



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 23, 2024 – 02:05 AM EDT

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

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

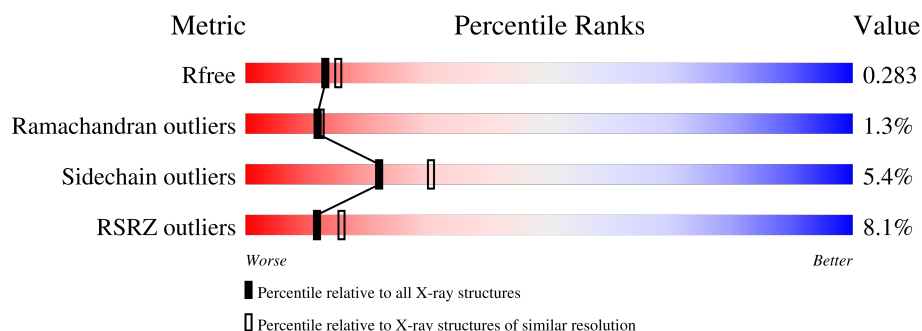
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5042 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 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	<div> <div>18%</div> <div> <div>94%</div> <div>5%</div> </div> </div>
1	B	163	<div> <div>6%</div> <div> <div>96%</div> <div>•</div> </div> </div>
1	C	163	<div> <div>9%</div> <div> <div>96%</div> <div>••</div> </div> </div>
1	D	163	<div> <div>13%</div> <div> <div>90%</div> <div>8%</div> </div> </div>
1	E	163	<div> <div>5%</div> <div> <div>90%</div> <div>9%</div> </div> </div>
1	F	163	<div> <div>18%</div> <div> <div>90%</div> <div>8%</div> </div> </div>

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

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	2AN	A	204	-	-	-	X
2	2AN	F	206	-	-	-	X
2	2AN	I	205	-	-	-	X
2	2AN	N	203	-	-	-	X
2	2AN	S	204	-	-	-	X
2	2AN	U	202	-	-	-	X
2	2AN	d	204	-	-	-	X
2	2AN	f	203	-	-	-	X
2	2AN	h	205	-	-	-	X
2	2AN	j	207	-	-	-	X
3	SO4	A	205	-	-	-	X
6	FLC	G	206	-	X	-	-

2 Entry composition

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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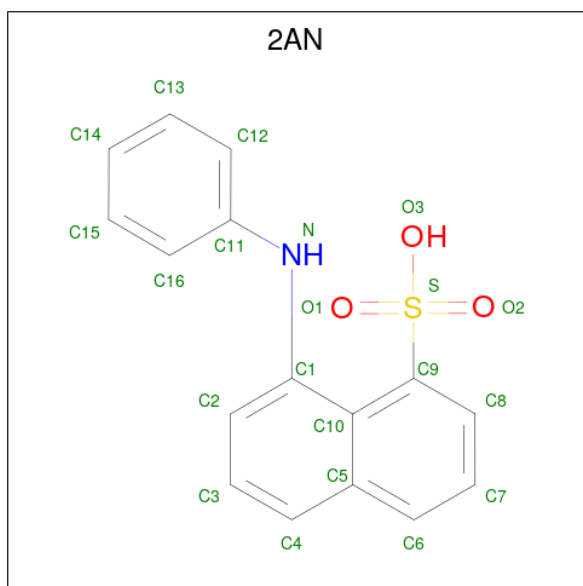
Chain	Residue	Modelled	Actual	Comment	Reference
c	-2	PRO	-	expression tag	UNP A0A160HRF0
c	-1	PHE	-	expression tag	UNP A0A160HRF0
c	0	THR	-	expression tag	UNP A0A160HRF0
b	-3	ASP	-	expression tag	UNP A0A160HRF0
b	-2	PRO	-	expression tag	UNP A0A160HRF0
b	-1	PHE	-	expression tag	UNP A0A160HRF0
b	0	THR	-	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 (three-letter code: 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	C	N	O	S	0	0
			21	16	1	3	1		
2	Z	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	Z	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	Y	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	Y	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	Y	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	Y	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	X	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	X	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	X	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	X	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	X	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	X	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	W	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	V	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	V	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	V	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	V	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	V	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	V	1	Total	C	N	O	S	0	0
			21	16	1	3	1		

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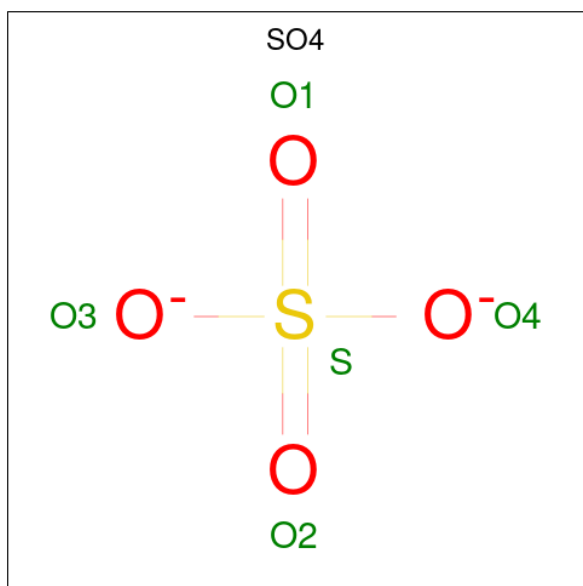
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	V	1	Total 21	C 16	N 1	O 3	S 1	0	0
2	U	1	Total 21	C 16	N 1	O 3	S 1	0	0
2	U	1	Total 21	C 16	N 1	O 3	S 1	0	0
2	T	1	Total 21	C 16	N 1	O 3	S 1	0	0
2	T	1	Total 21	C 16	N 1	O 3	S 1	0	0
2	T	1	Total 21	C 16	N 1	O 3	S 1	0	0
2	T	1	Total 21	C 16	N 1	O 3	S 1	0	0
2	T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

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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 (three-letter code: SO4) (formula: O₄S).



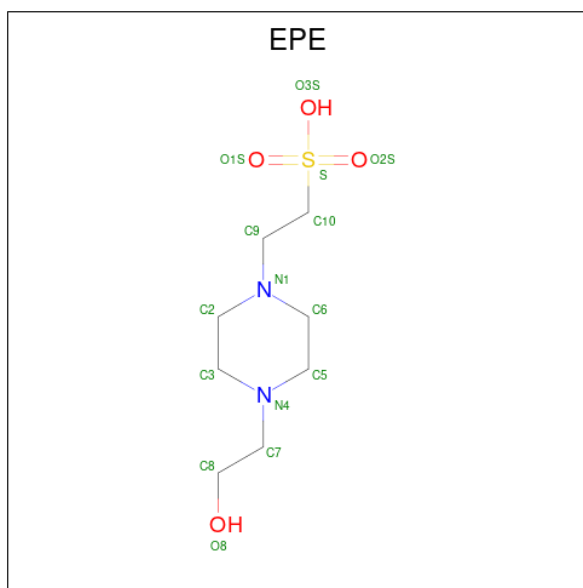
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	Q	1	Total	O	S	0	0
			5	4	1		
3	I	1	Total	O	S	0	0
			5	4	1		

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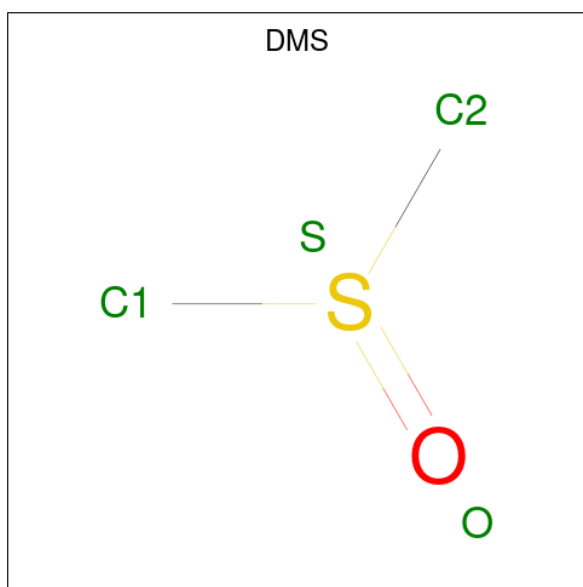
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	G	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	c	1	Total	O	S	0	0
			5	4	1		
3	c	1	Total	O	S	0	0
			5	4	1		
3	c	1	Total	O	S	0	0
			5	4	1		
3	Y	1	Total	O	S	0	0
			5	4	1		
3	g	1	Total	O	S	0	0
			5	4	1		

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



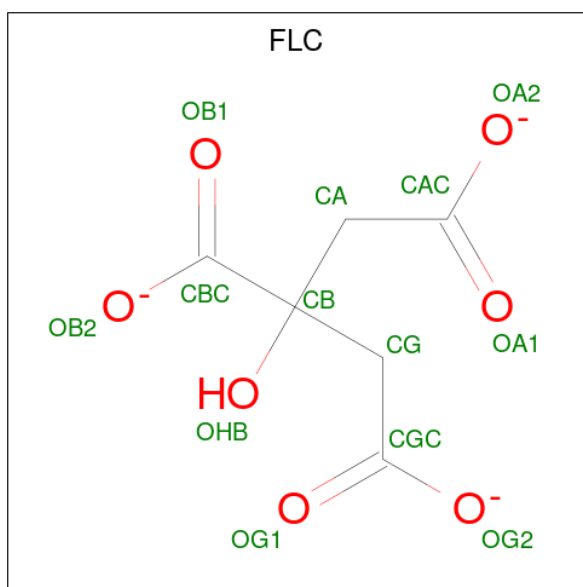
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	P	1	Total	C	N	O	S	0
			15	8	2	4	1	0

- Molecule 5 is DIMETHYL SULFOXIDE (three-letter code: 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 (three-letter code: FLC) (formula: $C_6H_5O_7$).



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

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

- Molecule 7 is water.

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

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

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

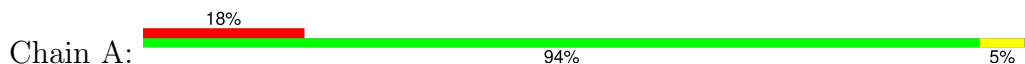
3 Residue-property plots [i](#)

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

- Molecule 1: PR-10 protein



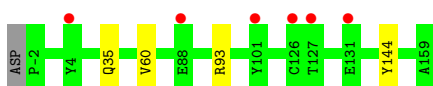
- Molecule 1: PR-10 protein



- Molecule 1: PR-10 protein



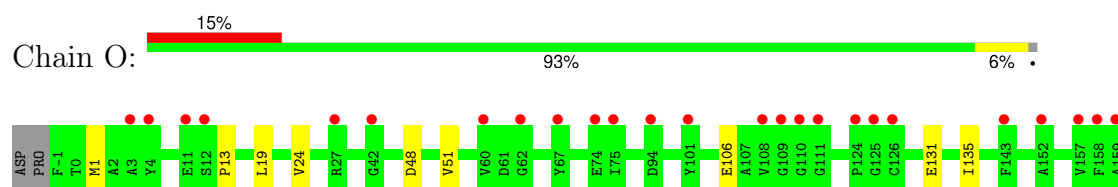
- Molecule 1: PR-10 protein



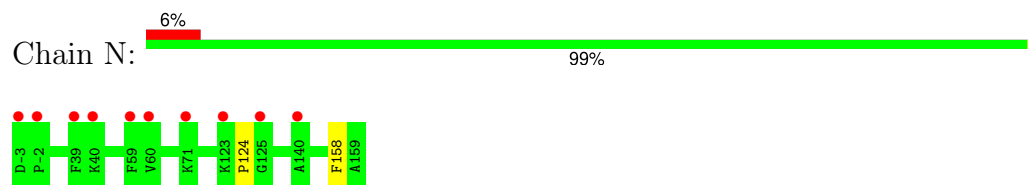
- Molecule 1: PR-10 protein



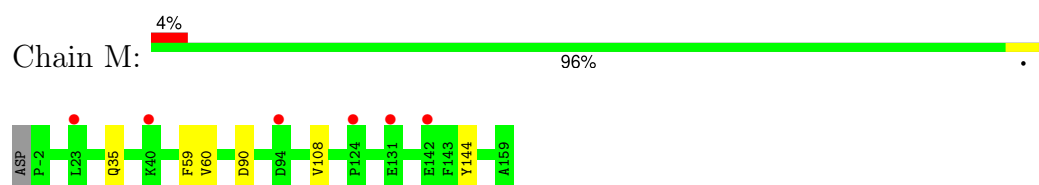
- Molecule 1: PR-10 protein



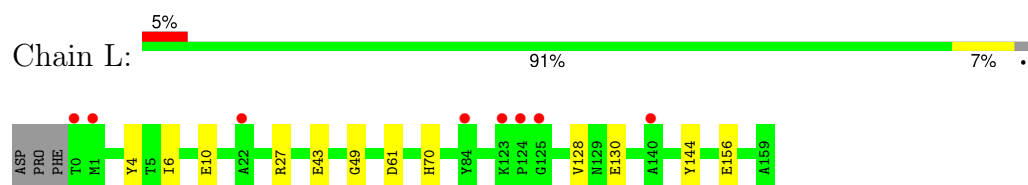
- Molecule 1: PR-10 protein



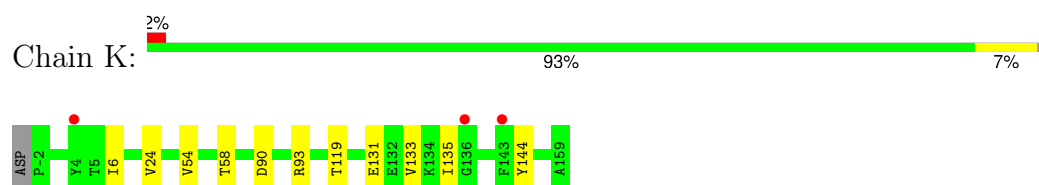
- Molecule 1: PR-10 protein



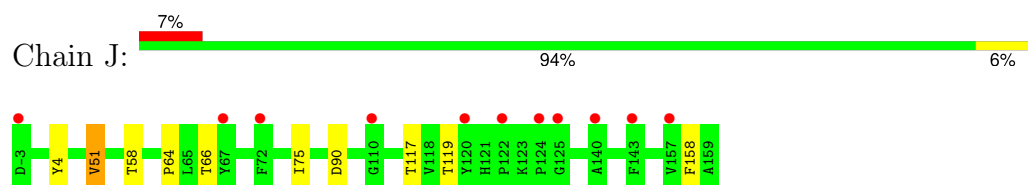
- Molecule 1: PR-10 protein



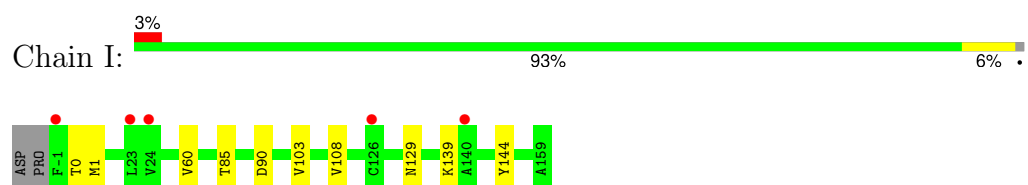
- Molecule 1: PR-10 protein



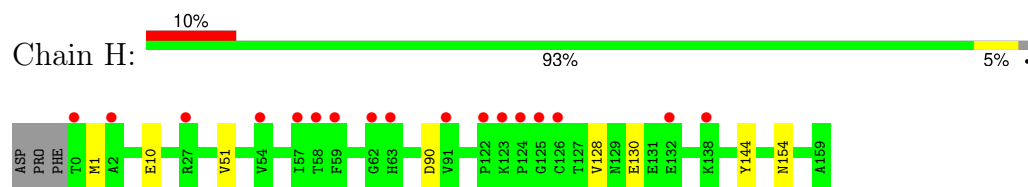
- Molecule 1: PR-10 protein



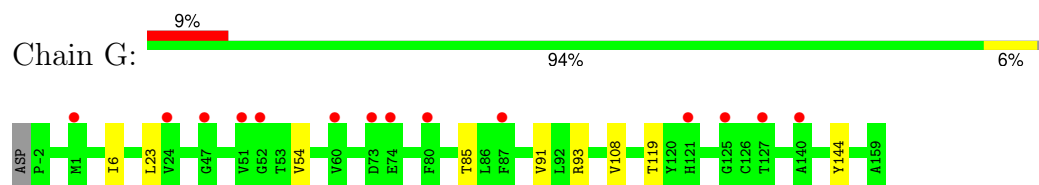
- Molecule 1: PR-10 protein



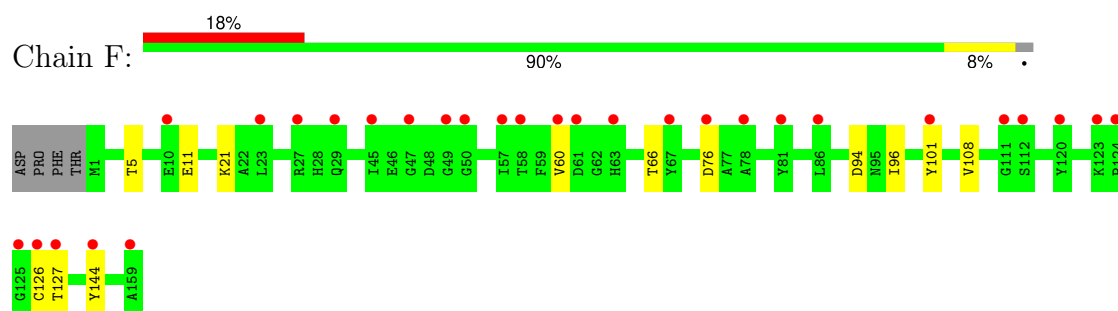
- Molecule 1: PR-10 protein



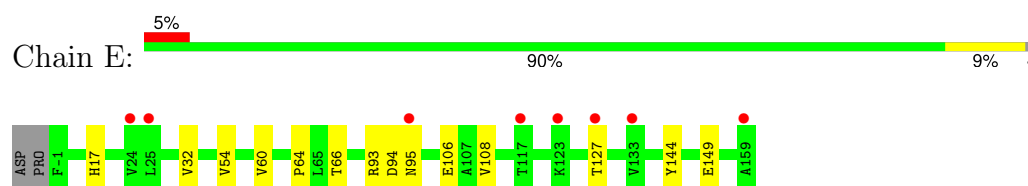
- Molecule 1: PR-10 protein



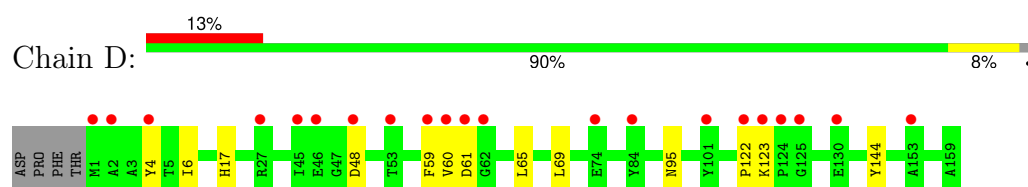
- Molecule 1: PR-10 protein



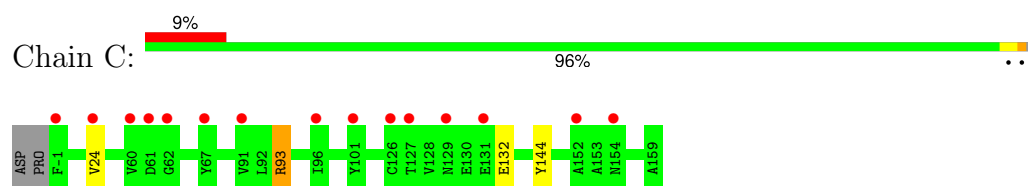
- Molecule 1: PR-10 protein



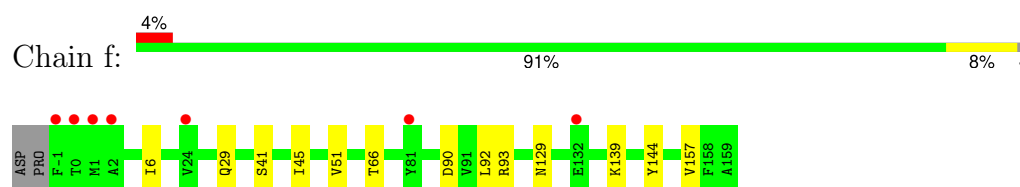
- Molecule 1: PR-10 protein



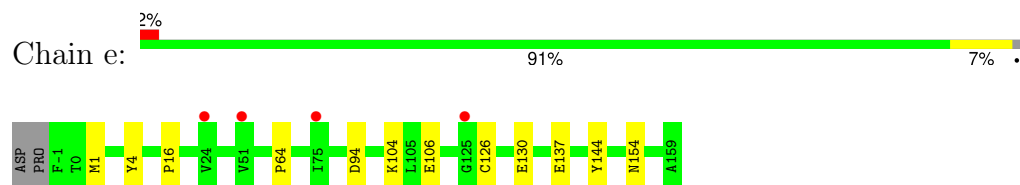
- Molecule 1: PR-10 protein



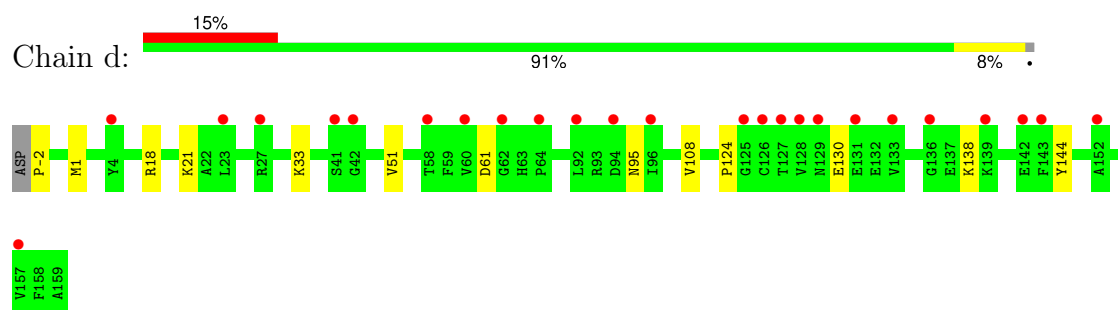
- Molecule 1: PR-10 protein



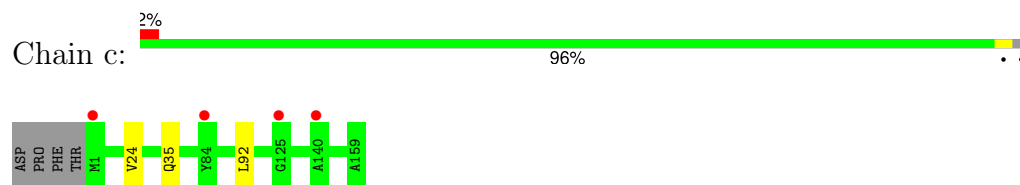
- Molecule 1: PR-10 protein



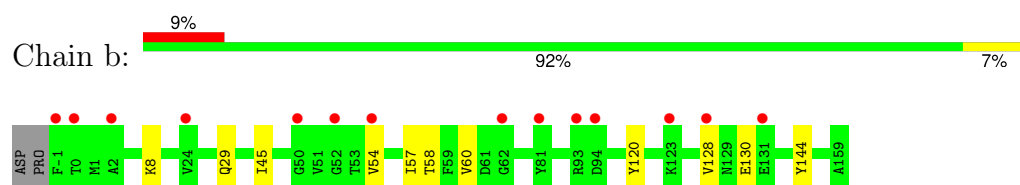
- Molecule 1: PR-10 protein



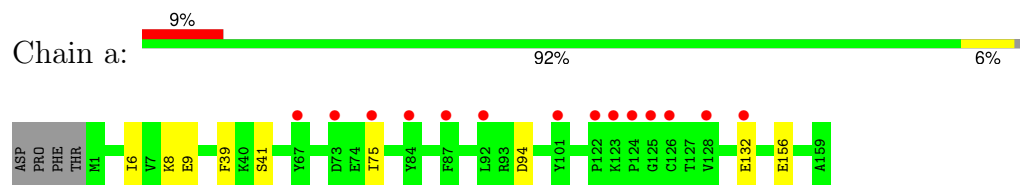
- Molecule 1: PR-10 protein



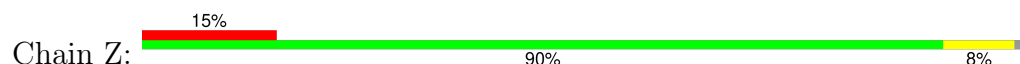
- Molecule 1: PR-10 protein

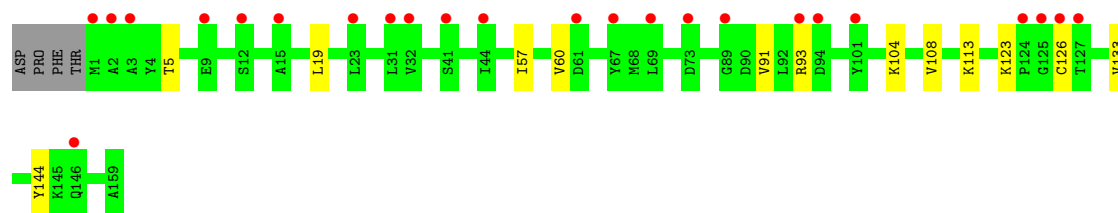


- Molecule 1: PR-10 protein

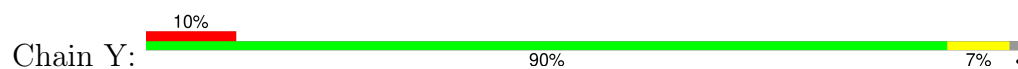


- Molecule 1: PR-10 protein

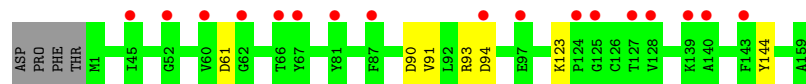
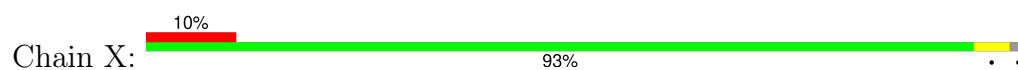




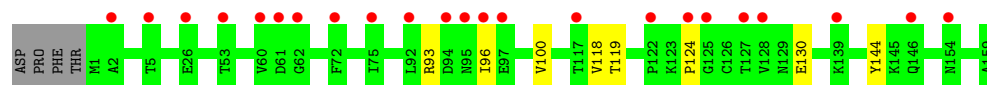
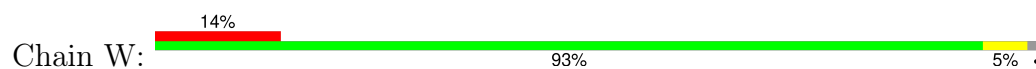
- Molecule 1: PR-10 protein



- Molecule 1: PR-10 protein



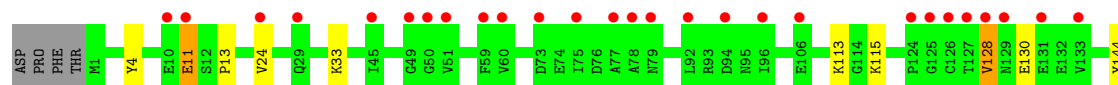
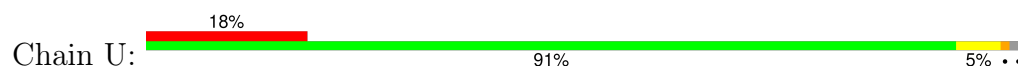
- Molecule 1: PR-10 protein



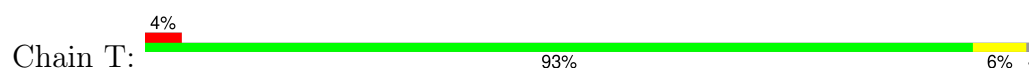
- Molecule 1: PR-10 protein



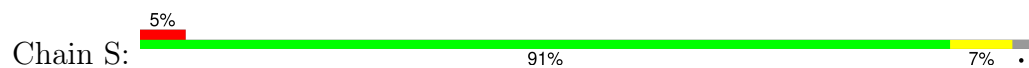
- Molecule 1: PR-10 protein



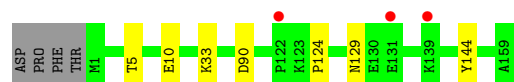
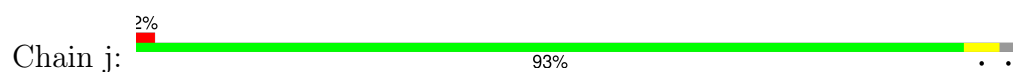
- Molecule 1: PR-10 protein



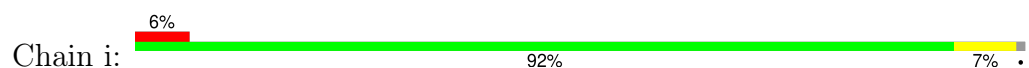
• Molecule 1: PR-10 protein



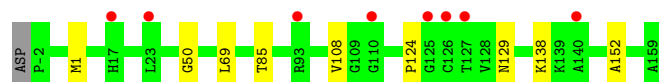
• Molecule 1: PR-10 protein



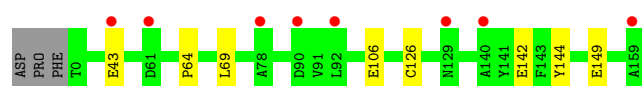
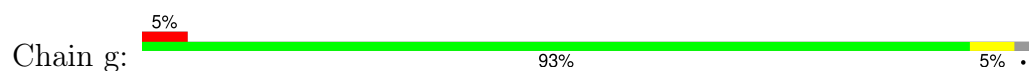
• Molecule 1: PR-10 protein



• Molecule 1: PR-10 protein



• Molecule 1: PR-10 protein



4 Data and refinement statistics

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) 99.3 (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 0.273 , 0.283	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)	0.29 , 54.3	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: FLC, SO4, 2AN, EPE, DMS

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

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

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

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

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

All (75) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	76	ASP

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Mol	Chain	Res	Type
1	O	51	VAL
1	F	94	ASP
1	X	123	LYS
1	O	24	VAL
1	M	60	VAL
1	K	24	VAL
1	J	51	VAL
1	F	76	ASP
1	f	93	ARG
1	f	129	ASN
1	d	108	VAL
1	Z	108	VAL
1	W	130	GLU
1	U	128	VAL
1	i	24	VAL
1	B	91	VAL
1	A	158	PHE
1	Q	60	VAL
1	P	50	GLY
1	O	19	LEU
1	I	90	ASP
1	G	93	ARG
1	D	59	PHE
1	Y	24	VAL
1	W	93	ARG
1	U	11	GLU
1	h	50	GLY
1	h	152	ALA
1	A	128	VAL
1	L	49	GLY
1	L	61	ASP
1	I	1	MET
1	E	32	VAL
1	D	65	LEU
1	C	24	VAL
1	C	93	ARG
1	f	139	LYS
1	d	51	VAL
1	a	75	ILE
1	X	94	ASP
1	W	96	ILE
1	U	13	PRO

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Mol	Chain	Res	Type
1	U	33	LYS
1	T	126	CYS
1	j	129	ASN
1	A	88	GLU
1	L	27	ARG
1	F	126	CYS
1	E	17	HIS
1	D	122	PRO
1	e	64	PRO
1	d	124	PRO
1	Z	93	ARG
1	V	93	ARG
1	O	135	ILE
1	E	60	VAL
1	D	6	ILE
1	d	130	GLU
1	Y	124	PRO
1	K	135	ILE
1	h	124	PRO
1	N	124	PRO
1	I	60	VAL
1	T	125	GLY
1	i	51	VAL
1	E	108	VAL
1	e	16	PRO
1	b	60	VAL
1	S	155	PRO
1	M	108	VAL
1	D	60	VAL
1	Z	123	LYS
1	W	124	PRO
1	V	124	PRO

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%)	109 (96%)	5 (4%)	28	39
1	B	130/138 (94%)	129 (99%)	1 (1%)	81	91
1	C	124/138 (90%)	121 (98%)	3 (2%)	49	66
1	D	123/138 (89%)	115 (94%)	8 (6%)	17	23
1	E	128/138 (93%)	118 (92%)	10 (8%)	12	16
1	F	114/138 (83%)	104 (91%)	10 (9%)	10	12
1	G	122/138 (88%)	114 (93%)	8 (7%)	16	22
1	H	125/138 (91%)	117 (94%)	8 (6%)	17	23
1	I	130/138 (94%)	123 (95%)	7 (5%)	22	30
1	J	128/138 (93%)	118 (92%)	10 (8%)	12	16
1	K	132/138 (96%)	123 (93%)	9 (7%)	16	21
1	L	132/138 (96%)	123 (93%)	9 (7%)	16	21
1	M	134/138 (97%)	130 (97%)	4 (3%)	41	57
1	N	131/138 (95%)	130 (99%)	1 (1%)	81	91
1	O	120/138 (87%)	115 (96%)	5 (4%)	30	42
1	P	131/138 (95%)	126 (96%)	5 (4%)	33	47
1	Q	132/138 (96%)	129 (98%)	3 (2%)	50	67
1	R	130/138 (94%)	127 (98%)	3 (2%)	50	67
1	S	131/138 (95%)	120 (92%)	11 (8%)	11	13
1	T	131/138 (95%)	123 (94%)	8 (6%)	18	25
1	U	123/138 (89%)	115 (94%)	8 (6%)	17	23
1	V	131/138 (95%)	128 (98%)	3 (2%)	50	67
1	W	121/138 (88%)	117 (97%)	4 (3%)	38	53
1	X	124/138 (90%)	119 (96%)	5 (4%)	31	44
1	Y	123/138 (89%)	113 (92%)	10 (8%)	11	15
1	Z	122/138 (88%)	112 (92%)	10 (8%)	11	14
1	a	123/138 (89%)	115 (94%)	8 (6%)	17	23
1	b	127/138 (92%)	117 (92%)	10 (8%)	12	15
1	c	130/138 (94%)	127 (98%)	3 (2%)	50	67
1	d	127/138 (92%)	118 (93%)	9 (7%)	14	19
1	e	129/138 (94%)	119 (92%)	10 (8%)	12	16
1	f	132/138 (96%)	122 (92%)	10 (8%)	13	16

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	g	132/138 (96%)	124 (94%)	8 (6%)	18	25
1	h	131/138 (95%)	125 (95%)	6 (5%)	27	38
1	i	129/138 (94%)	120 (93%)	9 (7%)	15	19
1	j	130/138 (94%)	124 (95%)	6 (5%)	27	38
All	All	4576/4968 (92%)	4329 (95%)	247 (5%)	22	30

All (247) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	80	PHE
1	A	1	MET
1	A	72	PHE
1	A	82	CYS
1	A	126	CYS
1	A	144	TYR
1	R	4	TYR
1	R	17	HIS
1	R	61	ASP
1	Q	35	GLN
1	Q	93	ARG
1	Q	144	TYR
1	P	4	TYR
1	P	71	LYS
1	P	80	PHE
1	P	131	GLU
1	P	156	GLU
1	O	1	MET
1	O	13	PRO
1	O	48	ASP
1	O	106	GLU
1	O	131	GLU
1	N	158	PHE
1	M	35	GLN
1	M	59	PHE
1	M	90	ASP
1	M	144	TYR
1	L	4	TYR
1	L	6	ILE
1	L	10	GLU
1	L	43	GLU
1	L	70	HIS

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Mol	Chain	Res	Type
1	L	128	VAL
1	L	130	GLU
1	L	144	TYR
1	L	156	GLU
1	K	6	ILE
1	K	54	VAL
1	K	58	THR
1	K	90	ASP
1	K	93	ARG
1	K	119	THR
1	K	131	GLU
1	K	133	VAL
1	K	144	TYR
1	J	4	TYR
1	J	51	VAL
1	J	58	THR
1	J	64	PRO
1	J	66	THR
1	J	75	ILE
1	J	90	ASP
1	J	117	THR
1	J	119	THR
1	J	158	PHE
1	I	0	THR
1	I	85	THR
1	I	103	VAL
1	I	108	VAL
1	I	129	ASN
1	I	139	LYS
1	I	144	TYR
1	H	1	MET
1	H	10	GLU
1	H	51	VAL
1	H	90	ASP
1	H	128	VAL
1	H	130	GLU
1	H	144	TYR
1	H	154	ASN
1	G	6	ILE
1	G	23	LEU
1	G	54	VAL
1	G	85	THR

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Mol	Chain	Res	Type
1	G	91	VAL
1	G	108	VAL
1	G	119	THR
1	G	144	TYR
1	F	5	THR
1	F	11	GLU
1	F	21	LYS
1	F	60	VAL
1	F	66	THR
1	F	96	ILE
1	F	101	TYR
1	F	108	VAL
1	F	127	THR
1	F	144	TYR
1	E	54	VAL
1	E	64	PRO
1	E	66	THR
1	E	93	ARG
1	E	94	ASP
1	E	95	ASN
1	E	106	GLU
1	E	127	THR
1	E	144	TYR
1	E	149	GLU
1	D	4	TYR
1	D	17	HIS
1	D	48	ASP
1	D	61	ASP
1	D	69	LEU
1	D	95	ASN
1	D	123	LYS
1	D	144	TYR
1	C	93	ARG
1	C	132	GLU
1	C	144	TYR
1	f	6	ILE
1	f	29	GLN
1	f	41	SER
1	f	45	ILE
1	f	51	VAL
1	f	66	THR
1	f	90	ASP

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Mol	Chain	Res	Type
1	f	92	LEU
1	f	144	TYR
1	f	157	VAL
1	e	1	MET
1	e	4	TYR
1	e	94	ASP
1	e	104	LYS
1	e	106	GLU
1	e	126	CYS
1	e	130	GLU
1	e	137	GLU
1	e	144	TYR
1	e	154	ASN
1	d	-2	PRO
1	d	1	MET
1	d	18	ARG
1	d	21	LYS
1	d	33	LYS
1	d	61	ASP
1	d	95	ASN
1	d	138	LYS
1	d	144	TYR
1	c	24	VAL
1	c	35	GLN
1	c	92	LEU
1	b	8	LYS
1	b	29	GLN
1	b	45	ILE
1	b	54	VAL
1	b	57	ILE
1	b	58	THR
1	b	120	TYR
1	b	128	VAL
1	b	130	GLU
1	b	144	TYR
1	a	6	ILE
1	a	8	LYS
1	a	9	GLU
1	a	39	PHE
1	a	41	SER
1	a	94	ASP
1	a	132	GLU

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Mol	Chain	Res	Type
1	a	156	GLU
1	Z	5	THR
1	Z	19	LEU
1	Z	57	ILE
1	Z	60	VAL
1	Z	91	VAL
1	Z	104	LYS
1	Z	113	LYS
1	Z	126	CYS
1	Z	133	VAL
1	Z	144	TYR
1	Y	4	TYR
1	Y	23	LEU
1	Y	43	GLU
1	Y	54	VAL
1	Y	61	ASP
1	Y	67	TYR
1	Y	82	CYS
1	Y	90	ASP
1	Y	106	GLU
1	Y	144	TYR
1	X	61	ASP
1	X	90	ASP
1	X	91	VAL
1	X	93	ARG
1	X	144	TYR
1	W	100	VAL
1	W	118	VAL
1	W	119	THR
1	W	144	TYR
1	V	1	MET
1	V	90	ASP
1	V	144	TYR
1	U	4	TYR
1	U	11	GLU
1	U	24	VAL
1	U	113	LYS
1	U	115	LYS
1	U	128	VAL
1	U	130	GLU
1	U	144	TYR
1	T	0	THR

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Mol	Chain	Res	Type
1	T	19	LEU
1	T	65	LEU
1	T	67	TYR
1	T	69	LEU
1	T	92	LEU
1	T	95	ASN
1	T	144	TYR
1	S	0	THR
1	S	6	ILE
1	S	11	GLU
1	S	58	THR
1	S	67	TYR
1	S	90	ASP
1	S	127	THR
1	S	130	GLU
1	S	135	ILE
1	S	137	GLU
1	S	144	TYR
1	j	5	THR
1	j	10	GLU
1	j	33	LYS
1	j	90	ASP
1	j	124	PRO
1	j	144	TYR
1	i	0	THR
1	i	4	TYR
1	i	17	HIS
1	i	25	LEU
1	i	48	ASP
1	i	79	ASN
1	i	94	ASP
1	i	95	ASN
1	i	144	TYR
1	h	1	MET
1	h	69	LEU
1	h	85	THR
1	h	108	VAL
1	h	129	ASN
1	h	138	LYS
1	g	43	GLU
1	g	64	PRO
1	g	69	LEU

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Mol	Chain	Res	Type
1	g	106	GLU
1	g	126	CYS
1	g	142	GLU
1	g	144	TYR
1	g	149	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	R	95	ASN
1	R	154	ASN
1	P	79	ASN
1	M	70	HIS
1	L	35	GLN
1	L	79	ASN
1	K	17	HIS
1	K	121	HIS
1	J	79	ASN
1	H	35	GLN
1	H	70	HIS
1	H	154	ASN
1	G	70	HIS
1	F	79	ASN
1	E	95	ASN
1	f	79	ASN
1	f	146	GLN
1	e	35	GLN
1	e	70	HIS
1	d	146	GLN
1	d	154	ASN
1	c	17	HIS
1	c	146	GLN
1	X	63	HIS
1	W	154	ASN
1	V	129	ASN
1	U	79	ASN
1	T	63	HIS
1	T	95	ASN
1	S	146	GLN
1	i	79	ASN
1	i	129	ASN
1	h	35	GLN

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Mol	Chain	Res	Type
1	h	154	ASN
1	g	28	HIS
1	g	146	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

178 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	2AN	S	203	-	22,23,23	1.72	4 (18%)	29,33,33	1.08	2 (6%)
3	SO4	E	205	-	4,4,4	0.19	0	6,6,6	0.13	0
2	2AN	B	203	-	22,23,23	1.71	5 (22%)	29,33,33	1.53	4 (13%)
2	2AN	b	202	-	22,23,23	1.86	5 (22%)	29,33,33	1.24	3 (10%)
2	2AN	M	201	-	22,23,23	2.11	4 (18%)	29,33,33	2.09	9 (31%)
2	2AN	S	201	-	22,23,23	2.06	4 (18%)	29,33,33	1.84	4 (13%)
2	2AN	N	201	-	22,23,23	1.39	4 (18%)	29,33,33	1.22	2 (6%)
2	2AN	V	207	-	22,23,23	1.74	5 (22%)	29,33,33	0.90	1 (3%)
2	2AN	b	204	-	22,23,23	1.73	3 (13%)	29,33,33	1.11	2 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	DMS	G	208	-	3,3,3	0.52	0	3,3,3	1.10	0
2	2AN	Q	202	-	22,23,23	1.80	4 (18%)	29,33,33	1.24	2 (6%)
2	2AN	L	203	-	22,23,23	1.60	4 (18%)	29,33,33	1.92	8 (27%)
2	2AN	X	201	-	22,23,23	2.00	5 (22%)	29,33,33	1.63	4 (13%)
2	2AN	V	204	-	22,23,23	1.74	5 (22%)	29,33,33	1.37	3 (10%)
6	FLC	i	202	-	12,12,12	1.34	2 (16%)	17,17,17	1.21	1 (5%)
2	2AN	P	202	-	22,23,23	1.84	7 (31%)	29,33,33	1.96	10 (34%)
2	2AN	j	207	-	22,23,23	2.30	5 (22%)	29,33,33	1.13	2 (6%)
2	2AN	R	205	-	22,23,23	1.83	5 (22%)	29,33,33	1.36	2 (6%)
2	2AN	W	201	-	22,23,23	2.06	5 (22%)	29,33,33	1.63	5 (17%)
5	DMS	X	207	-	3,3,3	0.56	0	3,3,3	0.62	0
2	2AN	V	205	-	22,23,23	1.58	7 (31%)	29,33,33	1.65	6 (20%)
2	2AN	H	202	-	22,23,23	1.82	4 (18%)	29,33,33	1.55	5 (17%)
2	2AN	P	204	-	22,23,23	1.81	5 (22%)	29,33,33	1.51	3 (10%)
3	SO4	I	208	-	4,4,4	0.32	0	6,6,6	0.90	0
2	2AN	H	204	-	22,23,23	2.01	5 (22%)	29,33,33	1.41	2 (6%)
2	2AN	X	206	-	22,23,23	1.81	5 (22%)	29,33,33	0.90	2 (6%)
2	2AN	d	202	-	22,23,23	1.96	5 (22%)	29,33,33	1.41	2 (6%)
2	2AN	I	205	-	22,23,23	2.69	5 (22%)	29,33,33	1.61	7 (24%)
2	2AN	K	201	-	22,23,23	1.70	5 (22%)	29,33,33	1.79	7 (24%)
2	2AN	f	206	-	22,23,23	1.87	4 (18%)	29,33,33	1.28	2 (6%)
2	2AN	X	202	-	22,23,23	1.82	6 (27%)	29,33,33	1.33	2 (6%)
2	2AN	S	204	-	22,23,23	1.69	6 (27%)	29,33,33	2.56	4 (13%)
2	2AN	j	202	-	22,23,23	1.39	3 (13%)	29,33,33	1.99	8 (27%)
2	2AN	j	206	-	22,23,23	1.94	6 (27%)	29,33,33	1.36	3 (10%)
6	FLC	G	206	-	12,12,12	1.04	0	17,17,17	1.93	5 (29%)
2	2AN	j	204	-	22,23,23	1.68	5 (22%)	29,33,33	1.50	4 (13%)
2	2AN	b	206	-	22,23,23	2.33	5 (22%)	29,33,33	1.60	4 (13%)
2	2AN	F	202	-	22,23,23	2.04	4 (18%)	29,33,33	2.07	13 (44%)
2	2AN	V	201	-	22,23,23	1.83	5 (22%)	29,33,33	1.58	6 (20%)
2	2AN	a	204	-	22,23,23	1.90	5 (22%)	29,33,33	1.21	2 (6%)
2	2AN	L	202	-	22,23,23	1.76	4 (18%)	29,33,33	1.29	3 (10%)
2	2AN	A	202	-	22,23,23	2.07	7 (31%)	29,33,33	1.79	8 (27%)
2	2AN	Y	203	-	22,23,23	1.71	5 (22%)	29,33,33	1.54	6 (20%)
2	2AN	M	202	-	22,23,23	1.58	5 (22%)	29,33,33	2.09	9 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	2AN	B	205	-	22,23,23	1.71	4 (18%)	29,33,33	1.31	4 (13%)
2	2AN	L	204	-	22,23,23	1.98	5 (22%)	29,33,33	1.55	6 (20%)
6	FLC	i	203	-	12,12,12	1.39	1 (8%)	17,17,17	2.32	5 (29%)
2	2AN	F	201	-	22,23,23	1.55	4 (18%)	29,33,33	1.45	6 (20%)
2	2AN	I	202	-	22,23,23	1.78	5 (22%)	29,33,33	1.36	4 (13%)
2	2AN	d	201	-	22,23,23	1.58	3 (13%)	29,33,33	1.59	5 (17%)
2	2AN	a	201	-	22,23,23	1.98	5 (22%)	29,33,33	2.21	8 (27%)
2	2AN	U	202	-	22,23,23	1.79	5 (22%)	29,33,33	1.30	2 (6%)
4	EPE	P	205	-	15,15,15	2.10	1 (6%)	19,20,20	1.74	7 (36%)
2	2AN	V	206	-	22,23,23	1.71	4 (18%)	29,33,33	1.87	8 (27%)
2	2AN	G	201	-	22,23,23	1.71	4 (18%)	29,33,33	1.38	5 (17%)
2	2AN	Z	202	-	22,23,23	2.01	5 (22%)	29,33,33	1.55	5 (17%)
2	2AN	a	203	-	22,23,23	2.19	7 (31%)	29,33,33	1.51	3 (10%)
2	2AN	c	203	-	22,23,23	1.69	3 (13%)	29,33,33	1.19	2 (6%)
2	2AN	E	202	-	22,23,23	1.44	3 (13%)	29,33,33	1.68	7 (24%)
2	2AN	F	203	-	22,23,23	1.45	4 (18%)	29,33,33	1.36	4 (13%)
2	2AN	c	205	-	22,23,23	1.66	5 (22%)	29,33,33	1.09	2 (6%)
2	2AN	V	208	-	22,23,23	2.11	6 (27%)	29,33,33	3.43	10 (34%)
2	2AN	B	206	-	22,23,23	1.81	4 (18%)	29,33,33	0.96	1 (3%)
2	2AN	N	202	-	22,23,23	1.73	6 (27%)	29,33,33	1.59	6 (20%)
2	2AN	h	202	-	22,23,23	1.63	5 (22%)	29,33,33	1.68	6 (20%)
2	2AN	Y	204	-	22,23,23	1.68	4 (18%)	29,33,33	0.90	2 (6%)
2	2AN	P	201	-	22,23,23	1.68	3 (13%)	29,33,33	1.16	3 (10%)
2	2AN	G	203	-	22,23,23	1.39	4 (18%)	29,33,33	1.23	3 (10%)
2	2AN	e	201	-	22,23,23	2.01	6 (27%)	29,33,33	1.59	6 (20%)
6	FLC	a	206	-	12,12,12	1.15	0	17,17,17	1.43	3 (17%)
2	2AN	f	204	-	22,23,23	1.67	7 (31%)	29,33,33	1.35	2 (6%)
3	SO4	c	207	-	4,4,4	0.43	0	6,6,6	0.45	0
3	SO4	c	208	-	4,4,4	0.45	0	6,6,6	0.38	0
2	2AN	X	204	-	22,23,23	1.91	4 (18%)	29,33,33	1.41	5 (17%)
2	2AN	R	201	-	22,23,23	1.84	5 (22%)	29,33,33	1.00	1 (3%)
2	2AN	g	202	-	22,23,23	1.63	4 (18%)	29,33,33	1.86	7 (24%)
2	2AN	O	202	-	22,23,23	2.12	4 (18%)	29,33,33	1.29	4 (13%)
2	2AN	O	203	-	22,23,23	2.08	4 (18%)	29,33,33	1.52	3 (10%)
2	2AN	F	204	-	22,23,23	1.77	4 (18%)	29,33,33	1.29	4 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	2AN	D	201	-	22,23,23	1.77	6 (27%)	29,33,33	1.56	5 (17%)
2	2AN	c	204	-	22,23,23	1.44	4 (18%)	29,33,33	1.52	4 (13%)
2	2AN	A	203	-	22,23,23	2.11	4 (18%)	29,33,33	1.39	4 (13%)
2	2AN	I	207	-	22,23,23	2.37	4 (18%)	29,33,33	1.69	10 (34%)
2	2AN	I	204	-	22,23,23	2.03	5 (22%)	29,33,33	1.43	4 (13%)
2	2AN	H	201	-	22,23,23	1.60	5 (22%)	29,33,33	1.38	3 (10%)
2	2AN	R	202	-	22,23,23	2.09	8 (36%)	29,33,33	1.30	5 (17%)
2	2AN	C	203[A]	-	22,23,23	0.61	0	29,33,33	1.44	5 (17%)
2	2AN	V	202	-	22,23,23	1.48	5 (22%)	29,33,33	1.71	7 (24%)
3	SO4	Q	204	-	4,4,4	0.53	0	6,6,6	0.58	0
6	FLC	e	202	-	12,12,12	1.54	1 (8%)	17,17,17	1.85	3 (17%)
2	2AN	K	202	-	22,23,23	1.63	4 (18%)	29,33,33	1.10	4 (13%)
2	2AN	F	205	-	22,23,23	1.71	4 (18%)	29,33,33	1.27	3 (10%)
2	2AN	f	202	-	22,23,23	1.36	2 (9%)	29,33,33	1.52	4 (13%)
2	2AN	G	205	-	22,23,23	1.88	4 (18%)	29,33,33	1.19	3 (10%)
2	2AN	c	201	-	22,23,23	1.69	6 (27%)	29,33,33	1.52	4 (13%)
6	FLC	a	205	-	12,12,12	1.33	1 (8%)	17,17,17	1.47	5 (29%)
2	2AN	C	202	-	22,23,23	1.75	5 (22%)	29,33,33	1.02	1 (3%)
2	2AN	h	204	-	22,23,23	1.51	4 (18%)	29,33,33	1.58	2 (6%)
2	2AN	E	203	-	22,23,23	1.91	4 (18%)	29,33,33	1.87	8 (27%)
2	2AN	b	203	-	22,23,23	1.75	5 (22%)	29,33,33	1.06	2 (6%)
3	SO4	G	209	-	4,4,4	0.52	0	6,6,6	0.20	0
2	2AN	Q	203	-	22,23,23	2.14	5 (22%)	29,33,33	1.75	5 (17%)
2	2AN	a	202	-	22,23,23	1.96	4 (18%)	29,33,33	1.54	6 (20%)
2	2AN	c	206	-	22,23,23	1.35	3 (13%)	29,33,33	1.25	3 (10%)
2	2AN	Y	201	-	22,23,23	2.49	6 (27%)	29,33,33	2.18	12 (41%)
3	SO4	A	205	-	4,4,4	0.41	0	6,6,6	0.78	0
2	2AN	J	202	-	22,23,23	1.49	4 (18%)	29,33,33	0.99	2 (6%)
2	2AN	A	201	-	22,23,23	1.67	6 (27%)	29,33,33	1.40	6 (20%)
2	2AN	h	205	-	22,23,23	2.11	5 (22%)	29,33,33	1.30	2 (6%)
2	2AN	H	203	-	22,23,23	1.69	5 (22%)	29,33,33	1.29	2 (6%)
2	2AN	G	202	-	22,23,23	1.51	4 (18%)	29,33,33	1.62	5 (17%)
2	2AN	h	203	-	22,23,23	2.21	6 (27%)	29,33,33	1.84	8 (27%)
2	2AN	Z	204	-	22,23,23	1.78	4 (18%)	29,33,33	1.42	3 (10%)
2	2AN	G	204	-	22,23,23	2.05	5 (22%)	29,33,33	1.39	5 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	2AN	T	204	-	22,23,23	2.27	5 (22%)	29,33,33	1.64	9 (31%)
2	2AN	j	201	-	22,23,23	1.66	4 (18%)	29,33,33	1.60	5 (17%)
2	2AN	X	203	-	22,23,23	1.79	5 (22%)	29,33,33	0.90	1 (3%)
2	2AN	j	203	-	22,23,23	1.71	6 (27%)	29,33,33	1.73	8 (27%)
2	2AN	T	202	-	22,23,23	2.00	4 (18%)	29,33,33	1.58	3 (10%)
5	DMS	N	206	-	3,3,3	0.50	0	3,3,3	0.85	0
2	2AN	h	201	-	22,23,23	2.23	4 (18%)	29,33,33	1.35	6 (20%)
6	FLC	j	208	-	12,12,12	2.27	1 (8%)	17,17,17	2.39	6 (35%)
2	2AN	E	204	-	22,23,23	2.09	6 (27%)	29,33,33	1.89	5 (17%)
2	2AN	B	204	-	22,23,23	1.60	4 (18%)	29,33,33	1.49	4 (13%)
2	2AN	M	203	-	22,23,23	1.87	7 (31%)	29,33,33	1.84	6 (20%)
2	2AN	B	202	-	22,23,23	1.65	3 (13%)	29,33,33	0.95	1 (3%)
2	2AN	h	206	-	22,23,23	2.03	4 (18%)	29,33,33	1.63	6 (20%)
2	2AN	R	204	-	22,23,23	2.16	4 (18%)	29,33,33	1.56	6 (20%)
2	2AN	D	202	-	22,23,23	1.81	6 (27%)	29,33,33	1.21	2 (6%)
3	SO4	c	209	-	4,4,4	0.49	0	6,6,6	0.62	0
2	2AN	K	203	-	22,23,23	1.74	4 (18%)	29,33,33	1.26	1 (3%)
2	2AN	b	205	-	22,23,23	2.00	5 (22%)	29,33,33	1.57	5 (17%)
2	2AN	D	204	-	22,23,23	2.40	5 (22%)	29,33,33	2.15	10 (34%)
2	2AN	N	204	-	22,23,23	1.56	5 (22%)	29,33,33	1.90	5 (17%)
2	2AN	f	203	-	22,23,23	1.81	5 (22%)	29,33,33	0.91	2 (6%)
2	2AN	S	202	-	22,23,23	1.85	4 (18%)	29,33,33	1.85	9 (31%)
2	2AN	N	205	-	22,23,23	2.42	7 (31%)	29,33,33	1.65	5 (17%)
2	2AN	d	204	-	22,23,23	1.64	4 (18%)	29,33,33	2.01	5 (17%)
2	2AN	F	206	-	22,23,23	1.88	5 (22%)	29,33,33	1.61	7 (24%)
2	2AN	X	205	-	22,23,23	2.06	5 (22%)	29,33,33	1.30	3 (10%)
2	2AN	j	205	-	22,23,23	1.80	4 (18%)	29,33,33	1.87	10 (34%)
2	2AN	c	202	-	22,23,23	2.14	5 (22%)	29,33,33	1.80	10 (34%)
2	2AN	N	203	-	22,23,23	1.97	5 (22%)	29,33,33	2.66	9 (31%)
2	2AN	Q	201	-	22,23,23	1.94	5 (22%)	29,33,33	1.73	6 (20%)
2	2AN	G	207	-	22,23,23	2.04	5 (22%)	29,33,33	1.05	1 (3%)
2	2AN	T	205	-	22,23,23	2.27	6 (27%)	29,33,33	2.23	10 (34%)
3	SO4	Y	205	-	4,4,4	0.31	0	6,6,6	0.63	0
2	2AN	f	201	-	22,23,23	2.07	6 (27%)	29,33,33	1.92	9 (31%)
2	2AN	f	205	-	22,23,23	1.68	4 (18%)	29,33,33	1.29	5 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	2AN	A	204	-	22,23,23	1.81	5 (22%)	29,33,33	0.88	2 (6%)
2	2AN	i	201	-	22,23,23	1.75	4 (18%)	29,33,33	1.72	6 (20%)
2	2AN	b	201	-	22,23,23	1.78	4 (18%)	29,33,33	1.01	1 (3%)
2	2AN	C	201	-	22,23,23	1.64	5 (22%)	29,33,33	1.39	4 (13%)
3	SO4	g	204	-	4,4,4	0.60	0	6,6,6	0.47	0
2	2AN	Z	203	-	22,23,23	1.90	5 (22%)	29,33,33	1.64	7 (24%)
2	2AN	d	203	-	22,23,23	1.74	5 (22%)	29,33,33	0.92	1 (3%)
2	2AN	g	203	-	22,23,23	1.79	6 (27%)	29,33,33	1.55	4 (13%)
2	2AN	E	201	-	22,23,23	1.71	4 (18%)	29,33,33	1.14	2 (6%)
2	2AN	I	206	-	22,23,23	2.36	6 (27%)	29,33,33	1.81	7 (24%)
2	2AN	J	203	-	22,23,23	1.76	4 (18%)	29,33,33	1.63	6 (20%)
2	2AN	B	201	-	22,23,23	1.80	5 (22%)	29,33,33	2.02	12 (41%)
2	2AN	Z	205	-	22,23,23	1.63	4 (18%)	29,33,33	1.61	5 (17%)
2	2AN	I	201	-	22,23,23	1.32	3 (13%)	29,33,33	1.89	7 (24%)
2	2AN	U	201	-	22,23,23	1.94	5 (22%)	29,33,33	1.26	1 (3%)
2	2AN	T	203	-	22,23,23	1.60	5 (22%)	29,33,33	1.92	7 (24%)
2	2AN	L	201	-	22,23,23	1.62	5 (22%)	29,33,33	1.25	2 (6%)
2	2AN	J	201	-	22,23,23	1.48	3 (13%)	29,33,33	1.01	1 (3%)
2	2AN	Z	201	-	22,23,23	2.32	6 (27%)	29,33,33	1.60	8 (27%)
2	2AN	R	203	-	22,23,23	1.84	6 (27%)	29,33,33	1.36	3 (10%)
2	2AN	Y	202	-	22,23,23	1.85	6 (27%)	29,33,33	1.42	6 (20%)
2	2AN	V	203	-	22,23,23	1.97	6 (27%)	29,33,33	1.59	6 (20%)
2	2AN	T	201	-	22,23,23	1.77	7 (31%)	29,33,33	1.31	2 (6%)
2	2AN	D	203	-	22,23,23	1.87	6 (27%)	29,33,33	1.62	5 (17%)
2	2AN	Z	206	-	22,23,23	2.02	5 (22%)	29,33,33	1.73	6 (20%)
2	2AN	g	201	-	22,23,23	1.96	6 (27%)	29,33,33	1.75	8 (27%)
2	2AN	P	203	-	22,23,23	1.65	6 (27%)	29,33,33	1.57	4 (13%)
2	2AN	I	203	-	22,23,23	1.92	5 (22%)	29,33,33	1.26	3 (10%)
2	2AN	O	201	-	22,23,23	1.44	2 (9%)	29,33,33	1.42	3 (10%)

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

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

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

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

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	2AN	J	201	-	-	0/10/10/10	0/3/3/3
2	2AN	Z	201	-	-	2/10/10/10	0/3/3/3
2	2AN	R	203	-	-	6/10/10/10	0/3/3/3
2	2AN	Y	202	-	-	6/10/10/10	0/3/3/3
2	2AN	V	203	-	-	1/10/10/10	0/3/3/3
2	2AN	T	201	-	-	0/10/10/10	0/3/3/3
2	2AN	D	203	-	-	6/10/10/10	0/3/3/3
2	2AN	Z	206	-	-	6/10/10/10	0/3/3/3
2	2AN	g	201	-	-	0/10/10/10	0/3/3/3
2	2AN	P	203	-	-	6/10/10/10	0/3/3/3
2	2AN	I	203	-	-	0/10/10/10	0/3/3/3
2	2AN	O	201	-	-	5/10/10/10	0/3/3/3

All (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
2	I	207	2AN	C1-C10	7.45	1.52	1.43
6	j	208	FLC	CB-CBC	-7.01	1.46	1.53
2	b	206	2AN	C1-C10	6.81	1.51	1.43
2	h	206	2AN	C1-C10	6.80	1.51	1.43
2	T	204	2AN	C1-C10	6.73	1.51	1.43
2	I	206	2AN	C1-C10	6.72	1.51	1.43
2	D	204	2AN	C1-C10	6.72	1.51	1.43
2	h	201	2AN	C1-C10	6.69	1.51	1.43
2	R	204	2AN	C1-C10	6.69	1.51	1.43
2	Z	201	2AN	C1-C10	6.65	1.51	1.43
2	T	202	2AN	C1-C10	6.51	1.51	1.43
2	I	204	2AN	C1-C10	6.51	1.51	1.43
2	a	202	2AN	C1-C10	6.43	1.51	1.43
2	a	201	2AN	C1-C10	6.42	1.51	1.43
2	N	205	2AN	C1-C10	6.39	1.51	1.43
2	X	205	2AN	C1-C10	6.37	1.51	1.43
2	Z	206	2AN	C1-C10	6.27	1.51	1.43
2	f	201	2AN	C1-C10	6.27	1.51	1.43
2	O	202	2AN	C1-C10	6.26	1.51	1.43
2	b	205	2AN	C1-C10	6.24	1.51	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	h	205	2AN	C1-C10	6.22	1.51	1.43
2	Z	202	2AN	C1-C10	6.20	1.51	1.43
2	G	204	2AN	C1-C10	6.11	1.51	1.43
2	A	203	2AN	C1-C10	6.07	1.50	1.43
2	S	201	2AN	C1-C10	6.05	1.50	1.43
2	X	201	2AN	C1-C10	6.04	1.50	1.43
2	H	204	2AN	C1-C10	5.99	1.50	1.43
2	c	202	2AN	C1-C10	5.97	1.50	1.43
2	e	201	2AN	C1-C10	5.95	1.50	1.43
2	V	203	2AN	C1-C10	5.93	1.50	1.43
2	Q	203	2AN	C1-C10	5.92	1.50	1.43
2	U	201	2AN	C1-C10	5.86	1.50	1.43
2	F	202	2AN	C1-C10	5.84	1.50	1.43
2	T	205	2AN	C1-C10	5.83	1.50	1.43
2	Q	201	2AN	C1-C10	5.81	1.50	1.43
2	G	207	2AN	C1-C10	5.80	1.50	1.43
2	S	202	2AN	C1-C10	5.75	1.50	1.43
2	I	202	2AN	C1-C10	5.75	1.50	1.43
2	a	203	2AN	C1-C10	5.74	1.50	1.43
2	g	201	2AN	C1-C10	5.70	1.50	1.43
2	O	203	2AN	C1-C10	5.61	1.50	1.43
2	X	204	2AN	C1-C10	5.60	1.50	1.43
2	L	204	2AN	C1-C10	5.57	1.50	1.43
2	d	202	2AN	C1-C10	5.56	1.50	1.43
2	i	201	2AN	C1-C10	5.48	1.50	1.43
2	A	202	2AN	C1-C10	5.45	1.50	1.43
2	F	206	2AN	C1-C10	5.45	1.50	1.43
2	R	201	2AN	C1-C10	5.45	1.50	1.43
2	W	201	2AN	C1-C10	5.43	1.50	1.43
2	R	205	2AN	C1-C10	5.40	1.50	1.43
2	I	205	2AN	C10-C5	5.34	1.53	1.42
2	E	204	2AN	C1-C10	5.34	1.50	1.43
2	B	202	2AN	C1-C10	5.27	1.49	1.43
2	G	205	2AN	C1-C10	5.27	1.49	1.43
2	H	202	2AN	C1-C10	5.26	1.49	1.43
2	j	206	2AN	C1-C10	5.23	1.49	1.43
2	f	206	2AN	C1-C10	5.17	1.49	1.43
2	Q	202	2AN	C1-C10	5.16	1.49	1.43
2	E	201	2AN	C1-C10	5.16	1.49	1.43
2	c	203	2AN	C1-C10	5.16	1.49	1.43
2	P	201	2AN	C1-C10	5.16	1.49	1.43
2	V	208	2AN	C1-C10	5.15	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	204	2AN	C1-C10	5.14	1.49	1.43
2	b	201	2AN	C1-C10	5.12	1.49	1.43
2	K	203	2AN	C1-C10	5.12	1.49	1.43
2	b	203	2AN	C1-C10	5.06	1.49	1.43
2	N	203	2AN	C1-N	-5.05	1.23	1.38
2	h	203	2AN	C1-C10	5.02	1.49	1.43
2	B	206	2AN	C1-C10	4.99	1.49	1.43
2	D	204	2AN	C9-C10	4.93	1.54	1.44
2	D	201	2AN	C1-C10	4.90	1.49	1.43
2	I	203	2AN	C1-C10	4.88	1.49	1.43
2	c	202	2AN	C9-C10	4.87	1.53	1.44
2	F	205	2AN	C1-C10	4.85	1.49	1.43
2	Y	203	2AN	C1-C10	4.78	1.49	1.43
2	O	203	2AN	O1-S	4.77	1.66	1.43
2	I	205	2AN	C9-C10	4.76	1.53	1.44
2	Y	202	2AN	C1-C10	4.75	1.49	1.43
2	b	206	2AN	C9-C10	4.75	1.53	1.44
2	E	204	2AN	O2-S	4.74	1.66	1.43
2	B	201	2AN	C1-C10	4.74	1.49	1.43
2	Z	204	2AN	C1-C10	4.70	1.49	1.43
2	E	203	2AN	C1-C10	4.69	1.49	1.43
2	Y	201	2AN	C9-C10	4.68	1.53	1.44
2	C	202	2AN	C1-C10	4.67	1.49	1.43
2	L	202	2AN	C1-C10	4.67	1.49	1.43
2	R	203	2AN	C1-C10	4.67	1.49	1.43
2	A	204	2AN	C1-C10	4.63	1.49	1.43
2	A	202	2AN	O1-S	4.57	1.65	1.43
2	f	203	2AN	C1-C10	4.57	1.49	1.43
2	X	206	2AN	C1-C10	4.56	1.49	1.43
2	V	207	2AN	C1-C10	4.55	1.49	1.43
2	W	201	2AN	O2-S	4.55	1.65	1.43
2	j	203	2AN	C1-C10	4.54	1.48	1.43
2	d	203	2AN	C1-C10	4.53	1.48	1.43
2	I	206	2AN	C9-C10	4.52	1.53	1.44
2	I	207	2AN	O2-S	4.52	1.65	1.43
2	L	202	2AN	O2-S	4.48	1.65	1.43
2	g	201	2AN	O1-S	4.47	1.65	1.43
2	Z	201	2AN	O1-S	4.46	1.65	1.43
2	Z	203	2AN	C1-C10	4.44	1.48	1.43
2	X	203	2AN	C1-C10	4.44	1.48	1.43
2	G	207	2AN	O2-S	4.42	1.65	1.43
2	E	203	2AN	O1-S	4.42	1.65	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	M	202	2AN	C1-C10	4.42	1.48	1.43
2	R	202	2AN	C11-N	-4.41	1.31	1.40
2	g	203	2AN	C1-C10	4.40	1.48	1.43
2	I	205	2AN	O1-S	4.40	1.64	1.43
2	b	204	2AN	C1-C10	4.39	1.48	1.43
2	V	204	2AN	O1-S	4.39	1.64	1.43
2	S	203	2AN	O1-S	4.38	1.64	1.43
2	c	205	2AN	O1-S	4.37	1.64	1.43
2	X	205	2AN	O1-S	4.37	1.64	1.43
2	D	202	2AN	O2-S	4.35	1.64	1.43
2	I	207	2AN	C9-C10	4.34	1.52	1.44
2	J	203	2AN	C1-C10	4.33	1.48	1.43
2	C	201	2AN	O1-S	4.32	1.64	1.43
2	N	205	2AN	C10-C5	4.32	1.51	1.42
2	Q	203	2AN	O2-S	4.32	1.64	1.43
2	R	202	2AN	C1-C10	4.32	1.48	1.43
2	T	204	2AN	C10-C5	4.31	1.51	1.42
2	F	206	2AN	O1-S	4.31	1.64	1.43
2	S	204	2AN	O2-S	4.30	1.64	1.43
2	V	201	2AN	O1-S	4.30	1.64	1.43
2	I	203	2AN	O1-S	4.29	1.64	1.43
2	K	201	2AN	O1-S	4.29	1.64	1.43
2	b	202	2AN	C1-C10	4.29	1.48	1.43
2	h	201	2AN	C9-C10	4.29	1.52	1.44
2	a	204	2AN	O1-S	4.28	1.64	1.43
2	V	201	2AN	C1-C10	4.28	1.48	1.43
2	g	202	2AN	C1-C10	4.28	1.48	1.43
2	G	204	2AN	O1-S	4.27	1.64	1.43
2	G	201	2AN	O1-S	4.27	1.64	1.43
2	b	206	2AN	O1-S	4.26	1.64	1.43
2	U	202	2AN	O2-S	4.26	1.64	1.43
2	A	201	2AN	C1-C10	4.24	1.48	1.43
2	L	204	2AN	O2-S	4.24	1.64	1.43
2	N	205	2AN	C9-C10	4.24	1.52	1.44
2	d	201	2AN	O1-S	4.24	1.64	1.43
2	X	201	2AN	O2-S	4.23	1.64	1.43
2	g	203	2AN	O2-S	4.23	1.64	1.43
2	a	204	2AN	C1-C10	4.23	1.48	1.43
2	Y	201	2AN	O2-S	4.21	1.64	1.43
2	O	202	2AN	O1-S	4.21	1.64	1.43
2	f	203	2AN	O2-S	4.20	1.64	1.43
2	Z	201	2AN	C9-C10	4.20	1.52	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	b	202	2AN	O1-S	4.20	1.64	1.43
2	a	203	2AN	O1-S	4.20	1.64	1.43
2	A	204	2AN	O2-S	4.20	1.63	1.43
2	T	205	2AN	O2-S	4.19	1.63	1.43
2	h	201	2AN	O1-S	4.19	1.63	1.43
2	h	205	2AN	O1-S	4.19	1.63	1.43
2	E	202	2AN	O1-S	4.19	1.63	1.43
2	X	203	2AN	O1-S	4.18	1.63	1.43
2	D	204	2AN	C10-C5	4.18	1.51	1.42
2	X	206	2AN	O2-S	4.18	1.63	1.43
2	j	207	2AN	O1-S	4.18	1.63	1.43
2	S	201	2AN	O1-S	4.18	1.63	1.43
2	d	204	2AN	O2-S	4.17	1.63	1.43
2	B	203	2AN	O1-S	4.17	1.63	1.43
2	S	203	2AN	C1-C10	4.17	1.48	1.43
2	K	202	2AN	C11-N	-4.16	1.31	1.40
2	K	201	2AN	C1-C10	4.16	1.48	1.43
2	e	201	2AN	C9-C10	4.16	1.52	1.44
2	j	205	2AN	C12-C11	-4.16	1.32	1.39
2	d	201	2AN	C1-C10	4.15	1.48	1.43
2	a	202	2AN	C9-C10	4.15	1.52	1.44
2	A	203	2AN	O1-S	4.14	1.63	1.43
2	D	202	2AN	C1-C10	4.14	1.48	1.43
2	H	202	2AN	O2-S	4.14	1.63	1.43
2	N	203	2AN	C11-N	-4.13	1.31	1.40
2	Z	206	2AN	O1-S	4.13	1.63	1.43
2	a	201	2AN	O2-S	4.13	1.63	1.43
6	e	202	FLC	CB-CBC	-4.12	1.49	1.53
2	B	205	2AN	C1-C10	4.11	1.48	1.43
2	Z	202	2AN	O1-S	4.11	1.63	1.43
2	Y	201	2AN	C10-C5	4.11	1.51	1.42
2	X	202	2AN	O1-S	4.10	1.63	1.43
2	X	204	2AN	O2-S	4.08	1.63	1.43
2	U	202	2AN	C1-C10	4.08	1.48	1.43
2	H	203	2AN	O2-S	4.07	1.63	1.43
2	B	204	2AN	O1-S	4.07	1.63	1.43
2	D	204	2AN	O1-S	4.07	1.63	1.43
2	Y	204	2AN	C1-C10	4.06	1.48	1.43
2	H	203	2AN	C1-C10	4.06	1.48	1.43
2	j	206	2AN	O2-S	4.06	1.63	1.43
2	T	202	2AN	O1-S	4.06	1.63	1.43
2	B	205	2AN	O1-S	4.04	1.63	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	R	204	2AN	O2-S	4.03	1.63	1.43
2	D	203	2AN	O2-S	4.02	1.63	1.43
2	b	204	2AN	O1-S	4.02	1.63	1.43
2	f	205	2AN	O1-S	4.02	1.63	1.43
2	T	205	2AN	C9-C10	4.02	1.52	1.44
2	Q	203	2AN	C9-C10	4.01	1.52	1.44
2	H	201	2AN	C1-C10	4.01	1.48	1.43
2	B	206	2AN	O2-S	3.99	1.63	1.43
2	Y	204	2AN	O2-S	3.99	1.63	1.43
2	P	203	2AN	C1-C10	3.99	1.48	1.43
2	T	205	2AN	C10-C5	3.99	1.50	1.42
2	d	204	2AN	C1-C10	3.98	1.48	1.43
2	R	204	2AN	C9-C10	3.97	1.52	1.44
2	M	203	2AN	O2-S	3.96	1.62	1.43
2	J	201	2AN	O1-S	3.95	1.62	1.43
2	j	204	2AN	O1-S	3.95	1.62	1.43
2	T	201	2AN	O2-S	3.95	1.62	1.43
2	I	206	2AN	O2-S	3.94	1.62	1.43
2	h	203	2AN	C11-N	-3.92	1.32	1.40
2	A	203	2AN	C9-C10	3.92	1.52	1.44
2	X	202	2AN	C1-C10	3.91	1.48	1.43
2	Q	201	2AN	O1-S	3.90	1.62	1.43
2	h	202	2AN	C1-C10	3.90	1.48	1.43
2	L	201	2AN	C1-C10	3.88	1.48	1.43
2	V	206	2AN	C1-C10	3.87	1.48	1.43
2	G	205	2AN	C11-N	-3.87	1.32	1.40
2	d	202	2AN	O1-S	3.87	1.62	1.43
2	c	205	2AN	C1-C10	3.84	1.48	1.43
2	P	202	2AN	C11-N	-3.84	1.32	1.40
2	T	201	2AN	C1-C10	3.83	1.48	1.43
2	a	203	2AN	C10-C5	3.82	1.50	1.42
2	A	201	2AN	O2-S	3.80	1.62	1.43
2	I	207	2AN	C10-C5	3.80	1.50	1.42
2	a	203	2AN	C9-C10	3.80	1.51	1.44
2	b	206	2AN	C10-C5	3.79	1.50	1.42
2	Z	203	2AN	O2-S	3.79	1.62	1.43
2	I	206	2AN	C10-C5	3.79	1.50	1.42
2	Y	202	2AN	O2-S	3.78	1.62	1.43
2	c	203	2AN	O3-S	3.77	1.65	1.45
2	f	206	2AN	O2-S	3.77	1.61	1.43
2	f	205	2AN	C11-N	-3.76	1.32	1.40
2	V	204	2AN	C1-C10	3.75	1.47	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	205	2AN	O1-S	3.74	1.61	1.43
2	c	202	2AN	C10-C5	3.74	1.50	1.42
2	G	201	2AN	C1-C10	3.74	1.47	1.43
2	F	203	2AN	O1-S	3.73	1.61	1.43
2	S	204	2AN	C1-C10	3.73	1.47	1.43
2	V	208	2AN	C9-C10	3.73	1.51	1.44
2	D	203	2AN	C11-N	-3.71	1.32	1.40
2	V	208	2AN	O3-S	3.70	1.64	1.45
2	c	202	2AN	O2-S	3.70	1.61	1.43
2	Q	202	2AN	O2-S	3.69	1.61	1.43
2	D	203	2AN	C1-C10	3.68	1.47	1.43
2	F	202	2AN	C9-C10	3.68	1.51	1.44
2	O	201	2AN	O2-S	3.68	1.61	1.43
2	P	204	2AN	C4-C5	-3.67	1.34	1.42
2	J	203	2AN	O2-S	3.67	1.61	1.43
2	V	208	2AN	C11-N	-3.67	1.32	1.40
2	Z	205	2AN	O3-S	3.66	1.64	1.45
2	T	204	2AN	O2-S	3.66	1.61	1.43
2	U	201	2AN	O3-S	3.66	1.64	1.45
2	V	206	2AN	C10-C5	3.66	1.50	1.42
2	f	202	2AN	O1-S	3.65	1.61	1.43
2	Z	204	2AN	O3-S	3.65	1.64	1.45
2	Q	203	2AN	C10-C5	3.64	1.50	1.42
2	I	204	2AN	O3-S	3.64	1.64	1.45
2	V	203	2AN	O2-S	3.64	1.61	1.43
2	a	204	2AN	C11-N	-3.63	1.32	1.40
2	B	201	2AN	O1-S	3.63	1.61	1.43
2	W	201	2AN	C9-C10	3.62	1.51	1.44
2	E	203	2AN	C10-C5	3.62	1.49	1.42
2	A	202	2AN	C9-C10	3.62	1.51	1.44
2	Z	203	2AN	C10-C5	3.62	1.49	1.42
2	E	201	2AN	O2-S	3.61	1.61	1.43
2	S	201	2AN	C9-C10	3.61	1.51	1.44
2	H	204	2AN	O3-S	3.61	1.64	1.45
2	R	203	2AN	O3-S	3.60	1.64	1.45
2	F	202	2AN	C10-C5	3.59	1.49	1.42
2	h	201	2AN	C10-C5	3.59	1.49	1.42
2	f	204	2AN	C1-C10	3.59	1.47	1.43
2	V	205	2AN	C1-C10	3.58	1.47	1.43
2	T	203	2AN	O3-S	3.58	1.64	1.45
2	F	201	2AN	O2-S	3.58	1.61	1.43
2	N	205	2AN	O3-S	3.57	1.64	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	j	207	2AN	C9-C10	3.56	1.51	1.44
2	C	202	2AN	O3-S	3.55	1.64	1.45
2	P	202	2AN	O2-S	3.55	1.60	1.43
2	G	205	2AN	O3-S	3.55	1.63	1.45
2	d	203	2AN	O3-S	3.55	1.63	1.45
2	A	203	2AN	C10-C5	3.55	1.49	1.42
2	P	204	2AN	O3-S	3.55	1.63	1.45
2	M	203	2AN	C9-C10	3.55	1.51	1.44
2	c	201	2AN	C4-C5	-3.54	1.34	1.42
2	V	207	2AN	O3-S	3.54	1.63	1.45
2	G	202	2AN	C1-C10	3.54	1.47	1.43
2	M	203	2AN	C1-C10	3.54	1.47	1.43
2	L	203	2AN	C1-C10	3.53	1.47	1.43
2	h	202	2AN	O2-S	3.53	1.60	1.43
2	c	204	2AN	O2-S	3.52	1.60	1.43
2	R	205	2AN	O3-S	3.52	1.63	1.45
2	e	201	2AN	C10-C5	3.52	1.49	1.42
2	J	201	2AN	C1-C10	3.50	1.47	1.43
2	J	202	2AN	O3-S	3.50	1.63	1.45
2	Z	203	2AN	C9-C10	3.50	1.51	1.44
2	M	202	2AN	O3-S	3.49	1.63	1.45
2	V	202	2AN	O1-S	3.49	1.60	1.43
2	i	201	2AN	C10-C5	3.49	1.49	1.42
2	h	203	2AN	O1-S	3.48	1.60	1.43
2	N	202	2AN	C1-C10	3.48	1.47	1.43
2	G	202	2AN	O3-S	3.48	1.63	1.45
2	L	203	2AN	O2-S	3.47	1.60	1.43
2	H	204	2AN	C10-C5	3.47	1.49	1.42
2	R	204	2AN	C10-C5	3.47	1.49	1.42
2	K	203	2AN	O3-S	3.46	1.63	1.45
2	S	202	2AN	C9-C10	3.45	1.51	1.44
2	P	204	2AN	C1-C10	3.45	1.47	1.43
2	j	204	2AN	C1-C10	3.45	1.47	1.43
2	N	202	2AN	O2-S	3.45	1.60	1.43
2	I	201	2AN	O1-S	3.45	1.60	1.43
2	O	203	2AN	C9-C10	3.44	1.51	1.44
2	P	203	2AN	C11-N	-3.44	1.33	1.40
2	T	203	2AN	C4-C5	-3.43	1.34	1.42
2	j	201	2AN	C4-C5	-3.43	1.34	1.42
2	j	201	2AN	C1-C10	3.43	1.47	1.43
2	K	202	2AN	C1-C10	3.42	1.47	1.43
2	B	203	2AN	C11-N	-3.42	1.33	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Y	203	2AN	O3-S	3.42	1.63	1.45
2	b	205	2AN	O3-S	3.41	1.63	1.45
2	T	204	2AN	C8-C9	3.41	1.41	1.37
2	G	207	2AN	C9-C10	3.41	1.50	1.44
2	Z	201	2AN	C10-C5	3.40	1.49	1.42
2	j	202	2AN	O1-S	3.40	1.60	1.43
2	F	201	2AN	C1-C10	3.39	1.47	1.43
2	j	205	2AN	O1-S	3.39	1.60	1.43
2	h	205	2AN	C10-C5	3.38	1.49	1.42
2	j	201	2AN	O2-S	3.38	1.60	1.43
2	B	204	2AN	C1-C10	3.37	1.47	1.43
2	R	203	2AN	C11-N	-3.37	1.33	1.40
2	I	203	2AN	C10-C5	3.37	1.49	1.42
2	X	202	2AN	C11-N	-3.37	1.33	1.40
2	N	204	2AN	C4-C5	-3.37	1.34	1.42
2	U	202	2AN	C11-N	-3.36	1.33	1.40
2	L	201	2AN	C4-C5	-3.35	1.34	1.42
2	L	203	2AN	C10-C5	3.35	1.49	1.42
2	V	202	2AN	C1-C10	3.34	1.47	1.43
2	S	202	2AN	C10-C5	3.33	1.49	1.42
2	N	205	2AN	C8-C9	3.33	1.41	1.37
2	h	206	2AN	O3-S	3.33	1.62	1.45
2	c	201	2AN	O1-S	3.33	1.59	1.43
2	h	205	2AN	C9-C10	3.33	1.50	1.44
2	Q	201	2AN	C9-C10	3.32	1.50	1.44
2	O	202	2AN	C10-C5	3.32	1.49	1.42
2	T	204	2AN	C9-C10	3.30	1.50	1.44
2	G	201	2AN	C9-C10	3.30	1.50	1.44
2	b	202	2AN	C11-N	-3.29	1.33	1.40
2	D	201	2AN	C10-C5	3.28	1.49	1.42
2	L	204	2AN	C10-C5	3.28	1.49	1.42
2	F	204	2AN	O3-S	3.28	1.62	1.45
2	F	202	2AN	O3-S	3.27	1.62	1.45
2	h	203	2AN	C9-C10	3.26	1.50	1.44
2	Z	202	2AN	C10-C5	3.26	1.49	1.42
2	Z	205	2AN	C1-C10	3.26	1.47	1.43
2	h	204	2AN	C1-C10	3.23	1.47	1.43
2	j	207	2AN	C10-C5	3.23	1.49	1.42
2	D	203	2AN	C9-C10	3.23	1.50	1.44
2	Z	206	2AN	C10-C5	3.23	1.49	1.42
2	M	201	2AN	O2-S	3.21	1.59	1.43
2	h	203	2AN	C10-C5	3.21	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	j	206	2AN	C11-N	-3.20	1.33	1.40
2	P	201	2AN	O3-S	3.20	1.62	1.45
2	b	205	2AN	C10-C5	3.20	1.49	1.42
2	N	204	2AN	O3-S	3.19	1.62	1.45
2	h	206	2AN	C9-C10	3.19	1.50	1.44
2	c	204	2AN	C1-C10	3.19	1.47	1.43
2	I	204	2AN	C10-C5	3.19	1.49	1.42
2	E	204	2AN	C9-C10	3.17	1.50	1.44
2	h	204	2AN	C6-C5	-3.17	1.35	1.42
2	L	204	2AN	C9-C10	3.17	1.50	1.44
2	Y	202	2AN	C10-C5	3.17	1.49	1.42
2	i	201	2AN	O3-S	3.16	1.61	1.45
2	P	203	2AN	O3-S	3.16	1.61	1.45
2	d	202	2AN	C10-C5	3.16	1.49	1.42
2	T	202	2AN	C9-C10	3.15	1.50	1.44
2	W	201	2AN	C10-C5	3.14	1.48	1.42
2	j	206	2AN	C10-C5	3.14	1.48	1.42
2	U	201	2AN	C10-C5	3.14	1.48	1.42
2	R	205	2AN	C4-C5	-3.14	1.35	1.42
2	S	202	2AN	O3-S	3.14	1.61	1.45
2	X	201	2AN	C9-C10	3.13	1.50	1.44
2	b	205	2AN	C9-C10	3.13	1.50	1.44
2	b	203	2AN	O3-S	3.13	1.61	1.45
2	F	204	2AN	C9-C10	3.12	1.50	1.44
2	K	201	2AN	C9-C10	3.12	1.50	1.44
2	b	202	2AN	C10-C5	3.11	1.48	1.42
2	X	205	2AN	C9-C10	3.11	1.50	1.44
2	N	202	2AN	C9-C10	3.11	1.50	1.44
2	E	204	2AN	C10-C5	3.10	1.48	1.42
2	E	204	2AN	C11-N	-3.10	1.34	1.40
2	c	201	2AN	C6-C5	-3.10	1.35	1.42
2	R	202	2AN	C4-C5	-3.10	1.35	1.42
2	A	202	2AN	C10-C5	3.09	1.48	1.42
2	f	201	2AN	C4-C5	-3.09	1.35	1.42
2	B	202	2AN	O3-S	3.09	1.61	1.45
2	I	202	2AN	O2-S	3.09	1.58	1.43
2	X	204	2AN	C10-C5	3.09	1.48	1.42
2	Y	203	2AN	C10-C5	3.08	1.48	1.42
2	G	207	2AN	C10-C5	3.08	1.48	1.42
2	O	202	2AN	C9-C10	3.07	1.50	1.44
2	Z	206	2AN	C9-C10	3.07	1.50	1.44
2	V	201	2AN	C4-C5	-3.05	1.35	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	203	2AN	C9-C10	3.05	1.50	1.44
2	M	203	2AN	C10-C5	3.04	1.48	1.42
2	C	201	2AN	C1-C10	3.04	1.47	1.43
2	a	204	2AN	C9-C10	3.04	1.50	1.44
2	f	206	2AN	C10-C5	3.04	1.48	1.42
2	J	202	2AN	C4-C5	-3.04	1.35	1.42
2	Z	201	2AN	C8-C9	3.03	1.41	1.37
2	b	201	2AN	O2-S	3.03	1.58	1.43
2	V	204	2AN	C10-C5	3.02	1.48	1.42
2	J	202	2AN	C11-N	-3.01	1.34	1.40
2	N	202	2AN	C11-N	-3.00	1.34	1.40
2	c	206	2AN	O3-S	3.00	1.61	1.45
2	X	205	2AN	C10-C5	3.00	1.48	1.42
2	V	208	2AN	C10-C5	3.00	1.48	1.42
2	O	203	2AN	C10-C5	2.99	1.48	1.42
2	X	204	2AN	C9-C10	2.99	1.50	1.44
2	X	202	2AN	C9-C10	2.99	1.50	1.44
2	d	202	2AN	C9-C10	2.98	1.50	1.44
2	b	203	2AN	C9-C10	2.98	1.50	1.44
2	f	206	2AN	C9-C10	2.97	1.50	1.44
2	Y	201	2AN	C8-C9	2.96	1.41	1.37
2	D	202	2AN	C9-C10	2.96	1.50	1.44
2	E	203	2AN	C9-C10	2.96	1.50	1.44
2	d	202	2AN	C11-N	-2.95	1.34	1.40
2	R	201	2AN	O3-S	2.95	1.60	1.45
2	N	203	2AN	O3-S	2.95	1.60	1.45
2	C	202	2AN	C9-C10	2.95	1.50	1.44
2	g	202	2AN	C10-C5	2.94	1.48	1.42
2	j	202	2AN	C1-C10	2.94	1.46	1.43
2	c	205	2AN	C10-C5	2.93	1.48	1.42
2	B	204	2AN	C10-C5	2.93	1.48	1.42
2	D	201	2AN	O3-S	2.93	1.60	1.45
2	h	204	2AN	O3-S	2.93	1.60	1.45
2	Z	204	2AN	C9-C10	2.92	1.49	1.44
2	N	205	2AN	C11-N	-2.92	1.34	1.40
2	N	201	2AN	C6-C5	-2.92	1.35	1.42
2	Z	205	2AN	C10-C5	2.91	1.48	1.42
2	Z	204	2AN	C10-C5	2.90	1.48	1.42
2	h	206	2AN	C10-C5	2.88	1.48	1.42
2	b	202	2AN	C9-C10	2.88	1.49	1.44
2	H	204	2AN	C9-C10	2.87	1.49	1.44
2	T	203	2AN	C1-C10	2.86	1.46	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	P	202	2AN	C10-C5	2.86	1.48	1.42
2	R	202	2AN	C6-C5	-2.86	1.35	1.42
2	C	201	2AN	C9-C10	2.86	1.49	1.44
2	Y	203	2AN	C9-C10	2.86	1.49	1.44
2	X	206	2AN	C10-C5	2.86	1.48	1.42
2	f	203	2AN	C10-C5	2.85	1.48	1.42
2	V	207	2AN	C10-C5	2.85	1.48	1.42
2	C	202	2AN	C10-C5	2.85	1.48	1.42
2	D	202	2AN	C11-N	-2.84	1.34	1.40
2	j	207	2AN	C8-C9	2.84	1.41	1.37
2	A	204	2AN	C10-C5	2.84	1.48	1.42
2	e	201	2AN	C8-C9	2.84	1.41	1.37
2	Y	204	2AN	C11-N	-2.84	1.34	1.40
2	I	201	2AN	C1-C10	2.83	1.46	1.43
2	b	201	2AN	C11-N	-2.83	1.34	1.40
2	G	203	2AN	C11-N	-2.83	1.34	1.40
2	K	202	2AN	O3-S	2.83	1.60	1.45
2	B	206	2AN	C10-C5	2.83	1.48	1.42
2	H	202	2AN	C10-C5	2.83	1.48	1.42
2	U	201	2AN	C9-C10	2.83	1.49	1.44
2	I	203	2AN	C9-C10	2.83	1.49	1.44
2	V	205	2AN	O3-S	2.82	1.60	1.45
2	X	203	2AN	C10-C5	2.82	1.48	1.42
2	d	203	2AN	C10-C5	2.82	1.48	1.42
2	N	203	2AN	C9-C10	2.82	1.49	1.44
2	S	203	2AN	C10-C5	2.81	1.48	1.42
2	D	203	2AN	C10-C5	2.81	1.48	1.42
2	V	206	2AN	O3-S	2.81	1.60	1.45
2	a	202	2AN	O2-S	2.80	1.57	1.43
2	K	203	2AN	C10-C5	2.80	1.48	1.42
2	Y	202	2AN	C9-C10	2.80	1.49	1.44
2	j	203	2AN	C10-C5	2.80	1.48	1.42
2	F	203	2AN	C11-N	-2.80	1.34	1.40
2	A	201	2AN	C9-C10	2.80	1.49	1.44
2	S	201	2AN	C10-C5	2.80	1.48	1.42
2	N	204	2AN	C6-C5	-2.79	1.35	1.42
2	j	205	2AN	C11-N	-2.79	1.34	1.40
2	I	204	2AN	C9-C10	2.78	1.49	1.44
2	N	201	2AN	O3-S	2.78	1.59	1.45
2	g	202	2AN	O3-S	2.78	1.59	1.45
2	F	206	2AN	C11-N	-2.78	1.34	1.40
2	P	204	2AN	C9-C10	2.77	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	T	201	2AN	C8-C9	2.76	1.41	1.37
2	G	204	2AN	C10-C5	2.76	1.48	1.42
2	R	203	2AN	C9-C10	2.76	1.49	1.44
2	D	204	2AN	C8-C9	2.75	1.41	1.37
2	V	203	2AN	C9-C10	2.75	1.49	1.44
2	H	201	2AN	O3-S	2.75	1.59	1.45
2	I	206	2AN	C8-C9	2.74	1.41	1.37
2	B	201	2AN	C10-C5	2.74	1.48	1.42
2	H	201	2AN	C10-C5	2.74	1.48	1.42
2	P	203	2AN	C6-C5	-2.73	1.36	1.42
2	a	203	2AN	C11-N	-2.73	1.34	1.40
2	G	205	2AN	C9-C10	2.72	1.49	1.44
2	G	203	2AN	O1-S	2.71	1.56	1.43
2	G	203	2AN	C4-C5	-2.70	1.36	1.42
2	V	204	2AN	C11-N	-2.70	1.34	1.40
2	f	204	2AN	O3-S	2.70	1.59	1.45
2	I	206	2AN	C11-N	-2.70	1.34	1.40
2	L	201	2AN	O3-S	2.70	1.59	1.45
2	J	203	2AN	C10-C5	2.70	1.48	1.42
2	f	202	2AN	C9-C10	2.69	1.49	1.44
2	Z	202	2AN	C9-C10	2.68	1.49	1.44
2	f	204	2AN	C12-C11	-2.68	1.34	1.39
2	T	201	2AN	C11-N	-2.68	1.35	1.40
2	F	204	2AN	C10-C5	2.68	1.48	1.42
2	B	203	2AN	C1-C10	2.68	1.46	1.43
2	h	205	2AN	C8-C9	2.67	1.40	1.37
2	M	203	2AN	C11-N	-2.67	1.35	1.40
2	F	205	2AN	C10-C5	2.66	1.47	1.42
2	V	203	2AN	C10-C5	2.66	1.47	1.42
2	T	203	2AN	C10-C5	2.66	1.47	1.42
2	N	201	2AN	C11-N	-2.66	1.35	1.40
2	j	203	2AN	O2-S	2.66	1.56	1.43
2	V	206	2AN	C9-C10	2.66	1.49	1.44
2	G	207	2AN	C8-C9	2.65	1.40	1.37
2	h	204	2AN	C4-C5	-2.65	1.36	1.42
2	I	201	2AN	C4-C5	-2.64	1.36	1.42
2	b	203	2AN	C11-N	-2.64	1.35	1.40
2	Q	202	2AN	C10-C5	2.64	1.47	1.42
2	f	204	2AN	C11-N	-2.64	1.35	1.40
2	a	204	2AN	C10-C5	2.64	1.47	1.42
2	L	204	2AN	C8-C9	2.63	1.40	1.37
2	f	201	2AN	O2-S	2.63	1.56	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	203	2AN	C4-C5	-2.63	1.36	1.42
2	Q	202	2AN	C11-N	-2.61	1.35	1.40
2	G	204	2AN	C9-C10	2.61	1.49	1.44
2	T	205	2AN	C8-C9	2.60	1.40	1.37
2	I	202	2AN	C10-C5	2.60	1.47	1.42
2	R	201	2AN	C9-C10	2.60	1.49	1.44
2	F	206	2AN	C10-C5	2.60	1.47	1.42
2	T	201	2AN	C4-C5	-2.59	1.36	1.42
2	V	202	2AN	C10-C5	2.59	1.47	1.42
2	N	201	2AN	C4-C5	-2.59	1.36	1.42
2	f	201	2AN	C9-C10	2.59	1.49	1.44
2	E	202	2AN	C6-C5	-2.58	1.36	1.42
2	F	201	2AN	C10-C5	2.58	1.47	1.42
2	M	201	2AN	C9-C10	2.58	1.49	1.44
2	g	202	2AN	C6-C5	-2.57	1.36	1.42
2	E	201	2AN	C9-C10	2.57	1.49	1.44
2	I	203	2AN	C8-C9	2.57	1.40	1.37
2	a	201	2AN	C10-C5	2.56	1.47	1.42
2	V	205	2AN	C10-C5	2.56	1.47	1.42
2	B	205	2AN	C10-C5	2.56	1.47	1.42
2	D	201	2AN	C9-C10	2.55	1.49	1.44
2	d	204	2AN	C10-C5	2.55	1.47	1.42
2	R	205	2AN	C8-C9	2.54	1.40	1.37
6	a	205	FLC	CB-CBC	-2.54	1.50	1.53
2	I	202	2AN	C9-C10	2.54	1.49	1.44
2	R	202	2AN	O2-S	2.53	1.56	1.43
2	B	201	2AN	C11-N	-2.53	1.35	1.40
2	g	201	2AN	C10-C5	2.53	1.47	1.42
2	F	201	2AN	C9-C10	2.51	1.49	1.44
2	R	201	2AN	C10-C5	2.51	1.47	1.42
2	B	204	2AN	C9-C10	2.51	1.49	1.44
2	H	203	2AN	C10-C5	2.51	1.47	1.42
2	j	201	2AN	C11-N	-2.51	1.35	1.40
2	Z	206	2AN	C11-N	-2.50	1.35	1.40
2	i	201	2AN	C9-C10	2.49	1.49	1.44
2	f	201	2AN	C10-C5	2.49	1.47	1.42
2	M	202	2AN	C10-C5	2.48	1.47	1.42
2	S	203	2AN	C9-C10	2.48	1.49	1.44
2	f	203	2AN	C11-N	-2.47	1.35	1.40
2	Q	201	2AN	C10-C5	2.47	1.47	1.42
2	Y	204	2AN	C10-C5	2.47	1.47	1.42
2	d	203	2AN	C11-N	-2.47	1.35	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	X	203	2AN	C11-N	-2.46	1.35	1.40
2	b	204	2AN	C11-N	-2.46	1.35	1.40
2	D	201	2AN	C4-C5	-2.46	1.36	1.42
2	X	206	2AN	C11-N	-2.45	1.35	1.40
2	b	206	2AN	C8-C9	2.45	1.40	1.37
2	X	203	2AN	C9-C10	2.45	1.49	1.44
2	f	201	2AN	C7-C8	2.45	1.43	1.38
2	X	206	2AN	C9-C10	2.45	1.49	1.44
2	g	201	2AN	C8-C9	2.45	1.40	1.37
2	V	207	2AN	C11-N	-2.45	1.35	1.40
2	O	201	2AN	C11-N	-2.44	1.35	1.40
2	j	204	2AN	C11-N	-2.44	1.35	1.40
2	A	204	2AN	C11-N	-2.44	1.35	1.40
2	d	203	2AN	C9-C10	2.43	1.49	1.44
2	P	202	2AN	C8-C9	-2.43	1.34	1.37
2	R	201	2AN	C4-C5	-2.43	1.36	1.42
2	f	203	2AN	C9-C10	2.42	1.48	1.44
2	R	203	2AN	C10-C5	2.42	1.47	1.42
2	f	205	2AN	C1-C10	2.42	1.46	1.43
2	V	207	2AN	C9-C10	2.42	1.48	1.44
2	c	204	2AN	C6-C5	-2.41	1.36	1.42
2	E	202	2AN	C1-C10	2.41	1.46	1.43
2	G	204	2AN	C8-C9	2.40	1.40	1.37
2	H	203	2AN	C4-C5	-2.40	1.36	1.42
2	P	204	2AN	C8-C9	-2.40	1.34	1.37
2	B	203	2AN	C6-C5	-2.39	1.36	1.42
2	X	201	2AN	C4-C5	-2.39	1.36	1.42
2	D	203	2AN	C6-C5	-2.39	1.36	1.42
2	b	205	2AN	C8-C9	2.39	1.40	1.37
2	L	201	2AN	C9-C10	2.39	1.48	1.44
2	c	202	2AN	C8-C9	2.38	1.40	1.37
2	L	203	2AN	C9-C10	2.38	1.48	1.44
2	H	201	2AN	C11-N	-2.38	1.35	1.40
2	D	202	2AN	C10-C5	2.38	1.47	1.42
2	L	202	2AN	C8-C9	2.37	1.40	1.37
2	A	204	2AN	C9-C10	2.37	1.48	1.44
2	N	204	2AN	C10-C5	2.36	1.47	1.42
2	j	203	2AN	C6-C5	-2.36	1.36	1.42
2	a	202	2AN	C10-C5	2.36	1.47	1.42
2	d	204	2AN	C11-N	-2.36	1.35	1.40
2	F	203	2AN	C1-C10	2.34	1.46	1.43
2	T	205	2AN	C11-N	-2.34	1.35	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	h	202	2AN	C10-C5	2.34	1.47	1.42
2	W	201	2AN	C8-C9	2.34	1.40	1.37
2	N	202	2AN	C6-C5	-2.33	1.36	1.42
2	c	201	2AN	C1-N	-2.33	1.31	1.38
2	X	202	2AN	C10-C5	2.33	1.47	1.42
2	c	201	2AN	C1-C10	2.33	1.46	1.43
2	b	201	2AN	C10-C5	2.33	1.47	1.42
2	G	201	2AN	C6-C5	-2.32	1.36	1.42
2	c	204	2AN	C10-C5	2.32	1.47	1.42
2	H	204	2AN	C8-C9	2.32	1.40	1.37
2	V	205	2AN	C4-C5	-2.32	1.36	1.42
2	j	202	2AN	C9-C10	2.32	1.48	1.44
2	j	206	2AN	C9-C10	2.32	1.48	1.44
2	R	203	2AN	C6-C5	-2.32	1.36	1.42
2	S	204	2AN	C1-N	-2.31	1.31	1.38
6	i	203	FLC	OB1-CBC	2.31	1.29	1.22
2	A	201	2AN	C6-C5	-2.31	1.37	1.42
2	H	203	2AN	C11-N	-2.31	1.35	1.40
2	M	203	2AN	C8-C9	2.30	1.40	1.37
2	A	201	2AN	C10-C5	2.30	1.47	1.42
2	P	201	2AN	C9-C10	2.30	1.48	1.44
2	I	202	2AN	C6-C5	-2.30	1.37	1.42
2	N	202	2AN	C4-C5	-2.30	1.37	1.42
2	j	204	2AN	C1-N	-2.30	1.31	1.38
2	I	205	2AN	C8-C9	2.30	1.40	1.37
2	I	204	2AN	C8-C9	2.29	1.40	1.37
2	L	202	2AN	C10-C5	2.29	1.47	1.42
2	d	201	2AN	C4-C5	-2.29	1.37	1.42
2	e	201	2AN	C11-N	-2.29	1.35	1.40
2	V	205	2AN	C8-C9	2.28	1.40	1.37
2	Q	203	2AN	C8-C9	2.28	1.40	1.37
2	B	206	2AN	C3-C4	2.27	1.41	1.36
2	Z	201	2AN	C11-N	-2.27	1.35	1.40
2	g	203	2AN	C11-N	-2.27	1.35	1.40
2	g	201	2AN	C4-C5	-2.26	1.37	1.42
2	U	202	2AN	C10-C5	2.26	1.47	1.42
2	c	203	2AN	C9-C10	2.26	1.48	1.44
2	M	202	2AN	C6-C5	-2.26	1.37	1.42
2	Y	202	2AN	C11-N	-2.25	1.35	1.40
2	f	204	2AN	C8-C9	2.25	1.40	1.37
2	M	202	2AN	C4-C5	-2.24	1.37	1.42
2	H	202	2AN	C9-C10	2.24	1.48	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	205	2AN	C9-C10	2.24	1.48	1.44
2	a	201	2AN	C9-C10	2.24	1.48	1.44
2	h	203	2AN	C4-C5	-2.23	1.37	1.42
2	h	202	2AN	C4-C5	-2.23	1.37	1.42
2	B	205	2AN	C9-C10	2.23	1.48	1.44
2	j	205	2AN	C4-C5	-2.22	1.37	1.42
2	X	201	2AN	C8-C9	2.22	1.40	1.37
2	N	204	2AN	C11-N	-2.22	1.36	1.40
2	K	201	2AN	C6-C5	-2.22	1.37	1.42
2	G	203	2AN	C6-C5	-2.21	1.37	1.42
2	V	203	2AN	C4-C5	-2.21	1.37	1.42
2	j	203	2AN	C4-C5	-2.21	1.37	1.42
2	f	204	2AN	C4-C5	-2.21	1.37	1.42
2	X	205	2AN	C8-C9	2.21	1.40	1.37
2	J	201	2AN	C4-C5	-2.20	1.37	1.42
2	c	201	2AN	C11-N	-2.20	1.36	1.40
2	S	204	2AN	C11-N	-2.20	1.36	1.40
2	h	202	2AN	C11-N	-2.19	1.36	1.40
6	i	202	FLC	CB-CBC	-2.19	1.51	1.53
2	Z	202	2AN	C8-C9	2.19	1.40	1.37
2	B	201	2AN	C4-C5	-2.18	1.37	1.42
2	D	202	2AN	C6-C5	-2.18	1.37	1.42
2	B	202	2AN	C4-C5	-2.17	1.37	1.42
2	P	202	2AN	C6-C5	-2.17	1.37	1.42
2	A	202	2AN	C11-N	-2.17	1.36	1.40
2	C	201	2AN	C8-C9	2.17	1.40	1.37
2	P	202	2AN	C12-C11	-2.17	1.35	1.39
2	f	204	2AN	C15-C14	-2.17	1.33	1.38
2	A	202	2AN	C4-C5	-2.17	1.37	1.42
2	N	205	2AN	C7-C6	2.16	1.41	1.36
2	Z	203	2AN	C8-C9	2.16	1.40	1.37
2	c	206	2AN	C8-C9	-2.16	1.34	1.37
2	T	201	2AN	C9-C10	2.16	1.48	1.44
2	N	203	2AN	C16-C11	-2.15	1.35	1.39
2	V	205	2AN	C6-C5	-2.15	1.37	1.42
2	a	203	2AN	C8-C9	2.14	1.40	1.37
6	i	202	FLC	OG2-CGC	-2.14	1.23	1.30
2	M	203	2AN	C1-N	-2.14	1.32	1.38
2	J	202	2AN	C1-N	-2.14	1.32	1.38
2	R	202	2AN	C9-C10	2.13	1.48	1.44
2	V	205	2AN	C11-N	-2.13	1.36	1.40
2	Y	202	2AN	C4-C5	-2.13	1.37	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	V	208	2AN	C3-C2	-2.13	1.35	1.38
2	g	203	2AN	C4-C5	-2.12	1.37	1.42
2	R	205	2AN	C9-C10	2.12	1.48	1.44
2	g	203	2AN	C9-C10	2.12	1.48	1.44
2	C	201	2AN	C10-C5	2.11	1.46	1.42
2	g	201	2AN	C9-C10	2.11	1.48	1.44
2	g	203	2AN	C1-N	-2.11	1.32	1.38
2	a	201	2AN	C4-C5	-2.11	1.37	1.42
2	V	201	2AN	C11-N	-2.11	1.36	1.40
2	V	201	2AN	C8-C9	2.11	1.40	1.37
2	V	204	2AN	C9-C10	2.11	1.48	1.44
2	b	203	2AN	C4-C5	-2.10	1.37	1.42
2	U	202	2AN	C9-C10	2.10	1.48	1.44
2	F	206	2AN	C9-C10	2.10	1.48	1.44
2	T	202	2AN	C10-C5	2.09	1.46	1.42
2	c	205	2AN	C11-N	-2.09	1.36	1.40
2	f	205	2AN	C10-C5	2.09	1.46	1.42
2	A	201	2AN	C11-N	-2.09	1.36	1.40
2	C	202	2AN	C11-N	-2.08	1.36	1.40
2	G	202	2AN	C4-C5	-2.08	1.37	1.42
2	T	203	2AN	C11-N	-2.07	1.36	1.40
2	H	201	2AN	C9-C10	2.07	1.48	1.44
2	j	203	2AN	C9-C10	2.06	1.48	1.44
2	F	203	2AN	C10-C5	2.06	1.46	1.42
2	c	206	2AN	C6-C5	-2.06	1.37	1.42
2	V	203	2AN	C7-C6	2.05	1.41	1.36
2	K	202	2AN	C4-C5	-2.05	1.37	1.42
2	P	202	2AN	C1-C10	2.05	1.45	1.43
2	V	202	2AN	C4-C5	-2.05	1.37	1.42
2	Q	201	2AN	C11-N	-2.05	1.36	1.40
2	D	201	2AN	C11-N	-2.04	1.36	1.40
2	K	201	2AN	C11-N	-2.04	1.36	1.40
2	Y	201	2AN	C4-C5	-2.04	1.37	1.42
2	K	203	2AN	C9-C10	2.04	1.48	1.44
2	E	201	2AN	C11-N	-2.04	1.36	1.40
2	c	205	2AN	C9-C10	2.04	1.48	1.44
2	L	201	2AN	C11-N	-2.04	1.36	1.40
2	e	201	2AN	O3-S	2.04	1.56	1.45
2	S	204	2AN	C4-C5	-2.03	1.37	1.42
2	V	202	2AN	C11-N	-2.03	1.36	1.40
2	Z	205	2AN	C11-N	-2.03	1.36	1.40
2	A	202	2AN	C8-C9	2.03	1.40	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	T	201	2AN	C10-C5	2.03	1.46	1.42
2	M	201	2AN	C4-C5	-2.03	1.37	1.42
2	j	206	2AN	C8-C9	2.03	1.40	1.37
2	Y	203	2AN	C11-N	-2.02	1.36	1.40
2	X	202	2AN	C7-C6	2.02	1.41	1.36
2	P	203	2AN	C9-C10	2.02	1.48	1.44
2	P	203	2AN	C4-C5	-2.02	1.37	1.42
2	R	202	2AN	C7-C8	-2.02	1.35	1.38
2	G	202	2AN	C10-C5	2.02	1.46	1.42
2	S	204	2AN	C6-C5	-2.02	1.37	1.42
2	a	203	2AN	C4-C5	-2.02	1.37	1.42
2	E	204	2AN	C1-N	-2.01	1.32	1.38
2	U	201	2AN	C4-C5	-2.01	1.37	1.42
2	j	204	2AN	C10-C5	2.01	1.46	1.42
2	R	202	2AN	C1-N	-2.01	1.32	1.38

