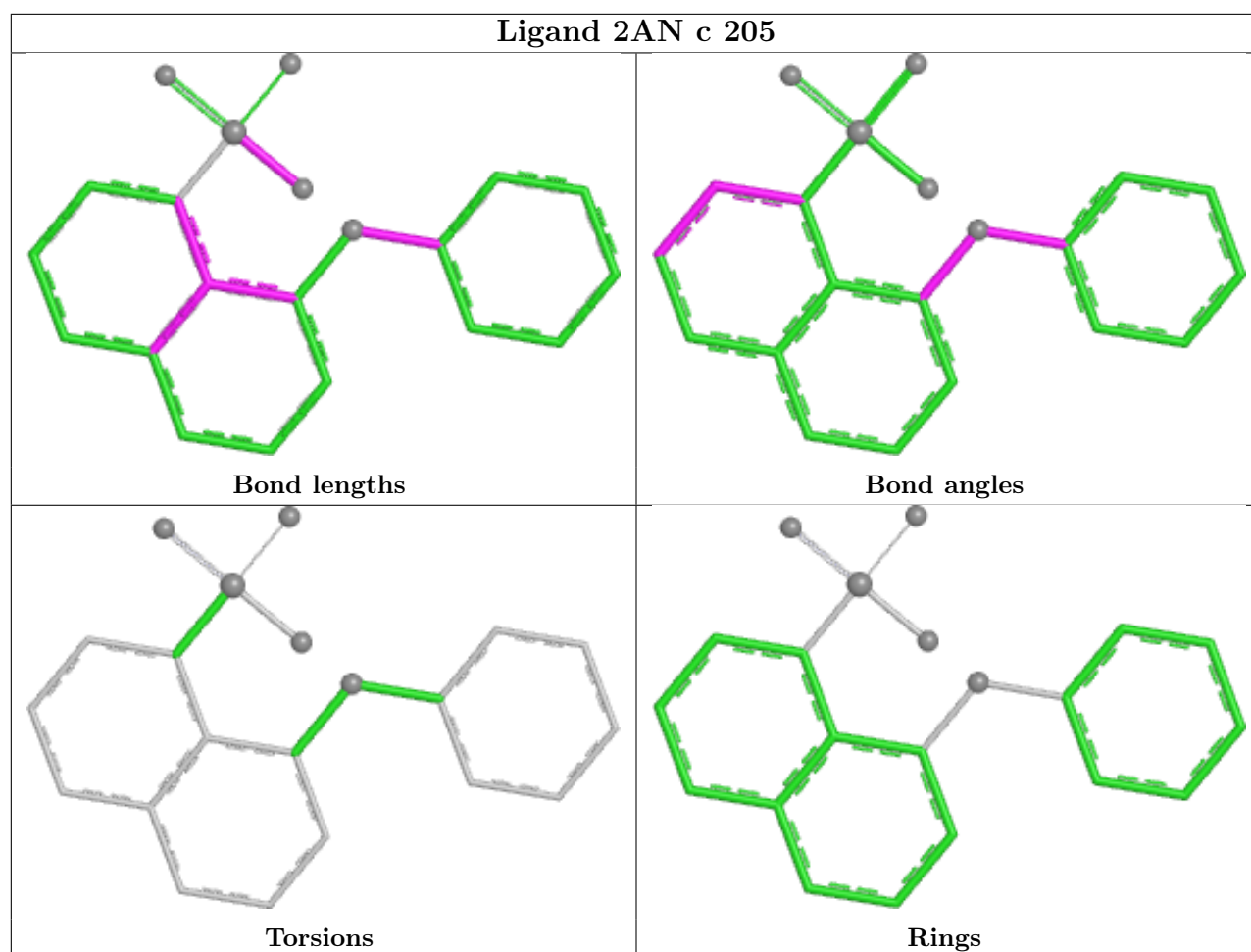


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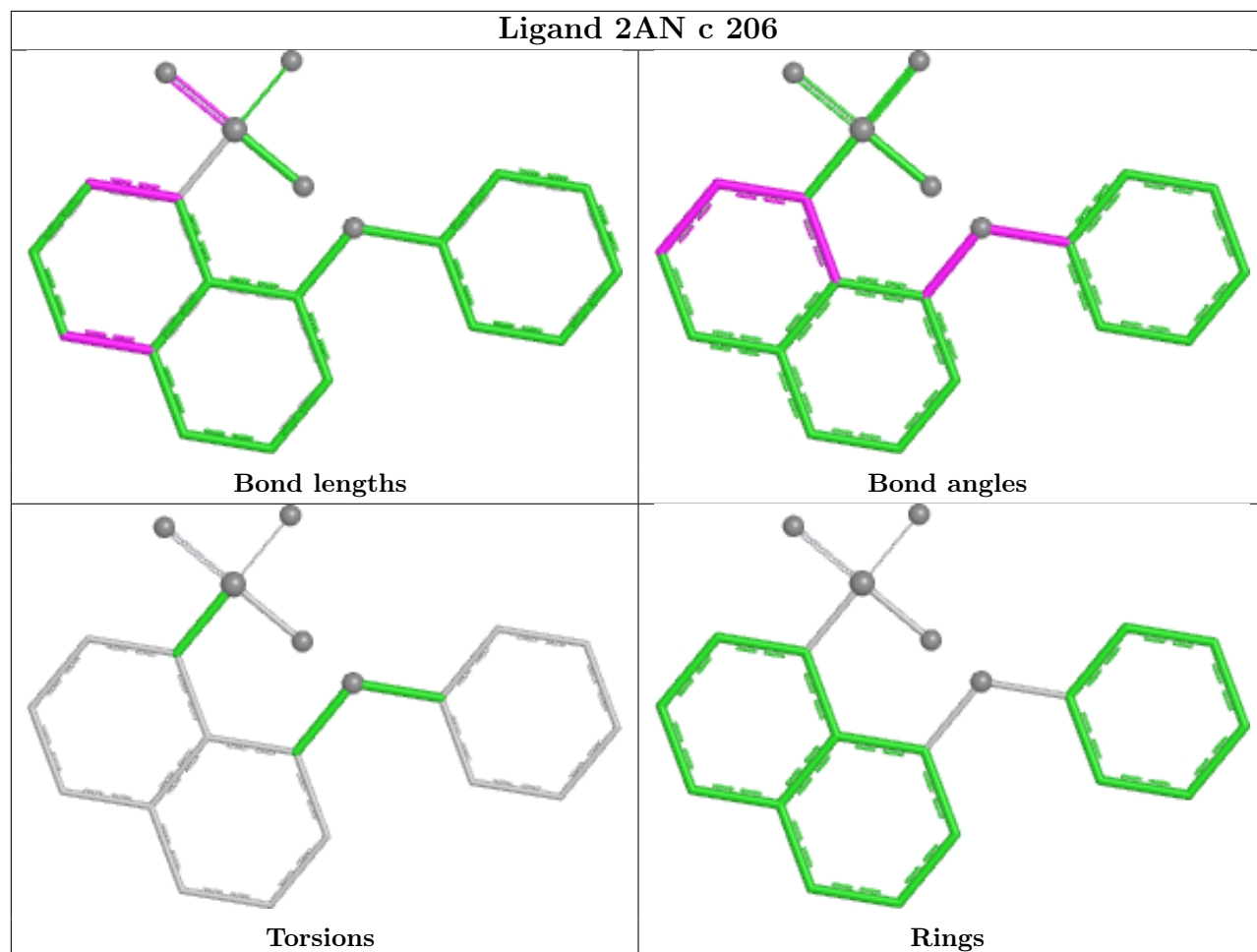


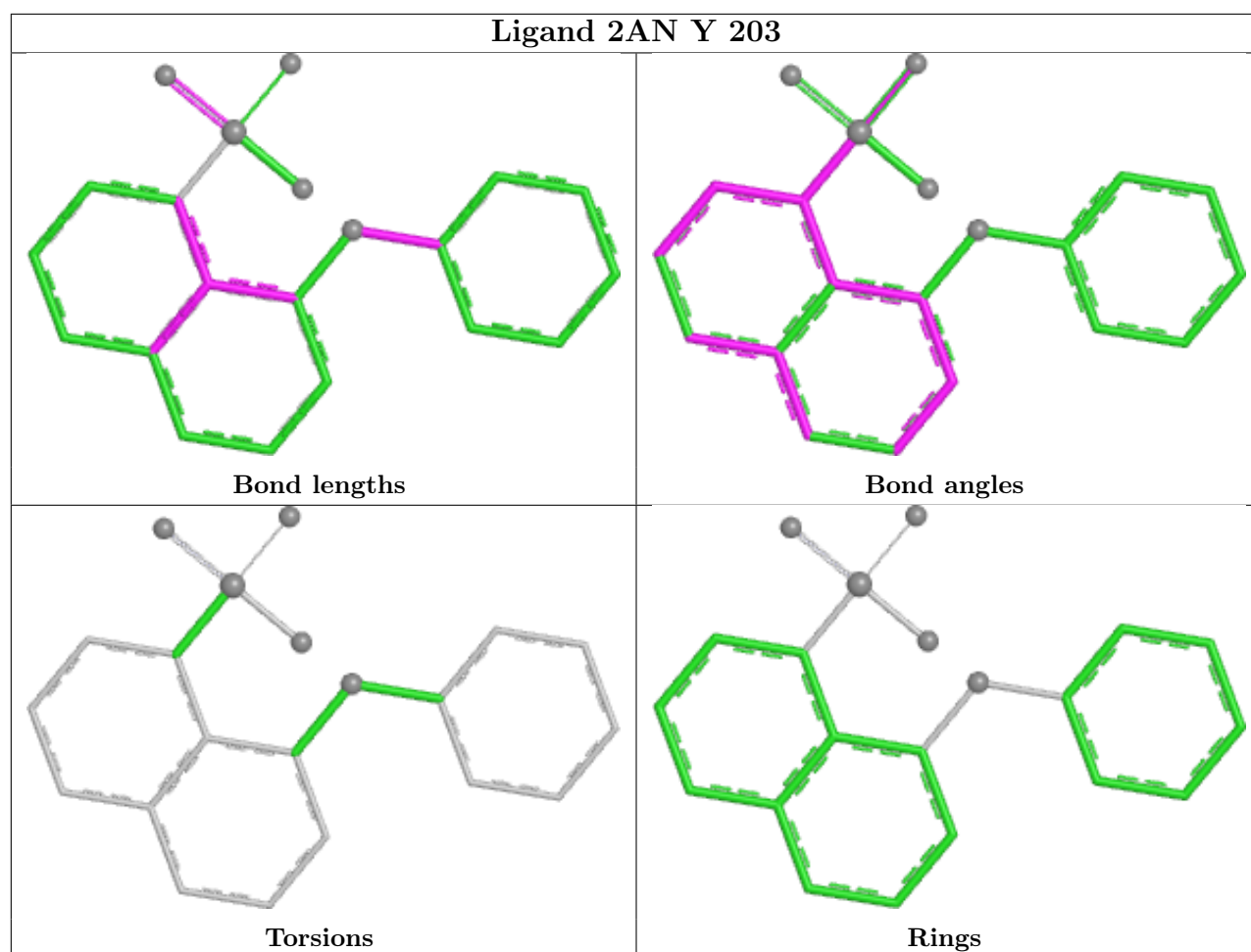


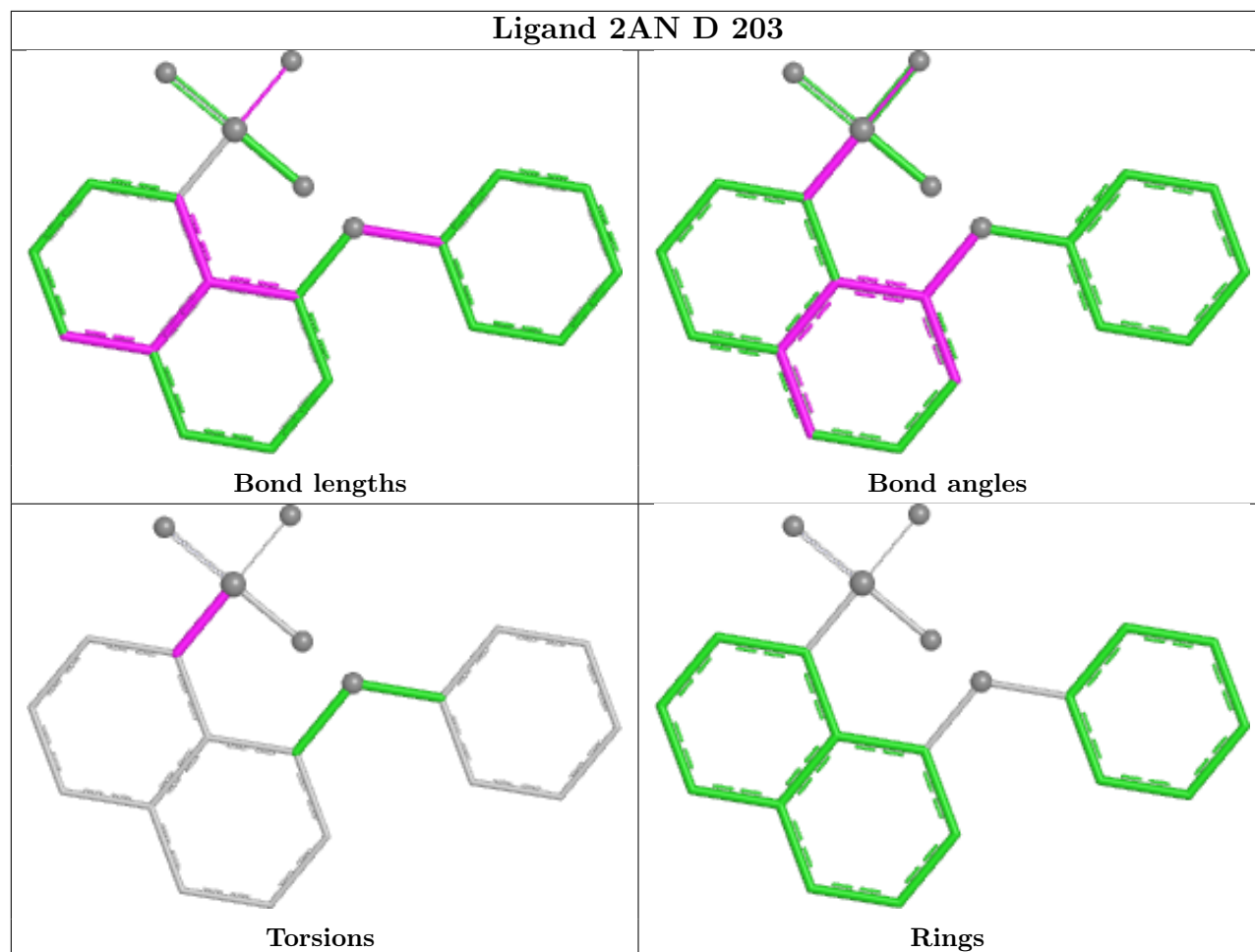




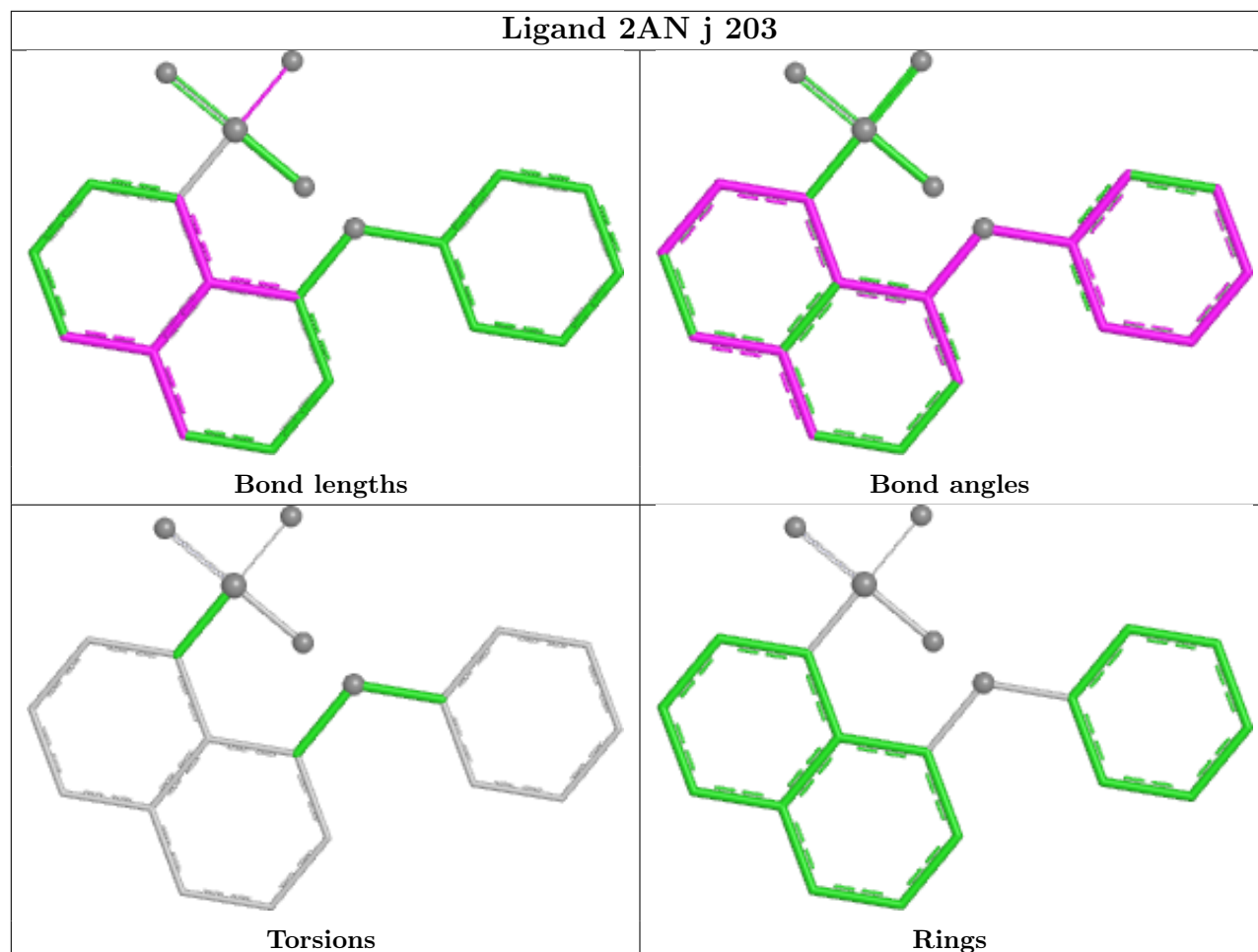
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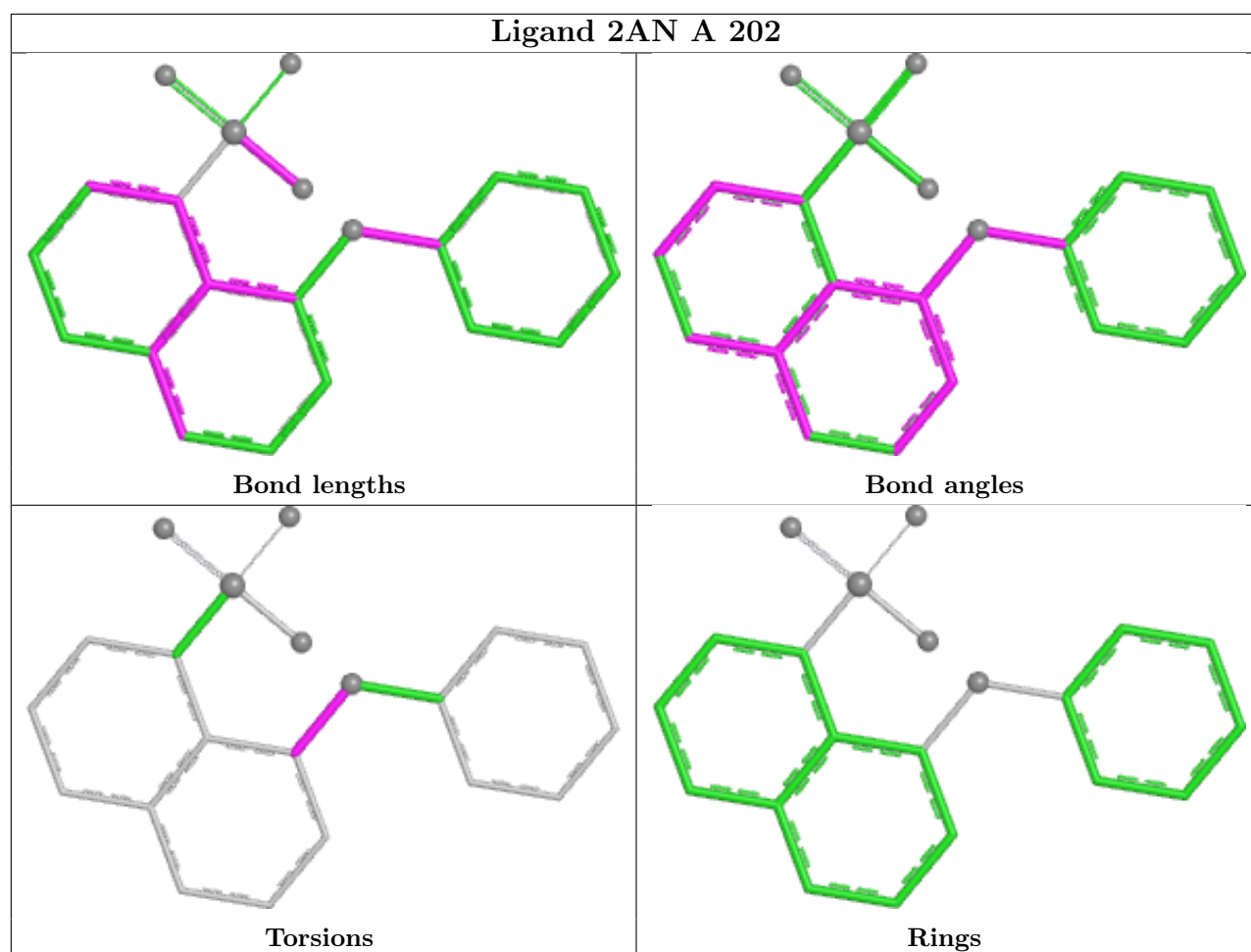


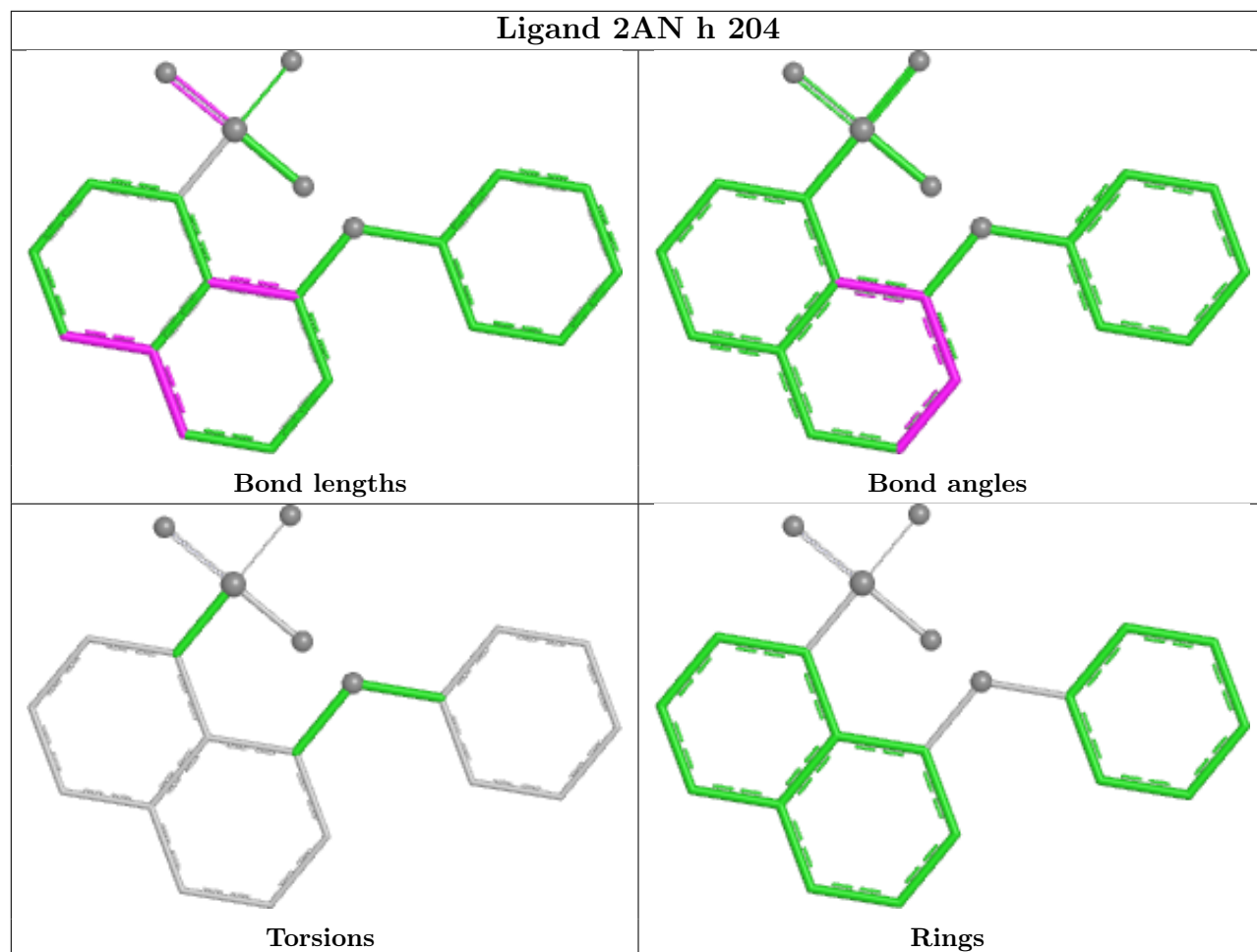




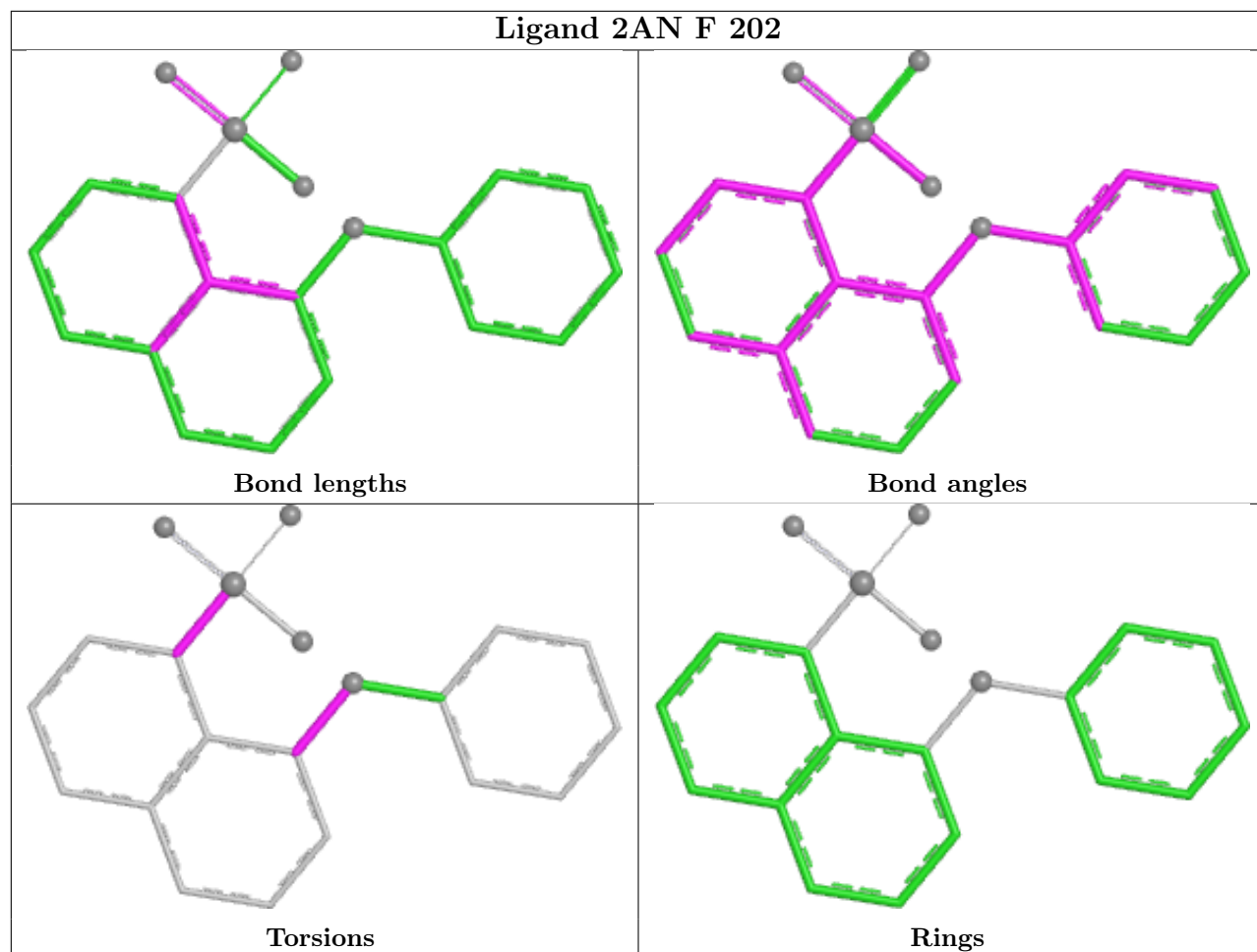
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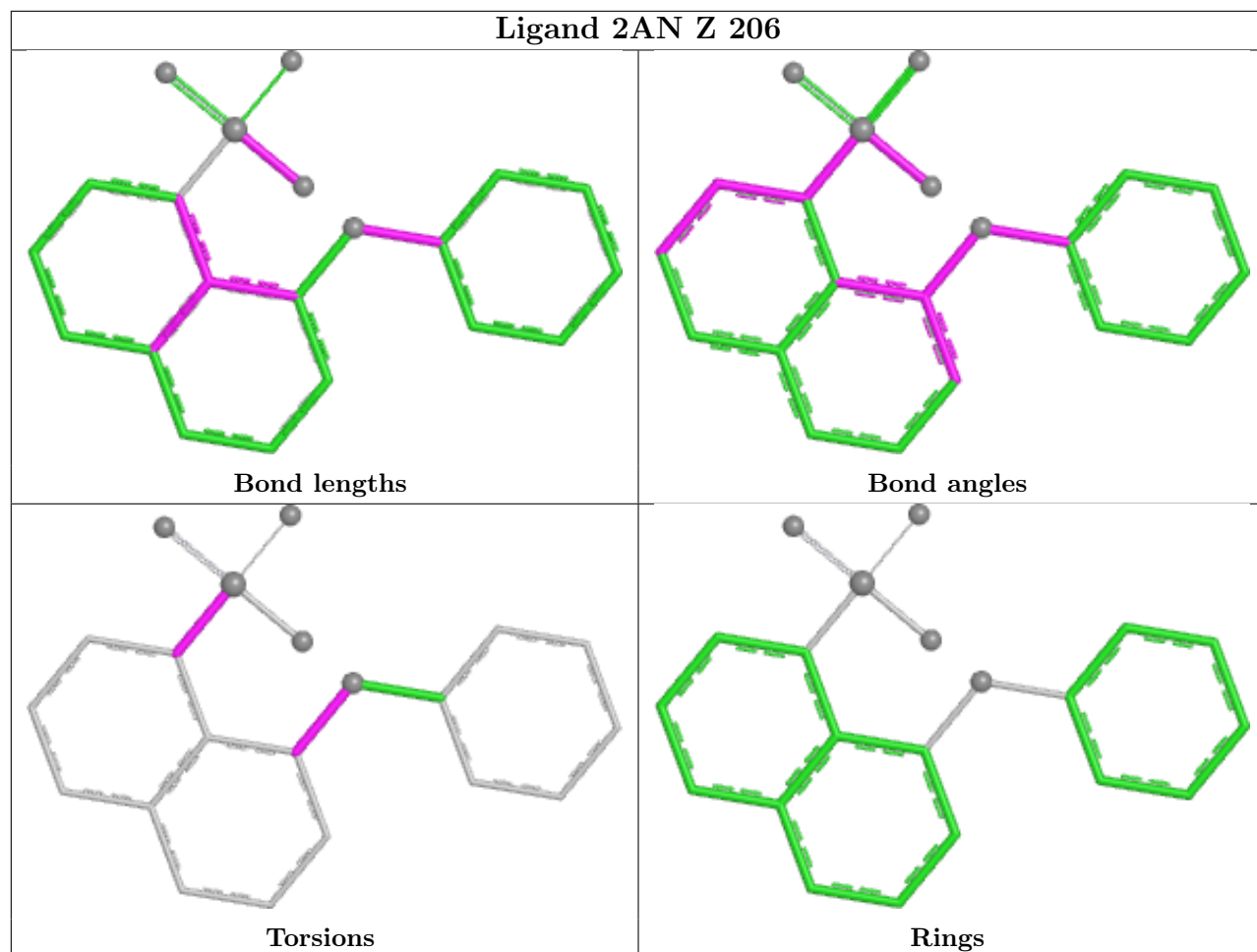




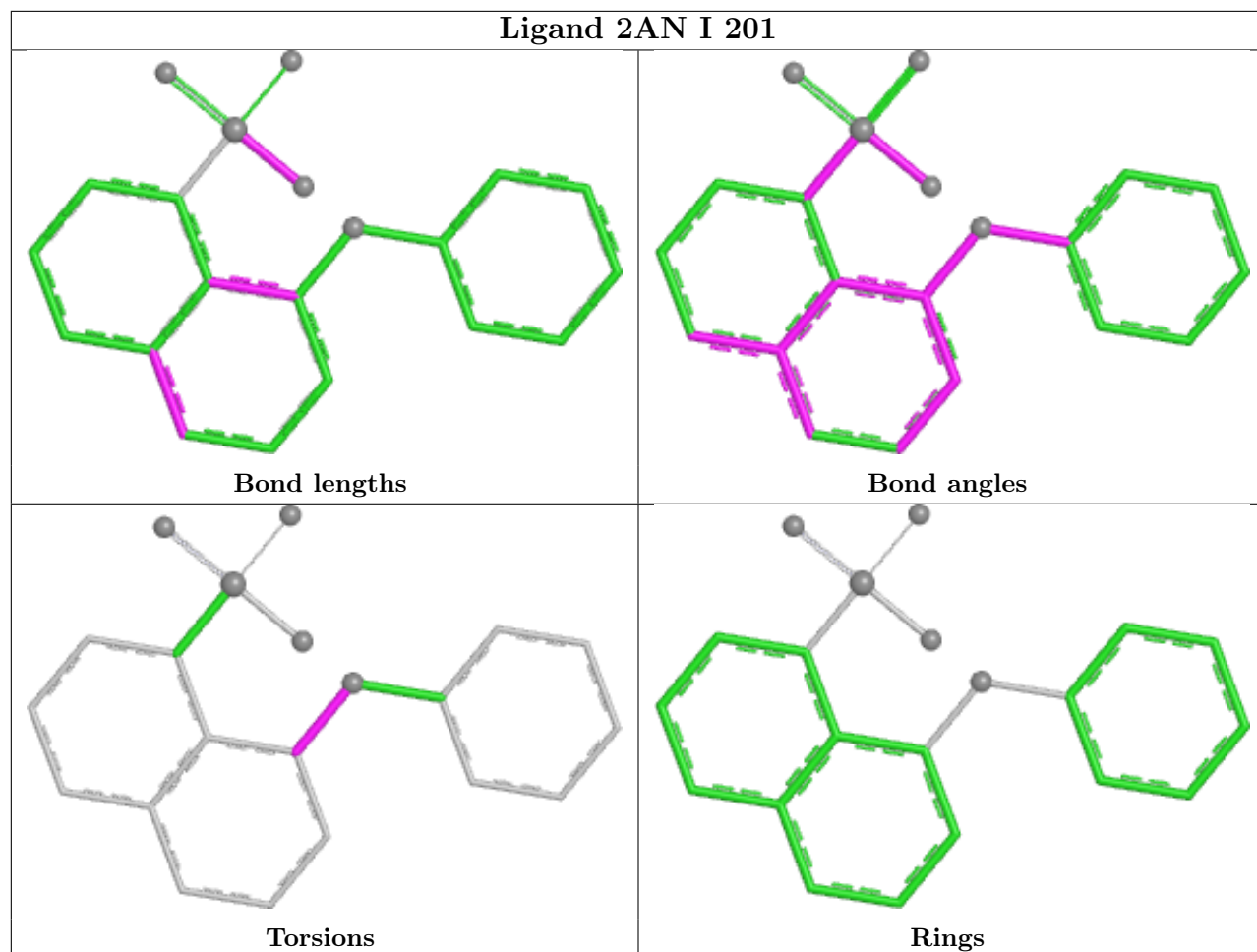
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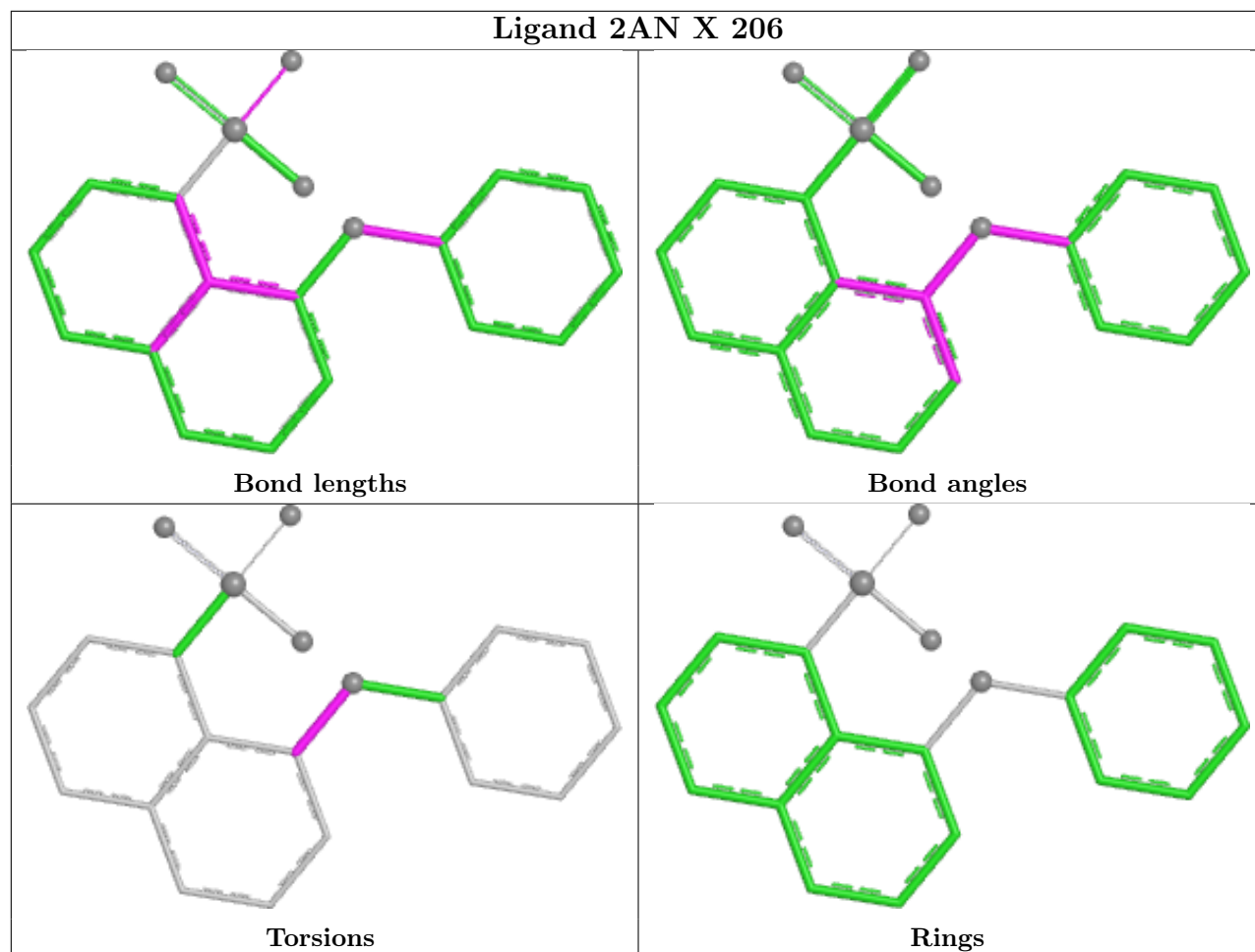


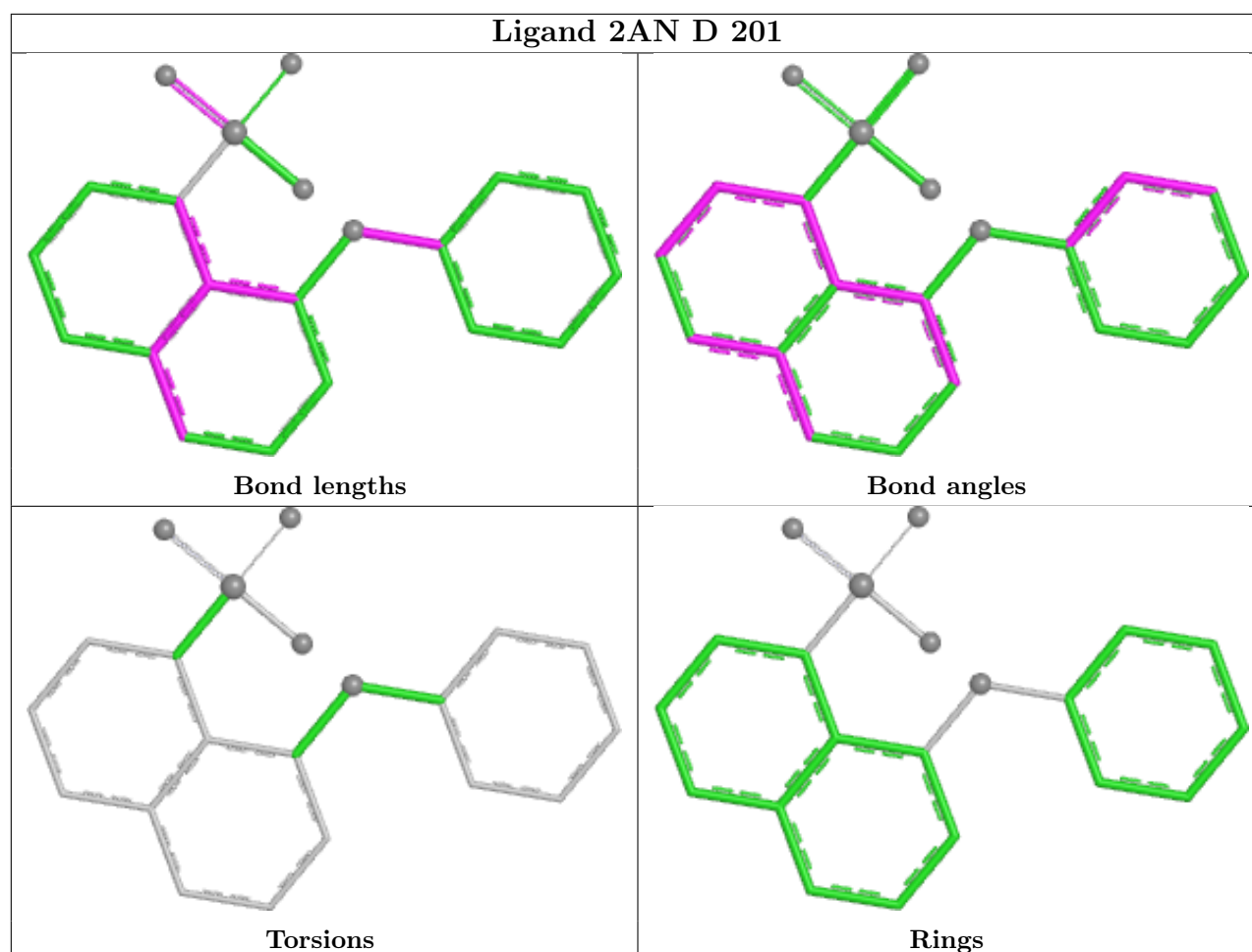
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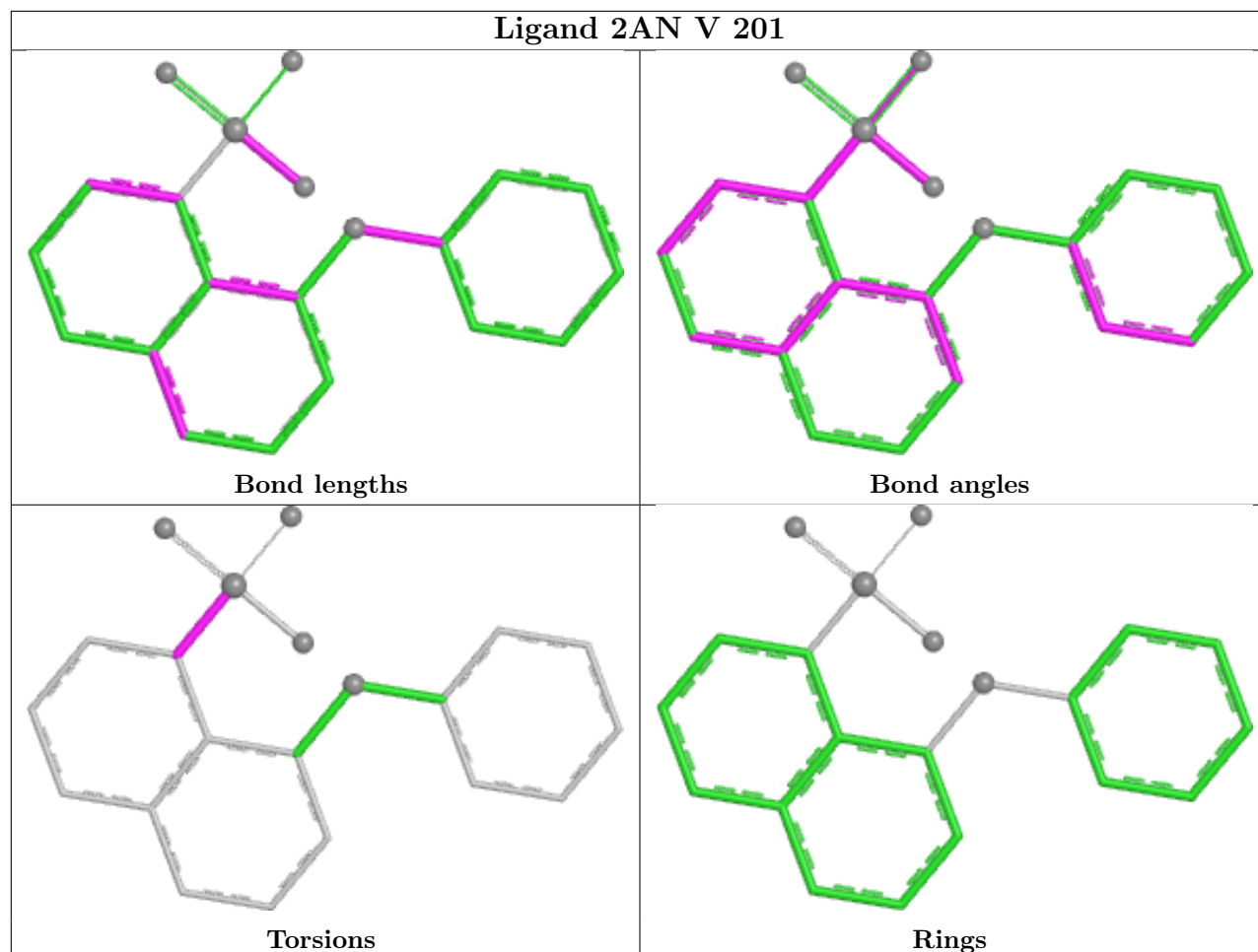
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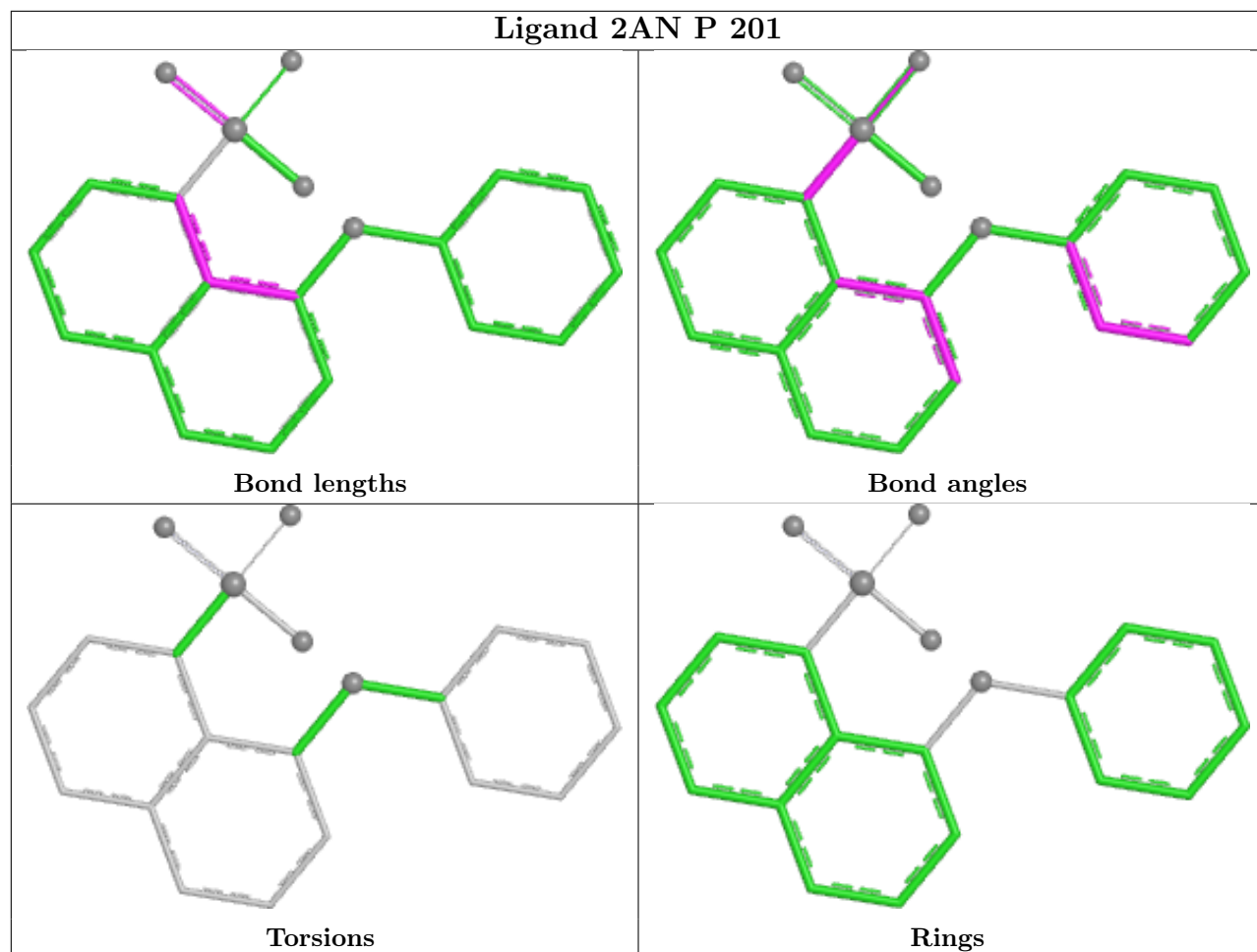


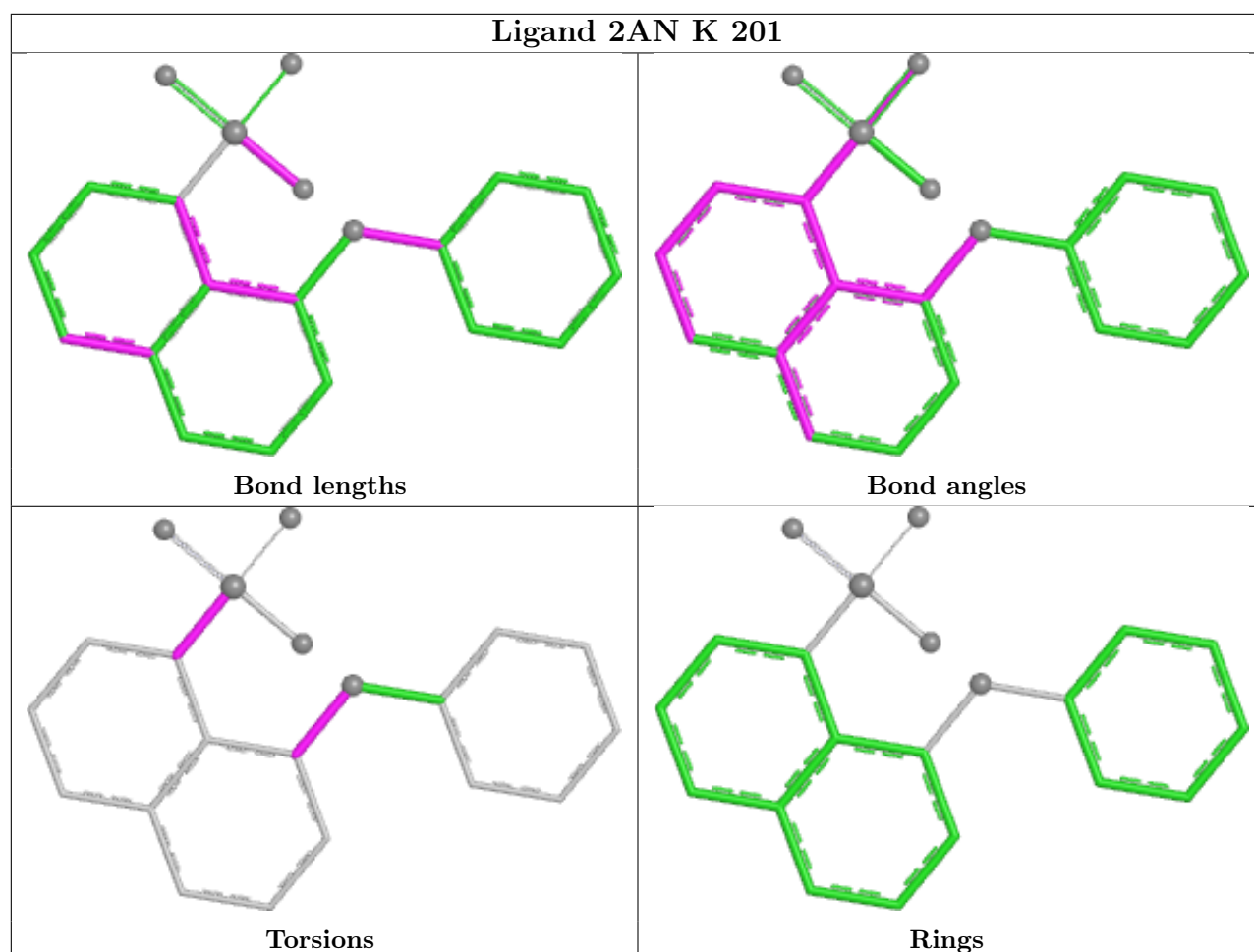




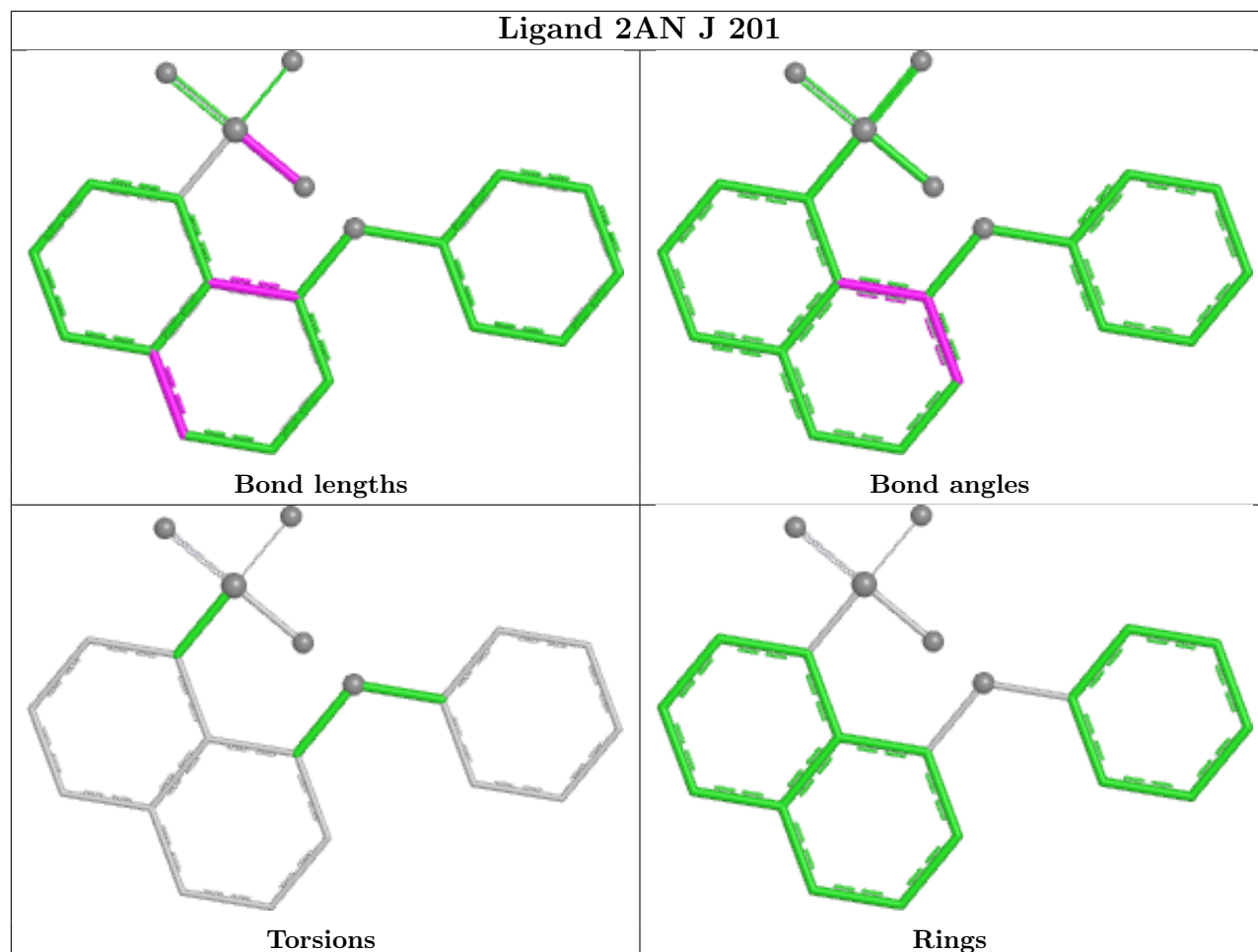
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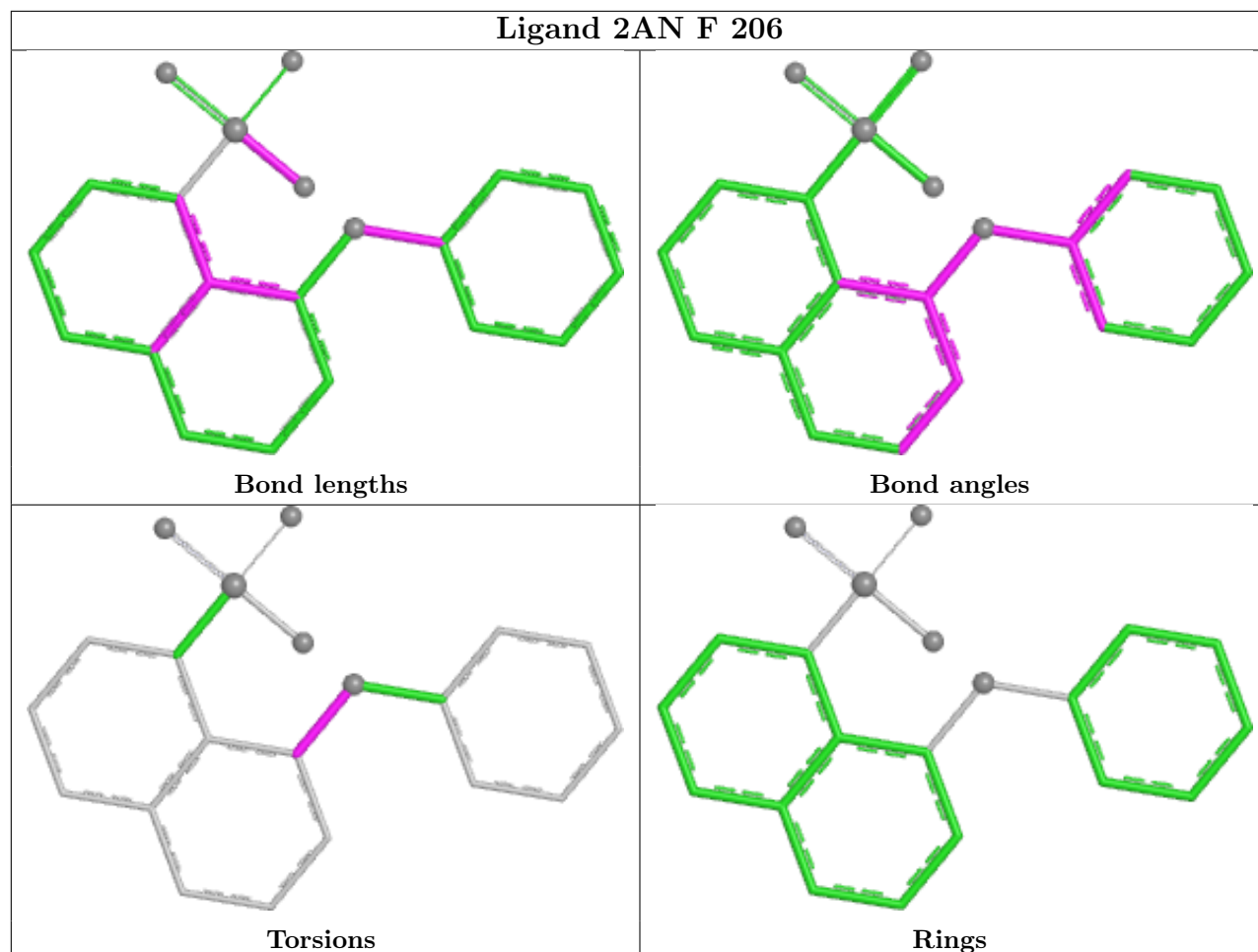


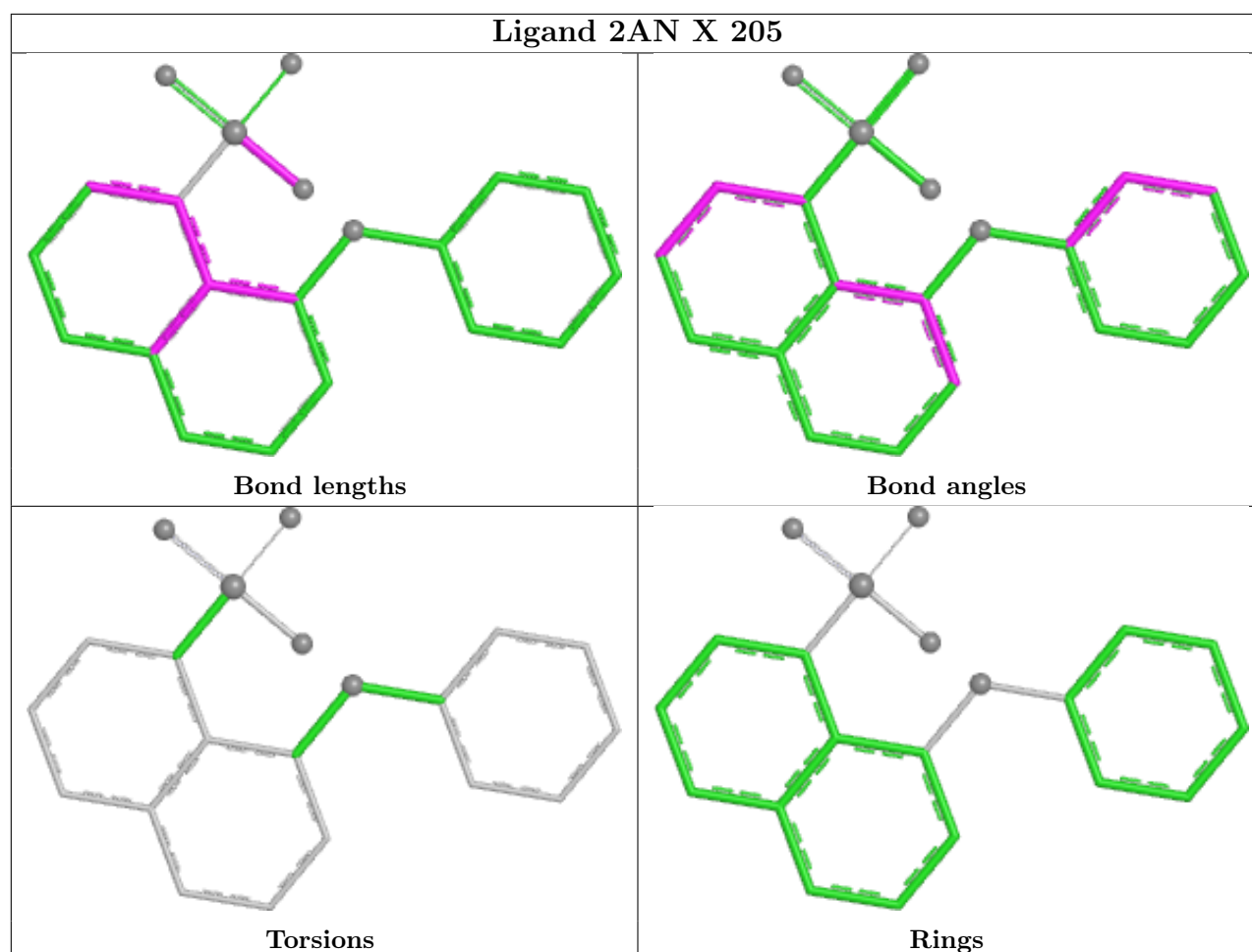


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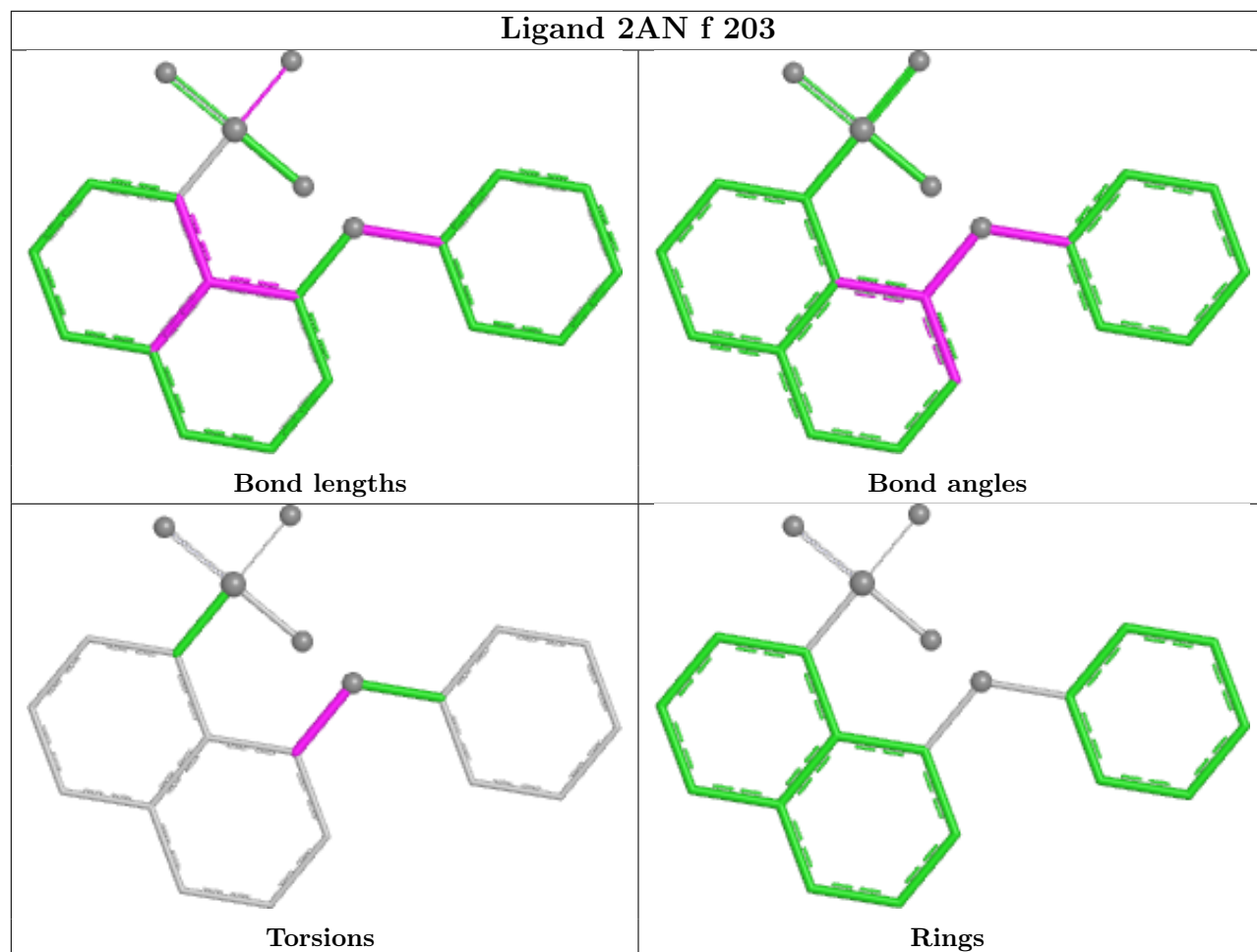


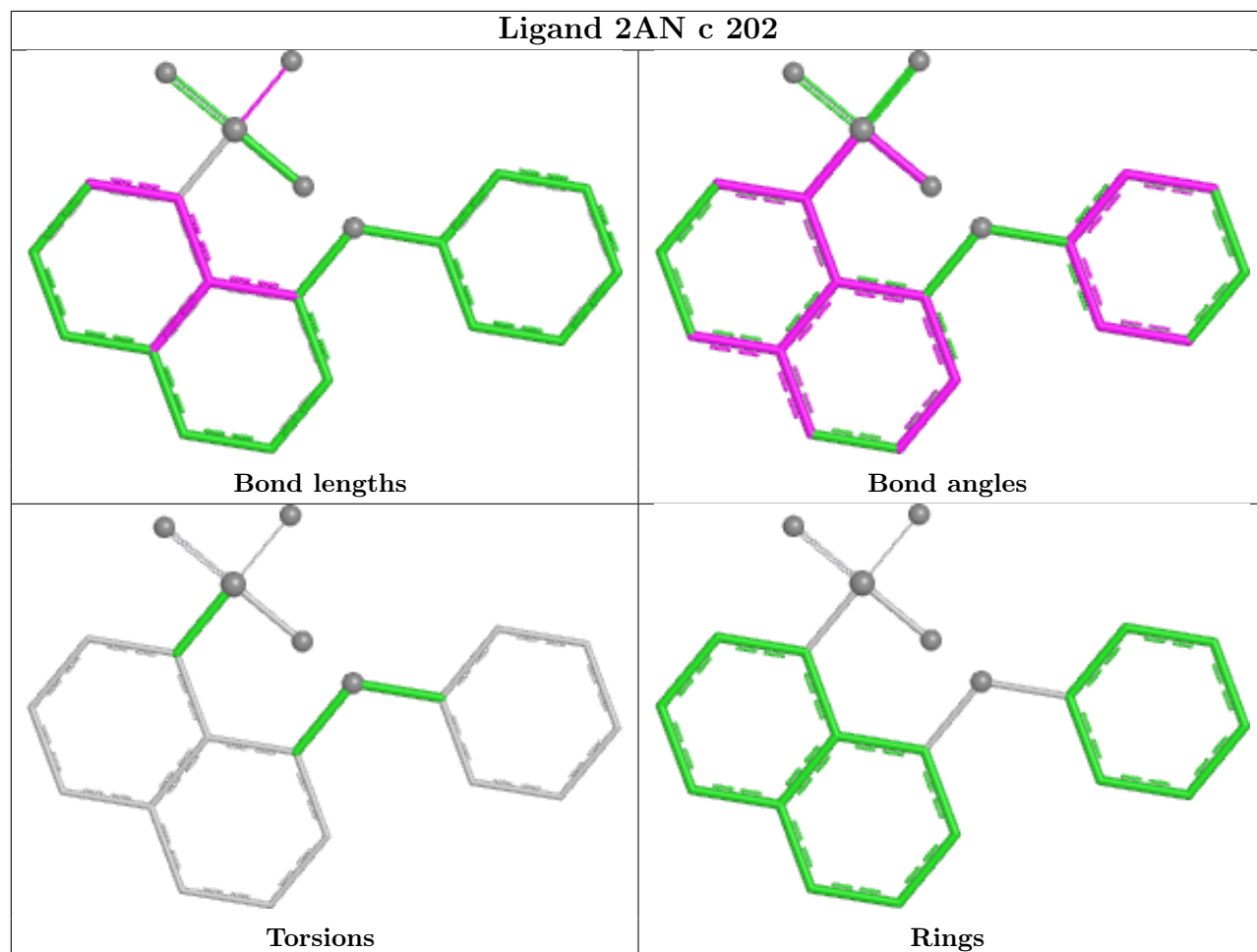
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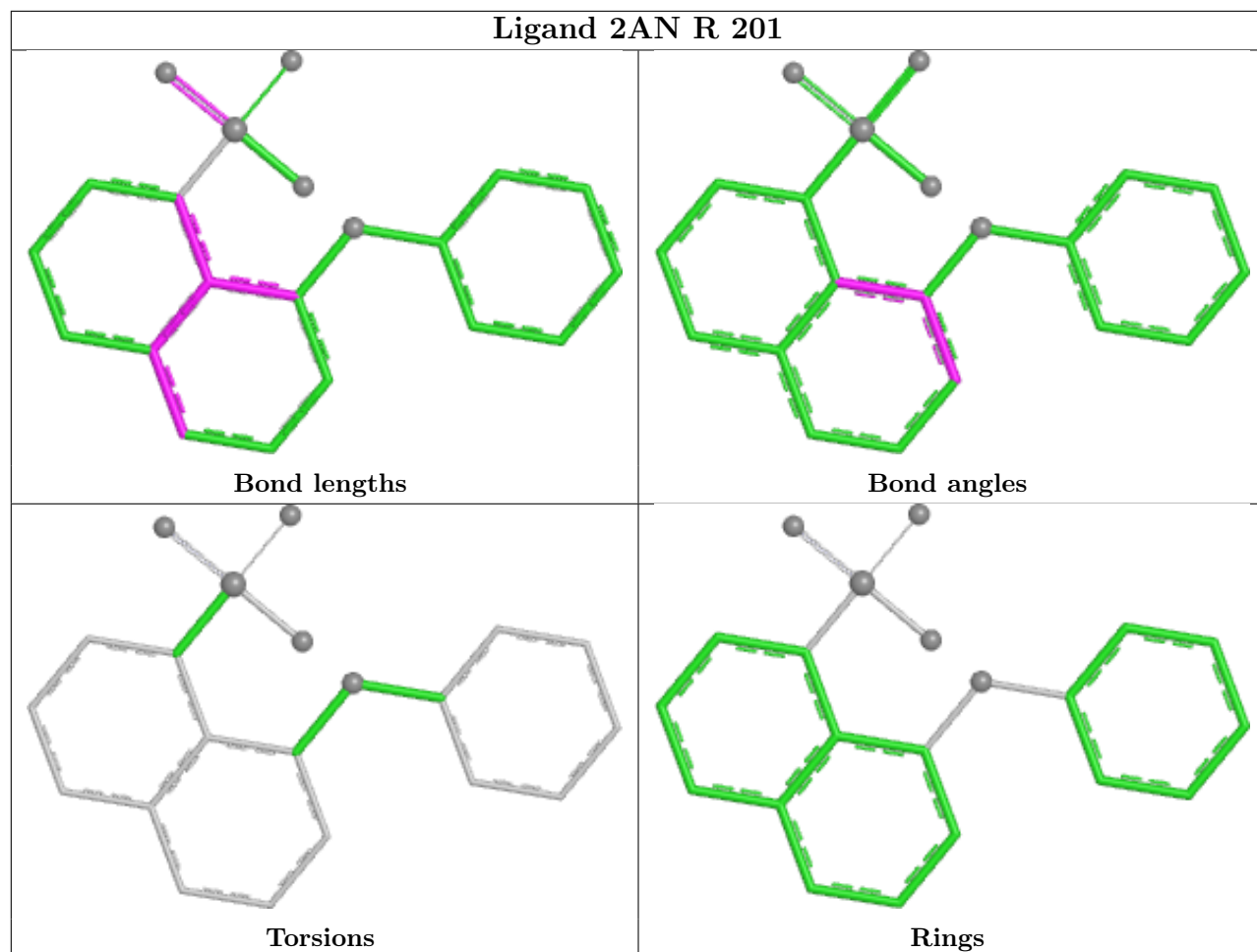


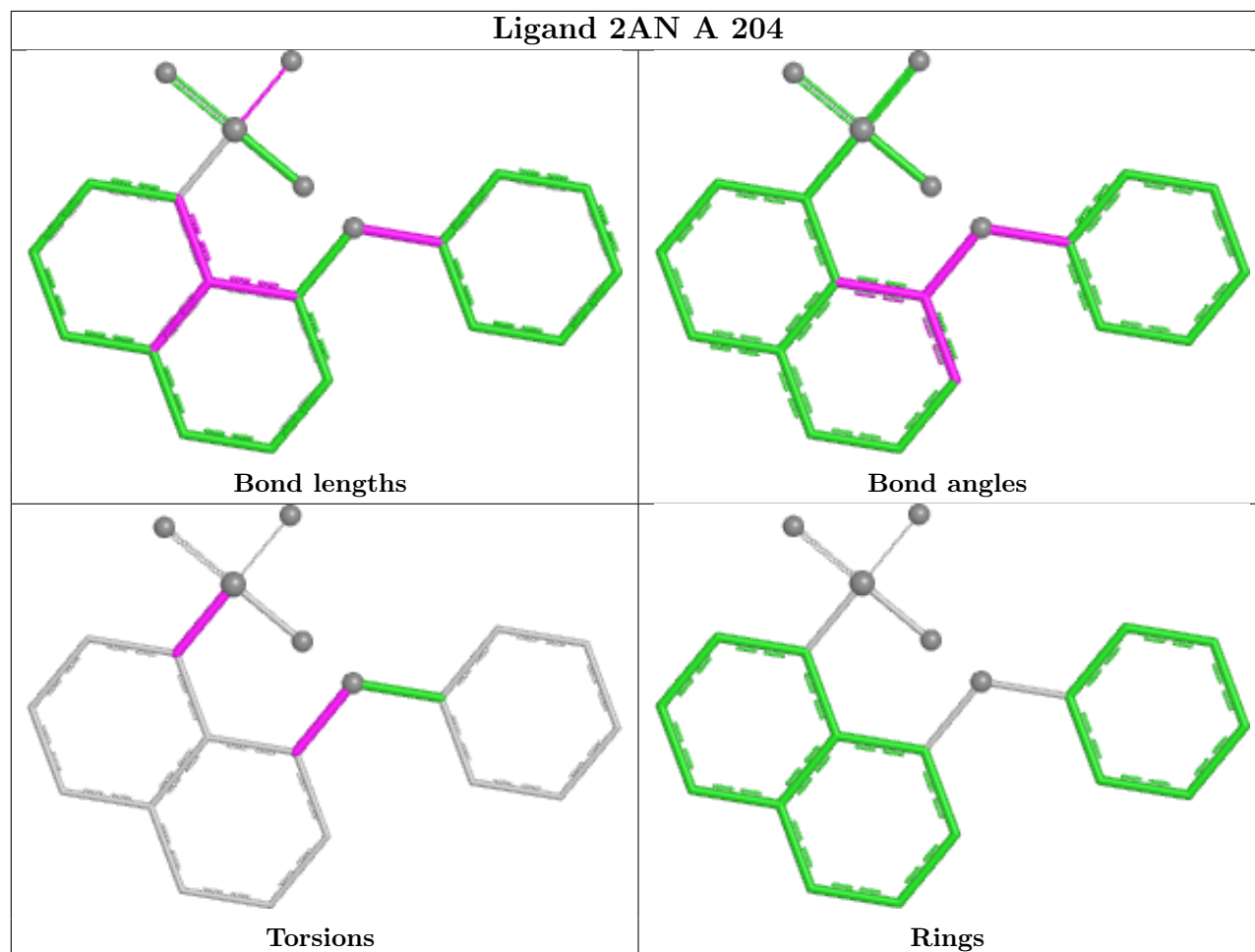


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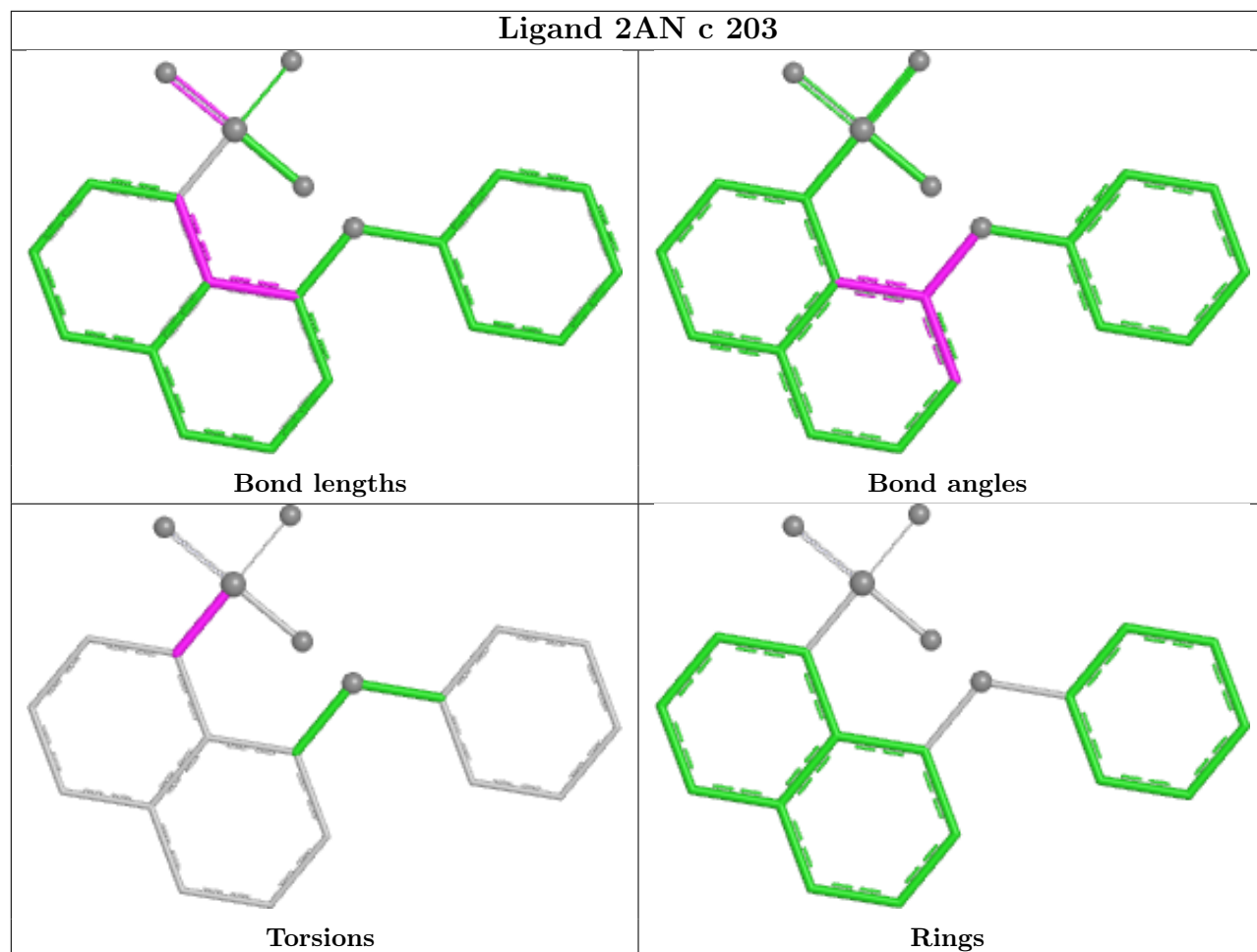


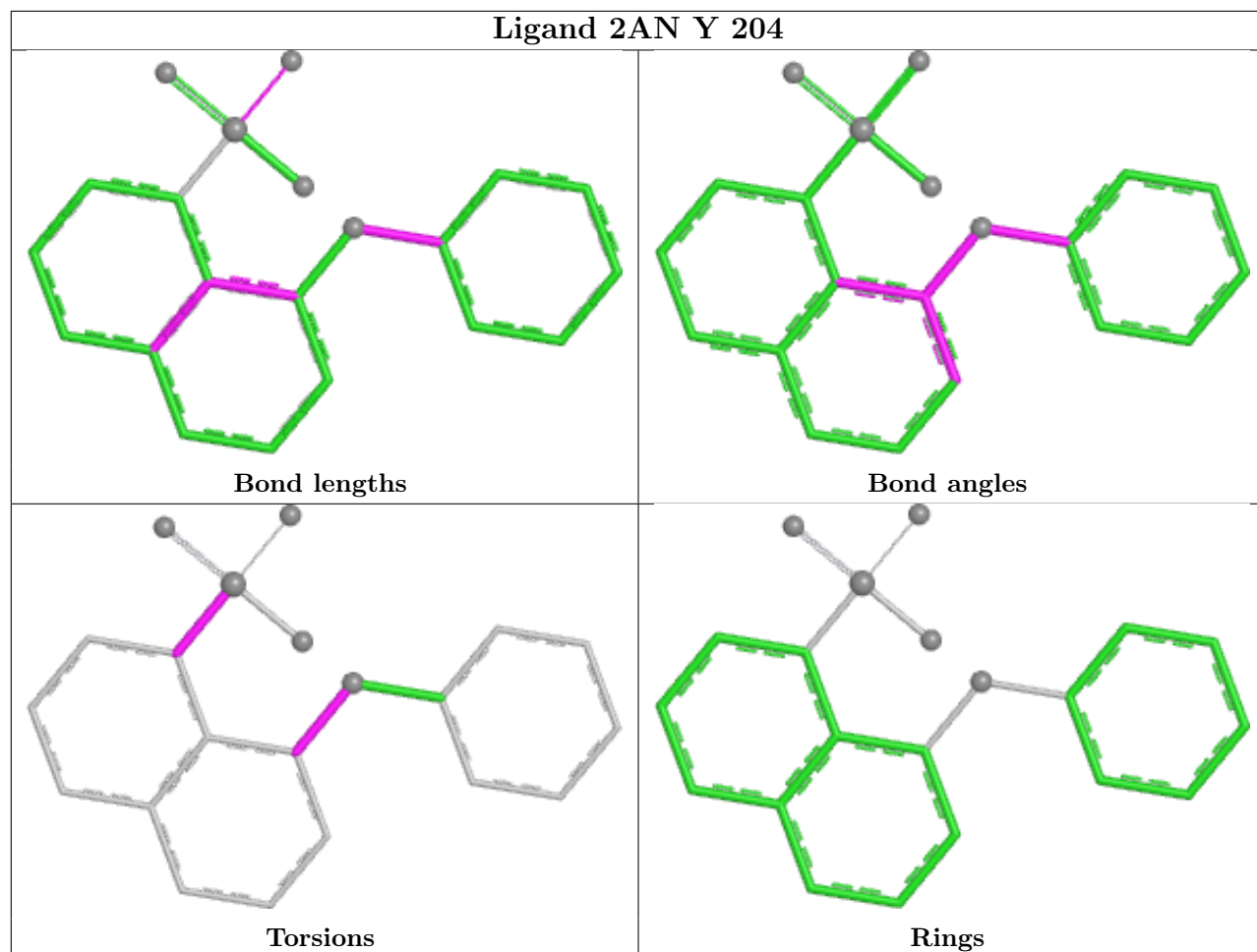




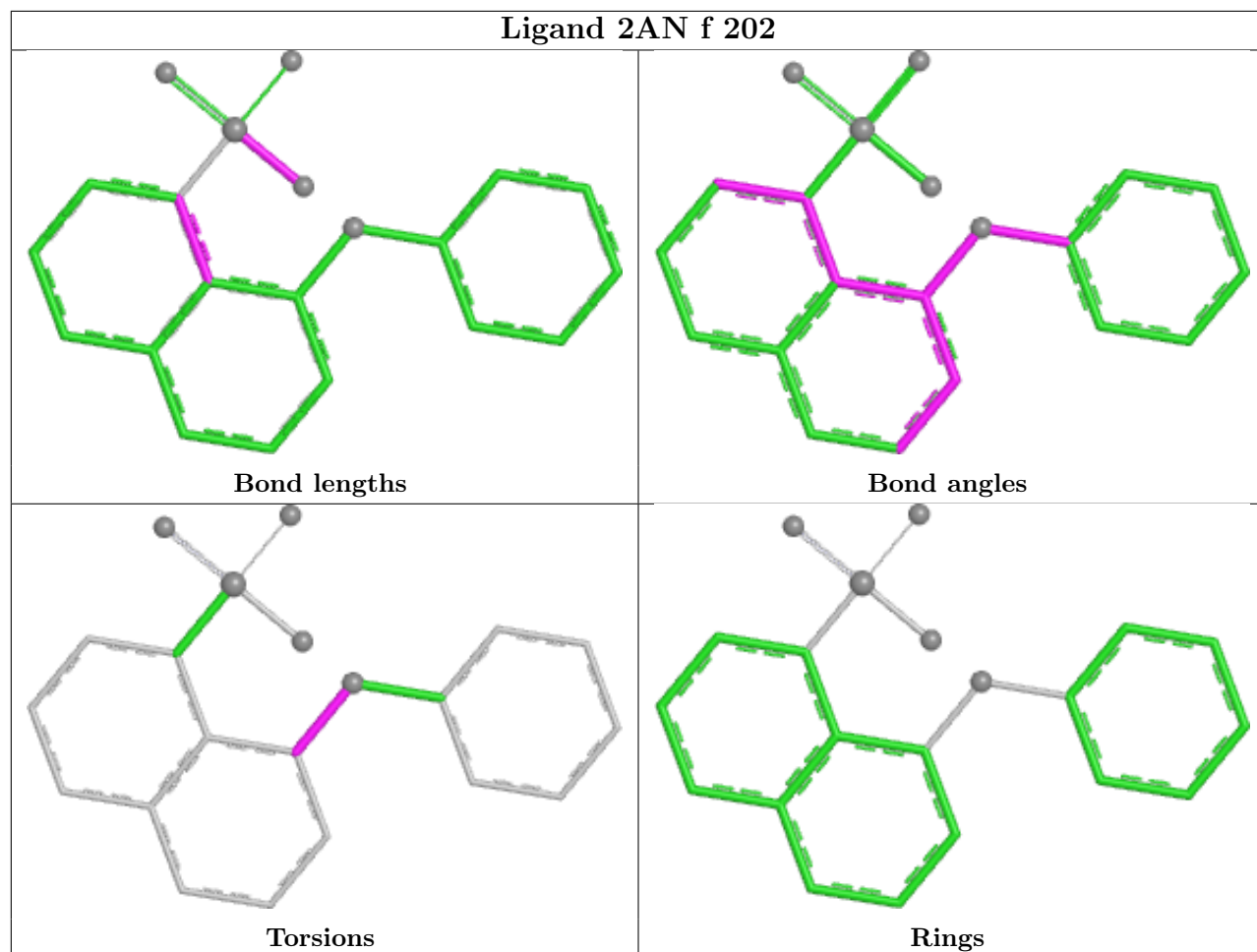


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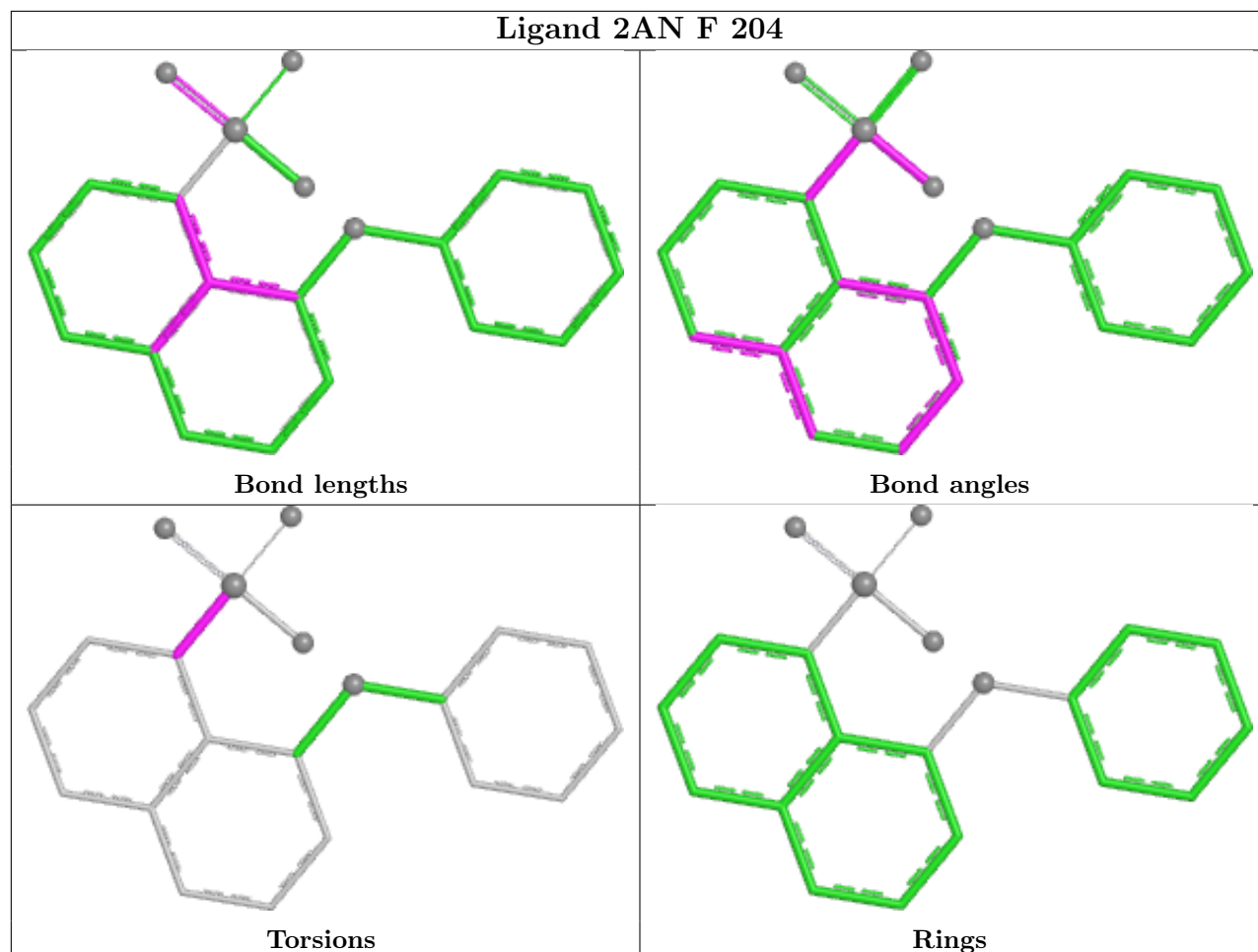




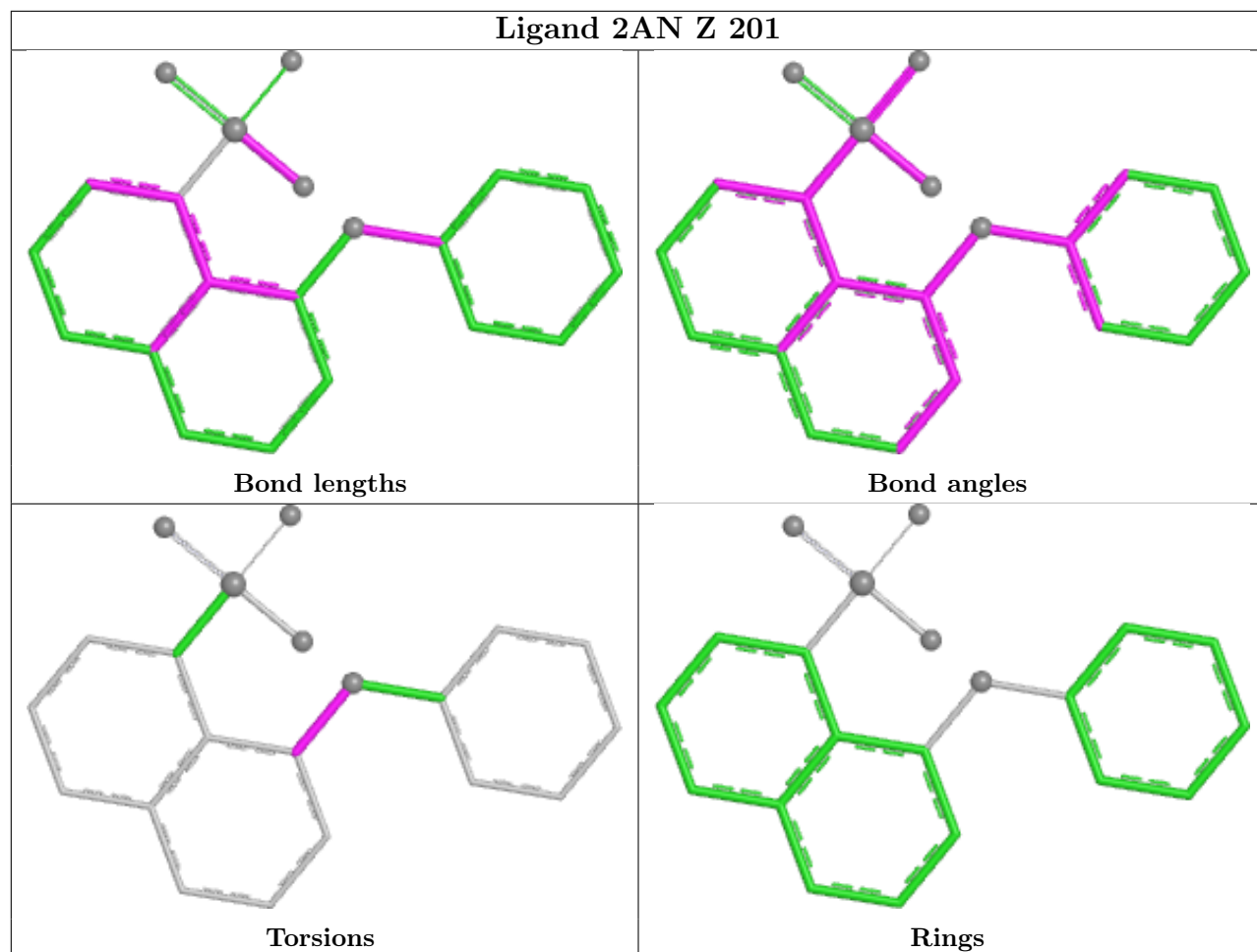
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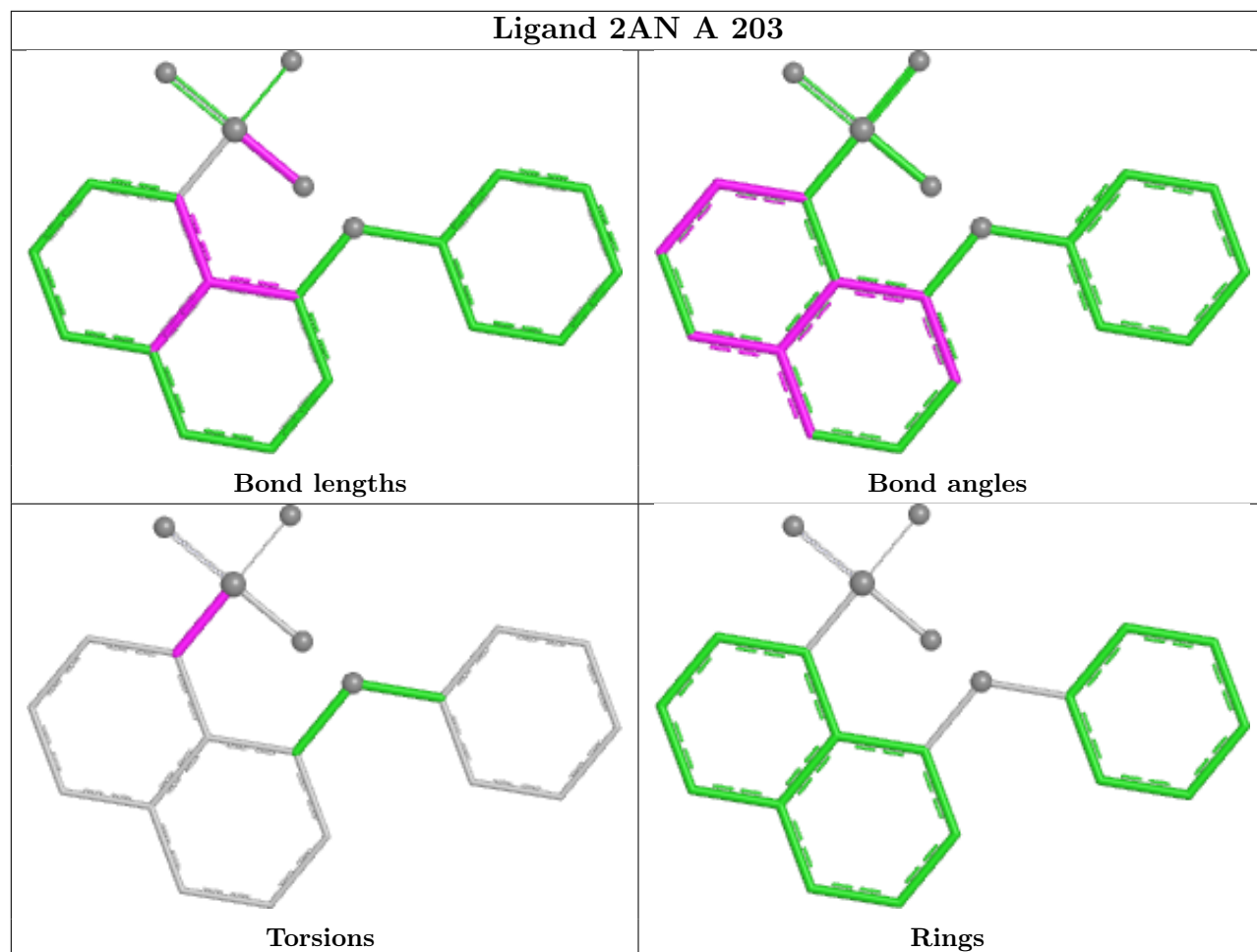