All (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
2	N	204	2AN	C2-C1-C10	-6.93	113.79	120.21
2	S	201	2AN	C11-N-C1	-6.83	111.45	126.36
2	D	204	2AN	C11-N-C1	-6.79	111.56	126.36
2	T	203	2AN	C2-C1-C10	-6.54	114.15	120.21
2	T	205	2AN	C2-C1-C10	-6.37	114.32	120.21
2	M	203	2AN	C11-N-C1	-6.36	112.49	126.36
2	Q	203	2AN	C11-N-C1	-6.33	112.56	126.36
6	j	208	FLC	OHB-CB-CBC	-6.30	100.03	108.96
2	d	204	2AN	C10-C1-N	6.23	129.48	120.39
2	a	201	2AN	C11-N-C1	-6.20	112.85	126.36
2	V	208	2AN	C11-N-C1	6.19	139.86	126.36
2	N	203	2AN	C1-C10-C5	-6.16	110.68	118.91
2	N	203	2AN	C11-N-C1	-6.09	113.08	126.36
6	i	203	FLC	OHB-CB-CBC	5.79	117.16	108.96
2	g	203	2AN	C11-N-C1	-5.64	114.06	126.36
2	d	204	2AN	C11-N-C1	-5.59	114.16	126.36
2	d	202	2AN	C2-C1-C10	-5.48	115.14	120.21
2	h	204	2AN	C2-C1-C10	-5.48	115.14	120.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Z	205	2AN	C2-C1-C10	-5.47	115.15	120.21
2	I	206	2AN	C11-N-C1	-5.46	114.44	126.36
2	g	201	2AN	C2-C1-C10	-5.46	115.16	120.21
6	e	202	FLC	OHB-CB-CBC	-5.45	101.23	108.96
2	Z	202	2AN	C2-C1-C10	-5.40	115.21	120.21
2	V	206	2AN	C2-C1-C10	-5.31	115.30	120.21
2	G	202	2AN	C11-N-C1	-5.28	114.84	126.36
2	V	208	2AN	C1-C10-C5	-5.26	111.88	118.91
2	T	202	2AN	C2-C1-C10	-5.22	115.38	120.21
2	O	201	2AN	C10-C1-N	-5.14	112.89	120.39
2	U	202	2AN	C11-N-C1	-5.13	115.17	126.36
2	M	202	2AN	C2-C1-C10	-5.13	115.46	120.21
2	W	201	2AN	O2-S-C9	5.12	121.22	106.37
2	M	202	2AN	C11-N-C1	-5.04	115.37	126.36
2	K	203	2AN	C2-C1-C10	-5.03	115.55	120.21
2	X	202	2AN	C10-C1-N	-5.03	113.05	120.39
2	H	204	2AN	C2-C1-C10	-4.99	115.59	120.21
2	j	202	2AN	C2-C1-C10	-4.97	115.61	120.21
2	h	202	2AN	O2-S-C9	4.90	120.56	106.37
2	c	201	2AN	C11-N-C1	-4.87	115.74	126.36
2	K	201	2AN	O2-S-C9	4.83	120.36	106.37
2	D	201	2AN	C2-C1-C10	-4.83	115.74	120.21
2	S	204	2AN	C2-C1-N	-4.83	111.26	123.47
2	V	202	2AN	C2-C1-C10	-4.81	115.76	120.21
2	J	203	2AN	C11-N-C1	-4.78	115.93	126.36
2	I	201	2AN	C2-C1-C10	-4.78	115.79	120.21
2	Y	201	2AN	C13-C12-C11	4.77	125.23	119.73
2	D	203	2AN	O2-S-C9	4.75	120.13	106.37
2	X	201	2AN	C2-C1-C10	-4.66	115.90	120.21
2	Z	206	2AN	C11-N-C1	-4.62	116.28	126.36
2	P	202	2AN	C2-C1-C10	-4.62	115.94	120.21
2	h	203	2AN	O3-S-O2	-4.60	90.19	111.55
2	E	203	2AN	C2-C1-C10	-4.58	115.97	120.21
2	d	204	2AN	C2-C1-N	-4.57	111.90	123.47
2	d	201	2AN	O1-S-C9	4.55	119.56	106.37
2	L	203	2AN	C2-C1-C10	-4.54	116.01	120.21
2	Y	203	2AN	C2-C1-C10	-4.53	116.02	120.21
2	j	205	2AN	C2-C1-C10	-4.51	116.03	120.21
2	a	203	2AN	C2-C1-C10	-4.49	116.06	120.21
2	S	204	2AN	C10-C1-N	4.48	126.94	120.39
2	b	205	2AN	C2-C1-C10	-4.42	116.12	120.21
2	j	204	2AN	O1-S-C9	4.37	119.04	106.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	X	204	2AN	C2-C1-C10	-4.34	116.19	120.21
2	a	201	2AN	C2-C1-C10	-4.33	116.21	120.21
2	f	201	2AN	C10-C1-N	4.31	126.69	120.39
2	j	201	2AN	O1-S-C9	-4.27	94.01	106.37
2	i	201	2AN	C2-C1-C10	-4.24	116.29	120.21
2	j	202	2AN	O2-S-O1	-4.22	91.65	112.88
2	V	201	2AN	O1-S-C9	-4.21	94.18	106.37
2	L	204	2AN	C2-C1-C10	-4.20	116.32	120.21
2	V	205	2AN	C2-C1-C10	-4.19	116.33	120.21
2	j	202	2AN	C3-C2-C1	4.19	126.66	120.05
2	E	203	2AN	C7-C8-C9	4.17	125.01	120.37
2	g	202	2AN	C2-C1-C10	-4.16	116.36	120.21
2	M	201	2AN	C10-C1-N	4.15	126.44	120.39
2	M	201	2AN	C15-C16-C11	4.14	124.51	119.73
2	T	204	2AN	C2-C1-C10	-4.14	116.38	120.21
2	B	201	2AN	C7-C8-C9	4.13	124.97	120.37
2	c	204	2AN	C2-C1-C10	-4.13	116.39	120.21
2	N	201	2AN	C11-N-C1	-4.13	117.36	126.36
2	B	201	2AN	C2-C1-C10	-4.11	116.40	120.21
2	O	202	2AN	C2-C1-C10	-4.08	116.43	120.21
2	S	201	2AN	C2-C1-N	-4.08	113.15	123.47
2	f	204	2AN	C2-C1-C10	-4.07	116.45	120.21
2	a	201	2AN	C10-C1-N	4.04	126.29	120.39
2	Q	201	2AN	C10-C1-N	4.03	126.28	120.39
2	B	203	2AN	C2-C1-C10	-4.00	116.50	120.21
2	B	204	2AN	C2-C1-C10	-4.00	116.50	120.21
2	f	201	2AN	C13-C12-C11	4.00	124.34	119.73
2	Y	201	2AN	C10-C1-N	4.00	126.23	120.39
2	N	202	2AN	O1-S-C9	3.99	117.93	106.37
2	M	201	2AN	C16-C11-C12	-3.98	113.76	119.04
2	h	205	2AN	C2-C1-C10	-3.96	116.55	120.21
6	i	203	FLC	OB2-CBC-CB	3.95	120.73	113.14
2	R	205	2AN	C2-C1-C10	-3.92	116.58	120.21
2	j	203	2AN	C13-C12-C11	3.92	124.25	119.73
2	Z	204	2AN	C2-C1-C10	-3.92	116.58	120.21
2	F	206	2AN	C10-C1-N	3.90	126.08	120.39
2	T	201	2AN	O2-S-C9	3.89	117.63	106.37
2	D	204	2AN	C1-C10-C5	-3.88	113.72	118.91
2	H	203	2AN	C2-C1-C10	-3.88	116.62	120.21
2	j	206	2AN	C2-C1-C10	-3.88	116.62	120.21
2	g	202	2AN	C7-C8-C9	3.87	124.67	120.37
2	j	205	2AN	C11-N-C1	-3.86	117.94	126.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	U	201	2AN	C2-C1-C10	-3.85	116.64	120.21
2	P	203	2AN	O1-S-C9	3.84	117.50	106.37
2	G	204	2AN	C2-C1-C10	-3.84	116.66	120.21
2	f	201	2AN	C2-C1-N	-3.84	113.76	123.47
2	T	205	2AN	C11-N-C1	-3.80	118.07	126.36
2	Q	201	2AN	C2-C1-N	-3.77	113.92	123.47
2	F	205	2AN	O1-S-C9	3.76	117.26	106.37
2	e	201	2AN	O1-S-C9	3.74	117.22	106.37
2	b	206	2AN	C11-N-C1	-3.74	118.20	126.36
2	h	203	2AN	C8-C9-C10	-3.74	114.50	120.18
2	F	202	2AN	C2-C1-N	-3.72	114.06	123.47
2	Z	203	2AN	O2-S-C9	3.72	117.14	106.37
2	B	201	2AN	C10-C1-N	3.71	125.80	120.39
2	G	205	2AN	C10-C1-N	-3.70	114.98	120.39
2	D	204	2AN	C2-C1-N	-3.70	114.10	123.47
2	S	202	2AN	C10-C1-N	3.70	125.79	120.39
2	T	205	2AN	C3-C2-C1	3.65	125.81	120.05
2	M	201	2AN	C15-C14-C13	-3.64	114.88	119.87
6	G	206	FLC	OHB-CB-CBC	3.63	114.11	108.96
2	V	208	2AN	C6-C5-C4	-3.62	114.75	123.01
2	C	203[A]	2AN	C11-N-C1	3.62	134.26	126.36
2	f	202	2AN	C2-C1-C10	-3.61	116.87	120.21
2	P	203	2AN	C10-C1-N	-3.60	115.13	120.39
2	H	202	2AN	C2-C1-C10	-3.60	116.88	120.21
2	P	202	2AN	O1-S-C9	3.60	116.79	106.37
2	K	201	2AN	C8-C9-C10	-3.59	114.72	120.18
2	X	201	2AN	C15-C16-C11	3.59	123.86	119.73
2	f	205	2AN	O1-S-C9	3.58	116.75	106.37
2	M	202	2AN	C13-C12-C11	3.56	123.83	119.73
2	i	201	2AN	C7-C8-C9	3.55	124.32	120.37
6	i	203	FLC	OB1-CBC-CB	-3.55	115.22	122.09
2	M	201	2AN	C2-C1-C10	-3.54	116.93	120.21
2	V	204	2AN	C2-C1-C10	-3.54	116.94	120.21
2	S	202	2AN	C2-C1-C10	-3.53	116.94	120.21
2	j	201	2AN	O2-S-C9	3.51	116.55	106.37
2	Y	201	2AN	C16-C11-C12	-3.50	114.39	119.04
2	I	206	2AN	O2-S-C9	3.50	116.51	106.37
2	N	205	2AN	O2-S-C9	3.50	116.50	106.37
2	A	202	2AN	C2-C1-C10	-3.49	116.98	120.21
2	A	202	2AN	C10-C1-N	3.49	125.48	120.39
2	F	202	2AN	C10-C1-N	3.48	125.47	120.39
2	L	203	2AN	C11-N-C1	-3.48	118.77	126.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	203	2AN	C2-C1-C10	-3.48	116.99	120.21
2	h	206	2AN	C15-C16-C11	3.45	123.71	119.73
2	R	203	2AN	C10-C1-N	-3.45	115.36	120.39
2	F	206	2AN	C2-C1-C10	-3.45	117.02	120.21
2	P	202	2AN	C7-C8-C9	3.44	124.20	120.37
2	X	205	2AN	C2-C1-C10	-3.44	117.03	120.21
2	N	205	2AN	C10-C1-N	-3.43	115.38	120.39
2	E	201	2AN	O1-S-C9	3.42	116.29	106.37
6	j	208	FLC	CB-CA-CAC	-3.42	104.56	113.92
2	j	204	2AN	O2-S-C9	-3.42	96.45	106.37
2	c	204	2AN	O2-S-C9	3.42	116.27	106.37
2	V	208	2AN	C3-C2-C1	3.42	125.45	120.05
2	f	202	2AN	C11-N-C1	-3.42	118.91	126.36
2	B	205	2AN	O2-S-C9	3.41	116.25	106.37
2	h	203	2AN	C7-C8-C9	3.41	124.17	120.37
2	Z	201	2AN	C1-C10-C5	-3.41	114.35	118.91
2	C	203[A]	2AN	C10-C1-N	3.41	125.36	120.39
2	N	203	2AN	C7-C6-C5	3.39	125.20	120.48
2	c	203	2AN	C2-C1-C10	-3.39	117.08	120.21
2	Z	206	2AN	C2-C1-N	-3.36	114.96	123.47
2	F	202	2AN	C11-N-C1	-3.36	119.03	126.36
2	F	202	2AN	O1-S-C9	3.36	116.10	106.37
2	P	204	2AN	C1-C10-C5	-3.36	114.42	118.91
2	a	201	2AN	C2-C1-N	-3.35	114.98	123.47
2	F	202	2AN	C7-C8-C9	3.35	124.10	120.37
2	L	201	2AN	C13-C12-C11	3.32	123.56	119.73
2	O	203	2AN	O2-S-C9	3.32	115.99	106.37
2	N	205	2AN	C2-C1-C10	-3.31	117.15	120.21
2	P	204	2AN	C2-C1-N	-3.30	115.11	123.47
6	G	206	FLC	OHB-CB-CG	-3.30	101.84	109.38
2	C	201	2AN	C2-C1-N	-3.29	115.14	123.47
2	F	206	2AN	C2-C1-N	-3.29	115.15	123.47
2	G	203	2AN	C10-C1-N	-3.28	115.60	120.39
6	j	208	FLC	CG-CB-CA	3.28	117.72	109.31
2	N	203	2AN	C2-C1-N	-3.28	115.18	123.47
2	Z	203	2AN	C2-C1-C10	-3.27	117.18	120.21
2	g	203	2AN	C2-C1-N	-3.27	115.19	123.47
2	C	203[A]	2AN	C2-C1-C10	-3.27	117.19	120.21
2	Y	201	2AN	C6-C5-C4	-3.26	115.56	123.01
4	P	205	EPE	C5-N4-C3	3.26	115.87	108.84
2	I	204	2AN	C13-C12-C11	3.26	123.49	119.73
2	b	206	2AN	C2-C1-N	-3.26	115.22	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	204	2AN	C2-C1-C10	-3.25	117.20	120.21
2	c	202	2AN	C1-C10-C5	-3.24	114.58	118.91
6	G	206	FLC	OB2-CBC-CB	3.24	119.36	113.14
2	V	205	2AN	C8-C9-C10	-3.24	115.25	120.18
2	E	202	2AN	C11-N-C1	-3.24	119.30	126.36
2	h	202	2AN	O1-S-C9	3.22	115.71	106.37
2	I	201	2AN	C6-C5-C4	-3.22	115.66	123.01
2	S	202	2AN	C7-C8-C9	3.22	123.95	120.37
2	T	205	2AN	C10-C1-N	3.21	125.08	120.39
2	c	206	2AN	C7-C8-C9	3.21	123.94	120.37
2	L	203	2AN	O3-S-O2	-3.21	96.68	111.55
2	c	202	2AN	C2-C1-C10	-3.20	117.25	120.21
2	Q	201	2AN	C13-C12-C11	3.19	123.40	119.73
2	a	202	2AN	C2-C1-C10	-3.18	117.26	120.21
2	j	201	2AN	C2-C1-C10	-3.18	117.27	120.21
2	V	203	2AN	C8-C9-C10	-3.17	115.36	120.18
2	T	201	2AN	C2-C1-C10	-3.14	117.30	120.21
2	j	203	2AN	C11-N-C1	-3.14	119.50	126.36
2	Z	205	2AN	C10-C1-N	-3.14	115.80	120.39
2	I	205	2AN	C2-C1-C10	-3.14	117.30	120.21
2	T	205	2AN	C15-C16-C11	3.13	123.34	119.73
2	I	206	2AN	C2-C1-N	-3.13	115.55	123.47
2	j	203	2AN	C8-C9-C10	-3.13	115.42	120.18
2	a	204	2AN	C10-C1-N	-3.13	115.82	120.39
2	Y	201	2AN	C2-C1-C10	-3.13	117.32	120.21
2	Y	201	2AN	C1-C10-C5	-3.12	114.73	118.91
2	b	204	2AN	C2-C1-C10	-3.12	117.32	120.21
2	V	202	2AN	C3-C2-C1	3.12	124.97	120.05
2	L	203	2AN	C7-C8-C9	3.11	123.83	120.37
2	C	201	2AN	C11-N-C1	-3.11	119.58	126.36
2	e	201	2AN	C2-C1-C10	-3.11	117.33	120.21
2	a	201	2AN	C16-C11-C12	-3.10	114.92	119.04
2	F	201	2AN	C13-C12-C11	3.10	123.30	119.73
2	a	202	2AN	O1-S-C9	3.09	115.33	106.37
2	J	203	2AN	O1-S-C9	3.09	115.32	106.37
2	h	206	2AN	C11-N-C1	-3.07	119.67	126.36
2	N	205	2AN	C8-C9-C10	-3.07	115.52	120.18
2	j	207	2AN	C2-C1-C10	-3.06	117.38	120.21
2	N	202	2AN	C11-N-C1	-3.06	119.69	126.36
2	A	203	2AN	C2-C1-C10	-3.06	117.38	120.21
2	N	204	2AN	C3-C2-C1	3.05	124.87	120.05
2	V	206	2AN	O2-S-C9	3.05	115.21	106.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Q	203	2AN	C2-C1-N	-3.05	115.75	123.47
2	A	202	2AN	C11-N-C1	-3.04	119.72	126.36
2	f	206	2AN	C2-C1-C10	-3.04	117.40	120.21
2	g	201	2AN	C13-C12-C11	3.04	123.23	119.73
2	N	203	2AN	C4-C3-C2	-3.03	116.33	121.00
2	D	204	2AN	C10-C1-N	3.03	124.82	120.39
2	d	201	2AN	C2-C1-C10	-3.03	117.41	120.21
2	F	202	2AN	O3-S-O1	-3.03	97.51	111.55
2	F	203	2AN	C10-C1-N	-3.02	115.98	120.39
2	G	202	2AN	C2-C1-N	-3.02	115.82	123.47
2	I	201	2AN	C11-N-C1	-3.02	119.78	126.36
2	a	203	2AN	C10-C1-N	-3.02	115.99	120.39
2	V	202	2AN	C10-C1-N	3.02	124.79	120.39
2	V	205	2AN	C11-N-C1	-3.02	119.78	126.36
2	Z	206	2AN	C10-C1-N	3.02	124.79	120.39
2	P	202	2AN	C3-C2-C1	3.01	124.81	120.05
2	I	204	2AN	C2-C1-C10	-3.01	117.42	120.21
2	d	204	2AN	C2-C1-C10	-3.00	117.43	120.21
2	R	204	2AN	C1-C10-C5	-3.00	114.90	118.91
2	j	205	2AN	C8-C9-C10	-2.99	115.63	120.18
2	d	203	2AN	C11-N-C1	-2.99	119.84	126.36
2	V	203	2AN	C2-C1-C10	-2.99	117.45	120.21
2	i	201	2AN	C8-C9-C10	-2.98	115.64	120.18
2	f	206	2AN	C11-N-C1	-2.97	119.89	126.36
2	M	201	2AN	C13-C12-C11	2.96	123.14	119.73
2	S	201	2AN	C1-C10-C5	-2.95	114.96	118.91
2	c	202	2AN	C3-C2-C1	2.95	124.71	120.05
6	j	208	FLC	OA1-CAC-CA	-2.95	114.60	122.95
2	D	202	2AN	O2-S-C9	2.95	114.91	106.37
6	i	203	FLC	OG1-CGC-CG	-2.94	114.61	122.95
2	M	203	2AN	O2-S-C9	2.94	114.88	106.37
2	j	202	2AN	C7-C8-C9	2.94	123.64	120.37
2	I	207	2AN	C1-C10-C5	-2.93	114.99	118.91
2	f	203	2AN	C11-N-C1	-2.93	119.97	126.36
2	b	206	2AN	C10-C1-N	2.93	124.66	120.39
2	X	203	2AN	C11-N-C1	-2.92	119.99	126.36
2	X	206	2AN	C11-N-C1	-2.91	120.02	126.36
2	E	203	2AN	C8-C9-C10	-2.91	115.76	120.18
2	h	202	2AN	C2-C1-C10	-2.90	117.53	120.21
2	Y	201	2AN	C2-C1-N	-2.90	116.14	123.47
2	V	207	2AN	C11-N-C1	-2.89	120.05	126.36
2	V	208	2AN	C4-C5-C10	2.89	123.99	118.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	201	2AN	O1-S-C9	2.89	114.73	106.37
2	Y	202	2AN	O1-S-C9	2.89	114.73	106.37
2	D	203	2AN	C10-C1-N	-2.88	116.18	120.39
2	j	201	2AN	C7-C8-C9	2.88	123.58	120.37
2	Y	203	2AN	C7-C8-C9	2.87	123.57	120.37
2	M	202	2AN	C10-C1-N	2.87	124.58	120.39
2	E	204	2AN	C2-C1-N	-2.87	116.20	123.47
2	Q	202	2AN	C2-C1-C10	-2.87	117.56	120.21
2	c	201	2AN	C2-C1-C10	-2.86	117.56	120.21
2	A	202	2AN	C2-C1-N	-2.86	116.23	123.47
2	h	203	2AN	C1-C10-C5	-2.86	115.08	118.91
2	G	201	2AN	C8-C9-C10	-2.86	115.83	120.18
2	V	206	2AN	C8-C9-C10	-2.86	115.83	120.18
2	D	201	2AN	C7-C8-C9	2.86	123.55	120.37
2	h	206	2AN	C10-C1-N	2.85	124.56	120.39
2	f	201	2AN	C15-C14-C13	-2.85	115.97	119.87
2	F	201	2AN	C2-C1-C10	-2.85	117.57	120.21
2	H	203	2AN	O2-S-C9	2.85	114.61	106.37
2	S	204	2AN	C7-C8-C9	2.84	123.53	120.37
2	h	201	2AN	C2-C1-C10	-2.84	117.58	120.21
2	e	201	2AN	C3-C2-C1	2.84	124.53	120.05
2	P	204	2AN	C11-N-C1	-2.84	120.17	126.36
2	I	205	2AN	C16-C11-C12	-2.83	115.28	119.04
2	j	206	2AN	C10-C1-N	-2.83	116.25	120.39
2	H	202	2AN	C11-N-C1	-2.83	120.19	126.36
2	I	201	2AN	C10-C1-N	2.83	124.52	120.39
2	E	203	2AN	O1-S-C9	2.83	114.56	106.37
2	O	203	2AN	C13-C12-C11	2.82	122.98	119.73
2	L	202	2AN	C2-C1-C10	-2.82	117.60	120.21
2	d	201	2AN	O2-S-C9	2.82	114.53	106.37
2	V	201	2AN	O2-S-C9	2.82	114.53	106.37
2	K	201	2AN	C6-C7-C8	2.82	125.32	121.00
2	N	203	2AN	C13-C12-C11	2.82	122.97	119.73
2	I	207	2AN	C6-C5-C4	-2.81	116.60	123.01
2	Z	206	2AN	C2-C1-C10	-2.81	117.61	120.21
2	H	201	2AN	C8-C9-C10	-2.81	115.91	120.18
2	G	203	2AN	C7-C8-C9	-2.80	117.24	120.37
2	j	202	2AN	C8-C9-C10	-2.80	115.92	120.18
2	Q	202	2AN	O1-S-C9	2.80	114.49	106.37
2	T	203	2AN	O3-S-O2	-2.80	98.57	111.55
2	F	205	2AN	C2-C1-C10	-2.80	117.62	120.21
2	I	207	2AN	C2-C1-C10	-2.80	117.62	120.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	203	2AN	C3-C2-C1	2.79	124.46	120.05
2	c	202	2AN	C13-C12-C11	2.79	122.95	119.73
2	P	202	2AN	O3-S-O2	-2.79	98.60	111.55
2	F	205	2AN	C10-C1-N	-2.79	116.32	120.39
2	W	201	2AN	C2-C1-C10	-2.78	117.64	120.21
2	M	202	2AN	C3-C2-C1	2.78	124.44	120.05
2	G	205	2AN	C16-C11-N	-2.77	111.22	120.61
2	I	205	2AN	C13-C12-C11	2.76	122.92	119.73
2	B	201	2AN	C2-C1-N	-2.76	116.47	123.47
2	b	206	2AN	C1-C10-C5	-2.76	115.22	118.91
2	S	203	2AN	C2-C1-C10	-2.76	117.66	120.21
2	M	201	2AN	C2-C1-N	-2.75	116.50	123.47
2	T	202	2AN	C3-C2-C1	2.75	124.40	120.05
2	T	202	2AN	C13-C12-C11	2.75	122.90	119.73
2	e	201	2AN	C1-C10-C5	-2.74	115.25	118.91
2	V	206	2AN	C7-C8-C9	2.73	123.41	120.37
2	V	208	2AN	C16-C11-N	-2.73	111.36	120.61
2	c	203	2AN	C10-C1-N	-2.73	116.41	120.39
2	f	201	2AN	C7-C8-C9	2.73	123.41	120.37
2	b	205	2AN	C15-C16-C11	2.73	122.88	119.73
2	L	204	2AN	C15-C16-C11	2.72	122.87	119.73
2	c	204	2AN	O1-S-C9	2.72	114.25	106.37
2	S	202	2AN	C2-C1-N	-2.72	116.59	123.47
2	T	203	2AN	C8-C9-C10	-2.71	116.05	120.18
4	P	205	EPE	C5-C6-N1	-2.71	105.19	110.65
2	A	204	2AN	C11-N-C1	-2.70	120.47	126.36
2	Z	206	2AN	O1-S-C9	2.69	114.18	106.37
2	j	203	2AN	C7-C8-C9	2.69	123.37	120.37
2	A	202	2AN	C6-C5-C4	-2.69	116.87	123.01
2	S	202	2AN	C3-C2-C1	2.69	124.29	120.05
2	G	202	2AN	C10-C1-N	2.68	124.30	120.39
2	V	208	2AN	O3-S-O2	-2.68	99.12	111.55
2	E	202	2AN	C6-C5-C4	-2.68	116.90	123.01
2	H	201	2AN	C13-C12-C11	2.67	122.81	119.73
2	a	203	2AN	C8-C9-C10	-2.67	116.11	120.18
2	Y	202	2AN	C2-C1-C10	-2.67	117.74	120.21
2	K	201	2AN	C1-C10-C5	-2.67	115.34	118.91
2	Z	203	2AN	C8-C9-C10	-2.66	116.13	120.18
2	V	205	2AN	C7-C8-C9	2.66	123.33	120.37
2	F	206	2AN	C16-C11-N	-2.66	111.62	120.61
2	e	201	2AN	C8-C9-C10	-2.66	116.14	120.18
2	V	201	2AN	C2-C1-C10	-2.65	117.76	120.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	g	202	2AN	C6-C5-C4	-2.65	116.96	123.01
2	B	201	2AN	C15-C16-C11	2.65	122.78	119.73
2	B	201	2AN	C6-C5-C4	-2.65	116.97	123.01
2	j	205	2AN	O2-S-C9	2.64	114.03	106.37
2	Z	204	2AN	O2-S-C9	2.64	114.03	106.37
2	E	202	2AN	C7-C8-C9	2.64	123.31	120.37
2	E	203	2AN	C6-C5-C4	-2.64	116.99	123.01
2	T	203	2AN	C7-C8-C9	2.64	123.30	120.37
2	d	202	2AN	C3-C2-C1	2.64	124.22	120.05
2	F	202	2AN	C6-C5-C4	-2.64	117.00	123.01
2	h	206	2AN	C2-C1-N	-2.63	116.80	123.47
2	h	202	2AN	O2-S-O1	-2.63	99.63	112.88
2	E	204	2AN	O2-S-C9	2.63	113.99	106.37
2	C	201	2AN	C10-C1-N	2.63	124.23	120.39
2	c	202	2AN	C16-C11-C12	-2.63	115.56	119.04
2	Y	201	2AN	C7-C8-C9	2.62	123.29	120.37
2	A	201	2AN	C2-C1-C10	-2.62	117.78	120.21
2	Z	201	2AN	O2-S-O1	-2.62	99.70	112.88
2	V	203	2AN	C7-C6-C5	-2.62	116.84	120.48
2	C	202	2AN	C2-C1-C10	-2.62	117.79	120.21
2	V	206	2AN	C15-C16-C11	2.61	122.74	119.73
2	R	204	2AN	C3-C2-C1	2.61	124.18	120.05
2	b	202	2AN	C2-C1-C10	-2.61	117.80	120.21
2	Z	201	2AN	O2-S-C9	2.61	113.92	106.37
2	c	202	2AN	O1-S-C9	2.59	113.89	106.37
2	V	206	2AN	C3-C2-C1	2.59	124.15	120.05
2	g	201	2AN	C10-C1-N	2.59	124.17	120.39
2	G	207	2AN	C2-C1-C10	-2.59	117.81	120.21
4	P	205	EPE	O3S-S-C10	2.59	111.07	106.00
2	b	205	2AN	O1-S-C9	2.59	113.87	106.37
2	O	203	2AN	C8-C9-C10	-2.59	116.25	120.18
2	c	205	2AN	C11-N-C1	-2.58	120.73	126.36
2	C	201	2AN	O1-S-C9	2.58	113.85	106.37
2	O	201	2AN	C8-C9-C10	-2.58	116.25	120.18
2	I	203	2AN	C7-C8-C9	2.58	123.24	120.37
6	e	202	FLC	OHB-CB-CA	2.58	115.26	109.38
2	K	202	2AN	O2-S-C9	2.58	113.84	106.37
6	a	205	FLC	CG-CB-CBC	2.58	115.73	110.03
2	B	201	2AN	O1-S-C9	2.57	113.83	106.37
2	j	206	2AN	C11-N-C1	2.57	131.97	126.36
2	D	204	2AN	C8-C9-C10	-2.57	116.27	120.18
2	R	202	2AN	C10-C1-N	2.57	124.14	120.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	205	2AN	O1-S-C9	2.57	113.80	106.37
2	g	202	2AN	C3-C2-C1	2.56	124.10	120.05
2	Y	202	2AN	C7-C8-C9	2.56	123.21	120.37
2	V	205	2AN	O1-S-C9	2.55	113.77	106.37
2	L	204	2AN	C7-C8-C9	2.55	123.21	120.37
2	b	205	2AN	C16-C11-C12	-2.55	115.66	119.04
2	a	201	2AN	C15-C16-C11	2.55	122.67	119.73
2	K	201	2AN	C10-C1-N	-2.55	116.67	120.39
2	I	201	2AN	C3-C2-C1	2.55	124.07	120.05
2	Y	202	2AN	C8-C9-C10	-2.55	116.31	120.18
2	f	201	2AN	O2-S-C9	-2.54	99.00	106.37
2	Q	201	2AN	C11-N-C1	-2.54	120.82	126.36
2	c	202	2AN	C6-C5-C4	-2.54	117.22	123.01
2	D	204	2AN	C3-C2-C1	2.54	124.06	120.05
4	P	205	EPE	O3S-S-O1S	-2.54	105.05	111.40
2	N	204	2AN	C8-C9-C10	-2.54	116.32	120.18
2	E	202	2AN	O1-S-C9	2.54	113.72	106.37
2	R	204	2AN	C6-C5-C4	-2.54	117.23	123.01
2	i	201	2AN	C3-C2-C1	2.53	124.05	120.05
2	f	205	2AN	O2-S-C9	-2.53	99.03	106.37
2	a	202	2AN	C4-C5-C10	2.53	123.29	118.27
2	Q	203	2AN	C1-C10-C5	-2.53	115.53	118.91
2	L	203	2AN	C8-C9-C10	-2.53	116.33	120.18
2	B	204	2AN	C11-N-C1	2.52	131.86	126.36
2	V	202	2AN	C6-C5-C4	-2.52	117.27	123.01
2	T	204	2AN	C6-C5-C4	-2.52	117.27	123.01
2	V	201	2AN	C13-C12-C11	2.51	122.63	119.73
4	P	205	EPE	C2-C3-N4	2.51	115.71	110.65
2	P	201	2AN	C2-C1-C10	-2.50	117.89	120.21
2	B	201	2AN	C11-N-C1	-2.50	120.90	126.36
2	Y	204	2AN	C2-C1-C10	-2.50	117.89	120.21
2	A	203	2AN	C7-C8-C9	2.50	123.15	120.37
2	F	202	2AN	C8-C9-C10	-2.50	116.38	120.18
2	V	203	2AN	O1-S-C9	2.49	113.60	106.37
2	g	201	2AN	C16-C11-C12	-2.49	115.73	119.04
2	I	207	2AN	C10-C1-N	2.49	124.03	120.39
2	K	201	2AN	C9-C10-C5	2.49	121.33	115.98
2	P	202	2AN	C4-C5-C10	2.49	123.21	118.27
2	g	202	2AN	C10-C1-N	2.49	124.03	120.39
2	G	204	2AN	C13-C12-C11	2.49	122.60	119.73
2	G	202	2AN	C15-C16-C11	2.49	122.60	119.73
2	b	204	2AN	O1-S-C9	2.49	113.57	106.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	b	202	2AN	O2-S-C9	2.49	113.57	106.37
2	S	202	2AN	C6-C5-C4	-2.48	117.34	123.01
2	Z	206	2AN	C7-C8-C9	2.48	123.13	120.37
2	f	204	2AN	C15-C16-C11	2.48	122.59	119.73
2	P	202	2AN	C16-C11-N	-2.48	112.22	120.61
2	Y	201	2AN	C3-C2-C1	2.48	123.96	120.05
2	X	204	2AN	C13-C12-C11	2.48	122.58	119.73
2	R	204	2AN	C2-C1-C10	-2.47	117.92	120.21
2	T	205	2AN	C6-C5-C4	-2.47	117.38	123.01
2	M	203	2AN	C2-C1-N	-2.47	117.23	123.47
2	V	203	2AN	C7-C8-C9	2.46	123.11	120.37
2	A	201	2AN	C1-C10-C5	-2.46	115.62	118.91
2	Q	201	2AN	O2-S-C9	2.46	113.49	106.37
2	M	202	2AN	C7-C8-C9	2.46	123.10	120.37
2	A	202	2AN	C3-C2-C1	2.46	123.93	120.05
2	M	202	2AN	C6-C5-C4	-2.46	117.41	123.01
2	I	206	2AN	C1-C10-C5	-2.45	115.63	118.91
6	a	206	FLC	OB2-CBC-CB	2.45	117.84	113.14
2	Z	202	2AN	C15-C16-C11	2.45	122.55	119.73
2	Y	201	2AN	C16-C11-N	2.45	128.90	120.61
2	b	201	2AN	C14-C15-C16	2.44	123.25	120.24
2	a	202	2AN	C1-C10-C5	-2.44	115.64	118.91
6	a	205	FLC	CA-CB-CBC	-2.44	104.64	110.03
2	f	202	2AN	C3-C2-C1	2.44	123.90	120.05
2	B	205	2AN	C11-N-C1	-2.44	121.05	126.36
2	J	201	2AN	C2-C1-C10	-2.44	117.95	120.21
2	W	201	2AN	C13-C12-C11	2.43	122.53	119.73
2	D	204	2AN	C6-C5-C4	-2.43	117.47	123.01
2	L	204	2AN	O2-S-C9	2.43	113.40	106.37
6	a	206	FLC	OHB-CB-CBC	-2.43	105.52	108.96
2	A	201	2AN	C3-C2-C1	2.43	123.88	120.05
2	N	205	2AN	C7-C8-C9	2.43	123.07	120.37
2	L	203	2AN	C3-C2-C1	2.43	123.88	120.05
2	I	202	2AN	C13-C12-C11	2.42	122.52	119.73
2	E	202	2AN	C8-C9-C10	-2.42	116.50	120.18
2	j	203	2AN	C15-C14-C13	-2.42	116.56	119.87
2	h	206	2AN	O2-S-C9	2.41	113.36	106.37
2	F	206	2AN	C3-C2-C1	2.41	123.86	120.05
2	B	204	2AN	C3-C2-C1	2.41	123.85	120.05
2	j	205	2AN	C6-C7-C8	2.41	124.69	121.00
2	J	202	2AN	C11-N-C1	-2.40	121.12	126.36
2	P	203	2AN	O2-S-O1	-2.40	100.78	112.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	h	202	2AN	C7-C8-C9	2.40	123.04	120.37
2	f	205	2AN	C2-C1-C10	-2.40	117.99	120.21
2	V	202	2AN	C7-C8-C9	2.40	123.04	120.37
2	a	201	2AN	C6-C5-C4	-2.40	117.54	123.01
2	W	201	2AN	C7-C8-C9	2.40	123.04	120.37
2	I	207	2AN	C3-C2-C1	2.40	123.84	120.05
2	M	202	2AN	C8-C9-C10	-2.39	116.54	120.18
2	g	203	2AN	O2-S-C9	2.39	113.30	106.37
2	M	201	2AN	C6-C5-C10	2.39	123.00	118.27
2	d	201	2AN	O2-S-O1	-2.39	100.85	112.88
2	N	202	2AN	C2-C1-C10	-2.39	118.00	120.21
2	N	202	2AN	C4-C5-C10	2.39	123.00	118.27
2	F	202	2AN	C2-C1-C10	-2.39	118.00	120.21
2	j	204	2AN	C2-C1-C10	-2.39	118.00	120.21
2	W	201	2AN	O3-S-O2	-2.39	100.48	111.55
2	C	203[A]	2AN	C2-C1-N	-2.38	117.44	123.47
2	I	205	2AN	C10-C1-N	2.38	123.87	120.39
2	Y	201	2AN	O3-S-O1	-2.38	100.50	111.55
2	h	203	2AN	O2-S-C9	2.38	113.27	106.37
2	P	203	2AN	C8-C9-C10	-2.38	116.56	120.18
2	c	204	2AN	C3-C2-C1	2.38	123.81	120.05
2	I	201	2AN	O1-S-C9	2.38	113.25	106.37
2	R	202	2AN	C2-C1-N	-2.37	117.46	123.47
2	c	201	2AN	C2-C1-N	-2.37	117.47	123.47
2	a	202	2AN	C6-C5-C4	-2.36	117.62	123.01
2	h	206	2AN	C2-C1-C10	-2.36	118.02	120.21
2	S	202	2AN	C13-C12-C11	2.36	122.45	119.73
2	Z	201	2AN	C8-C9-C10	-2.36	116.59	120.18
2	H	202	2AN	C13-C12-C11	2.36	122.45	119.73
2	S	201	2AN	C10-C1-N	2.36	123.83	120.39
2	b	203	2AN	C2-C1-C10	-2.36	118.03	120.21
2	S	202	2AN	C1-C10-C5	-2.36	115.76	118.91
2	I	206	2AN	C10-C1-N	2.35	123.83	120.39
2	f	201	2AN	C6-C5-C10	2.35	122.93	118.27
2	L	204	2AN	C16-C11-C12	-2.35	115.92	119.04
6	G	206	FLC	CB-CG-CGC	-2.35	107.49	113.92
2	X	204	2AN	C3-C2-C1	2.35	123.76	120.05
2	j	205	2AN	C7-C6-C5	-2.35	117.22	120.48
2	D	202	2AN	C2-C1-C10	-2.35	118.04	120.21
2	T	204	2AN	O3-S-O2	-2.35	100.67	111.55
2	F	206	2AN	C11-N-C1	-2.34	121.25	126.36
2	f	205	2AN	C10-C1-N	-2.34	116.97	120.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	203	2AN	C6-C5-C4	-2.34	117.67	123.01
2	a	201	2AN	C13-C12-C11	2.34	122.42	119.73
2	F	202	2AN	C15-C16-C11	2.34	122.42	119.73
2	B	202	2AN	C15-C16-C11	2.33	122.42	119.73
4	P	205	EPE	C6-N1-C2	-2.33	103.82	108.84
2	G	202	2AN	C2-C1-C10	-2.33	118.05	120.21
2	I	207	2AN	C16-C11-C12	-2.33	115.96	119.04
2	j	205	2AN	C1-C10-C5	2.32	122.01	118.91
2	E	203	2AN	C3-C2-C1	2.32	123.72	120.05
2	P	202	2AN	C11-N-C1	-2.32	121.30	126.36
2	F	201	2AN	C6-C5-C4	-2.32	117.71	123.01
2	J	203	2AN	C2-C1-N	-2.32	117.59	123.47
2	D	201	2AN	C15-C16-C11	2.31	122.40	119.73
2	I	204	2AN	C16-C11-N	2.31	128.44	120.61
2	c	206	2AN	C8-C9-C10	-2.31	116.67	120.18
2	B	204	2AN	C7-C8-C9	2.31	122.94	120.37
2	B	201	2AN	C8-C9-C10	-2.31	116.67	120.18
2	c	201	2AN	O2-S-C9	-2.31	99.69	106.37
2	R	205	2AN	C6-C5-C10	2.31	122.84	118.27
2	B	206	2AN	C2-C1-C10	-2.30	118.08	120.21
2	e	201	2AN	C7-C8-C9	2.30	122.93	120.37
6	i	203	FLC	CA-CB-CBC	-2.30	104.94	110.03
2	h	205	2AN	C11-N-C1	2.30	131.38	126.36
2	H	201	2AN	C7-C8-C9	2.30	122.93	120.37
2	H	204	2AN	C11-N-C1	2.30	131.37	126.36
2	D	204	2AN	C7-C8-C9	2.30	122.92	120.37
2	V	208	2AN	C12-C11-N	2.29	128.38	120.61
2	g	202	2AN	C15-C16-C11	2.29	122.37	119.73
2	G	204	2AN	C11-N-C1	2.29	131.35	126.36
2	U	202	2AN	C2-C1-N	-2.29	117.68	123.47
2	h	201	2AN	C8-C9-C10	-2.29	116.70	120.18
2	R	202	2AN	C7-C8-C9	2.29	122.91	120.37
2	M	203	2AN	C7-C8-C9	2.28	122.91	120.37
2	b	203	2AN	O1-S-C9	2.28	112.98	106.37
2	F	201	2AN	C3-C2-C1	2.28	123.64	120.05
2	R	203	2AN	O1-S-C9	2.27	112.96	106.37
2	I	207	2AN	O1-S-C9	2.27	112.96	106.37
2	Y	203	2AN	C3-C2-C1	2.27	123.64	120.05
2	T	203	2AN	C3-C4-C5	-2.27	117.33	120.48
2	f	202	2AN	C8-C9-C10	-2.27	116.73	120.18
2	j	205	2AN	O3-S-O2	-2.27	101.04	111.55
2	B	205	2AN	C2-C1-N	-2.27	117.74	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	202	2AN	C1-C10-C5	-2.26	115.88	118.91
2	E	203	2AN	O2-S-O1	-2.26	101.50	112.88
2	Z	203	2AN	O2-S-O1	-2.26	101.50	112.88
2	b	202	2AN	O2-S-O1	-2.25	101.53	112.88
2	J	203	2AN	C2-C1-C10	-2.25	118.13	120.21
2	j	203	2AN	C2-C1-C10	-2.25	118.13	120.21
2	g	201	2AN	C6-C5-C4	-2.25	117.88	123.01
2	R	202	2AN	O1-S-C9	2.25	112.88	106.37
2	O	202	2AN	C11-N-C1	2.25	131.26	126.36
2	A	202	2AN	C1-C10-C5	-2.24	115.91	118.91
2	P	202	2AN	C8-C9-C10	-2.24	116.77	120.18
2	F	206	2AN	C12-C11-N	2.23	128.18	120.61
2	R	204	2AN	O2-S-C9	2.23	112.84	106.37
2	h	202	2AN	C8-C9-C10	-2.23	116.78	120.18
2	i	201	2AN	O2-S-O1	-2.23	101.65	112.88
2	J	203	2AN	C8-C9-C10	-2.22	116.80	120.18
2	R	203	2AN	C2-C1-C10	-2.22	118.15	120.21
2	N	204	2AN	C6-C5-C4	-2.22	117.94	123.01
2	F	204	2AN	O1-S-C9	2.22	112.79	106.37
2	a	204	2AN	C2-C1-C10	-2.21	118.16	120.21
2	T	205	2AN	C8-C9-C10	-2.21	116.82	120.18
2	F	203	2AN	C3-C2-C1	2.21	123.54	120.05
2	j	201	2AN	C4-C3-C2	2.21	124.39	121.00
2	R	202	2AN	C2-C1-C10	-2.21	118.17	120.21
2	T	203	2AN	C6-C5-C4	-2.21	117.98	123.01
6	a	205	FLC	OA1-CAC-CA	-2.20	116.71	122.95
2	P	201	2AN	C13-C12-C11	2.20	122.27	119.73
2	M	201	2AN	C6-C5-C4	-2.20	117.98	123.01
2	V	206	2AN	C16-C11-C12	-2.20	116.12	119.04
2	j	203	2AN	C6-C5-C4	-2.20	117.99	123.01
2	Z	205	2AN	O1-S-C9	2.20	112.74	106.37
2	E	204	2AN	C1-C10-C5	-2.20	115.97	118.91
2	F	203	2AN	C2-C1-C10	-2.20	118.18	120.21
2	Q	203	2AN	O2-S-C9	2.20	112.74	106.37
2	j	205	2AN	C9-C10-C5	2.19	120.69	115.98
2	D	203	2AN	C2-C1-C10	-2.19	118.18	120.21
2	I	205	2AN	C3-C2-C1	2.19	123.51	120.05
2	I	204	2AN	C16-C11-C12	-2.19	116.14	119.04
2	S	202	2AN	O2-S-C9	2.19	112.71	106.37
2	Z	203	2AN	C7-C8-C9	2.19	122.80	120.37
2	Z	201	2AN	C12-C11-N	2.18	128.01	120.61
6	a	206	FLC	OA2-CAC-CA	2.18	121.27	114.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	V	203	2AN	C6-C5-C10	2.18	122.60	118.27
2	D	201	2AN	C8-C9-C10	-2.18	116.86	120.18
2	T	205	2AN	O1-S-C9	2.18	112.69	106.37
2	T	204	2AN	C6-C5-C10	2.18	122.59	118.27
2	G	201	2AN	C6-C5-C4	-2.18	118.03	123.01
2	D	204	2AN	C4-C5-C10	2.18	122.59	118.27
2	M	203	2AN	C1-C10-C5	-2.18	116.00	118.91
2	j	202	2AN	C4-C5-C10	2.17	122.58	118.27
2	V	206	2AN	C6-C5-C4	-2.17	118.06	123.01
2	f	205	2AN	C11-N-C1	-2.17	121.62	126.36
2	c	206	2AN	C11-N-C1	-2.17	121.63	126.36
2	h	204	2AN	C3-C2-C1	2.17	123.48	120.05
2	j	202	2AN	C6-C5-C4	-2.17	118.06	123.01
2	X	201	2AN	C16-C11-C12	-2.17	116.17	119.04
2	F	204	2AN	C3-C2-C1	2.16	123.47	120.05
2	j	204	2AN	C15-C16-C11	2.16	122.22	119.73
2	Y	202	2AN	C6-C5-C4	-2.16	118.08	123.01
2	Z	202	2AN	C16-C11-C12	-2.16	116.18	119.04
2	N	202	2AN	C1-C10-C5	-2.15	116.03	118.91
2	N	201	2AN	O1-S-C9	2.15	112.61	106.37
2	O	202	2AN	O2-S-C9	2.15	112.60	106.37
2	G	205	2AN	C12-C11-N	2.15	127.90	120.61
2	I	206	2AN	C7-C8-C9	2.15	122.76	120.37
2	j	207	2AN	O2-S-C9	2.15	112.59	106.37
2	V	204	2AN	O2-S-C9	2.15	112.59	106.37
2	g	202	2AN	C11-N-C1	-2.15	121.68	126.36
2	F	202	2AN	C12-C11-N	2.14	127.88	120.61
2	Z	205	2AN	C2-C1-N	2.14	128.89	123.47
2	J	203	2AN	C7-C8-C9	2.14	122.75	120.37
2	T	204	2AN	C15-C16-C11	2.14	122.20	119.73
2	Y	203	2AN	C8-C9-C10	-2.14	116.92	120.18
2	T	203	2AN	C4-C3-C2	2.14	124.29	121.00
2	B	201	2AN	C16-C11-N	-2.14	113.36	120.61
2	c	205	2AN	C7-C8-C9	2.14	122.75	120.37
2	Q	201	2AN	C16-C11-N	2.14	127.86	120.61
2	f	201	2AN	C11-N-C1	-2.14	121.69	126.36
2	Z	202	2AN	C13-C12-C11	2.14	122.19	119.73
6	e	202	FLC	OA1-CAC-CA	-2.14	116.89	122.95
2	X	205	2AN	C7-C8-C9	2.14	122.75	120.37
2	T	204	2AN	C7-C8-C9	2.14	122.75	120.37
6	j	208	FLC	OG1-CGC-CG	-2.13	116.91	122.95
2	h	203	2AN	C16-C11-C12	2.13	121.87	119.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Y	203	2AN	C6-C5-C4	-2.13	118.15	123.01
2	B	203	2AN	C11-N-C1	-2.13	121.72	126.36
2	c	202	2AN	C8-C9-C10	-2.13	116.95	120.18
2	F	201	2AN	C1-C10-C5	-2.12	116.07	118.91
2	A	202	2AN	C7-C8-C9	2.12	122.73	120.37
2	I	202	2AN	C2-C1-N	-2.12	118.10	123.47
2	A	201	2AN	C4-C5-C10	2.12	122.47	118.27
2	N	202	2AN	C6-C5-C4	-2.12	118.18	123.01
2	D	204	2AN	C13-C12-C11	2.12	122.17	119.73
2	V	202	2AN	C16-C11-N	2.12	127.78	120.61
2	A	203	2AN	C1-C10-C5	-2.12	116.08	118.91
2	h	201	2AN	C3-C2-C1	2.12	123.39	120.05
2	S	203	2AN	C11-N-C1	-2.11	121.75	126.36
2	V	201	2AN	C7-C8-C9	2.11	122.72	120.37
2	I	202	2AN	C6-C5-C4	-2.11	118.19	123.01
2	g	201	2AN	C6-C5-C10	2.11	122.45	118.27
2	L	202	2AN	O2-S-C9	2.11	112.49	106.37
2	R	201	2AN	C2-C1-C10	-2.11	118.26	120.21
2	N	204	2AN	C3-C4-C5	-2.11	117.55	120.48
2	P	202	2AN	C6-C5-C4	-2.11	118.20	123.01
2	I	207	2AN	C2-C1-N	-2.11	118.13	123.47
2	I	205	2AN	C15-C14-C13	-2.11	116.98	119.87
2	i	201	2AN	C6-C5-C4	-2.11	118.20	123.01
2	F	204	2AN	C6-C5-C4	-2.11	118.20	123.01
2	G	204	2AN	O2-S-C9	2.11	112.47	106.37
2	X	204	2AN	C16-C11-C12	-2.11	116.25	119.04
2	T	205	2AN	C4-C5-C10	2.10	122.44	118.27
2	T	204	2AN	O2-S-C9	2.10	112.46	106.37
2	h	201	2AN	C1-C10-C5	-2.10	116.10	118.91
2	I	206	2AN	C12-C11-N	-2.10	113.49	120.61
2	I	203	2AN	C8-C9-C10	-2.10	116.98	120.18
2	L	204	2AN	C3-C2-C1	2.10	123.37	120.05
2	Y	203	2AN	O2-S-C9	2.10	112.45	106.37
2	B	201	2AN	C12-C11-N	2.10	127.72	120.61
2	Y	204	2AN	C11-N-C1	-2.10	121.78	126.36
2	Z	205	2AN	C11-N-C1	2.10	130.94	126.36
2	P	201	2AN	O2-S-C9	2.09	112.44	106.37
2	E	202	2AN	O3-S-O2	-2.09	101.84	111.55
2	E	201	2AN	C1-C10-C5	-2.09	116.11	118.91
2	B	205	2AN	C12-C11-N	2.09	127.68	120.61
2	L	203	2AN	C10-C1-N	2.09	123.44	120.39
2	g	201	2AN	C7-C8-C9	2.09	122.69	120.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	203	2AN	C8-C9-C10	2.09	123.36	120.18
2	D	201	2AN	C6-C5-C4	-2.09	118.25	123.01
2	V	205	2AN	O3-S-O1	-2.09	101.87	111.55
2	G	204	2AN	C16-C11-N	2.09	127.67	120.61
2	E	204	2AN	O1-S-C9	2.08	112.41	106.37
2	f	201	2AN	C6-C5-C4	-2.08	118.26	123.01
2	N	203	2AN	O2-S-C9	2.08	112.40	106.37
2	B	201	2AN	C3-C2-C1	2.08	123.33	120.05
4	P	205	EPE	O3S-S-O2S	-2.08	106.20	111.40
2	j	202	2AN	O1-S-C9	2.08	112.38	106.37
6	i	202	FLC	CG-CB-CA	-2.07	103.99	109.31
2	I	201	2AN	C4-C5-C10	2.07	122.38	118.27
2	Y	202	2AN	O2-S-C9	2.07	112.37	106.37
2	a	202	2AN	O3-S-O2	-2.07	101.95	111.55
6	G	206	FLC	OG2-CGC-CG	2.07	120.90	114.35
2	D	203	2AN	C4-C5-C10	2.07	122.37	118.27
2	G	201	2AN	C3-C2-C1	2.07	123.32	120.05
2	A	204	2AN	C2-C1-C10	-2.07	118.30	120.21
2	I	207	2AN	C15-C16-C11	2.07	122.11	119.73
2	d	201	2AN	C13-C12-C11	2.07	122.11	119.73
2	Z	202	2AN	C3-C2-C1	2.07	123.31	120.05
2	E	203	2AN	C4-C5-C10	2.07	122.36	118.27
2	E	202	2AN	O2-S-C9	-2.07	100.38	106.37
2	T	204	2AN	C12-C11-N	2.07	127.61	120.61
2	b	205	2AN	C3-C2-C1	2.06	123.31	120.05
2	H	202	2AN	O1-S-C9	2.06	112.34	106.37
2	M	203	2AN	C8-C9-C10	-2.06	117.05	120.18
2	N	203	2AN	C14-C15-C16	2.06	122.78	120.24
2	L	203	2AN	C16-C11-N	2.06	127.58	120.61
2	Z	203	2AN	O1-S-C9	2.06	112.33	106.37
2	V	204	2AN	C13-C12-C11	2.05	122.10	119.73
2	h	203	2AN	C7-C6-C5	-2.05	117.63	120.48
2	I	207	2AN	C13-C12-C11	2.05	122.09	119.73
2	d	204	2AN	C3-C2-C1	2.05	123.29	120.05
2	j	203	2AN	C16-C11-C12	-2.05	116.32	119.04
6	j	208	FLC	CB-CG-CGC	-2.05	108.32	113.92
2	K	201	2AN	C4-C5-C10	2.05	122.33	118.27
2	F	203	2AN	C15-C16-C11	2.05	122.09	119.73
2	X	205	2AN	C15-C16-C11	2.05	122.09	119.73
2	A	201	2AN	C10-C1-N	-2.04	117.41	120.39
2	K	202	2AN	O3-S-O1	-2.04	102.08	111.55
2	F	201	2AN	C4-C5-C10	2.04	122.31	118.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	202	2AN	C14-C15-C16	2.04	122.75	120.24
2	D	203	2AN	C1-C10-C5	-2.04	116.18	118.91
2	O	202	2AN	C10-C1-N	-2.04	117.42	120.39
2	g	203	2AN	C10-C1-N	2.04	123.36	120.39
2	C	203[A]	2AN	C3-C2-C1	2.03	123.26	120.05
2	T	205	2AN	C14-C15-C16	-2.03	117.73	120.24
6	a	205	FLC	CG-CB-CA	2.03	114.53	109.31
2	V	202	2AN	C12-C11-N	-2.03	113.73	120.61
2	K	202	2AN	O1-S-C9	2.03	112.26	106.37
2	R	204	2AN	C13-C12-C11	2.03	122.07	119.73
2	M	202	2AN	C2-C1-N	-2.03	118.33	123.47
2	X	202	2AN	C16-C11-C12	2.03	121.73	119.04
2	F	202	2AN	C16-C11-N	-2.03	113.74	120.61
2	Y	201	2AN	C4-C5-C10	2.03	122.28	118.27
2	L	201	2AN	O3-S-O2	-2.03	102.15	111.55
2	L	202	2AN	C3-C2-C1	2.03	123.25	120.05
6	a	205	FLC	CB-CA-CAC	-2.03	108.38	113.92
2	B	203	2AN	C14-C13-C12	2.03	122.74	120.24
2	Z	204	2AN	C10-C1-N	-2.03	117.44	120.39
2	Q	203	2AN	C7-C8-C9	2.02	122.62	120.37
2	O	201	2AN	C9-C10-C5	2.02	120.32	115.98
2	G	201	2AN	C7-C8-C9	2.02	122.62	120.37
2	h	201	2AN	C13-C12-C11	2.02	122.06	119.73
2	f	203	2AN	C2-C1-C10	-2.02	118.34	120.21
2	h	203	2AN	C6-C5-C4	-2.02	118.40	123.01
2	X	204	2AN	C15-C16-C11	2.02	122.06	119.73
2	Z	201	2AN	C16-C11-N	-2.02	113.77	120.61
2	G	201	2AN	C1-C10-C5	-2.02	116.21	118.91
2	K	202	2AN	C2-C1-C10	-2.02	118.34	120.21
2	Z	201	2AN	C2-C1-N	-2.02	118.36	123.47
2	H	202	2AN	C7-C8-C9	2.02	122.61	120.37
2	j	205	2AN	C15-C16-C11	2.02	122.06	119.73
2	X	201	2AN	C12-C11-N	2.01	127.42	120.61
2	X	206	2AN	C2-C1-C10	-2.01	118.35	120.21
2	g	201	2AN	O1-S-C9	2.01	112.19	106.37
2	Z	203	2AN	C6-C5-C4	-2.01	118.42	123.01
2	c	202	2AN	C15-C16-C11	2.01	122.04	119.73
2	I	202	2AN	O2-S-C9	2.00	112.17	106.37
2	T	204	2AN	C16-C11-C12	-2.00	116.39	119.04
2	h	201	2AN	O2-S-O1	-2.00	102.80	112.88
2	c	202	2AN	C4-C5-C10	2.00	122.24	118.27
2	Z	201	2AN	C3-C2-C1	2.00	123.21	120.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	V	201	2AN	C6-C5-C10	2.00	122.23	118.27

There are no chirality outliers.

All (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
2	A	203	2AN	C10-C9-S-O1
2	A	203	2AN	C10-C9-S-O2
2	R	203	2AN	C8-C9-S-O1
2	R	203	2AN	C10-C9-S-O1
2	R	203	2AN	C10-C9-S-O2
2	R	203	2AN	C8-C9-S-O3
2	R	203	2AN	C10-C9-S-O3
2	R	204	2AN	C8-C9-S-O1
2	R	204	2AN	C10-C9-S-O2
2	R	204	2AN	C8-C9-S-O3
2	R	204	2AN	C10-C9-S-O3
2	P	203	2AN	C8-C9-S-O1
2	N	203	2AN	C8-C9-S-O1
2	N	203	2AN	C10-C9-S-O1
2	N	203	2AN	C10-C9-S-O2
2	M	203	2AN	C10-C1-N-C11
2	M	203	2AN	C8-C9-S-O1
2	M	203	2AN	C10-C9-S-O1
2	M	203	2AN	C8-C9-S-O3
2	M	203	2AN	C10-C9-S-O3
2	I	205	2AN	C8-C9-S-O1
2	I	205	2AN	C8-C9-S-O2
2	I	205	2AN	C10-C9-S-O2
2	I	205	2AN	C8-C9-S-O3
2	I	205	2AN	C10-C9-S-O3
2	I	207	2AN	C8-C9-S-O1
2	I	207	2AN	C8-C9-S-O3
2	G	205	2AN	C8-C9-S-O1
2	G	205	2AN	C10-C9-S-O1
2	G	205	2AN	C10-C9-S-O2
2	G	205	2AN	C8-C9-S-O3

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Mol	Chain	Res	Type	Atoms
2	G	205	2AN	C10-C9-S-O3
2	F	201	2AN	C8-C9-S-O3
2	F	201	2AN	C10-C9-S-O3
2	F	202	2AN	C8-C9-S-O1
2	F	202	2AN	C10-C9-S-O2
2	F	202	2AN	C8-C9-S-O3
2	F	202	2AN	C10-C9-S-O3
2	E	204	2AN	C8-C9-S-O2
2	E	204	2AN	C10-C9-S-O2
2	E	204	2AN	C8-C9-S-O3
2	E	204	2AN	C10-C9-S-O3
2	D	203	2AN	C10-C9-S-O1
2	D	203	2AN	C8-C9-S-O2
2	D	203	2AN	C10-C9-S-O2
2	D	203	2AN	C8-C9-S-O3
2	D	203	2AN	C10-C9-S-O3
2	D	204	2AN	C8-C9-S-O1
2	D	204	2AN	C10-C9-S-O2
2	D	204	2AN	C8-C9-S-O3
2	D	204	2AN	C10-C9-S-O3
2	e	201	2AN	C8-C9-S-O3
2	e	201	2AN	C10-C9-S-O3
2	d	202	2AN	C8-C9-S-O3
2	d	202	2AN	C10-C9-S-O3
2	b	203	2AN	C8-C9-S-O1
2	b	203	2AN	C10-C9-S-O1
2	b	203	2AN	C10-C9-S-O2
2	b	203	2AN	C8-C9-S-O3
2	b	203	2AN	C10-C9-S-O3
2	b	206	2AN	C10-C9-S-O1
2	b	206	2AN	C10-C9-S-O2
2	Z	206	2AN	C10-C9-S-O3
2	Y	202	2AN	C10-C9-S-O3
2	Y	204	2AN	C8-C9-S-O3
2	W	201	2AN	C10-C9-S-O3
2	V	208	2AN	C2-C1-N-C11
2	V	208	2AN	C10-C1-N-C11
2	V	208	2AN	C8-C9-S-O3
2	V	208	2AN	C10-C9-S-O3
2	U	201	2AN	C8-C9-S-O1
2	U	201	2AN	C10-C9-S-O2
2	U	201	2AN	C8-C9-S-O3

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Mol	Chain	Res	Type	Atoms
2	U	201	2AN	C10-C9-S-O3
2	U	202	2AN	C8-C9-S-O3
2	T	204	2AN	C10-C9-S-O1
2	T	204	2AN	C8-C9-S-O3
2	T	204	2AN	C10-C9-S-O3
2	T	205	2AN	C10-C9-S-O3
2	S	201	2AN	C10-C9-S-O2
2	S	201	2AN	C8-C9-S-O3
2	S	201	2AN	C10-C9-S-O3
2	S	202	2AN	C8-C9-S-O3
2	S	202	2AN	C10-C9-S-O3
2	S	204	2AN	C10-C9-S-O1
2	S	204	2AN	C8-C9-S-O2
2	S	204	2AN	C10-C9-S-O2
2	S	204	2AN	C8-C9-S-O3
2	S	204	2AN	C10-C9-S-O3
2	j	201	2AN	C8-C9-S-O1
2	j	201	2AN	C10-C9-S-O1
2	j	201	2AN	C8-C9-S-O2
2	j	201	2AN	C8-C9-S-O3
2	j	201	2AN	C10-C9-S-O3
2	j	204	2AN	C8-C9-S-O3
2	i	201	2AN	C8-C9-S-O3
2	h	203	2AN	C10-C9-S-O3
6	G	206	FLC	CAC-CA-CB-CBC
6	G	206	FLC	CAC-CA-CB-CG
6	G	206	FLC	CAC-CA-CB-OHB
6	G	206	FLC	CG-CB-CBC-OB1
6	G	206	FLC	CG-CB-CBC-OB2
6	G	206	FLC	OHB-CB-CBC-OB1
6	G	206	FLC	OHB-CB-CBC-OB2
6	G	206	FLC	CA-CB-CG-CGC
6	G	206	FLC	CBC-CB-CG-CGC
6	G	206	FLC	OHB-CB-CG-CGC
6	e	202	FLC	CA-CB-CG-CGC
6	e	202	FLC	CBC-CB-CG-CGC
6	a	205	FLC	CG-CB-CBC-OB1
6	a	205	FLC	CG-CB-CBC-OB2
6	a	205	FLC	OHB-CB-CBC-OB1
6	a	205	FLC	OHB-CB-CBC-OB2
6	a	206	FLC	CA-CB-CBC-OB1
6	a	206	FLC	CA-CB-CBC-OB2

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Mol	Chain	Res	Type	Atoms
6	a	206	FLC	OHB-CB-CBC-OB1
6	a	206	FLC	OHB-CB-CBC-OB2
6	j	208	FLC	CG-CB-CBC-OB1
6	j	208	FLC	CG-CB-CBC-OB2
6	j	208	FLC	OHB-CB-CBC-OB1
6	j	208	FLC	OHB-CB-CBC-OB2
6	i	202	FLC	CA-CB-CBC-OB2
6	i	202	FLC	OHB-CB-CBC-OB2
6	i	203	FLC	CAC-CA-CB-OHB
6	i	203	FLC	CBC-CB-CG-CGC
6	i	203	FLC	OHB-CB-CG-CGC
6	i	203	FLC	CA-CB-CG-CGC
6	e	202	FLC	OHB-CB-CG-CGC
6	i	203	FLC	CAC-CA-CB-CG
2	I	206	2AN	C10-C1-N-C11
2	g	203	2AN	C10-C1-N-C11
2	B	205	2AN	C10-C9-S-O2
2	R	204	2AN	C10-C9-S-O1
2	P	203	2AN	C10-C9-S-O1
2	P	203	2AN	C10-C9-S-O2
2	O	201	2AN	C10-C9-S-O2
2	O	203	2AN	C10-C9-S-O2
2	M	203	2AN	C10-C9-S-O2
2	L	204	2AN	C10-C9-S-O2
2	K	201	2AN	C10-C9-S-O2
2	I	205	2AN	C10-C9-S-O1
2	I	207	2AN	C10-C9-S-O1
2	H	203	2AN	C10-C9-S-O2
2	F	201	2AN	C10-C9-S-O1
2	F	201	2AN	C10-C9-S-O2
2	F	202	2AN	C10-C9-S-O1
2	F	205	2AN	C10-C9-S-O1
2	F	205	2AN	C10-C9-S-O2
2	E	203	2AN	C10-C9-S-O1
2	E	204	2AN	C10-C9-S-O1
2	D	204	2AN	C10-C9-S-O1
2	C	203[A]	2AN	C10-C9-S-O1
2	C	203[A]	2AN	C10-C9-S-O2
2	e	201	2AN	C10-C9-S-O1
2	d	202	2AN	C10-C9-S-O1
2	d	202	2AN	C10-C9-S-O2
2	c	203	2AN	C10-C9-S-O1

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Mol	Chain	Res	Type	Atoms
2	c	203	2AN	C10-C9-S-O2
2	Z	206	2AN	C10-C9-S-O2
2	Y	202	2AN	C10-C9-S-O1
2	Y	202	2AN	C10-C9-S-O2
2	Y	204	2AN	C10-C9-S-O1
2	W	201	2AN	C10-C9-S-O1
2	W	201	2AN	C10-C9-S-O2
2	U	201	2AN	C10-C9-S-O1
2	U	202	2AN	C10-C9-S-O1
2	U	202	2AN	C10-C9-S-O2
2	T	204	2AN	C10-C9-S-O2
2	T	205	2AN	C10-C9-S-O1
2	S	201	2AN	C10-C9-S-O1
2	S	202	2AN	C10-C9-S-O1
2	j	201	2AN	C10-C9-S-O2
2	j	204	2AN	C10-C9-S-O1
6	e	202	FLC	CAC-CA-CB-OHB
6	a	205	FLC	CAC-CA-CB-OHB
6	j	208	FLC	CBC-CB-CG-CGC
2	Q	203	2AN	C2-C1-N-C11
2	J	203	2AN	C2-C1-N-C11
2	I	206	2AN	C2-C1-N-C11
2	F	202	2AN	C2-C1-N-C11
2	F	206	2AN	C2-C1-N-C11
2	E	204	2AN	C2-C1-N-C11
2	C	203[A]	2AN	C2-C1-N-C11
2	Z	206	2AN	C2-C1-N-C11
2	Y	204	2AN	C2-C1-N-C11
2	S	201	2AN	C2-C1-N-C11
2	A	203	2AN	C8-C9-S-O1
2	A	203	2AN	C8-C9-S-O2
2	R	203	2AN	C8-C9-S-O2
2	R	204	2AN	C8-C9-S-O2
2	Q	203	2AN	C8-C9-S-O2
2	O	201	2AN	C8-C9-S-O2
2	M	203	2AN	C8-C9-S-O2
2	L	204	2AN	C8-C9-S-O2
2	H	203	2AN	C8-C9-S-O2
2	F	201	2AN	C8-C9-S-O2
2	F	202	2AN	C8-C9-S-O2
2	E	203	2AN	C8-C9-S-O1
2	E	204	2AN	C8-C9-S-O1

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Mol	Chain	Res	Type	Atoms
2	e	201	2AN	C8-C9-S-O1
2	d	202	2AN	C8-C9-S-O1
2	Y	202	2AN	C8-C9-S-O2
2	W	201	2AN	C8-C9-S-O1
2	W	201	2AN	C8-C9-S-O2
2	V	201	2AN	C8-C9-S-O2
2	V	203	2AN	C8-C9-S-O1
2	U	201	2AN	C8-C9-S-O2
2	U	202	2AN	C8-C9-S-O1
2	T	204	2AN	C8-C9-S-O2
2	S	201	2AN	C8-C9-S-O1
2	S	202	2AN	C8-C9-S-O1
2	j	204	2AN	C8-C9-S-O1
6	a	205	FLC	CAC-CA-CB-CG
6	e	202	FLC	CG-CB-CBC-OB2
6	i	202	FLC	CA-CB-CBC-OB1
6	e	202	FLC	CAC-CA-CB-CBC
6	e	202	FLC	CAC-CA-CB-CG
6	a	206	FLC	CAC-CA-CB-OHB
2	a	201	2AN	C2-C1-N-C11
2	B	201	2AN	C10-C1-N-C11
2	A	202	2AN	C10-C1-N-C11
2	A	204	2AN	C10-C1-N-C11
2	Q	203	2AN	C10-C1-N-C11
2	P	202	2AN	C10-C1-N-C11
2	N	203	2AN	C10-C1-N-C11
2	M	202	2AN	C10-C1-N-C11
2	L	203	2AN	C10-C1-N-C11
2	J	203	2AN	C10-C1-N-C11
2	I	201	2AN	C10-C1-N-C11
2	H	202	2AN	C10-C1-N-C11
2	G	202	2AN	C10-C1-N-C11
2	C	203[A]	2AN	C10-C1-N-C11
2	c	201	2AN	C10-C1-N-C11
2	a	201	2AN	C10-C1-N-C11
2	V	205	2AN	C10-C1-N-C11
2	S	204	2AN	C10-C1-N-C11
2	Q	203	2AN	C10-C9-S-O2
2	O	201	2AN	C10-C9-S-O1
2	O	203	2AN	C10-C9-S-O1
2	L	204	2AN	C10-C9-S-O1
2	K	201	2AN	C10-C9-S-O1

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Mol	Chain	Res	Type	Atoms
2	I	207	2AN	C10-C9-S-O2
2	H	203	2AN	C10-C9-S-O1
2	H	204	2AN	C10-C9-S-O1
2	H	204	2AN	C10-C9-S-O2
2	F	204	2AN	C10-C9-S-O1
2	F	204	2AN	C10-C9-S-O2
2	c	204	2AN	C10-C9-S-O1
2	Z	206	2AN	C10-C9-S-O1
2	Y	204	2AN	C10-C9-S-O2
2	X	204	2AN	C10-C9-S-O2
2	V	201	2AN	C10-C9-S-O2
2	S	202	2AN	C10-C9-S-O2
2	j	204	2AN	C10-C9-S-O2
2	i	201	2AN	C10-C9-S-O2
2	h	203	2AN	C10-C9-S-O1
2	g	202	2AN	C10-C9-S-O2
6	a	205	FLC	CB-CG-CGC-OG2
6	G	206	FLC	CA-CB-CBC-OB1
6	e	202	FLC	CA-CB-CBC-OB1
6	e	202	FLC	CG-CB-CBC-OB1
6	i	202	FLC	CG-CB-CBC-OB2
2	N	203	2AN	C2-C1-N-C11
2	M	203	2AN	C2-C1-N-C11
2	L	203	2AN	C2-C1-N-C11
2	G	202	2AN	C2-C1-N-C11
2	D	204	2AN	C2-C1-N-C11
2	b	206	2AN	C2-C1-N-C11
2	X	203	2AN	C2-C1-N-C11
2	X	206	2AN	C2-C1-N-C11
6	a	205	FLC	CB-CG-CGC-OG1
2	A	203	2AN	C8-C9-S-O3
2	P	203	2AN	C8-C9-S-O3
2	N	203	2AN	C8-C9-S-O3
2	L	204	2AN	C8-C9-S-O3
2	H	203	2AN	C8-C9-S-O3
2	C	203[A]	2AN	C8-C9-S-O3
2	Z	206	2AN	C8-C9-S-O3
2	Y	202	2AN	C8-C9-S-O3
2	X	204	2AN	C8-C9-S-O3
2	W	201	2AN	C8-C9-S-O3
2	T	205	2AN	C8-C9-S-O3
2	h	203	2AN	C8-C9-S-O3

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Mol	Chain	Res	Type	Atoms
2	g	202	2AN	C8-C9-S-O3
6	a	205	FLC	CAC-CA-CB-CBC
2	A	203	2AN	C10-C9-S-O3
2	P	203	2AN	C10-C9-S-O3
2	O	201	2AN	C10-C9-S-O3
2	N	203	2AN	C10-C9-S-O3
2	I	207	2AN	C10-C9-S-O3
2	H	203	2AN	C10-C9-S-O3
2	Y	204	2AN	C10-C9-S-O3
2	X	204	2AN	C10-C9-S-O3
2	U	202	2AN	C10-C9-S-O3
2	j	204	2AN	C10-C9-S-O3
2	i	201	2AN	C10-C9-S-O3
2	g	202	2AN	C10-C9-S-O3
2	O	203	2AN	C8-C9-S-O2
2	N	203	2AN	C8-C9-S-O2
2	G	205	2AN	C8-C9-S-O2
2	D	204	2AN	C8-C9-S-O2
2	C	203[A]	2AN	C8-C9-S-O1
2	b	206	2AN	C8-C9-S-O1
2	Y	204	2AN	C8-C9-S-O1
2	T	204	2AN	C8-C9-S-O1
2	S	201	2AN	C8-C9-S-O2
2	Q	201	2AN	C10-C1-N-C11
2	E	204	2AN	C10-C1-N-C11
2	f	206	2AN	C10-C1-N-C11
2	Z	206	2AN	C10-C1-N-C11
2	Y	204	2AN	C10-C1-N-C11
2	X	203	2AN	C10-C1-N-C11
2	S	201	2AN	C10-C1-N-C11
2	A	204	2AN	C2-C1-N-C11
2	R	202	2AN	C2-C1-N-C11
2	d	203	2AN	C2-C1-N-C11
2	g	203	2AN	C2-C1-N-C11
6	i	202	FLC	OHB-CB-CBC-OB1
6	G	206	FLC	CA-CB-CBC-OB2
6	e	202	FLC	CA-CB-CBC-OB2
6	j	208	FLC	CA-CB-CBC-OB2
6	i	202	FLC	CG-CB-CBC-OB1
2	A	204	2AN	C10-C9-S-O1
2	Q	203	2AN	C10-C9-S-O1
2	M	202	2AN	C10-C9-S-O2

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Mol	Chain	Res	Type	Atoms
2	c	204	2AN	C10-C9-S-O2
2	T	205	2AN	C10-C9-S-O2
2	B	201	2AN	C2-C1-N-C11
2	P	202	2AN	C2-C1-N-C11
2	M	202	2AN	C2-C1-N-C11
2	f	203	2AN	C2-C1-N-C11
2	S	204	2AN	C2-C1-N-C11
2	B	205	2AN	C10-C1-N-C11
2	R	202	2AN	C10-C1-N-C11
2	P	204	2AN	C10-C1-N-C11
2	O	203	2AN	C10-C1-N-C11
2	N	202	2AN	C10-C1-N-C11
2	F	202	2AN	C10-C1-N-C11
2	E	202	2AN	C10-C1-N-C11
2	D	202	2AN	C10-C1-N-C11
2	D	204	2AN	C10-C1-N-C11
2	C	201	2AN	C10-C1-N-C11
2	f	203	2AN	C10-C1-N-C11
2	d	203	2AN	C10-C1-N-C11
2	b	206	2AN	C10-C1-N-C11
2	Z	201	2AN	C10-C1-N-C11
2	X	206	2AN	C10-C1-N-C11
2	V	202	2AN	C10-C1-N-C11
2	j	202	2AN	C10-C1-N-C11
6	i	203	FLC	CA-CB-CBC-OB1
6	i	203	FLC	CA-CB-CBC-OB2
4	P	205	EPE	C9-C10-S-O2S
2	P	203	2AN	C8-C9-S-O2
2	O	203	2AN	C8-C9-S-O1
2	L	204	2AN	C8-C9-S-O1
2	K	201	2AN	C8-C9-S-O2
2	H	203	2AN	C8-C9-S-O1
2	F	201	2AN	C8-C9-S-O1
2	F	205	2AN	C8-C9-S-O2
2	D	203	2AN	C8-C9-S-O1
2	C	203[A]	2AN	C8-C9-S-O2
2	d	202	2AN	C8-C9-S-O2
2	c	203	2AN	C8-C9-S-O2
2	b	203	2AN	C8-C9-S-O2
2	b	206	2AN	C8-C9-S-O2
2	Y	202	2AN	C8-C9-S-O1
2	S	202	2AN	C8-C9-S-O2

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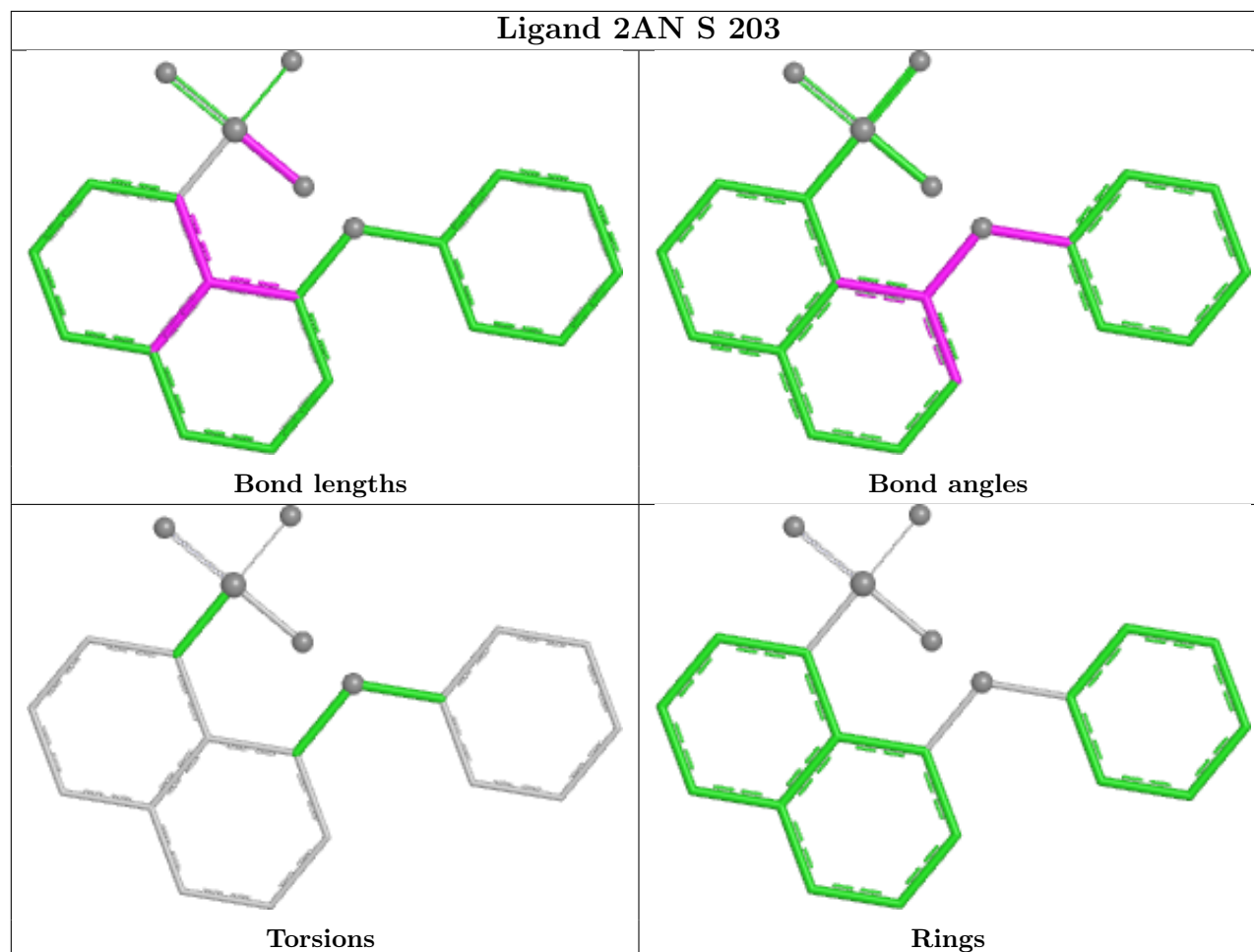
Mol	Chain	Res	Type	Atoms
2	S	204	2AN	C8-C9-S-O1
4	P	205	EPE	C8-C7-N4-C3
6	i	202	FLC	CB-CG-CGC-OG2
6	i	203	FLC	CB-CG-CGC-OG1
2	A	204	2AN	C10-C9-S-O2
2	E	203	2AN	C10-C9-S-O2
6	i	202	FLC	CB-CG-CGC-OG1
6	i	203	FLC	CB-CG-CGC-OG2
6	j	208	FLC	CA-CB-CBC-OB1
2	B	206	2AN	C10-C1-N-C11
2	K	201	2AN	C10-C1-N-C11
2	G	201	2AN	C10-C1-N-C11
2	F	206	2AN	C10-C1-N-C11
2	f	202	2AN	C10-C1-N-C11
2	T	202	2AN	C10-C1-N-C11
2	T	205	2AN	C10-C1-N-C11
2	j	205	2AN	C10-C1-N-C11
2	g	202	2AN	C10-C1-N-C11
6	a	206	FLC	CB-CA-CAC-OA1
2	A	202	2AN	C2-C1-N-C11
2	I	201	2AN	C2-C1-N-C11
2	H	202	2AN	C2-C1-N-C11
2	c	201	2AN	C2-C1-N-C11
2	Z	201	2AN	C2-C1-N-C11
2	V	205	2AN	C2-C1-N-C11
6	G	206	FLC	CB-CA-CAC-OA1
2	O	201	2AN	C8-C9-S-O3
2	O	203	2AN	C8-C9-S-O3
2	b	206	2AN	C8-C9-S-O3
6	G	206	FLC	CB-CA-CAC-OA2
6	e	202	FLC	CB-CG-CGC-OG2
6	a	206	FLC	CB-CA-CAC-OA2

There are no ring outliers.

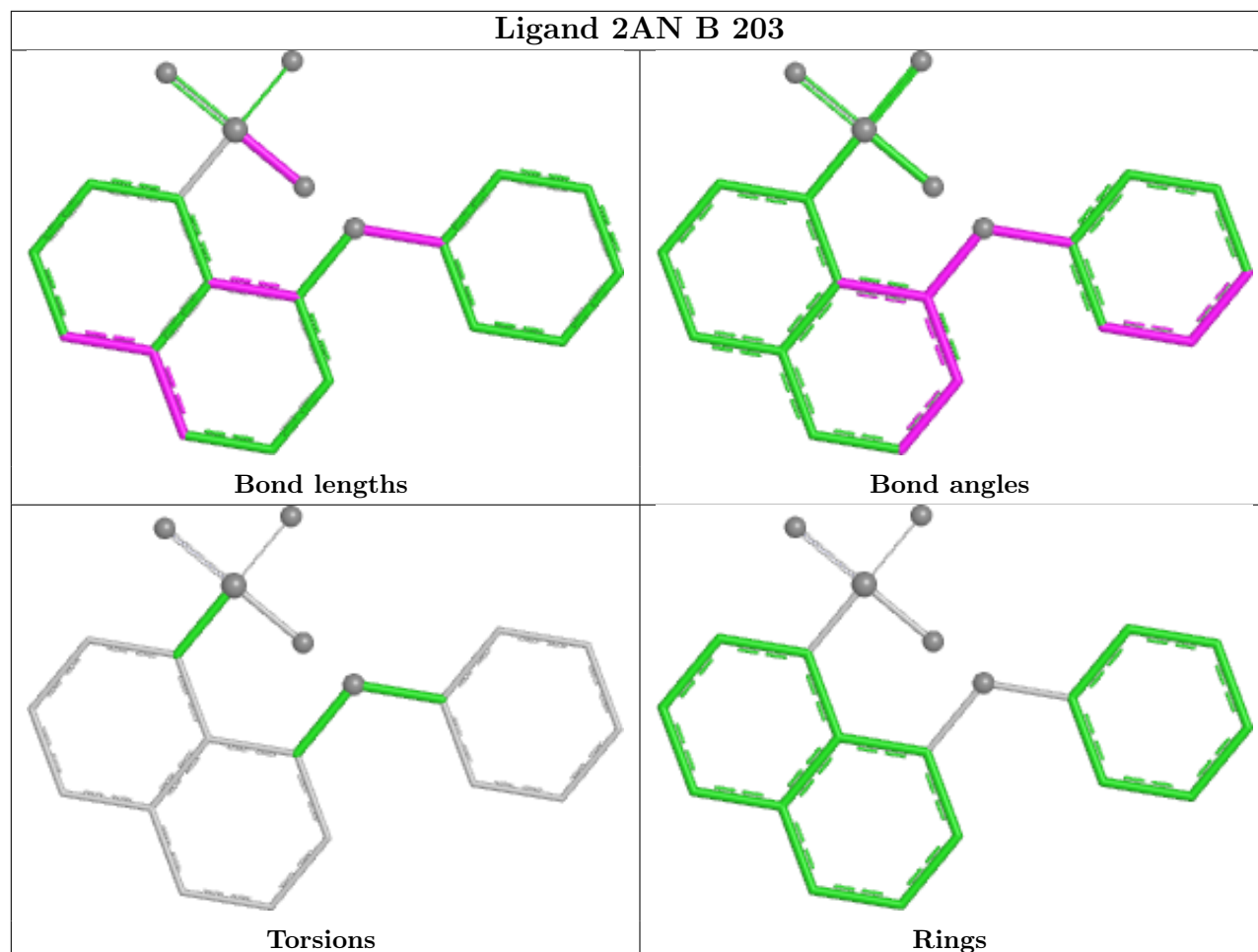
No monomer is involved in short contacts.

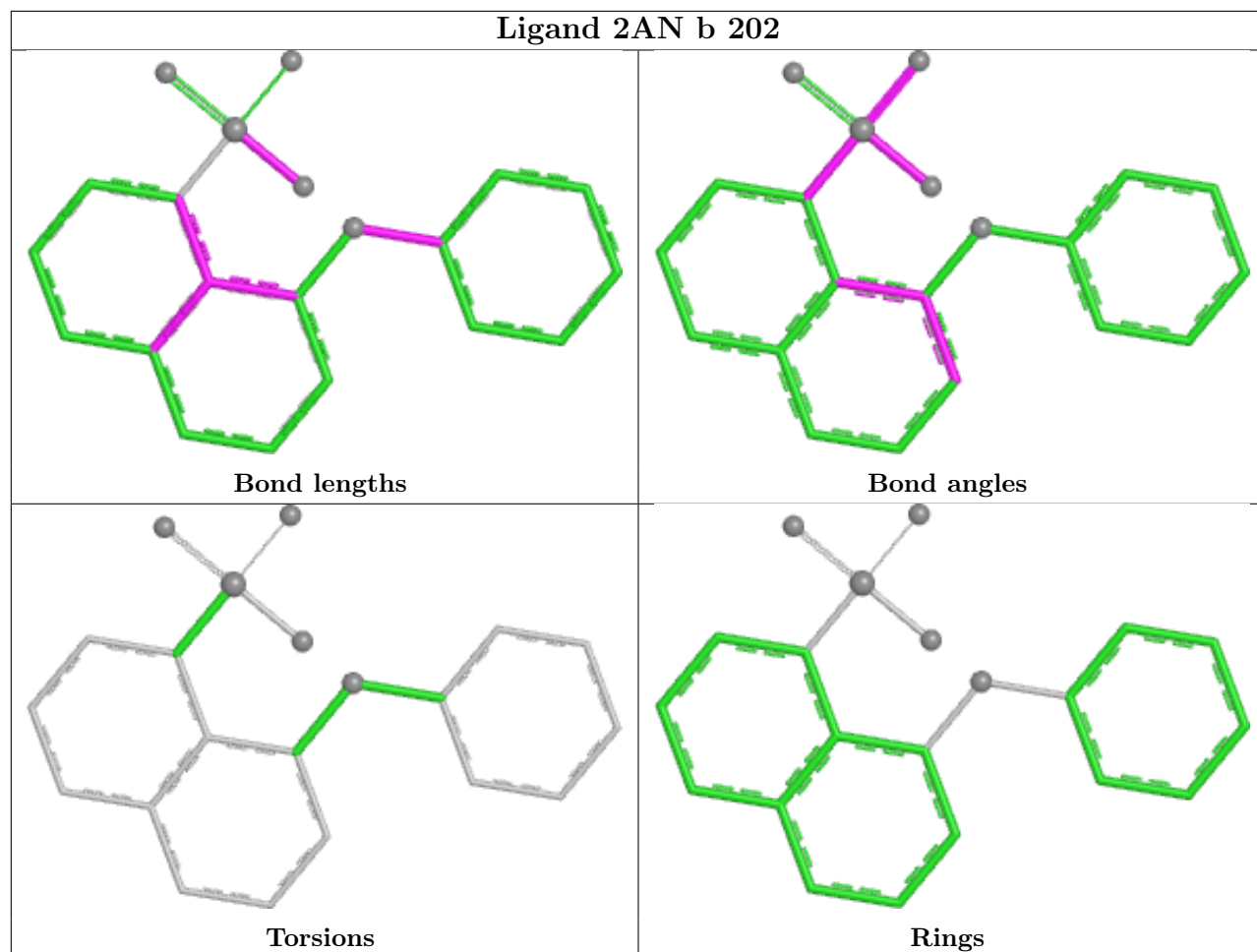
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

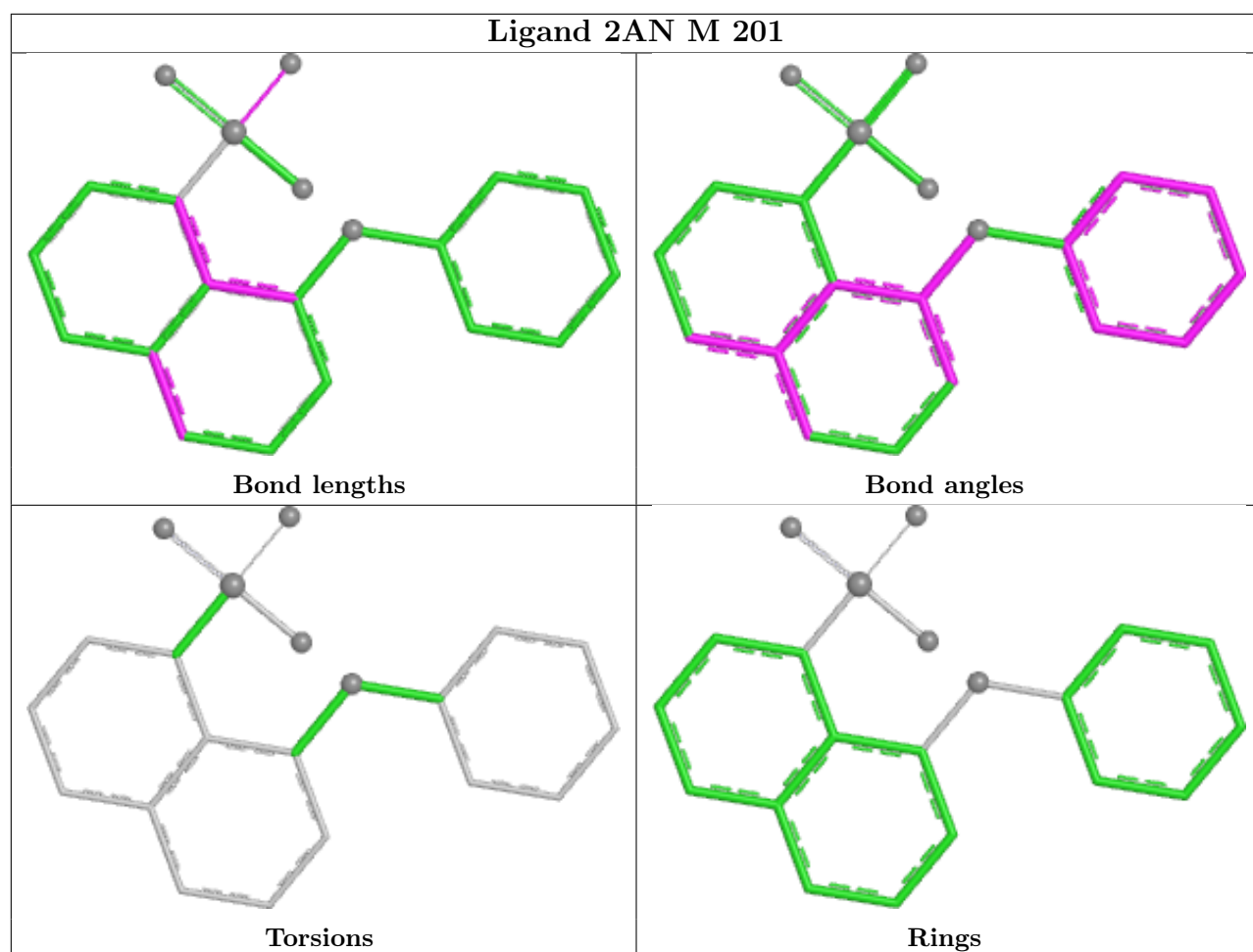
in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers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



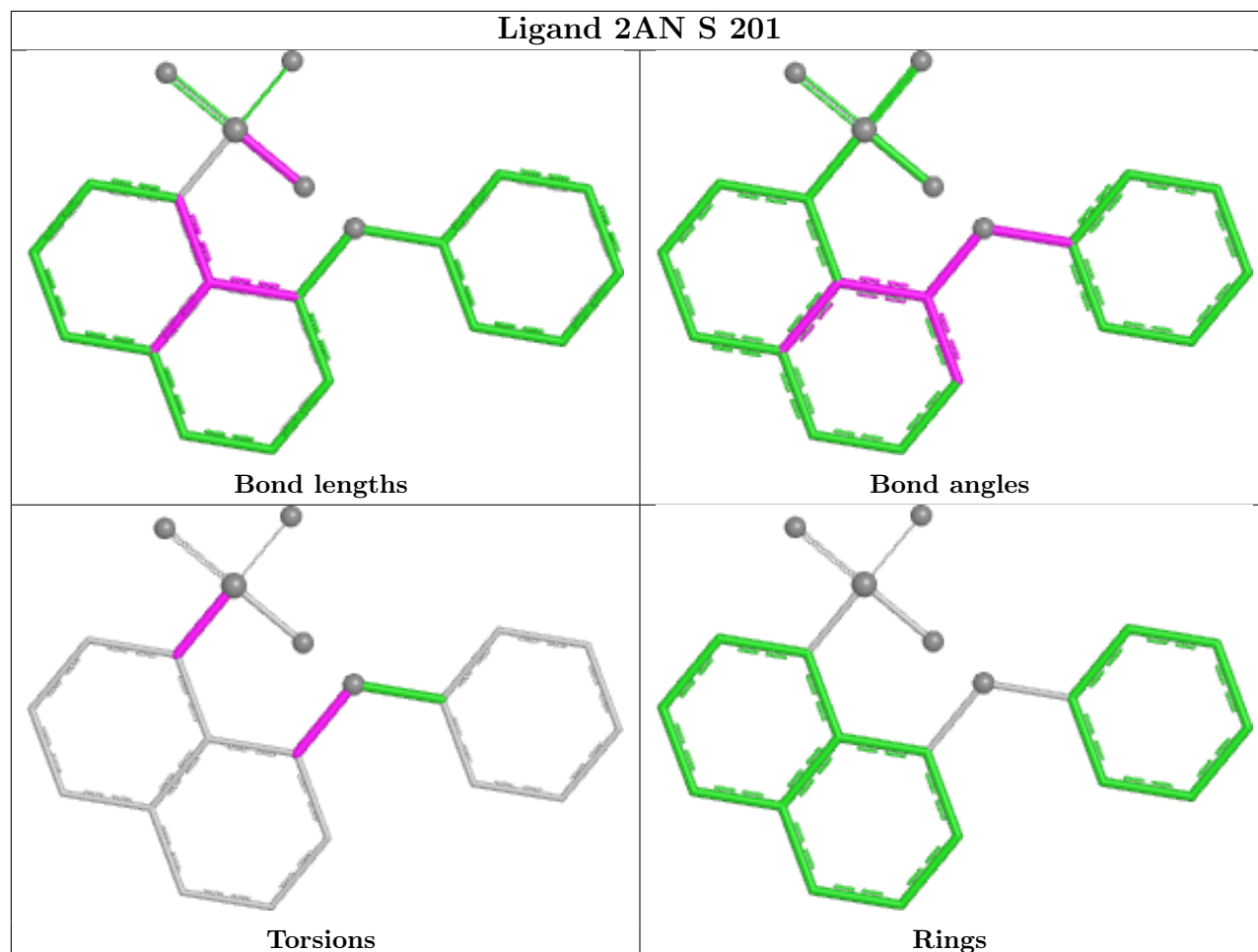
Ligand 2AN B 203

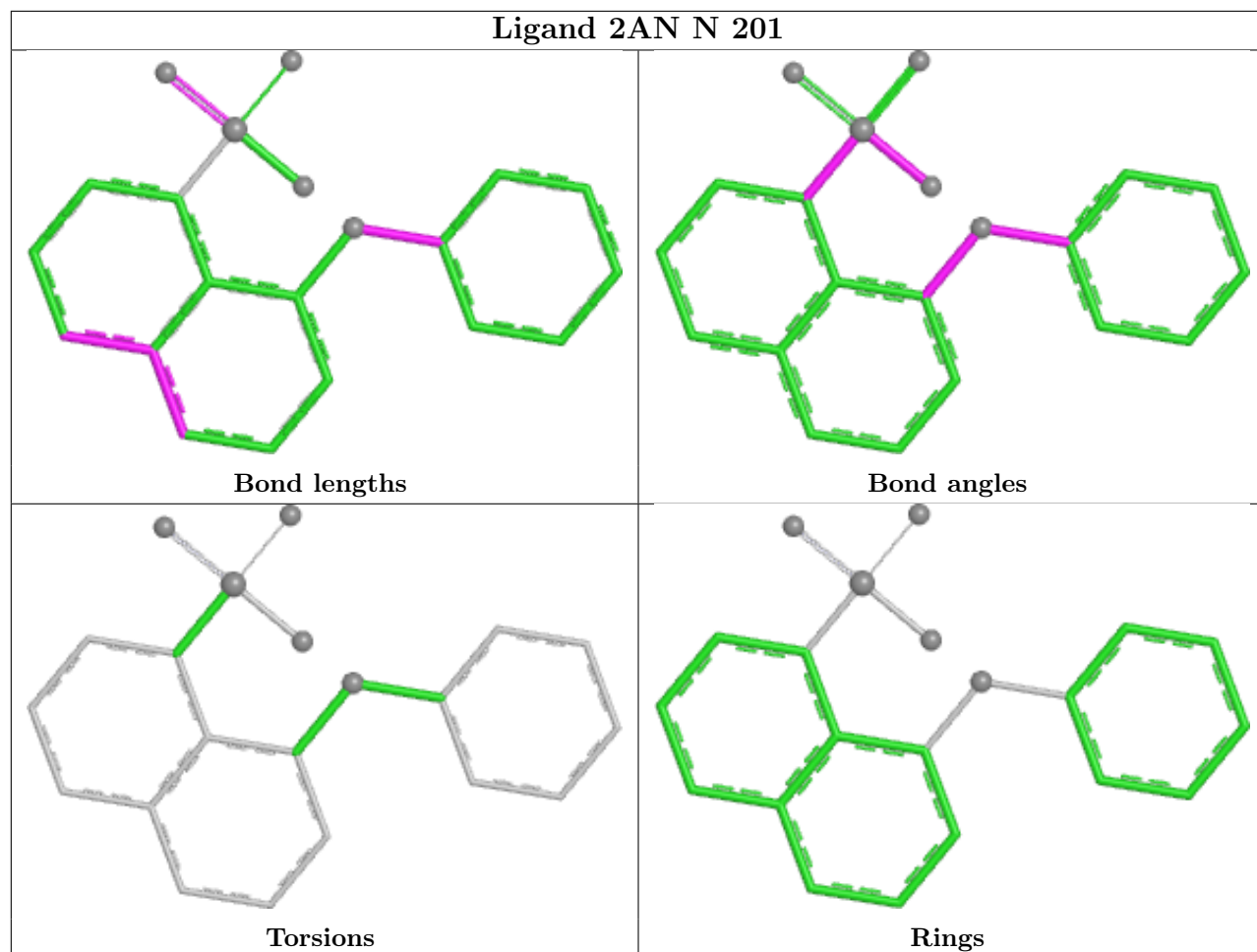


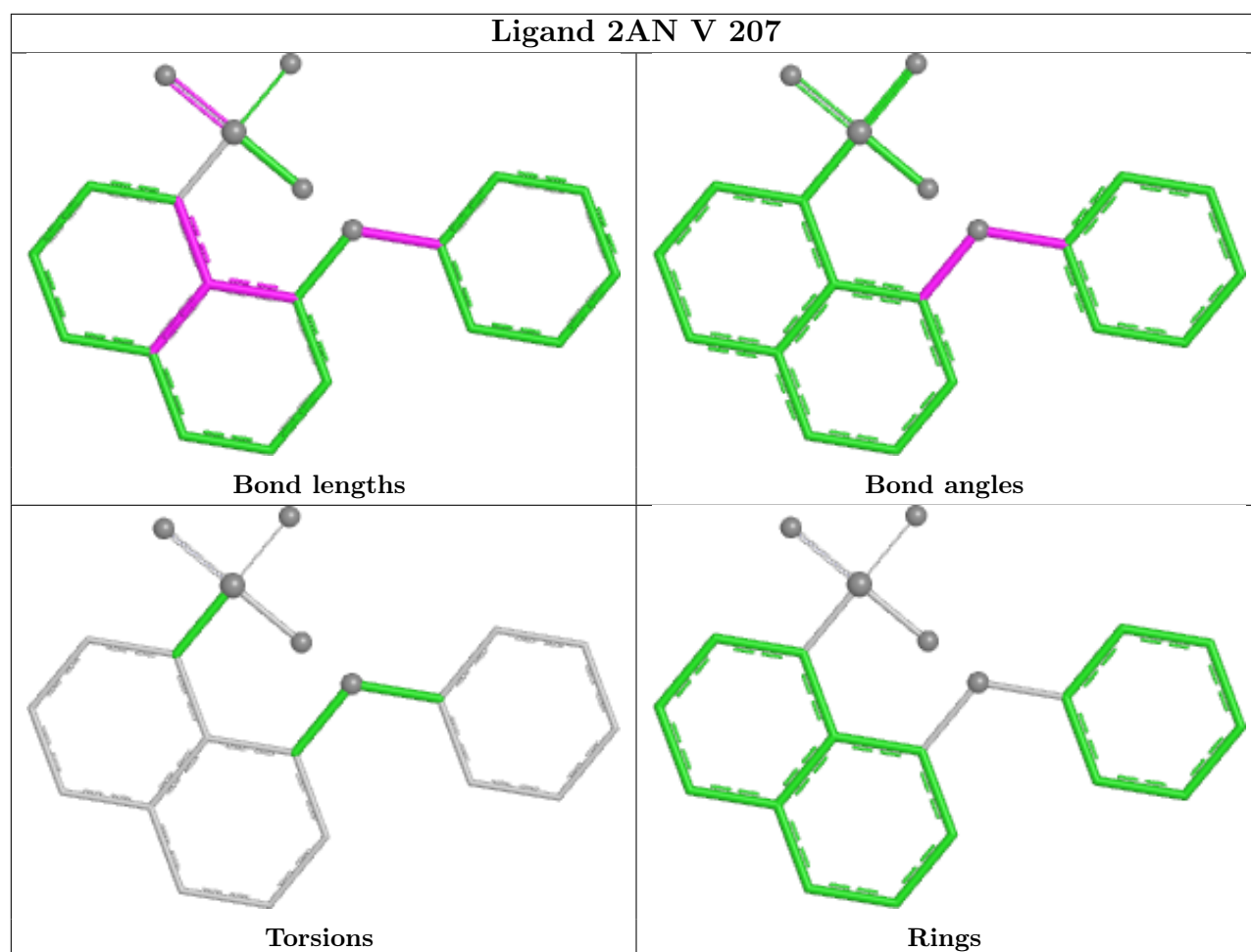


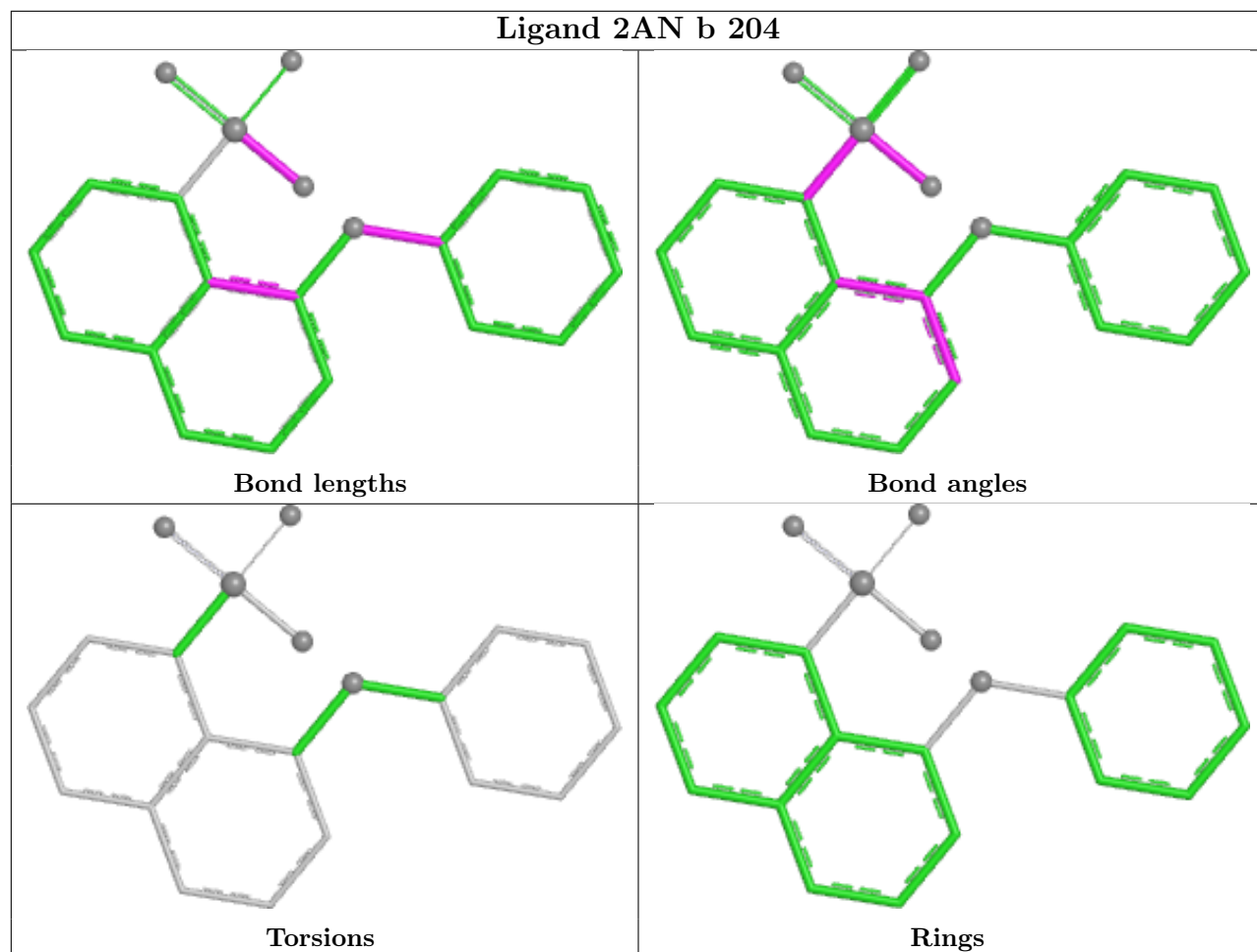


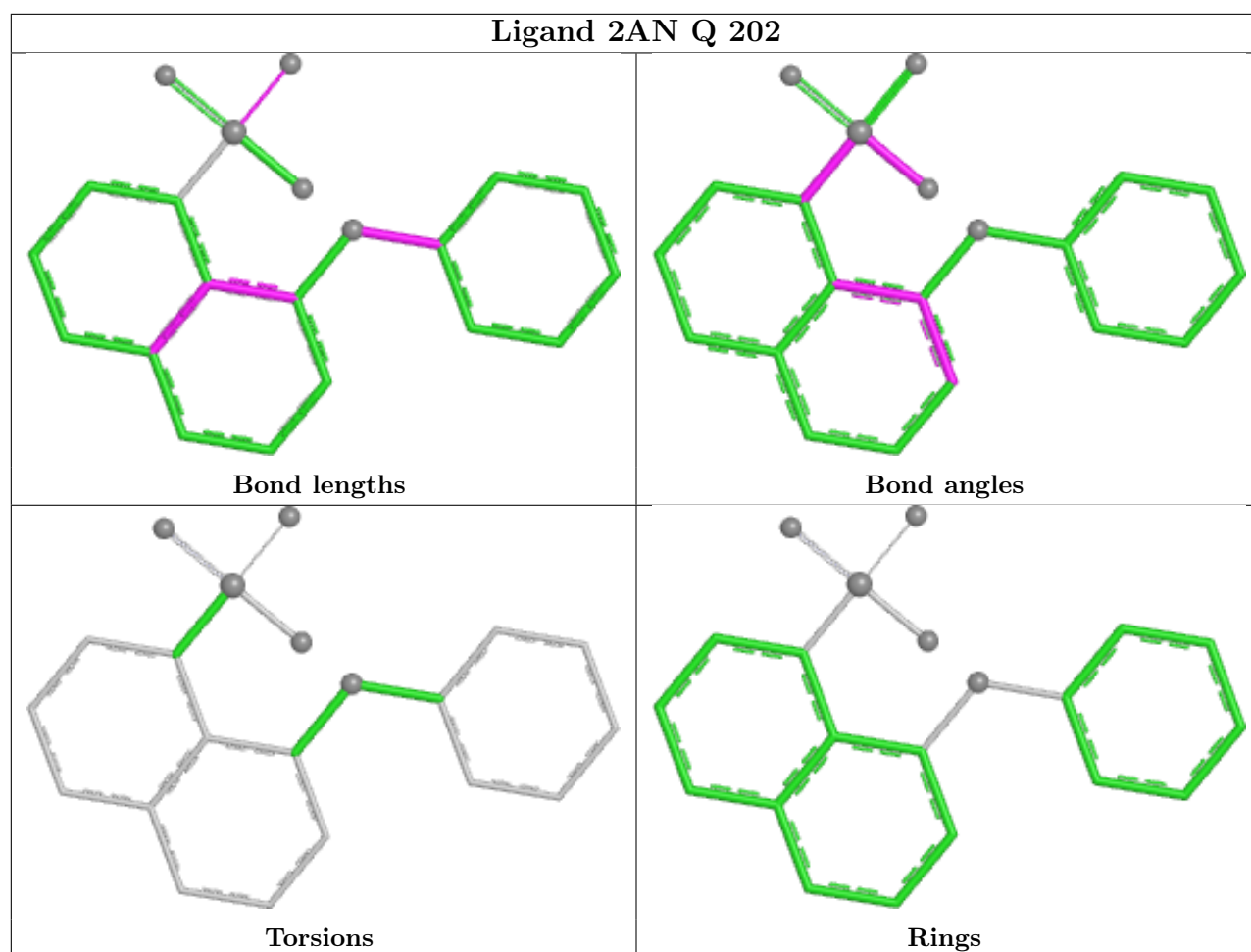
Ligand 2AN S 201



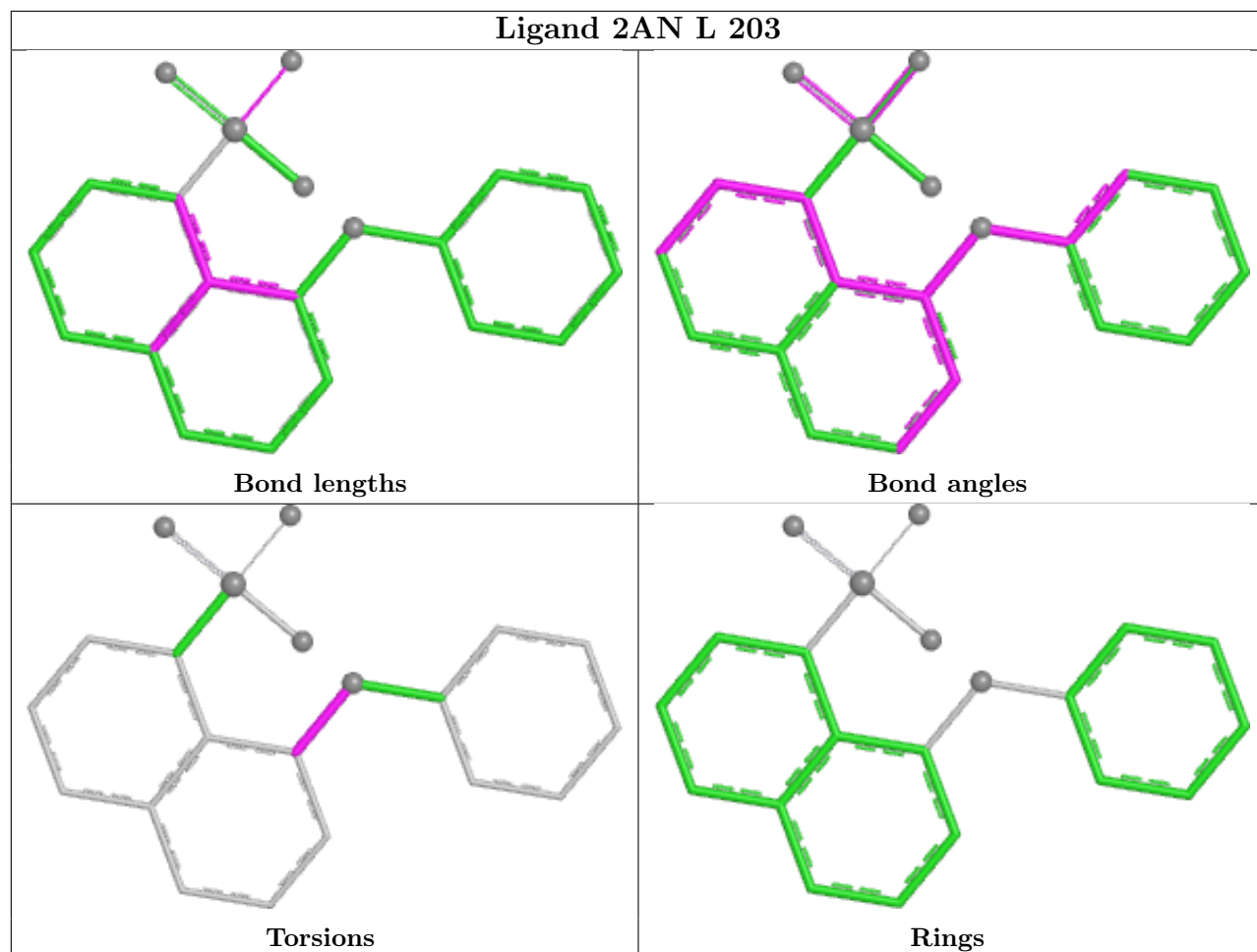


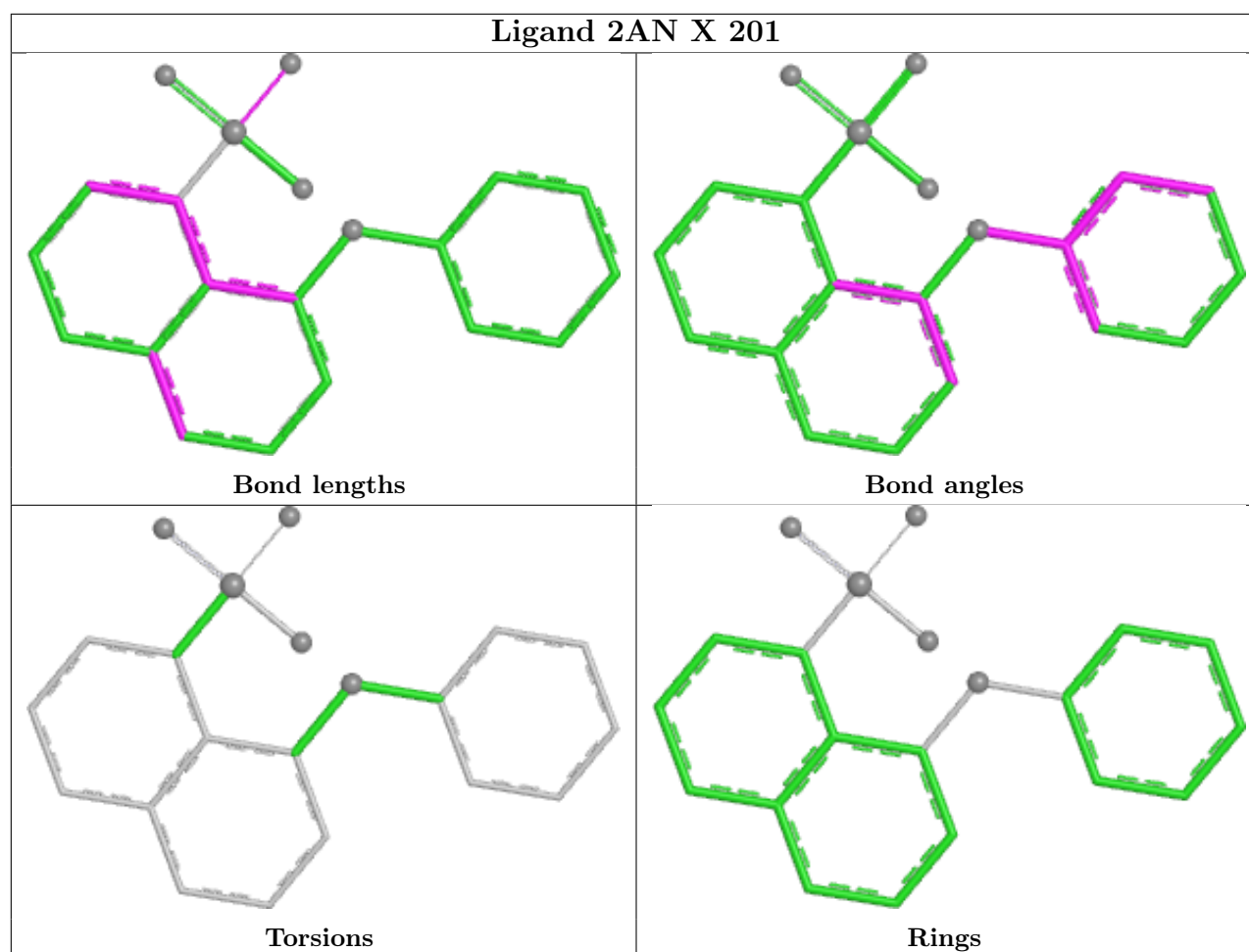


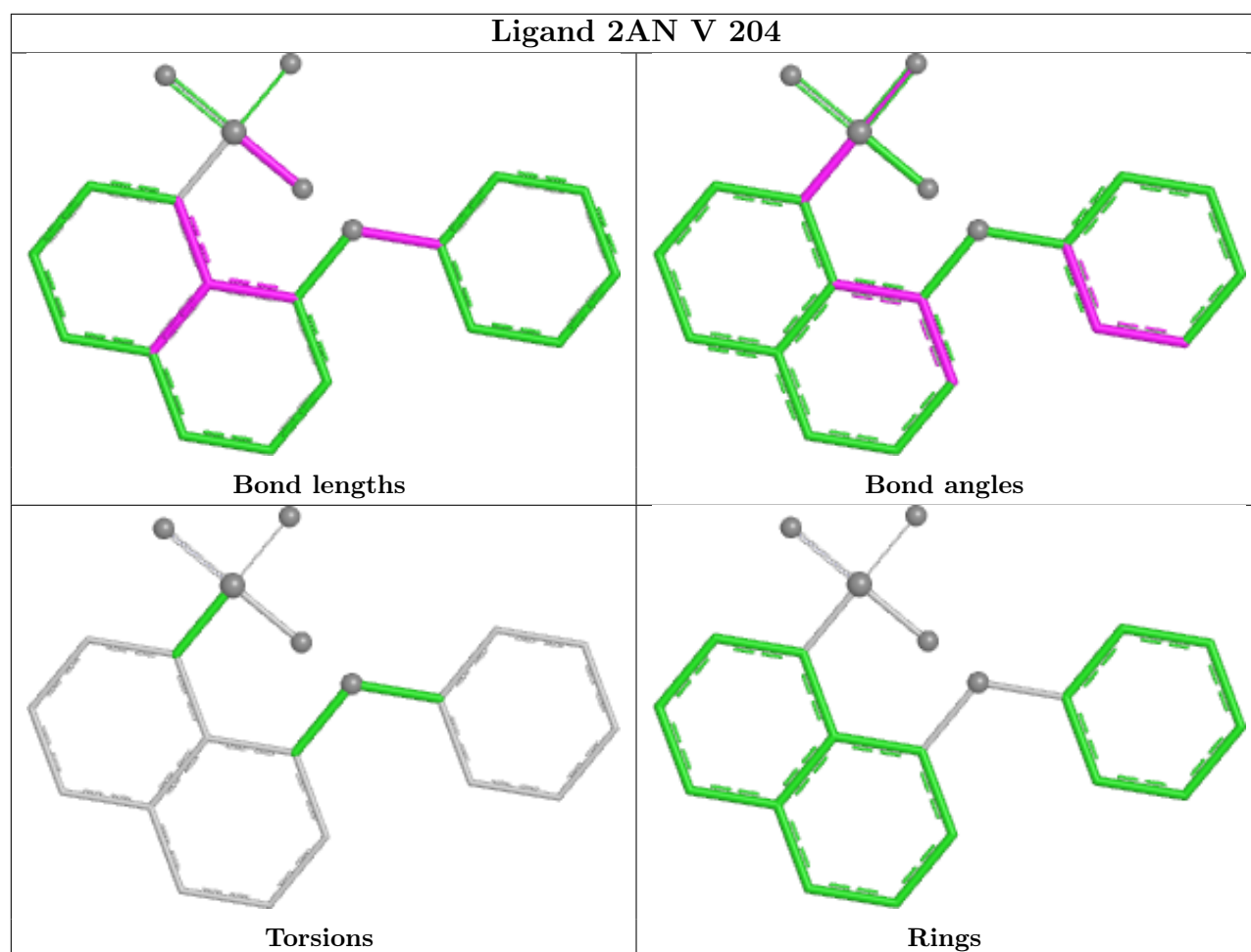




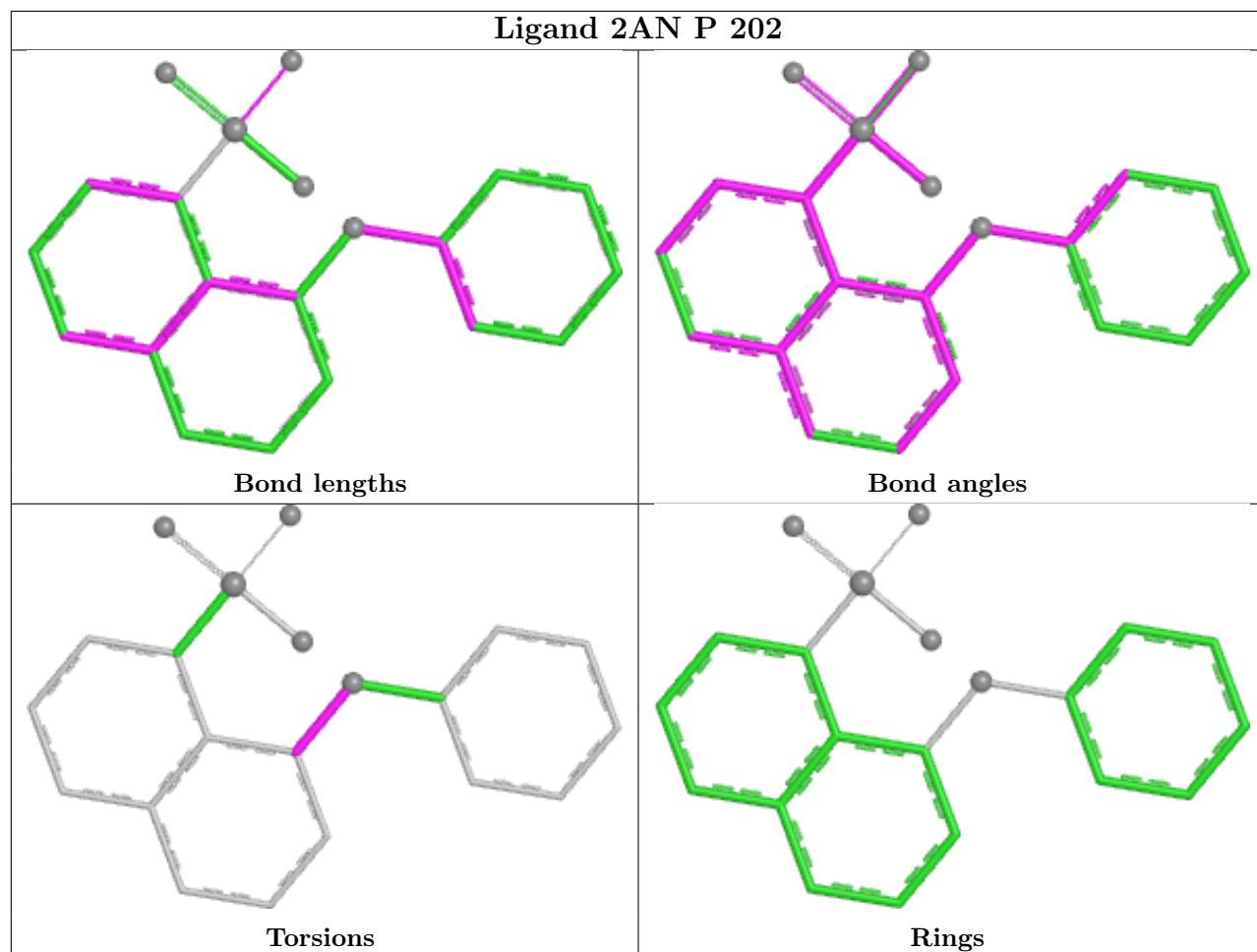
Ligand 2AN L 203

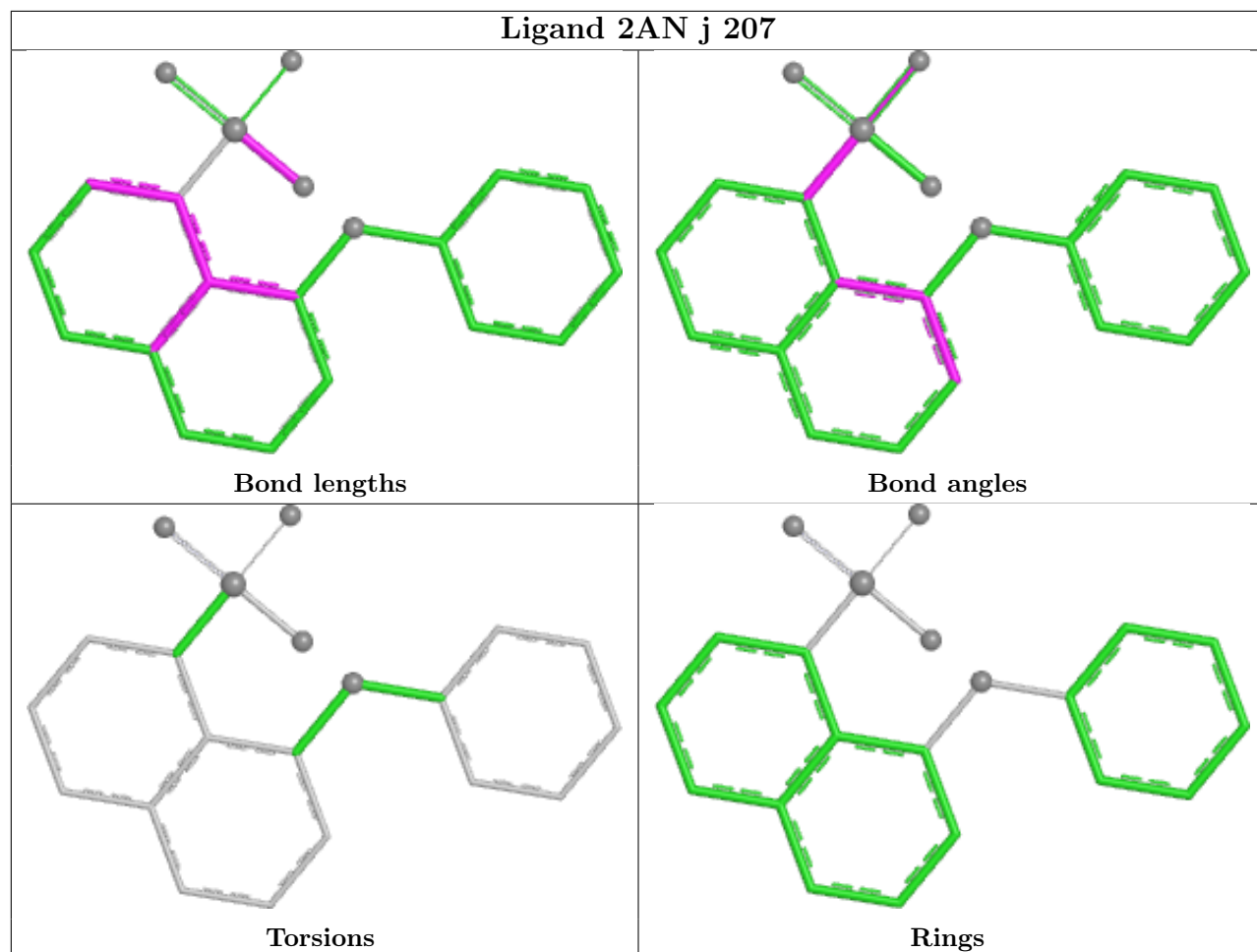




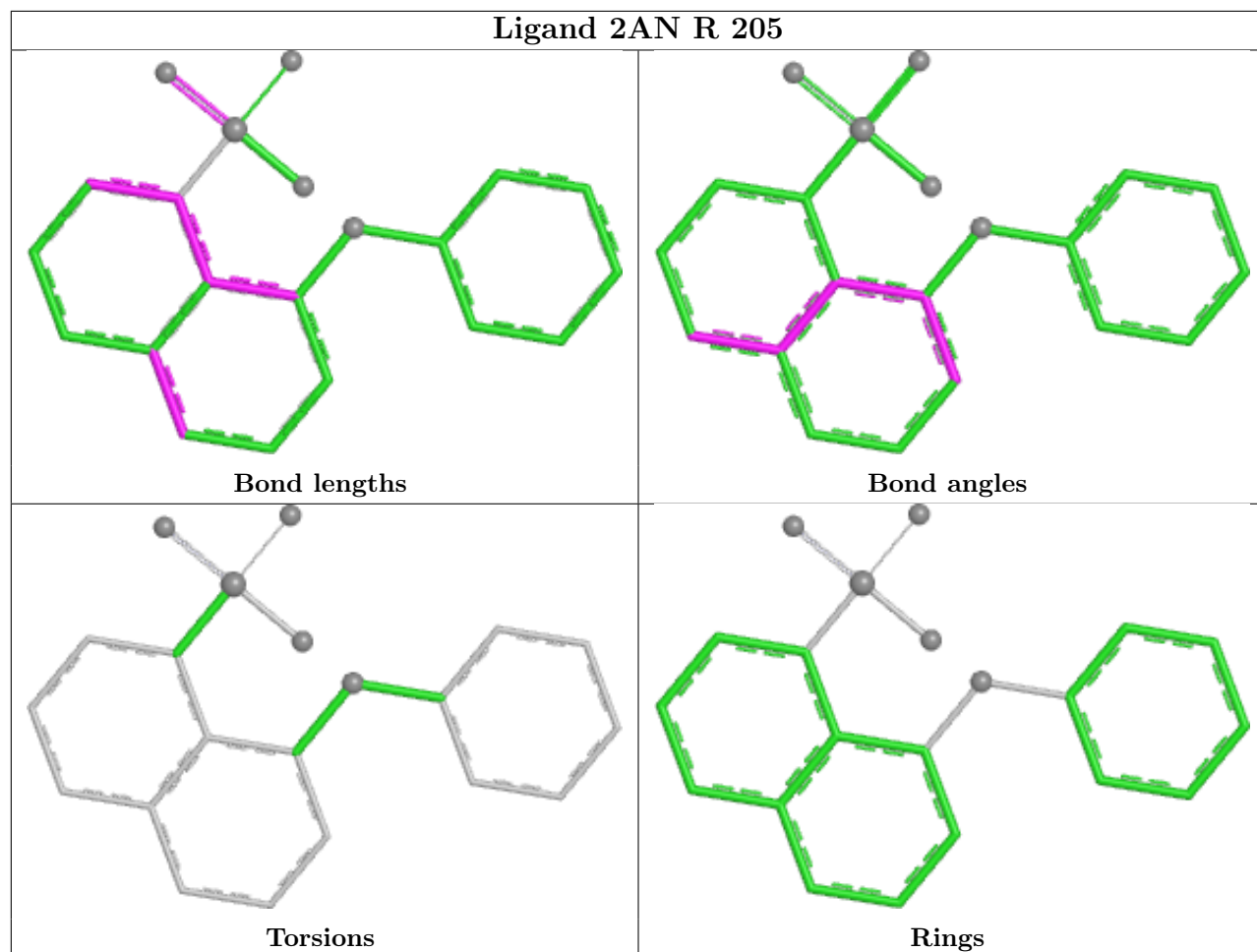


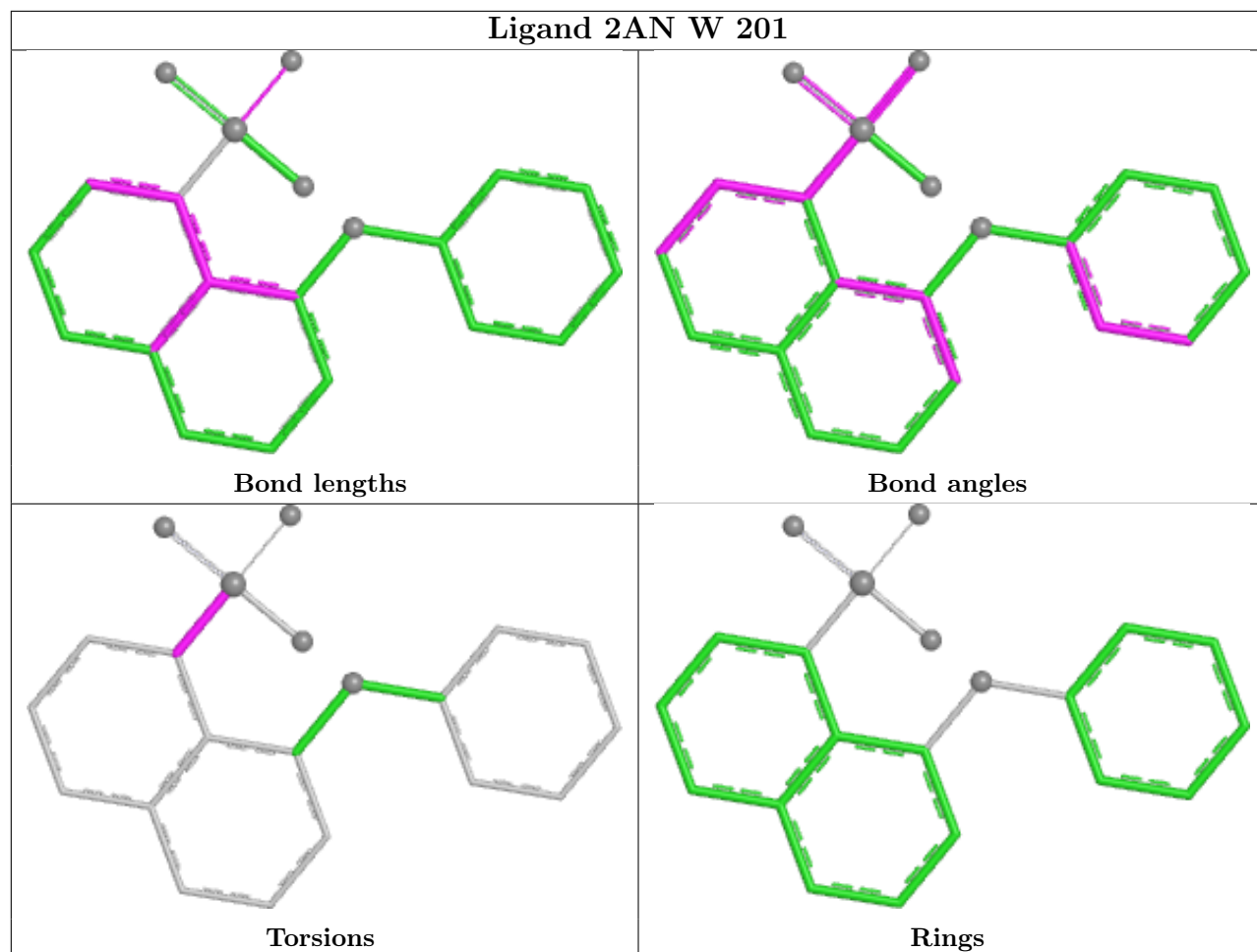
Ligand 2AN P 202



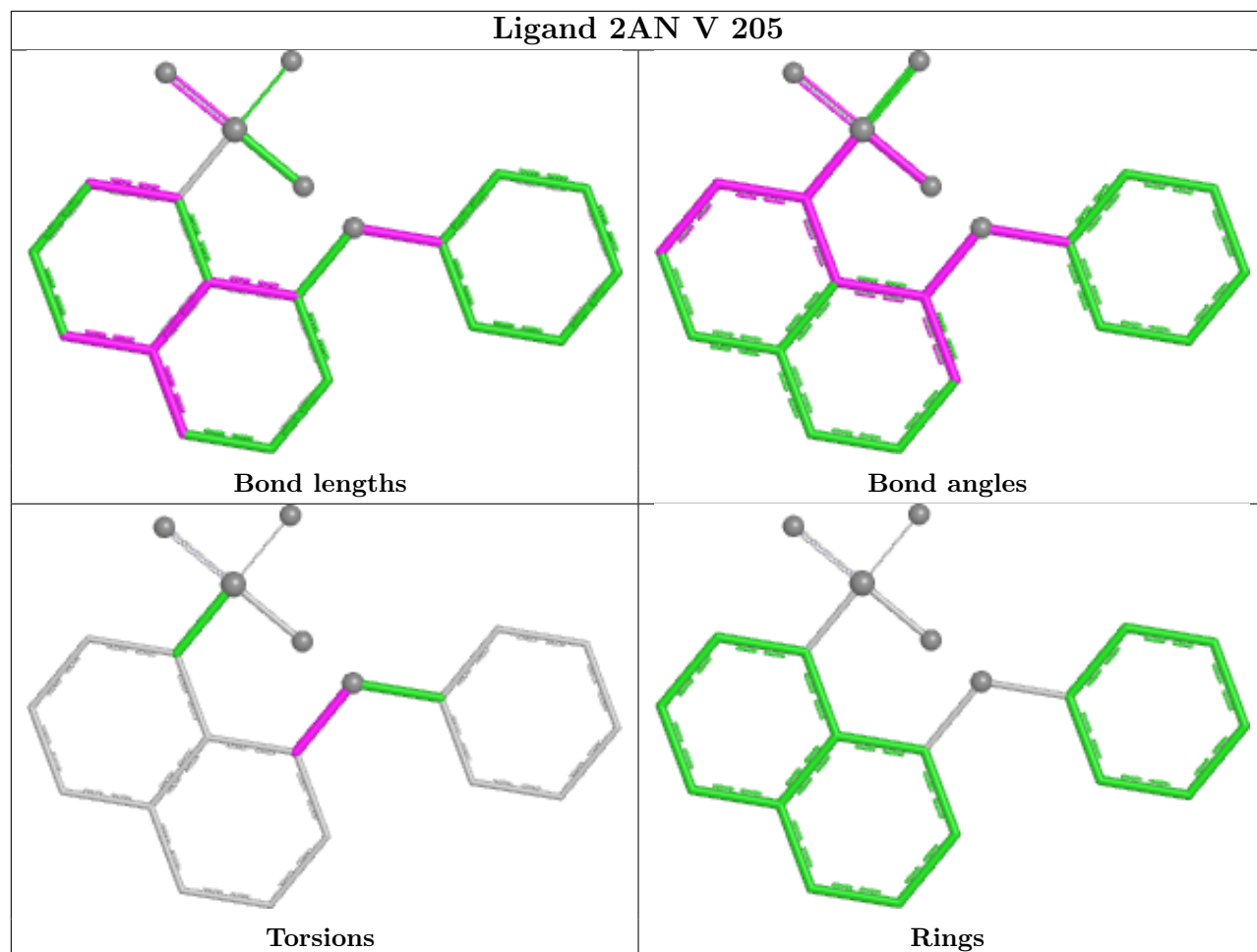


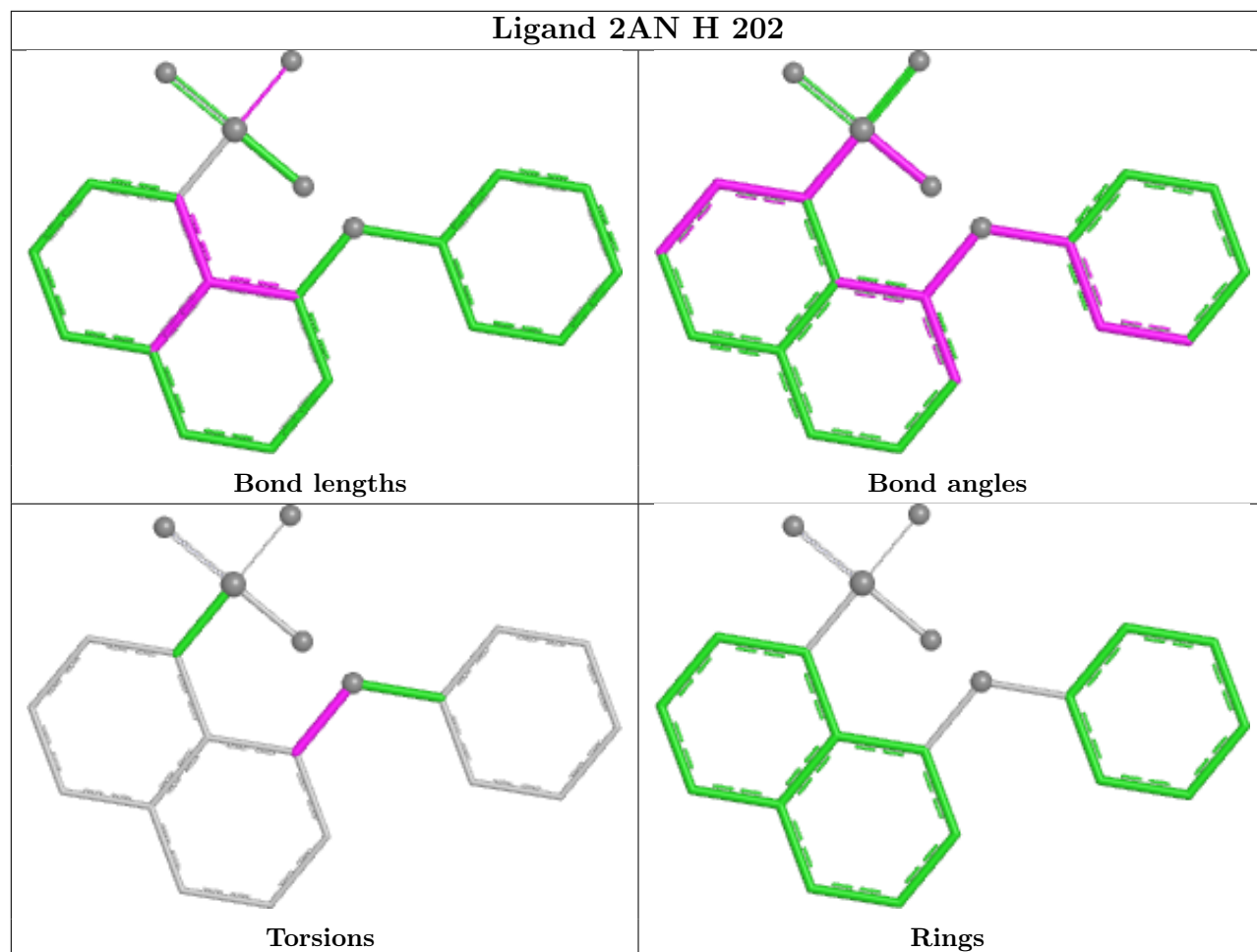
Ligand 2AN R 205



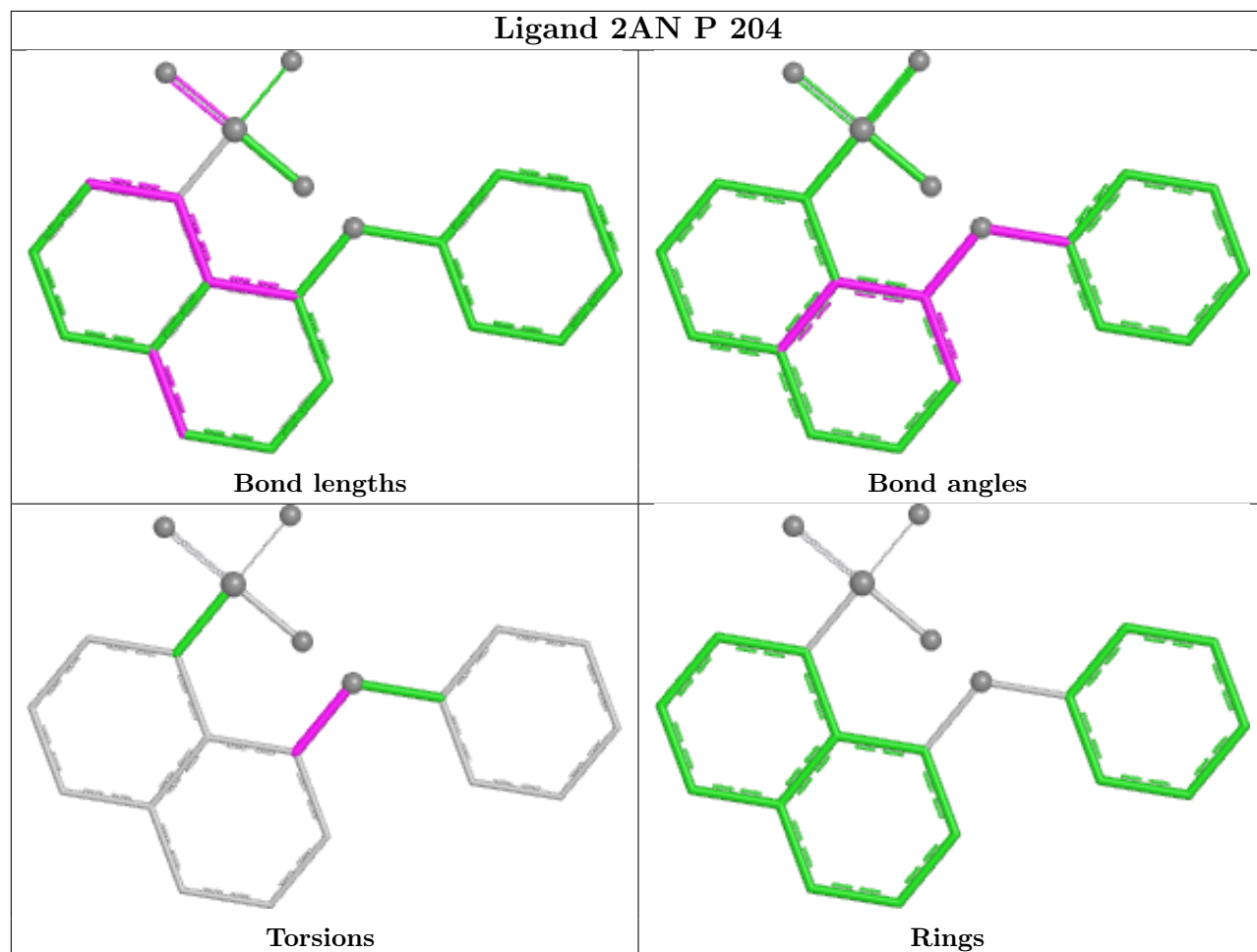


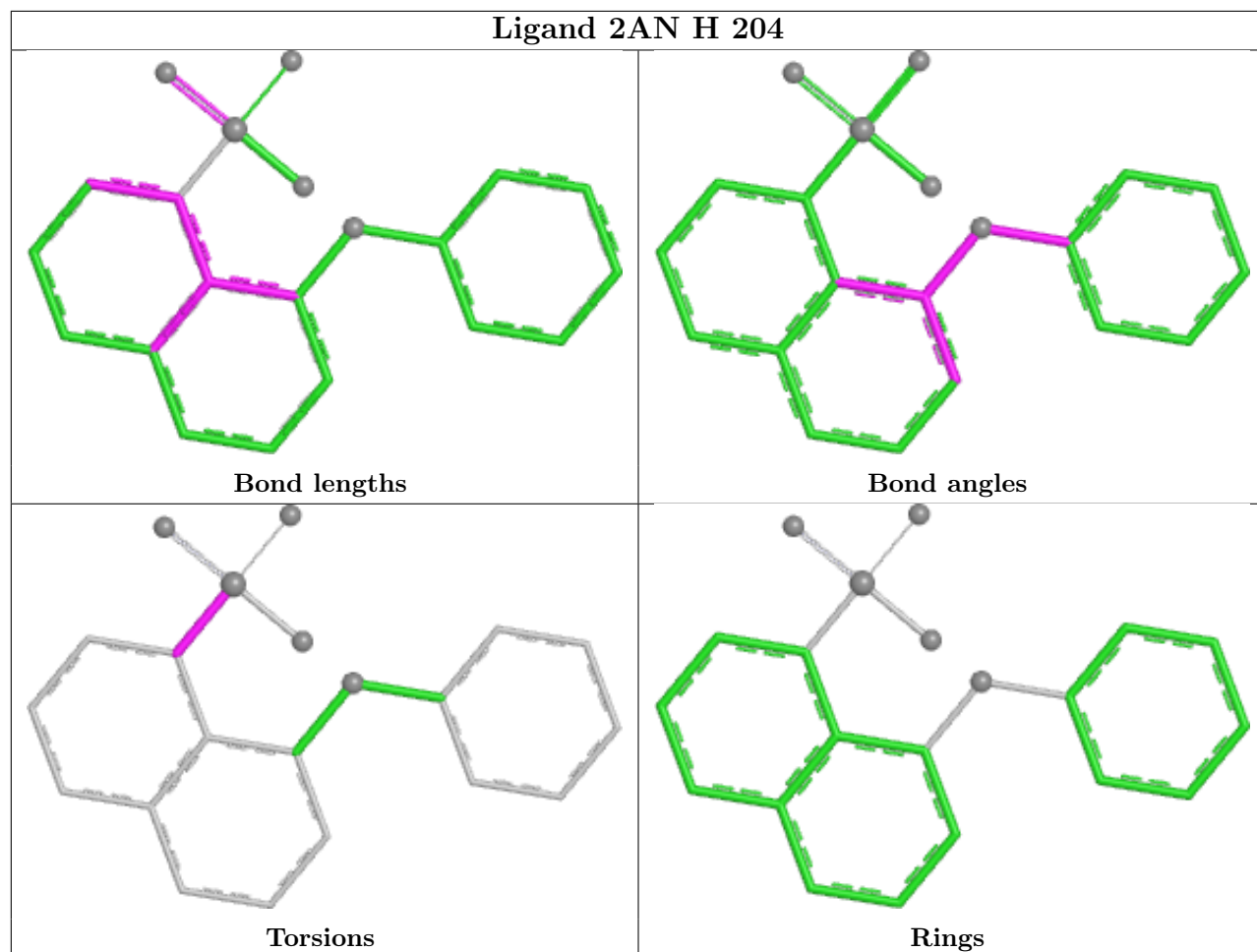
Ligand 2AN V 205

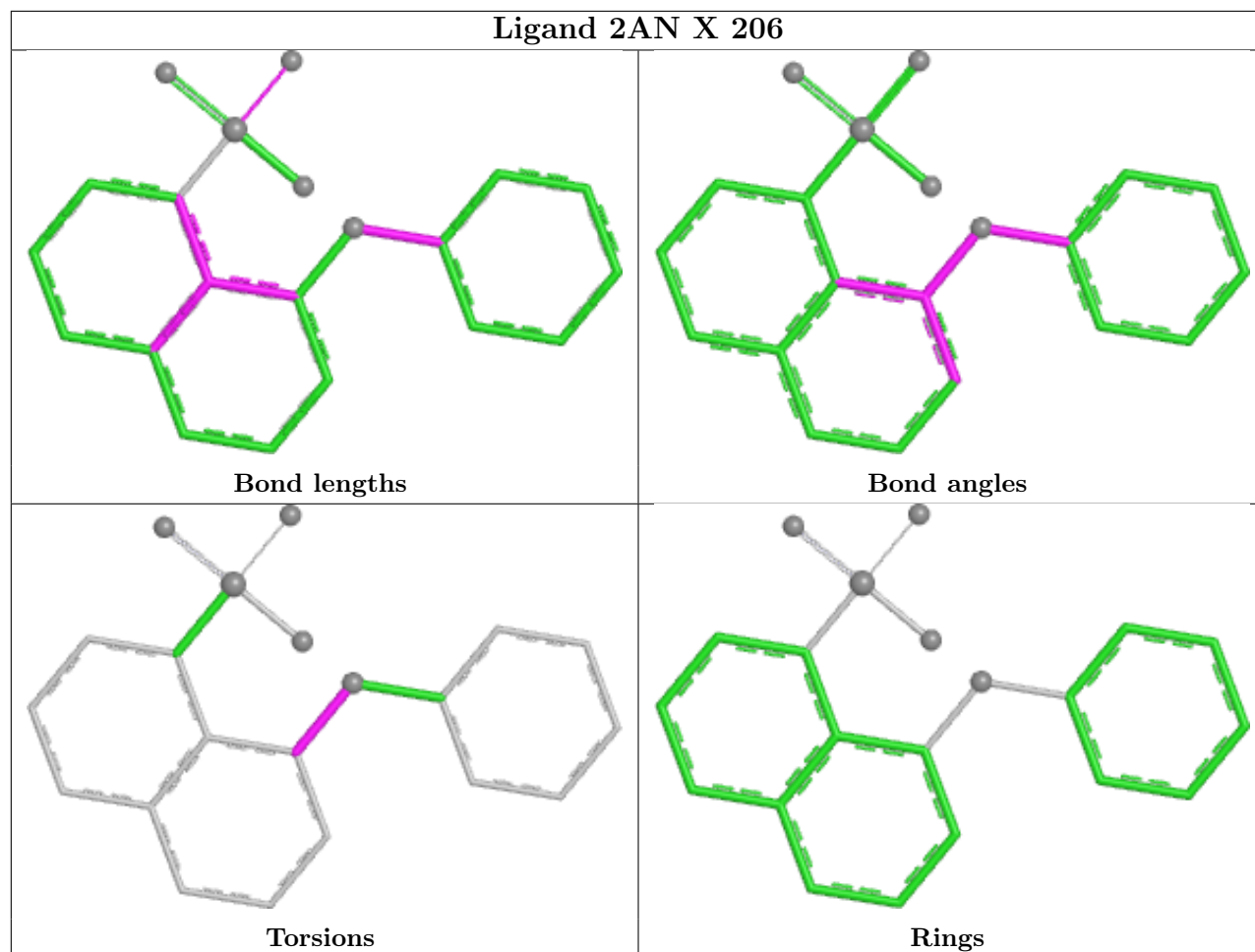


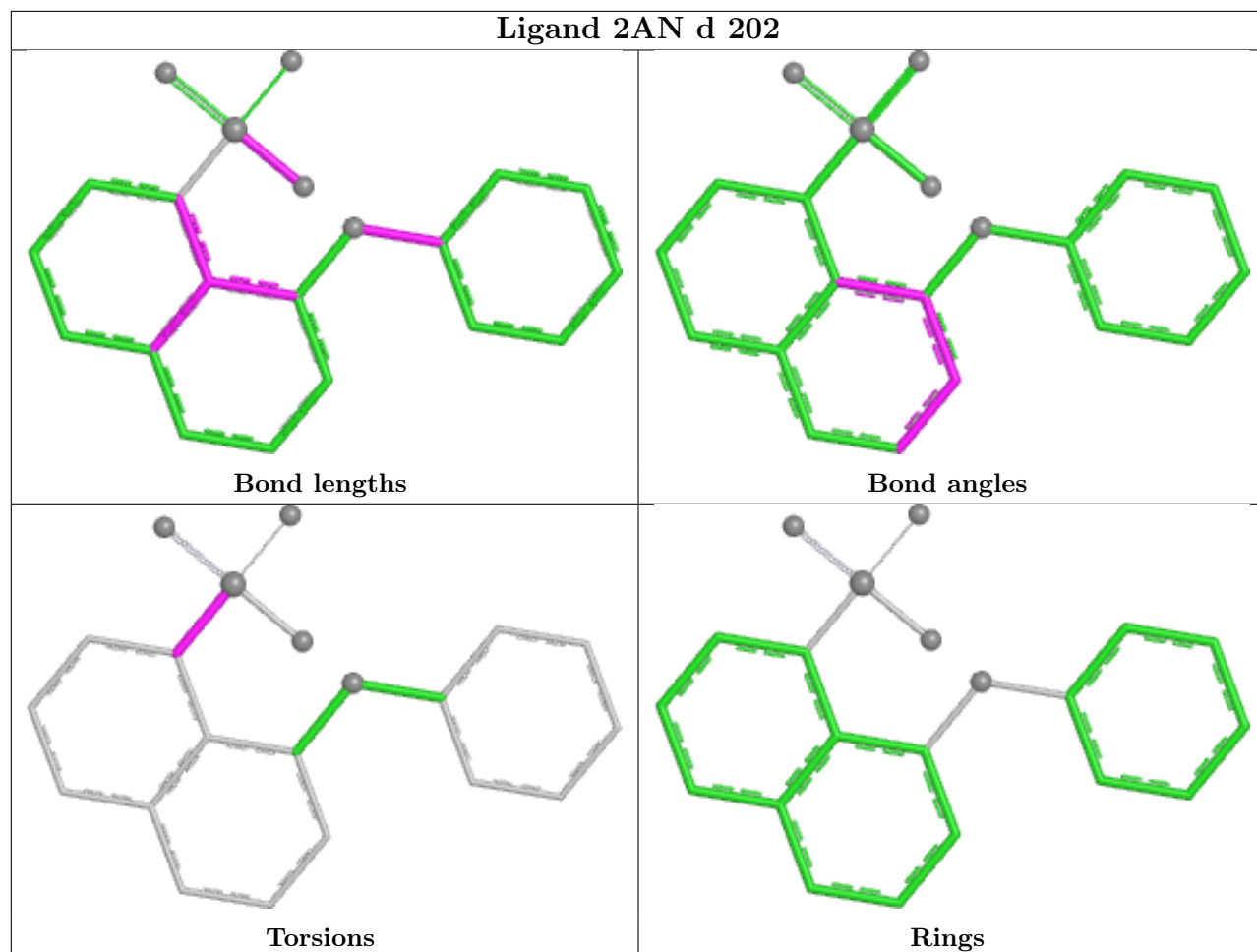


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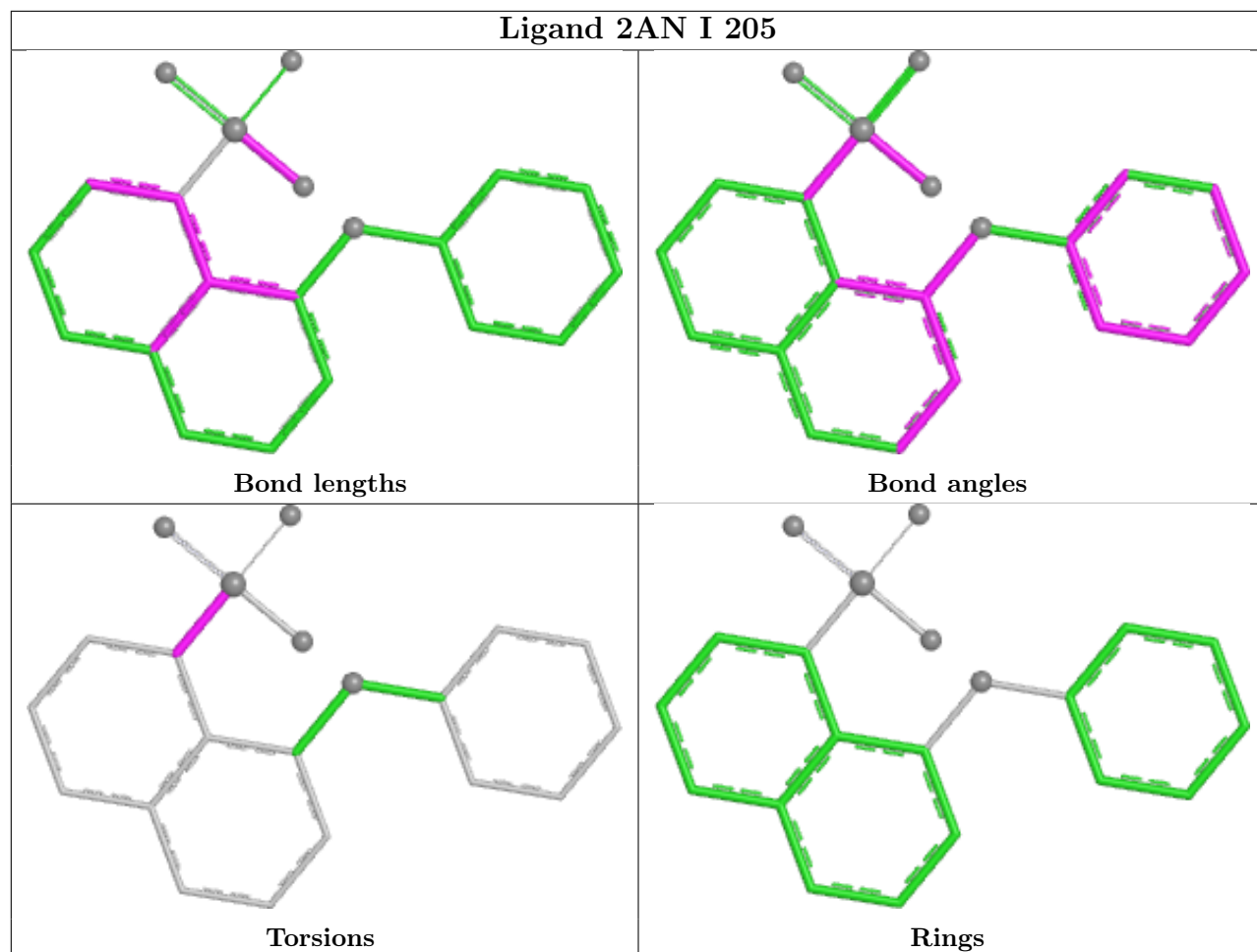


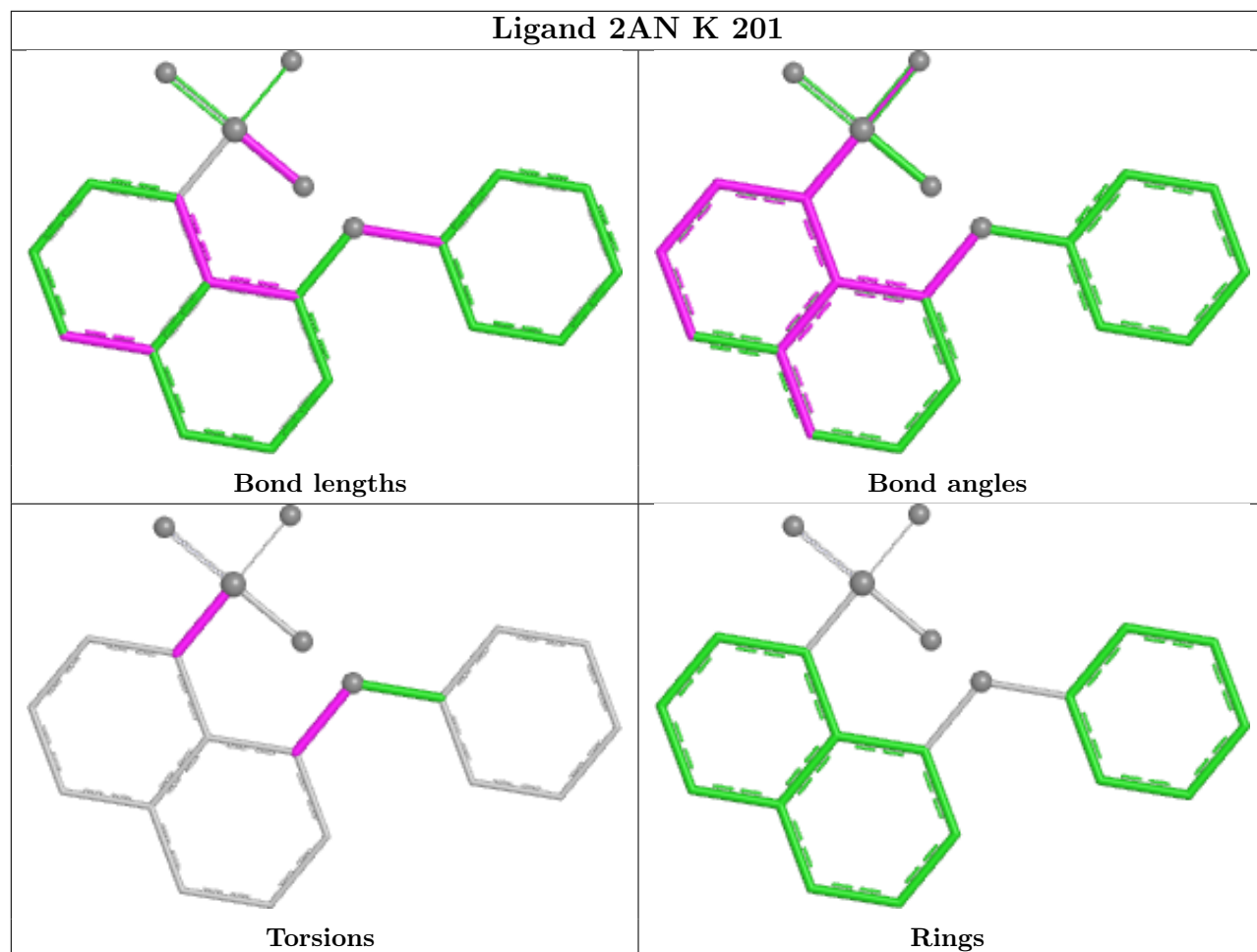




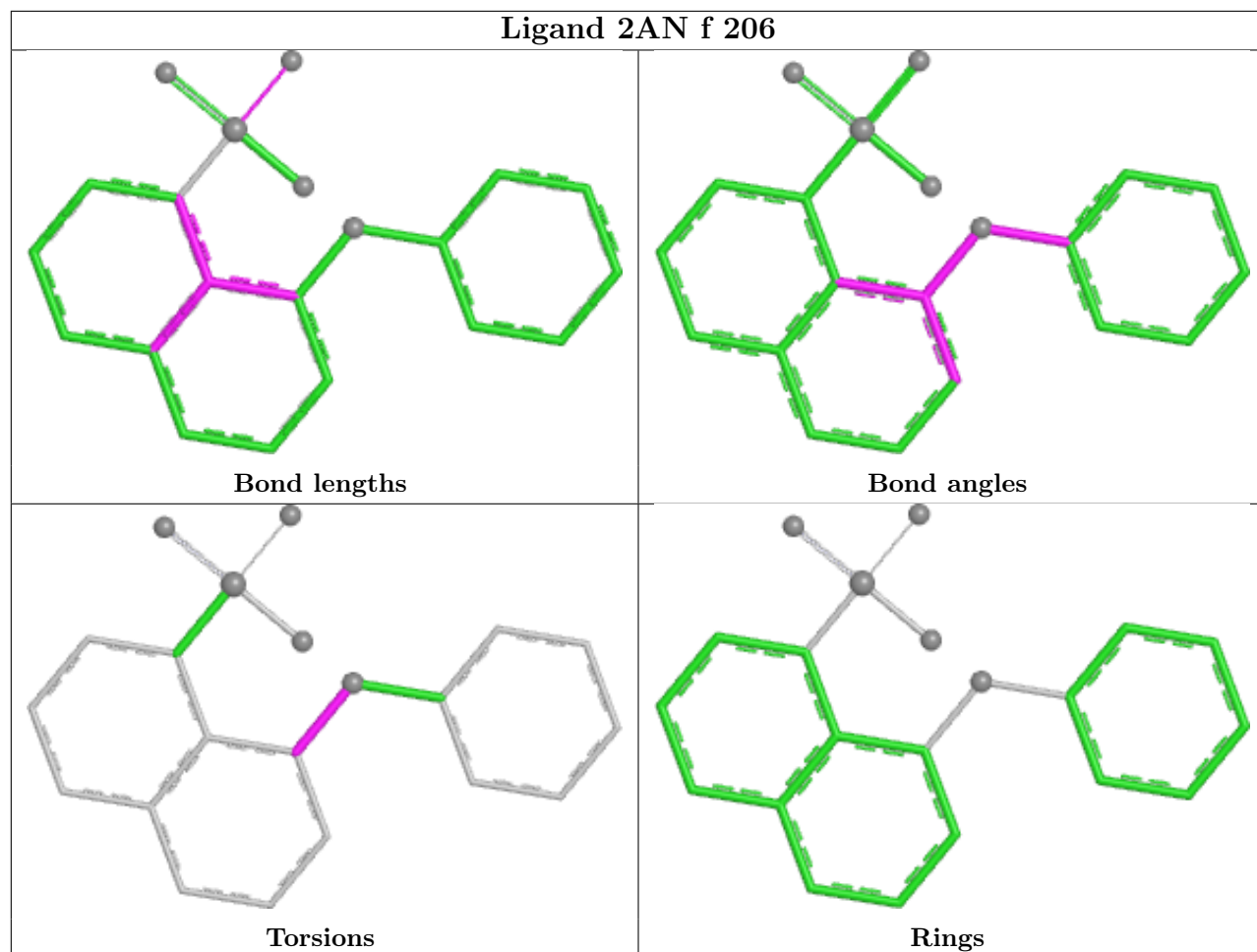


Ligand 2AN I 205

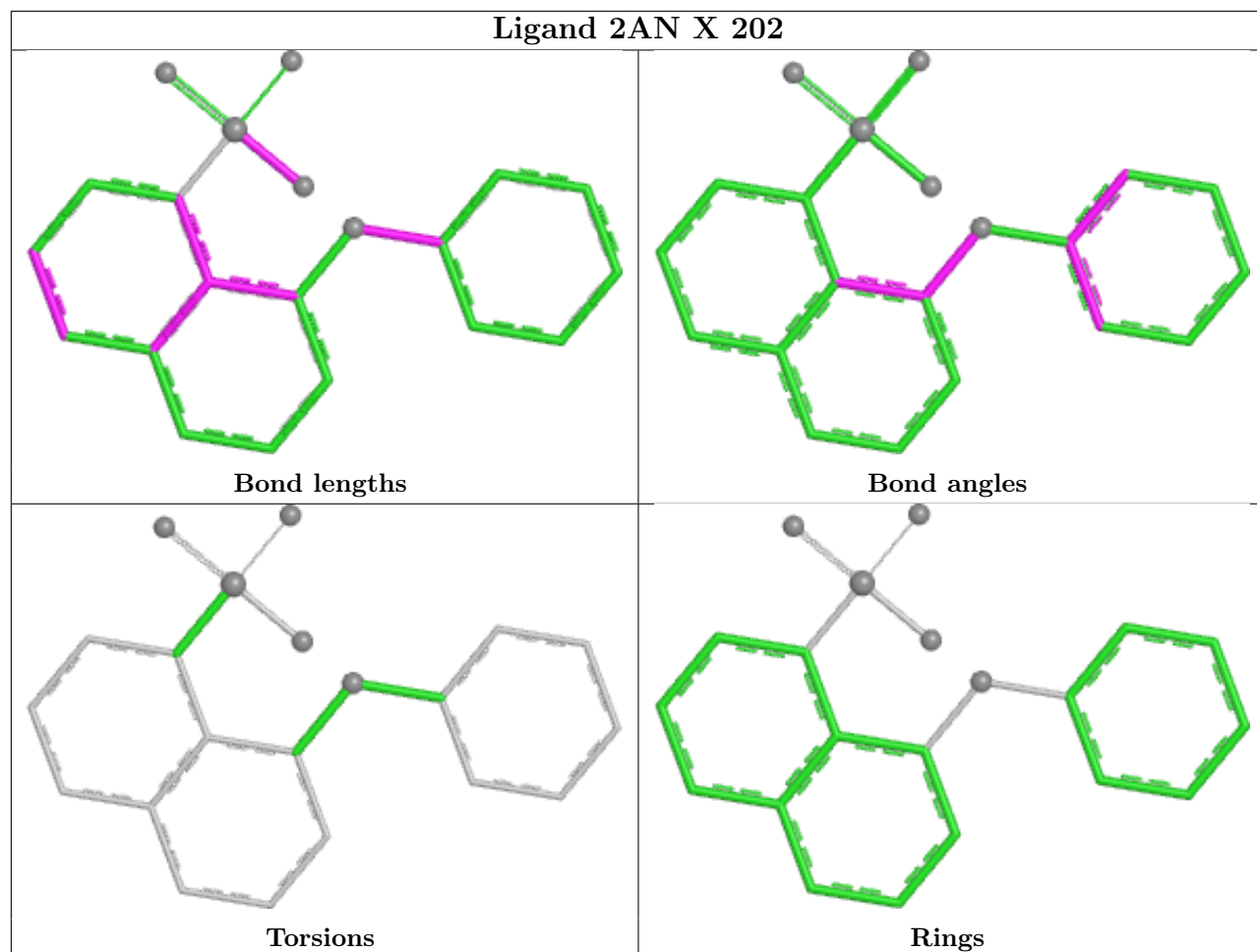




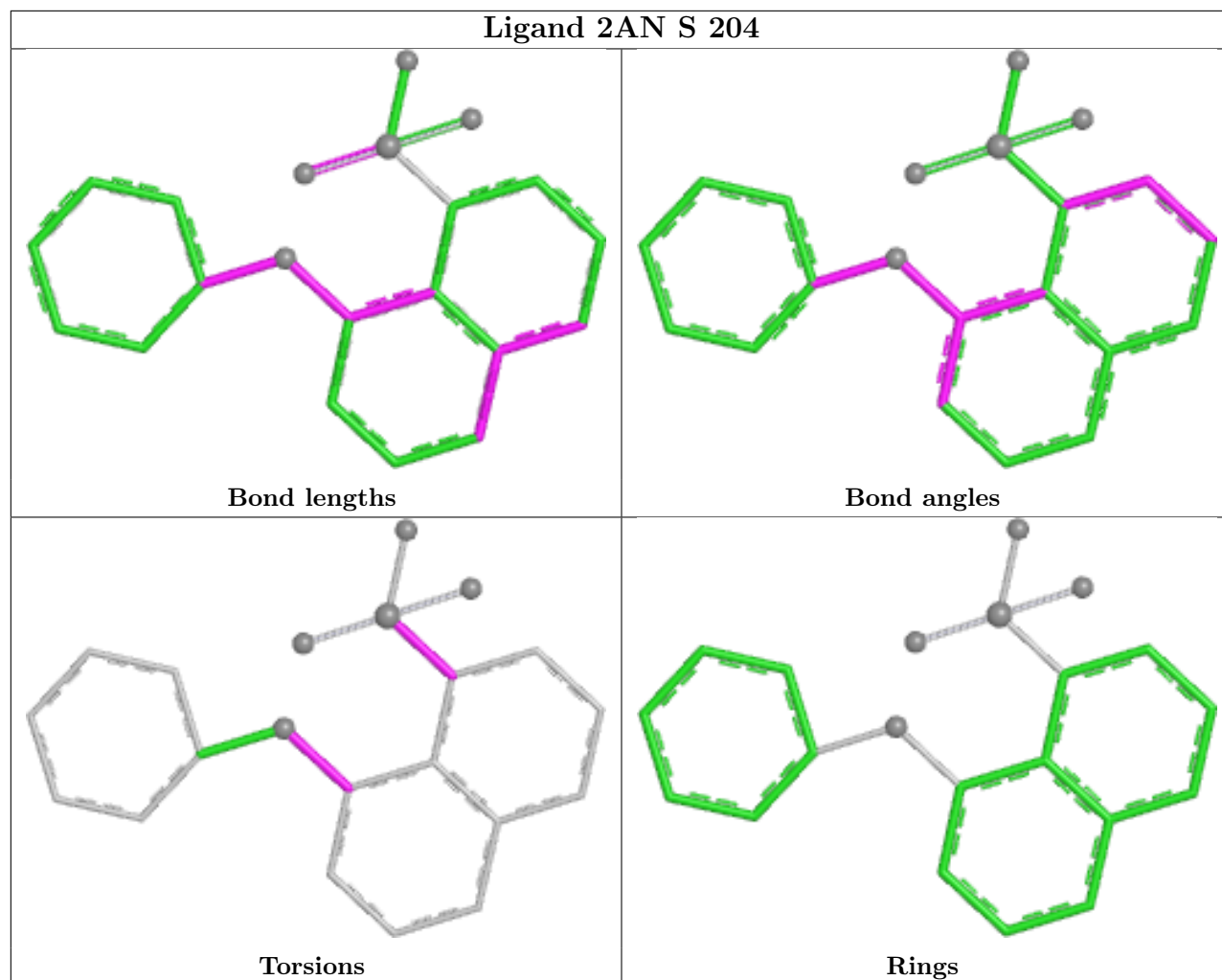
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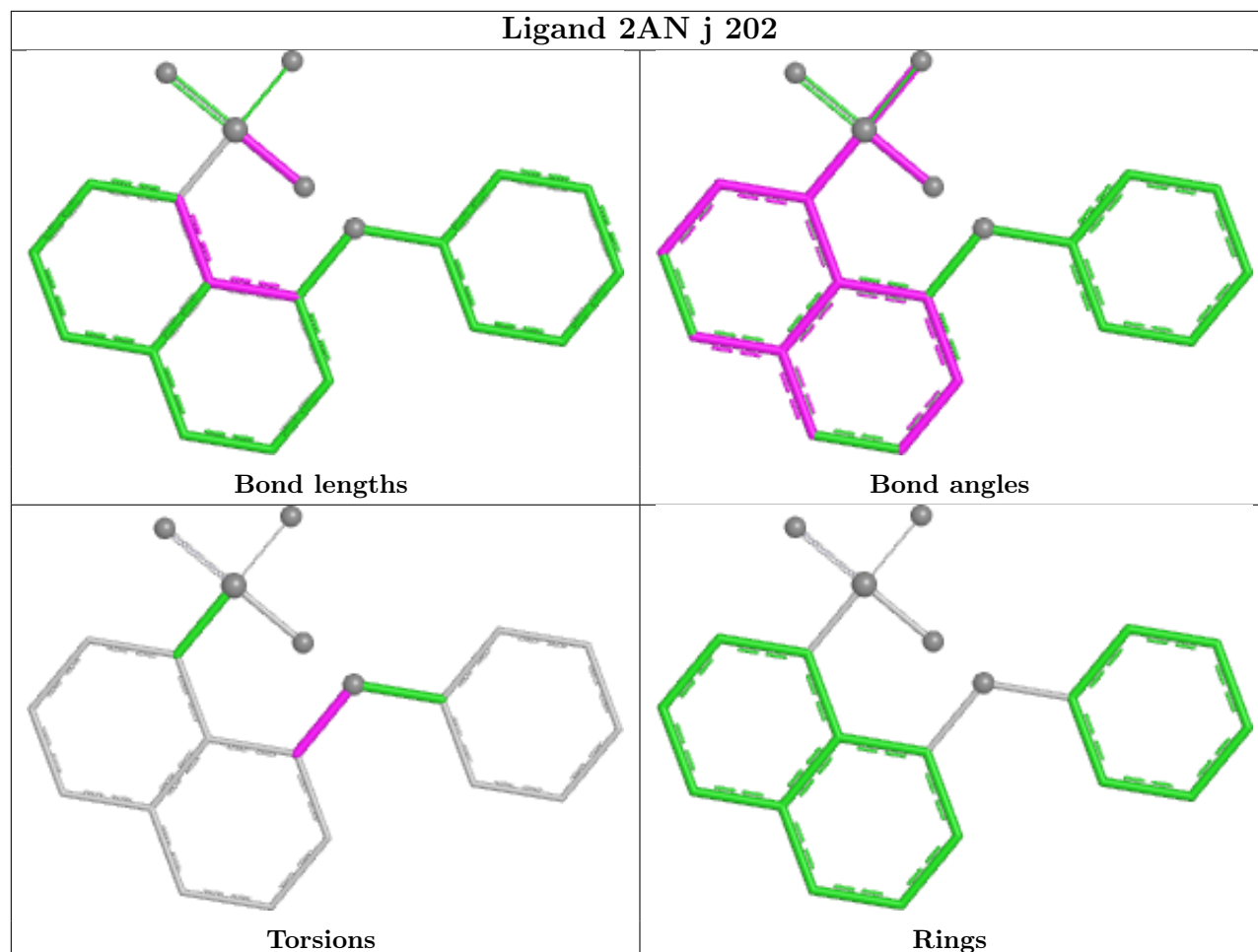
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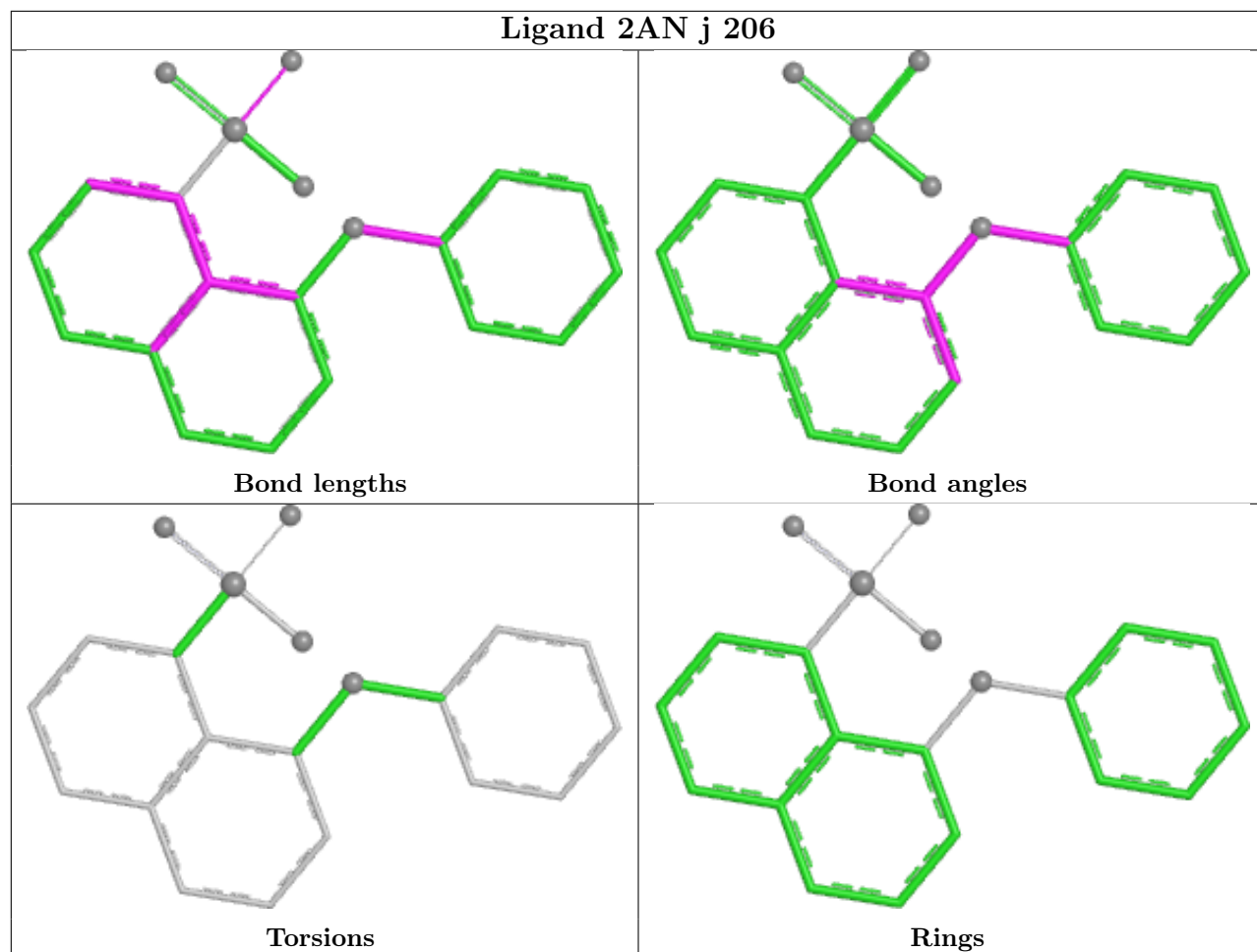


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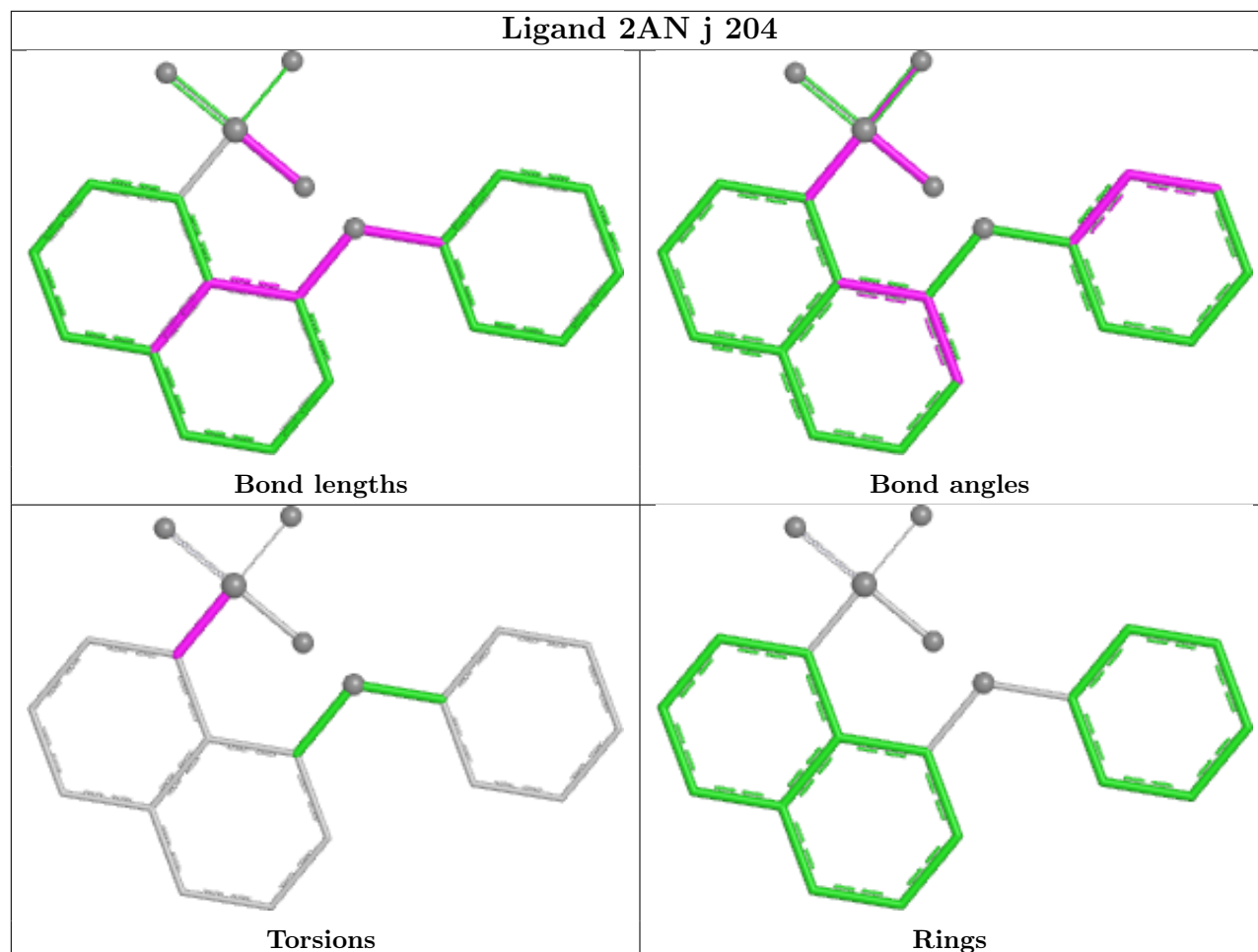


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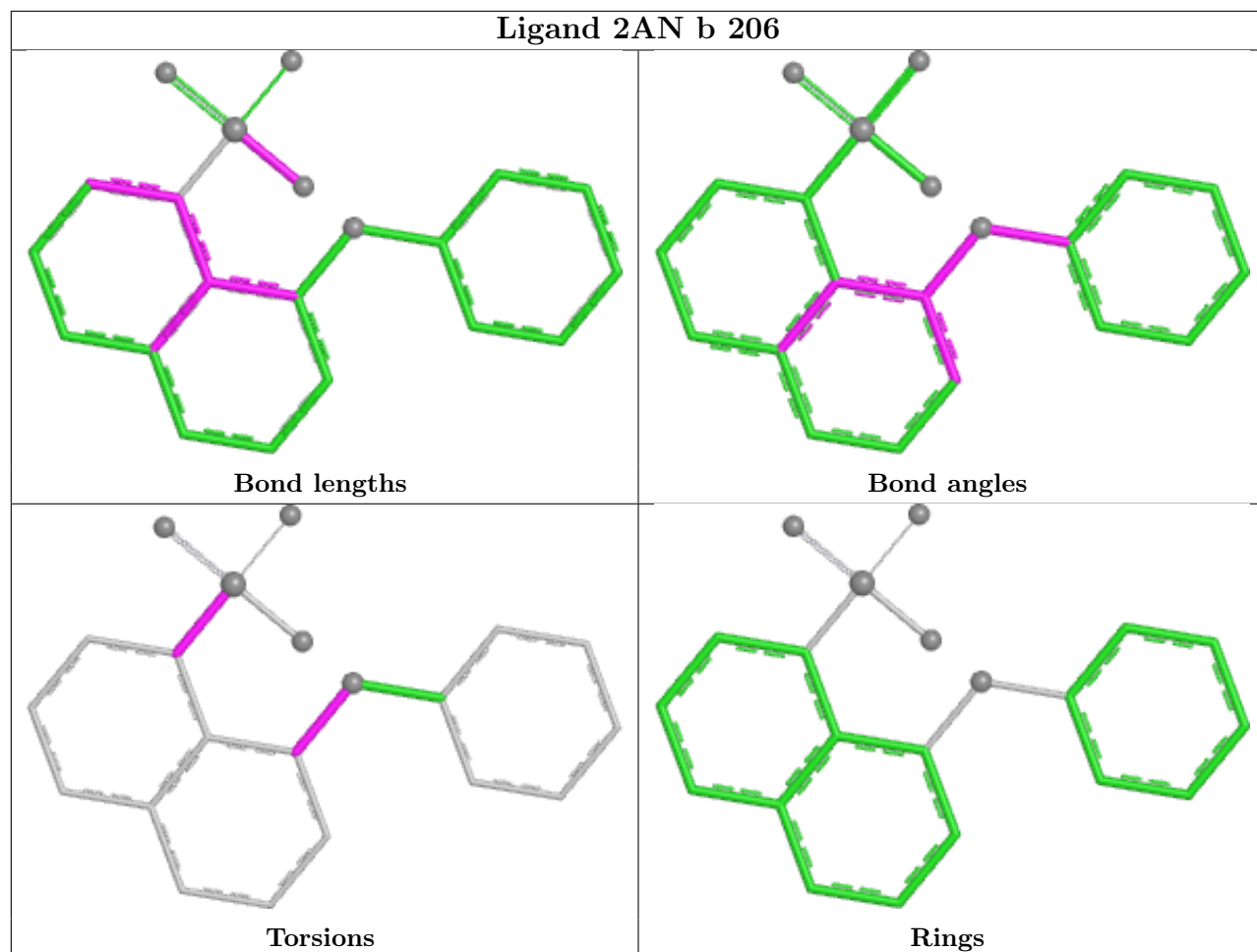




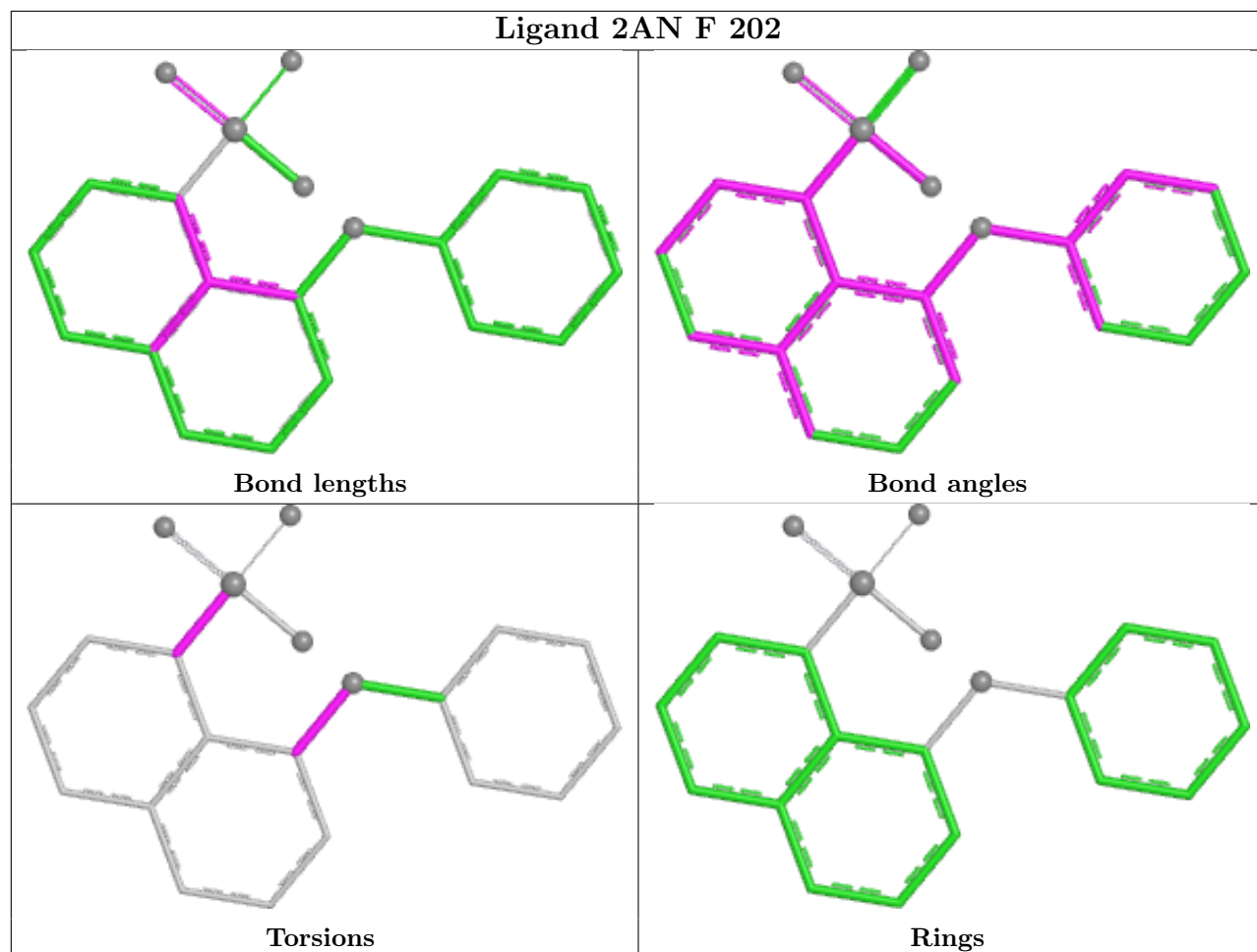
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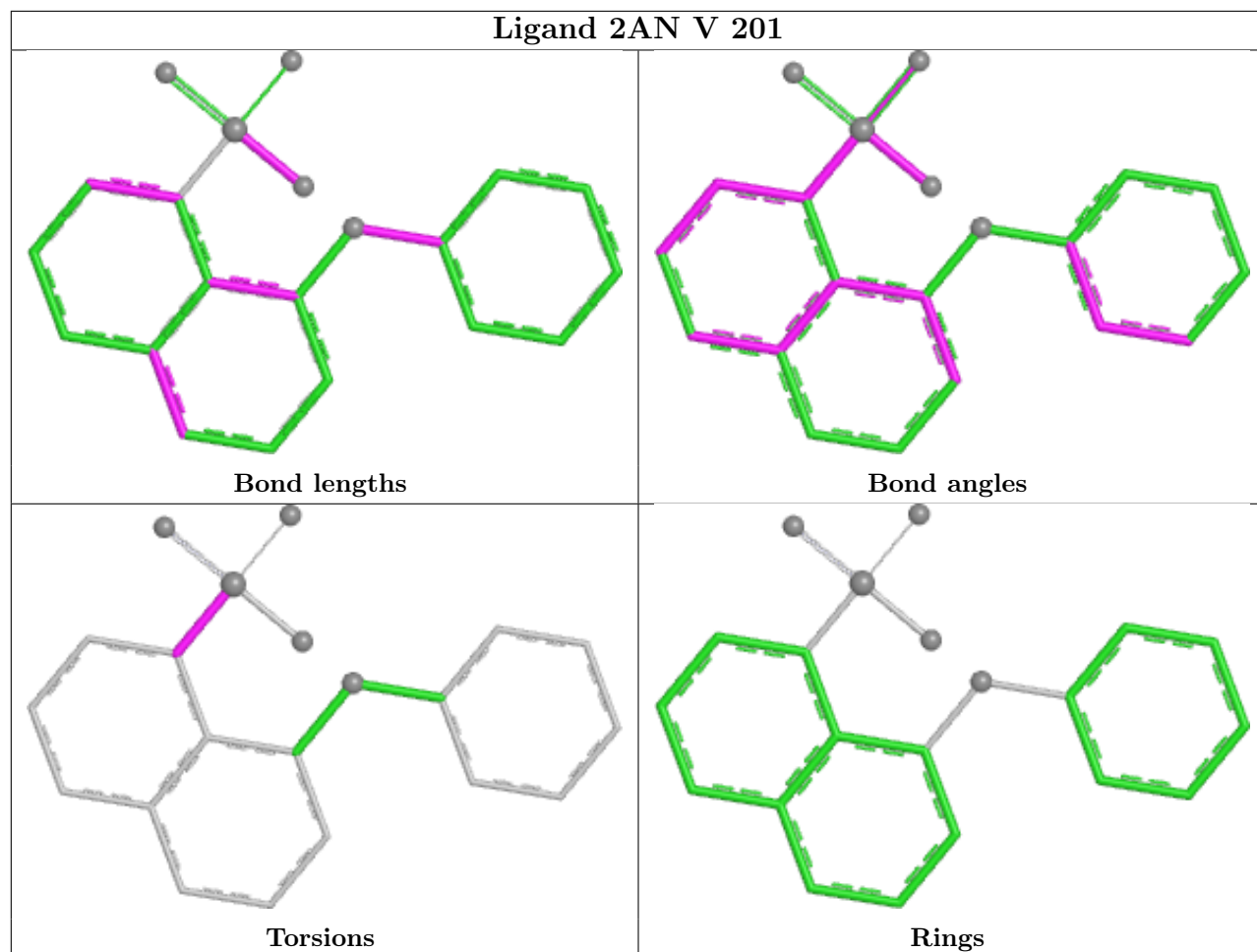
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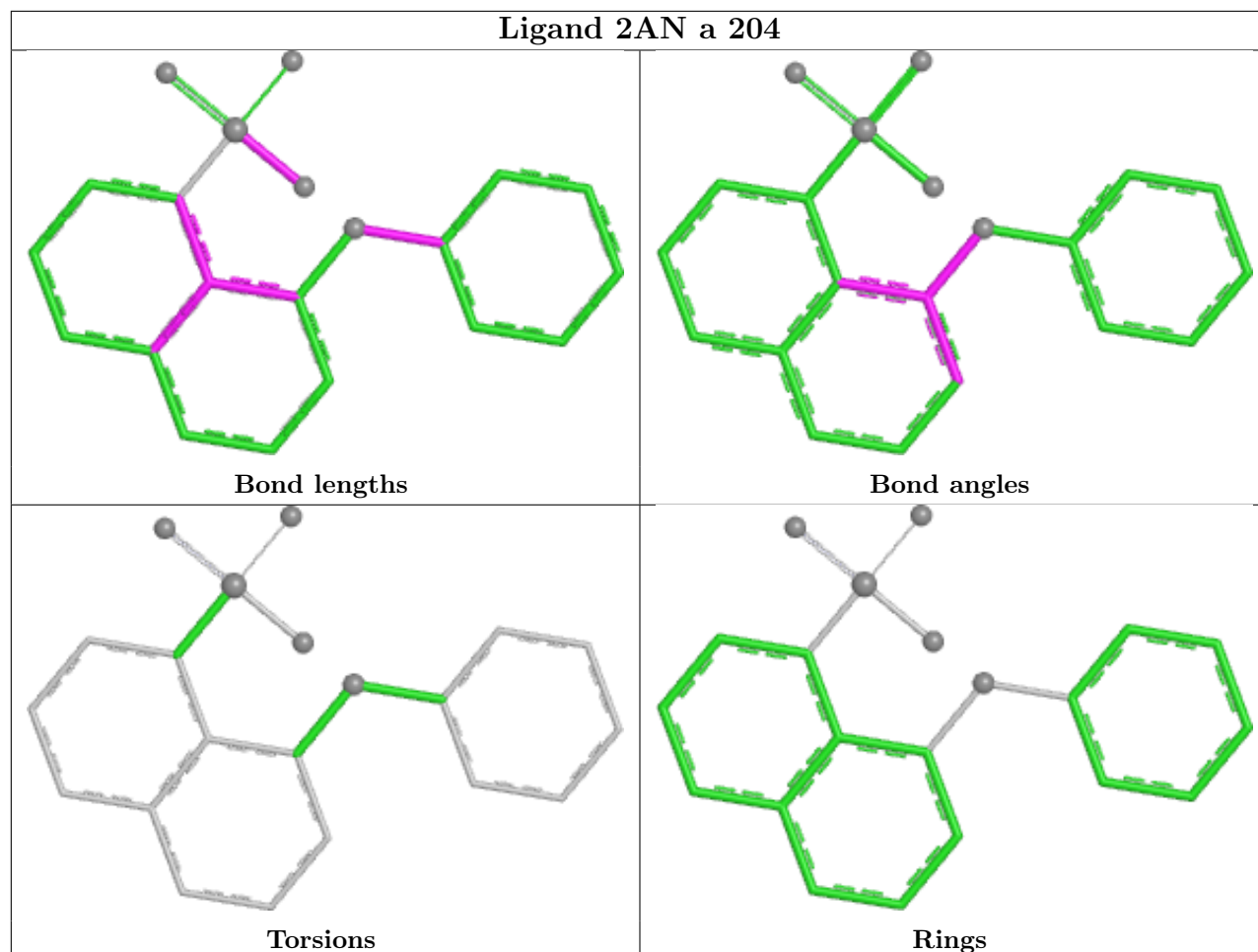
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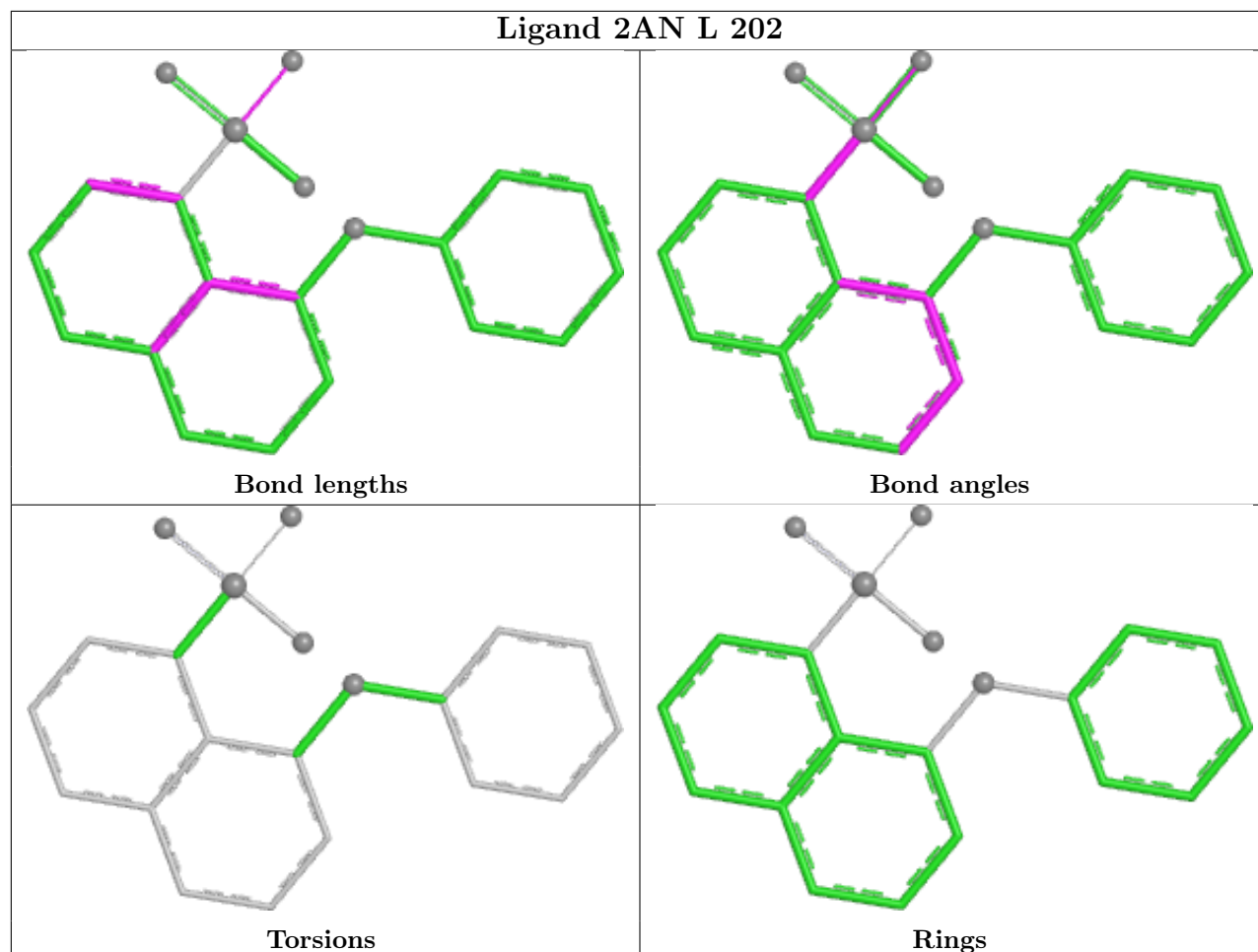
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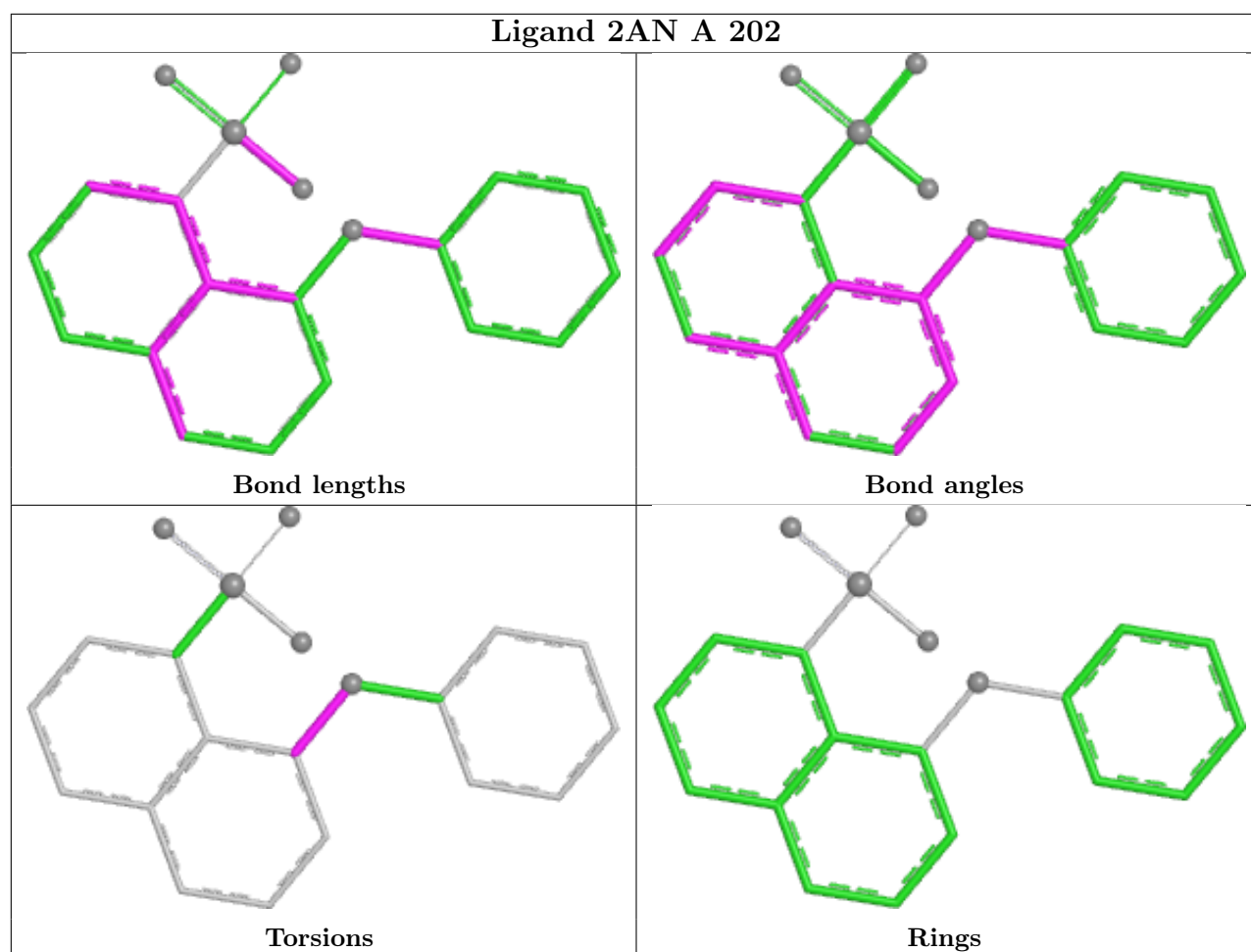


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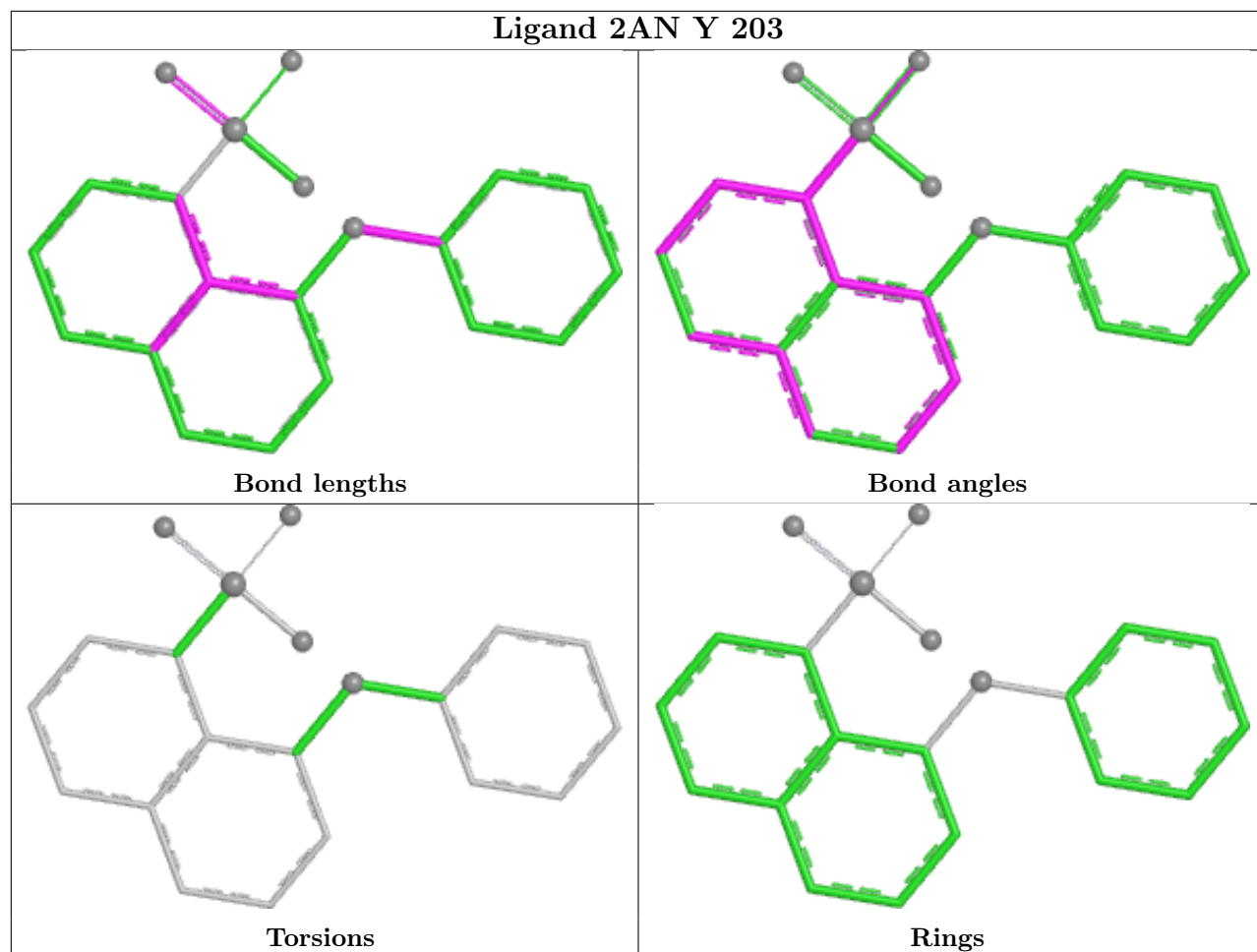


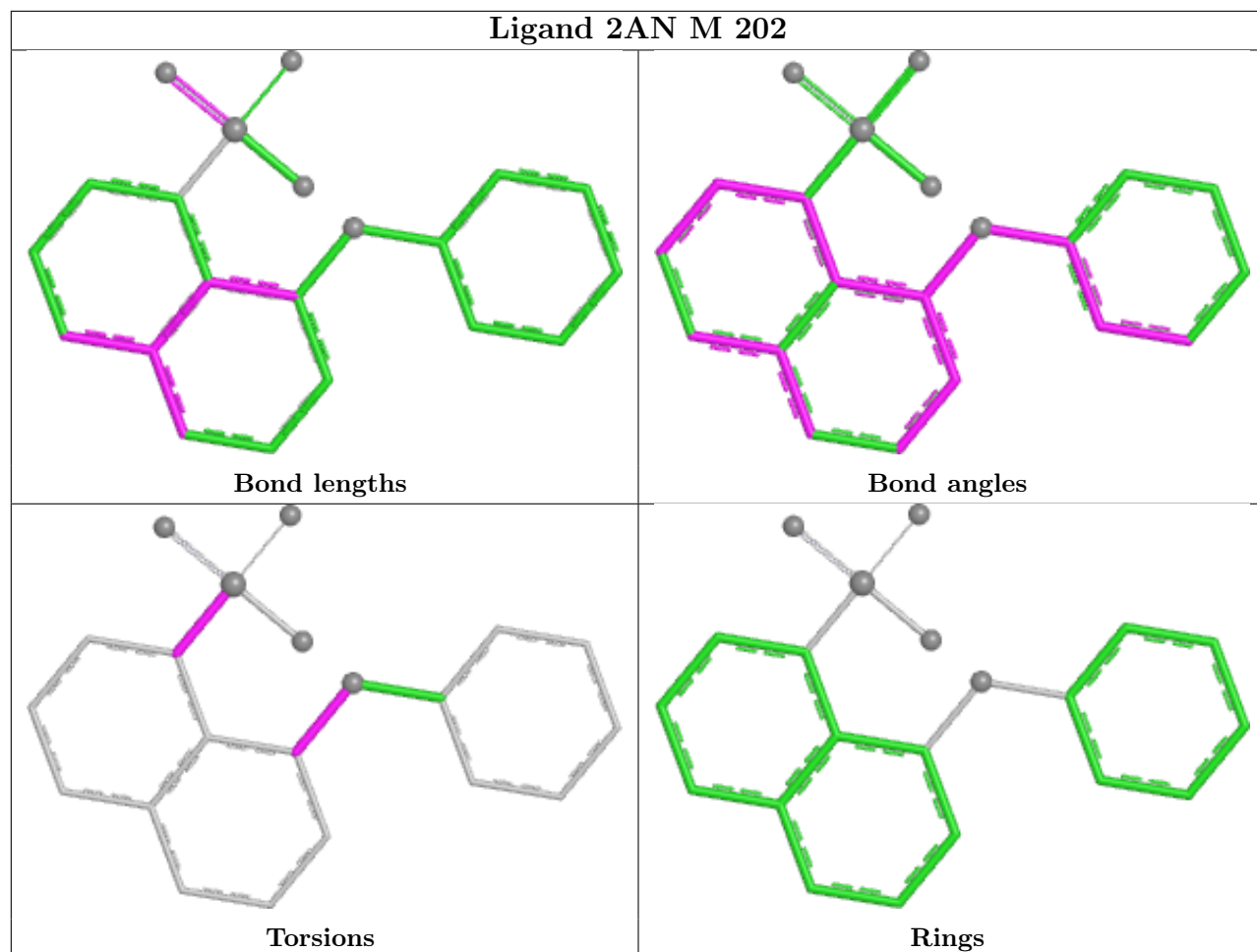
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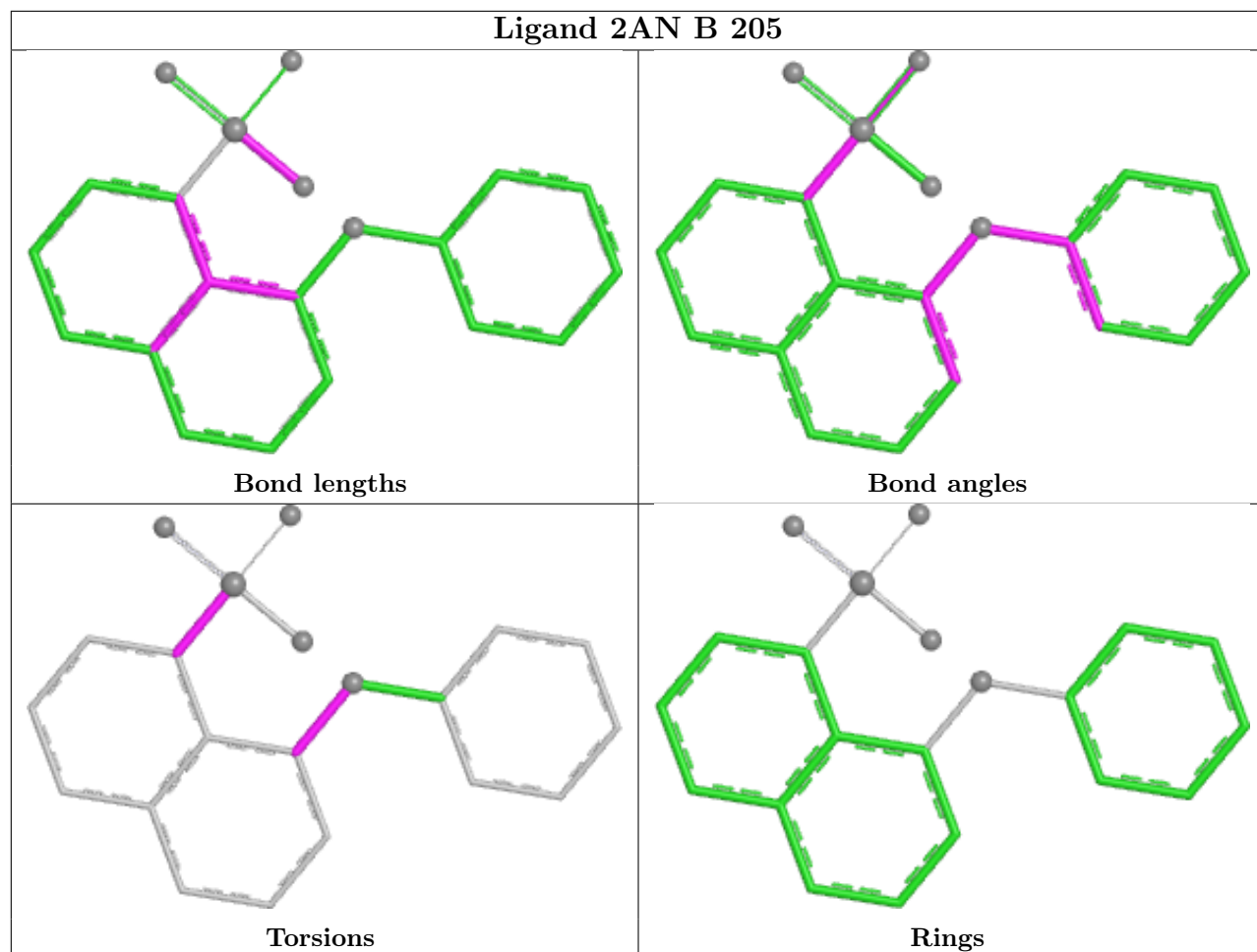


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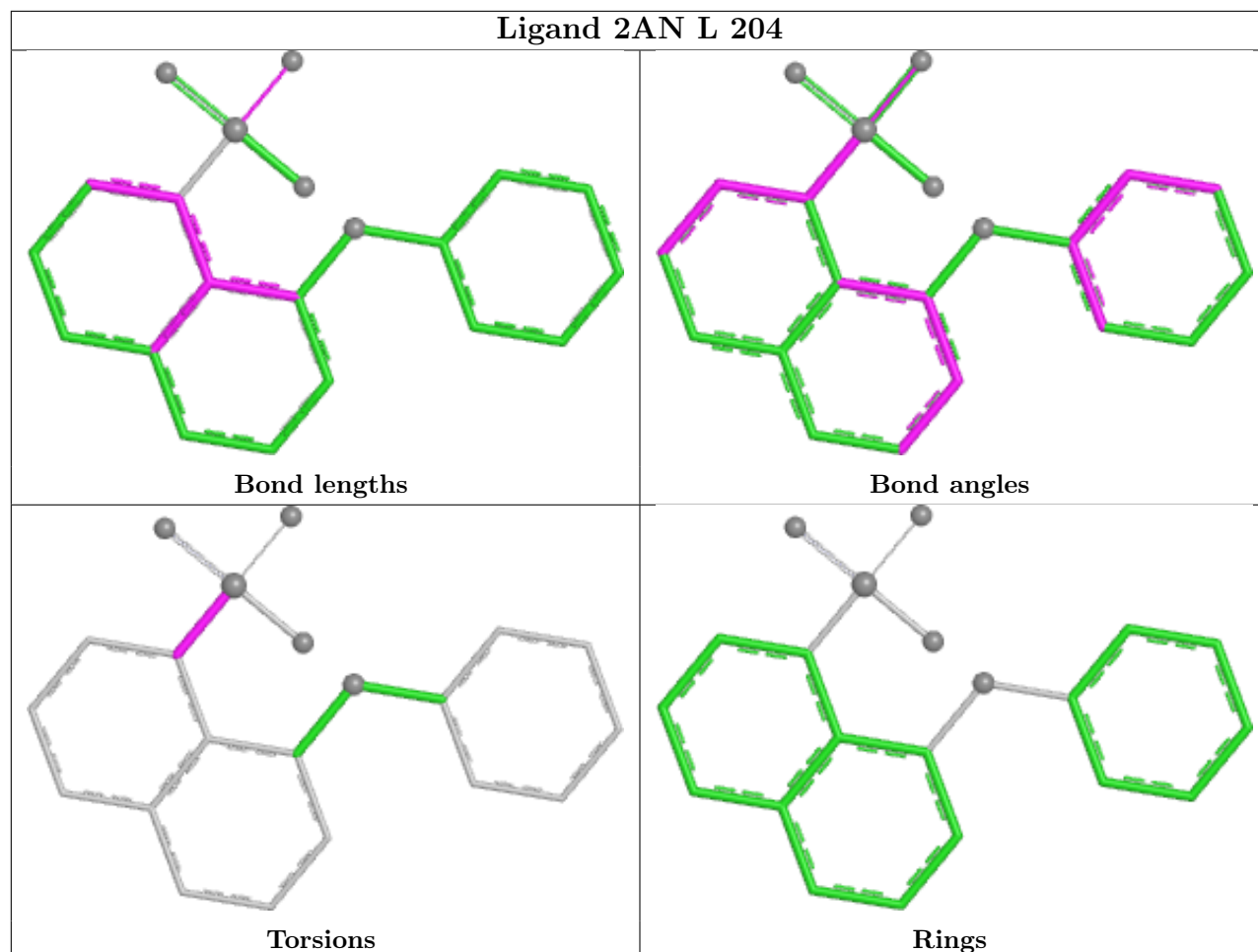




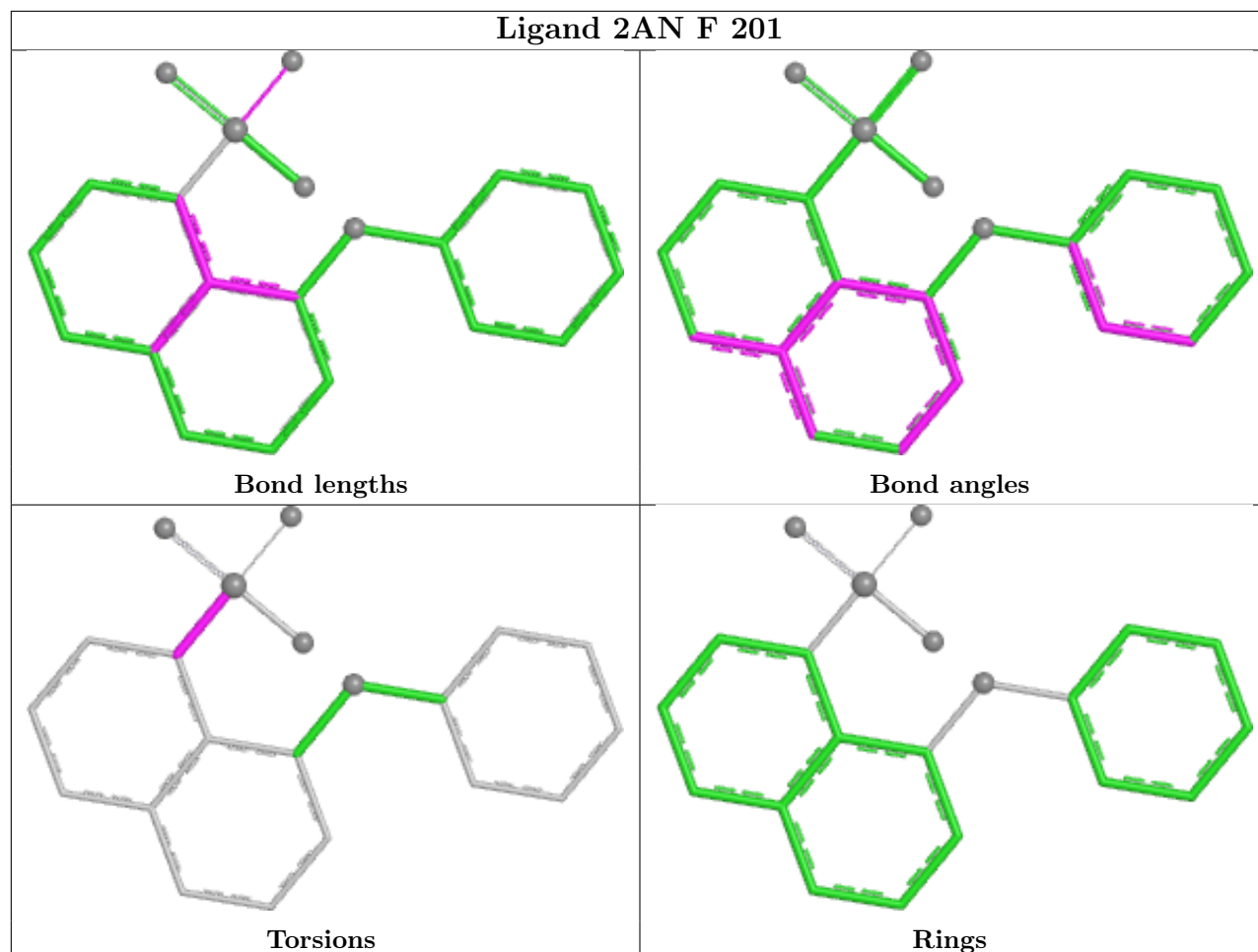
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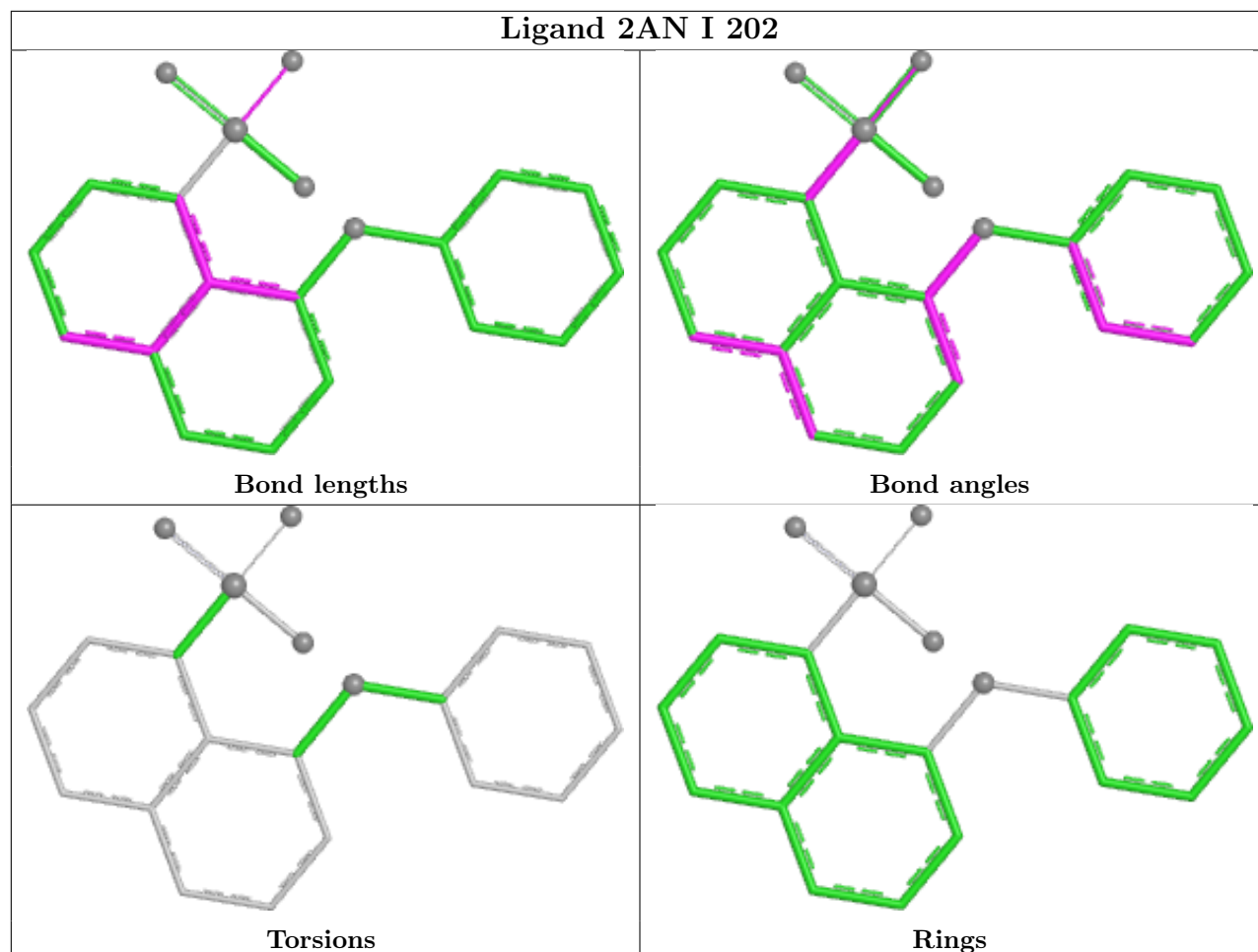
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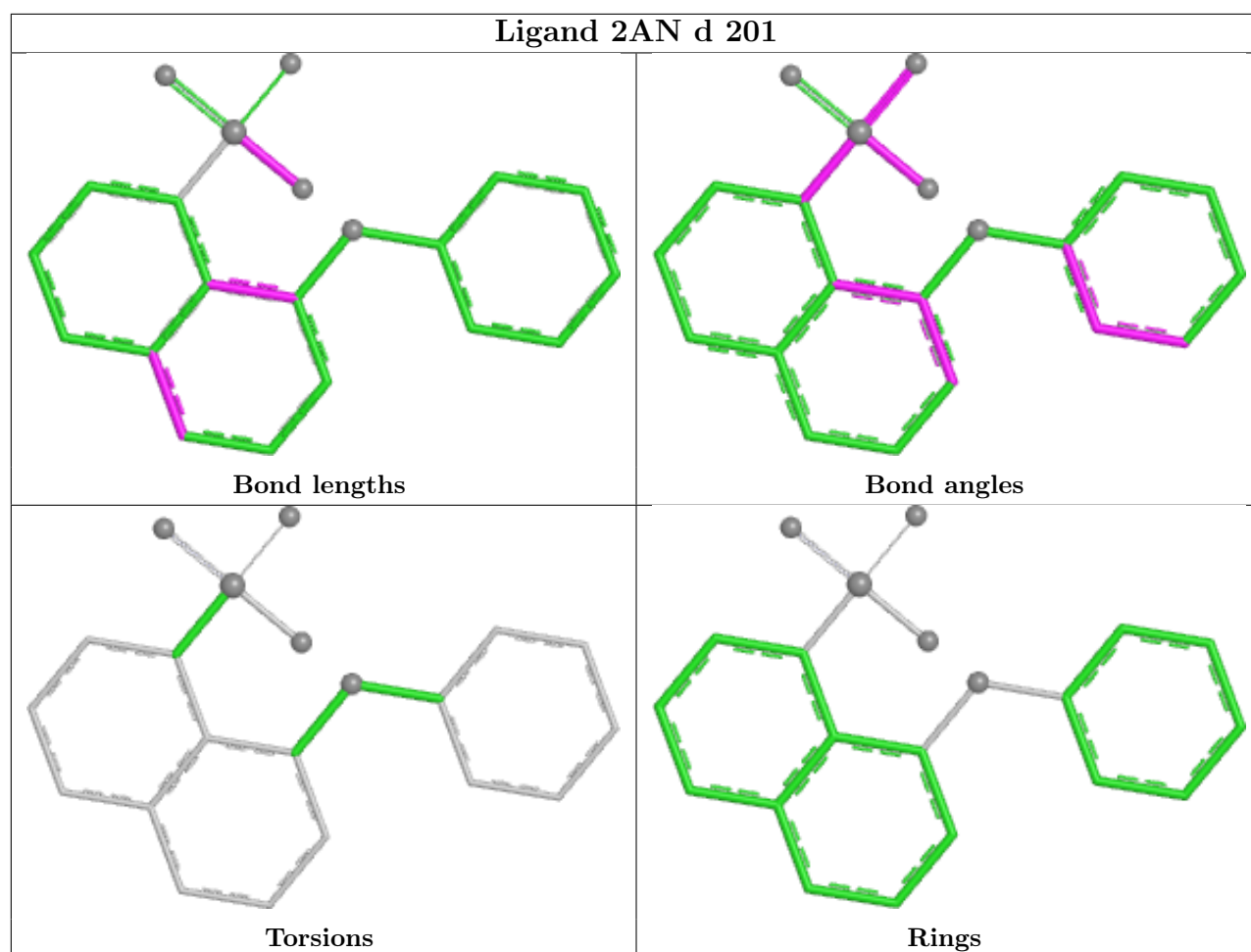


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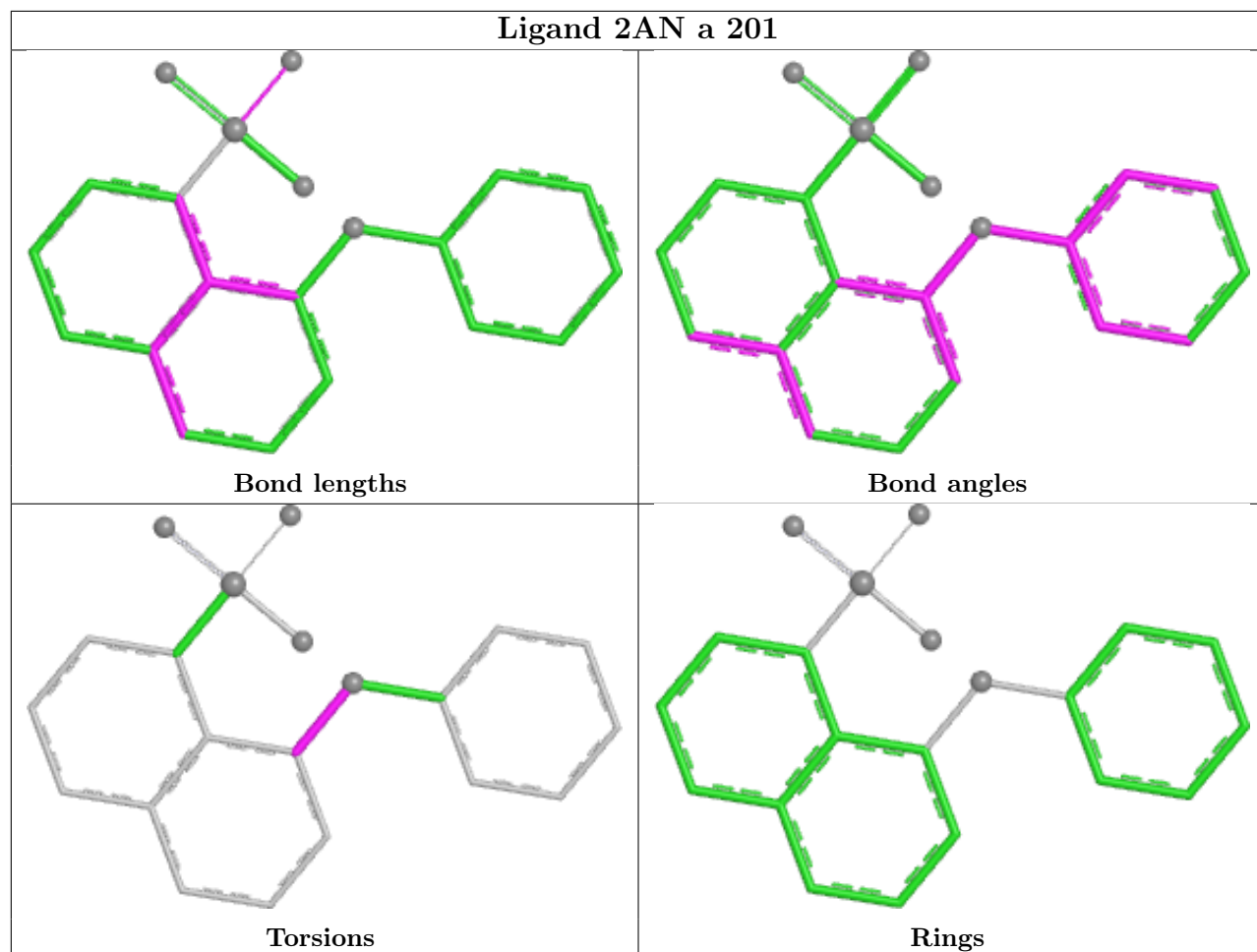