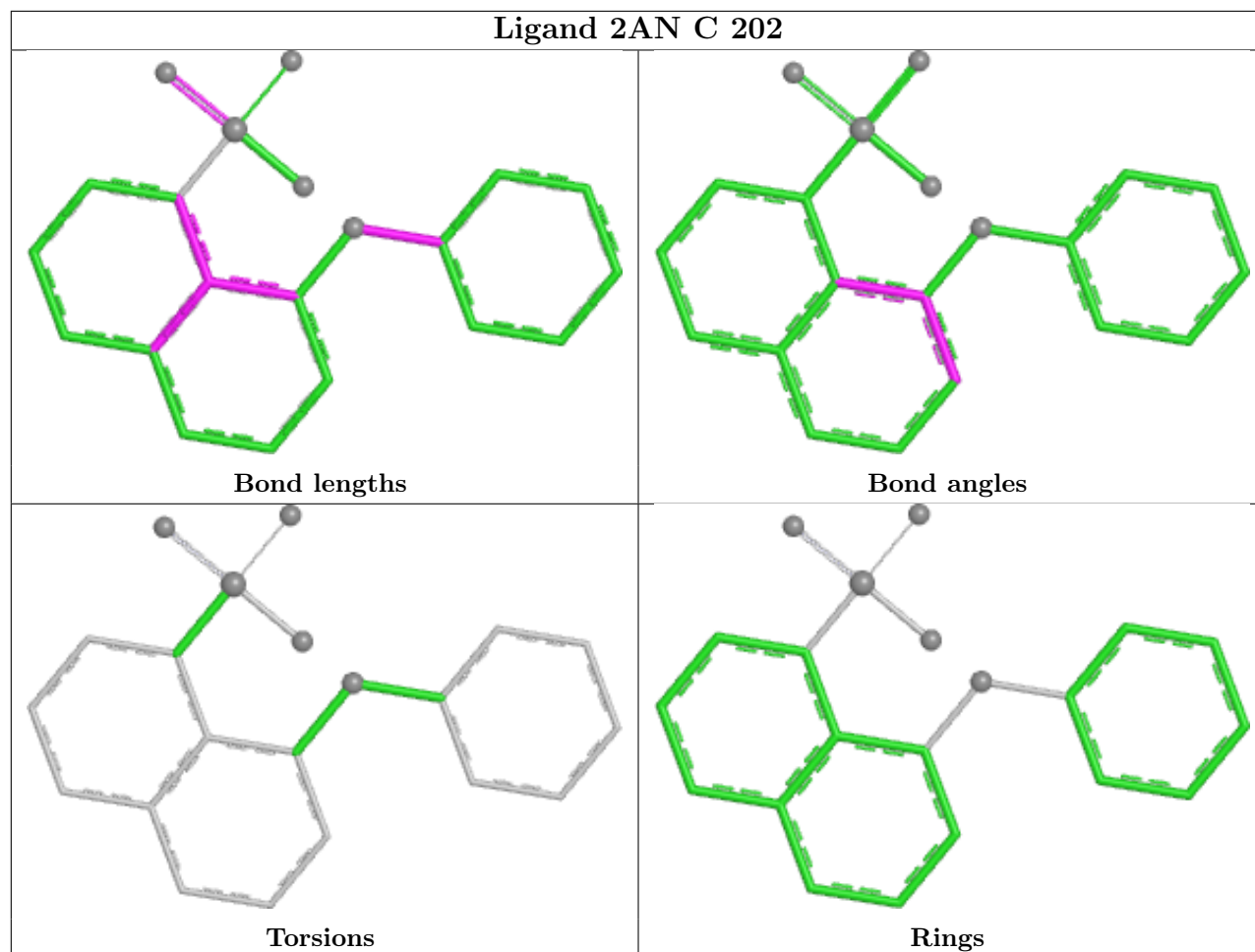
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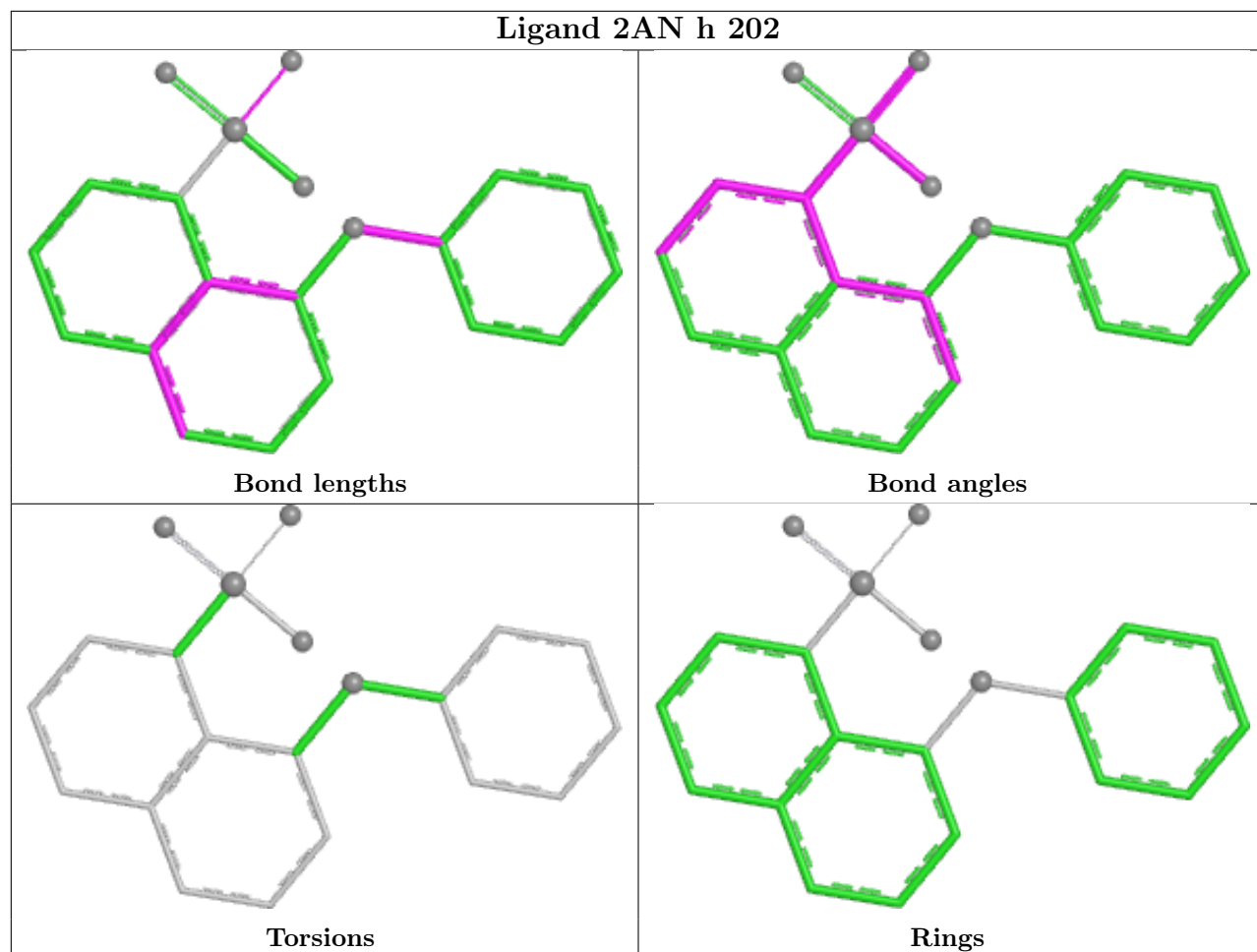


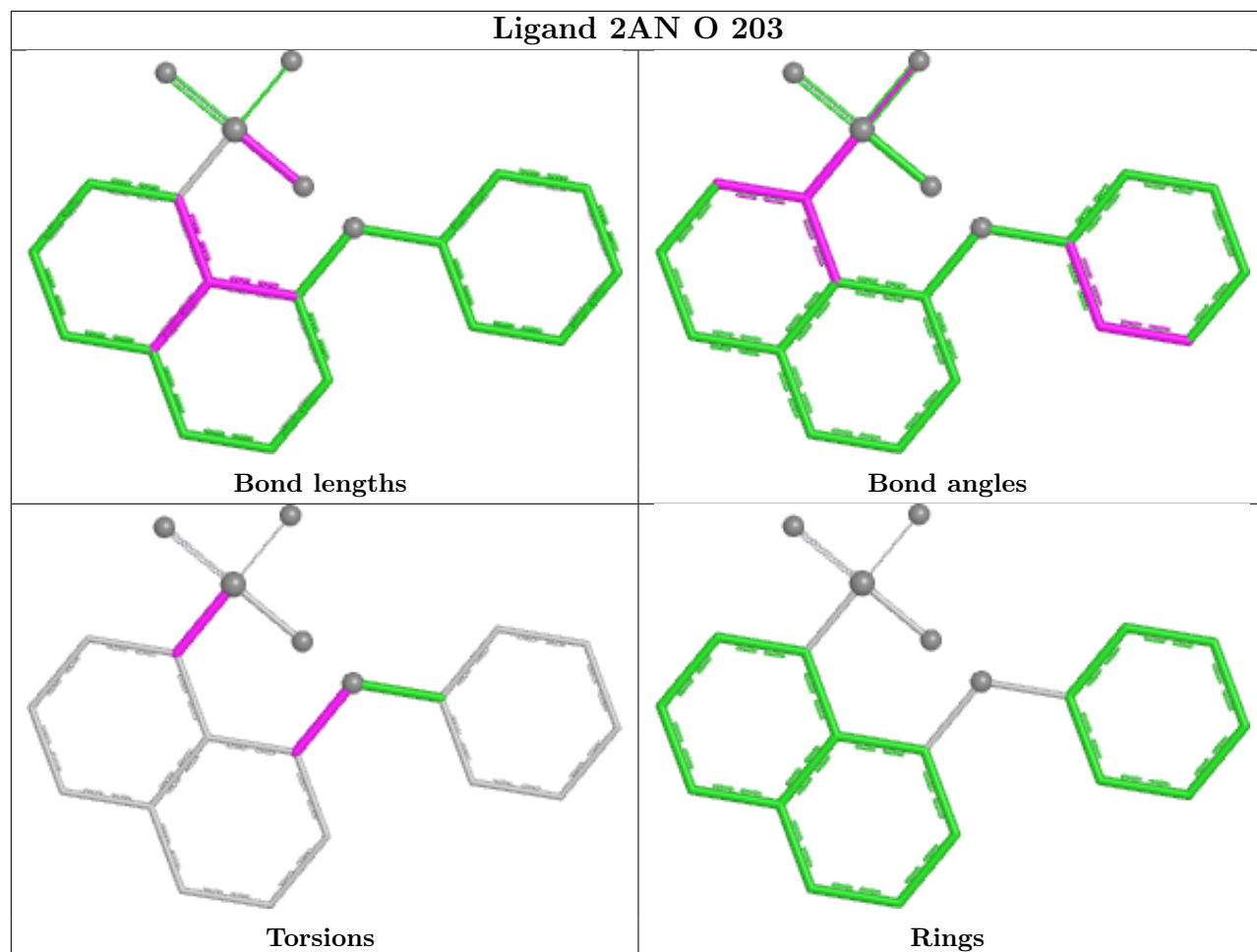
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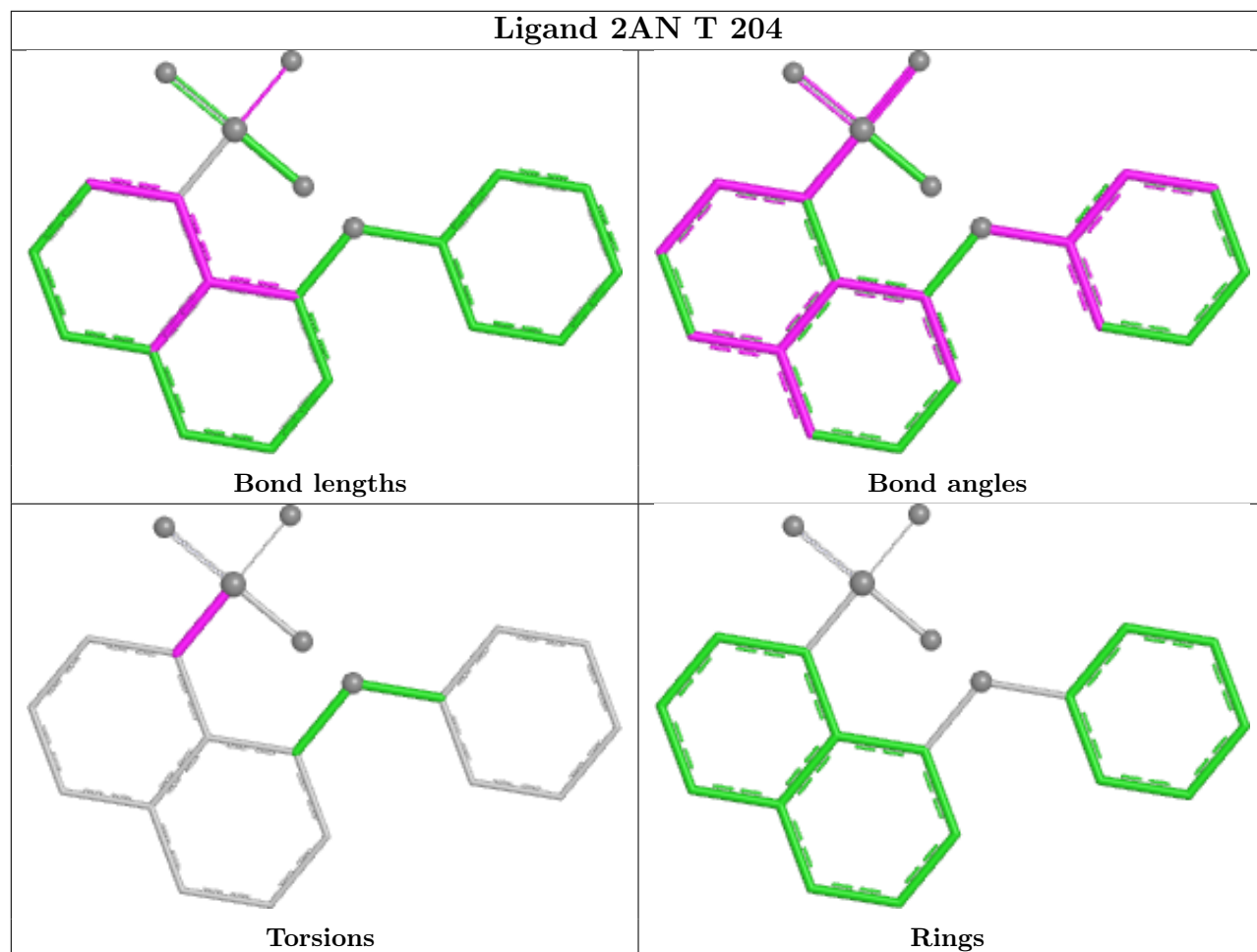


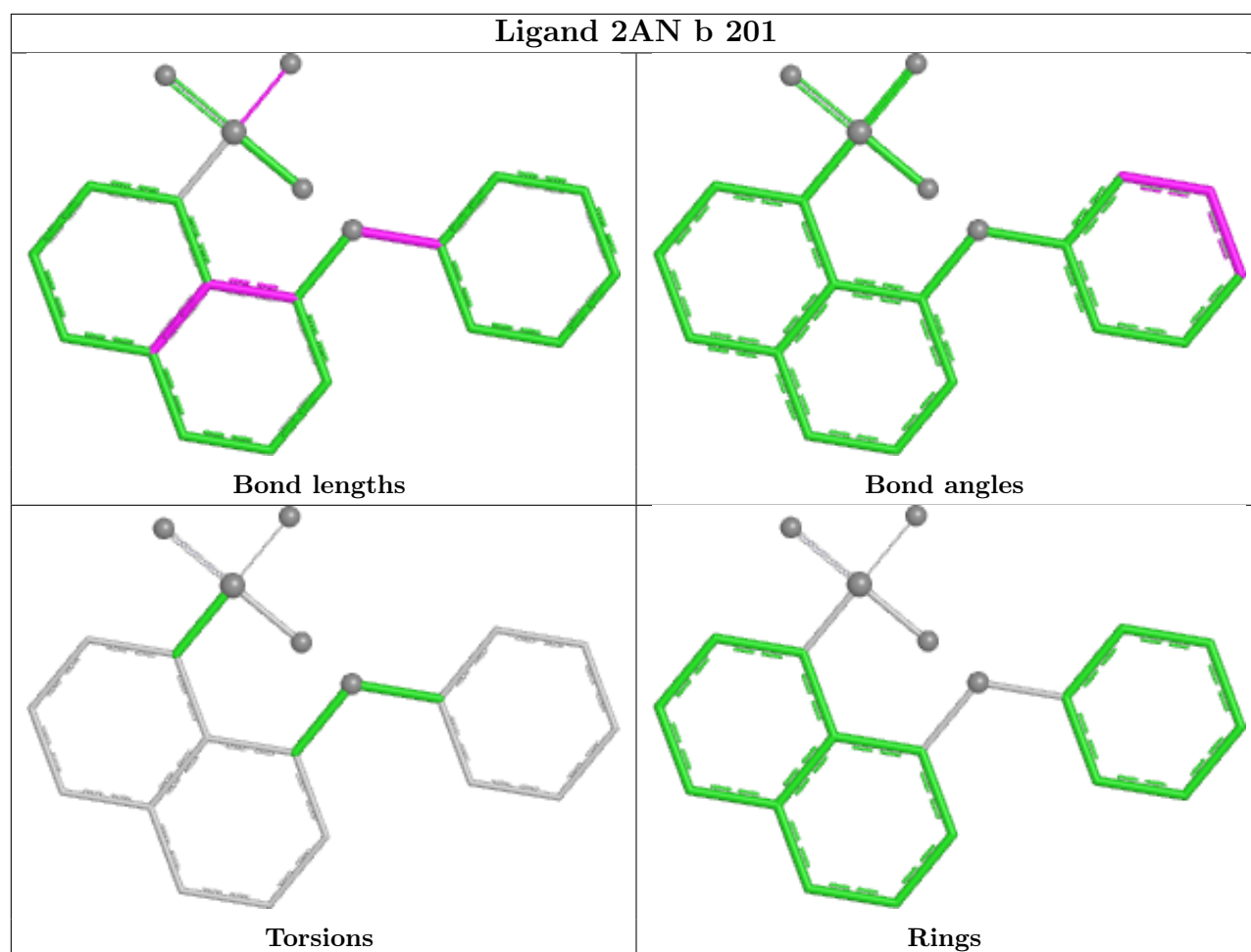




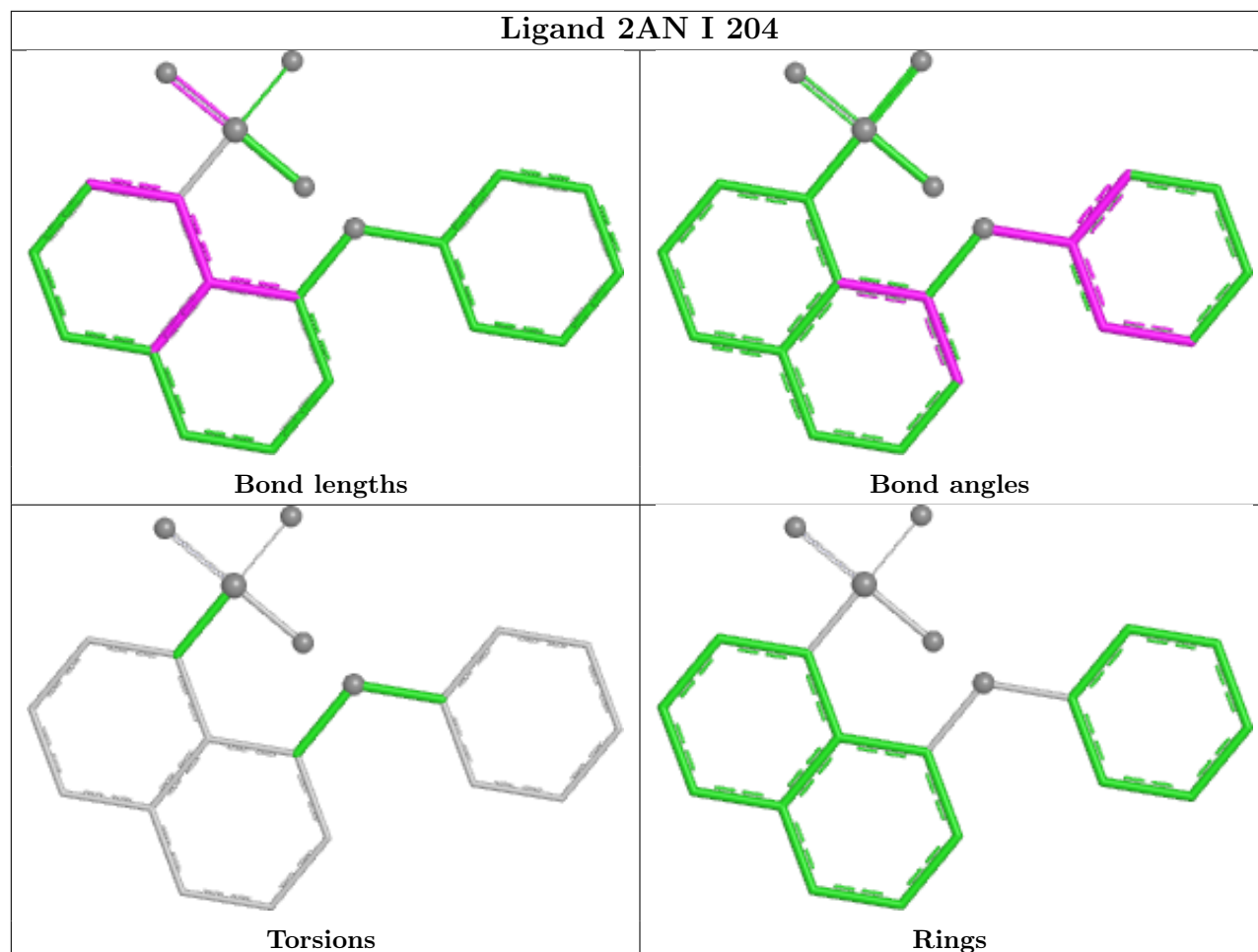


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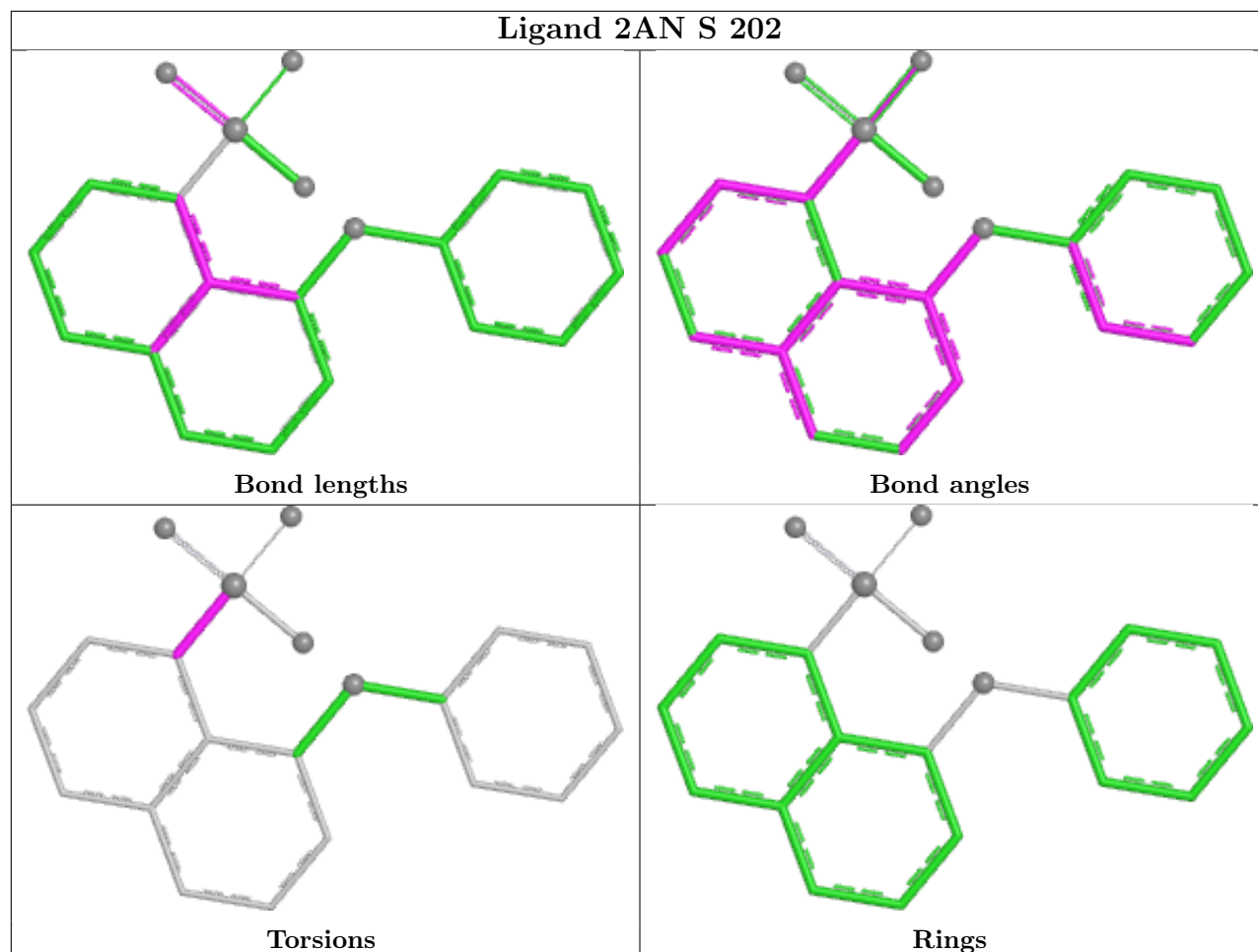




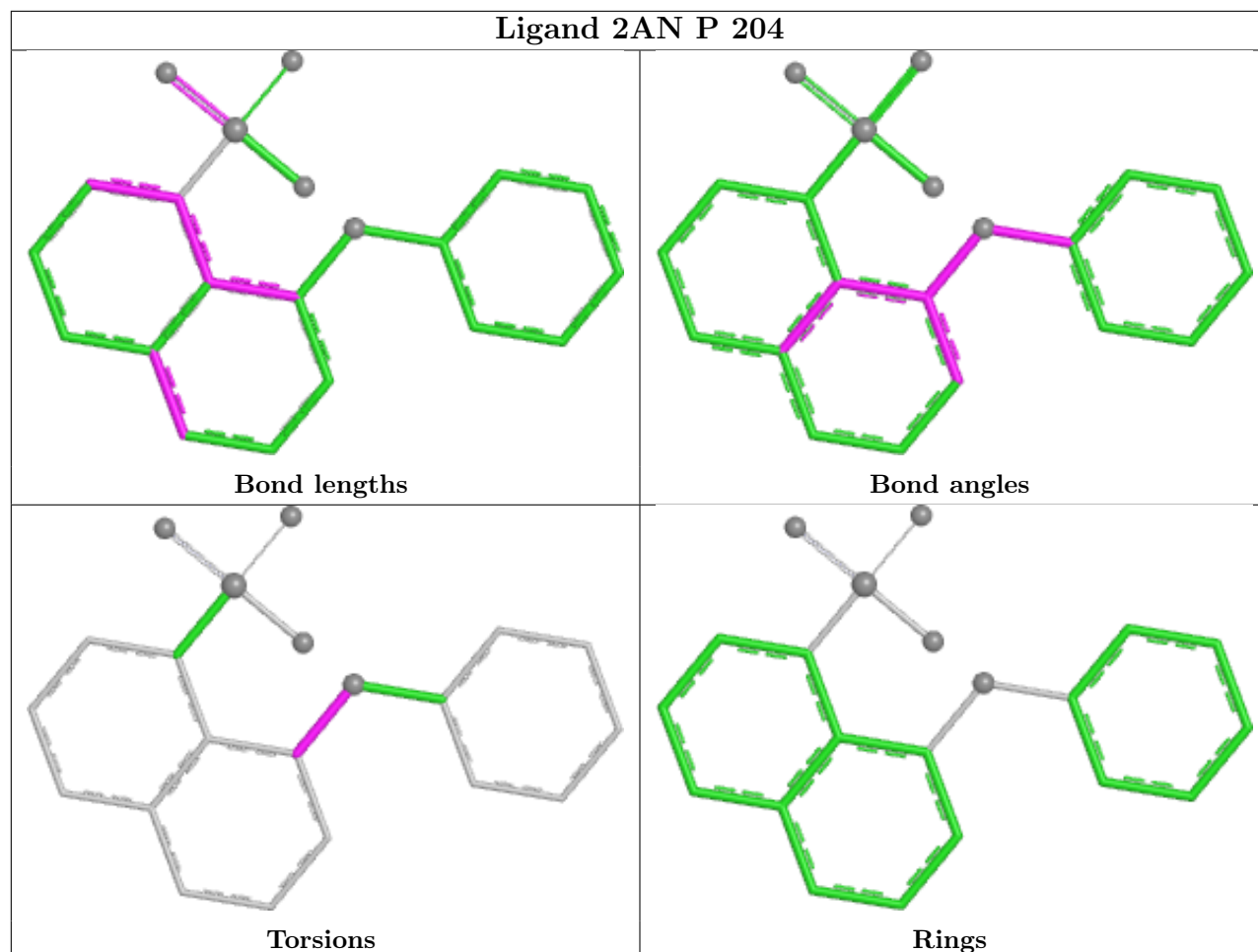
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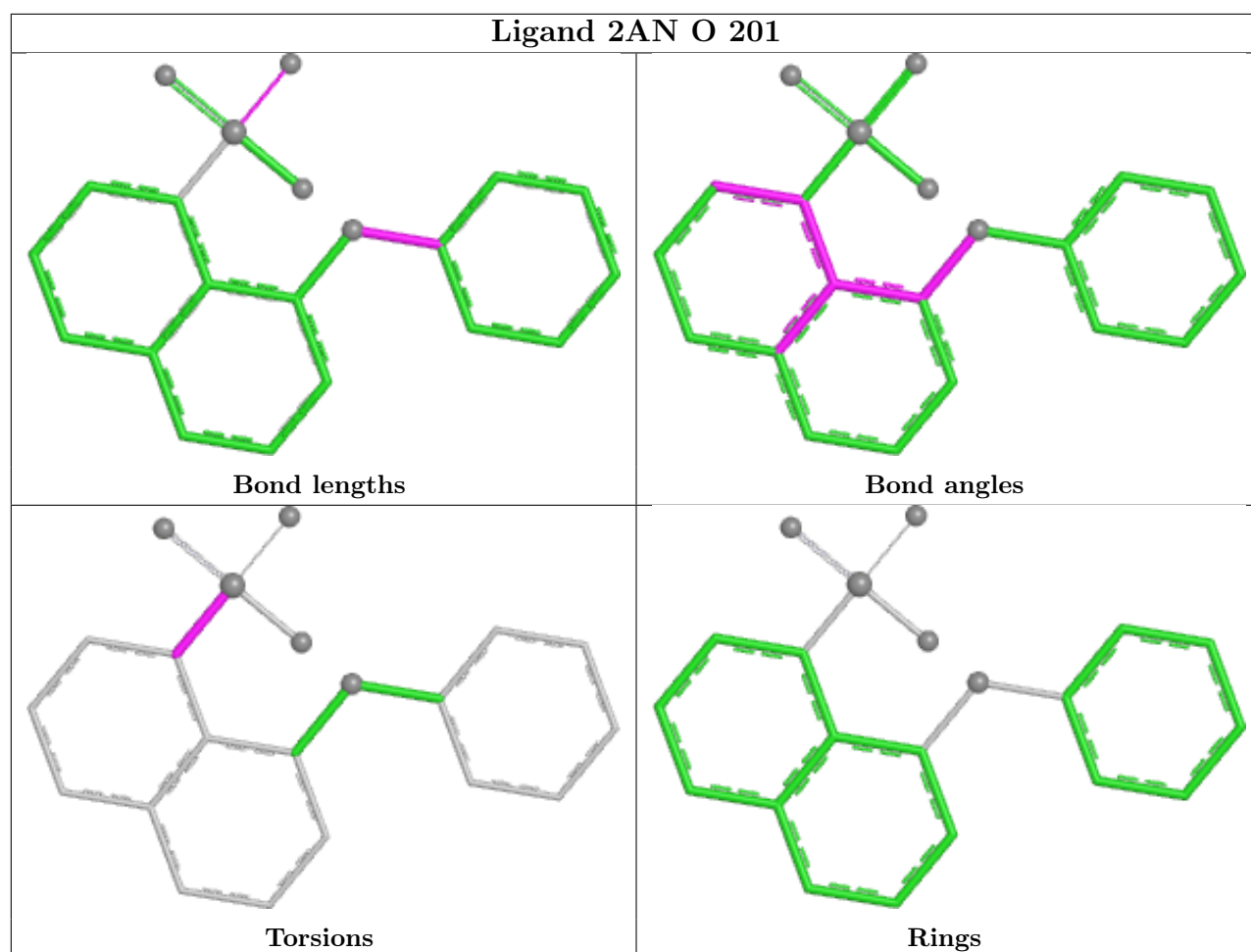


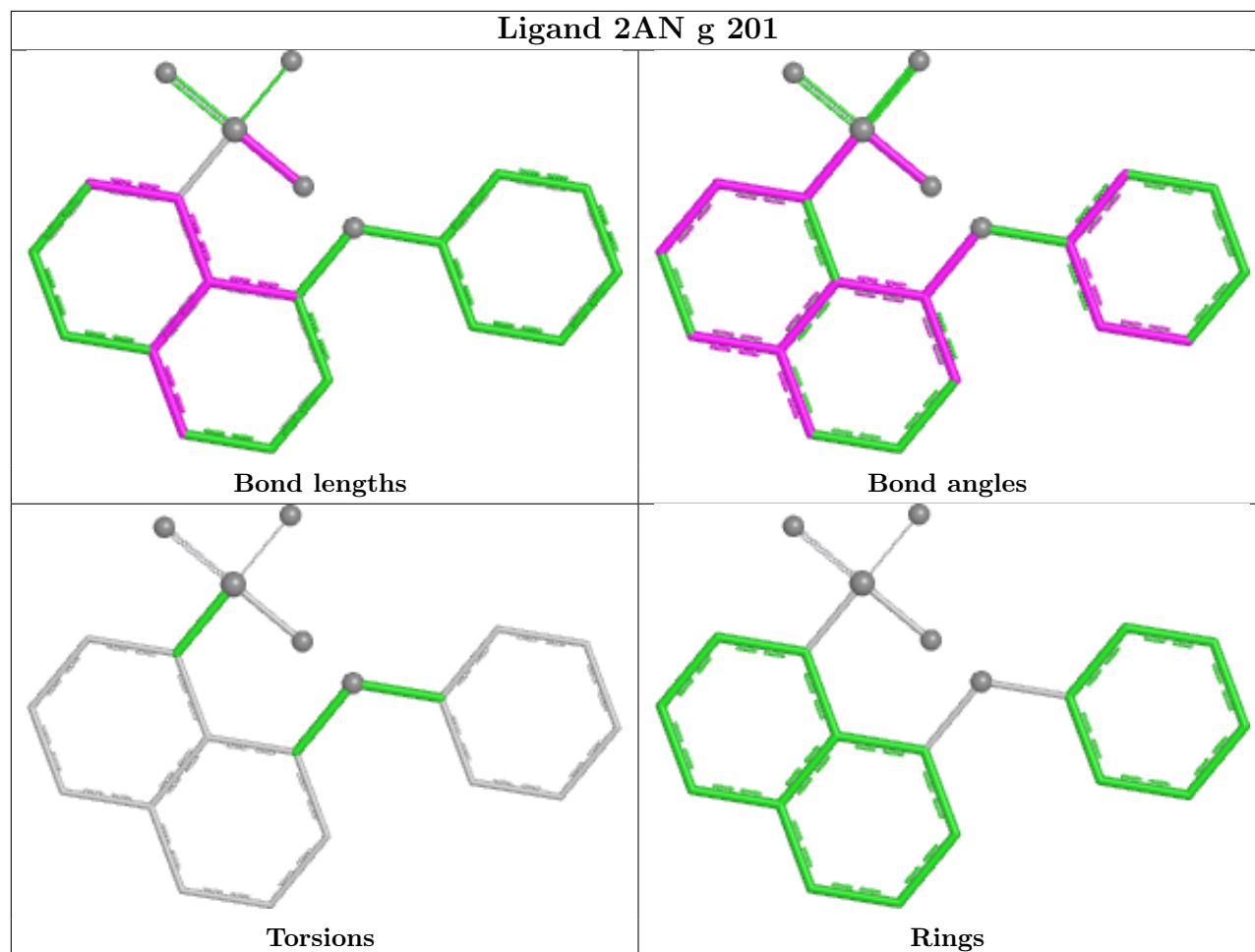
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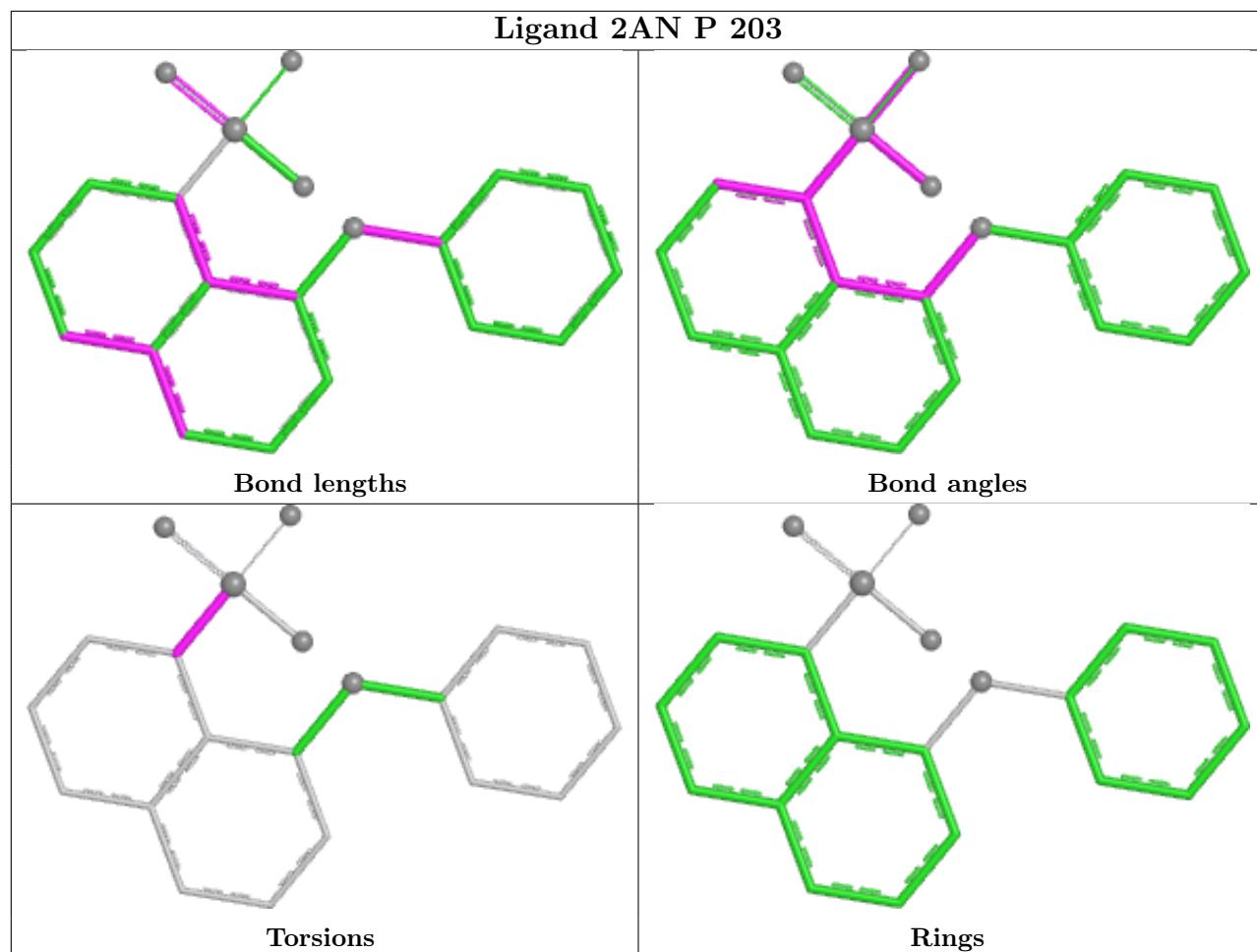
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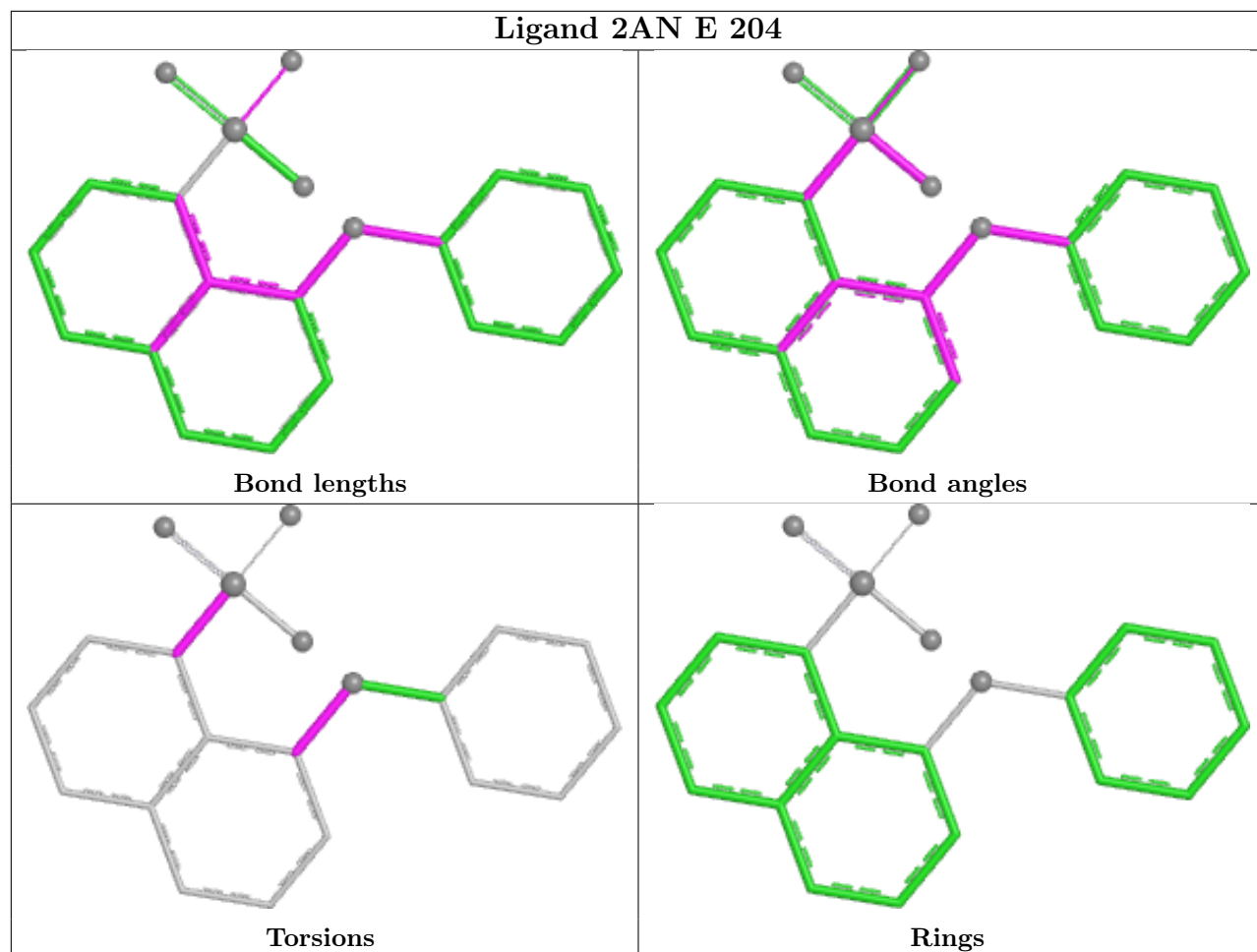


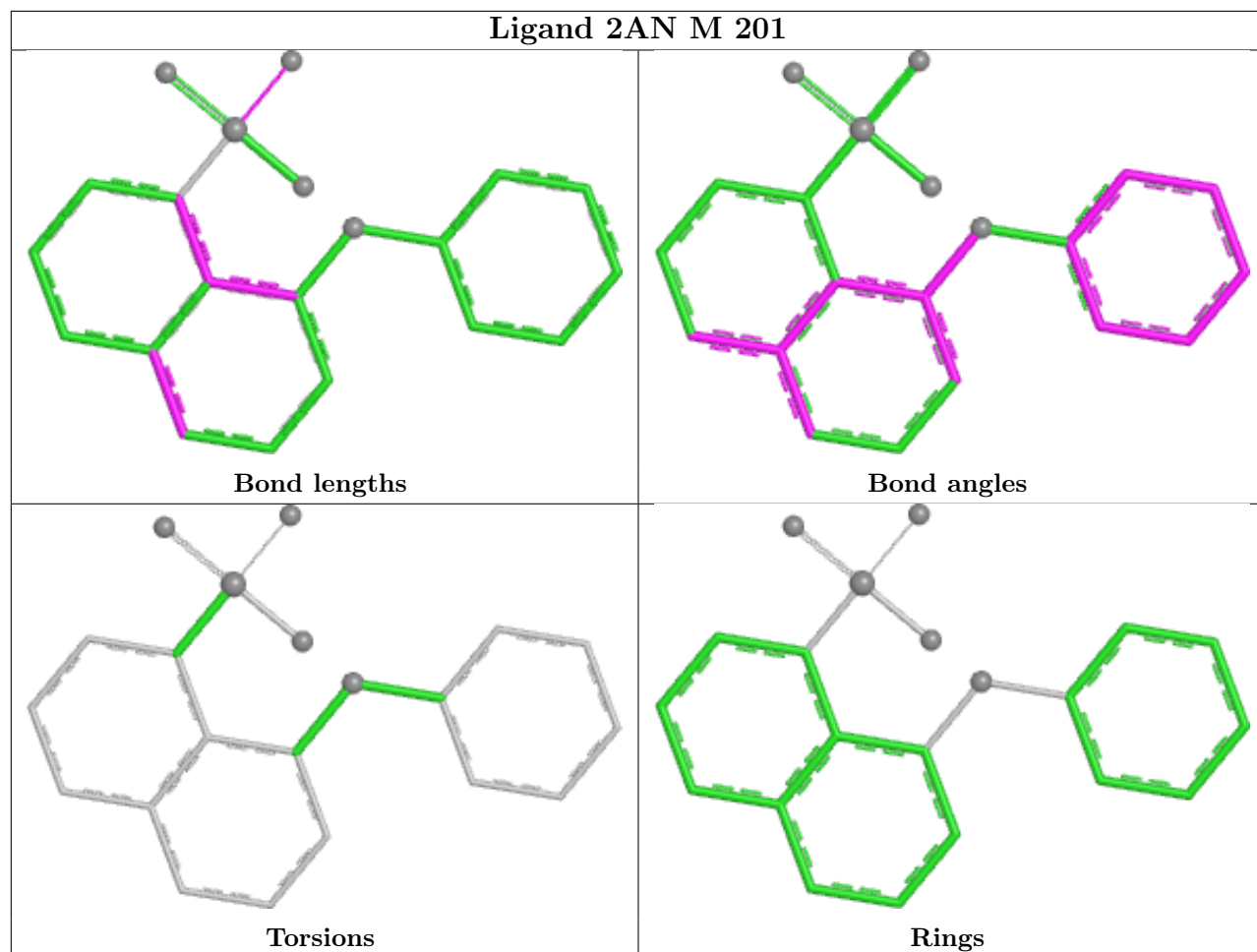


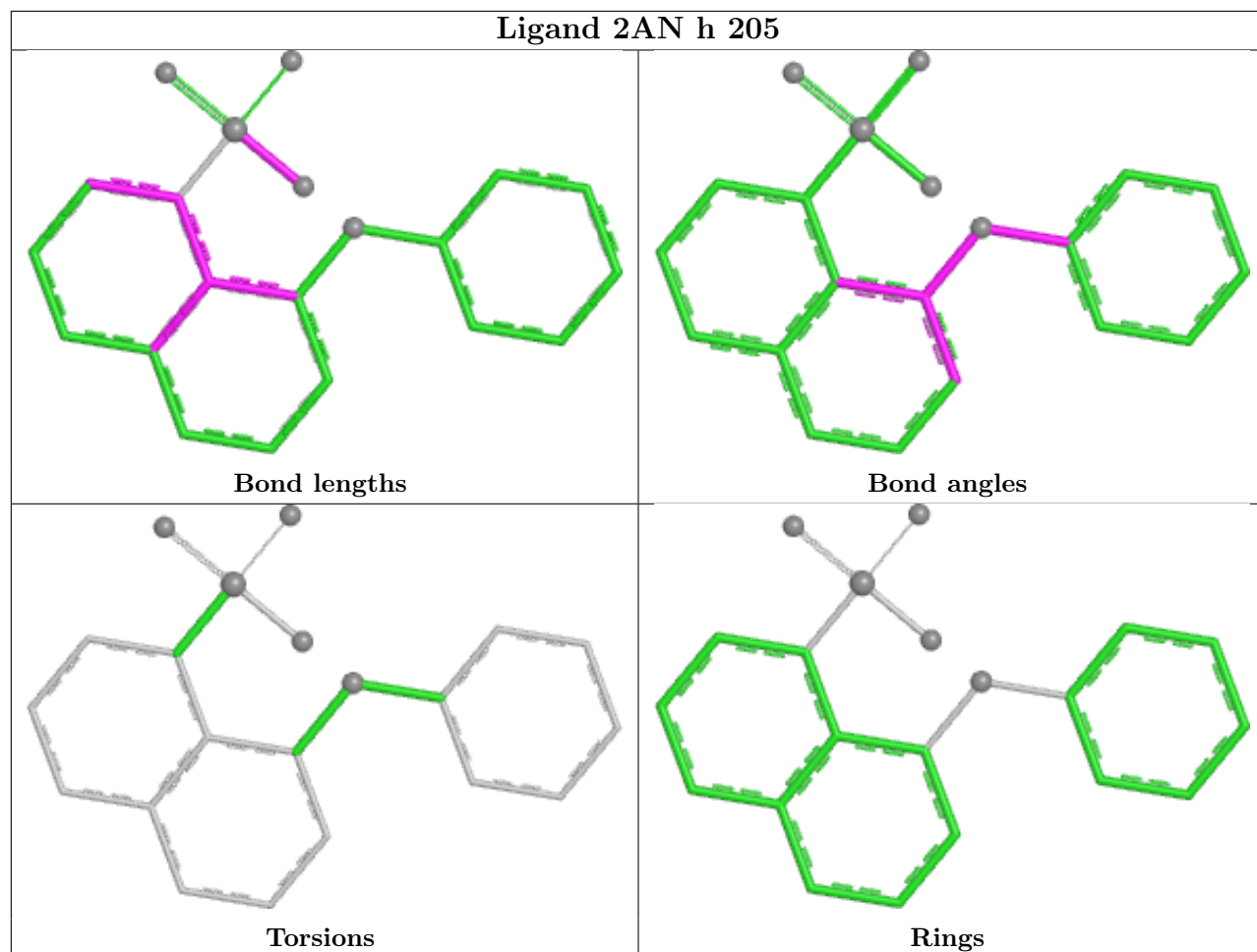
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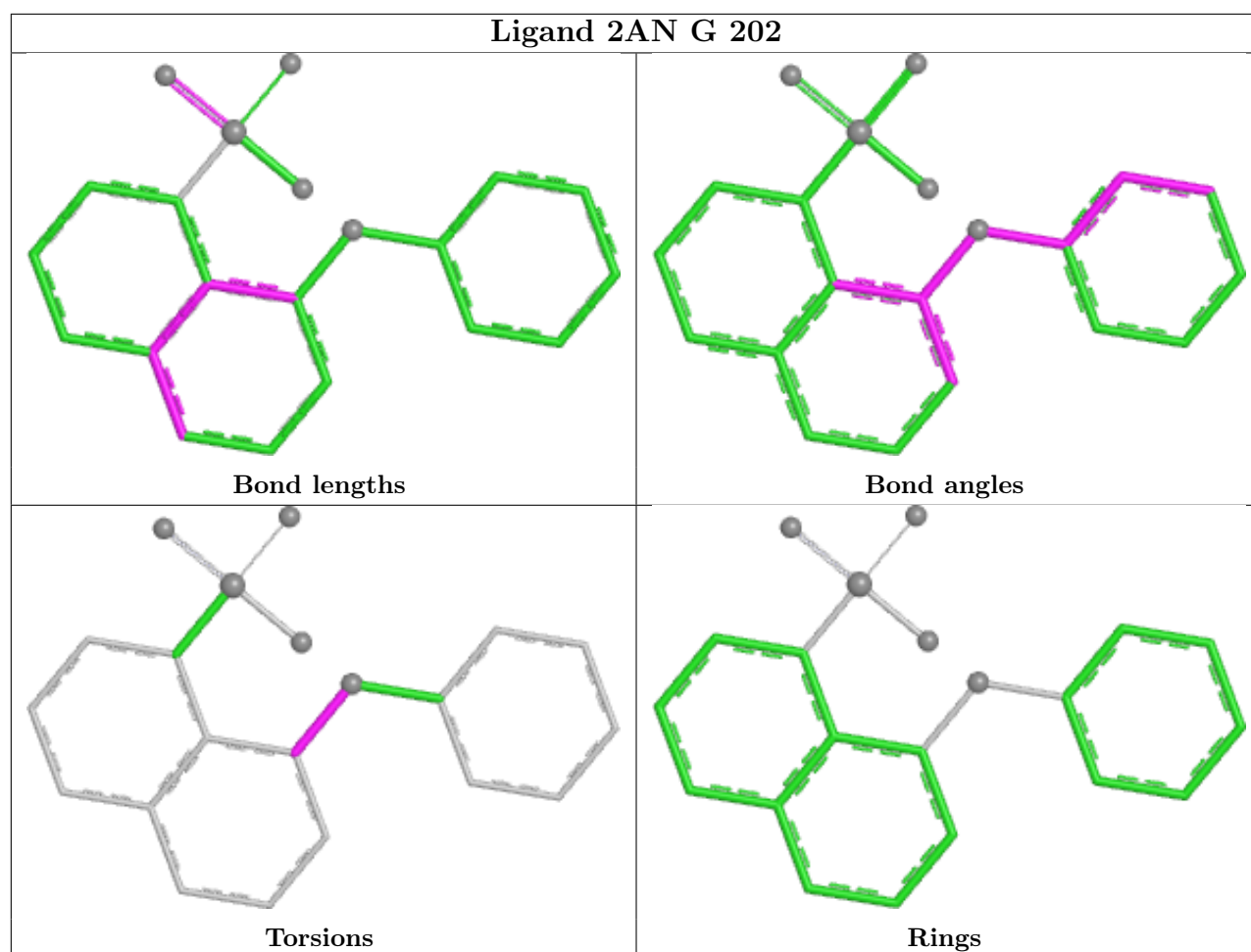


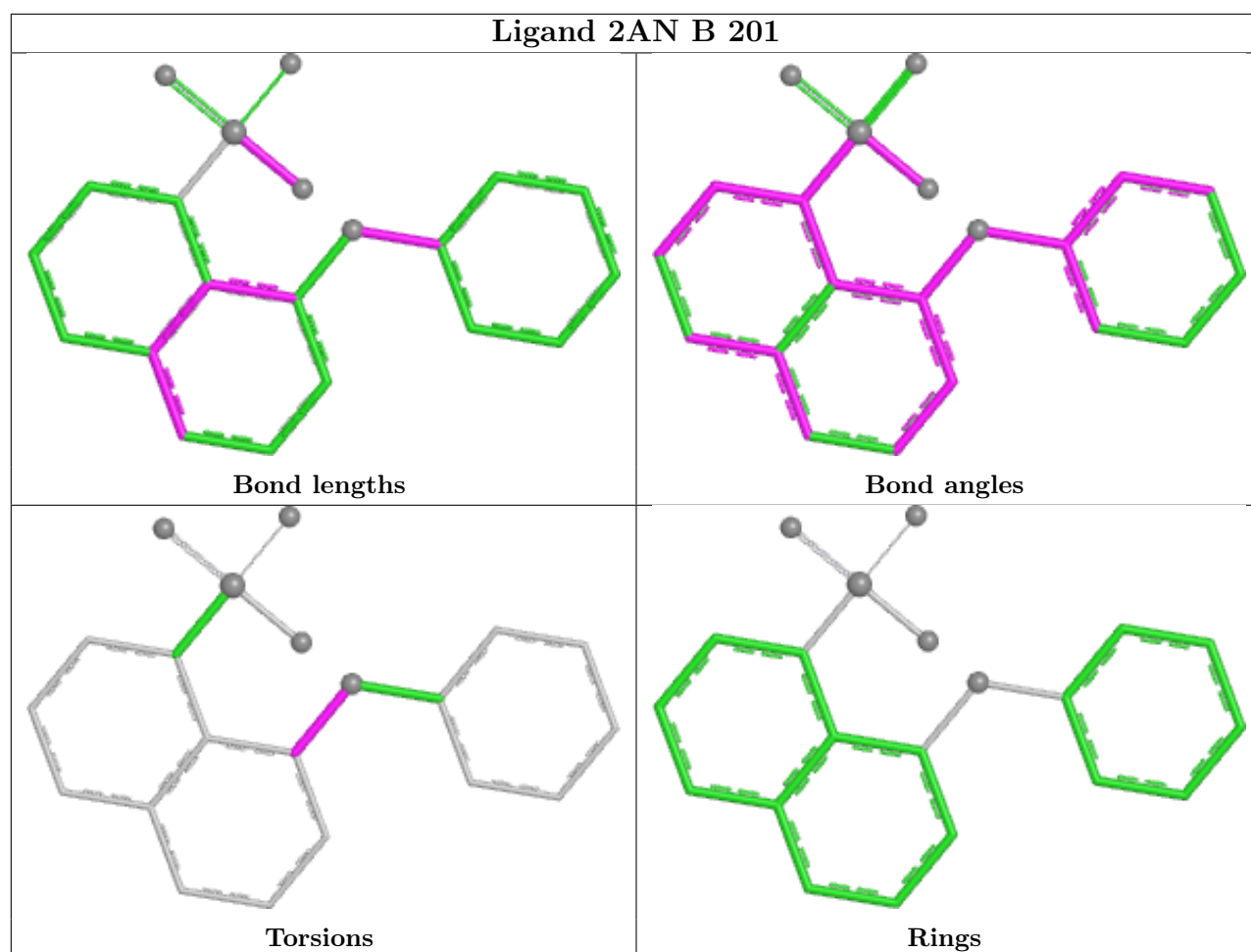
Ligand 2AN E 204



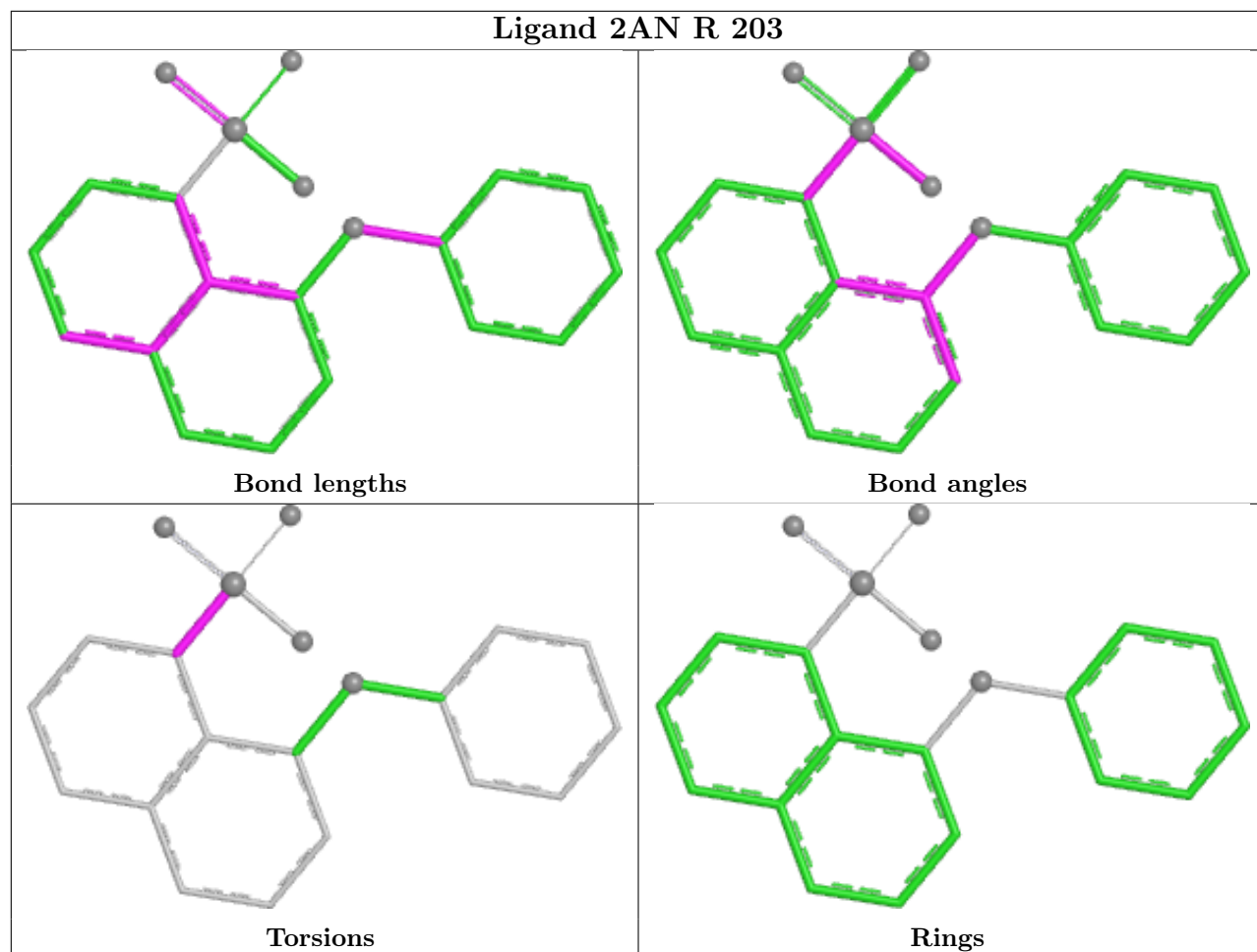


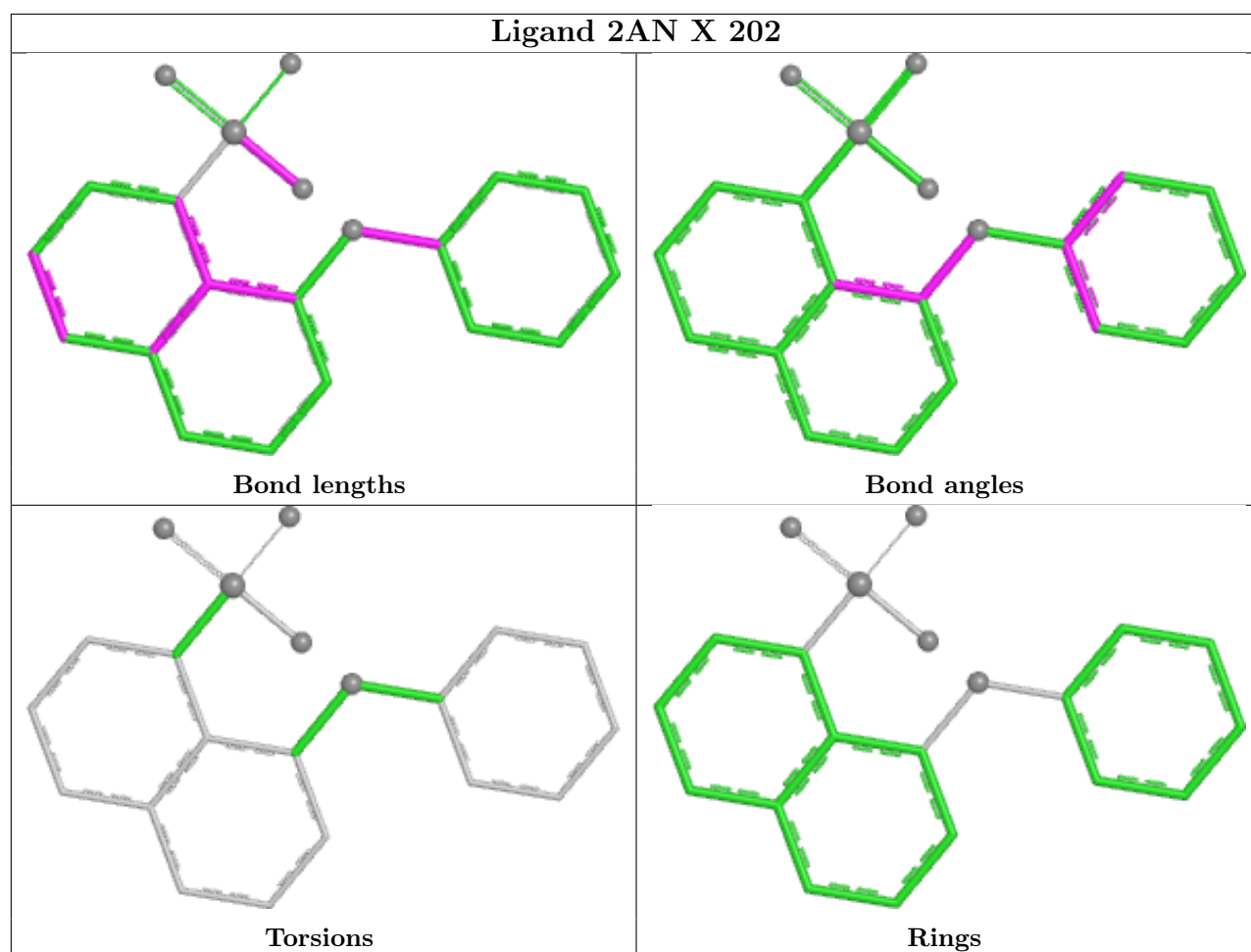




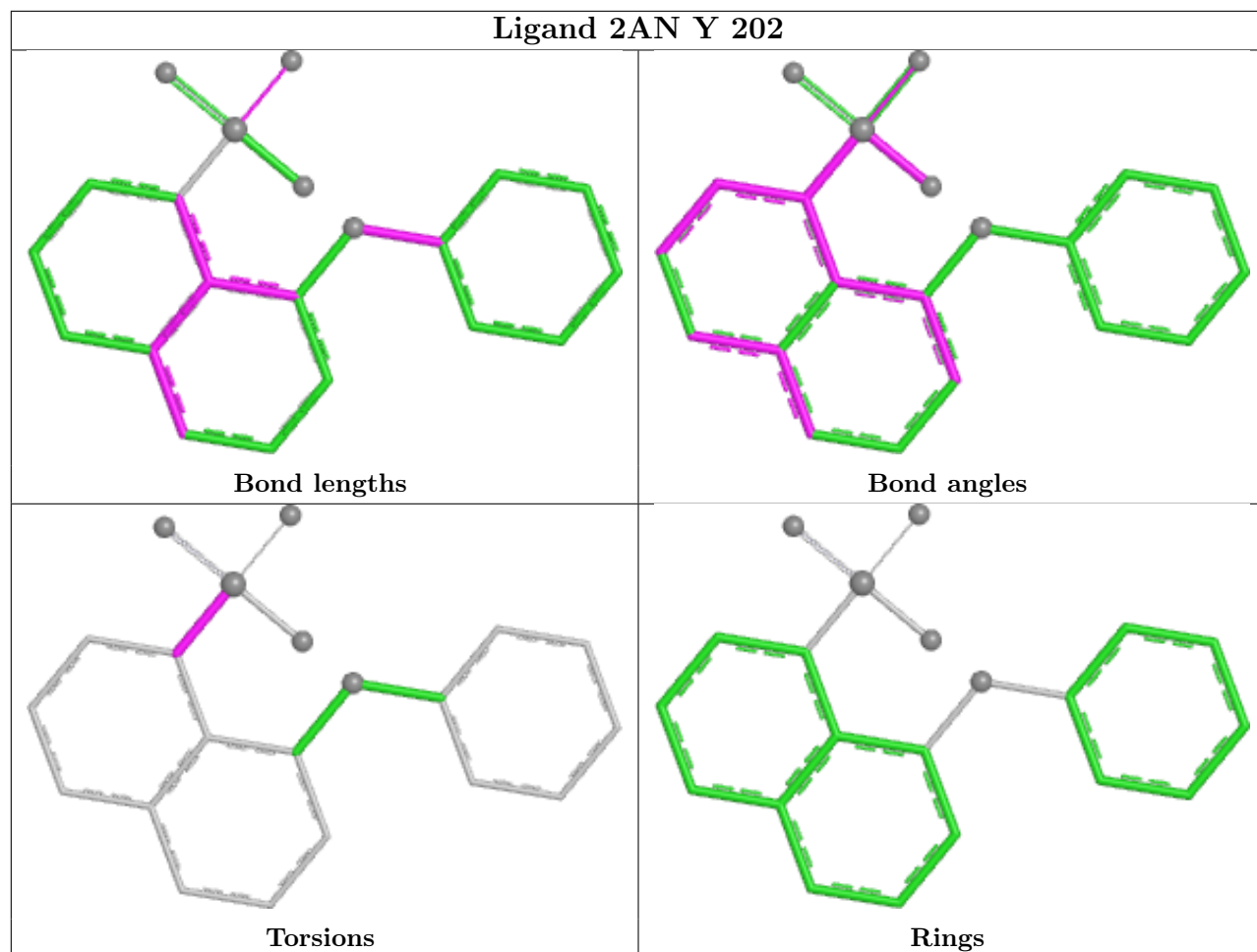


Ligand 2AN R 203

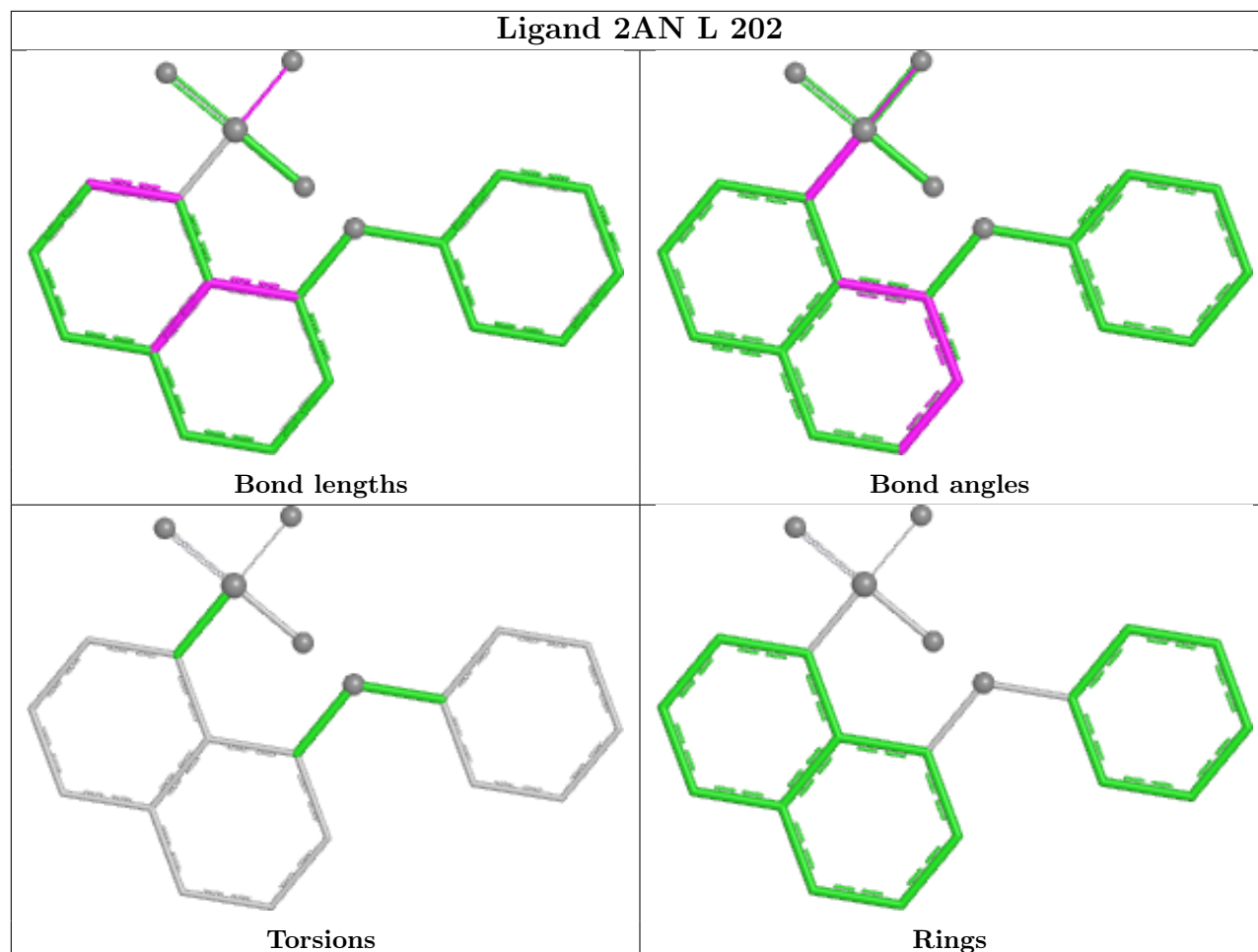


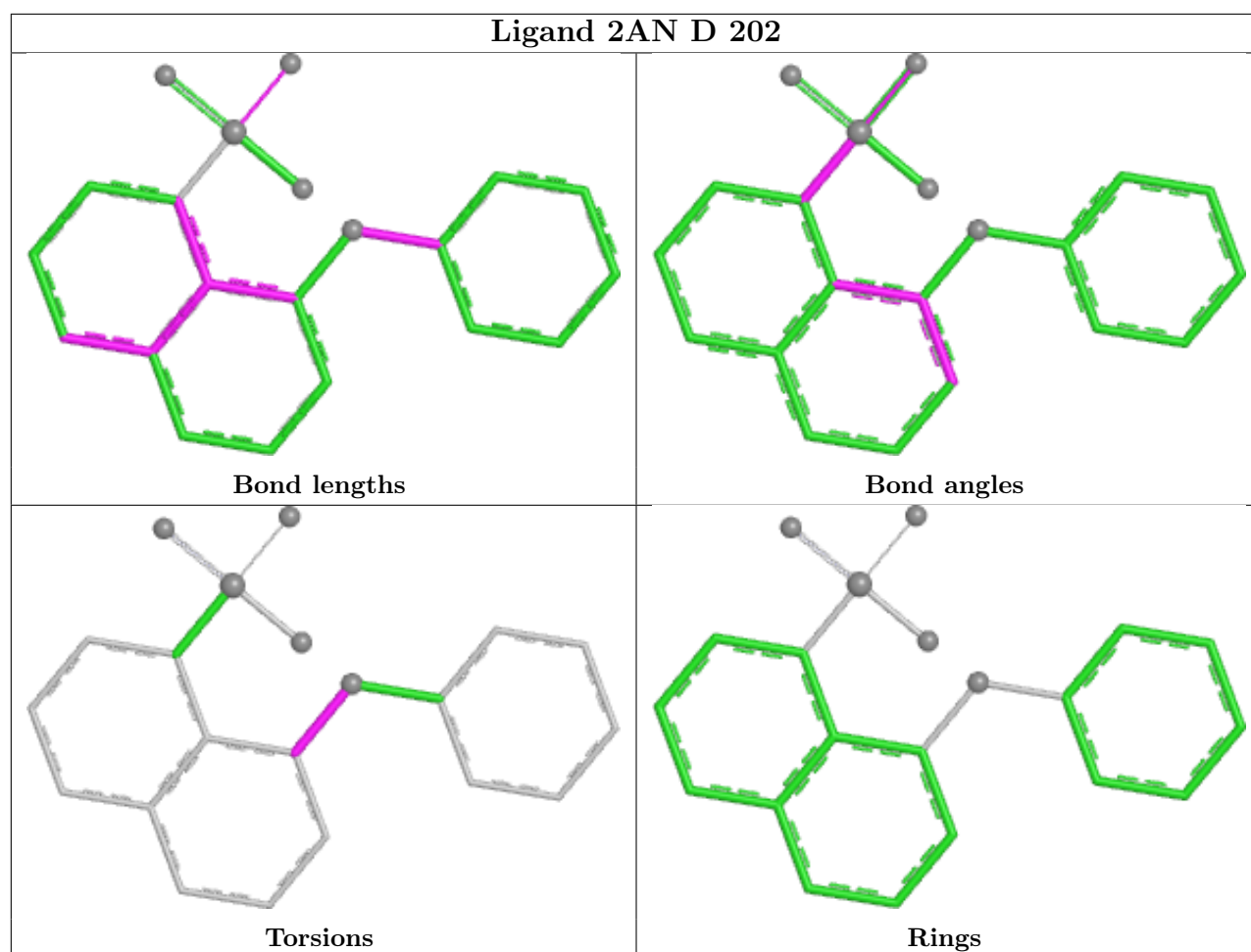


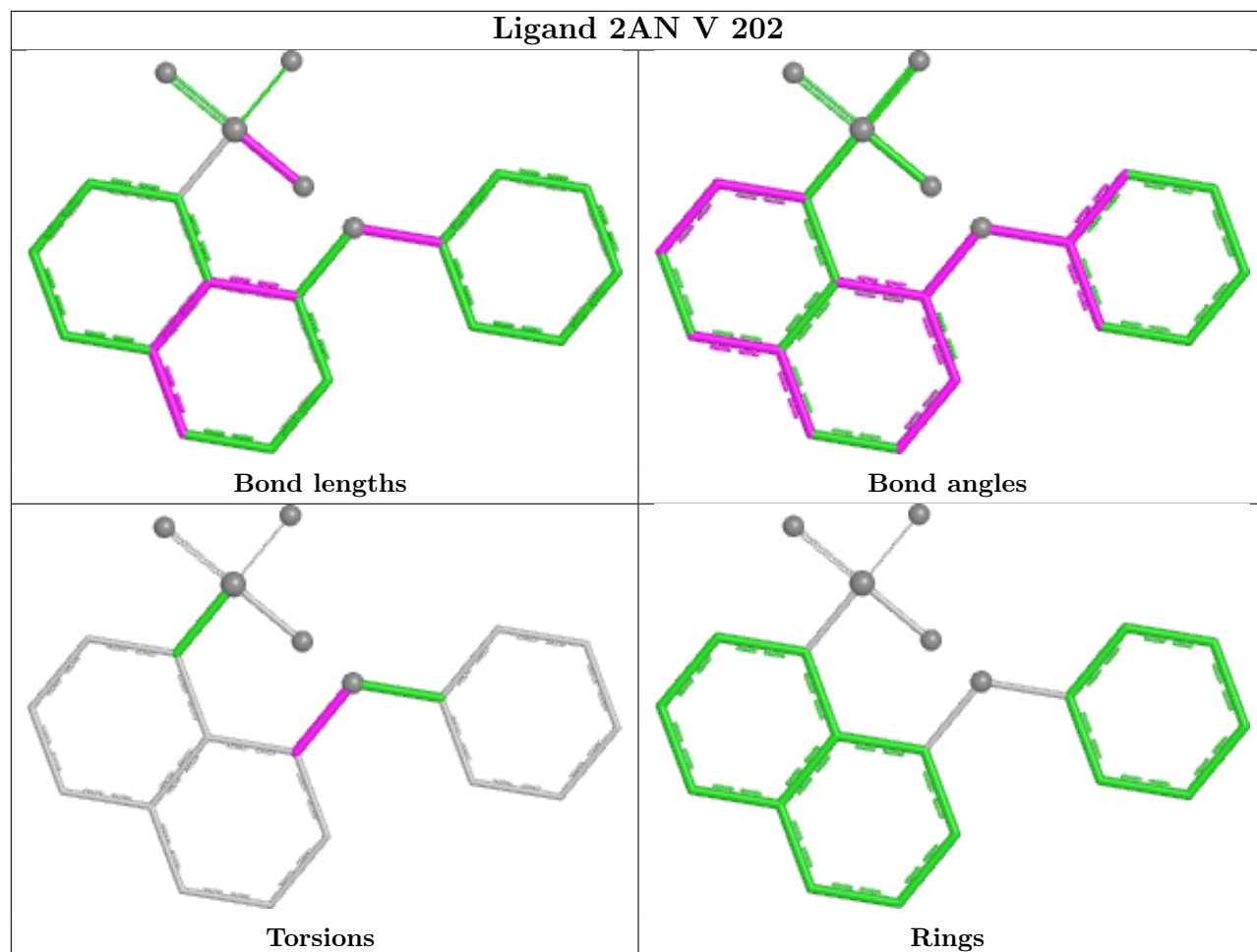
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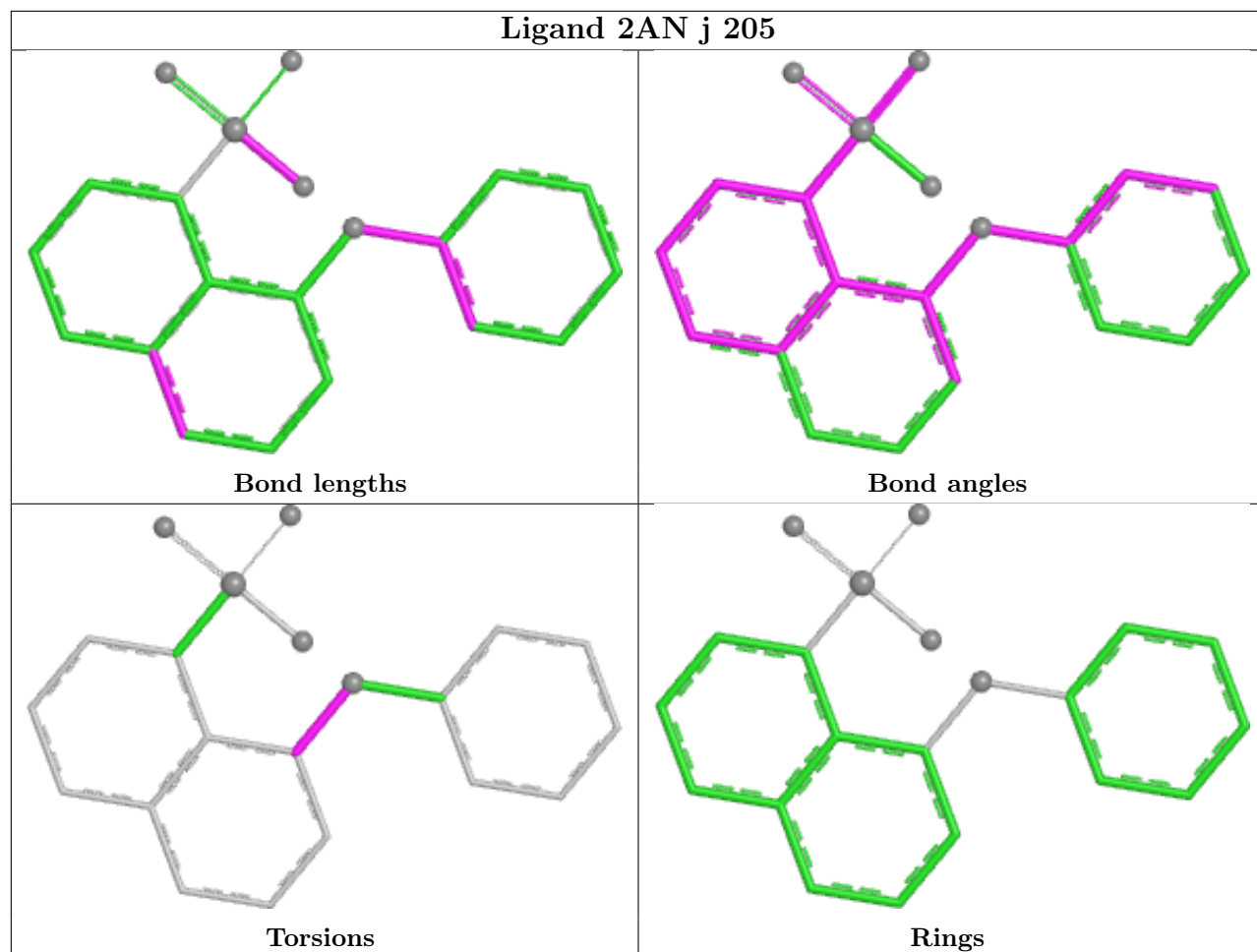
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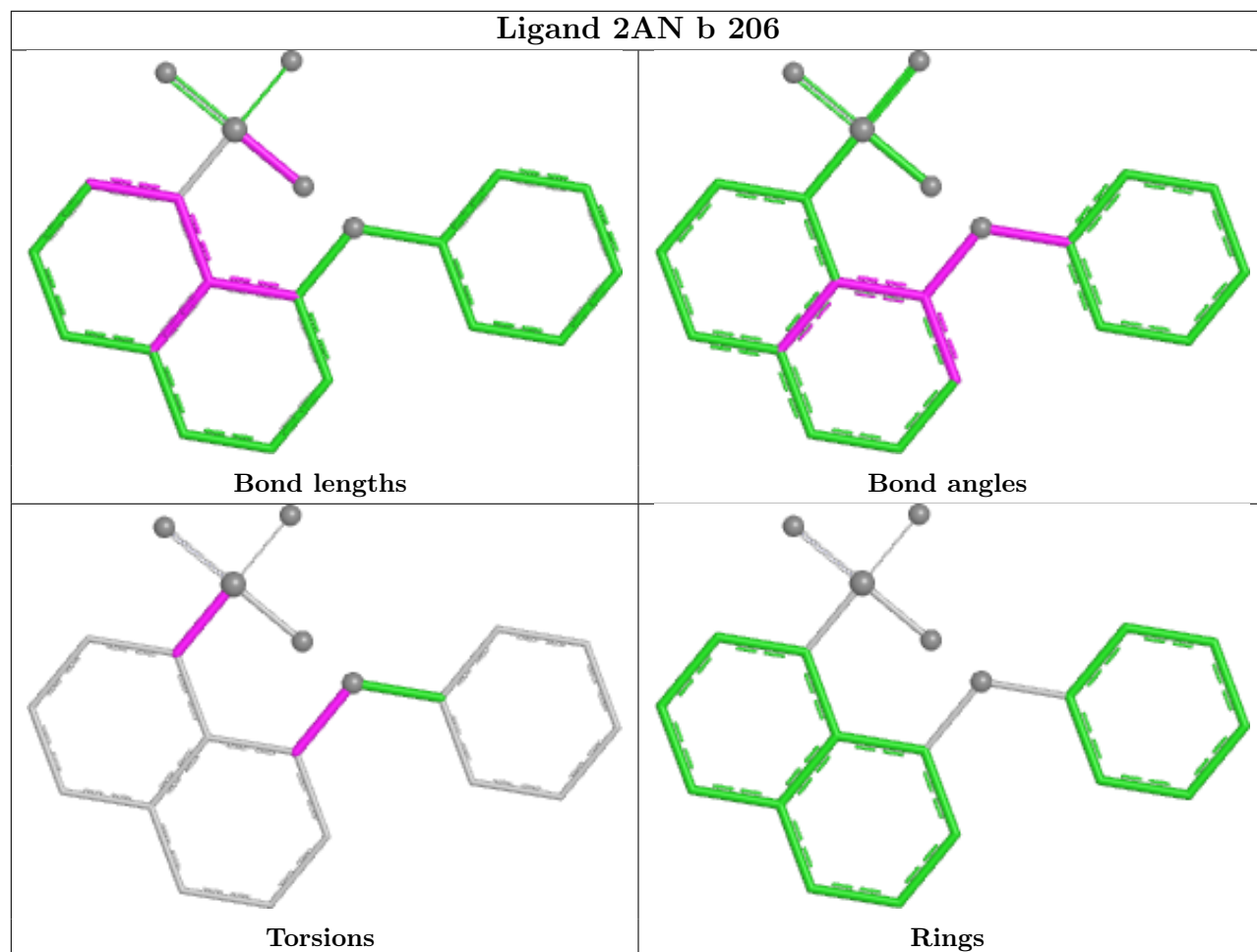


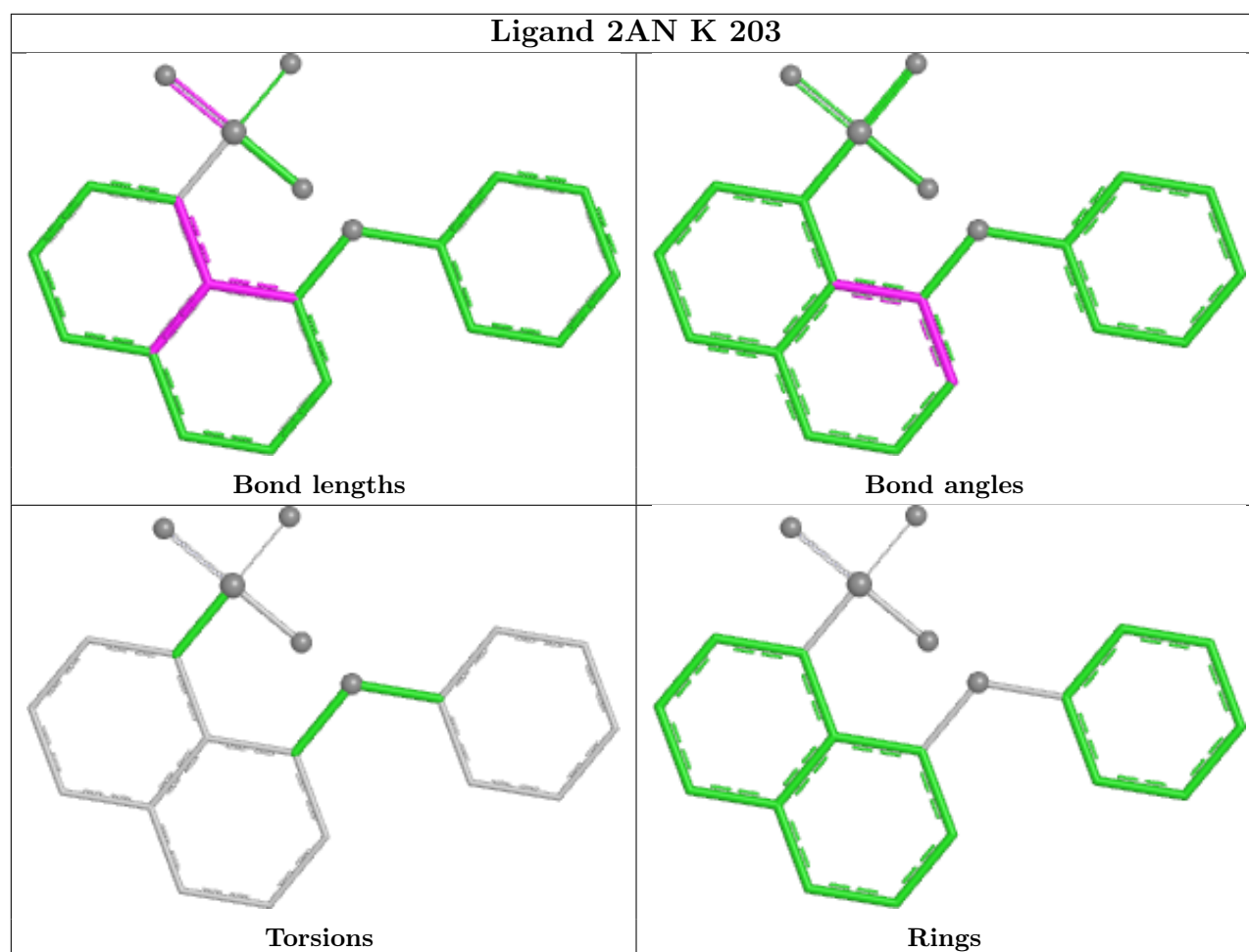


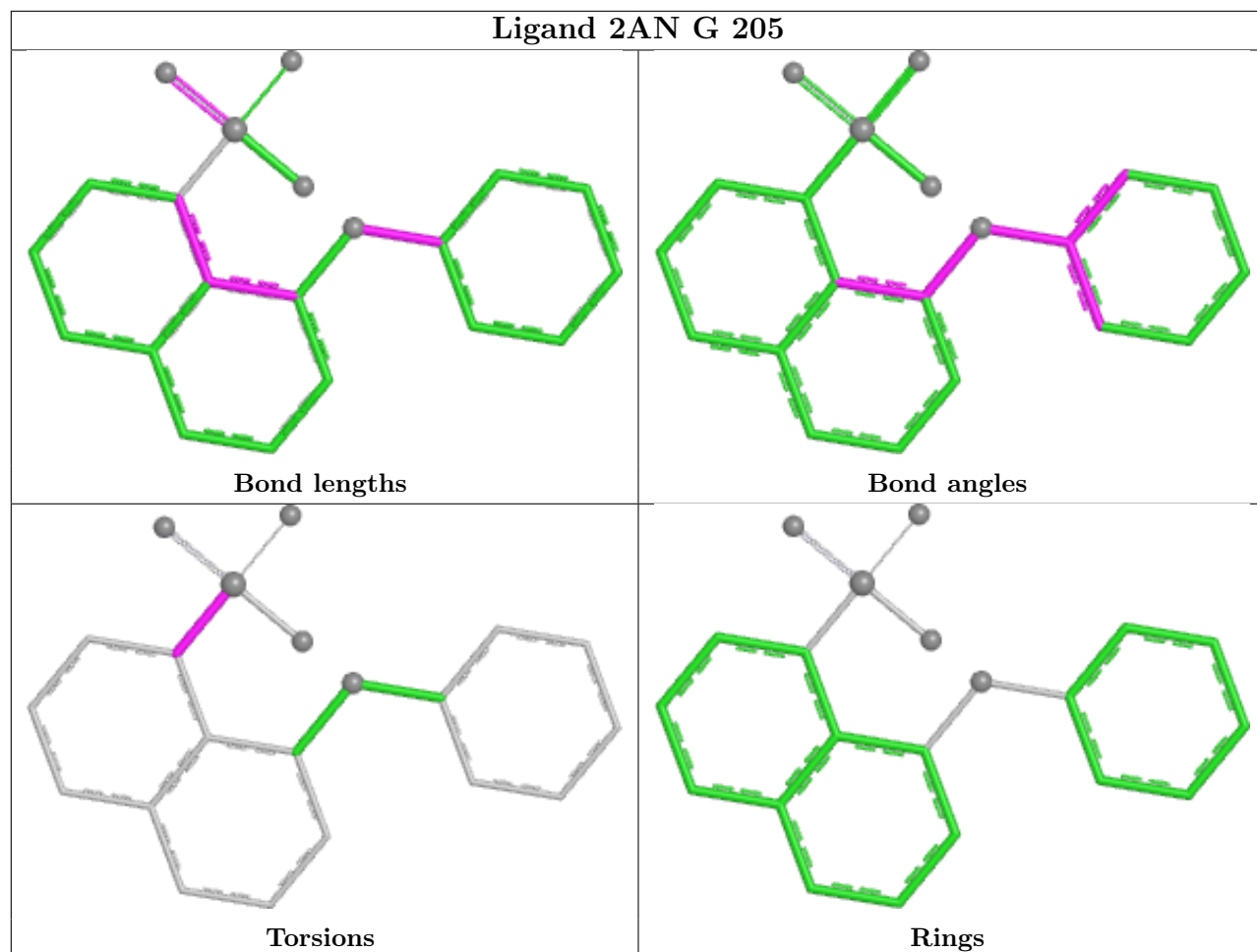
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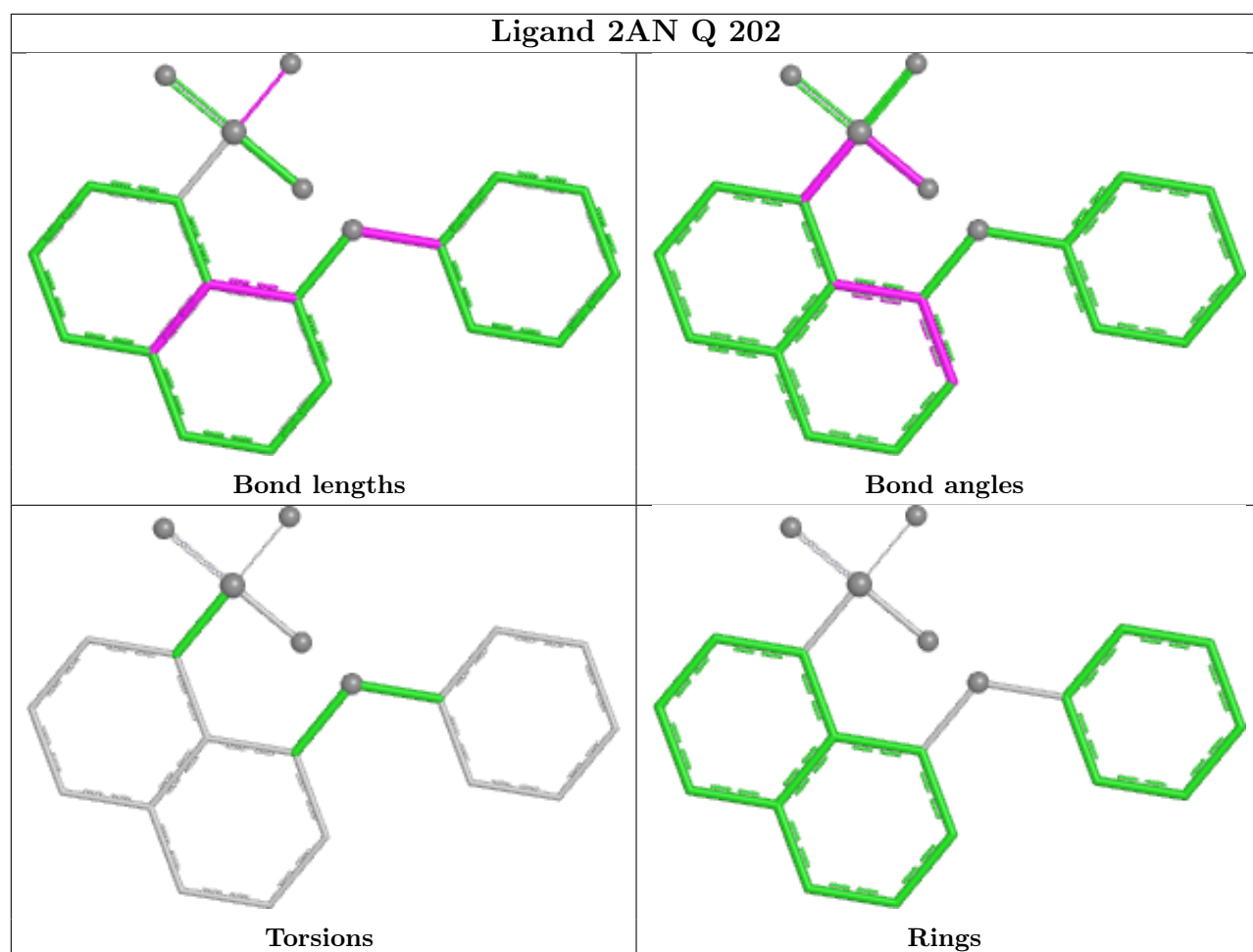


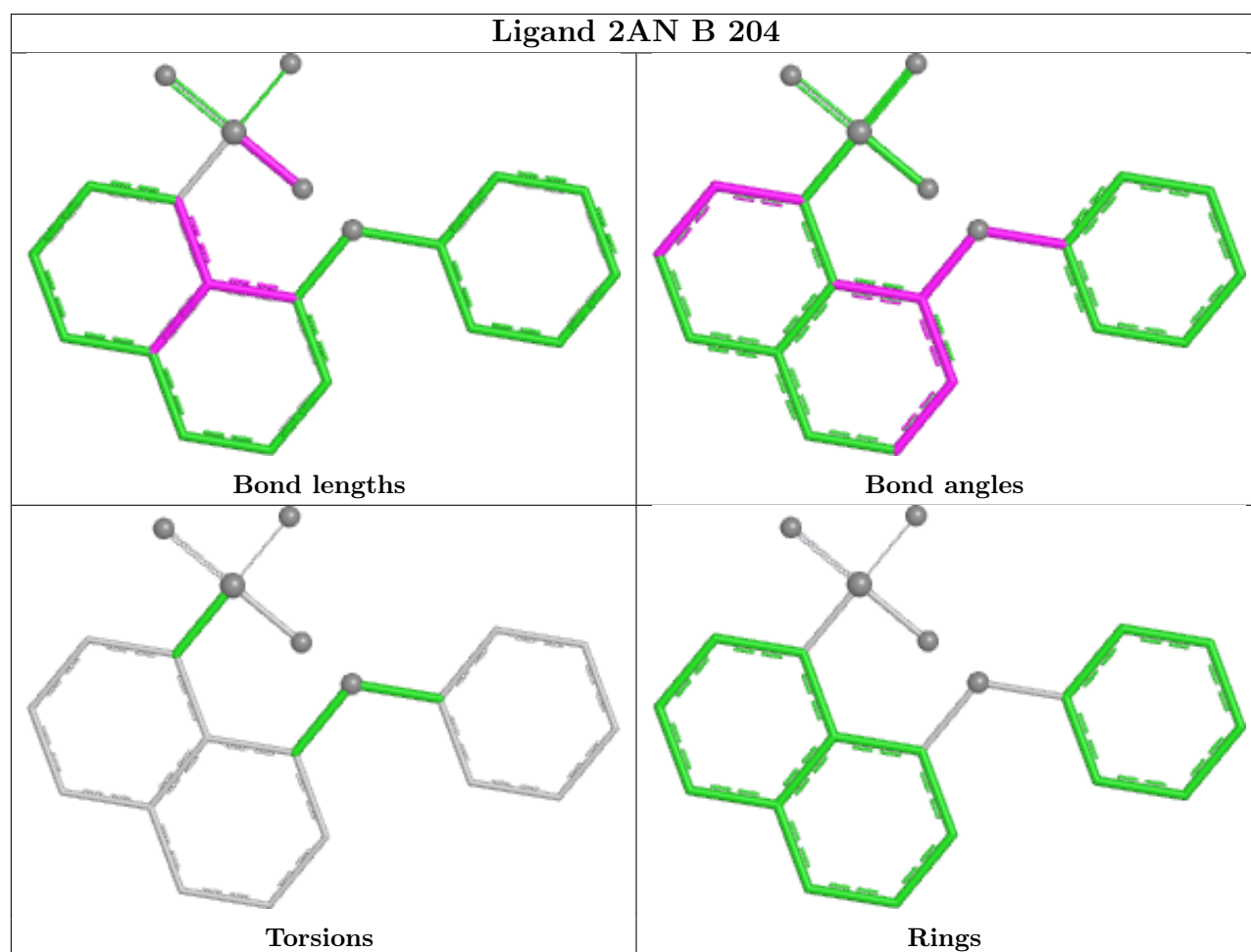
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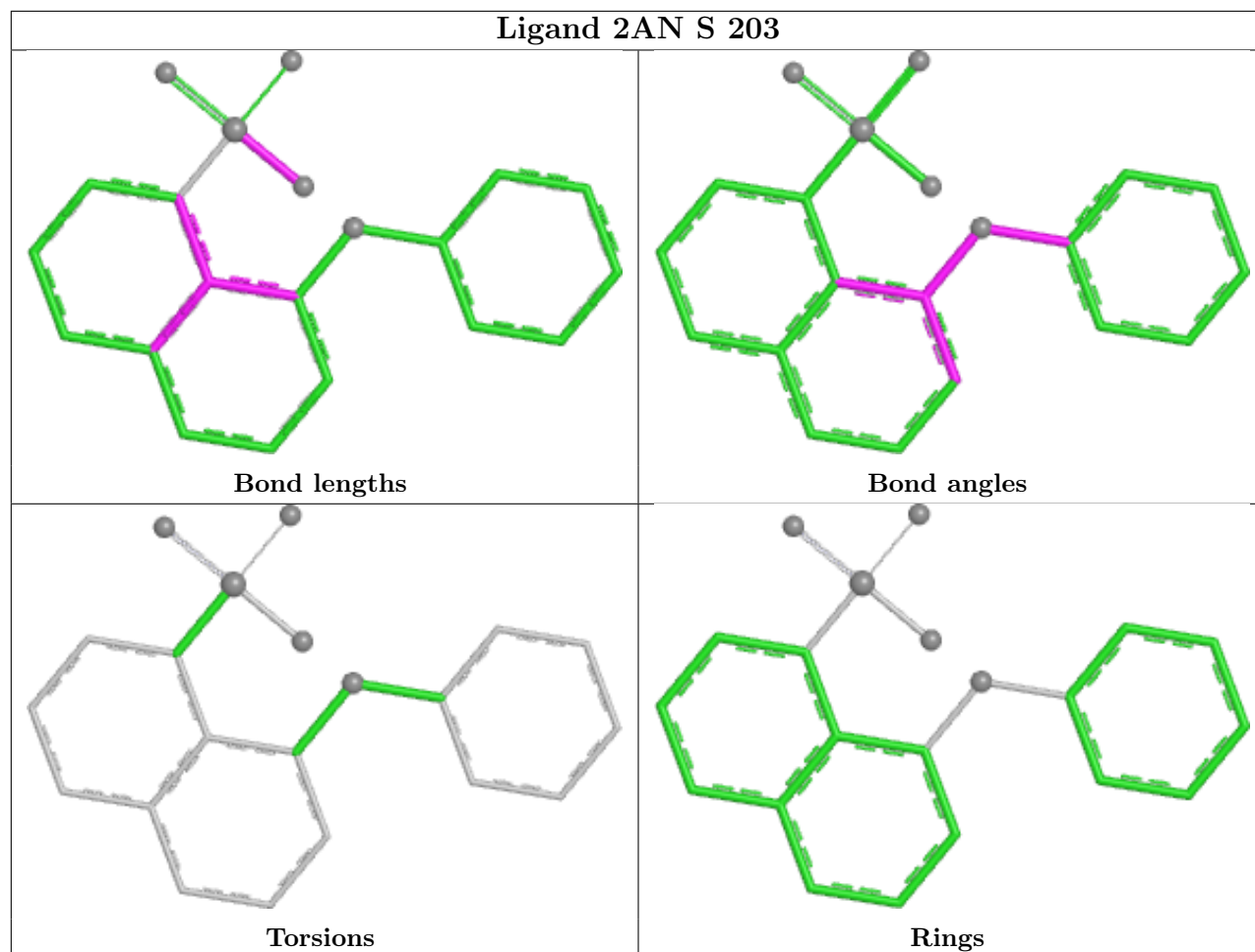