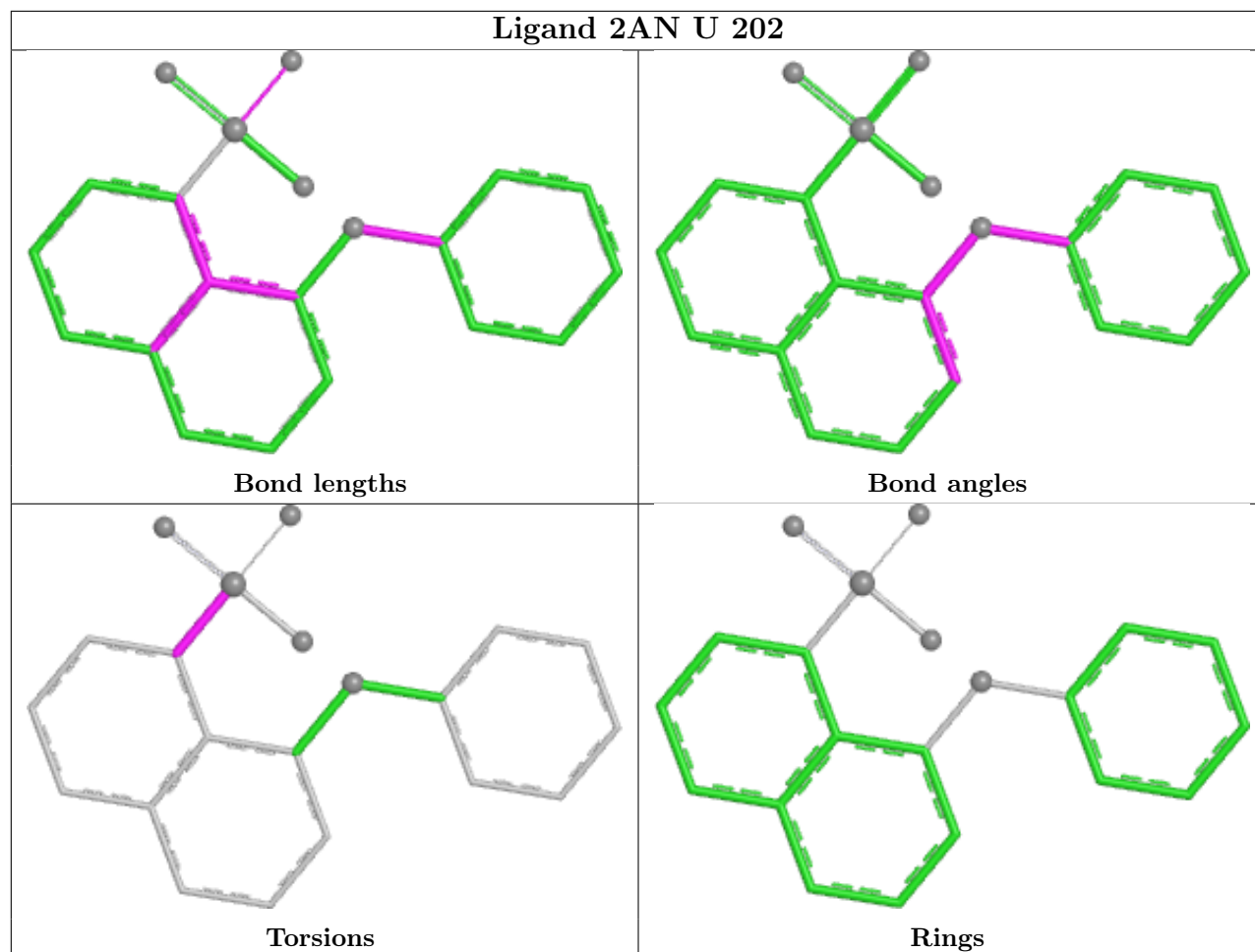
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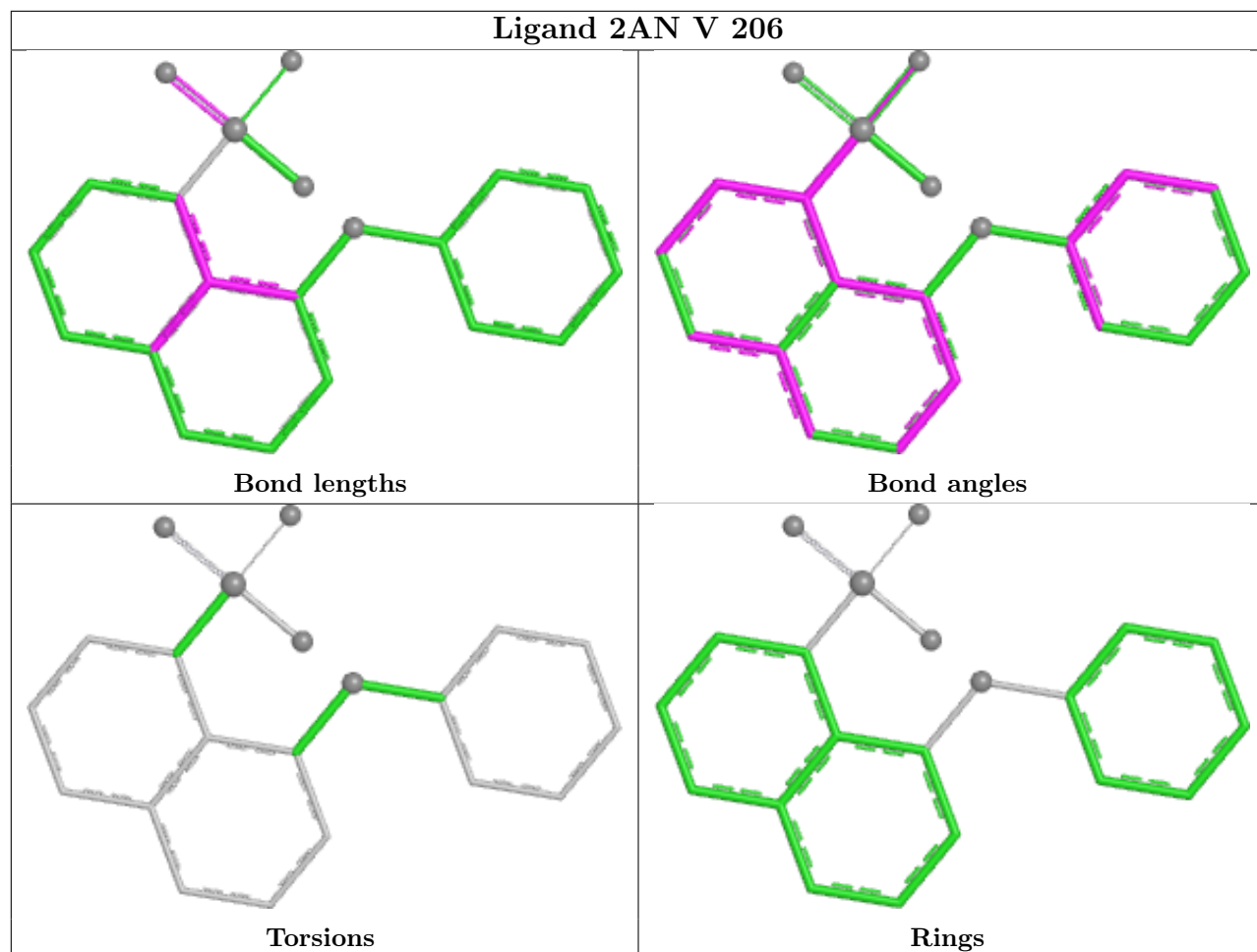


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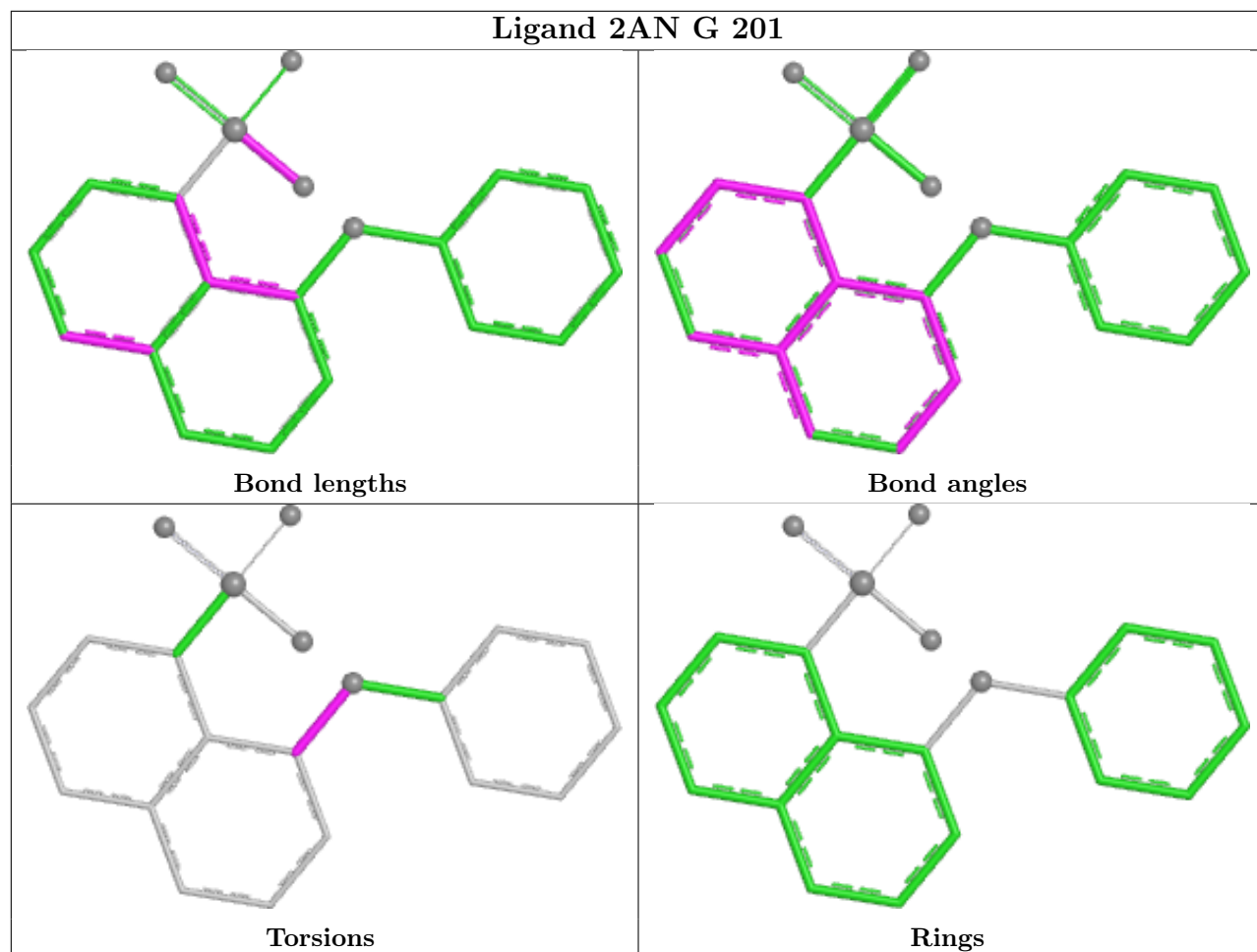




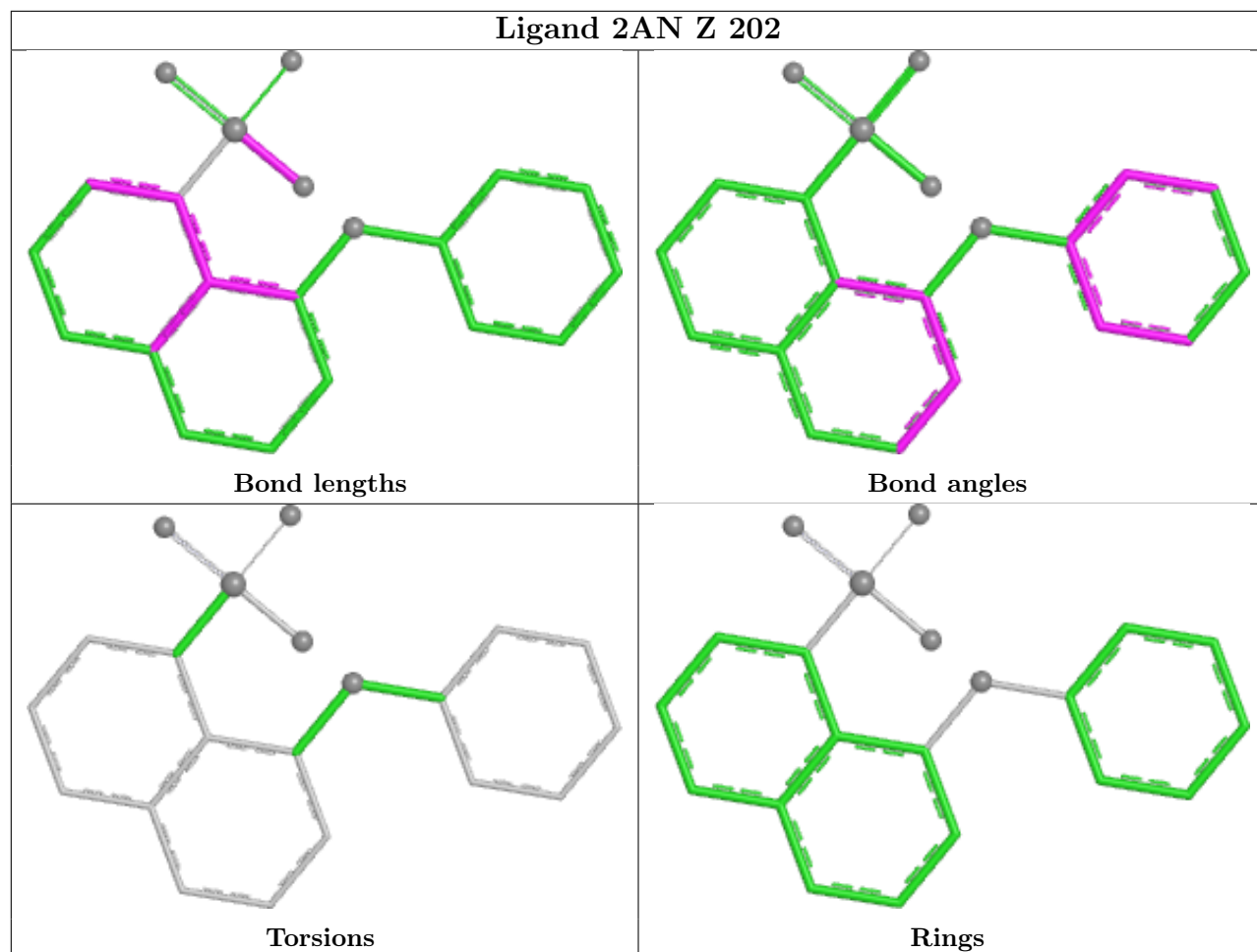
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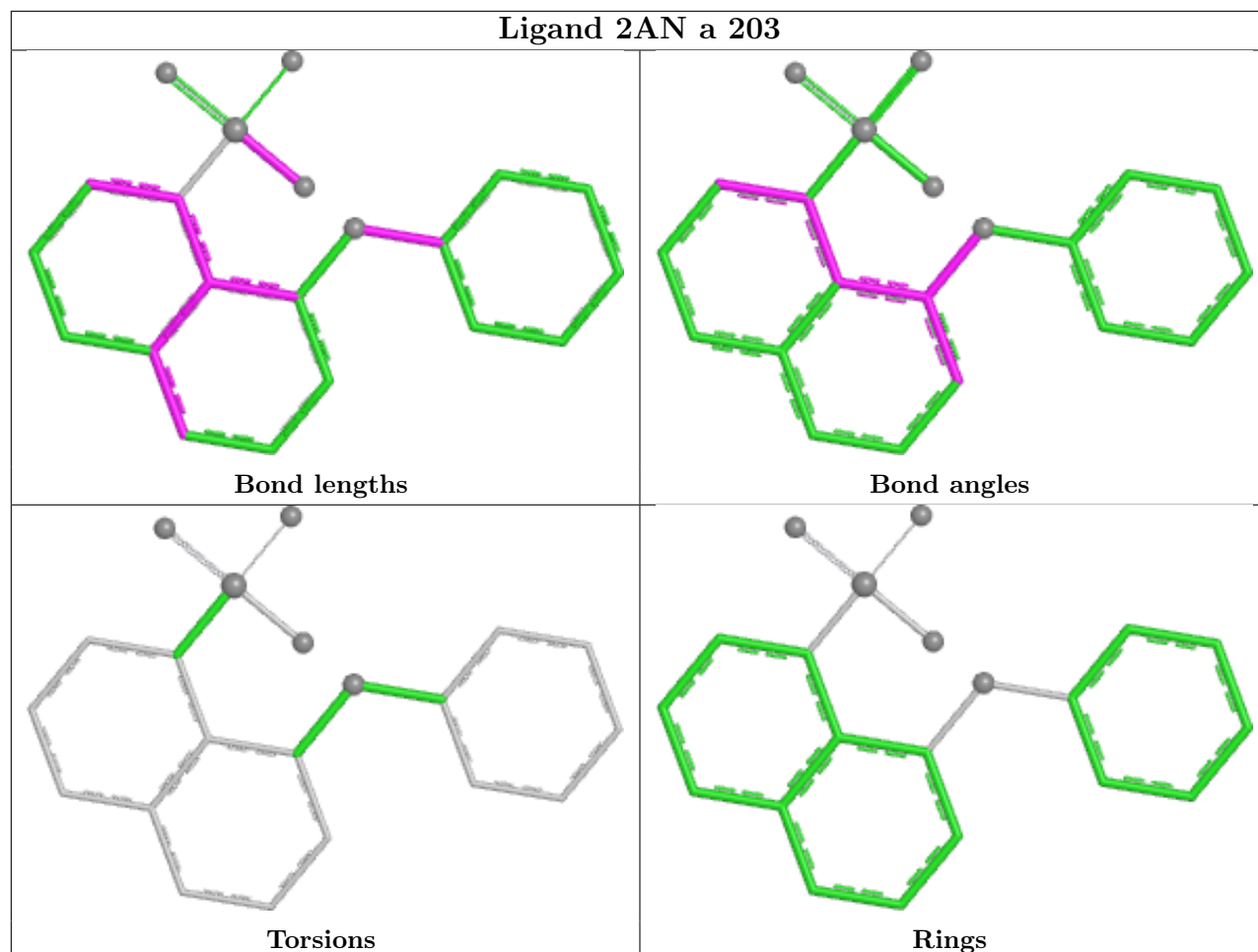
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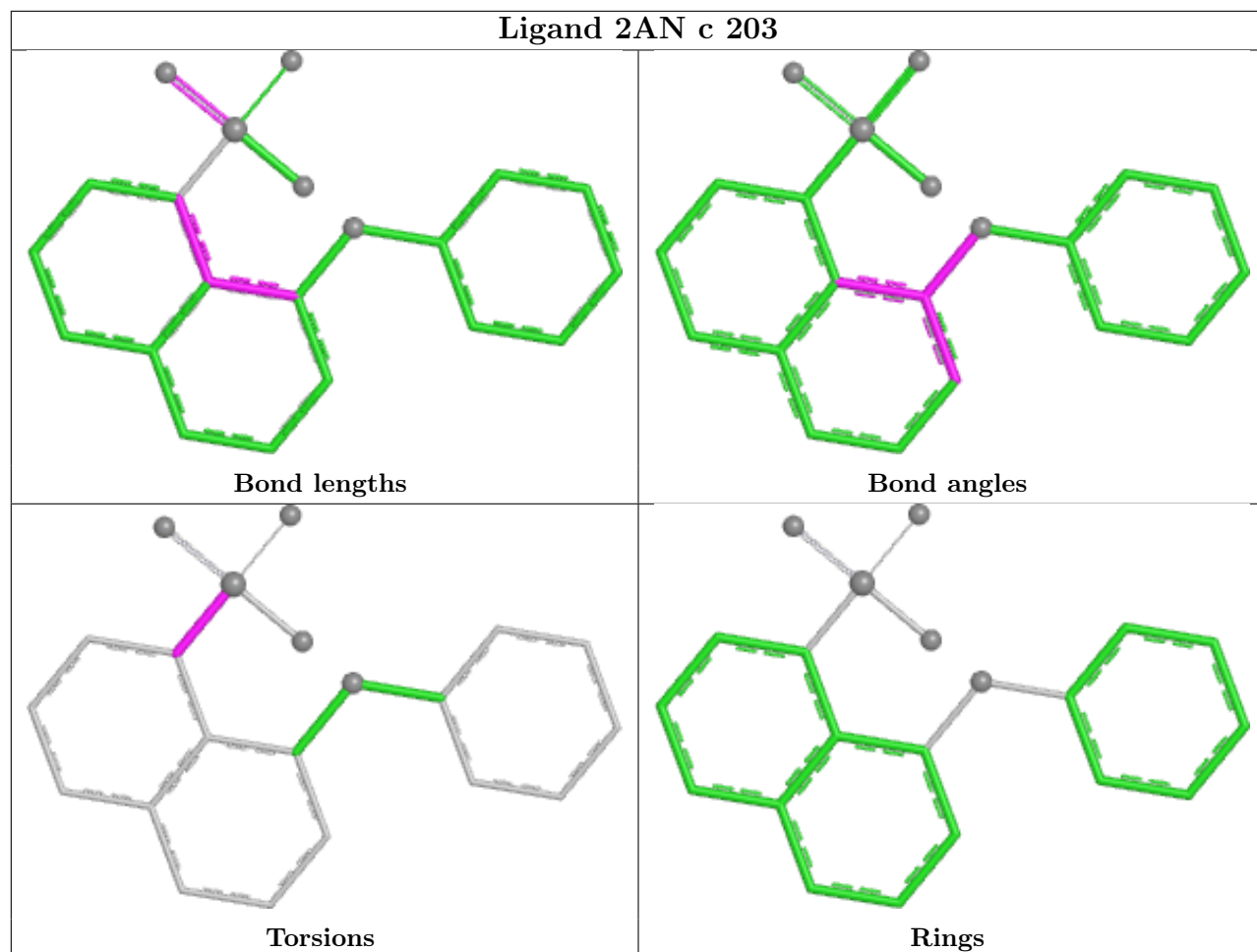
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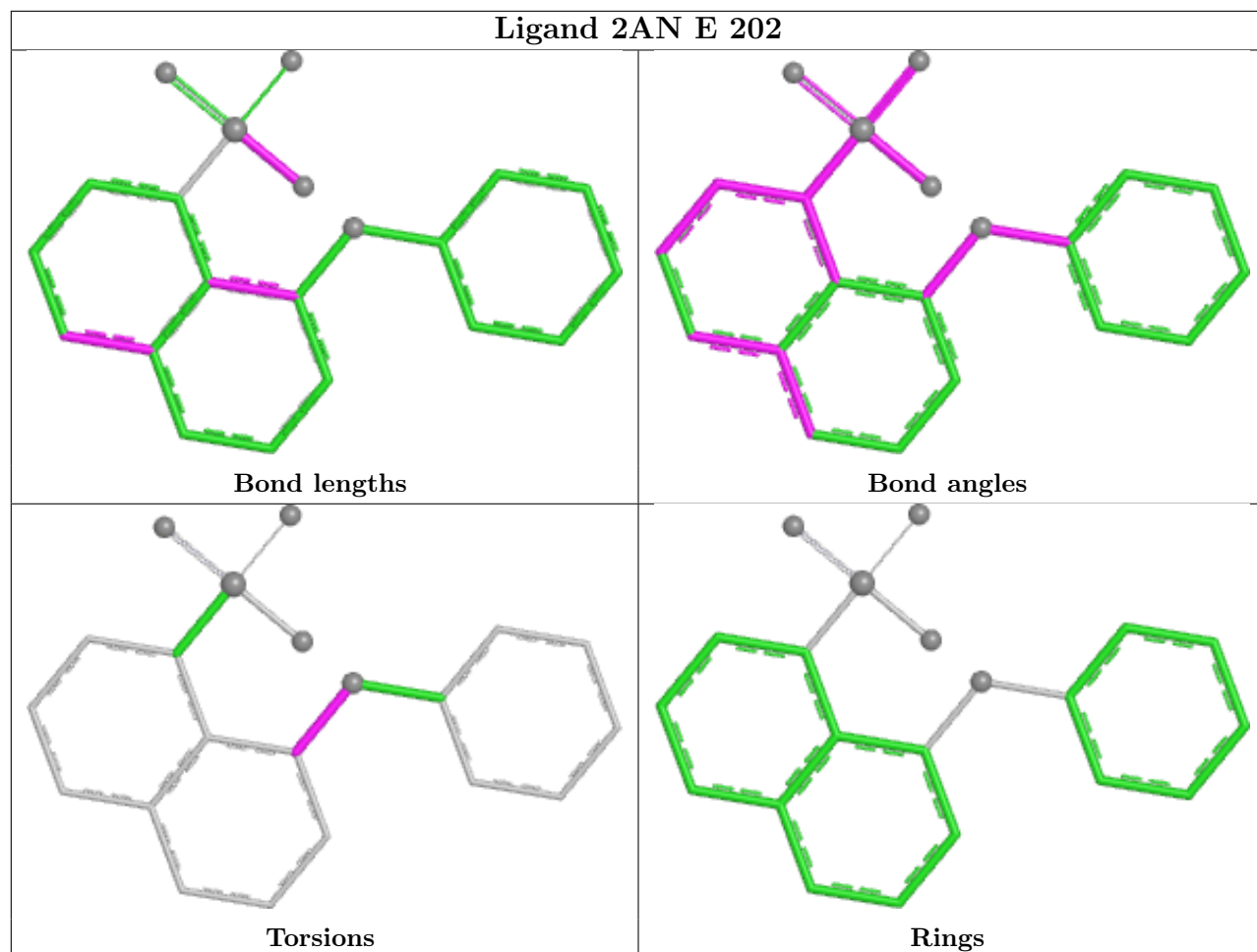
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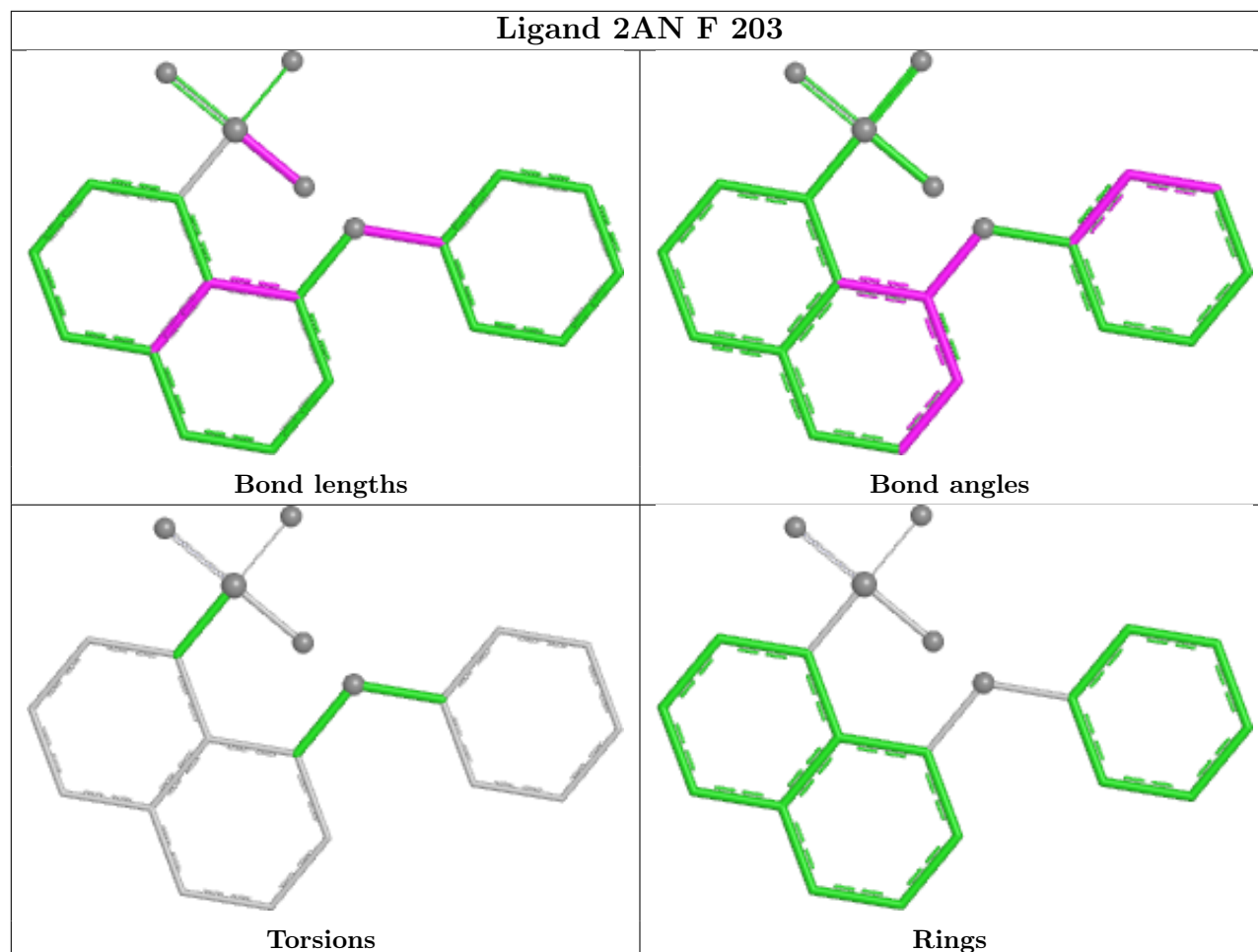
Ligand 2AN c 203

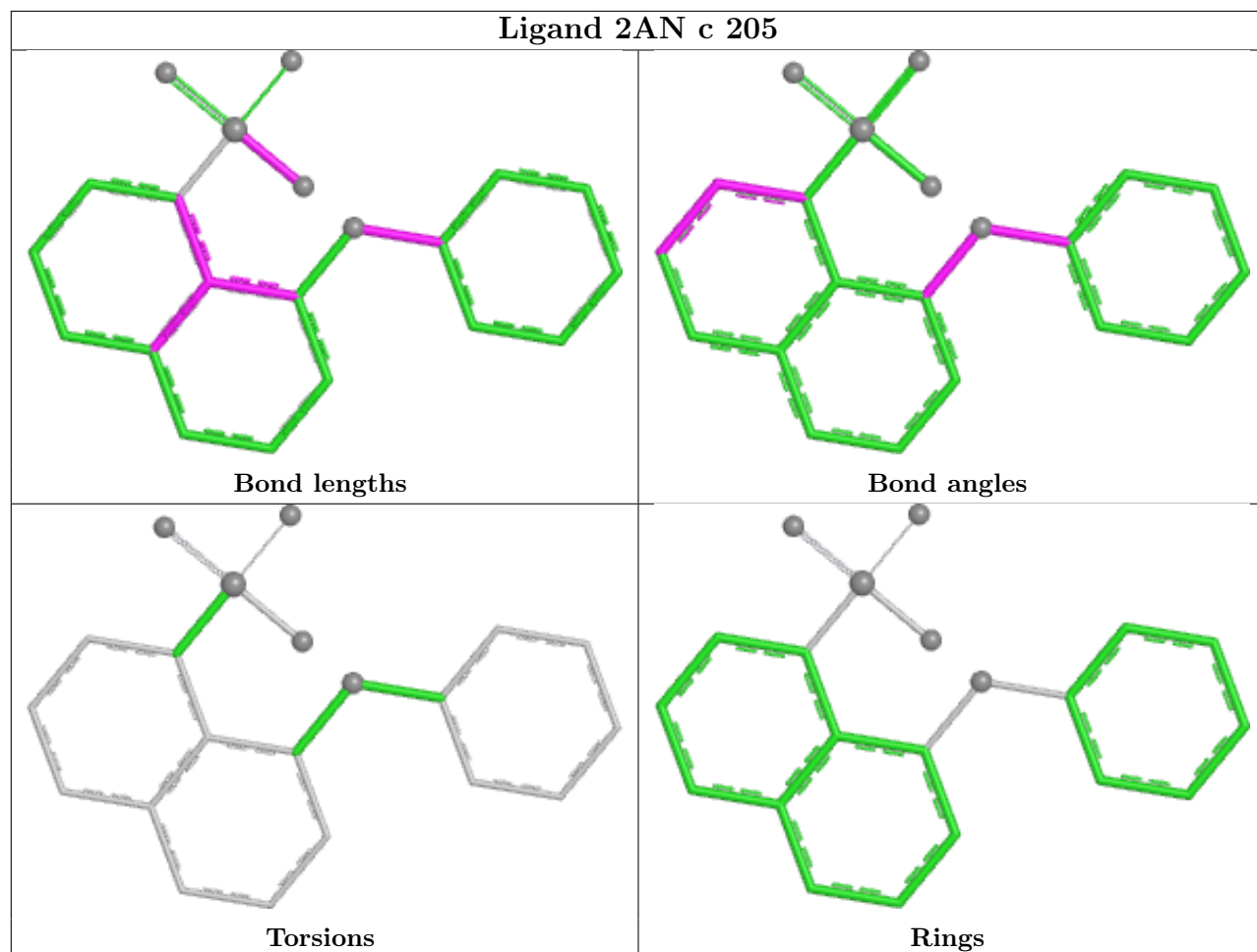


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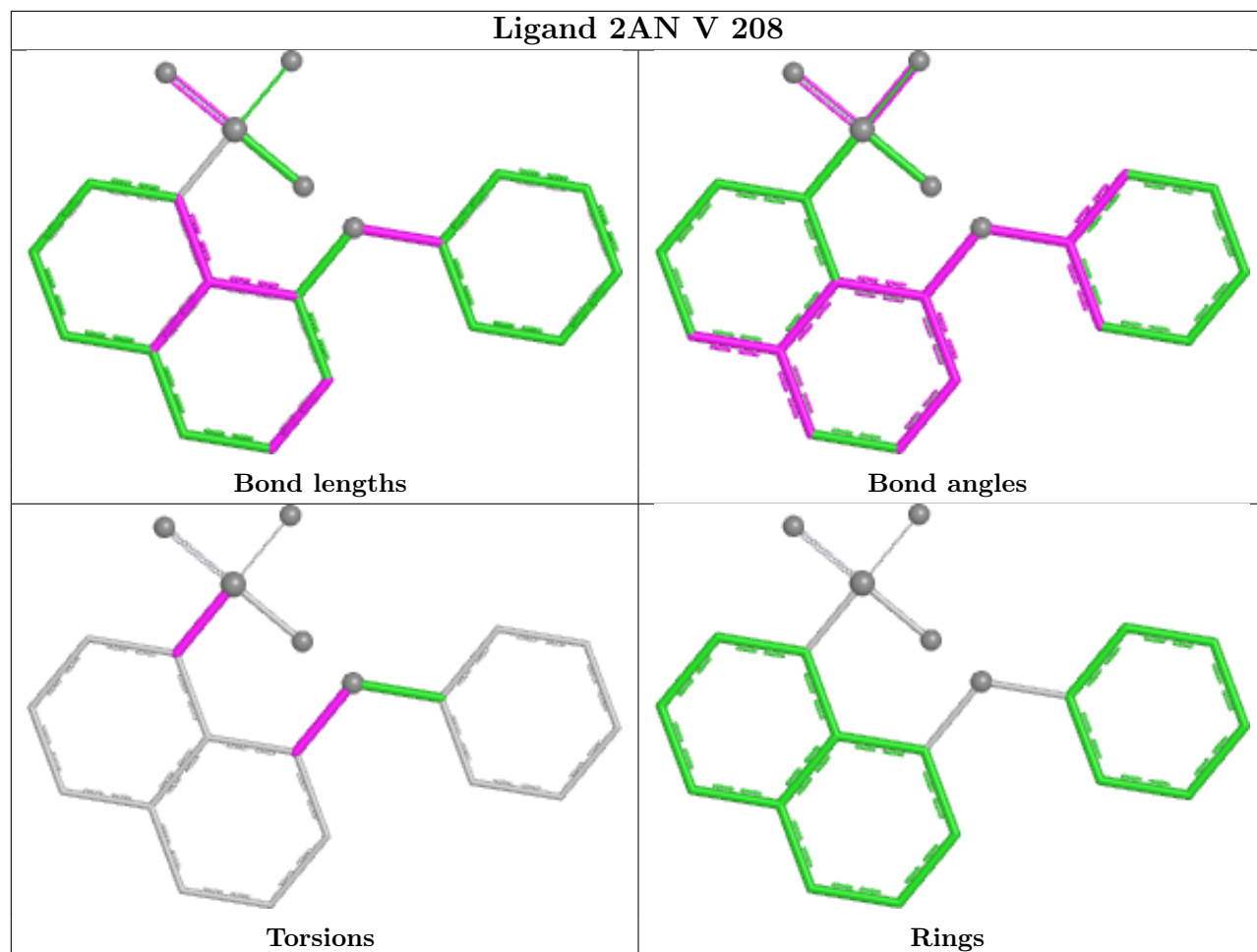


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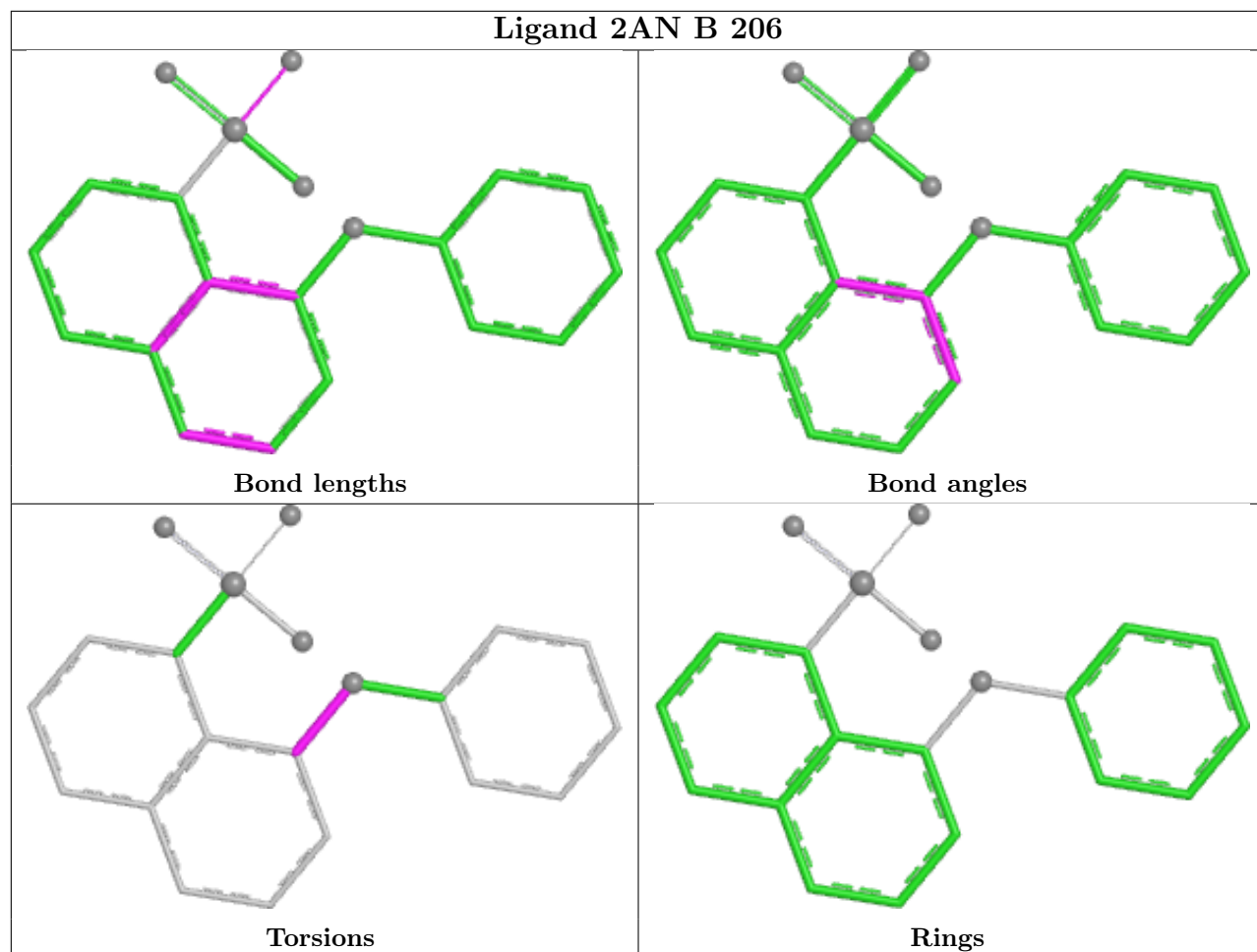


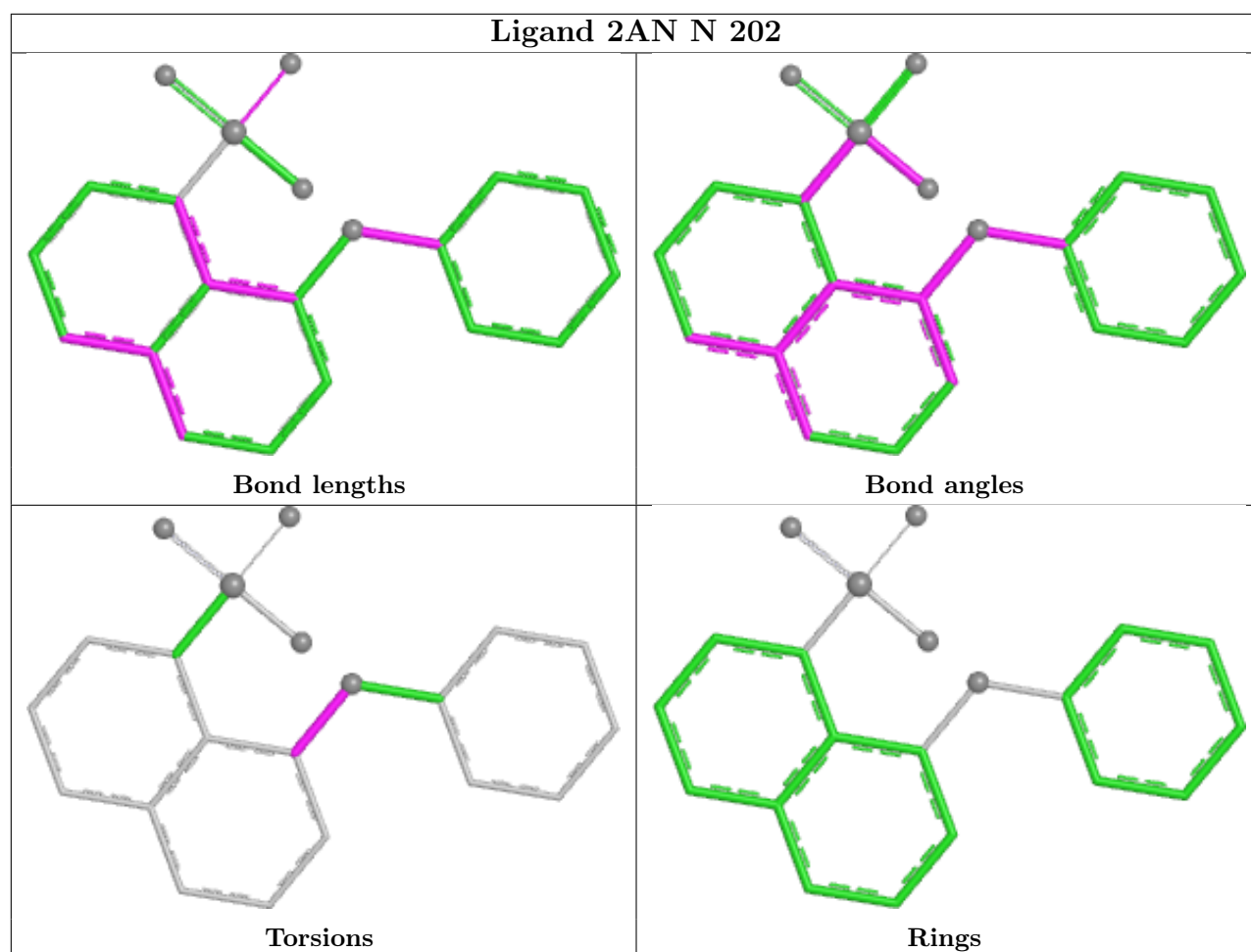


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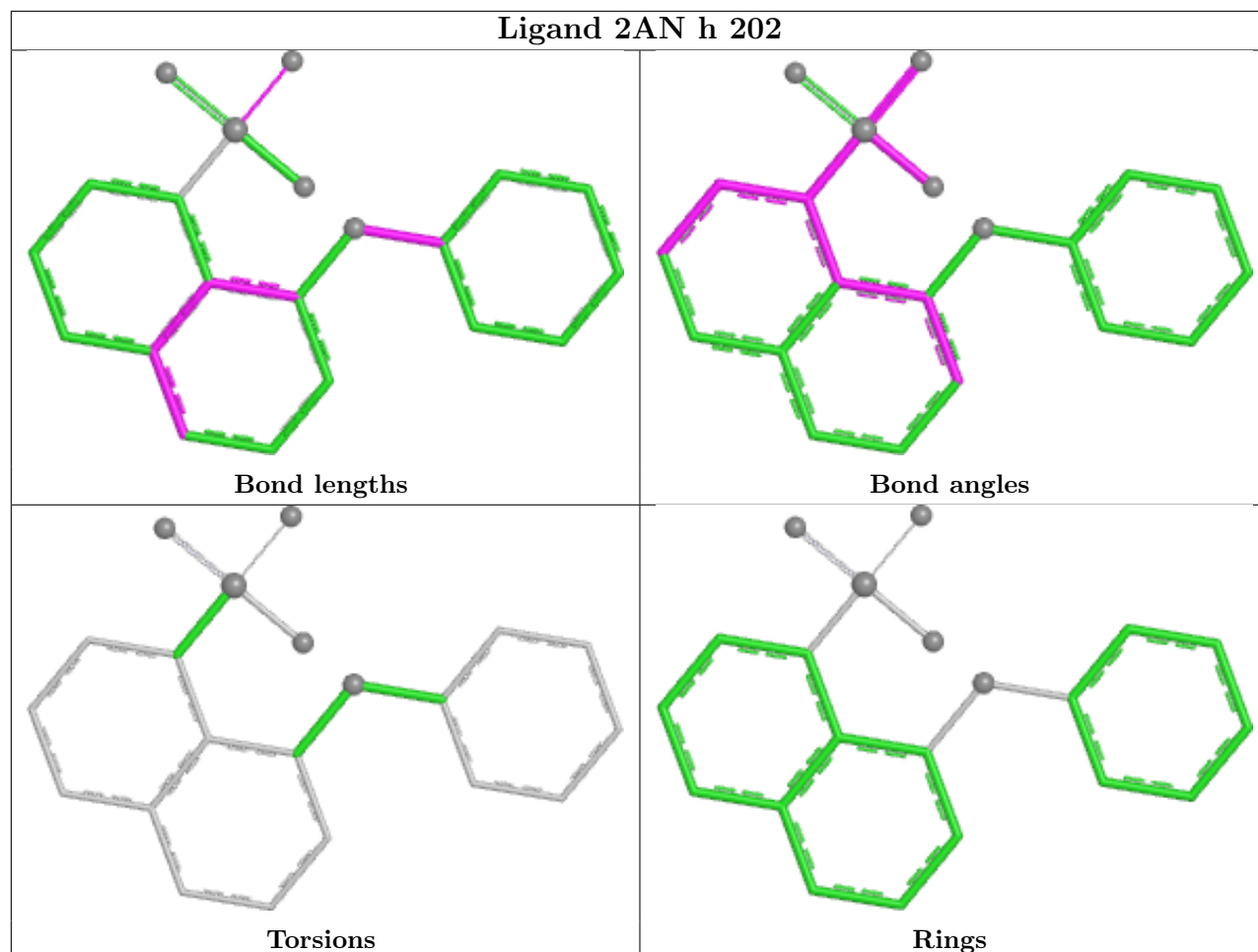


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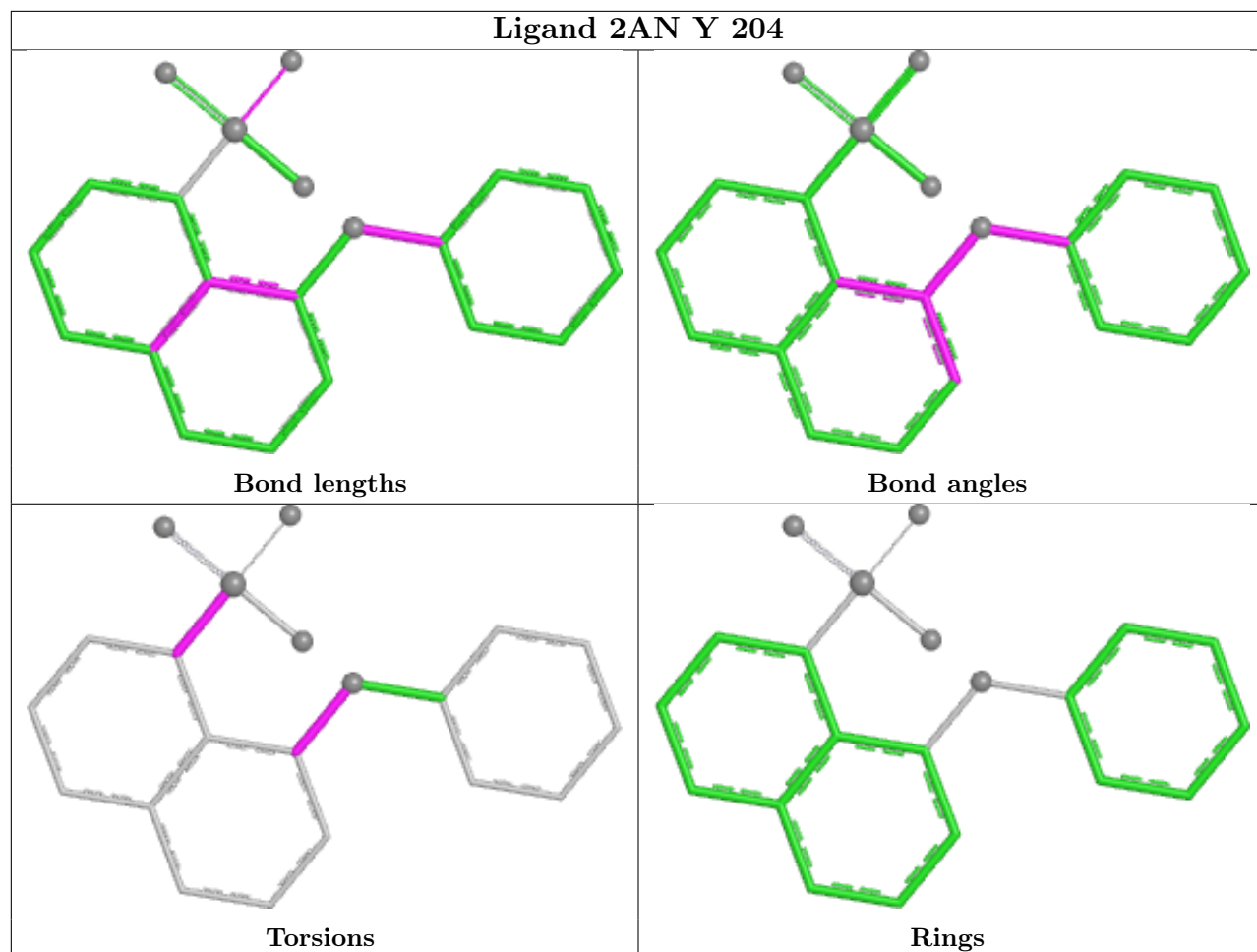




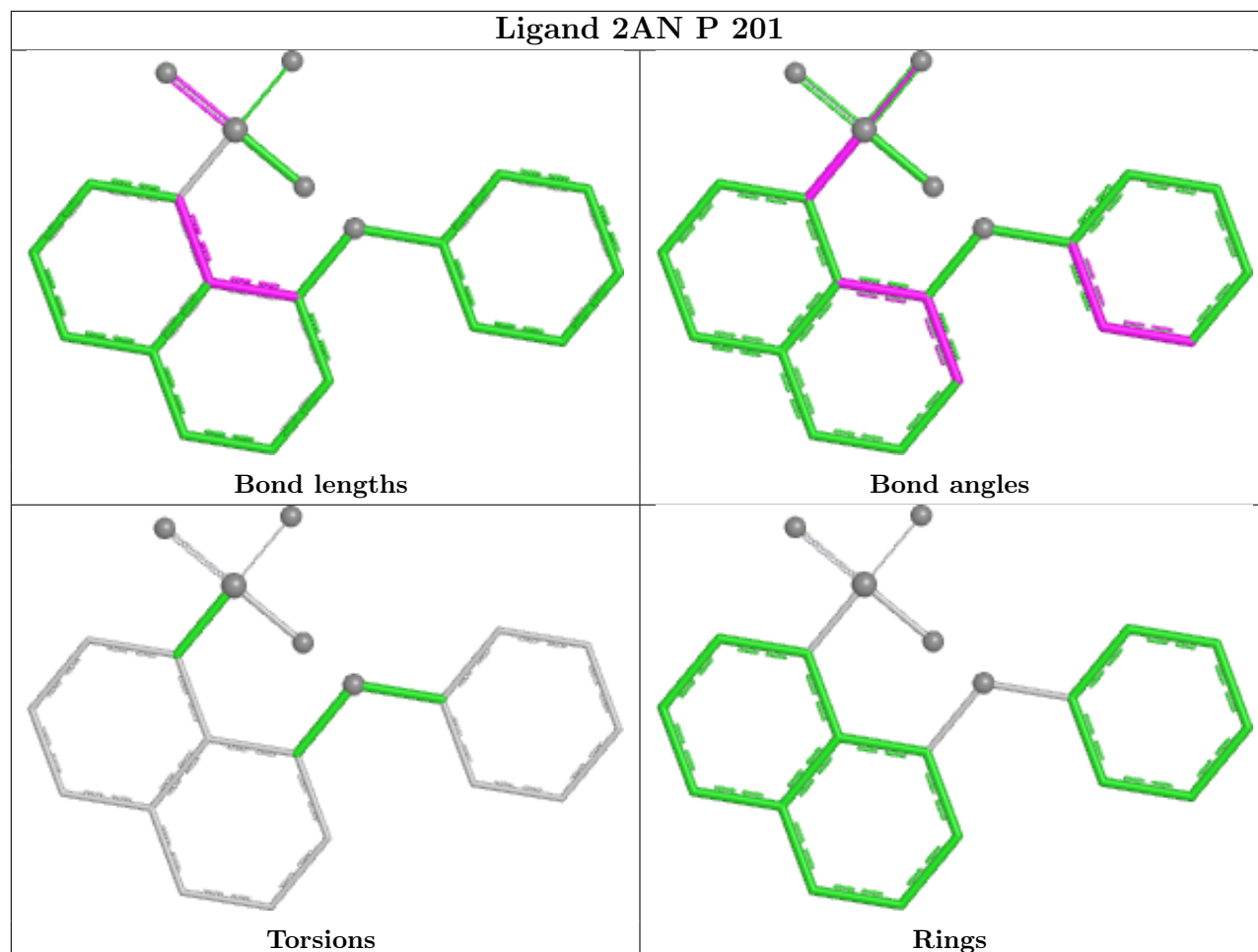
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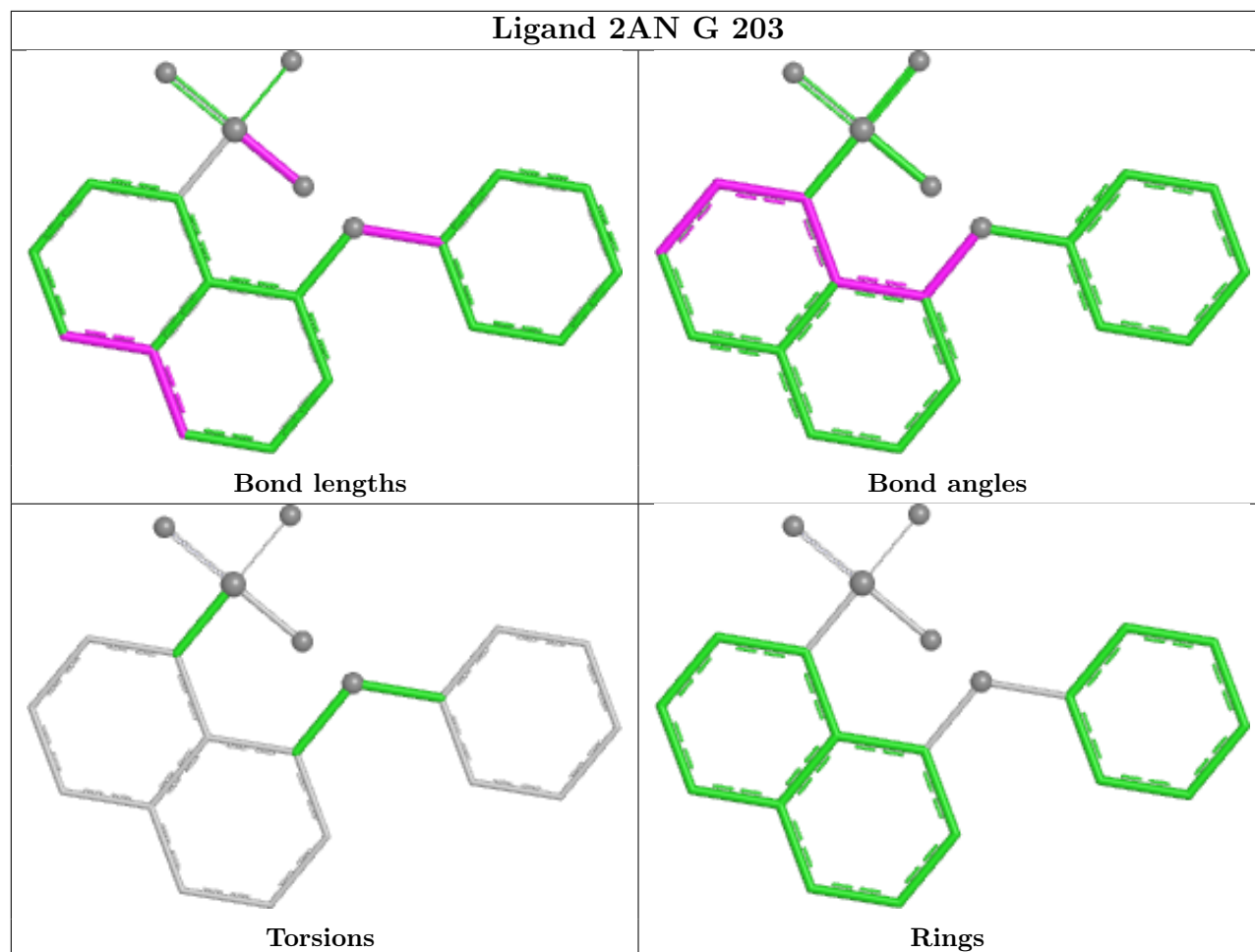


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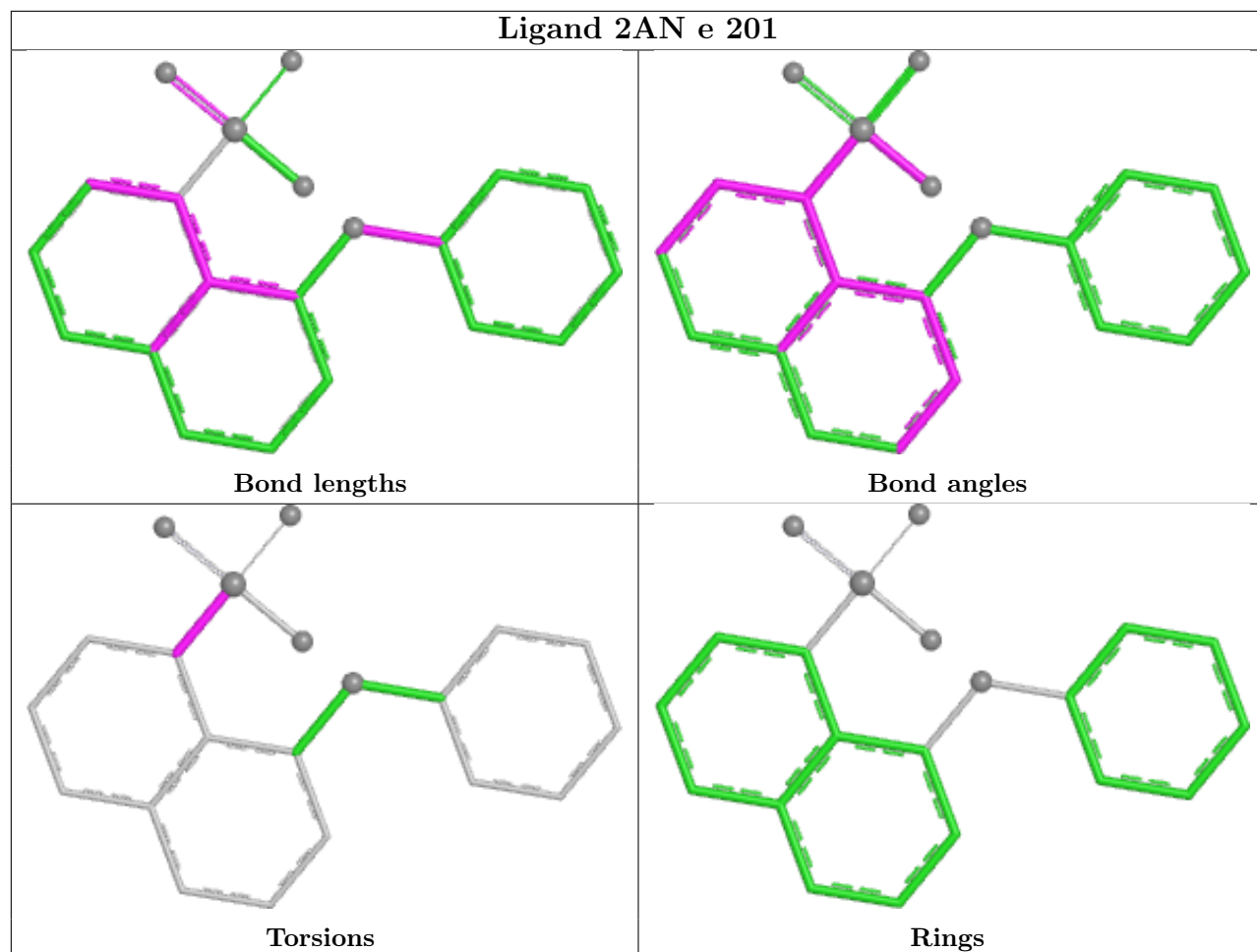


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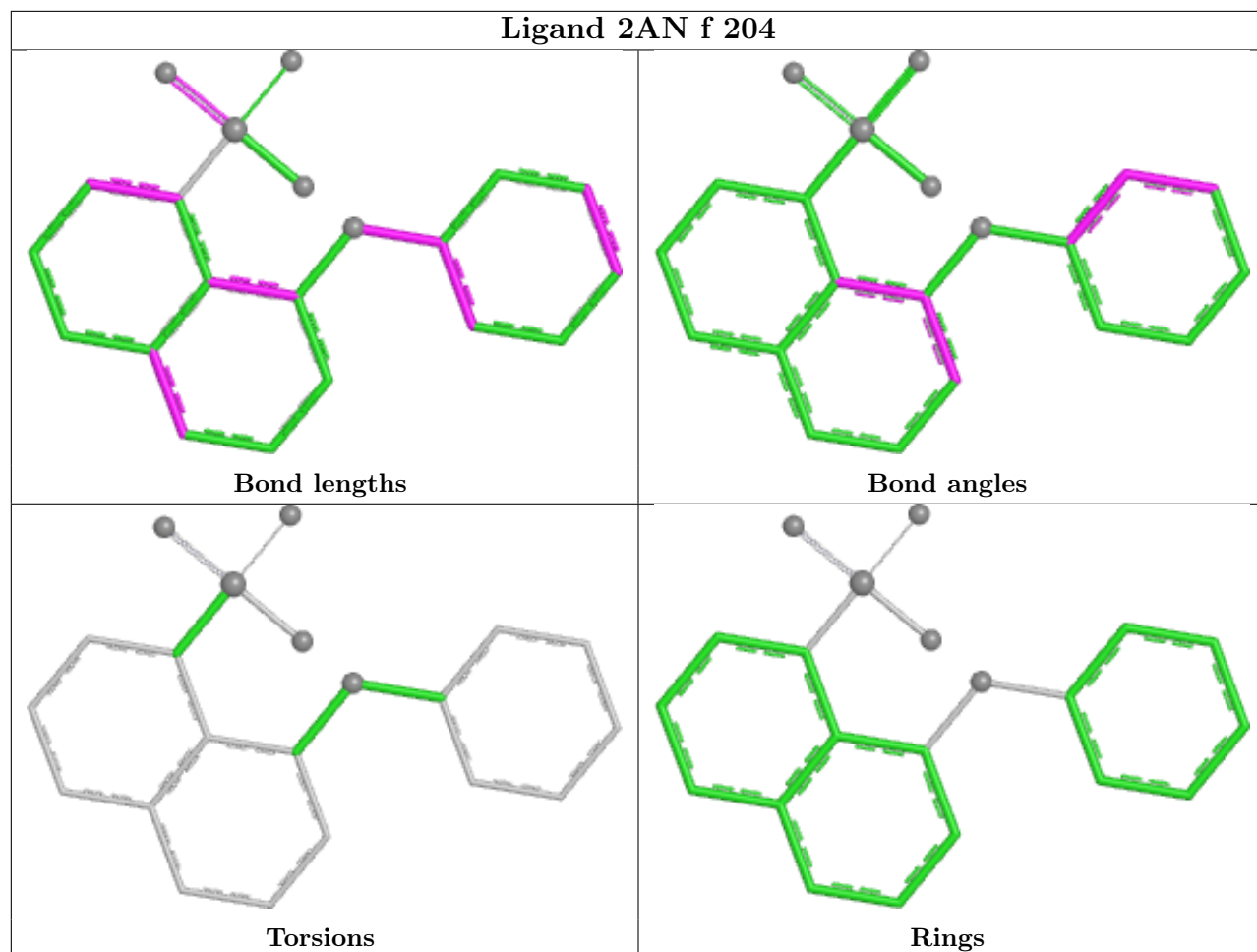




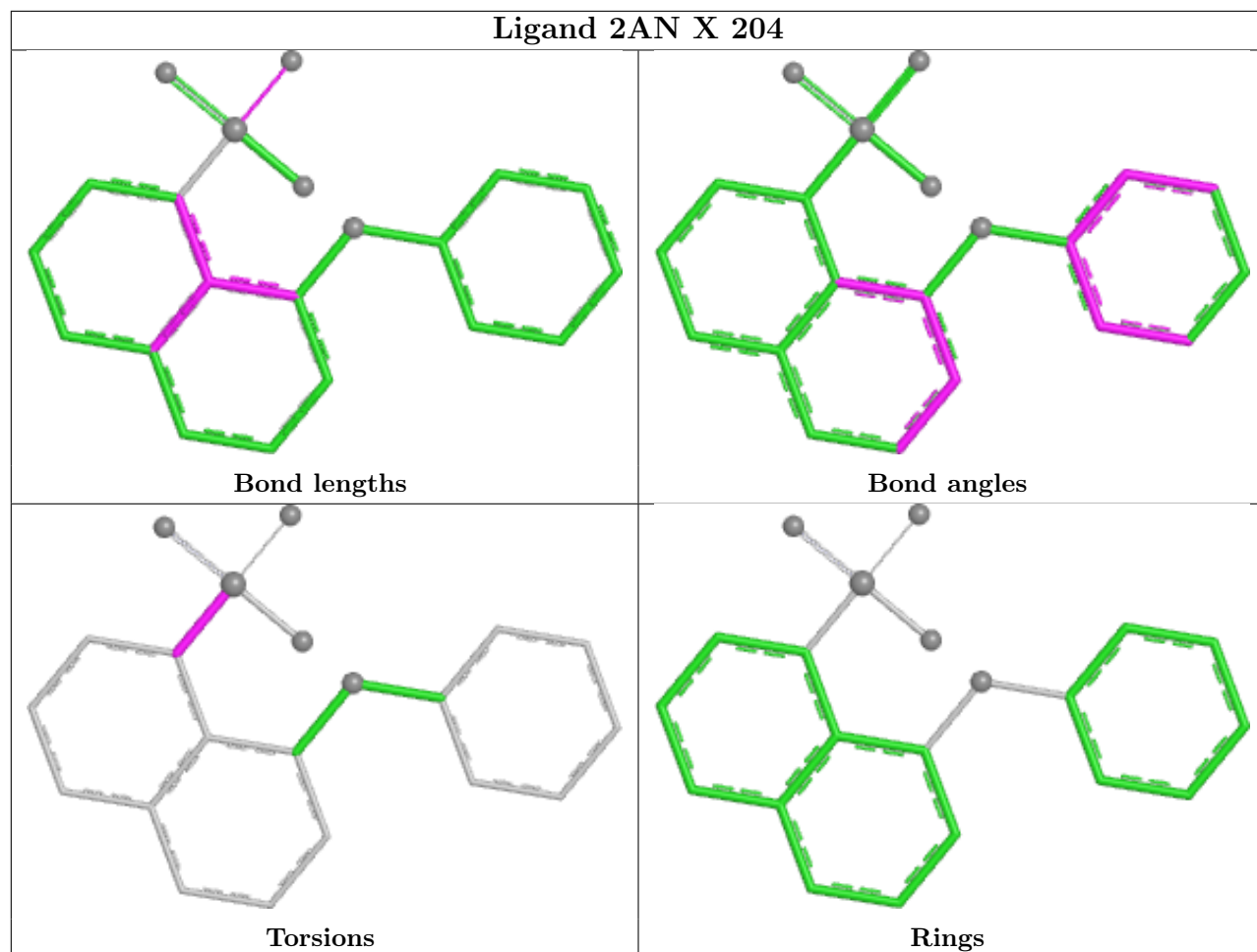
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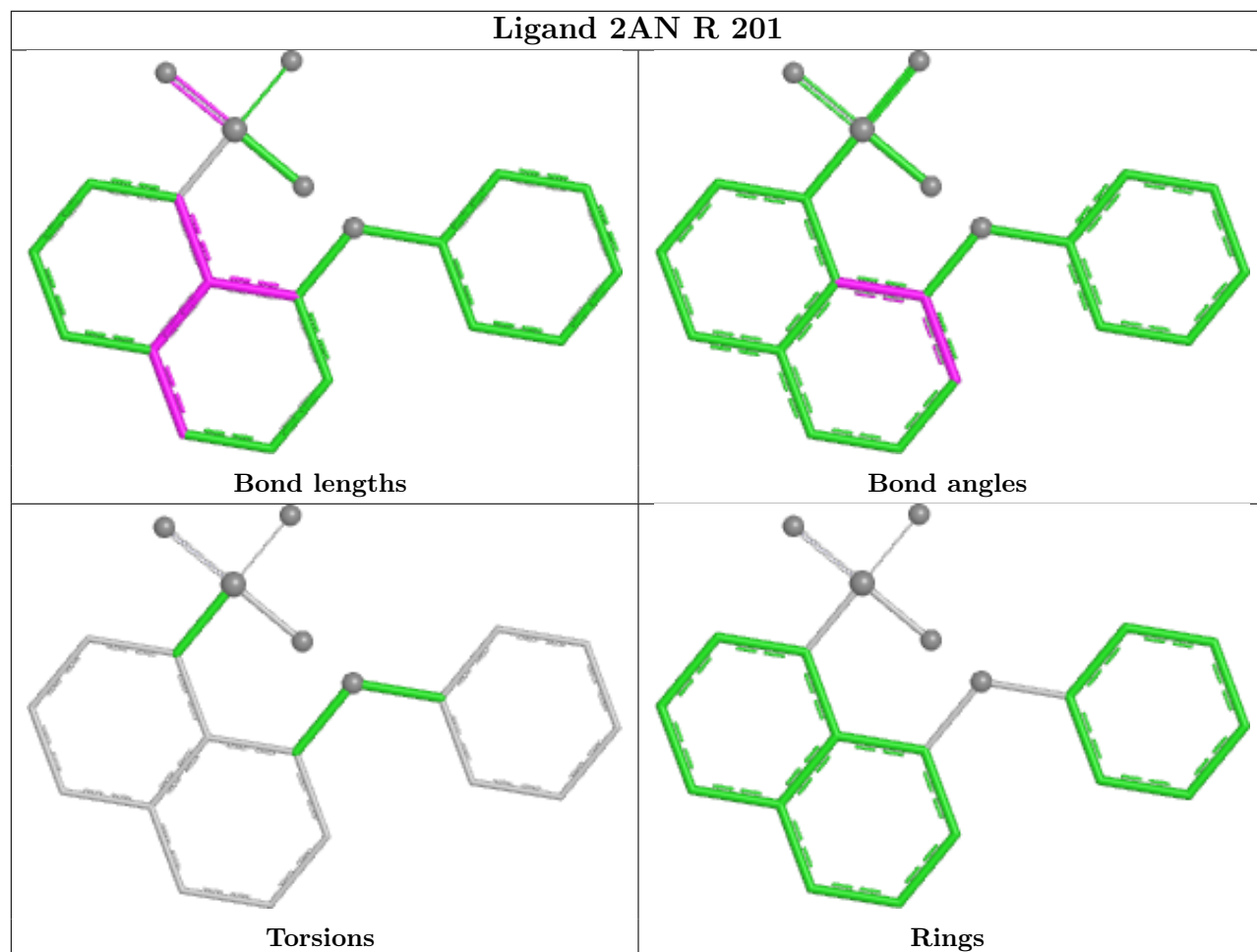
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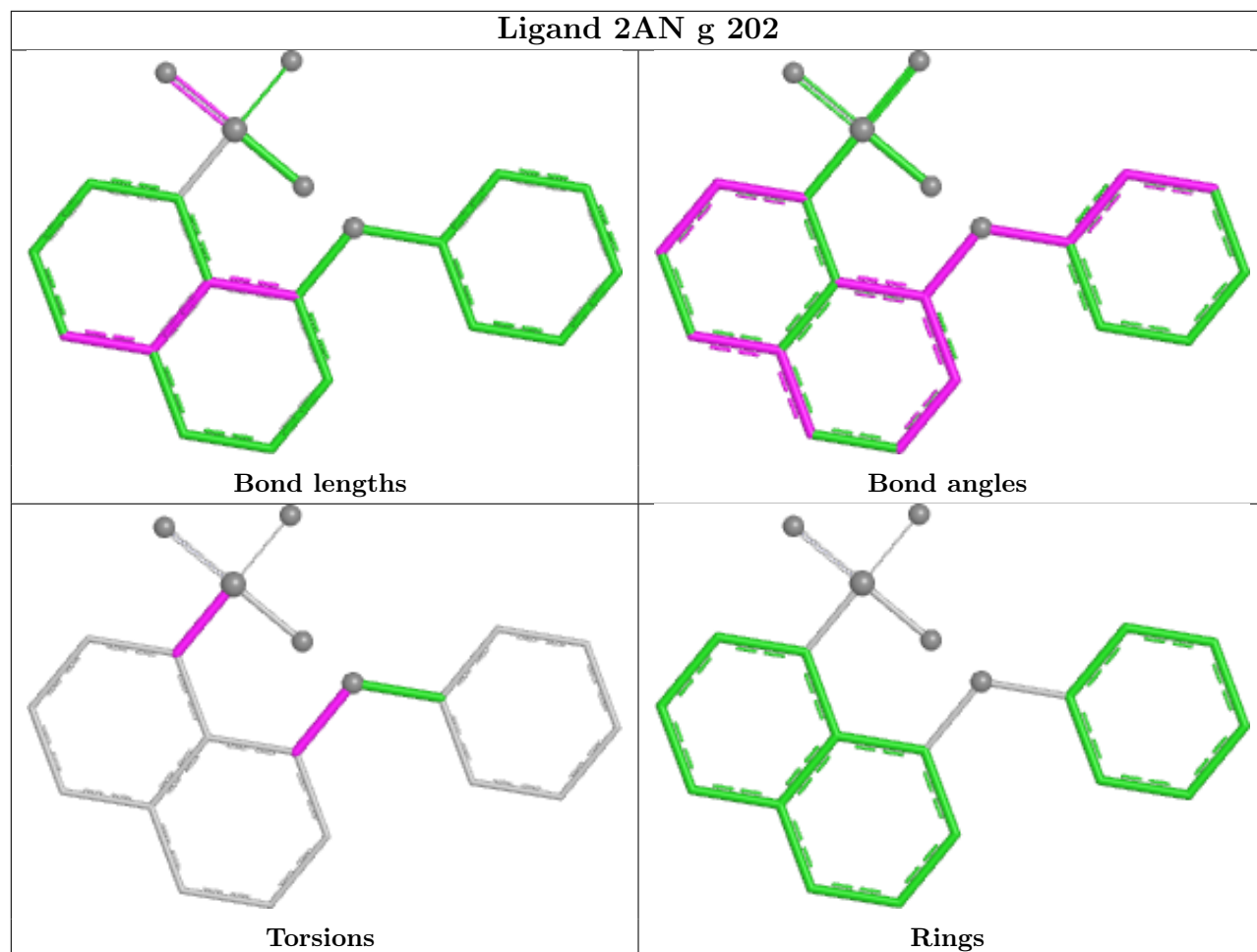
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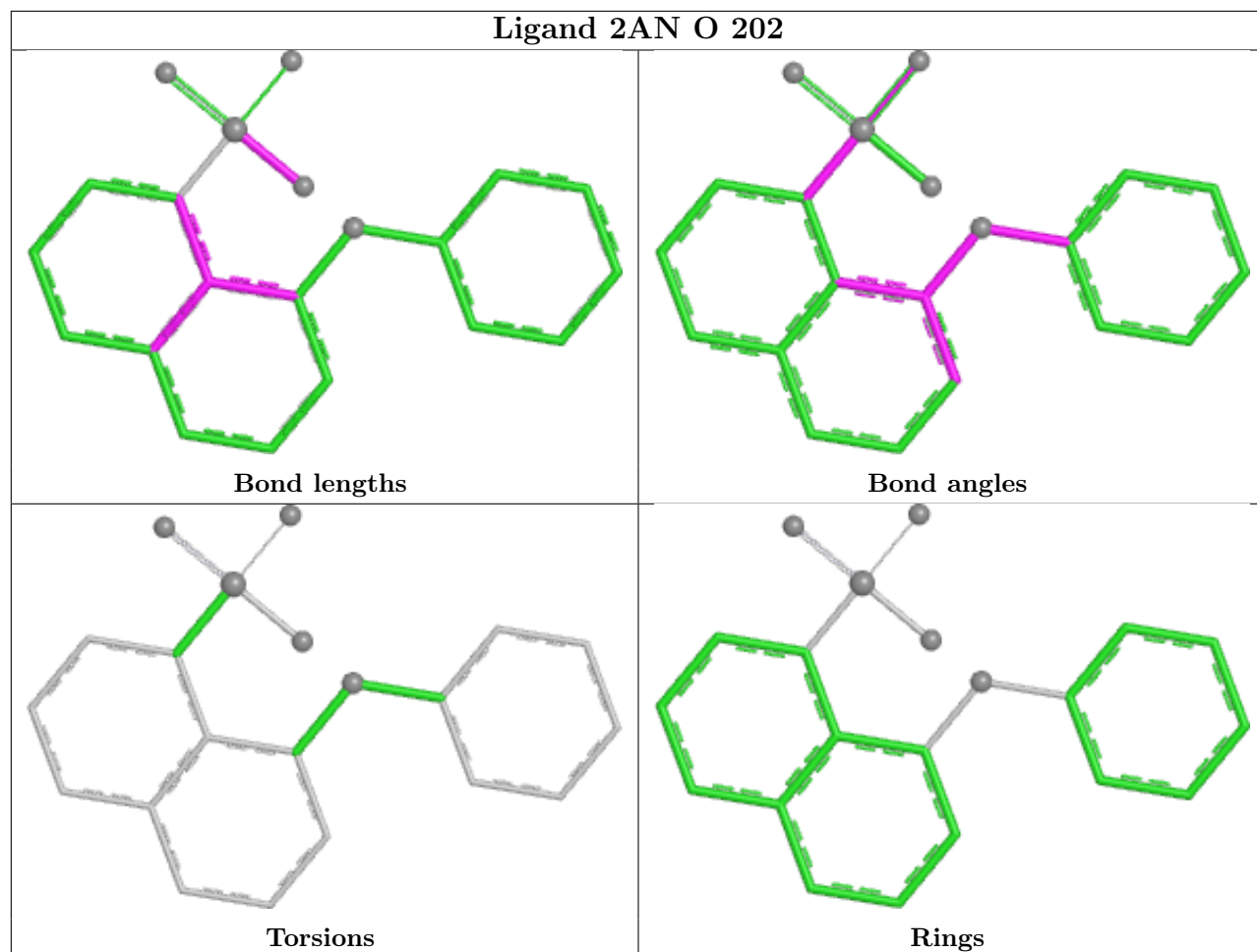
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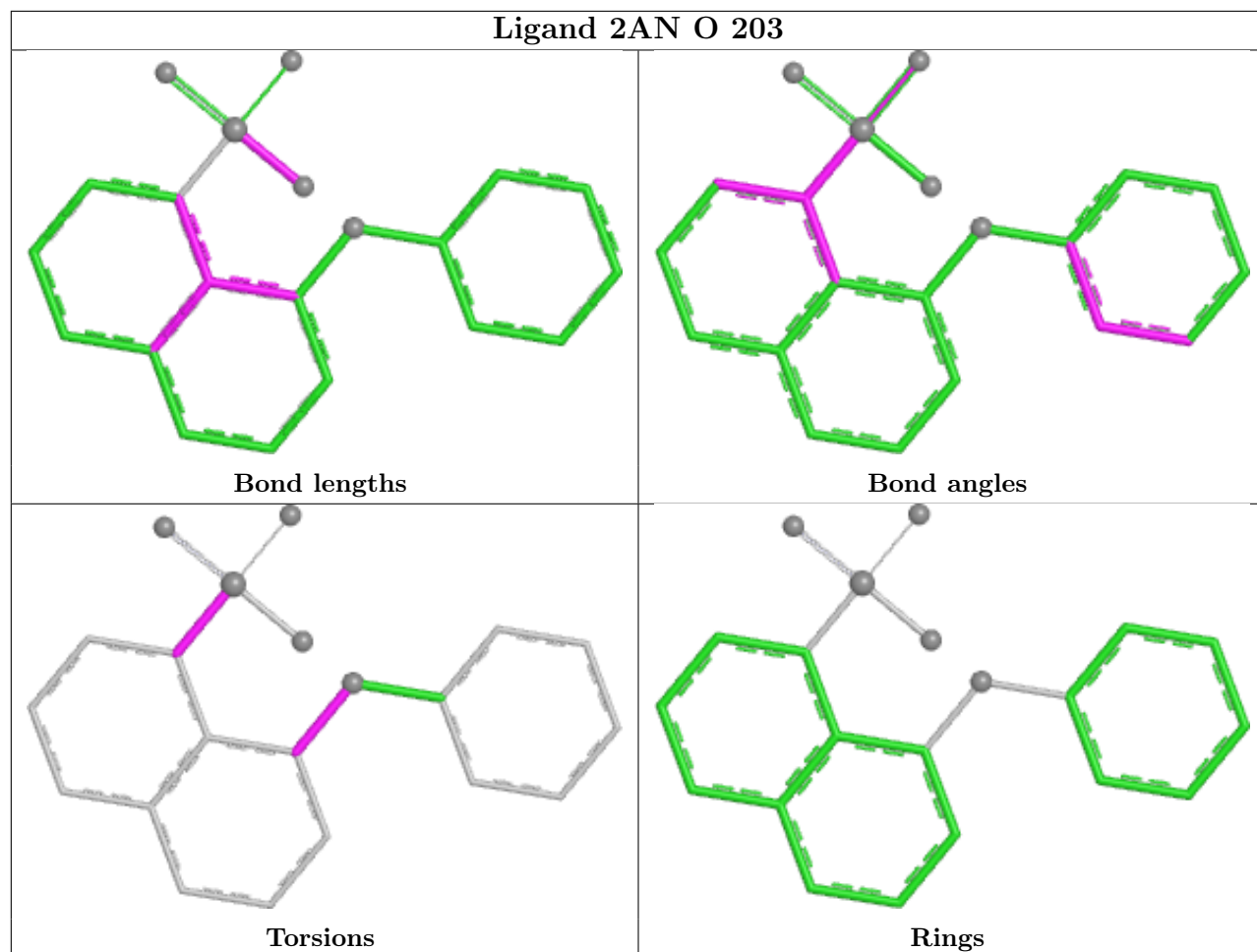


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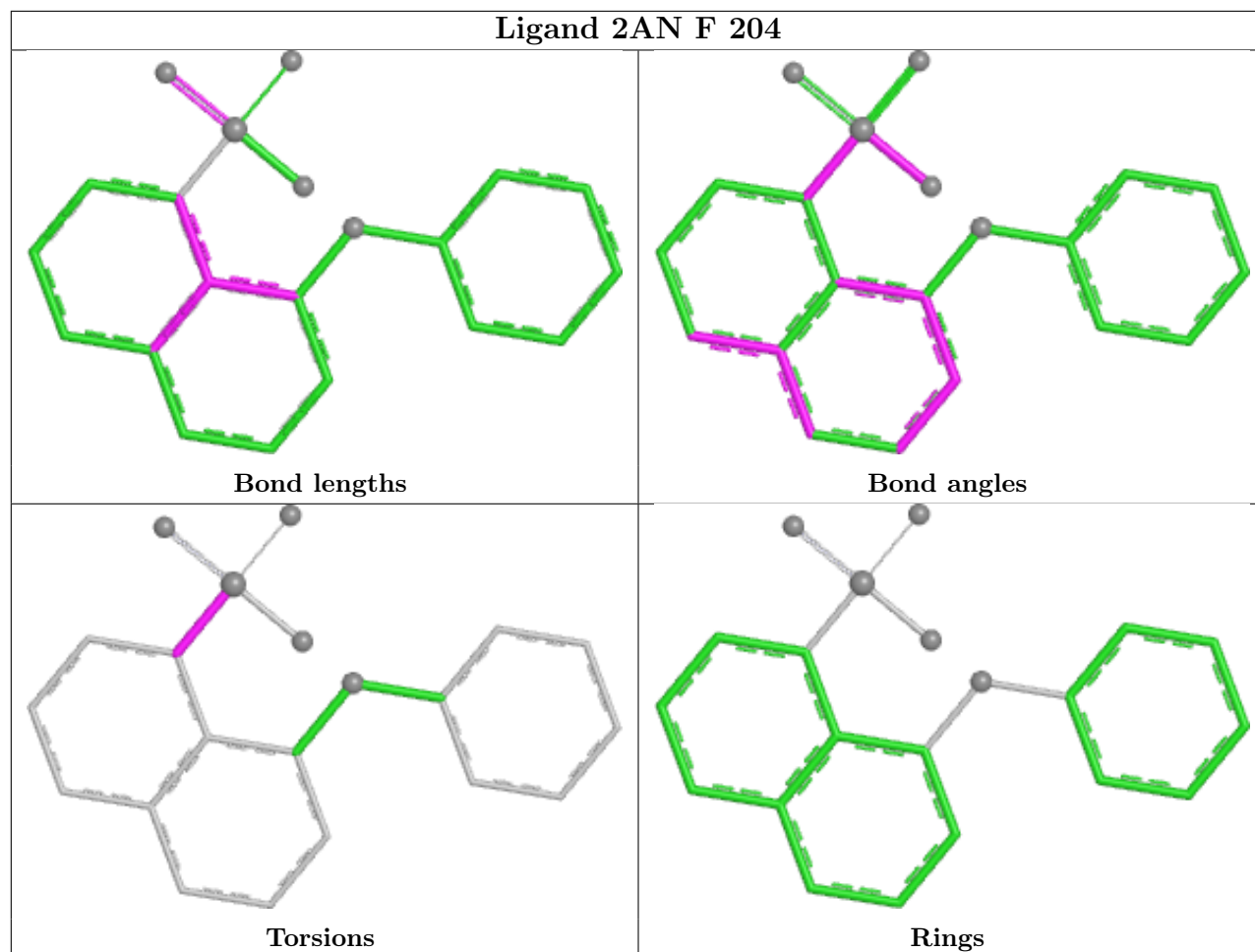


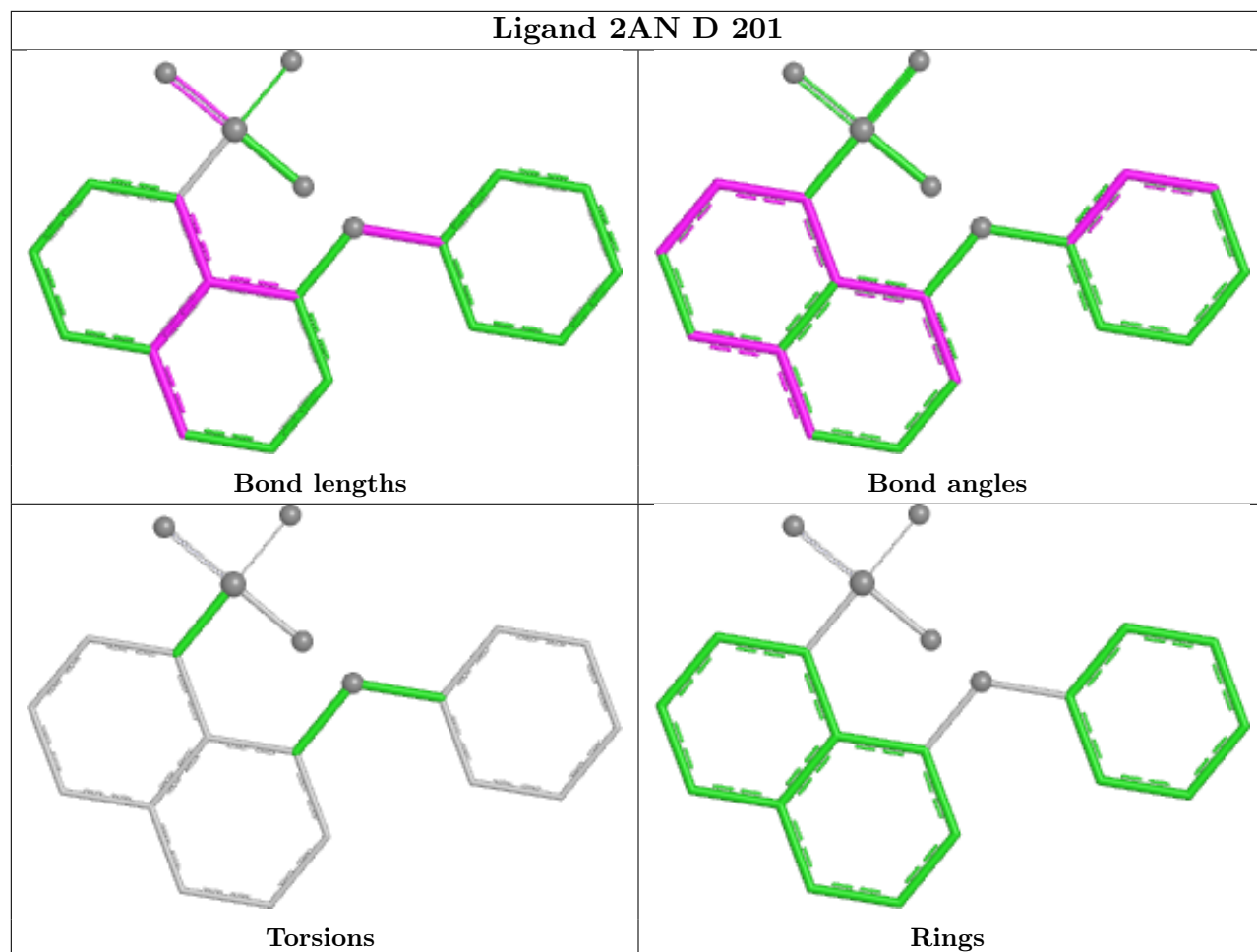
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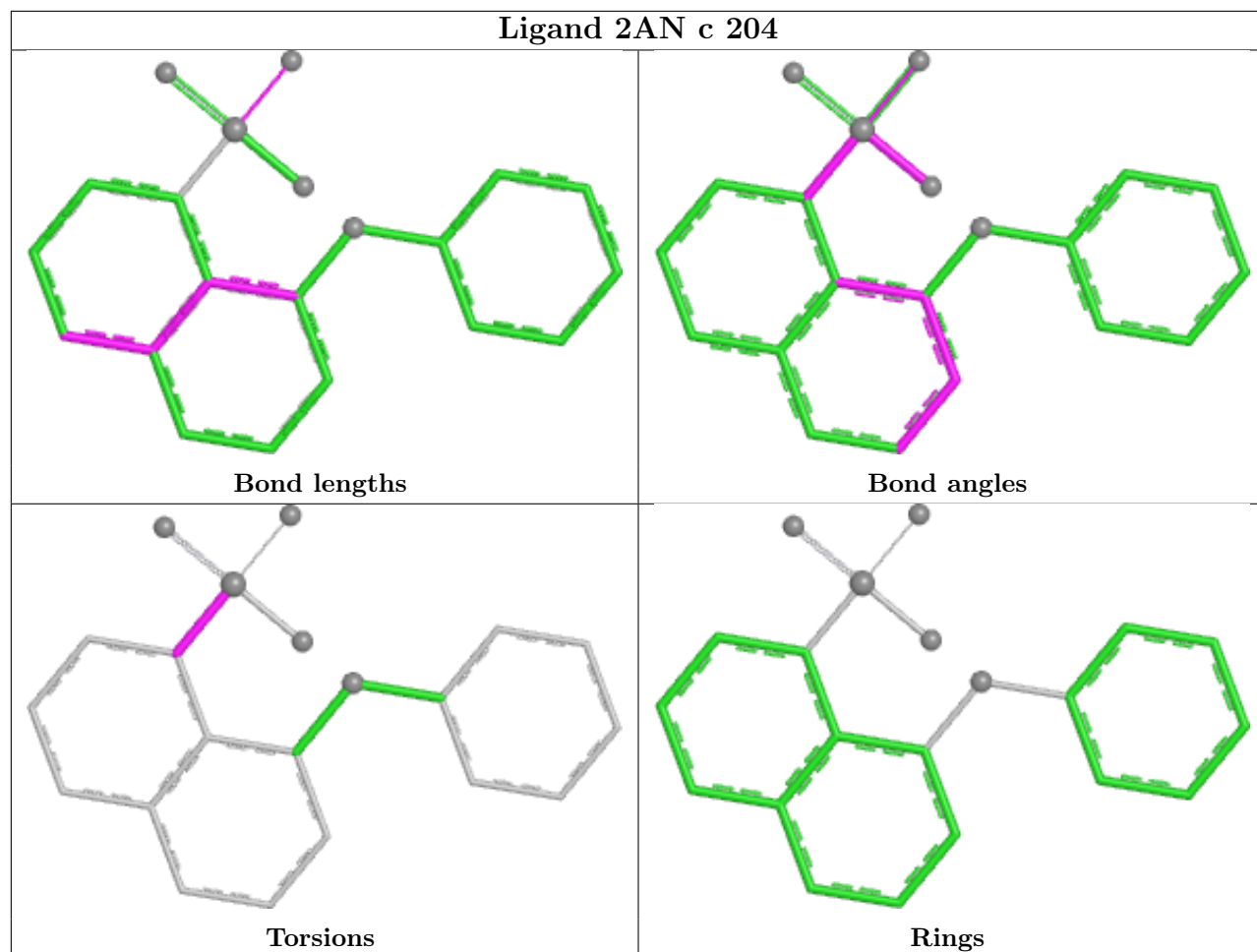




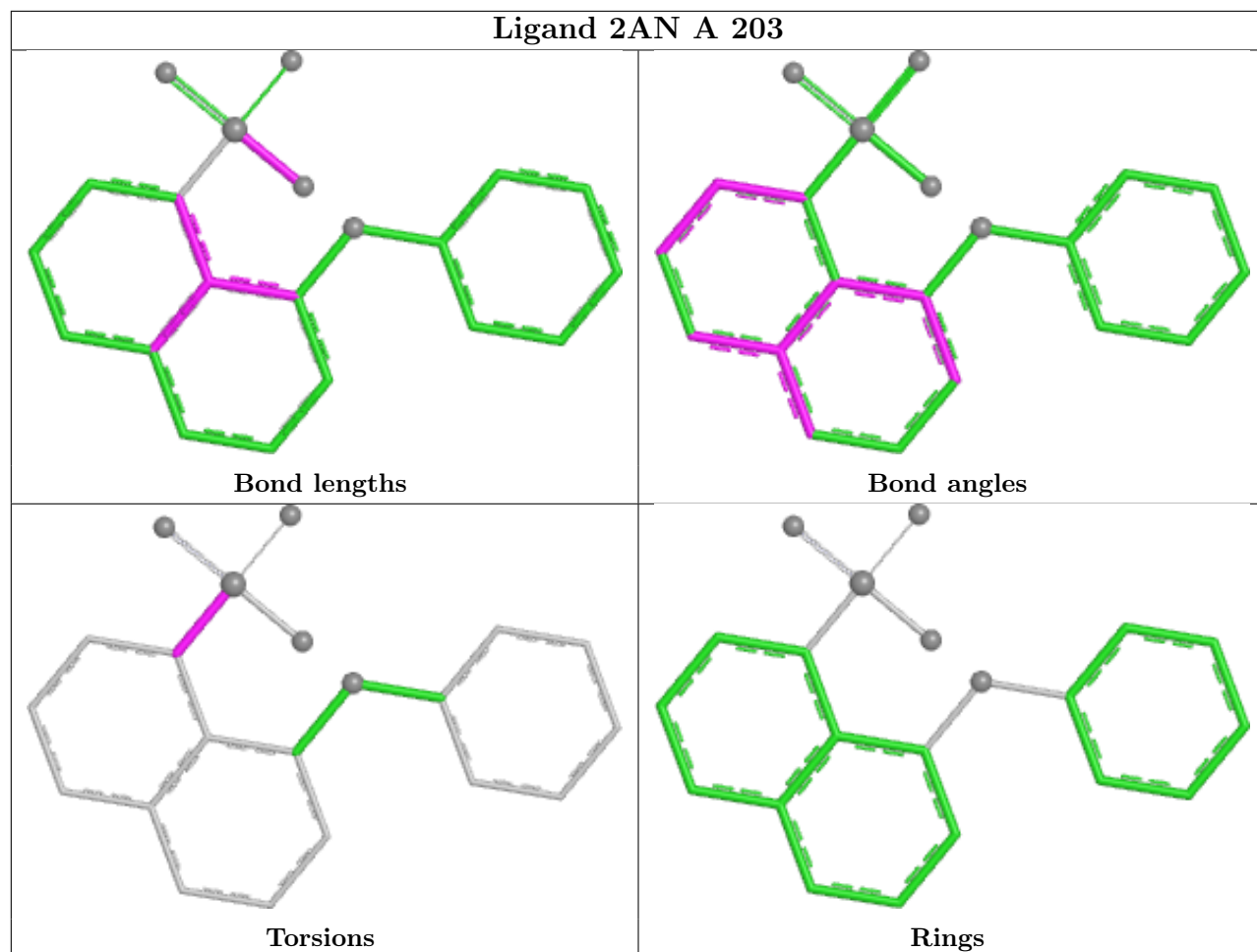
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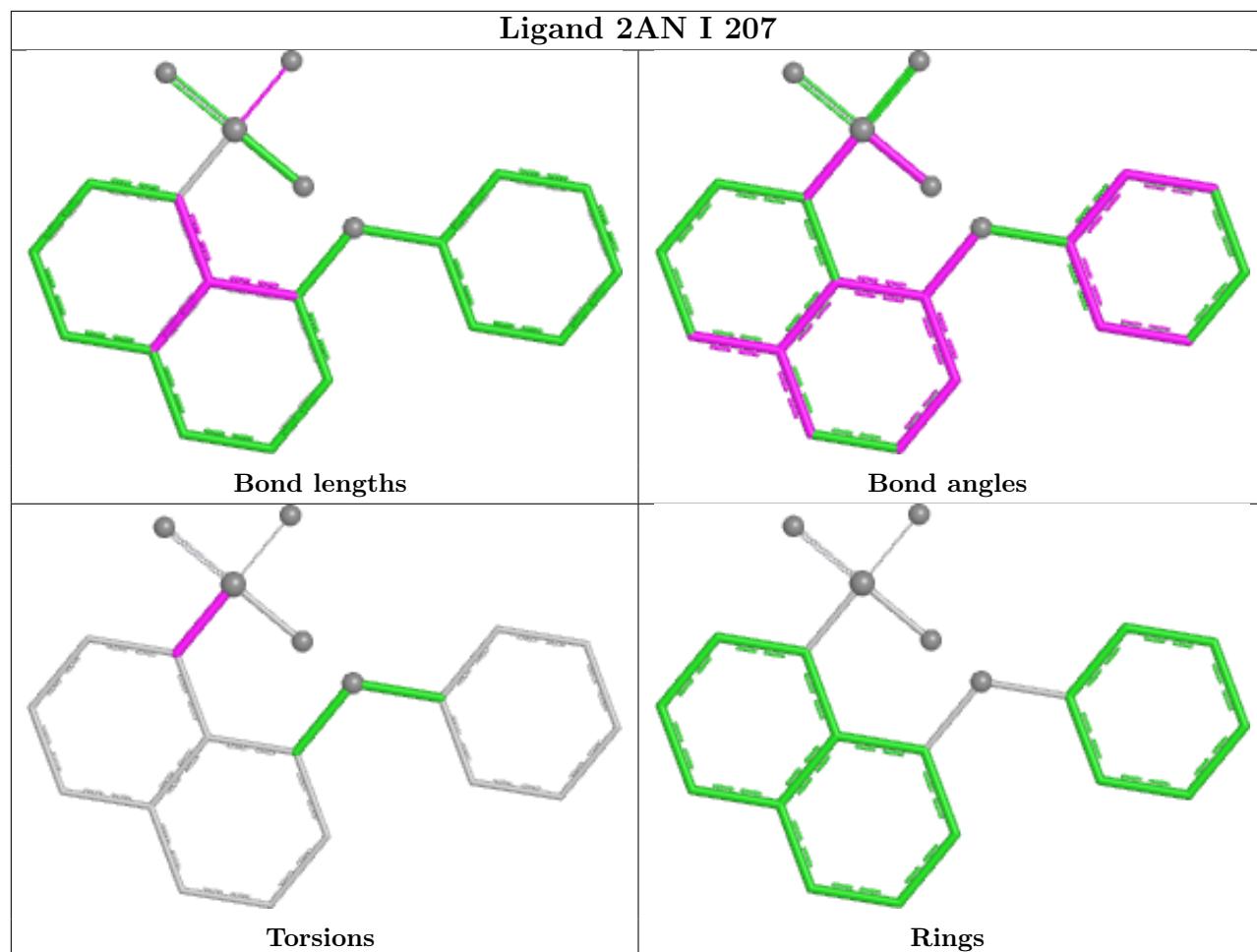




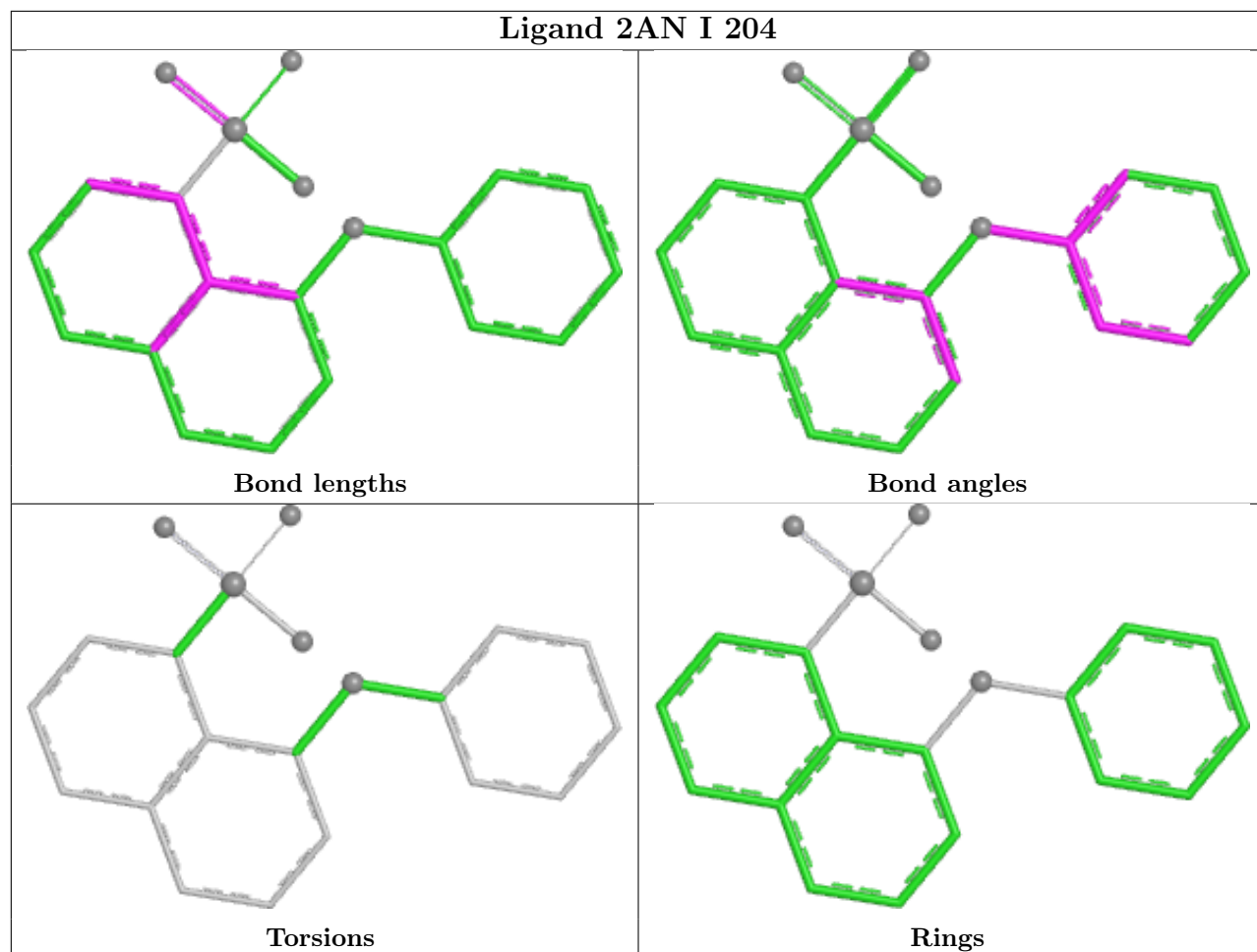
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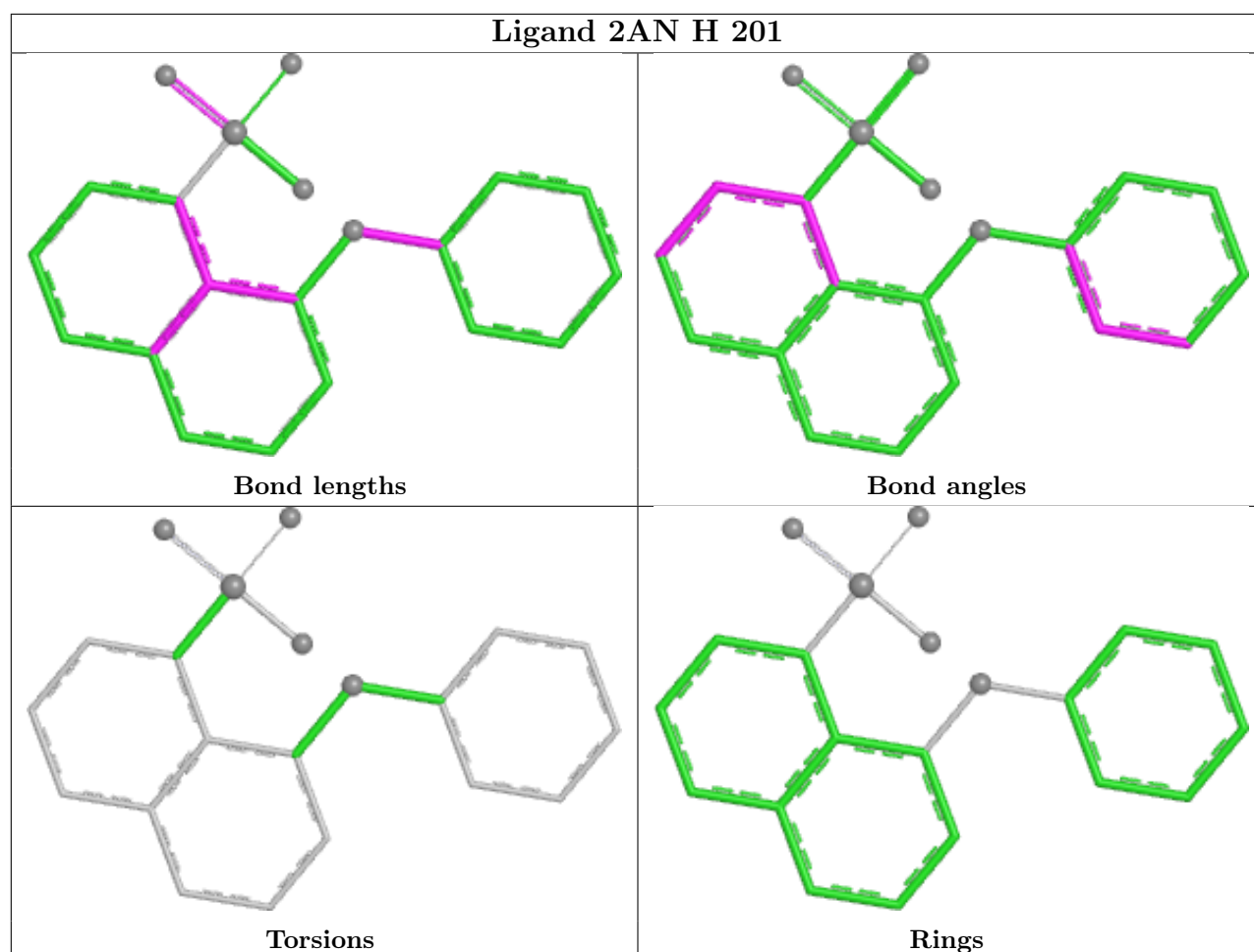


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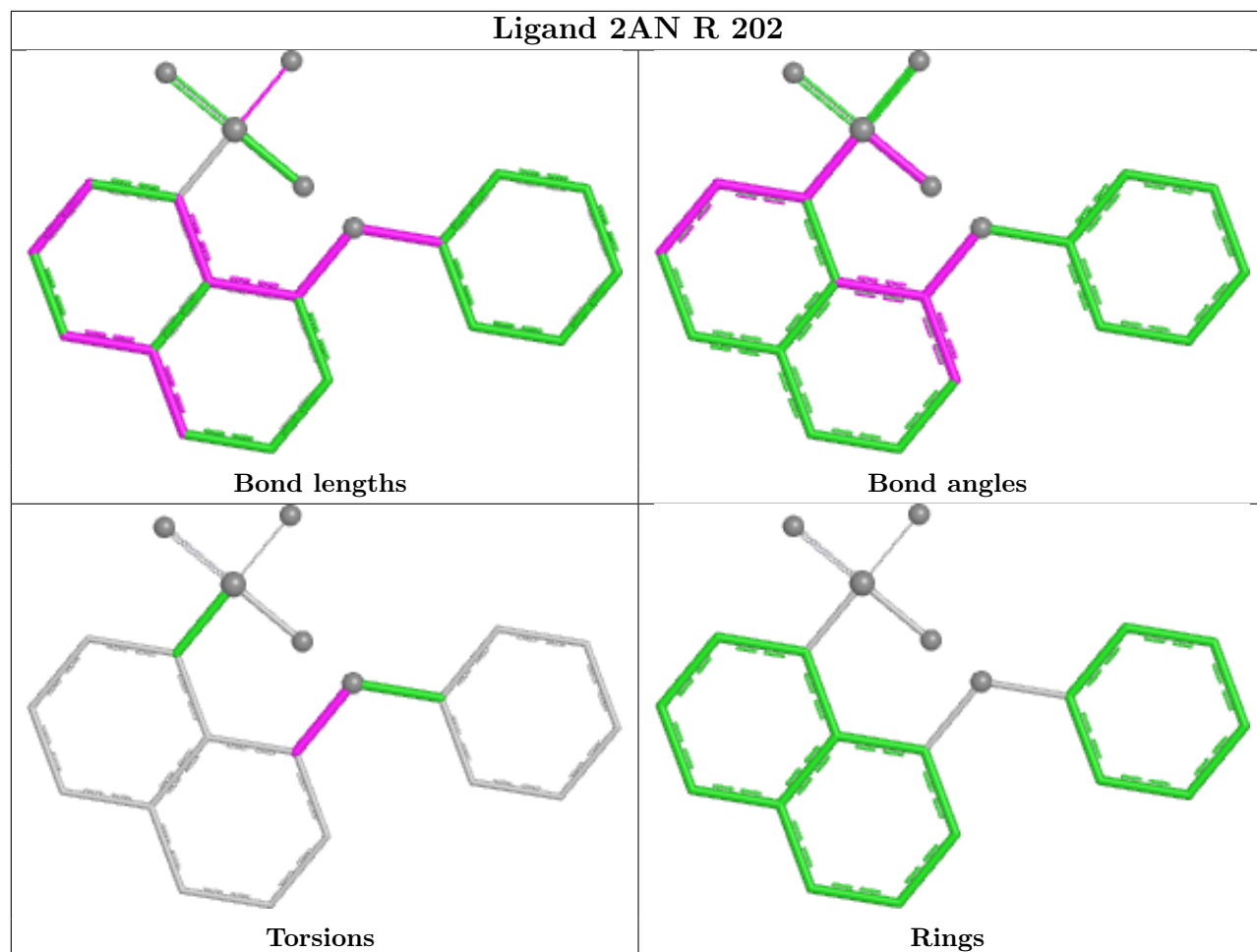


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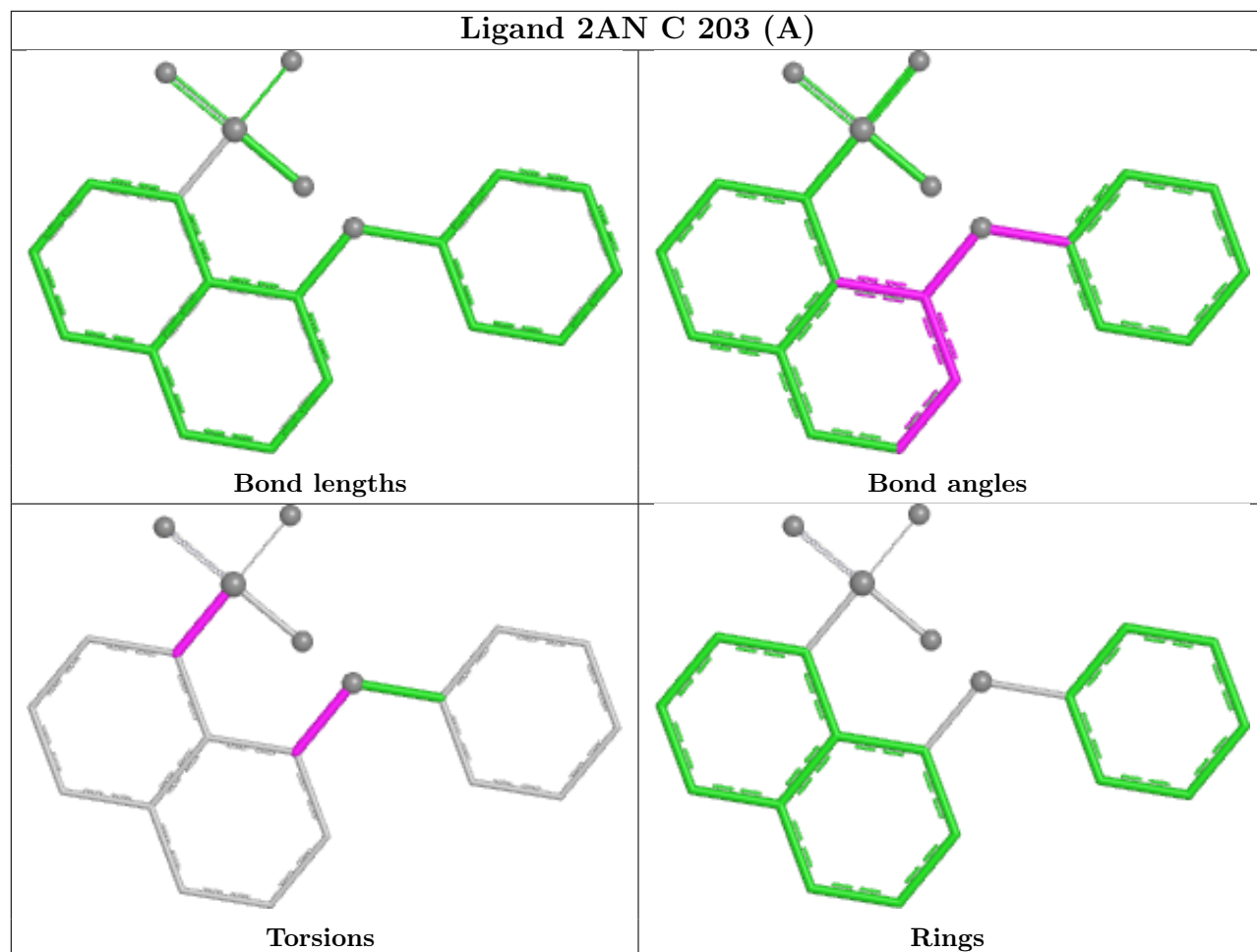