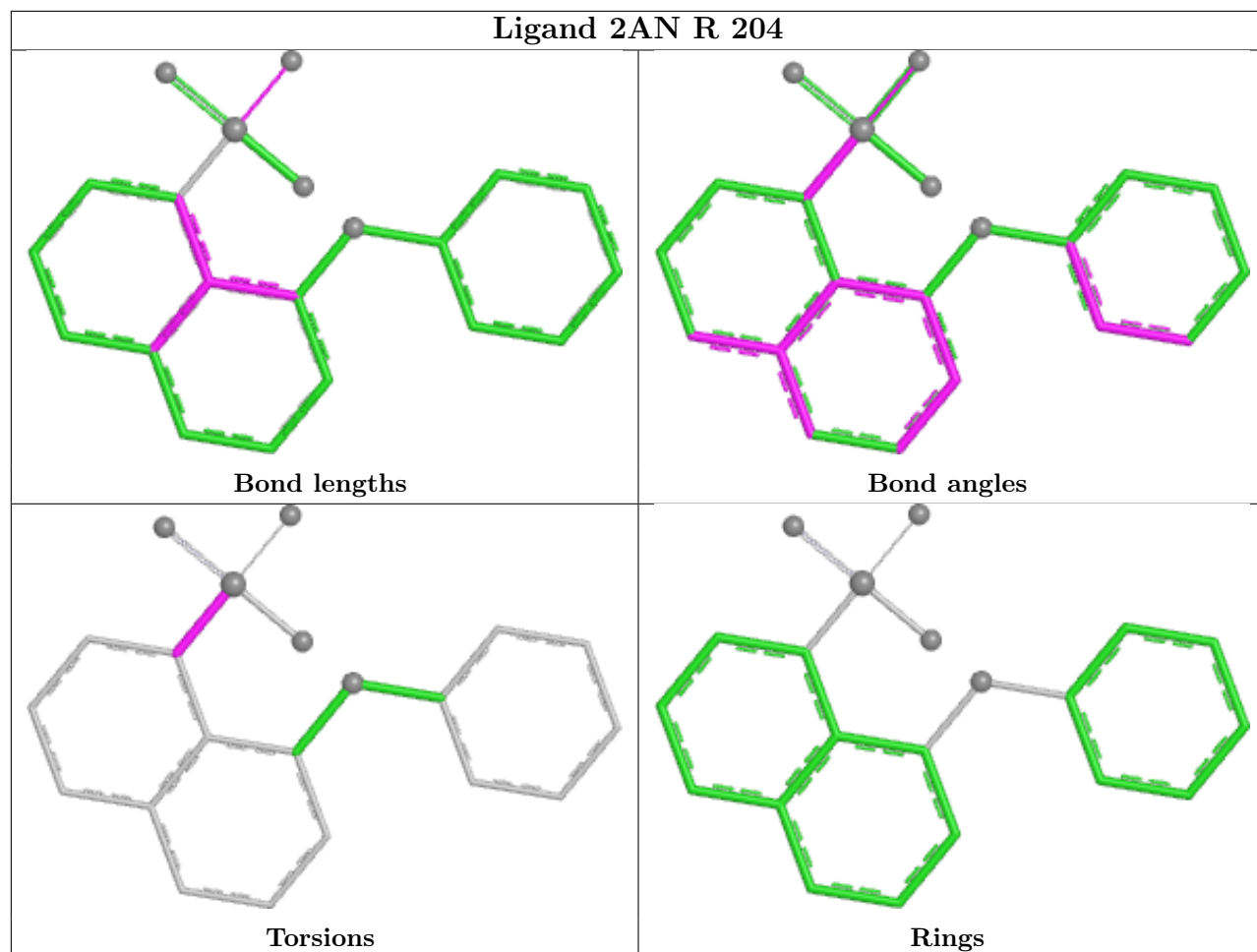




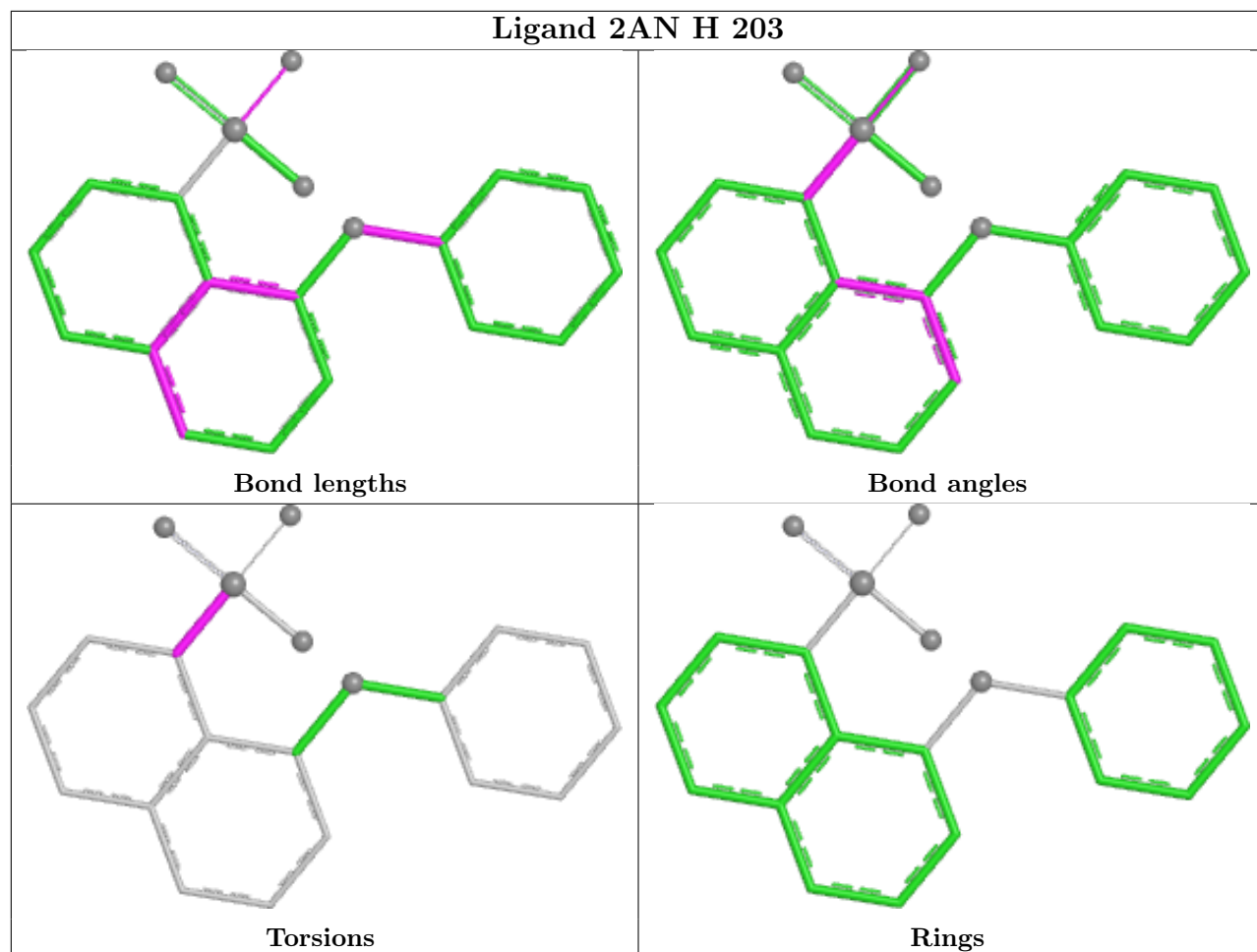


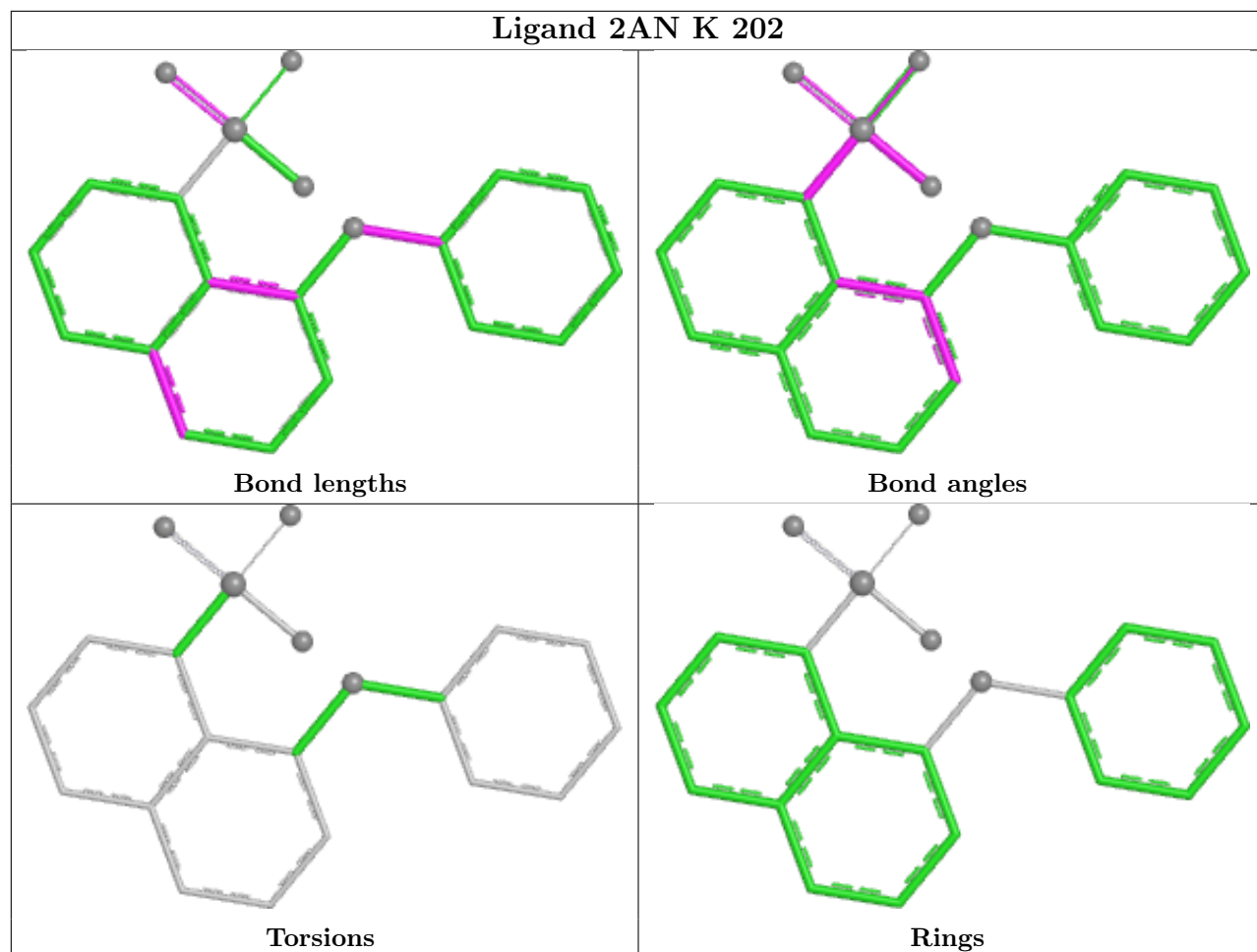


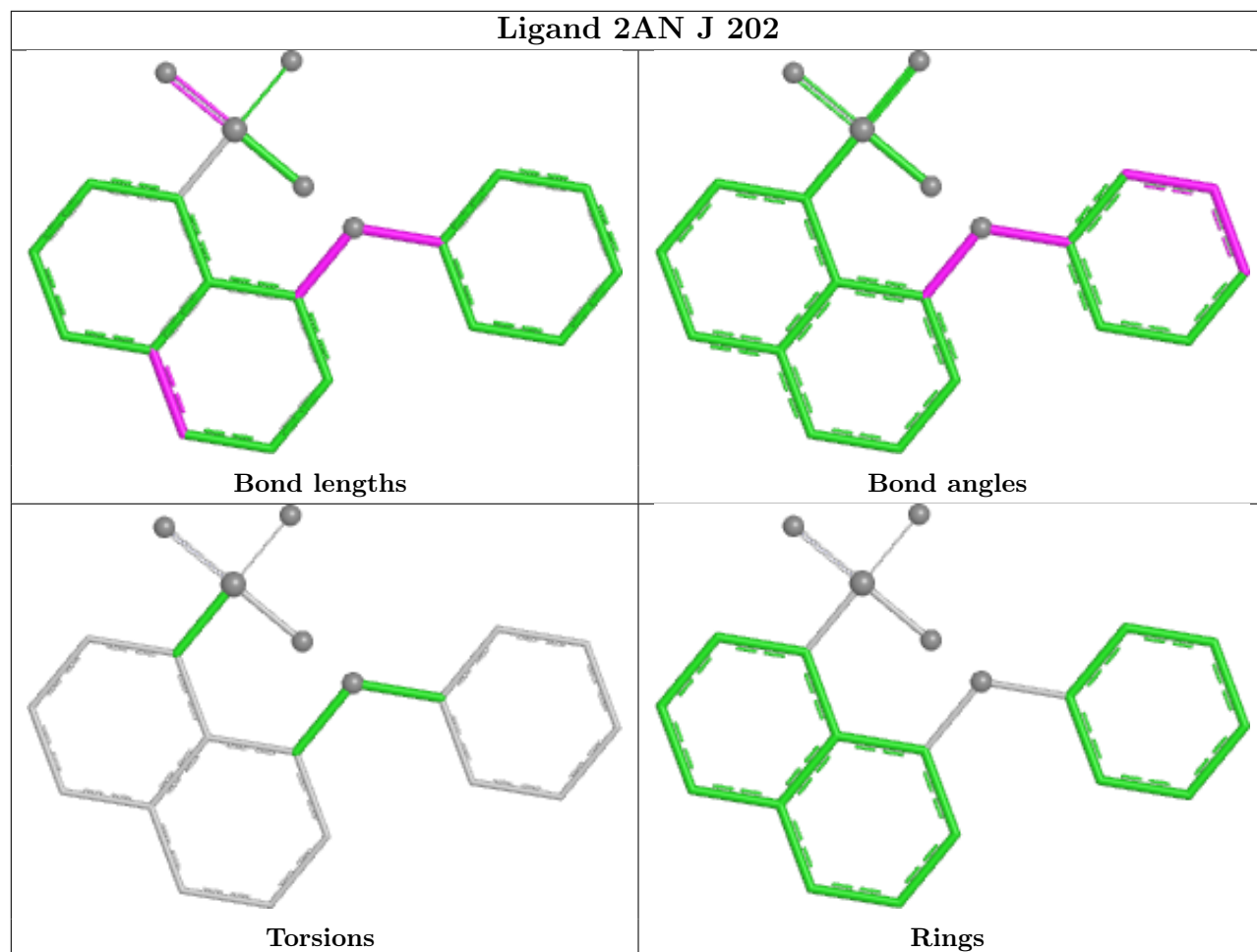
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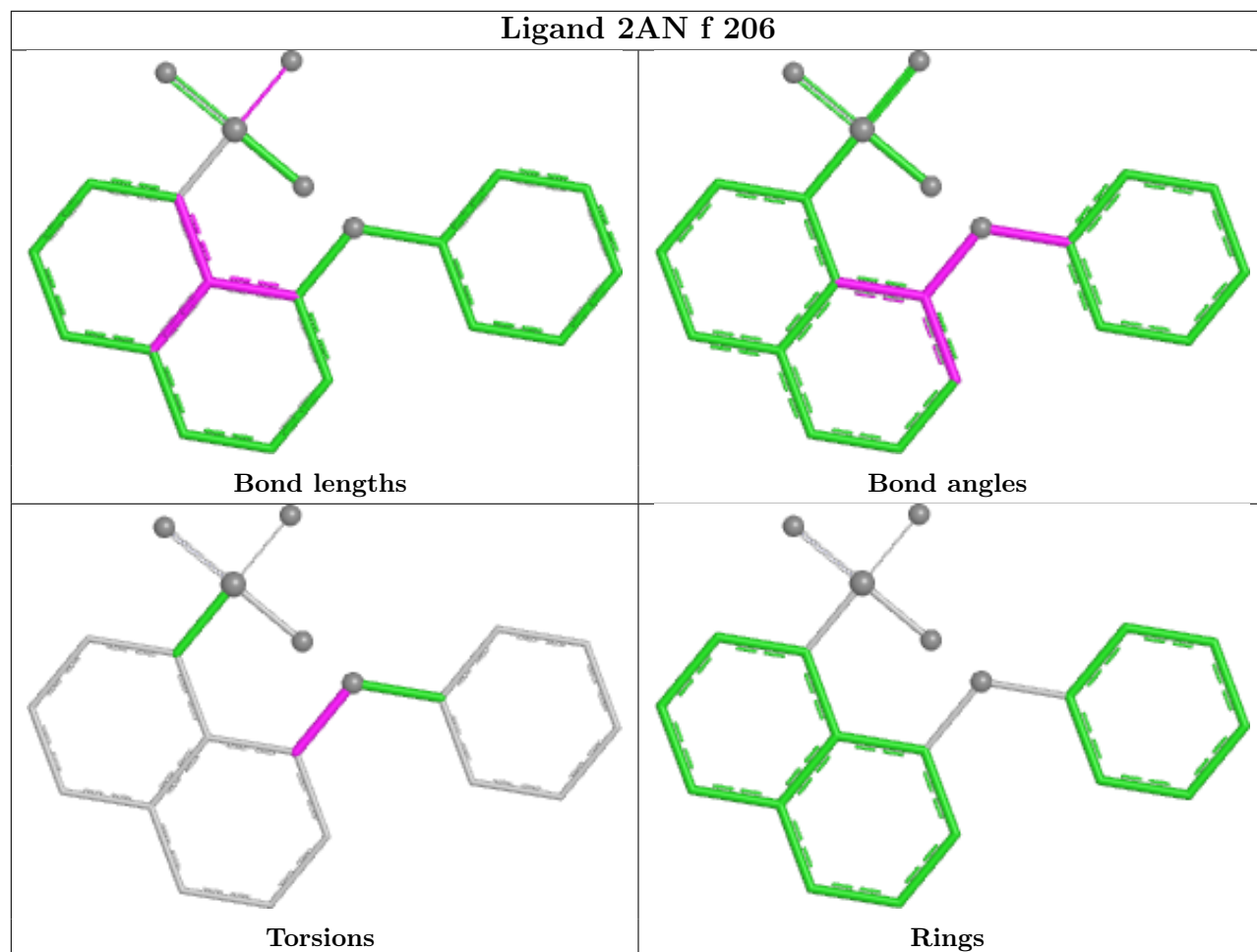
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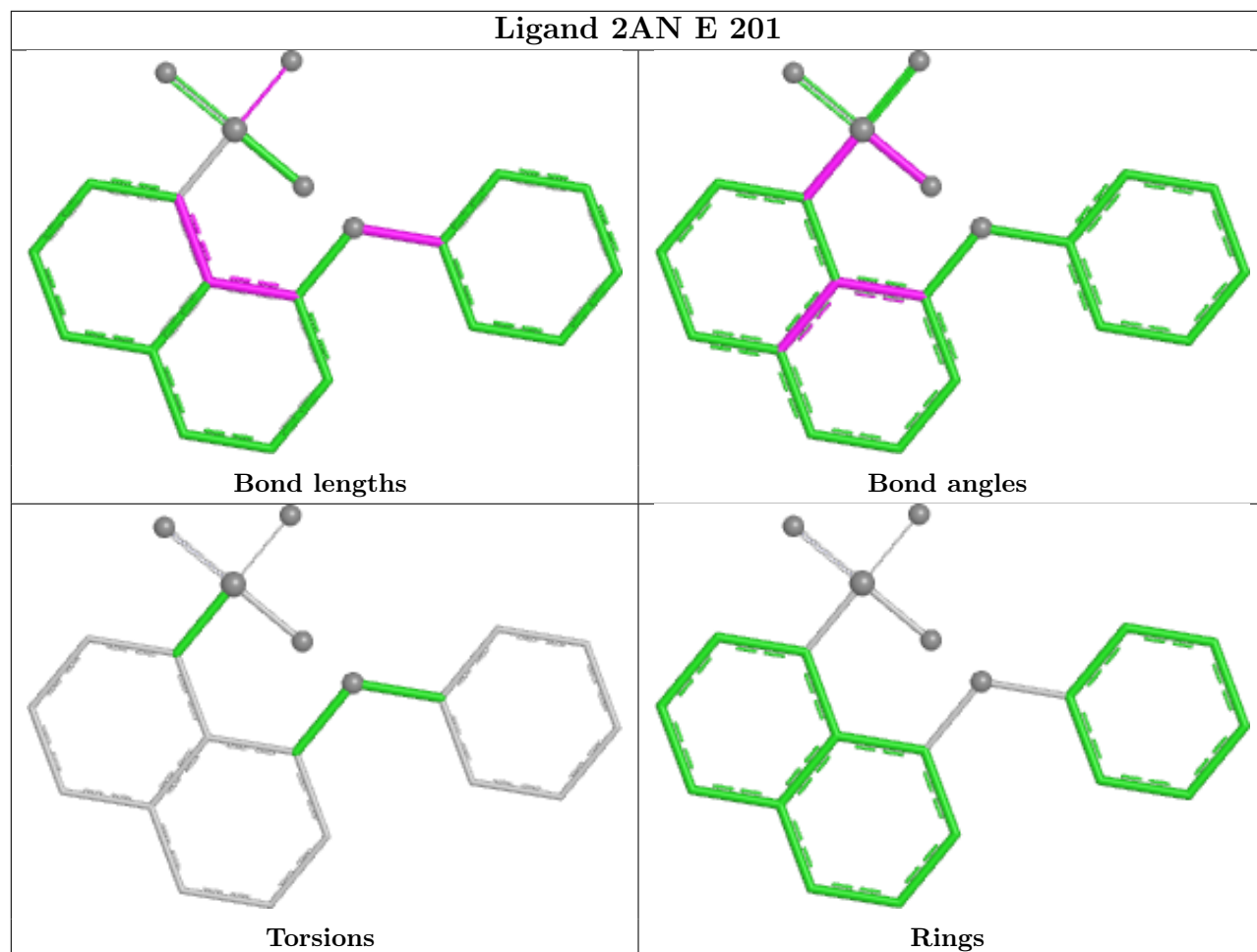




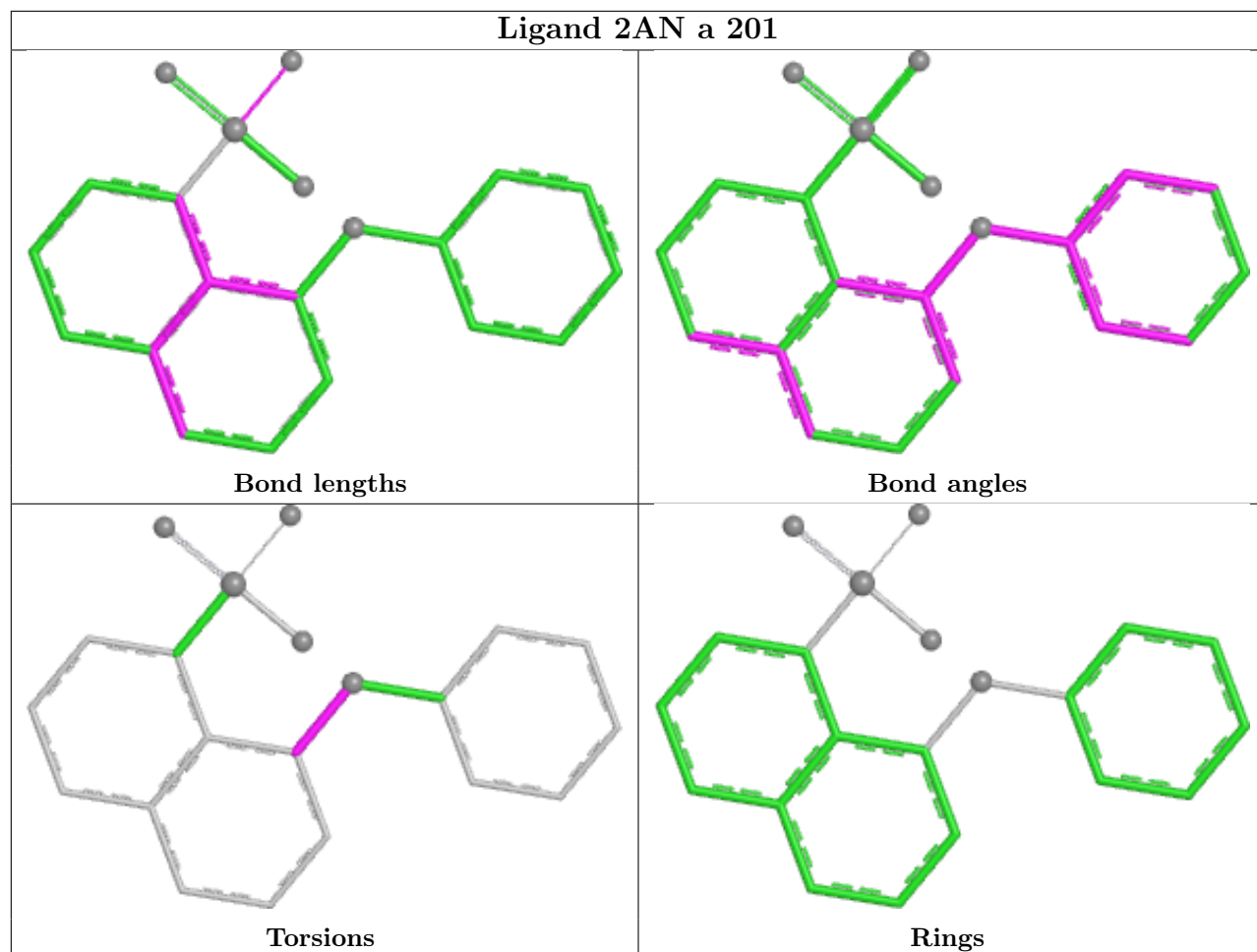


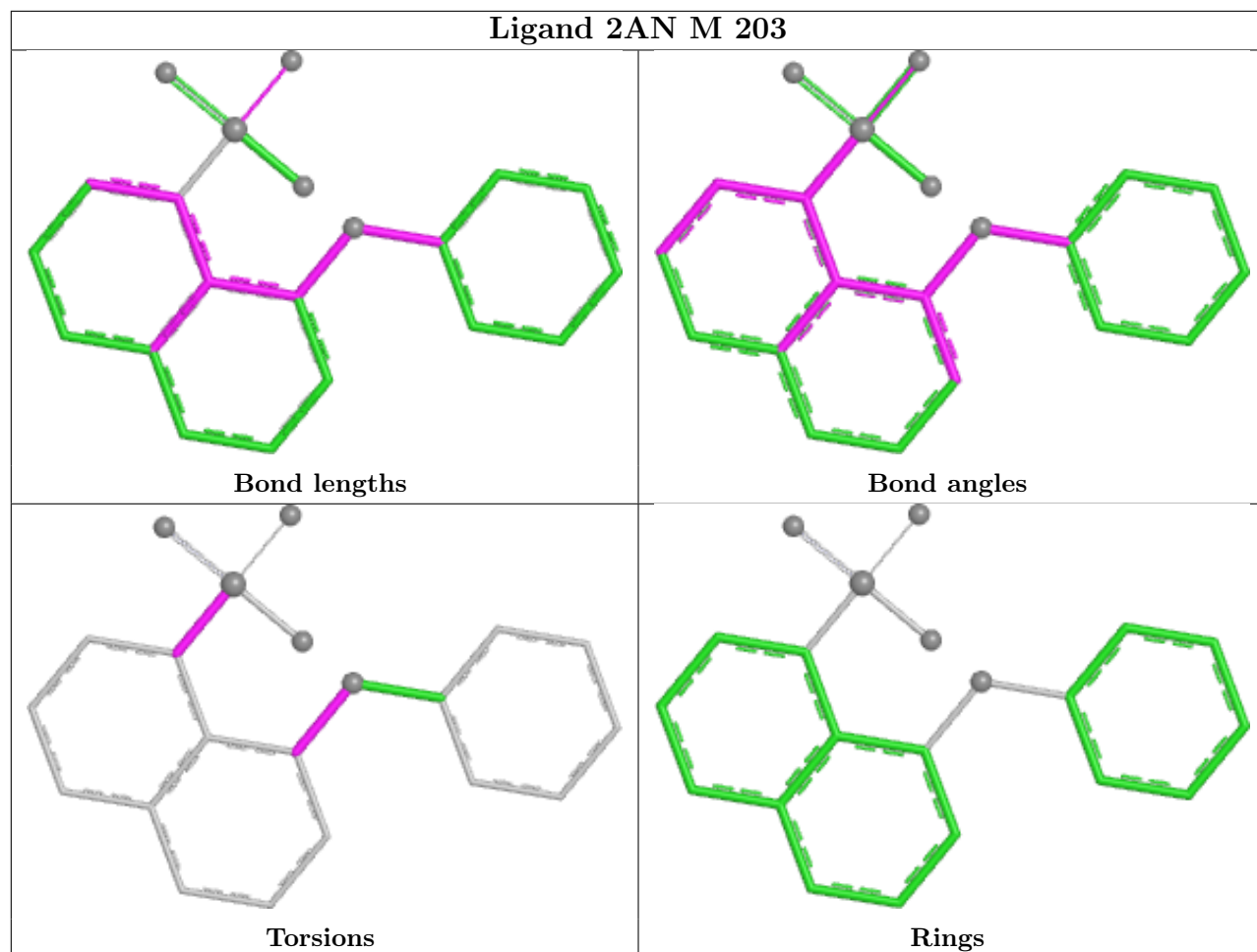
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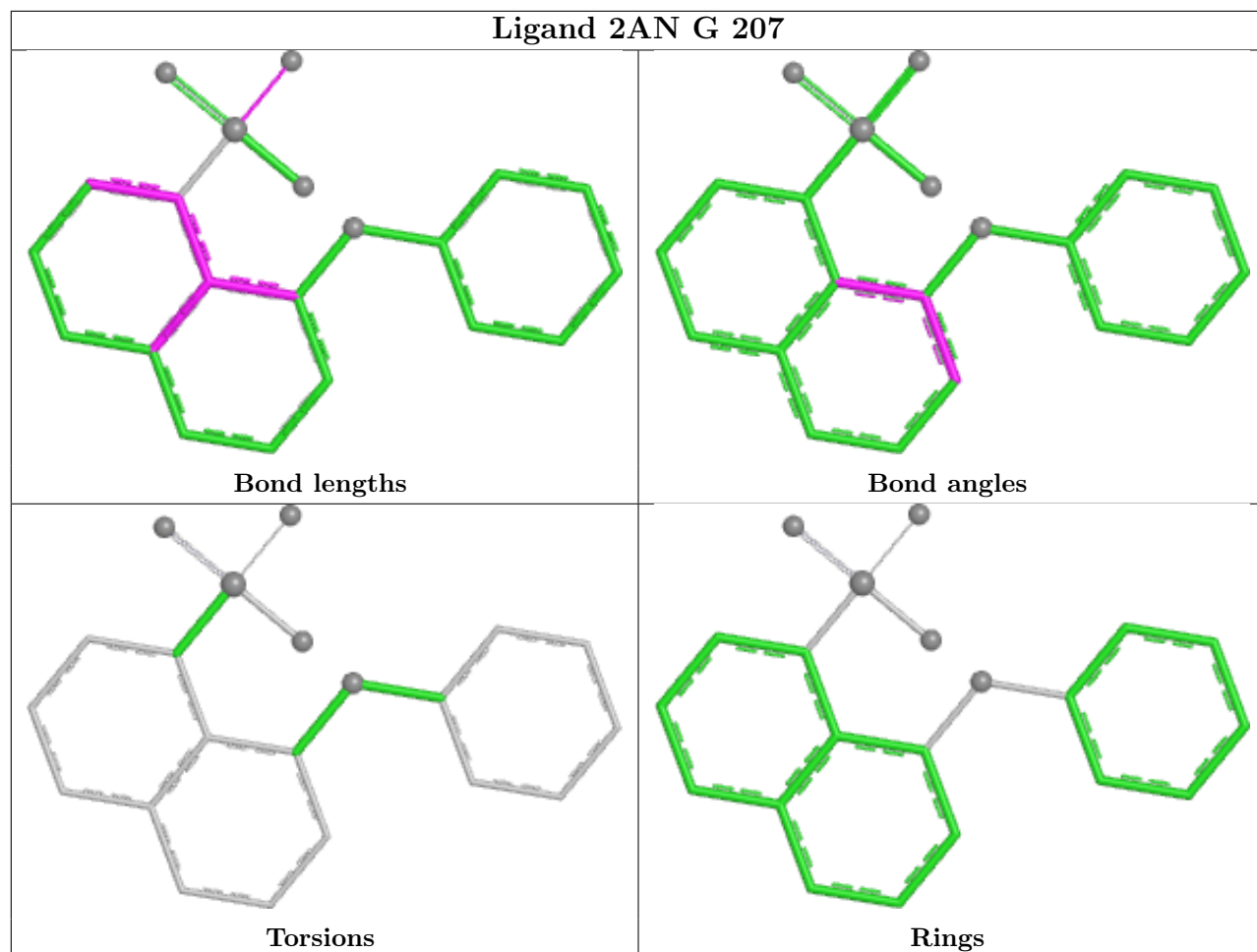


Ligand 2AN a 201

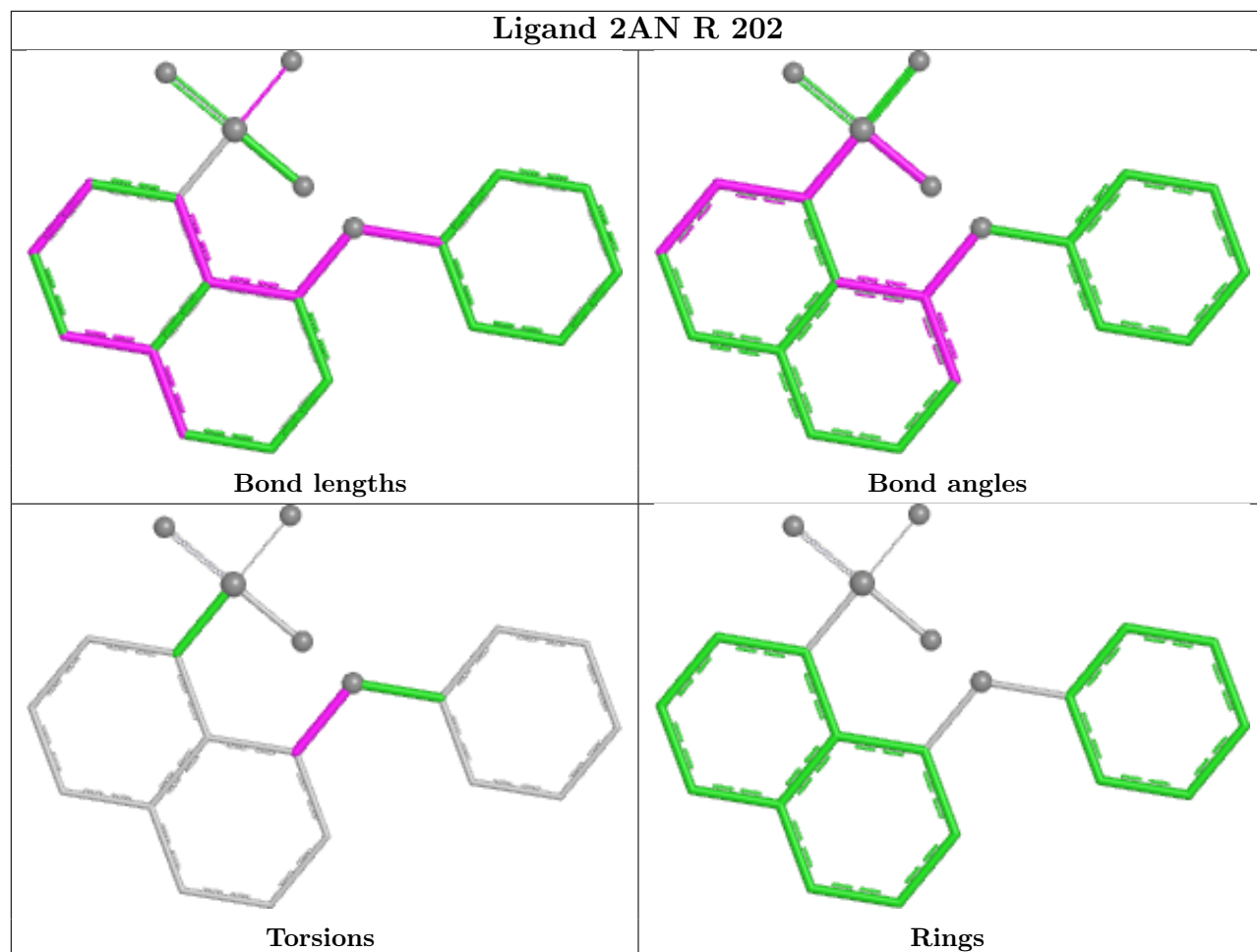


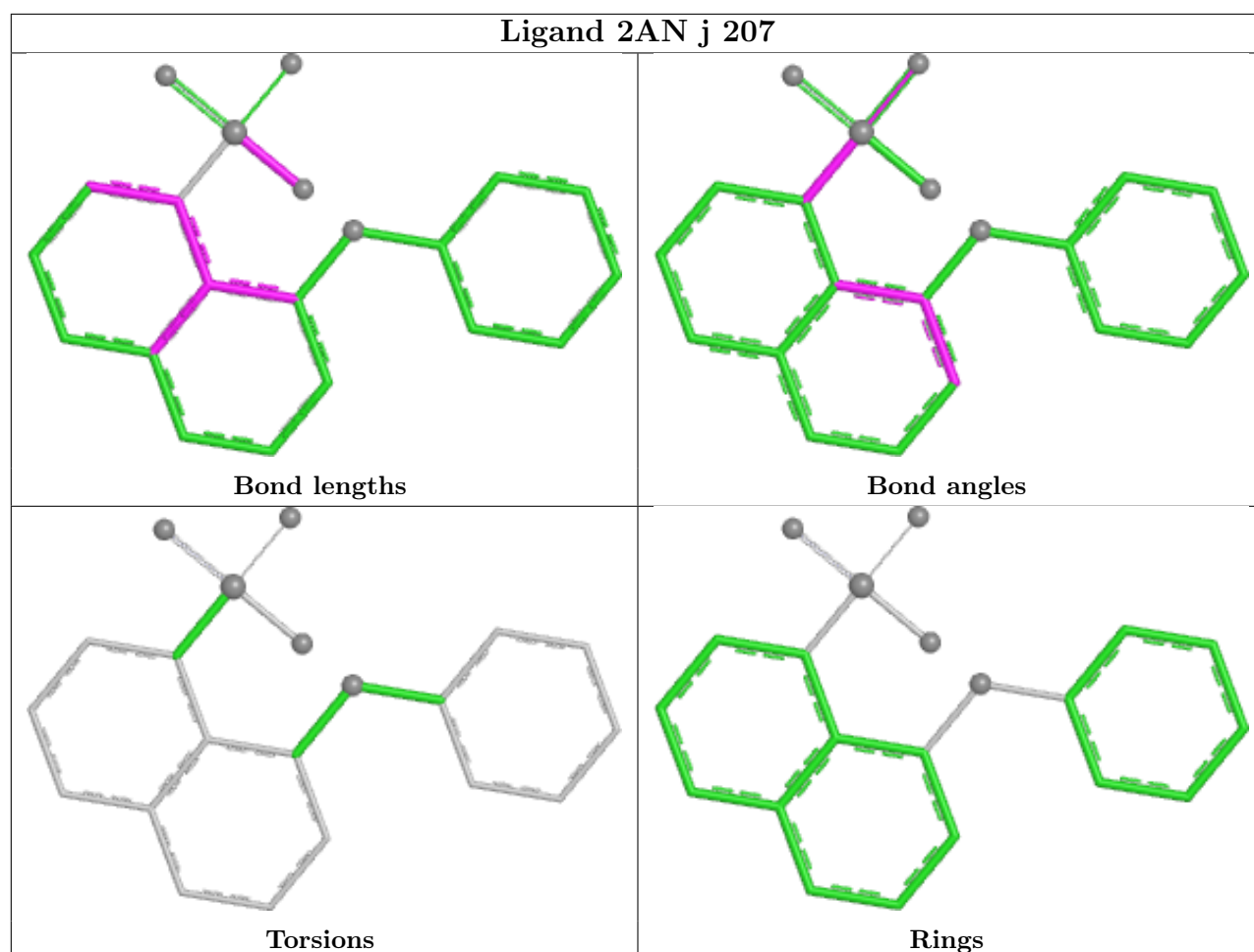


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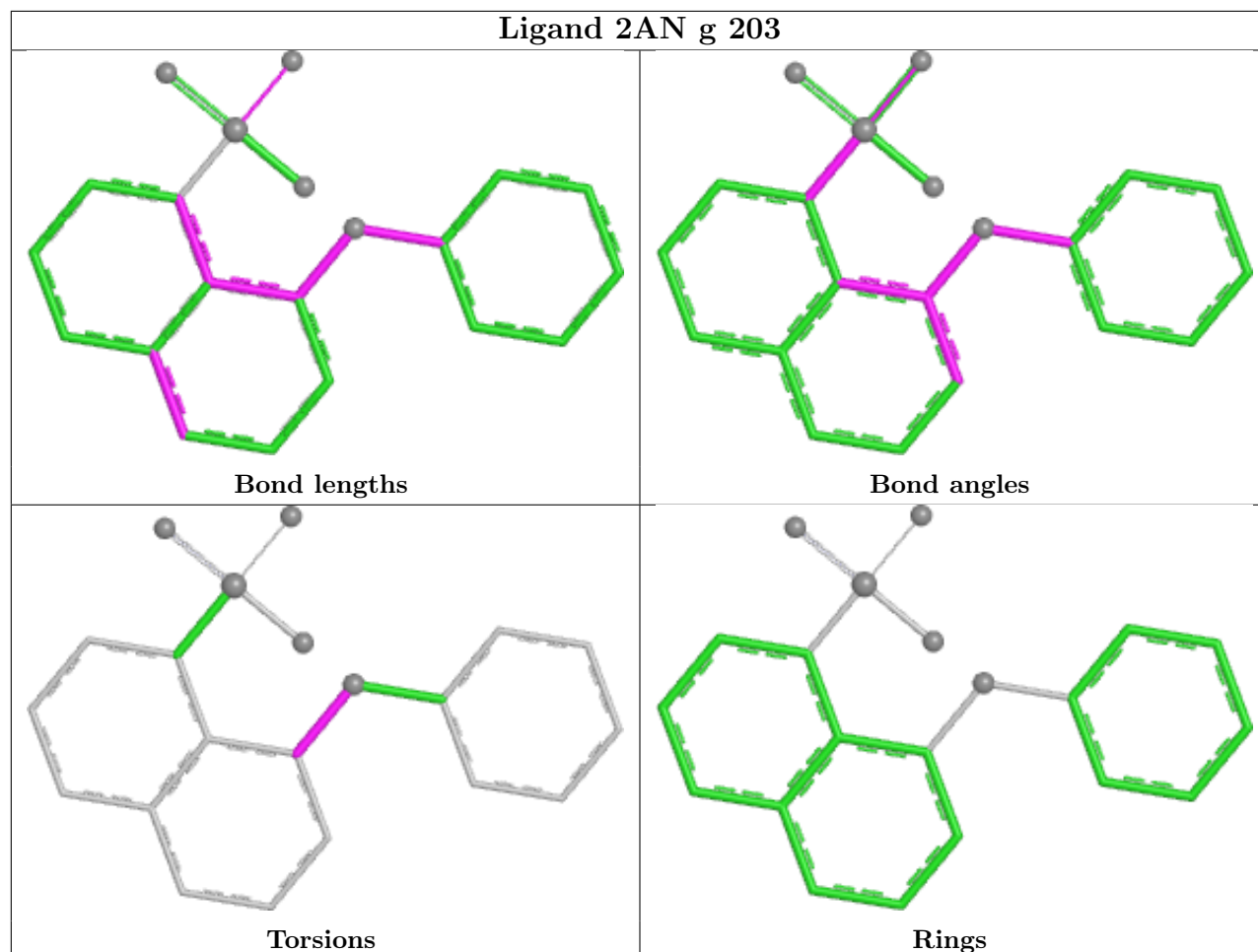


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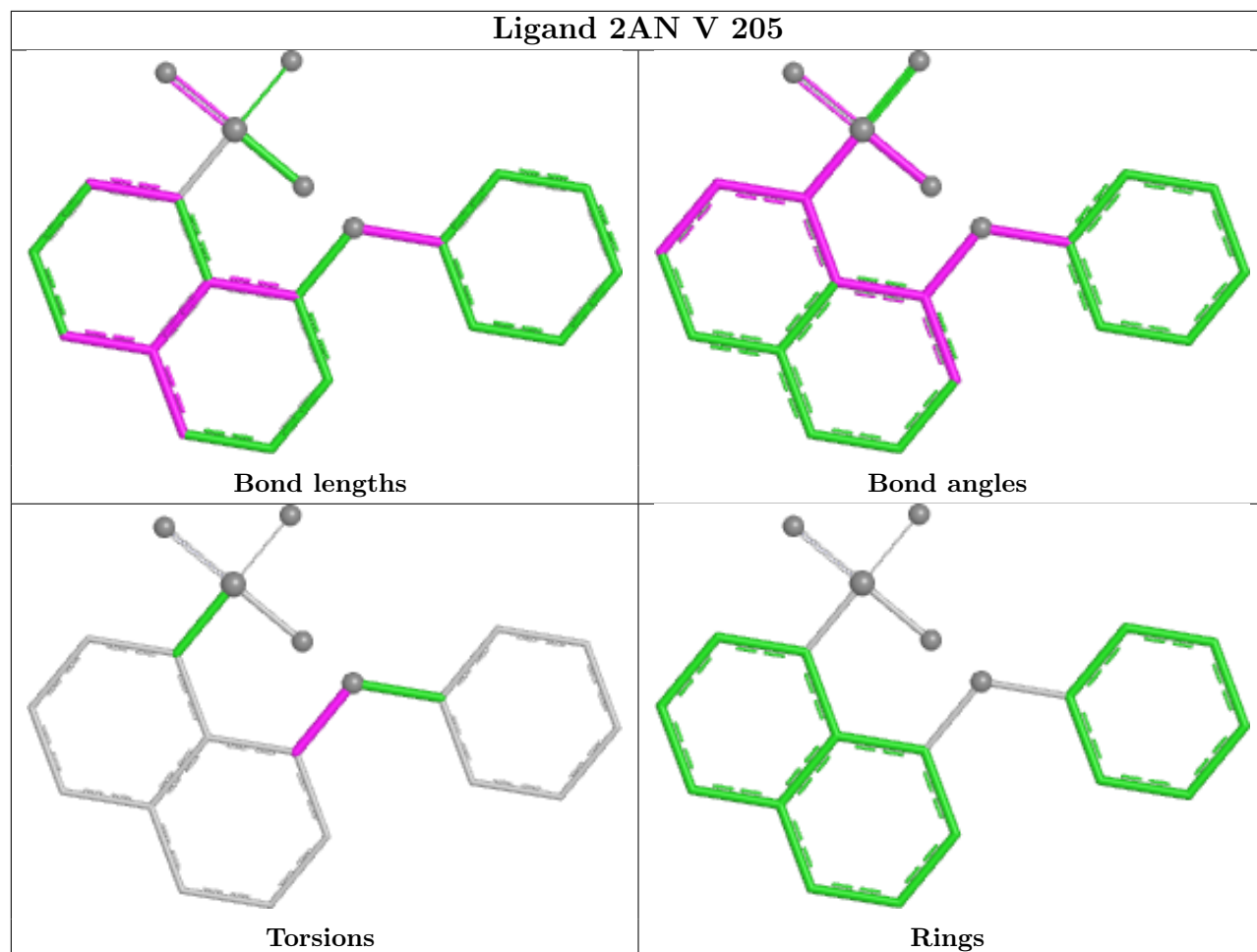




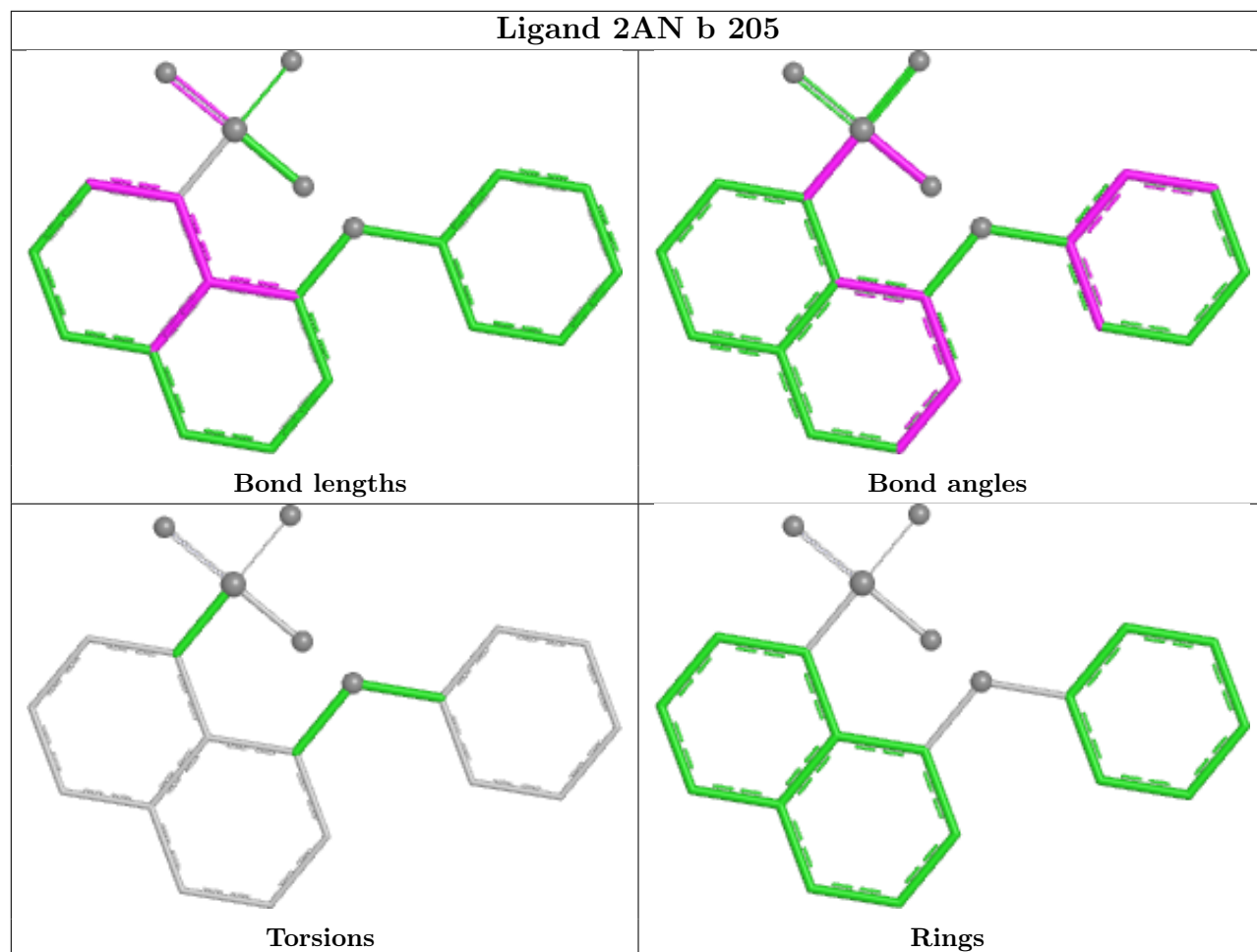
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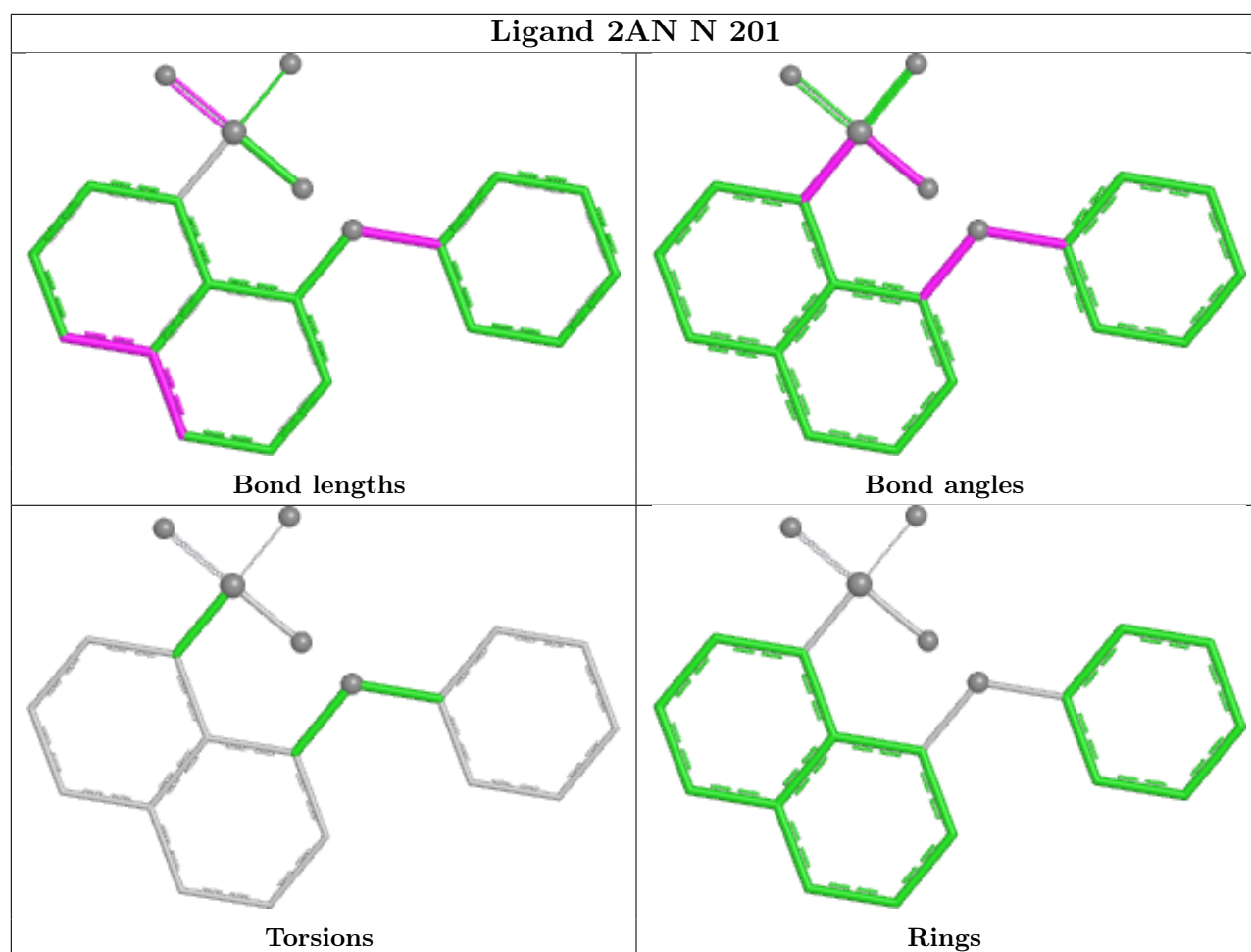


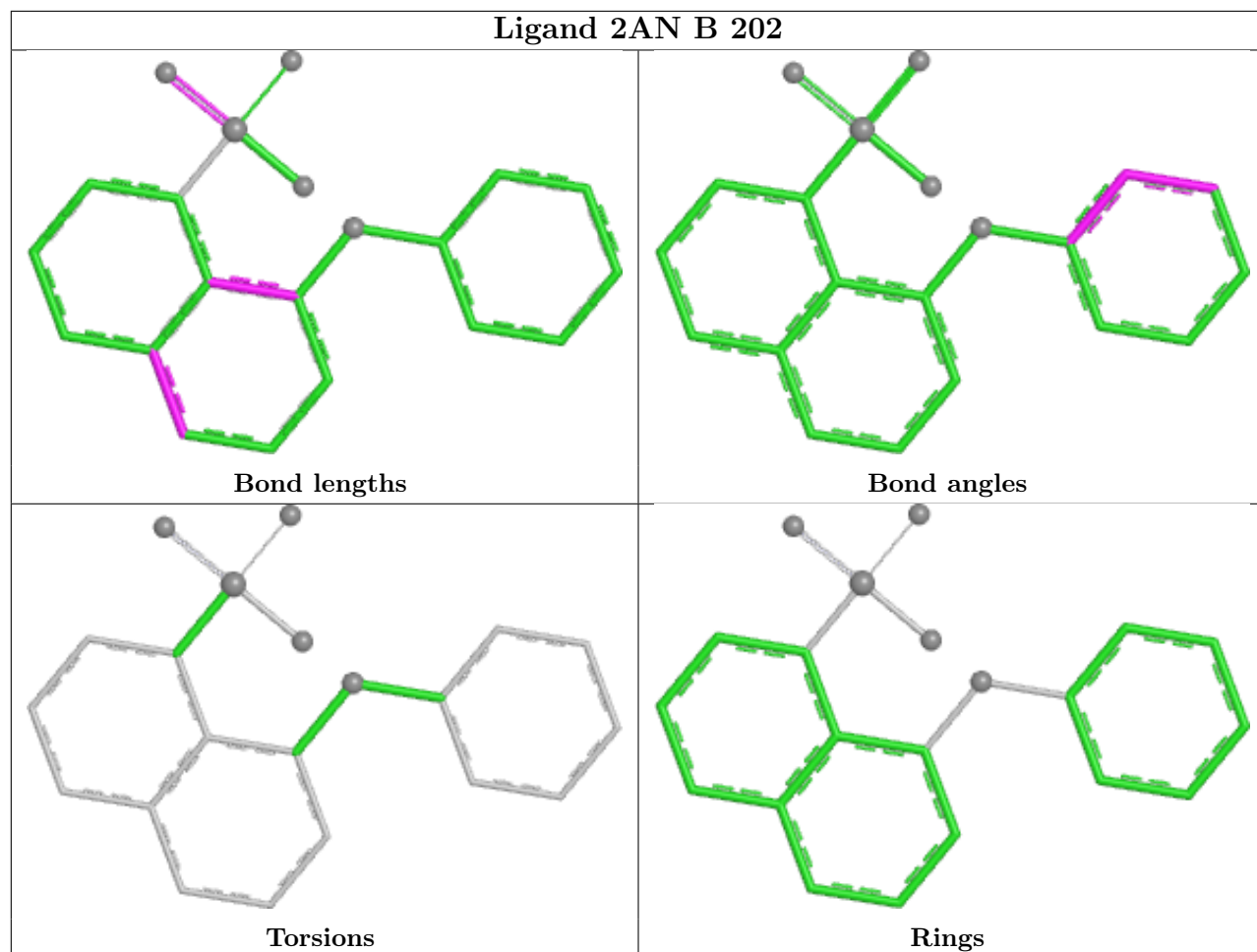
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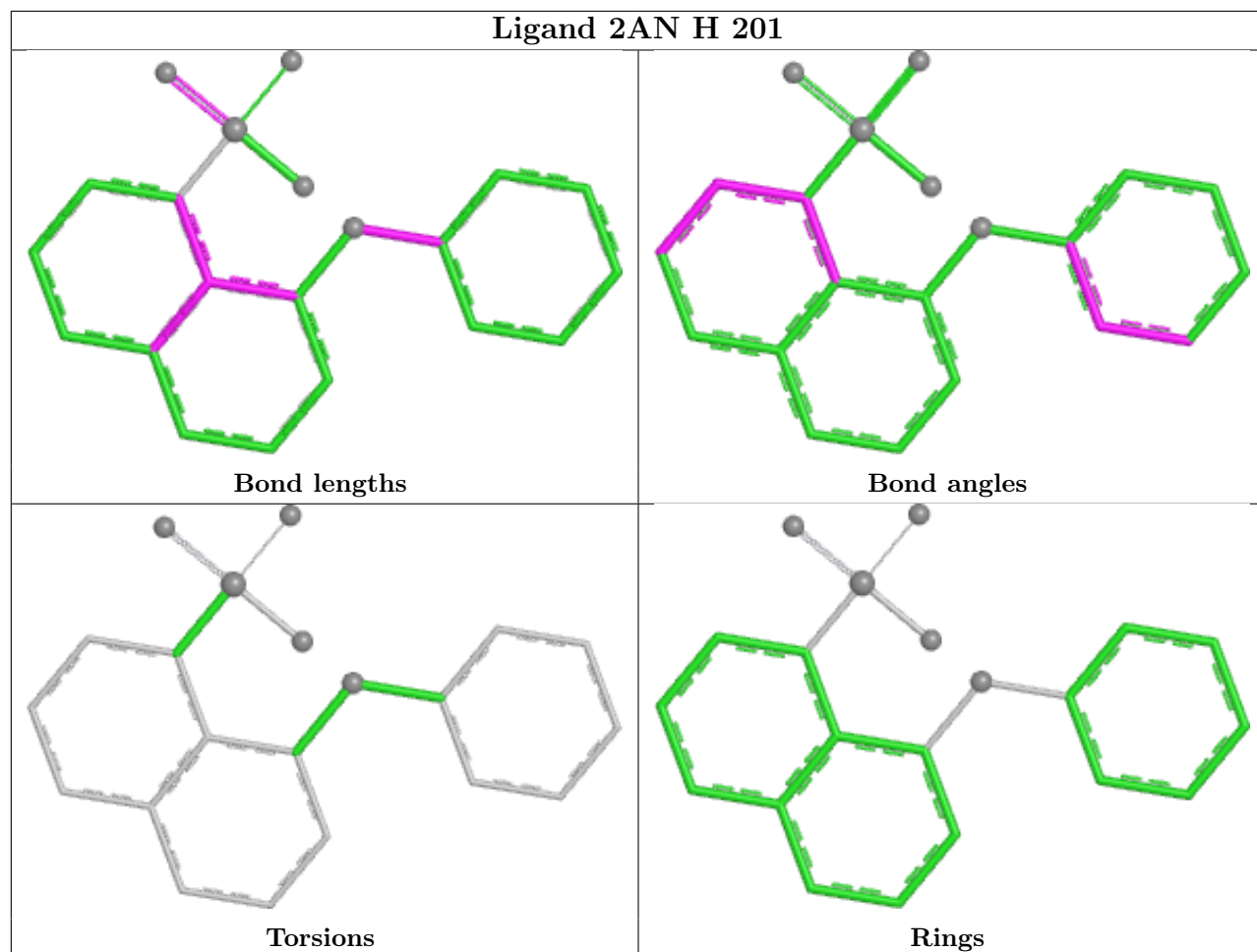


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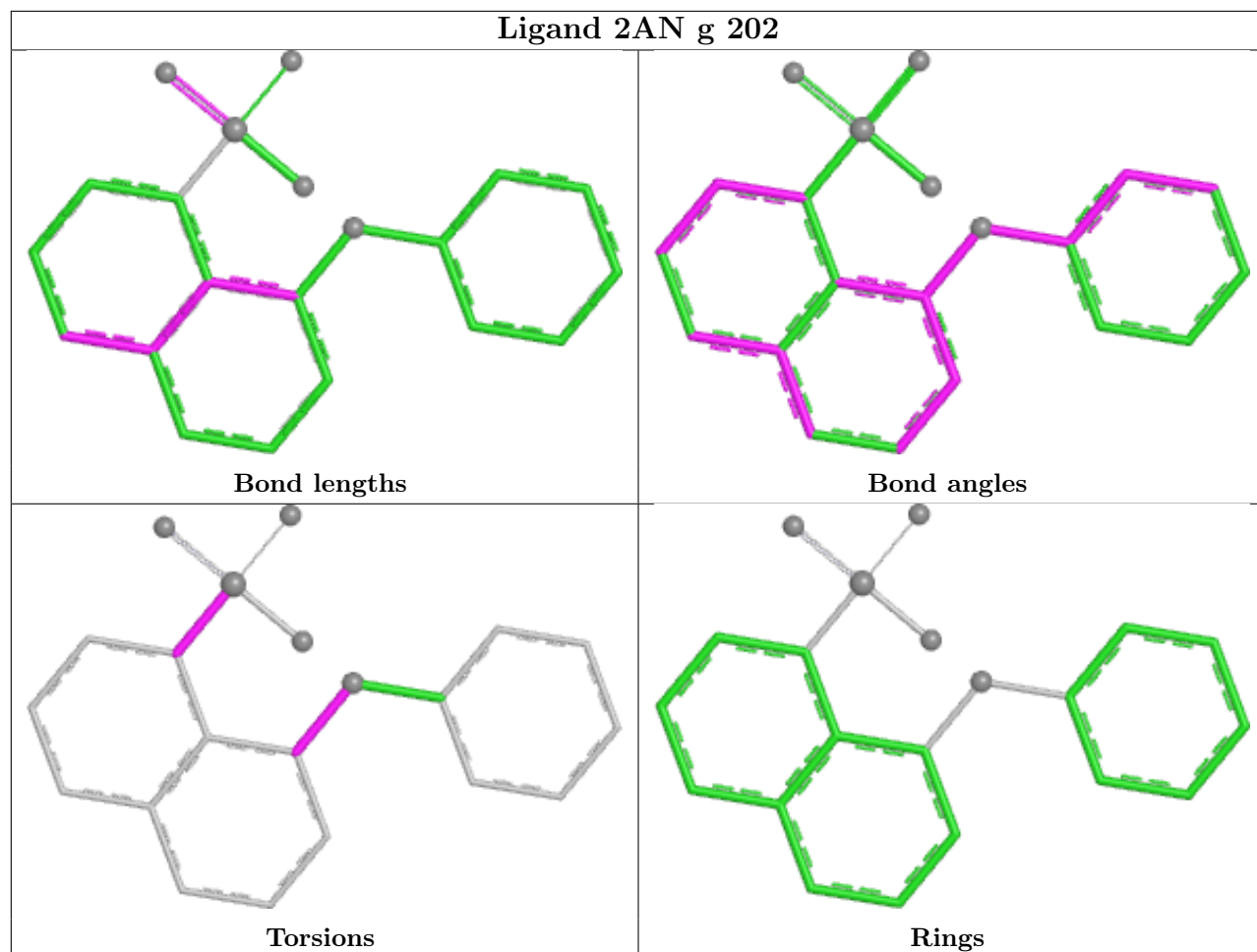


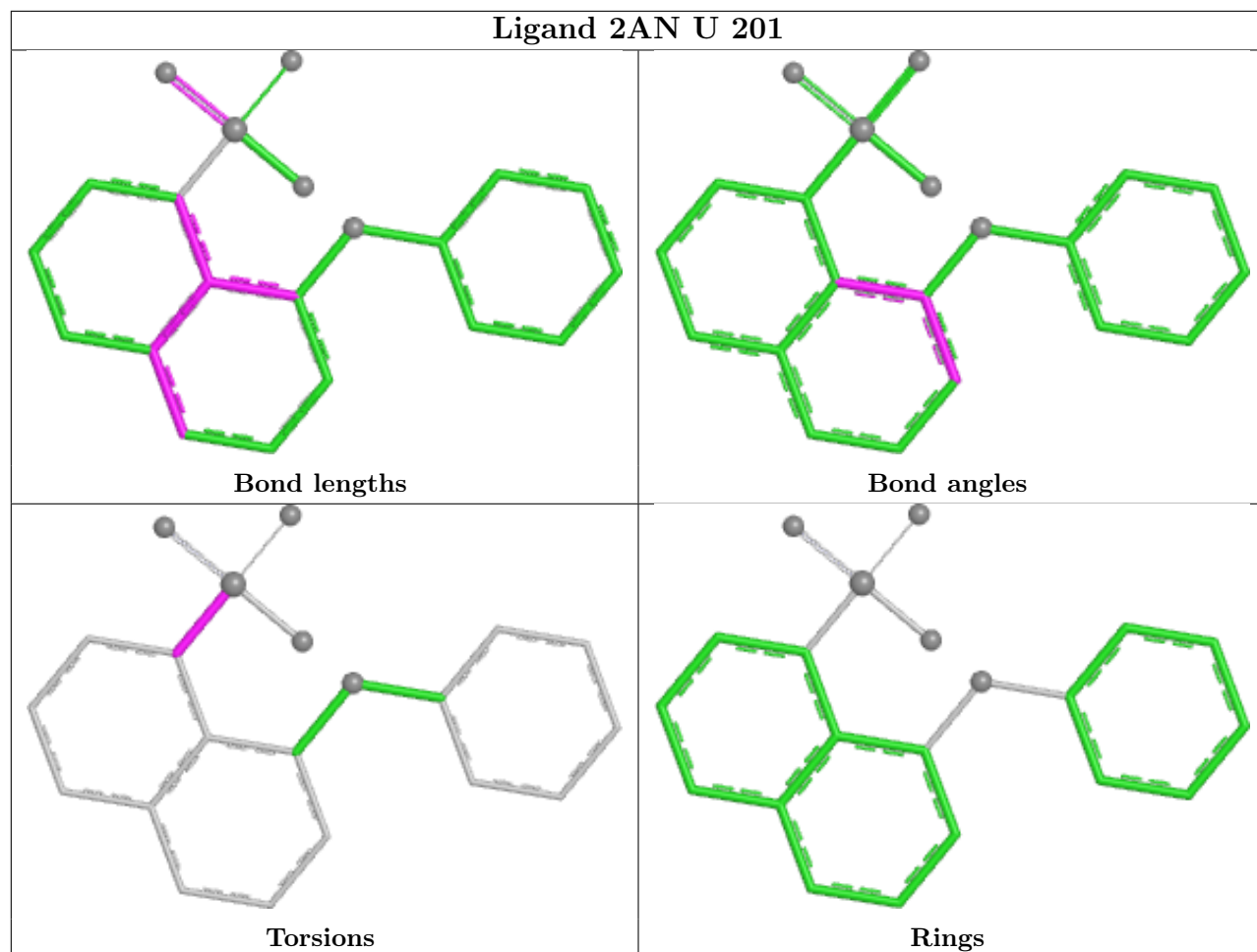




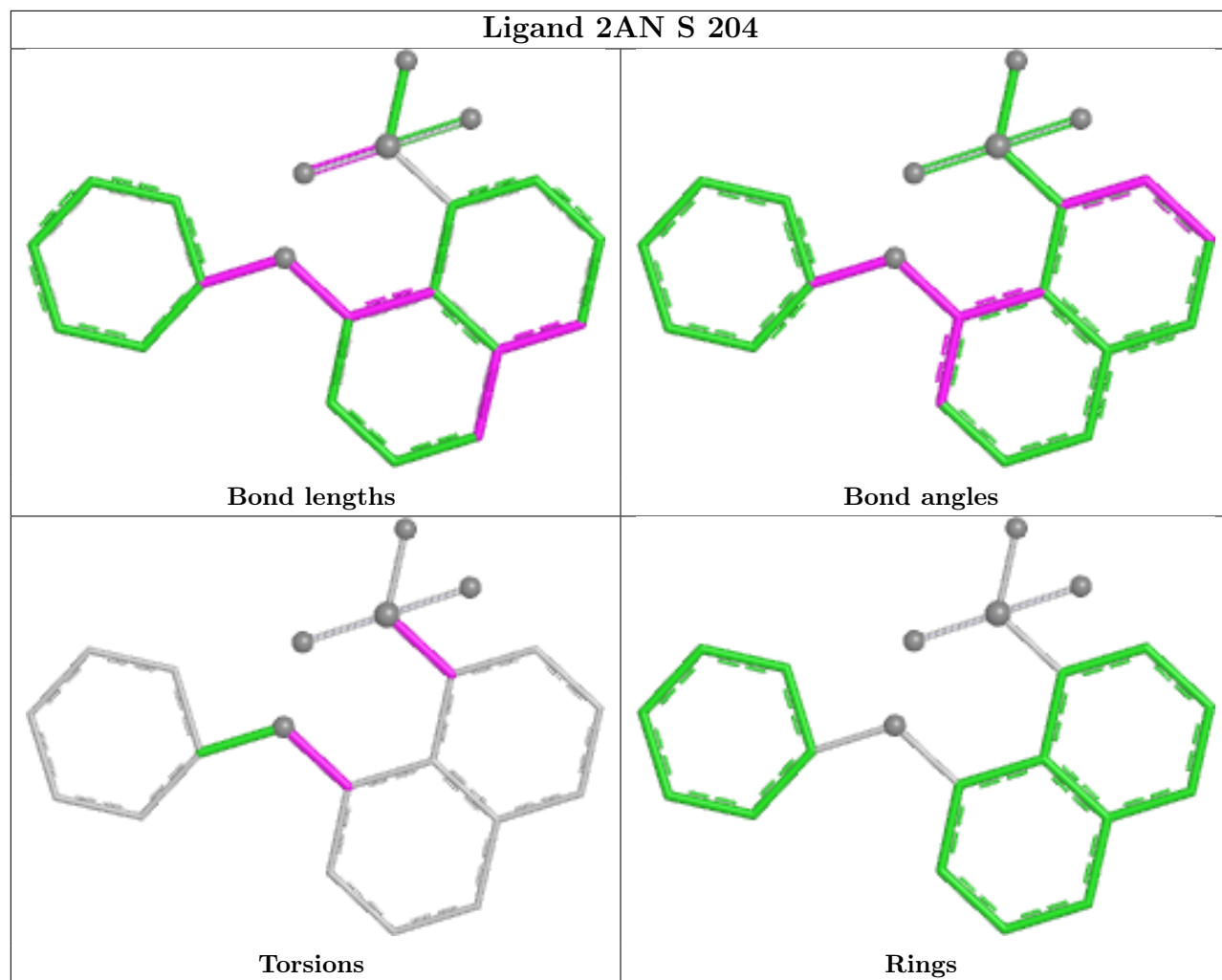


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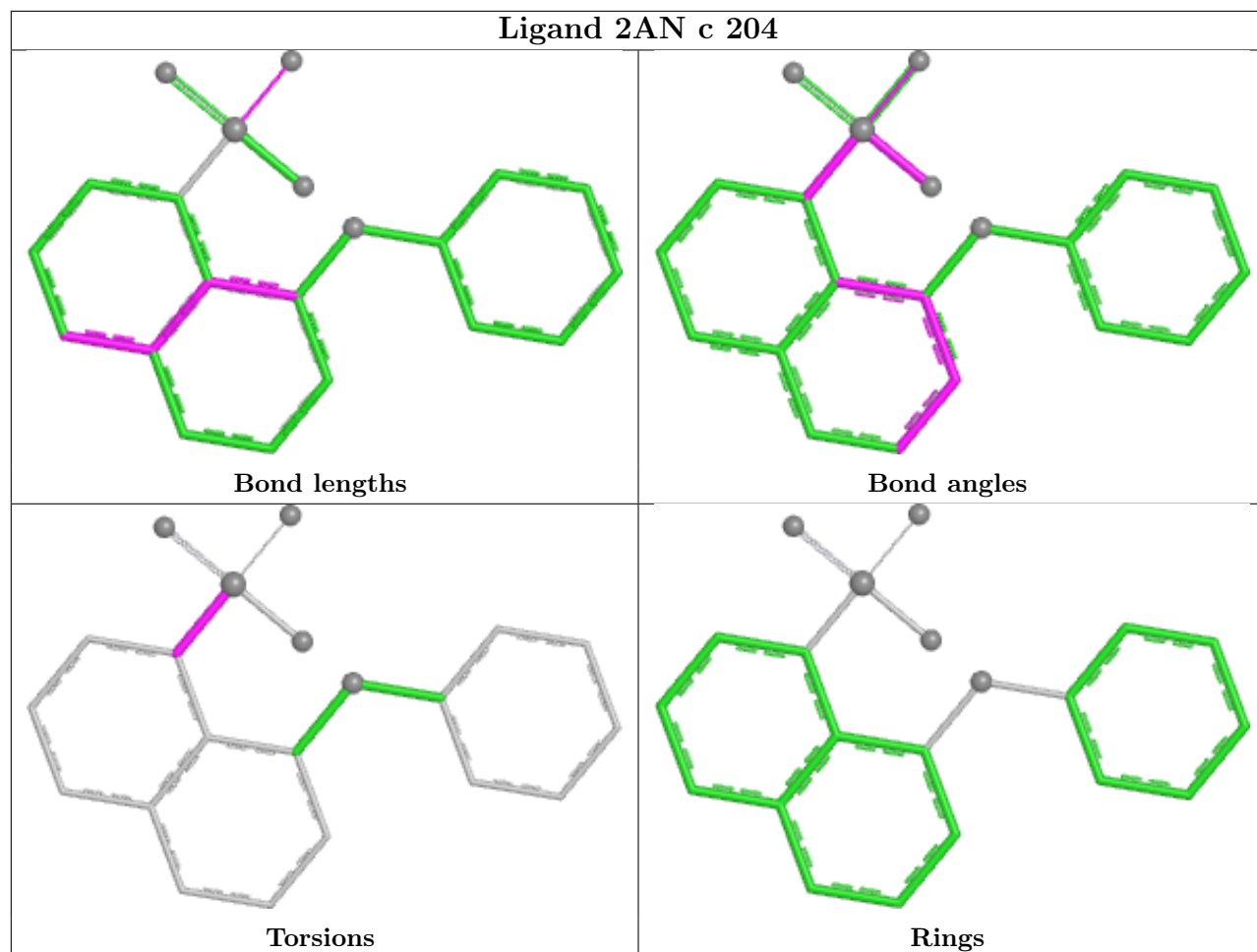




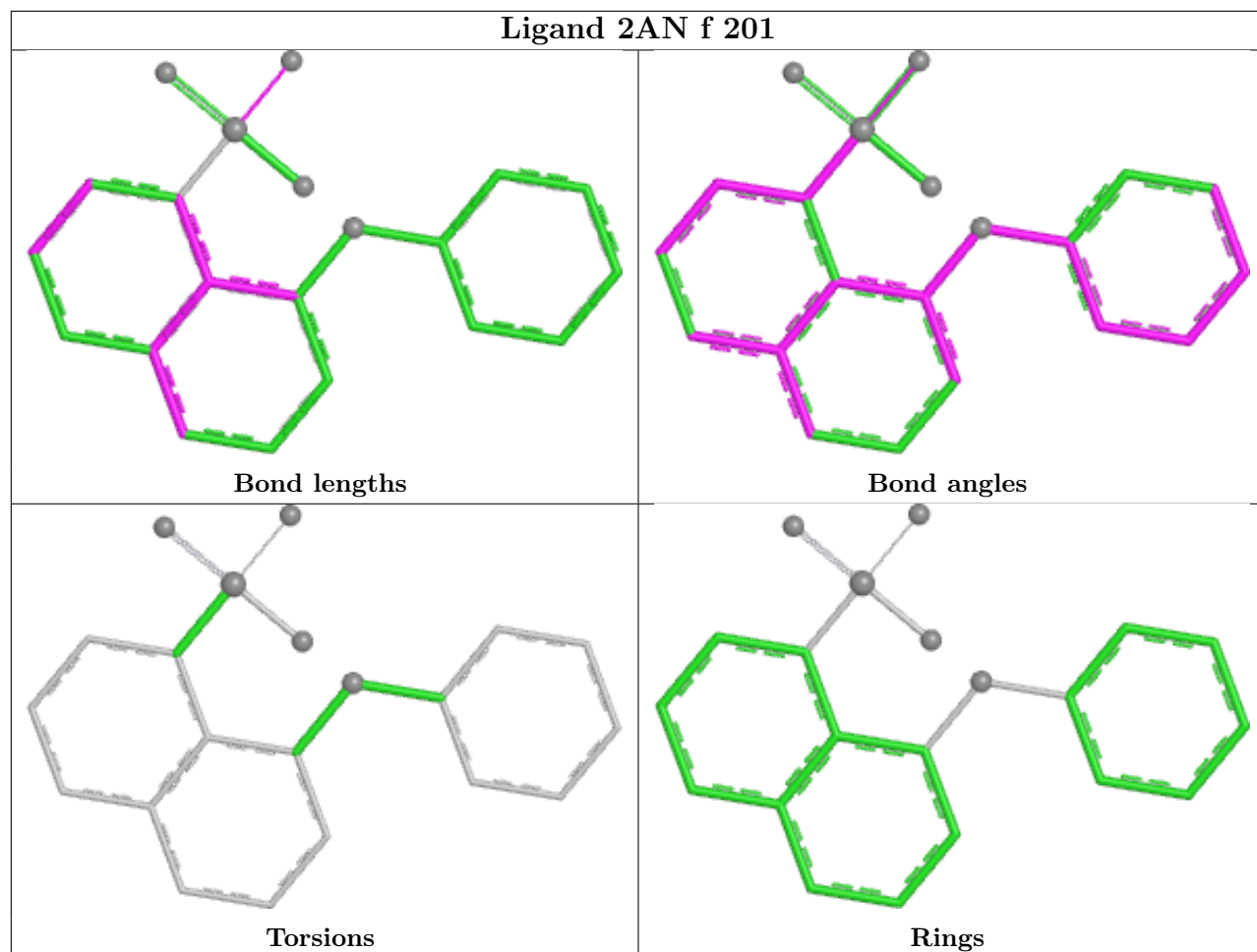
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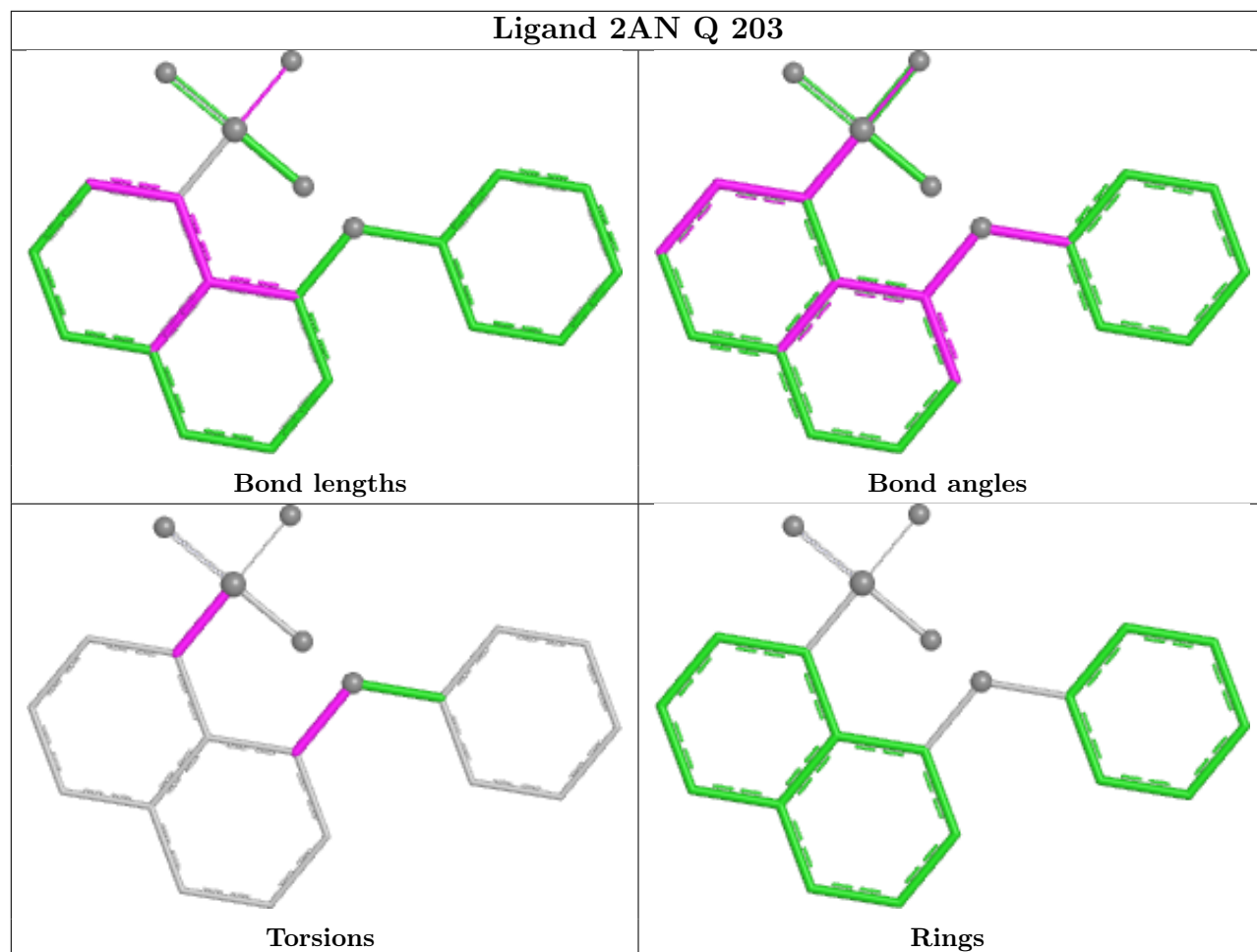


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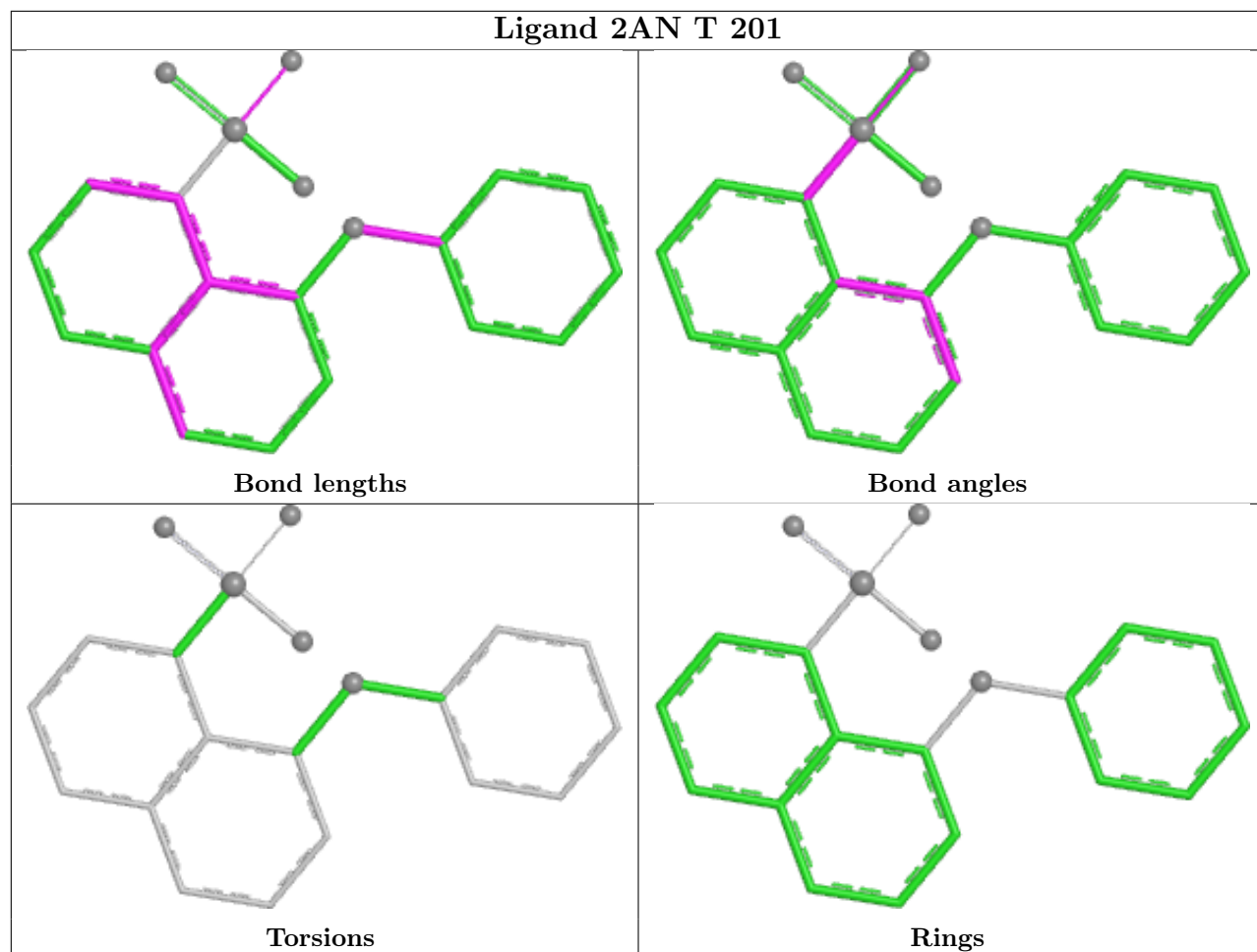


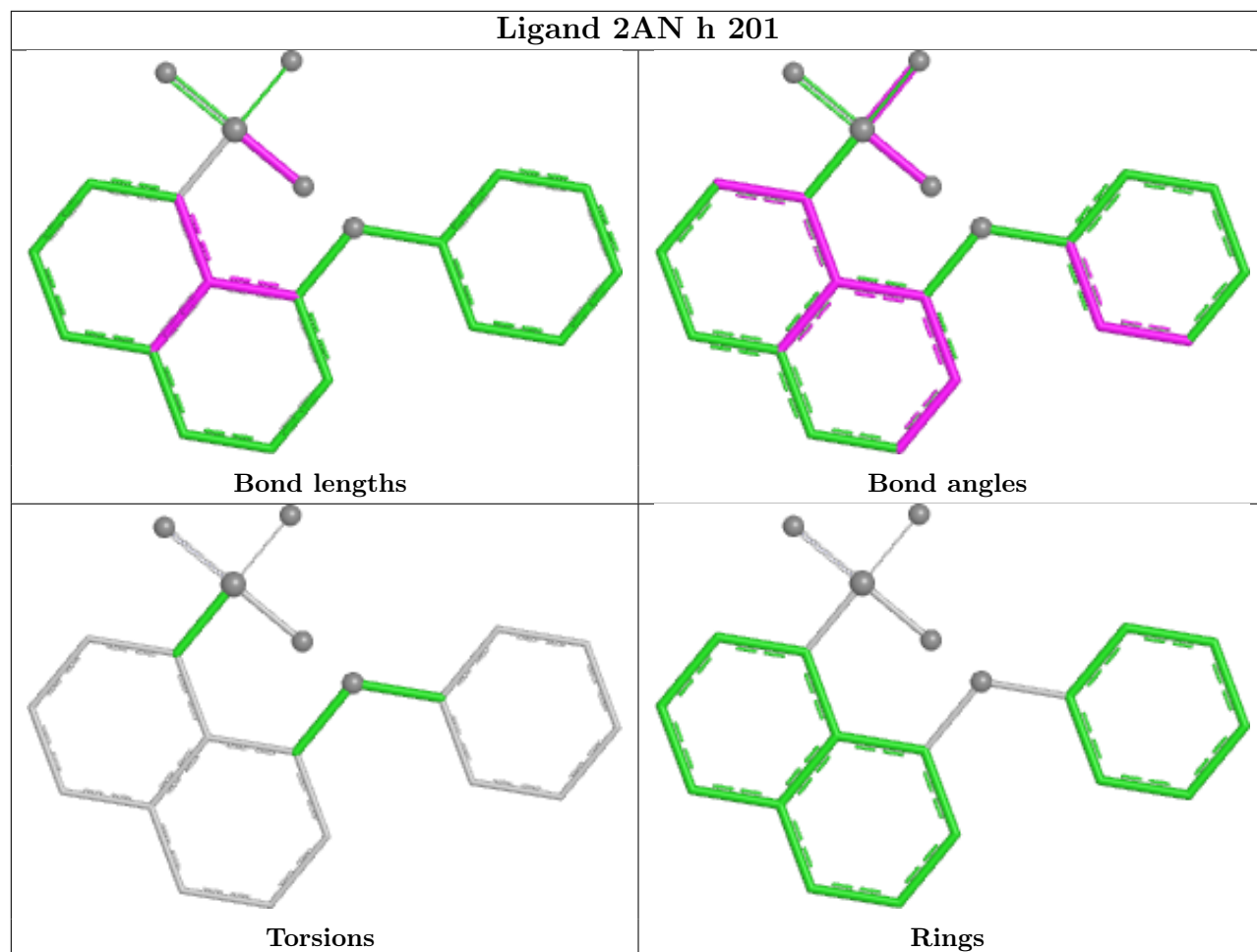
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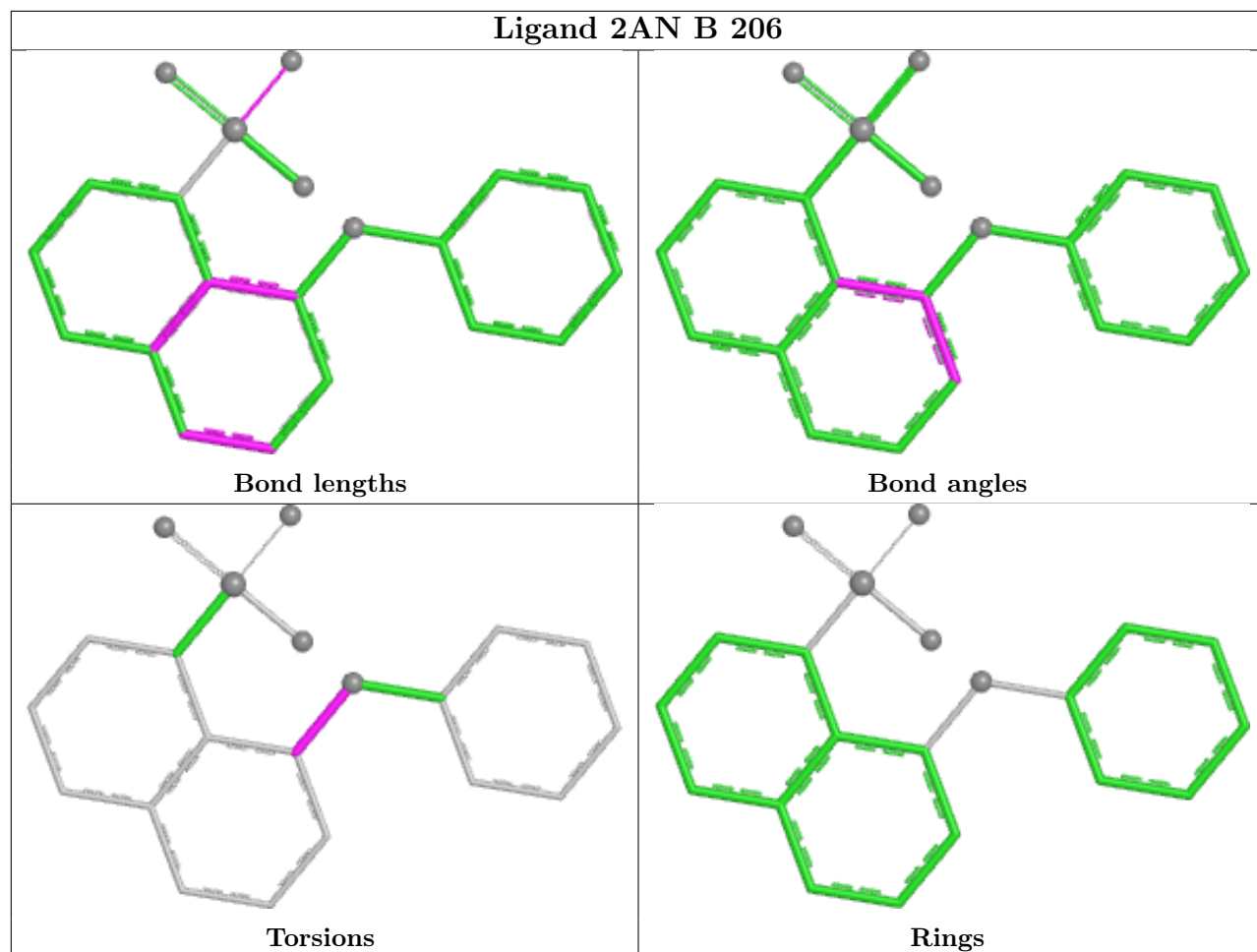


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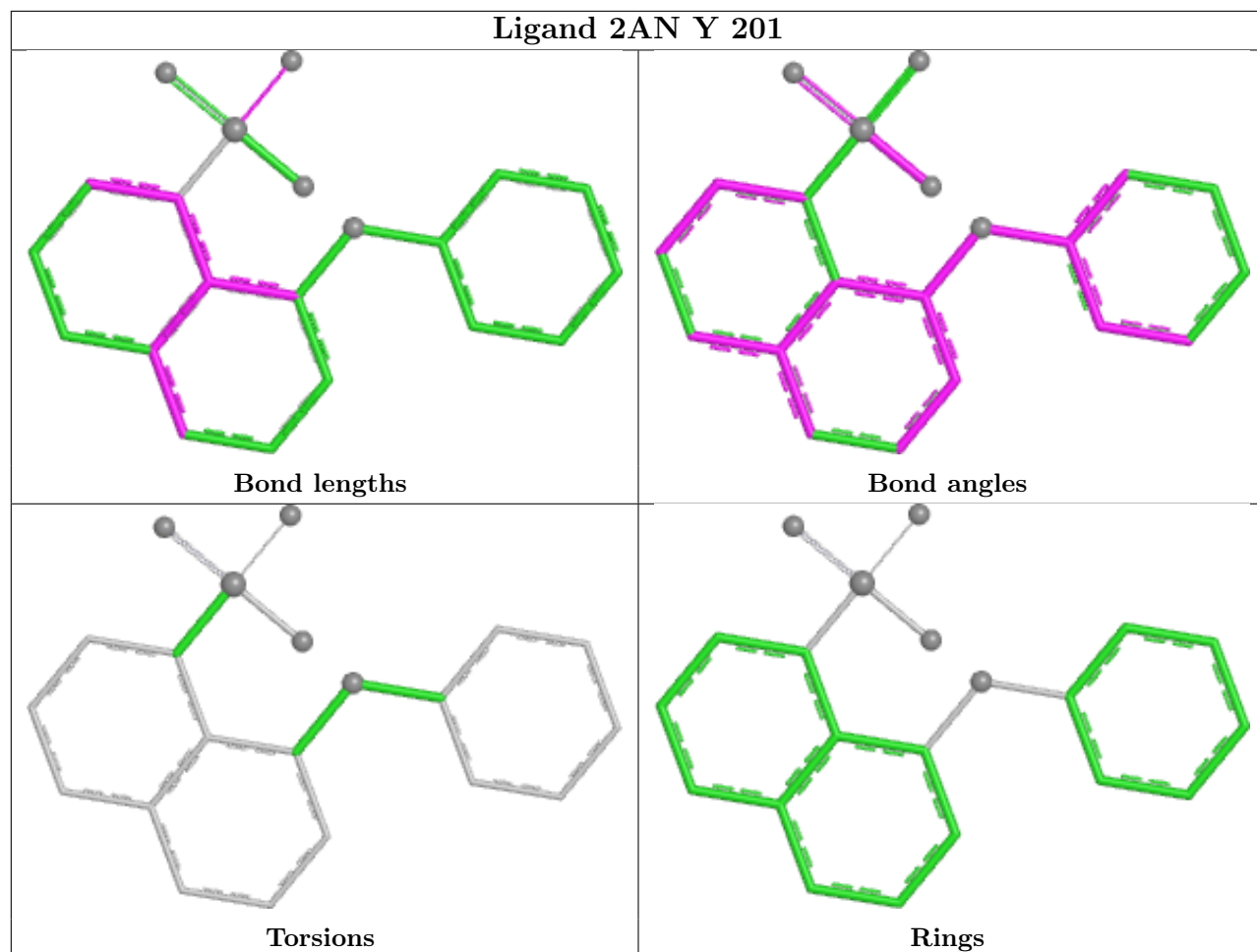




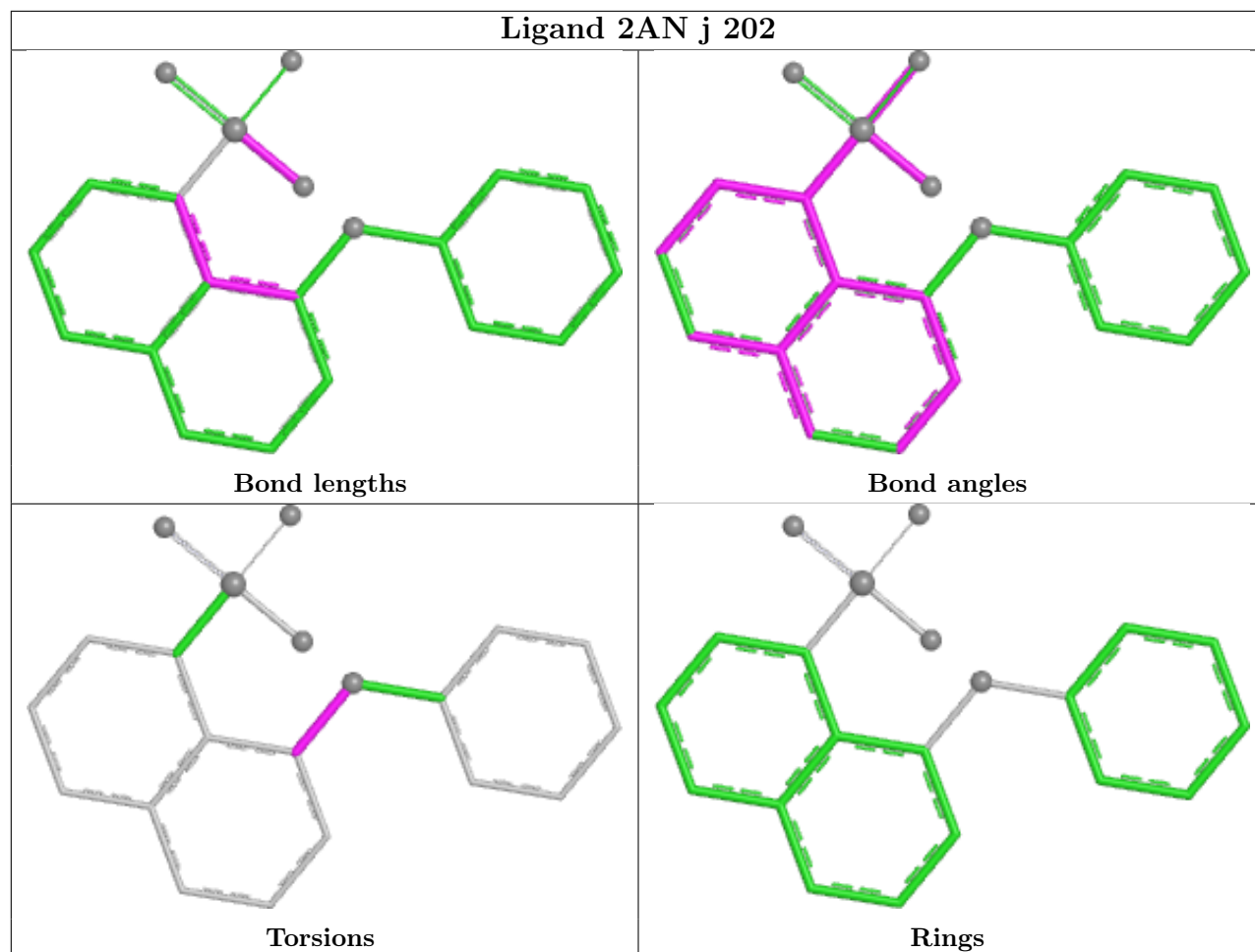
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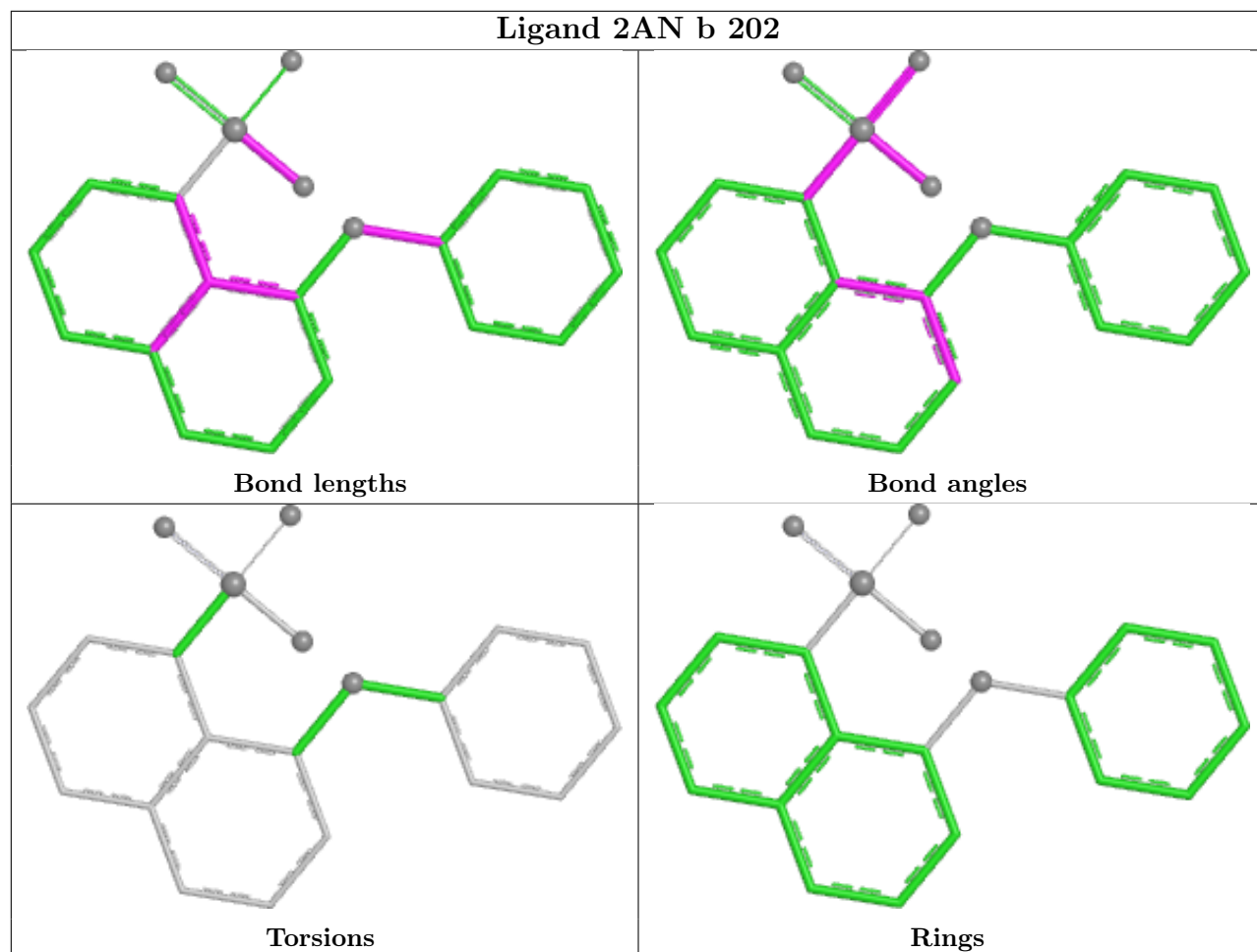
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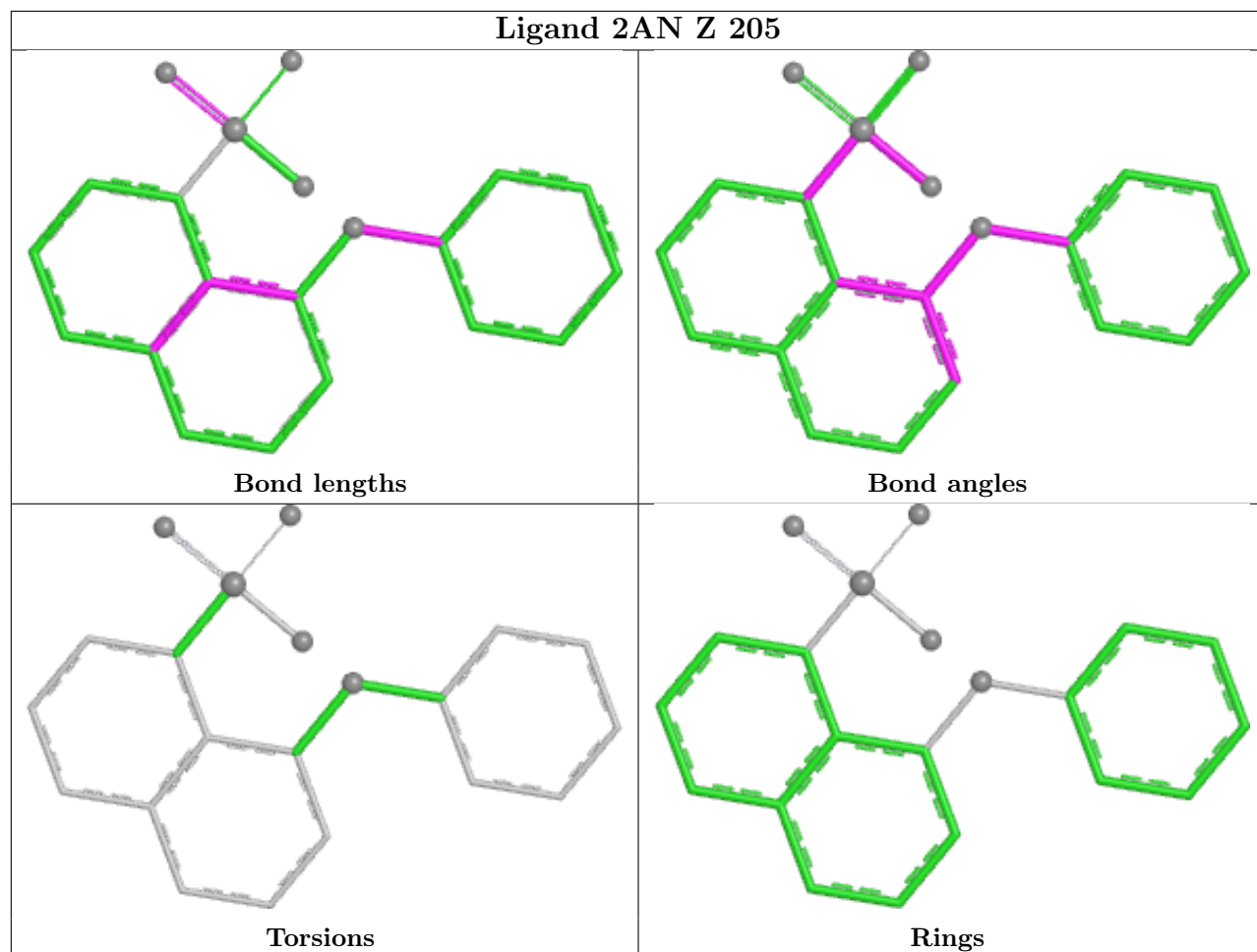
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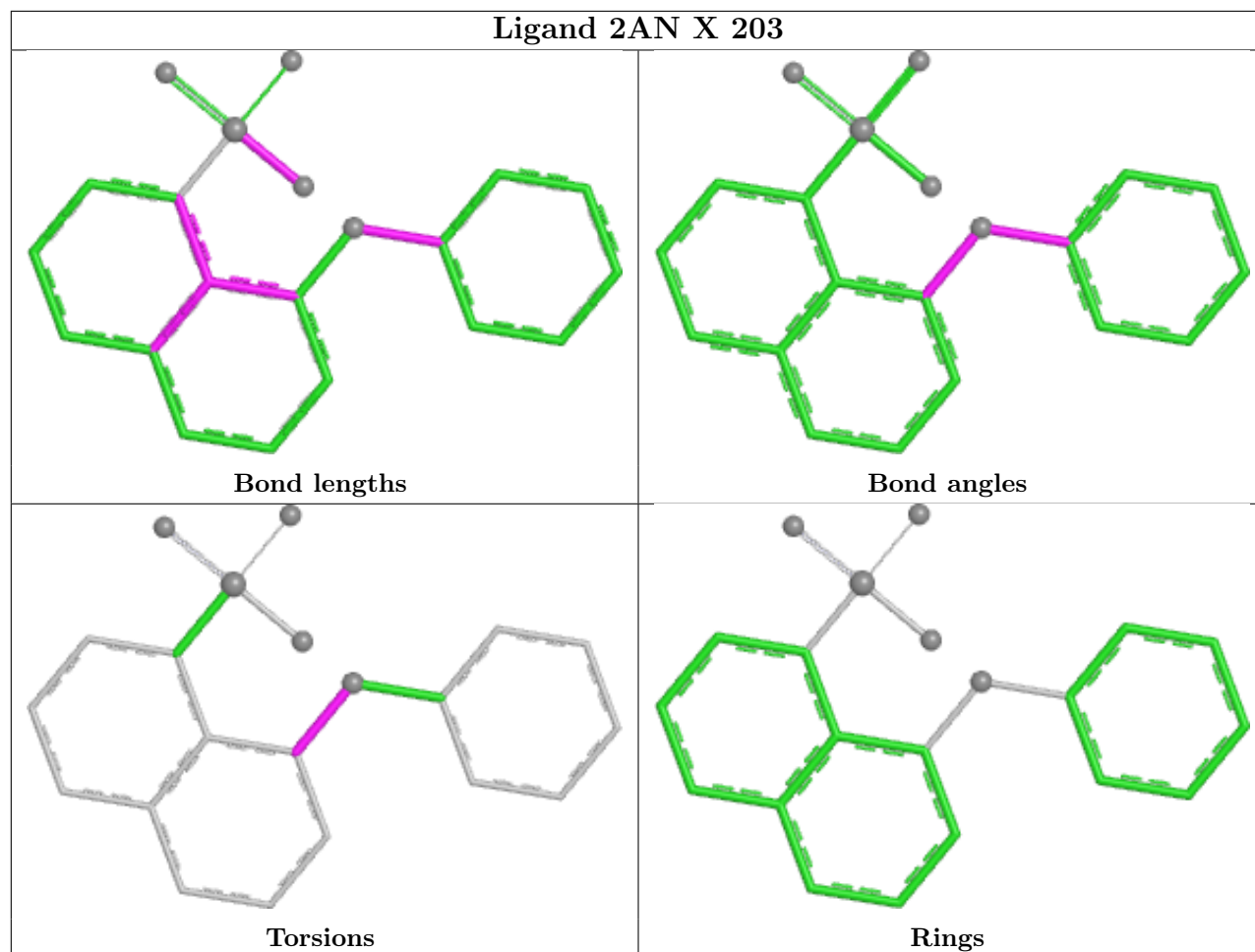