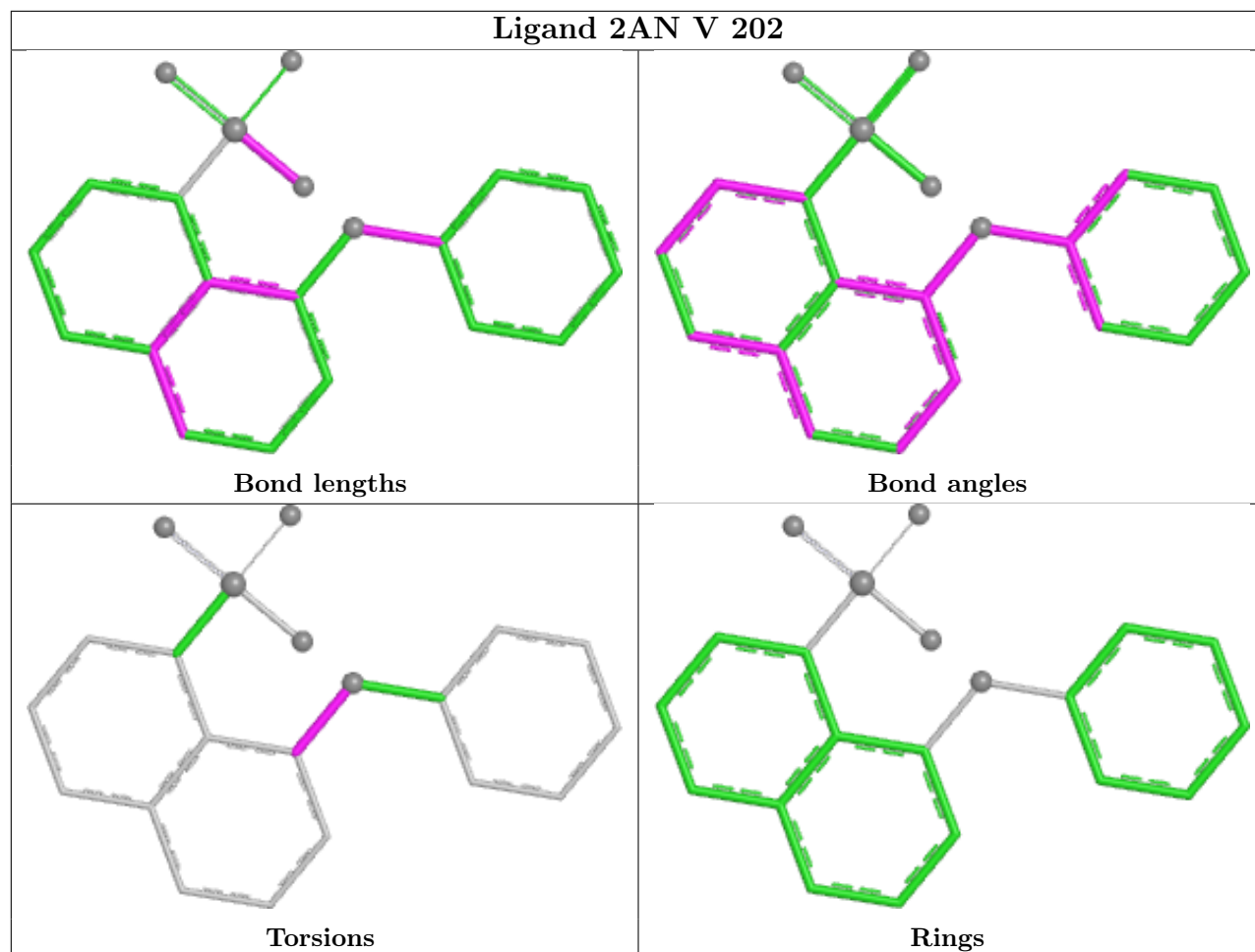
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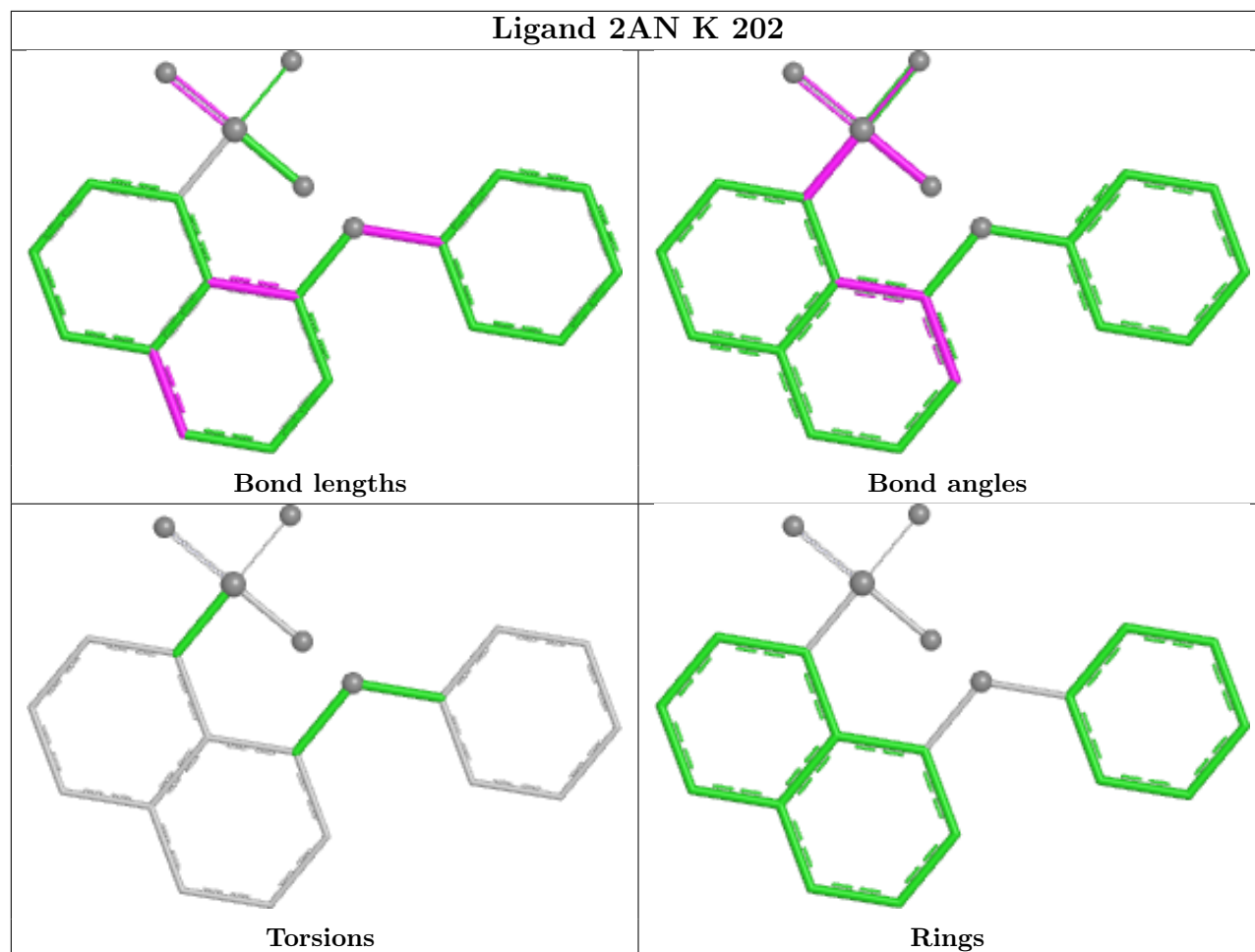
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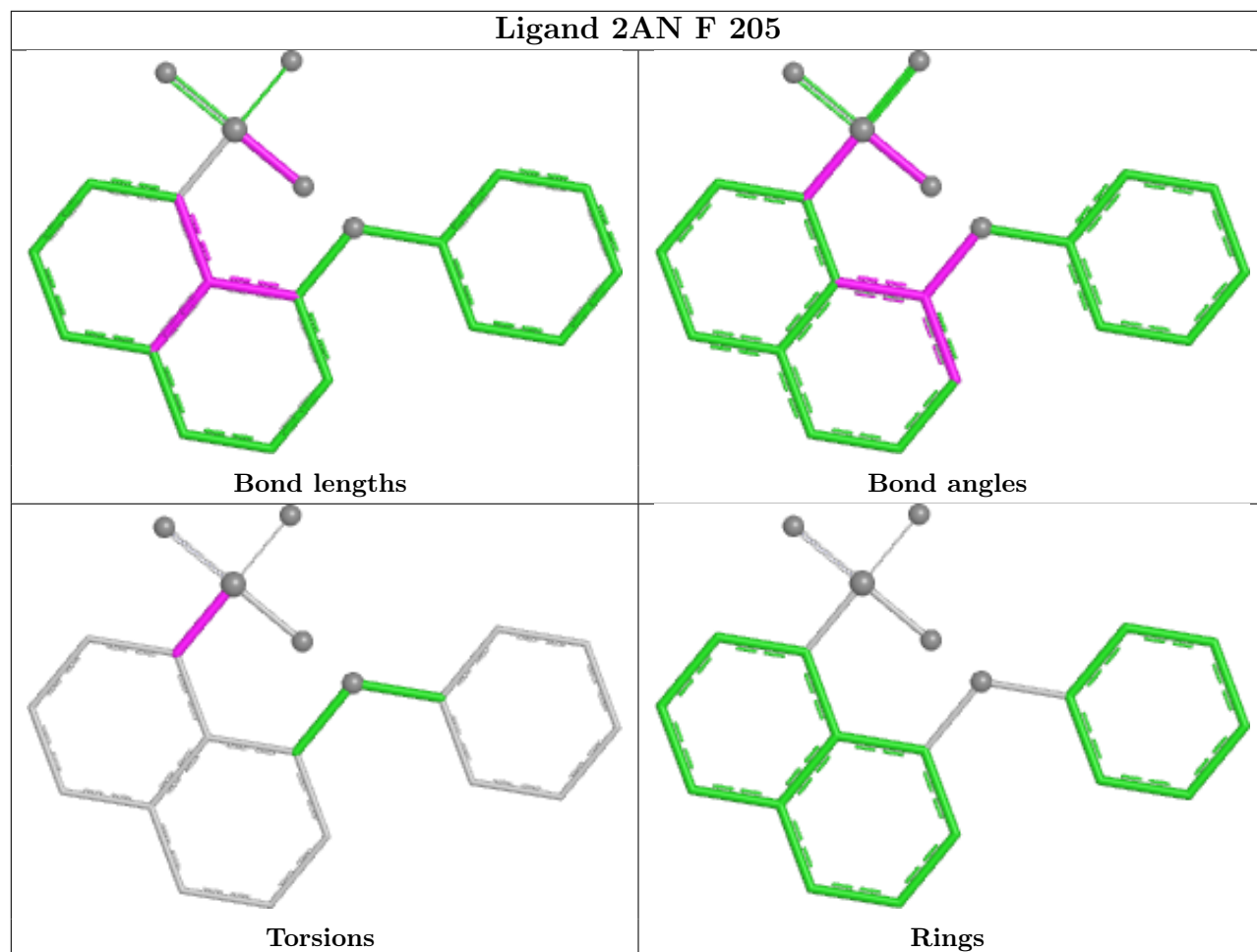
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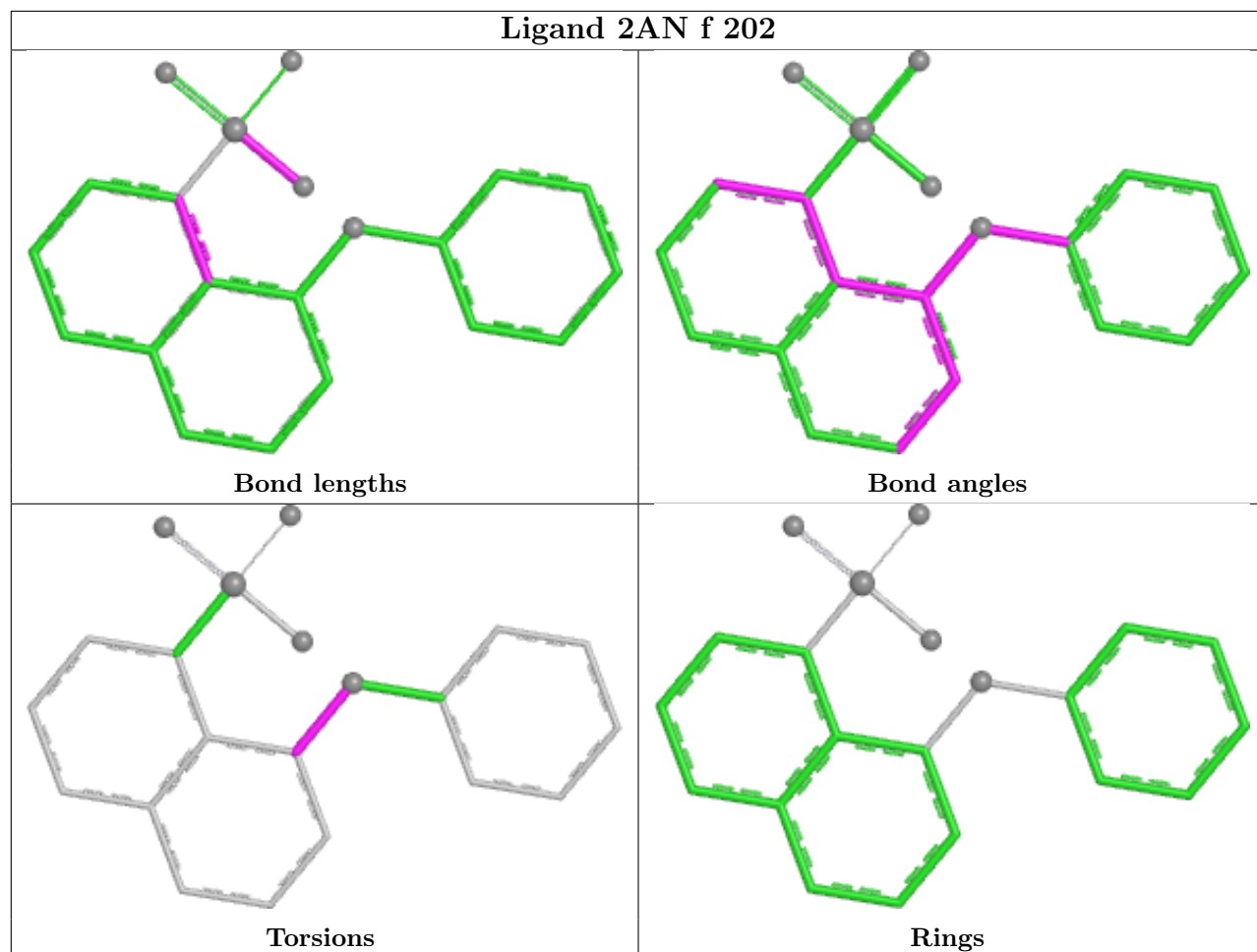
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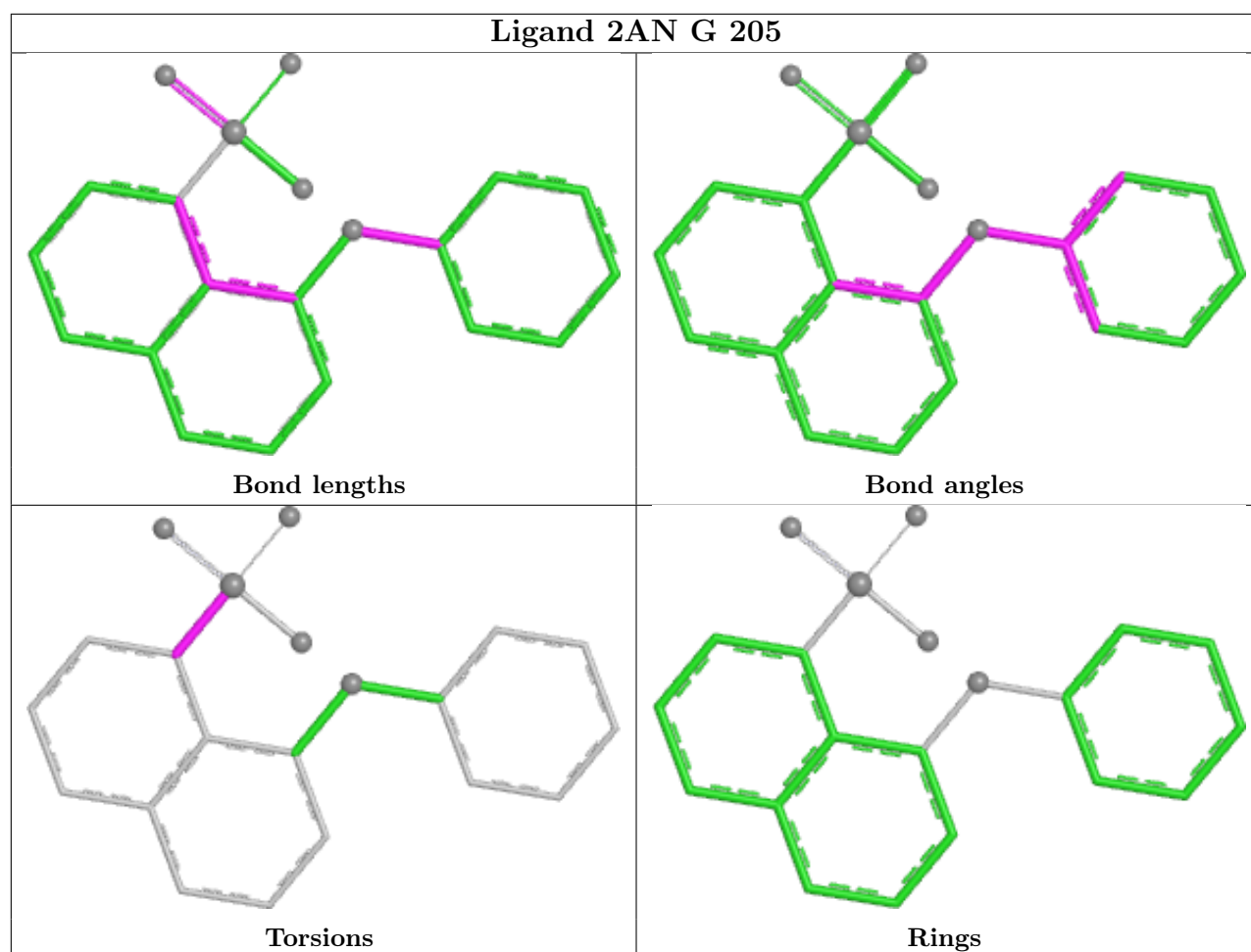


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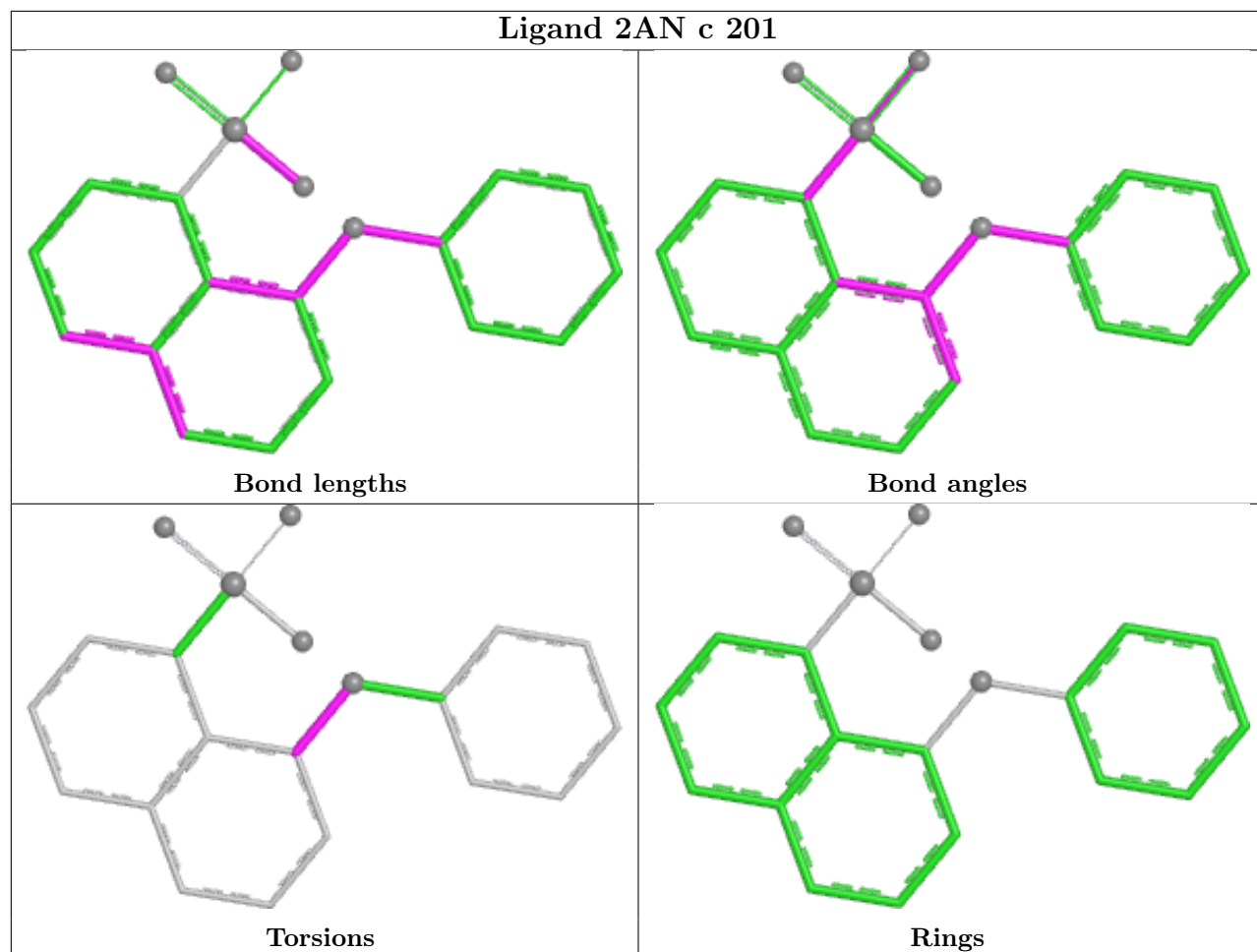


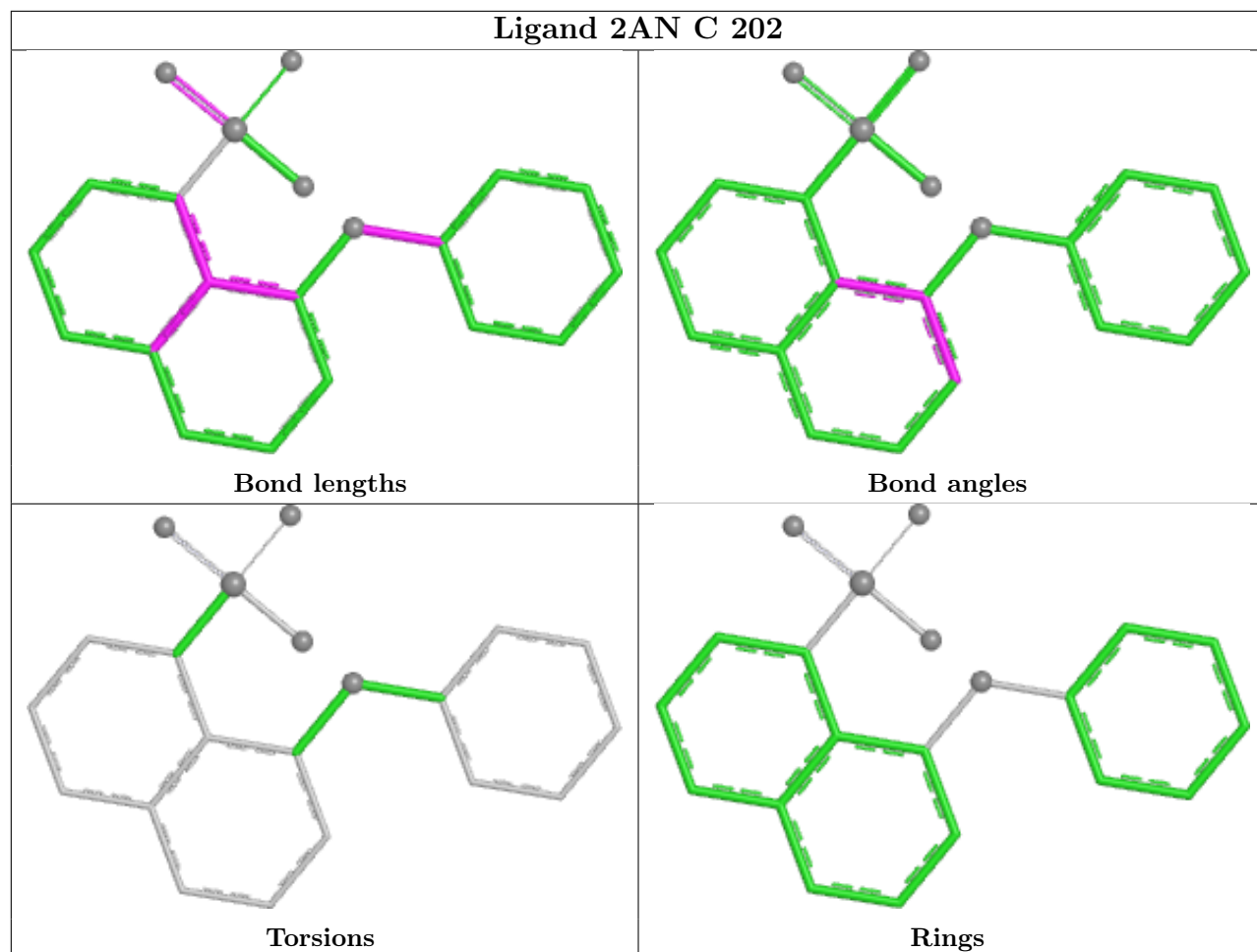
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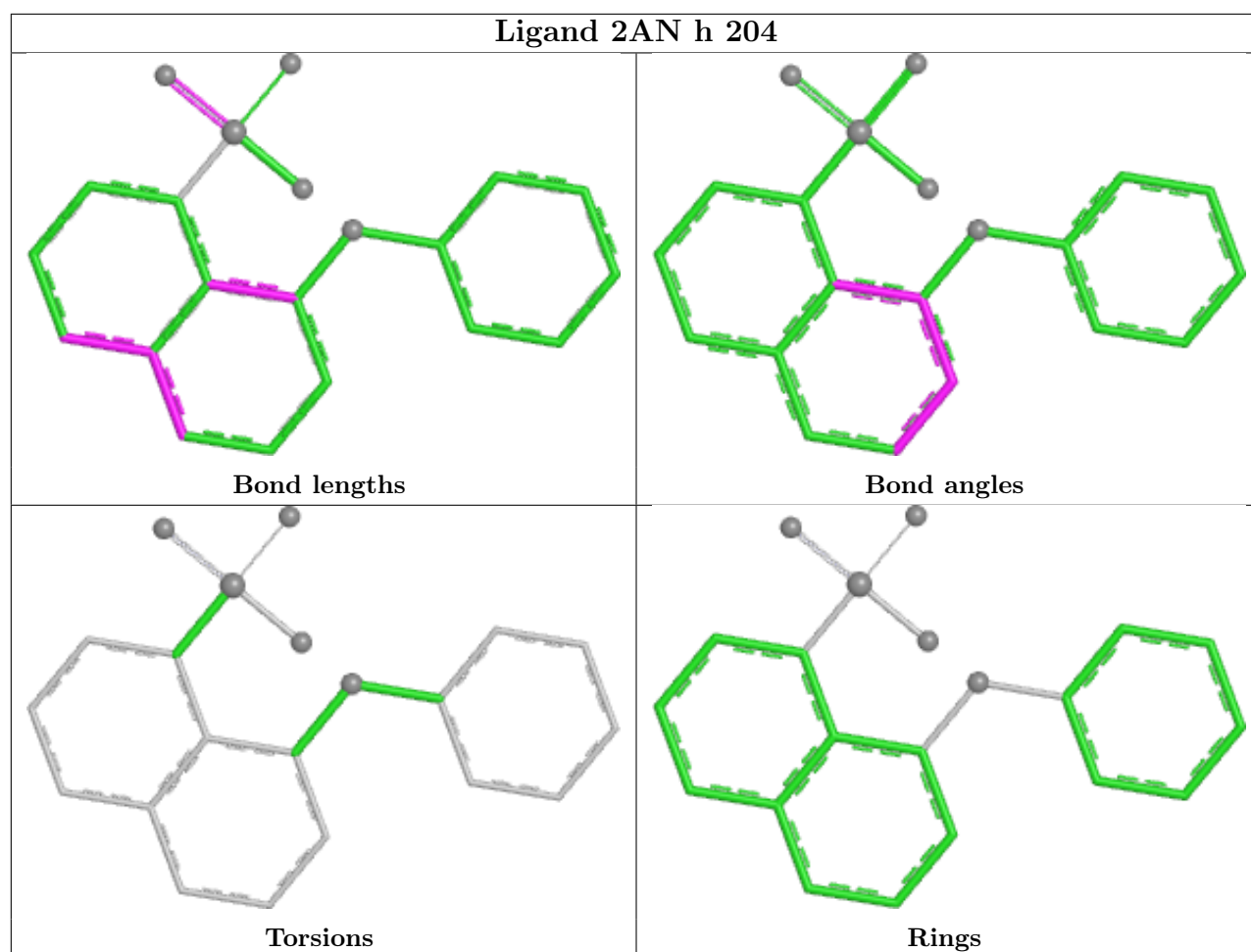




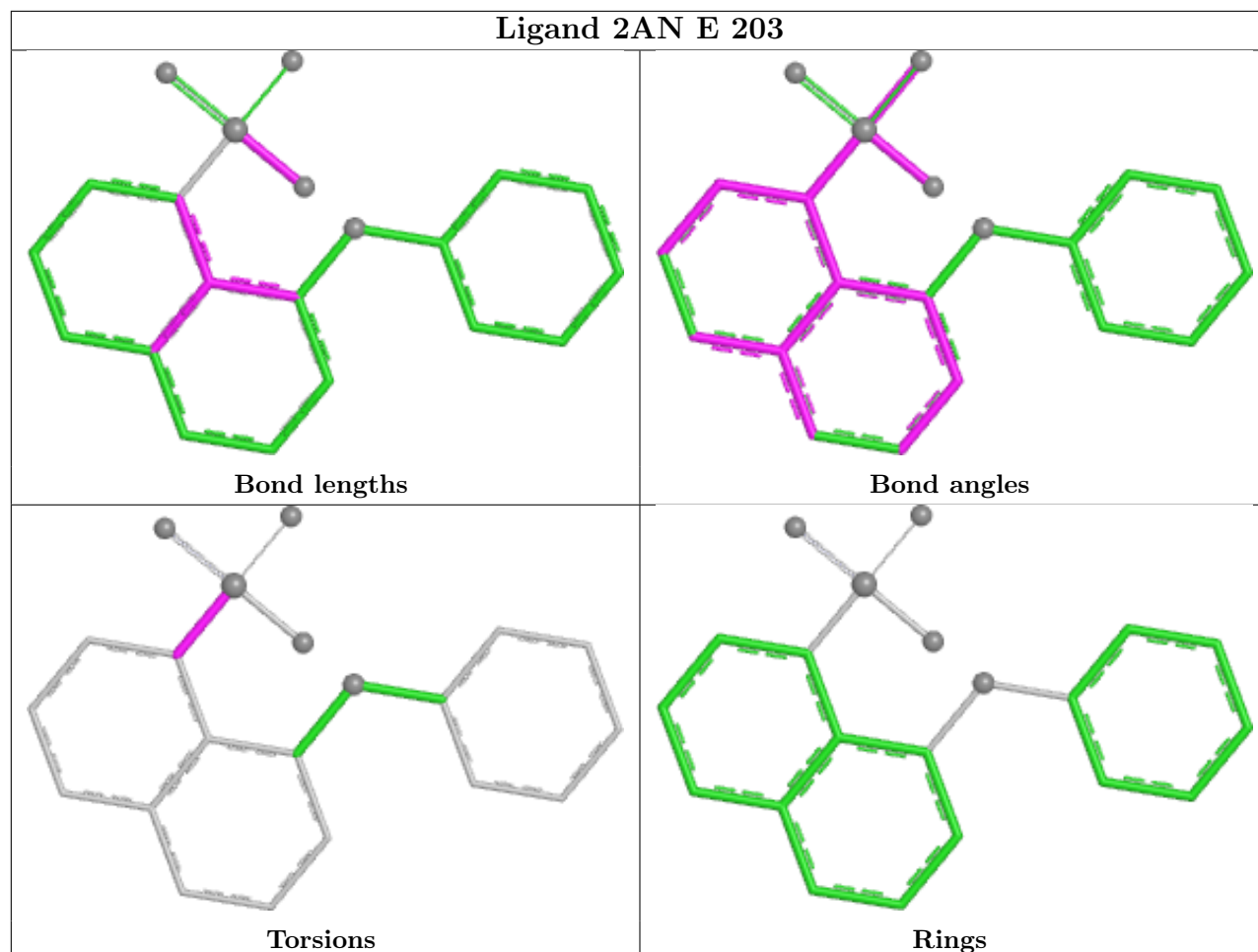
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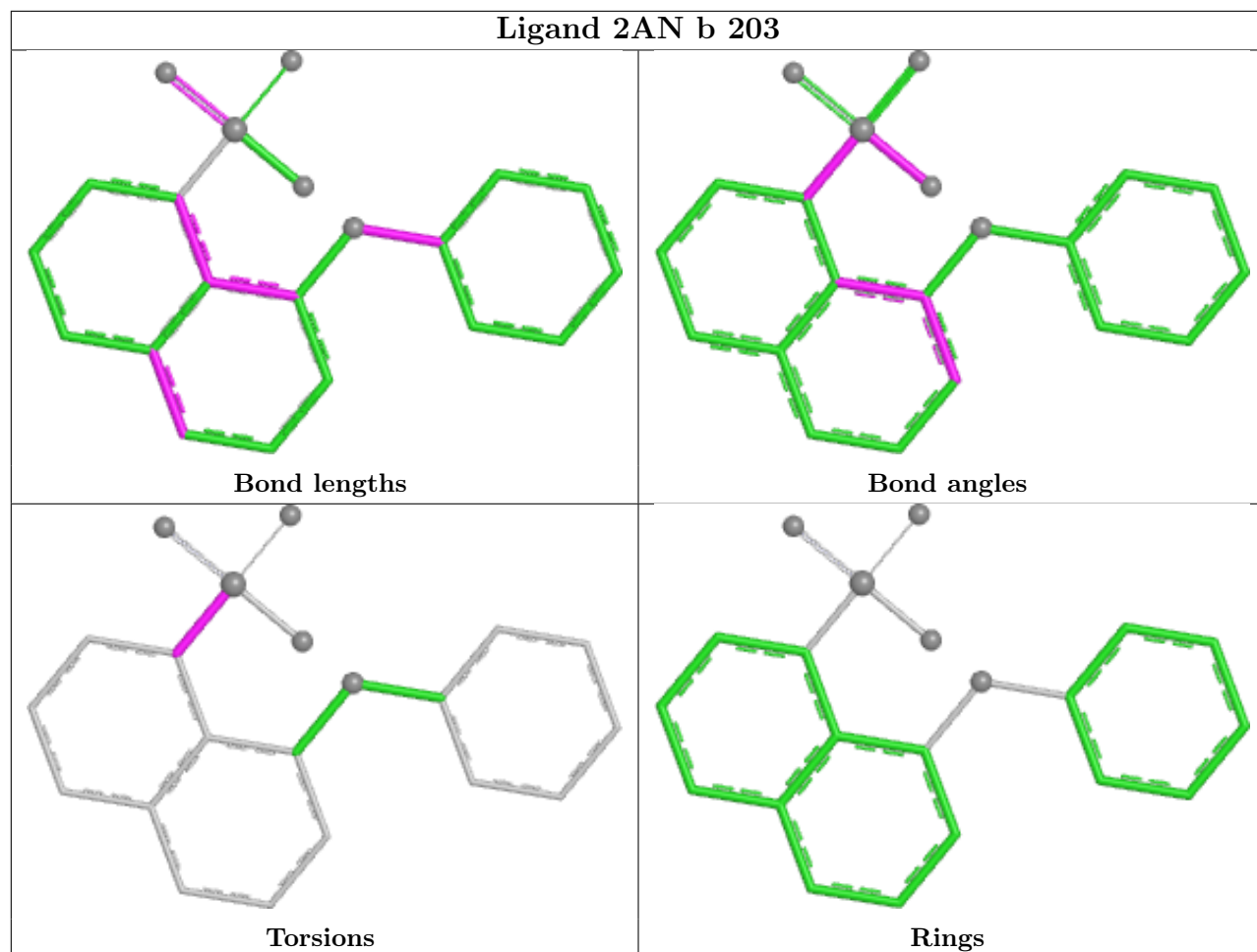




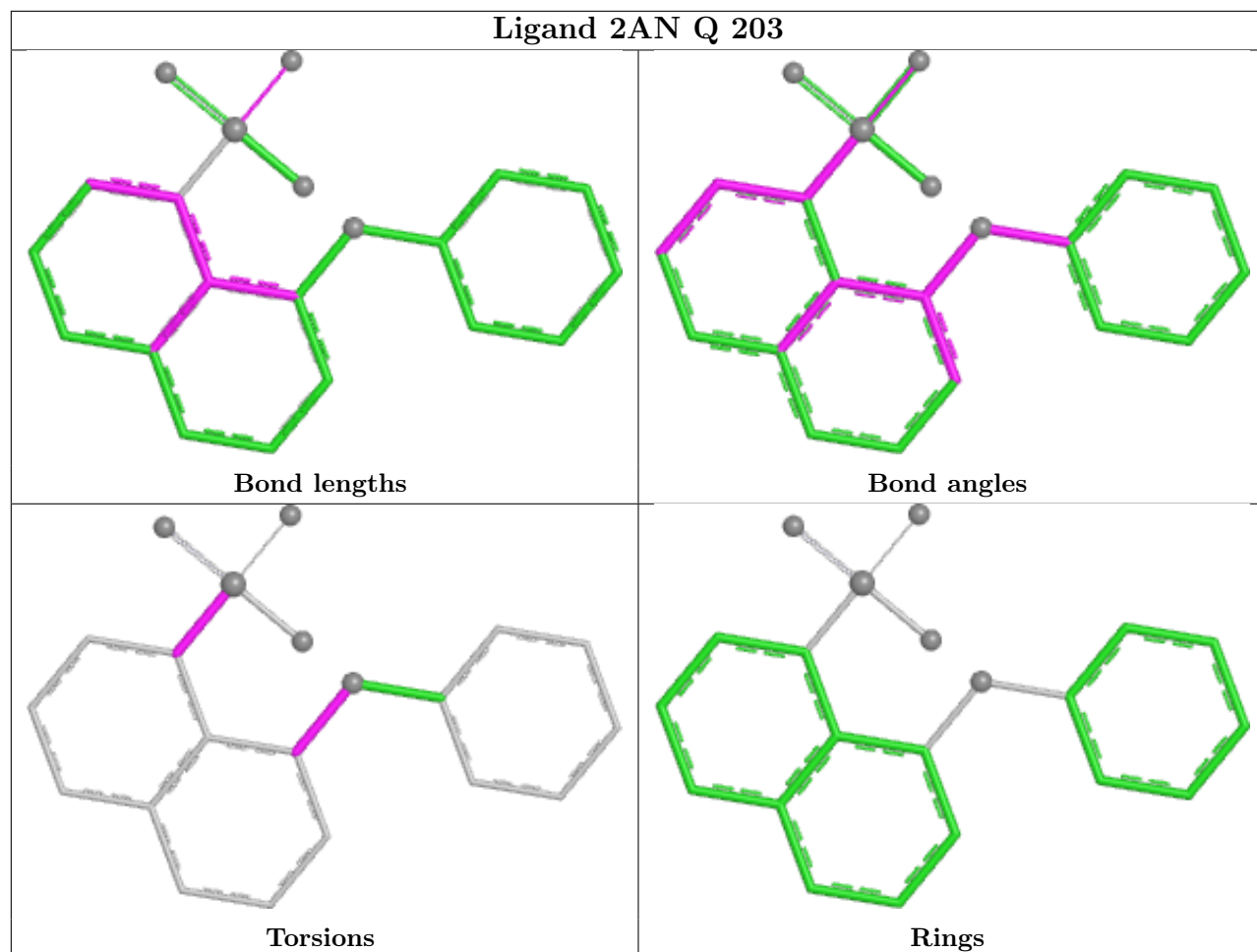
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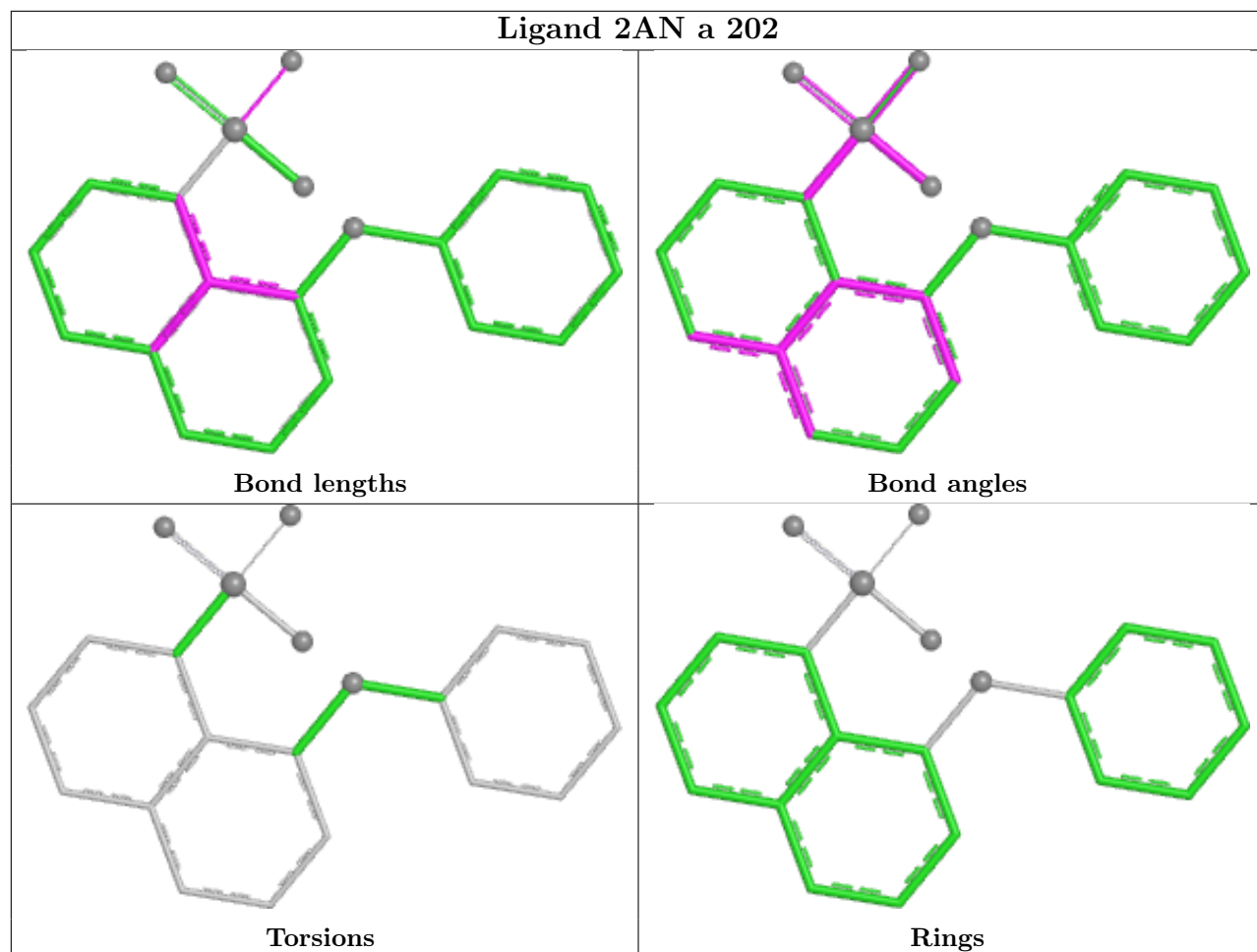
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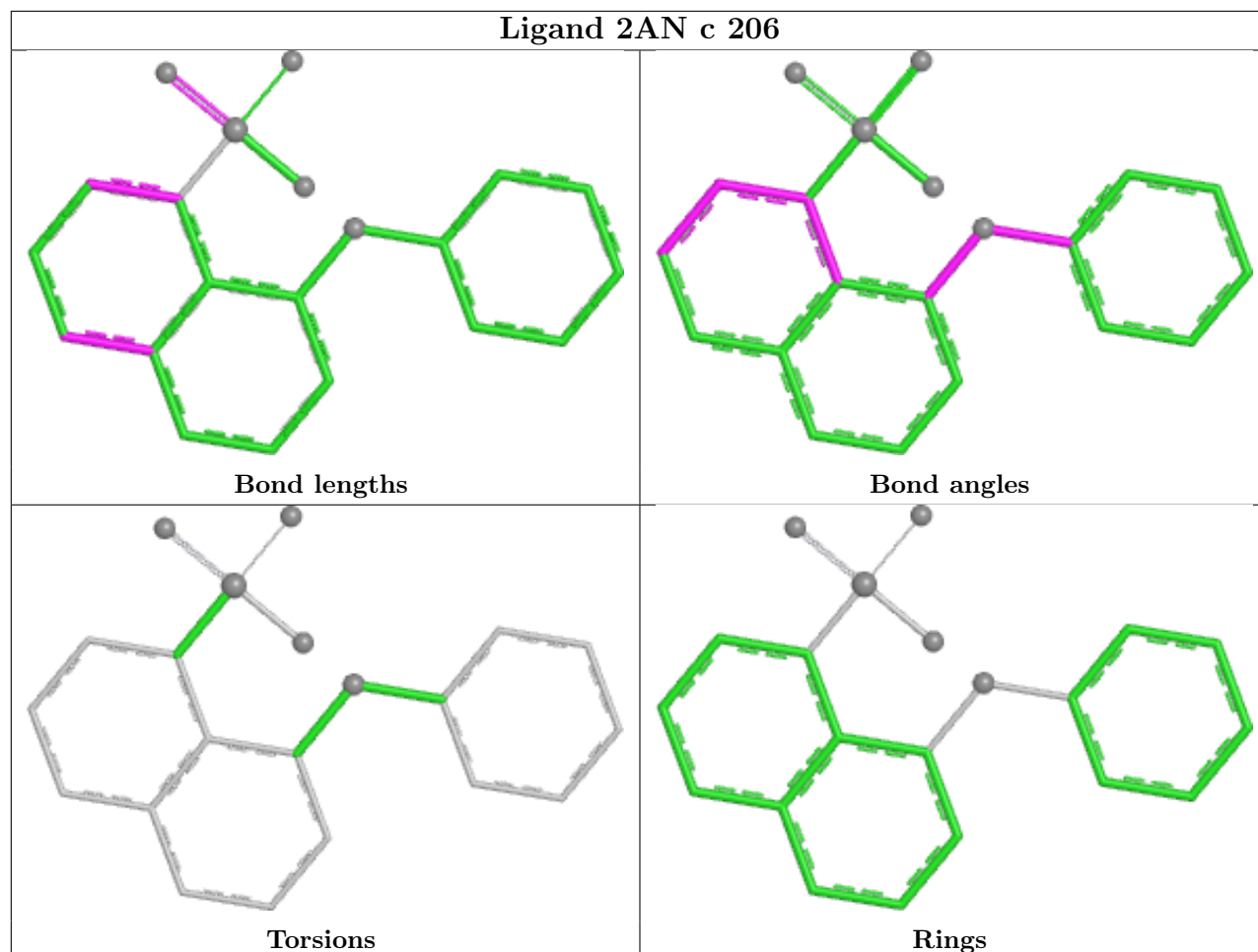
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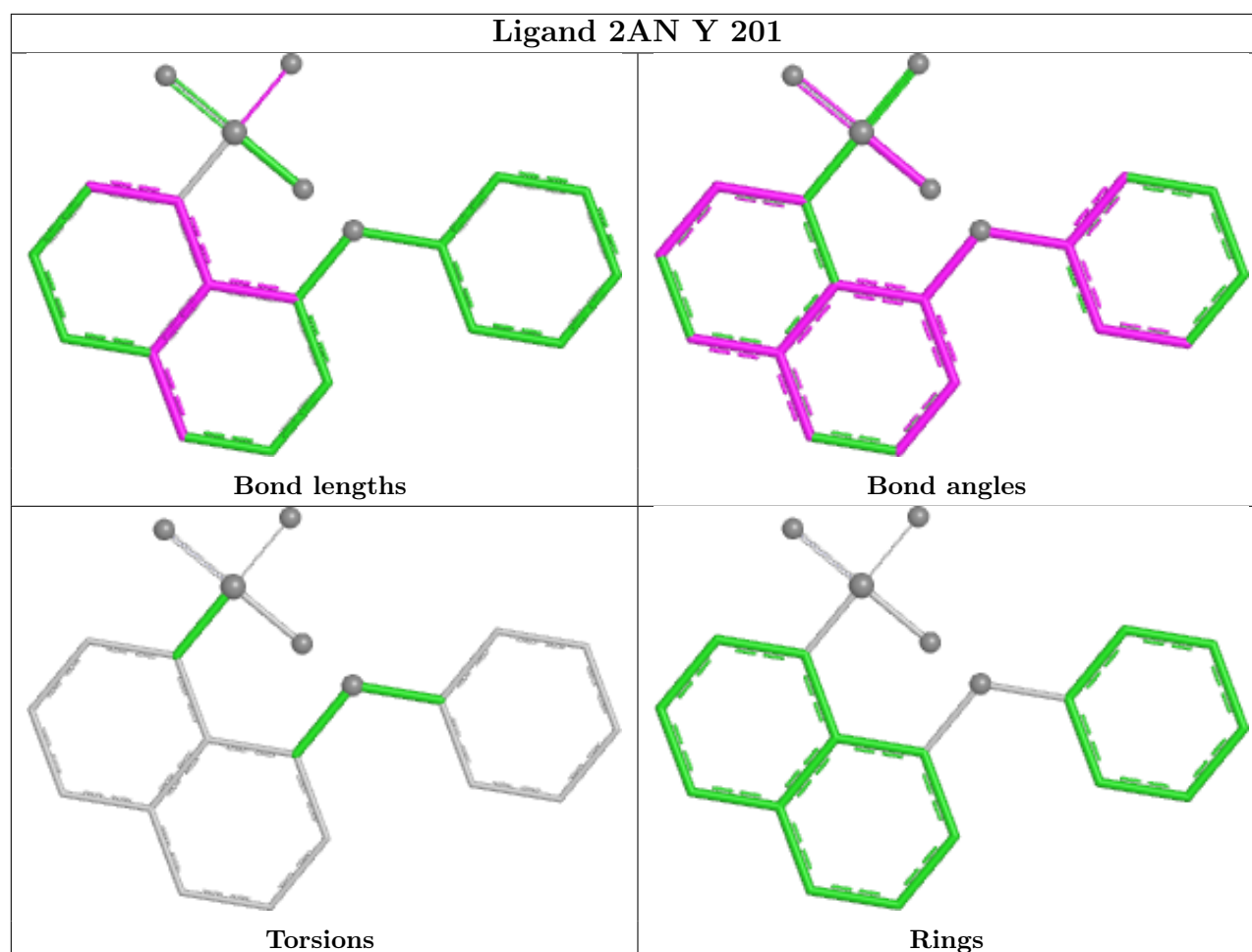


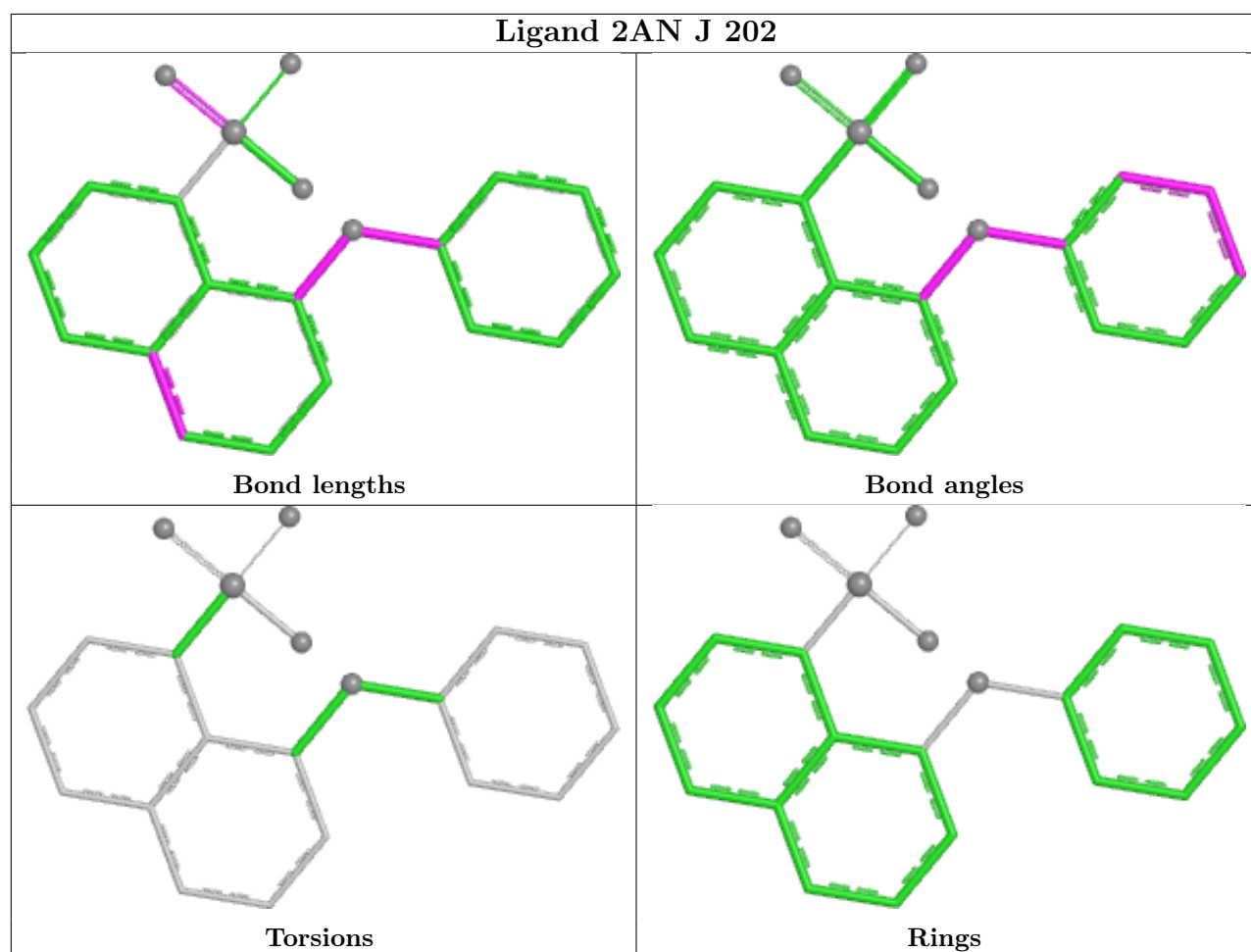
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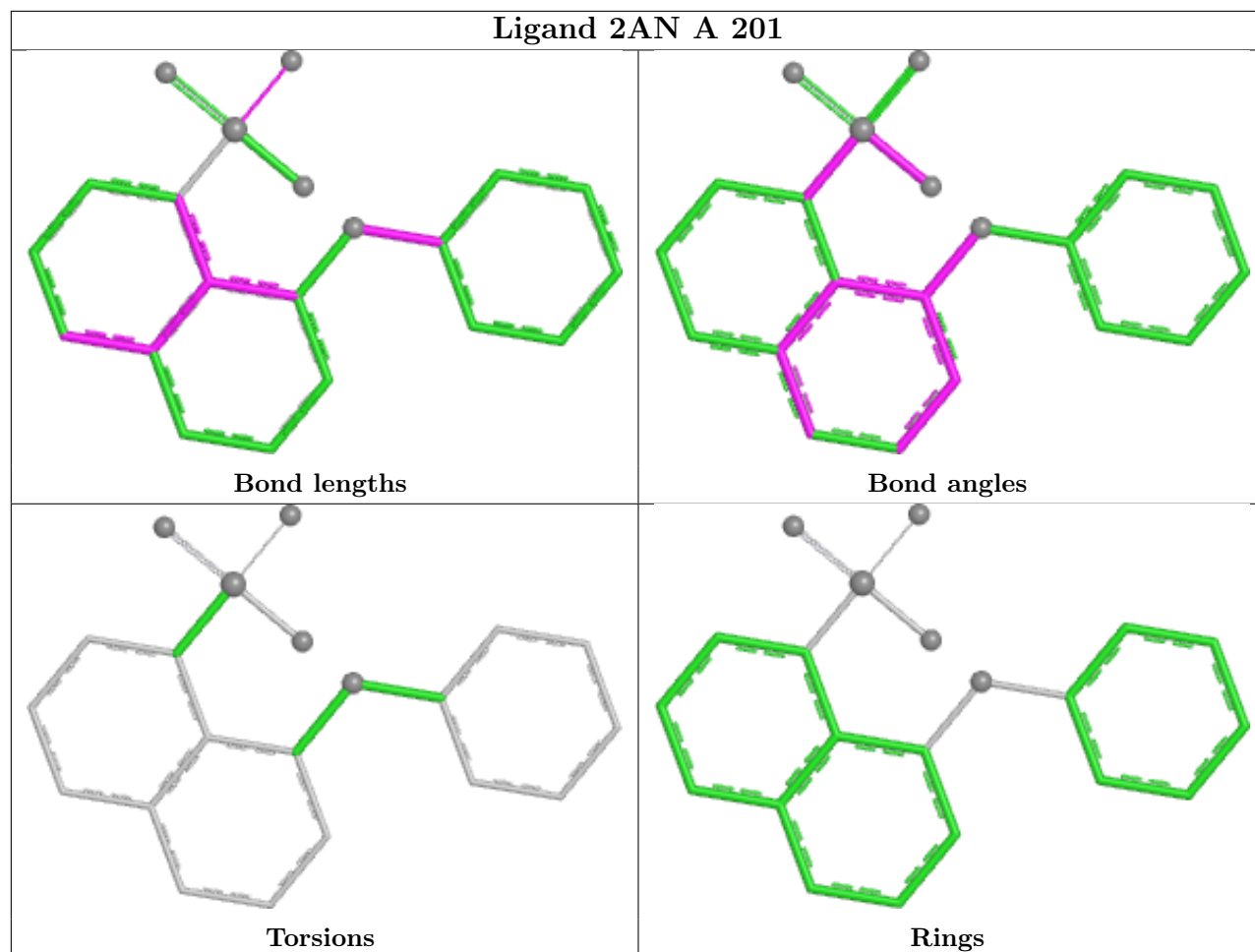
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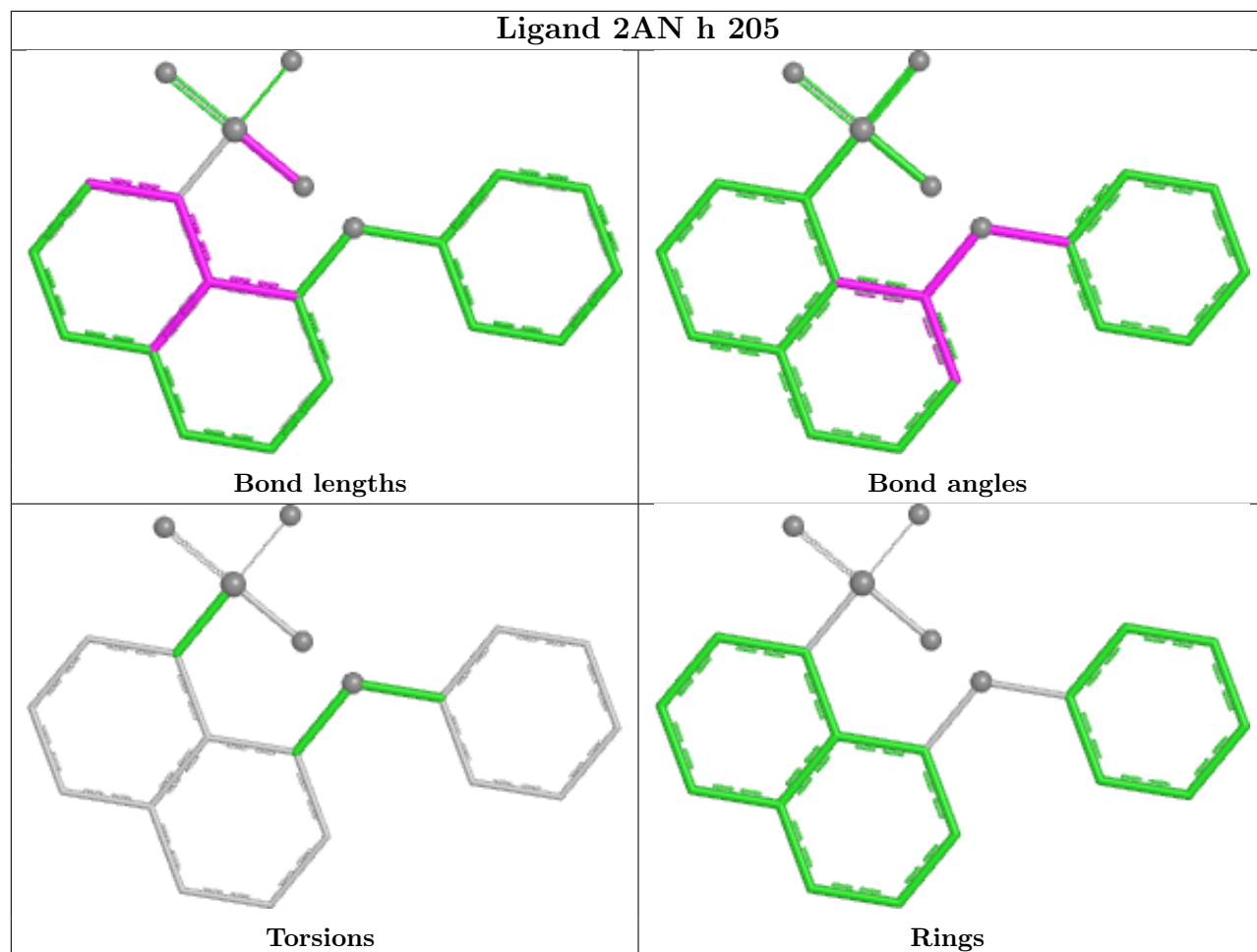




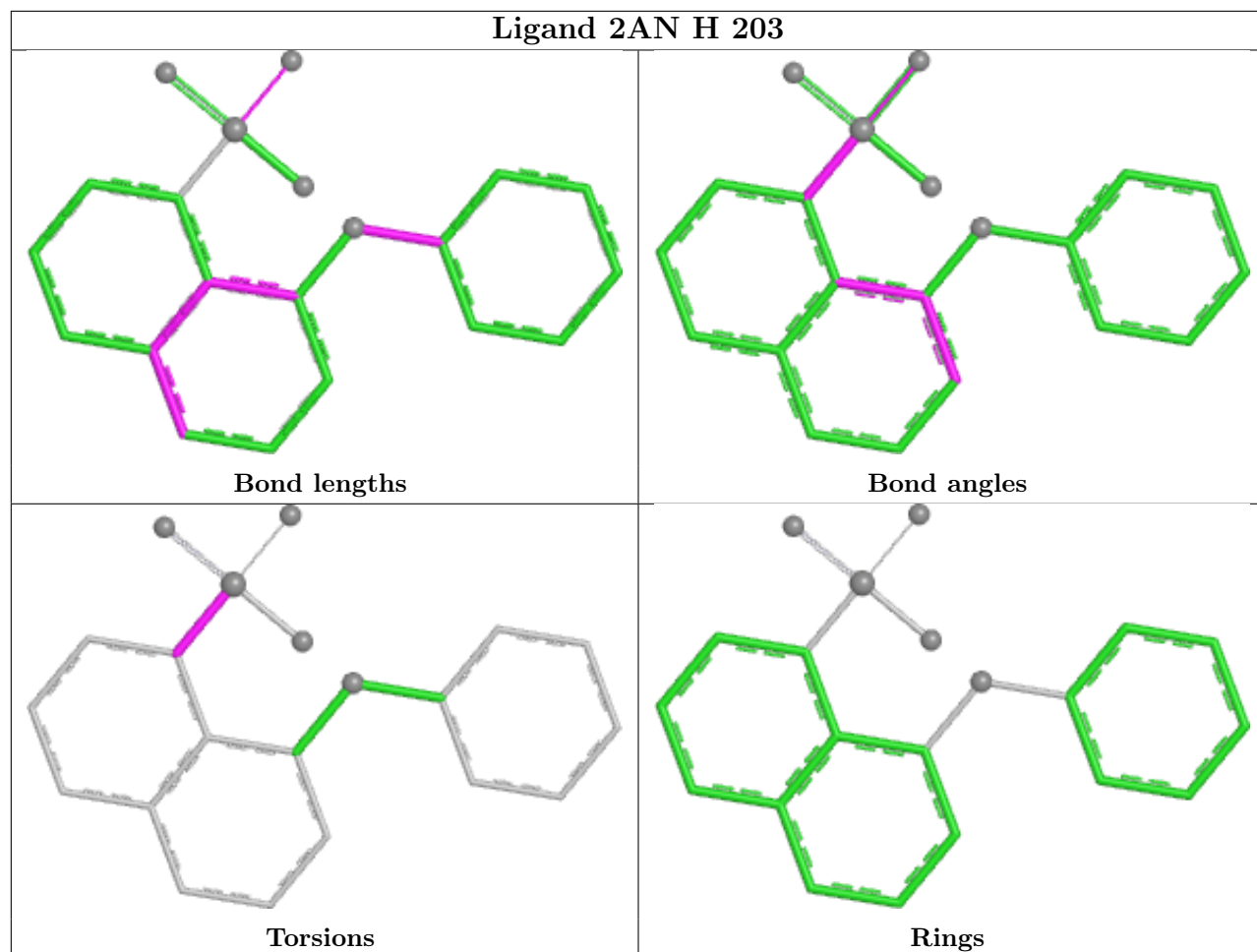
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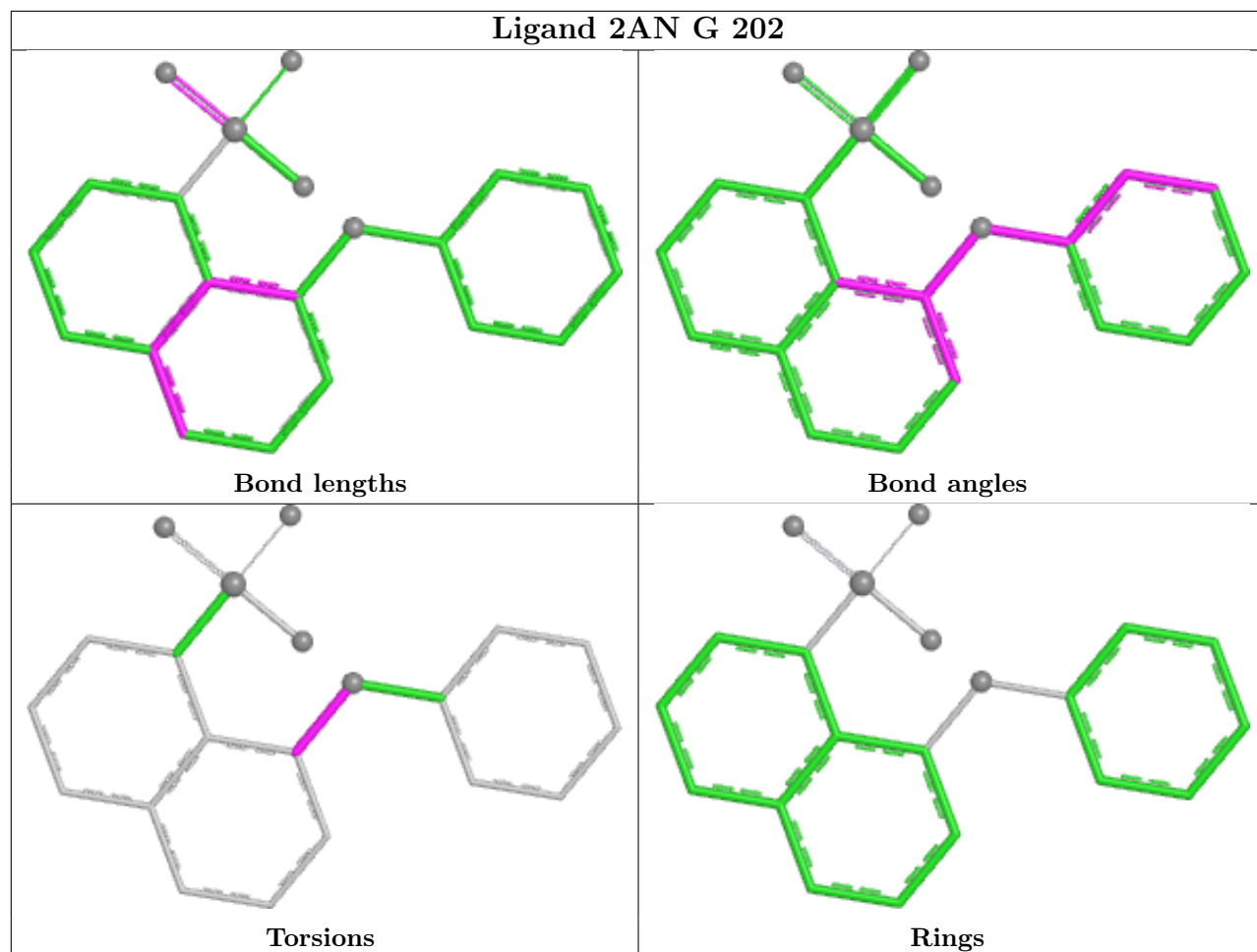
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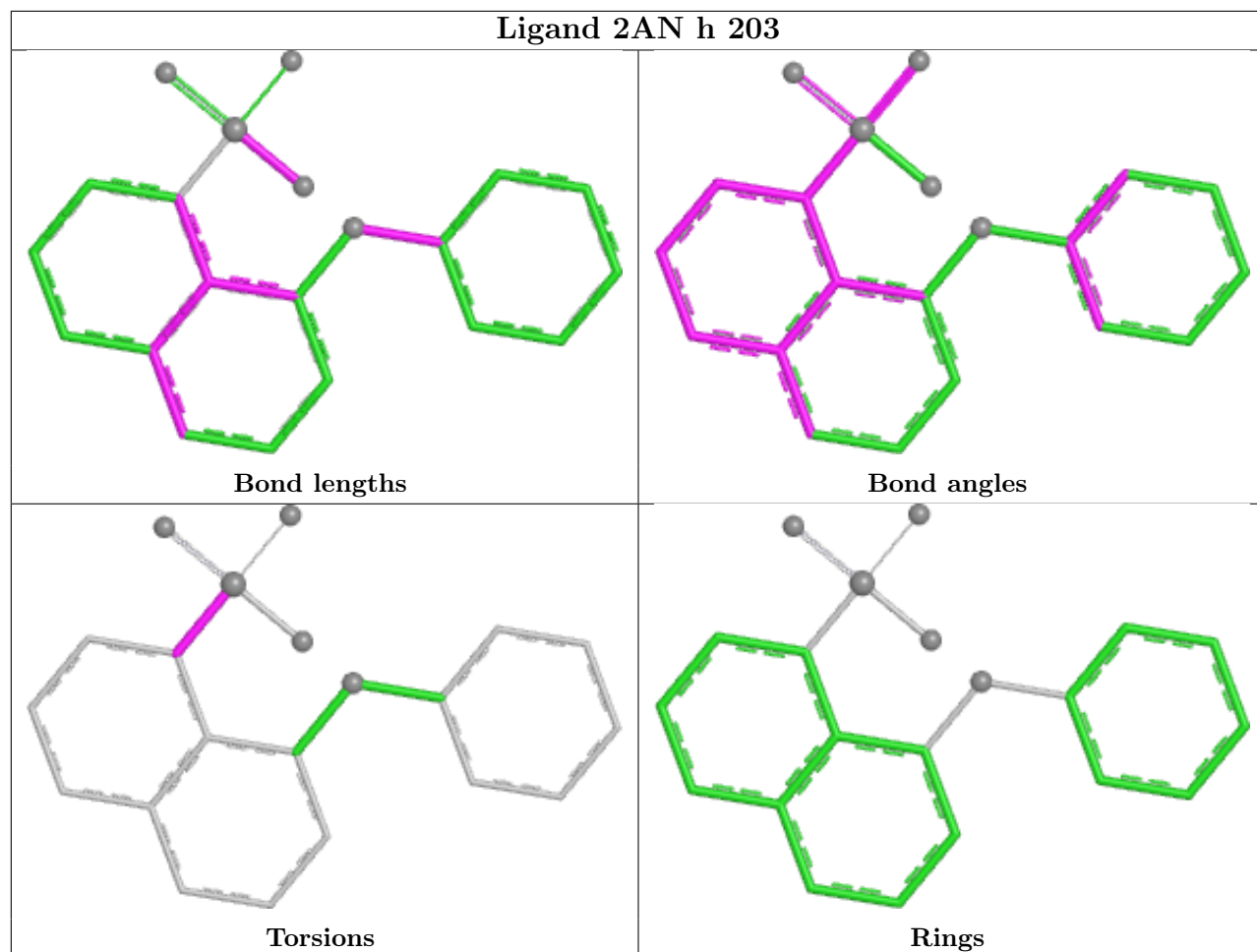
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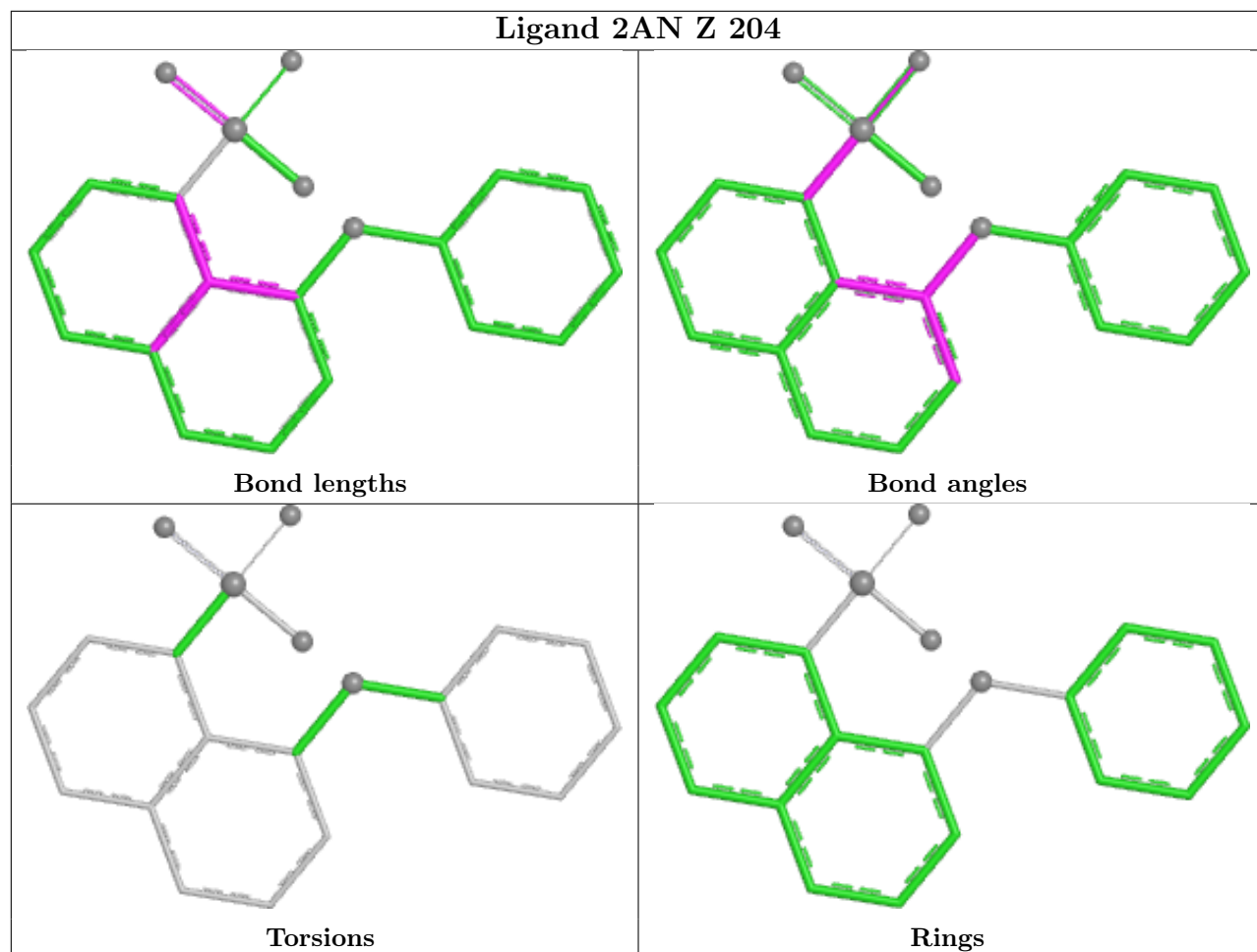
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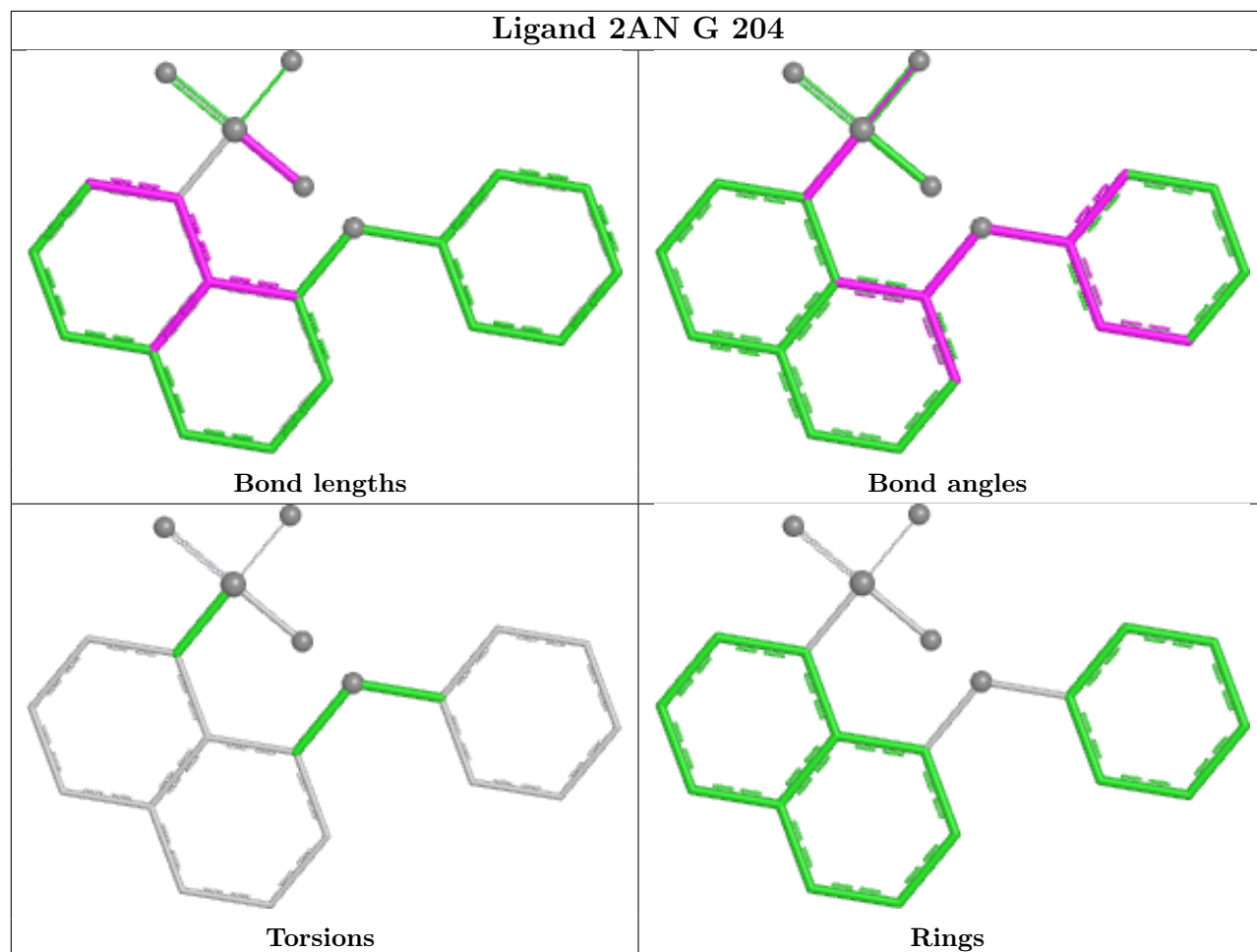
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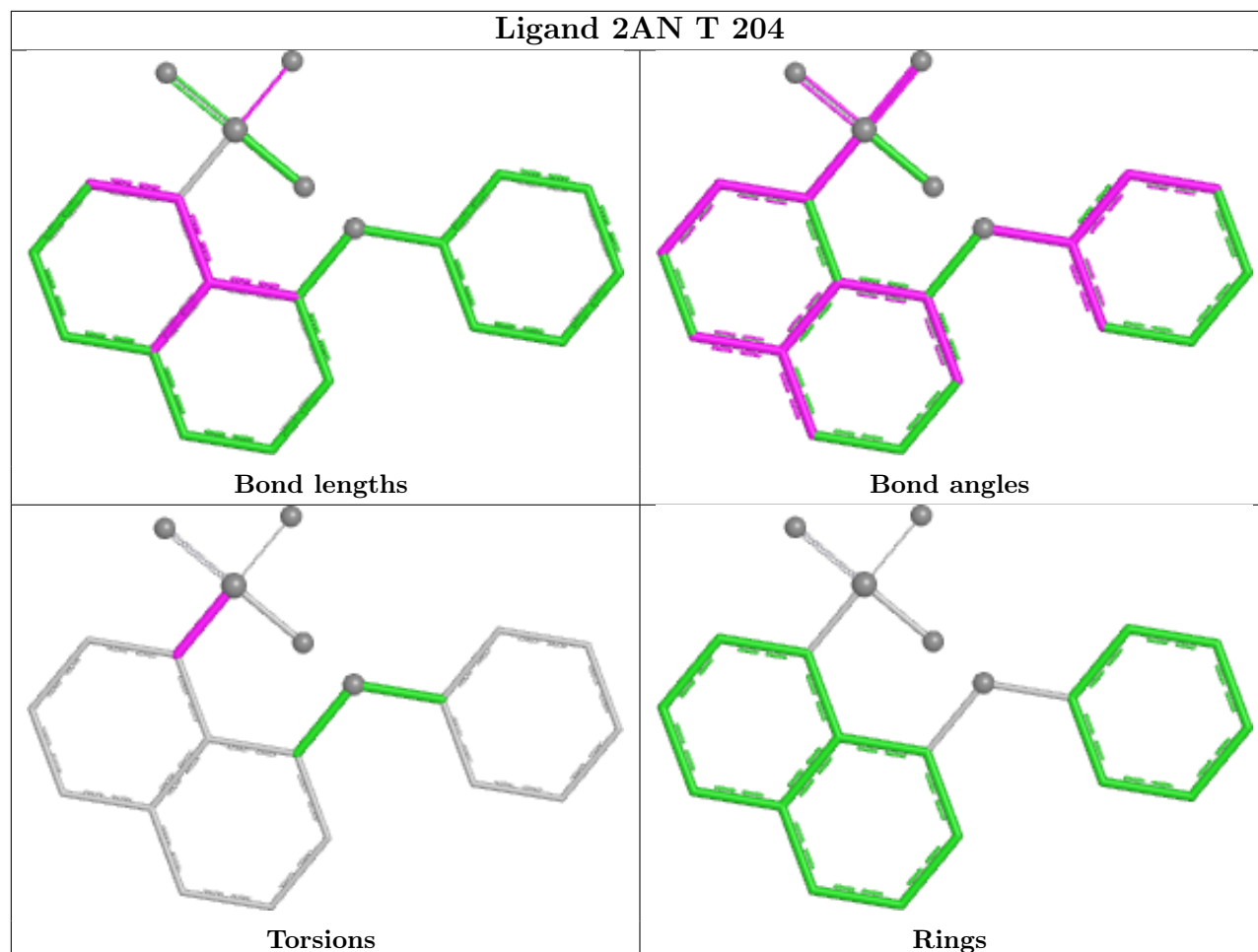
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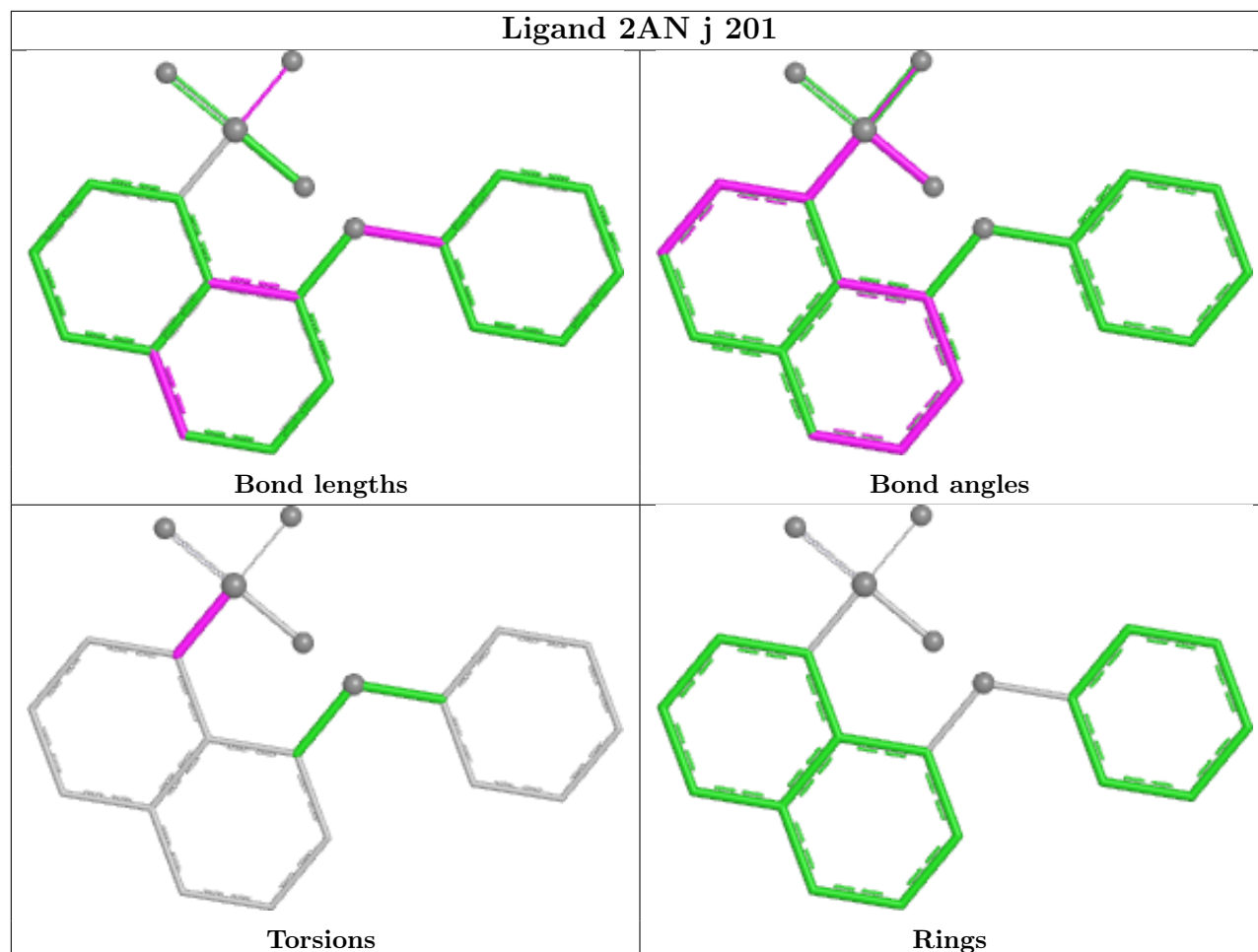
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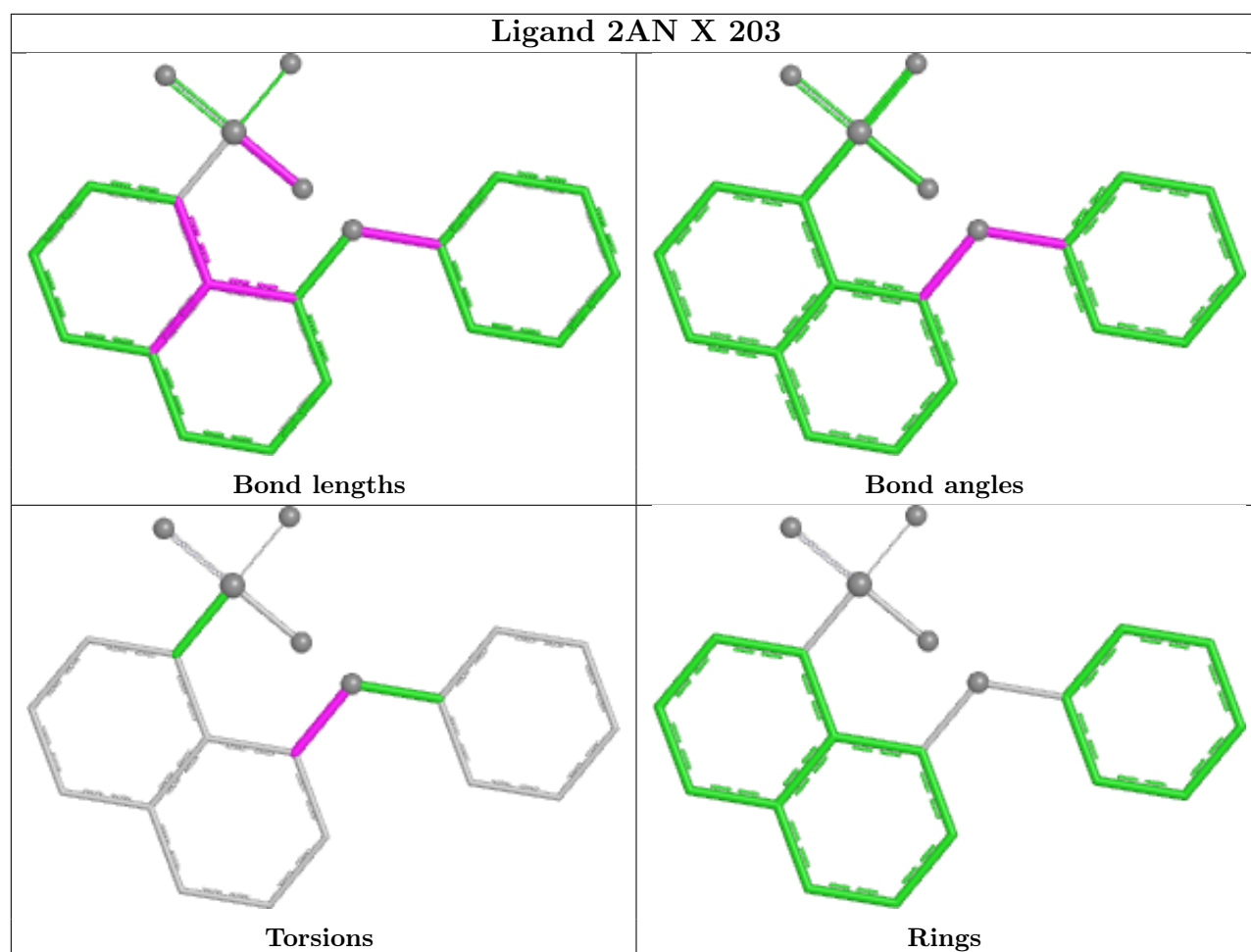


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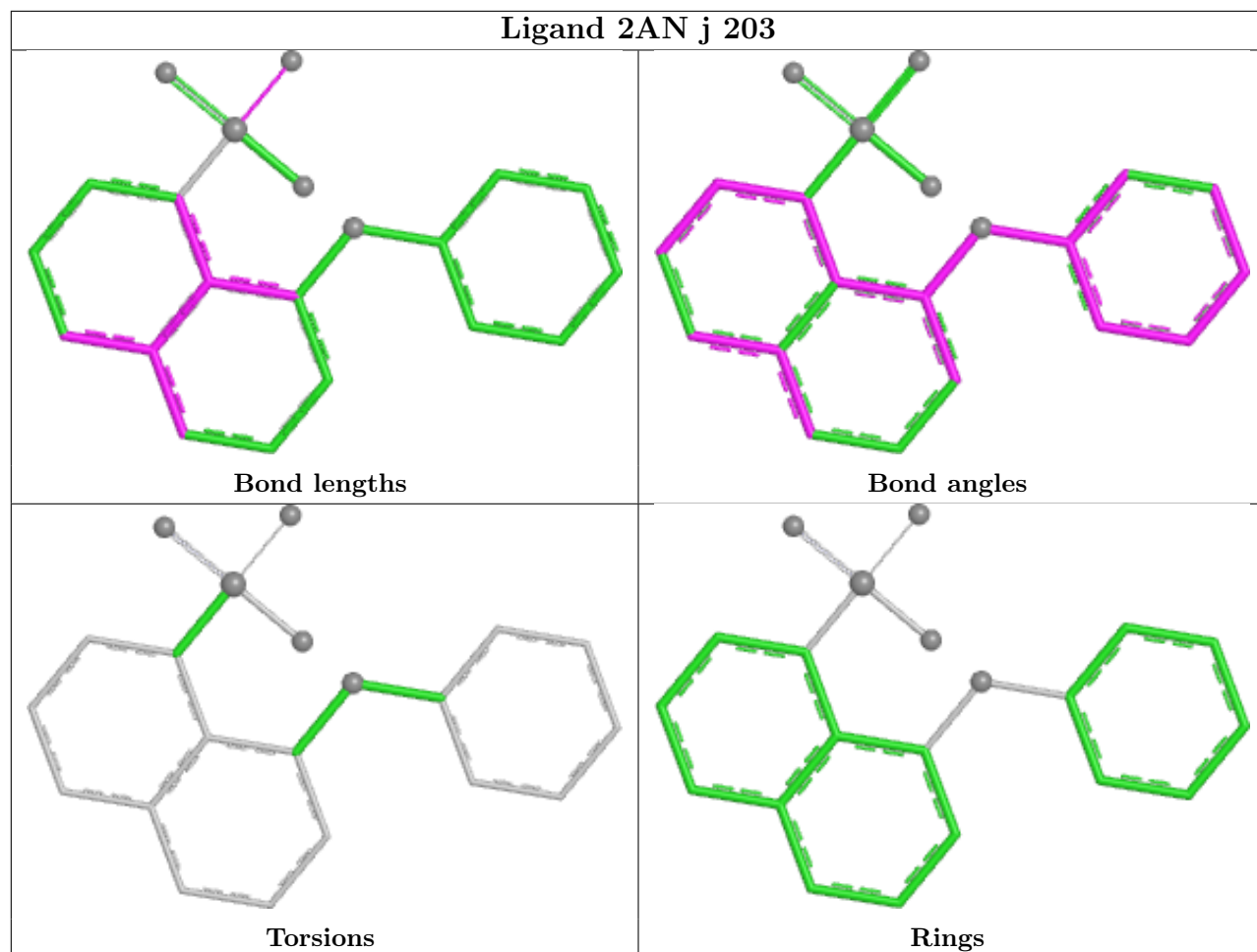


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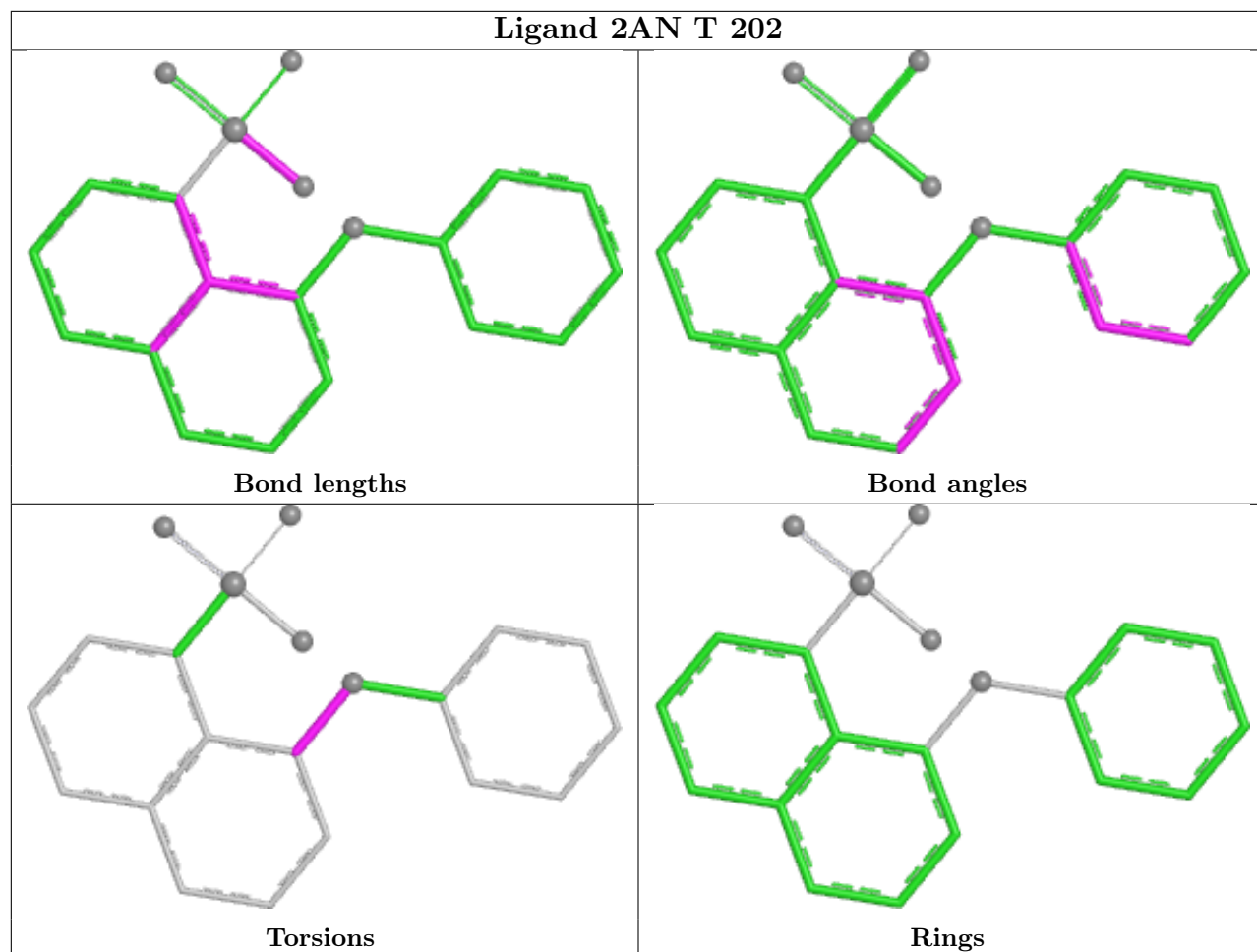




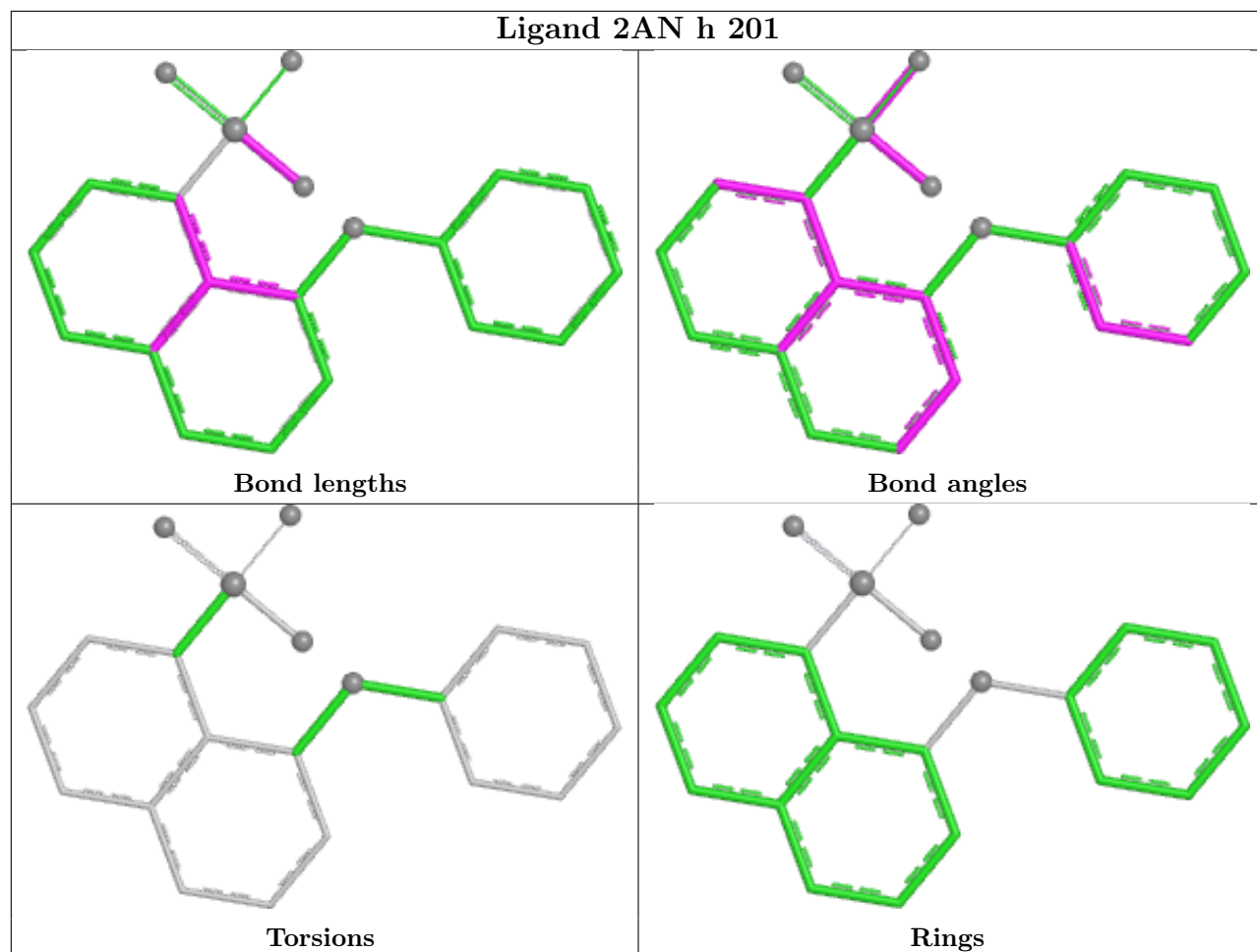
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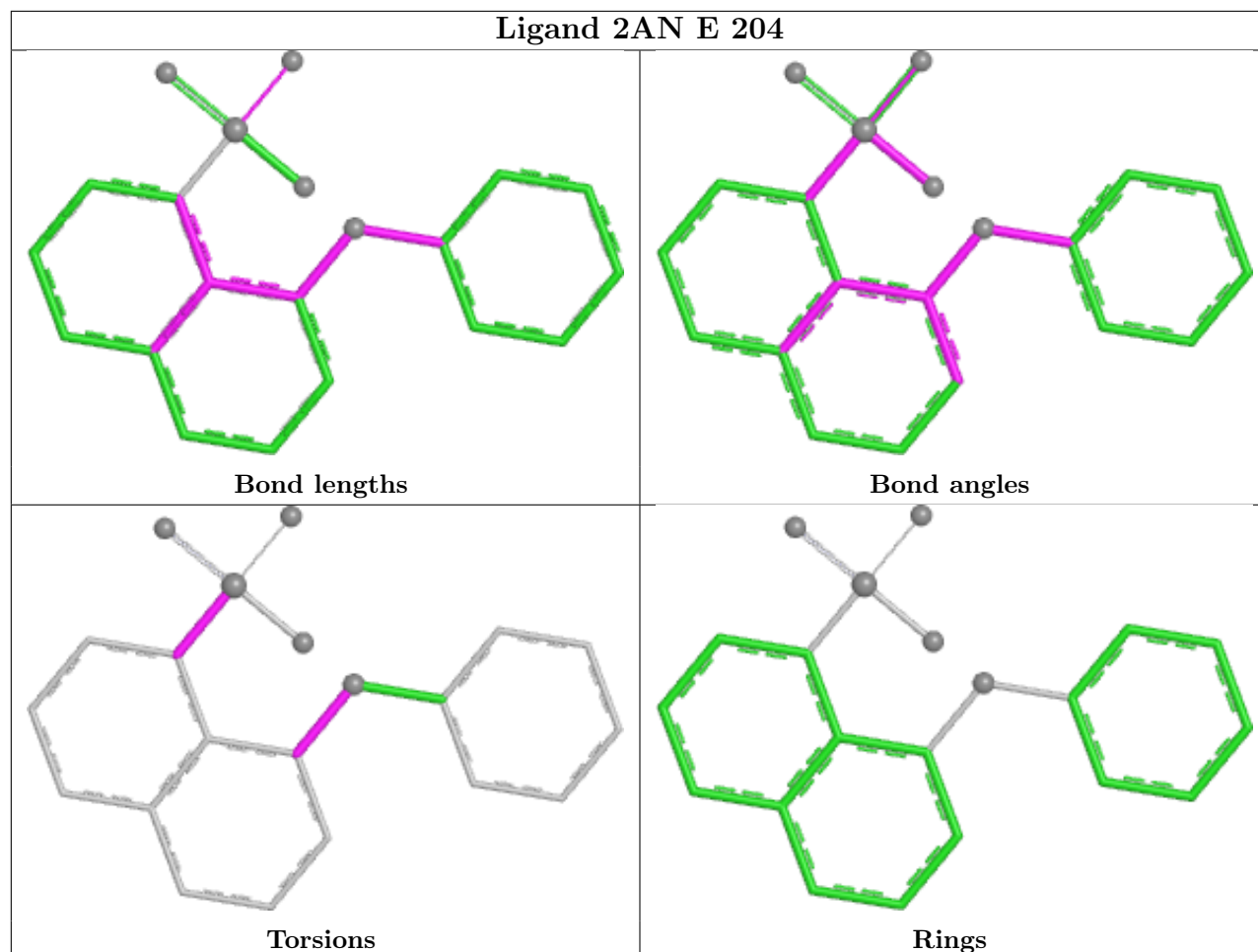
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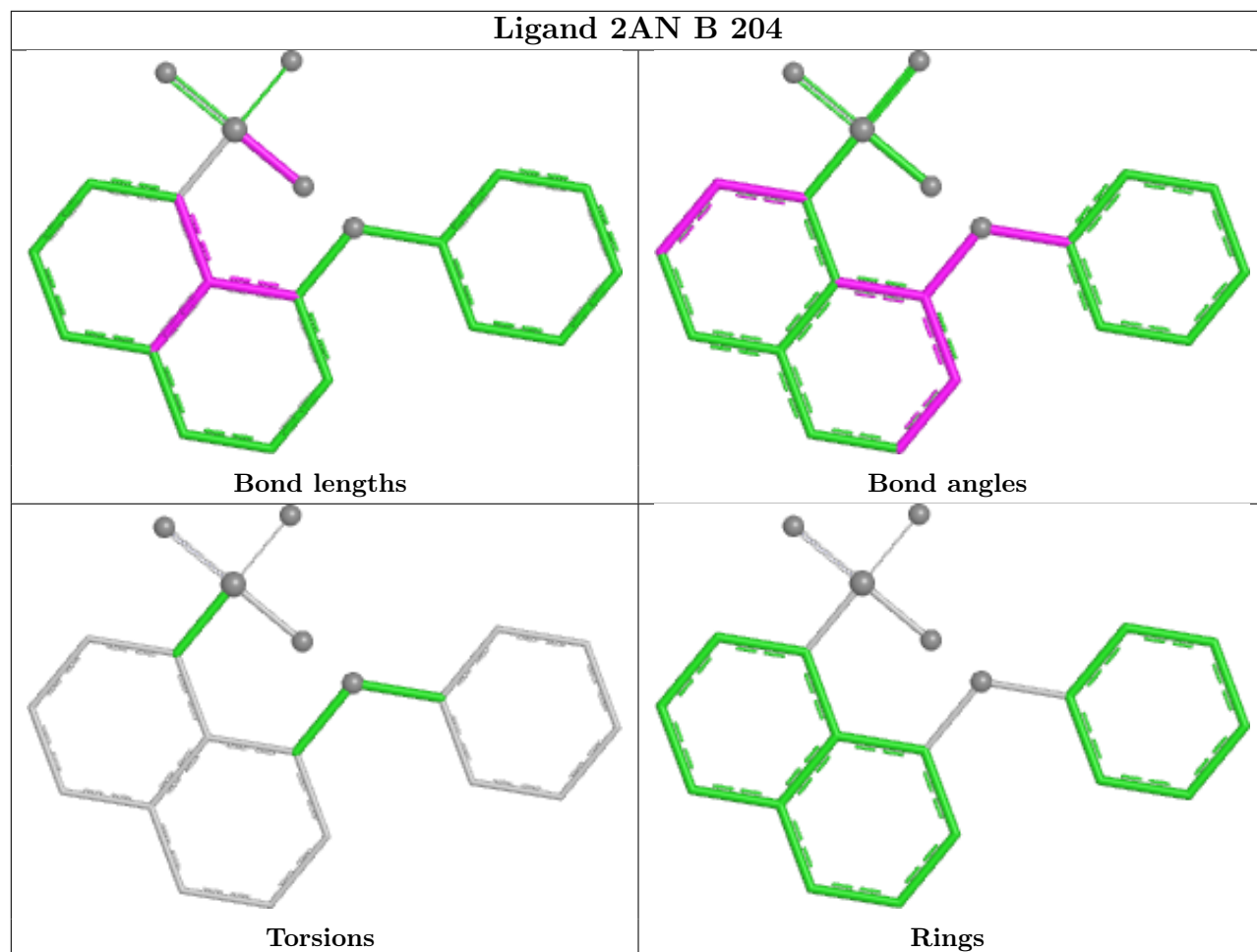
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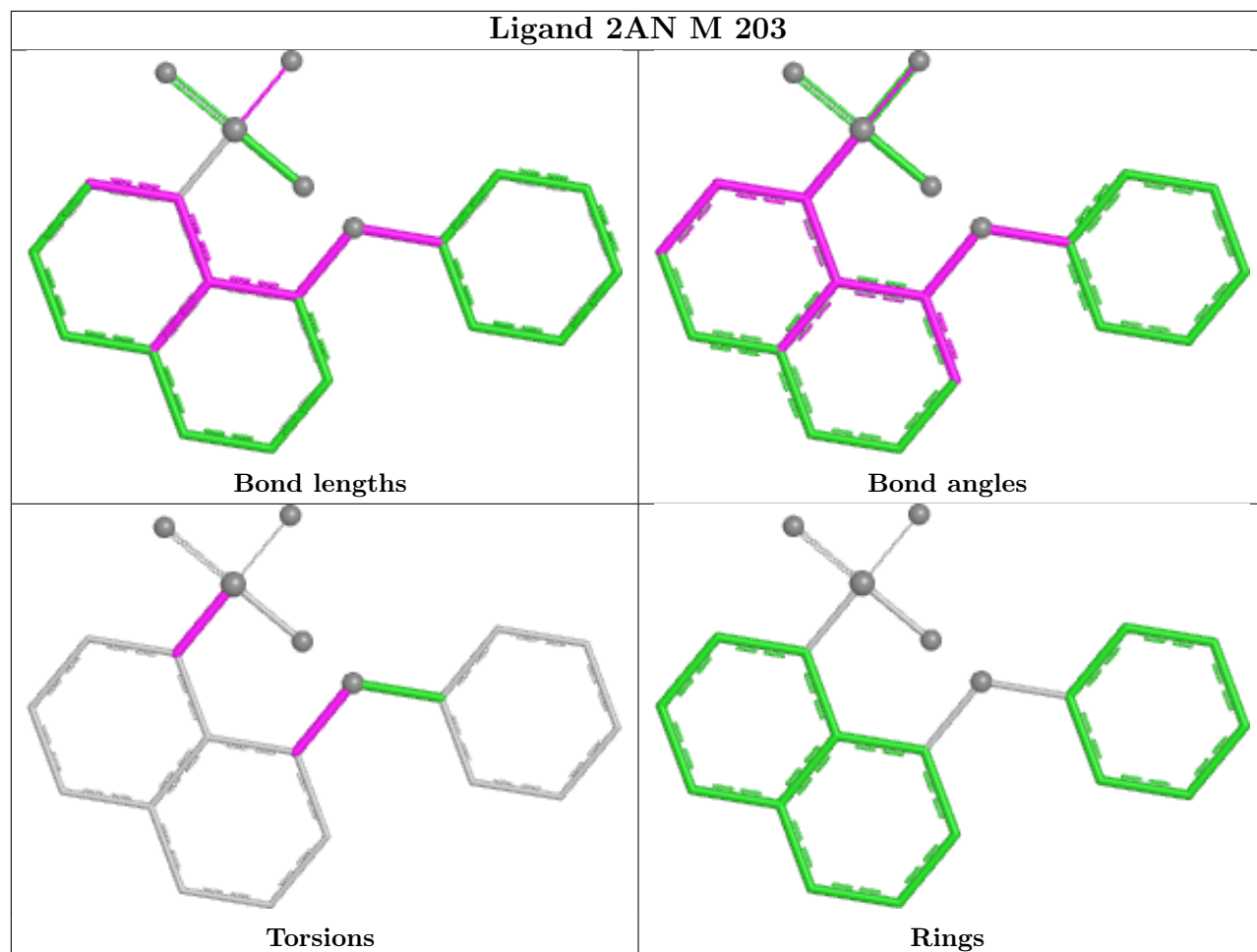


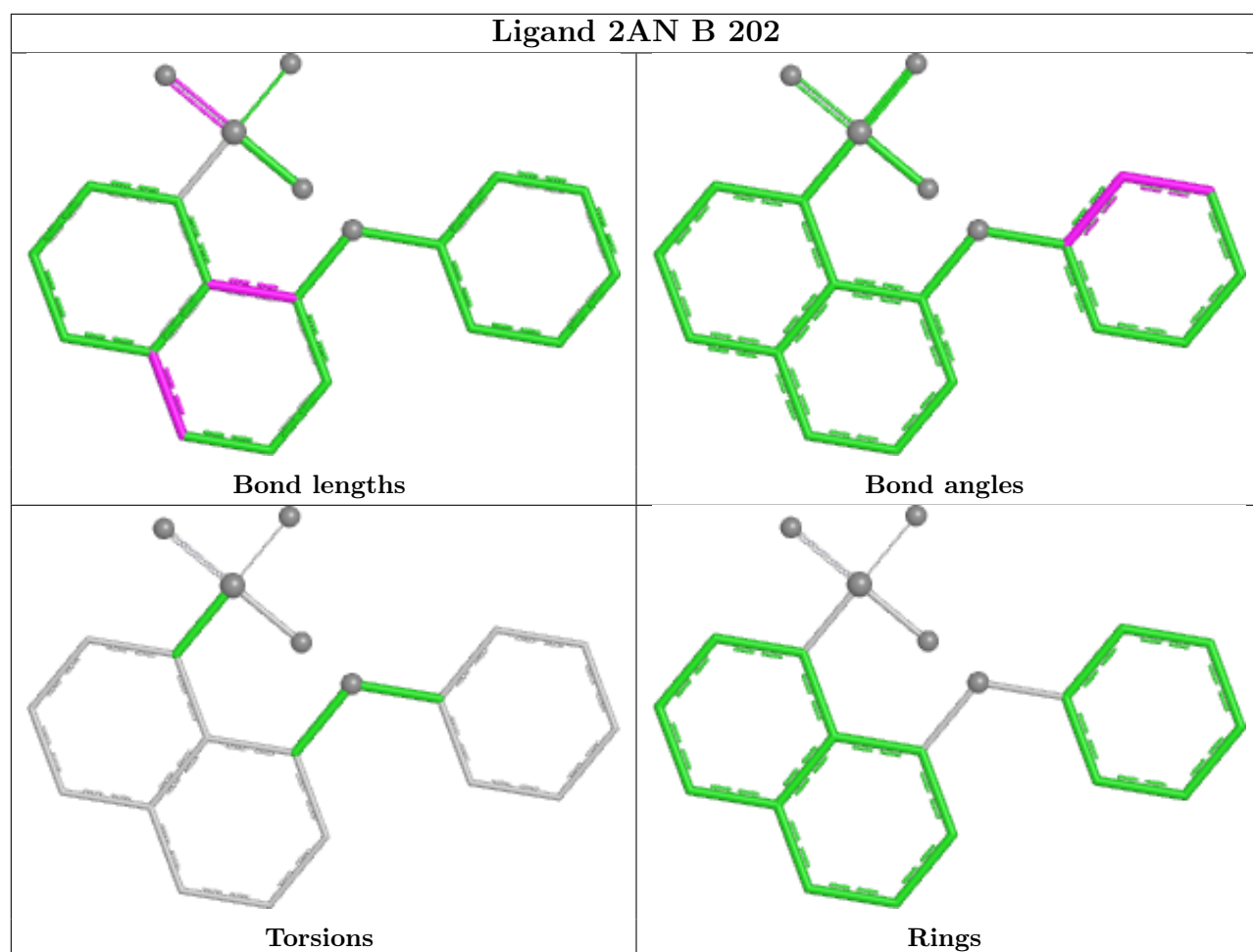
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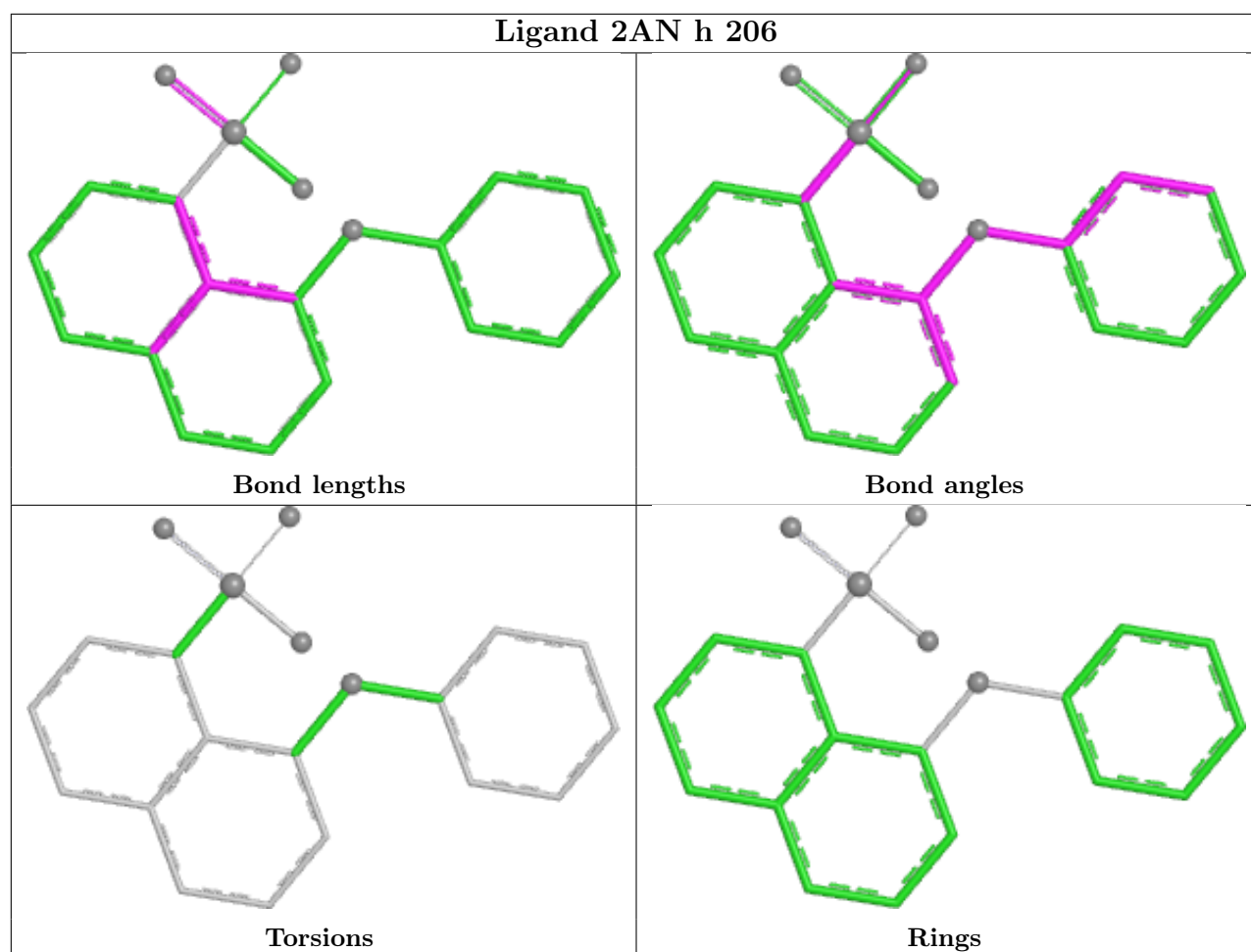


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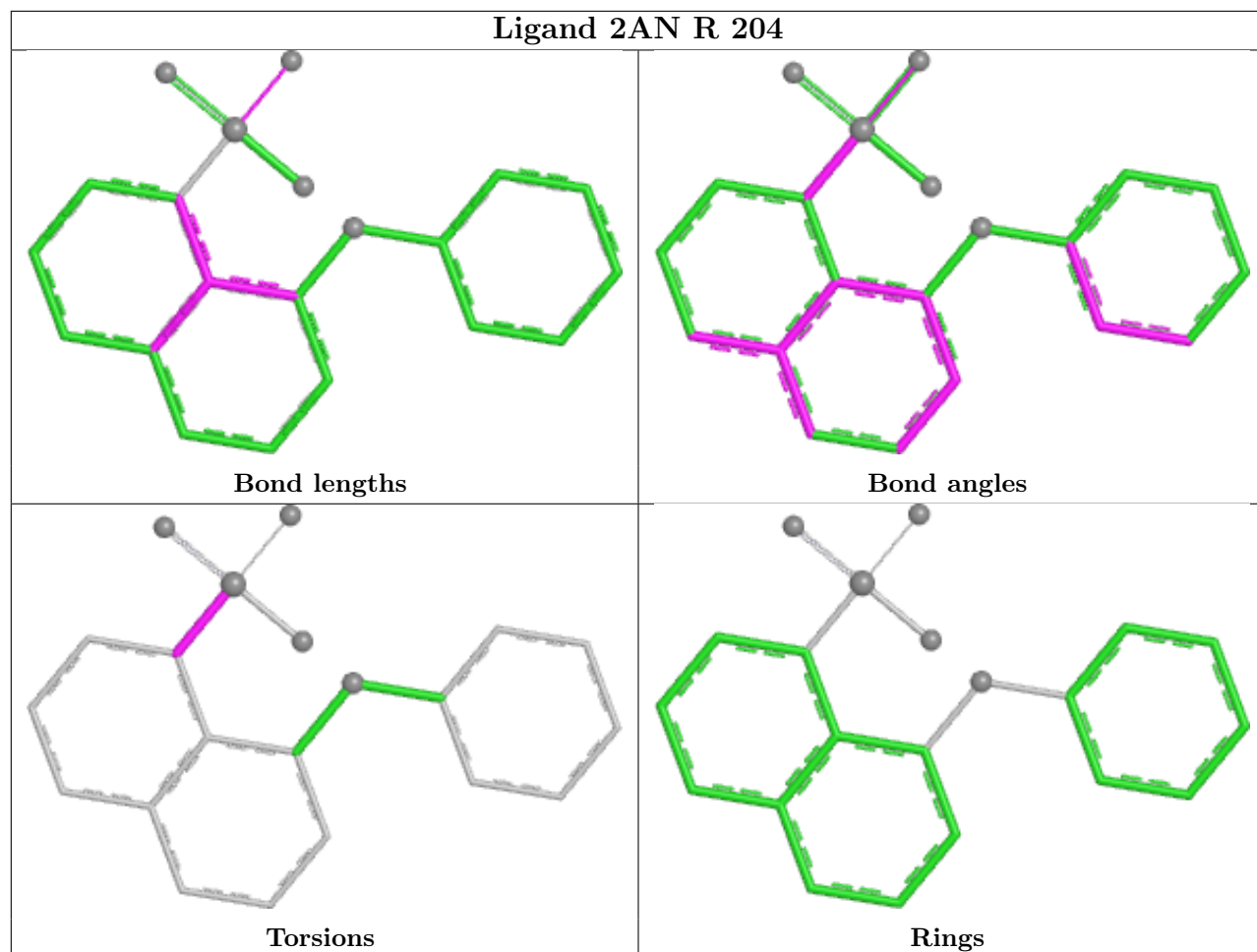


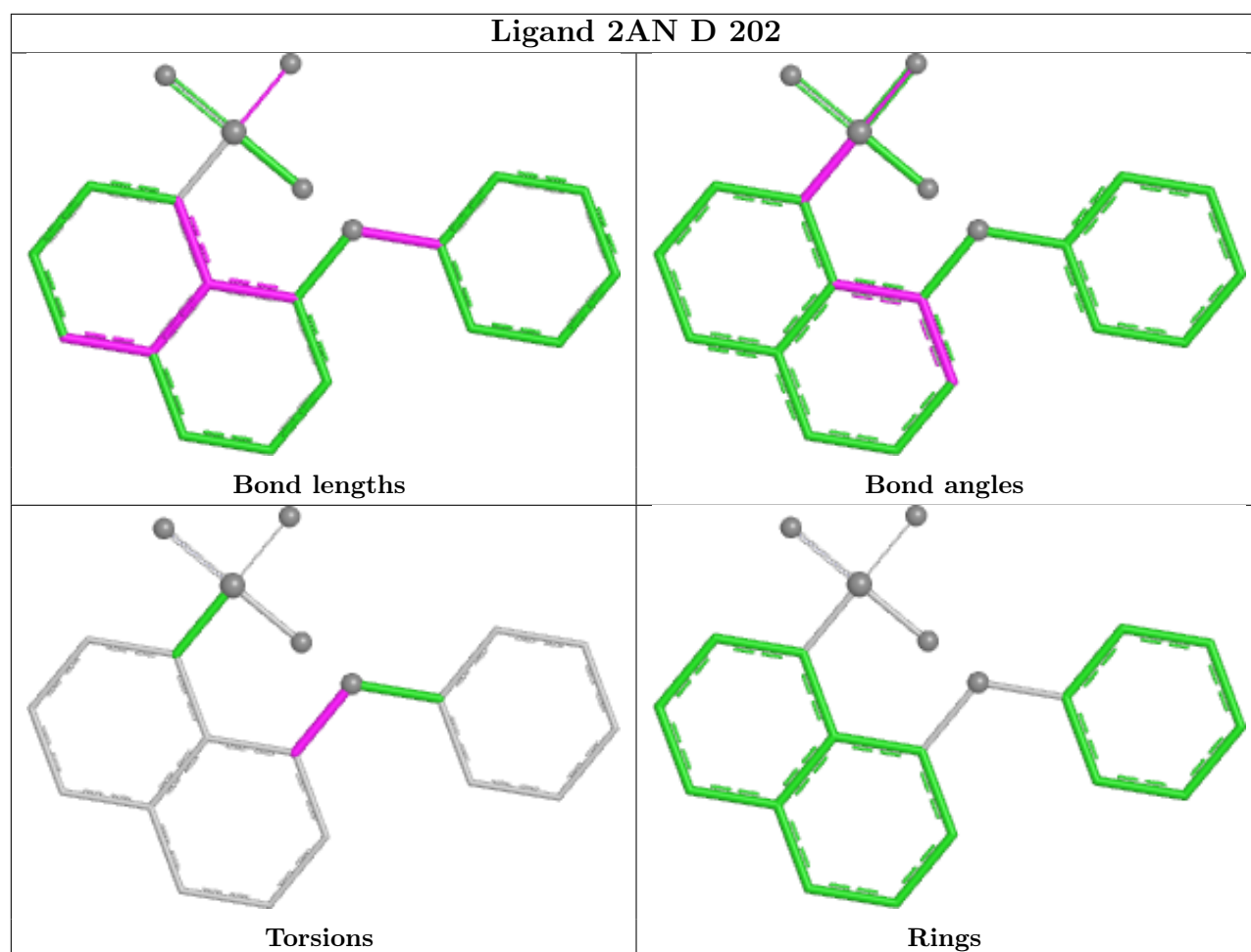




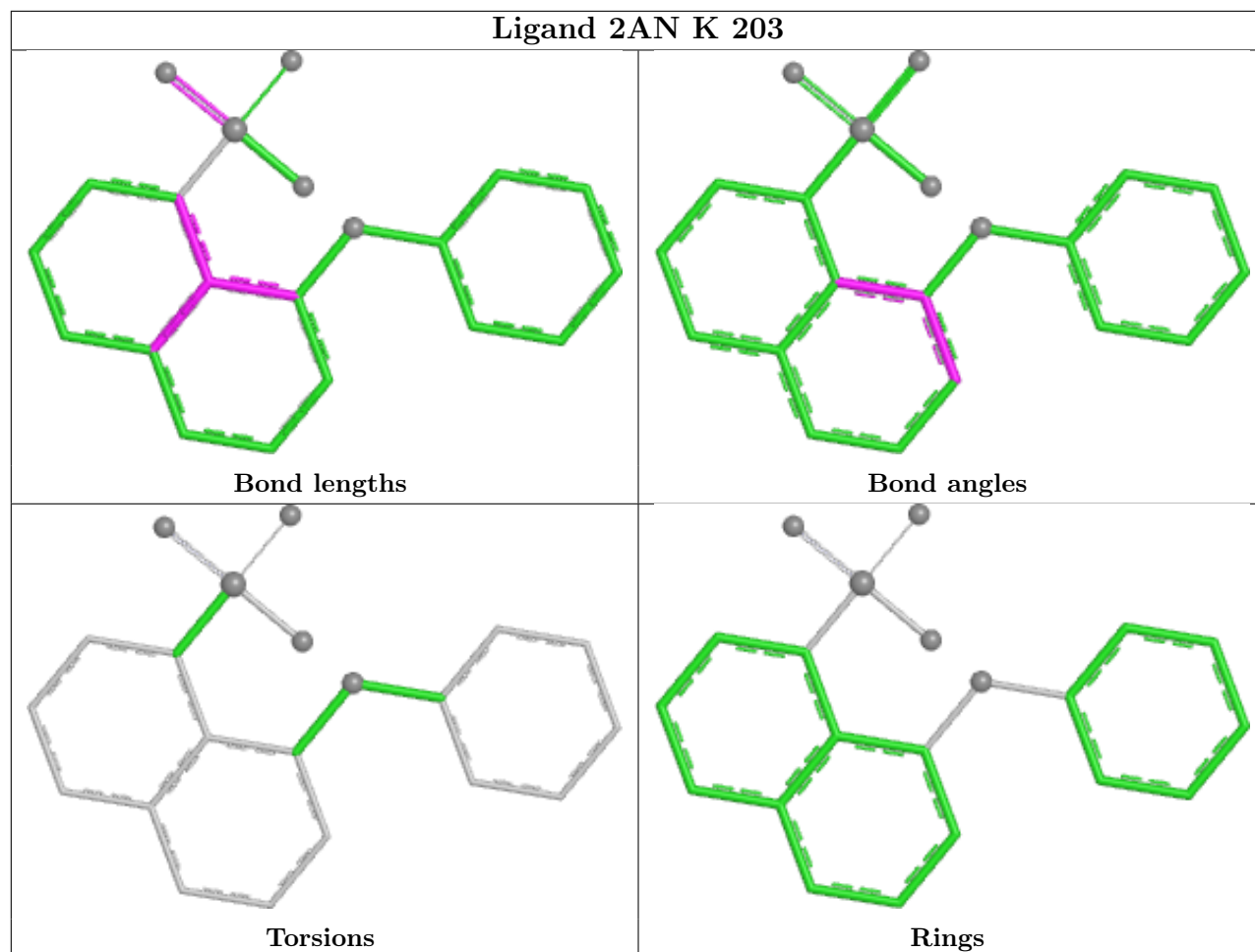


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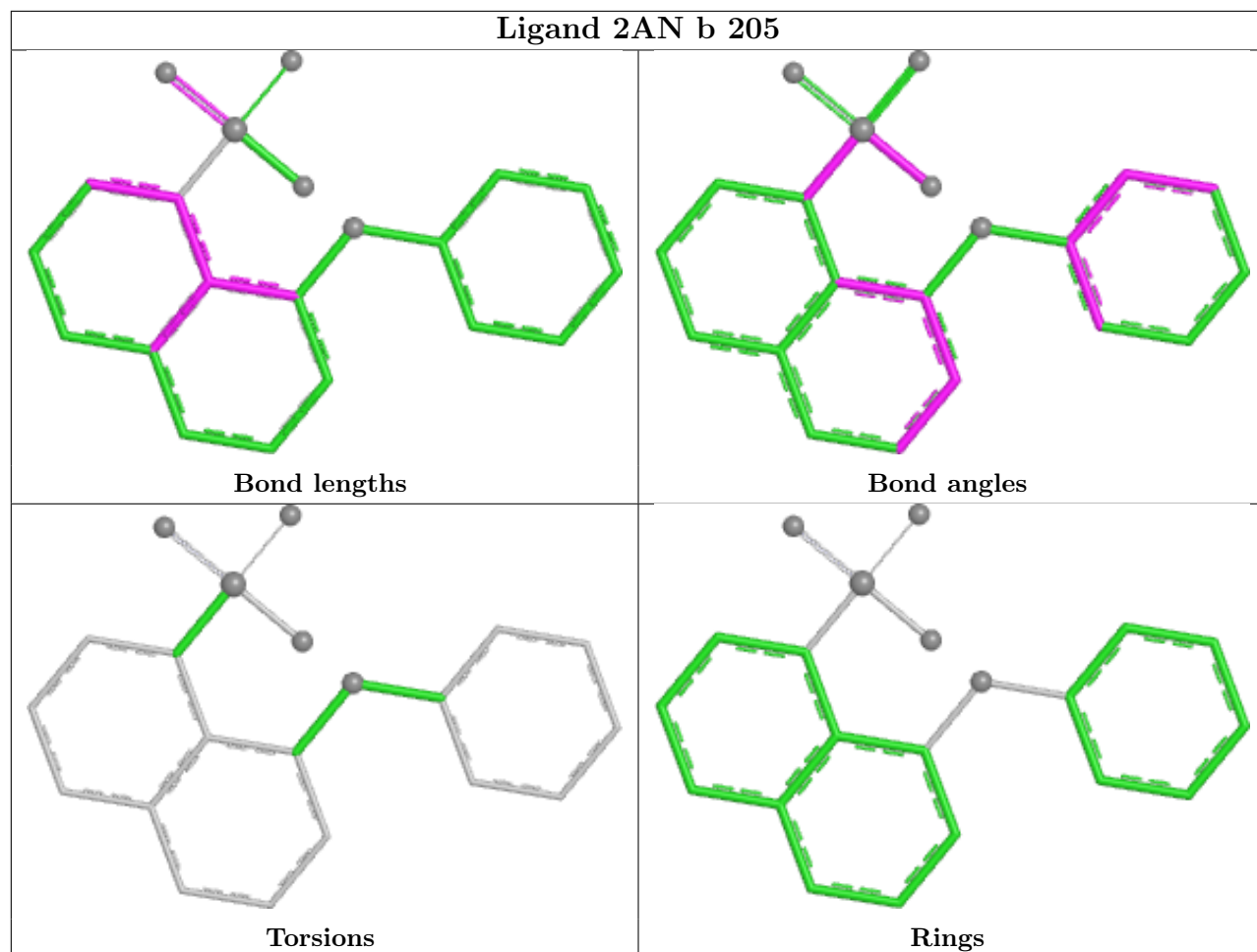




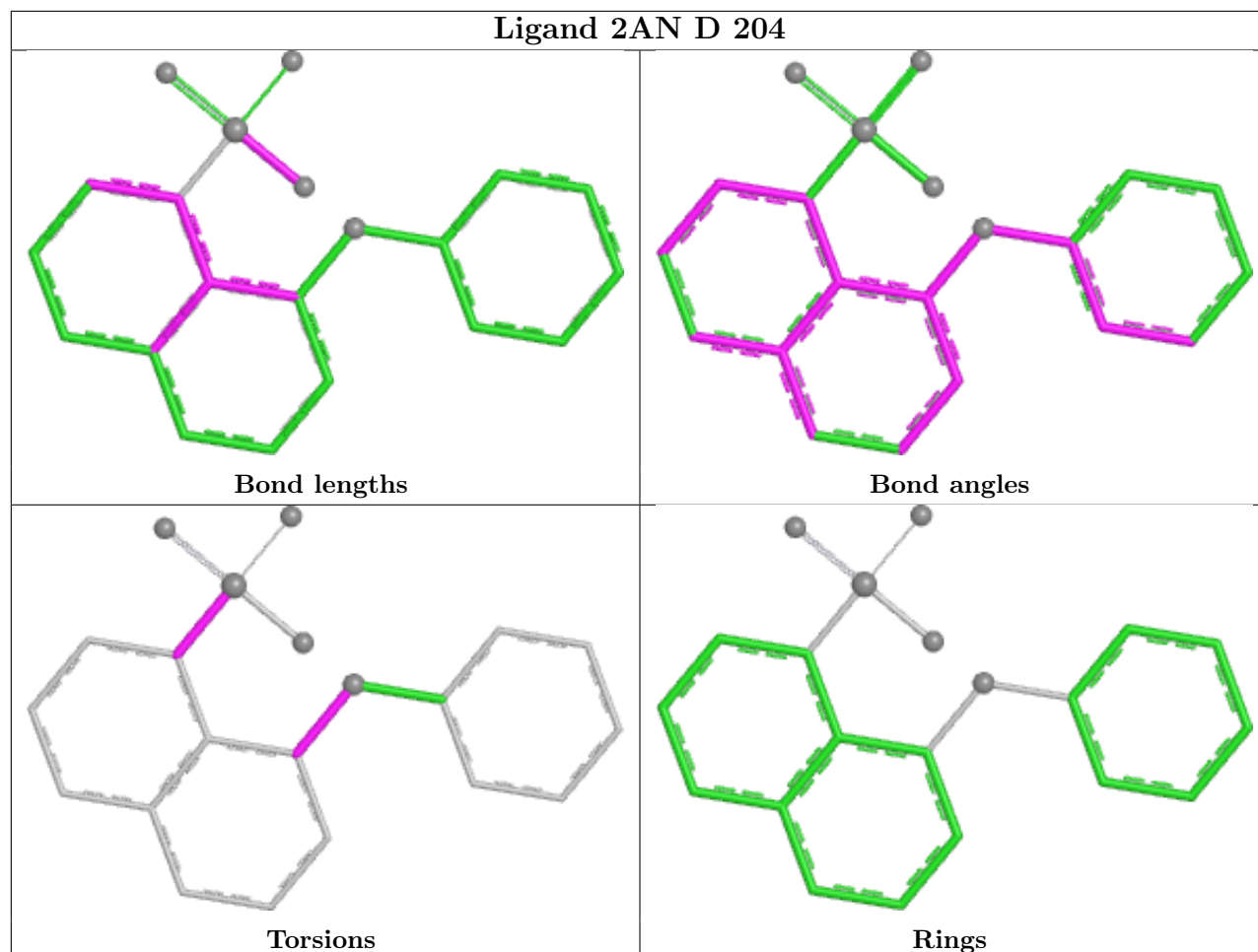
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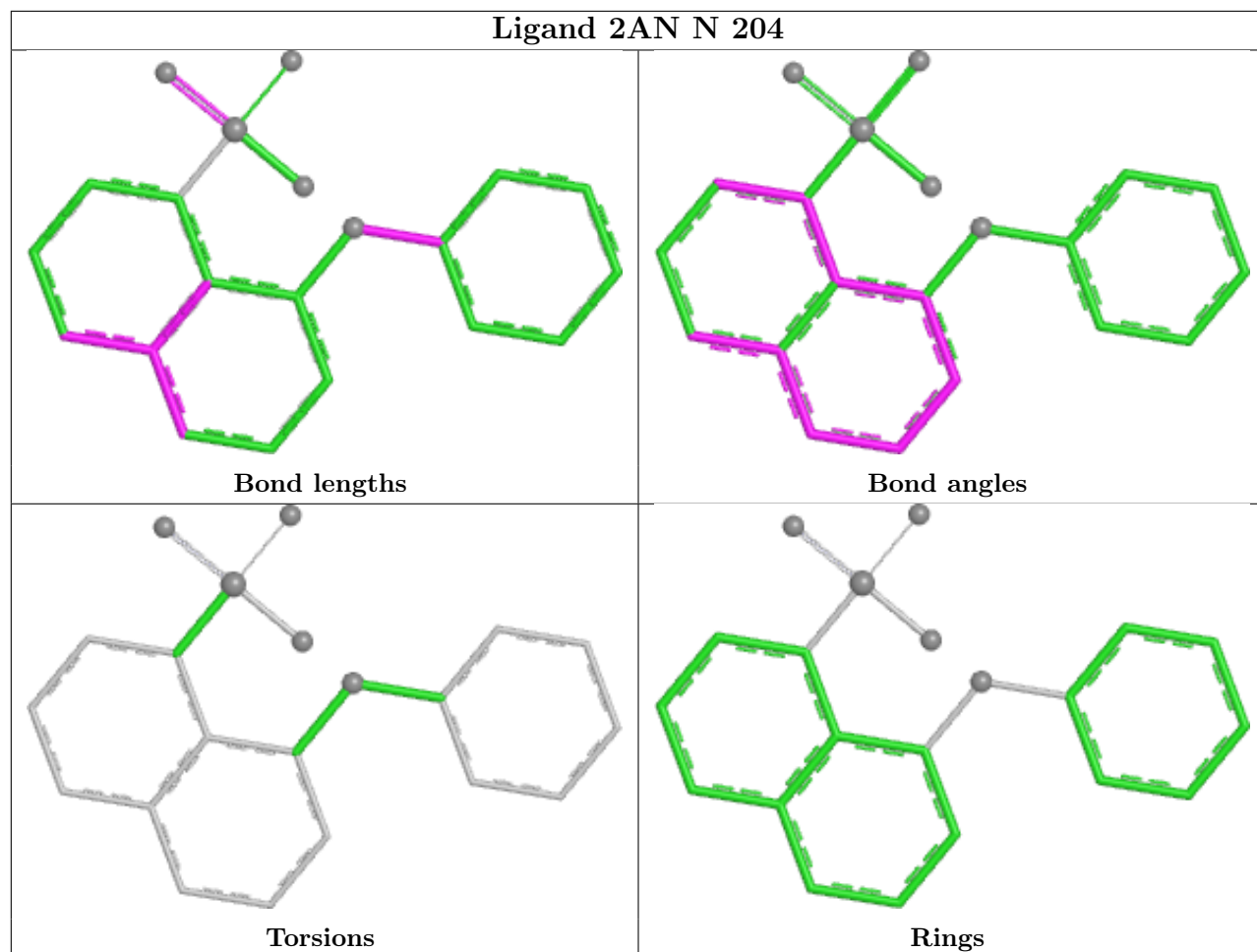


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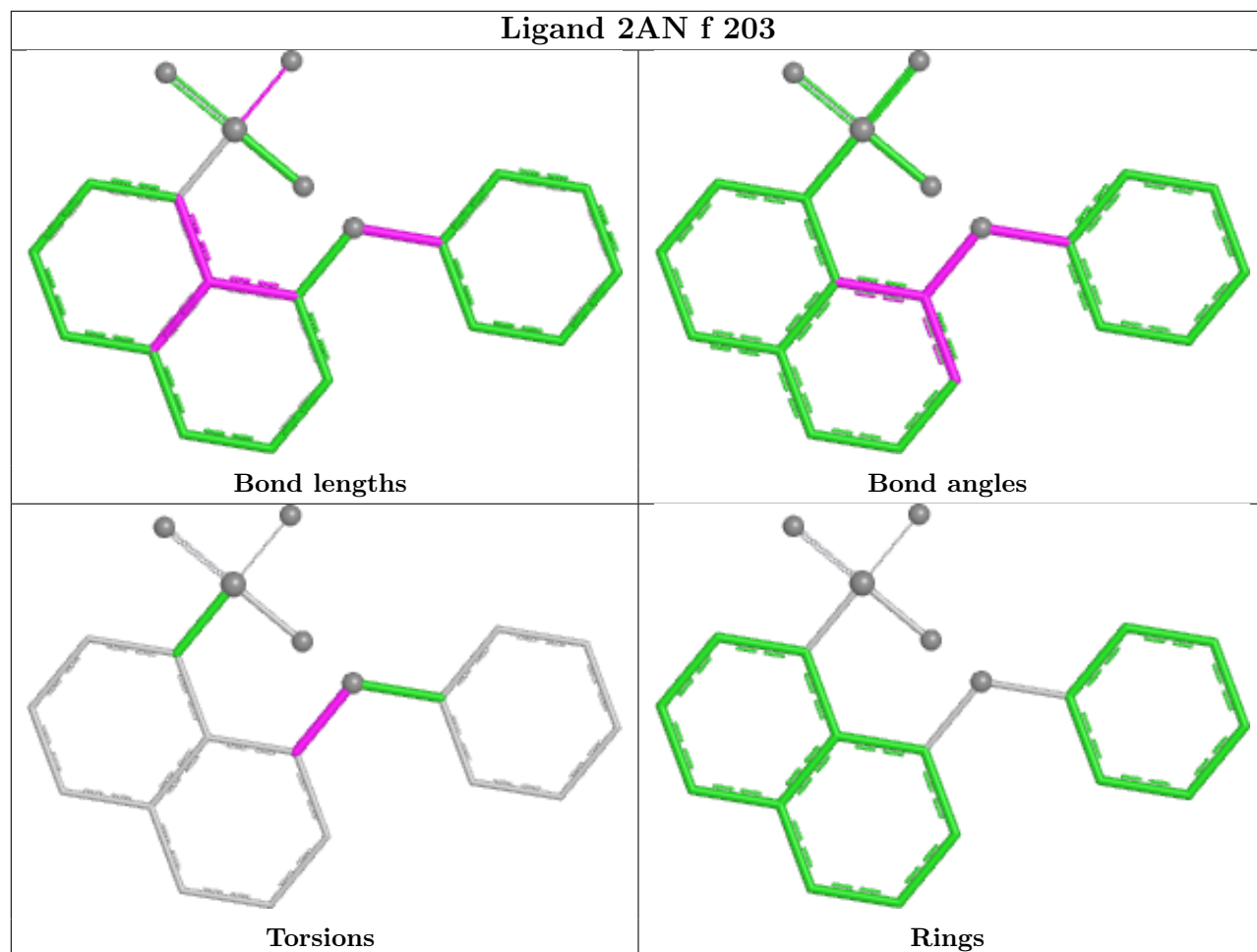