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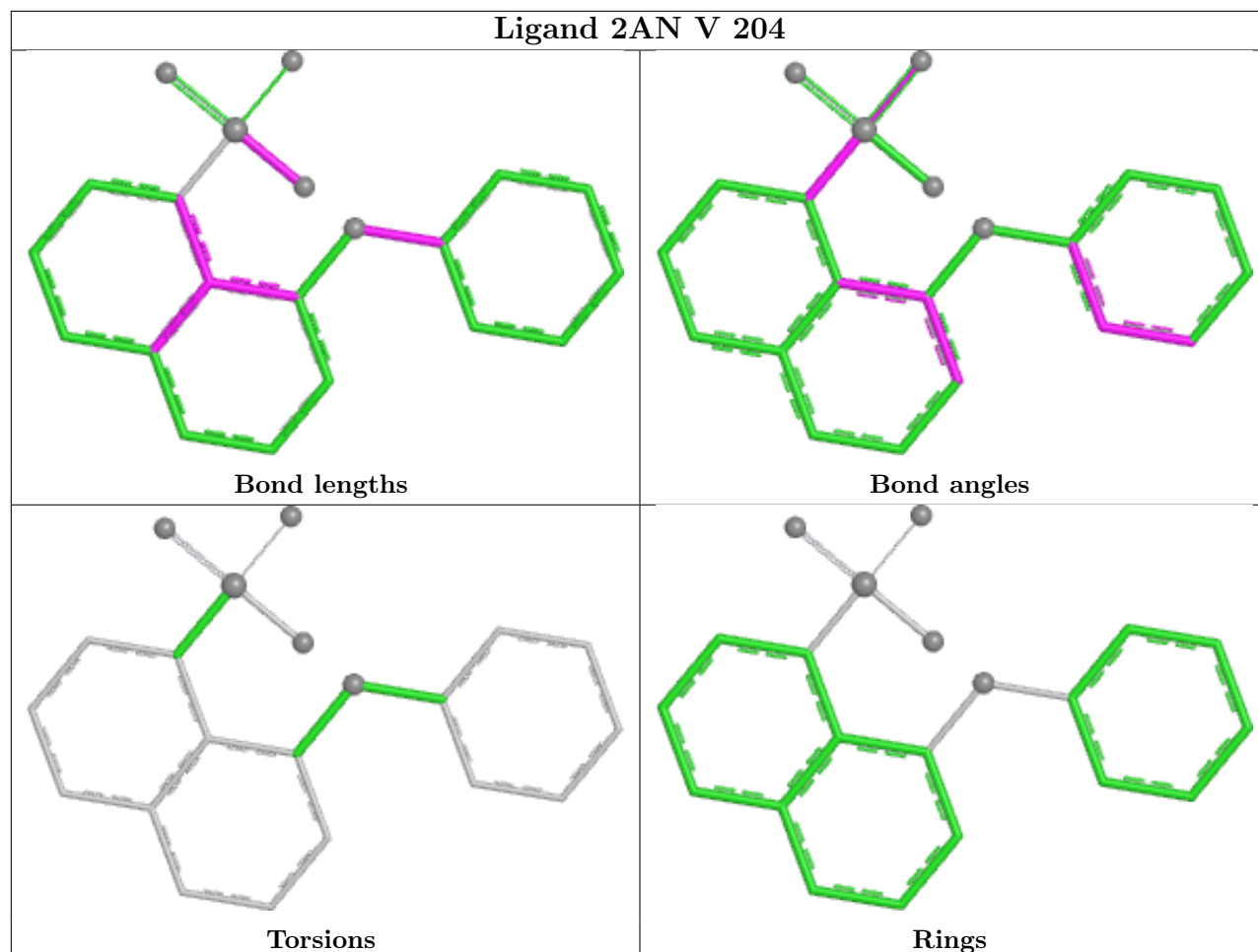


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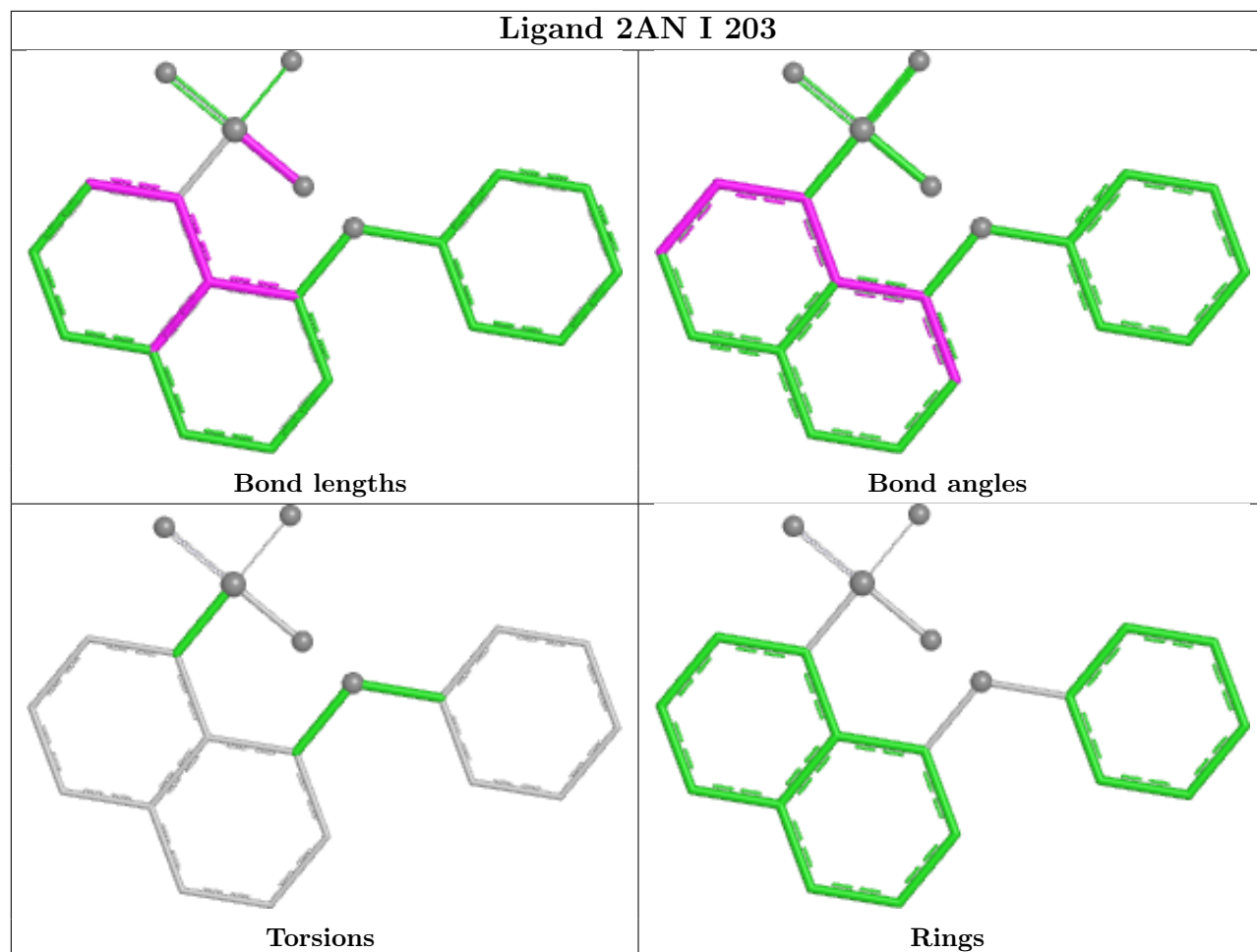


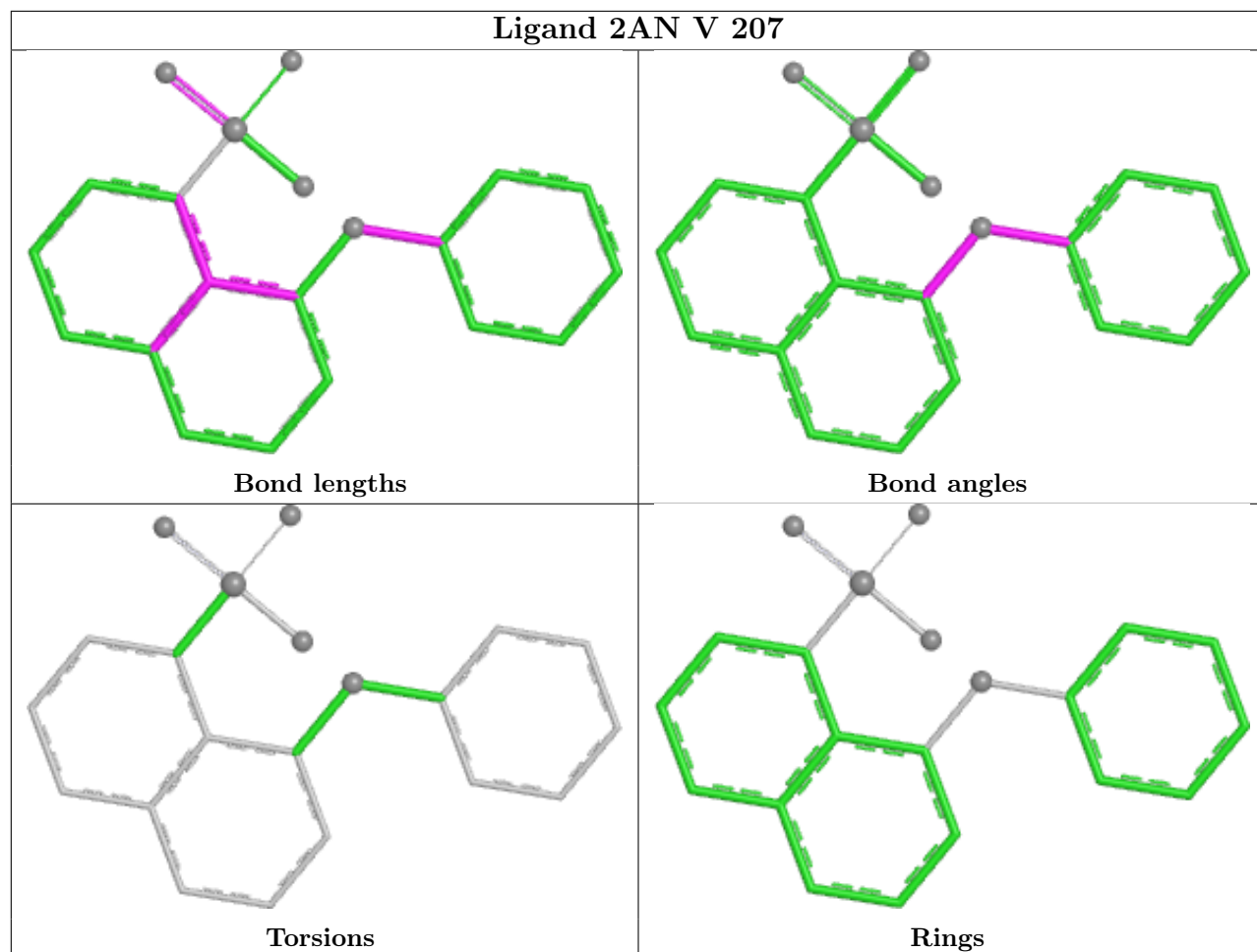


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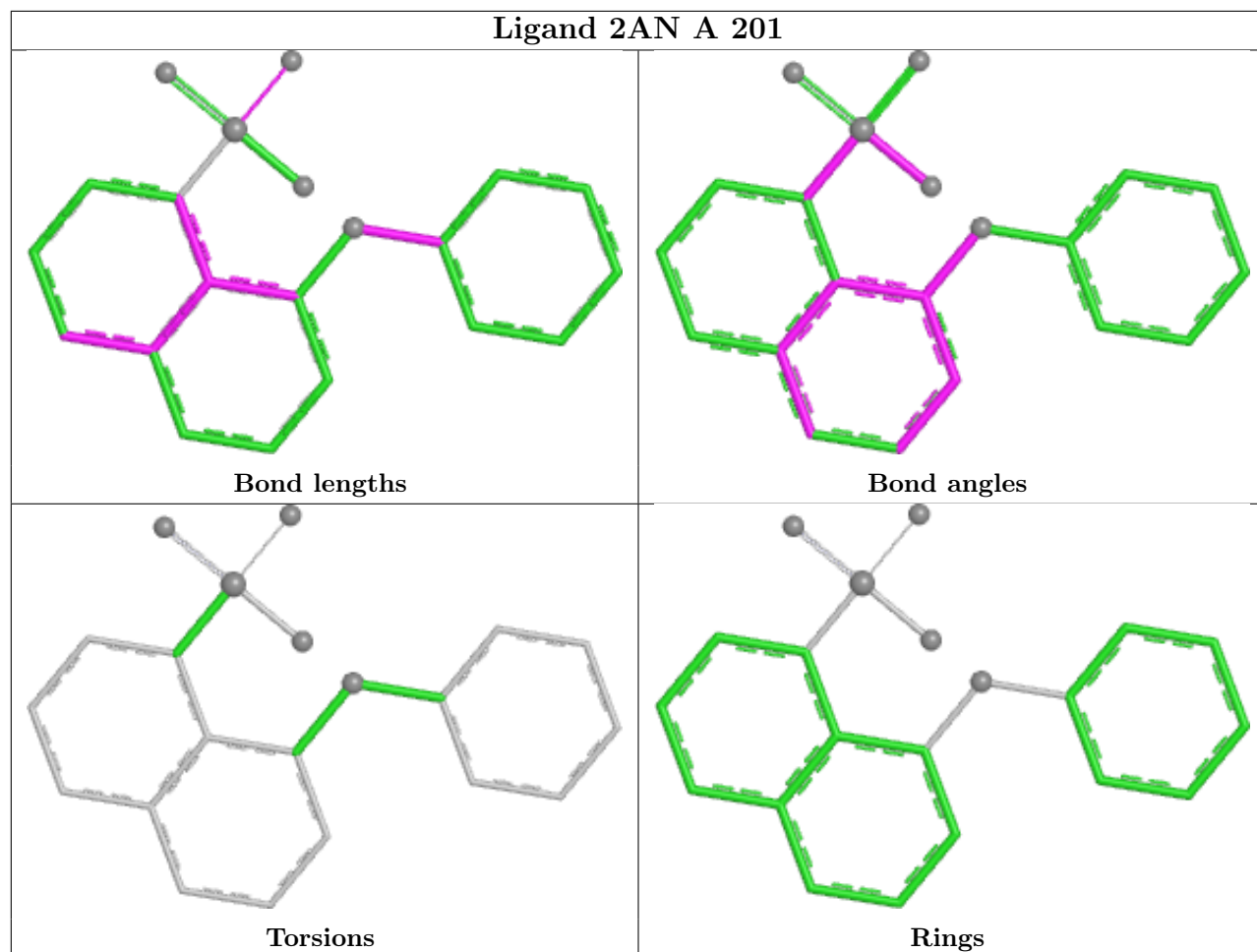


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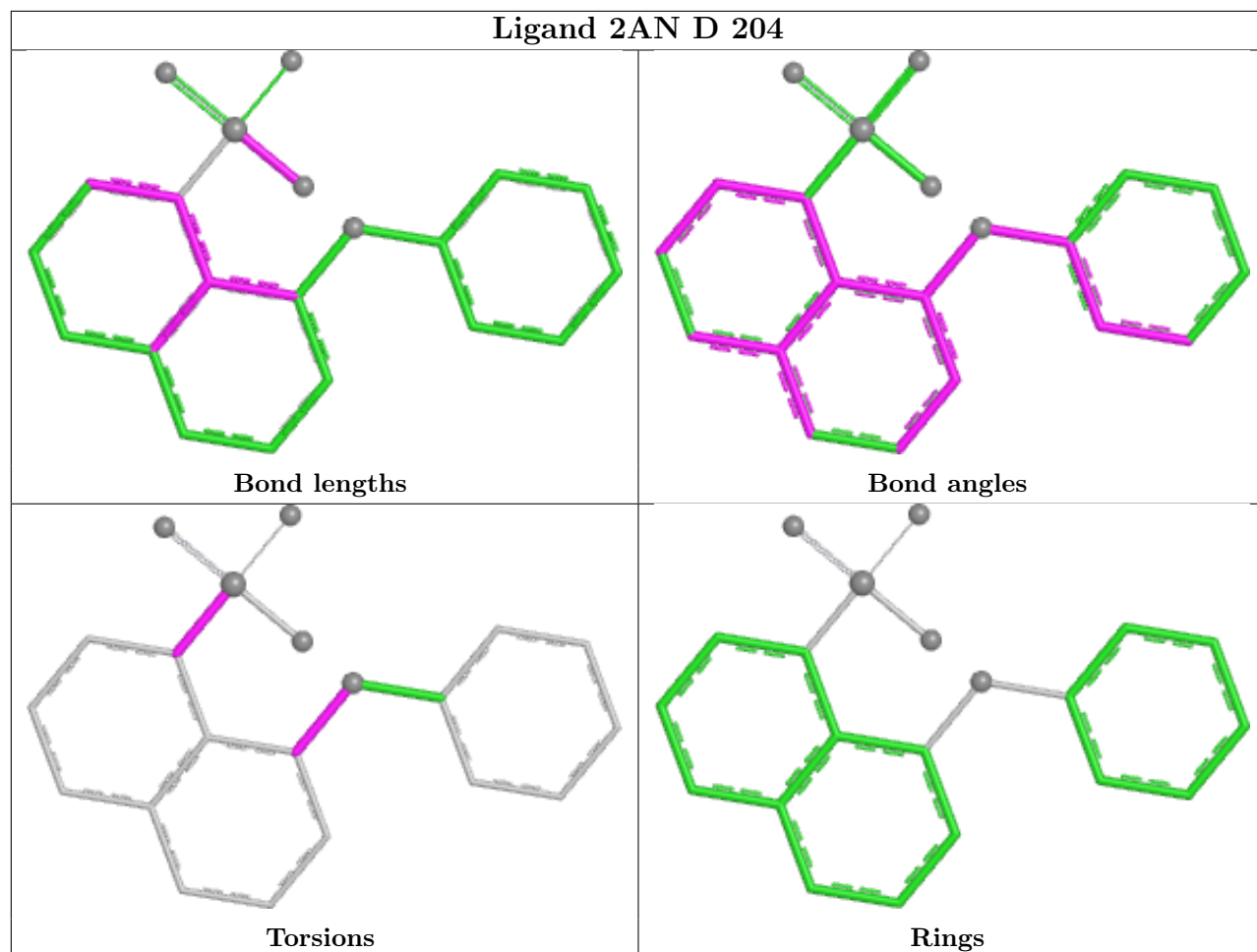


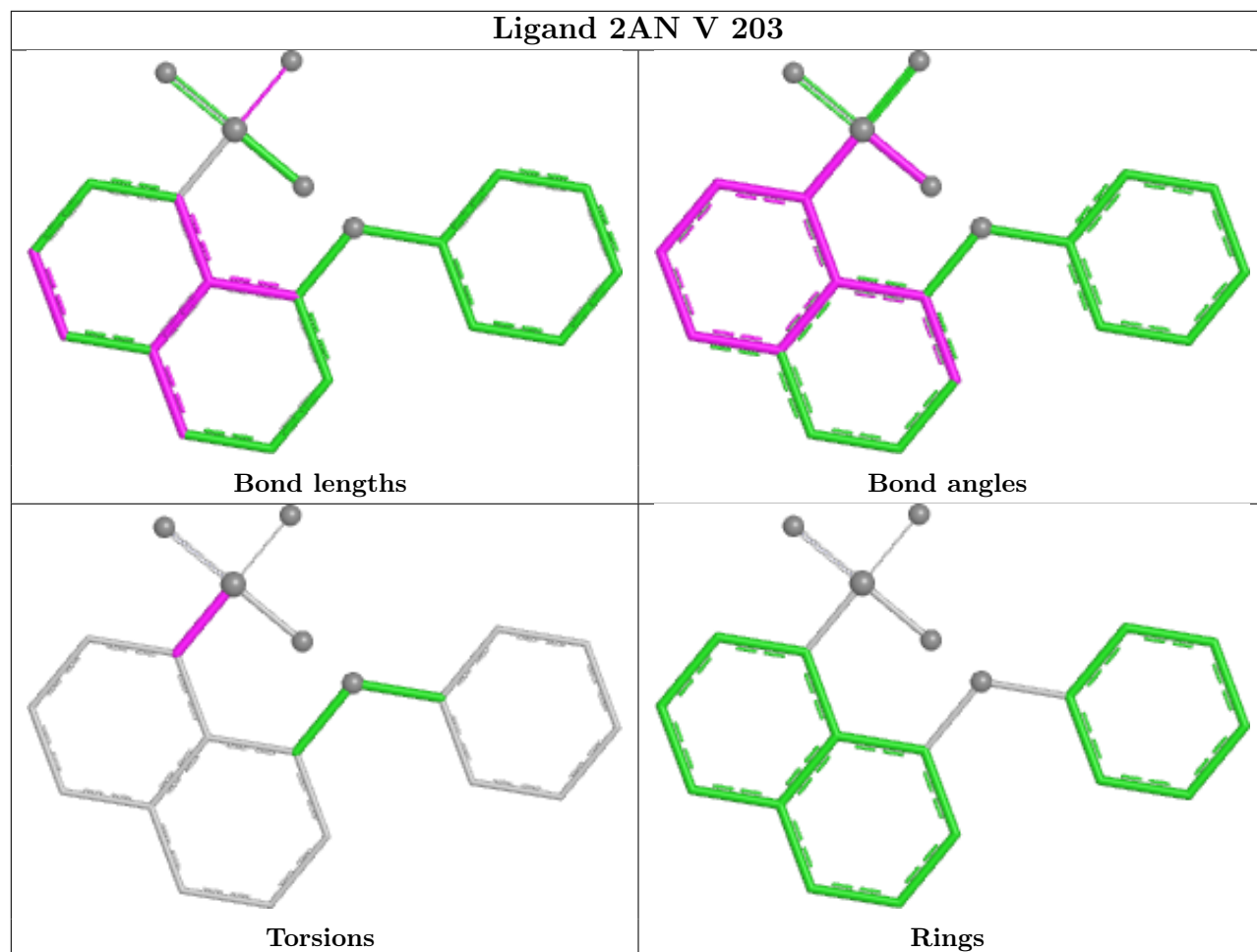


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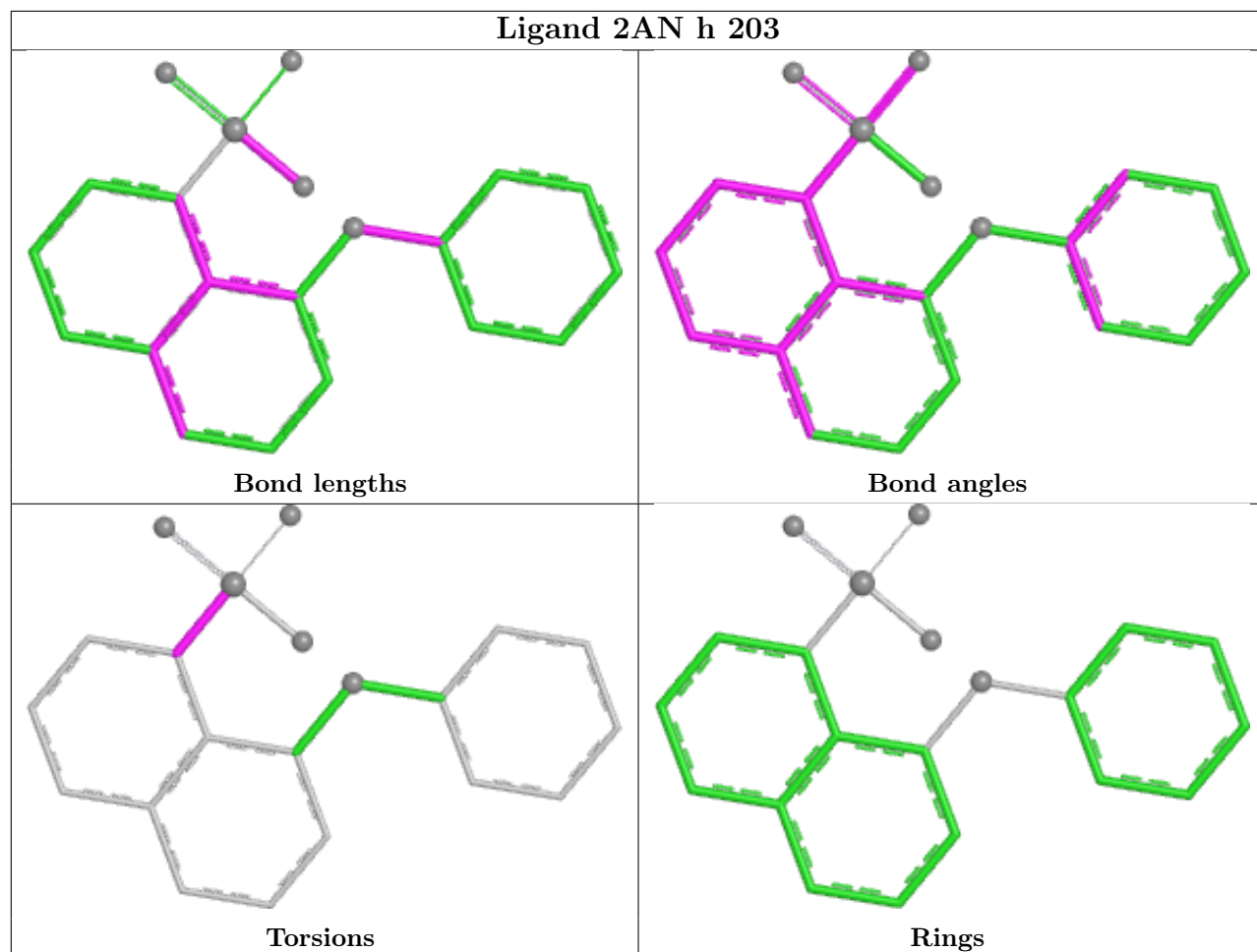


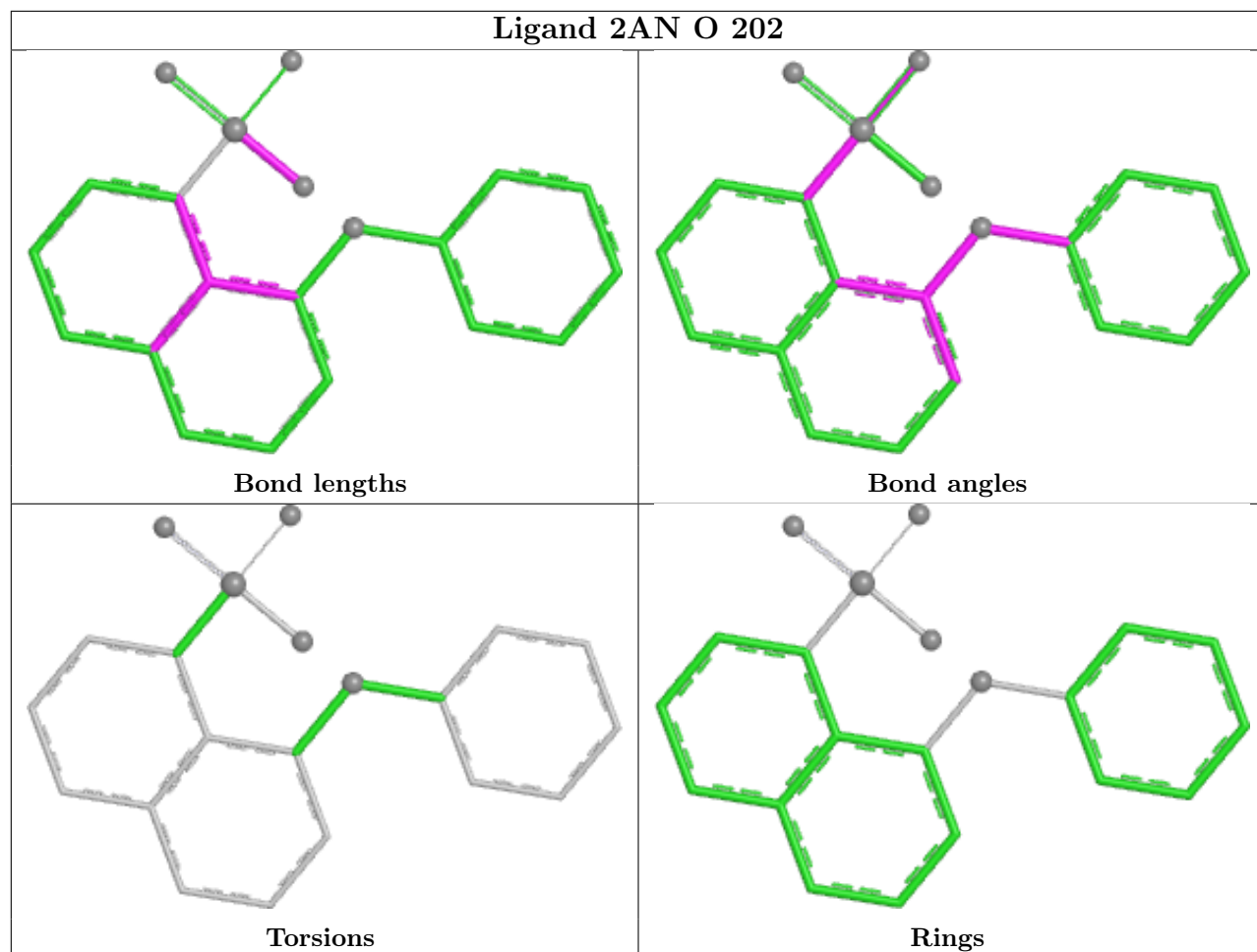
Ligand 2AN D 204



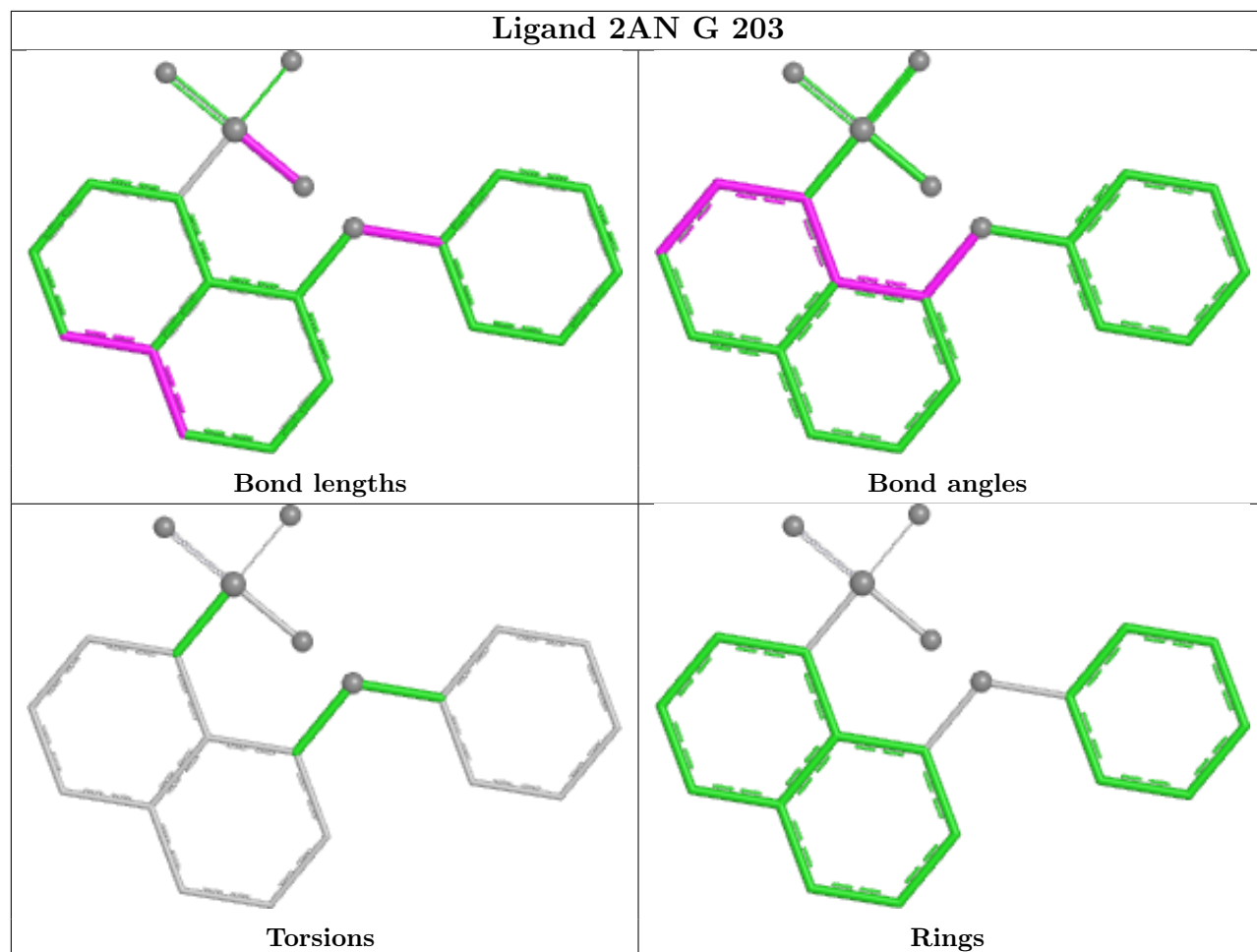


Ligand 2AN h 203

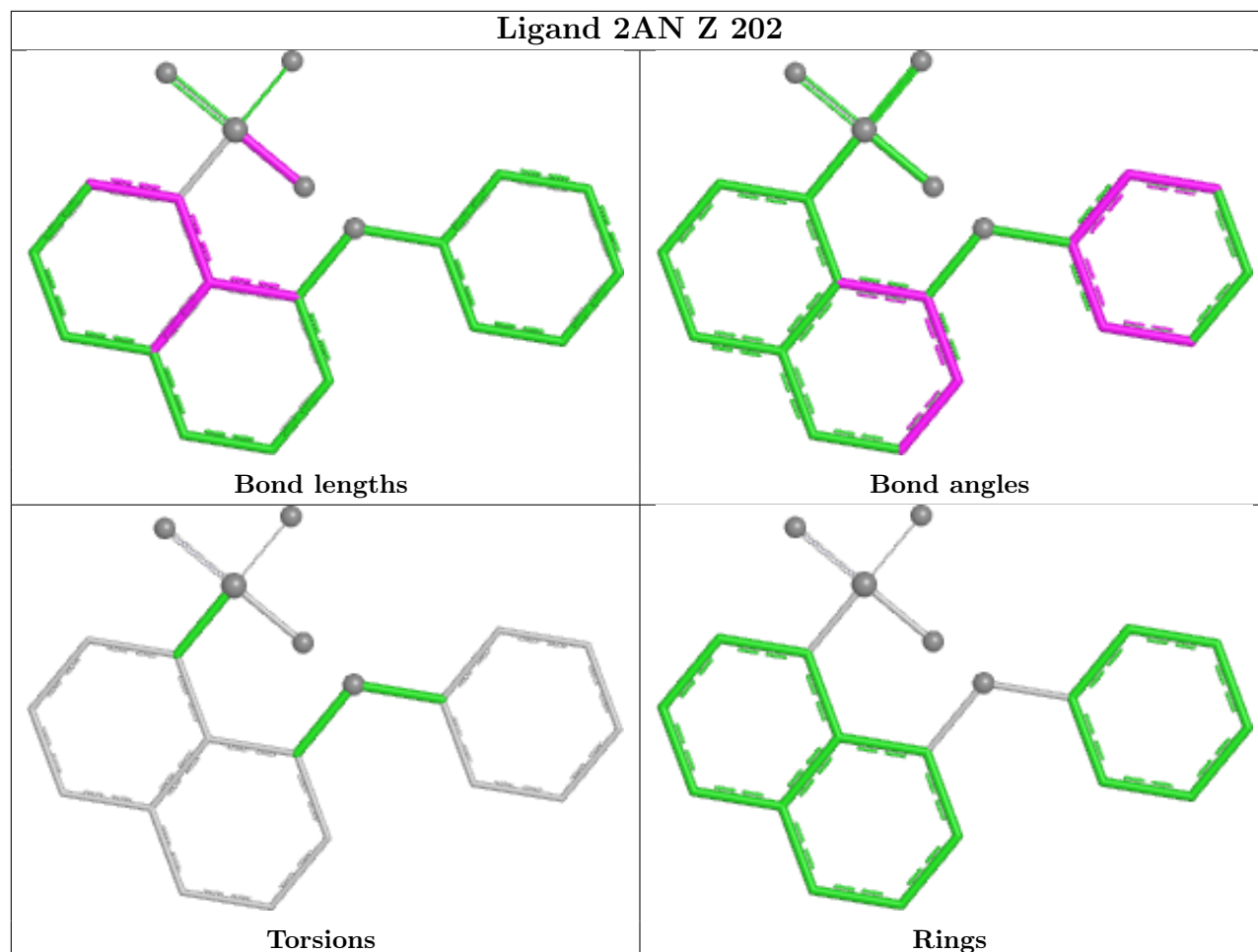




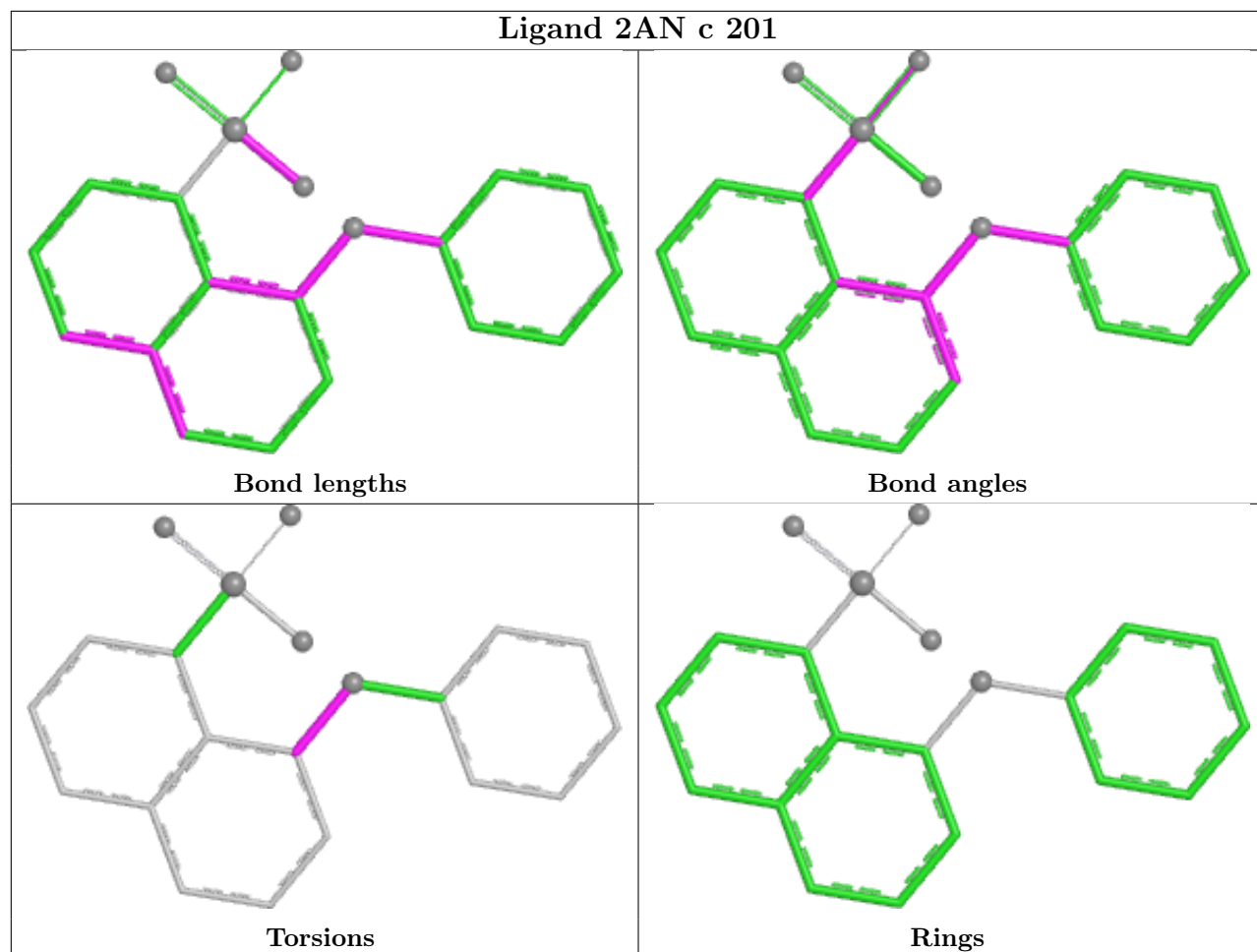
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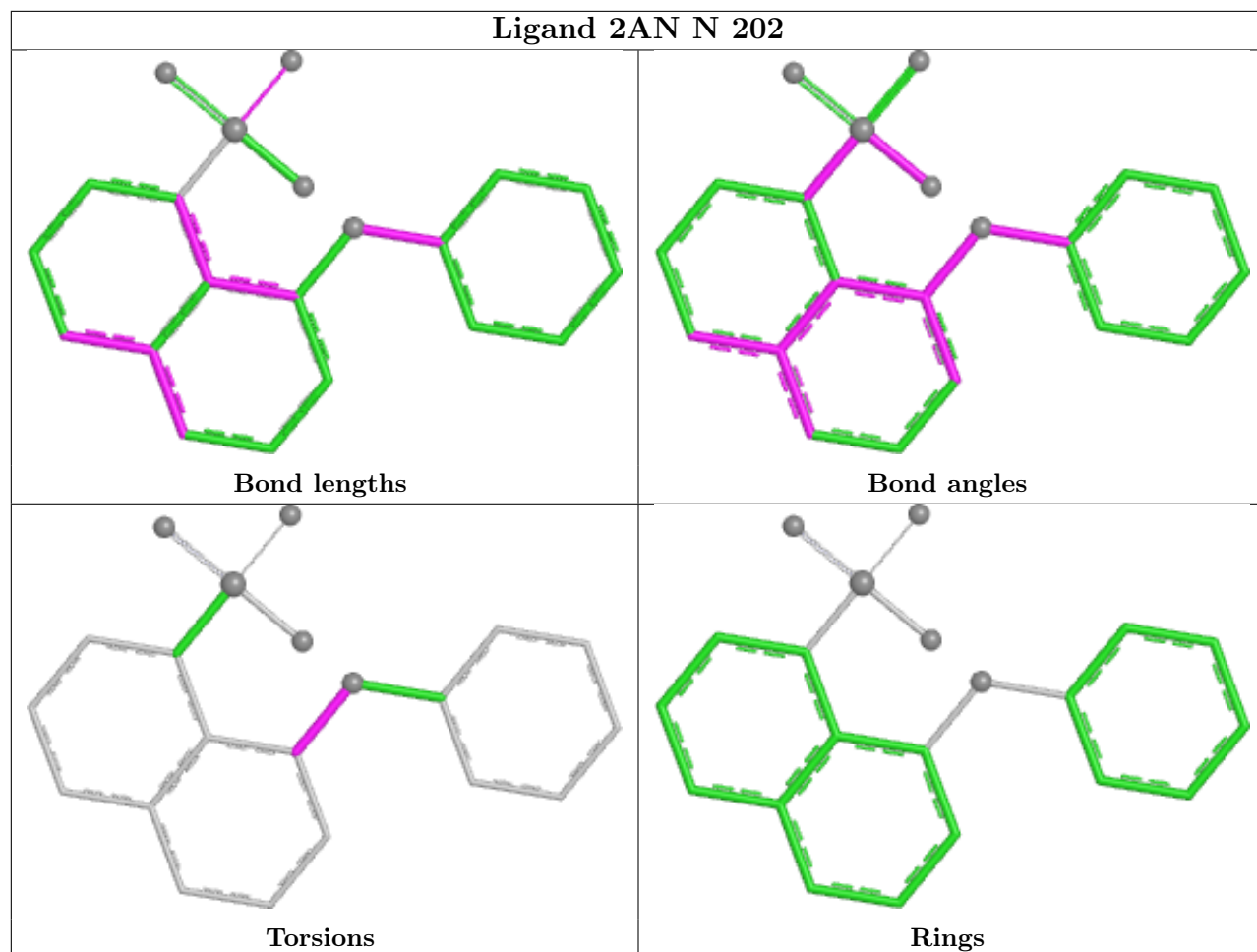


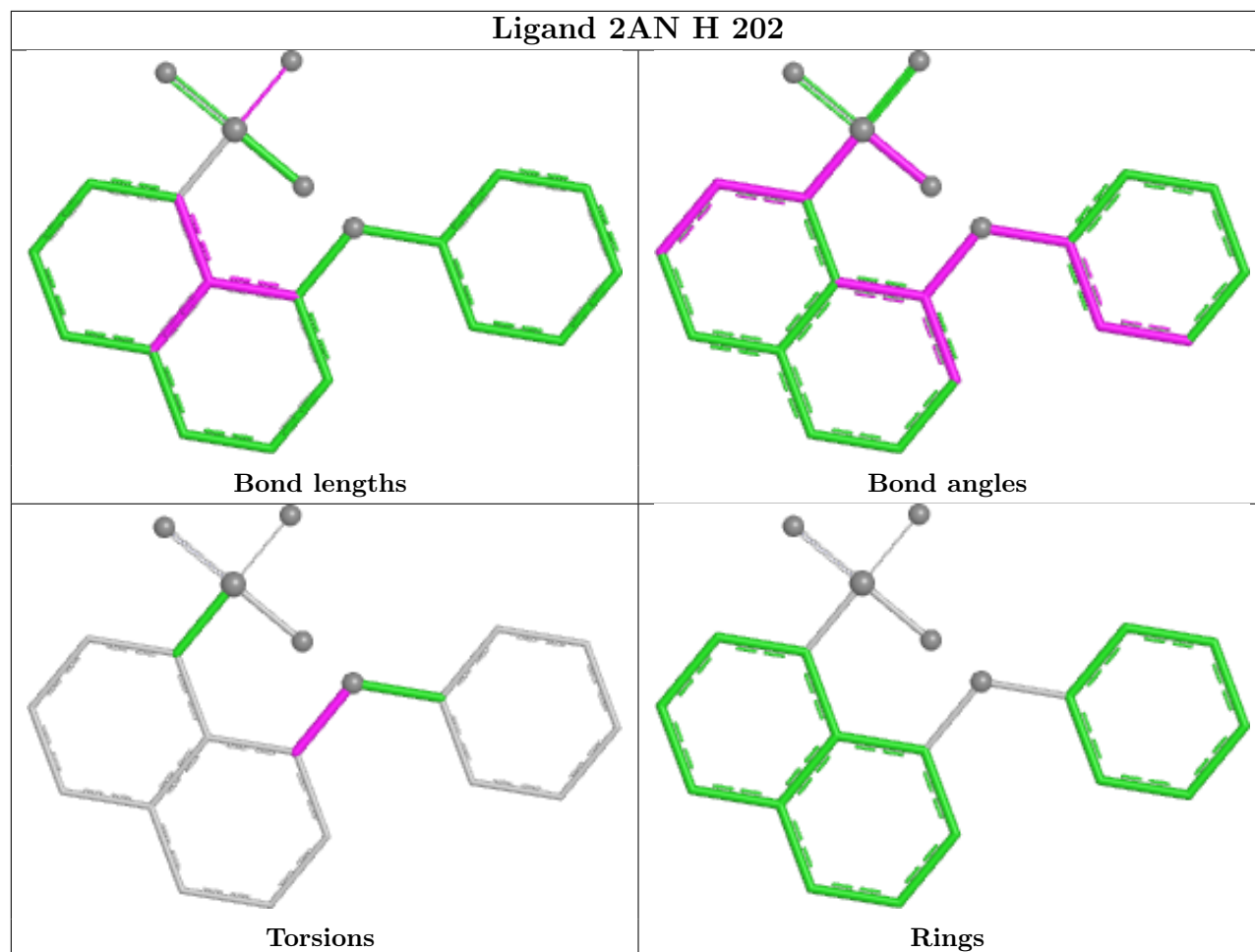
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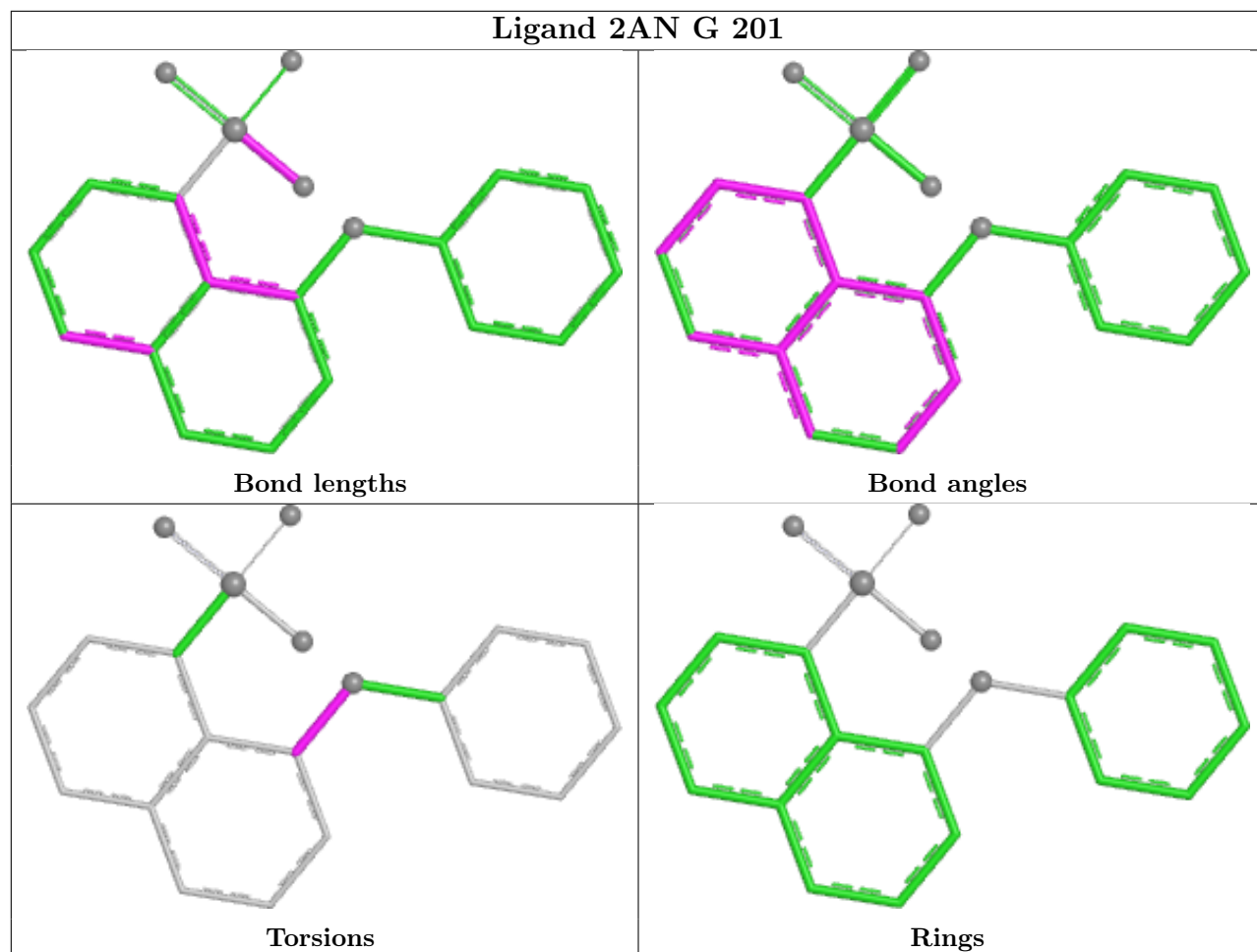


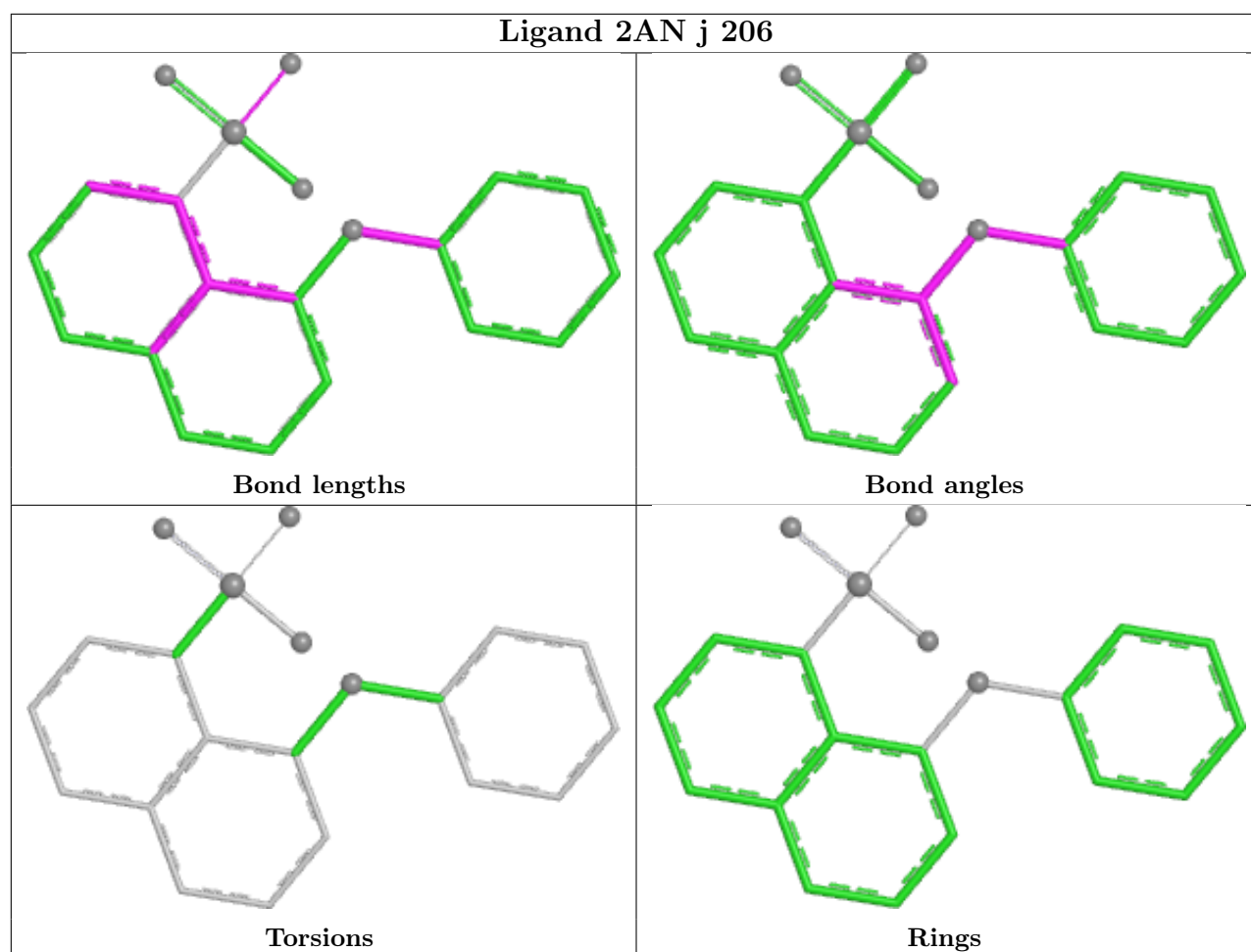
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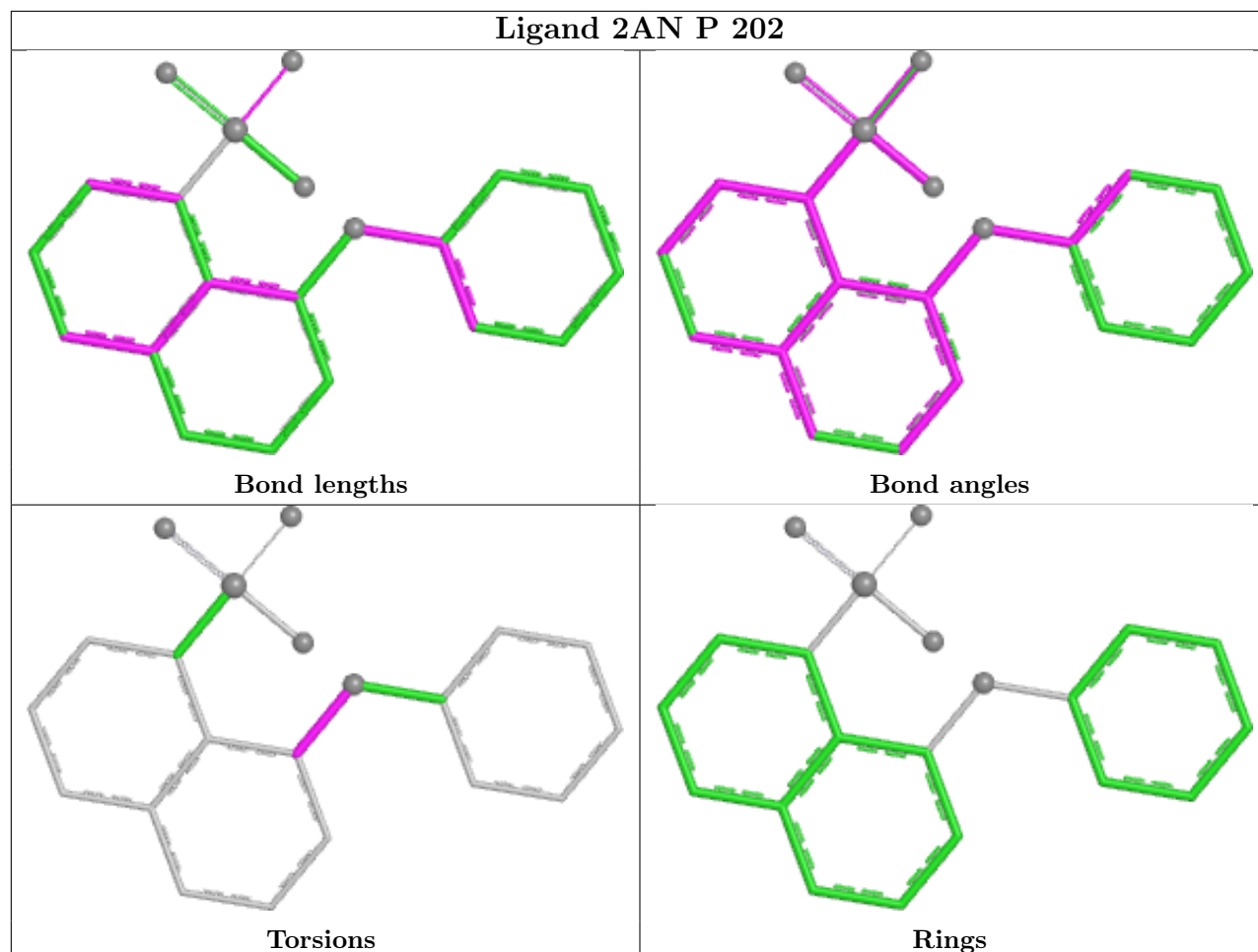


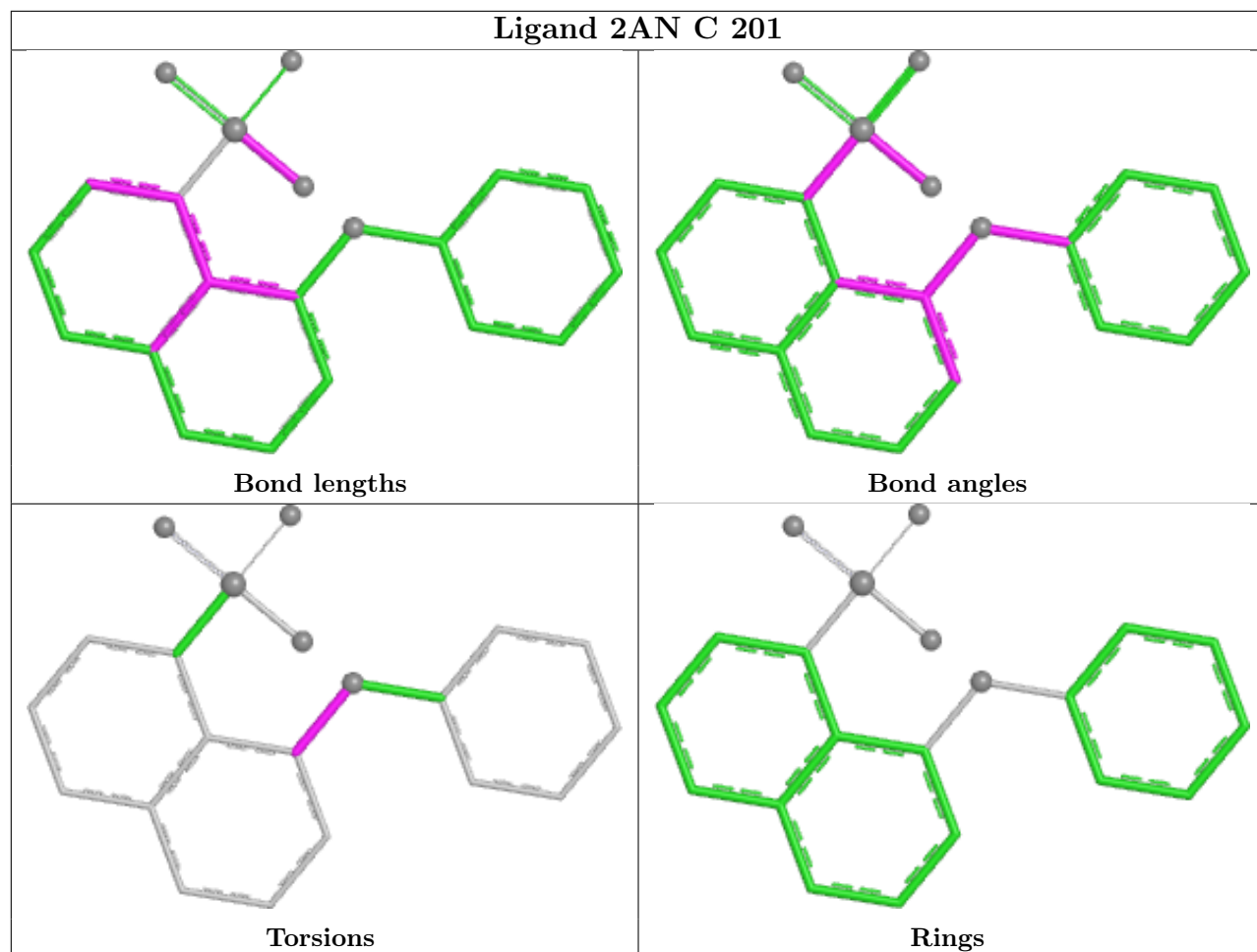


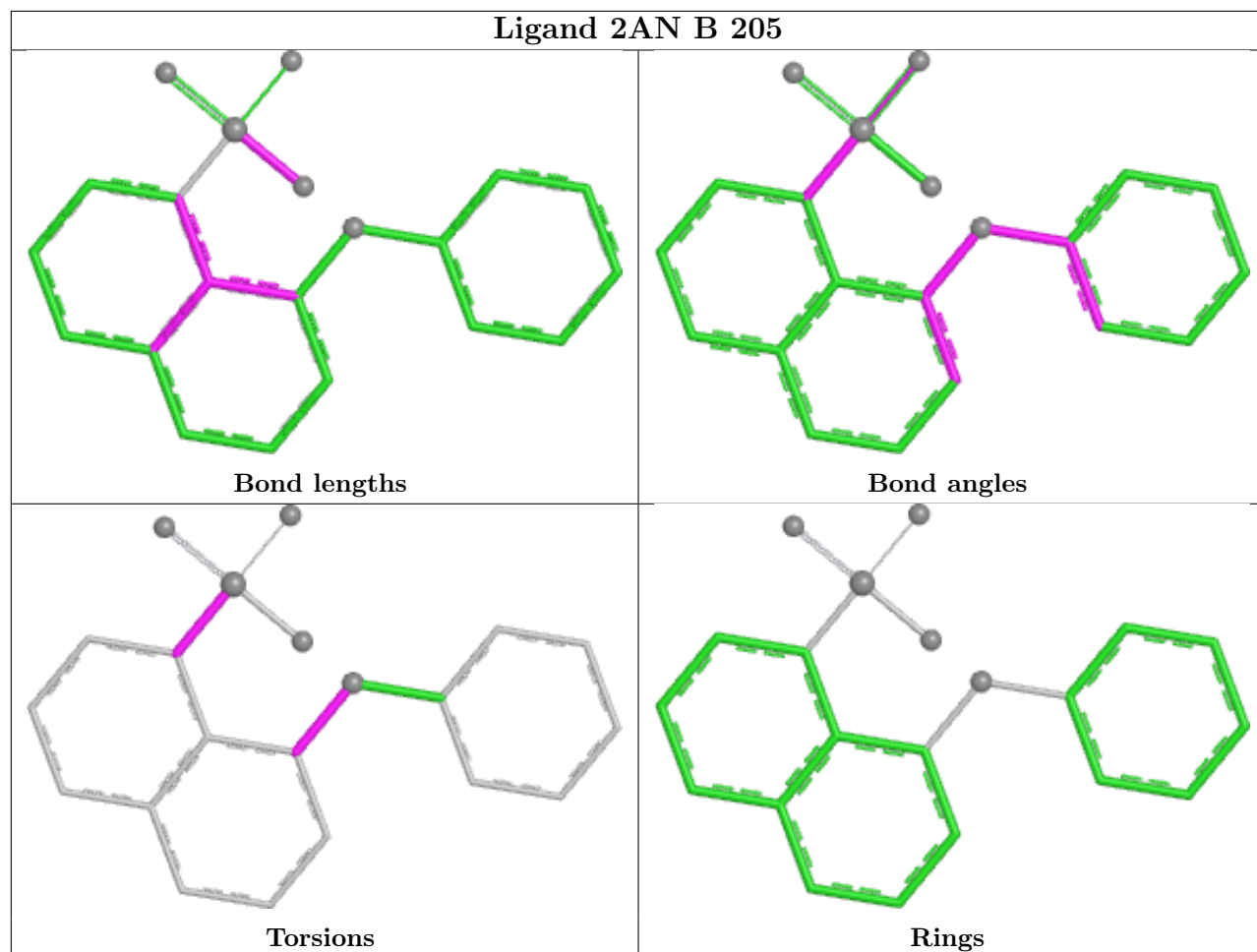


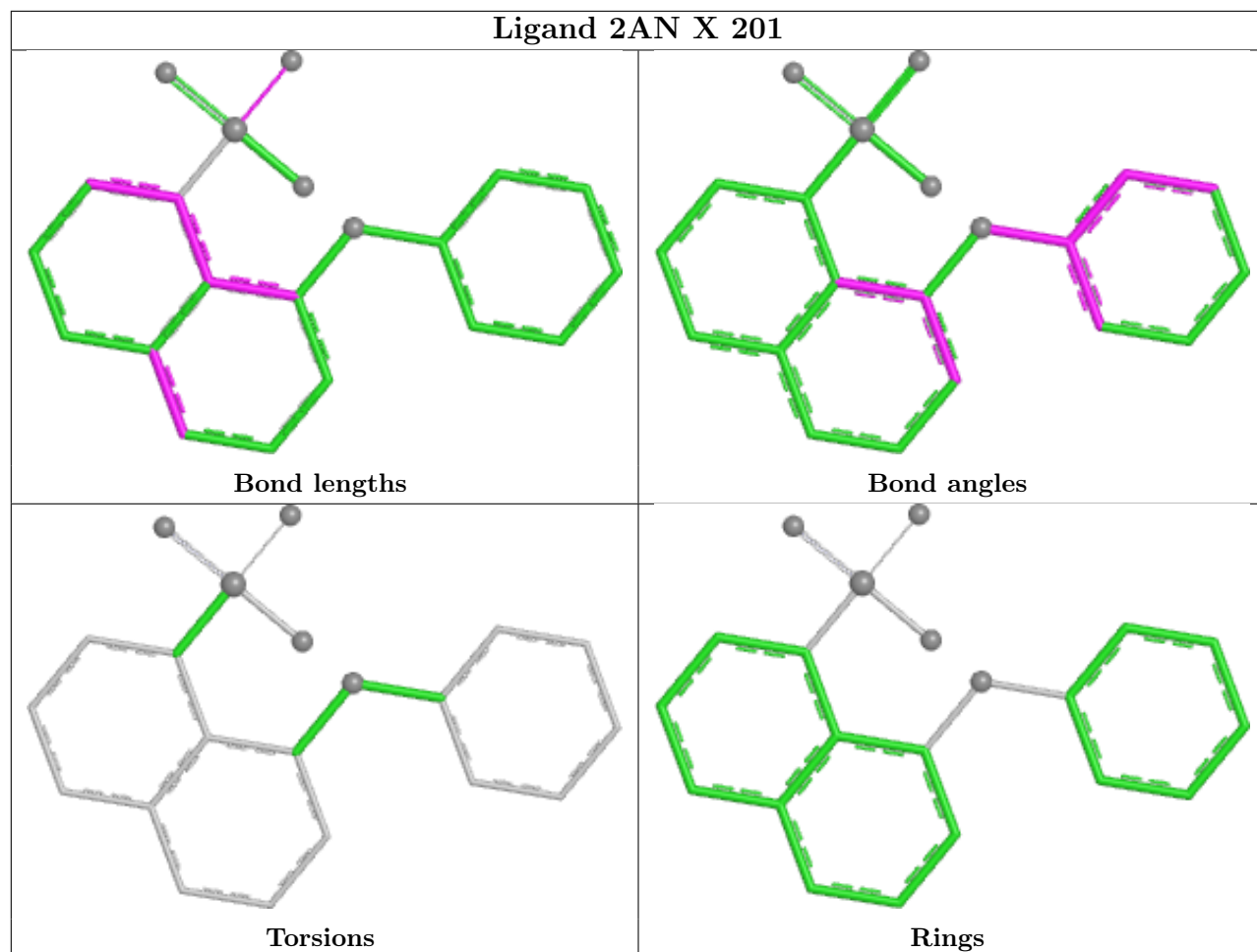


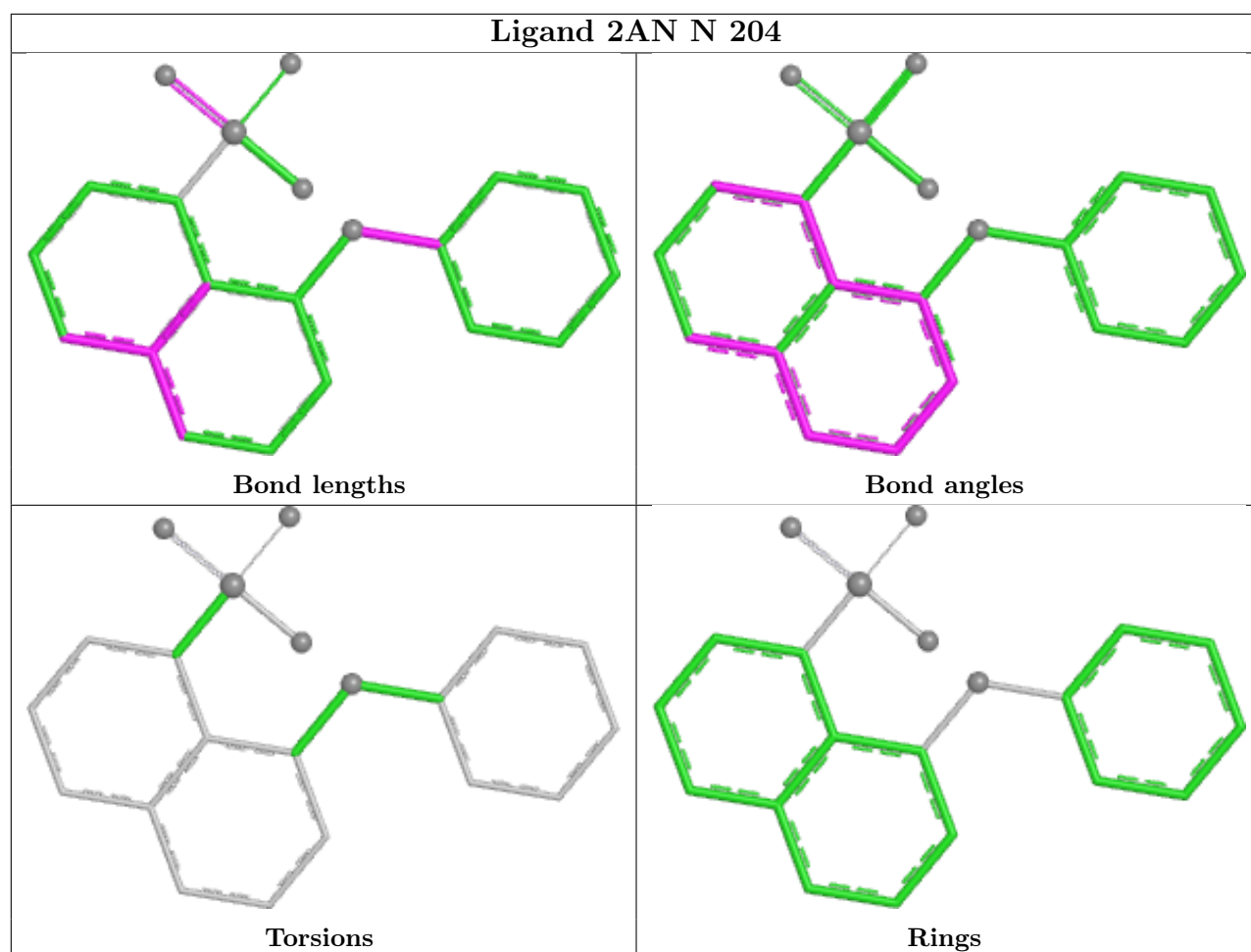
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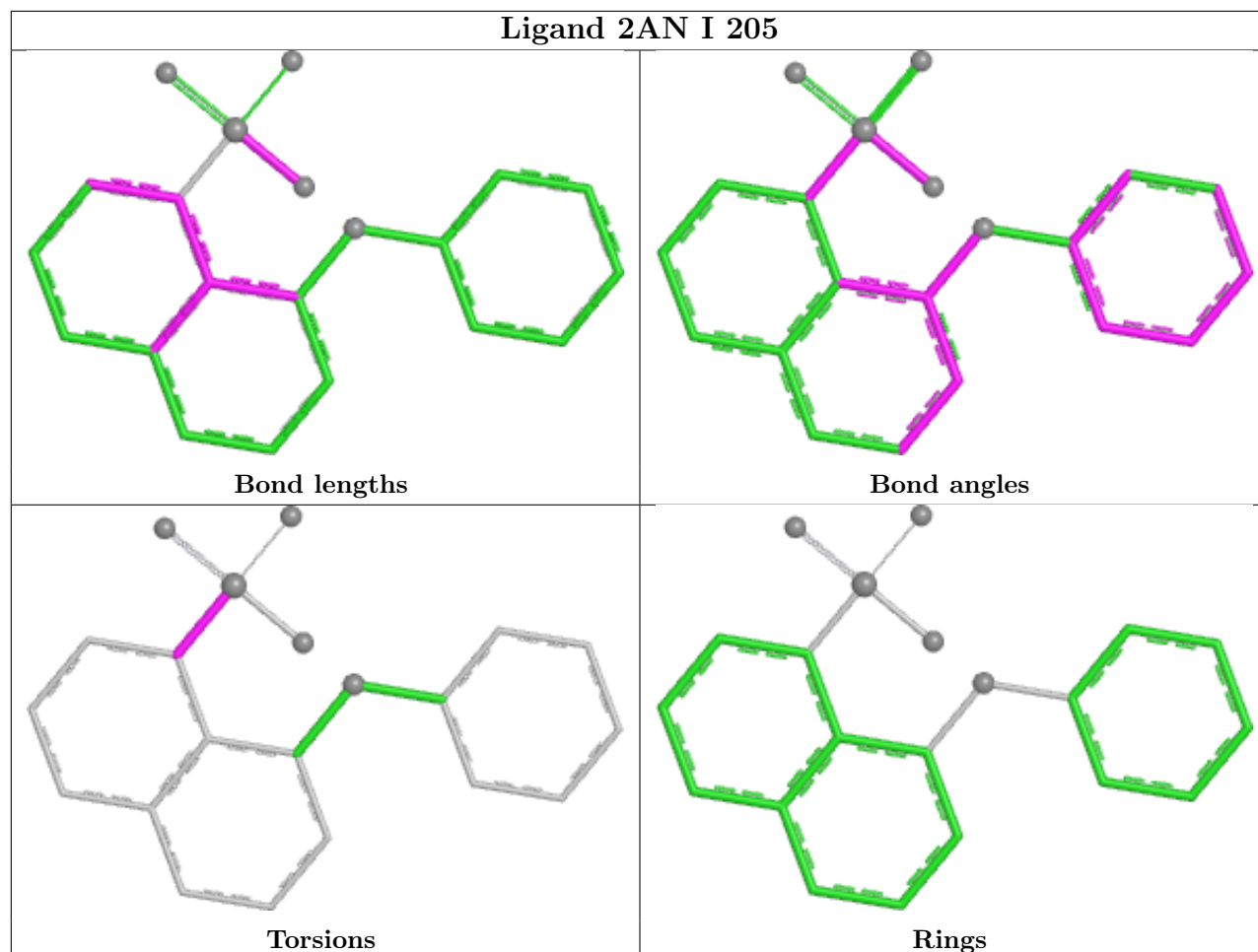




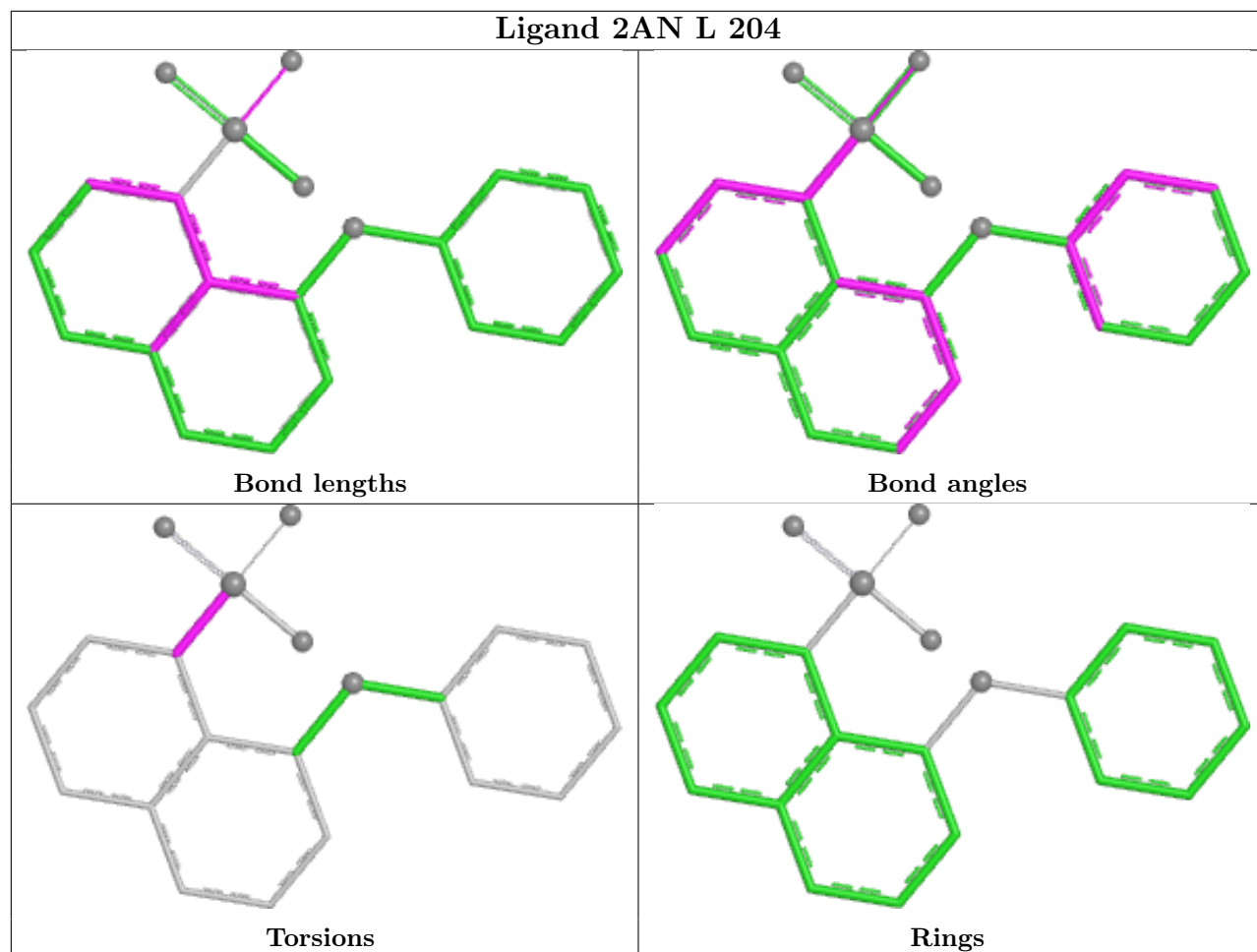


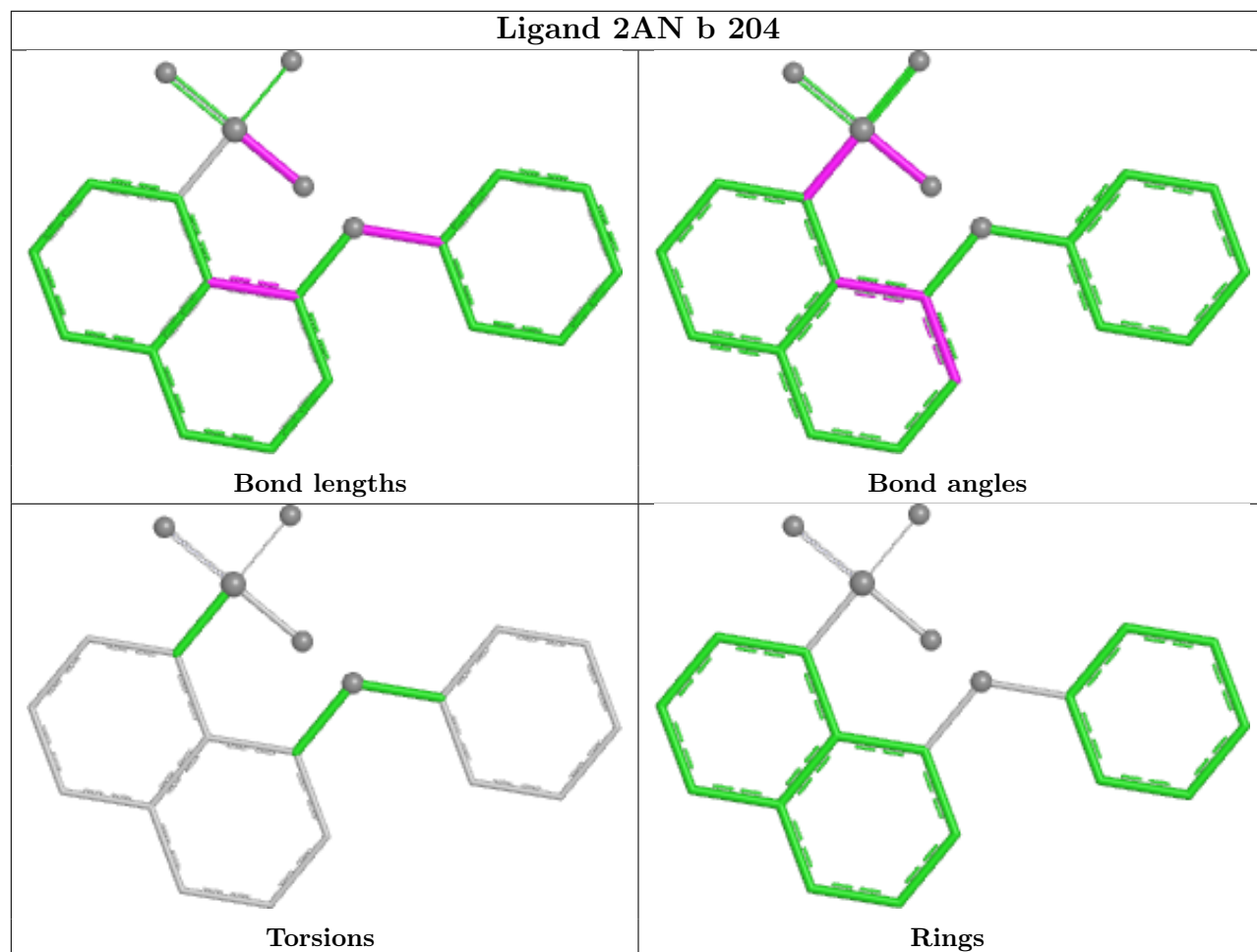


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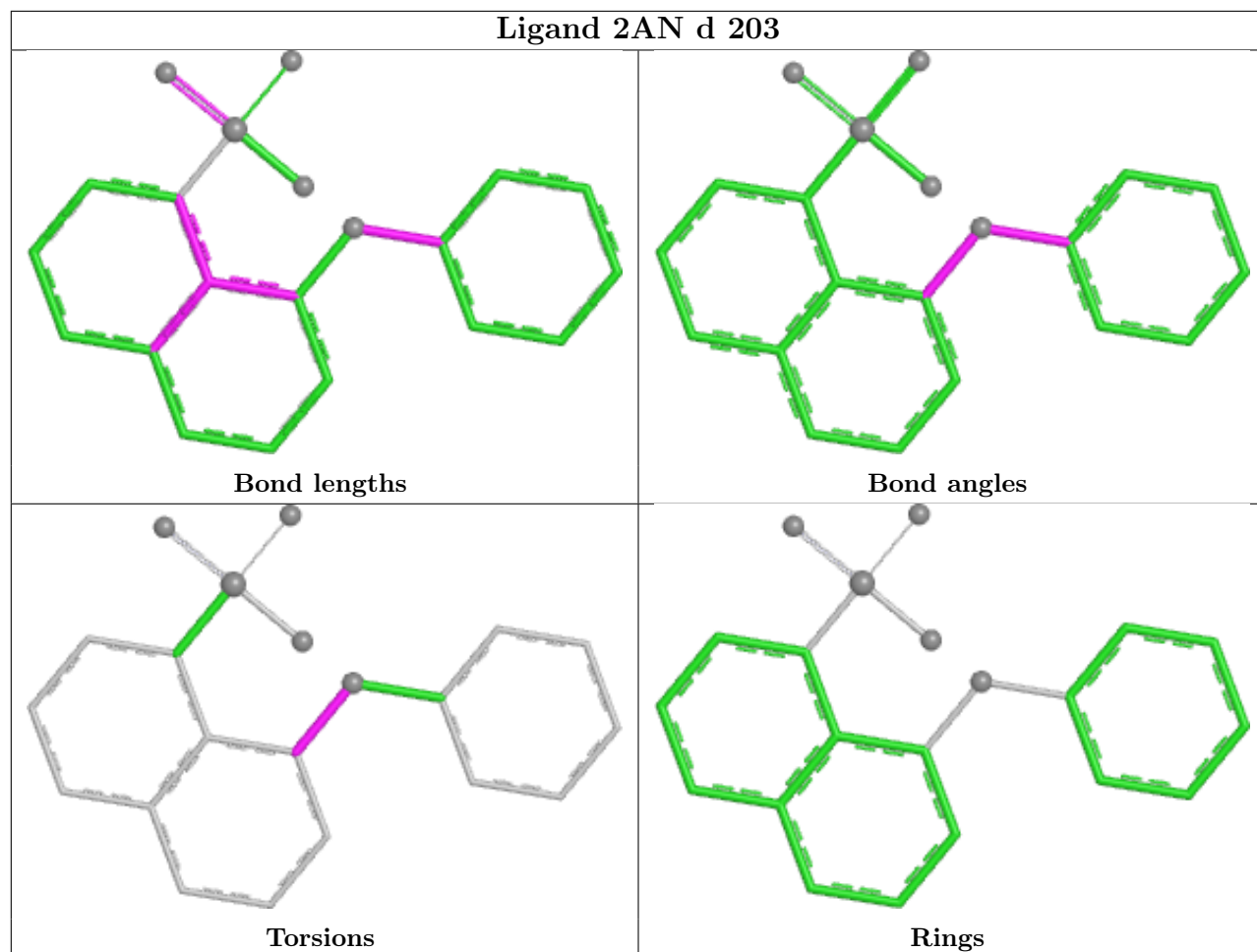


Ligand 2AN L 204

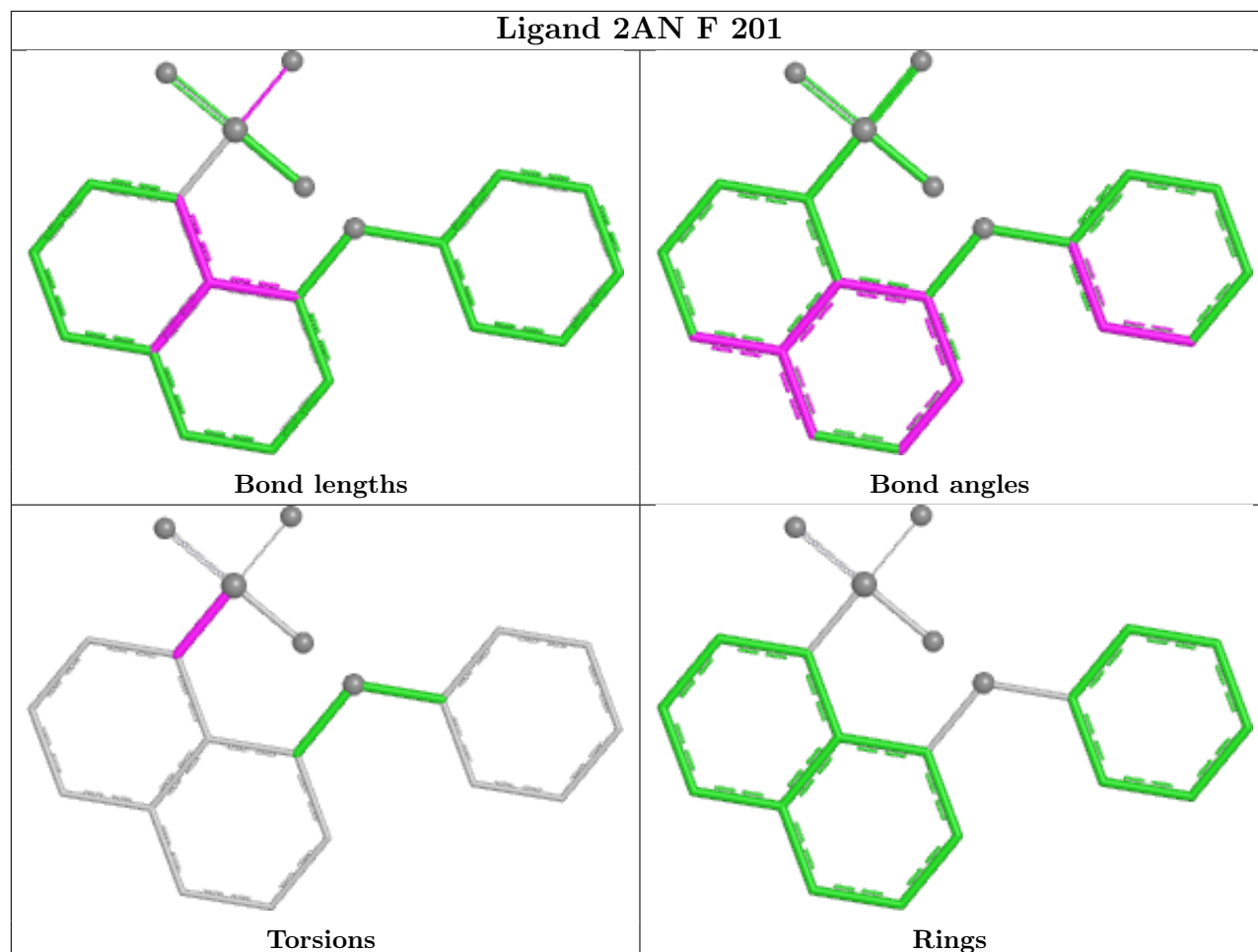




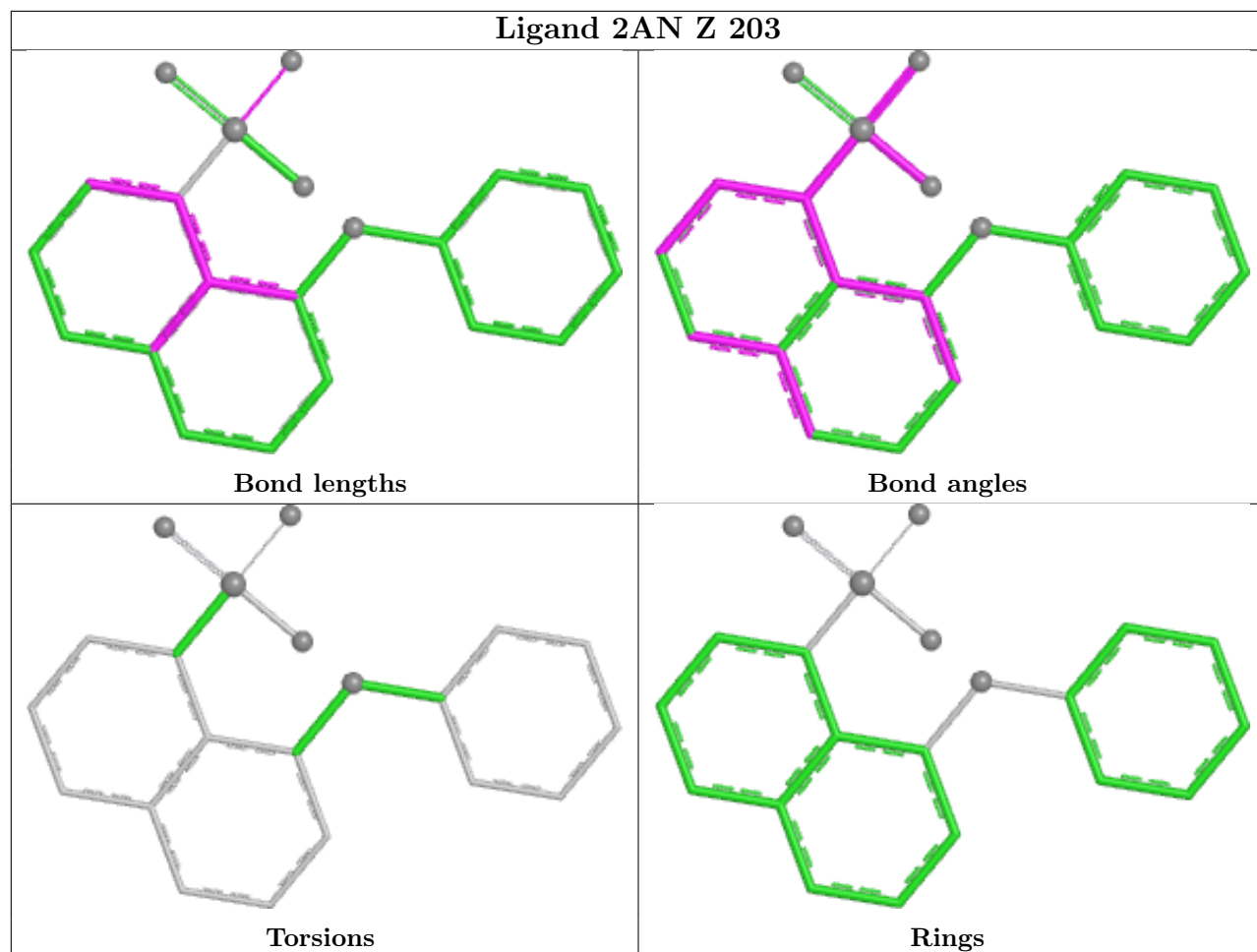
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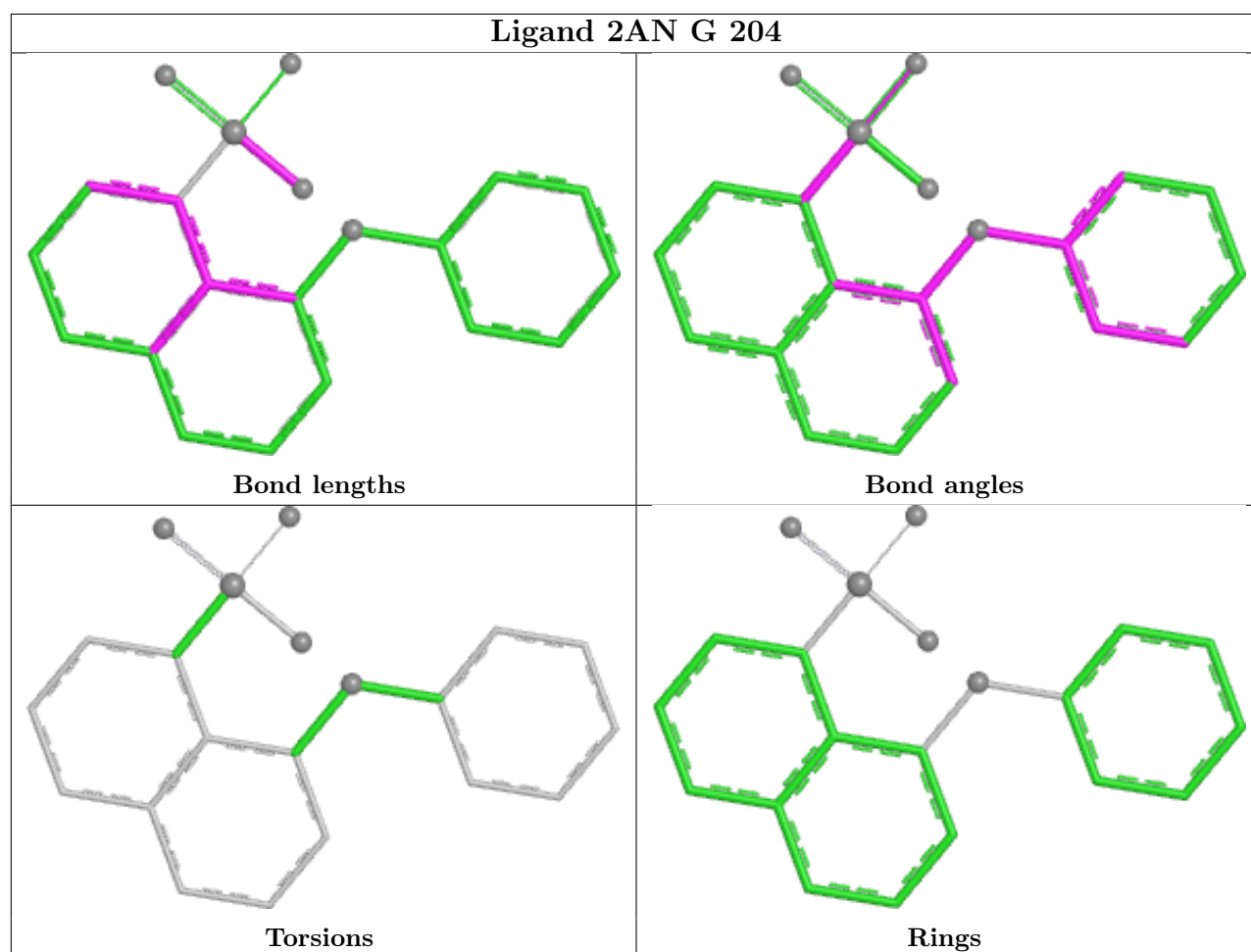


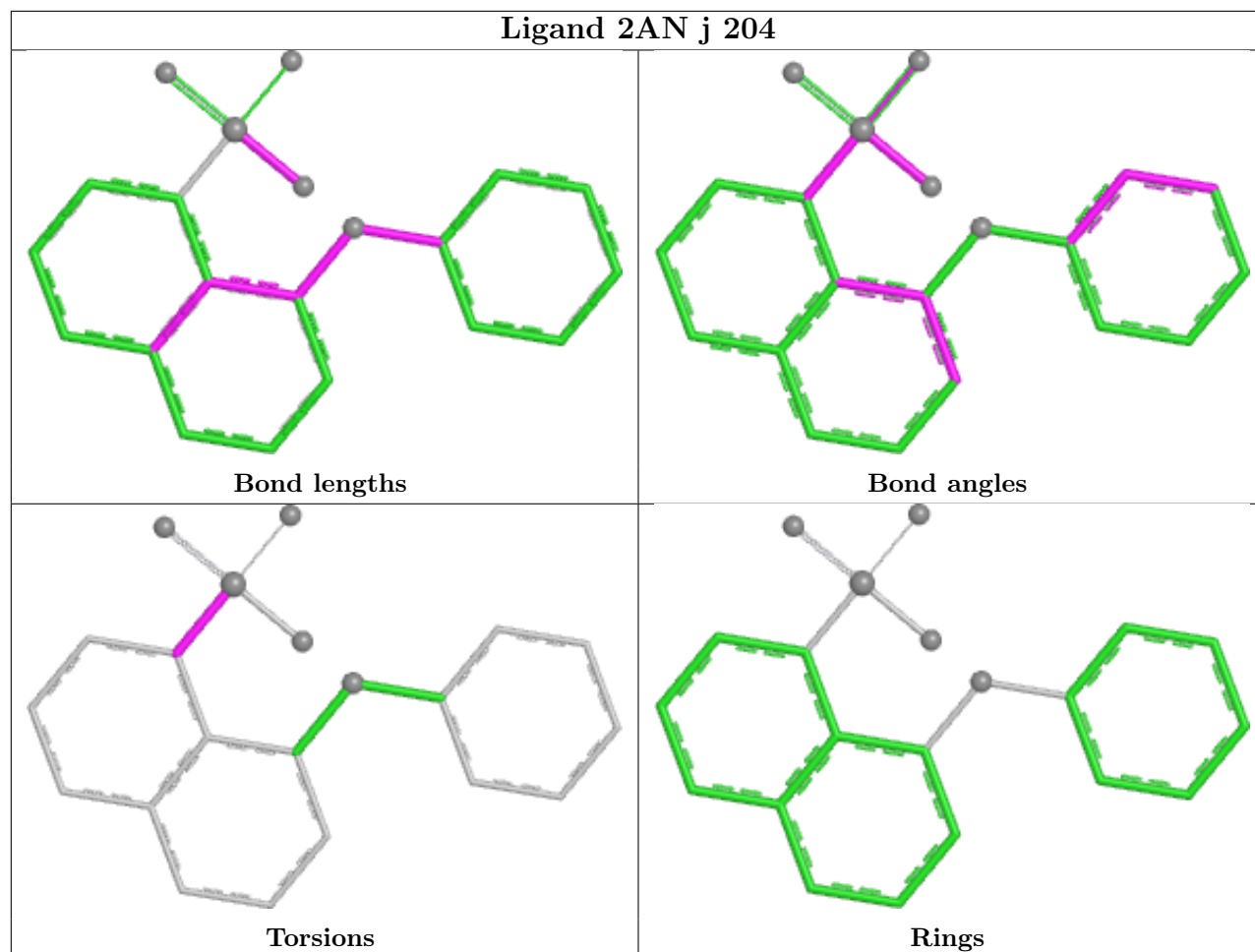
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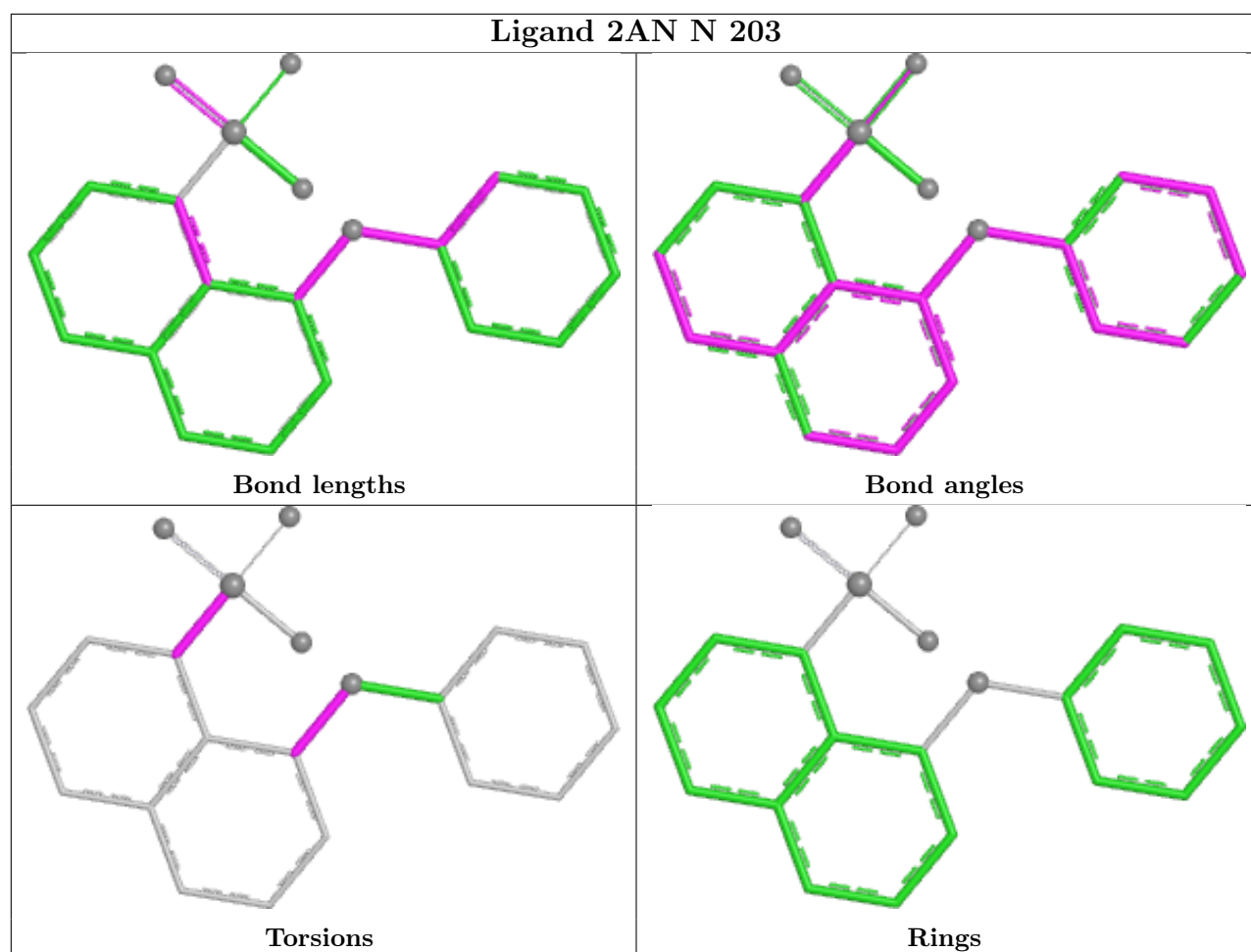


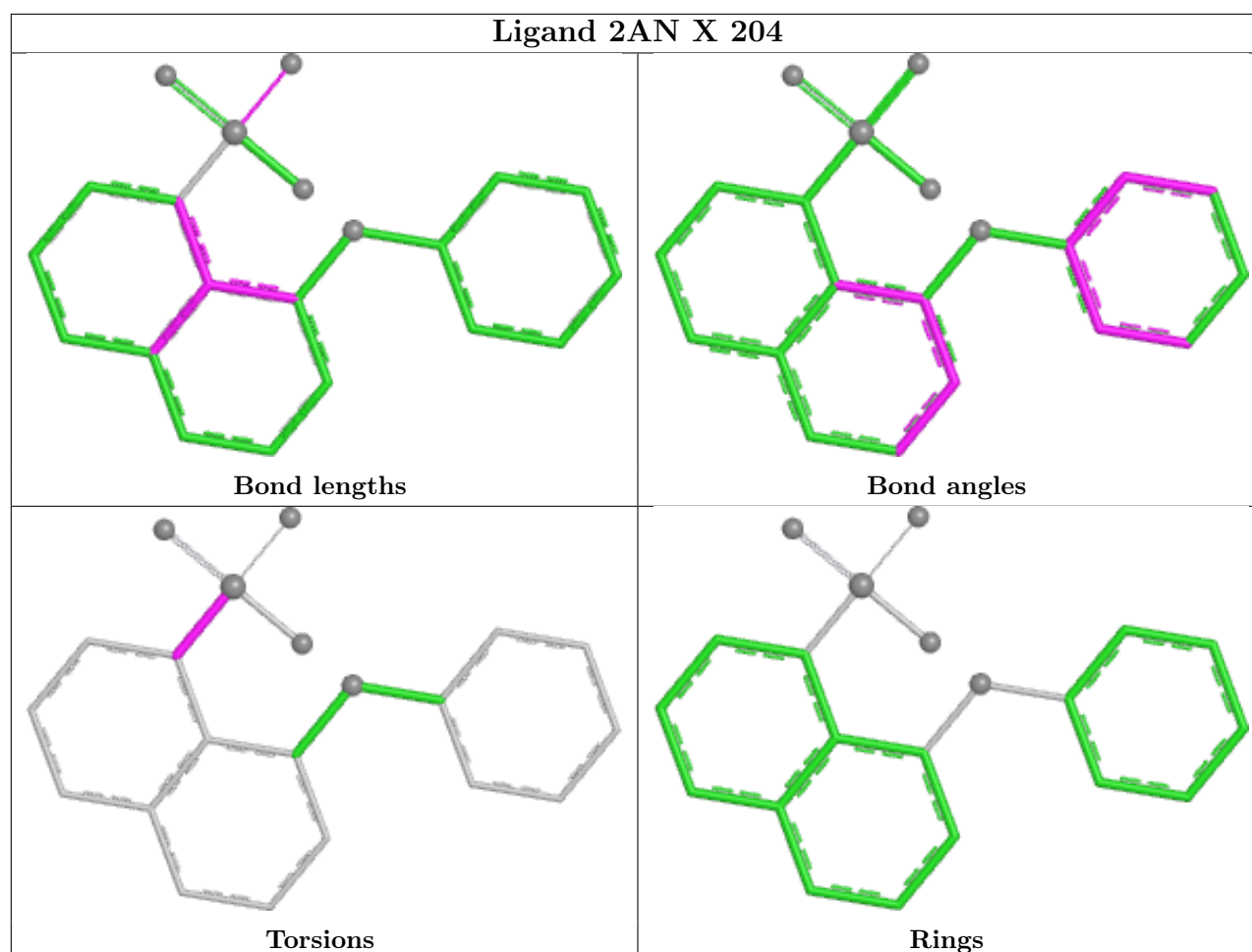
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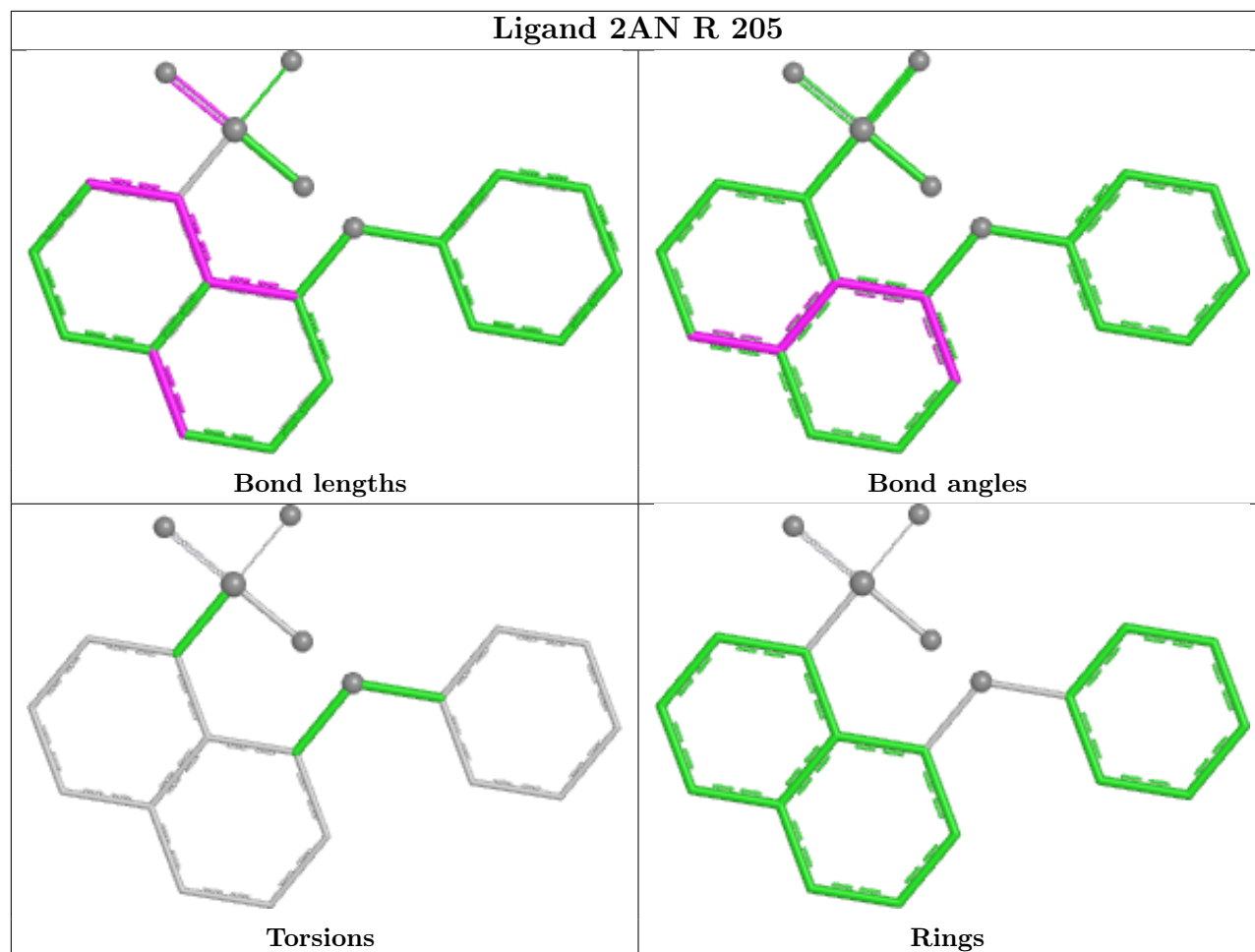




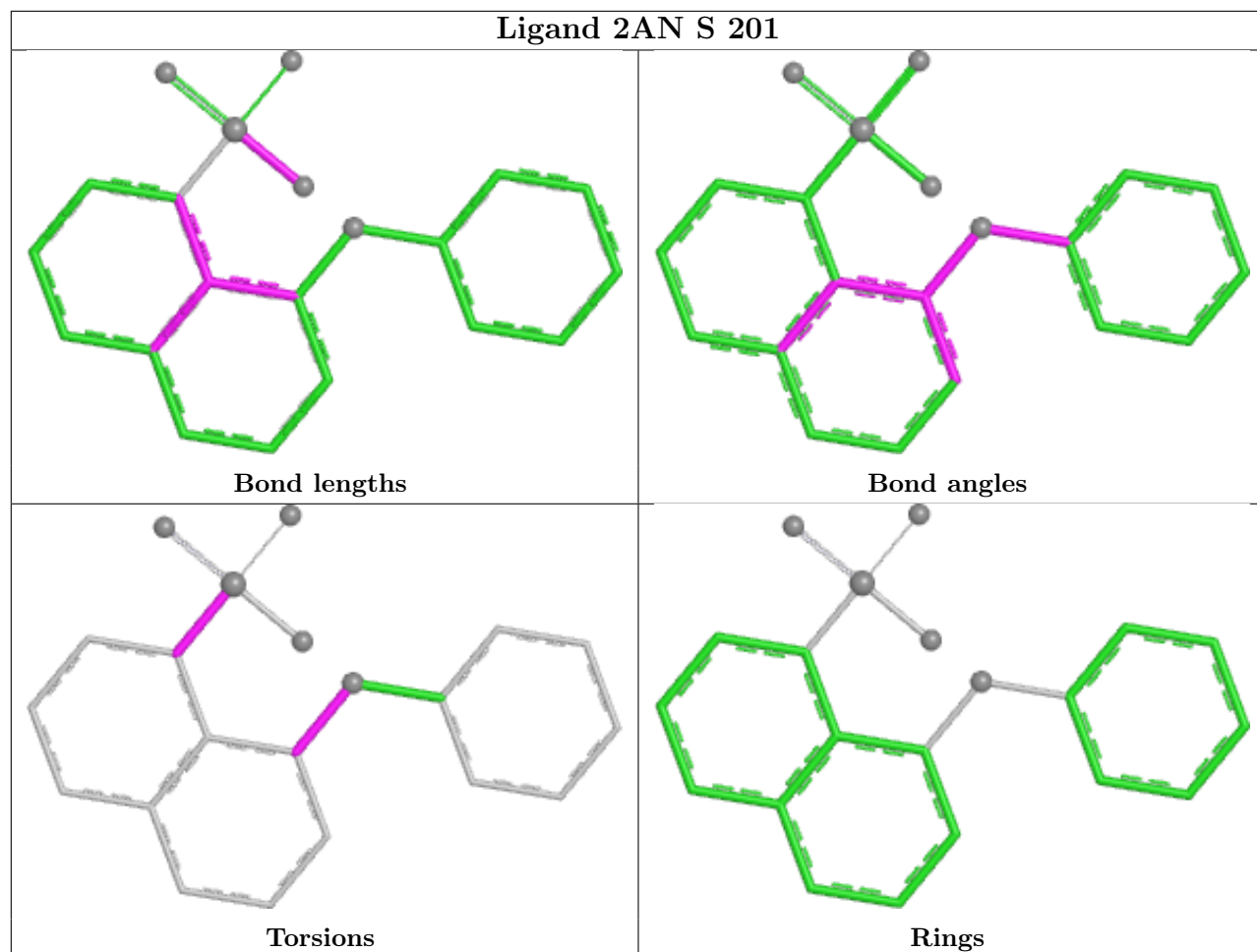


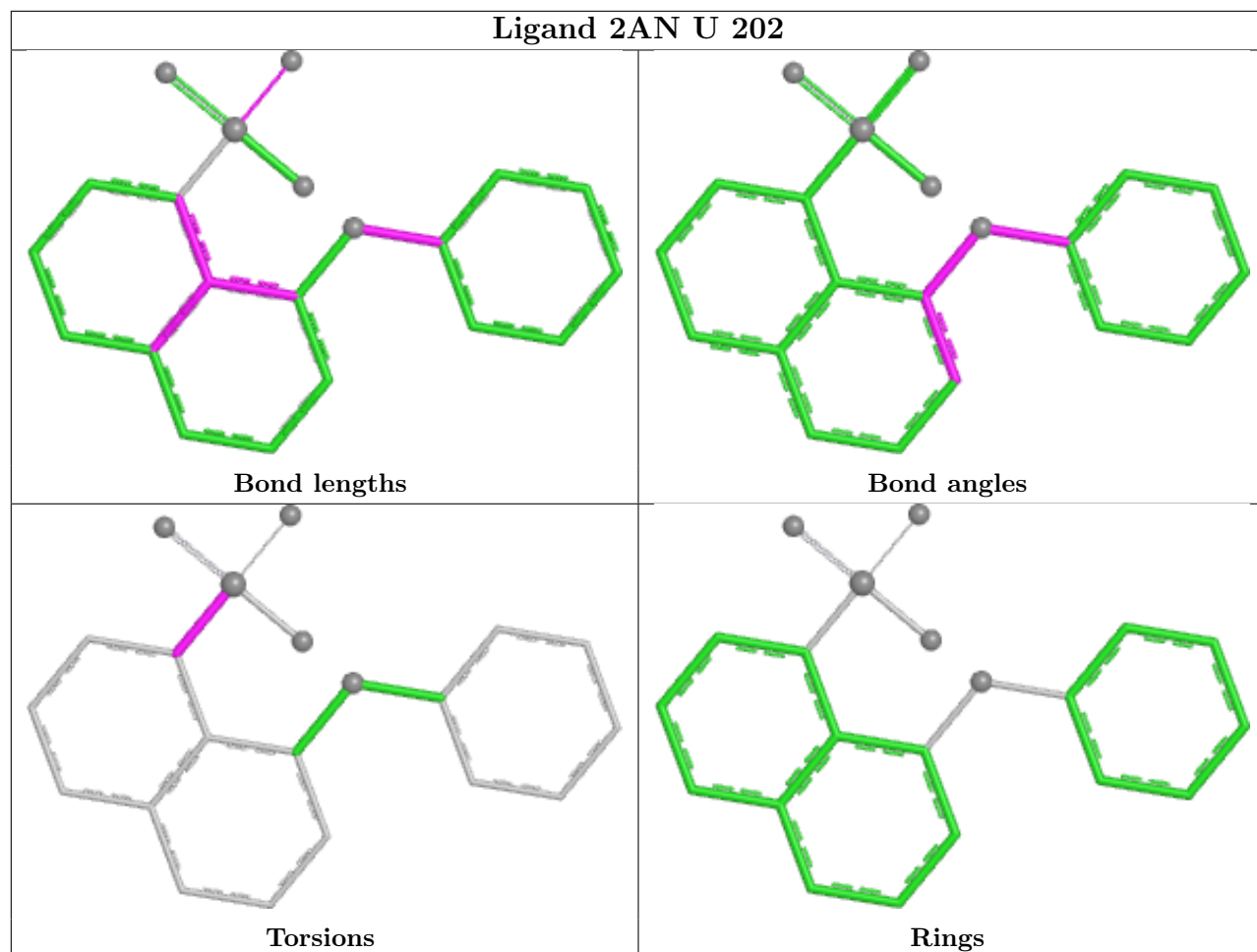


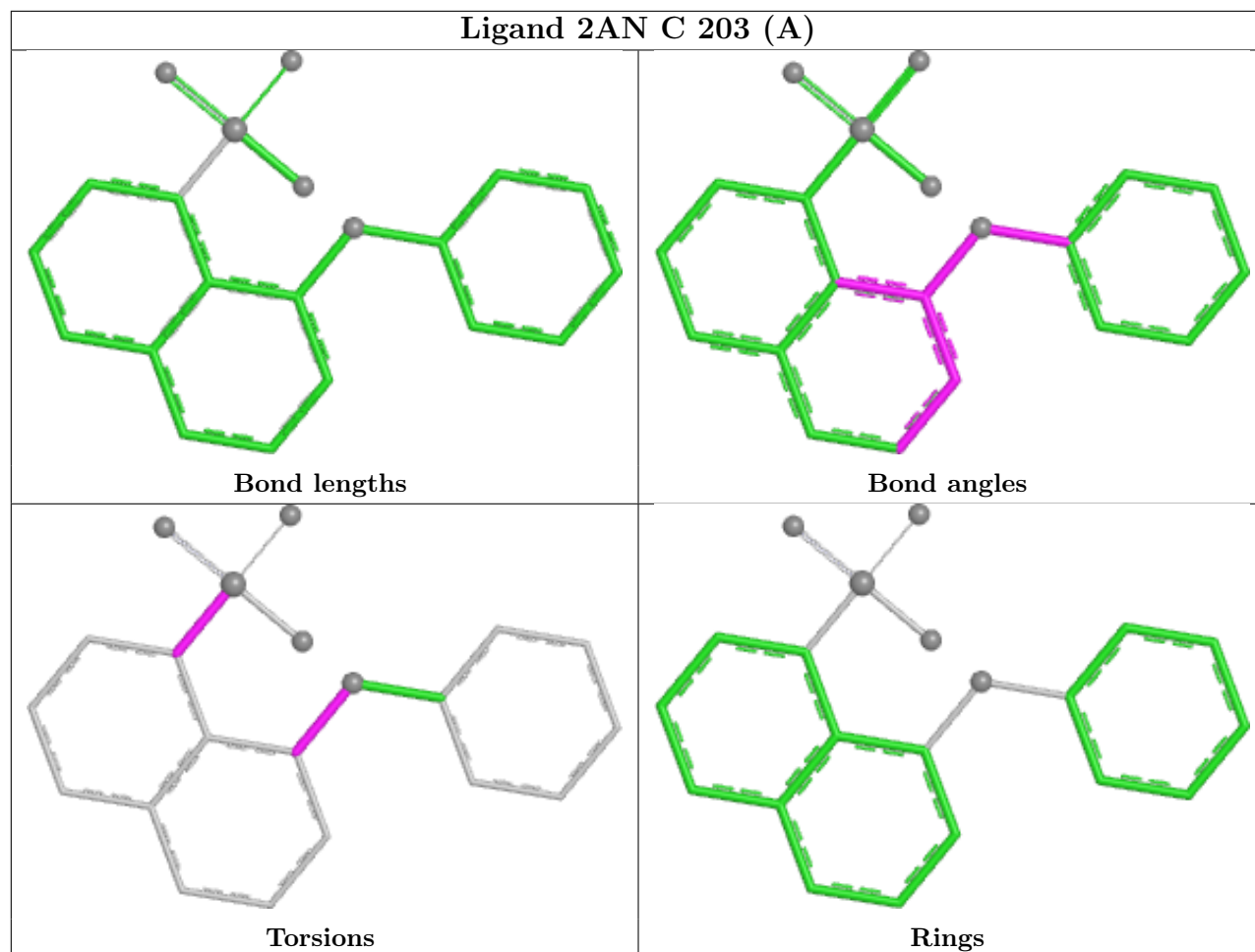


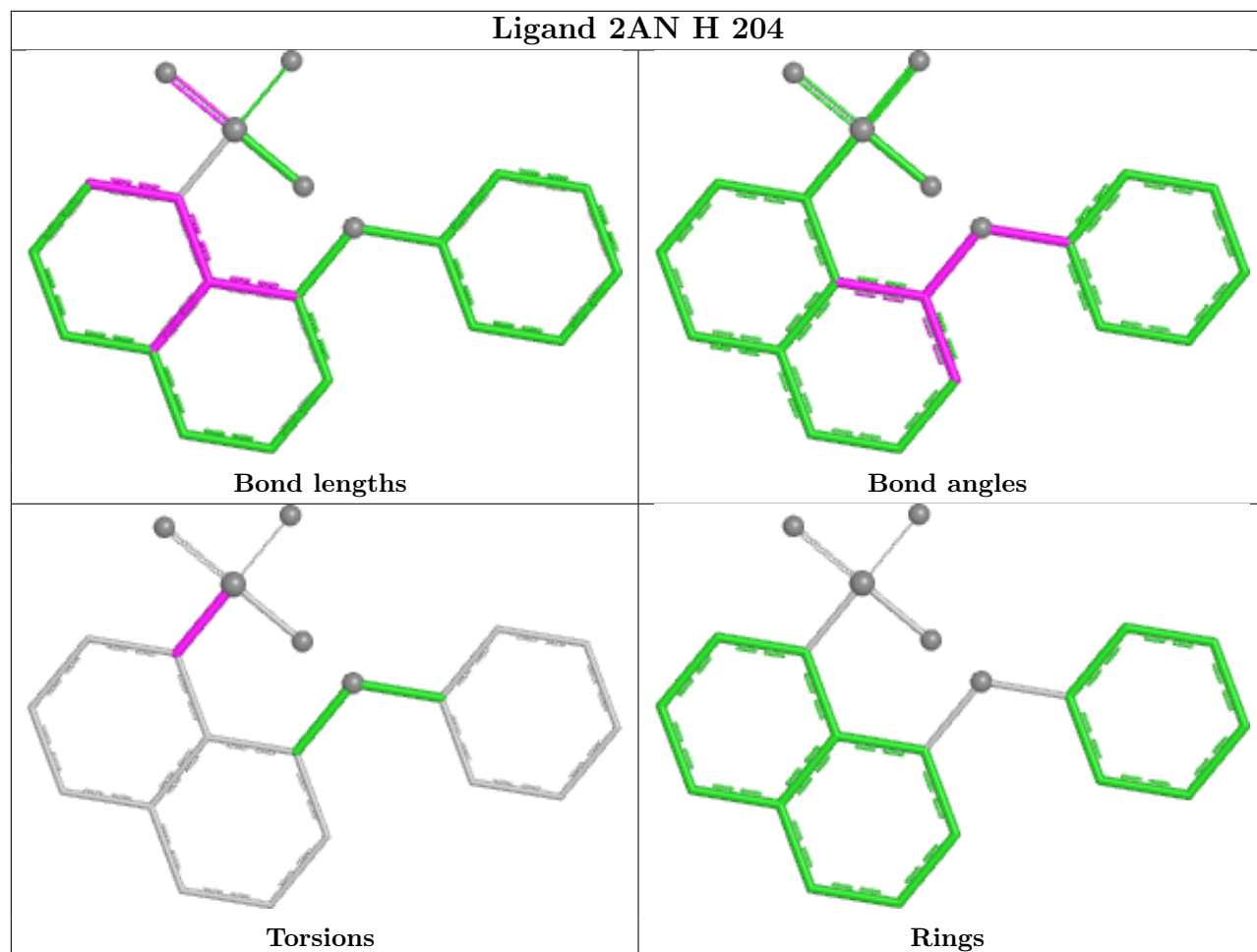


Ligand 2AN S 201

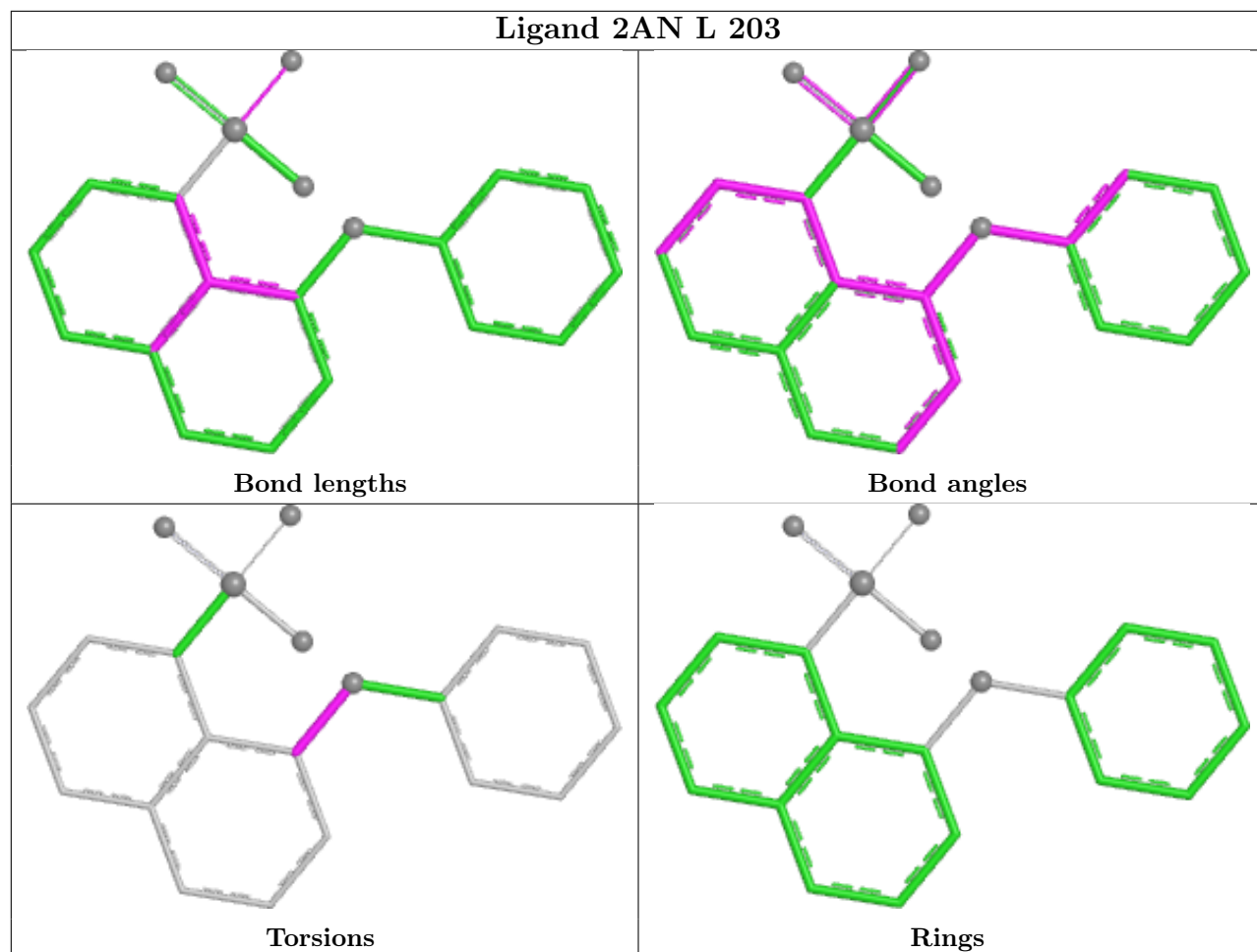




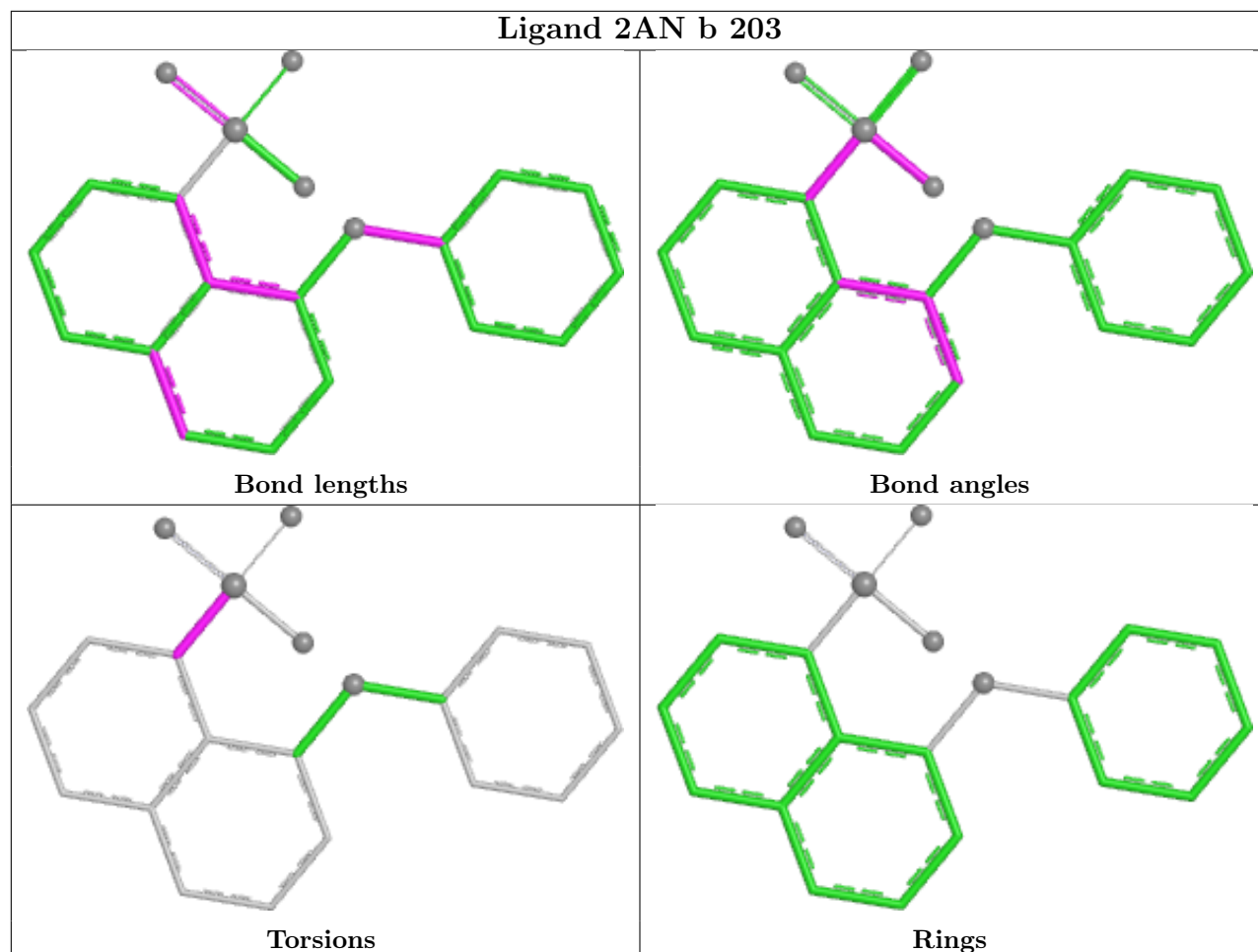




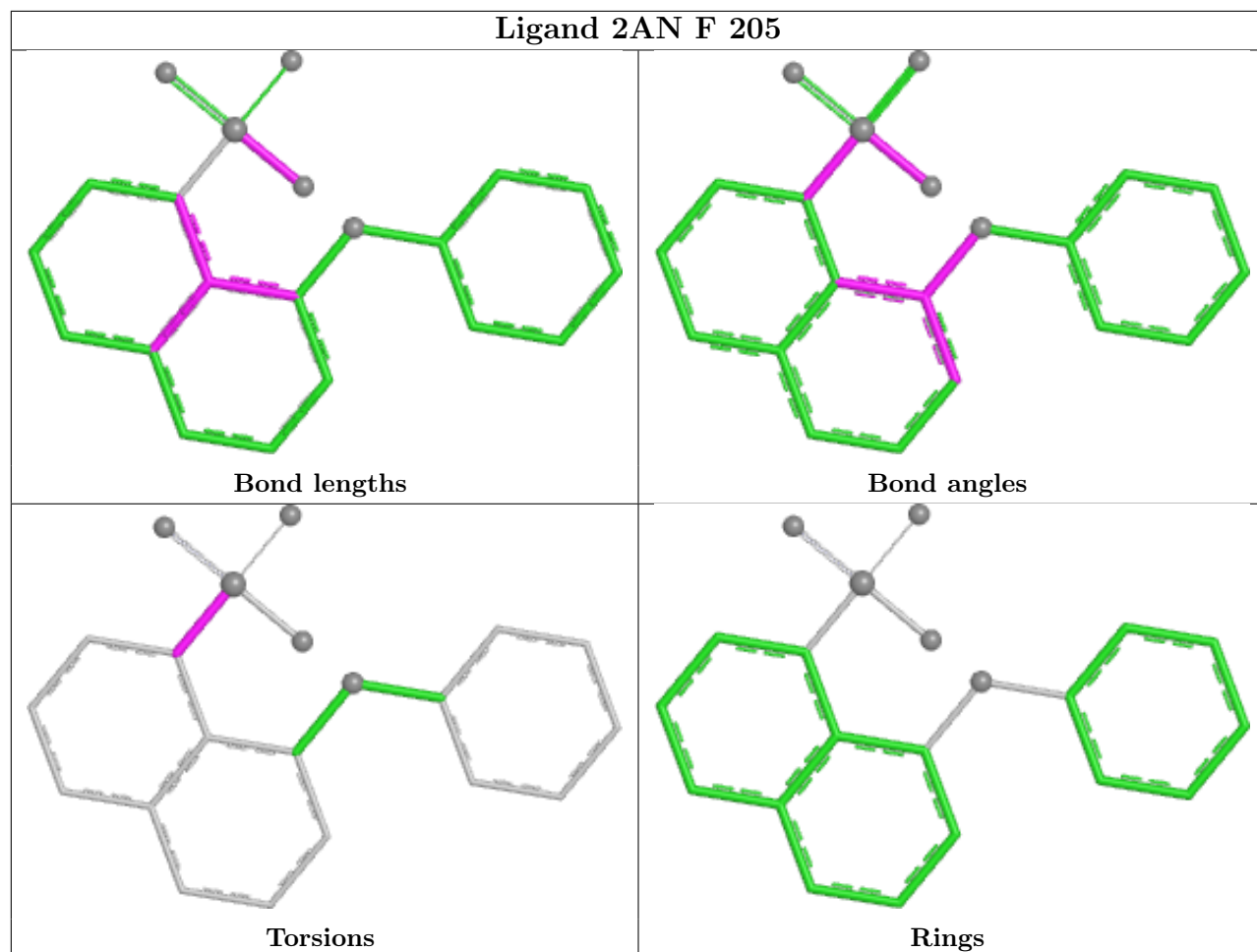
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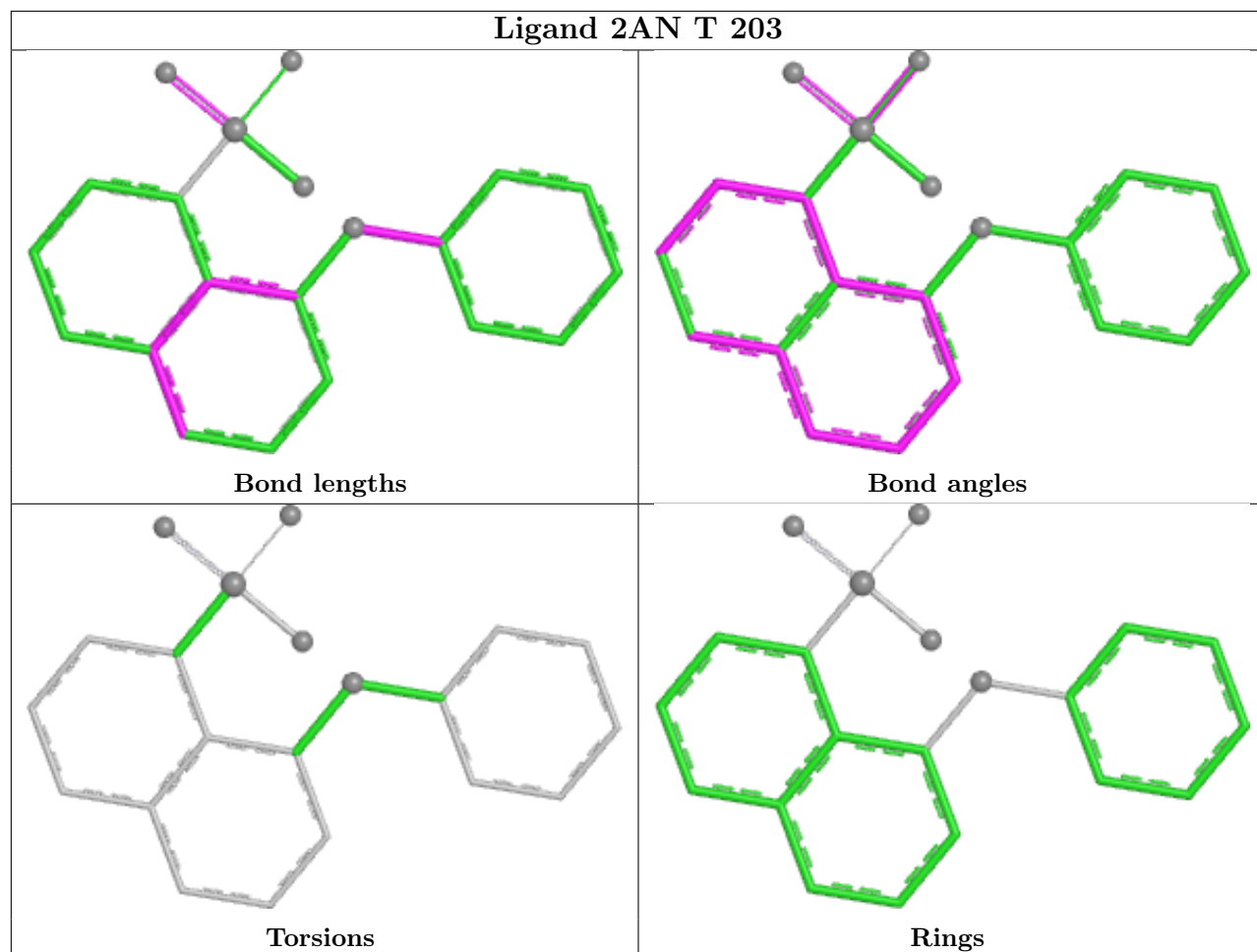
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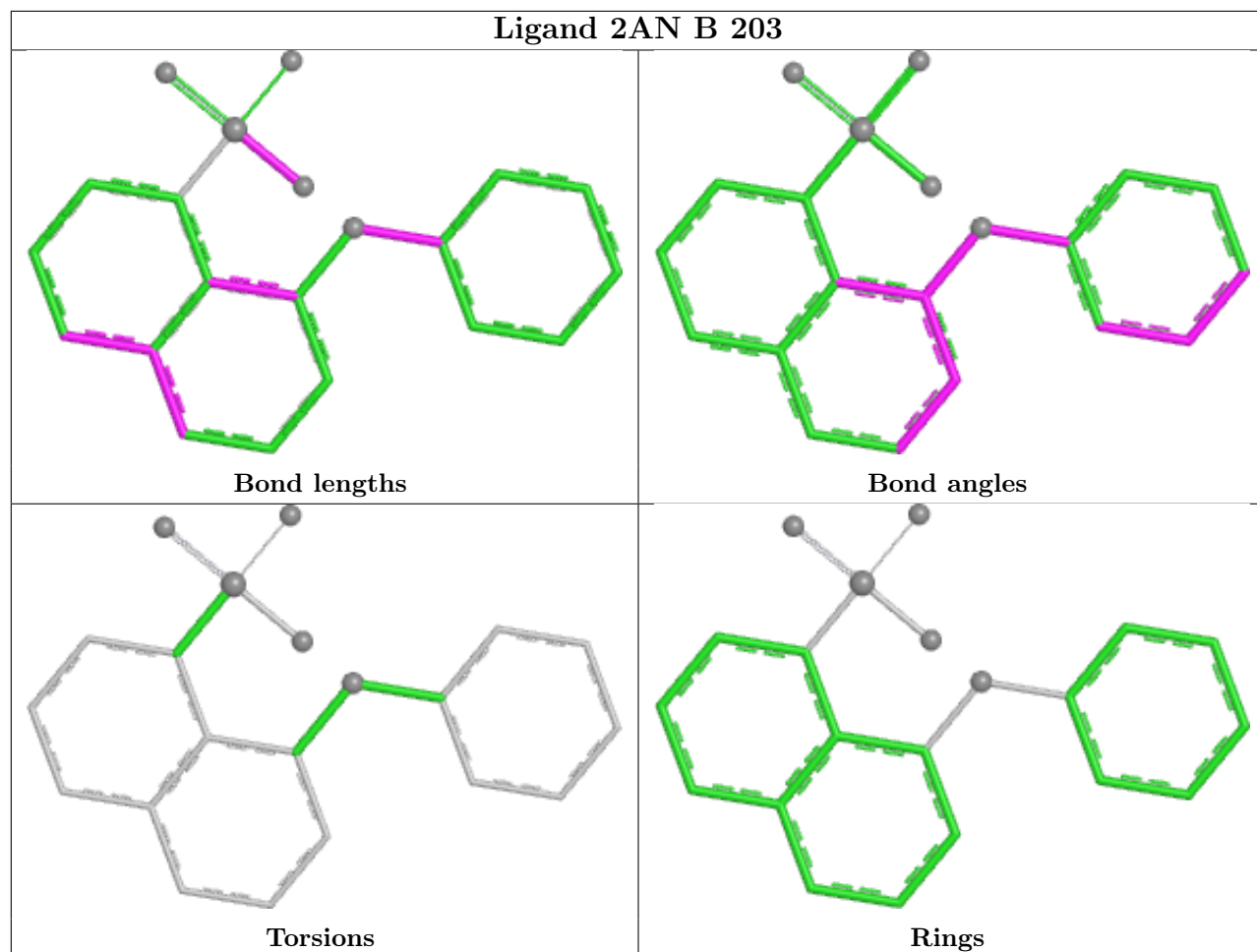


Ligand 2AN F 205

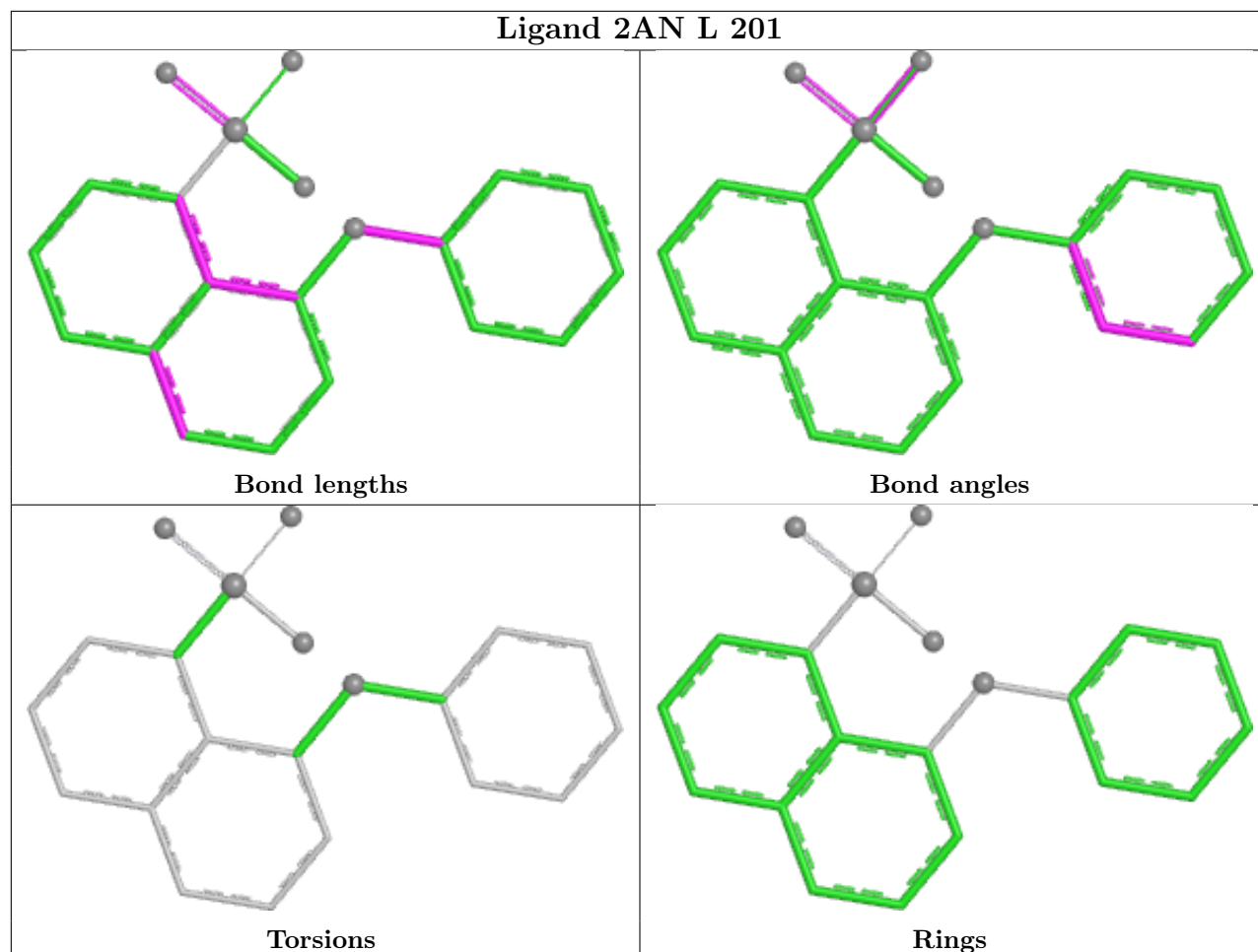


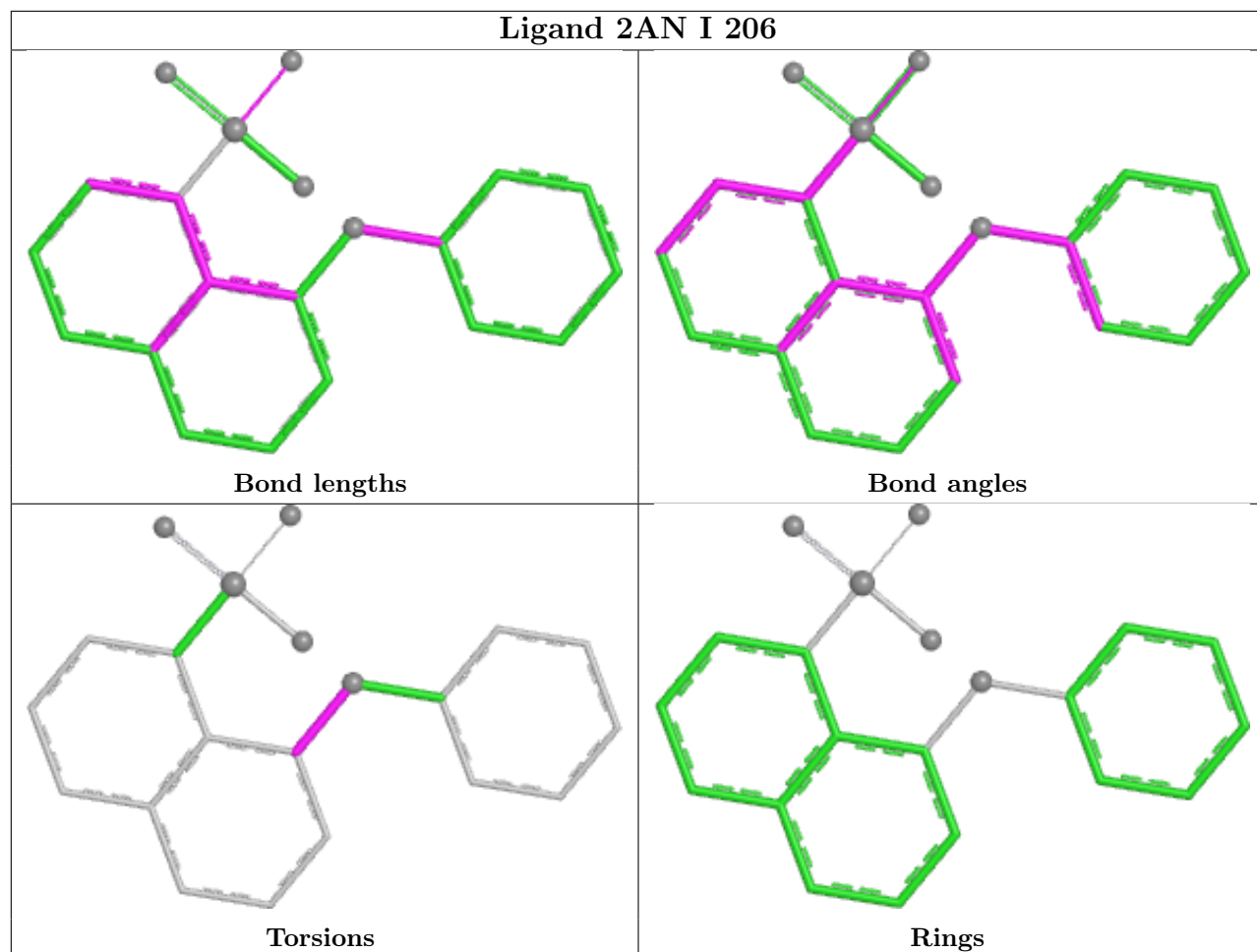
Ligand 2AN T 203



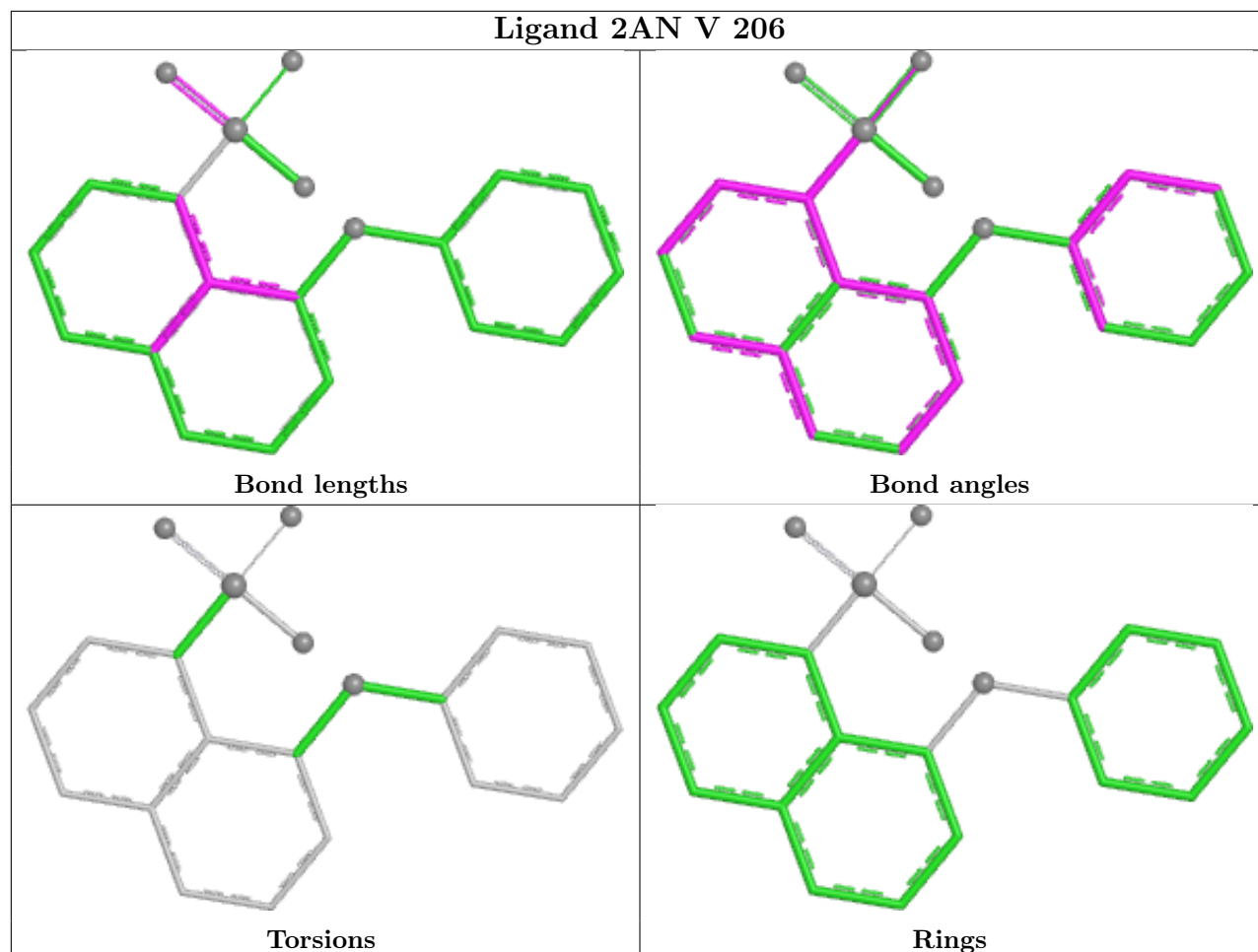


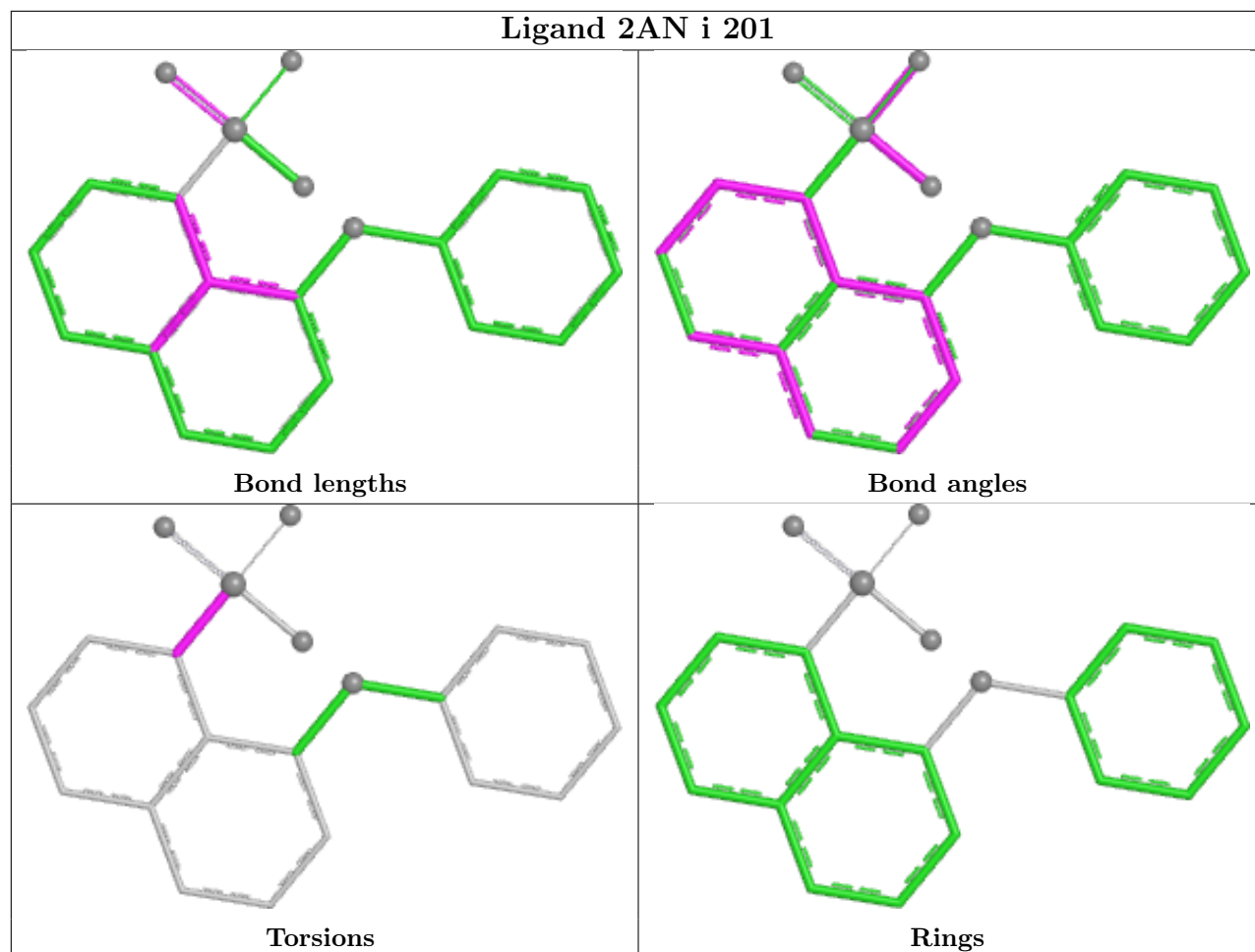
Ligand 2AN L 201





Ligand 2AN V 206





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

6.1 Protein, DNA and RNA chains

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, 95th 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 ²)	Q<0.9
1	A	162/163 (99%)	2.11	71 (43%) 0 0	56, 78, 120, 132	0
1	B	159/163 (97%)	1.57	40 (25%) 1 2	28, 62, 107, 131	2 (1%)
1	C	161/163 (98%)	2.11	78 (48%) 0 0	58, 82, 114, 139	0
1	D	159/163 (97%)	1.94	64 (40%) 0 0	46, 76, 120, 146	0
1	E	161/163 (98%)	1.67	55 (34%) 1 1	42, 63, 96, 114	0
1	F	159/163 (97%)	2.31	89 (55%) 0 0	50, 80, 115, 147	2 (1%)
1	G	162/163 (99%)	2.03	72 (44%) 0 0	37, 72, 103, 119	3 (1%)
1	H	160/163 (98%)	1.92	60 (37%) 1 1	45, 70, 112, 153	1 (0%)
1	I	161/163 (98%)	1.65	49 (30%) 1 1	39, 62, 90, 108	0
1	J	163/163 (100%)	1.93	66 (40%) 0 0	47, 72, 98, 259	1 (0%)
1	K	162/163 (99%)	1.73	50 (30%) 1 1	26, 63, 88, 111	2 (1%)
1	L	160/163 (98%)	1.50	37 (23%) 2 2	39, 61, 97, 124	4 (2%)
1	M	162/163 (99%)	1.60	44 (27%) 1 1	41, 64, 89, 131	1 (0%)
1	N	163/163 (100%)	1.62	45 (27%) 1 1	38, 61, 91, 131	0
1	O	161/163 (98%)	2.22	82 (50%) 0 0	58, 81, 105, 123	1 (0%)
1	P	159/163 (97%)	1.42	33 (20%) 2 3	22, 56, 89, 106	0
1	Q	162/163 (99%)	1.49	41 (25%) 1 2	40, 67, 100, 140	0
1	R	161/163 (98%)	1.66	46 (28%) 1 1	43, 65, 99, 120	0
1	S	160/163 (98%)	1.42	35 (21%) 2 2	35, 62, 95, 120	0
1	T	161/163 (98%)	1.60	47 (29%) 1 1	37, 61, 93, 146	3 (1%)
1	U	159/163 (97%)	2.22	81 (50%) 0 0	50, 85, 123, 163	0
1	V	159/163 (97%)	1.49	33 (20%) 2 3	34, 58, 88, 121	0
1	W	159/163 (97%)	1.95	58 (36%) 1 1	20, 73, 118, 148	7 (4%)
1	X	159/163 (97%)	2.02	74 (46%) 0 0	52, 79, 113, 135	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	Y	159/163 (97%)	1.83	60 (37%)	1	0	46, 72, 102, 124	1 (0%)
1	Z	159/163 (97%)	2.20	80 (50%)	0	0	50, 78, 104, 126	2 (1%)
1	a	159/163 (97%)	1.98	72 (45%)	0	0	40, 71, 104, 180	1 (0%)
1	b	161/163 (98%)	1.79	55 (34%)	1	1	49, 74, 102, 122	1 (0%)
1	c	159/163 (97%)	1.37	35 (22%)	2	2	36, 59, 89, 122	1 (0%)
1	d	162/163 (99%)	2.23	84 (51%)	0	0	26, 75, 108, 161	3 (1%)
1	e	161/163 (98%)	1.35	29 (18%)	3	4	32, 58, 85, 104	1 (0%)
1	f	161/163 (98%)	1.47	40 (24%)	2	2	33, 60, 91, 118	0
1	g	160/163 (98%)	1.38	33 (20%)	2	3	38, 60, 86, 115	0
1	h	162/163 (99%)	1.48	36 (22%)	2	2	25, 58, 86, 121	3 (1%)
1	i	161/163 (98%)	1.54	43 (26%)	1	1	40, 65, 93, 134	1 (0%)
1	j	159/163 (97%)	1.04	22 (13%)	6	7	30, 54, 78, 129	1 (0%)
All	All	5777/5868 (98%)	1.75	1939 (33%)	1	1	20, 68, 105, 259	42 (0%)

The worst 5 of 1939 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	59	PHE	11.8
1	R	95	ASN	9.4
1	V	130	GLU	8.9
1	R	60	VAL	8.4
1	V	129	ASN	8.4

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 oligosaccharides 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, 95th 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 ²)	Q<0.9
2	2AN	N	203	21/21	0.39	0.45	56,74,126,131	0
5	DMS	X	207	4/4	0.49	0.62	68,68,69,71	4
2	2AN	f	203	21/21	0.56	0.30	60,68,80,86	0
2	2AN	j	207	21/21	0.63	0.29	87,134,147,162	0
2	2AN	X	203	21/21	0.63	0.29	53,62,71,76	0
6	FLC	e	202	13/13	0.66	0.23	62,69,75,77	0
2	2AN	h	205	21/21	0.67	0.34	127,179,191,208	0
2	2AN	d	203	21/21	0.69	0.29	66,79,115,120	0
2	2AN	D	204	21/21	0.69	0.31	68,98,111,114	0
2	2AN	b	206	21/21	0.73	0.32	57,86,103,108	21
2	2AN	X	206	21/21	0.74	0.25	48,61,70,74	0
2	2AN	G	207	21/21	0.75	0.28	62,68,79,90	21
2	2AN	a	204	21/21	0.75	0.38	54,112,142,163	21
2	2AN	I	207	21/21	0.76	0.36	68,96,114,116	21
2	2AN	S	204	21/21	0.77	0.43	50,62,75,79	21
5	DMS	G	208	4/4	0.77	0.30	61,61,63,75	4
4	EPE	P	205	15/15	0.78	0.27	57,75,92,109	0
2	2AN	j	205	21/21	0.78	0.24	31,43,51,57	0
2	2AN	R	205	21/21	0.79	0.25	77,99,112,117	0
2	2AN	d	204	21/21	0.79	0.40	50,68,80,82	21
2	2AN	c	202	21/21	0.79	0.25	56,68,103,110	0
2	2AN	b	205	21/21	0.79	0.29	114,123,138,168	0
2	2AN	I	205	21/21	0.80	0.25	57,74,84,86	21
3	SO4	Q	204	5/5	0.80	0.18	47,67,73,75	5
2	2AN	A	204	21/21	0.80	0.58	58,79,92,95	21
2	2AN	R	204	21/21	0.80	0.22	61,75,82,83	0
2	2AN	F	206	21/21	0.80	0.34	49,63,97,104	21
2	2AN	Y	204	21/21	0.80	0.30	47,58,66,70	21
6	FLC	a	206	13/13	0.80	0.14	60,76,89,90	13
2	2AN	I	204	21/21	0.81	0.29	57,71,83,89	21
2	2AN	G	204	21/21	0.82	0.23	47,66,102,109	21
2	2AN	T	203	21/21	0.82	0.23	45,60,101,108	0
2	2AN	Y	201	21/21	0.83	0.21	63,72,89,91	0
5	DMS	N	206	4/4	0.83	0.28	36,47,47,48	4
2	2AN	U	202	21/21	0.83	0.46	76,90,110,117	21
6	FLC	i	202	13/13	0.83	0.17	47,60,64,70	13
2	2AN	f	206	21/21	0.84	0.23	62,76,97,101	21
2	2AN	T	204	21/21	0.84	0.20	50,64,70,85	0
2	2AN	S	203	21/21	0.84	0.28	46,51,80,83	21
2	2AN	H	204	21/21	0.84	0.23	71,79,107,109	21
6	FLC	j	208	13/13	0.84	0.27	30,38,45,59	13

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	2AN	G	205	21/21	0.84	0.23	32,40,50,55	21
2	2AN	j	206	21/21	0.85	0.20	52,69,105,107	0
2	2AN	I	203	21/21	0.85	0.20	63,75,83,91	21
2	2AN	F	204	21/21	0.86	0.27	74,96,127,138	0
2	2AN	O	202	21/21	0.86	0.21	74,83,90,94	21
2	2AN	c	203	21/21	0.86	0.19	58,78,115,123	0
2	2AN	F	202	21/21	0.86	0.19	50,81,108,112	0
6	FLC	i	203	13/13	0.86	0.08	45,52,60,62	0
3	SO4	Y	205	5/5	0.87	0.26	29,31,38,41	5
2	2AN	S	201	21/21	0.87	0.18	81,103,116,120	0
2	2AN	a	201	21/21	0.87	0.22	58,96,117,123	0
2	2AN	C	203[A]	21/21	0.87	0.30	51,60,72,76	21
2	2AN	V	208	21/21	0.87	0.25	54,67,114,129	21
6	FLC	G	206	13/13	0.87	0.24	45,60,64,69	13
2	2AN	Z	206	21/21	0.87	0.17	55,78,100,109	0
2	2AN	E	204	21/21	0.87	0.29	48,69,105,112	21
2	2AN	N	205	21/21	0.87	0.18	53,68,76,88	0
2	2AN	T	205	21/21	0.87	0.17	54,60,75,78	0
3	SO4	G	209	5/5	0.87	0.12	52,59,68,70	5
2	2AN	V	207	21/21	0.88	0.21	48,62,88,96	0
6	FLC	a	205	13/13	0.88	0.18	55,64,75,77	13
3	SO4	A	205	5/5	0.88	0.28	23,24,27,29	5
2	2AN	Z	202	21/21	0.88	0.18	88,99,106,119	0
2	2AN	I	206	21/21	0.88	0.19	54,78,87,90	0
2	2AN	W	201	21/21	0.88	0.20	45,60,69,73	21
2	2AN	X	202	21/21	0.89	0.17	70,81,106,111	0
2	2AN	h	203	21/21	0.89	0.16	36,44,58,66	0
2	2AN	A	202	21/21	0.89	0.16	54,71,83,94	0
2	2AN	c	205	21/21	0.89	0.23	38,48,57,61	21
2	2AN	Z	204	21/21	0.89	0.15	69,80,92,97	0
2	2AN	B	206	21/21	0.89	0.21	65,80,111,114	0
2	2AN	Q	203	21/21	0.89	0.17	81,100,118,121	0
2	2AN	U	201	21/21	0.89	0.21	89,112,138,139	0
2	2AN	K	203	21/21	0.89	0.20	45,61,72,73	21
2	2AN	V	206	21/21	0.90	0.16	50,64,84,93	0
2	2AN	a	203	21/21	0.90	0.17	58,67,76,81	0
2	2AN	j	204	21/21	0.90	0.16	44,54,66,71	0
2	2AN	Y	203	21/21	0.90	0.15	52,68,87,92	0
2	2AN	A	203	21/21	0.90	0.19	61,67,94,98	21
2	2AN	X	201	21/21	0.90	0.17	40,49,81,90	0
2	2AN	h	201	21/21	0.90	0.20	34,48,53,62	21
2	2AN	E	203	21/21	0.90	0.18	44,52,76,79	21

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	2AN	O	203	21/21	0.90	0.14	53,63,74,92	0
2	2AN	g	201	21/21	0.90	0.20	46,57,79,83	21
2	2AN	g	203	21/21	0.90	0.16	48,76,86,88	0
2	2AN	Z	205	21/21	0.90	0.17	68,75,126,139	0
2	2AN	D	203	21/21	0.90	0.16	72,78,87,91	0
2	2AN	P	203	21/21	0.91	0.17	44,55,68,85	0
2	2AN	F	205	21/21	0.91	0.18	67,91,99,104	0
2	2AN	Z	201	21/21	0.91	0.14	54,62,71,78	0
2	2AN	X	204	21/21	0.91	0.14	63,74,85,91	0
3	SO4	c	207	5/5	0.91	0.20	27,27,32,36	5
3	SO4	c	208	5/5	0.91	0.18	32,36,36,41	5
2	2AN	d	201	21/21	0.91	0.15	46,61,68,72	0
2	2AN	j	201	21/21	0.91	0.13	34,48,58,61	0
2	2AN	d	202	21/21	0.91	0.15	50,61,76,81	0
2	2AN	R	202	21/21	0.92	0.12	36,49,57,62	0
2	2AN	C	201	21/21	0.92	0.13	46,57,67,84	0
2	2AN	B	204	21/21	0.92	0.15	43,52,59,59	21
2	2AN	b	202	21/21	0.92	0.14	54,68,80,85	0
2	2AN	b	204	21/21	0.92	0.15	65,72,87,92	0
2	2AN	Y	202	21/21	0.92	0.18	45,53,56,59	21
2	2AN	G	201	21/21	0.92	0.14	48,55,82,93	0
2	2AN	B	205	21/21	0.92	0.15	48,62,80,82	0
2	2AN	h	206	21/21	0.92	0.13	39,57,75,82	0
2	2AN	M	203	21/21	0.92	0.17	57,73,80,81	0
2	2AN	L	204	21/21	0.92	0.12	65,75,91,95	0
2	2AN	D	202	21/21	0.92	0.13	50,59,76,79	0
2	2AN	F	201	21/21	0.92	0.17	61,70,79,84	0
2	2AN	X	205	21/21	0.92	0.13	55,66,81,86	0
2	2AN	f	204	21/21	0.93	0.14	38,50,60,72	0
2	2AN	J	201	21/21	0.93	0.18	53,69,97,103	0
2	2AN	b	203	21/21	0.93	0.11	47,55,66,72	0
2	2AN	B	203	21/21	0.93	0.16	38,49,74,80	0
2	2AN	i	201	21/21	0.93	0.16	40,48,51,52	21
2	2AN	N	204	21/21	0.93	0.17	53,64,92,95	0
2	2AN	V	201	21/21	0.93	0.14	46,58,79,93	0
2	2AN	c	204	21/21	0.94	0.16	39,46,53,55	21
2	2AN	P	204	21/21	0.94	0.16	36,52,60,62	0
2	2AN	b	201	21/21	0.94	0.14	44,52,58,60	0
2	2AN	T	202	21/21	0.94	0.16	31,39,49,52	21
2	2AN	J	202	21/21	0.94	0.16	44,52,71,73	0
2	2AN	G	203	21/21	0.94	0.18	42,52,92,100	0
2	2AN	f	205	21/21	0.94	0.13	41,54,66,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	2AN	O	201	21/21	0.94	0.14	42,62,79,92	0
3	SO4	c	209	5/5	0.94	0.12	47,52,58,61	5
2	2AN	S	202	21/21	0.94	0.13	46,56,69,70	21
2	2AN	e	201	21/21	0.94	0.14	39,50,52,57	0
2	2AN	Q	202	21/21	0.94	0.15	46,64,70,74	0
2	2AN	a	202	21/21	0.94	0.14	46,52,60,66	0
2	2AN	L	203	21/21	0.94	0.12	33,53,64,65	0
2	2AN	B	202	21/21	0.94	0.13	45,59,67,68	0
2	2AN	A	201	21/21	0.94	0.17	46,57,80,91	0
2	2AN	F	203	21/21	0.94	0.17	51,61,81,84	0
2	2AN	V	204	21/21	0.94	0.12	50,63,75,86	0
2	2AN	V	205	21/21	0.94	0.14	42,59,68,72	0
2	2AN	Z	203	21/21	0.94	0.14	60,69,82,90	0
2	2AN	C	202	21/21	0.94	0.16	66,99,110,116	0
2	2AN	P	202	21/21	0.95	0.12	29,43,52,57	0
2	2AN	L	202	21/21	0.95	0.13	46,54,67,71	0
3	SO4	I	208	5/5	0.95	0.10	35,36,41,46	5
2	2AN	H	202	21/21	0.95	0.12	48,67,79,83	0
2	2AN	V	203	21/21	0.95	0.12	44,52,61,62	0
2	2AN	f	202	21/21	0.95	0.12	33,49,57,62	0
2	2AN	H	203	21/21	0.95	0.13	53,66,79,84	0
2	2AN	B	201	21/21	0.95	0.12	35,51,62,63	0
2	2AN	J	203	21/21	0.95	0.12	43,69,75,80	0
2	2AN	E	201	21/21	0.95	0.13	40,49,68,76	0
2	2AN	E	202	21/21	0.95	0.12	34,41,50,65	0
2	2AN	G	202	21/21	0.95	0.13	56,64,68,75	0
2	2AN	T	201	21/21	0.95	0.12	38,49,58,65	0
2	2AN	h	204	21/21	0.95	0.15	48,67,91,97	0
2	2AN	I	202	21/21	0.95	0.15	37,47,59,69	0
2	2AN	R	203	21/21	0.95	0.14	54,73,82,84	0
2	2AN	K	201	21/21	0.95	0.11	38,44,66,82	0
2	2AN	g	202	21/21	0.95	0.11	37,51,60,64	0
2	2AN	K	202	21/21	0.95	0.19	45,54,83,89	0
2	2AN	V	202	21/21	0.96	0.12	26,40,56,62	0
2	2AN	h	202	21/21	0.96	0.12	37,52,59,61	0
2	2AN	D	201	21/21	0.96	0.13	38,69,79,84	0
3	SO4	g	204	5/5	0.96	0.11	24,30,34,38	5
2	2AN	N	201	21/21	0.96	0.12	36,44,54,58	0
2	2AN	H	201	21/21	0.96	0.14	44,58,62,65	0
2	2AN	M	201	21/21	0.96	0.15	40,49,59,60	0
2	2AN	c	206	21/21	0.96	0.13	30,44,58,62	0
2	2AN	N	202	21/21	0.96	0.14	37,52,61,64	0

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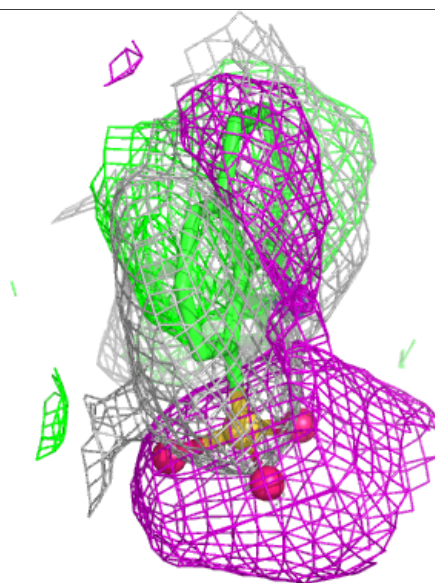
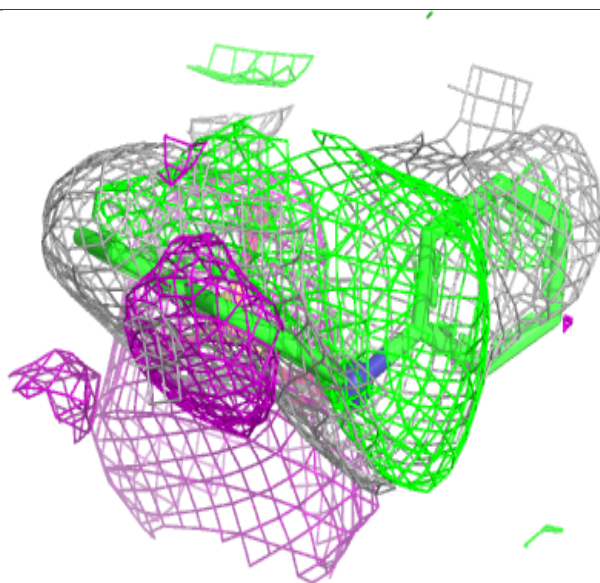
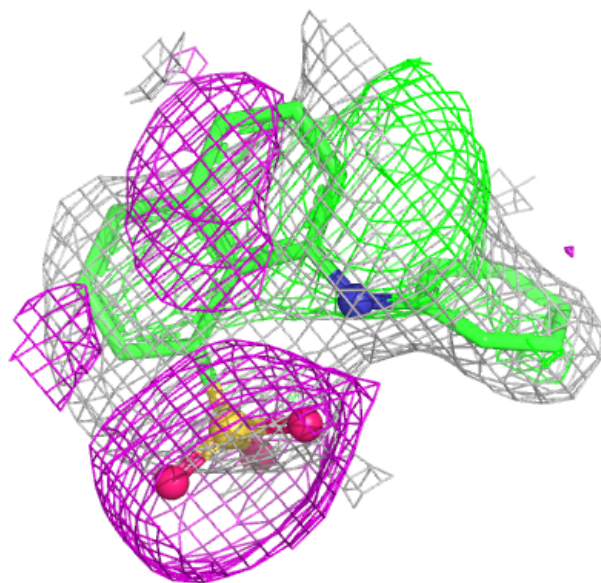
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	2AN	j	202	21/21	0.96	0.11	26,40,57,58	0
2	2AN	L	201	21/21	0.96	0.13	37,47,56,57	0
2	2AN	Q	201	21/21	0.96	0.12	40,50,60,67	0
2	2AN	f	201	21/21	0.96	0.12	34,40,48,49	0
2	2AN	P	201	21/21	0.96	0.10	38,50,59,61	0
2	2AN	c	201	21/21	0.96	0.12	35,45,58,59	0
2	2AN	M	202	21/21	0.97	0.10	38,48,54,56	0
2	2AN	I	201	21/21	0.97	0.11	28,39,57,62	0
2	2AN	j	203	21/21	0.97	0.11	32,40,49,58	0
3	SO4	E	205	5/5	0.97	0.12	34,41,51,56	5
2	2AN	R	201	21/21	0.98	0.10	29,52,60,61	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.

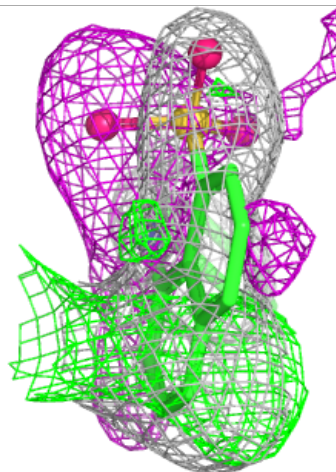
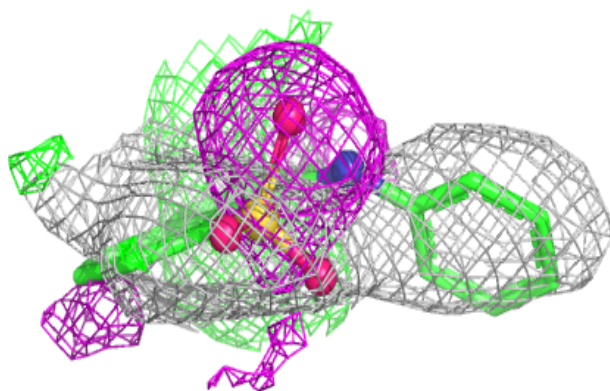
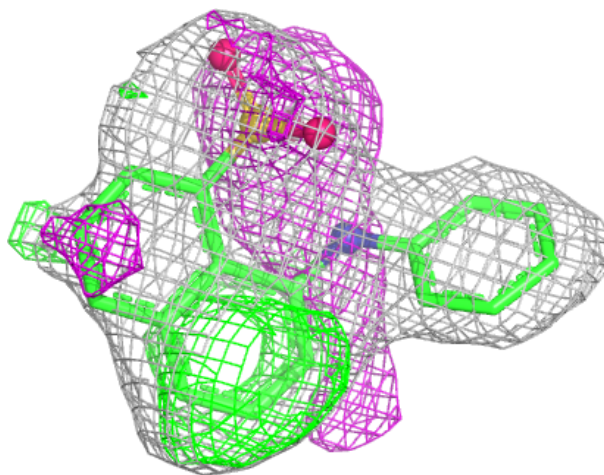
Electron density around 2AN N 203:

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



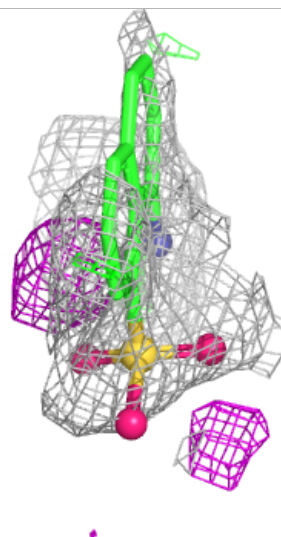
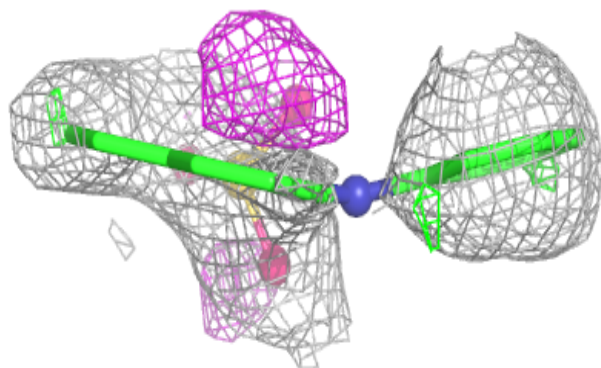
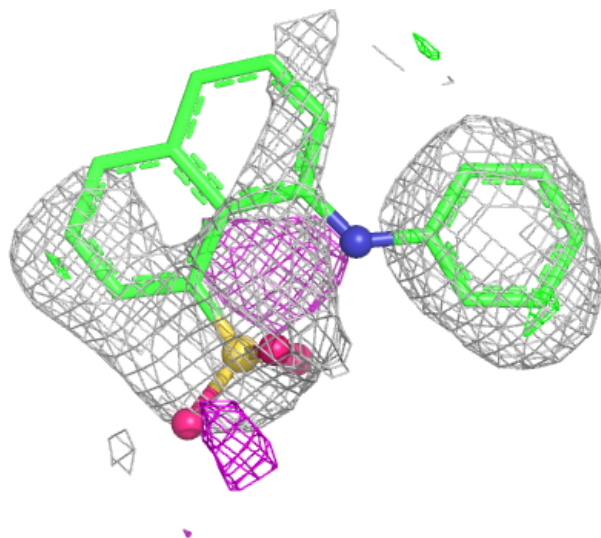
Electron density around 2AN f 203:

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



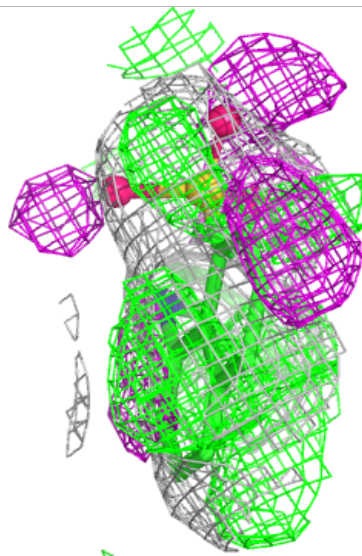
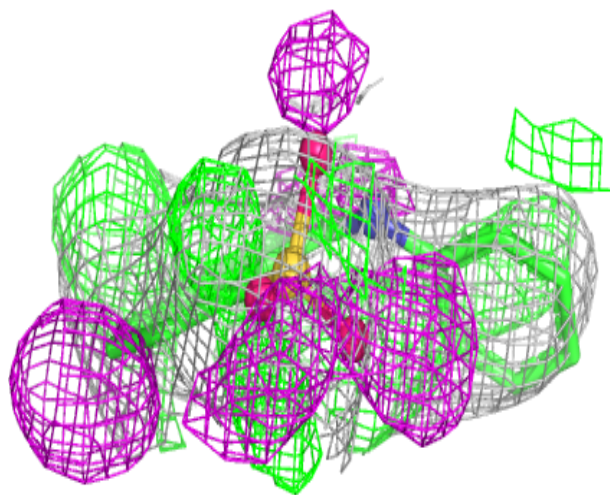
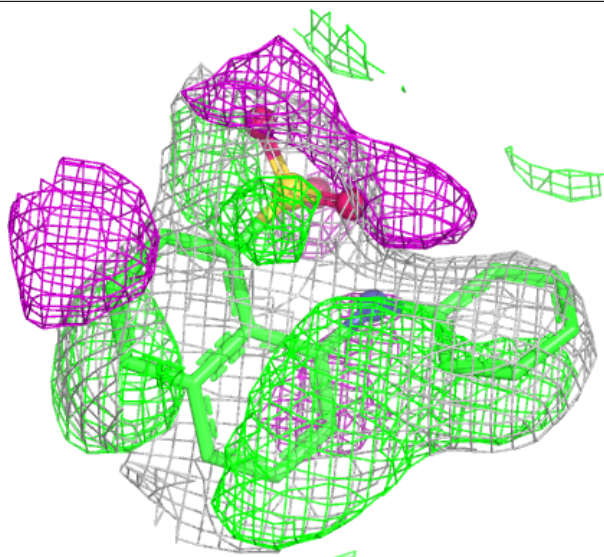
Electron density around 2AN j 207:

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



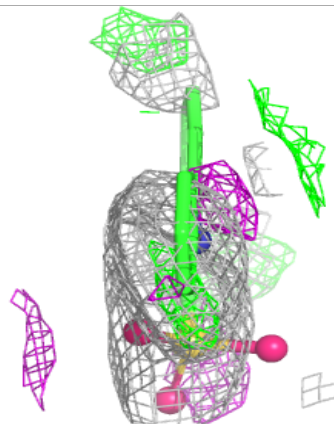
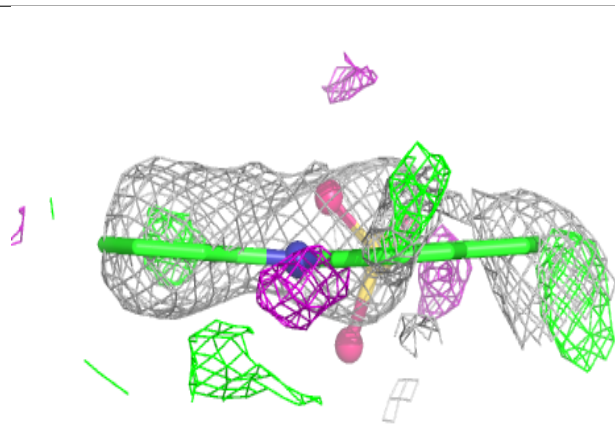
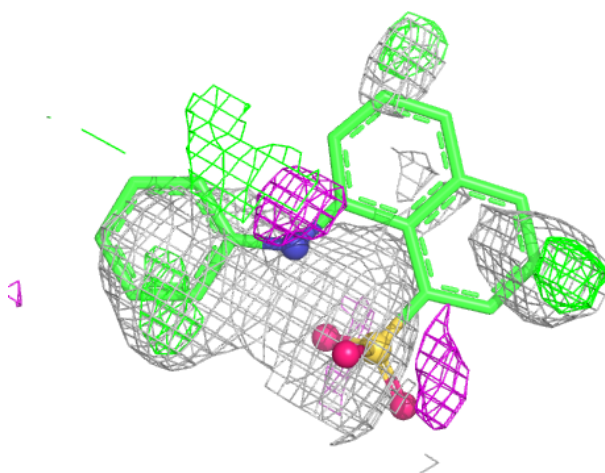
Electron density around 2AN X 203:

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



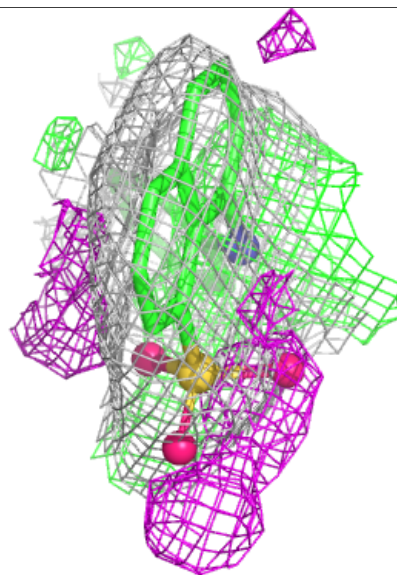
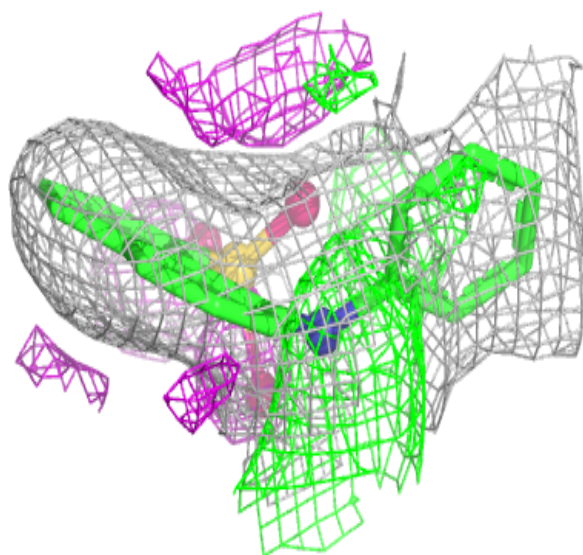
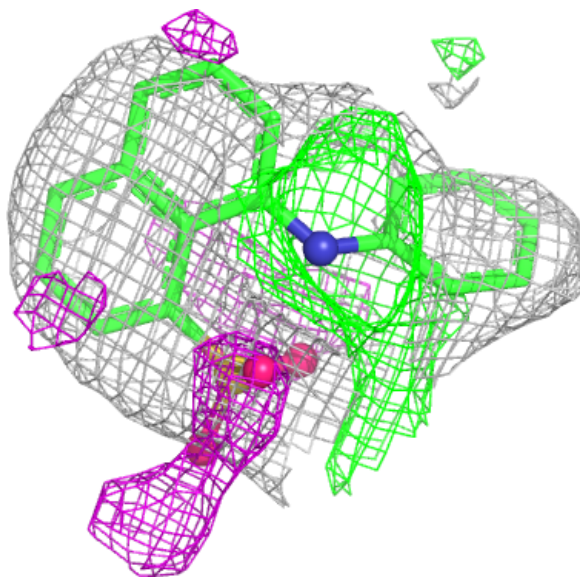
Electron density around 2AN h 205:

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



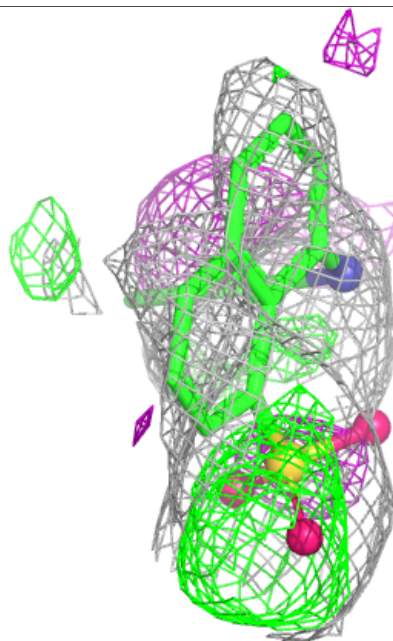
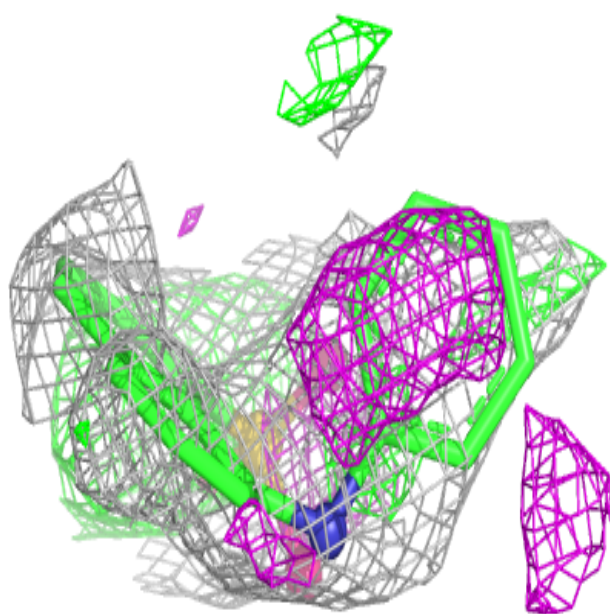
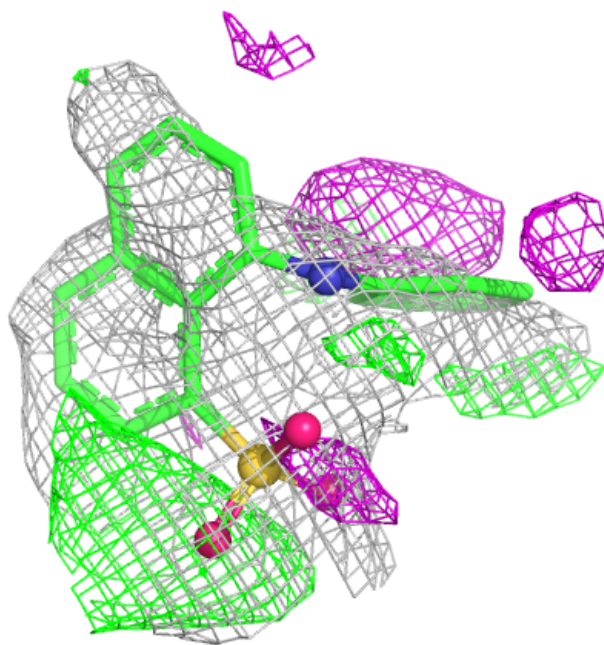
Electron density around 2AN d 203:

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



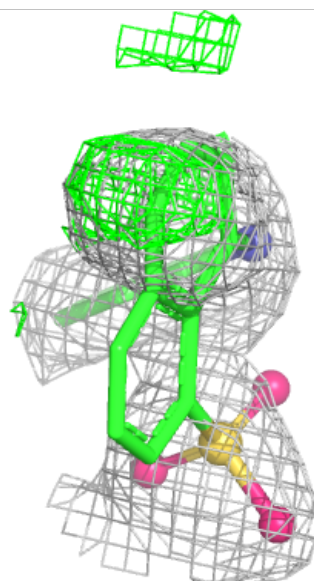
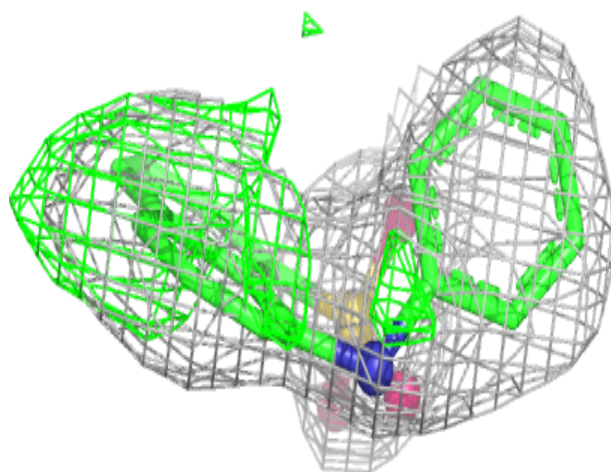
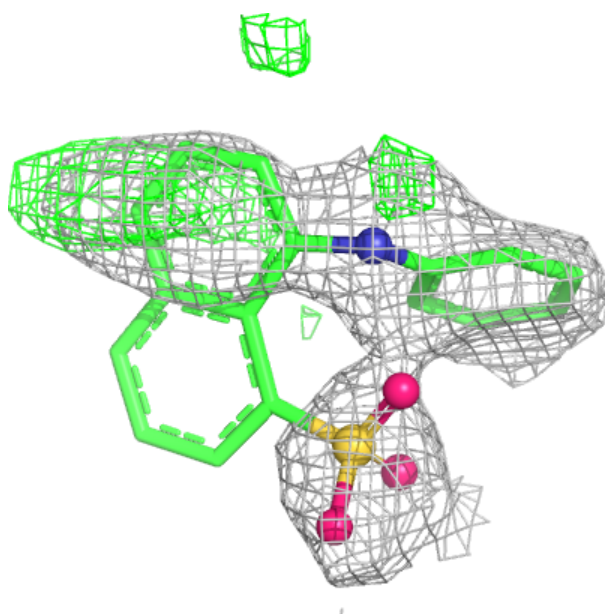
Electron density around 2AN D 204:

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



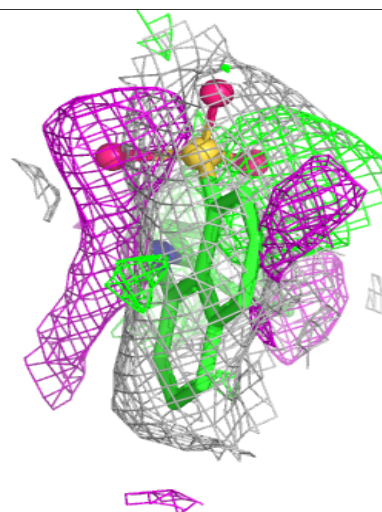
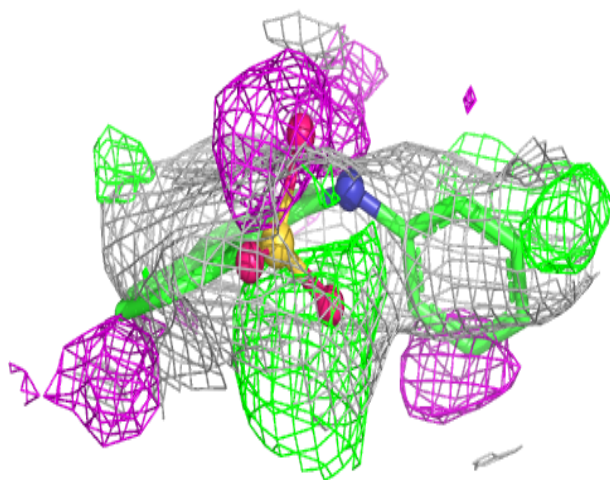
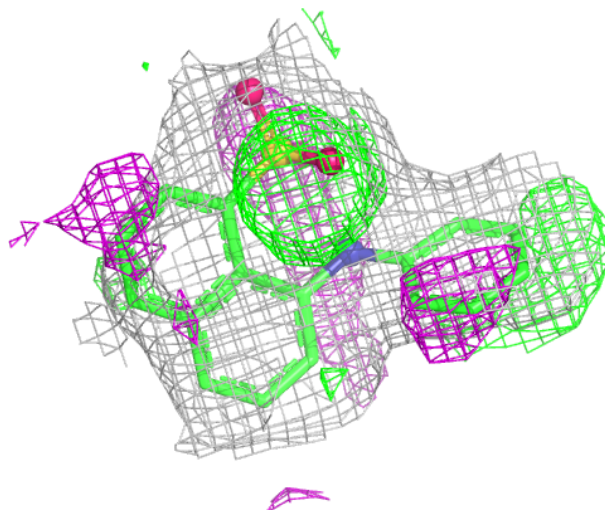
Electron density around 2AN b 206:

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



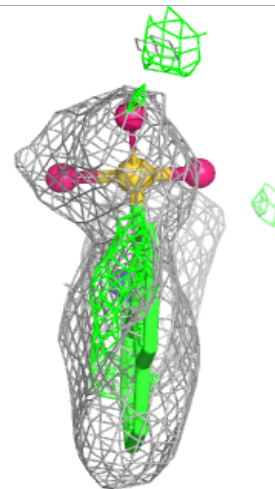
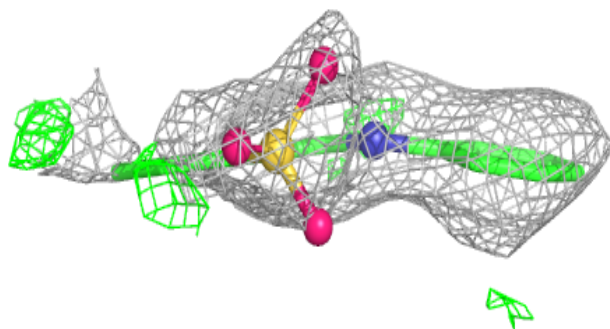
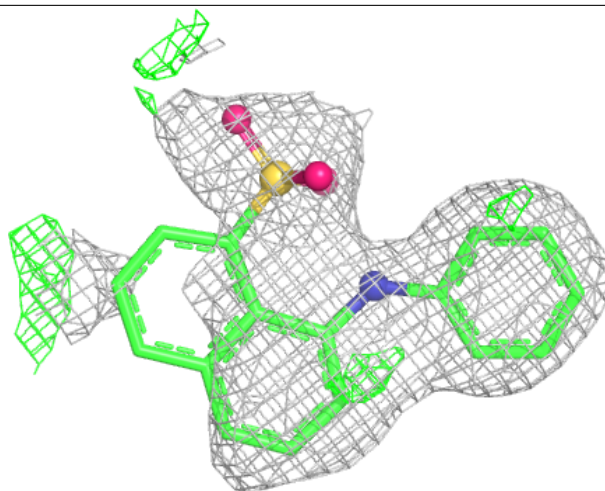
Electron density around 2AN X 206:

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



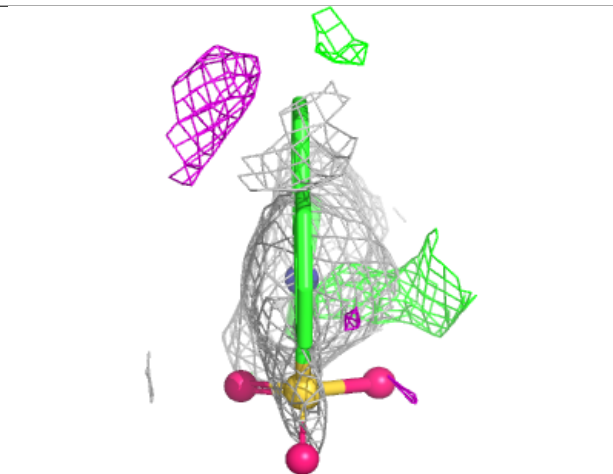
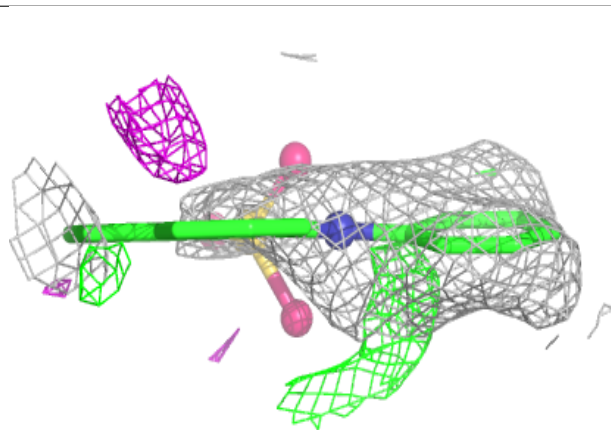
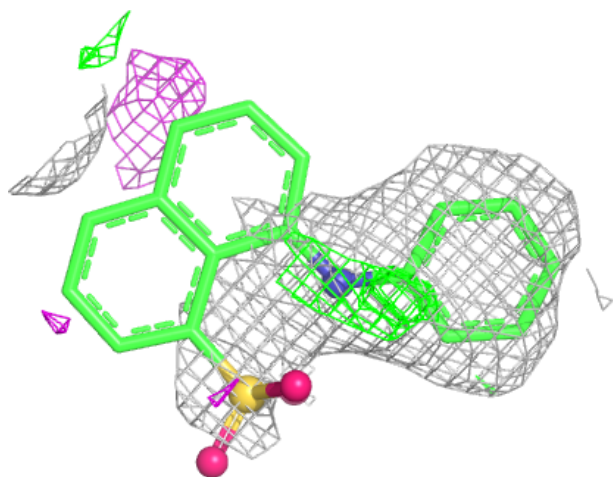
Electron density around 2AN G 207:

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



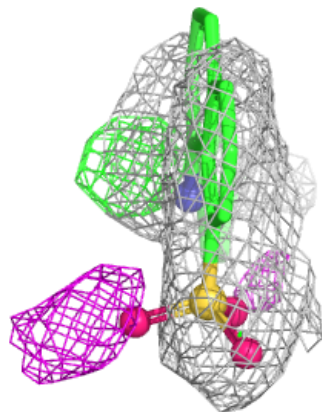
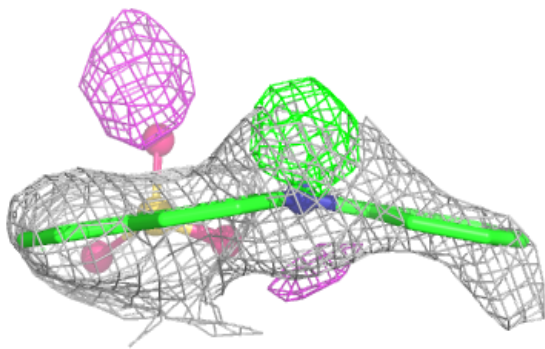
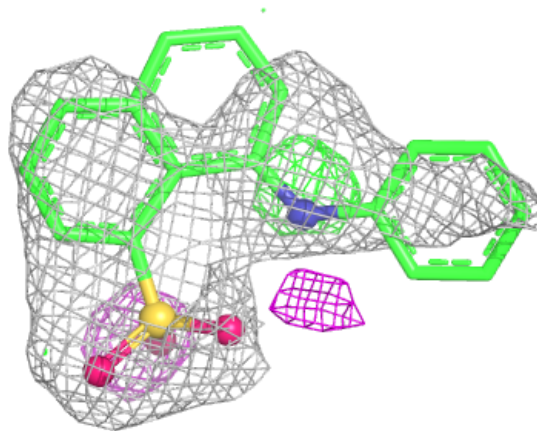
Electron density around 2AN a 204:

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



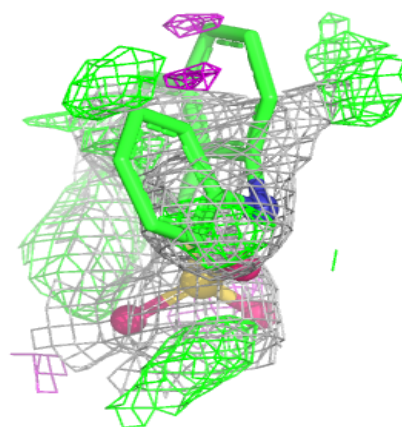
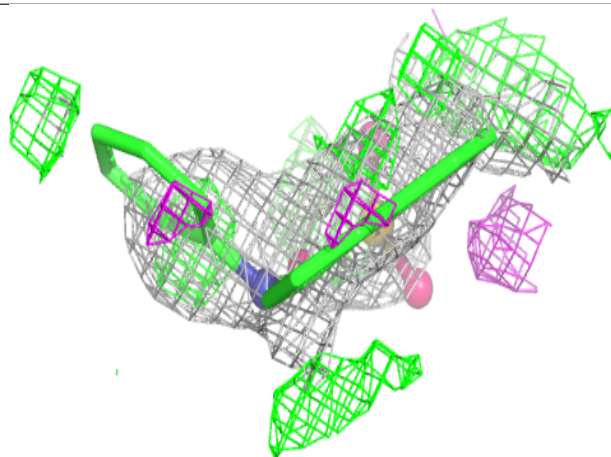
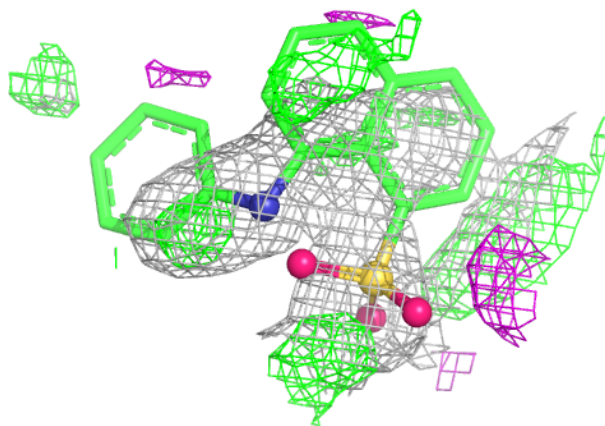
Electron density around 2AN I 207:

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



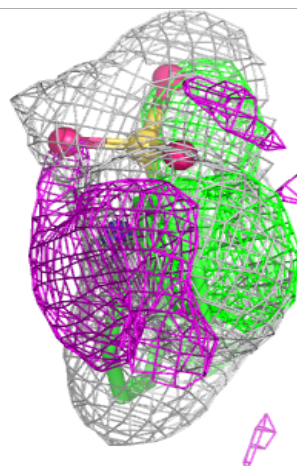
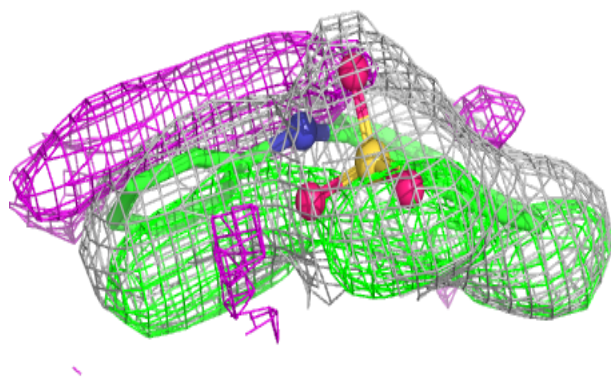
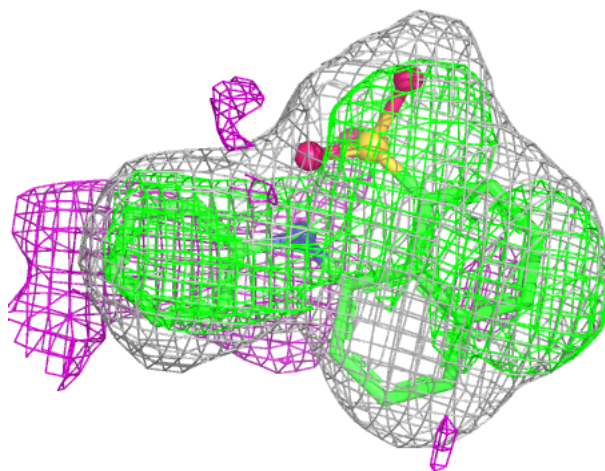
Electron density around 2AN S 204:

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



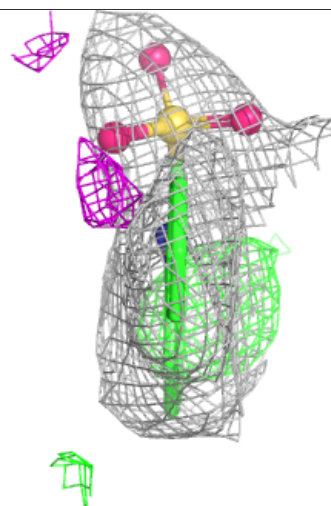
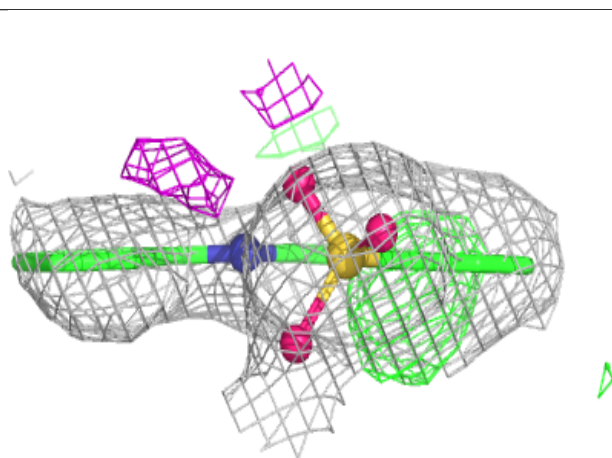
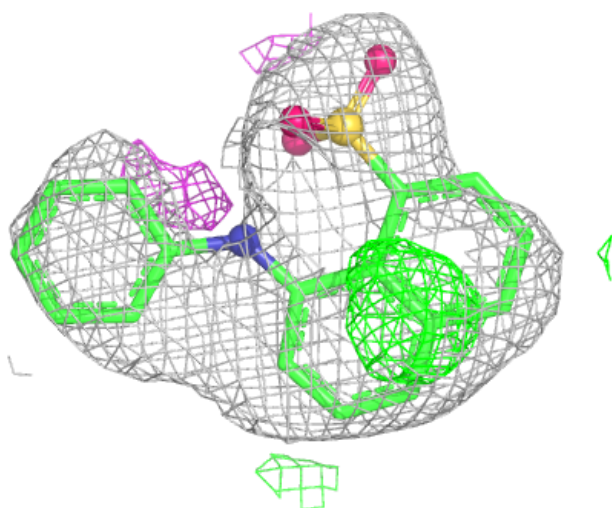
Electron density around 2AN j 205:

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



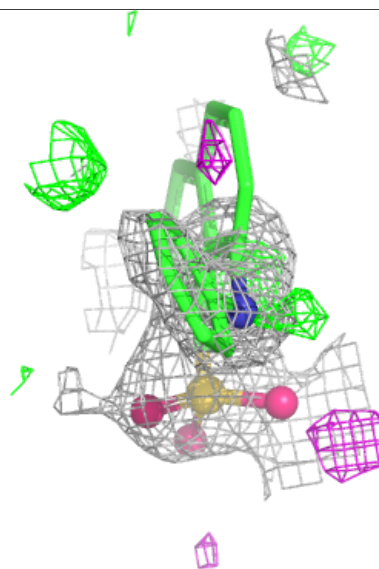
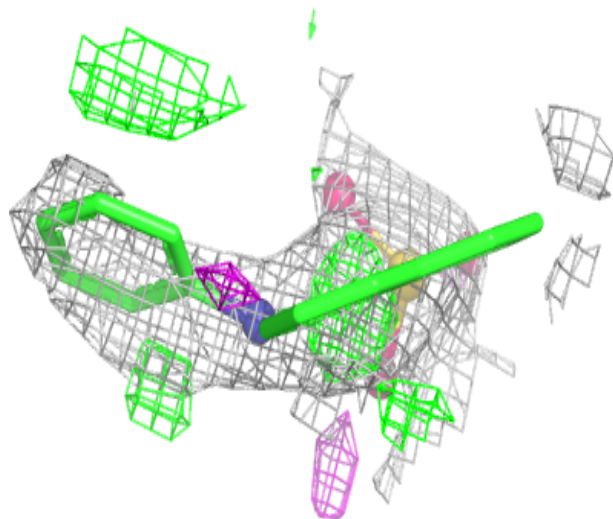
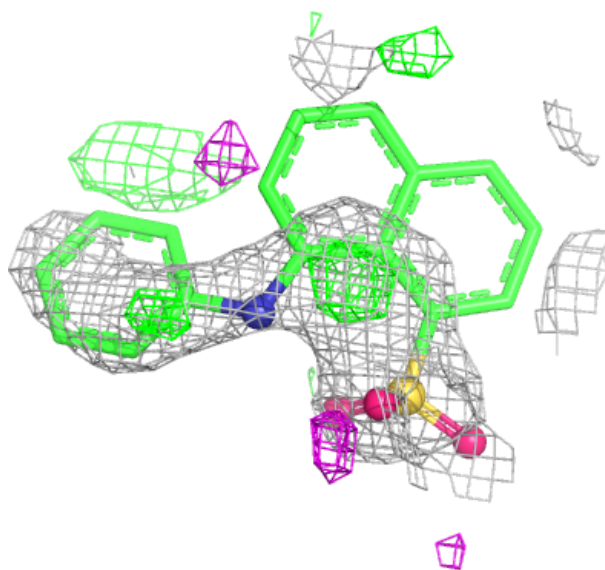
Electron density around 2AN R 205:

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



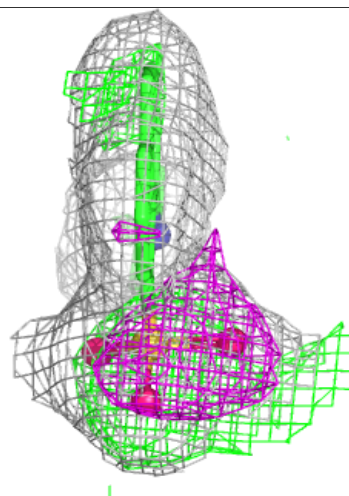
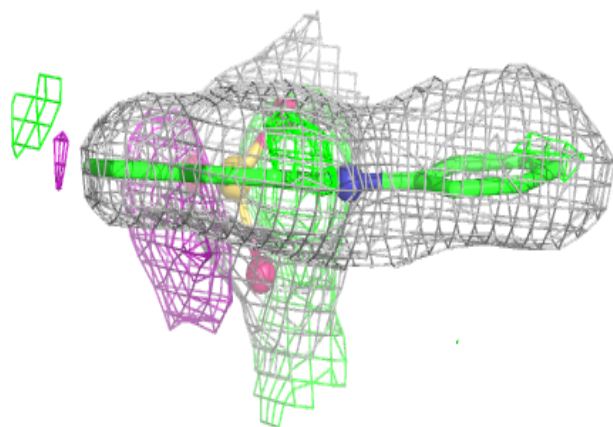
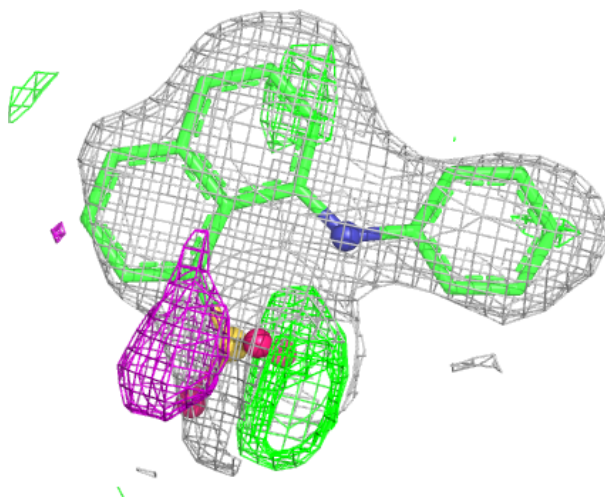
Electron density around 2AN d 204:

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



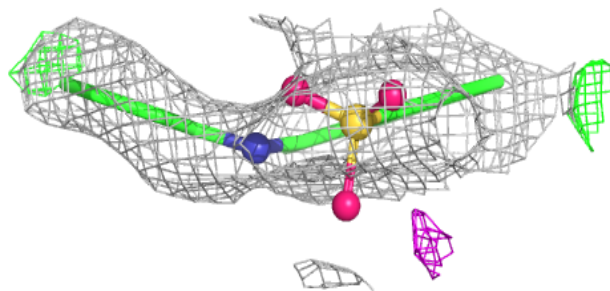
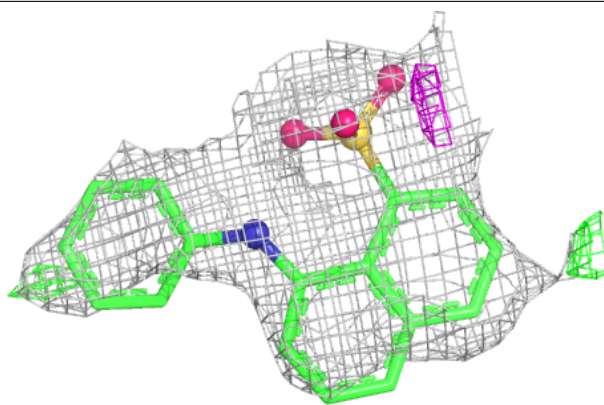
Electron density around 2AN c 202:

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



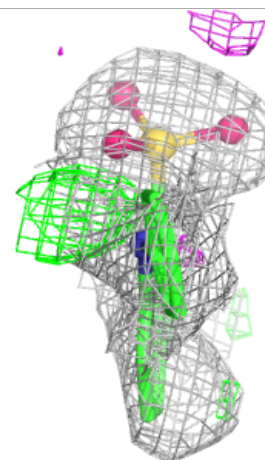
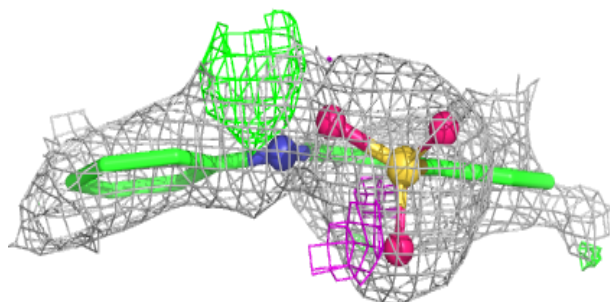
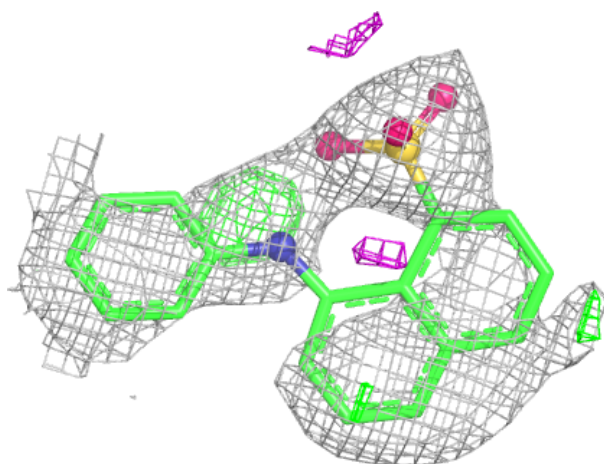
Electron density around 2AN b 205:

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



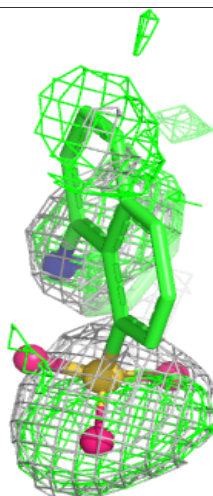
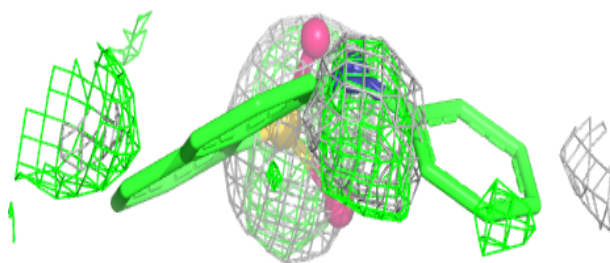
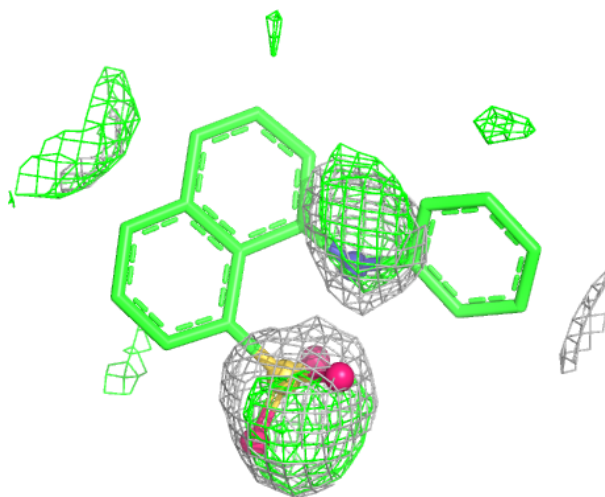
Electron density around 2AN I 205:

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



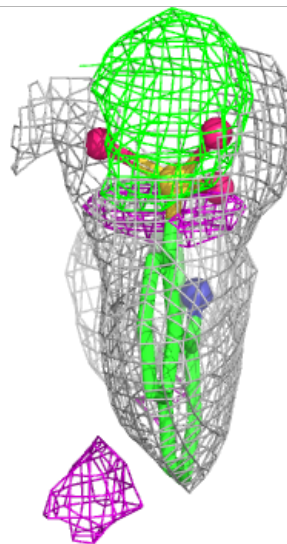
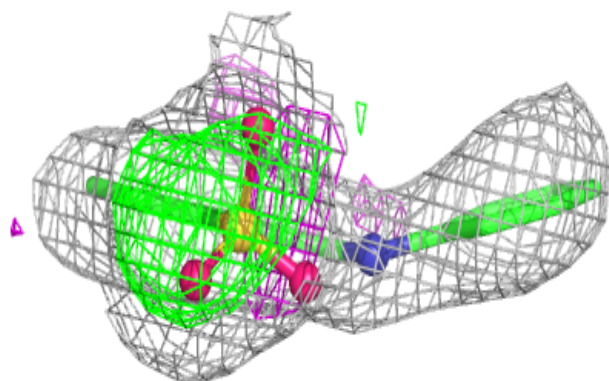
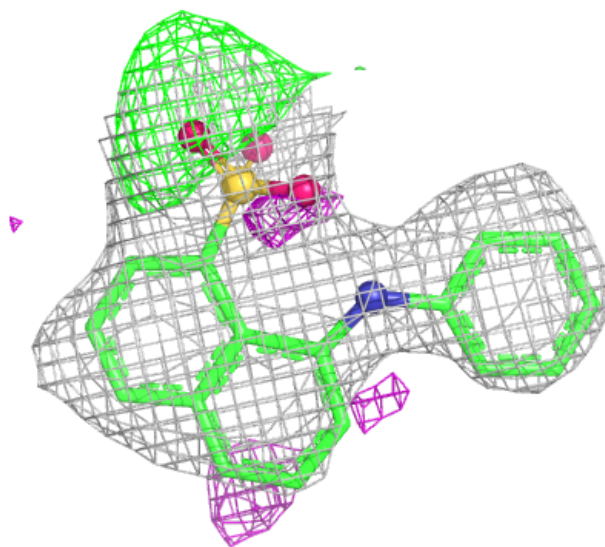
Electron density around 2AN A 204:

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



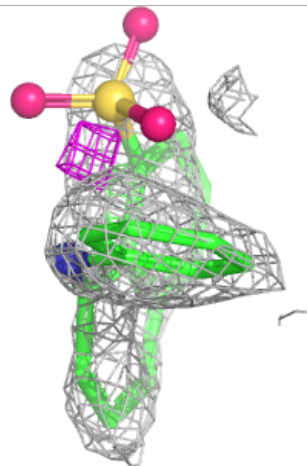
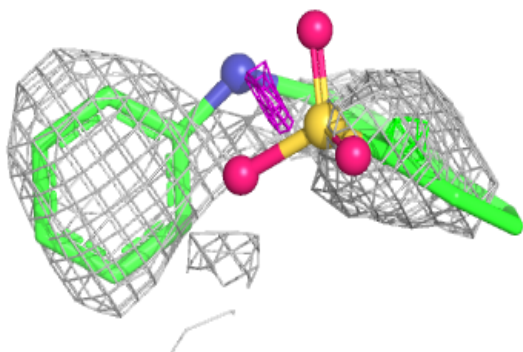
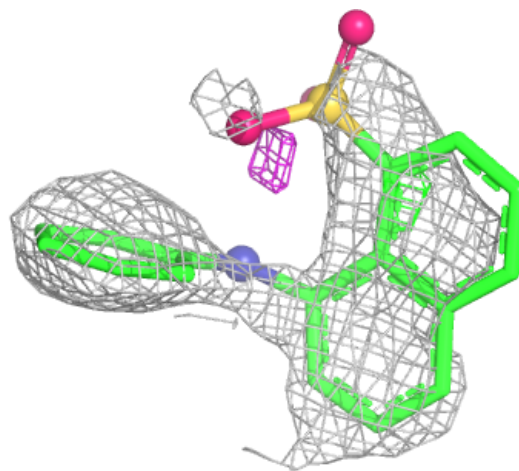
Electron density around 2AN R 204:

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



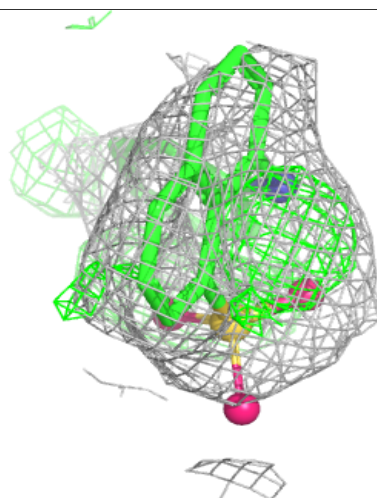
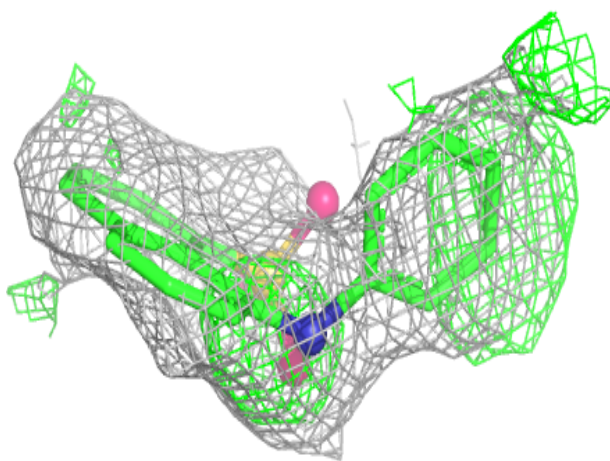
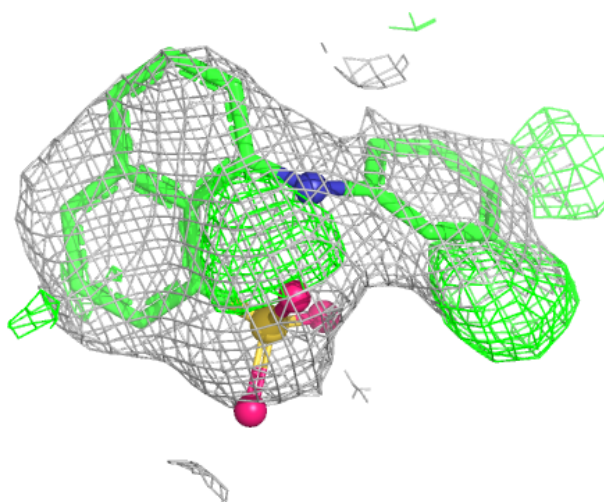
Electron density around 2AN F 206:

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



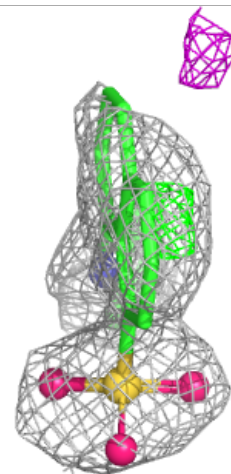
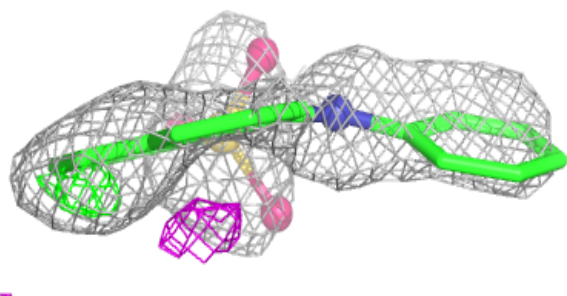
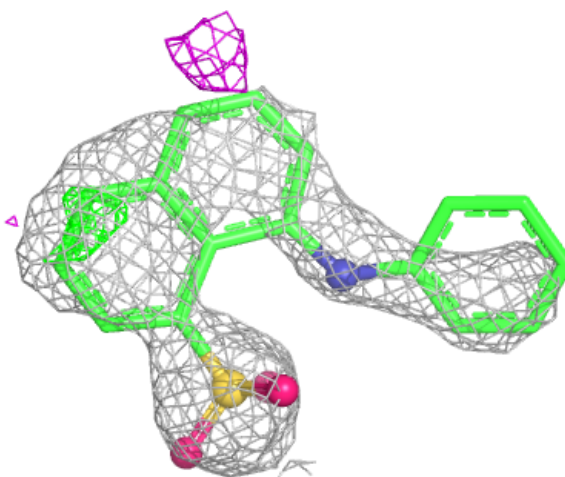
Electron density around 2AN Y 204:

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



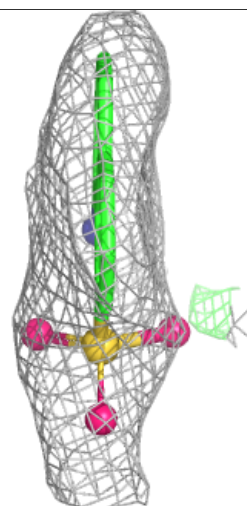
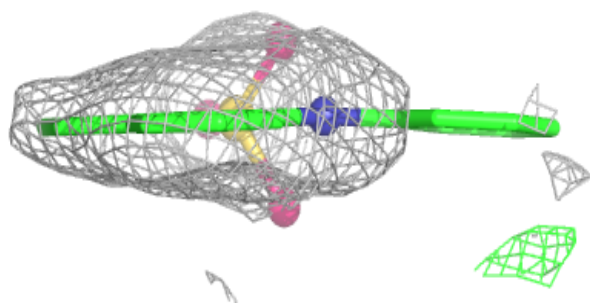
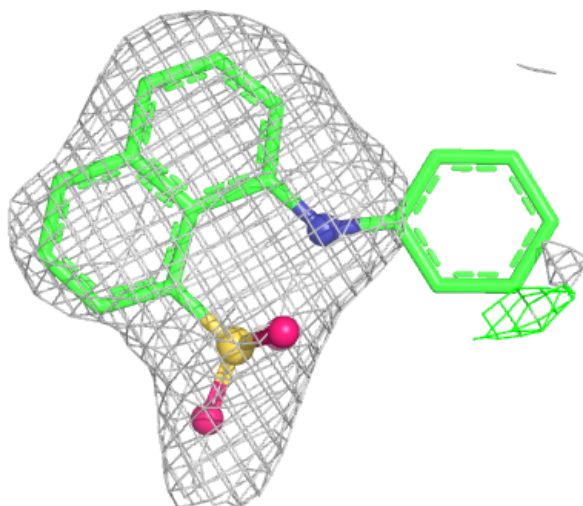
Electron density around 2AN I 204:

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



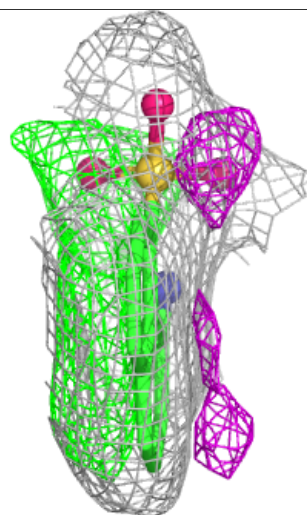
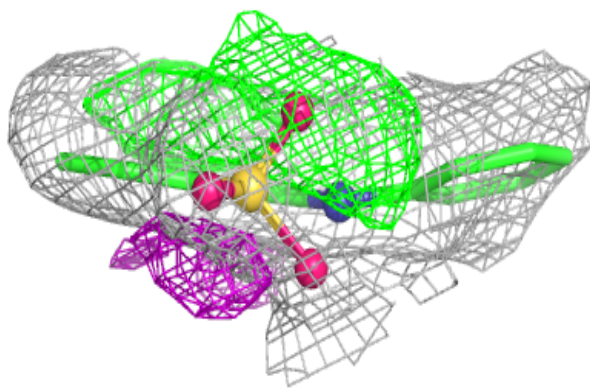
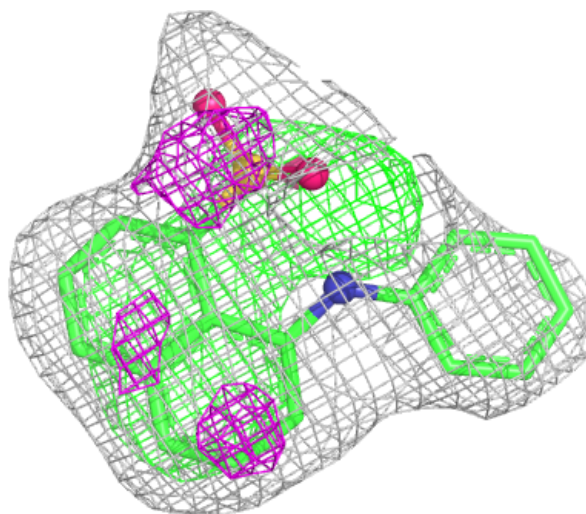
Electron density around 2AN G 204:

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



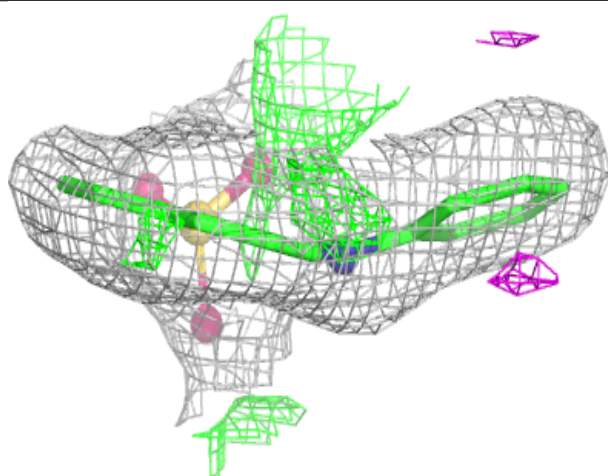
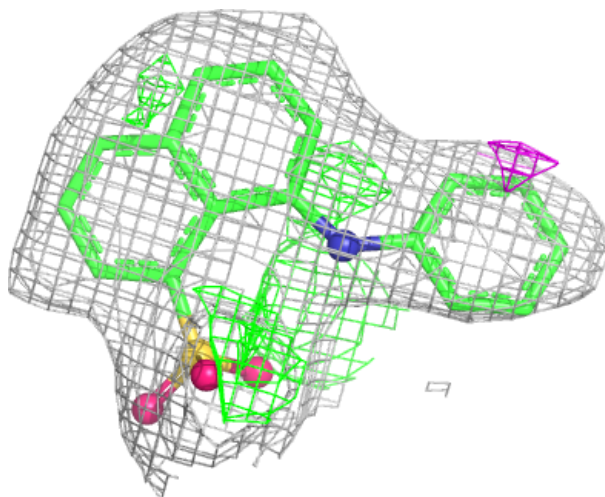
Electron density around 2AN T 203:

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



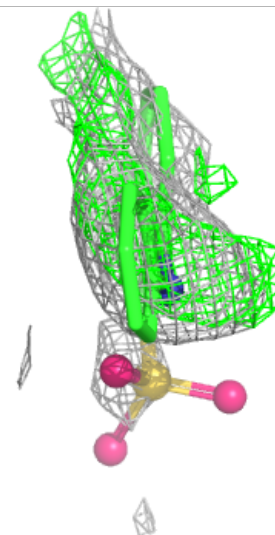
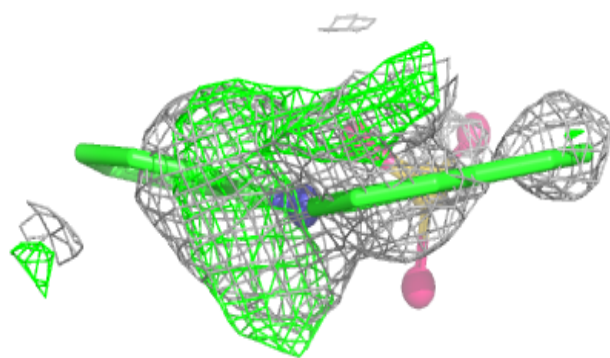
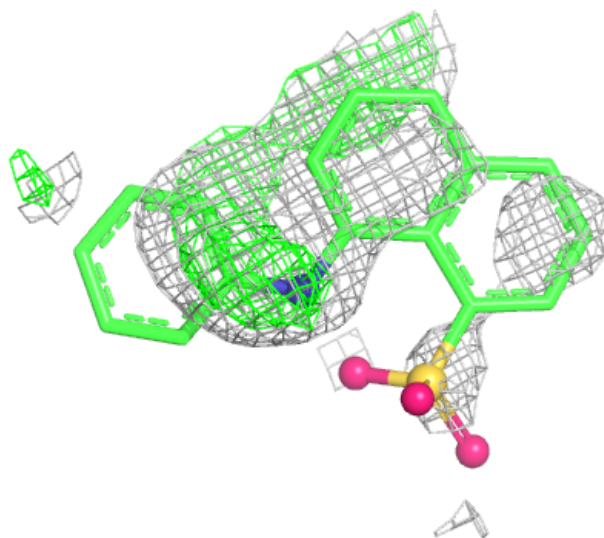
Electron density around 2AN Y 201:

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



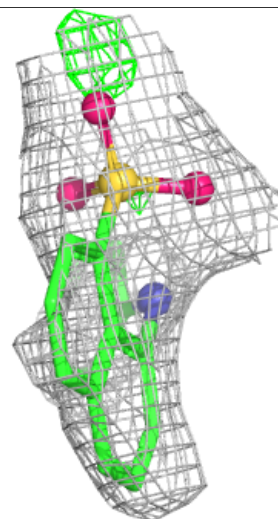
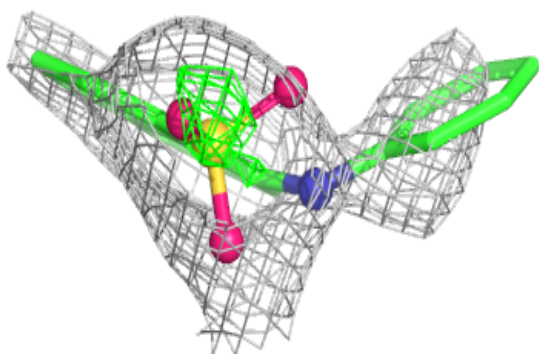
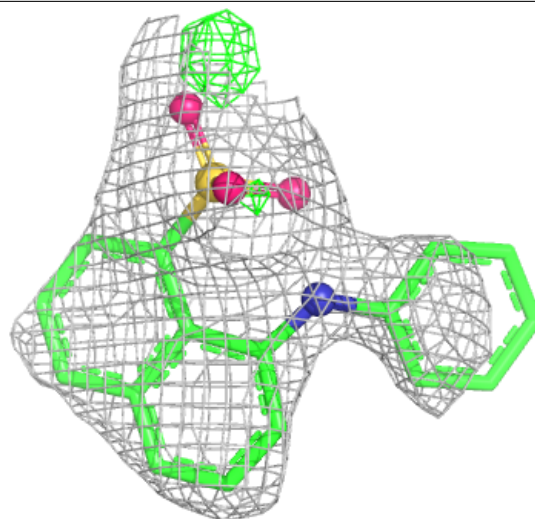
Electron density around 2AN U 202:

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



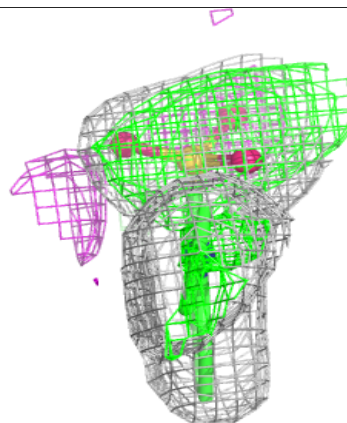
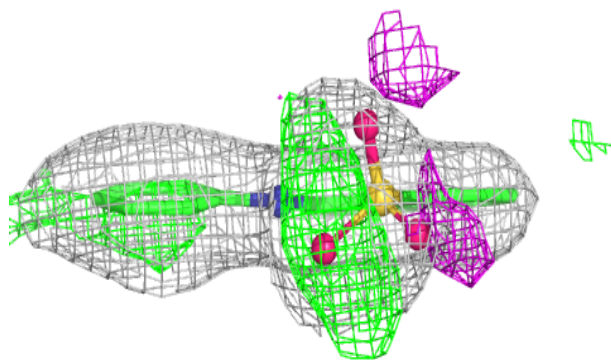
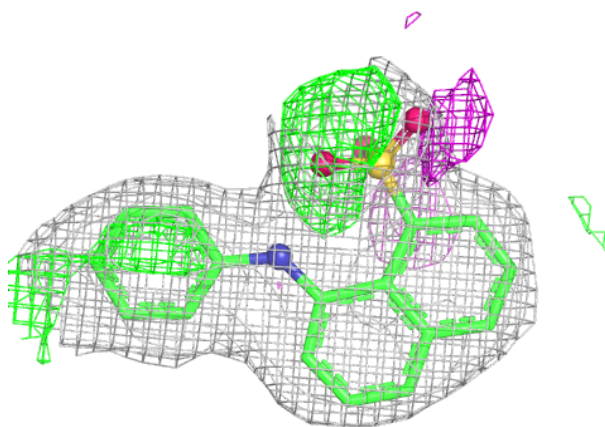
Electron density around 2AN f 206:

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



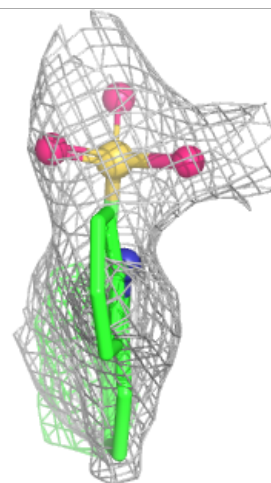
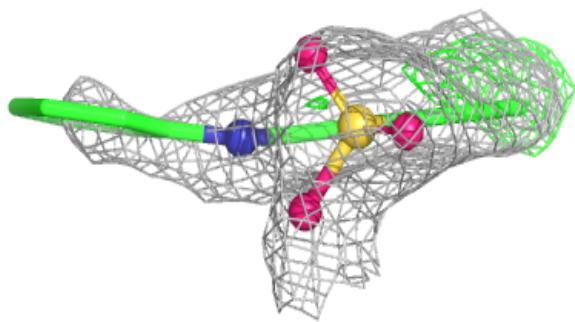
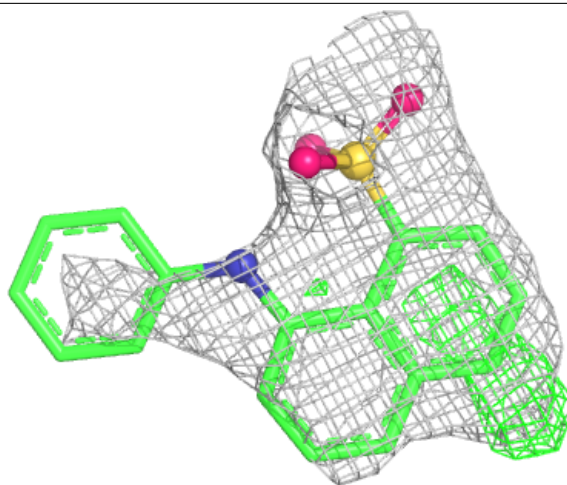
Electron density around 2AN T 204:

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



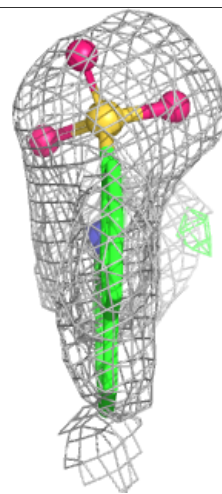
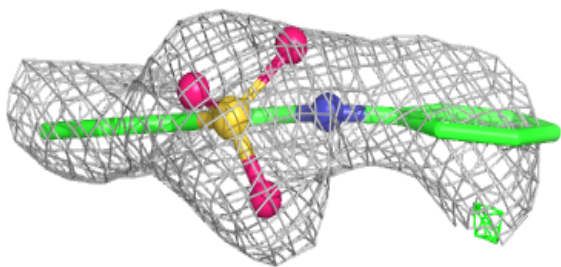
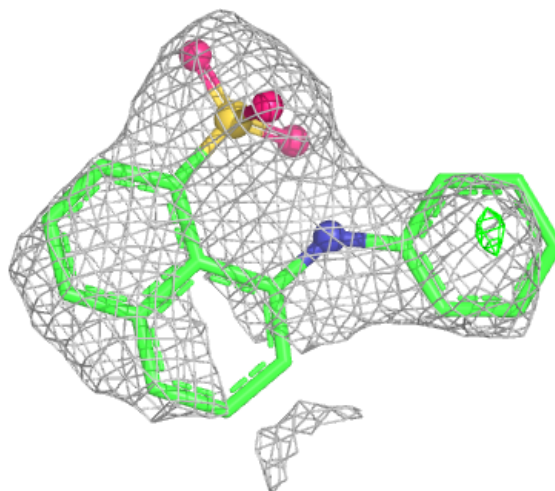
Electron density around 2AN S 203:

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



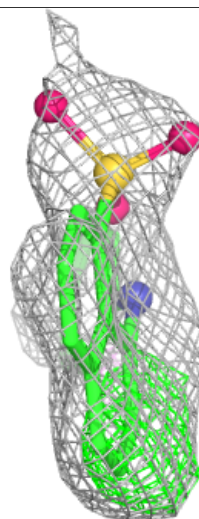
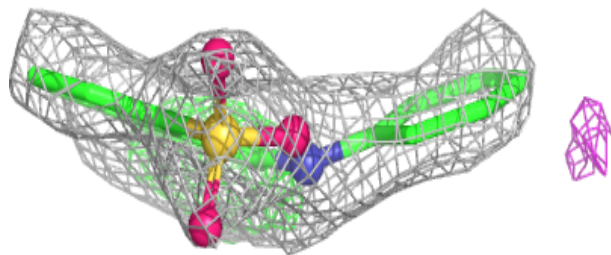
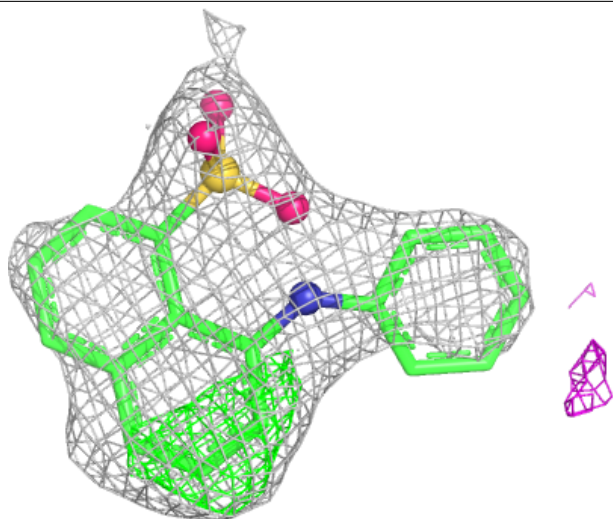
Electron density around 2AN H 204:

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



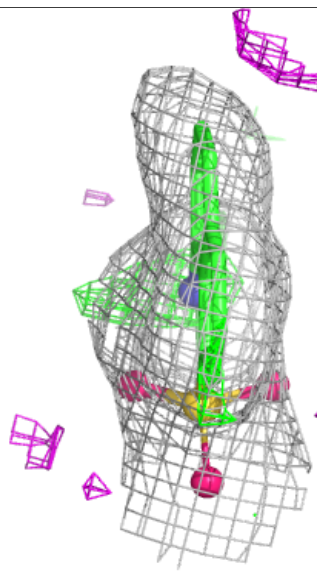
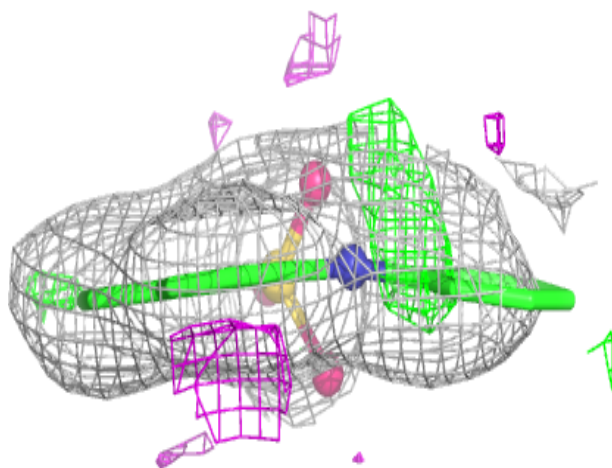
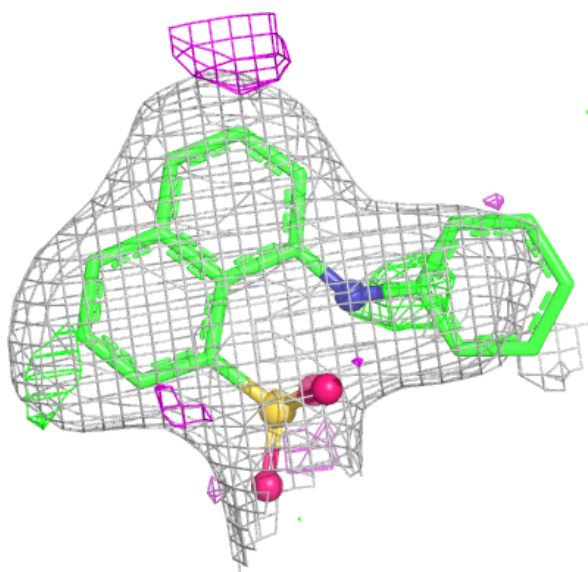
Electron density around 2AN G 205:

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



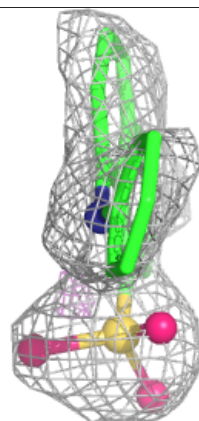
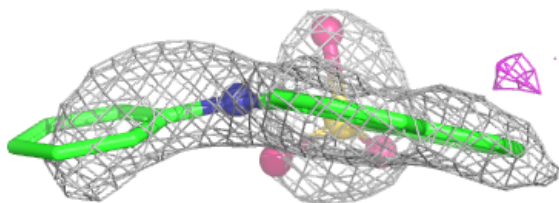
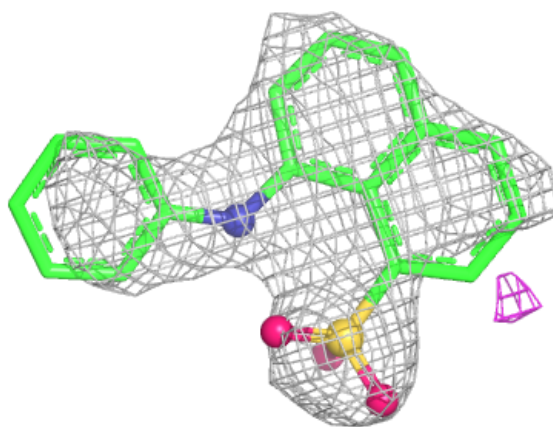
Electron density around 2AN j 206:

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



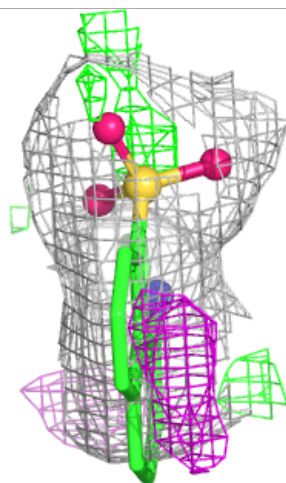
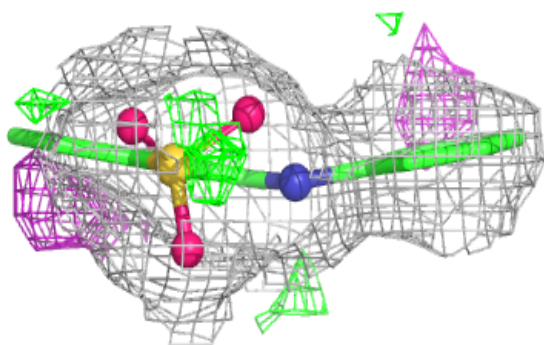
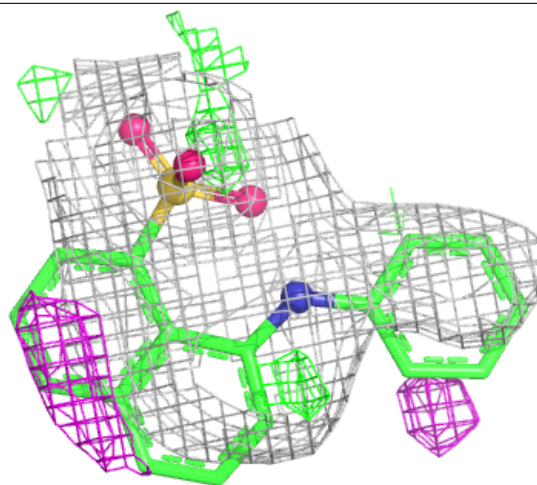
Electron density around 2AN I 203:

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



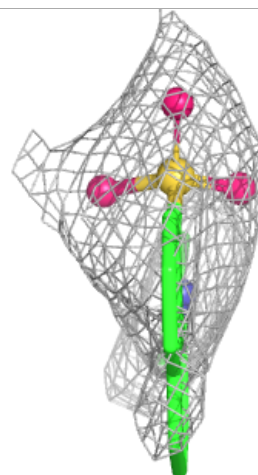
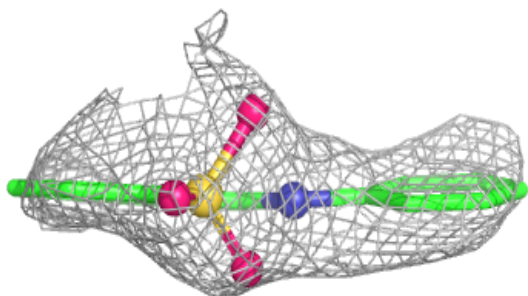
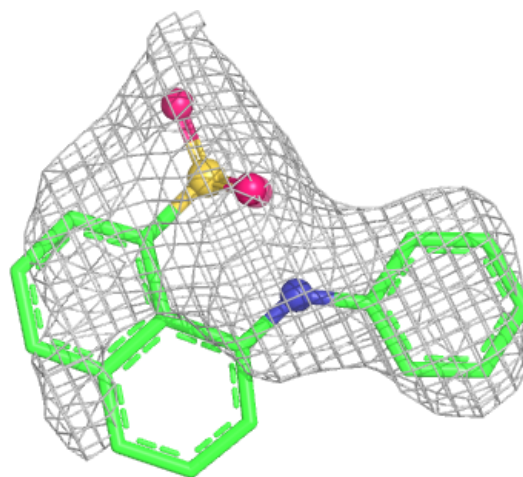
Electron density around 2AN F 204:

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



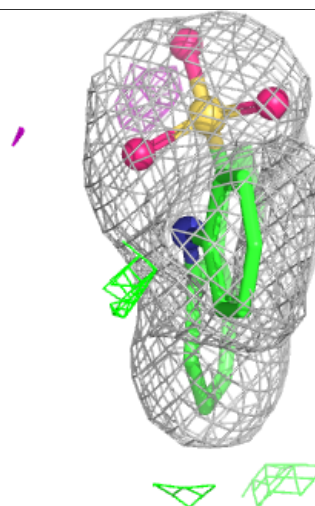
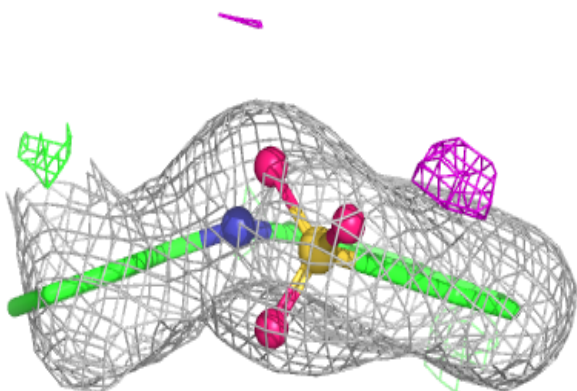
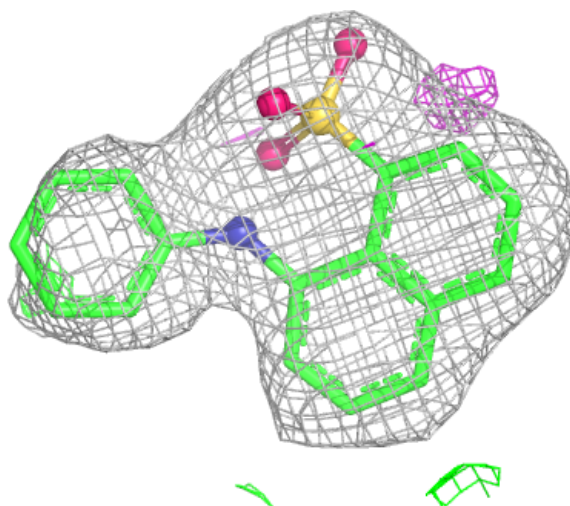
Electron density around 2AN O 202:

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



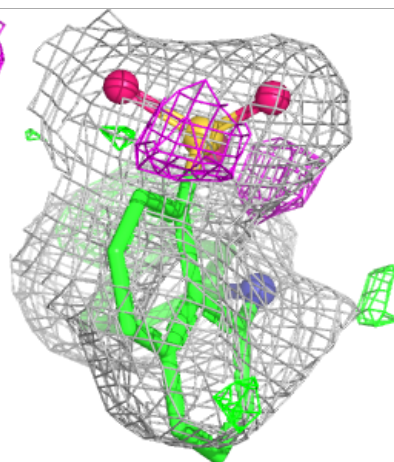
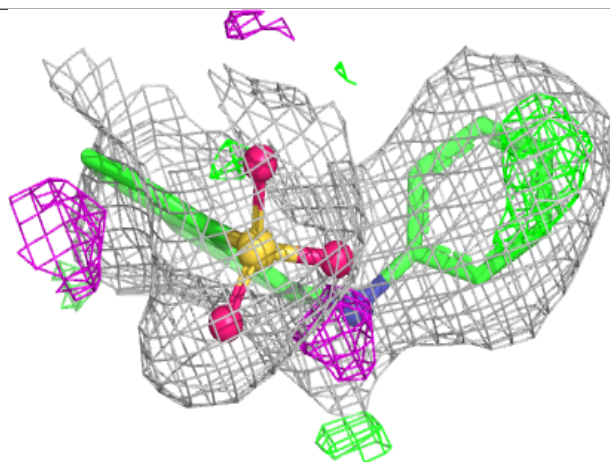
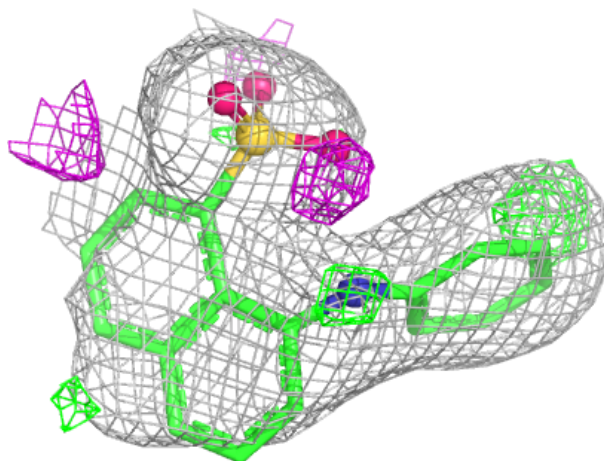
Electron density around 2AN c 203:

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



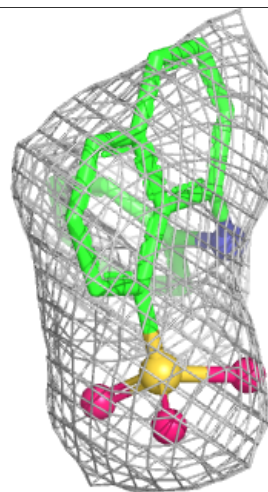
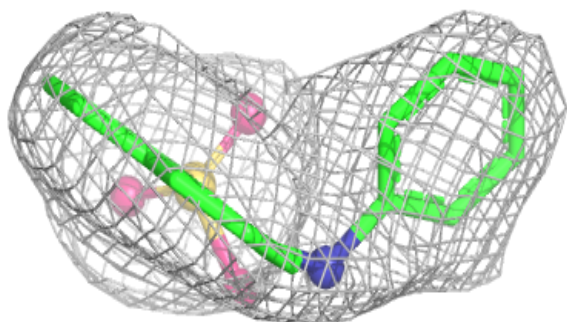
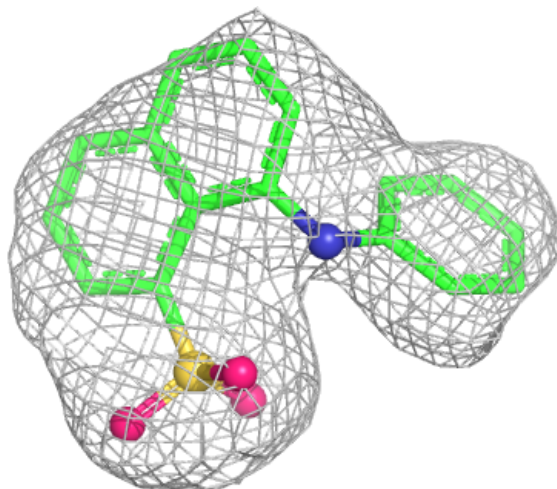
Electron density around 2AN F 202:

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



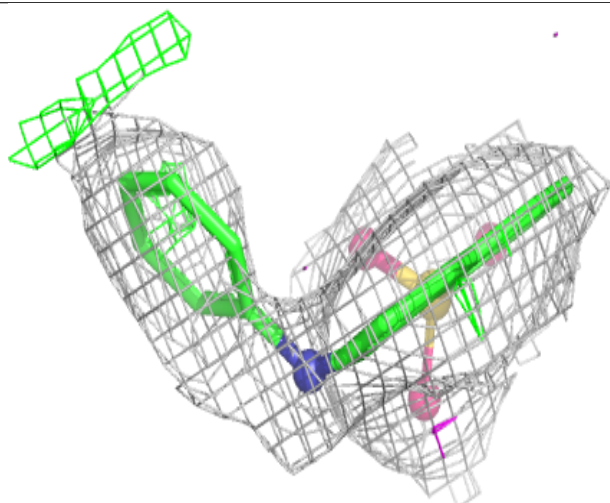
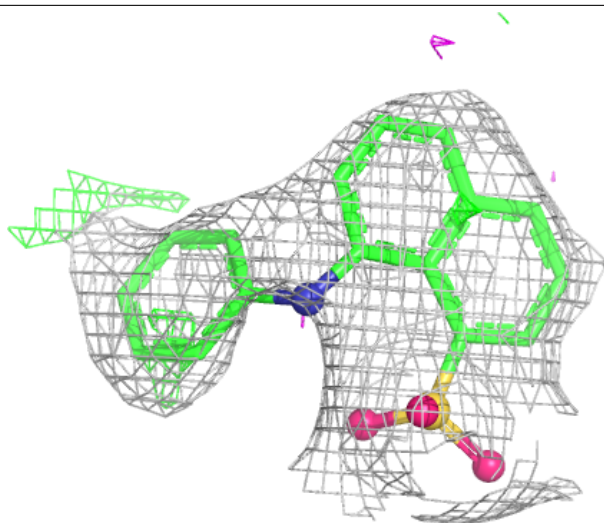
Electron density around 2AN S 201:

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



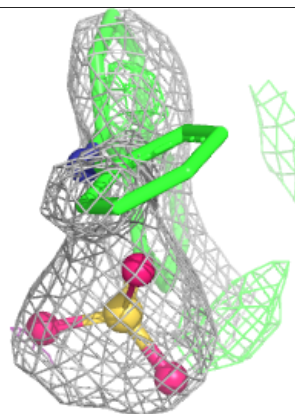
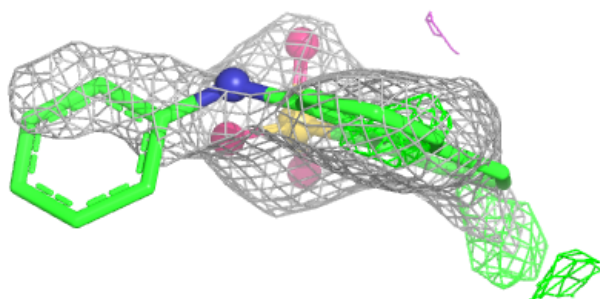
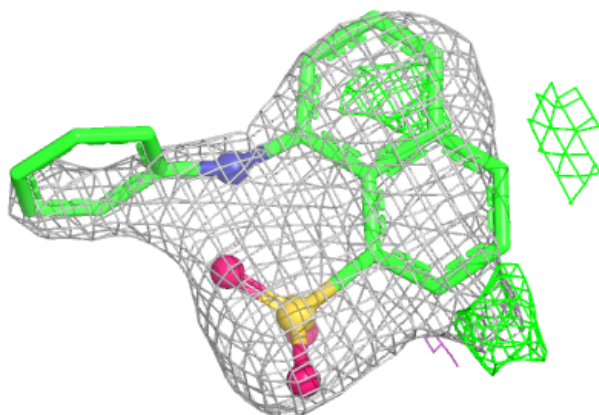
Electron density around 2AN a 201:

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



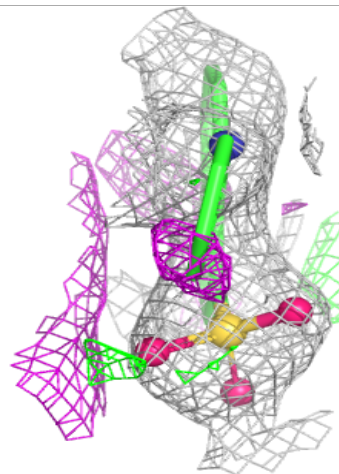
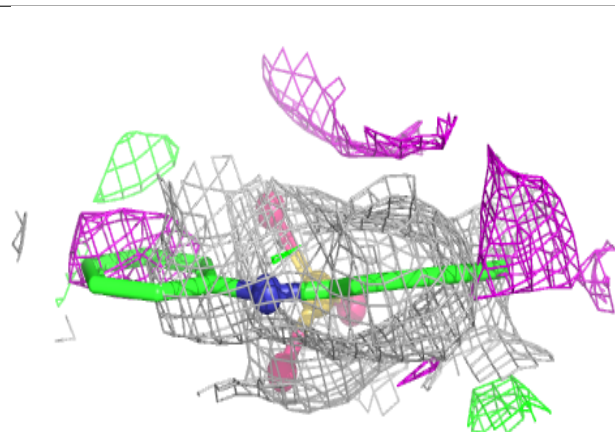
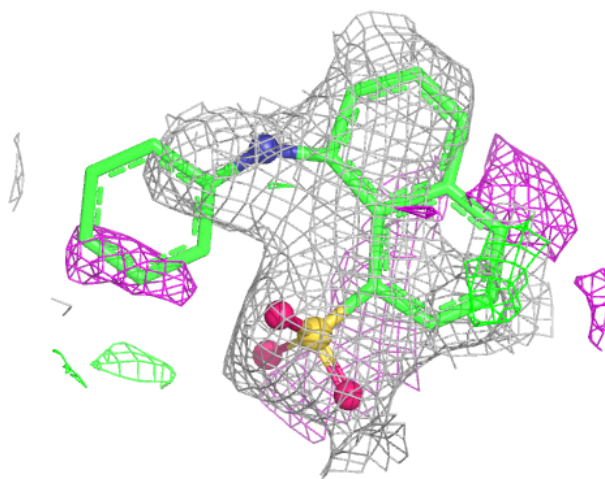
Electron density around 2AN C 203 (A):

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



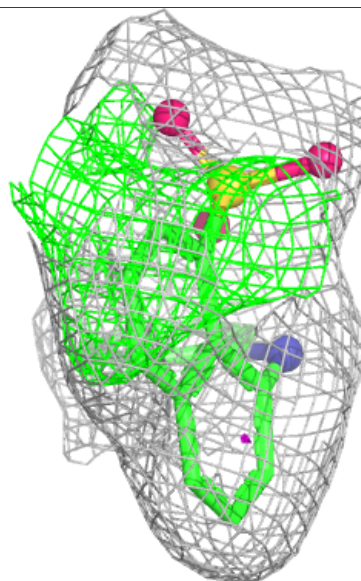
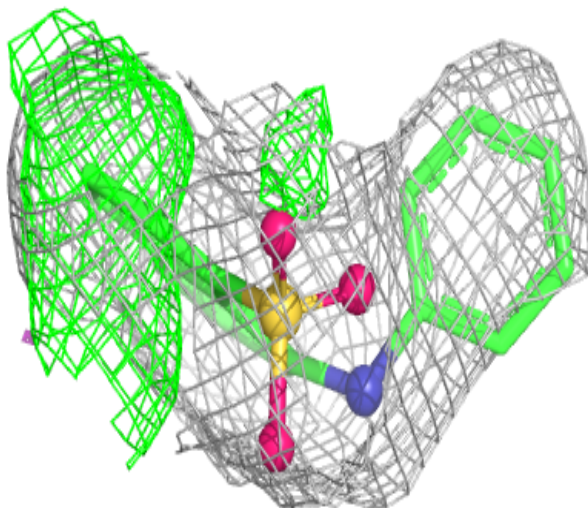
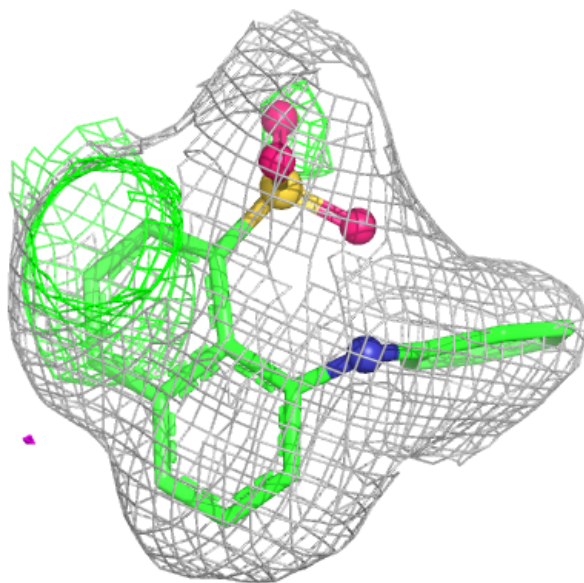
Electron density around 2AN V 208:

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



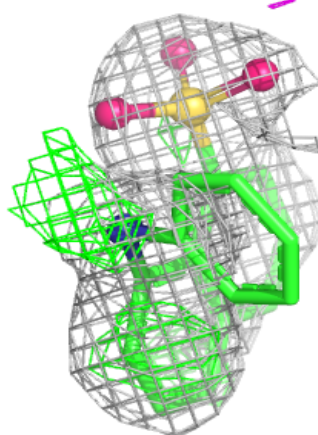
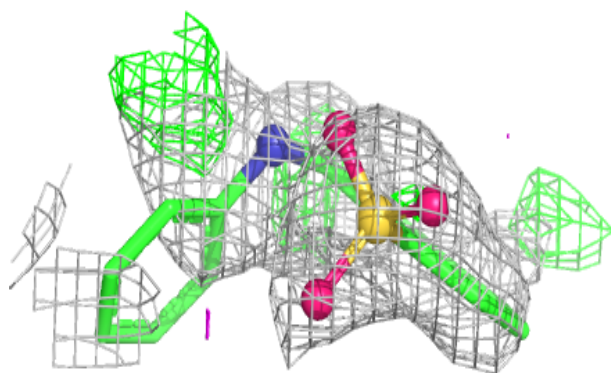
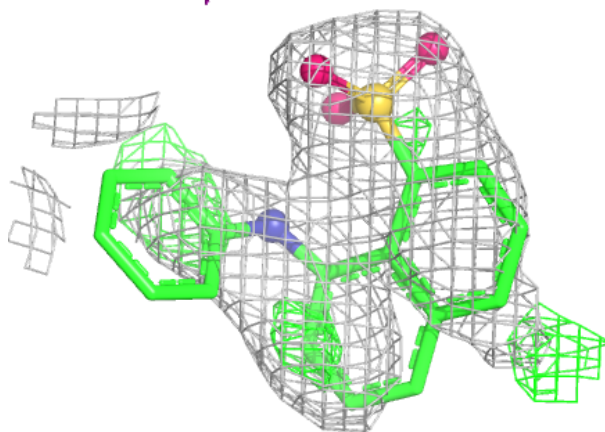
Electron density around 2AN Z 206:

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



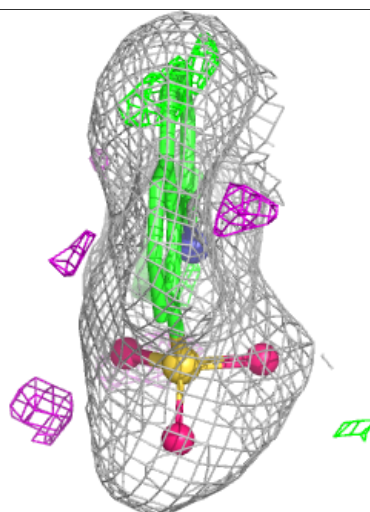
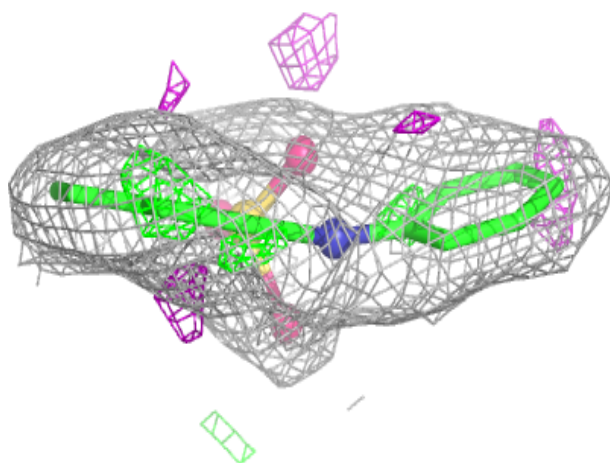
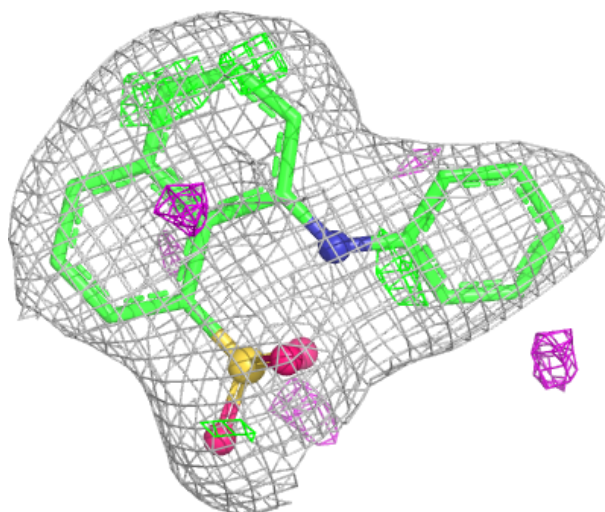
Electron density around 2AN E 204:

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



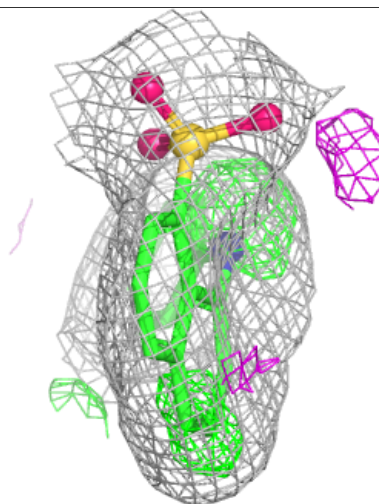
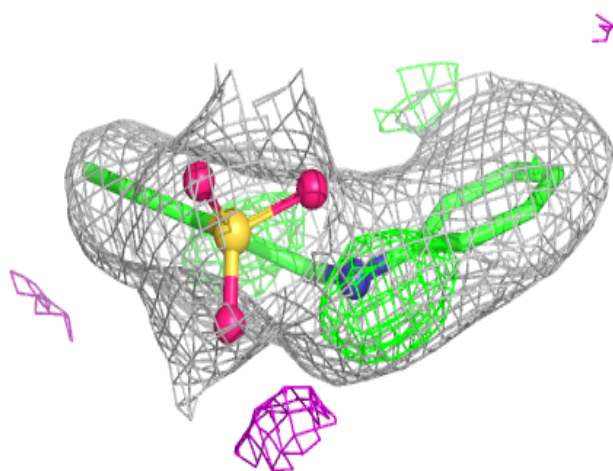
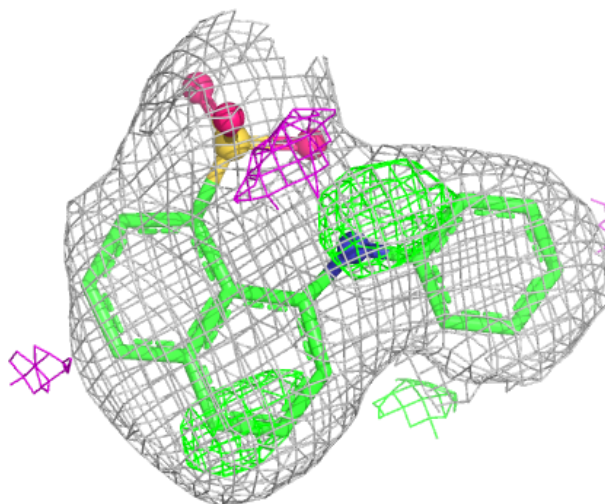
Electron density around 2AN N 205:

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



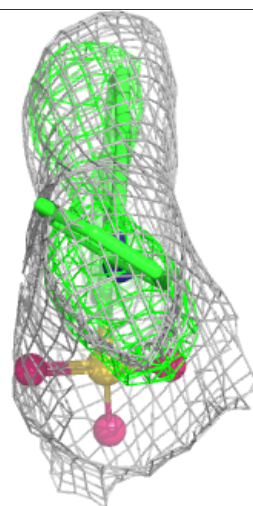
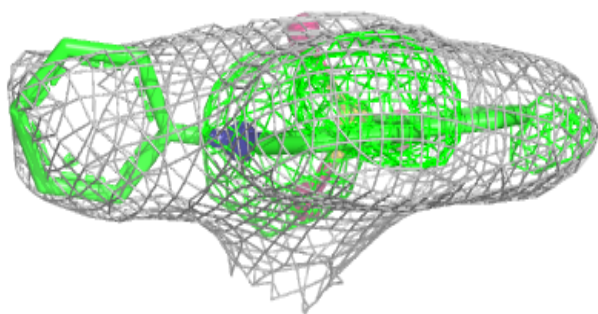
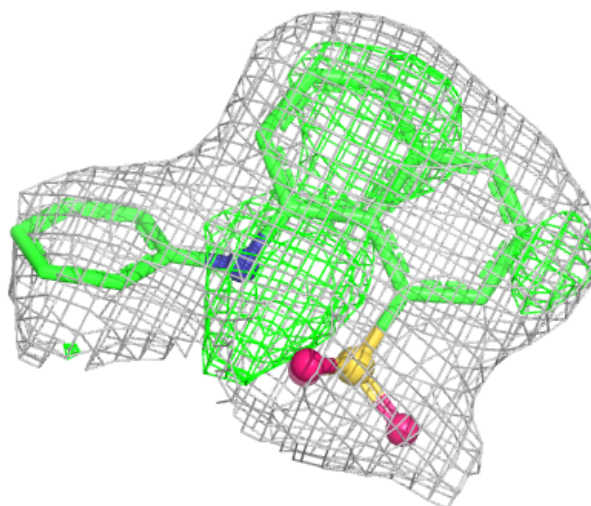
Electron density around 2AN T 205:

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



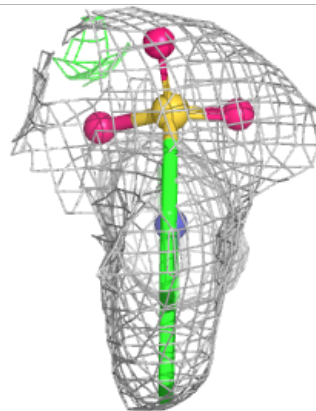
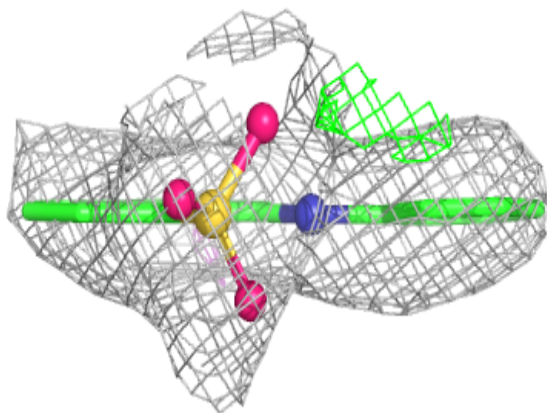
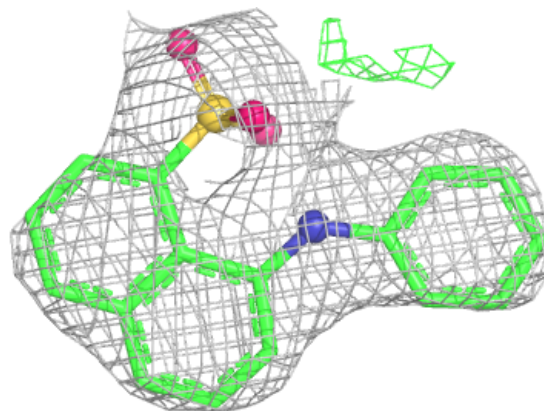
Electron density around 2AN V 207:

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



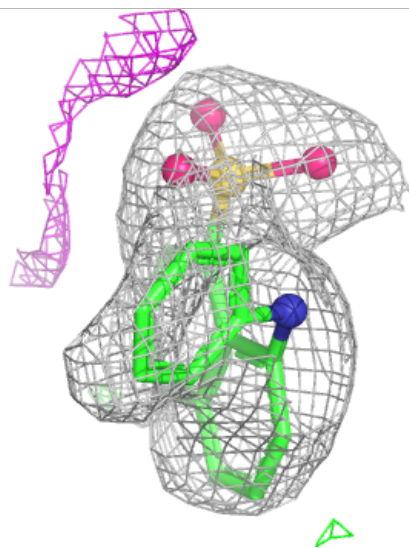
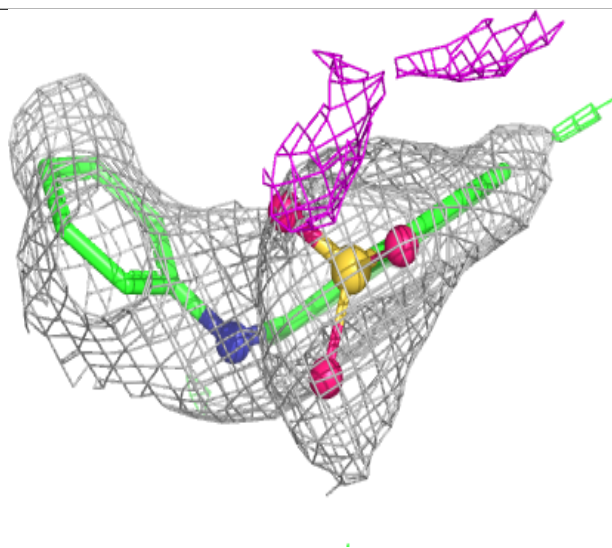
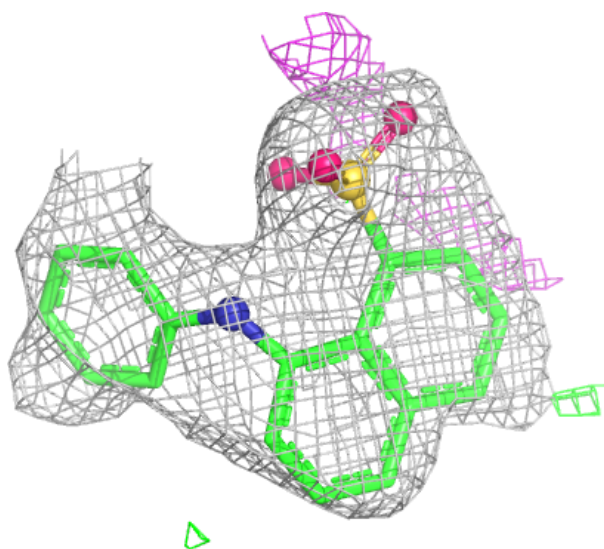
Electron density around 2AN Z 202:

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



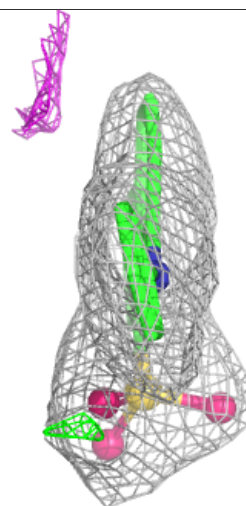
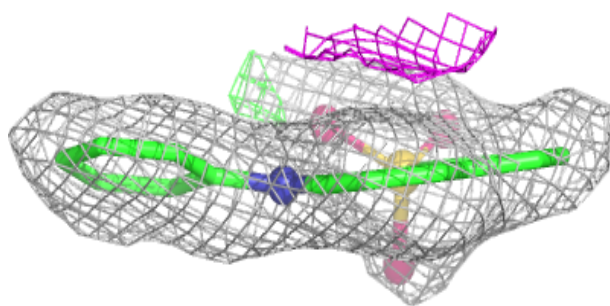
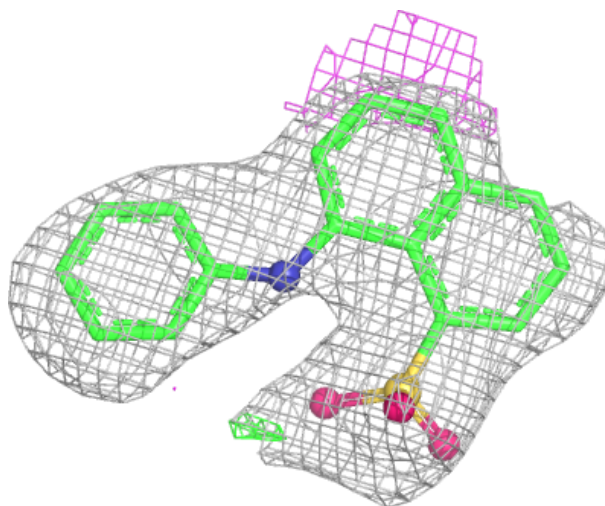
Electron density around 2AN I 206:

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



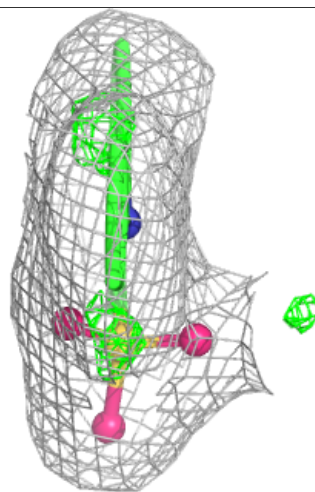
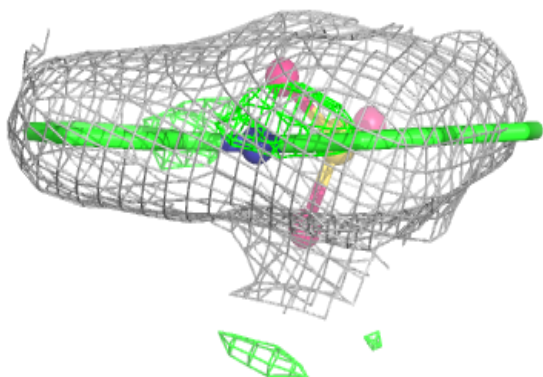
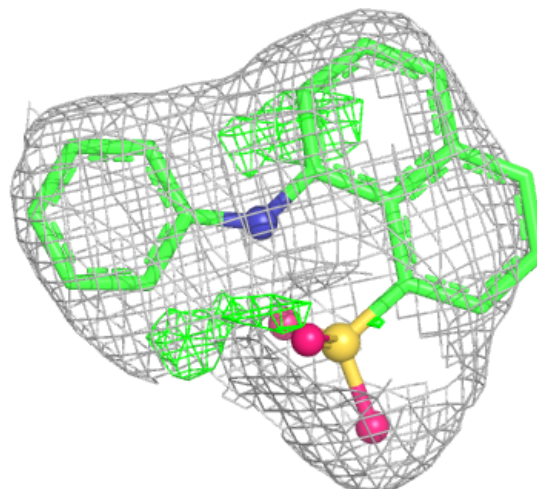
Electron density around 2AN W 201:

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



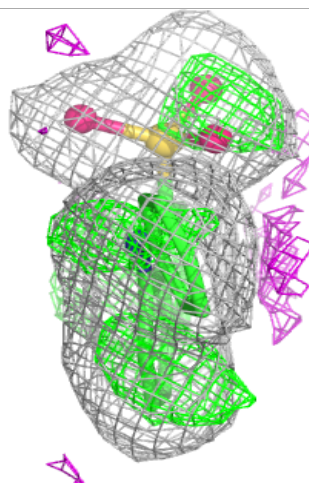
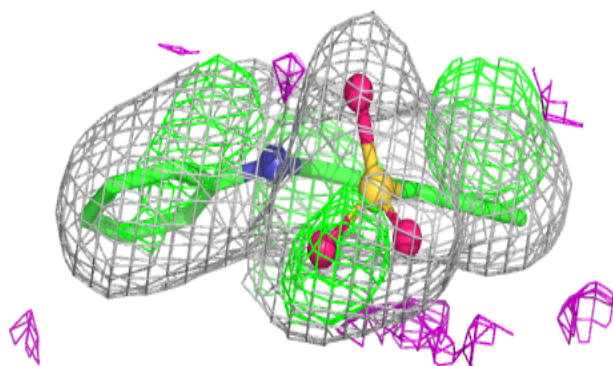
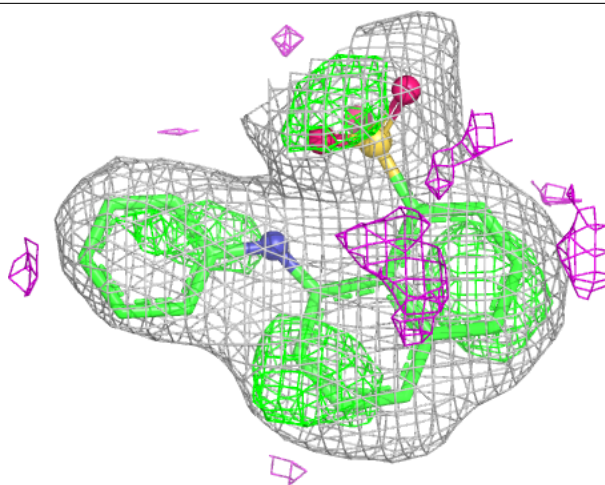
Electron density around 2AN X 202:

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



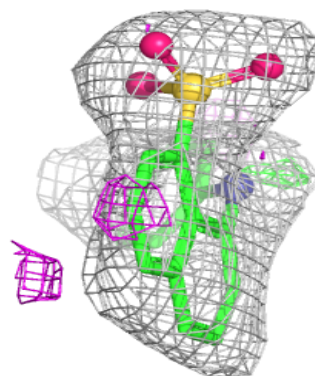
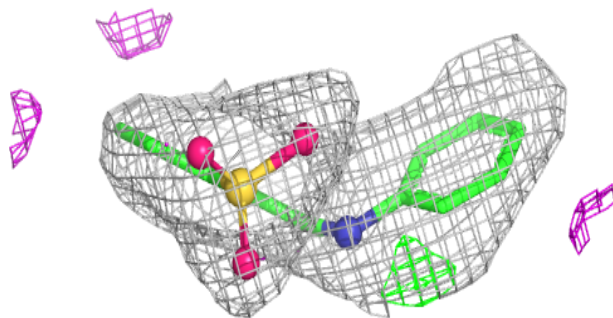
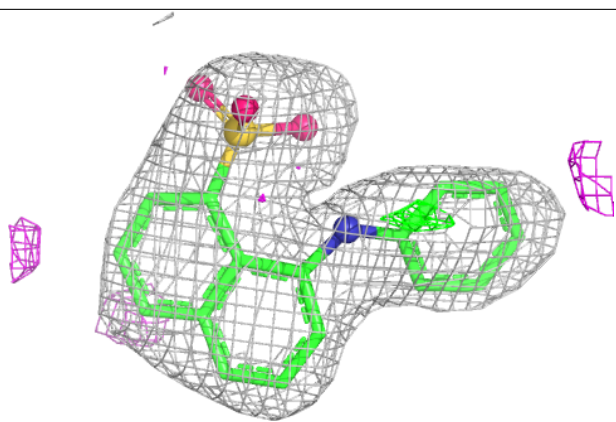
Electron density around 2AN h 203:

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



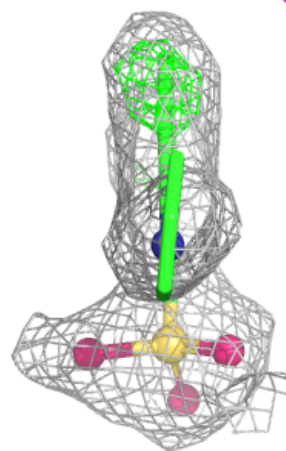
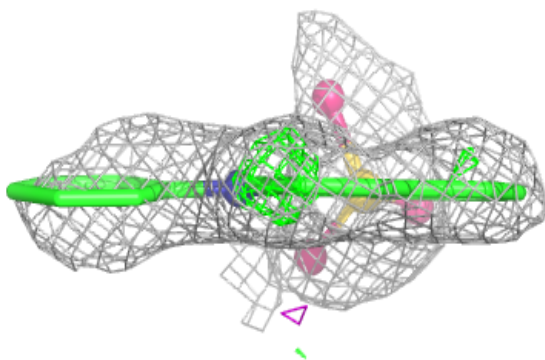
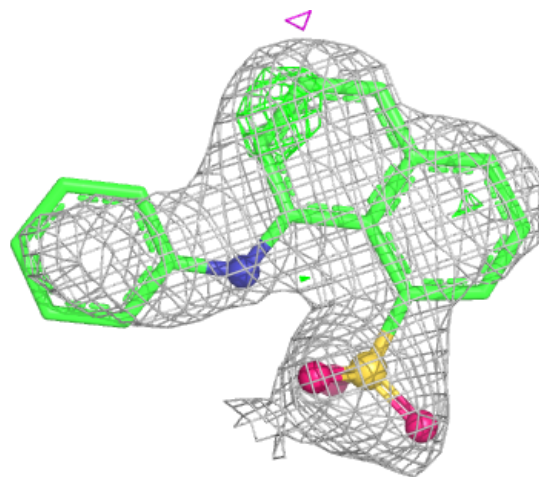
Electron density around 2AN A 202:

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



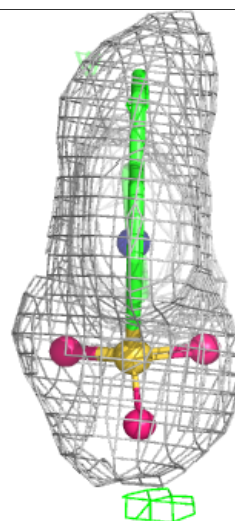
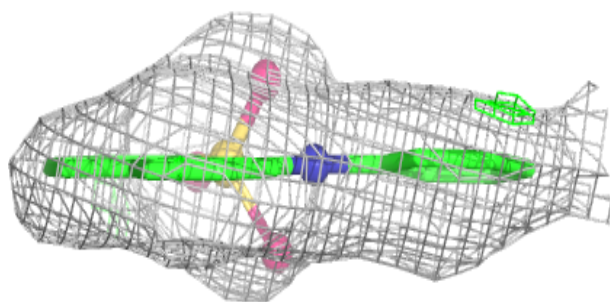
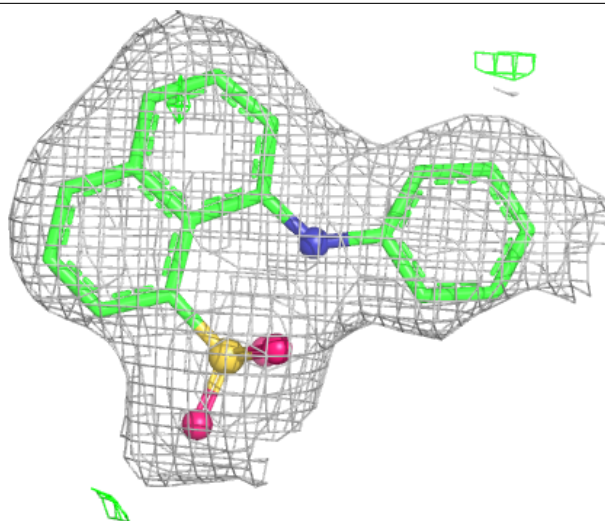
Electron density around 2AN c 205:

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



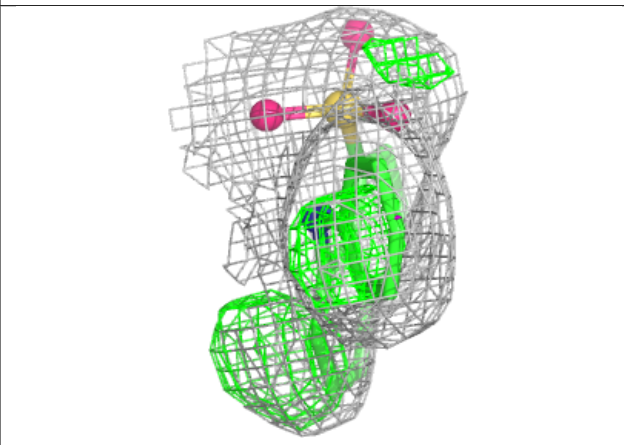
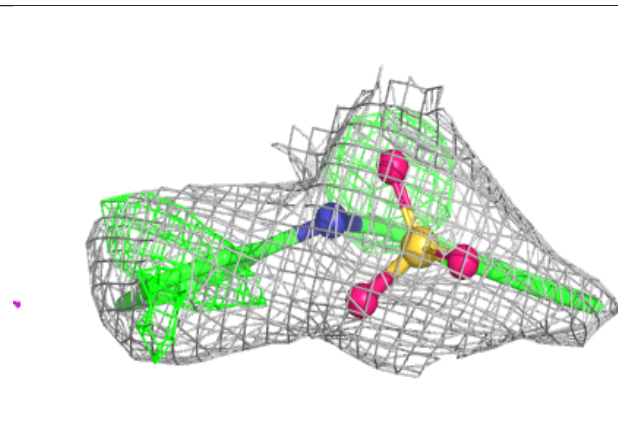
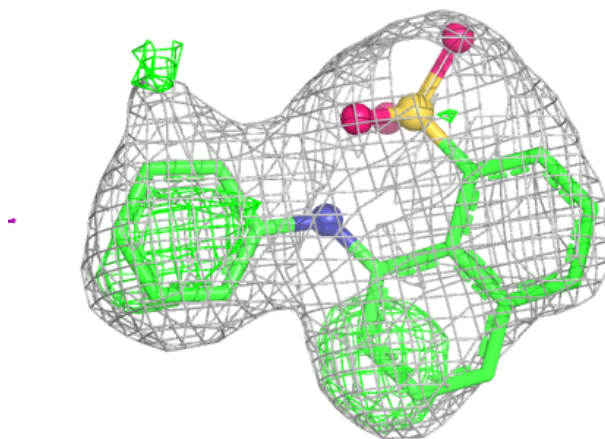
Electron density around 2AN Z 204:

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



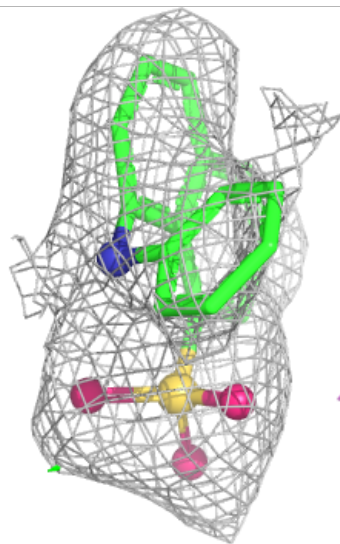
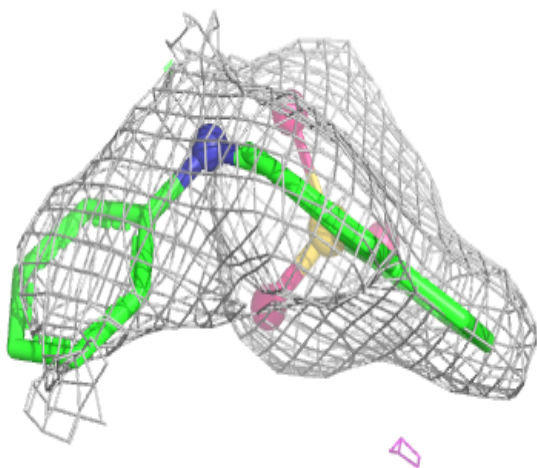
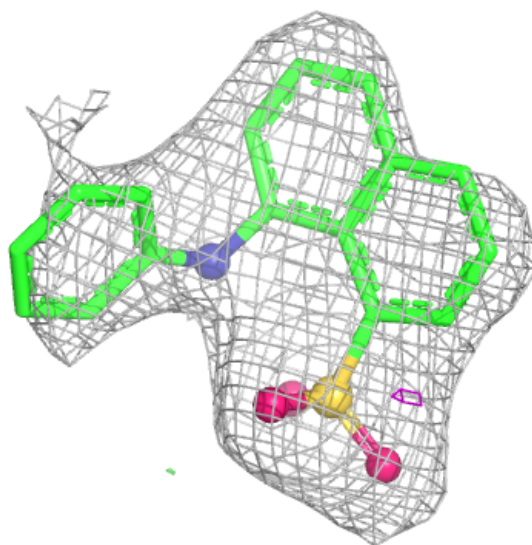
Electron density around 2AN B 206:

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



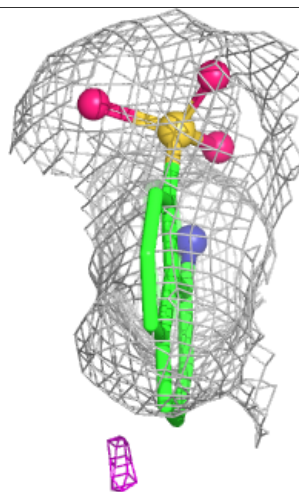
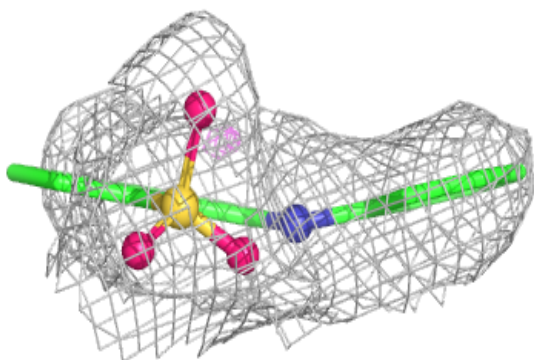
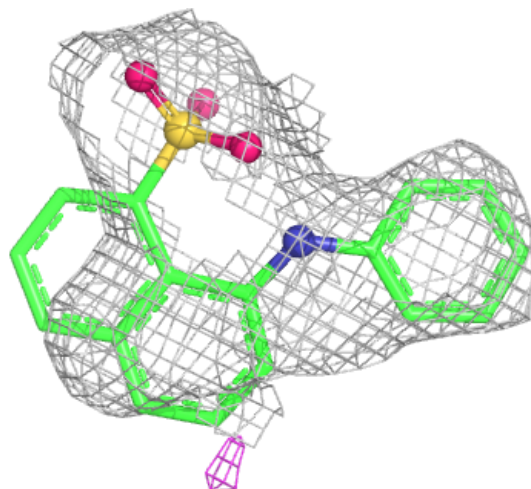
Electron density around 2AN Q 203:

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



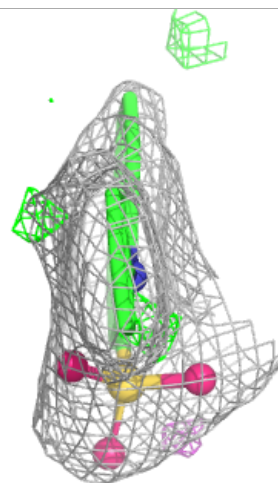
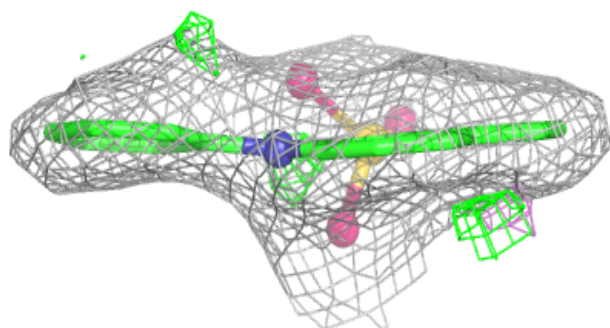
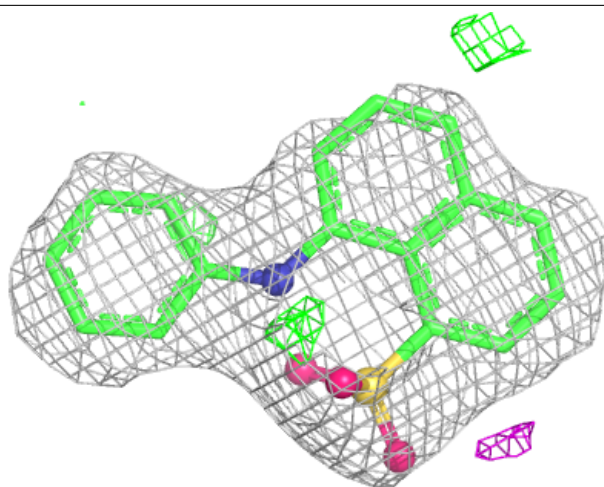
Electron density around 2AN U 201:

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



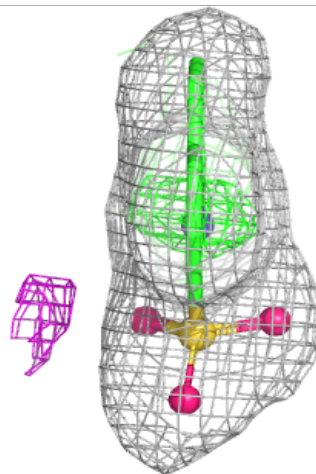
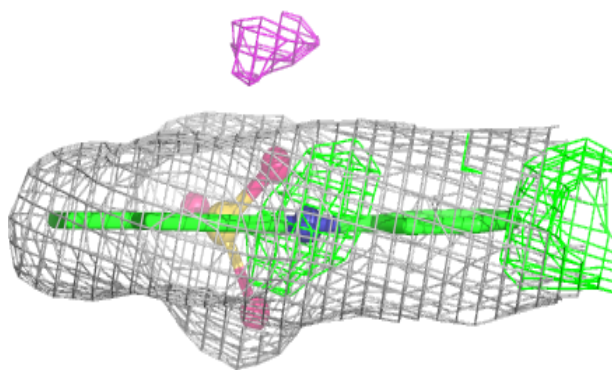
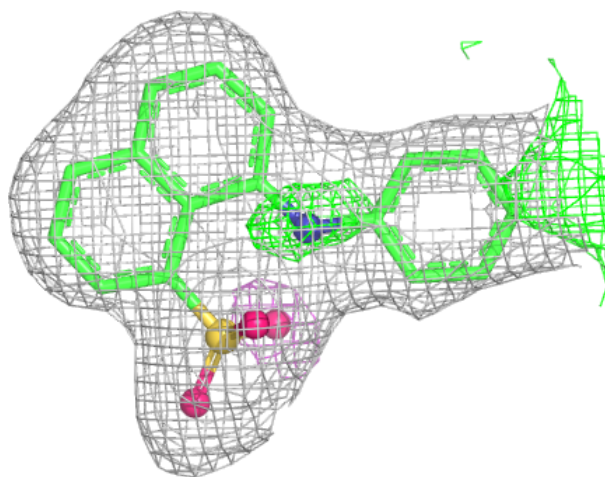
Electron density around 2AN K 203:

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



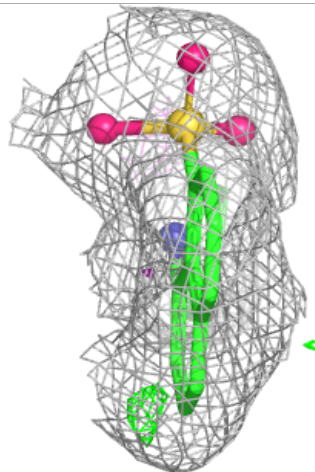
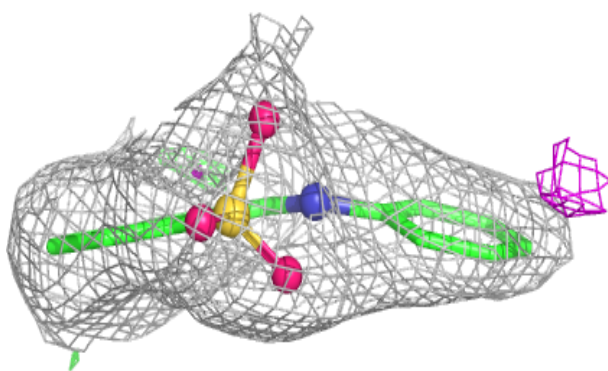
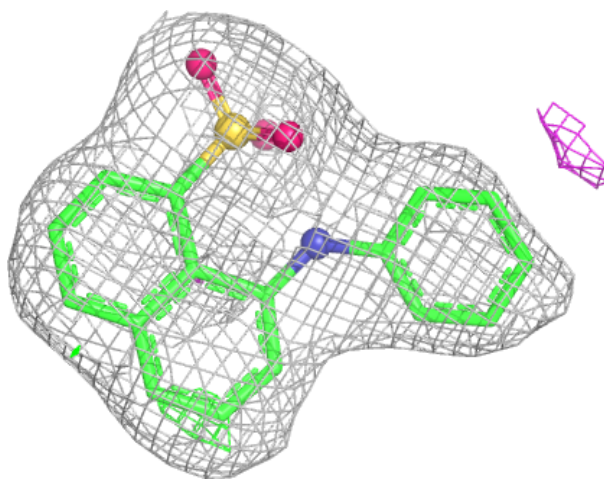
Electron density around 2AN V 206:

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



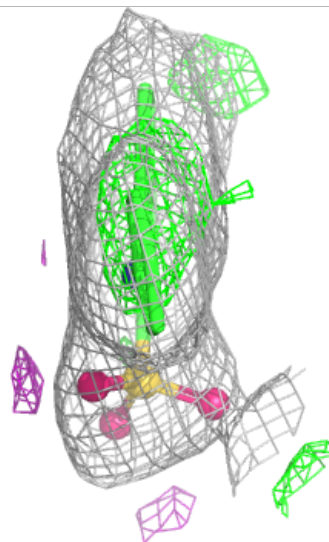
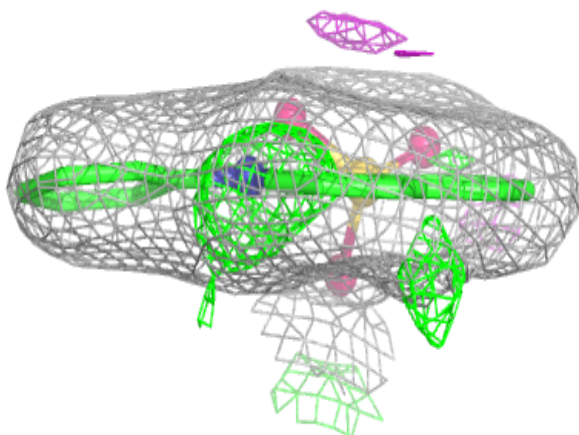
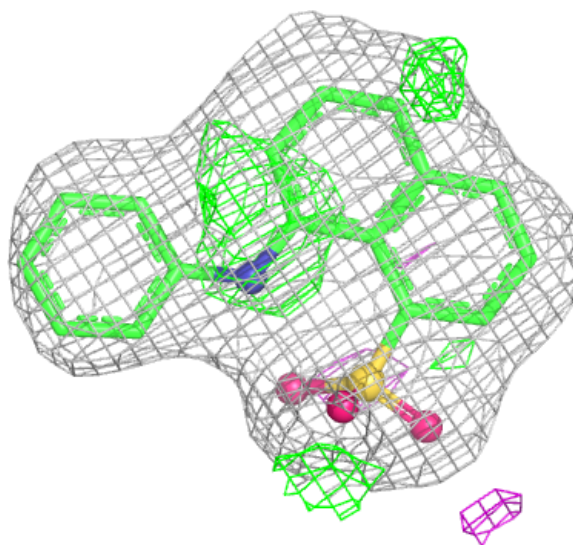
Electron density around 2AN a 203:

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



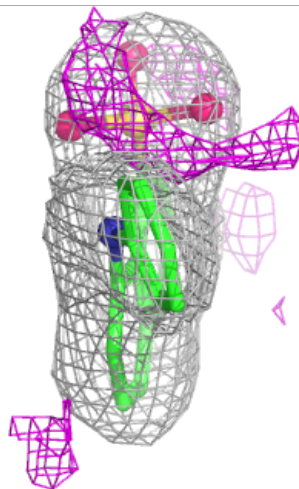
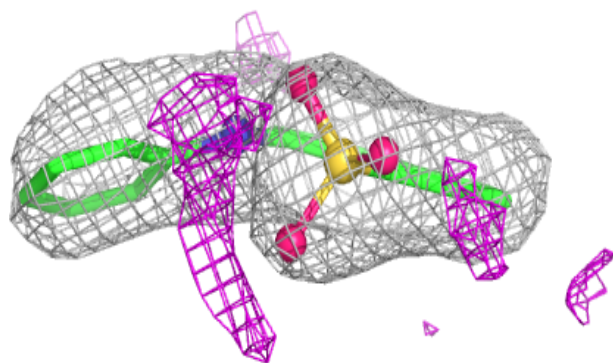
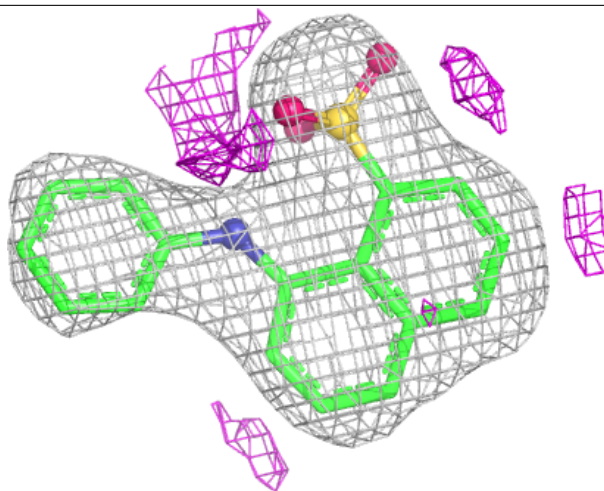
Electron density around 2AN j 204:

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



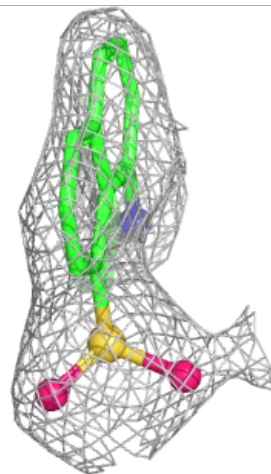
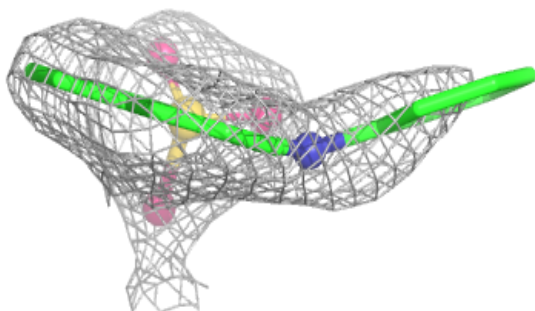
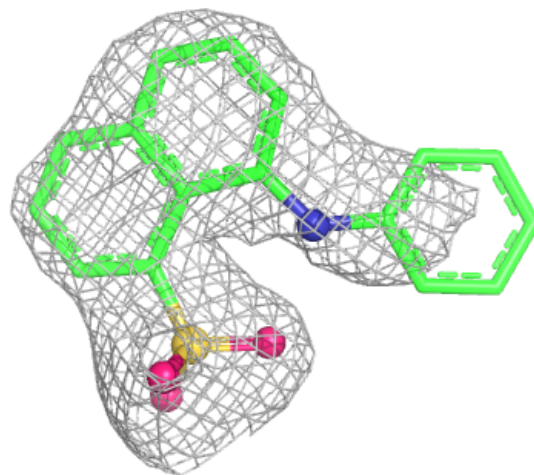
Electron density around 2AN Y 203:

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



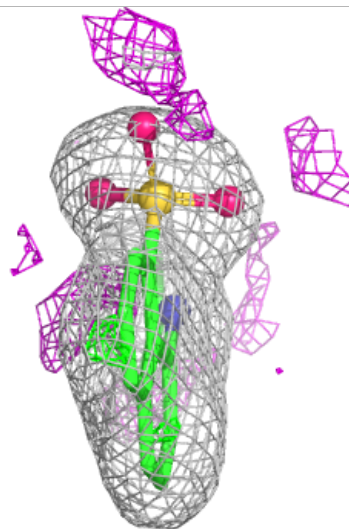
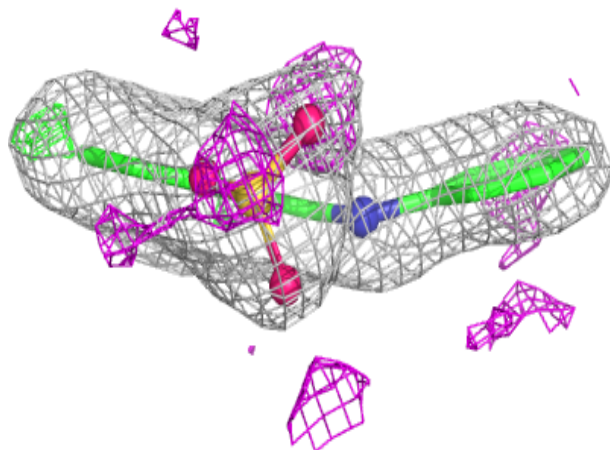
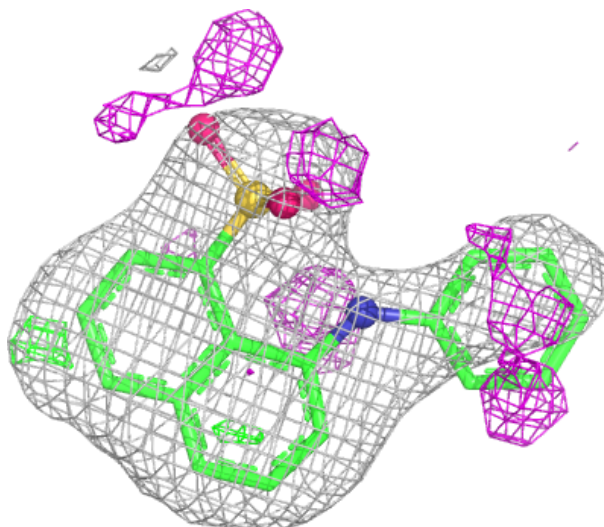
Electron density around 2AN A 203:

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



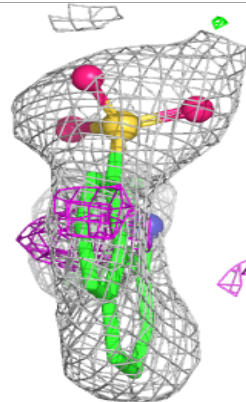
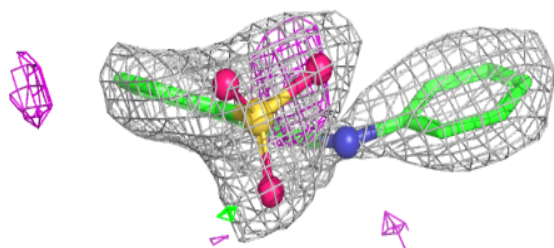
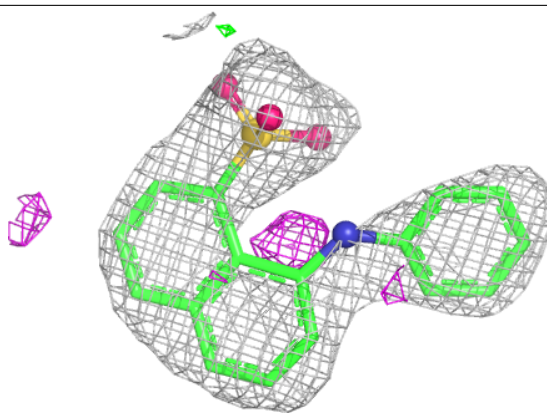
Electron density around 2AN X 201:

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



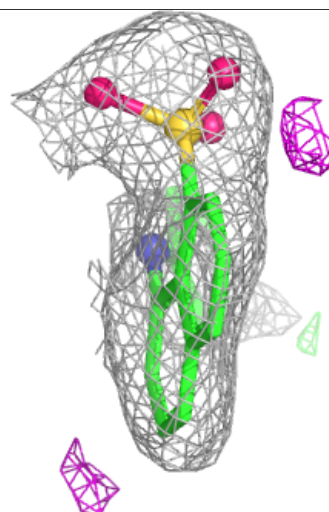
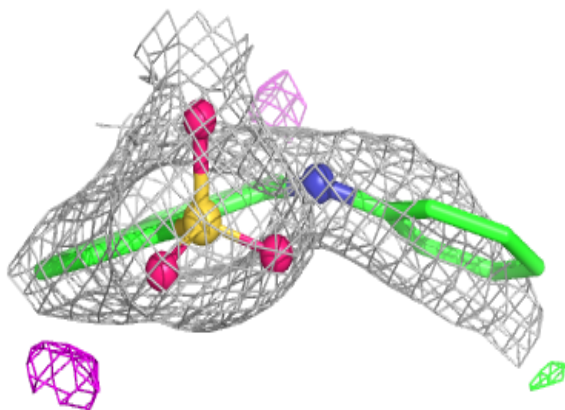
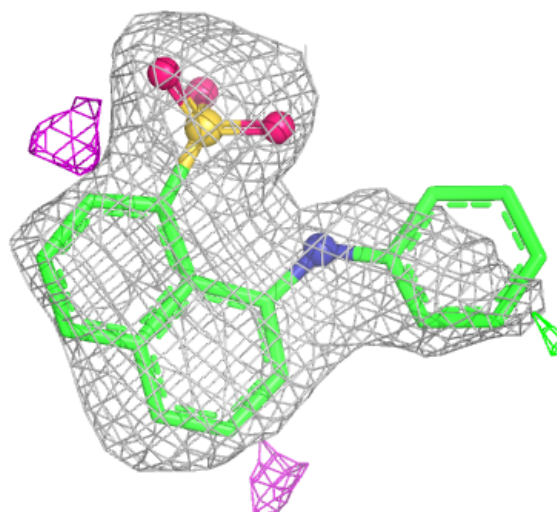
Electron density around 2AN h 201:

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



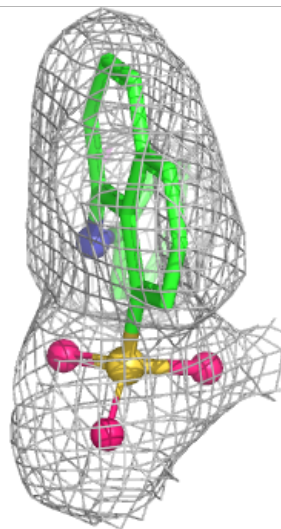
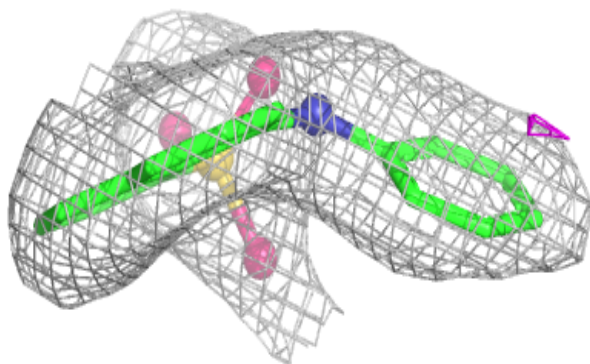
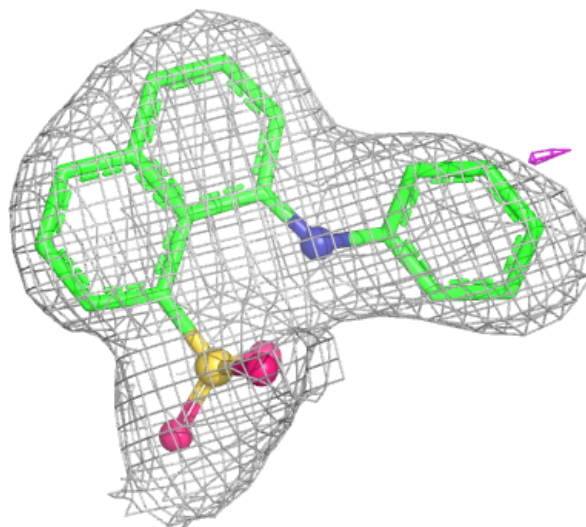
Electron density around 2AN E 203:

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



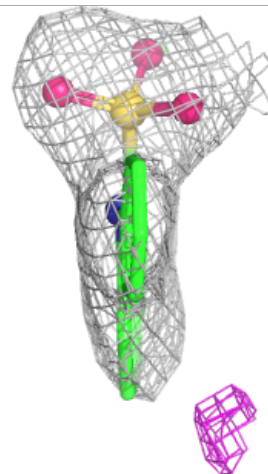
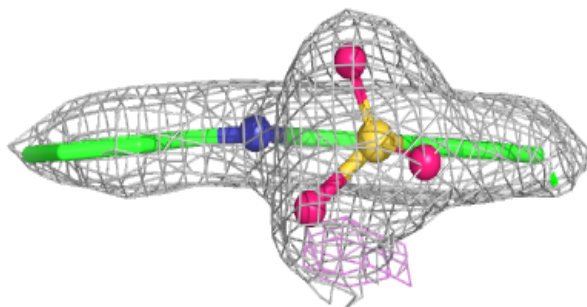
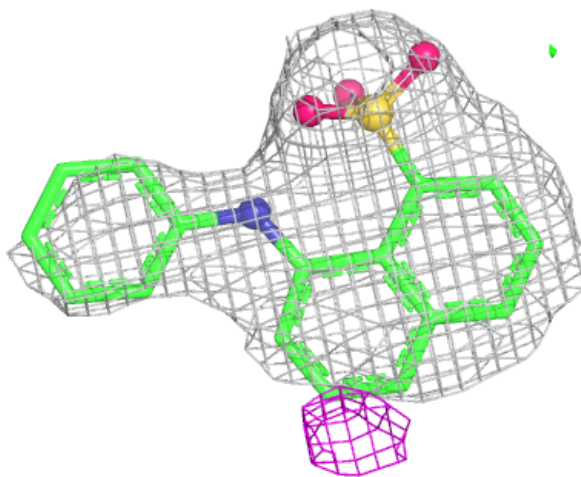
Electron density around 2AN O 203:

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



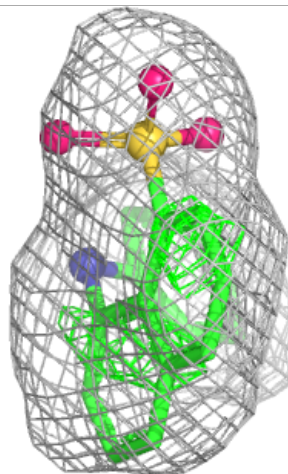
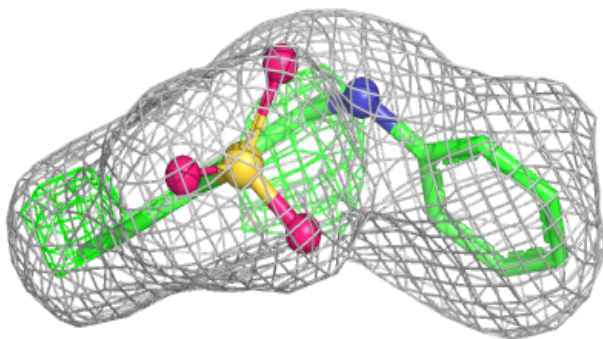
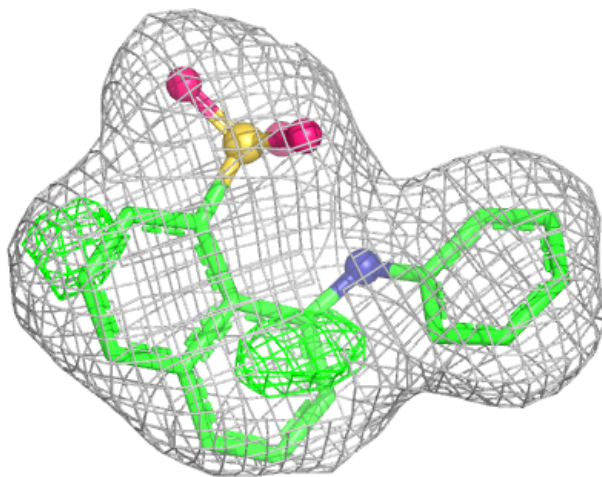
Electron density around 2AN g 201:

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



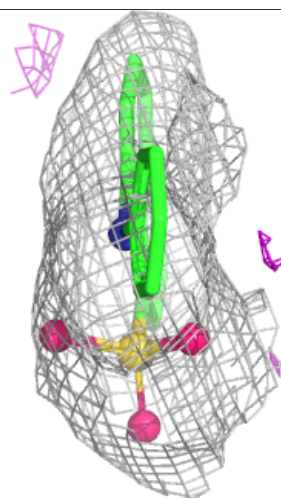
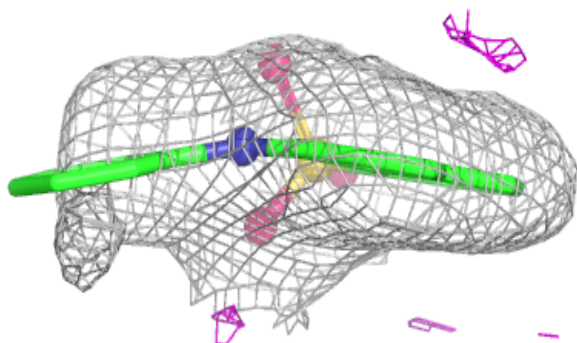
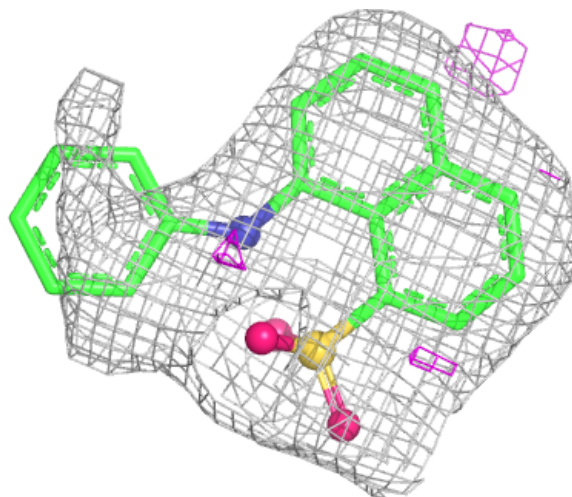
Electron density around 2AN g 203:

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



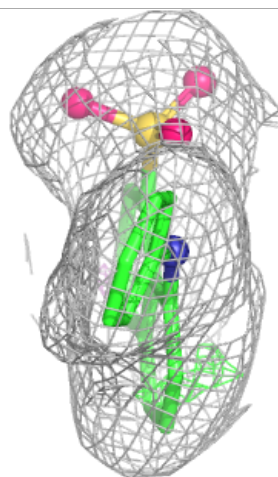
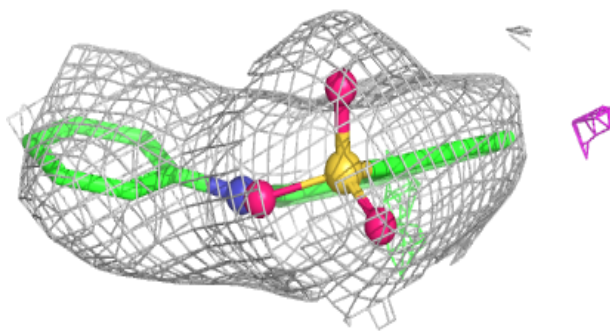
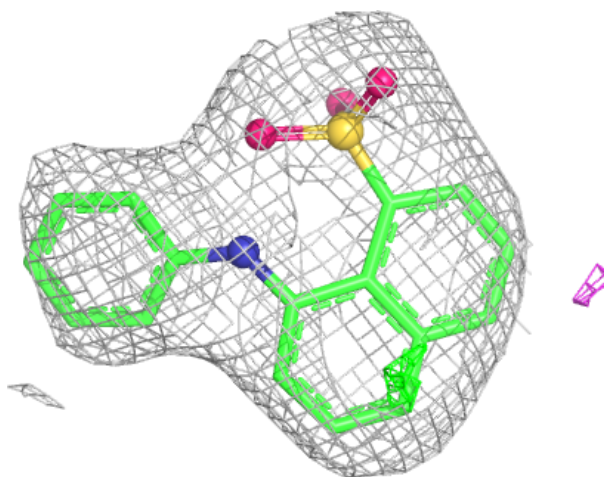
Electron density around 2AN Z 205:

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



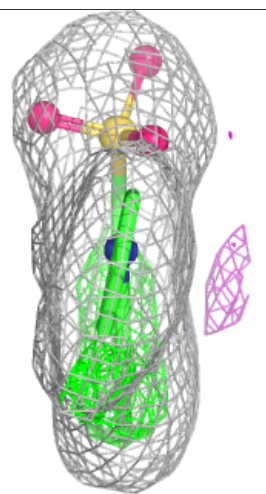
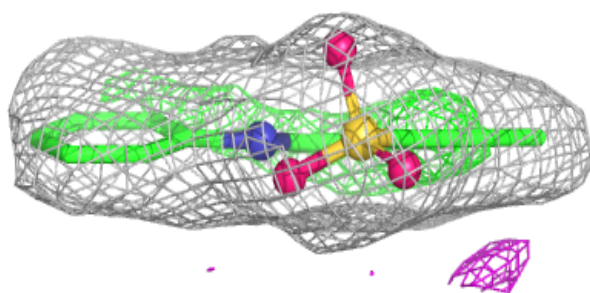
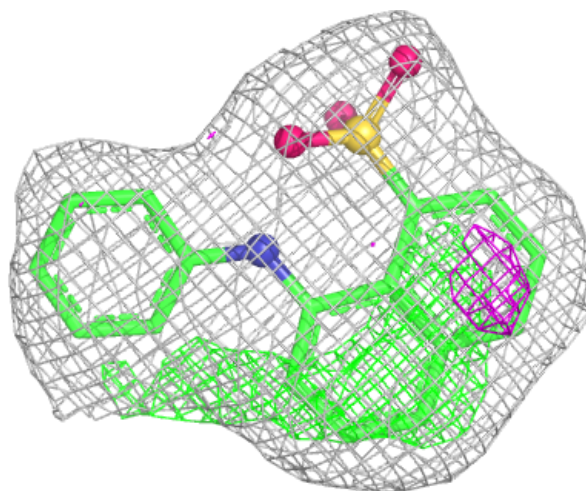
Electron density around 2AN D 203:

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



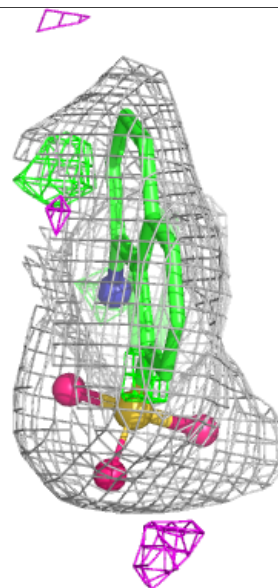
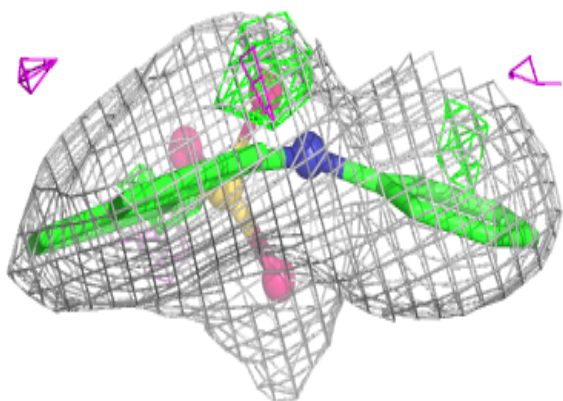
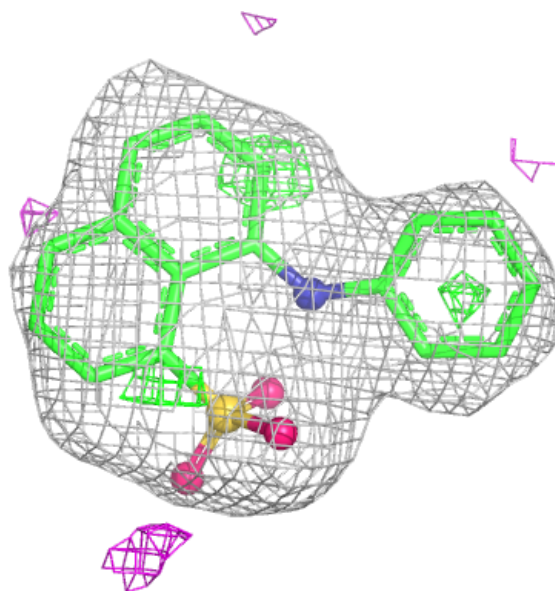
Electron density around 2AN P 203:

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



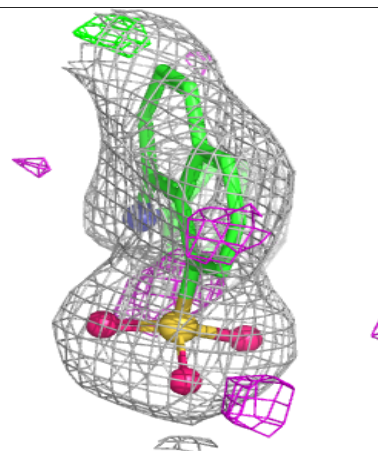
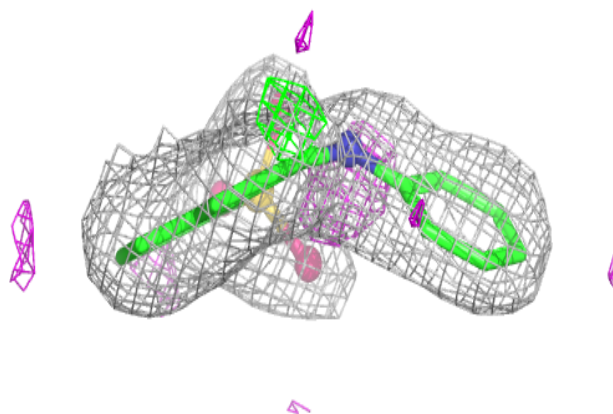
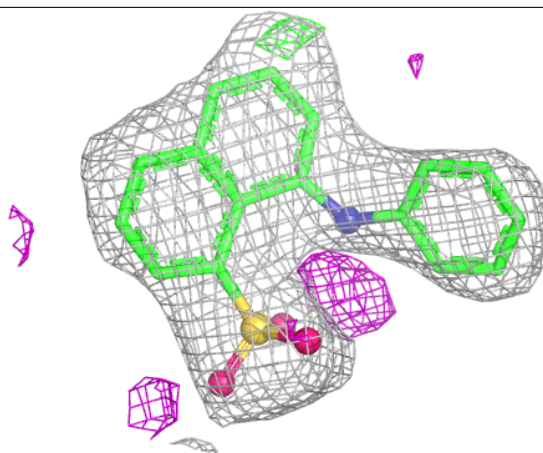
Electron density around 2AN F 205:

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



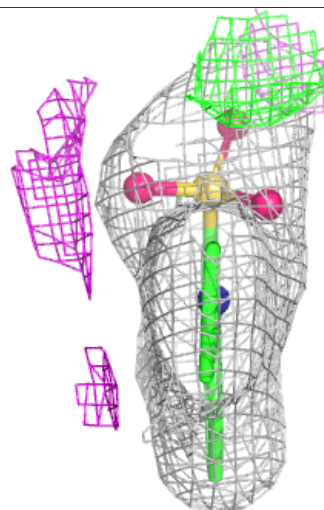
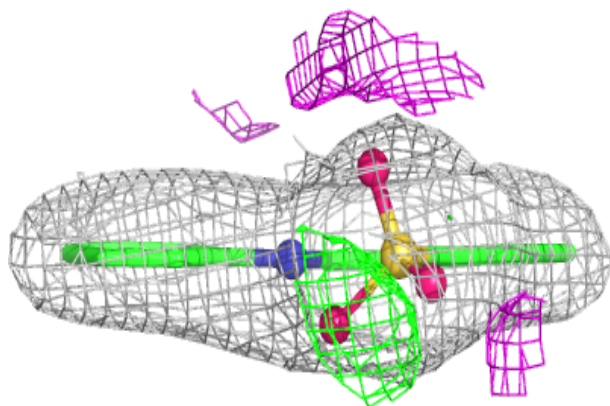
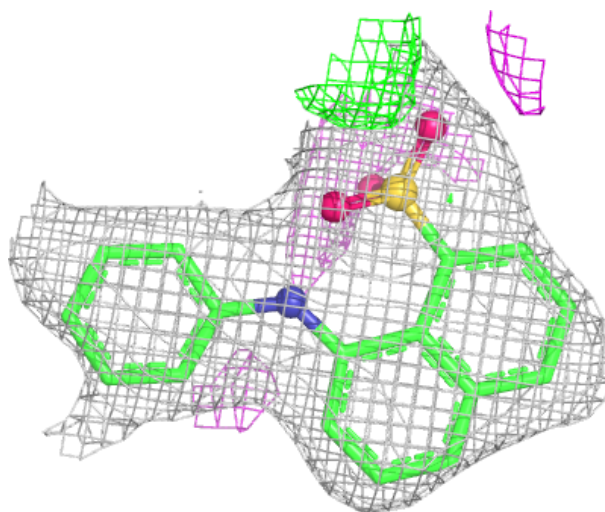
Electron density around 2AN Z 201:

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



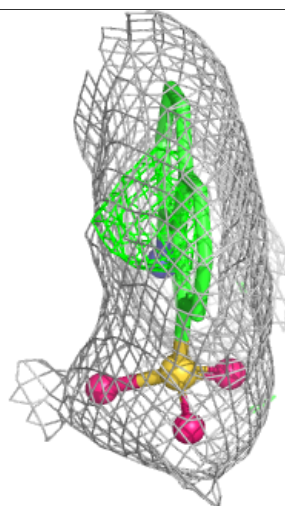
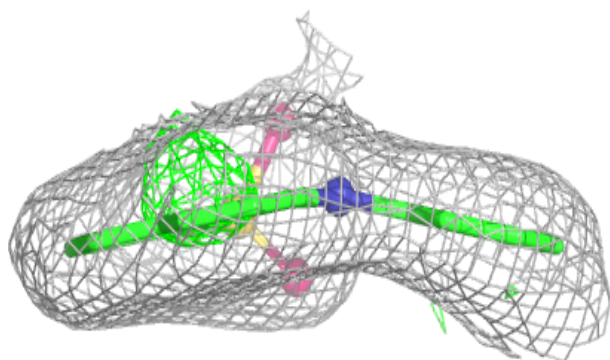
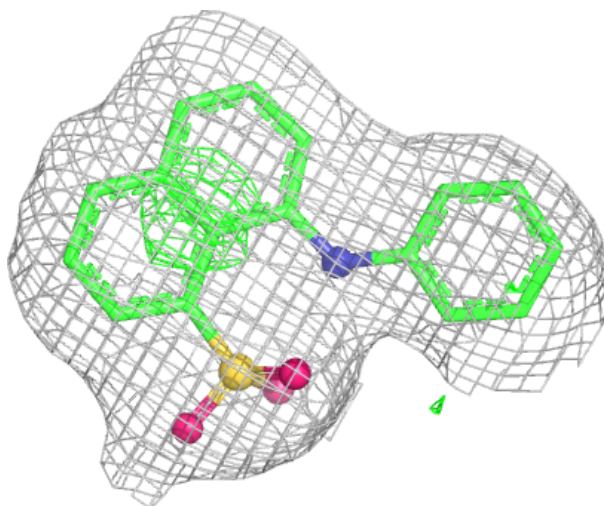
Electron density around 2AN X 204:

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



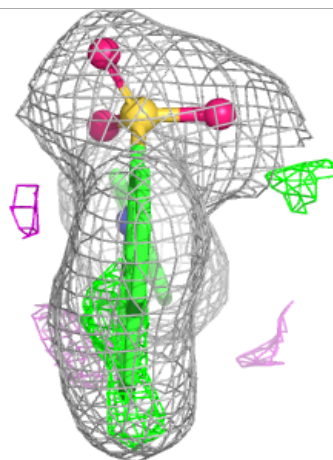
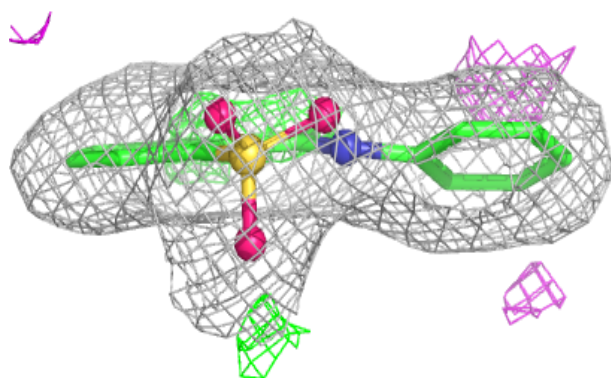
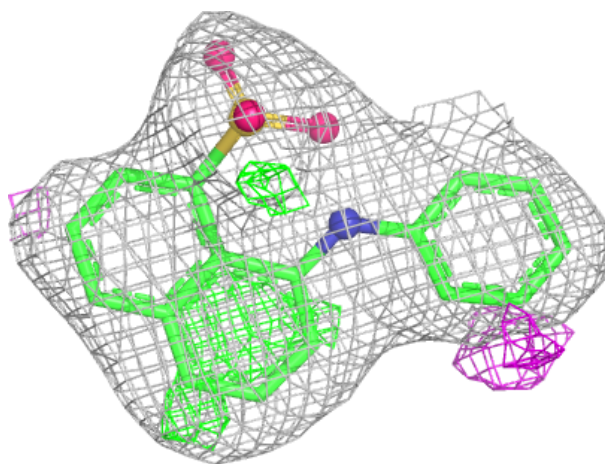
Electron density around 2AN d 201:

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



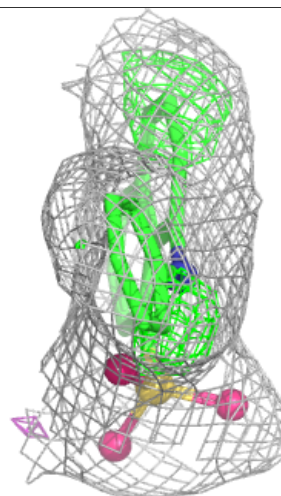
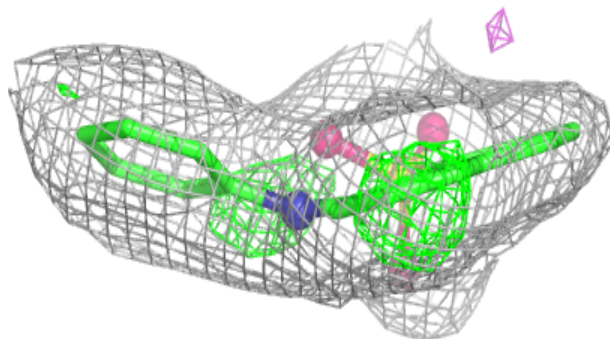
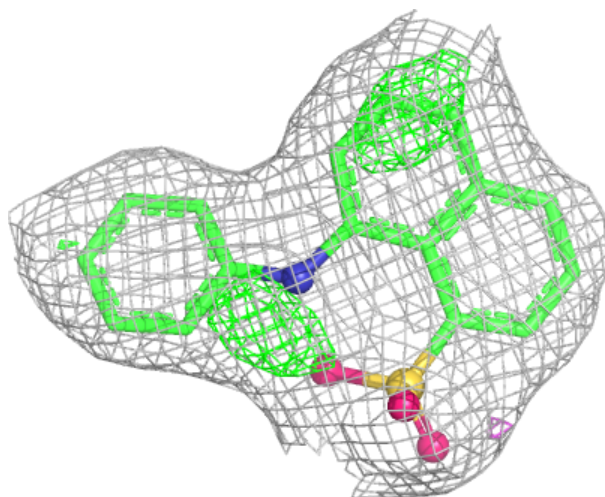
Electron density around 2AN j 201:

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



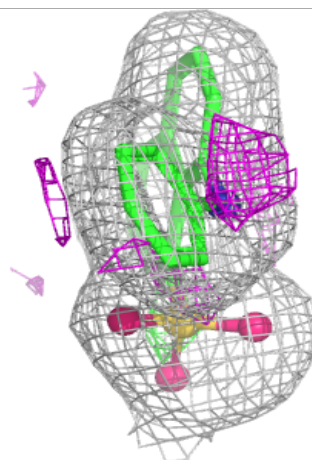
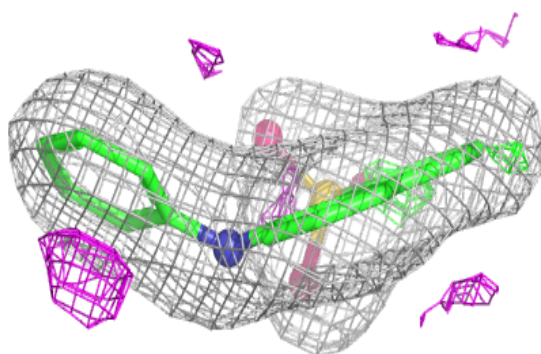
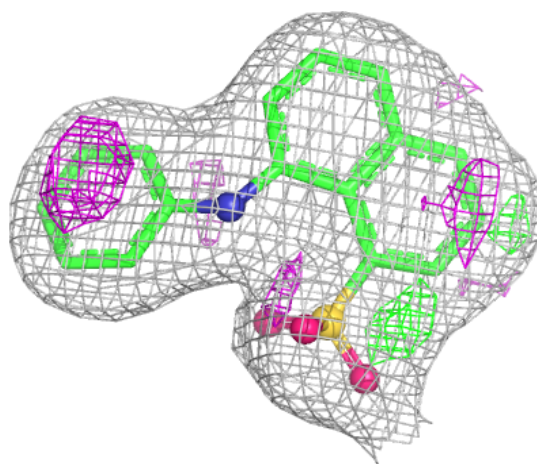
Electron density around 2AN d 202:

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



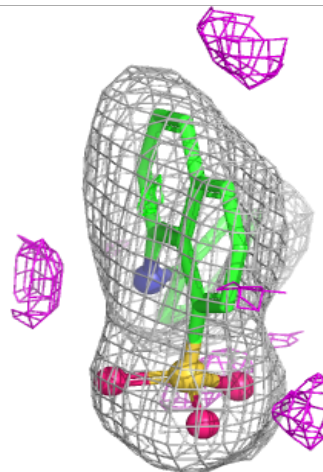
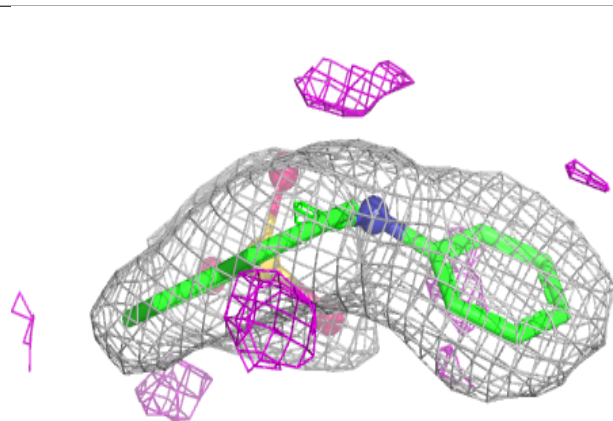
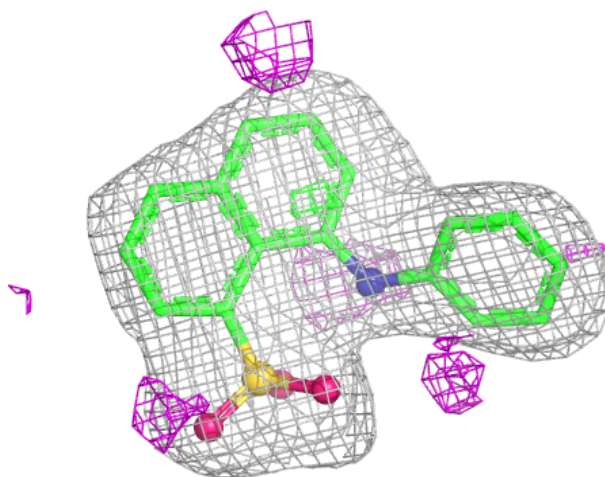
Electron density around 2AN R 202:

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



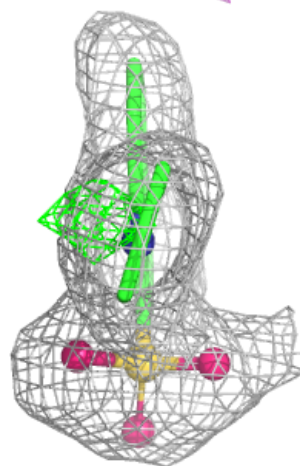
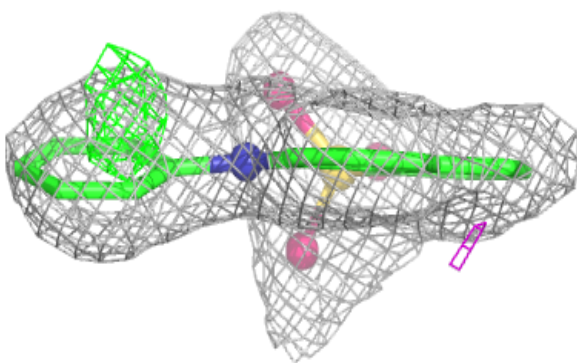
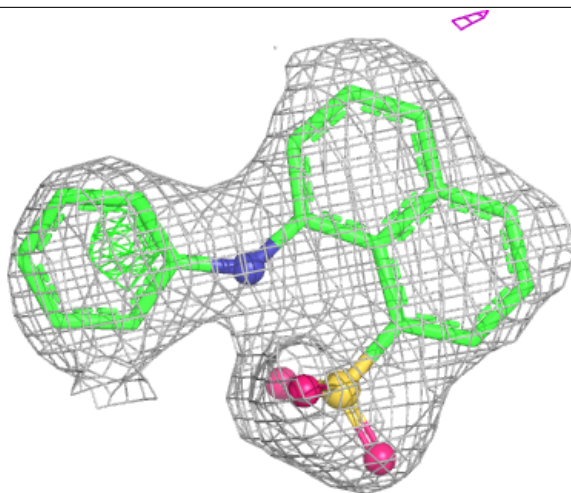
Electron density around 2AN C 201:

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



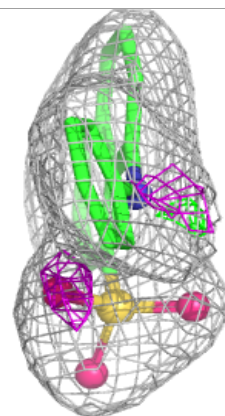
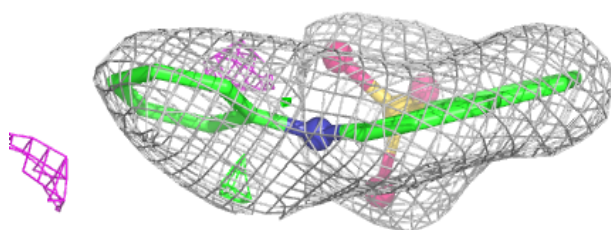
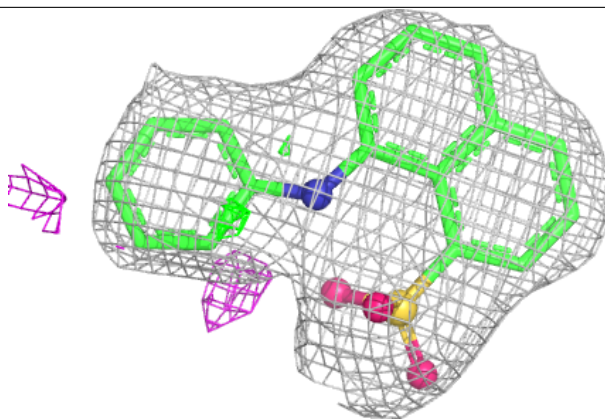
Electron density around 2AN B 204:

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



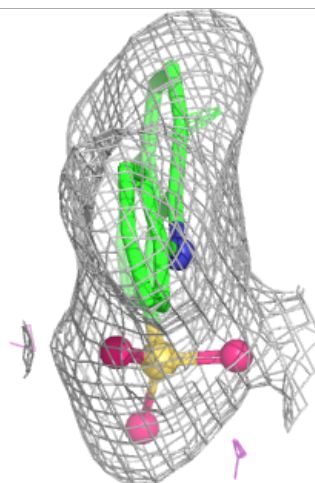
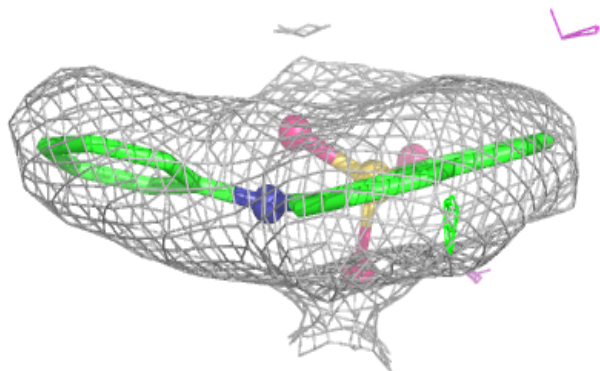
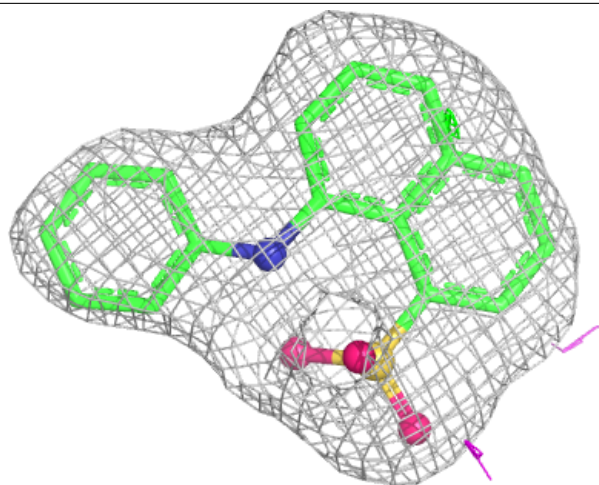
Electron density around 2AN b 202:

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



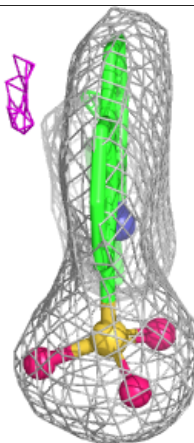
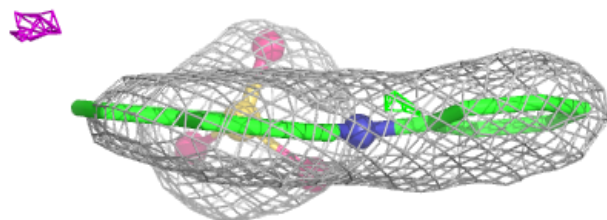
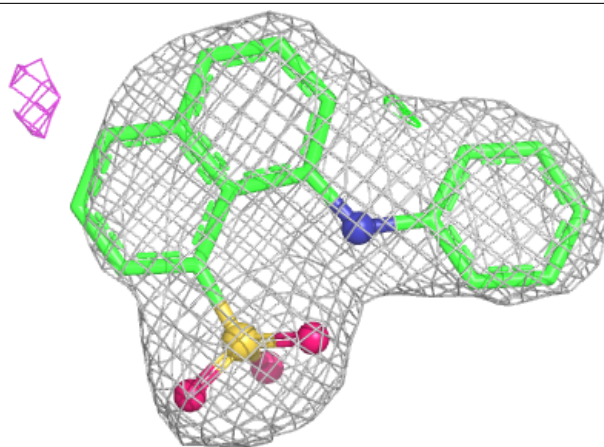
Electron density around 2AN b 204:

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



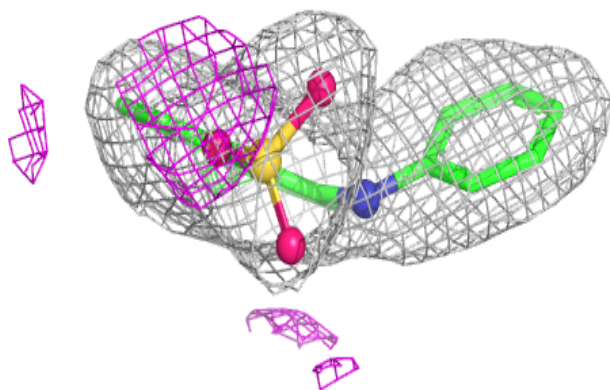
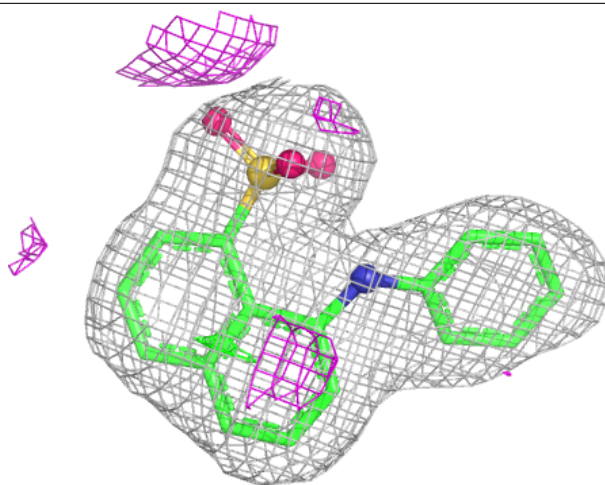
Electron density around 2AN Y 202:

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



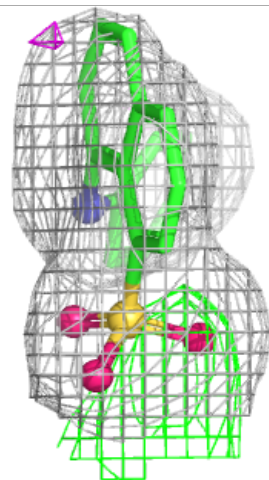
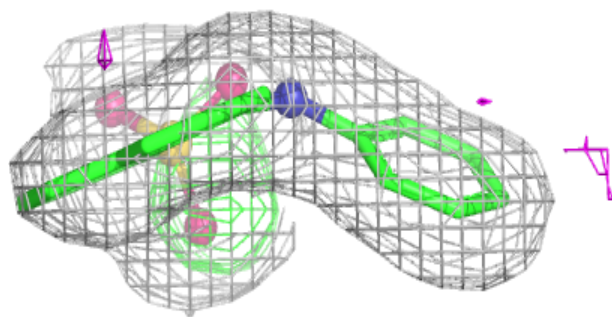
Electron density around 2AN G 201:

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



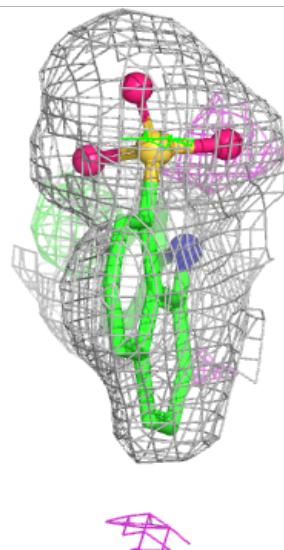
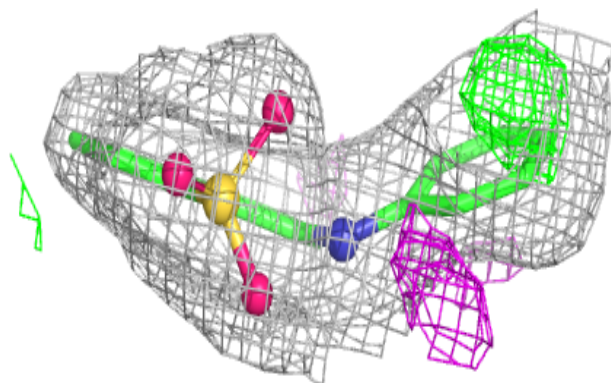
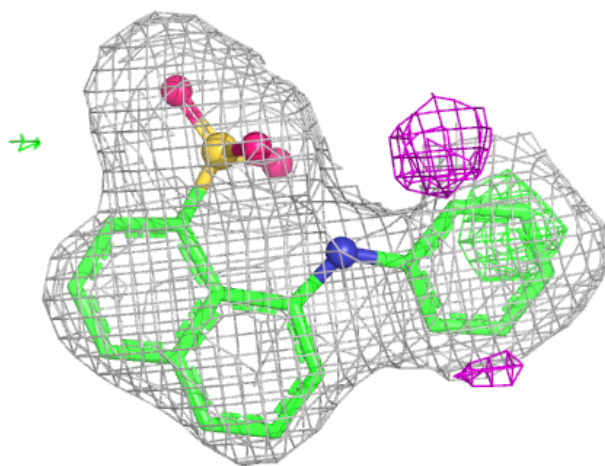
Electron density around 2AN B 205:

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



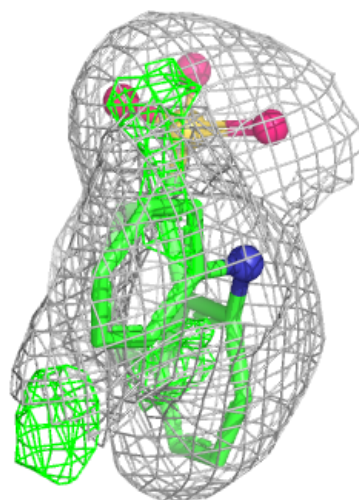
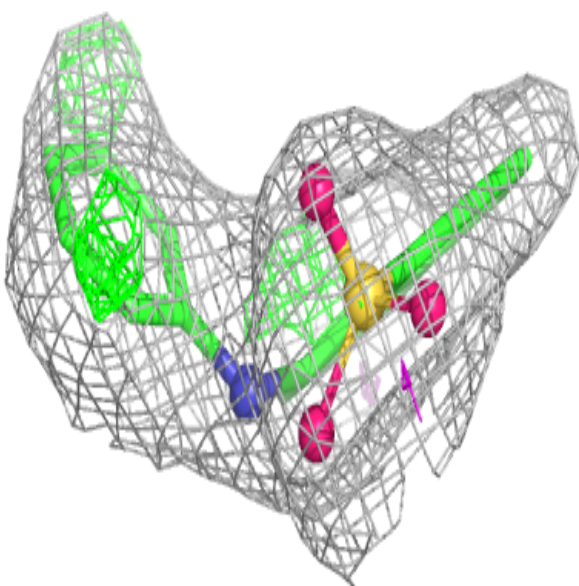
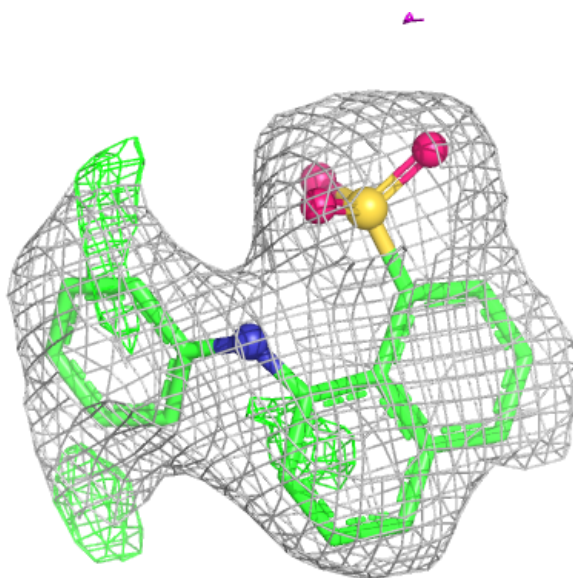
Electron density around 2AN h 206:

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



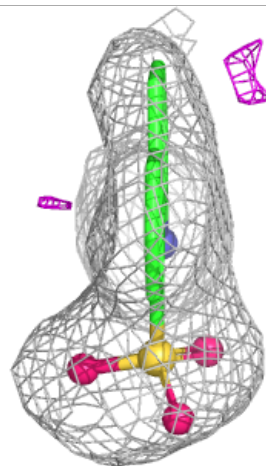
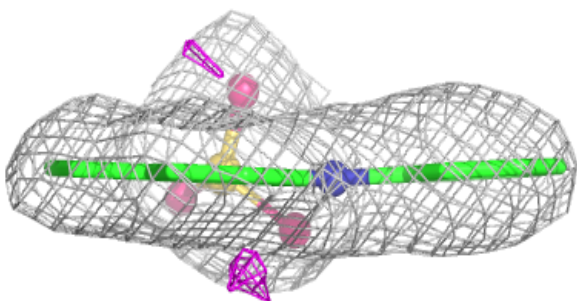
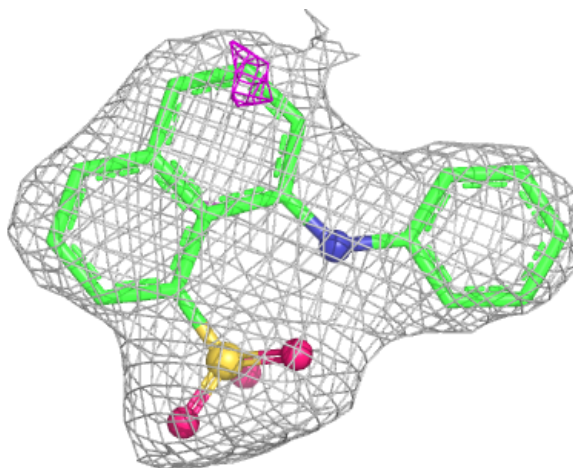
Electron density around 2AN M 203:

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



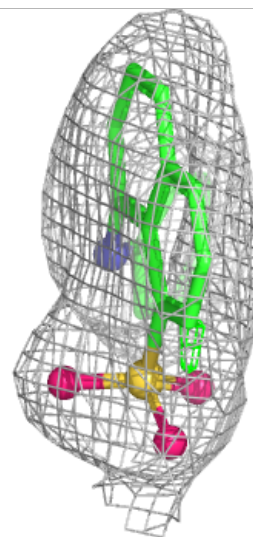
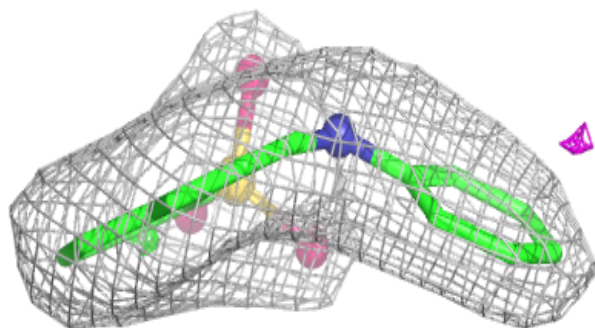
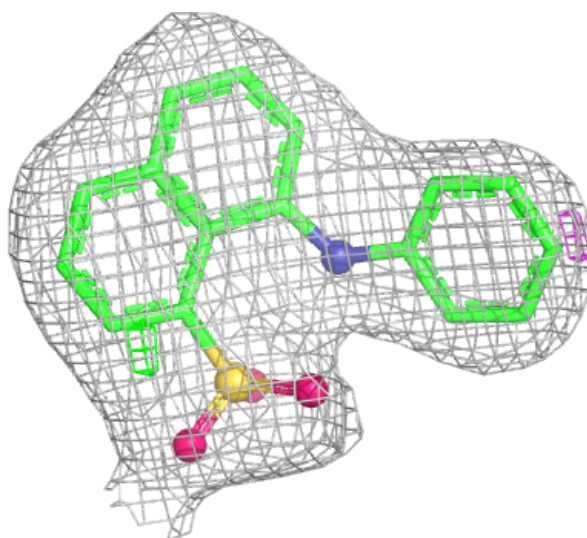
Electron density around 2AN L 204:

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



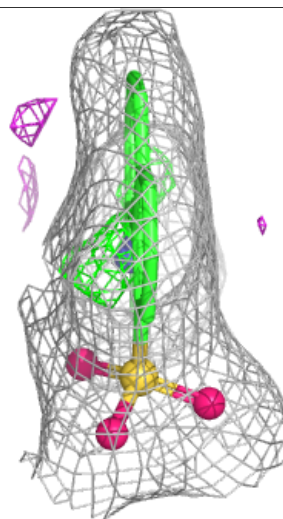
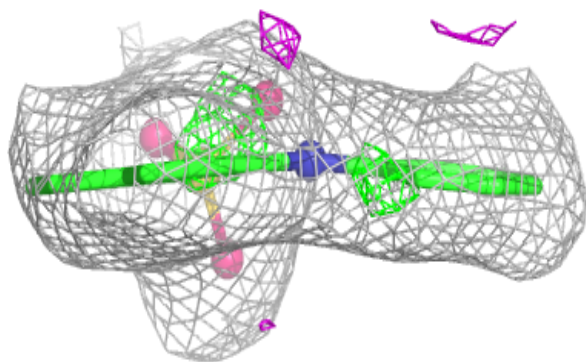
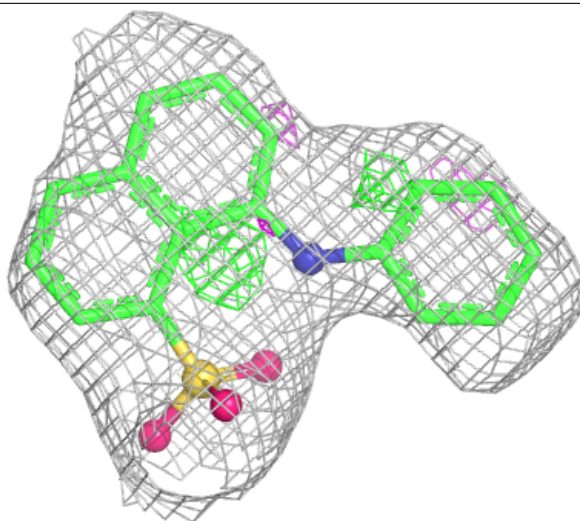
Electron density around 2AN D 202:

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



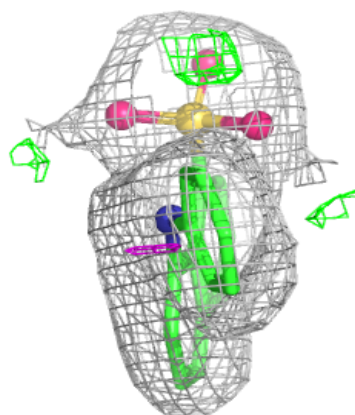
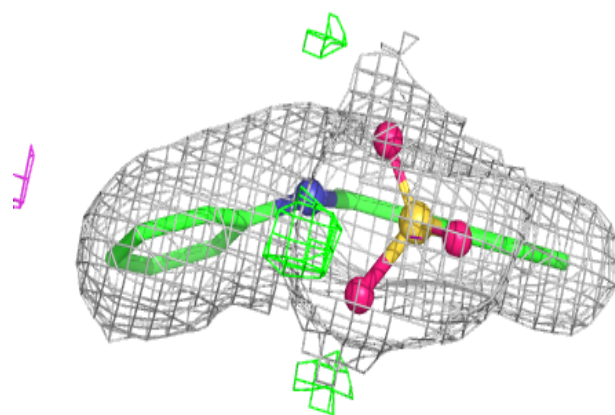
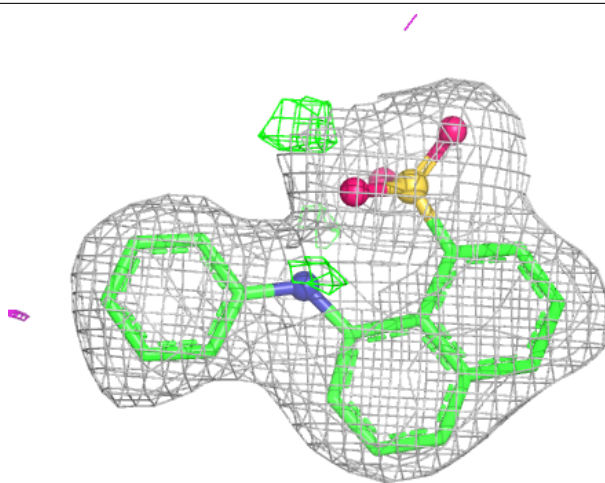
Electron density around 2AN F 201:

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



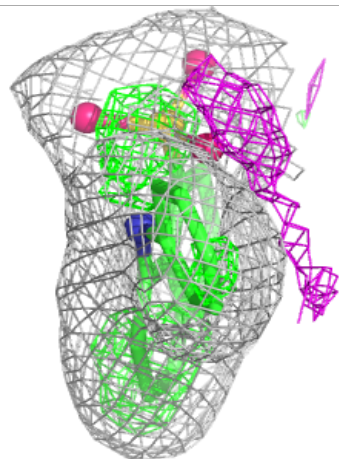
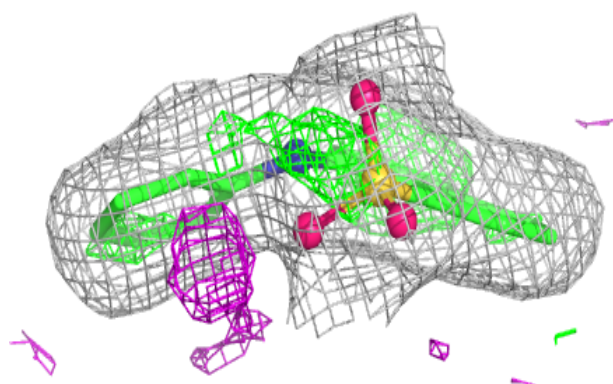
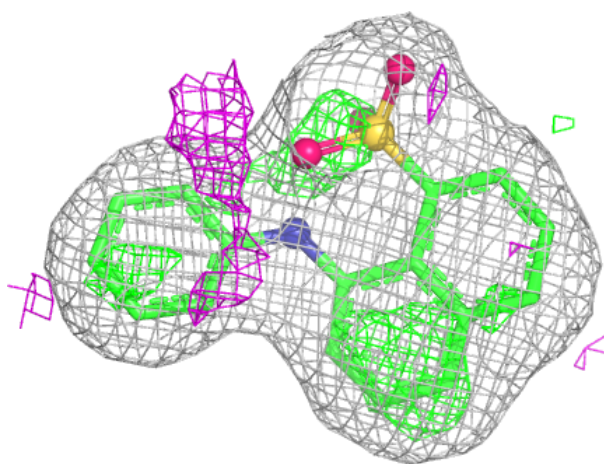
Electron density around 2AN X 205:

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



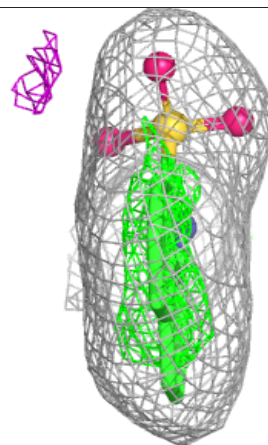
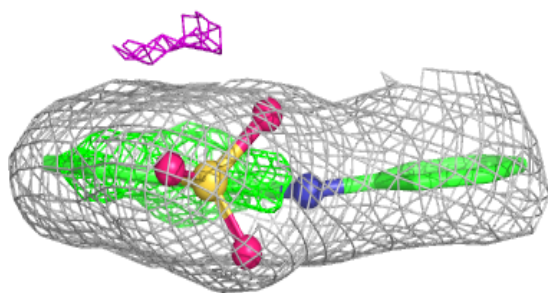
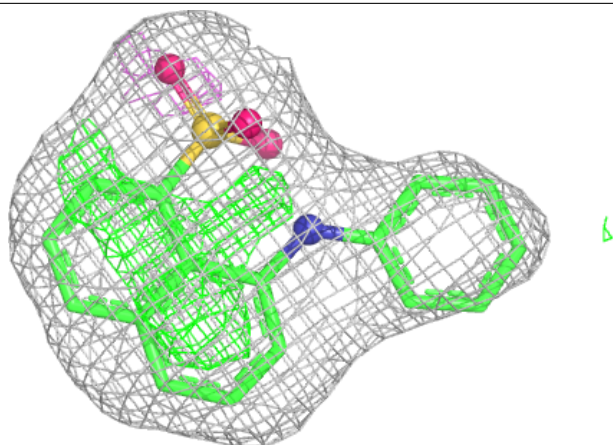
Electron density around 2AN f 204:

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



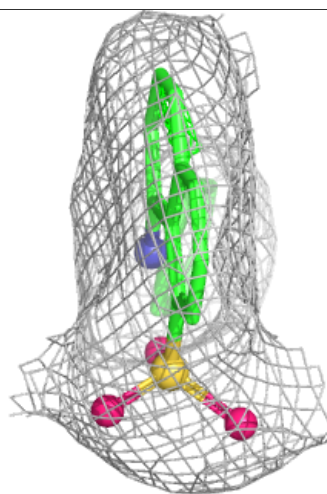
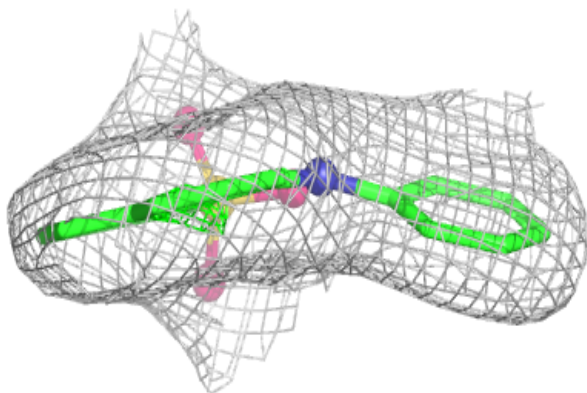
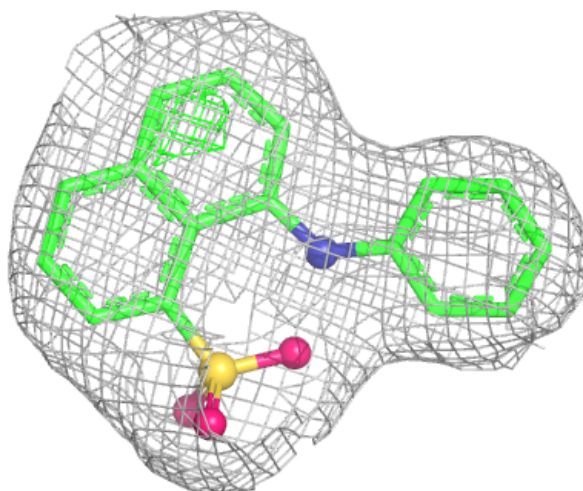
Electron density around 2AN J 201:

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



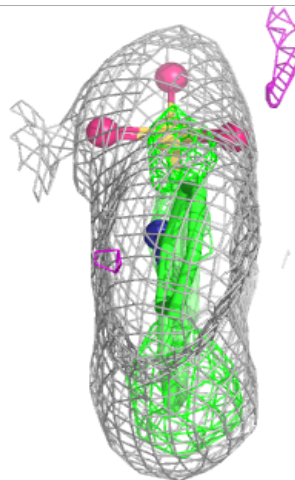
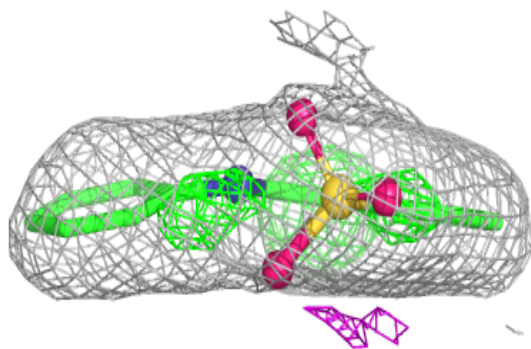
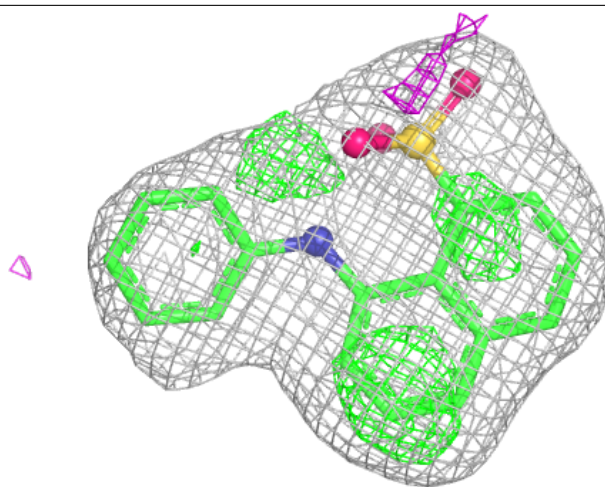
Electron density around 2AN b 203:

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



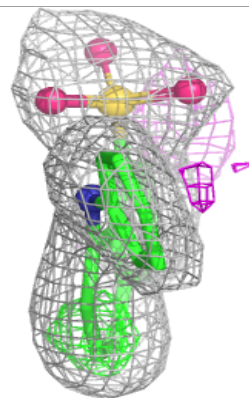
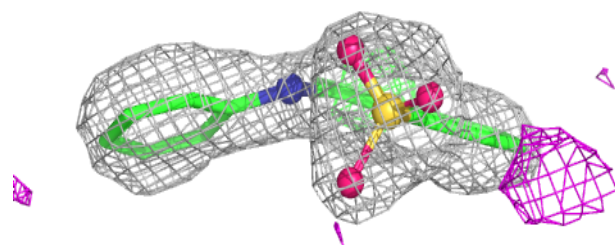
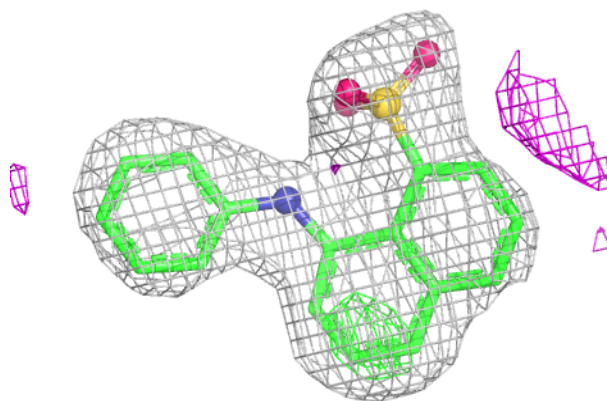
Electron density around 2AN B 203:

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

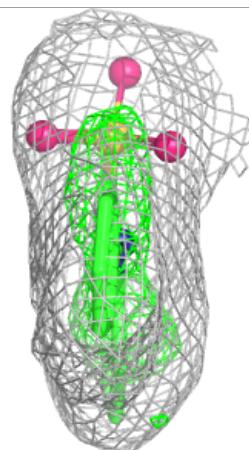
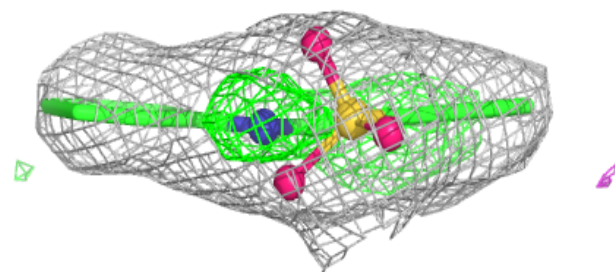
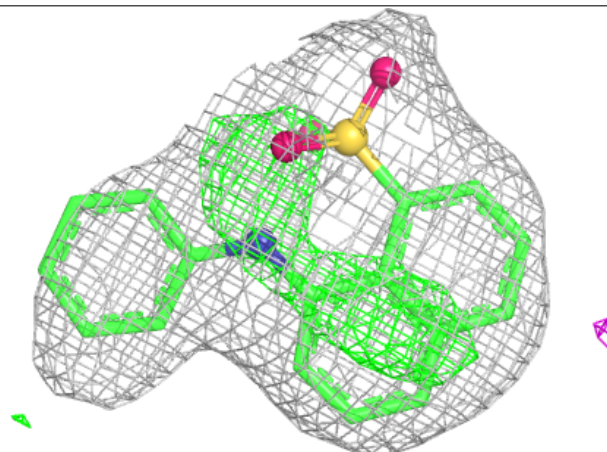


Electron density around 2AN i 201:

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

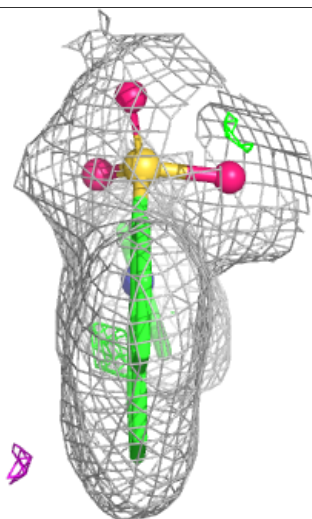
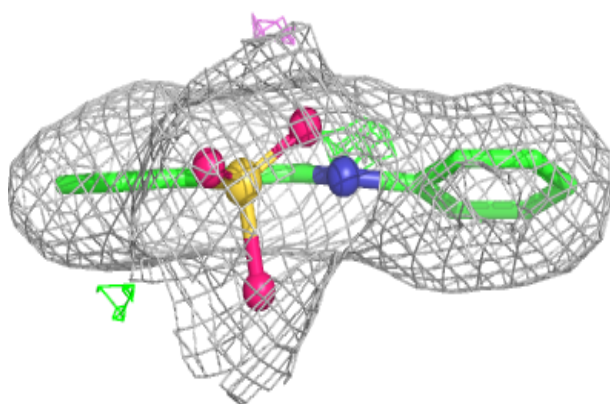
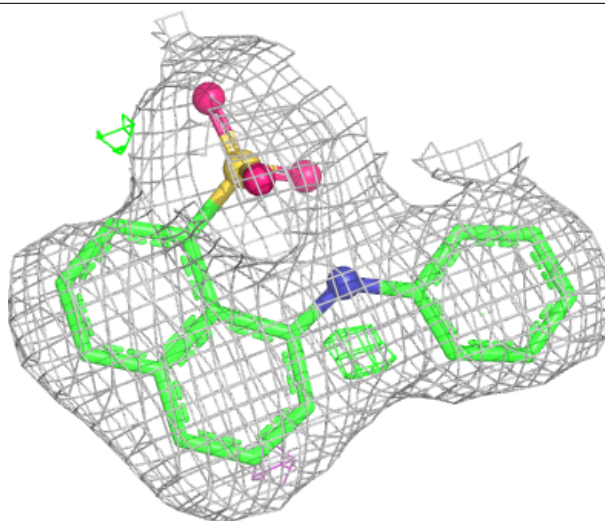
**Electron density around 2AN N 204:**

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



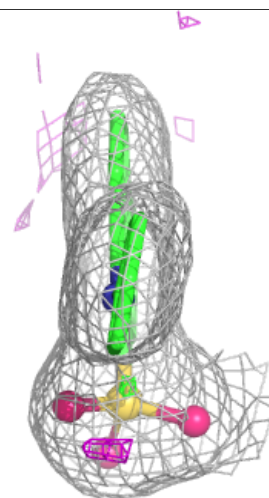
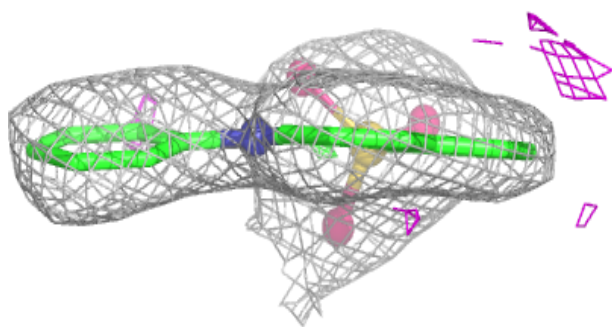
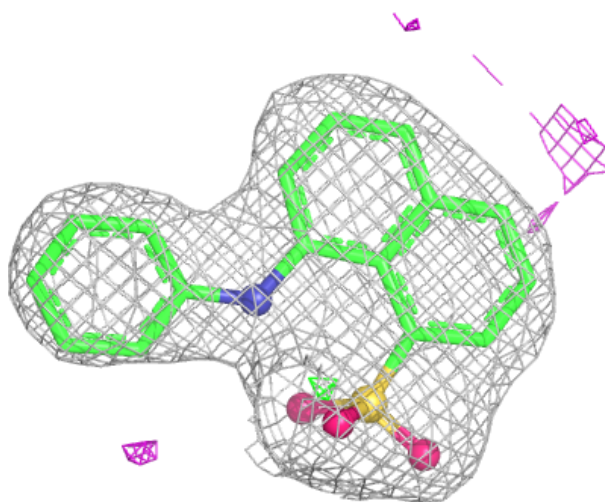
Electron density around 2AN V 201:

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



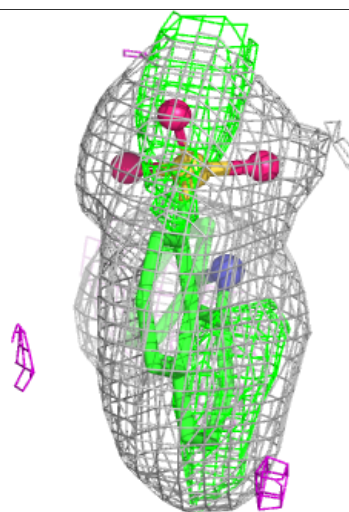
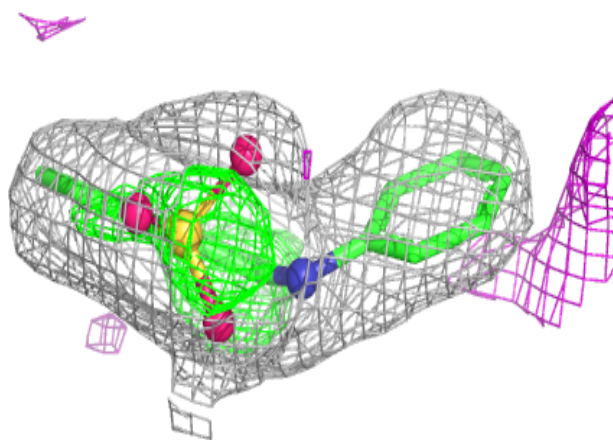
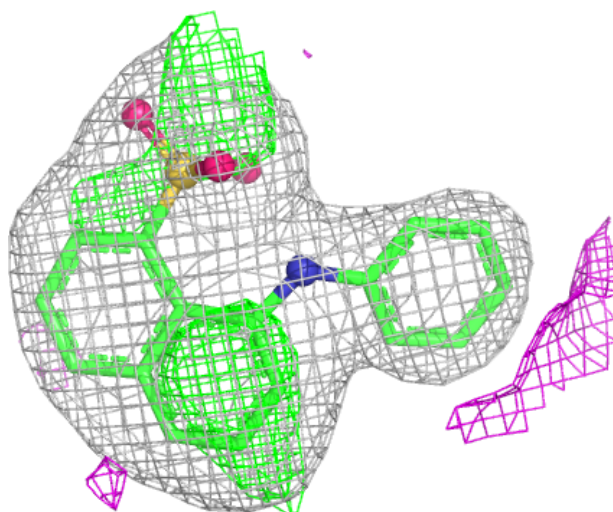
Electron density around 2AN c 204:

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



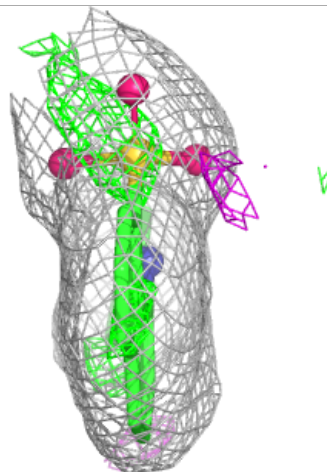
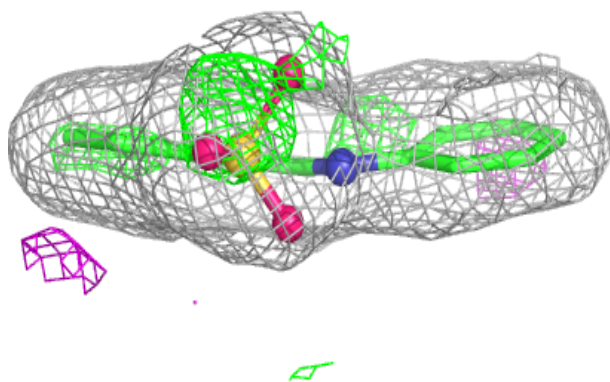
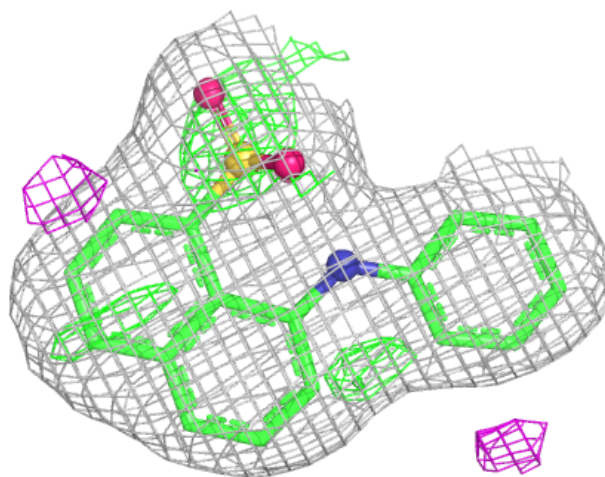
Electron density around 2AN P 204:

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



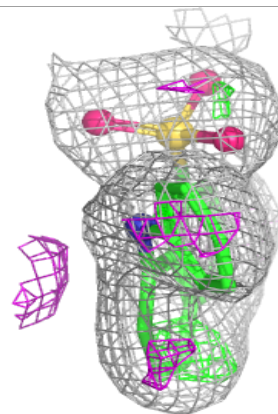
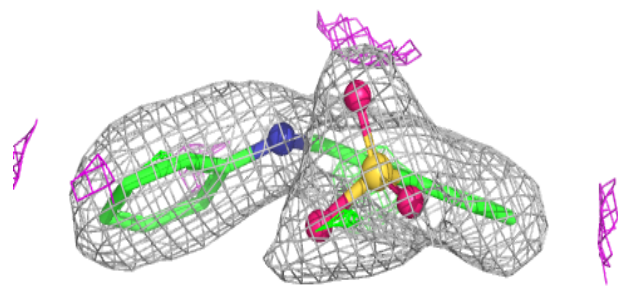
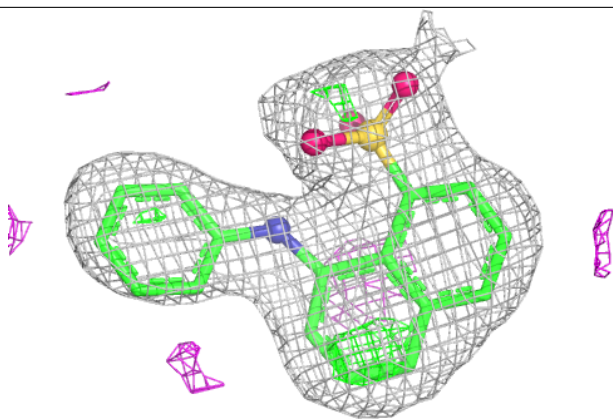
Electron density around 2AN b 201:

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



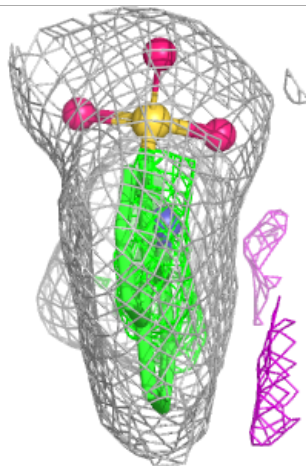
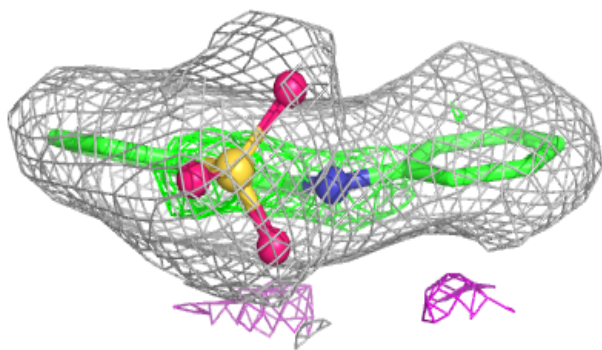
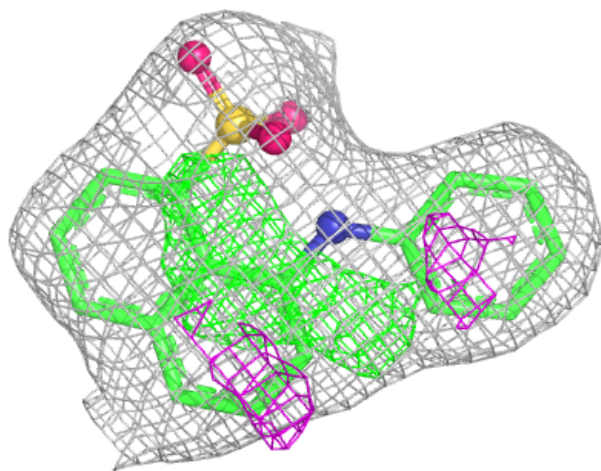
Electron density around 2AN T 202:

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



Electron density around 2AN J 202:

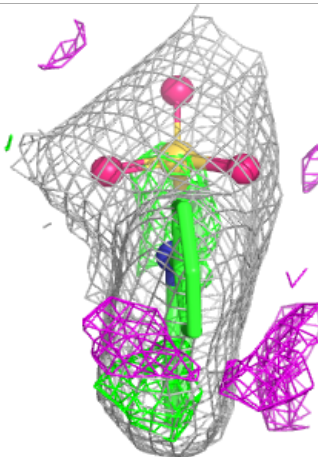
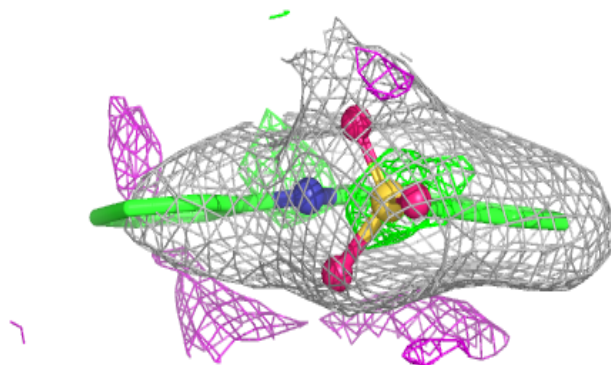
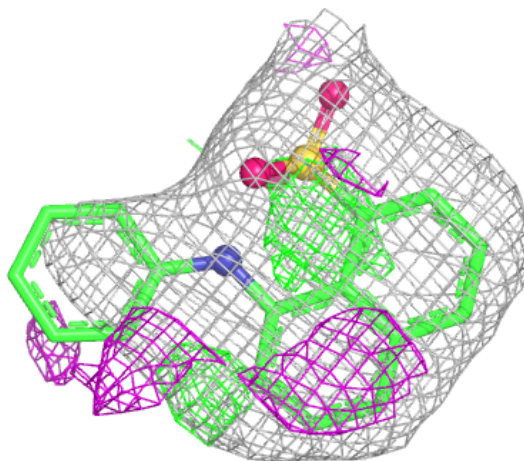
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around 2AN G 203:

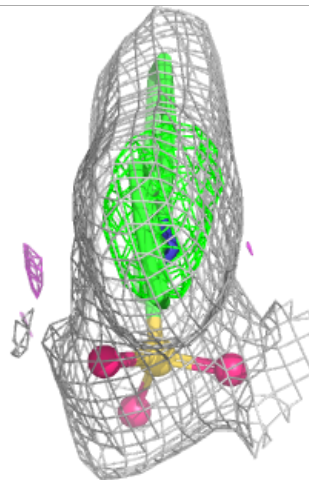
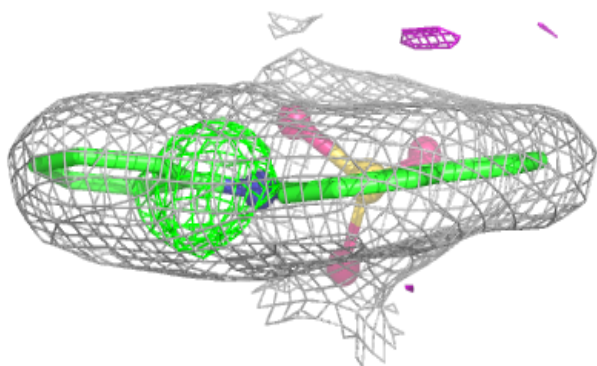
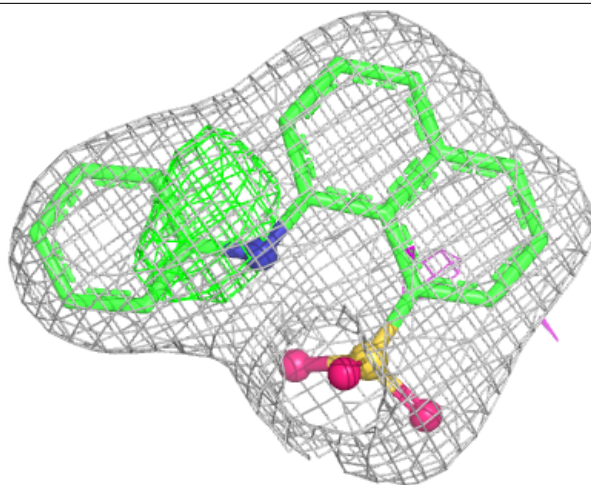
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

✓



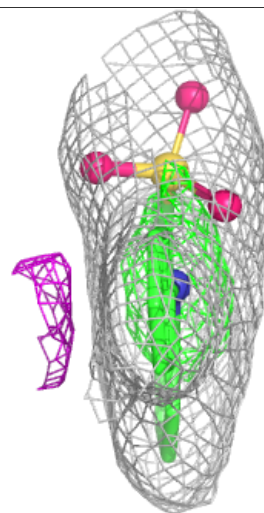
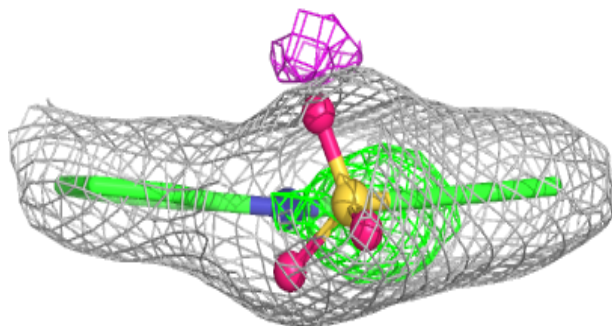
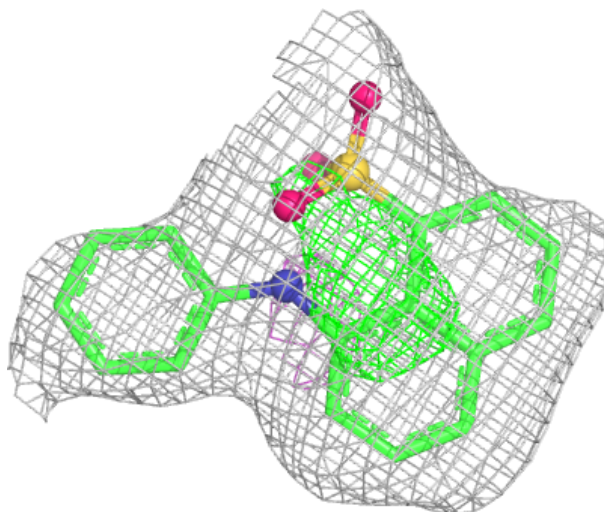
Electron density around 2AN f 205:

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



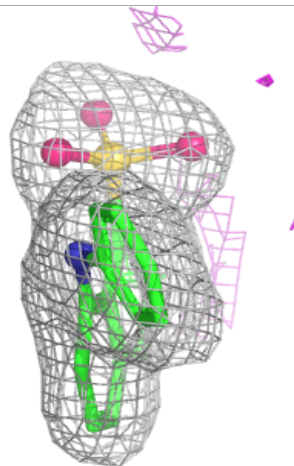
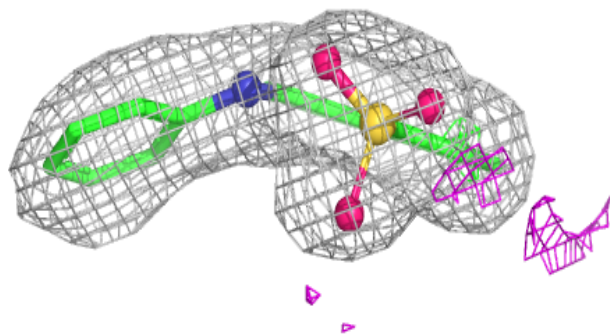
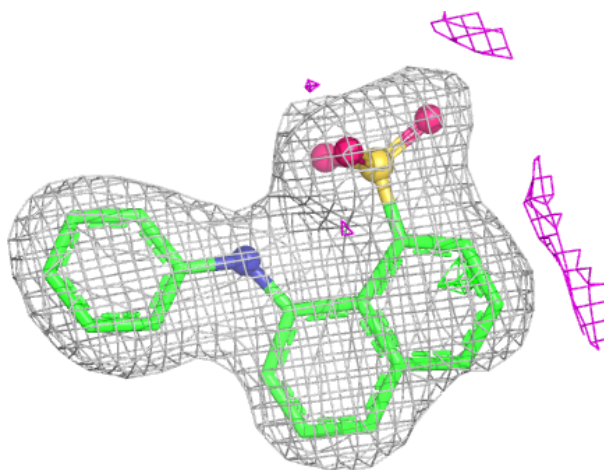
Electron density around 2AN O 201:

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



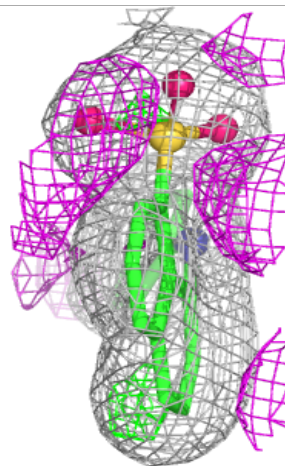
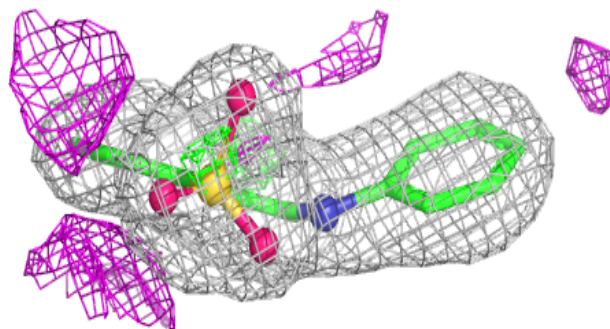
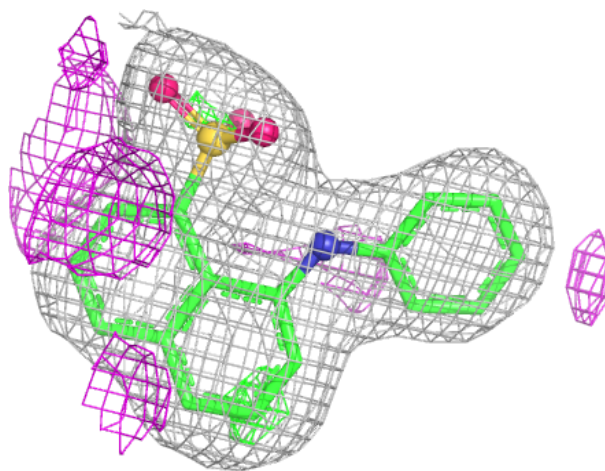
Electron density around 2AN S 202:

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



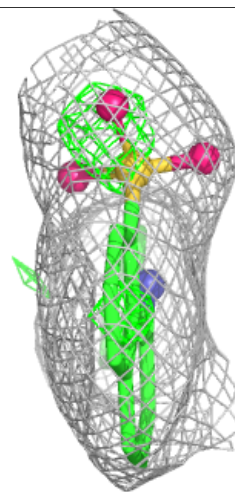
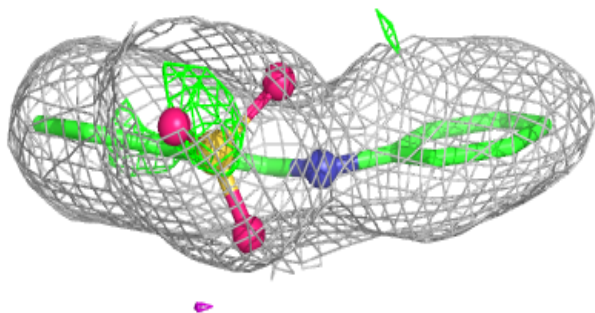
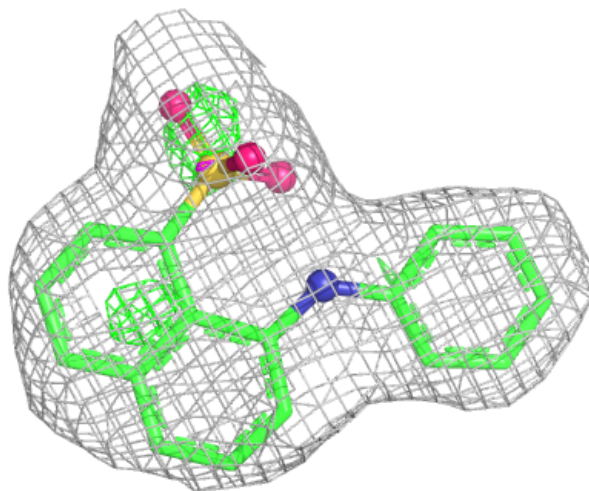
Electron density around 2AN e 201:

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



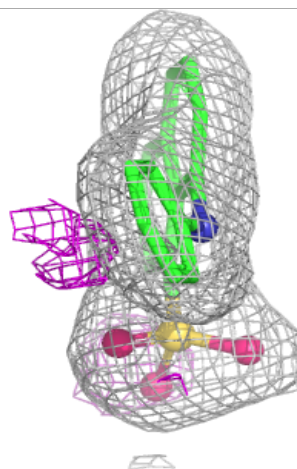
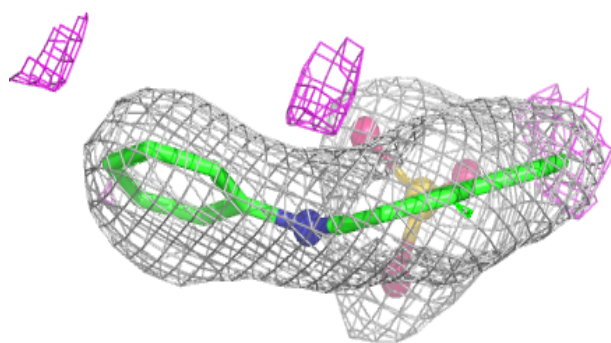
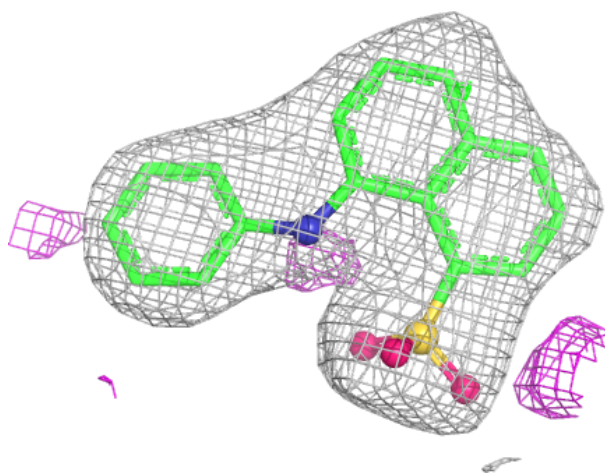
Electron density around 2AN Q 202:

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



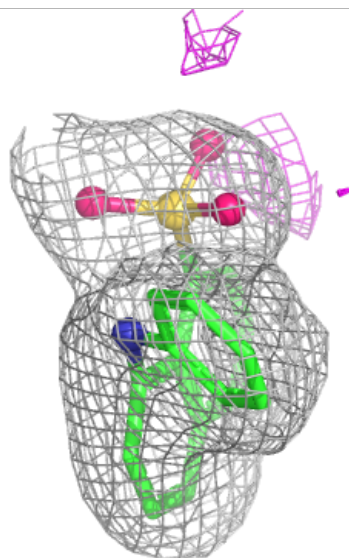
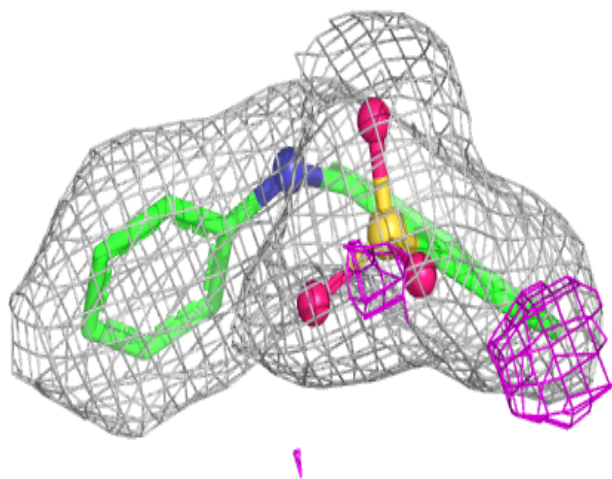
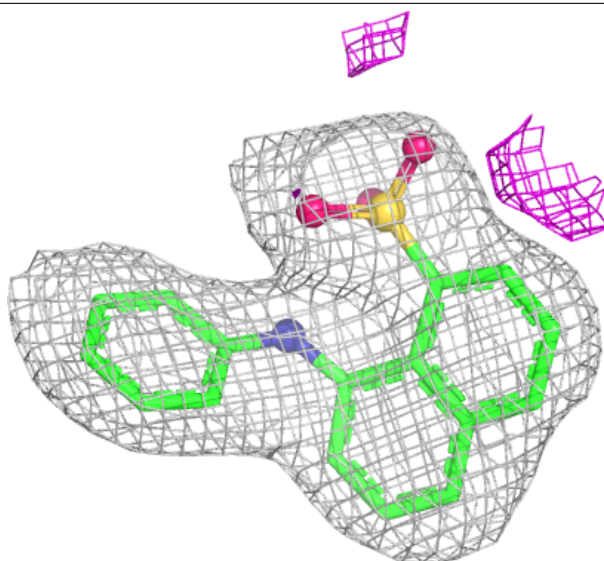
Electron density around 2AN a 202:

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



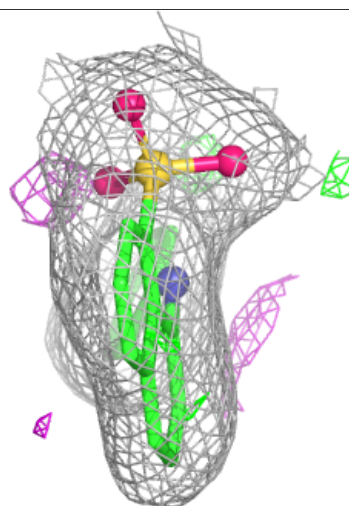
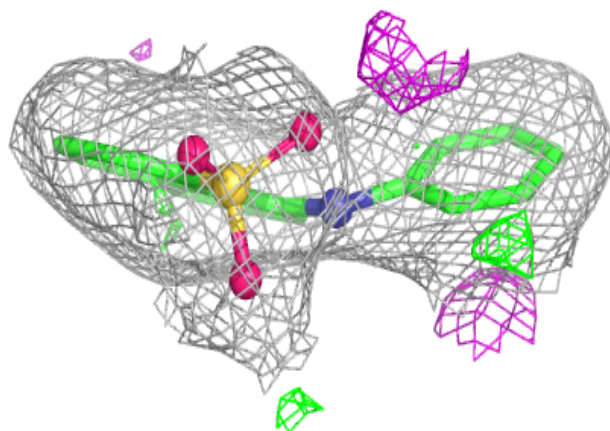
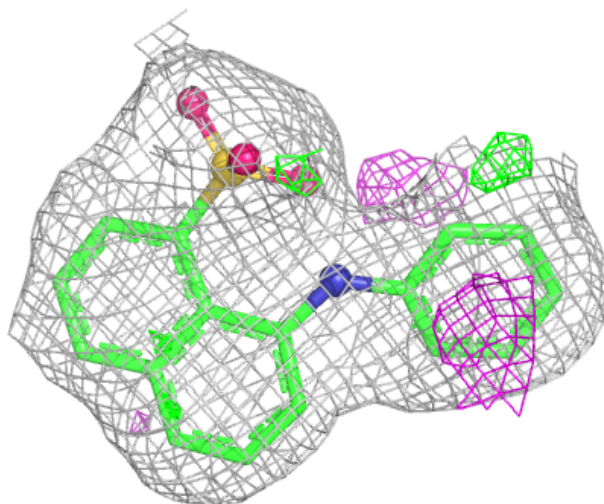
Electron density around 2AN L 203:

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



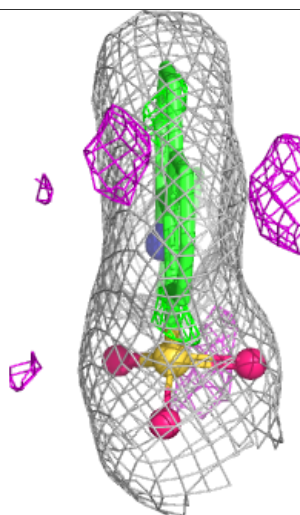
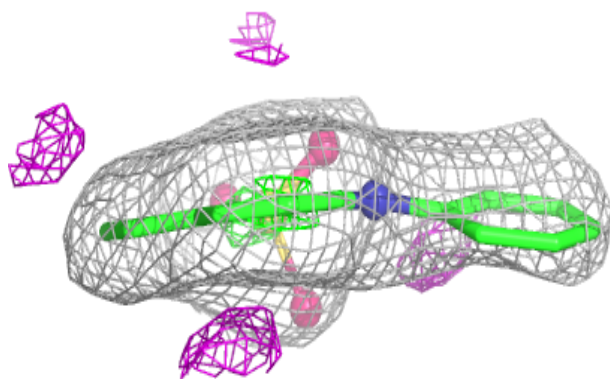
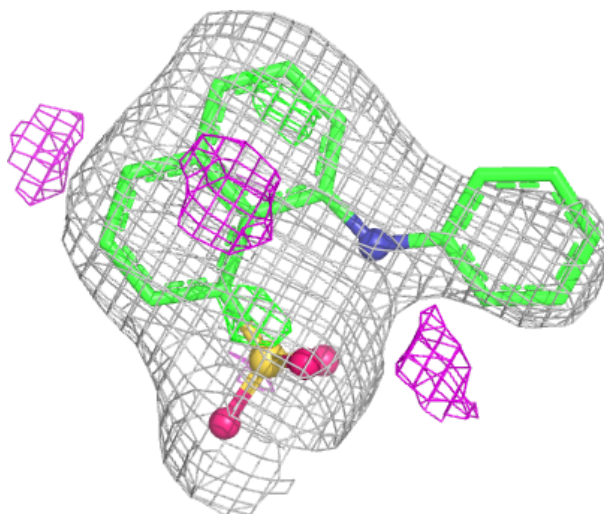
Electron density around 2AN B 202:

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



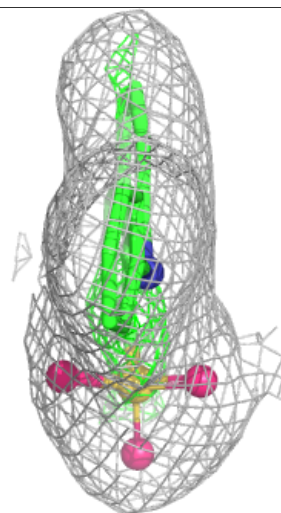
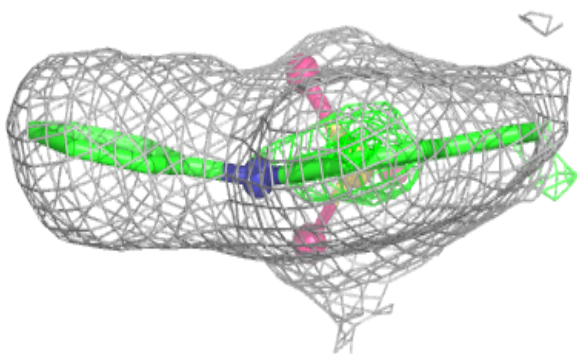
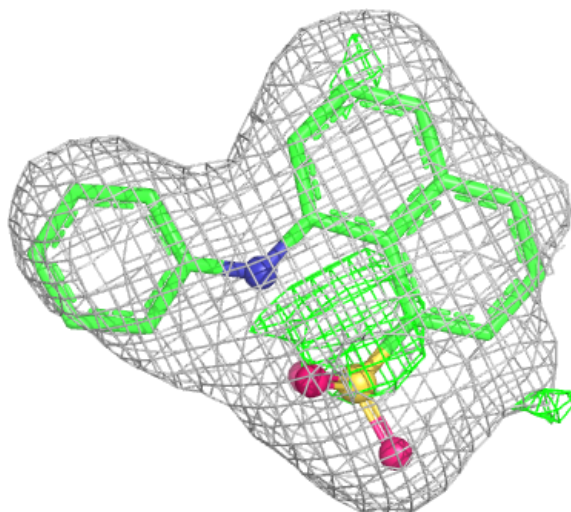
Electron density around 2AN A 201:

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



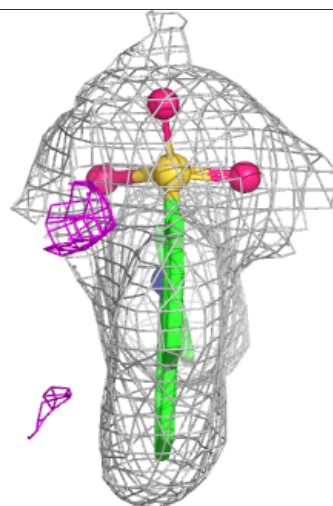
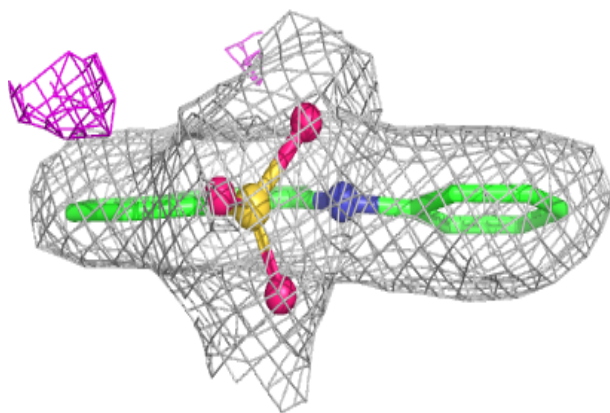
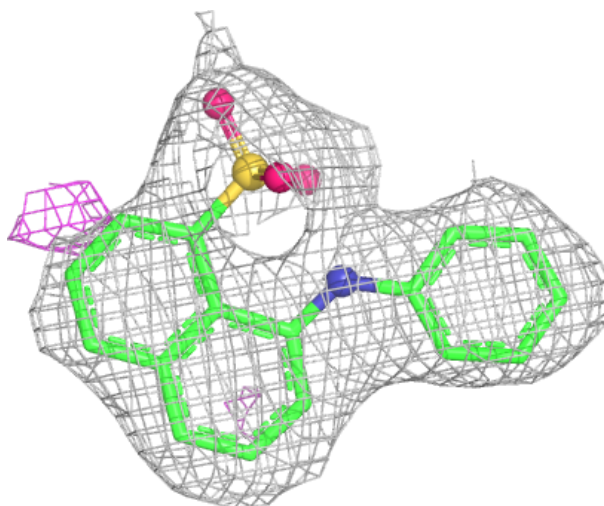
Electron density around 2AN F 203:

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



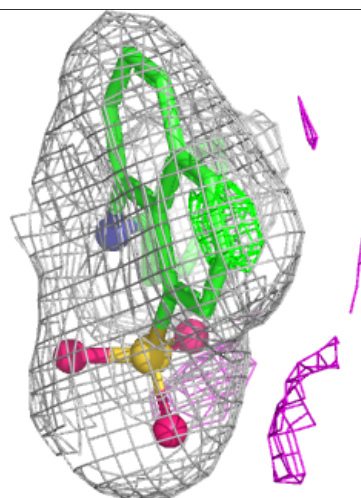
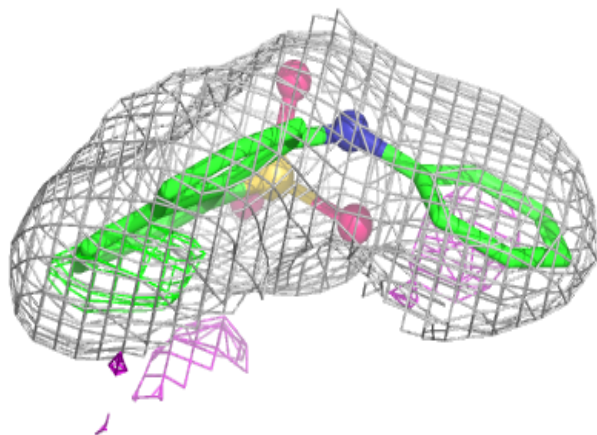
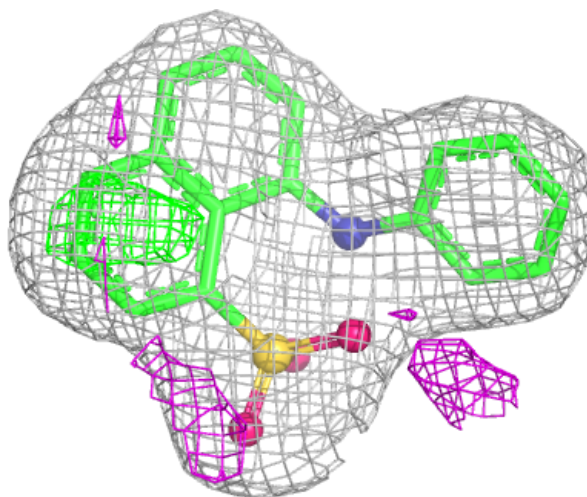
Electron density around 2AN V 204:

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



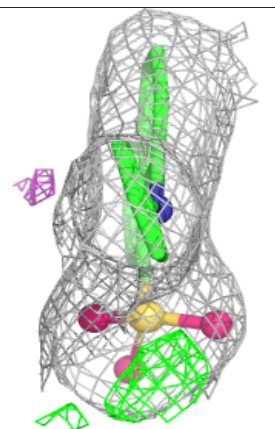
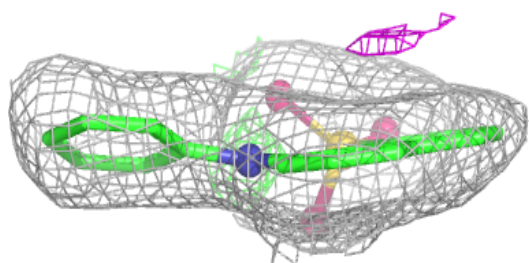
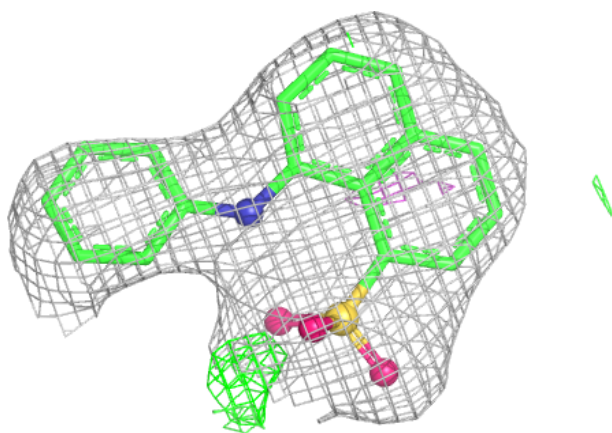
Electron density around 2AN V 205:

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



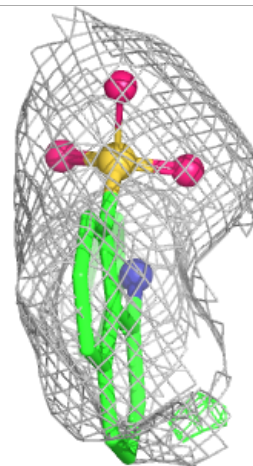
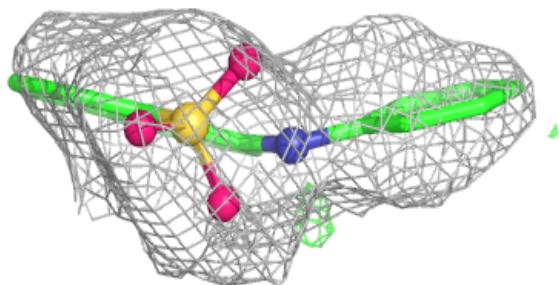
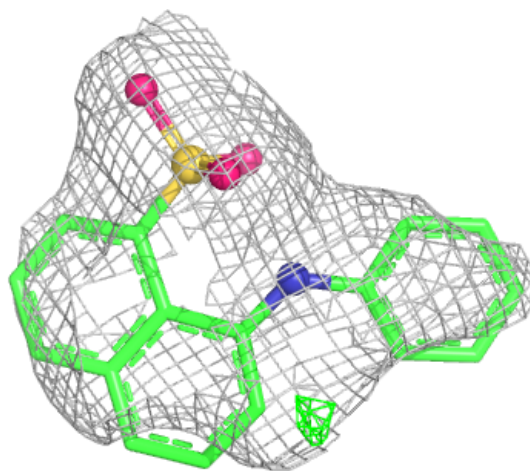
Electron density around 2AN Z 203:

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



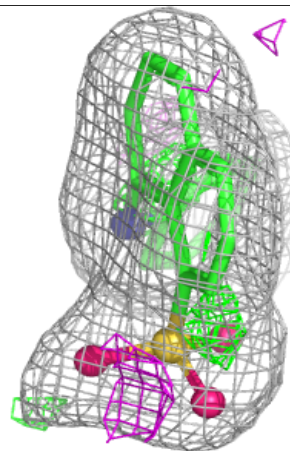
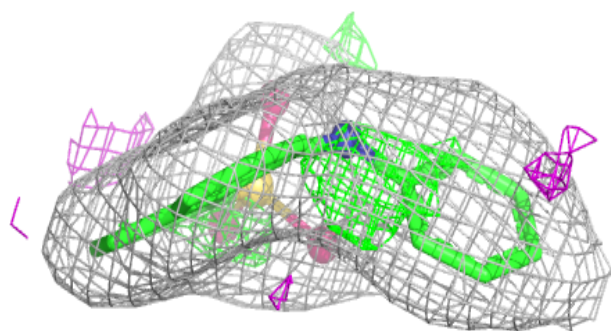
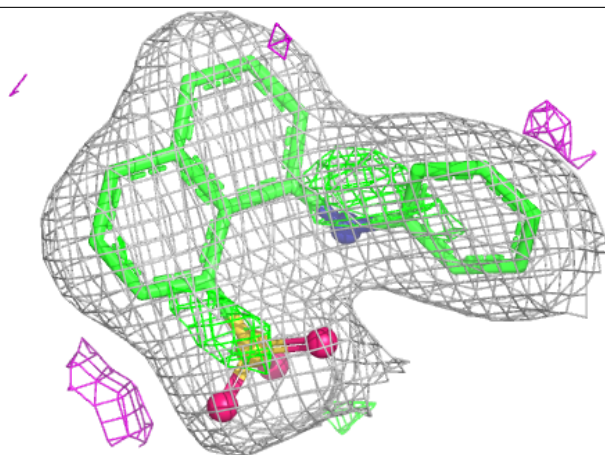
Electron density around 2AN C 202:

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



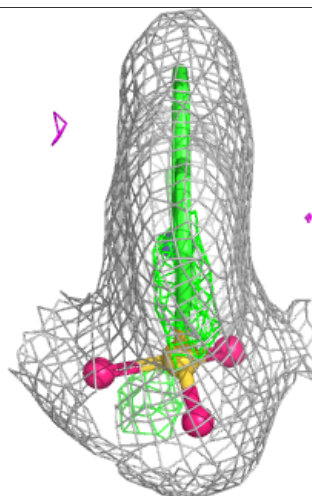
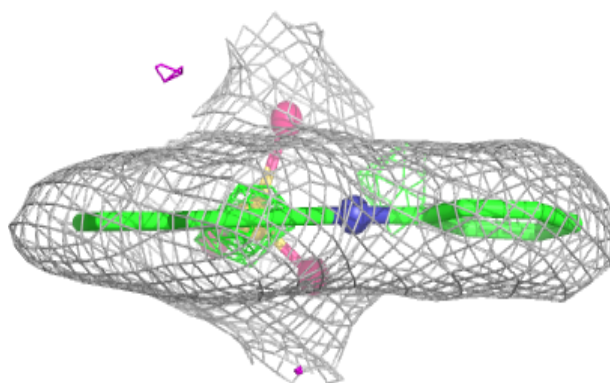
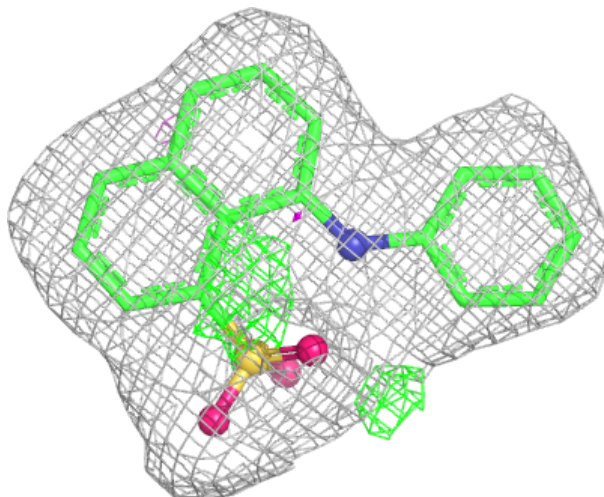
Electron density around 2AN P 202:

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



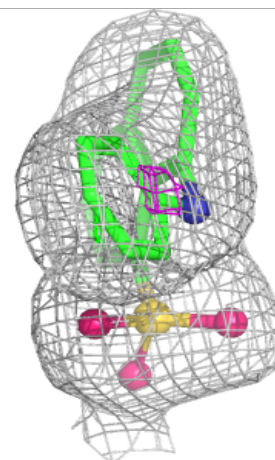
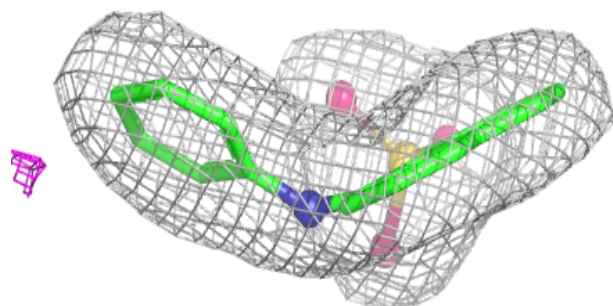
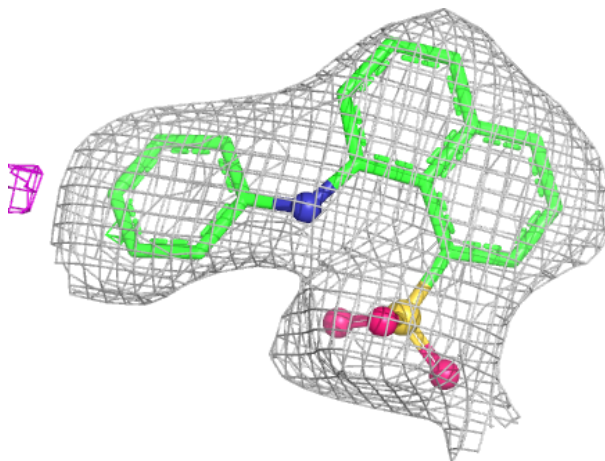
Electron density around 2AN L 202:

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



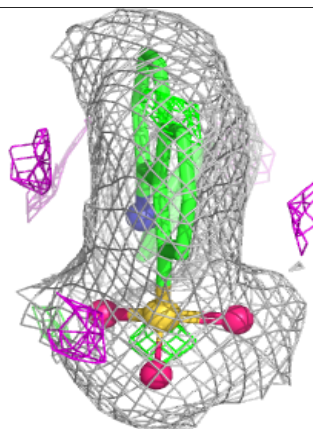
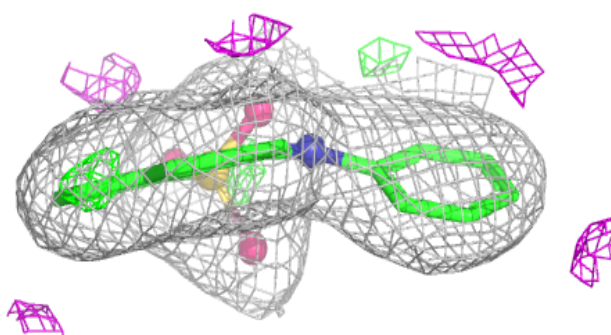
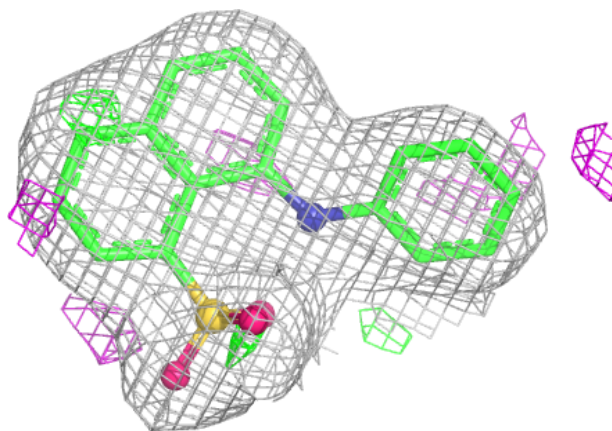
Electron density around 2AN H 202:

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



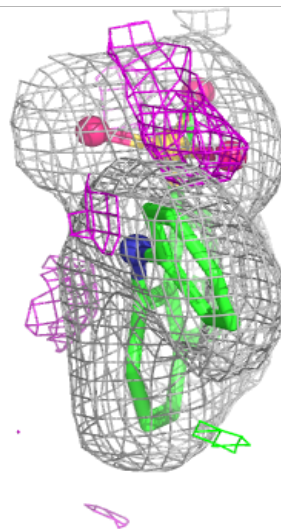
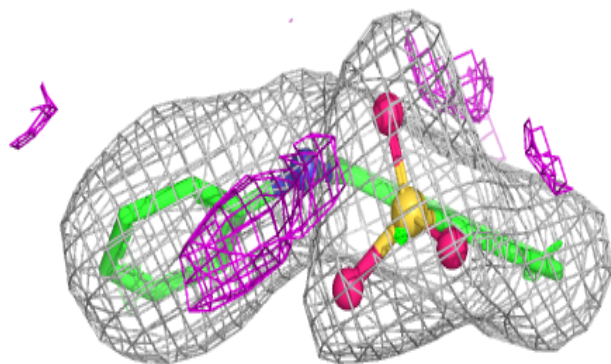
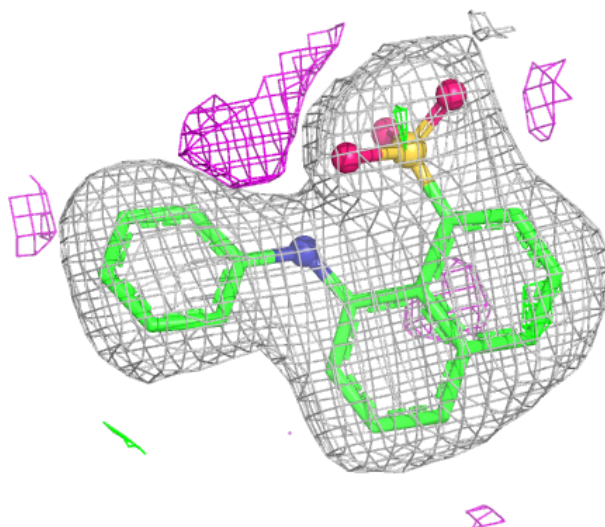
Electron density around 2AN V 203:

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



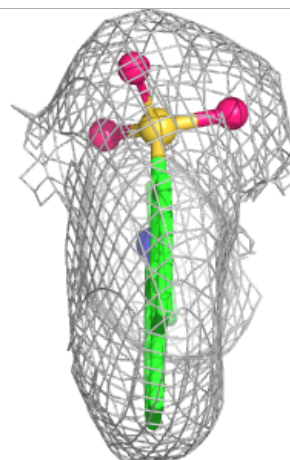
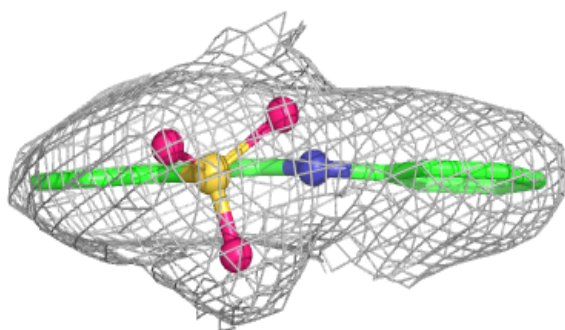
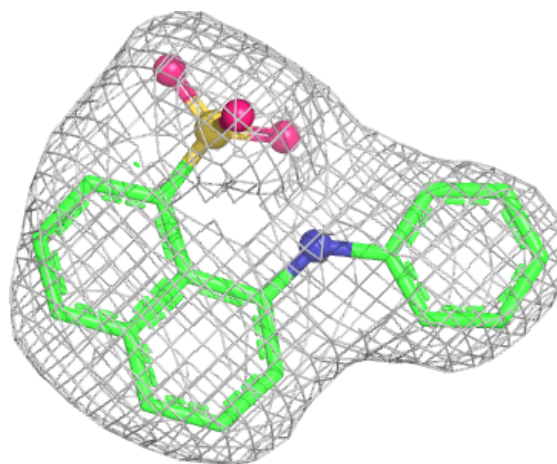
Electron density around 2AN f 202:

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



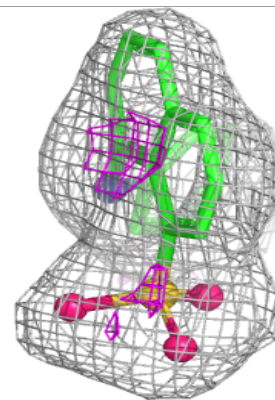
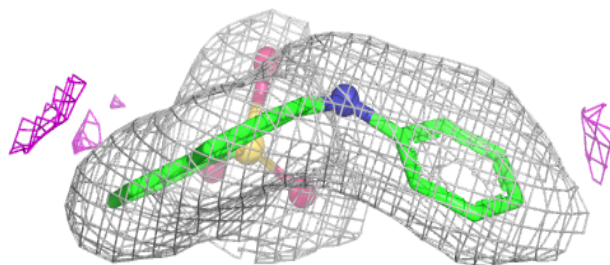
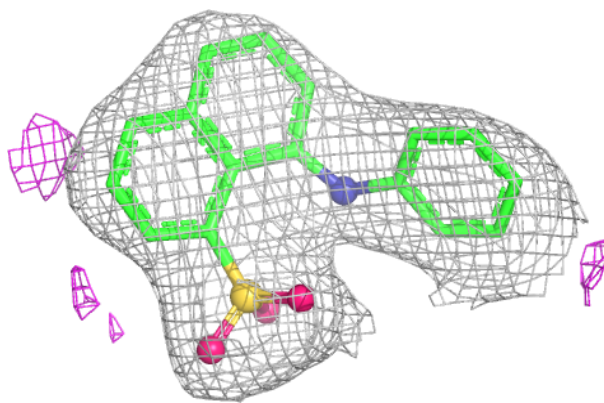
Electron density around 2AN H 203:

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



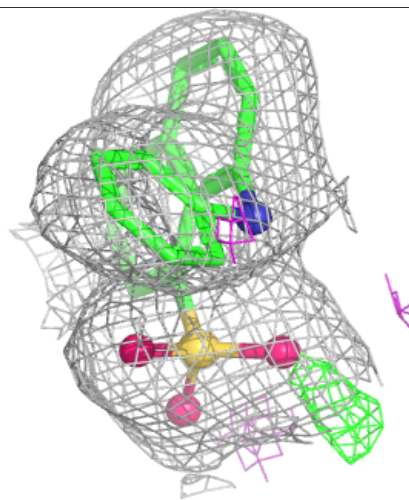
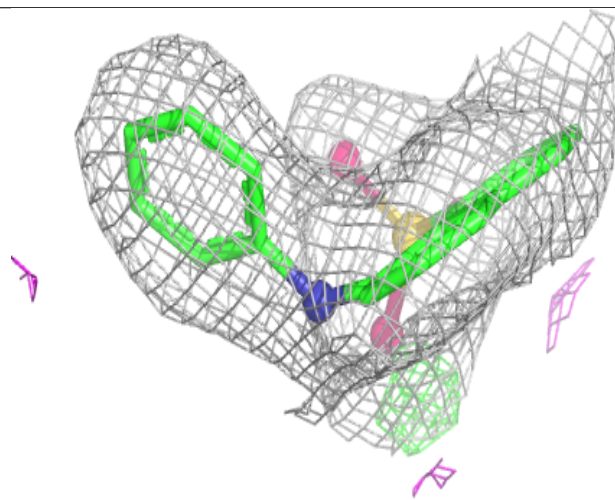
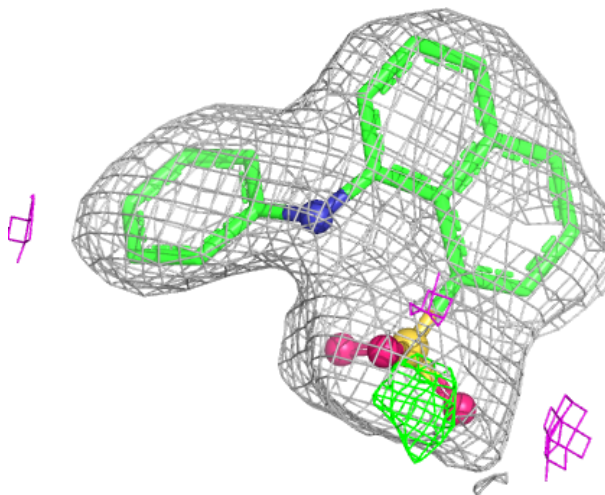
Electron density around 2AN B 201:

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



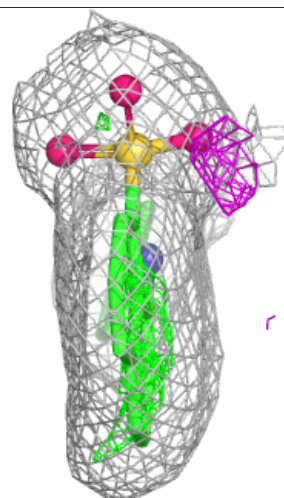
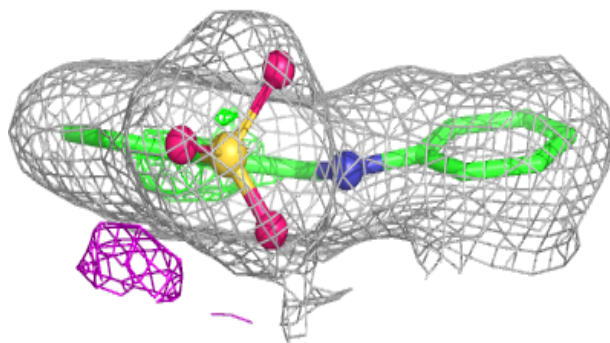
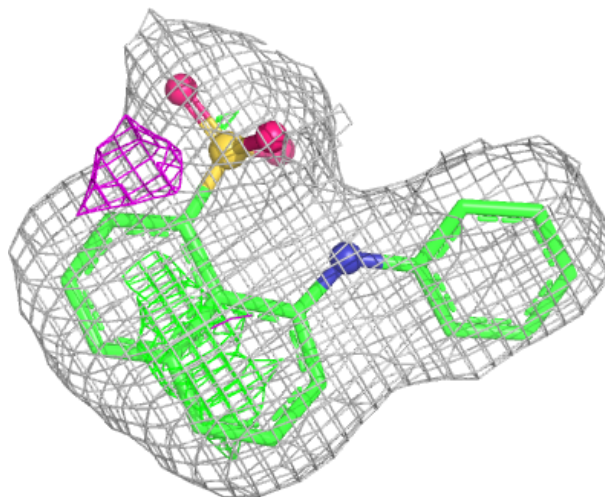
Electron density around 2AN J 203:

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



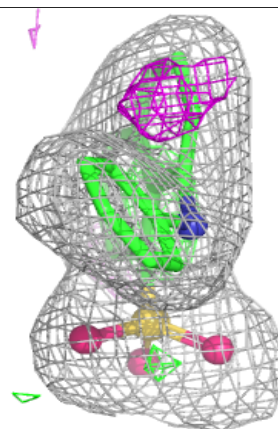
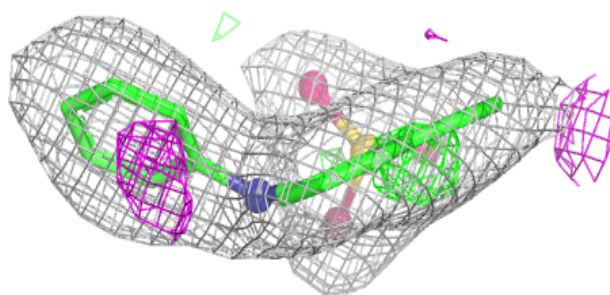
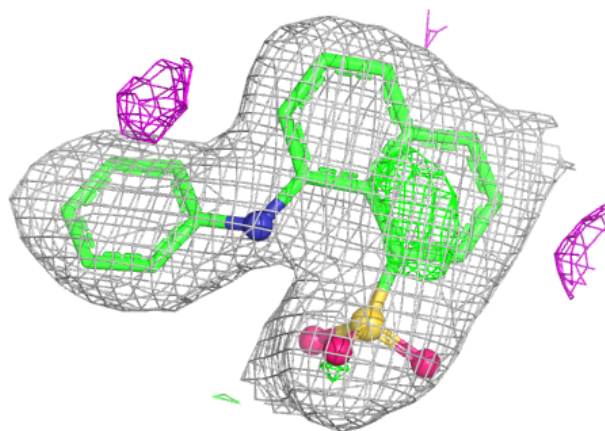
Electron density around 2AN E 201:

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



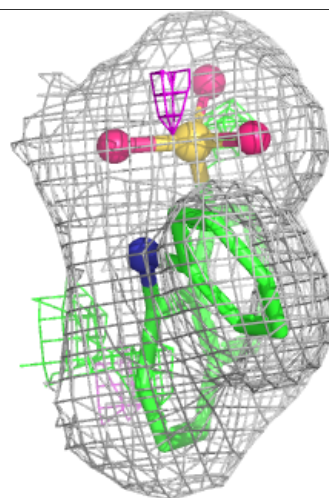
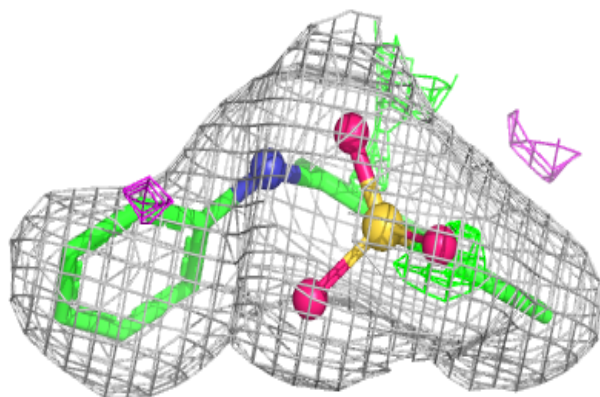
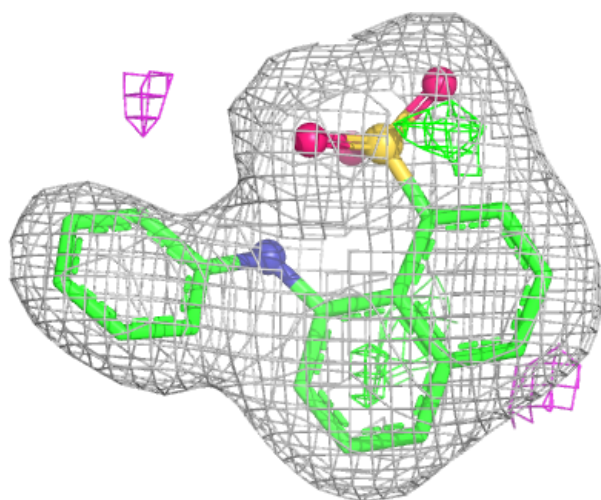
Electron density around 2AN E 202:

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



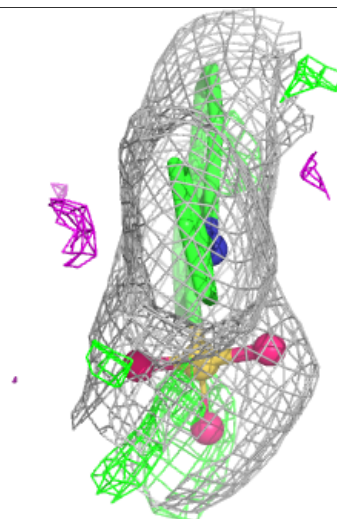
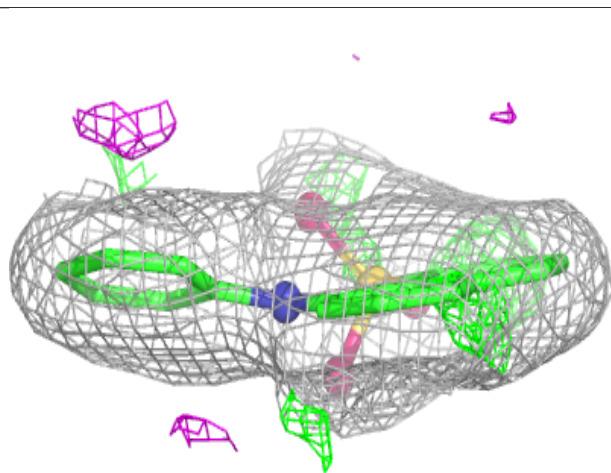
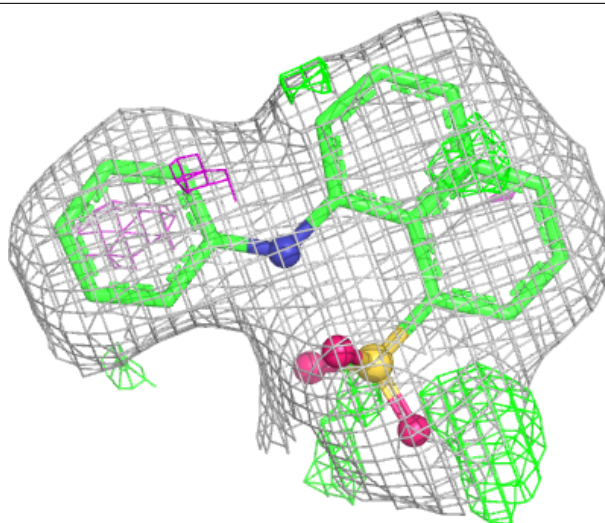
Electron density around 2AN G 202:

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



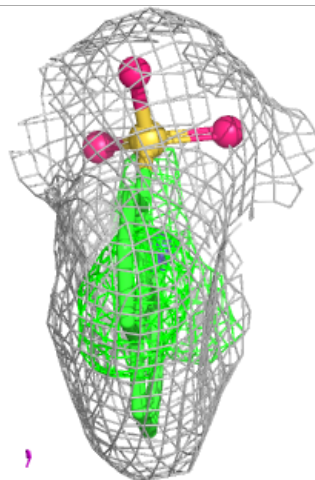
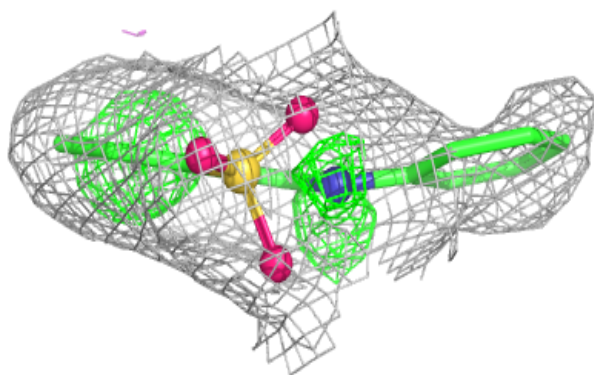
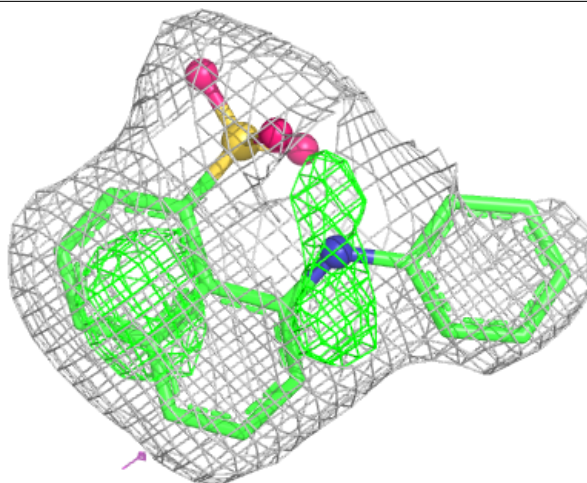
Electron density around 2AN T 201:

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



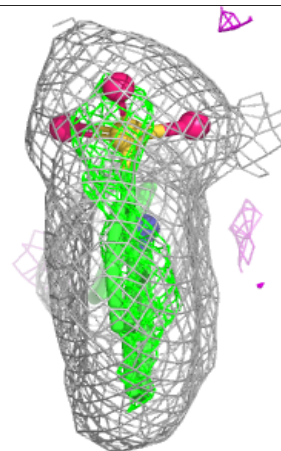
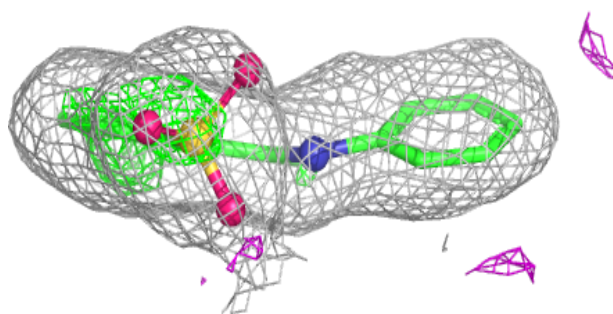
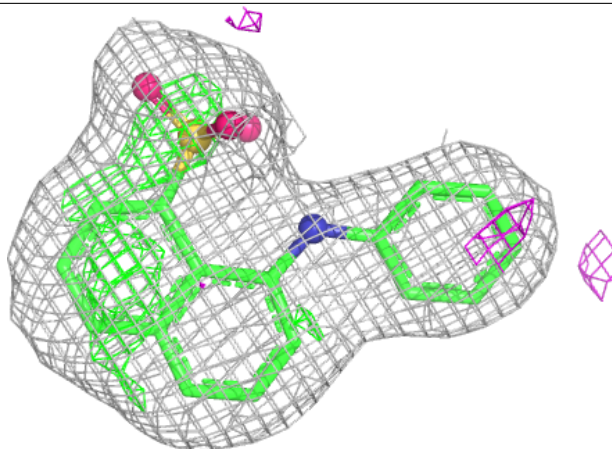
Electron density around 2AN h 204:

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



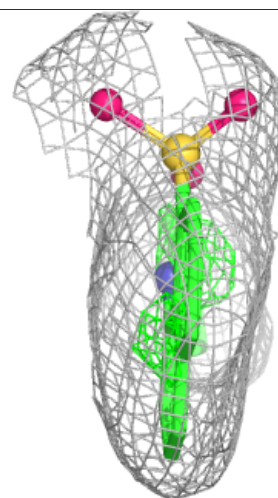
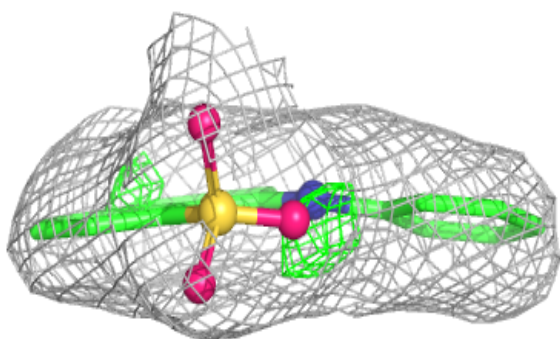
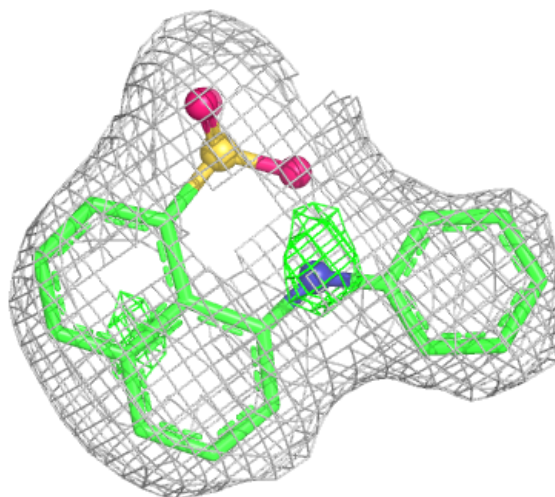
Electron density around 2AN I 202:

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



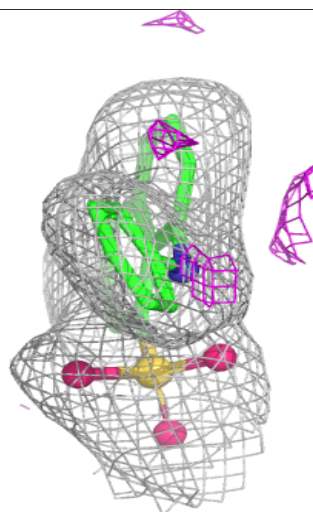
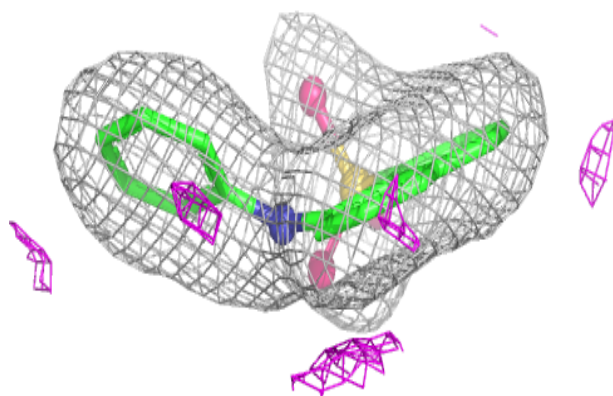
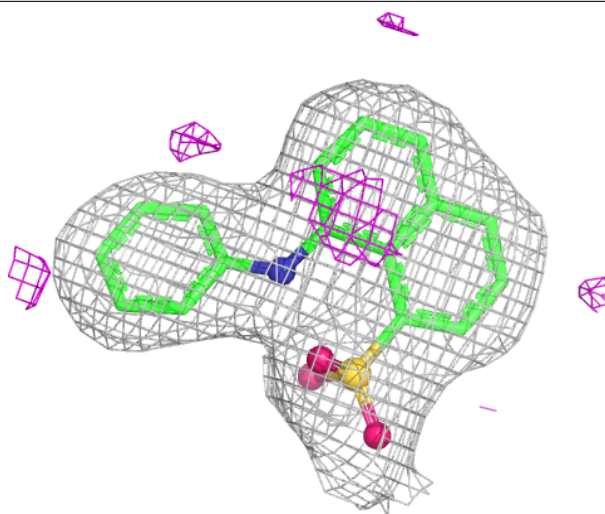
Electron density around 2AN R 203:

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



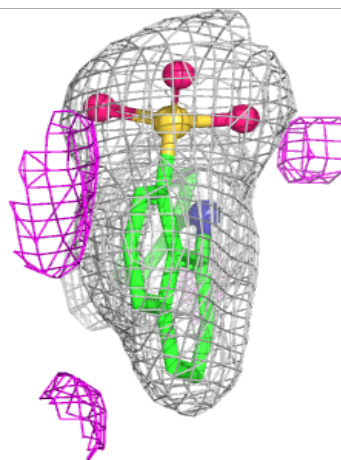
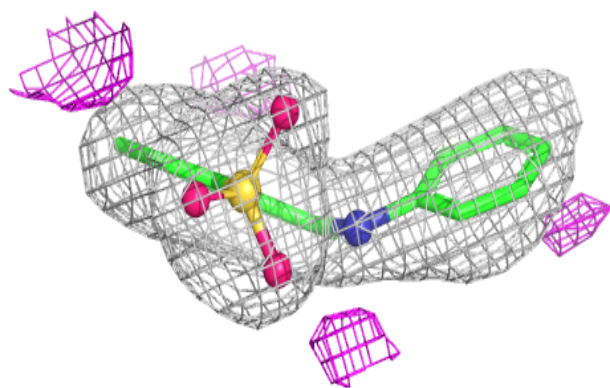
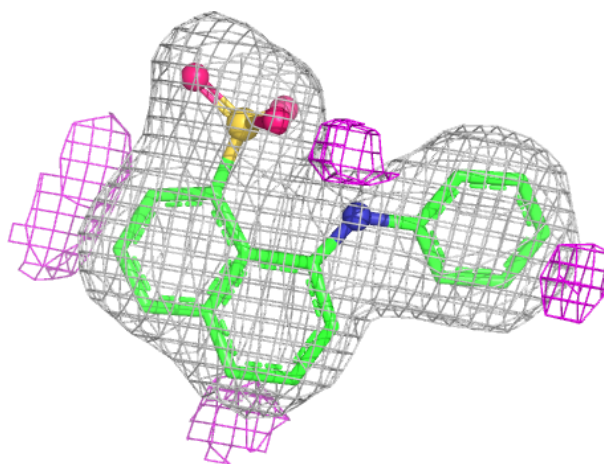
Electron density around 2AN K 201:

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



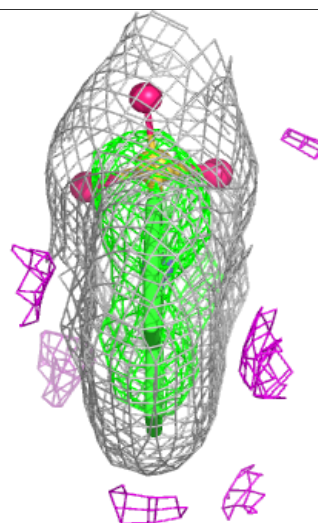
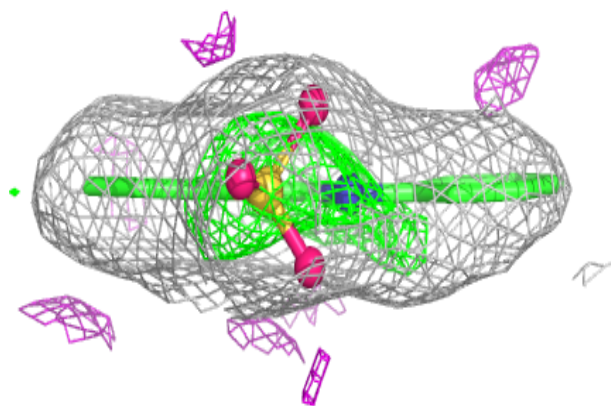
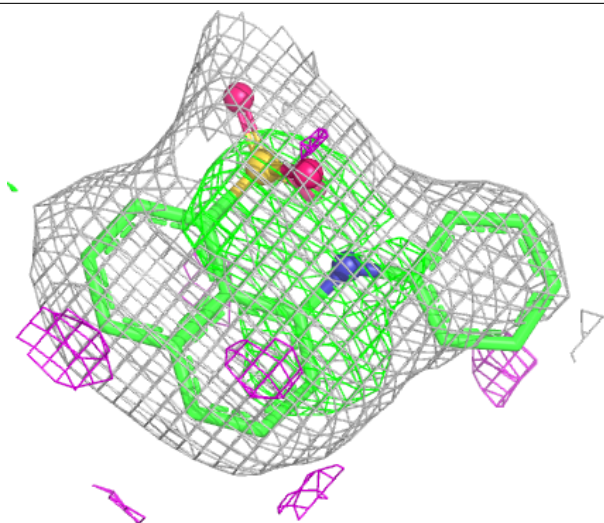
Electron density around 2AN g 202:

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



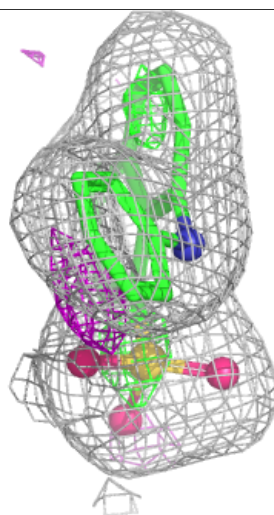
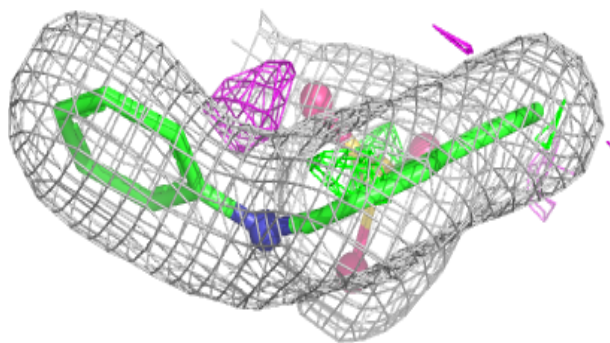
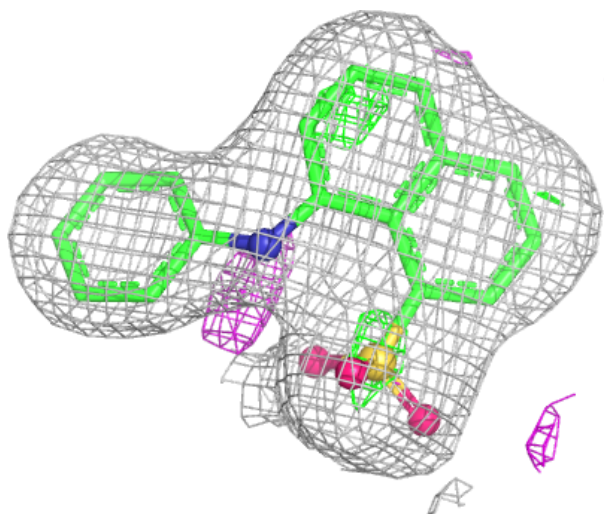
Electron density around 2AN K 202:

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



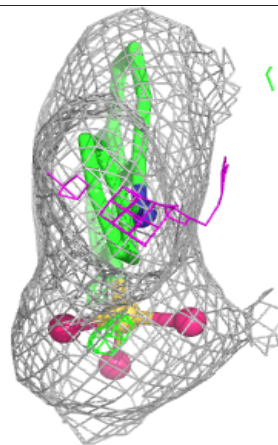
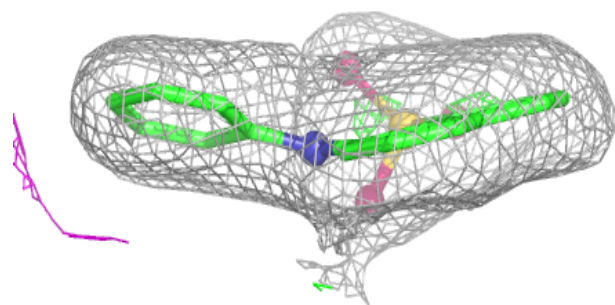
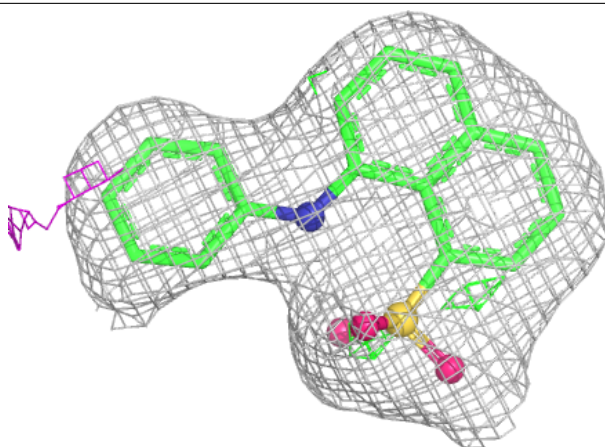
Electron density around 2AN V 202:

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



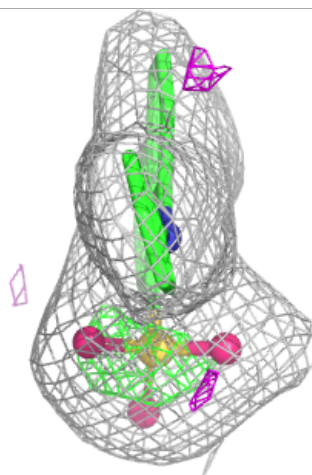
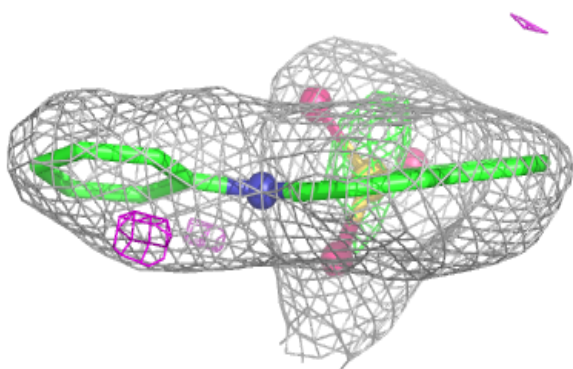
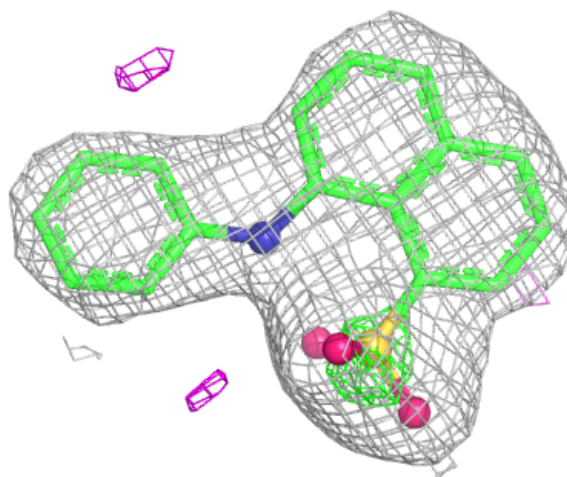
Electron density around 2AN h 202:

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



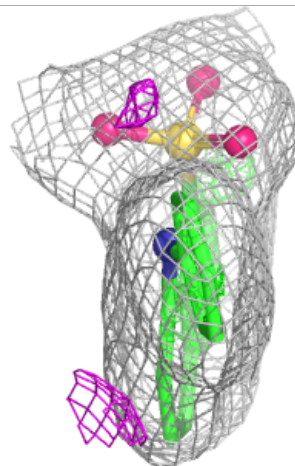
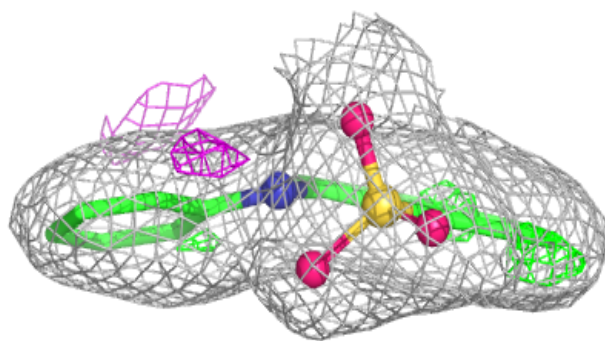
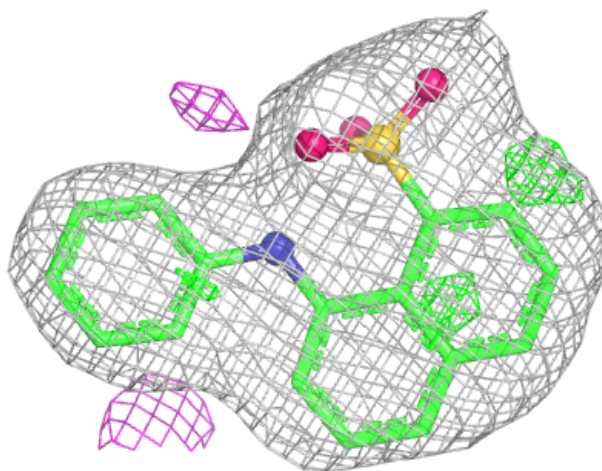
Electron density around 2AN D 201:

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



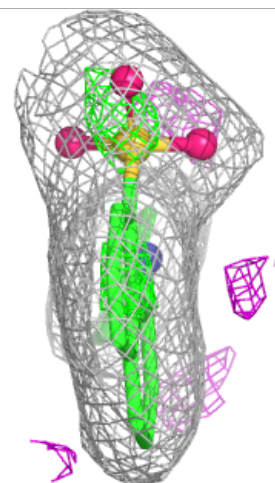
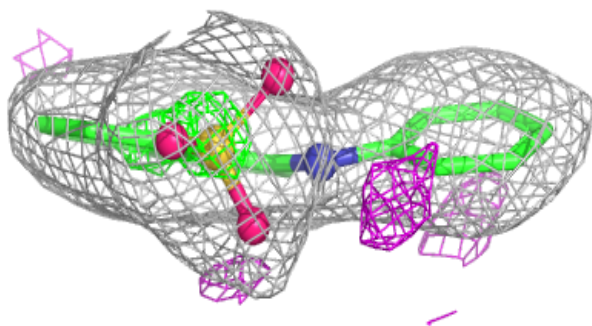
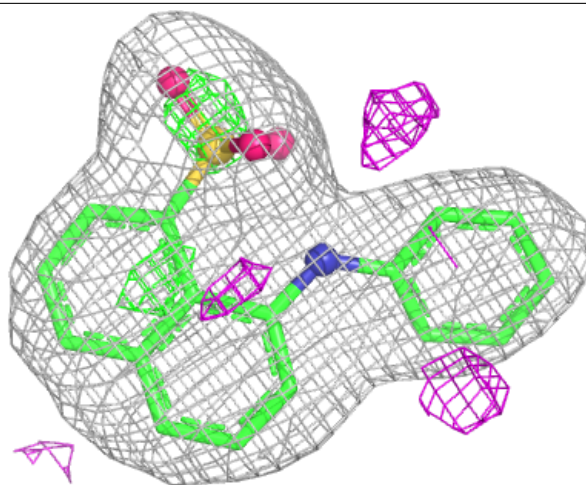
Electron density around 2AN N 201:

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



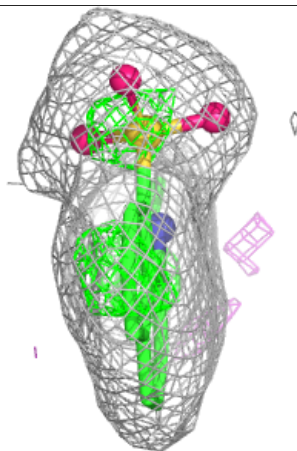
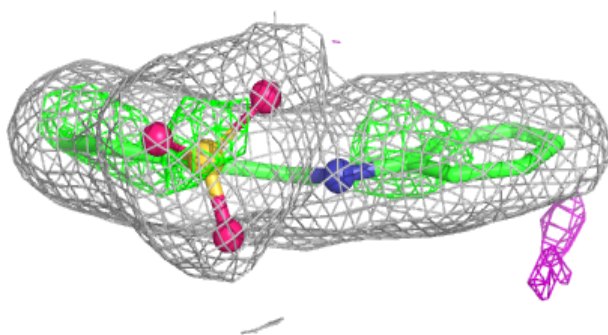
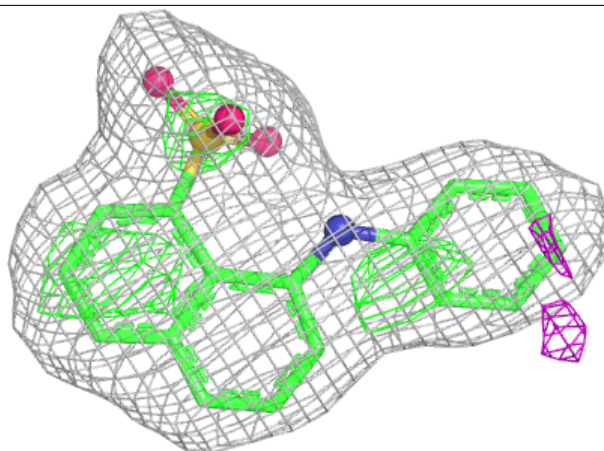
Electron density around 2AN H 201:

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



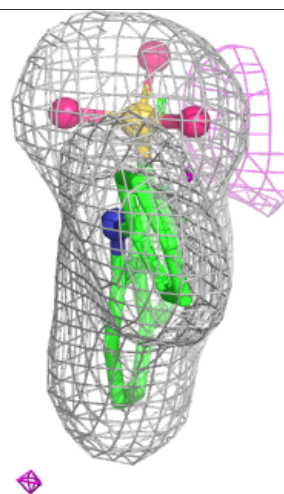
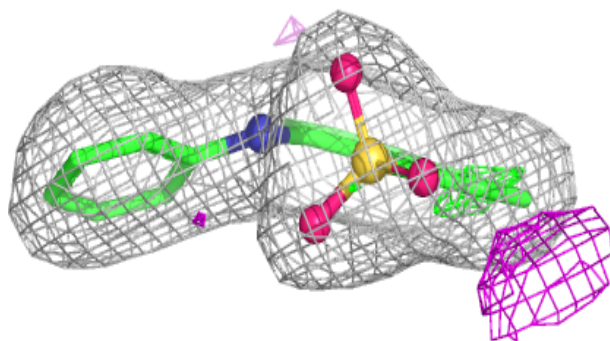
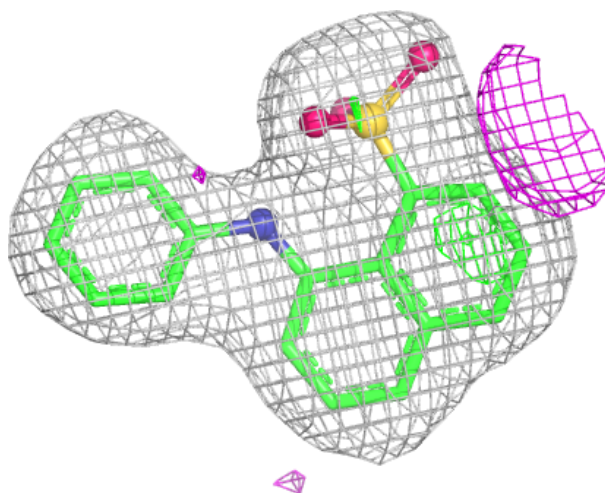
Electron density around 2AN M 201:

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



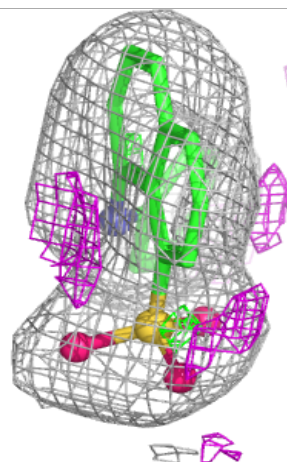
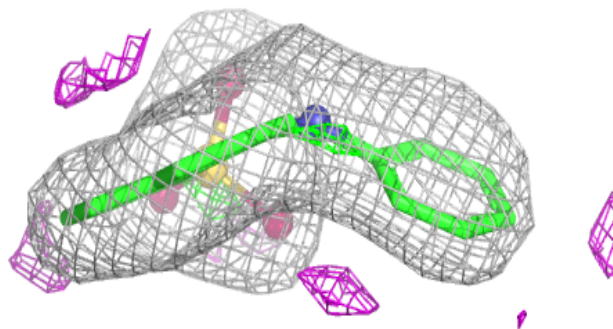
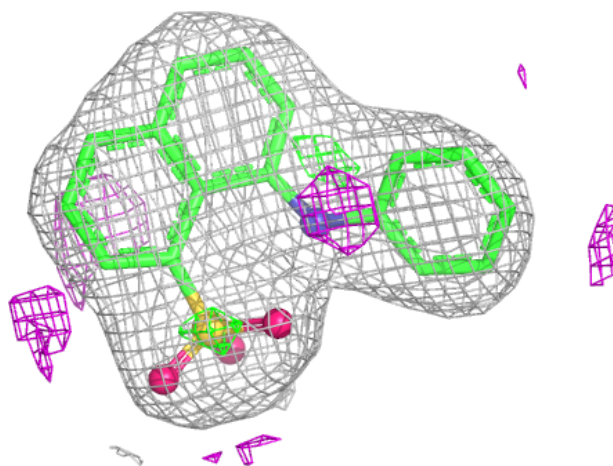
Electron density around 2AN c 206:

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



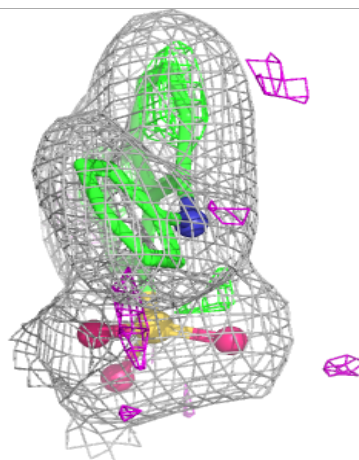
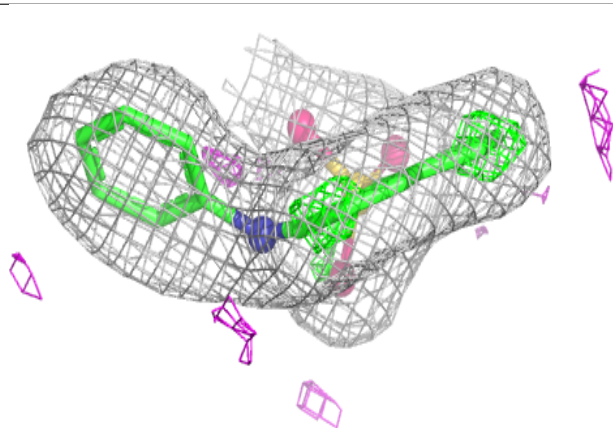
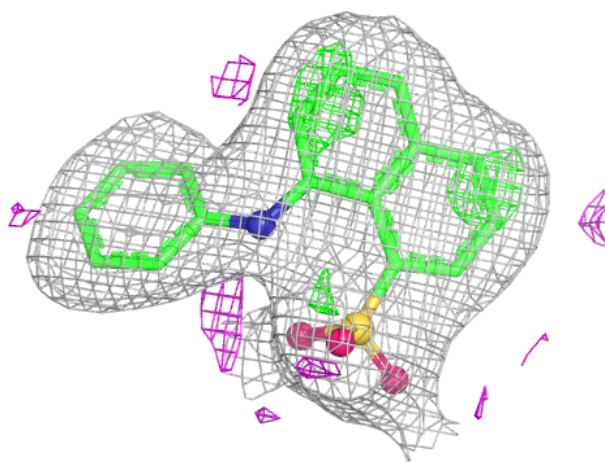
Electron density around 2AN N 202:

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



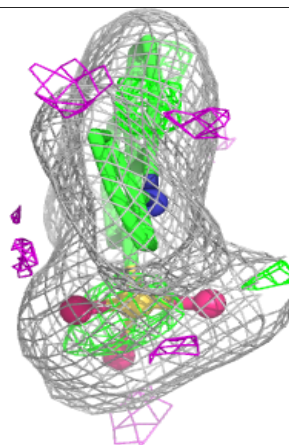
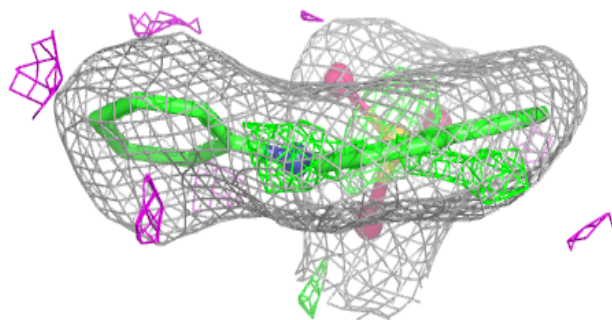
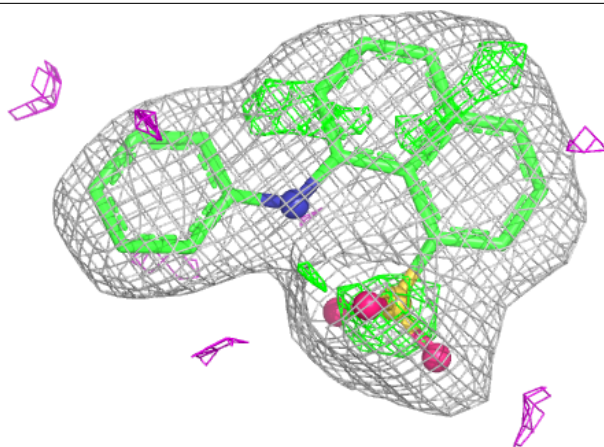
Electron density around 2AN j 202:

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



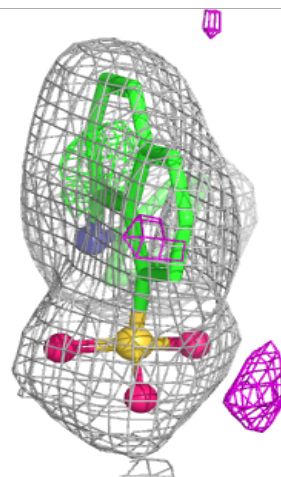
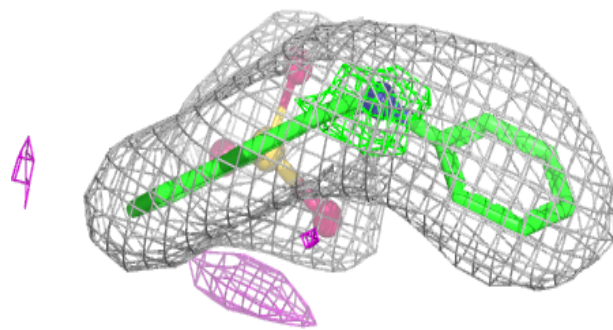
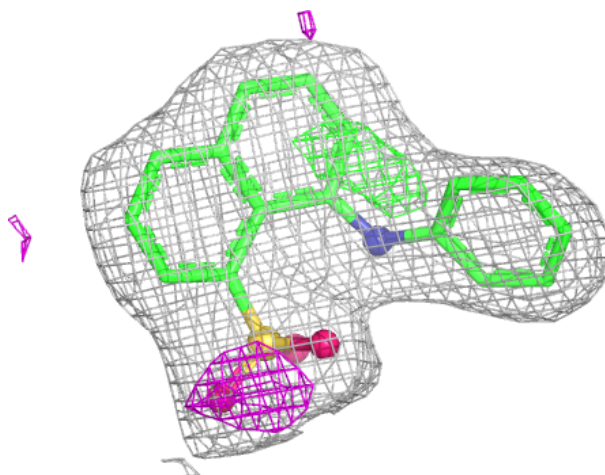
Electron density around 2AN L 201:

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



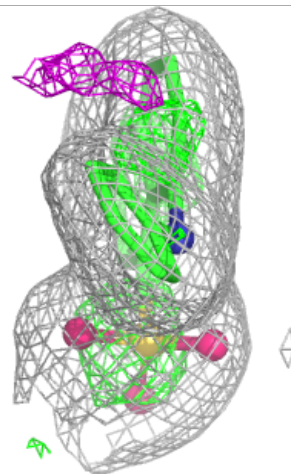
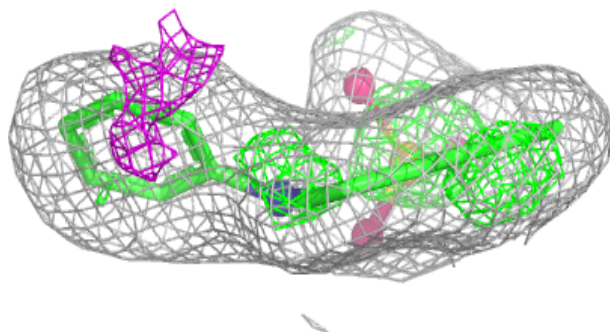
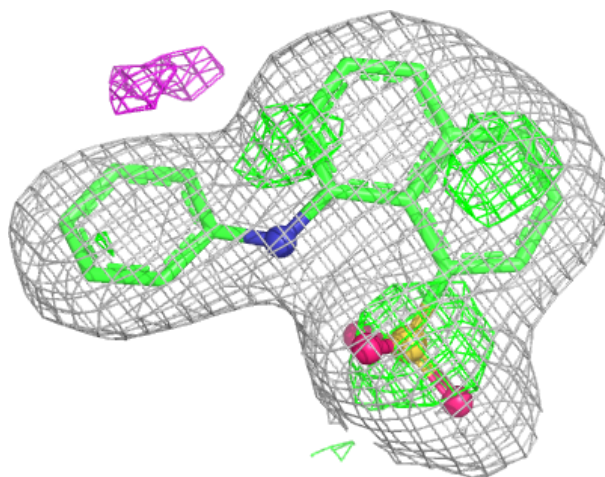
Electron density around 2AN Q 201:

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



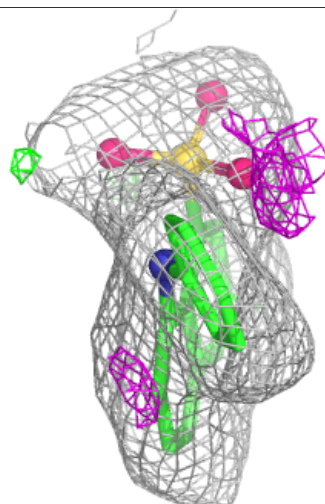
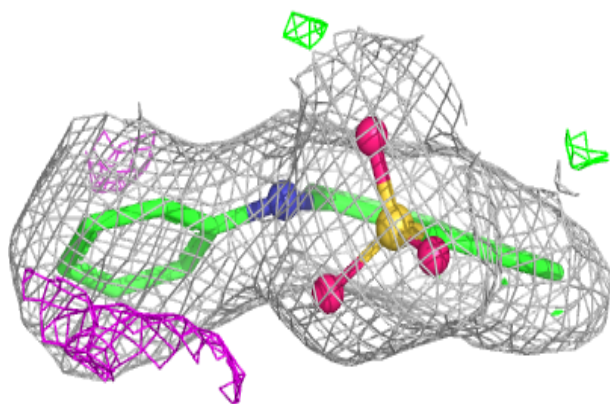
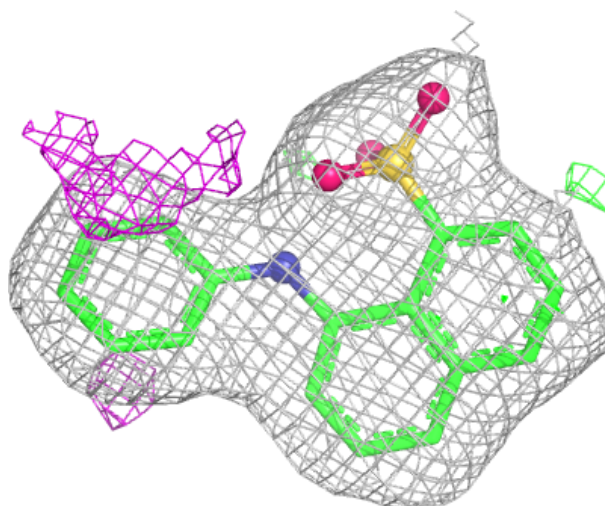
Electron density around 2AN f 201:

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



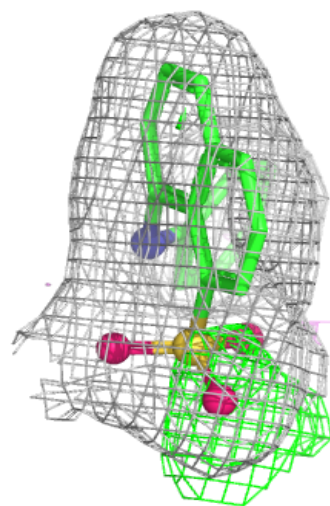
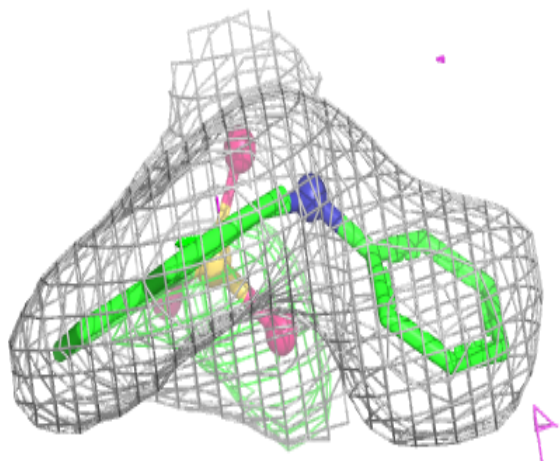
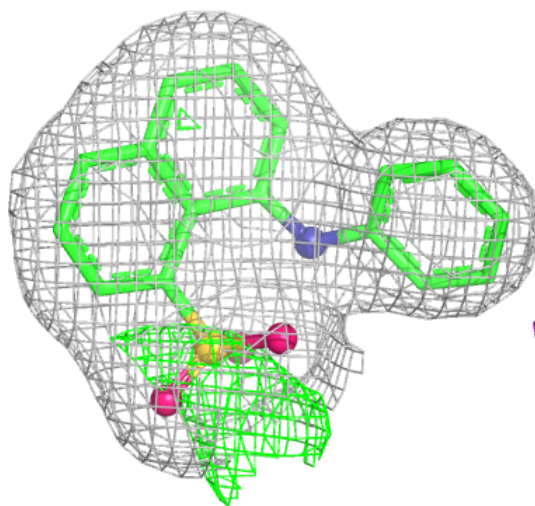
Electron density around 2AN P 201:

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



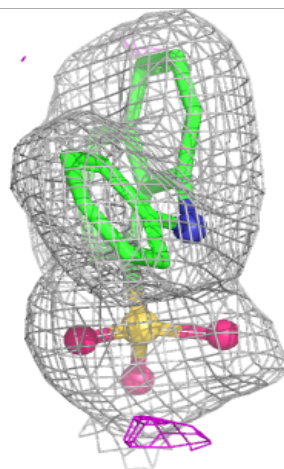
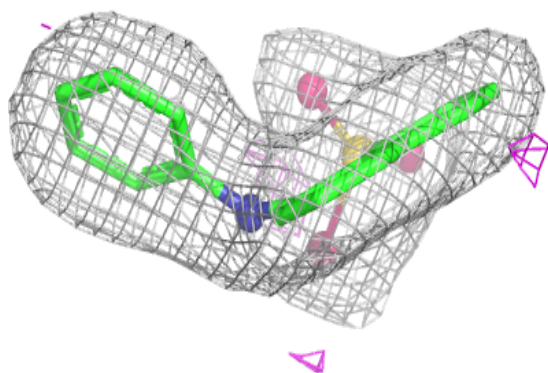
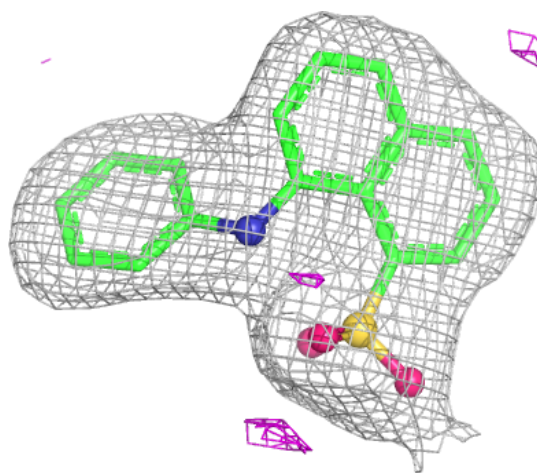
Electron density around 2AN c 201:

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



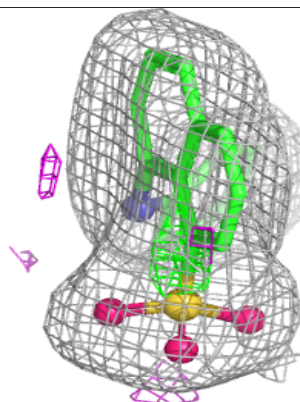
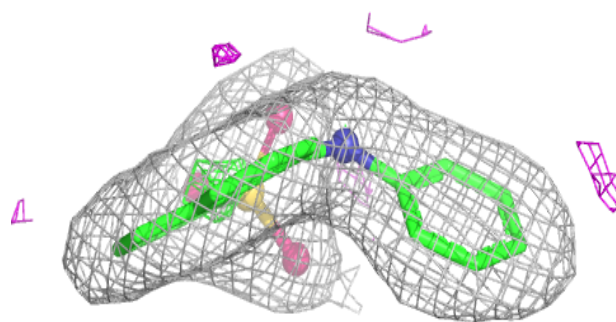
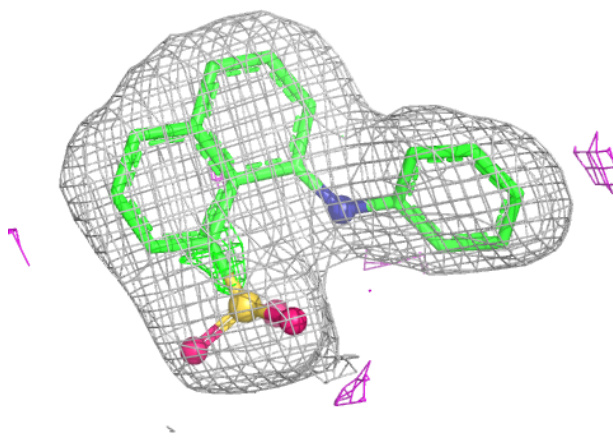
Electron density around 2AN M 202:

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



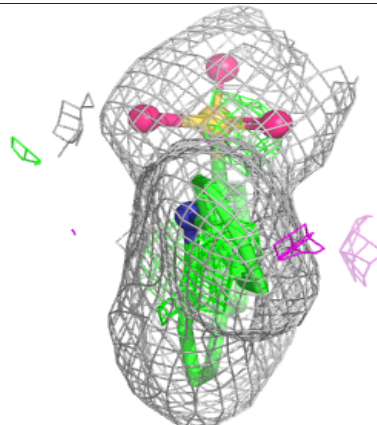
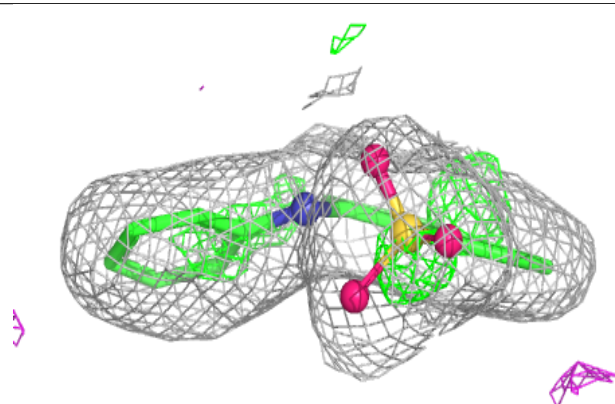
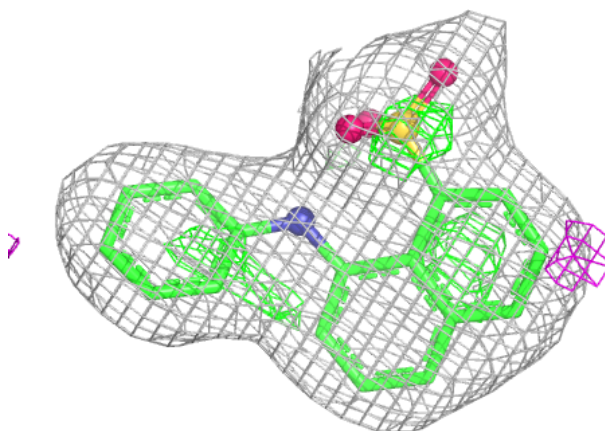
Electron density around 2AN I 201:

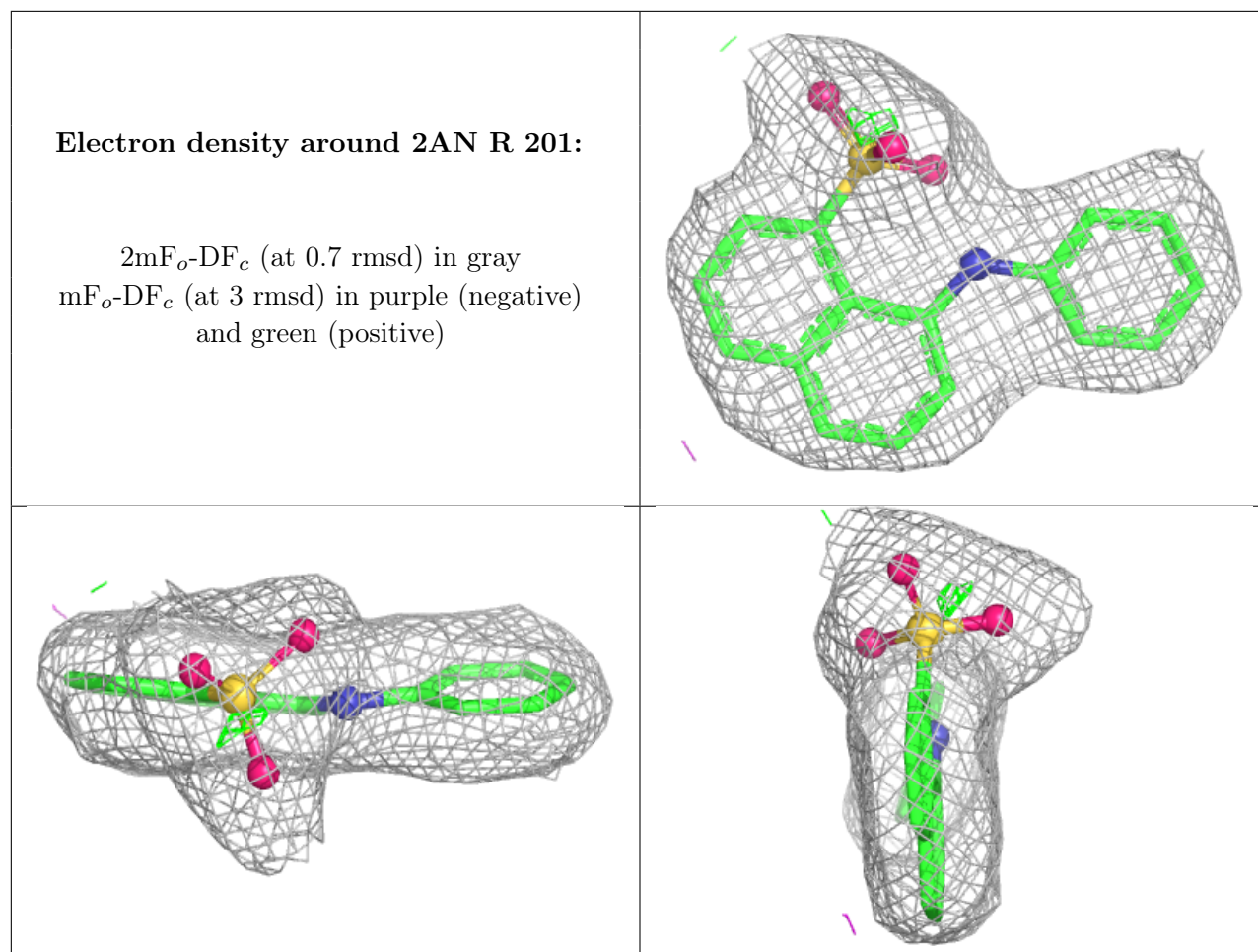
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around 2AN j 203:

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





6.5 Other polymers [i](#)

There are no such residues in this entry.