Ligand 2AN D 204

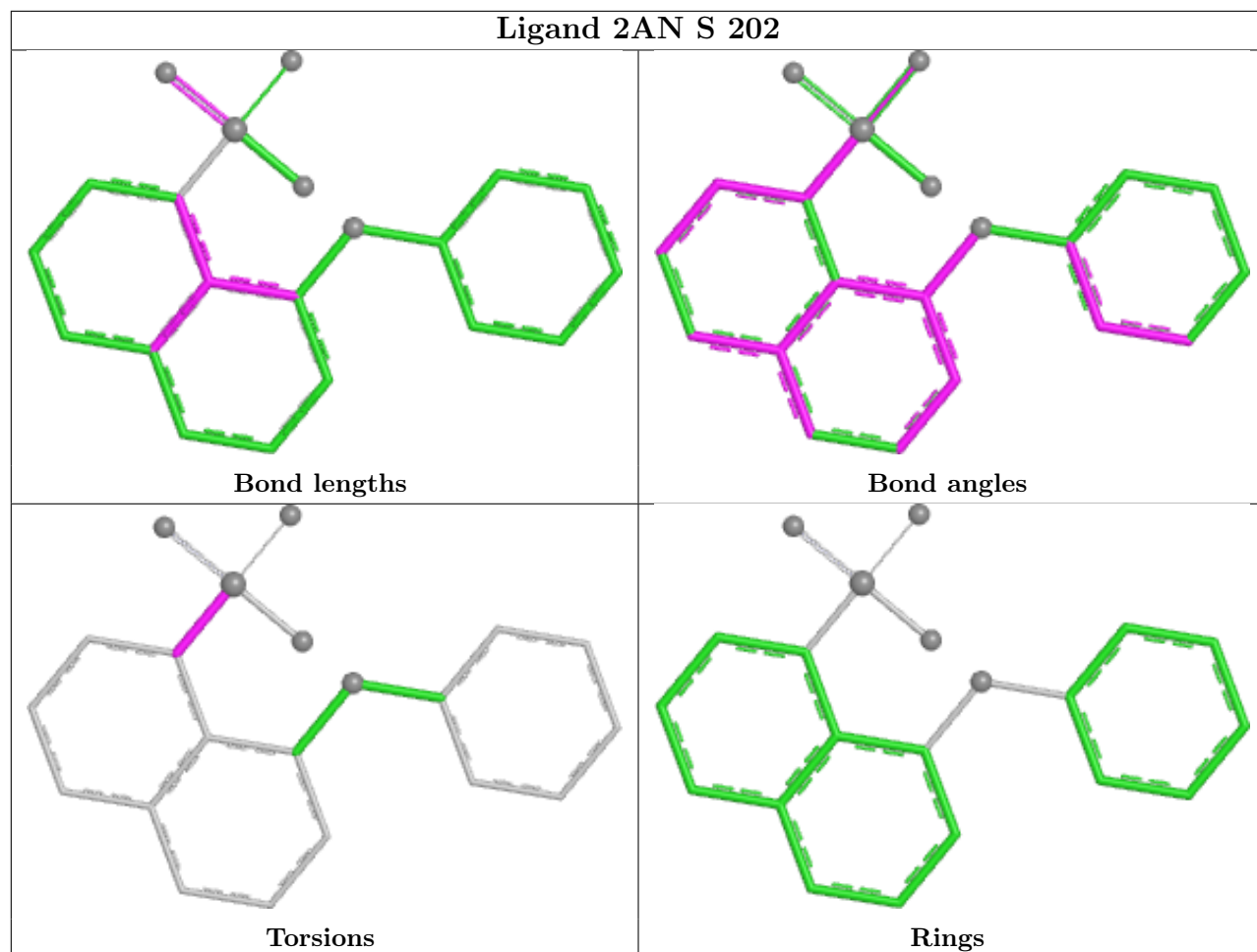


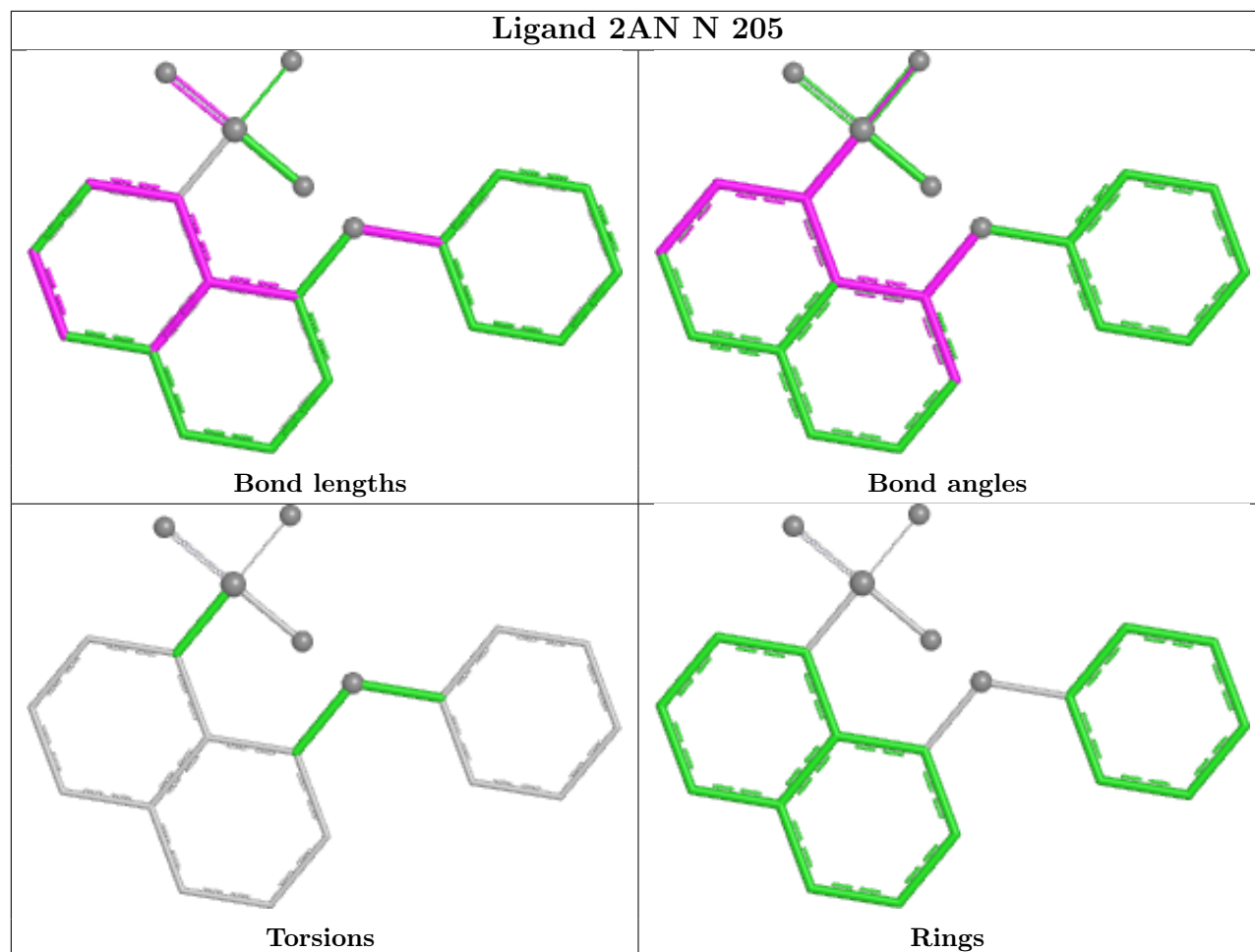


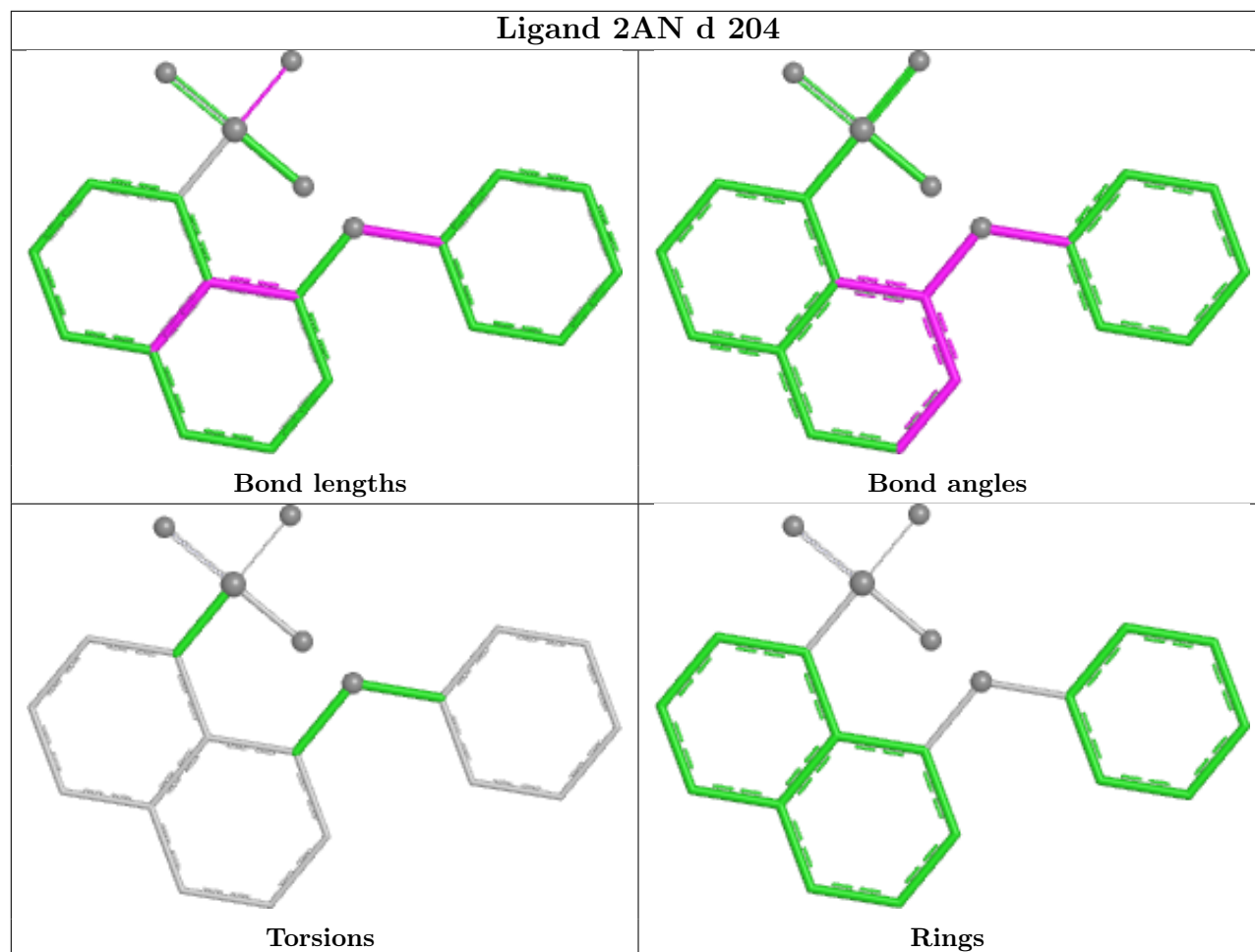
Ligand 2AN f 203



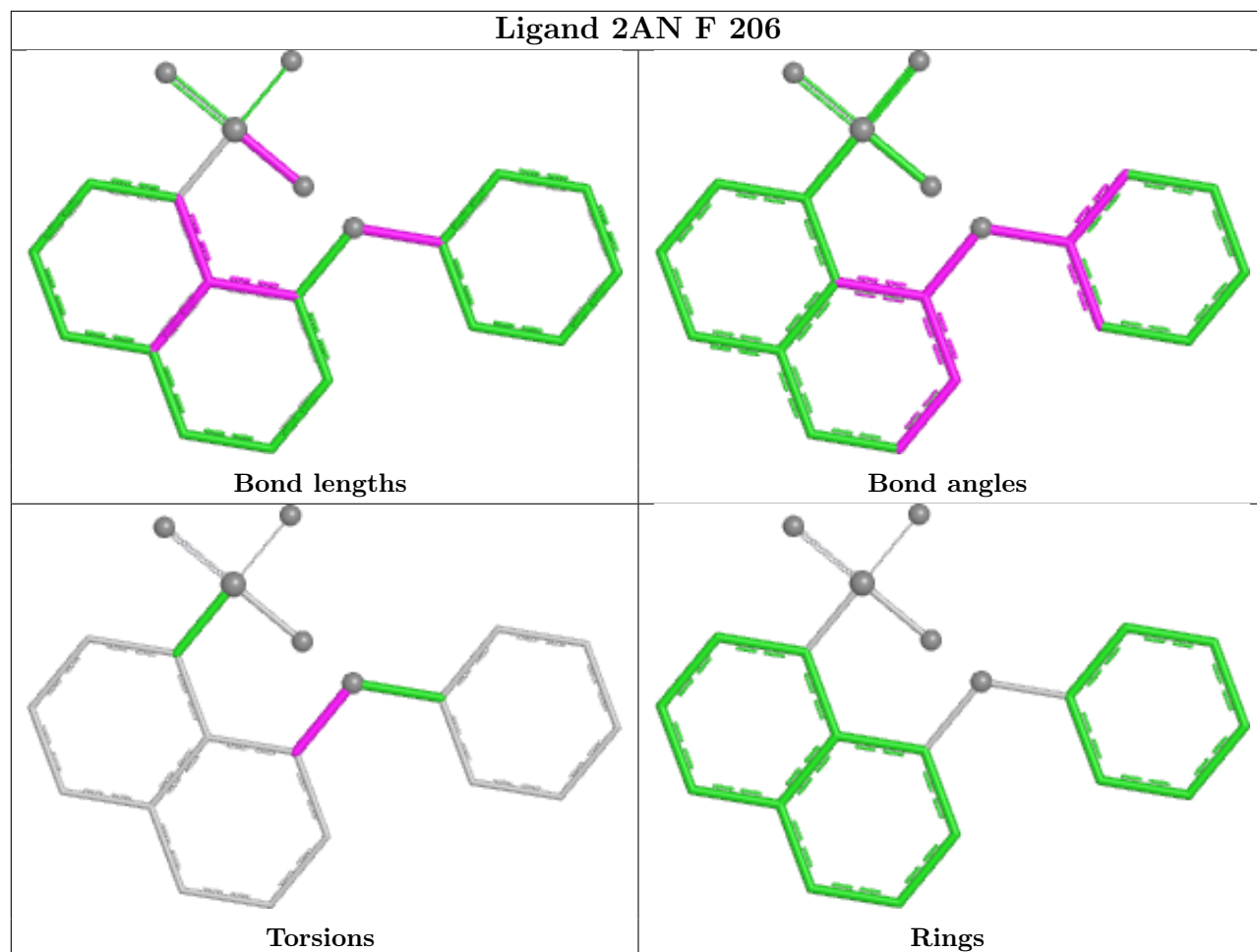
Ligand 2AN S 202

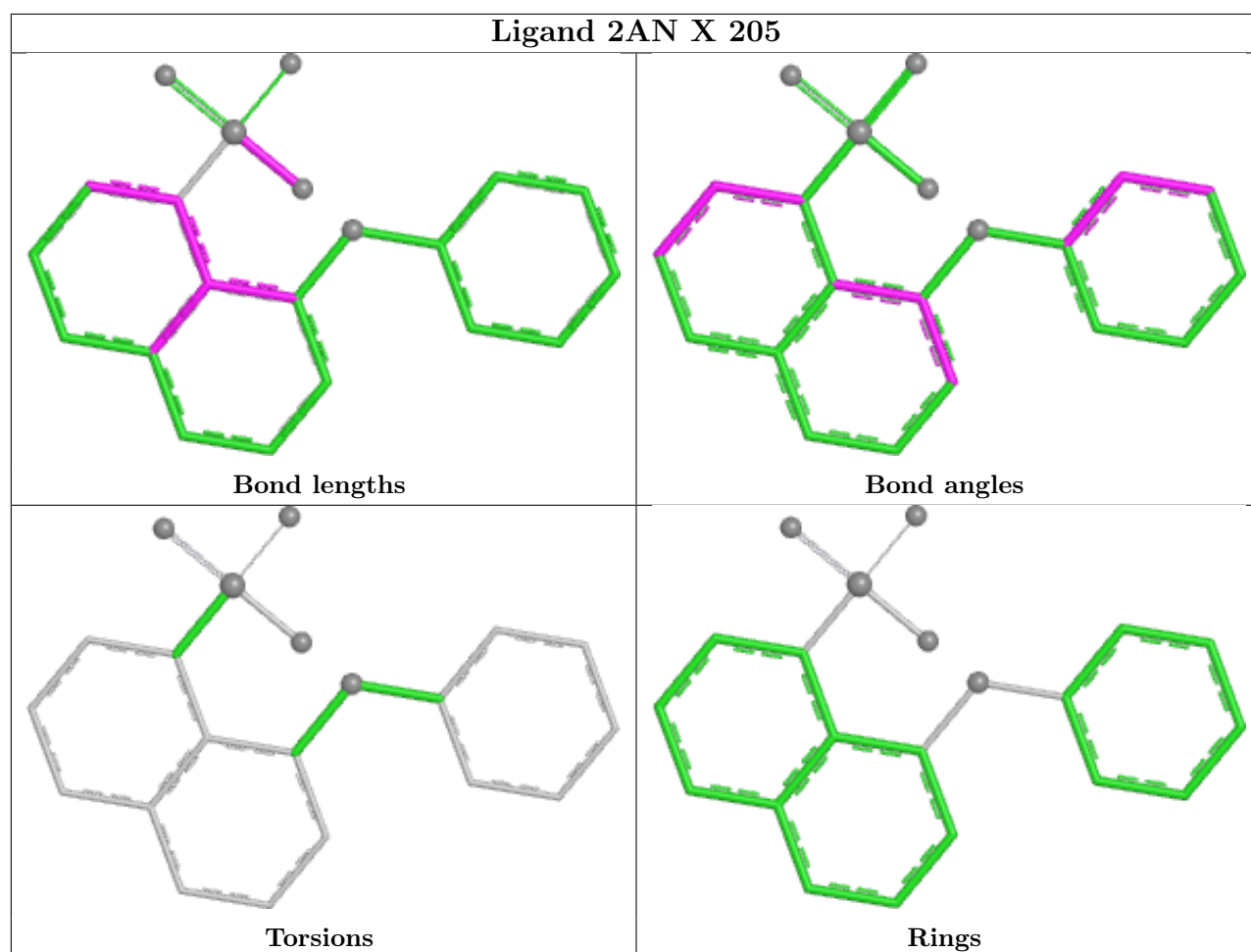




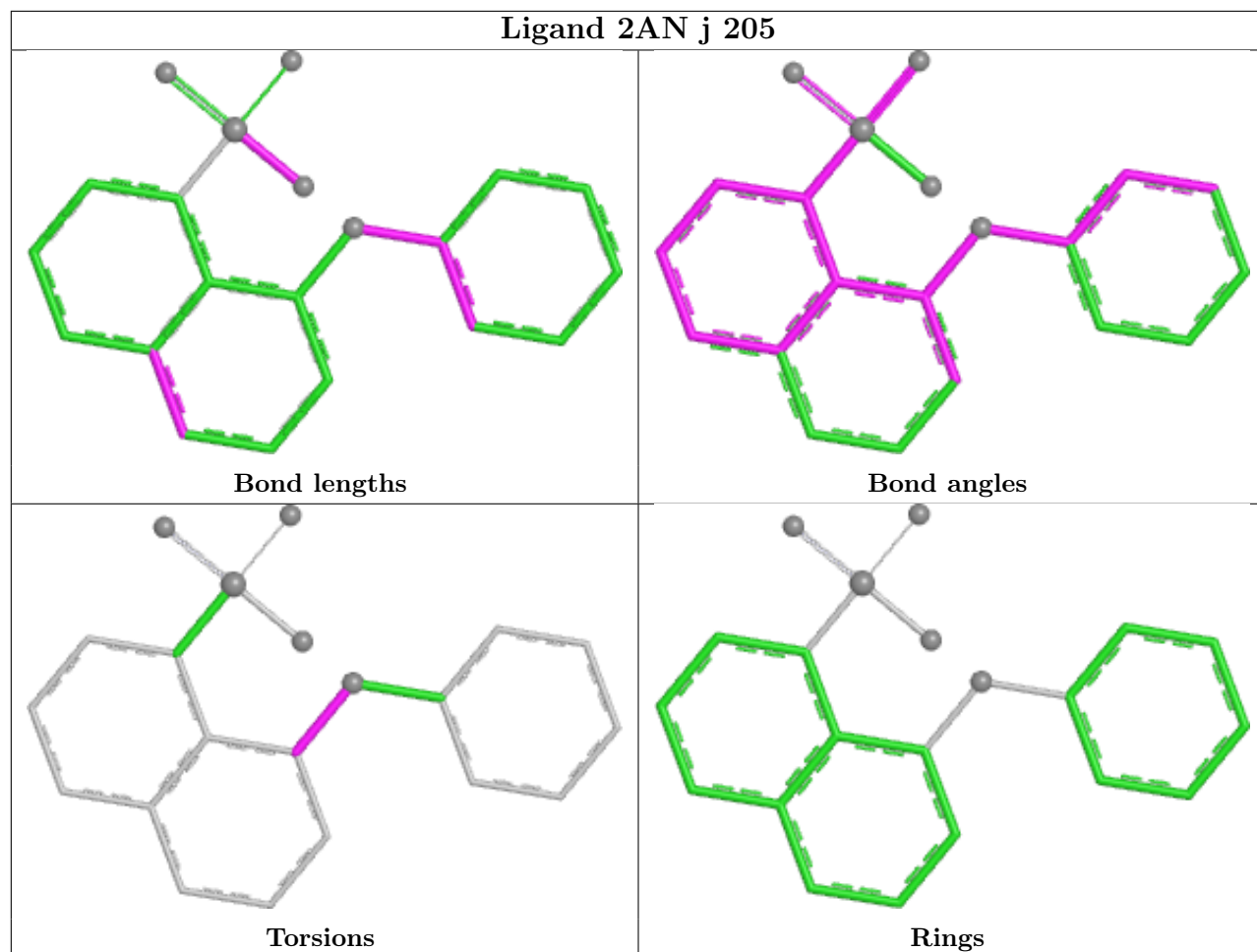


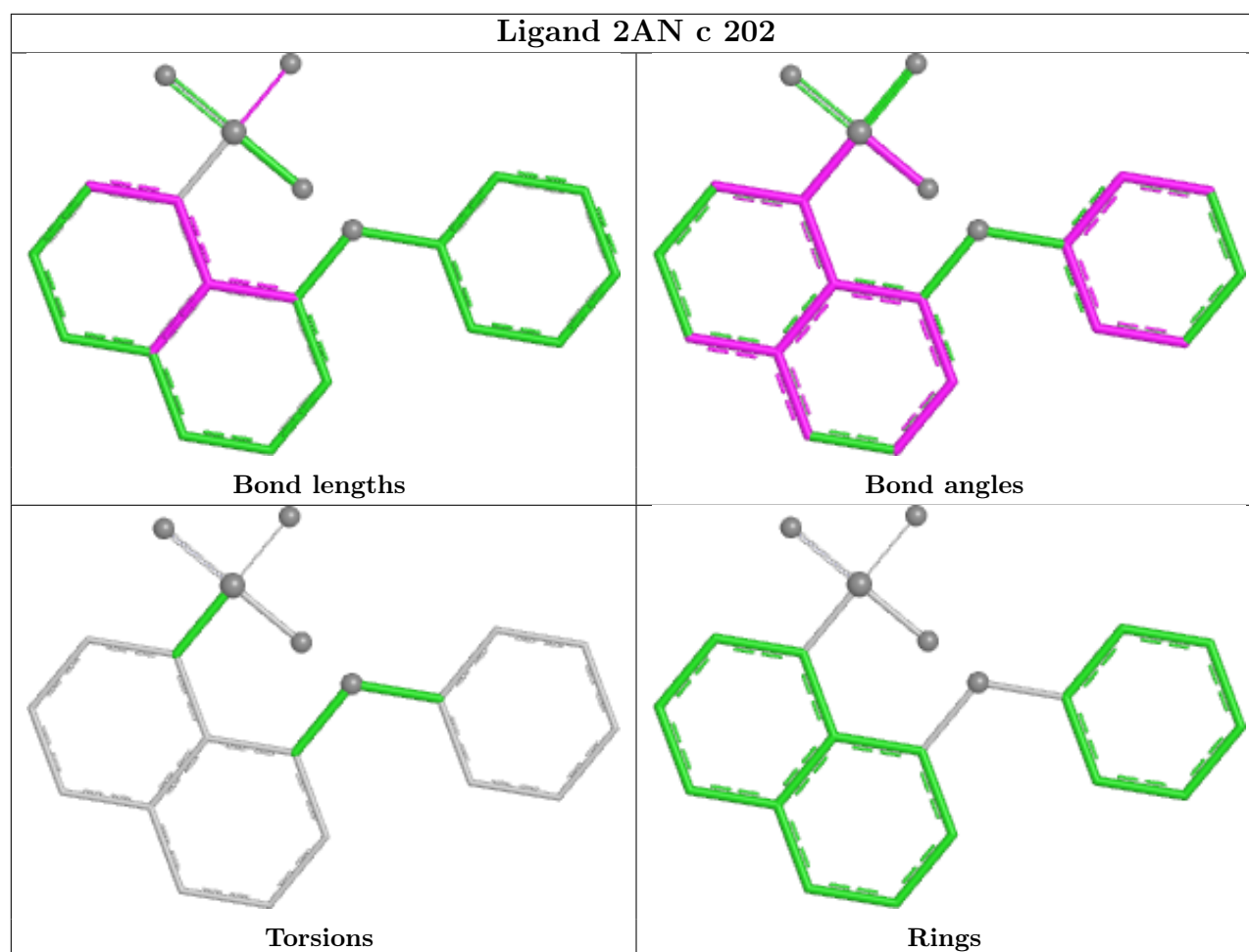
Ligand 2AN F 206

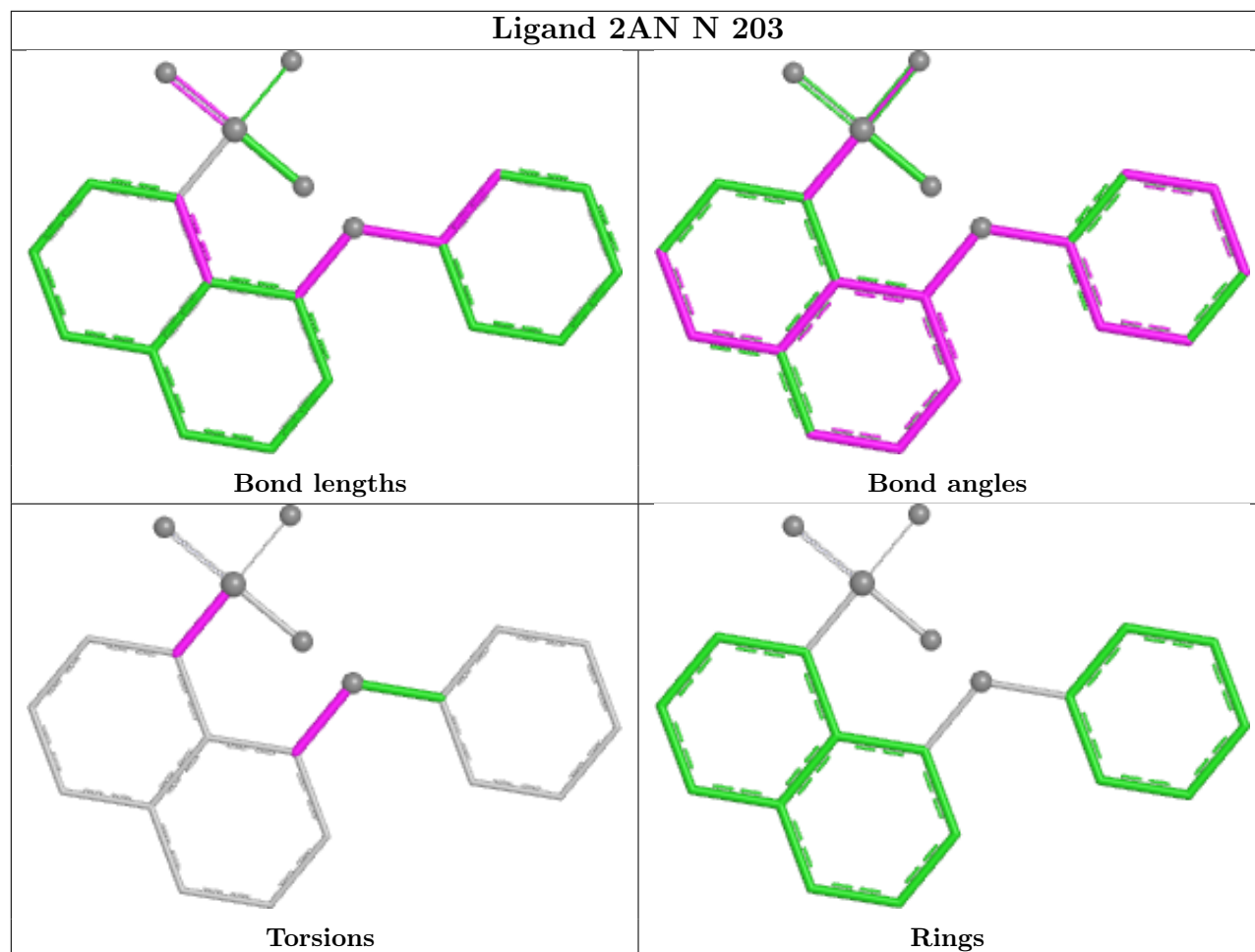


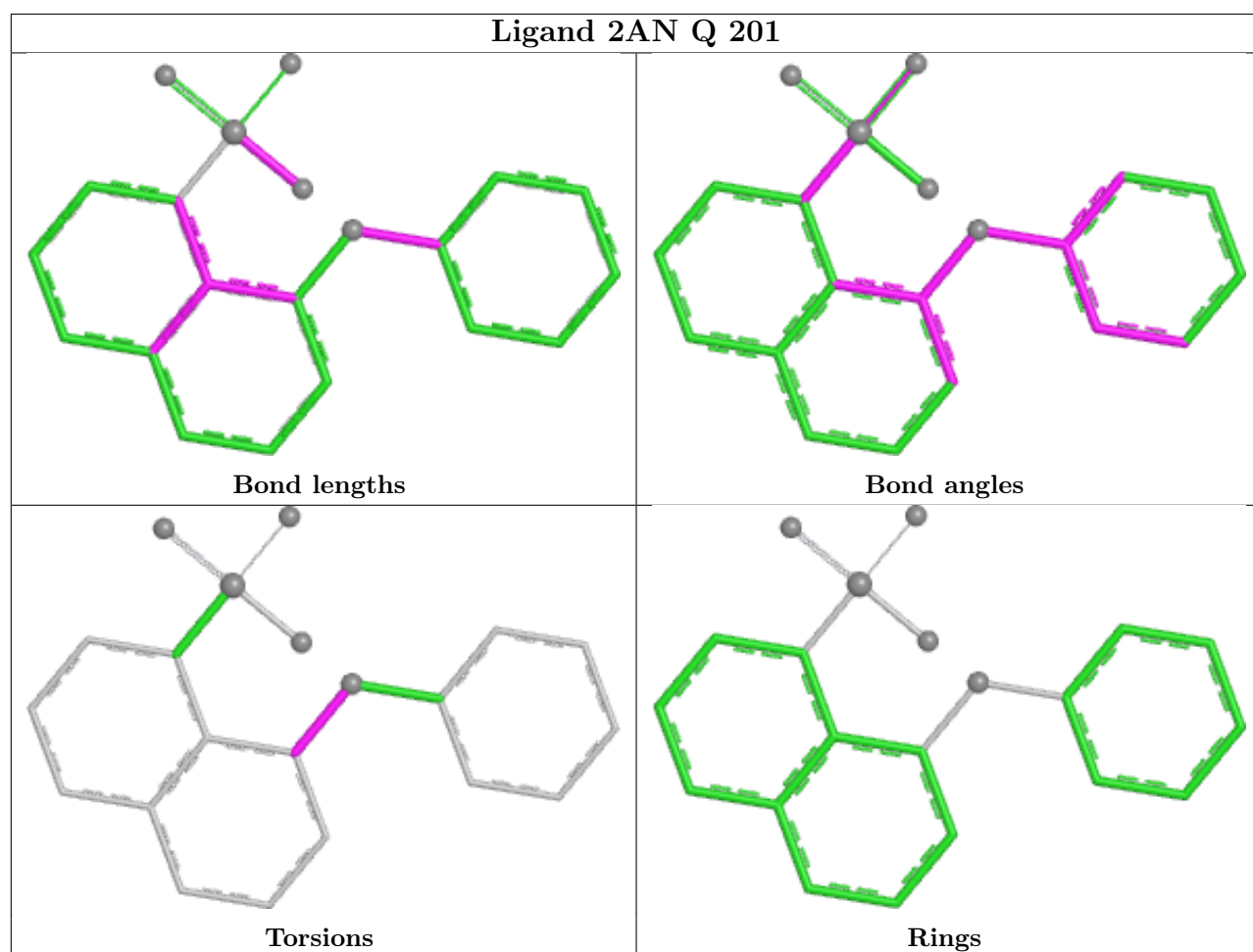


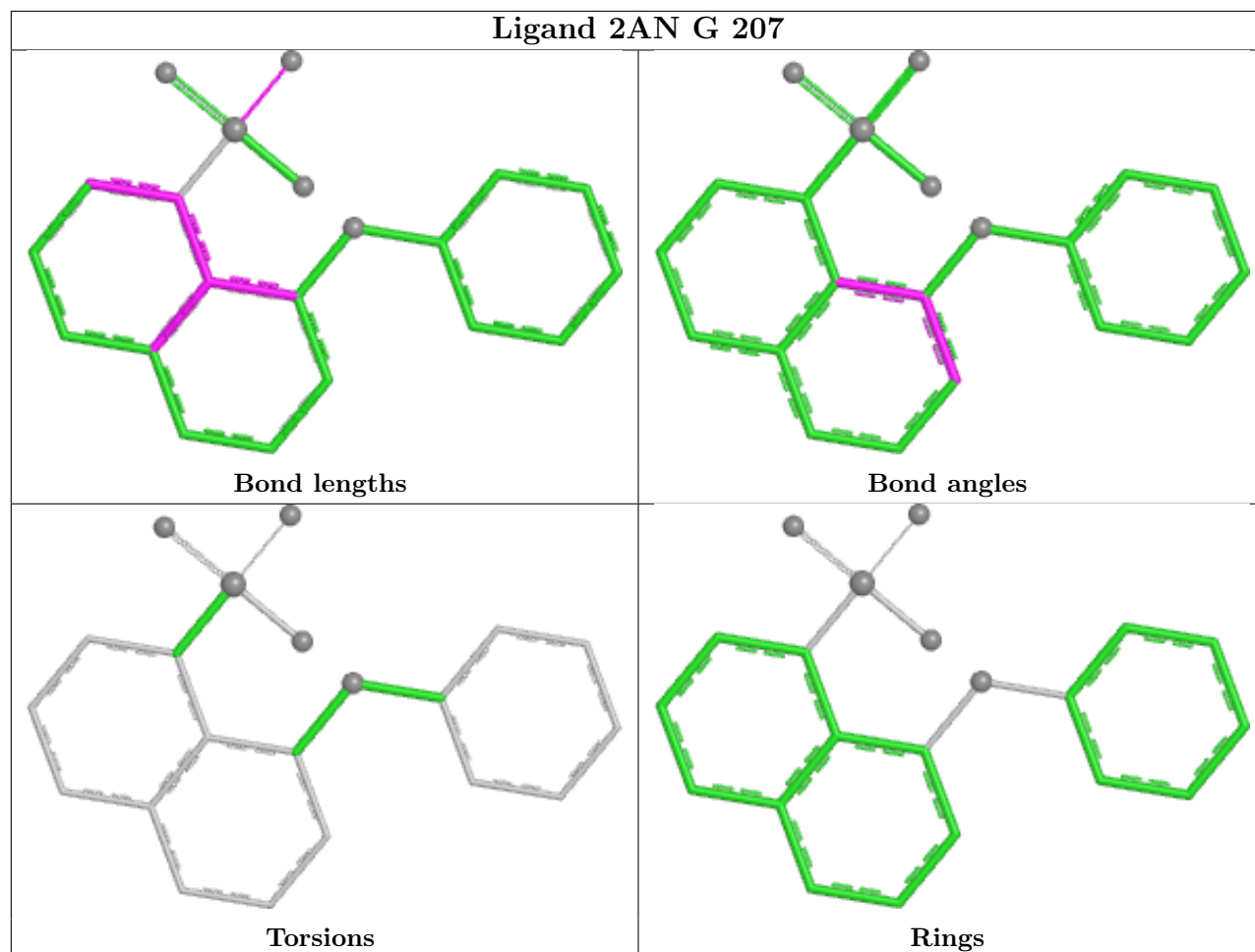
Ligand 2AN j 205



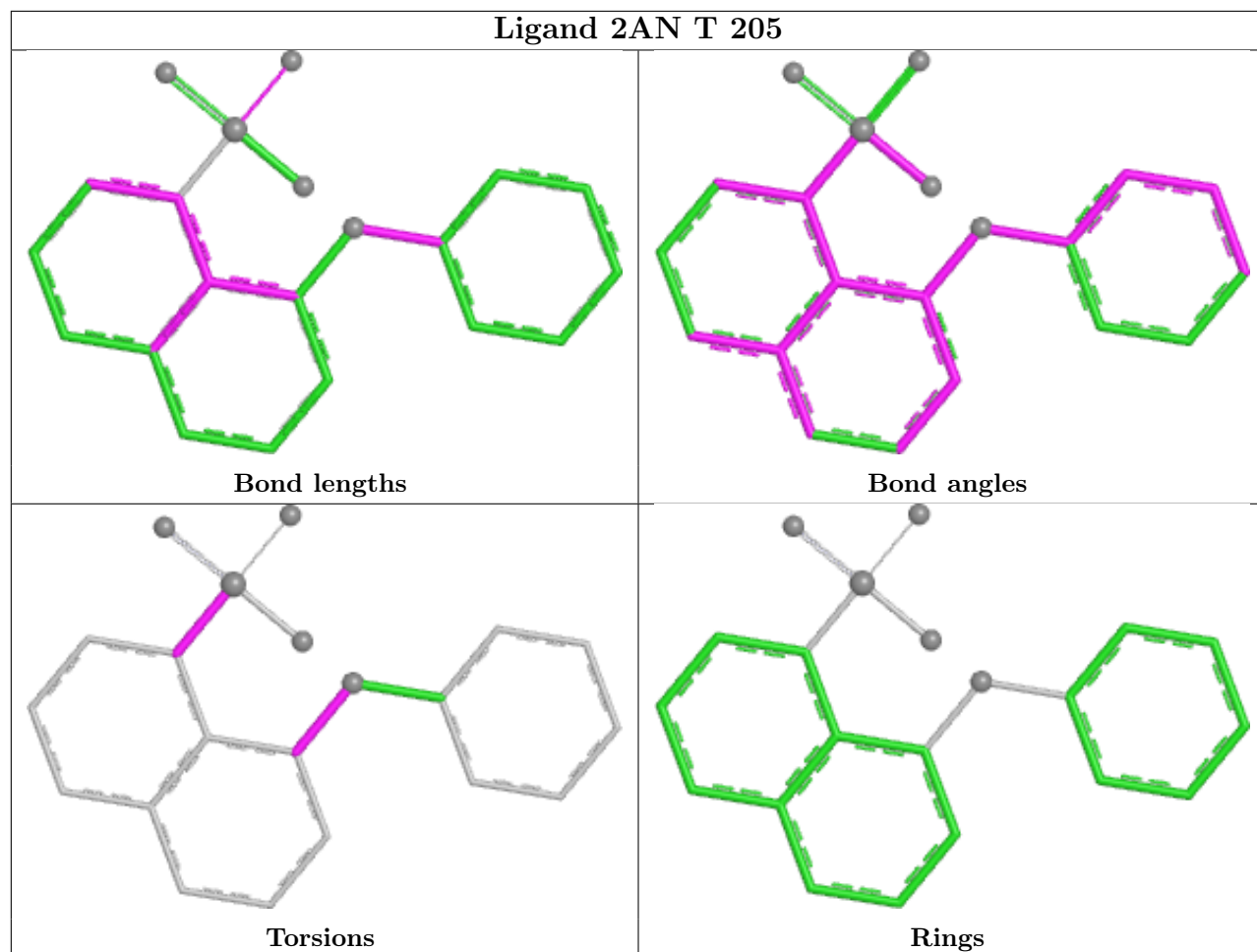




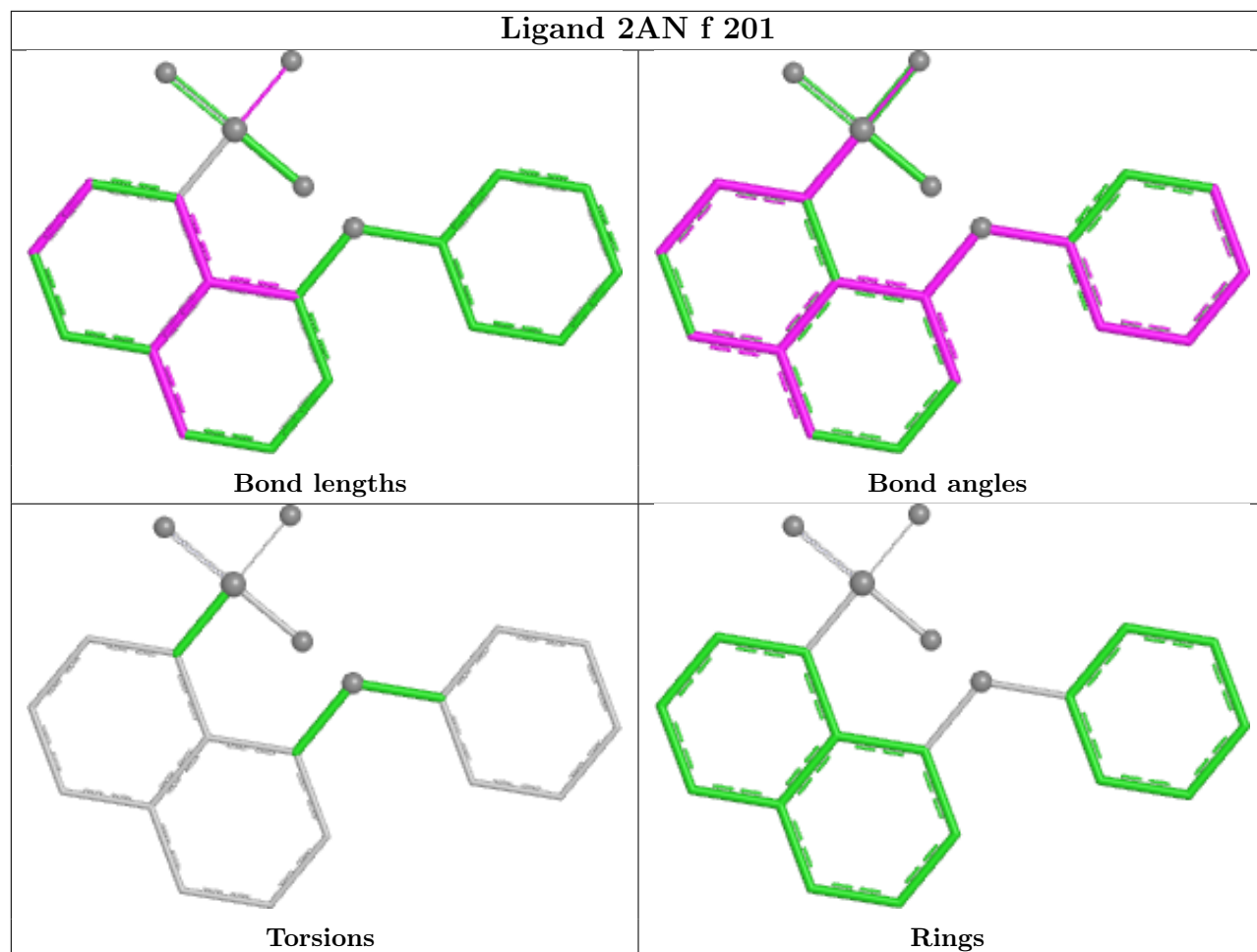




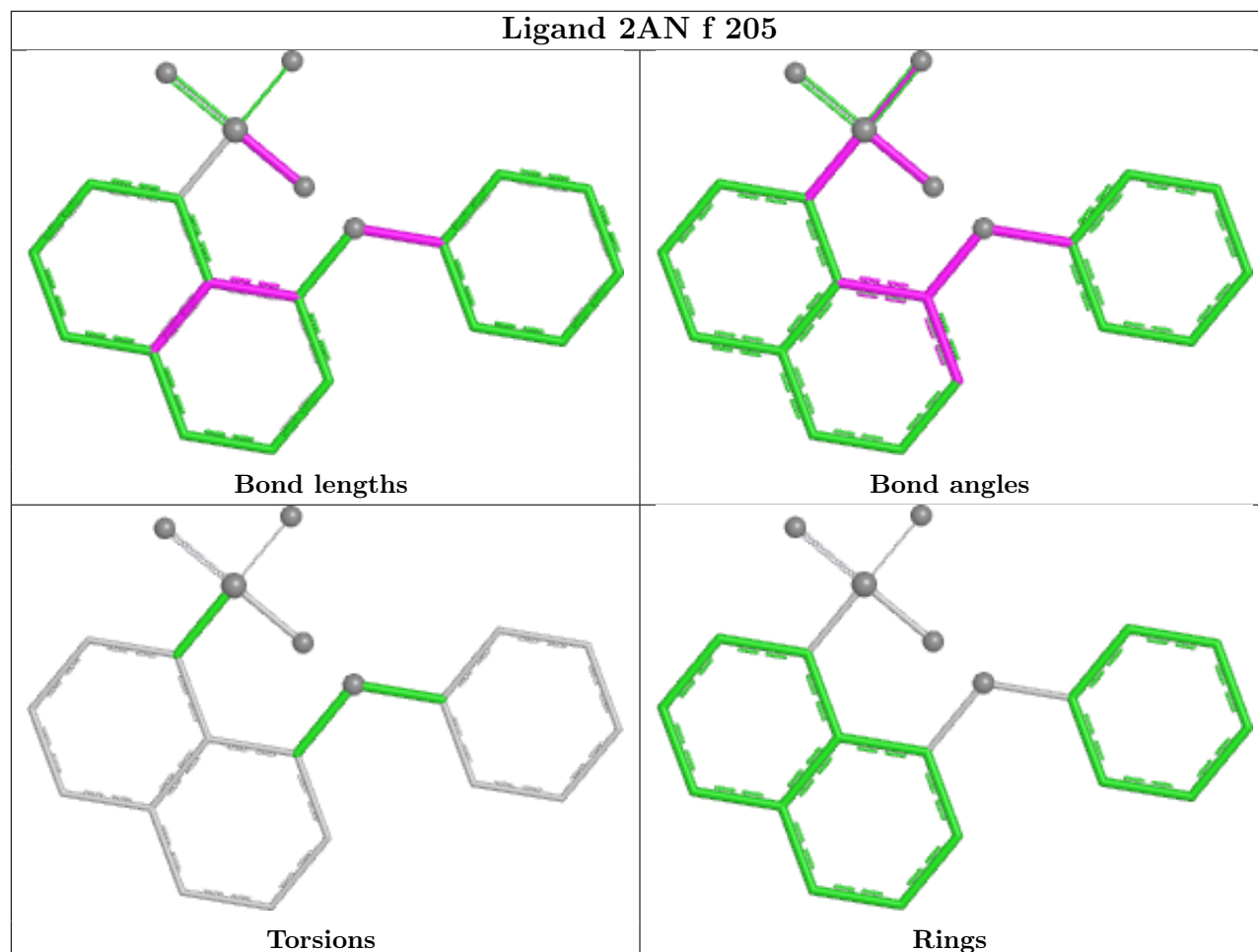
Ligand 2AN T 205

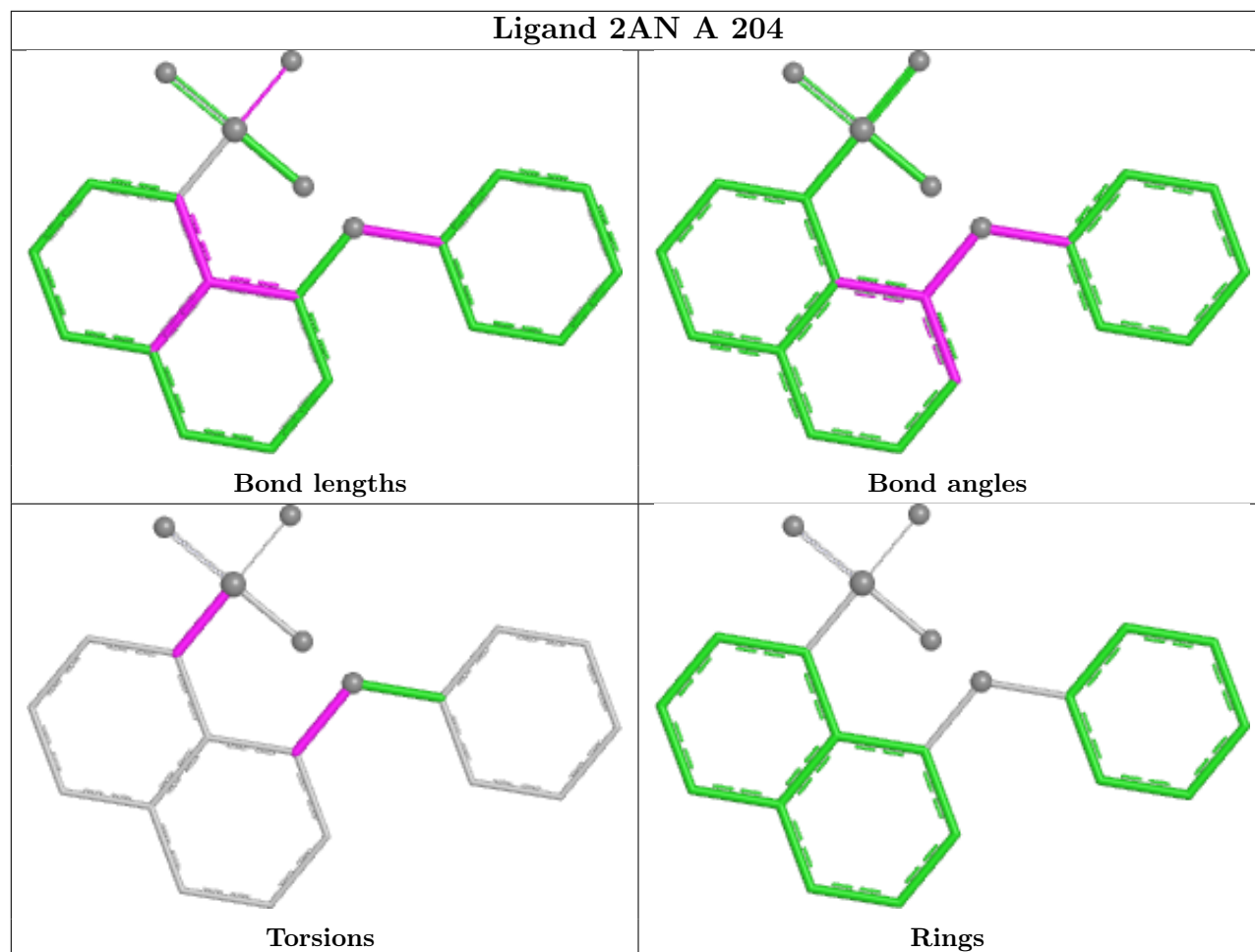


Ligand 2AN f 201

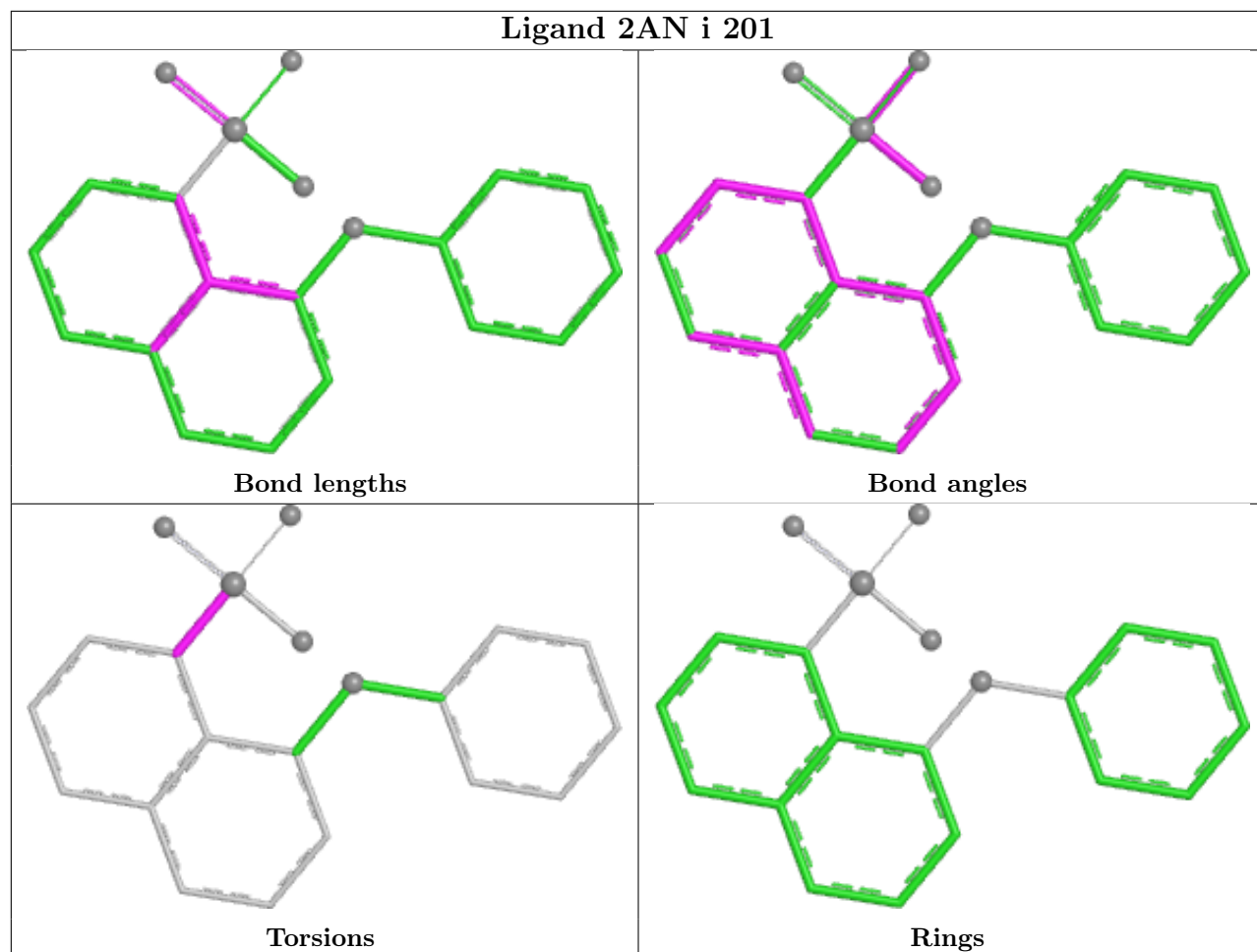


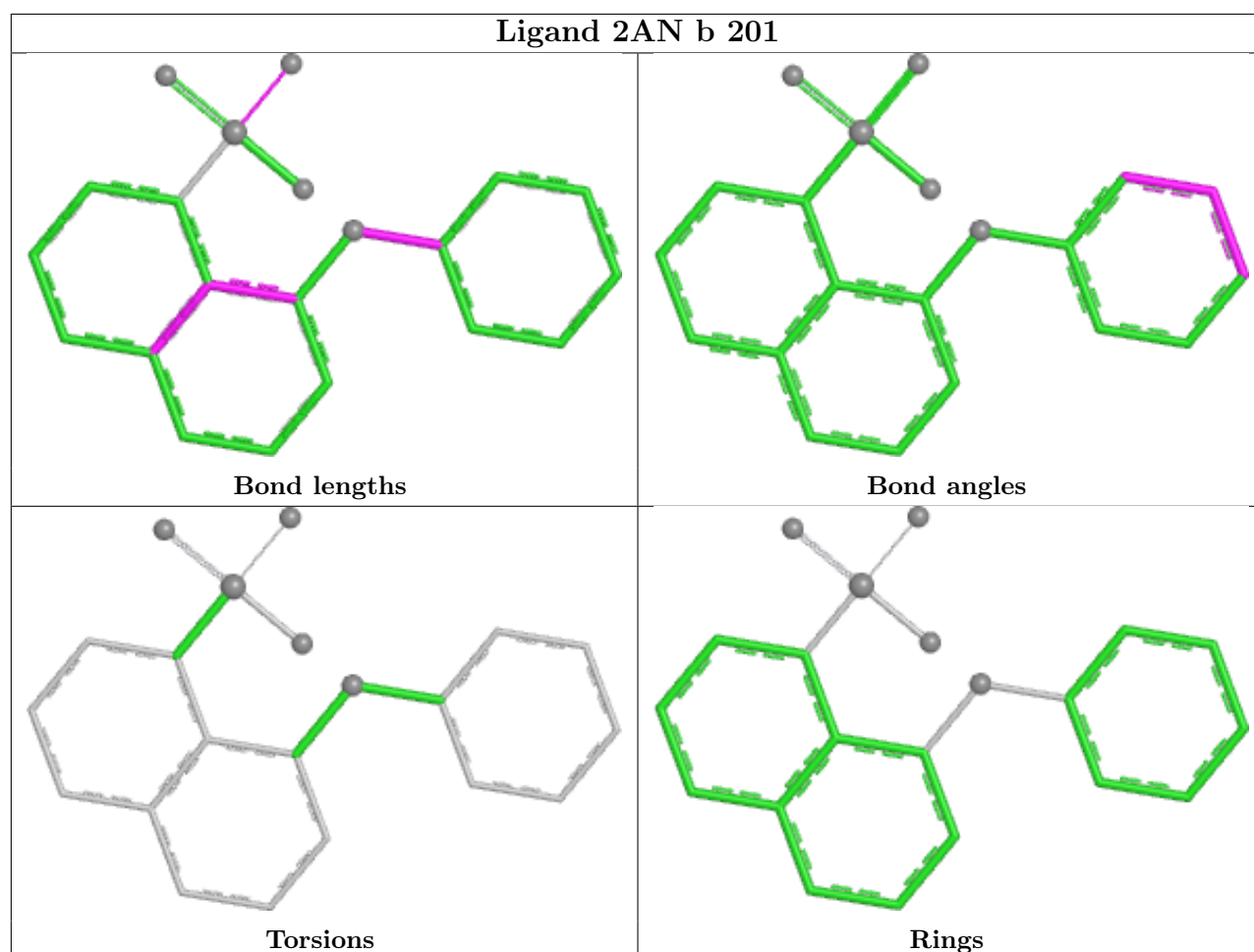
Ligand 2AN f 205



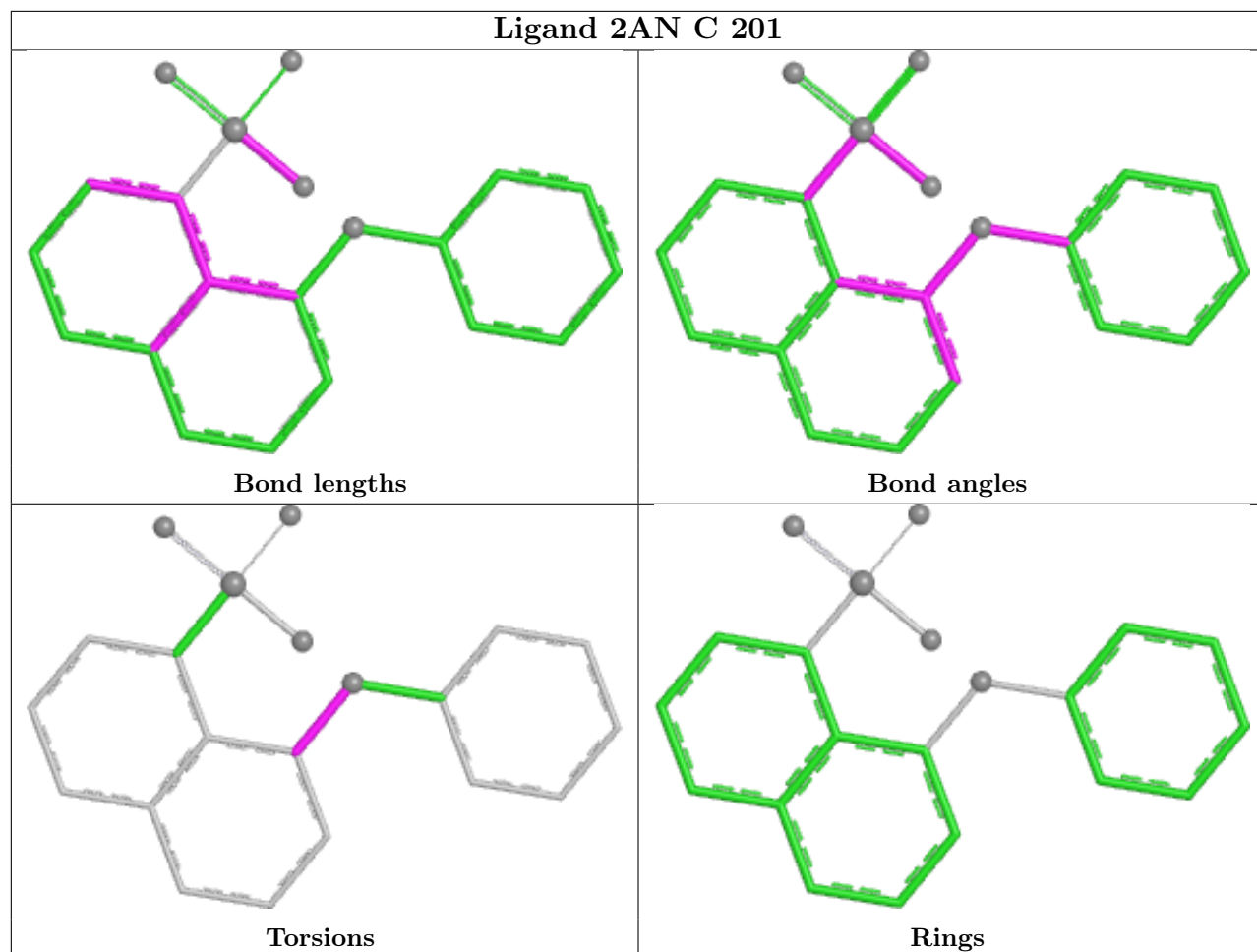


Ligand 2AN i 201

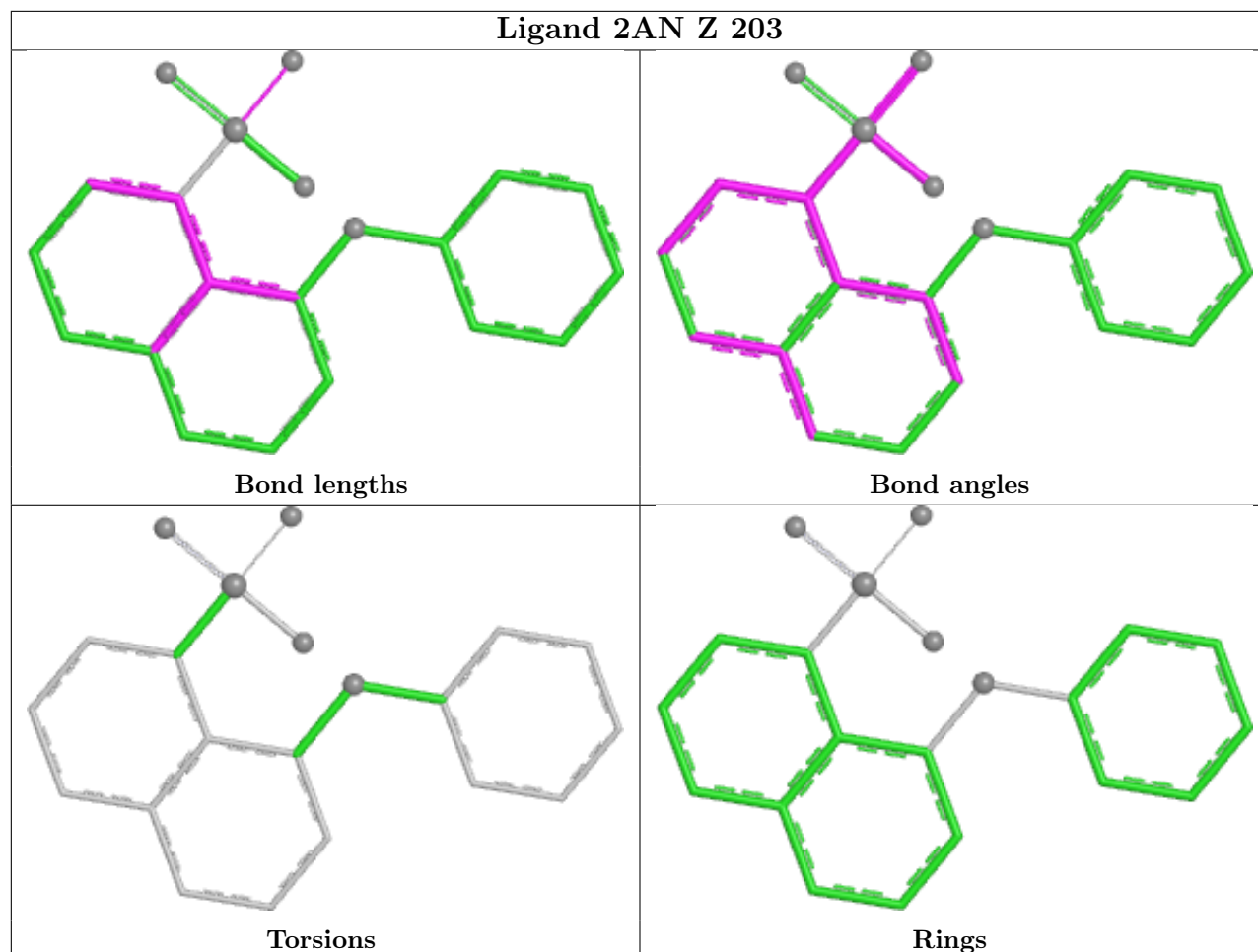




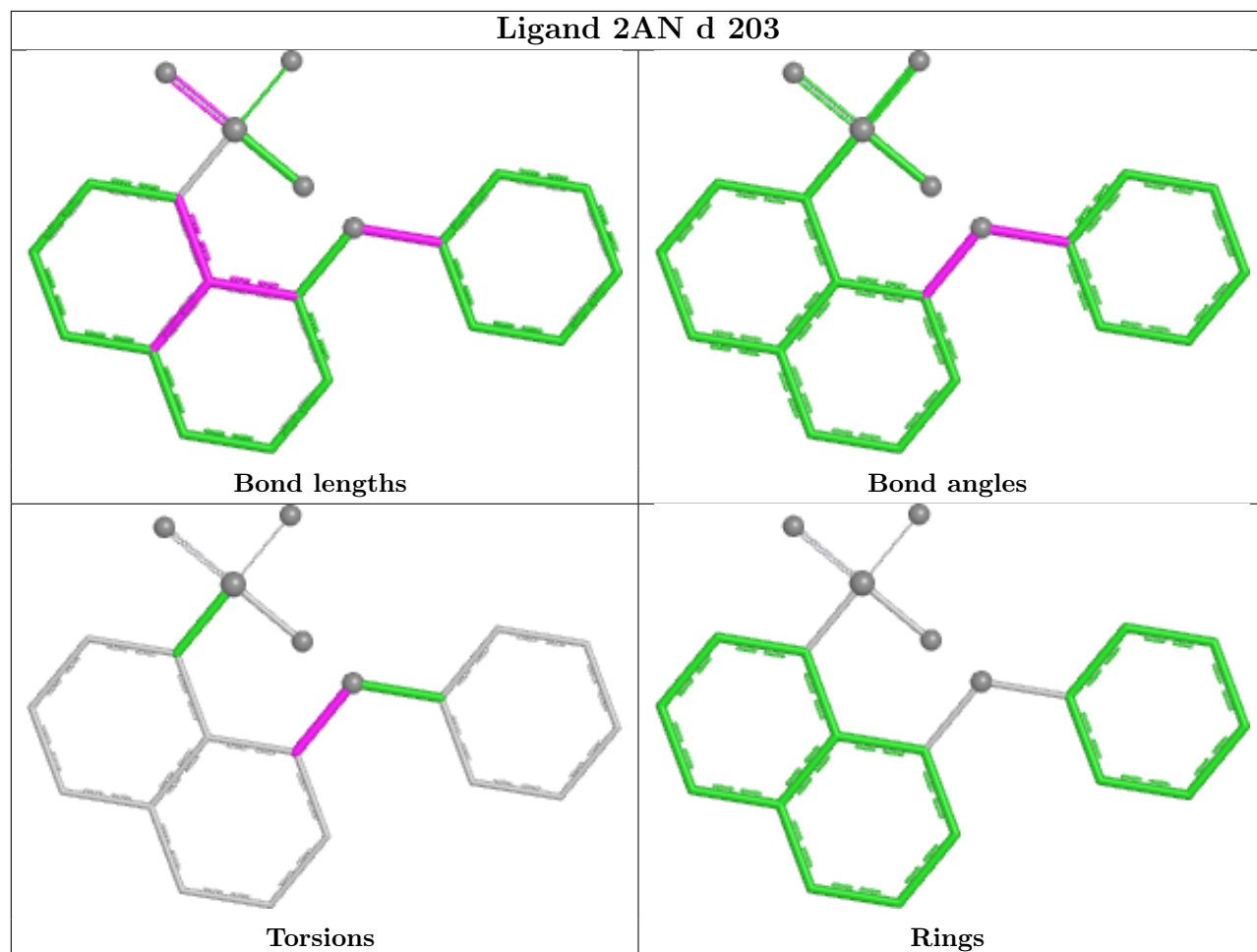
Ligand 2AN C 201



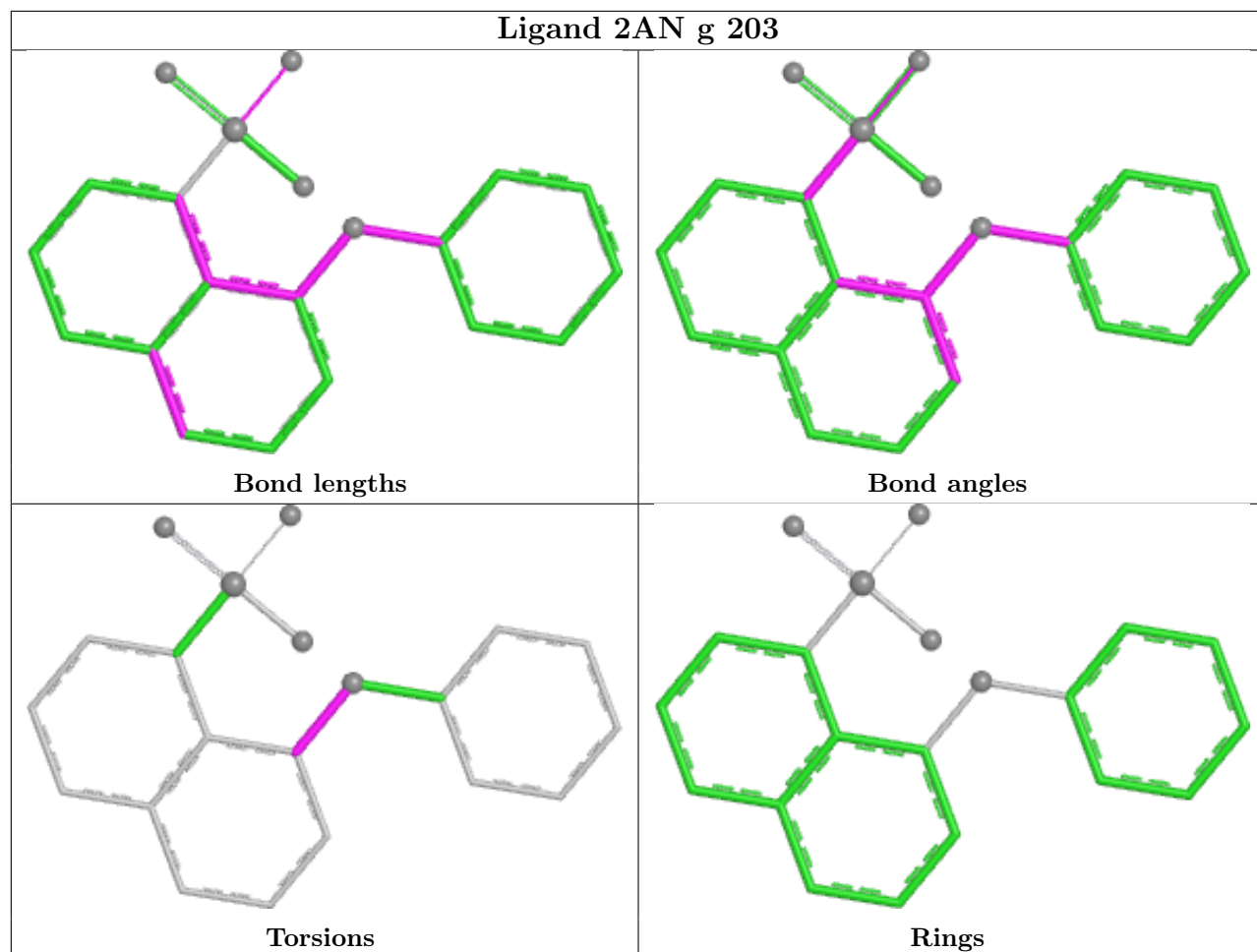
Ligand 2AN Z 203

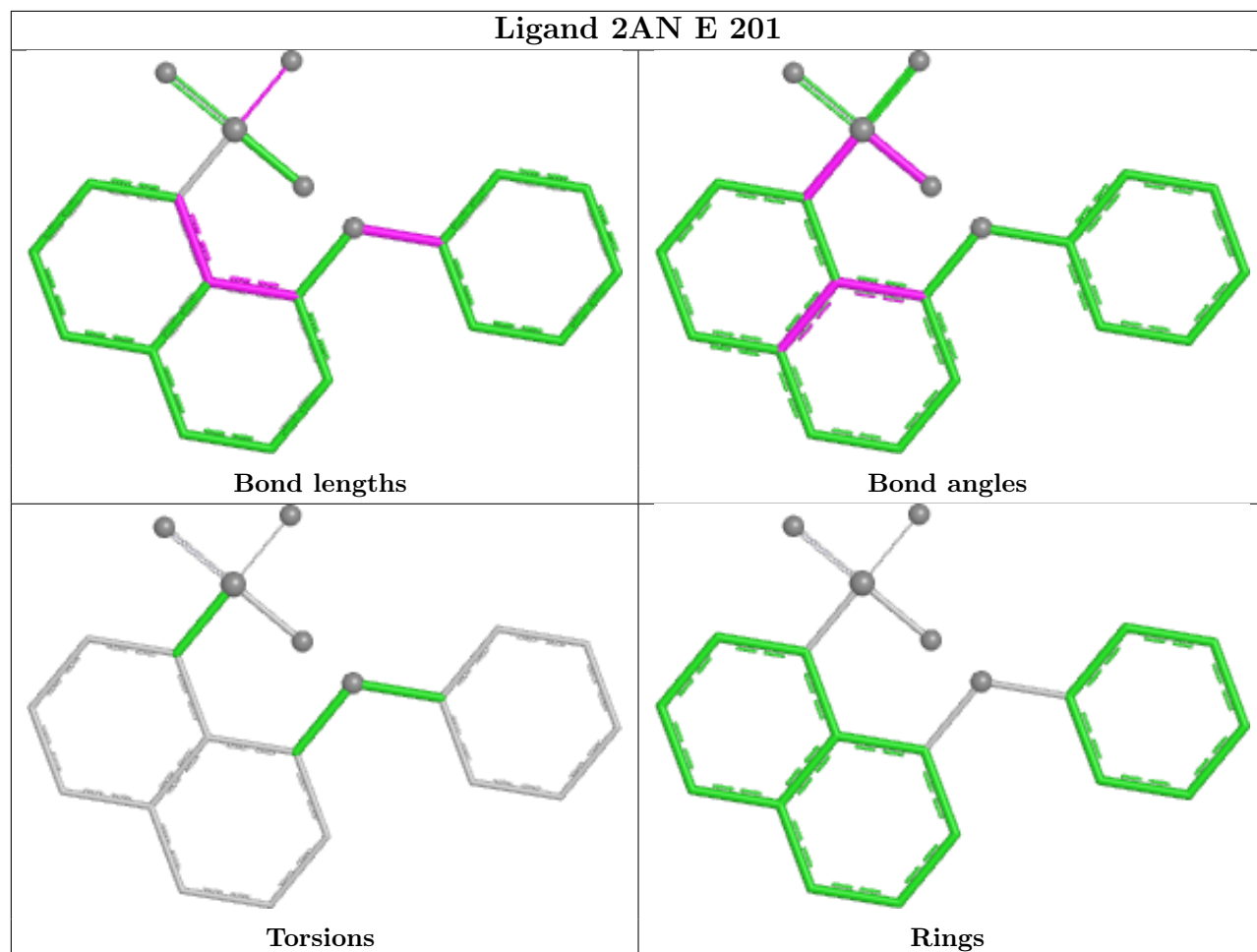


Ligand 2AN d 203

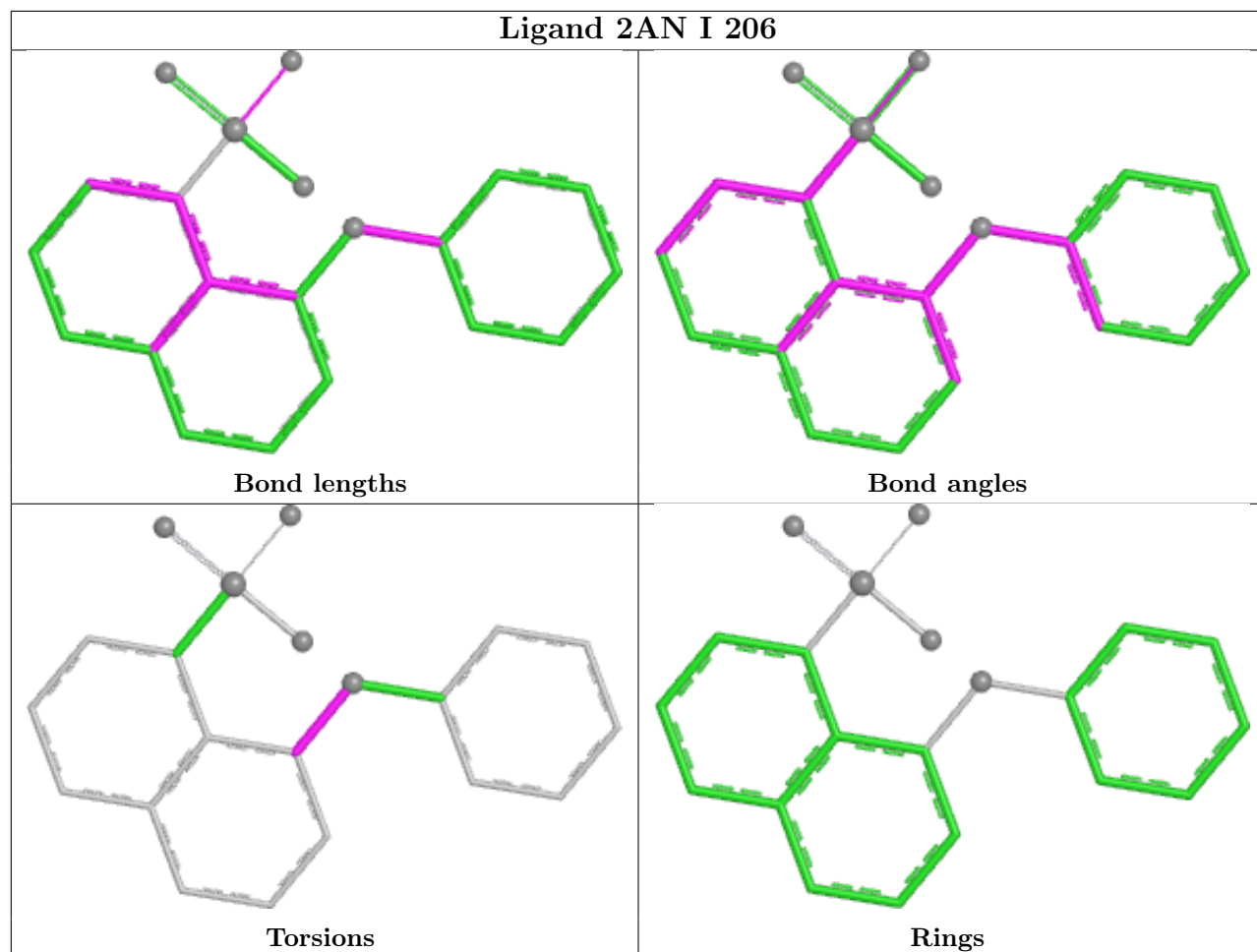


Ligand 2AN g 203

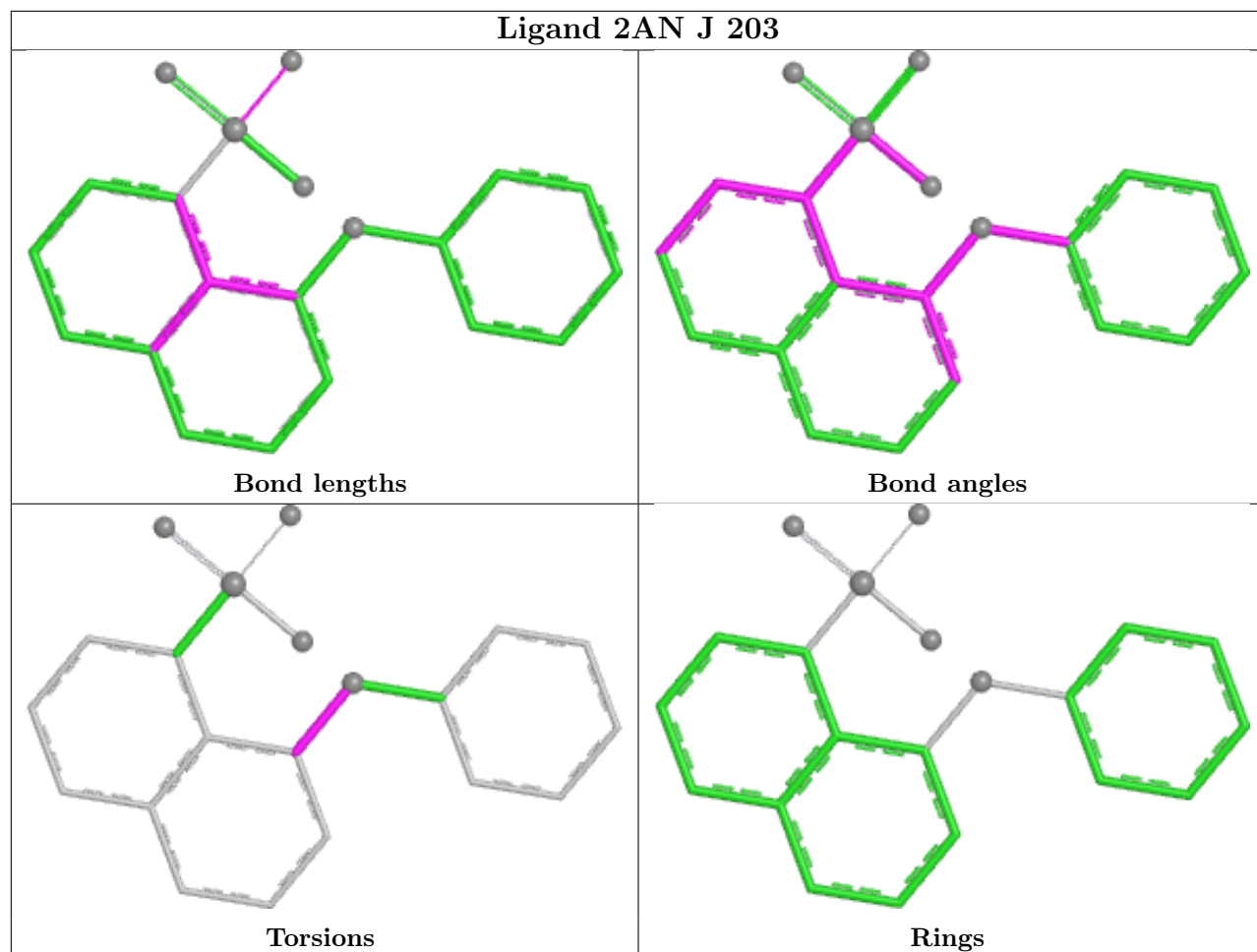




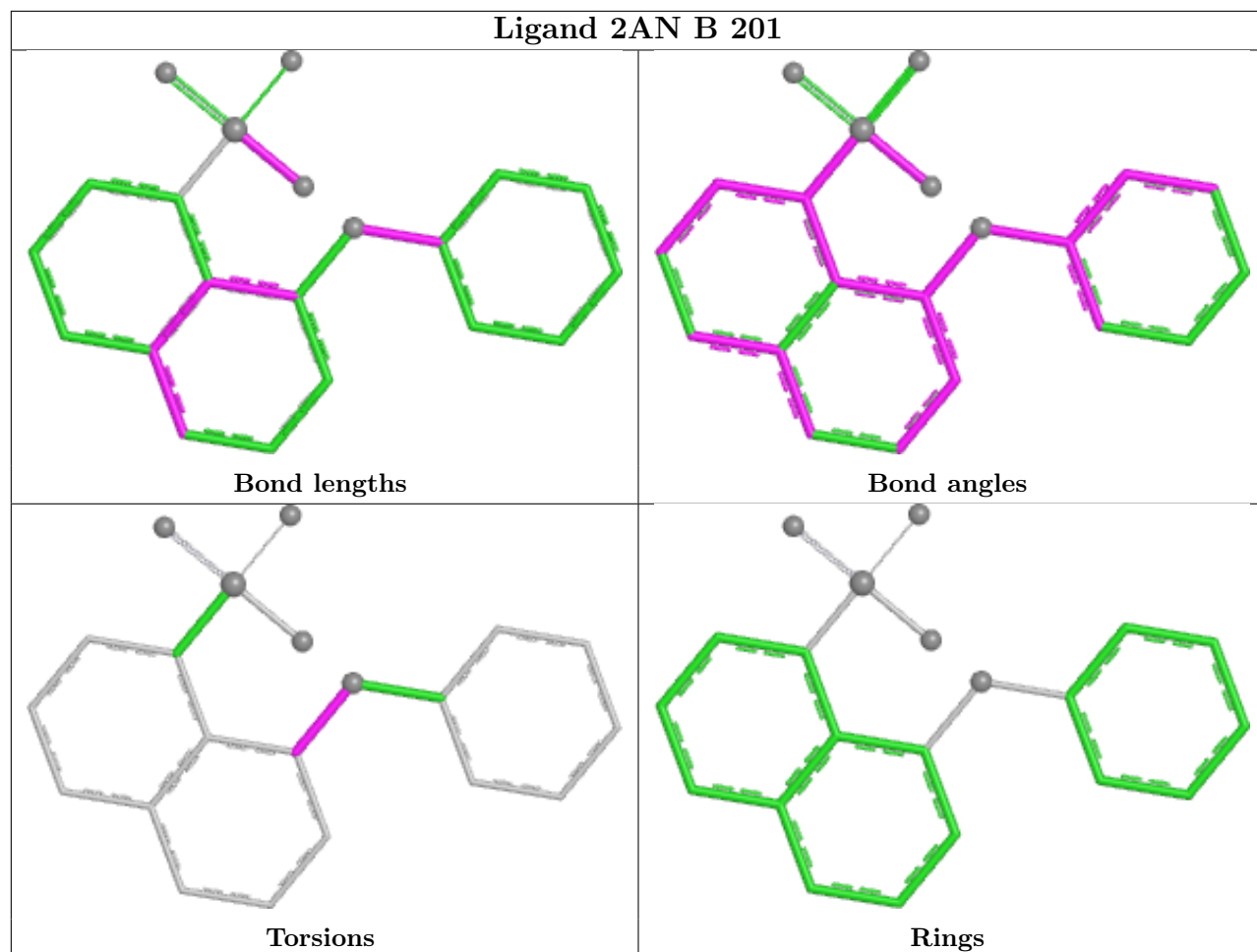
Ligand 2AN I 206



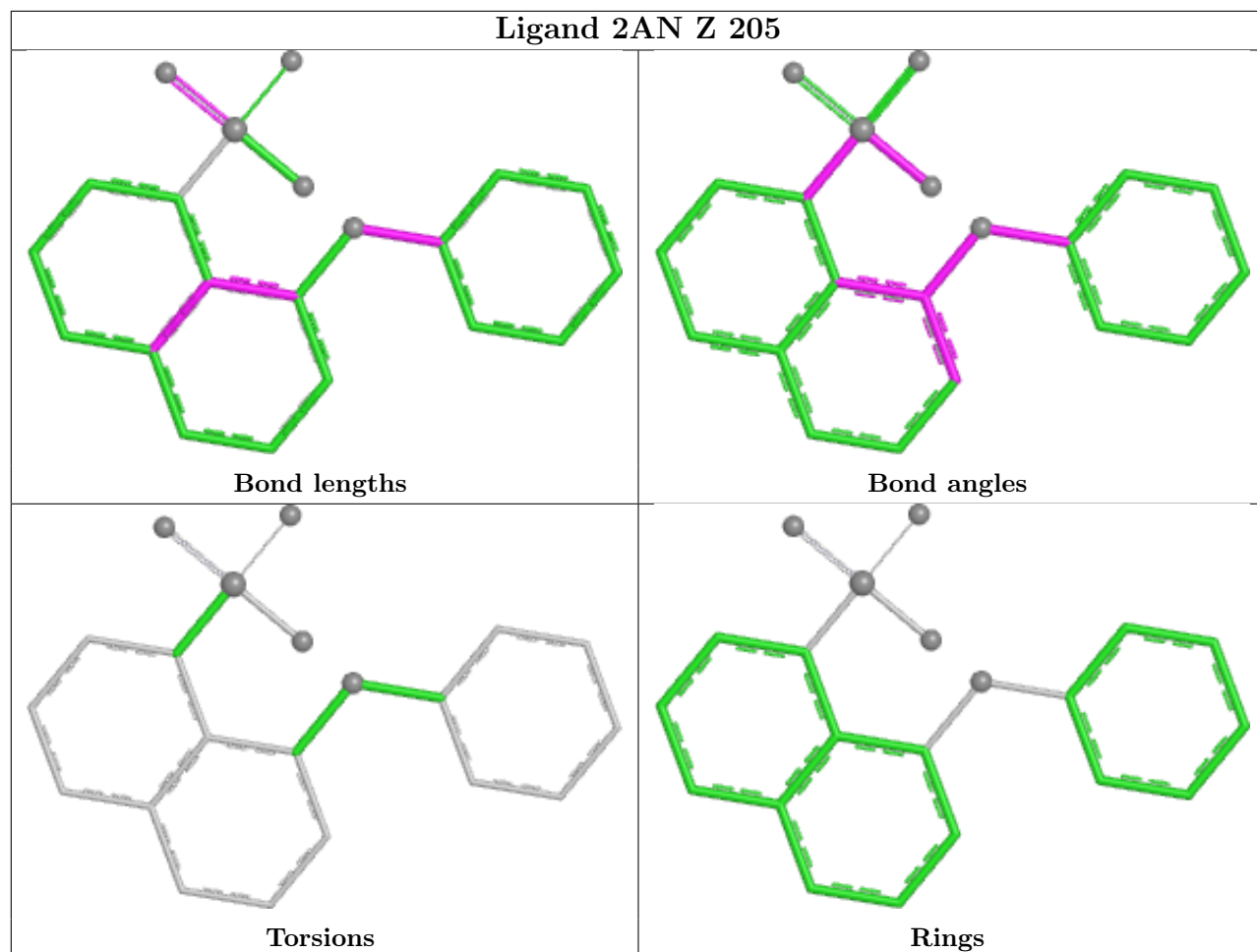
Ligand 2AN J 203



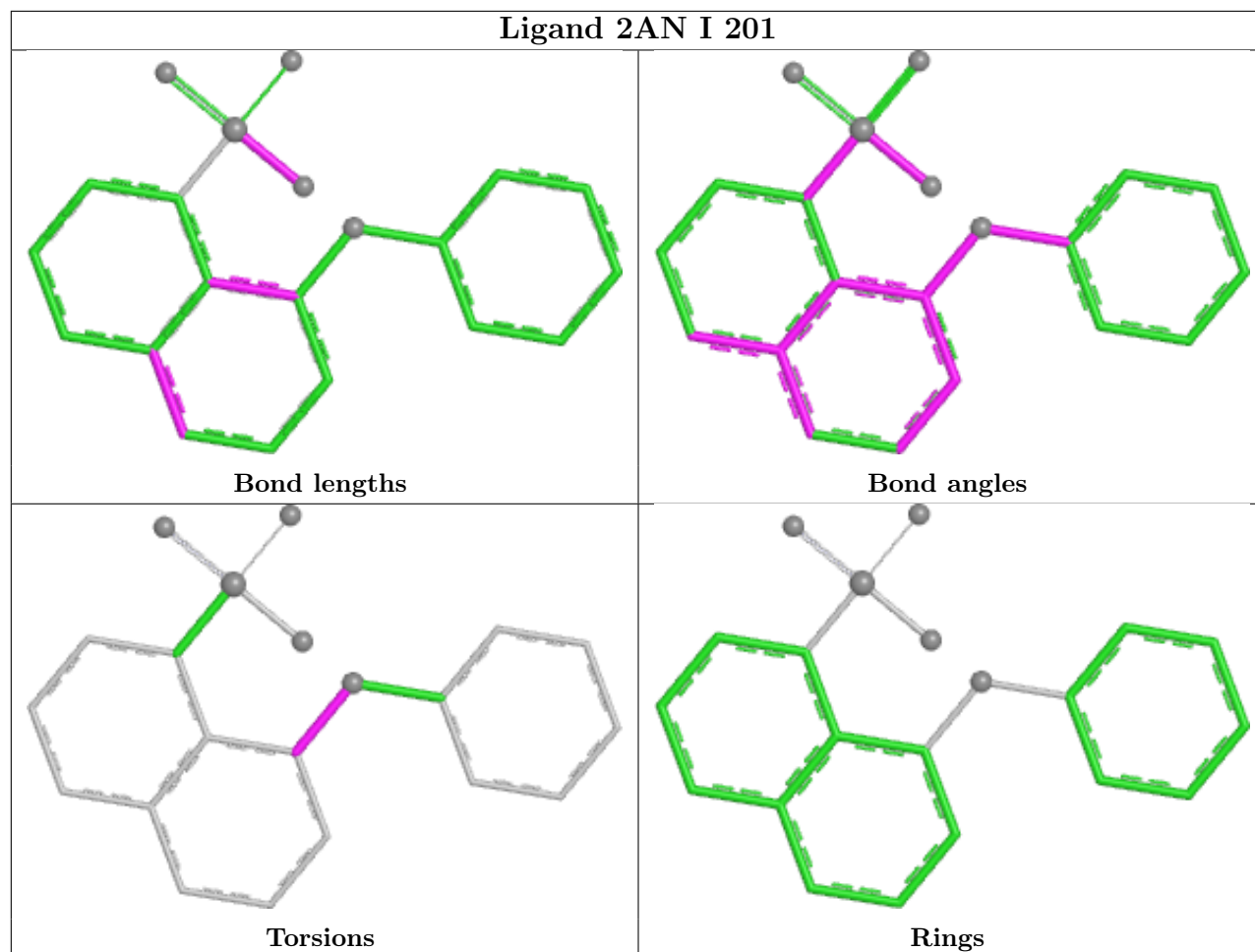
Ligand 2AN B 201

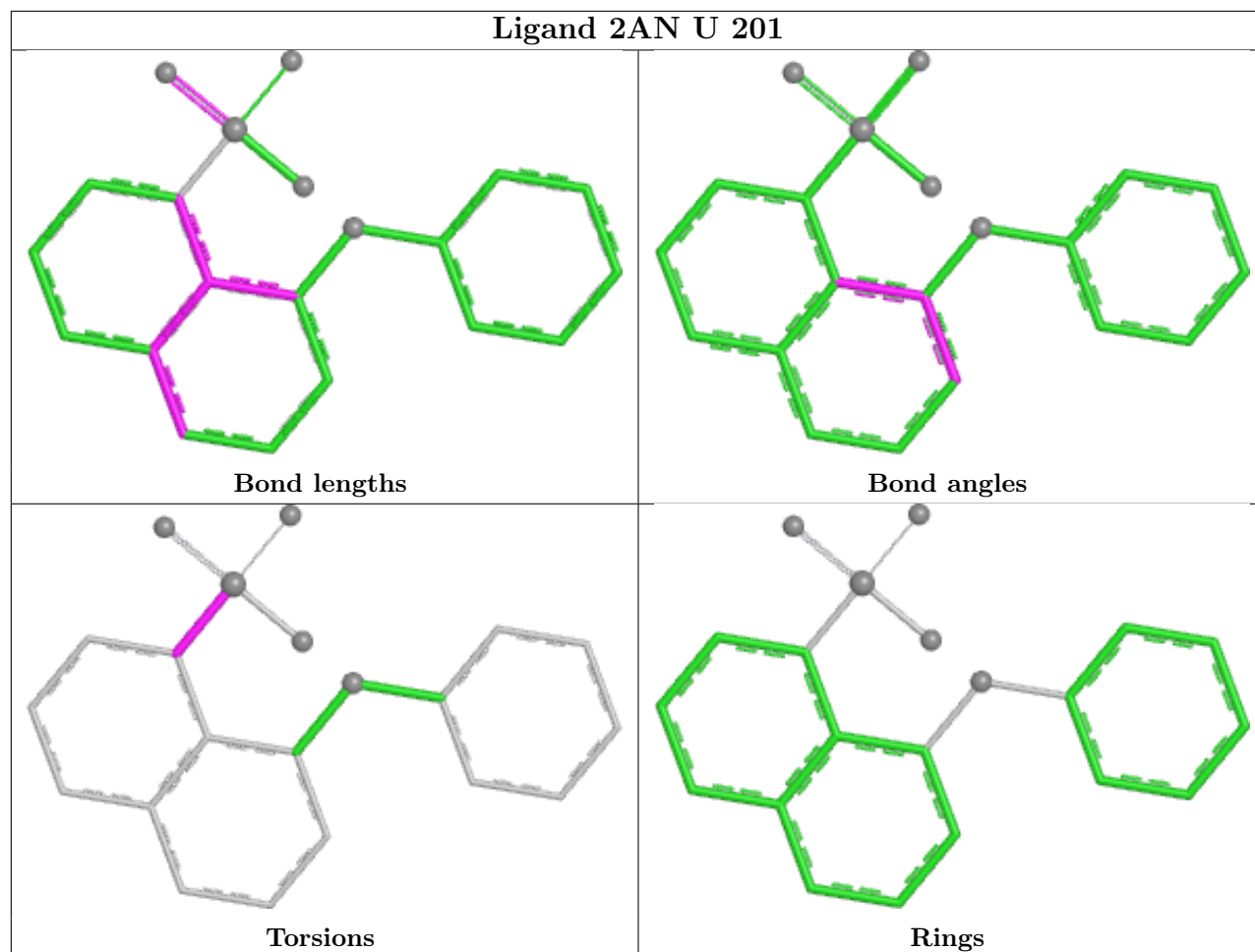


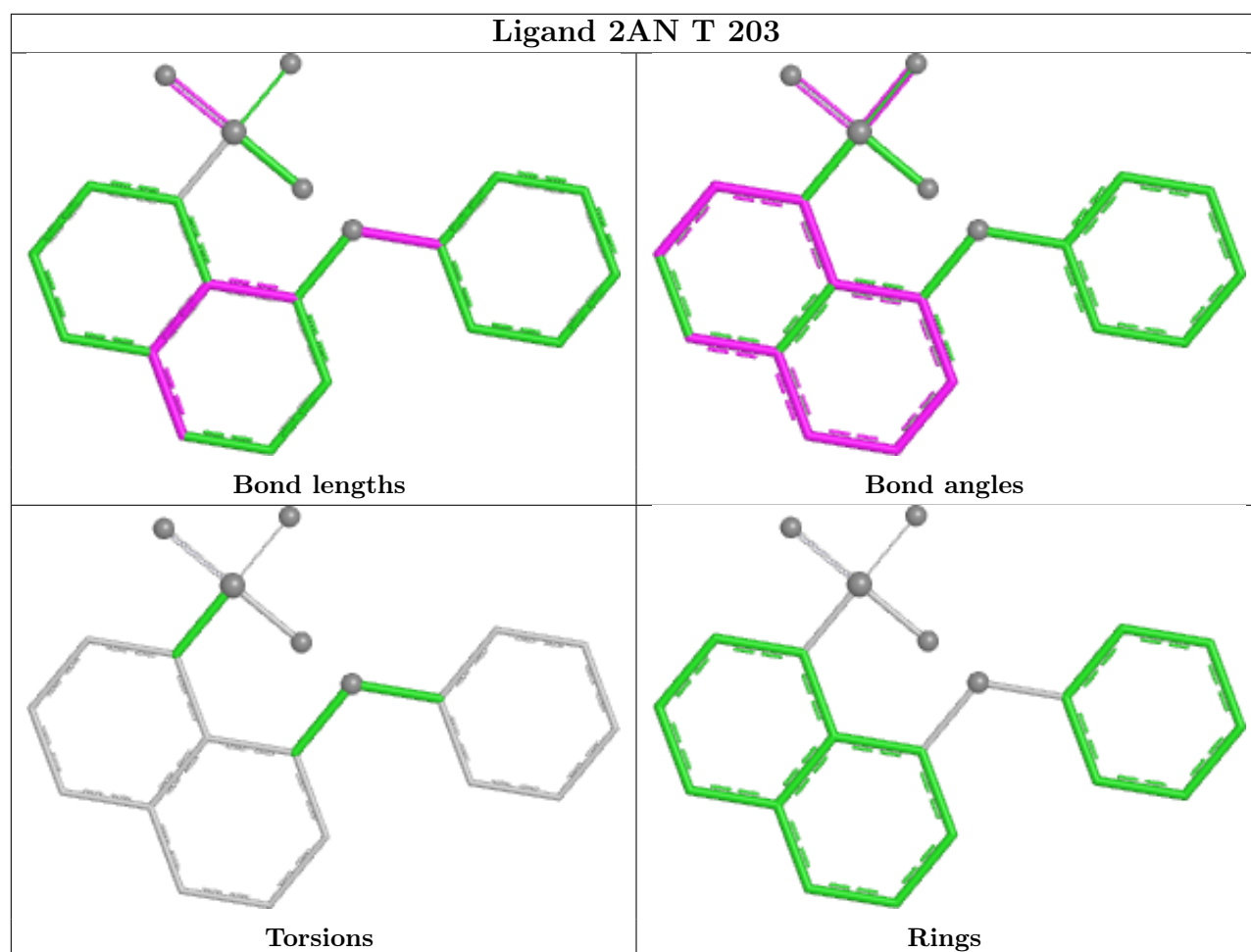
Ligand 2AN Z 205



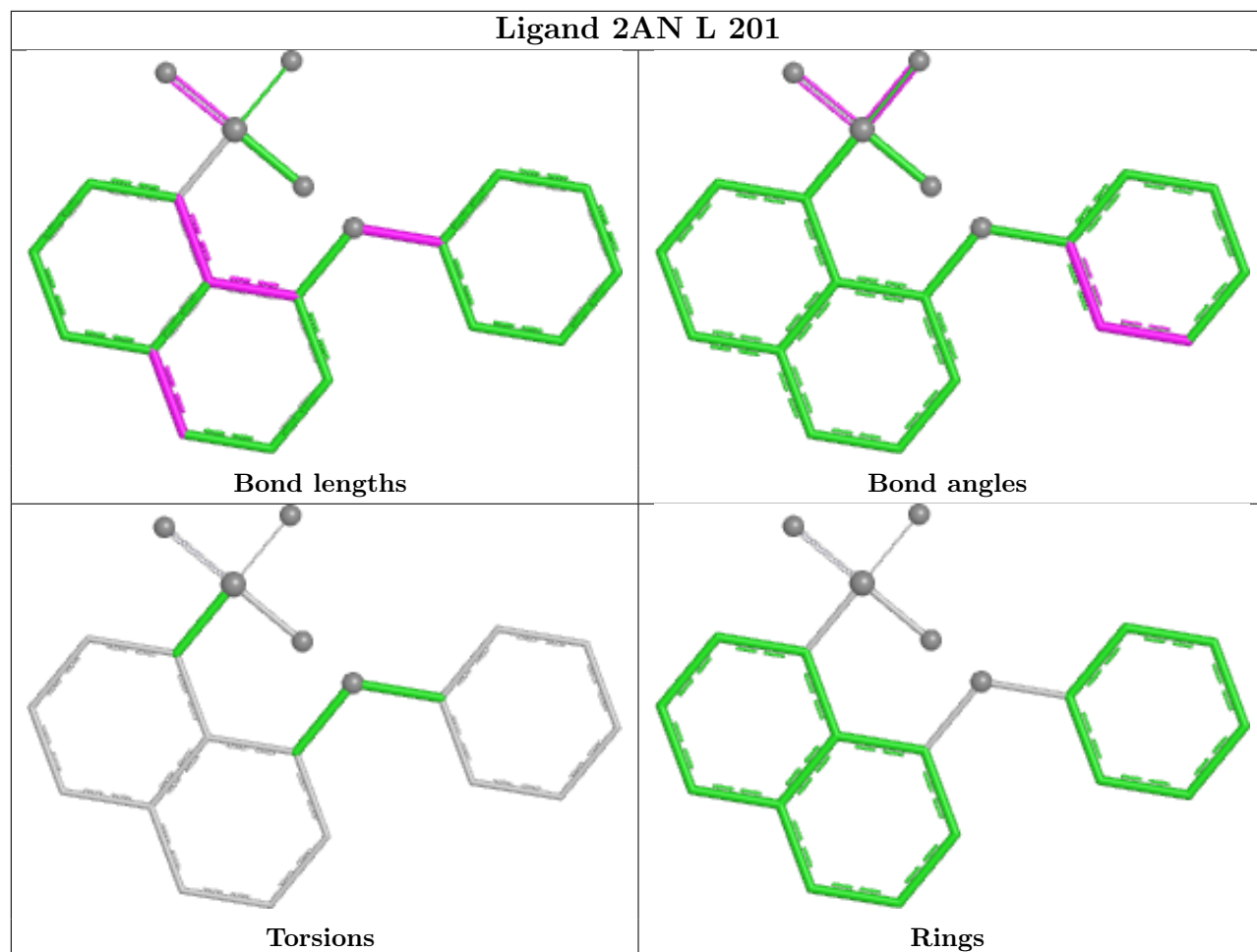
Ligand 2AN I 201



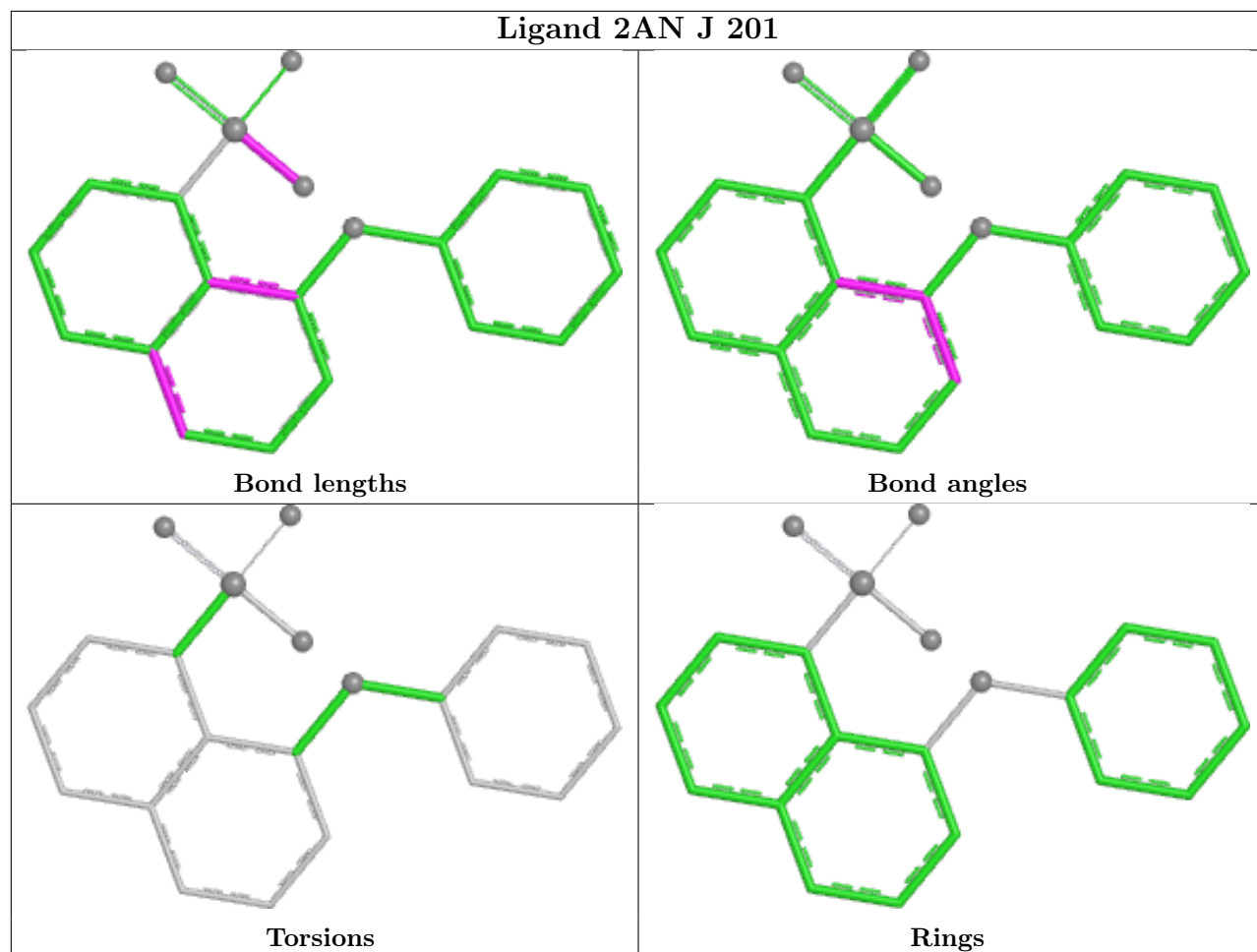




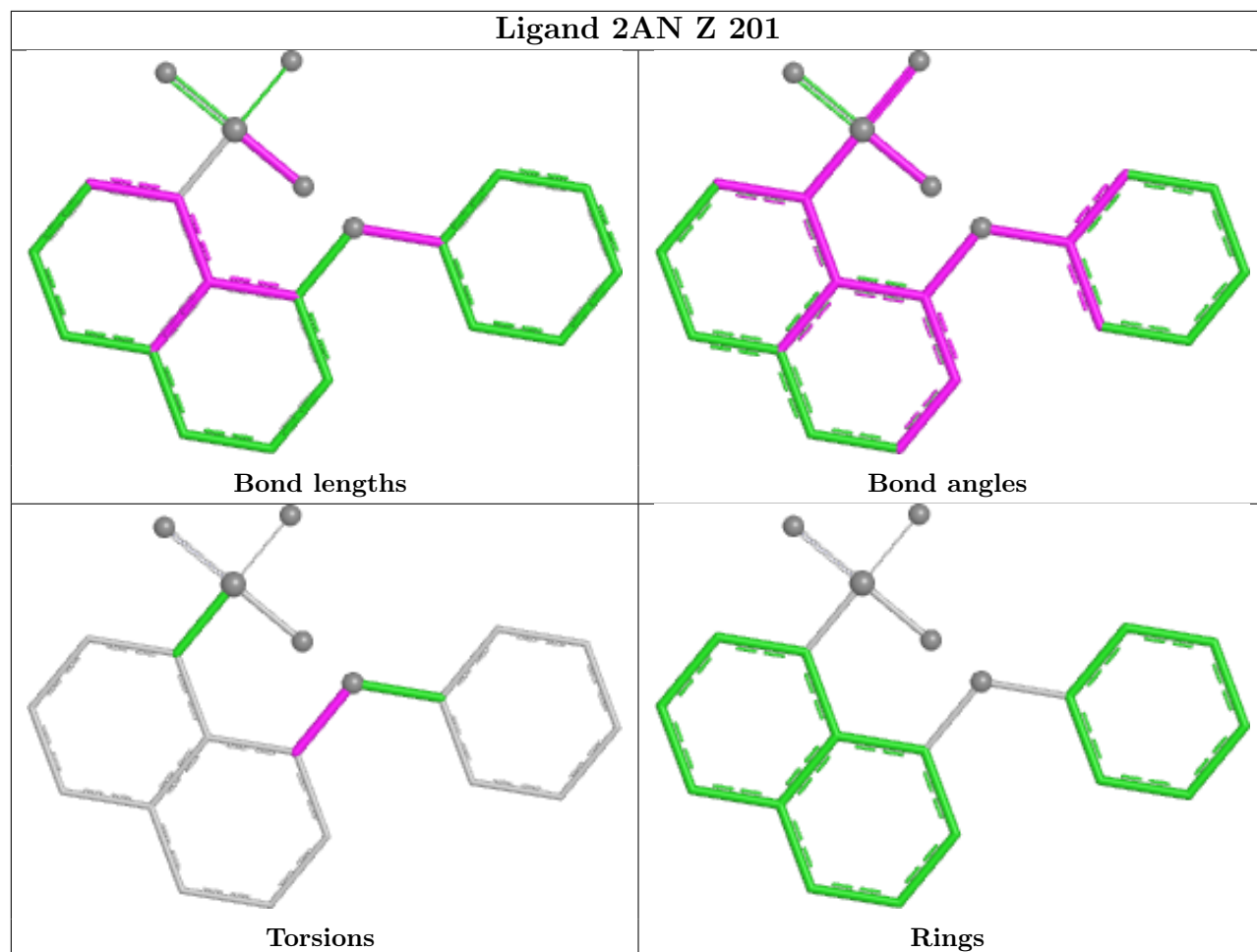
Ligand 2AN L 201



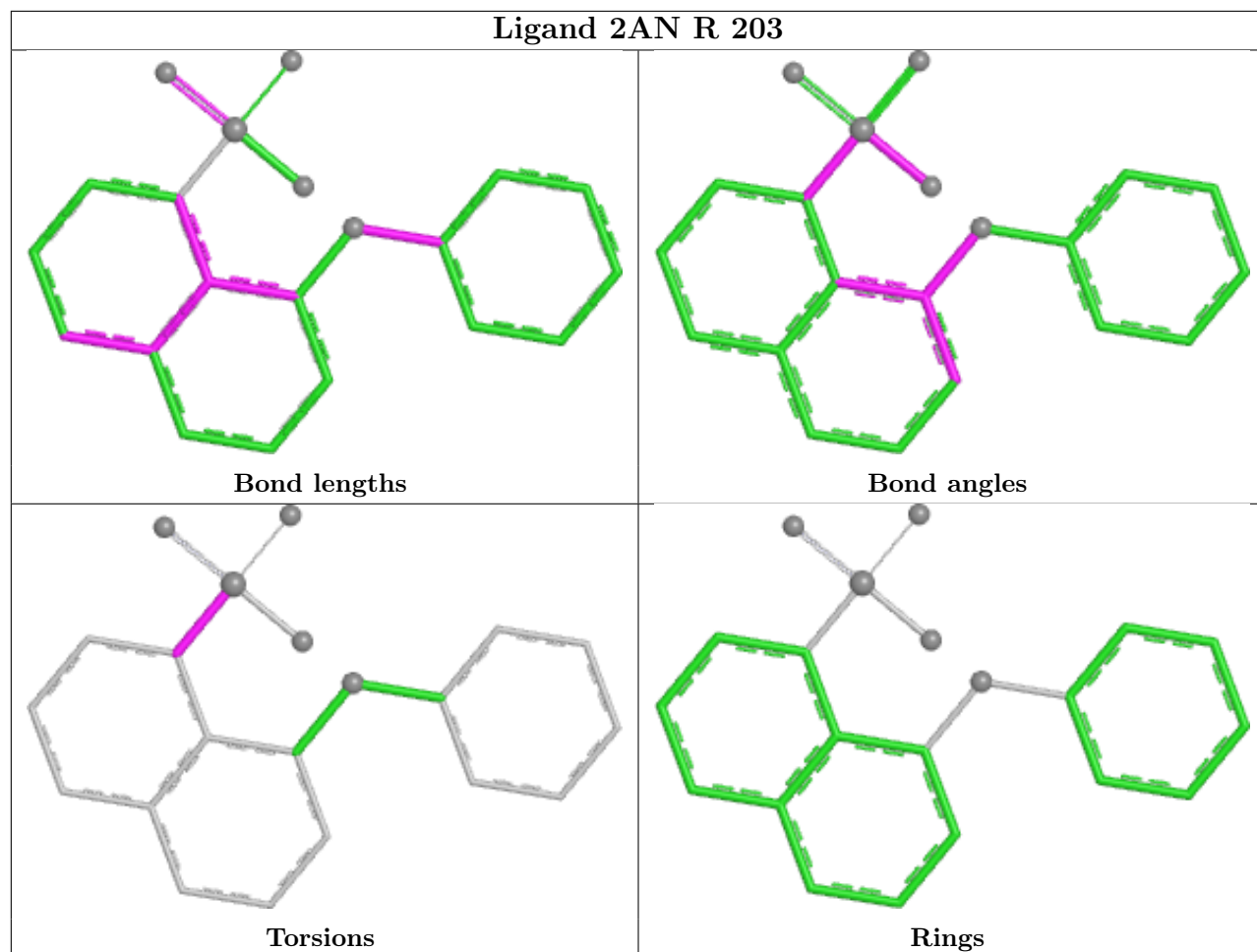
Ligand 2AN J 201

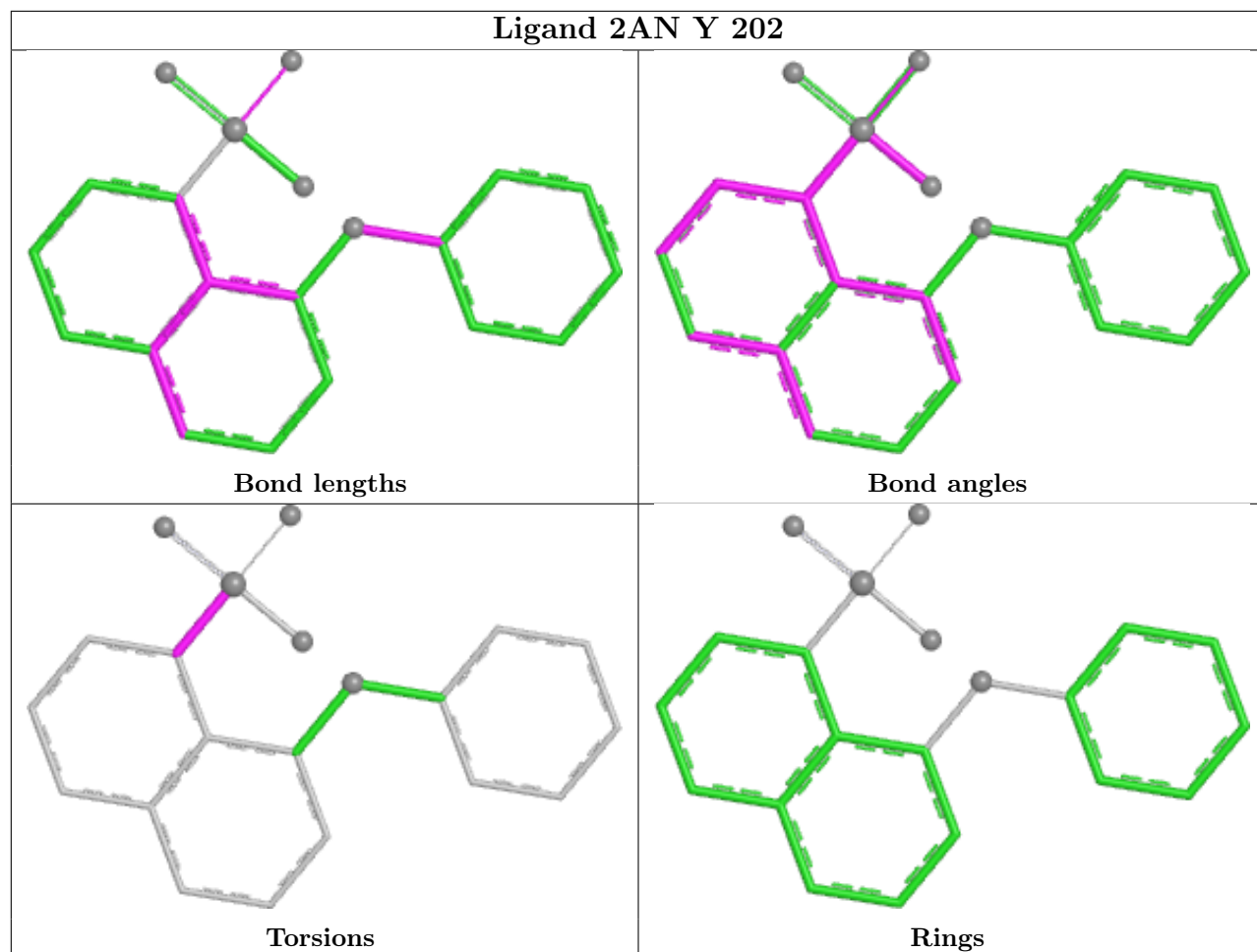


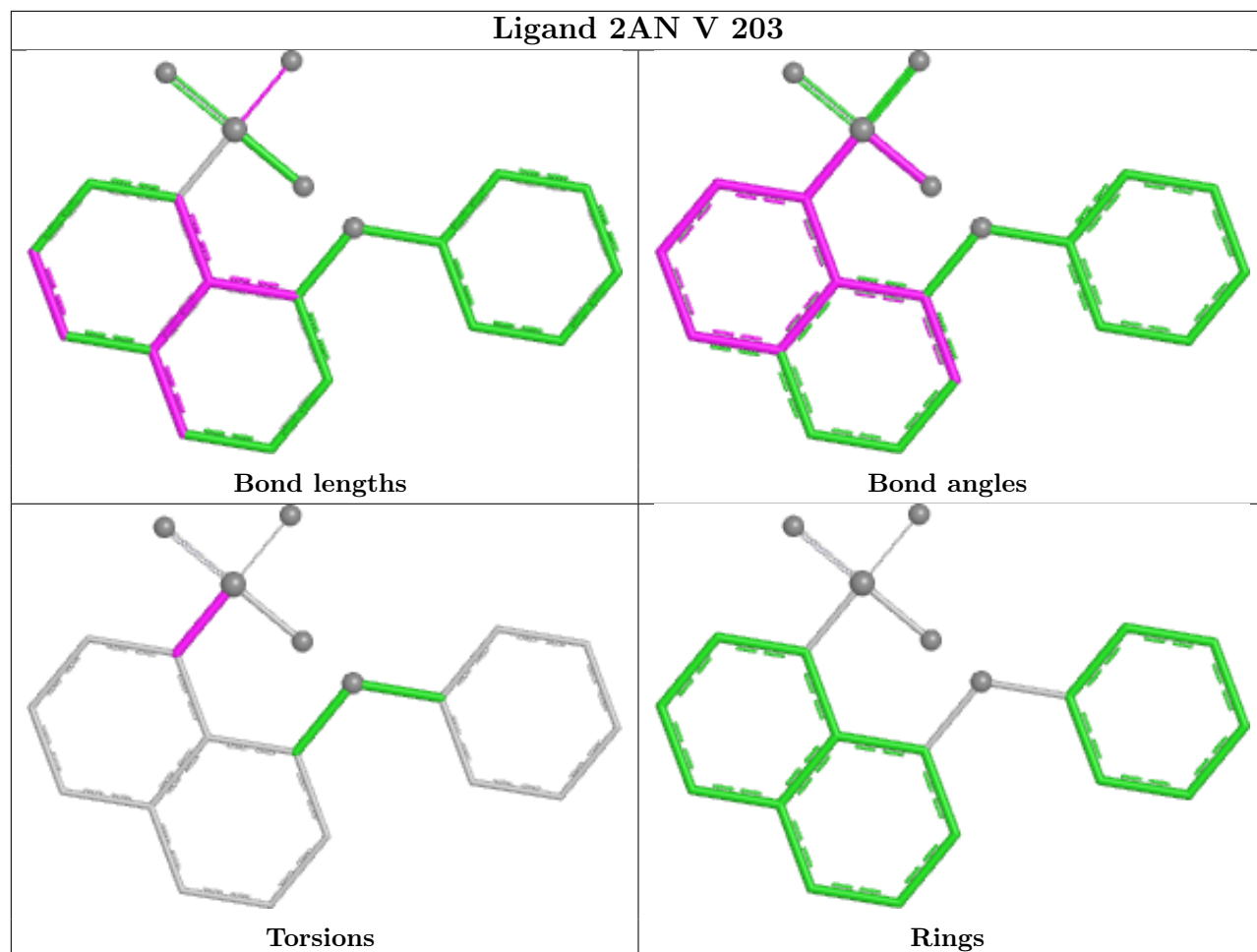
Ligand 2AN Z 201



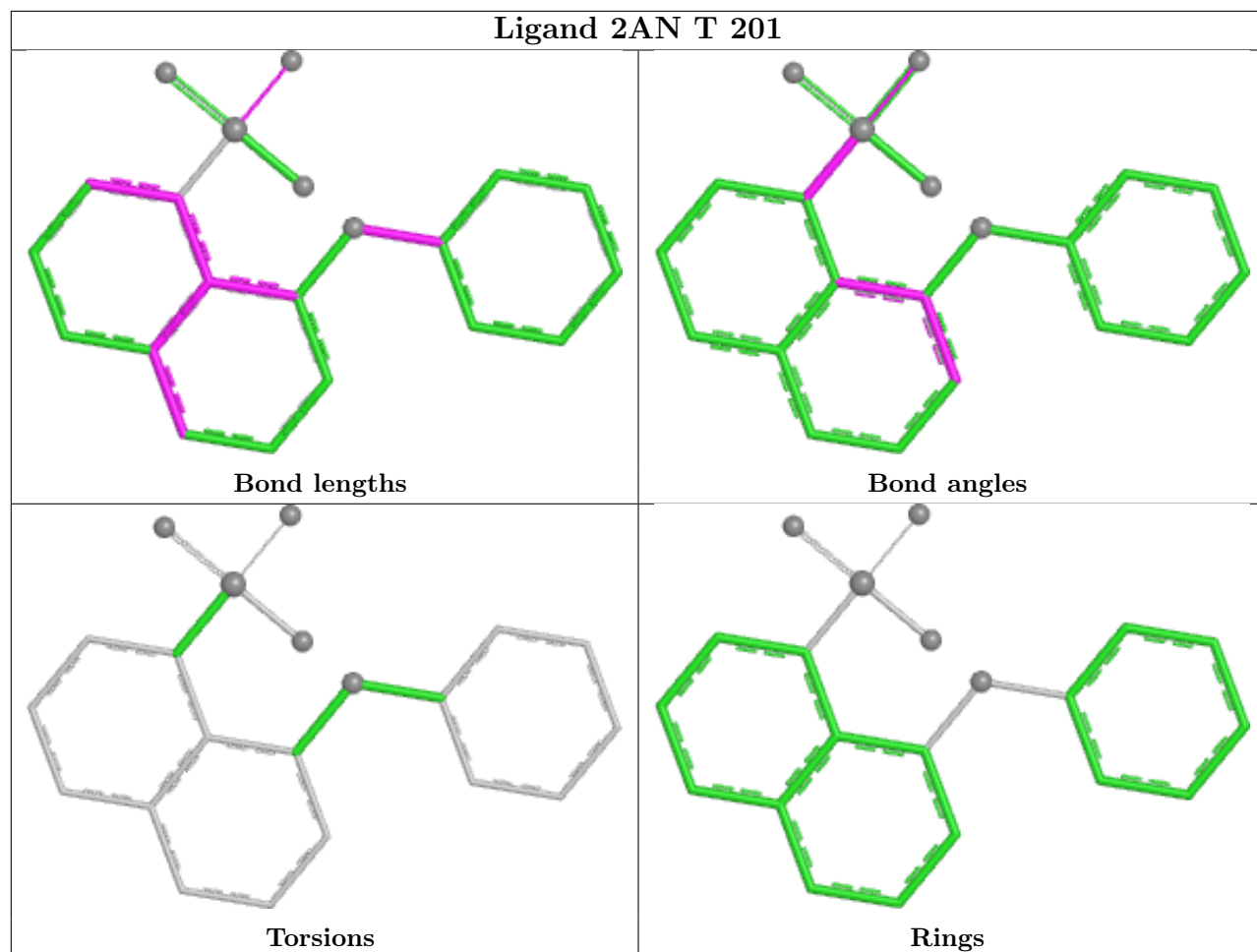
Ligand 2AN R 203



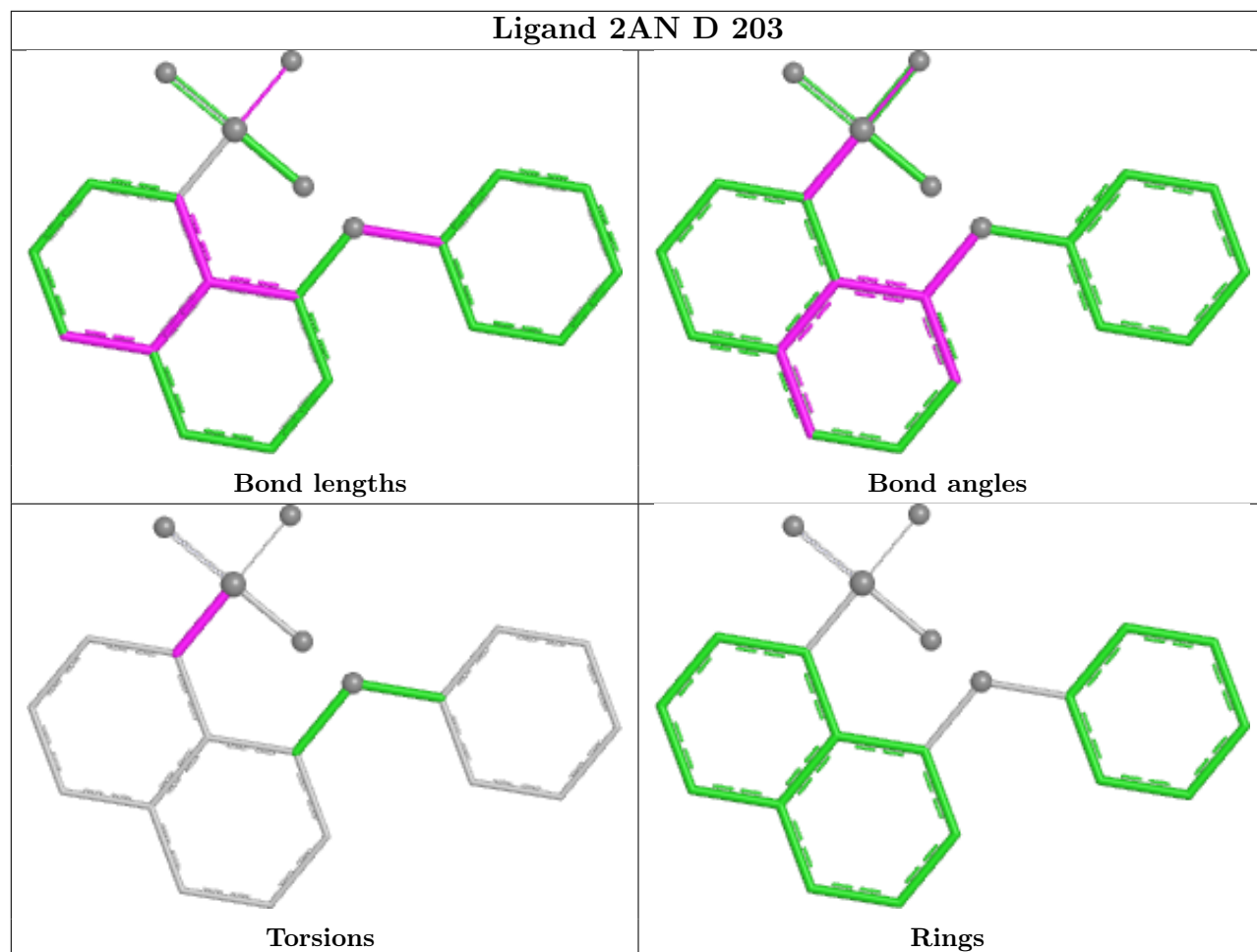




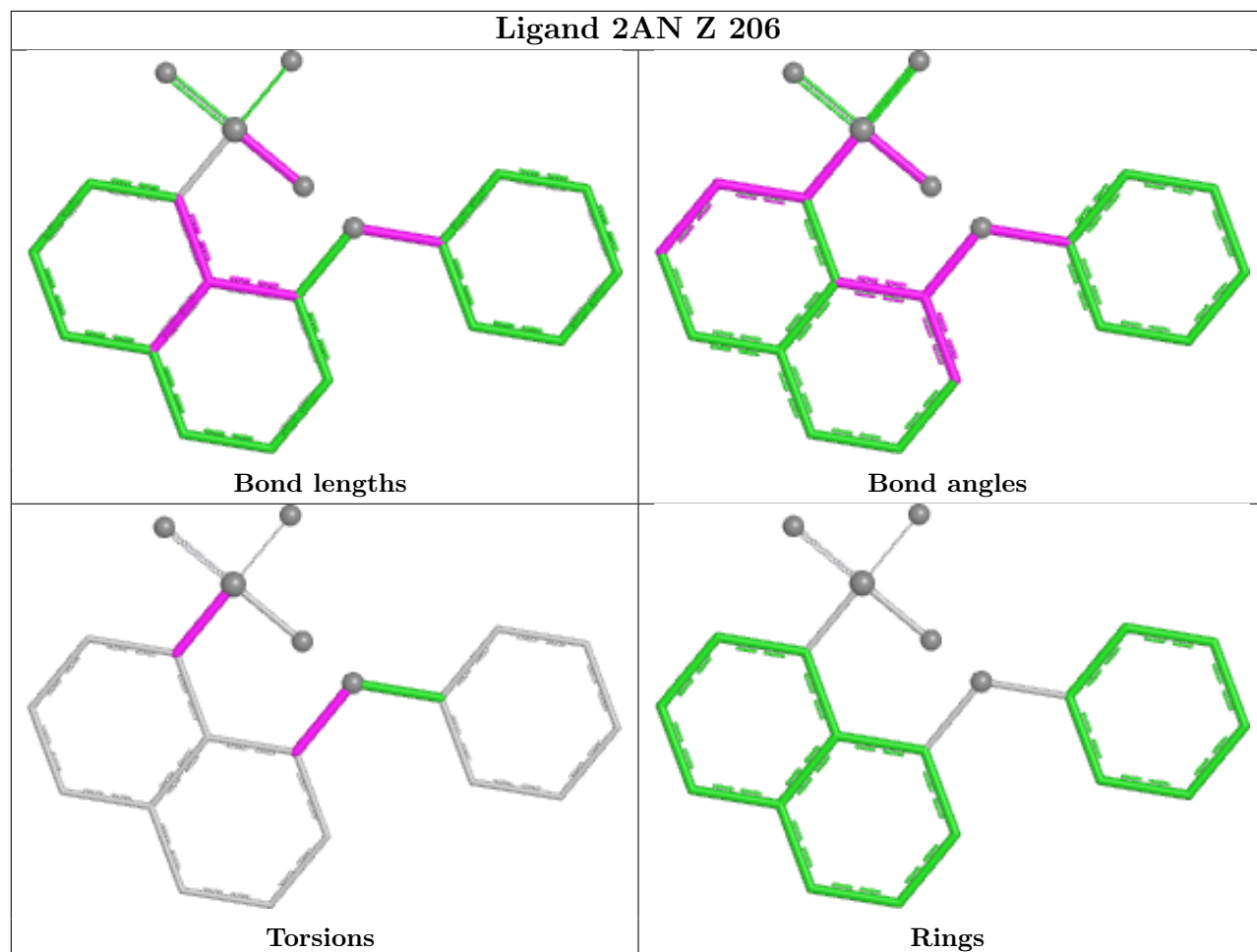
Ligand 2AN T 201



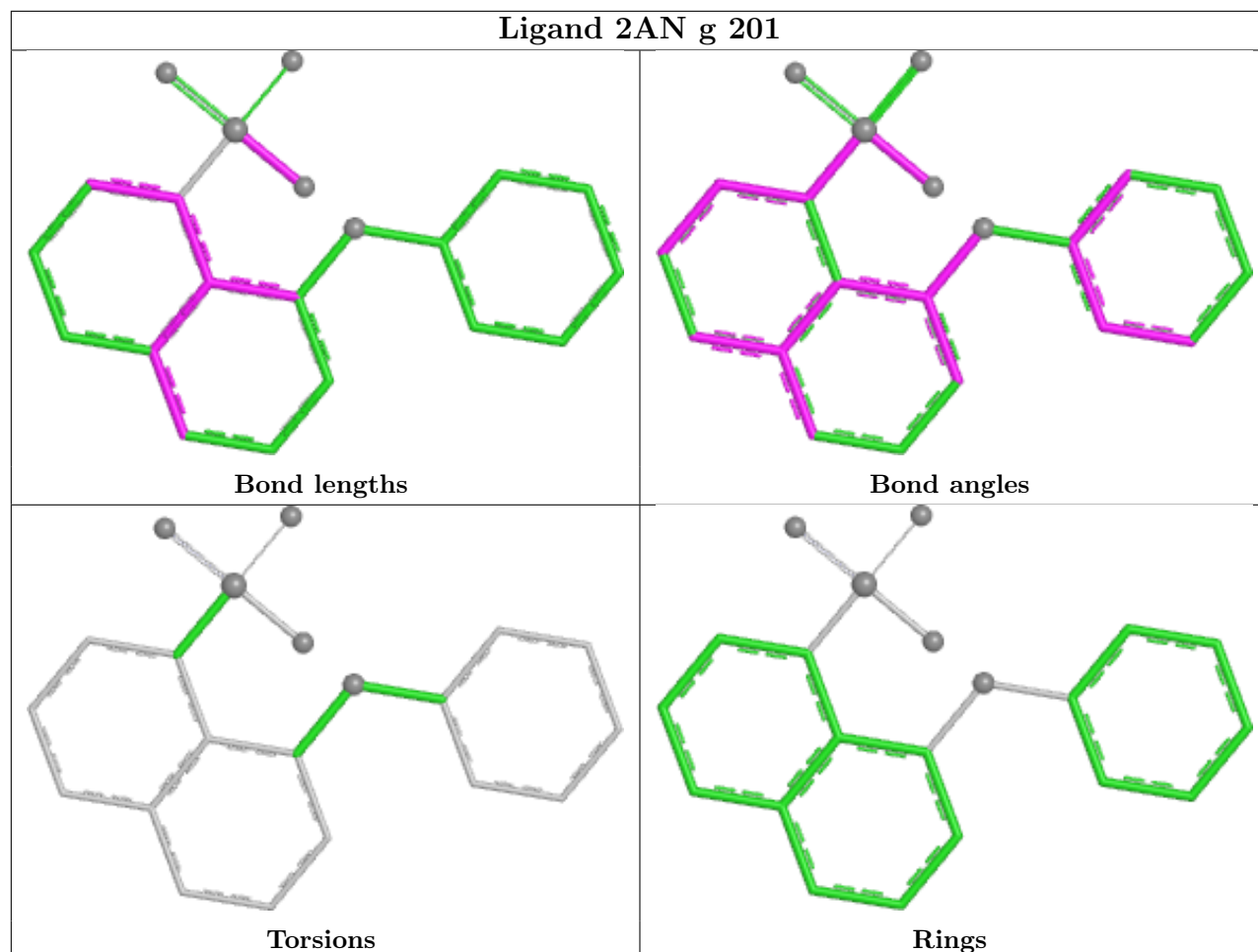
Ligand 2AN D 203



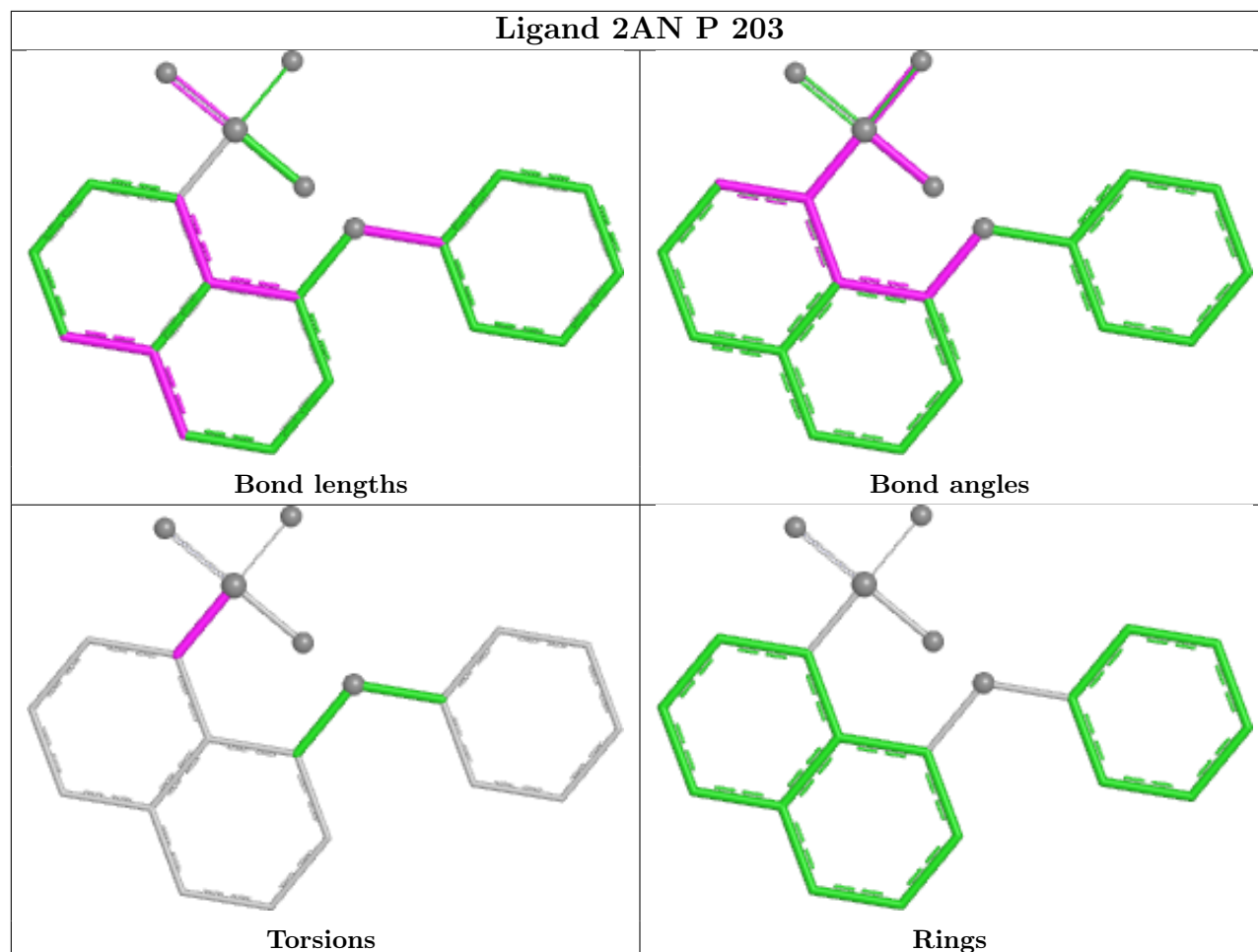
Ligand 2AN Z 206



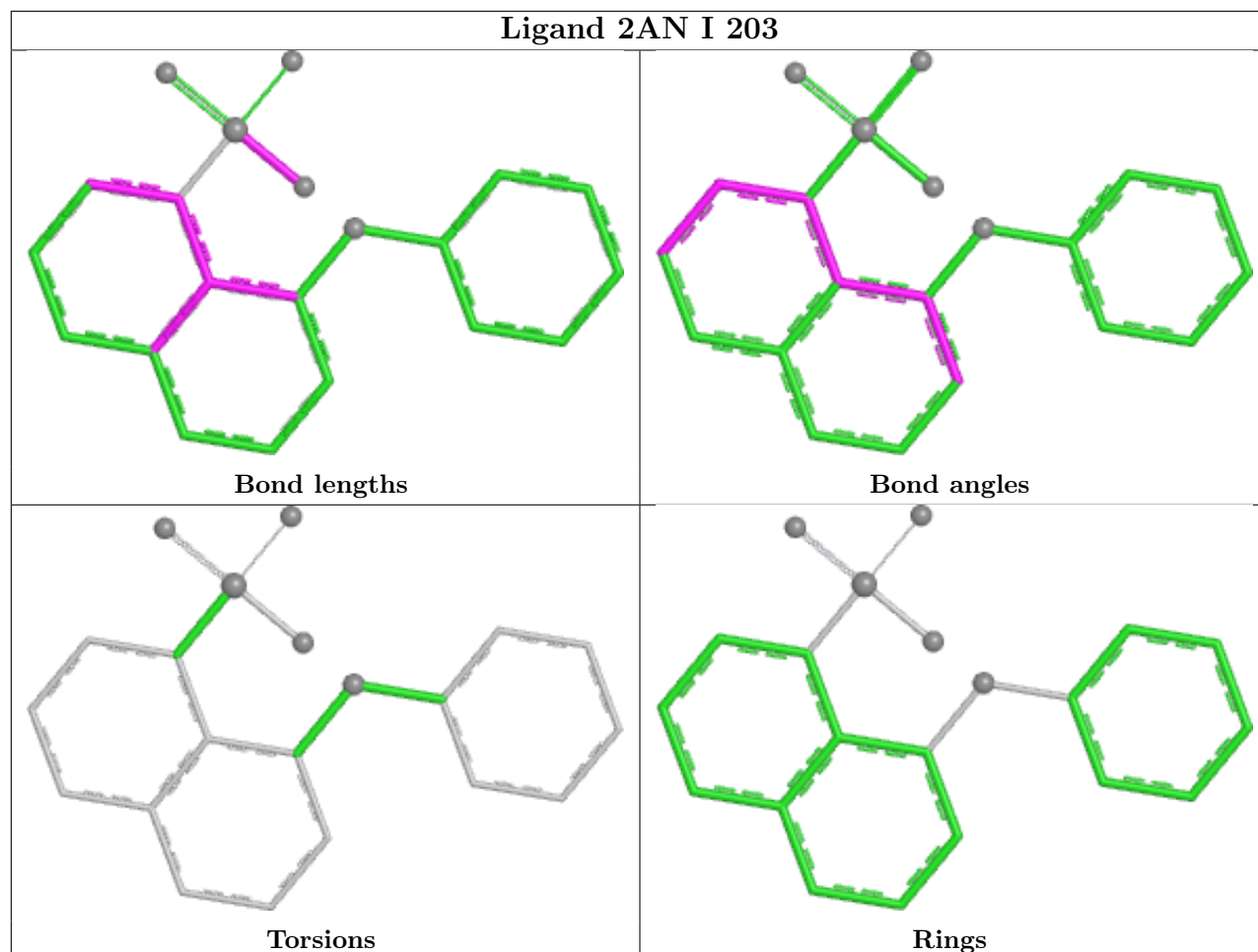
Ligand 2AN g 201

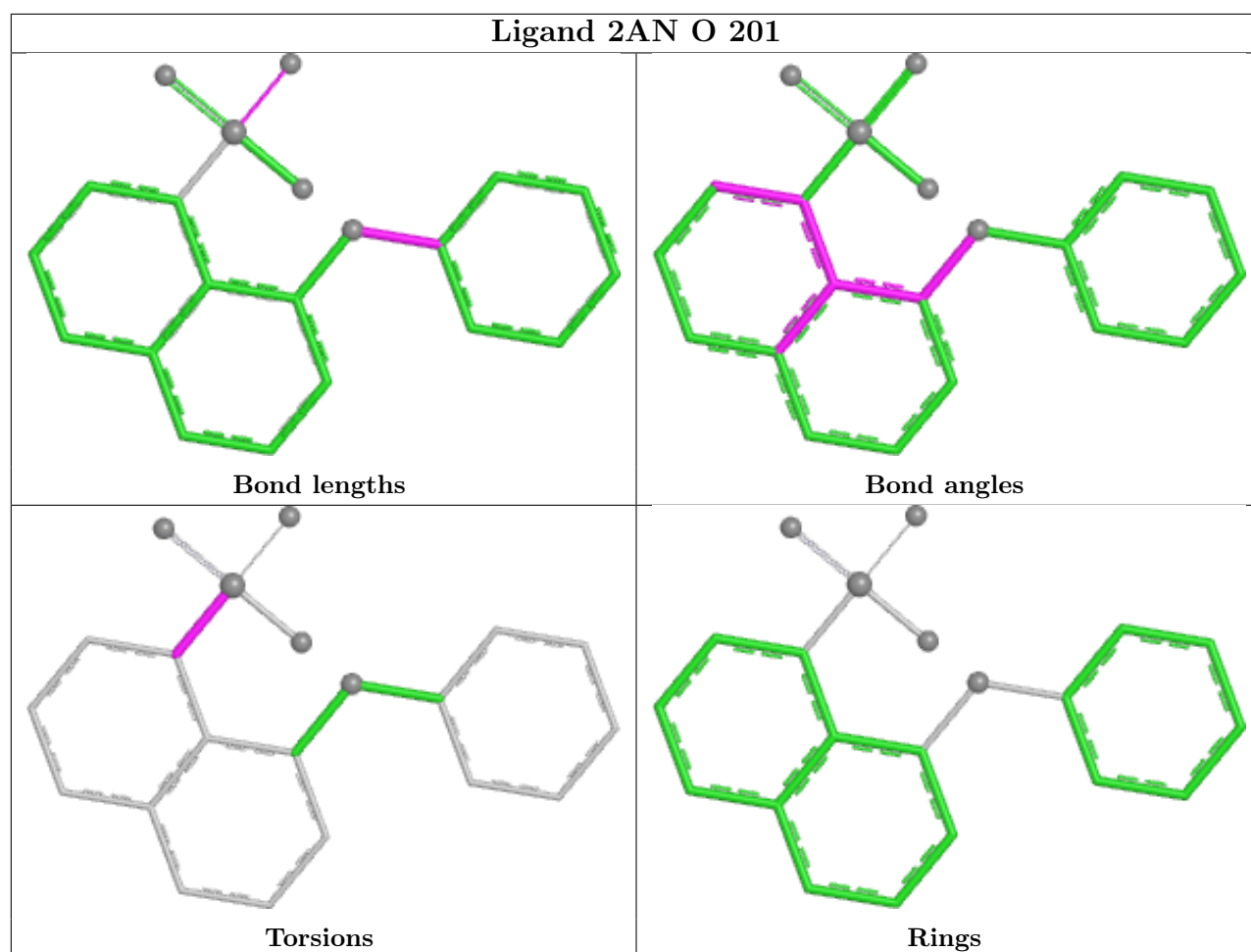


Ligand 2AN P 203



Ligand 2AN I 203





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

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

All (469) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	a	125	GLY	12.7
1	J	-3	ASP	11.4
1	T	128	VAL	10.6
1	H	59	PHE	9.0
1	H	124	PRO	8.0
1	U	128	VAL	8.0
1	A	78	ALA	7.6
1	h	93	ARG	7.2
1	N	-3	ASP	7.2
1	Y	124	PRO	7.0
1	A	47	GLY	7.0
1	U	127	THR	7.0
1	d	126	CYS	6.9
1	W	96	ILE	6.8
1	V	129	ASN	6.7
1	R	95	ASN	6.7
1	d	94	ASP	6.7
1	L	0	THR	6.4
1	W	124	PRO	6.4
1	O	152	ALA	6.3
1	F	124	PRO	6.3

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Mol	Chain	Res	Type	RSRZ
1	d	125	GLY	6.2
1	X	128	VAL	6.2
1	W	62	GLY	6.1
1	V	131	GLU	6.0
1	f	-1	PHE	6.0
1	U	11	GLU	5.9
1	R	60	VAL	5.9
1	B	124	PRO	5.9
1	d	127	THR	5.8
1	F	125	GLY	5.7
1	U	131	GLU	5.6
1	G	87	PHE	5.5
1	Z	2	ALA	5.5
1	W	127	THR	5.3
1	e	125	GLY	5.2
1	U	50	GLY	5.2
1	A	127	THR	5.1
1	D	124	PRO	5.1
1	H	58	THR	5.1
1	C	60	VAL	5.0
1	B	2	ALA	5.0
1	h	125	GLY	5.0
1	A	158	PHE	5.0
1	i	129	ASN	4.9
1	B	123	LYS	4.8
1	O	67	TYR	4.8
1	H	138	LYS	4.8
1	b	-1	PHE	4.7
1	D	45	ILE	4.7
1	B	122	PRO	4.6
1	f	2	ALA	4.5
1	Y	125	GLY	4.5
1	U	10	GLU	4.5
1	T	97	GLU	4.4
1	H	123	LYS	4.4
1	U	51	VAL	4.3
1	A	119	THR	4.3
1	L	123	LYS	4.3
1	D	122	PRO	4.3
1	C	127	THR	4.3
1	X	67	TYR	4.2
1	U	94	ASP	4.2

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Mol	Chain	Res	Type	RSRZ
1	D	53	THR	4.2
1	O	60	VAL	4.2
1	H	57	ILE	4.2
1	c	1	MET	4.2
1	R	61	ASP	4.2
1	R	58	THR	4.2
1	h	126	CYS	4.2
1	O	75	ILE	4.2
1	O	111	GLY	4.2
1	A	2	ALA	4.1
1	V	1	MET	4.1
1	X	87	PHE	4.1
1	f	0	THR	4.1
1	A	125	GLY	4.0
1	b	81	TYR	4.0
1	H	125	GLY	4.0
1	F	10	GLU	3.9
1	V	130	GLU	3.9
1	D	60	VAL	3.9
1	Z	124	PRO	3.9
1	I	126	CYS	3.9
1	D	125	GLY	3.9
1	c	125	GLY	3.9
1	D	74	GLU	3.8
1	A	18	ARG	3.8
1	D	2	ALA	3.8
1	K	4	TYR	3.8
1	O	158	PHE	3.8
1	R	159	ALA	3.8
1	b	52	GLY	3.8
1	F	47	GLY	3.8
1	U	126	CYS	3.7
1	A	124	PRO	3.7
1	D	4	TYR	3.7
1	M	131	GLU	3.7
1	Y	96	ILE	3.7
1	C	129	ASN	3.7
1	h	127	THR	3.7
1	P	122	PRO	3.7
1	D	153	ALA	3.6
1	D	62	GLY	3.6
1	F	111	GLY	3.6

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Mol	Chain	Res	Type	RSRZ
1	U	124	PRO	3.6
1	E	95	ASN	3.6
1	i	51	VAL	3.6
1	R	74	GLU	3.6
1	a	124	PRO	3.6
1	f	81	TYR	3.6
1	A	107	ALA	3.5
1	X	94	ASP	3.5
1	Q	126	CYS	3.5
1	L	125	GLY	3.5
1	U	159	ALA	3.5
1	D	46	GLU	3.5
1	G	127	THR	3.5
1	e	51	VAL	3.5
1	a	128	VAL	3.5
1	Z	15	ALA	3.5
1	d	143	PHE	3.4
1	b	24	VAL	3.4
1	f	132	GLU	3.4
1	b	62	GLY	3.4
1	U	92	LEU	3.4
1	Z	126	CYS	3.4
1	A	4	TYR	3.3
1	F	127	THR	3.3
1	A	140	ALA	3.3
1	F	123	LYS	3.3
1	Z	23	LEU	3.3
1	U	45	ILE	3.3
1	A	81	TYR	3.3
1	Z	67	TYR	3.3
1	J	157	VAL	3.3
1	F	101	TYR	3.3
1	h	17	HIS	3.3
1	C	131	GLU	3.3
1	e	75	ILE	3.3
1	d	58	THR	3.2
1	X	52	GLY	3.2
1	W	72	PHE	3.2
1	W	128	VAL	3.2
1	O	125	GLY	3.2
1	b	50	GLY	3.2
1	b	131	GLU	3.2

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Mol	Chain	Res	Type	RSRZ
1	X	139	LYS	3.2
1	Z	69	LEU	3.2
1	U	129	ASN	3.2
1	b	128	VAL	3.2
1	C	126	CYS	3.2
1	R	124	PRO	3.2
1	O	3	ALA	3.2
1	F	126	CYS	3.1
1	N	125	GLY	3.1
1	J	120	TYR	3.1
1	N	140	ALA	3.1
1	F	50	GLY	3.1
1	X	125	GLY	3.1
1	H	0	THR	3.1
1	A	87	PHE	3.1
1	K	143	PHE	3.1
1	Z	3	ALA	3.1
1	d	42	GLY	3.1
1	a	92	LEU	3.1
1	A	96	ILE	3.1
1	N	39	PHE	3.1
1	Q	131	GLU	3.1
1	O	42	GLY	3.1
1	J	143	PHE	3.1
1	F	81	TYR	3.1
1	D	1	MET	3.1
1	W	61	ASP	3.0
1	F	58	THR	3.0
1	Y	127	THR	3.0
1	F	60	VAL	3.0
1	O	74	GLU	3.0
1	d	60	VAL	3.0
1	d	133	VAL	3.0
1	J	124	PRO	3.0
1	O	12	SER	3.0
1	K	136	GLY	3.0
1	H	126	CYS	3.0
1	Z	1	MET	3.0
1	O	108	VAL	3.0
1	A	3	ALA	2.9
1	O	94	ASP	2.9
1	O	62	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
1	X	127	THR	2.9
1	U	106	GLU	2.9
1	G	1	MET	2.9
1	G	51	VAL	2.9
1	C	91	VAL	2.9
1	b	94	ASP	2.9
1	Z	89	GLY	2.9
1	f	1	MET	2.9
1	A	75	ILE	2.9
1	Y	123	LYS	2.9
1	W	60	VAL	2.9
1	R	96	ILE	2.8
1	X	45	ILE	2.8
1	d	128	VAL	2.8
1	G	121	HIS	2.8
1	F	63	HIS	2.8
1	Z	41	SER	2.8
1	i	159	ALA	2.8
1	Z	94	ASP	2.8
1	C	67	TYR	2.8
1	X	81	TYR	2.8
1	W	2	ALA	2.8
1	W	94	ASP	2.8
1	S	94	ASP	2.8
1	X	60	VAL	2.8
1	O	109	GLY	2.8
1	d	4	TYR	2.8
1	U	60	VAL	2.7
1	i	108	VAL	2.7
1	F	67	TYR	2.7
1	Y	61	ASP	2.7
1	L	124	PRO	2.7
1	W	5	THR	2.7
1	A	76	ASP	2.7
1	c	140	ALA	2.7
1	U	59	PHE	2.7
1	d	139	LYS	2.7
1	j	131	GLU	2.7
1	R	125	GLY	2.7
1	P	123	LYS	2.7
1	d	131	GLU	2.7
1	G	140	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	M	94	ASP	2.7
1	F	78	ALA	2.7
1	B	1	MET	2.7
1	P	126	CYS	2.7
1	N	40	LYS	2.7
1	W	146	GLN	2.7
1	O	110	GLY	2.7
1	A	120	TYR	2.7
1	C	62	GLY	2.7
1	a	75	ILE	2.6
1	U	75	ILE	2.6
1	W	92	LEU	2.6
1	W	125	GLY	2.6
1	g	90	ASP	2.6
1	O	124	PRO	2.6
1	A	123	LYS	2.6
1	Y	23	LEU	2.6
1	U	29	GLN	2.6
1	d	142	GLU	2.6
1	Z	93	ARG	2.6
1	W	117	THR	2.6
1	J	67	TYR	2.6
1	a	67	TYR	2.6
1	P	125	GLY	2.6
1	J	140	ALA	2.6
1	G	52	GLY	2.6
1	b	2	ALA	2.6
1	U	125	GLY	2.6
1	U	79	ASN	2.6
1	i	79	ASN	2.6
1	A	106	GLU	2.6
1	W	122	PRO	2.6
1	H	54	VAL	2.6
1	Z	12	SER	2.5
1	S	0	THR	2.5
1	e	24	VAL	2.5
1	P	84	TYR	2.5
1	F	144	TYR	2.5
1	a	101	TYR	2.5
1	V	127	THR	2.5
1	A	88	GLU	2.5
1	I	23	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	d	136	GLY	2.5
1	Y	24	VAL	2.5
1	T	127	THR	2.5
1	G	73	ASP	2.5
1	Y	47	GLY	2.5
1	Y	65	LEU	2.5
1	X	143	PHE	2.5
1	P	140	ALA	2.5
1	b	123	LYS	2.5
1	B	58	THR	2.5
1	F	57	ILE	2.5
1	g	129	ASN	2.5
1	E	133	VAL	2.5
1	d	157	VAL	2.5
1	a	132	GLU	2.5
1	d	96	ILE	2.5
1	Z	125	GLY	2.5
1	S	95	ASN	2.5
1	Z	31	LEU	2.5
1	H	27	ARG	2.5
1	H	122	PRO	2.5
1	V	101	TYR	2.5
1	W	95	ASN	2.5
1	d	41	SER	2.4
1	R	59	PHE	2.4
1	M	40	LYS	2.4
1	N	60	VAL	2.4
1	G	80	PHE	2.4
1	E	24	VAL	2.4
1	U	77	ALA	2.4
1	U	78	ALA	2.4
1	U	133	VAL	2.4
1	X	66	THR	2.4
1	d	23	LEU	2.4
1	g	78	ALA	2.4
1	A	133	VAL	2.4
1	J	122	PRO	2.4
1	T	125	GLY	2.4
1	C	61	ASP	2.4
1	V	23	LEU	2.4
1	A	74	GLU	2.4
1	D	61	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	N	123	LYS	2.4
1	Q	4	TYR	2.4
1	E	25	LEU	2.4
1	B	125	GLY	2.4
1	C	152	ALA	2.4
1	d	62	GLY	2.4
1	J	72	PHE	2.4
1	C	24	VAL	2.4
1	Q	88	GLU	2.4
1	i	148	GLU	2.4
1	B	120	TYR	2.4
1	D	101	TYR	2.4
1	S	141	TYR	2.4
1	X	124	PRO	2.4
1	Q	127	THR	2.4
1	a	126	CYS	2.4
1	O	27	ARG	2.3
1	D	48	ASP	2.3
1	Z	61	ASP	2.3
1	A	6	ILE	2.3
1	G	125	GLY	2.3
1	a	84	TYR	2.3
1	Z	101	TYR	2.3
1	O	11	GLU	2.3
1	F	159	ALA	2.3
1	d	152	ALA	2.3
1	W	26	GLU	2.3
1	Q	101	TYR	2.3
1	D	84	TYR	2.3
1	E	159	ALA	2.3
1	i	24	VAL	2.3
1	F	45	ILE	2.3
1	O	4	TYR	2.3
1	L	84	TYR	2.3
1	Z	73	ASP	2.3
1	Y	94	ASP	2.3
1	g	43	GLU	2.3
1	B	127	THR	2.3
1	h	23	LEU	2.3
1	A	1	MET	2.3
1	N	71	LYS	2.3
1	J	125	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	H	62	GLY	2.3
1	P	124	PRO	2.3
1	d	129	ASN	2.3
1	a	123	LYS	2.3
1	h	140	ALA	2.3
1	F	23	LEU	2.3
1	X	62	GLY	2.3
1	A	131	GLU	2.3
1	I	-1	PHE	2.3
1	Y	131	GLU	2.2
1	O	101	TYR	2.2
1	F	120	TYR	2.2
1	a	73	ASP	2.2
1	d	27	ARG	2.2
1	F	49	GLY	2.2
1	W	53	THR	2.2
1	X	97	GLU	2.2
1	J	110	GLY	2.2
1	Z	127	THR	2.2
1	W	75	ILE	2.2
1	g	61	ASP	2.2
1	A	67	TYR	2.2
1	M	142	GLU	2.2
1	H	132	GLU	2.2
1	D	130	GLU	2.2
1	F	27	ARG	2.2
1	H	91	VAL	2.2
1	f	24	VAL	2.2
1	O	159	ALA	2.2
1	C	96	ILE	2.2
1	b	0	THR	2.2
1	W	154	ASN	2.2
1	Z	146	GLN	2.2
1	R	129	ASN	2.2
1	Y	97	GLU	2.2
1	B	29	GLN	2.2
1	R	127	THR	2.2
1	L	140	ALA	2.2
1	E	117	THR	2.2
1	T	17	HIS	2.2
1	A	44	ILE	2.2
1	E	123	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	V	122	PRO	2.2
1	G	24	VAL	2.2
1	O	143	PHE	2.2
1	U	158	PHE	2.2
1	S	129	ASN	2.2
1	C	101	TYR	2.1
1	b	54	VAL	2.1
1	U	96	ILE	2.1
1	F	61	ASP	2.1
1	F	86	LEU	2.1
1	C	154	ASN	2.1
1	h	110	GLY	2.1
1	H	63	HIS	2.1
1	Z	9	GLU	2.1
1	U	24	VAL	2.1
1	A	159	ALA	2.1
1	I	140	ALA	2.1
1	D	59	PHE	2.1
1	a	87	PHE	2.1
1	g	159	ALA	2.1
1	Z	44	ILE	2.1
1	F	112	SER	2.1
1	d	64	PRO	2.1
1	d	92	LEU	2.1
1	Y	25	LEU	2.1
1	j	122	PRO	2.1
1	S	1	MET	2.1
1	L	22	ALA	2.1
1	G	60	VAL	2.1
1	W	139	LYS	2.1
1	i	60	VAL	2.1
1	C	-1	PHE	2.1
1	i	140	ALA	2.1
1	g	140	ALA	2.1
1	P	23	LEU	2.1
1	N	-2	PRO	2.1
1	M	23	LEU	2.1
1	W	97	GLU	2.1
1	D	123	LYS	2.1
1	S	123	LYS	2.1
1	S	24	VAL	2.1
1	Y	27	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	U	49	GLY	2.1
1	U	73	ASP	2.1
1	E	127	THR	2.1
1	O	157	VAL	2.1
1	c	84	TYR	2.1
1	T	4	TYR	2.1
1	D	27	ARG	2.1
1	H	2	ALA	2.1
1	I	24	VAL	2.1
1	G	47	GLY	2.1
1	Z	32	VAL	2.1
1	V	24	VAL	2.1
1	M	124	PRO	2.1
1	j	139	LYS	2.0
1	N	59	PHE	2.0
1	F	76	ASP	2.0
1	R	69	LEU	2.0
1	g	92	LEU	2.0
1	X	140	ALA	2.0
1	R	122	PRO	2.0
1	b	93	ARG	2.0
1	a	122	PRO	2.0
1	Y	87	PHE	2.0
1	O	126	CYS	2.0
1	G	74	GLU	2.0
1	L	1	MET	2.0
1	F	29	GLN	2.0
1	Y	85	THR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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

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

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

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

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

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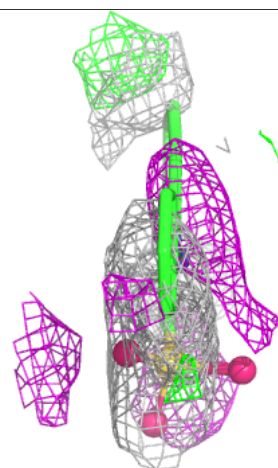
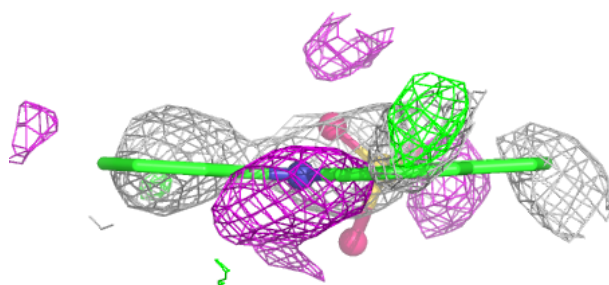
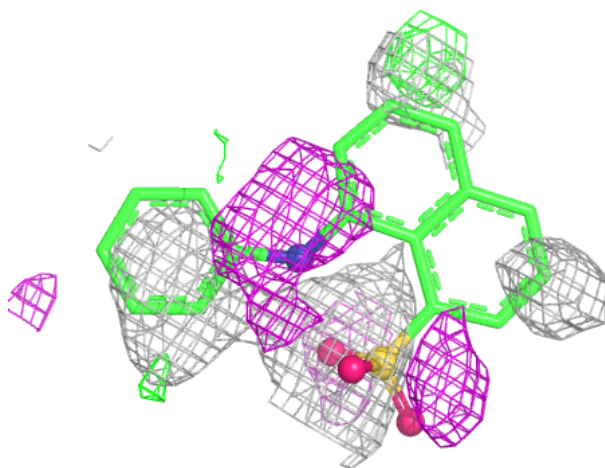
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	2AN	L	203	21/21	0.96	0.18	33,53,64,65	0
2	2AN	c	201	21/21	0.97	0.15	35,45,58,59	0
2	2AN	N	202	21/21	0.97	0.19	37,52,61,64	0
2	2AN	P	202	21/21	0.97	0.21	29,43,52,57	0
2	2AN	L	201	21/21	0.97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

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

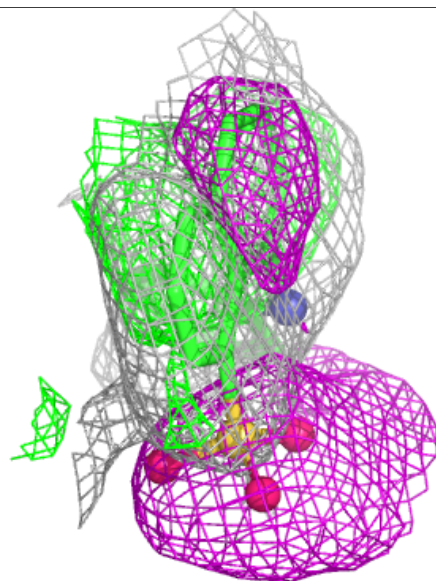
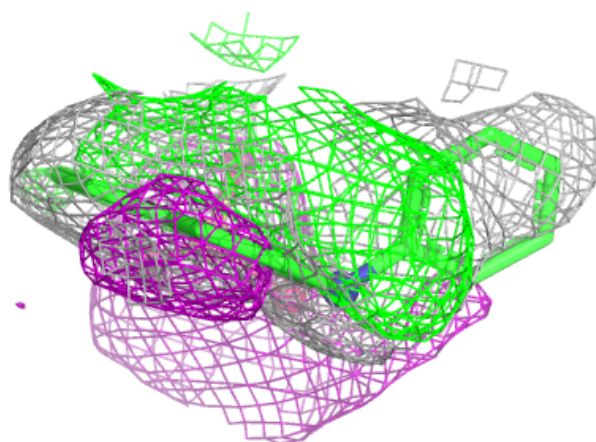
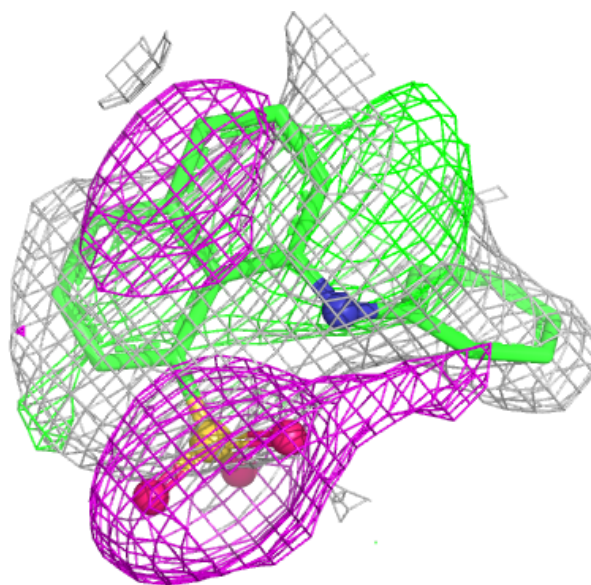
Electron density around 2AN h 205:

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



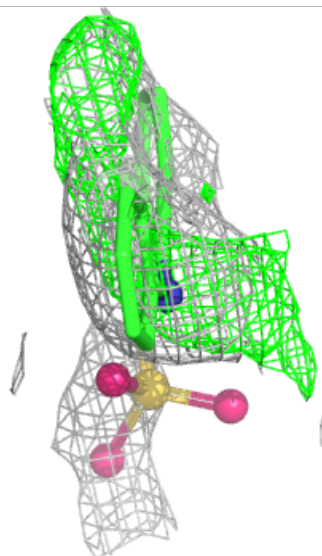
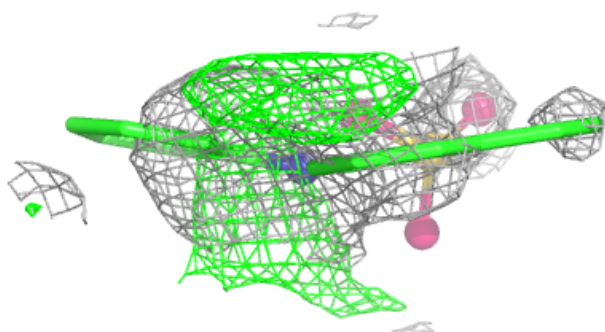
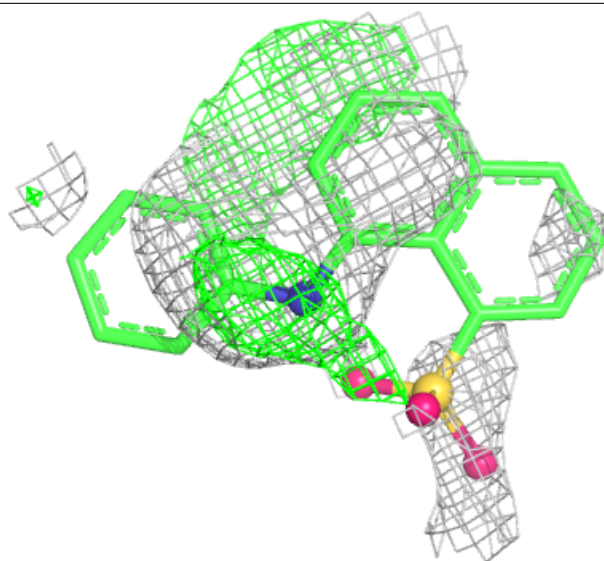
Electron density around 2AN N 203:

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



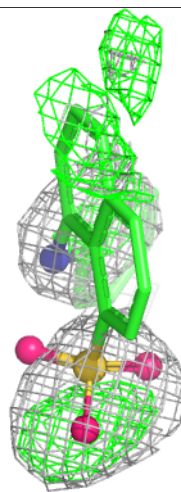
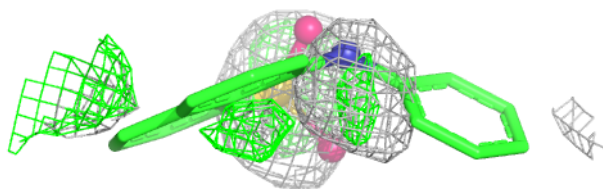
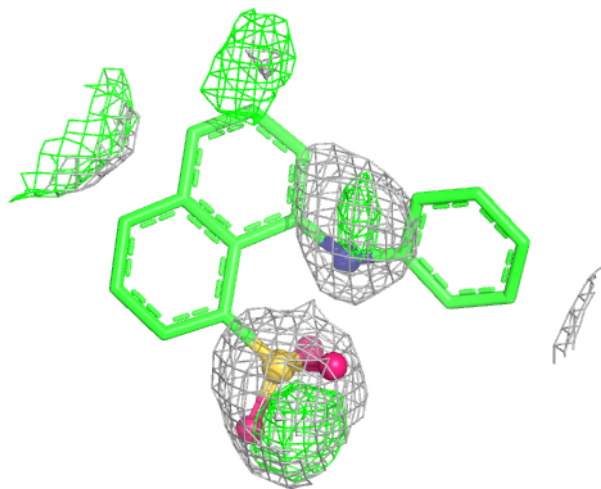
Electron density around 2AN U 202:

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



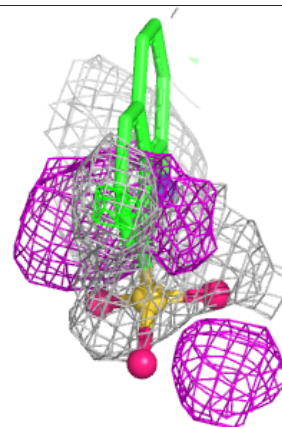
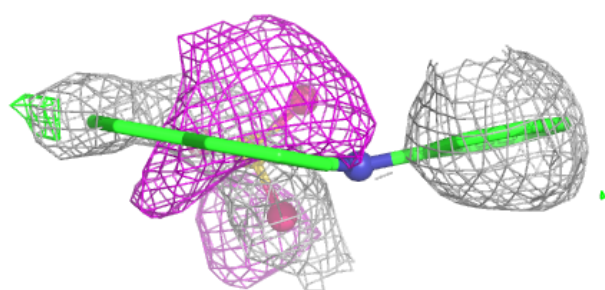
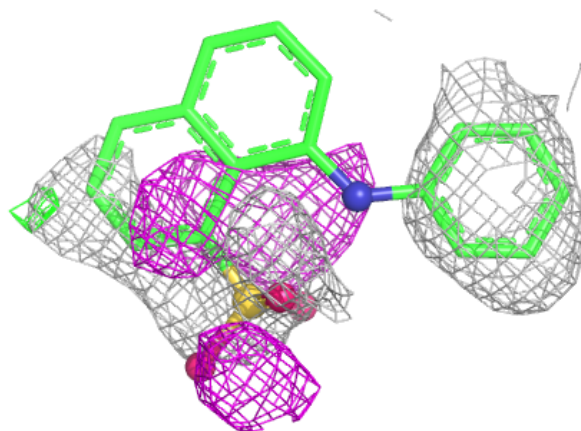
Electron density around 2AN A 204:

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



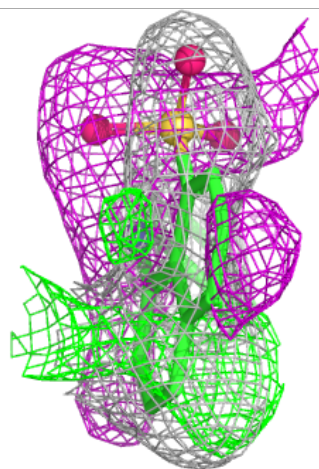
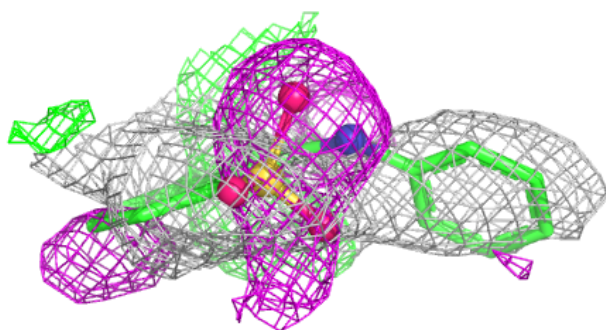
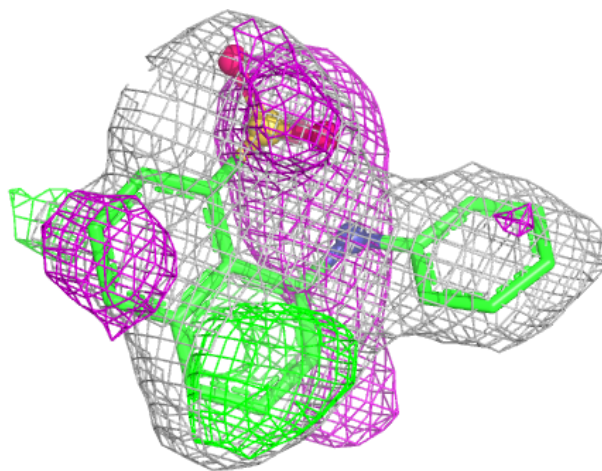
Electron density around 2AN j 207:

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



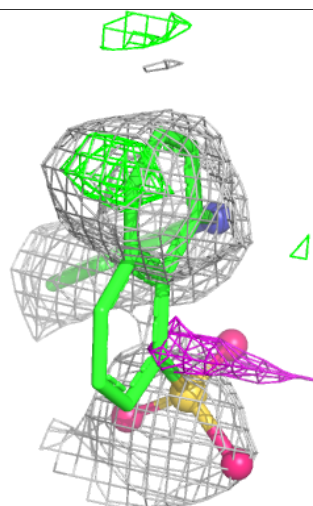
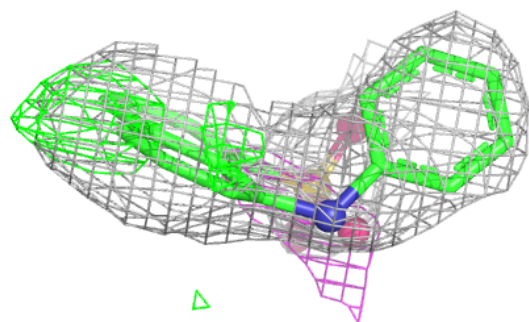
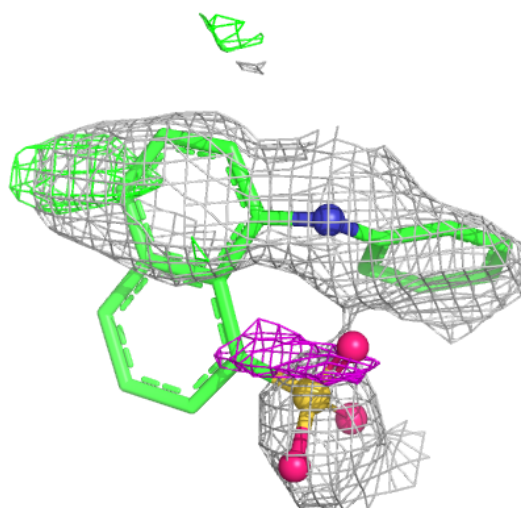
Electron density around 2AN f 203:

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



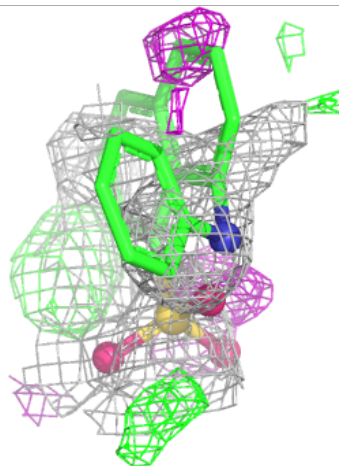
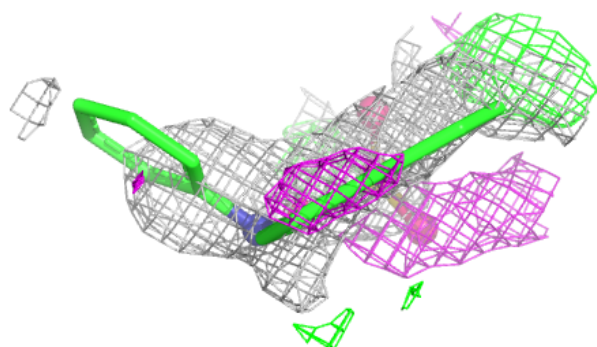
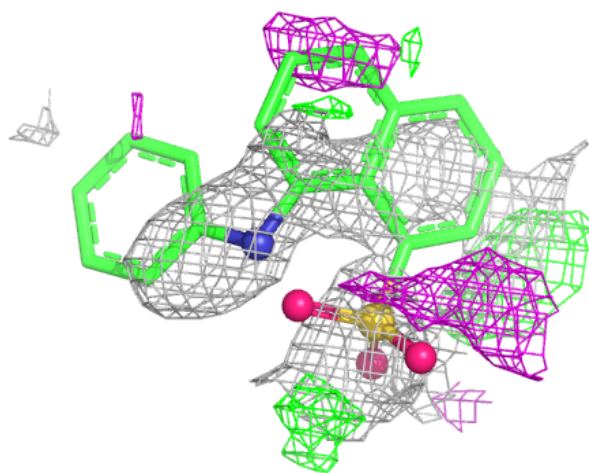
Electron density around 2AN b 206:

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



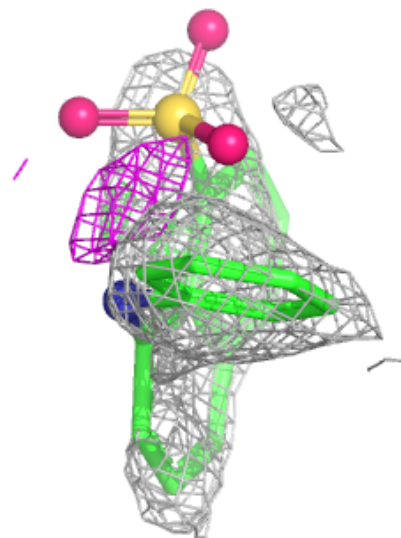
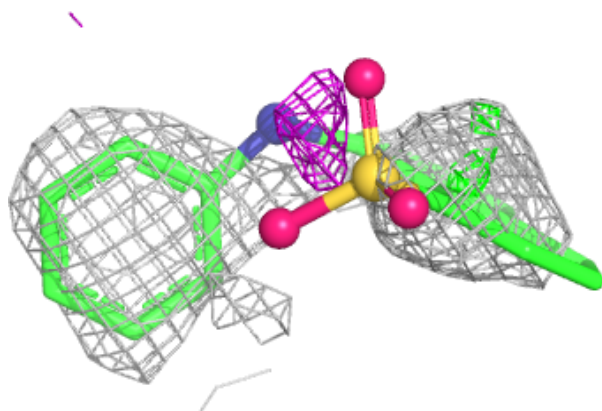
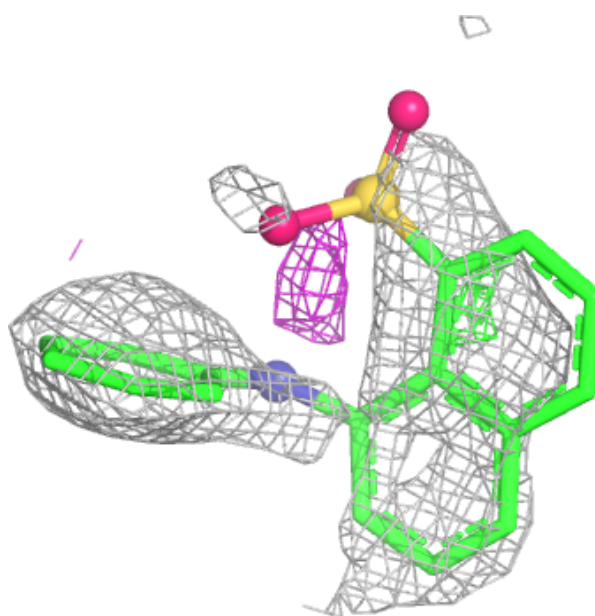
Electron density around 2AN S 204:

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



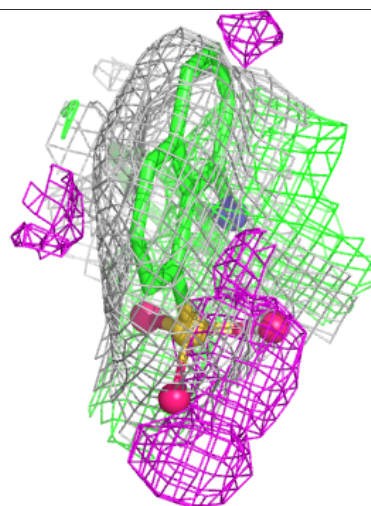
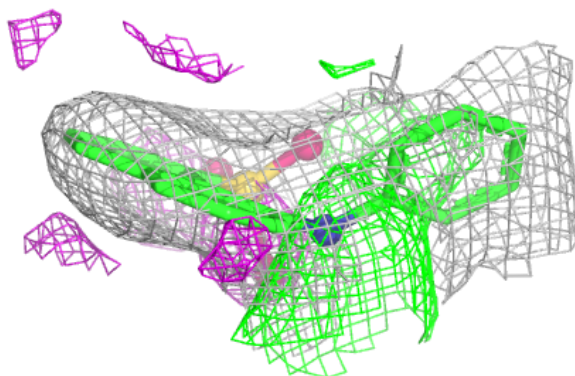
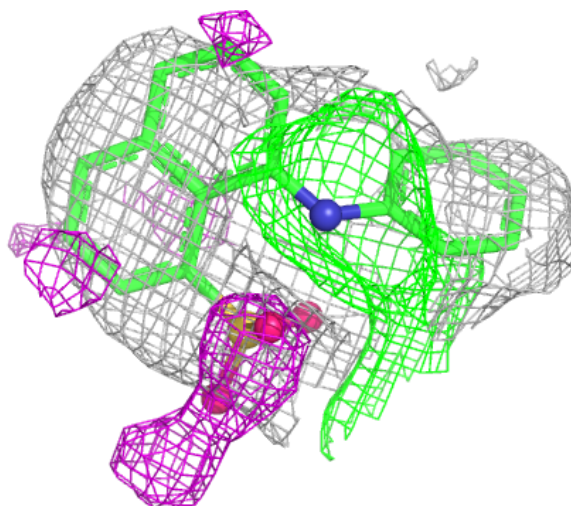
Electron density around 2AN F 206:

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



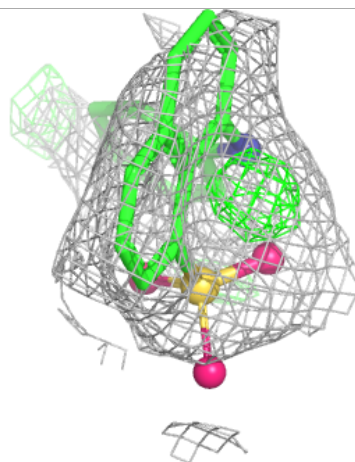
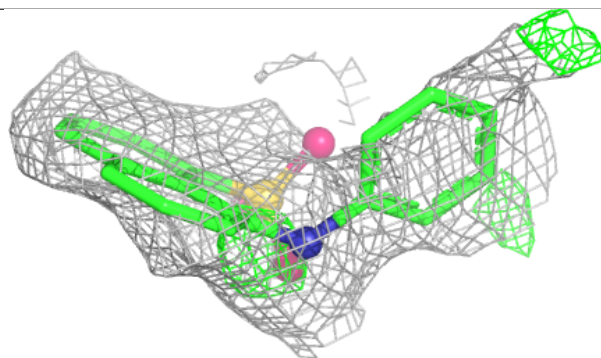
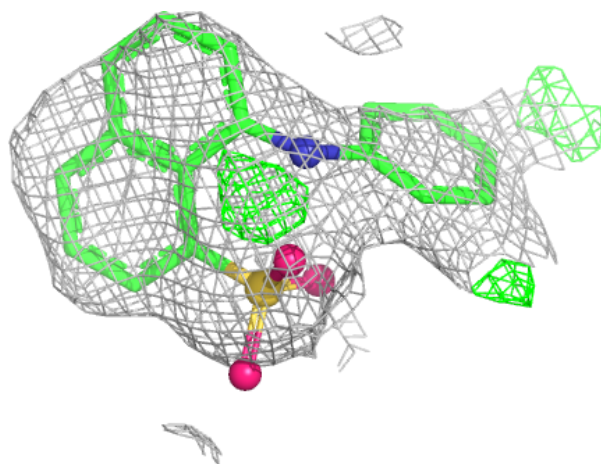
Electron density around 2AN d 203:

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



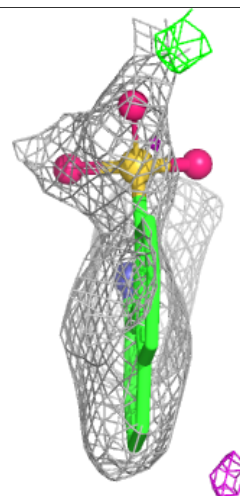
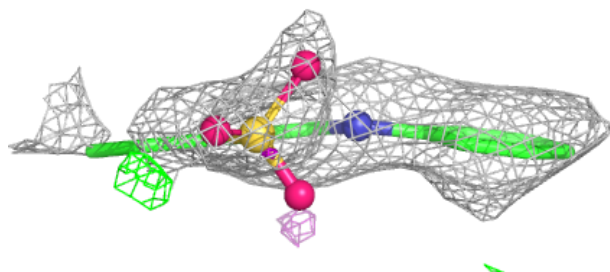
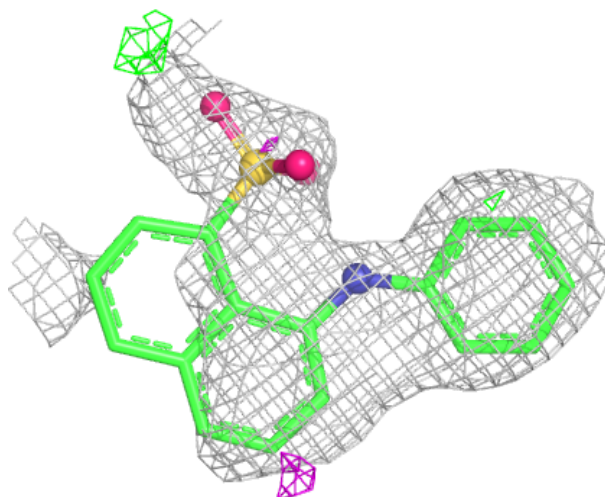
Electron density around 2AN Y 204:

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and green (positive)



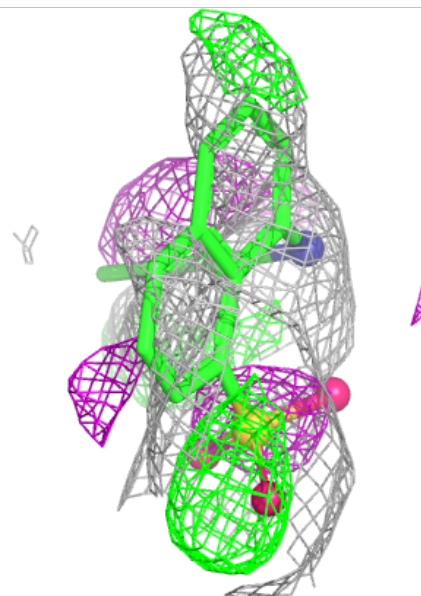
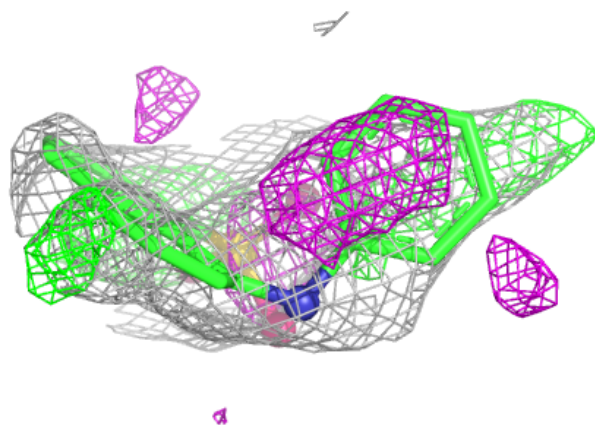
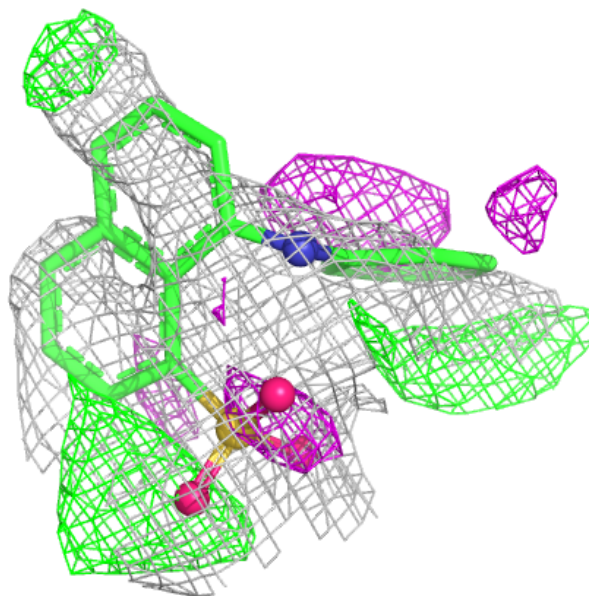
Electron density around 2AN G 207:

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



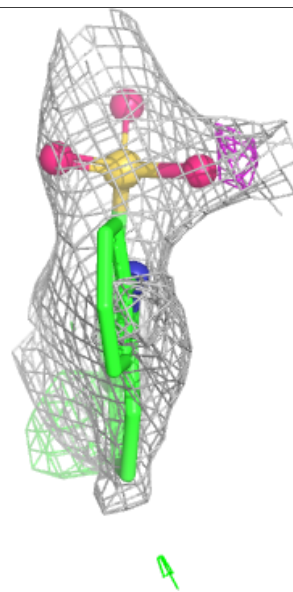
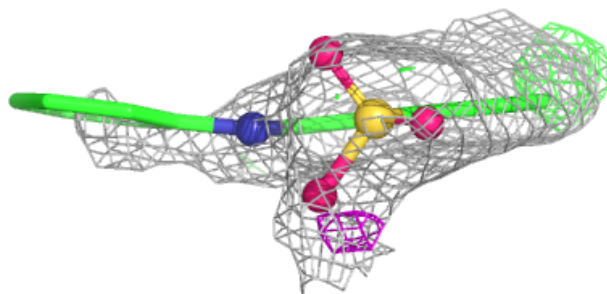
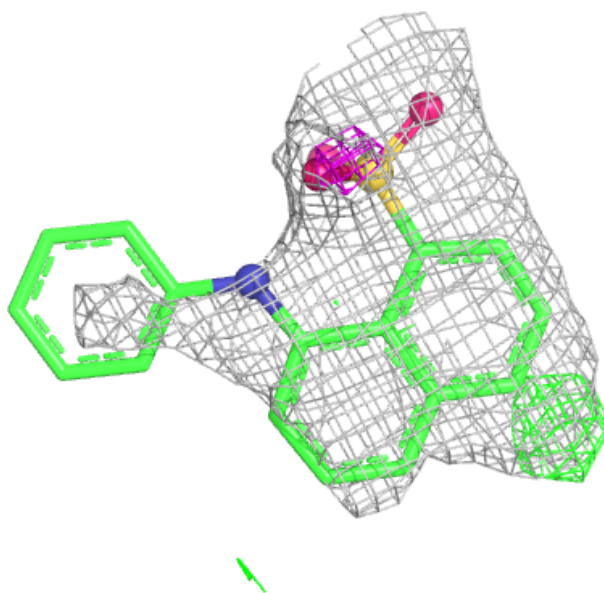
Electron density around 2AN D 204:

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and green (positive)



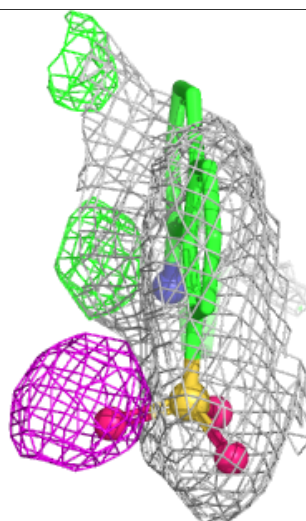
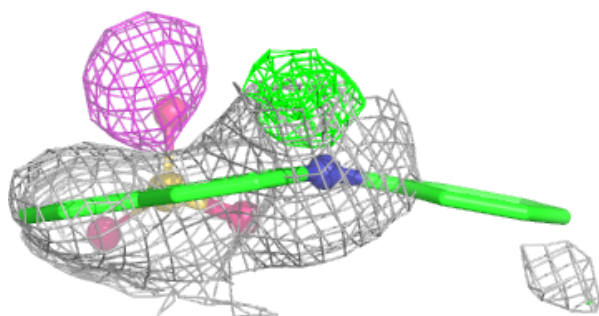
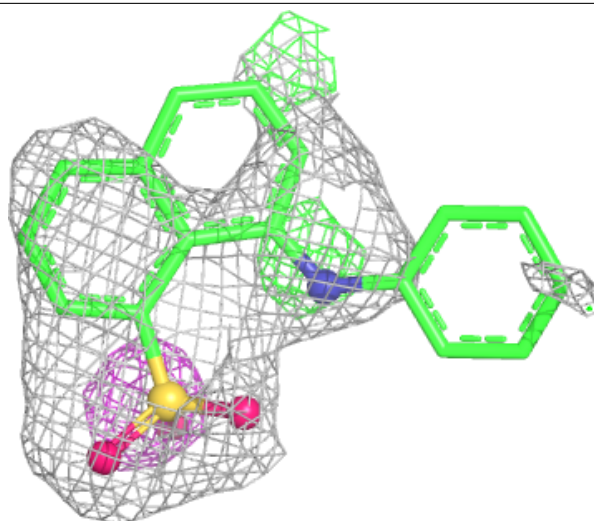
Electron density around 2AN S 203:

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



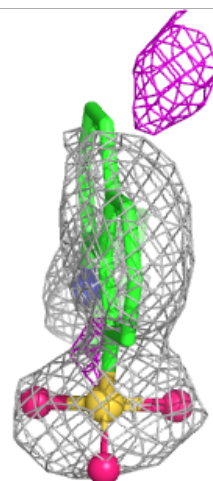
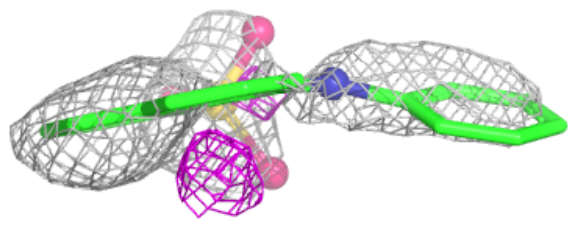
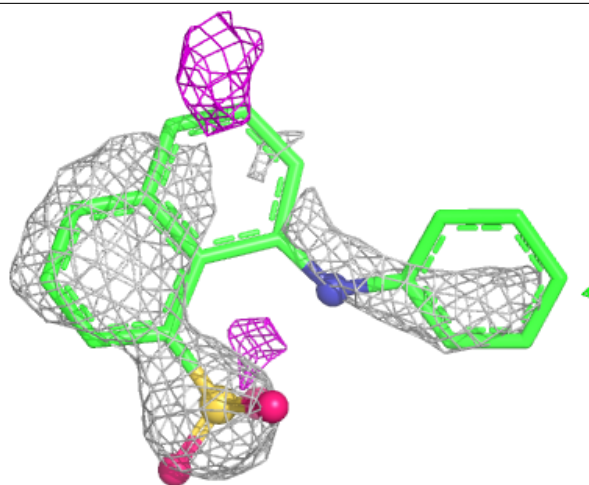
Electron density around 2AN I 207:

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



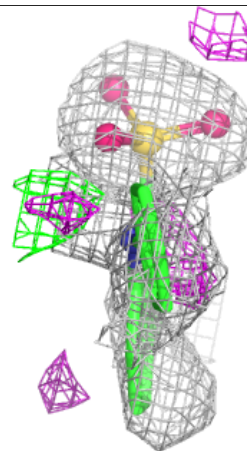
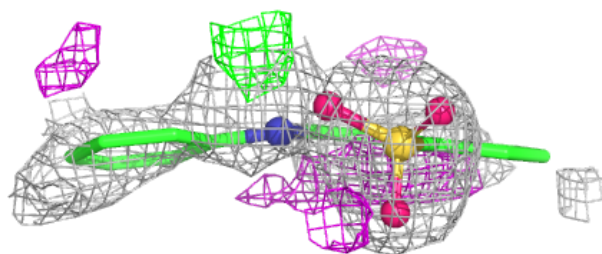
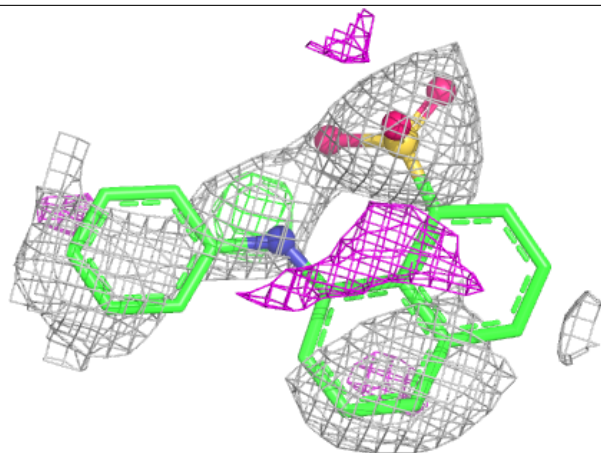
Electron density around 2AN I 204:

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and green (positive)



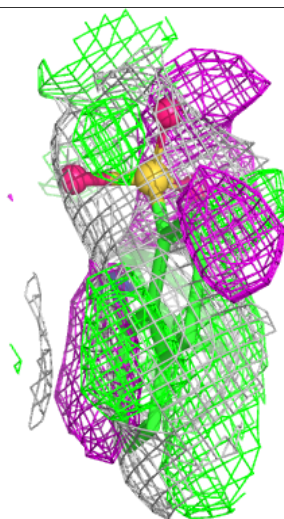
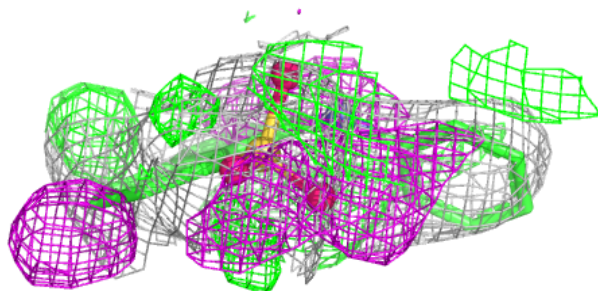
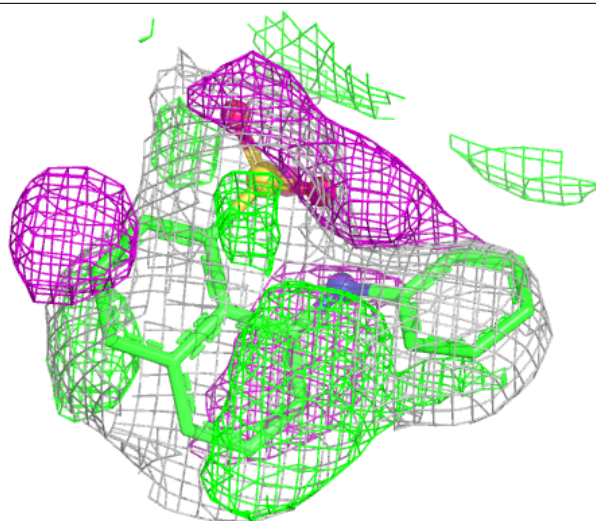
Electron density around 2AN I 205:

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and green (positive)



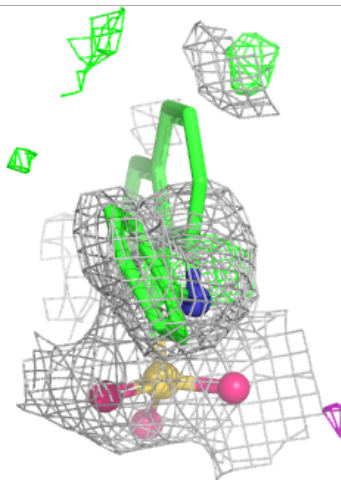
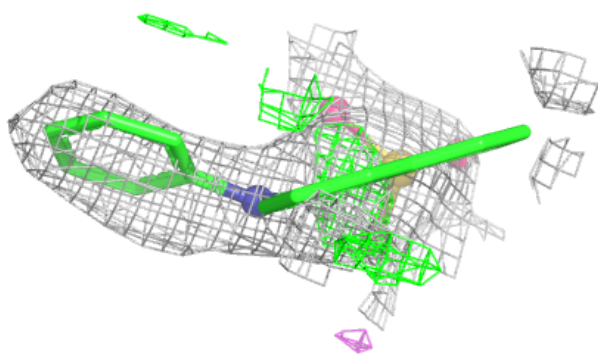
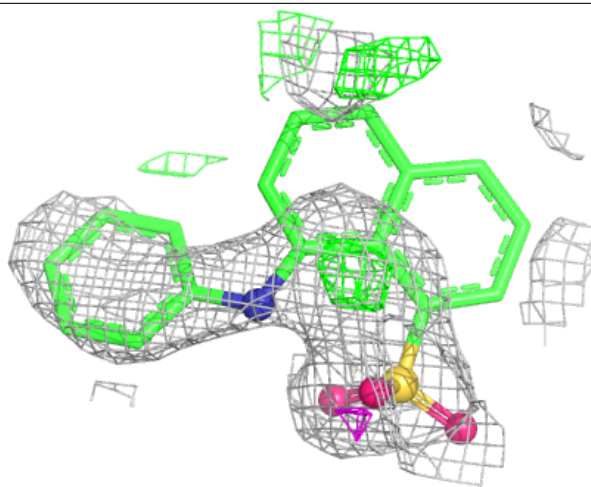
Electron density around 2AN X 203:

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and green (positive)



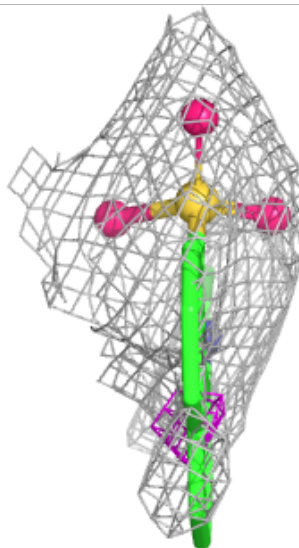
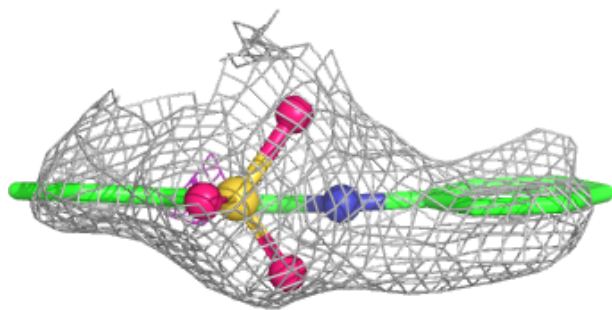
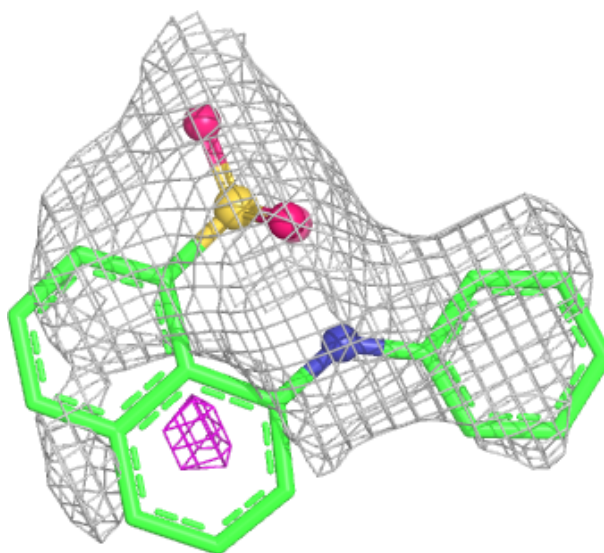
Electron density around 2AN d 204:

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



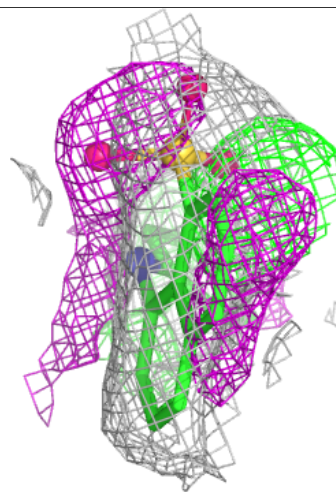
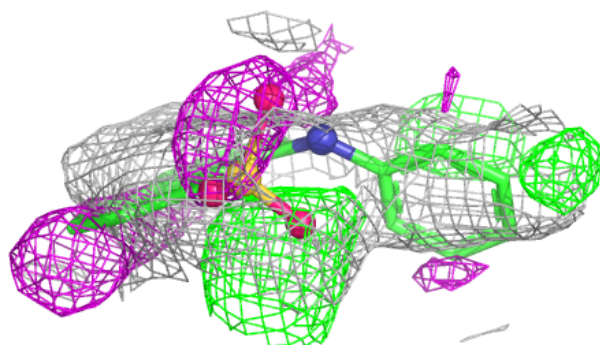
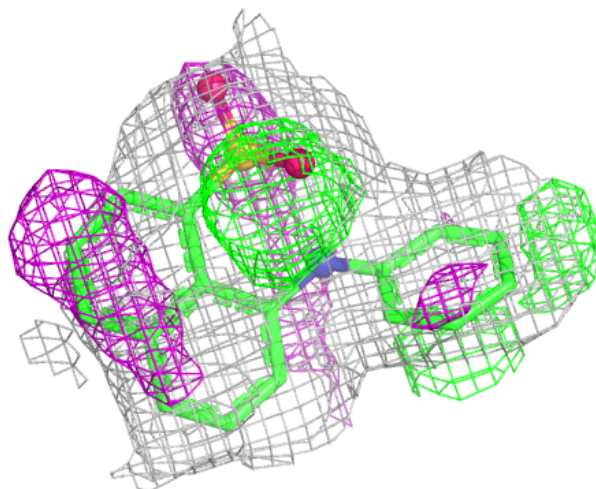
Electron density around 2AN O 202:

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



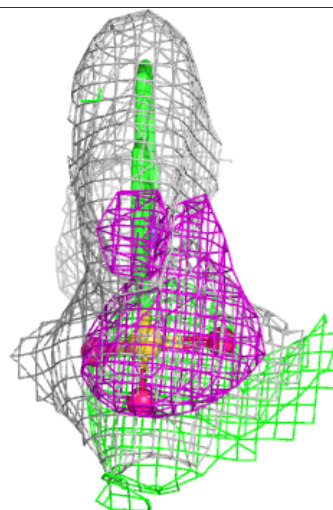
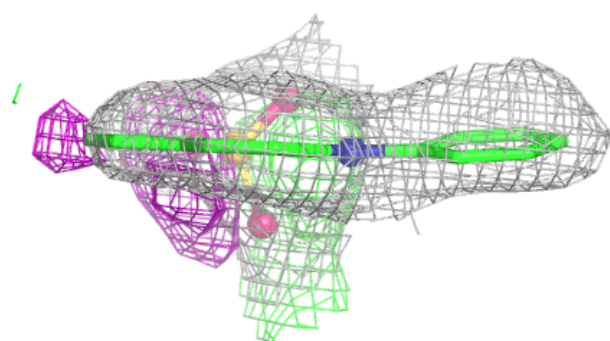
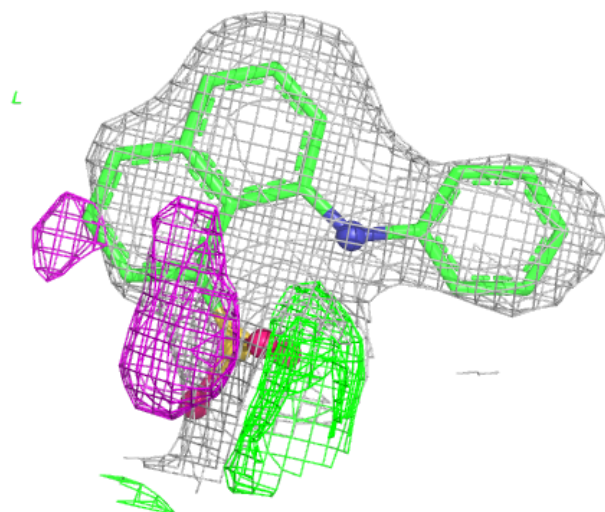
Electron density around 2AN X 206:

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



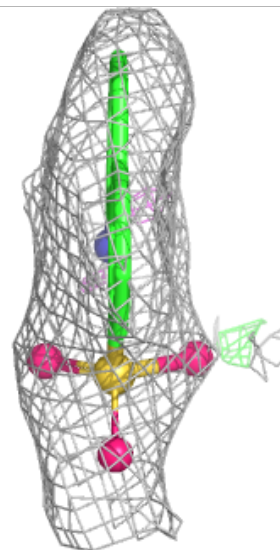
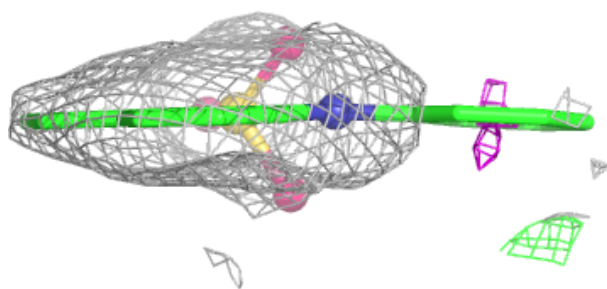
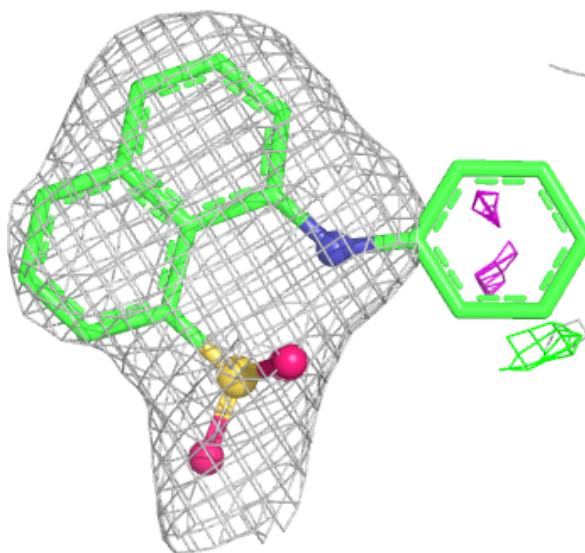
Electron density around 2AN c 202:

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



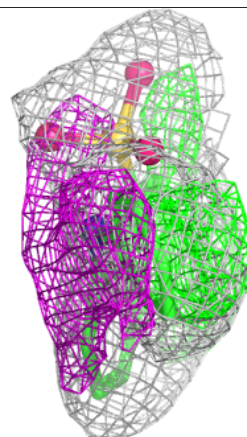
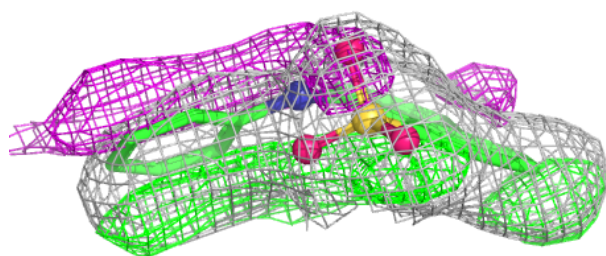
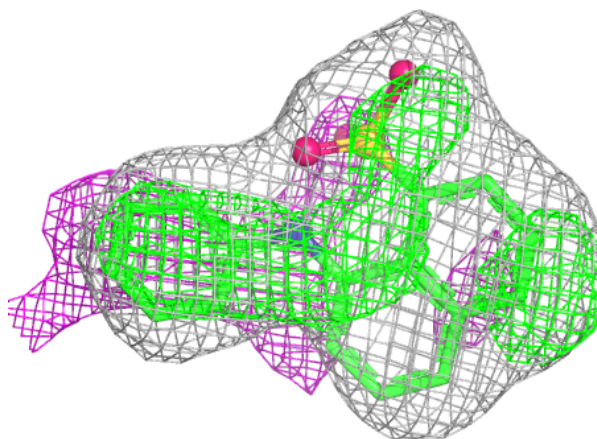
Electron density around 2AN G 204:

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

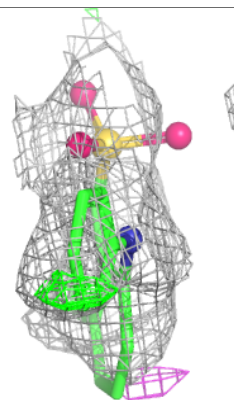
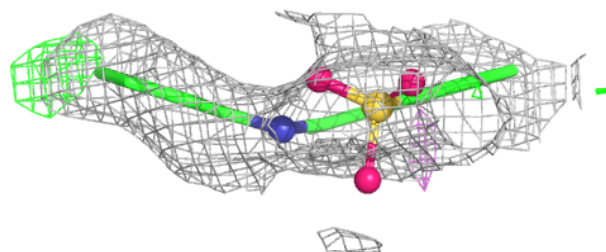
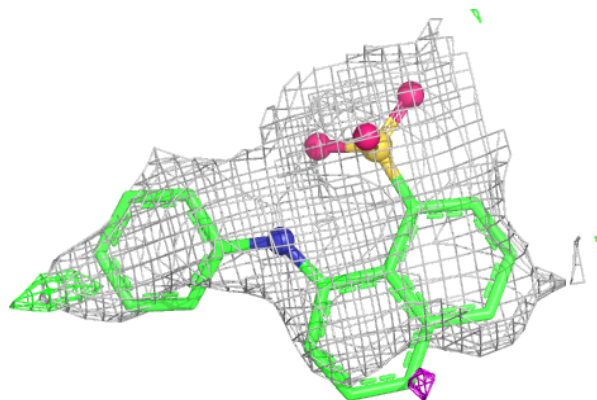


Electron density around 2AN j 205:

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

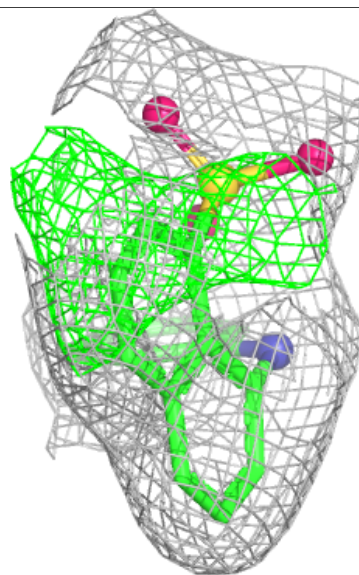
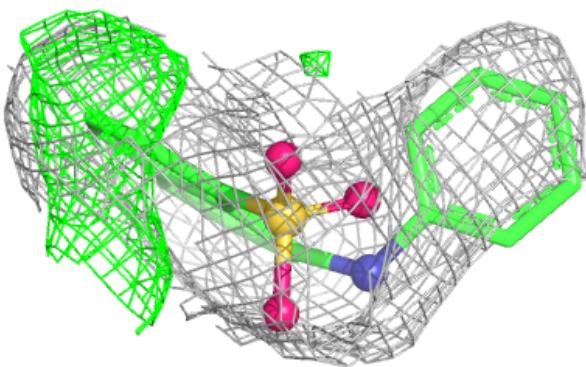
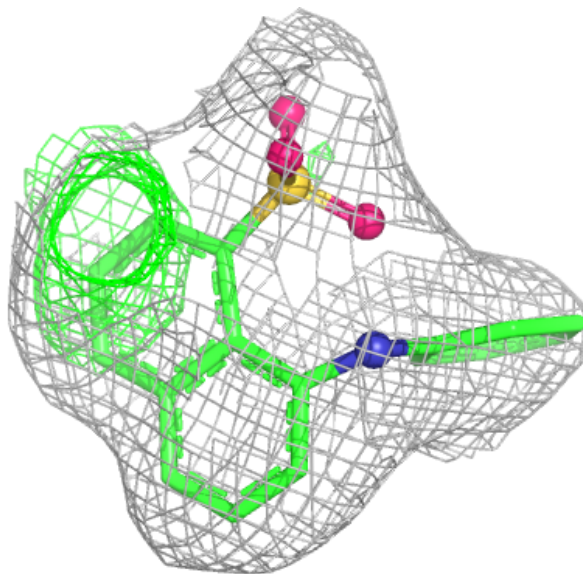
**Electron density around 2AN b 205:**

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



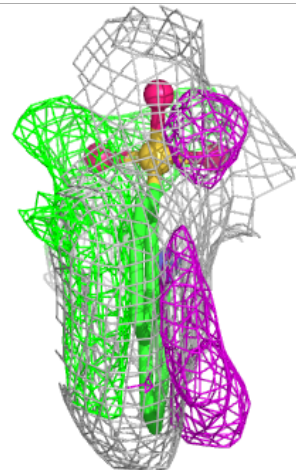
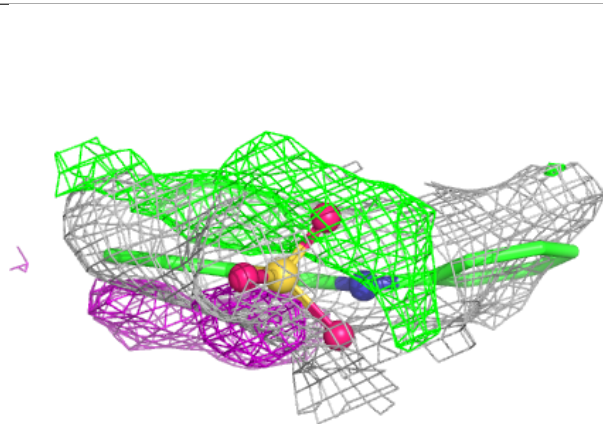
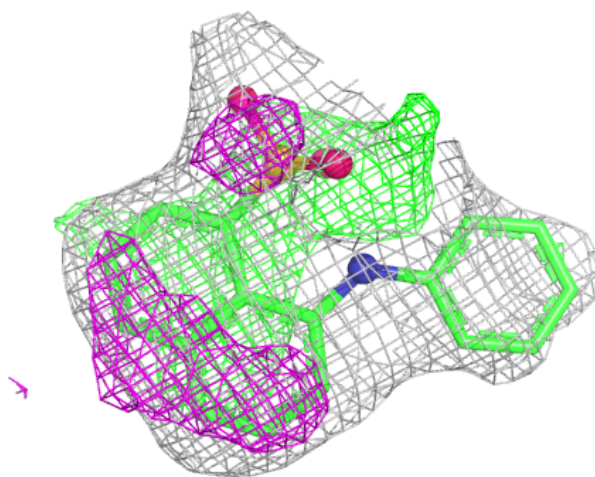
Electron density around 2AN Z 206:

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



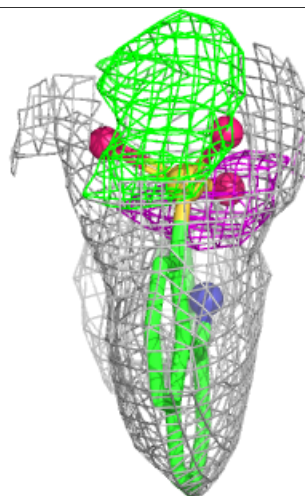
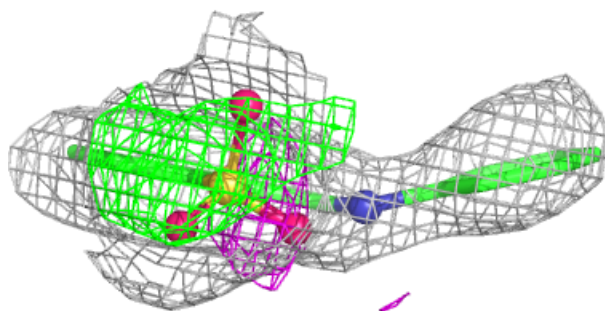
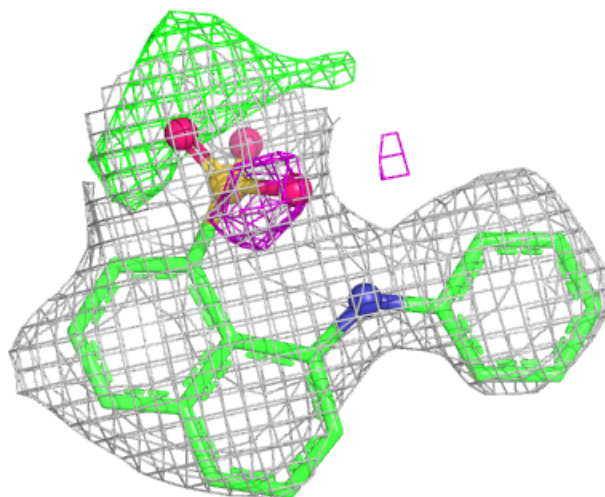
Electron density around 2AN T 203:

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



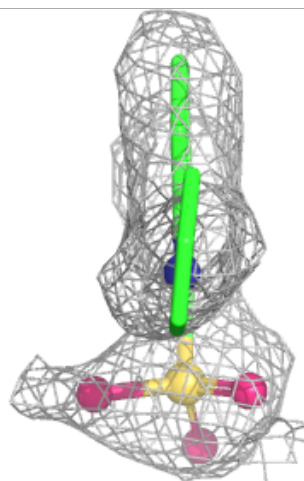
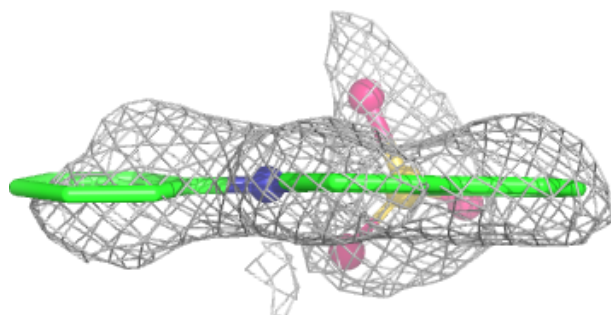
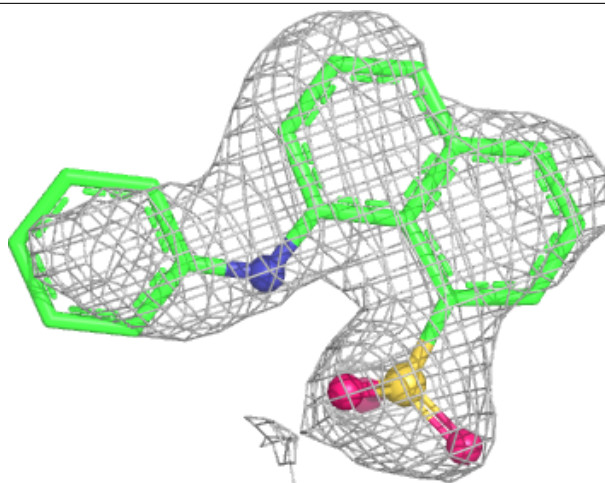
Electron density around 2AN R 204:

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



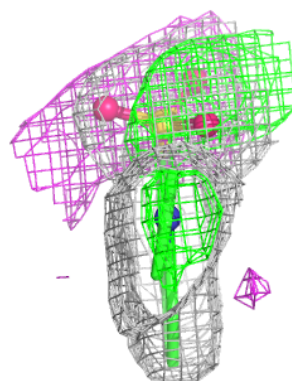
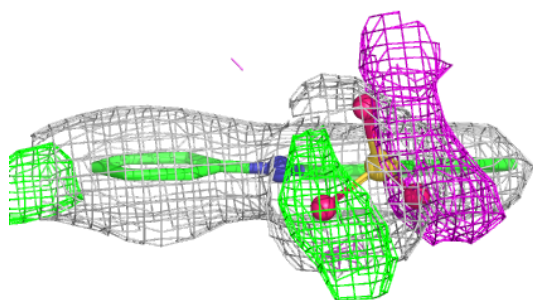
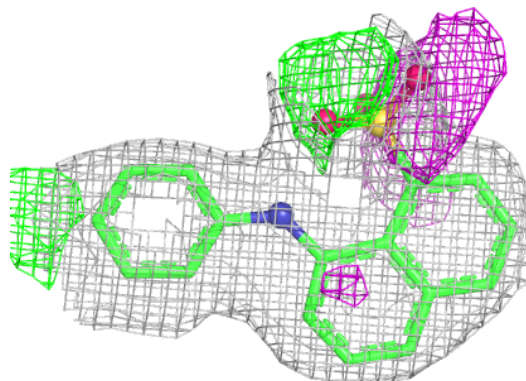
Electron density around 2AN c 205:

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



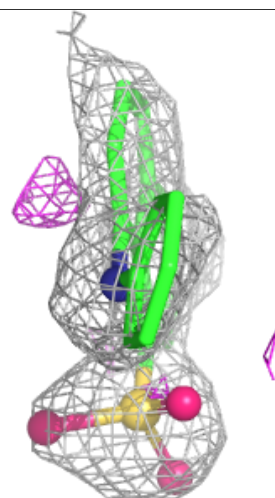
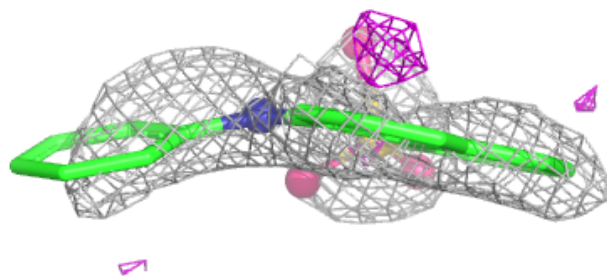
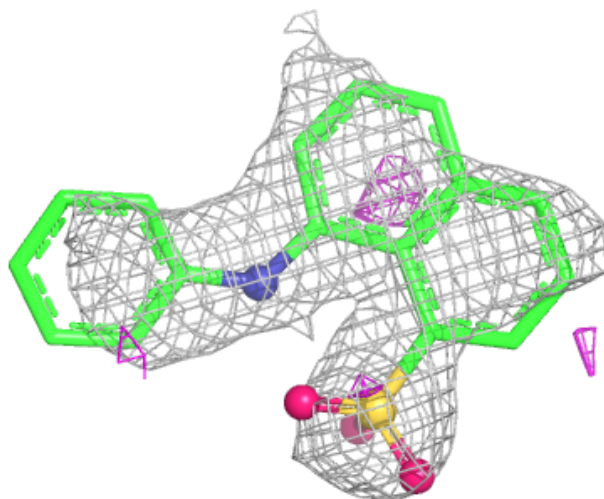
Electron density around 2AN T 204:

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



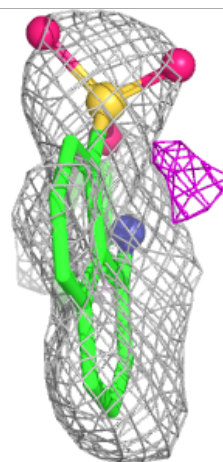
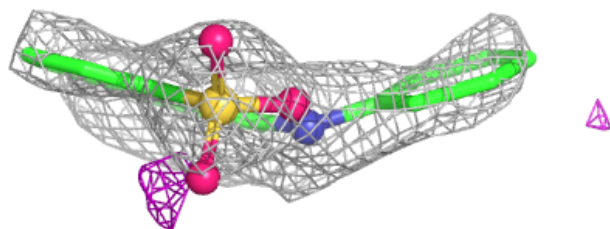
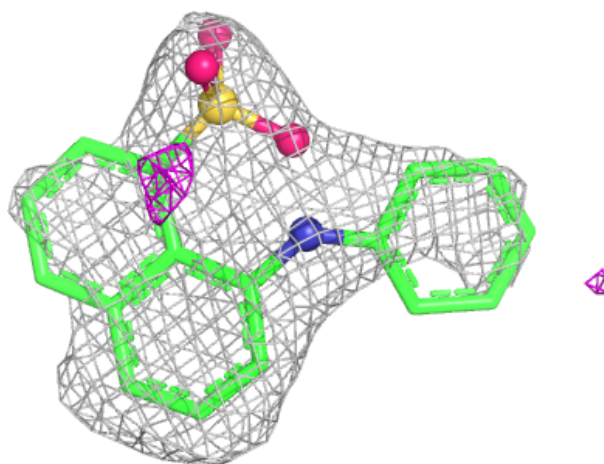
Electron density around 2AN I 203:

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



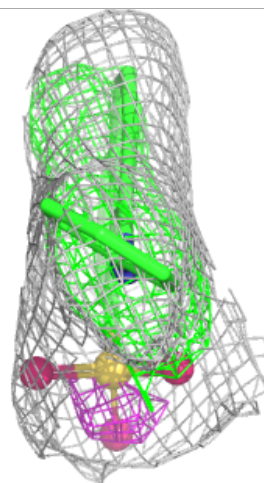
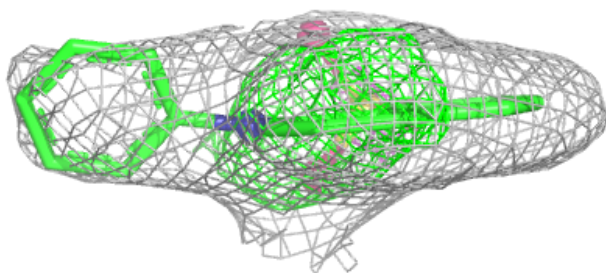
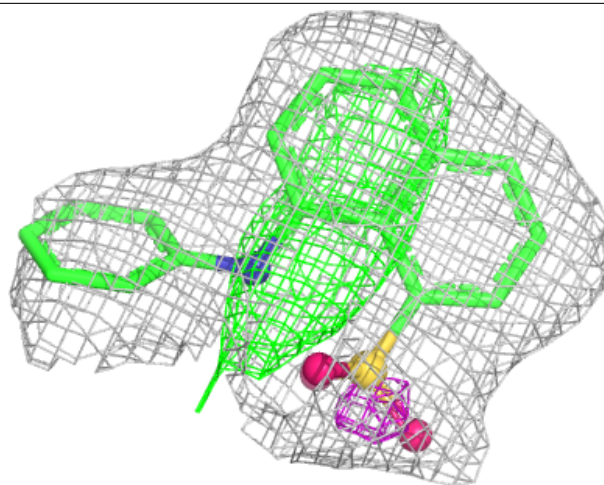
Electron density around 2AN G 205:

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



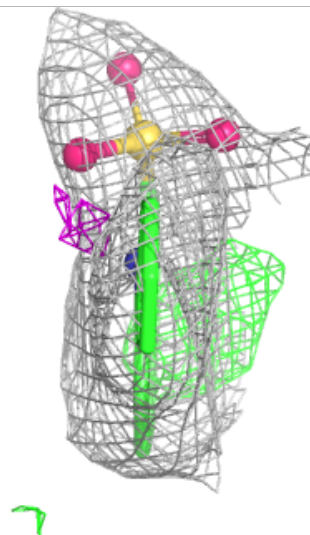
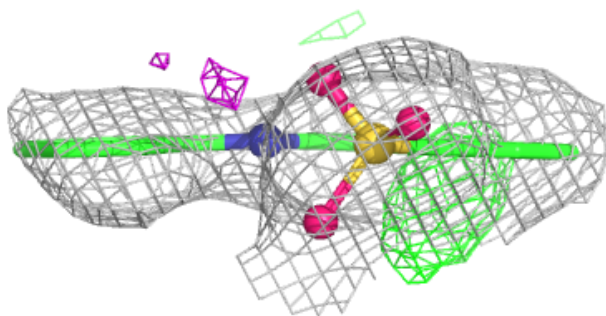
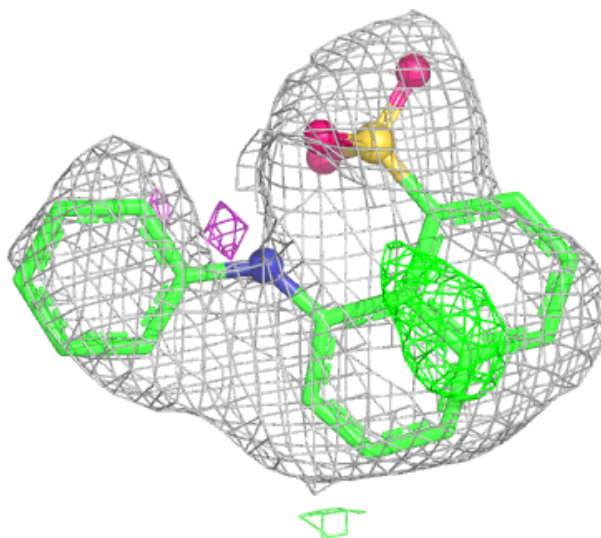
Electron density around 2AN V 207:

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



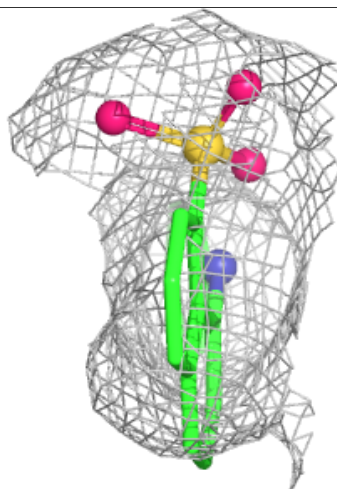
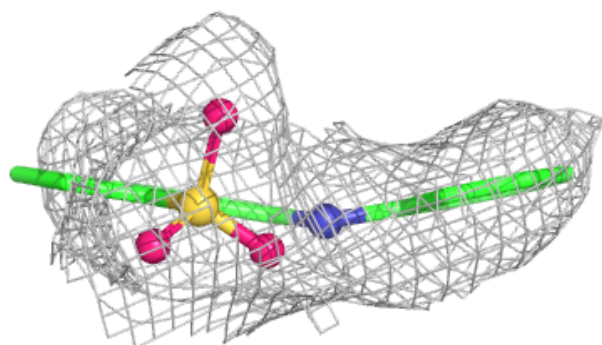
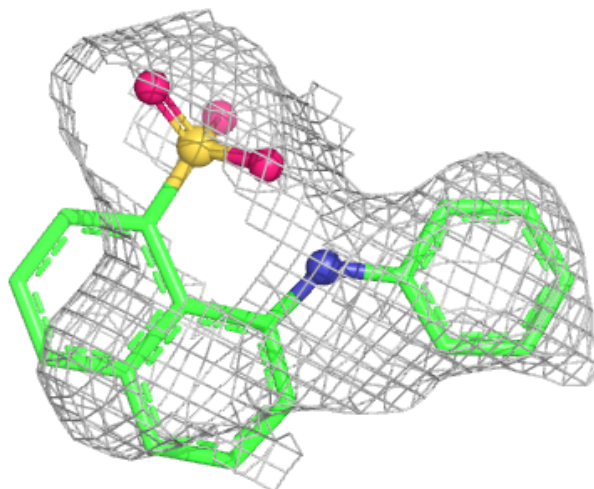
Electron density around 2AN R 205:

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



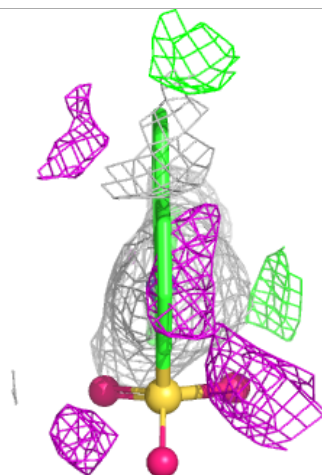
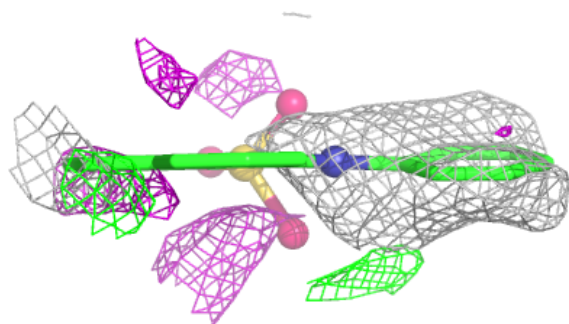
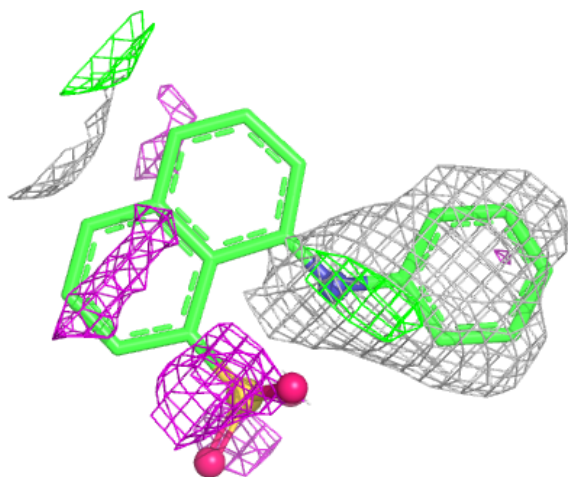
Electron density around 2AN U 201:

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



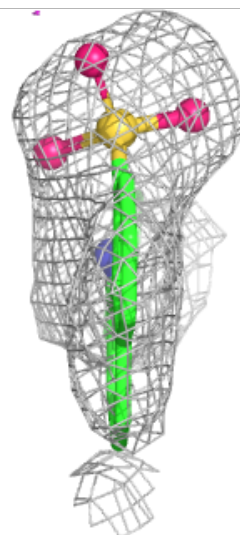
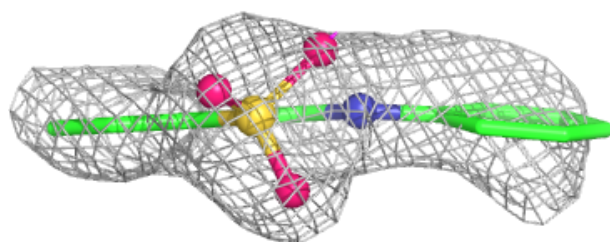
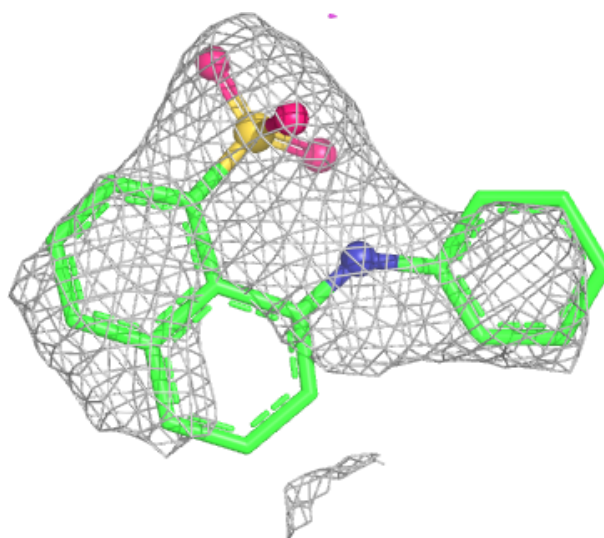
Electron density around 2AN a 204:

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



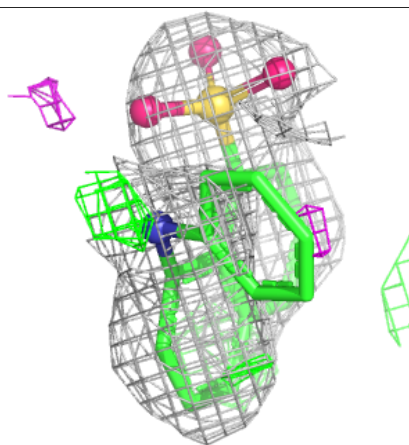
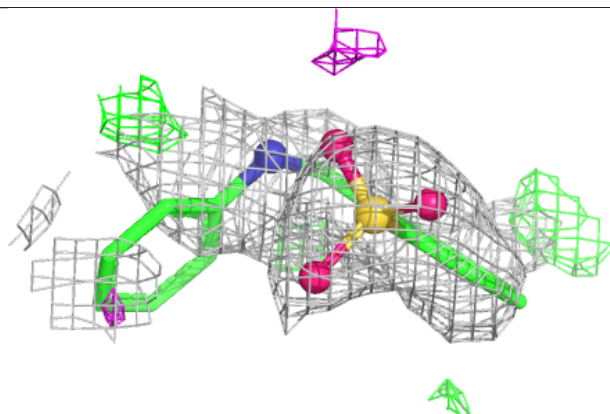
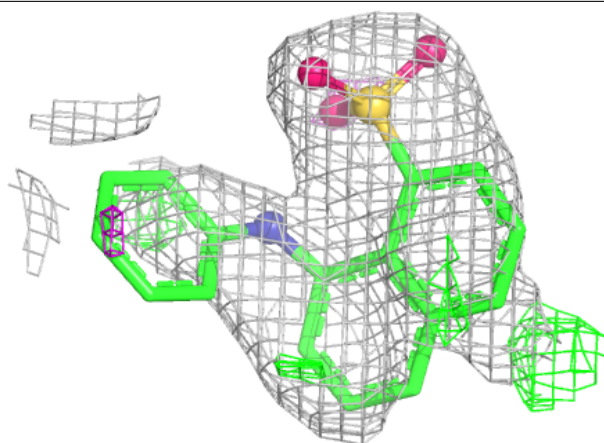
Electron density around 2AN H 204:

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



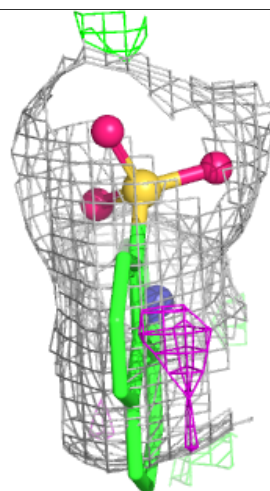
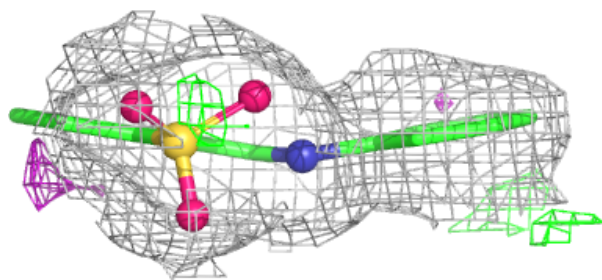
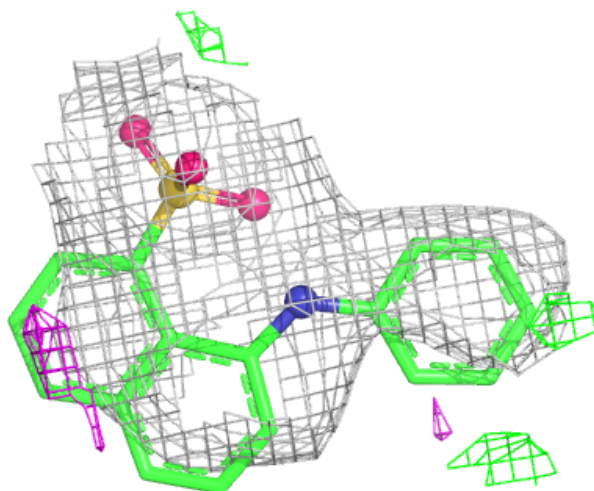
Electron density around 2AN E 204:

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



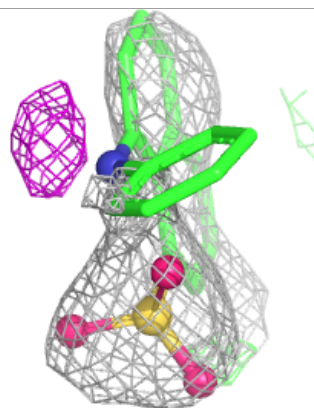
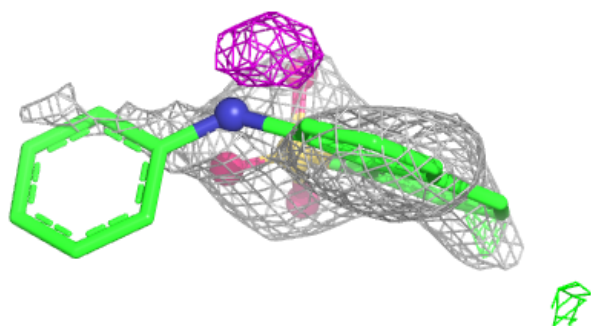
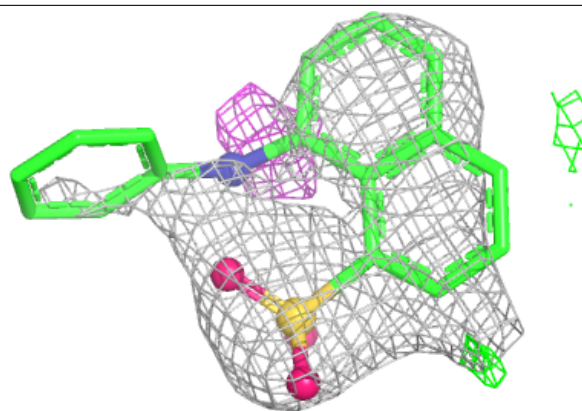
Electron density around 2AN F 204:

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



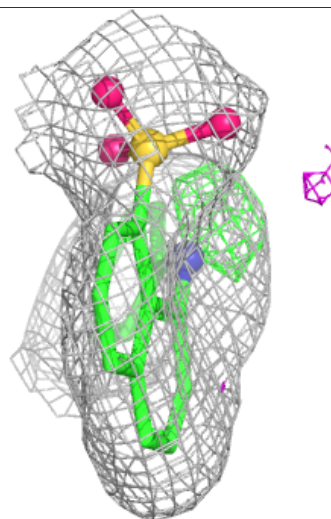
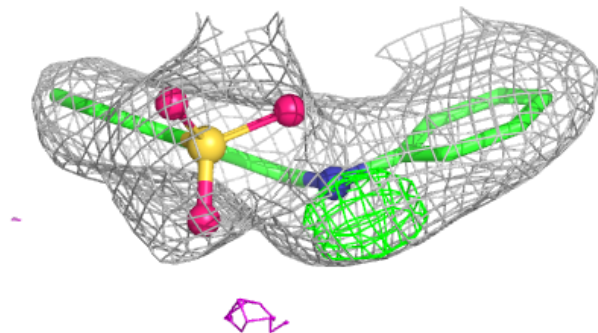
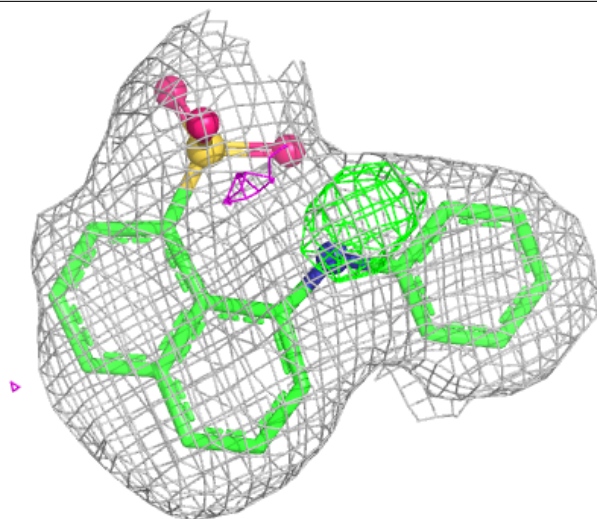
Electron density around 2AN C 203 (A):

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



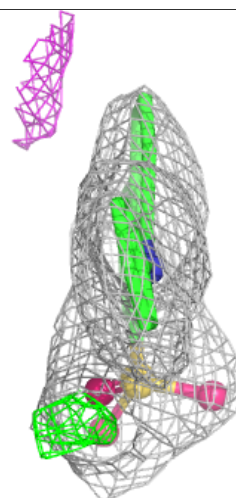
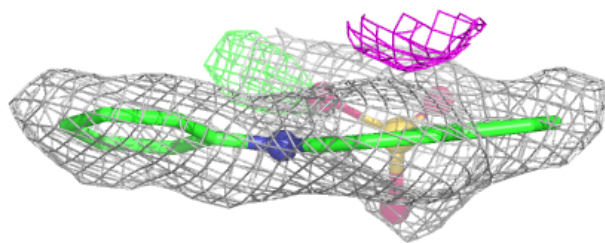
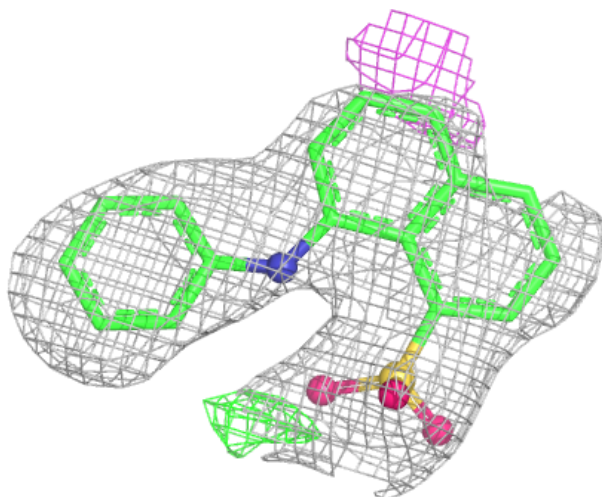
Electron density around 2AN T 205:

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



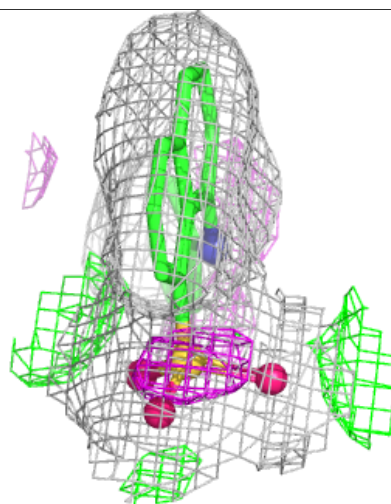
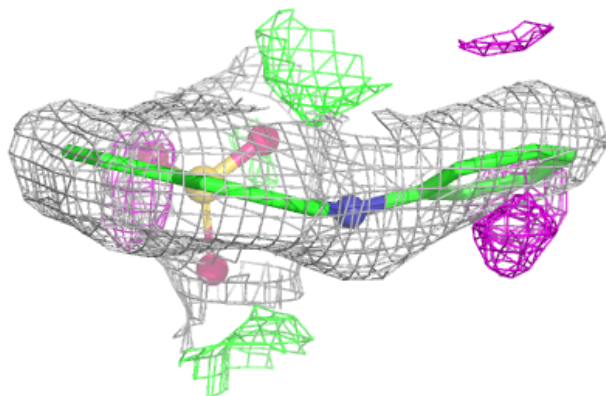
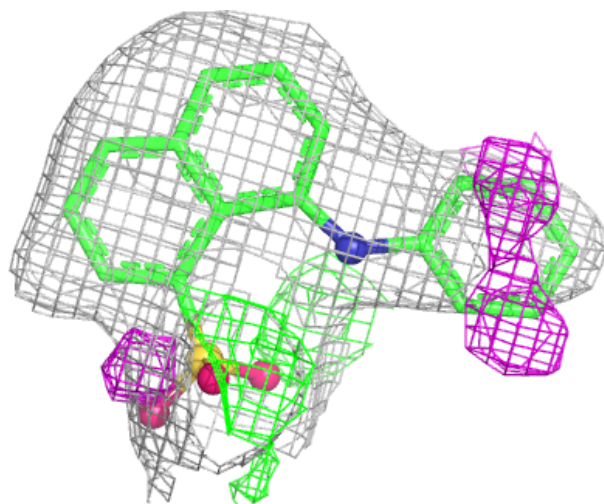
Electron density around 2AN W 201:

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



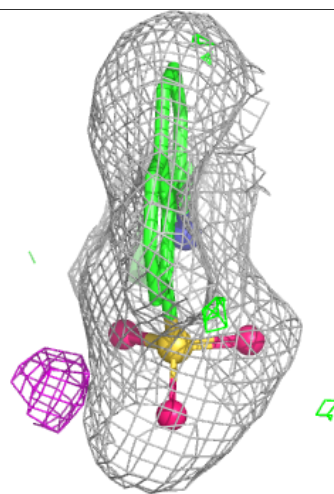
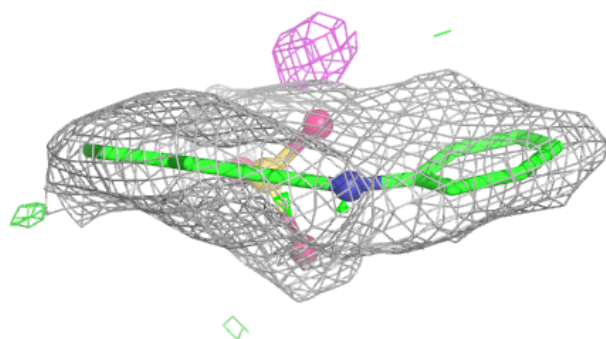
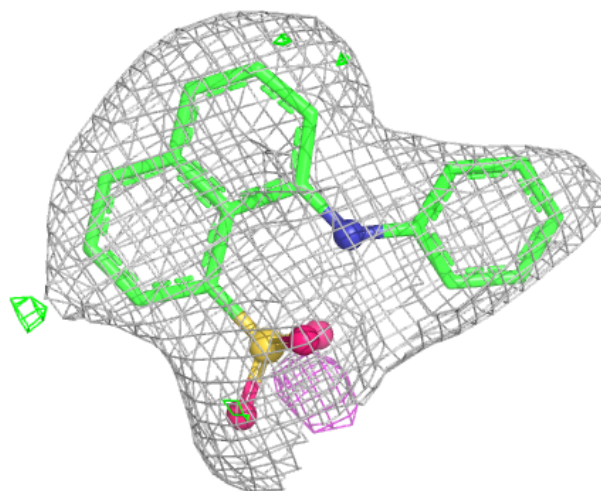
Electron density around 2AN Y 201:

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



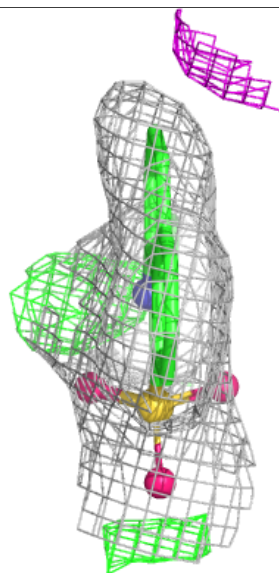
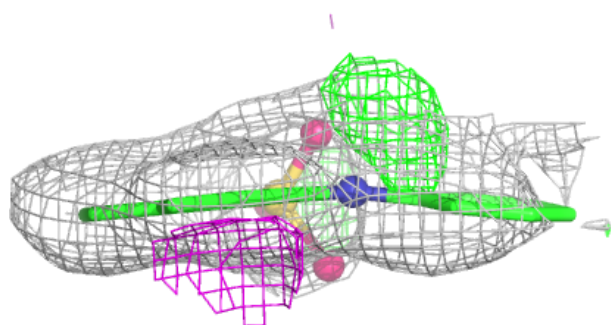
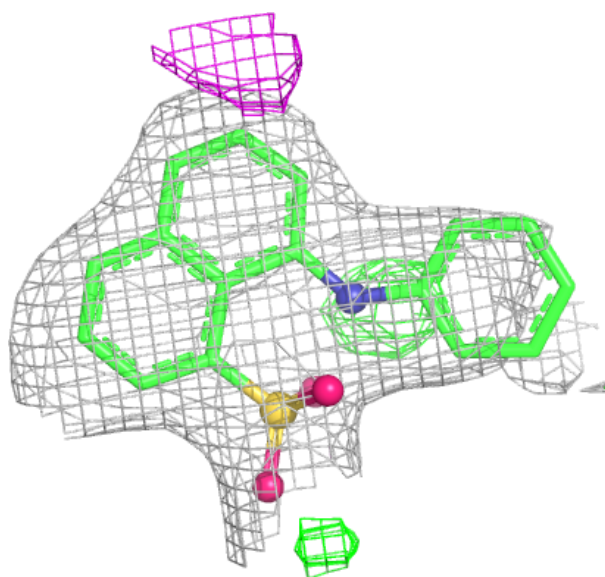
Electron density around 2AN N 205:

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



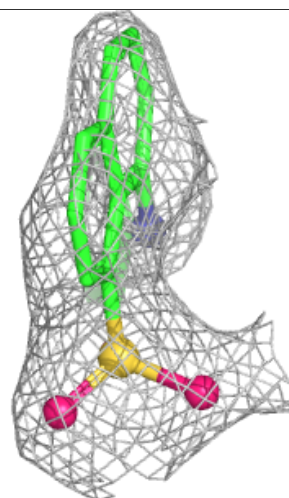
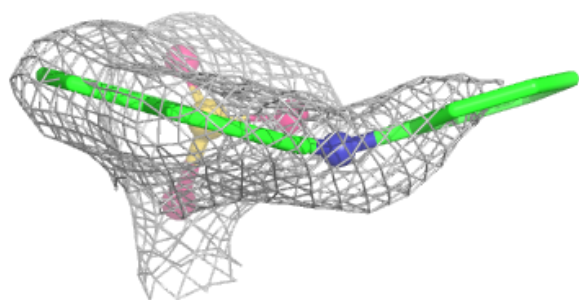
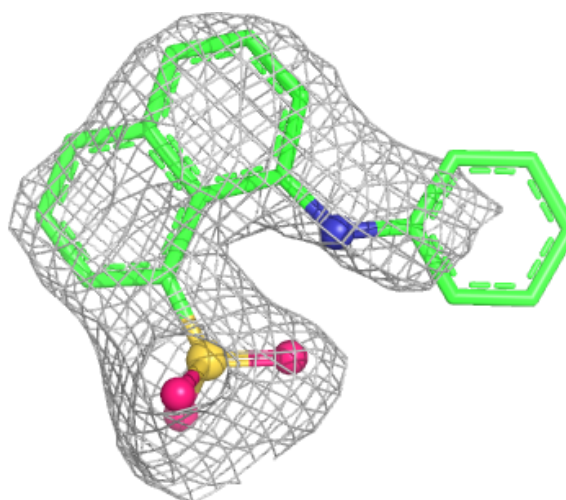
Electron density around 2AN j 206:

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



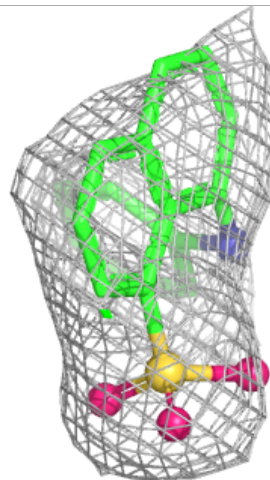
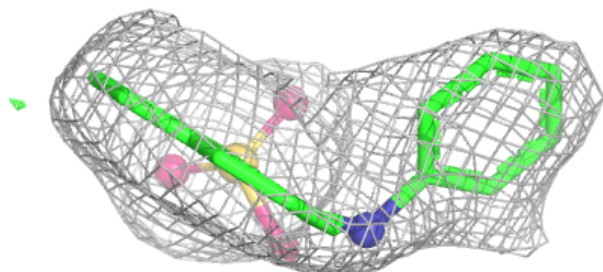
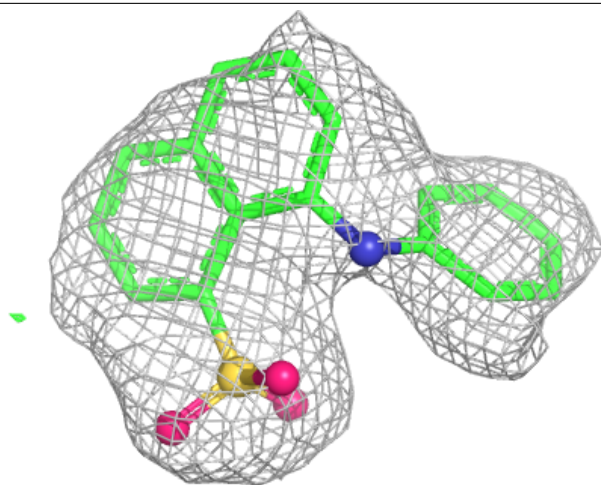
Electron density around 2AN A 203:

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



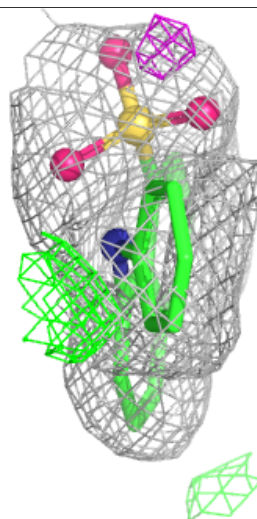
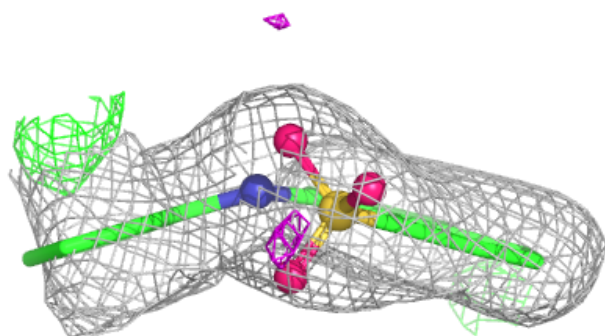
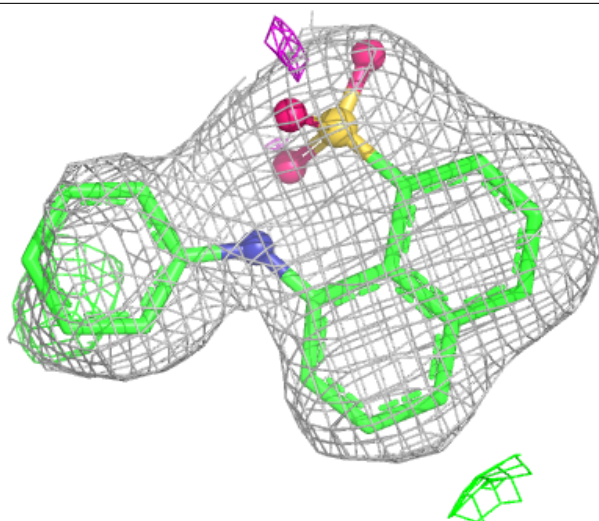
Electron density around 2AN S 201:

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



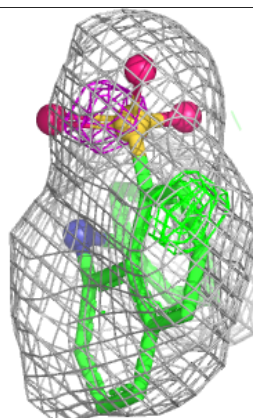
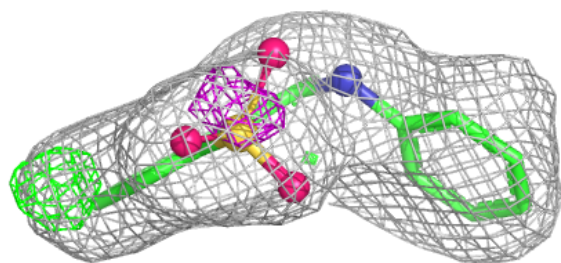
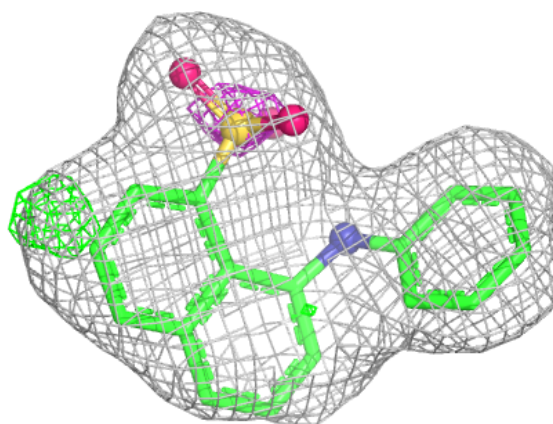
Electron density around 2AN c 203:

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



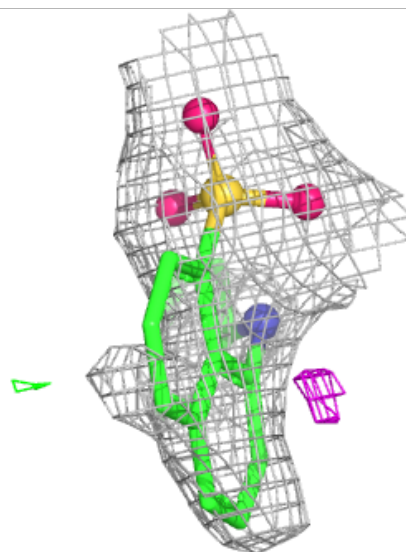
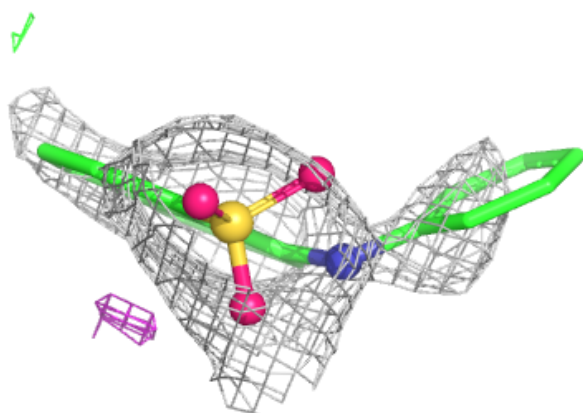
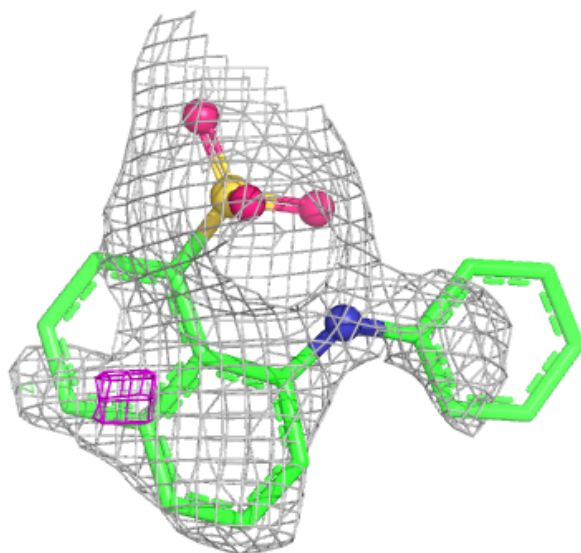
Electron density around 2AN g 203:

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



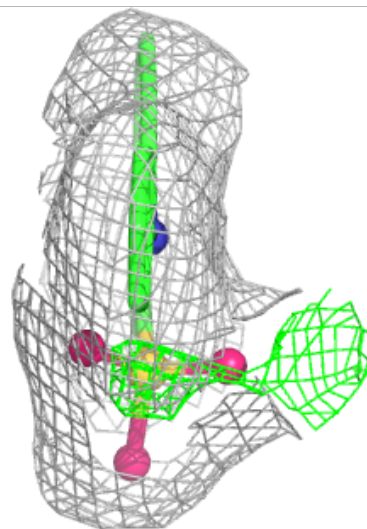
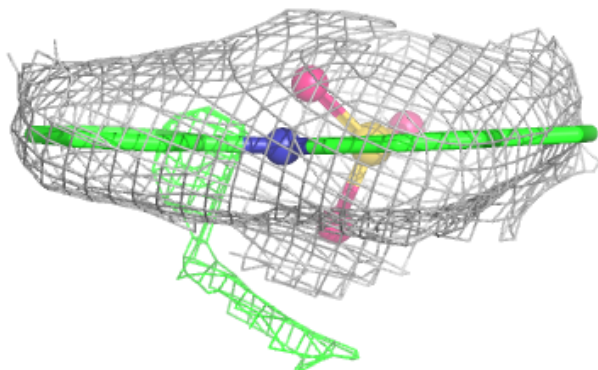
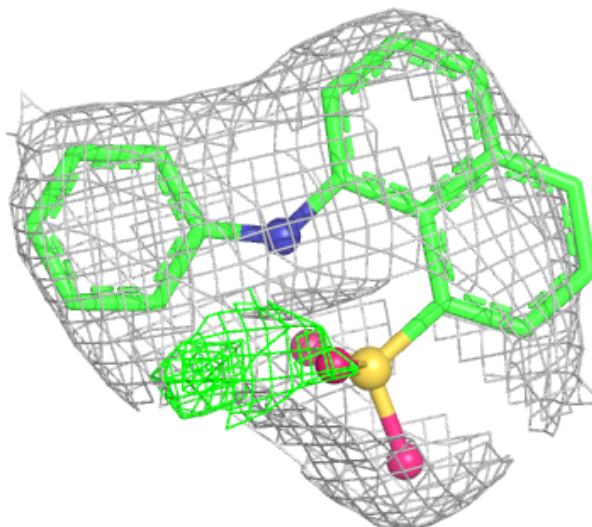
Electron density around 2AN f 206:

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



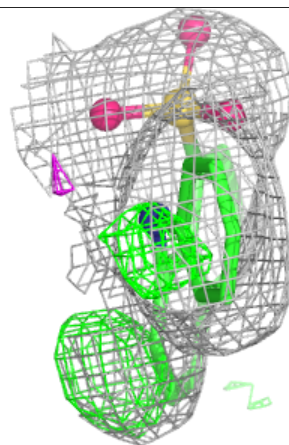
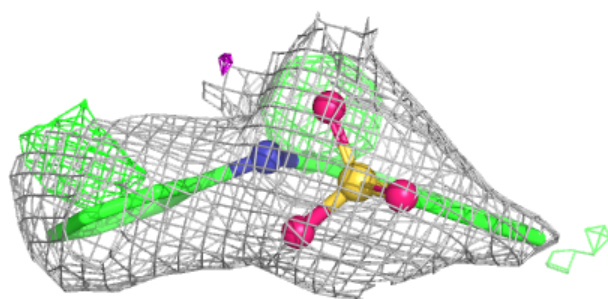
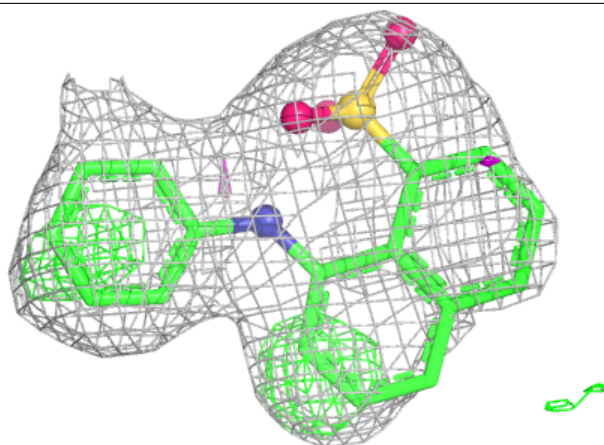
Electron density around 2AN X 202:

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



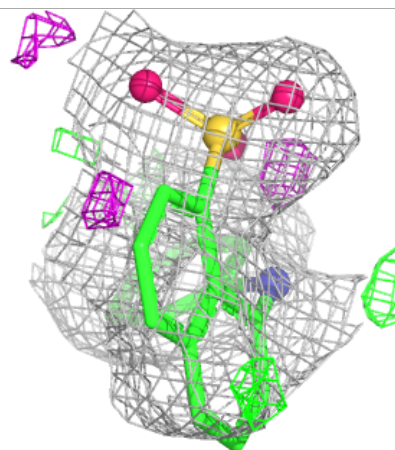
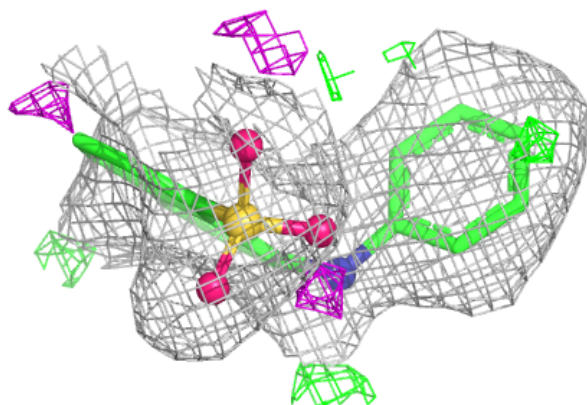
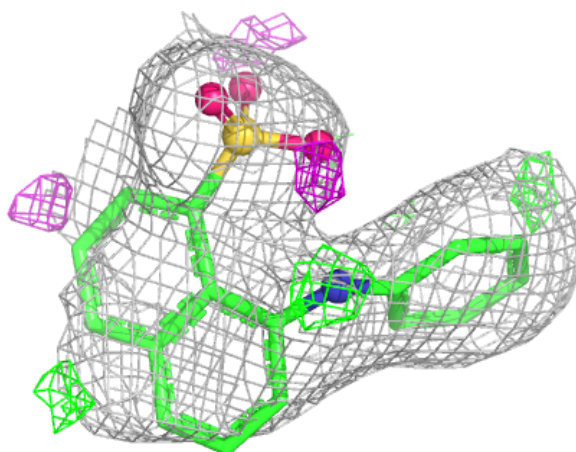
Electron density around 2AN B 206:

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



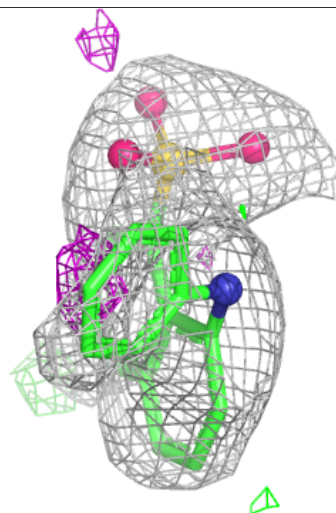
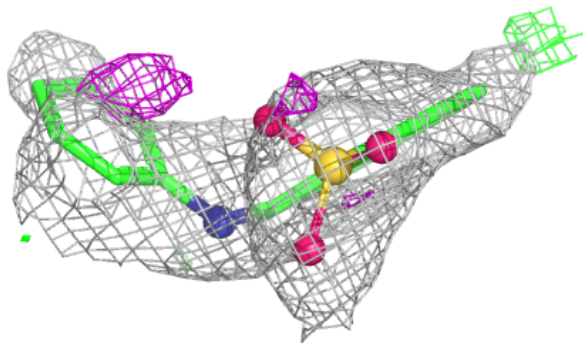
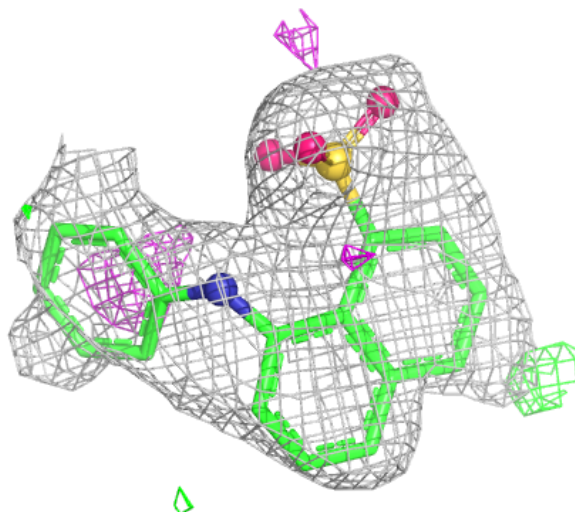
Electron density around 2AN F 202:

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



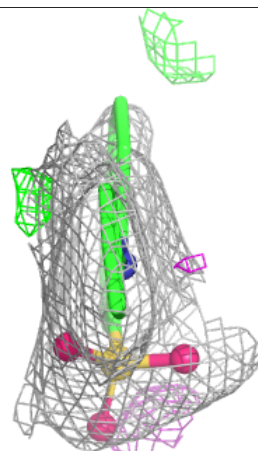
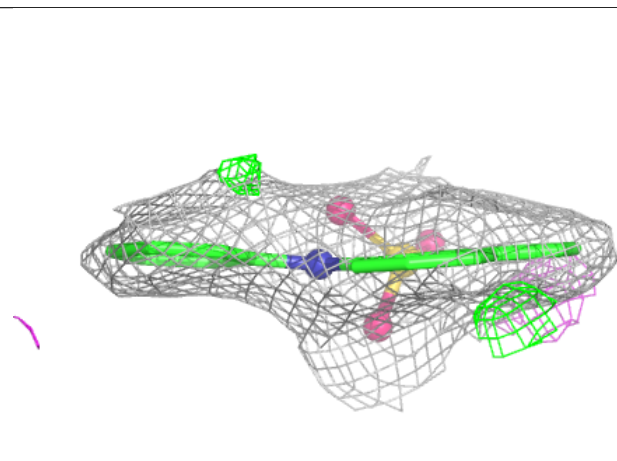
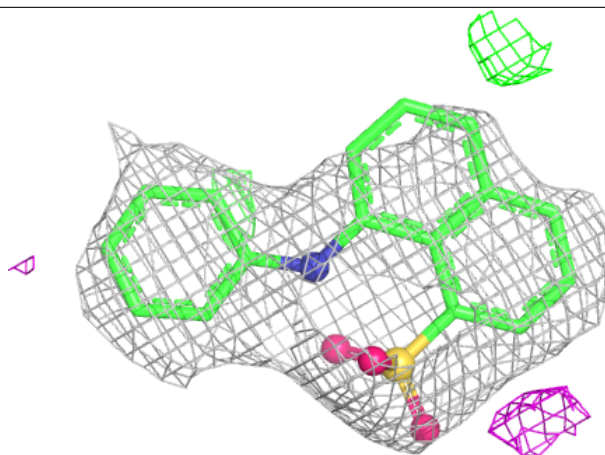
Electron density around 2AN I 206:

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



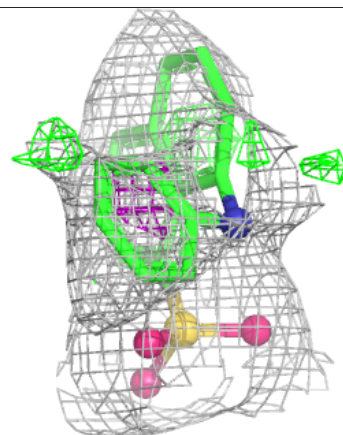
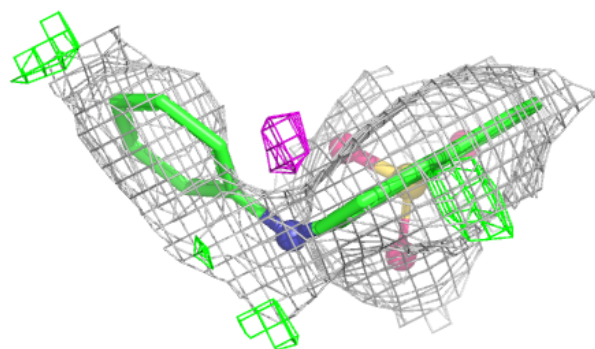
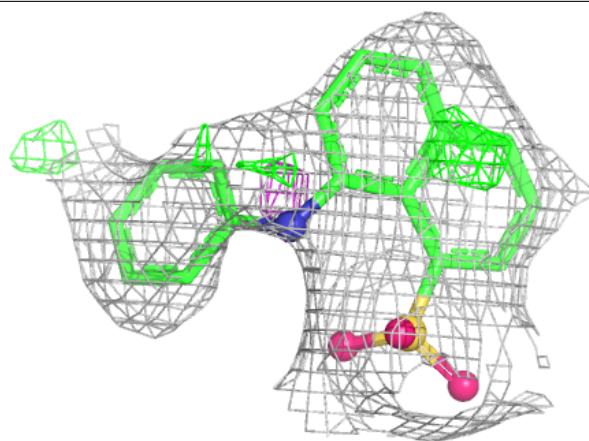
Electron density around 2AN K 203:

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



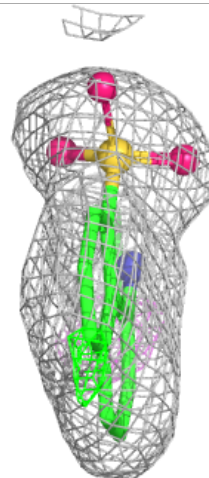
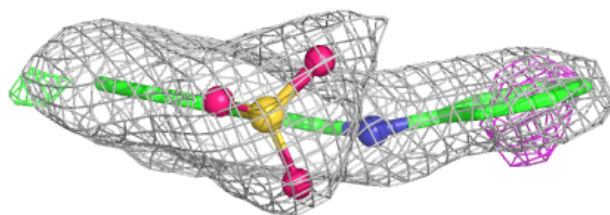
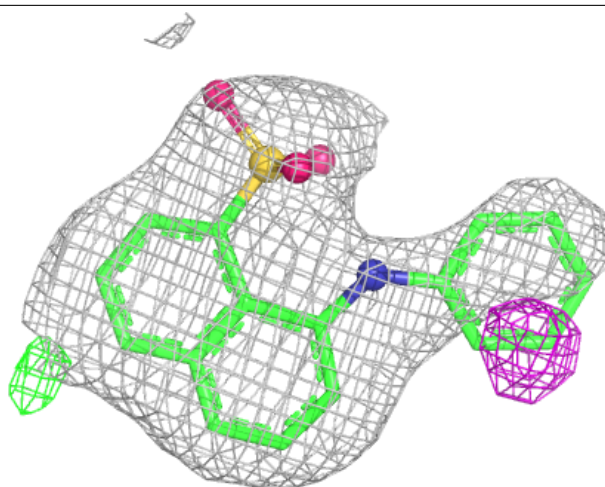
Electron density around 2AN a 201:

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



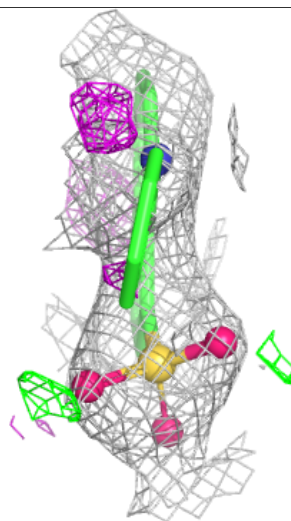
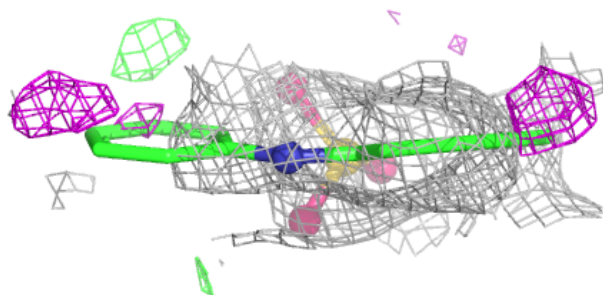
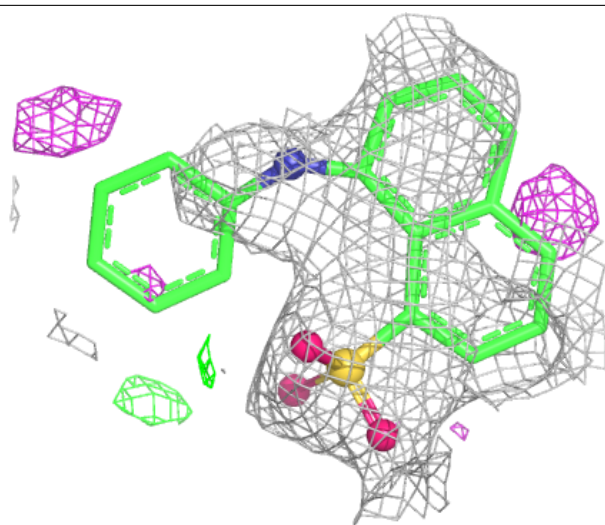
Electron density around 2AN X 201:

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



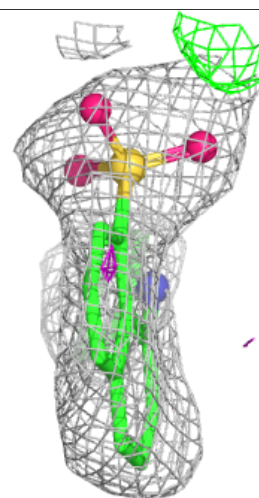
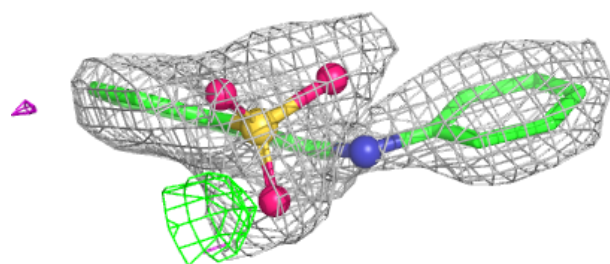
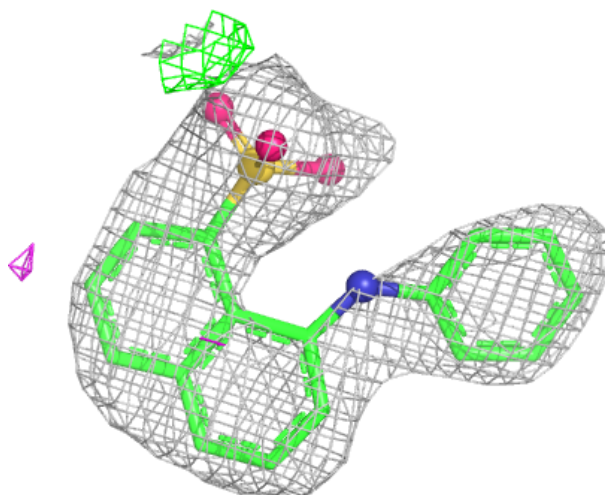
Electron density around 2AN V 208:

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



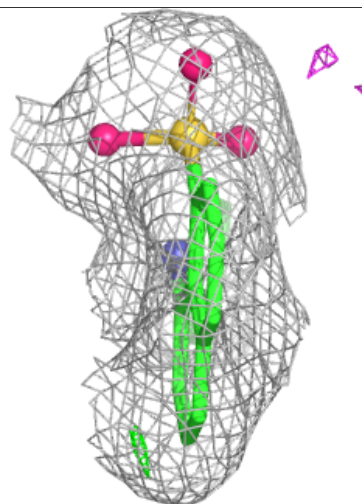
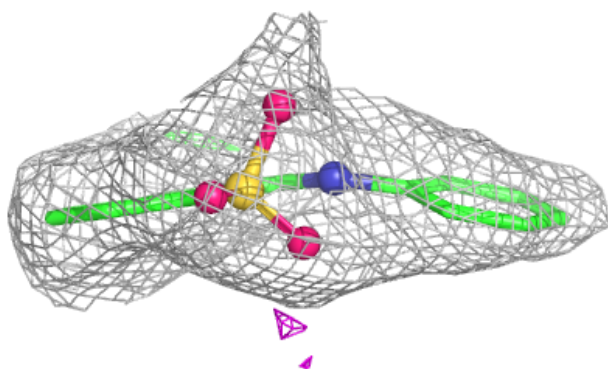
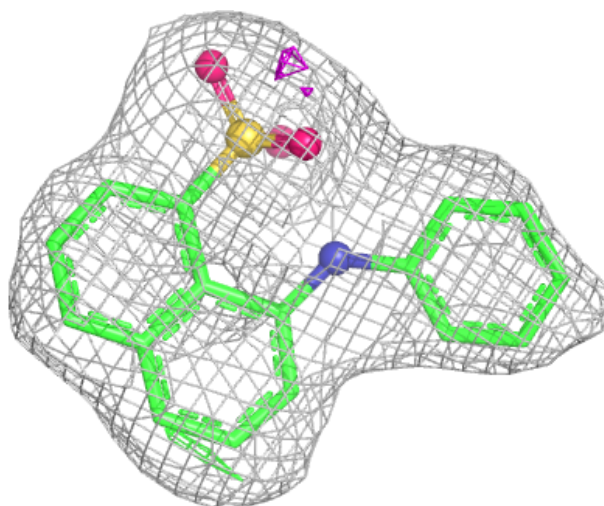
Electron density around 2AN h 201:

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



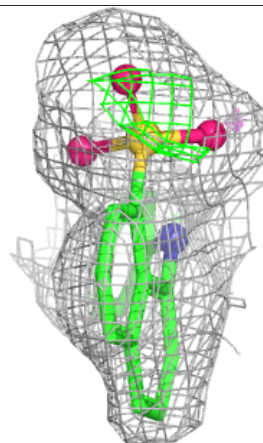
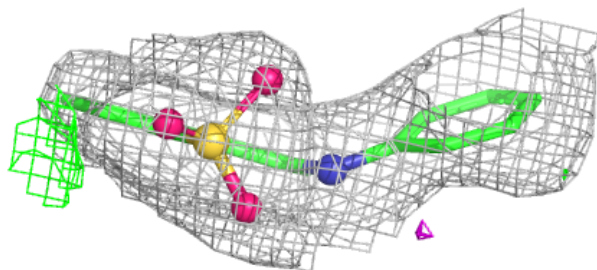
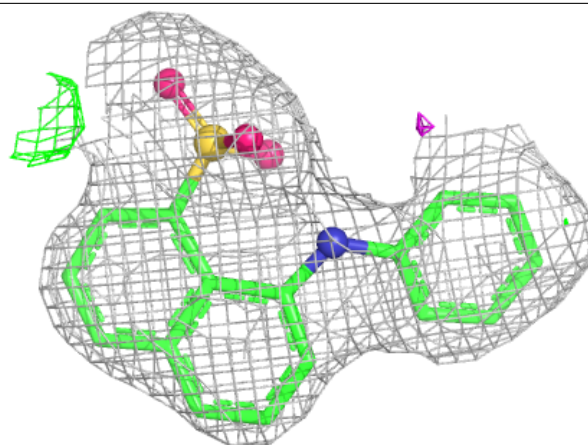
Electron density around 2AN a 203:

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



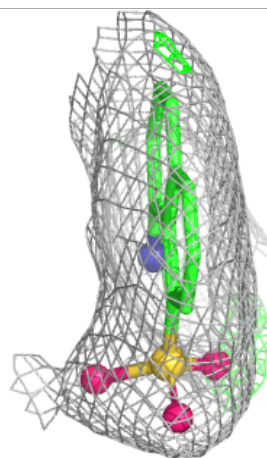
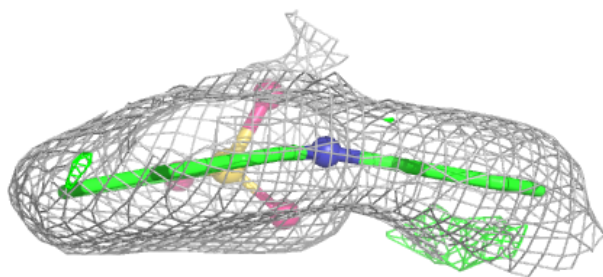
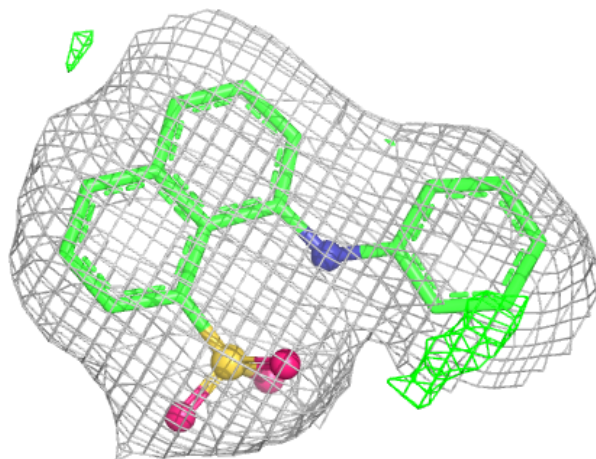
Electron density around 2AN h 206:

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



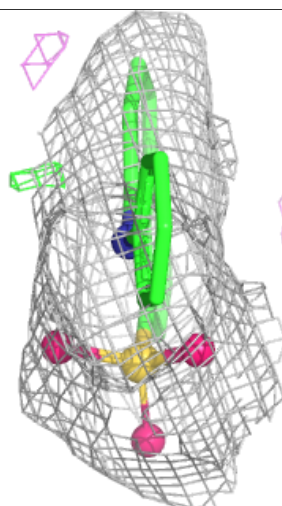
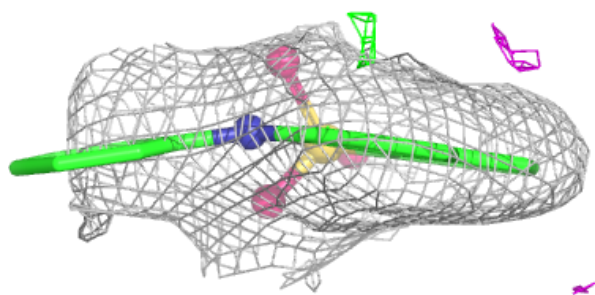
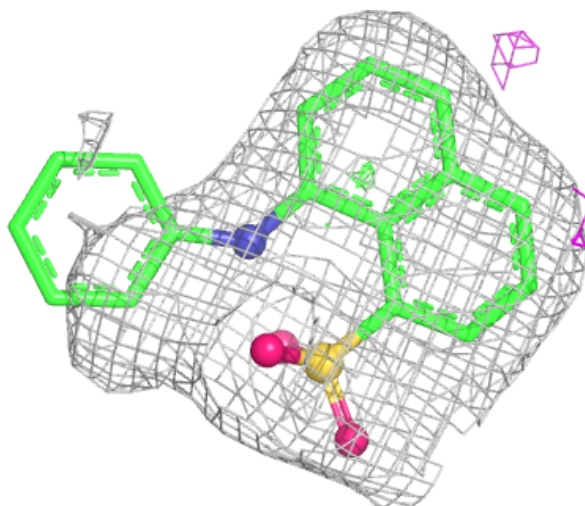
Electron density around 2AN d 201:

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



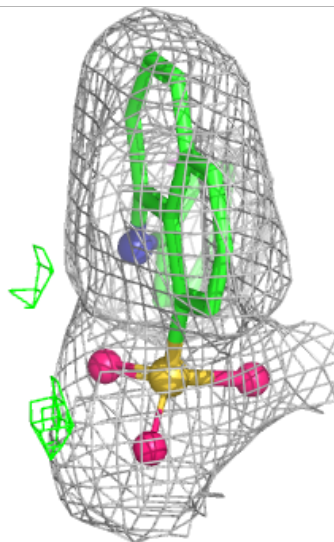
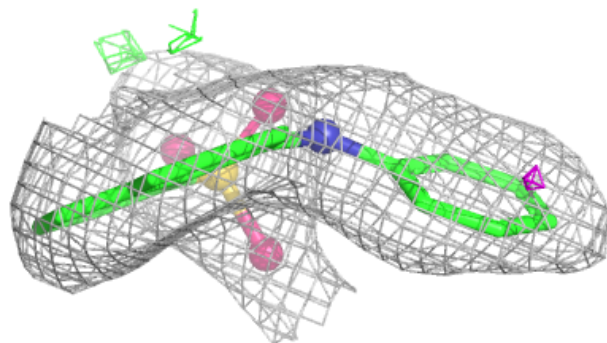
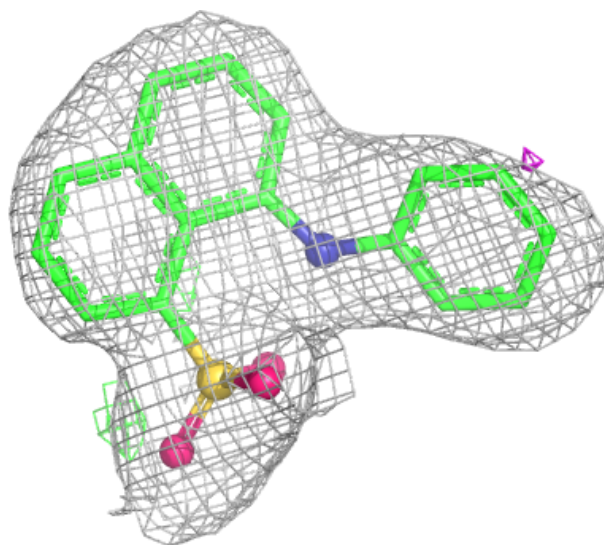
Electron density around 2AN Z 205:

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



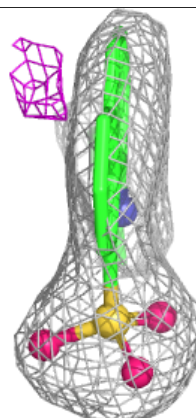
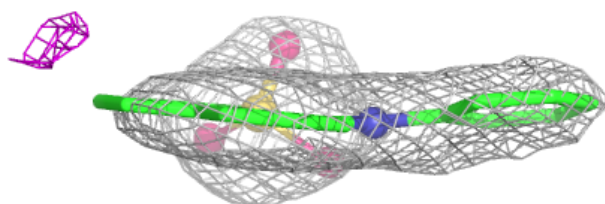
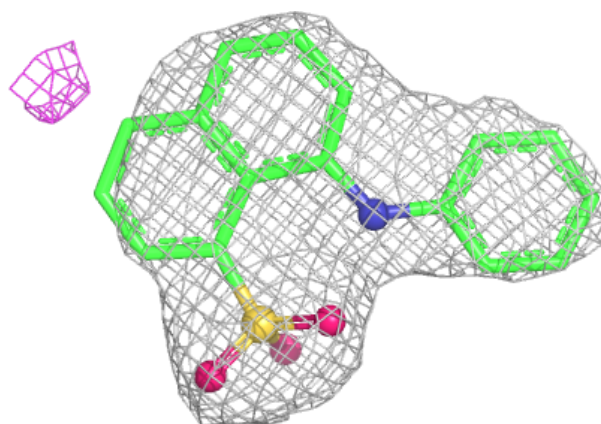
Electron density around 2AN O 203:

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



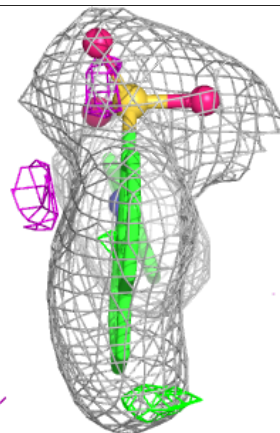
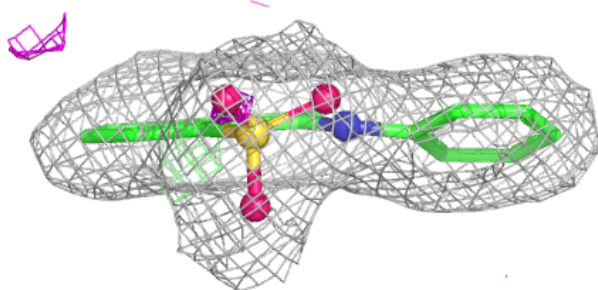
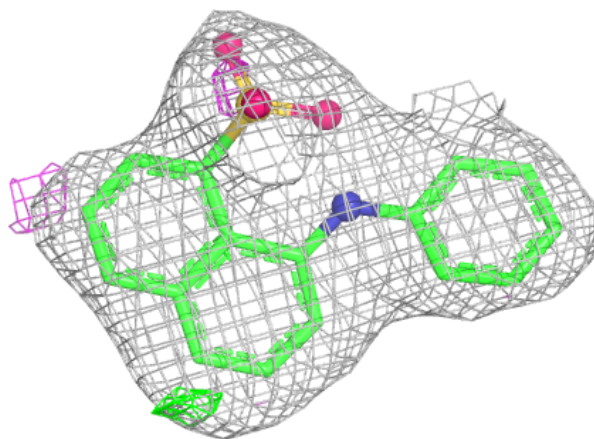
Electron density around 2AN Y 202:

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



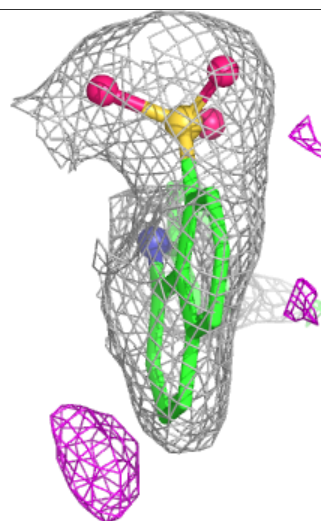
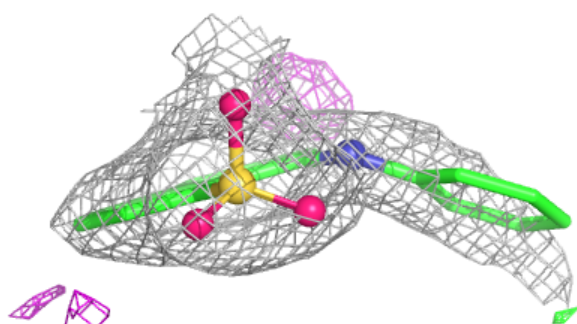
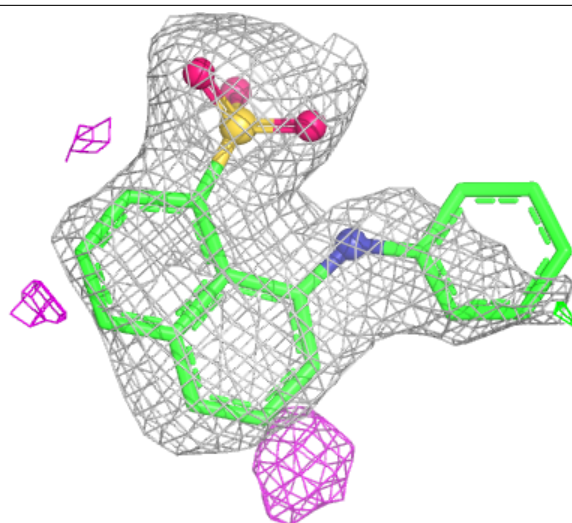
Electron density around 2AN j 201:

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



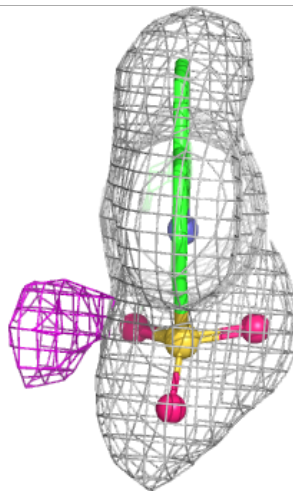
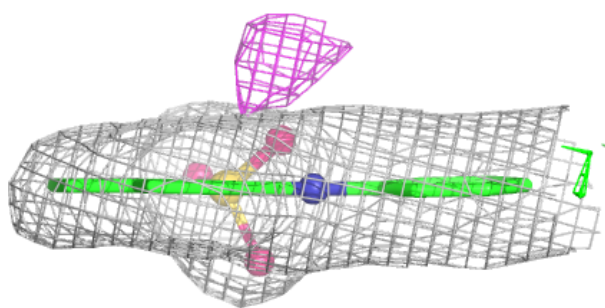
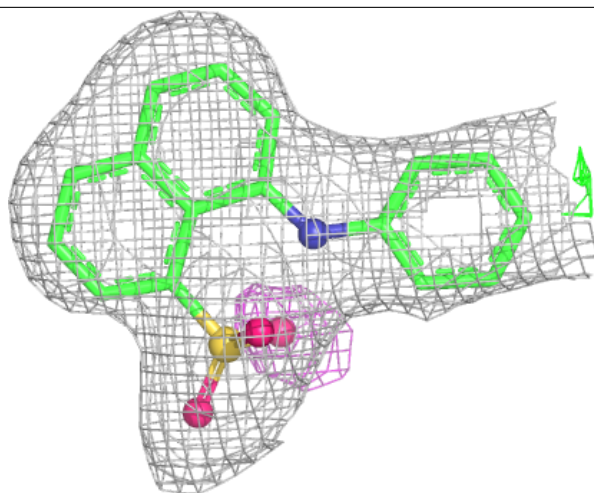
Electron density around 2AN E 203:

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



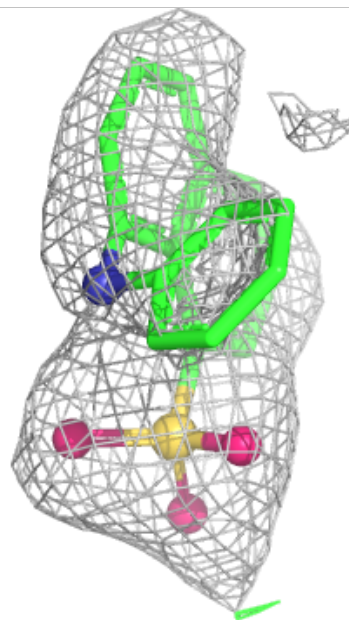
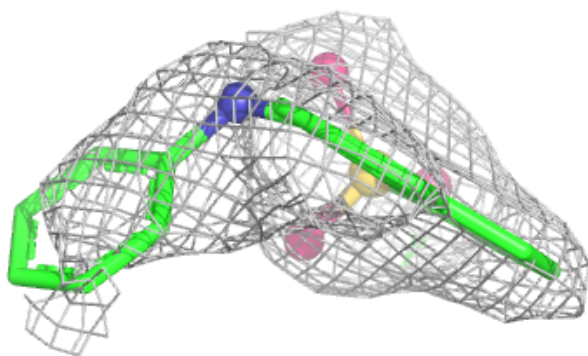
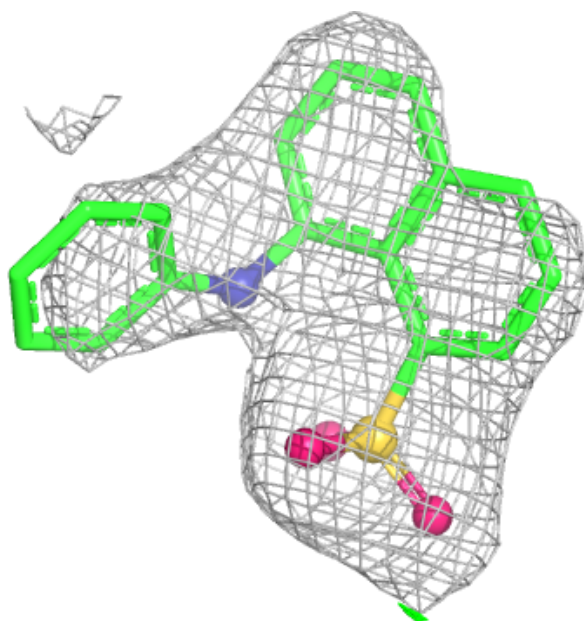
Electron density around 2AN V 206:

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



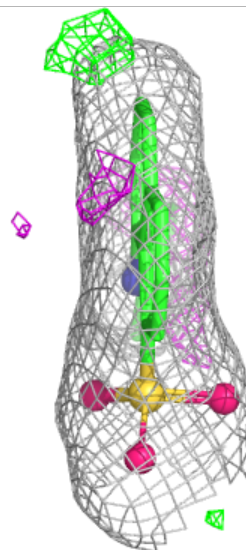
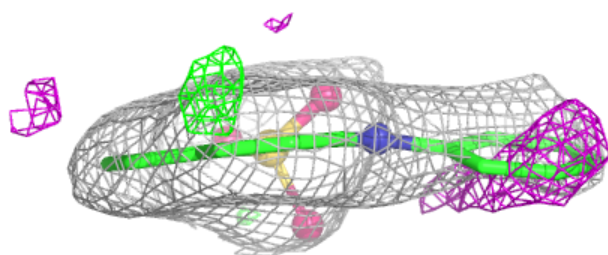
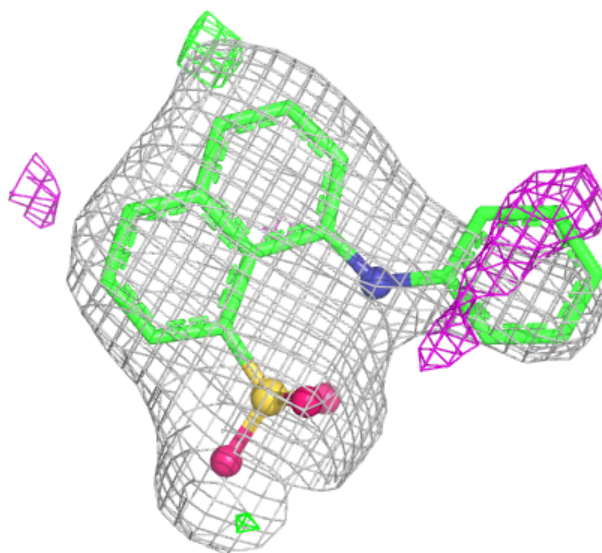
Electron density around 2AN Q 203:

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



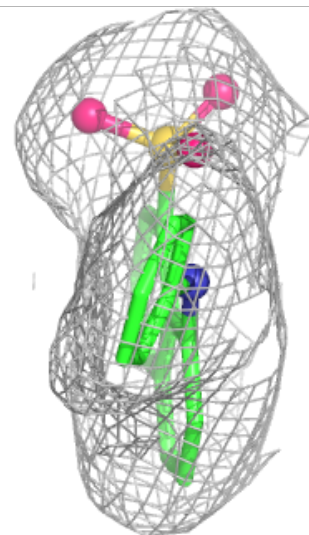
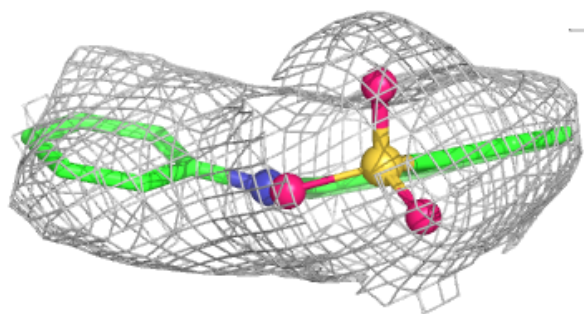
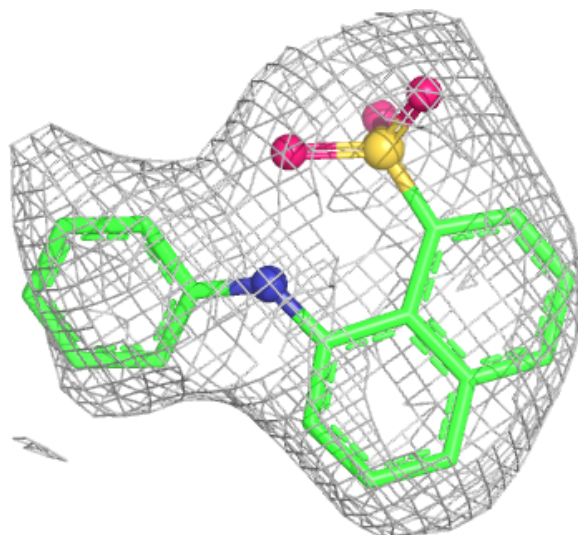
Electron density around 2AN A 201:

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



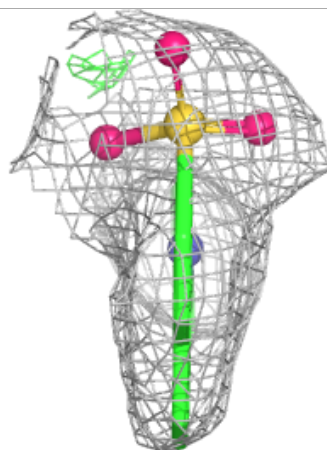
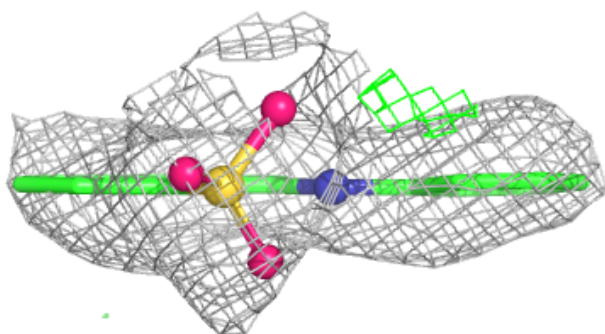
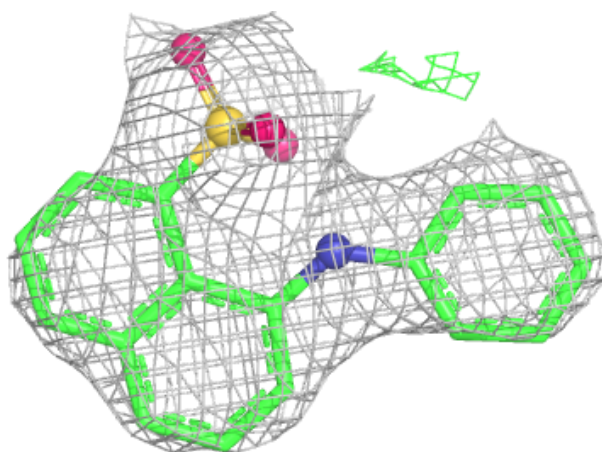
Electron density around 2AN D 203:

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



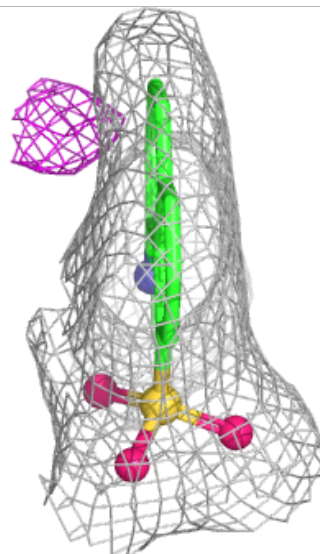
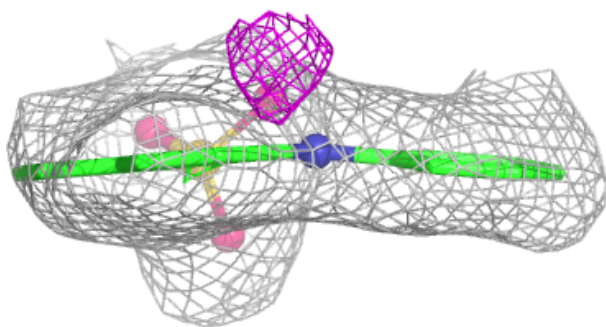
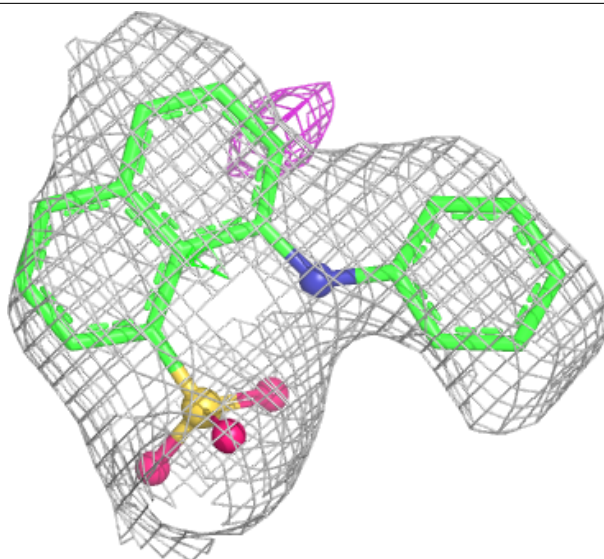
Electron density around 2AN Z 202:

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



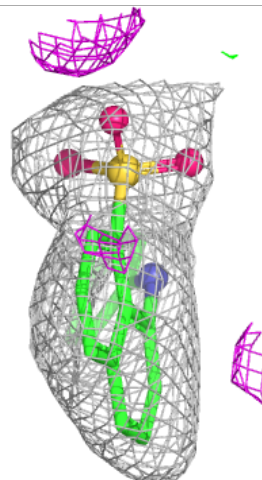
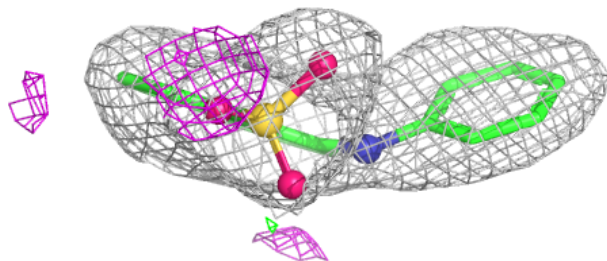
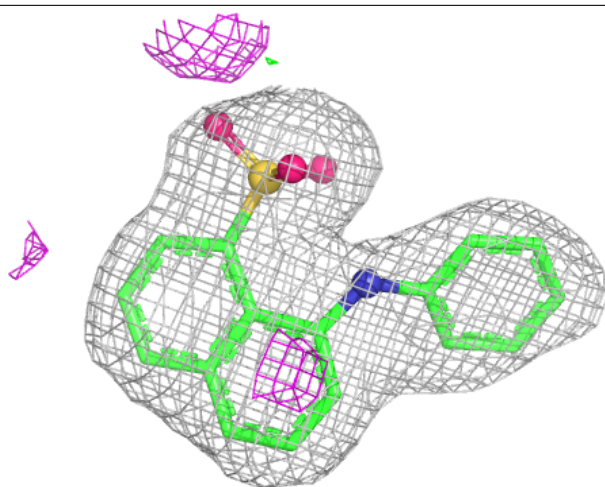
Electron density around 2AN F 201:

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



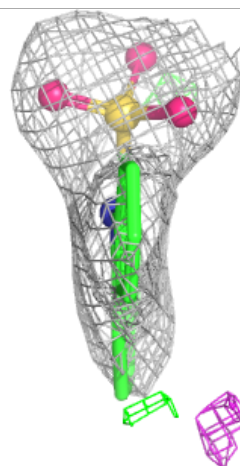
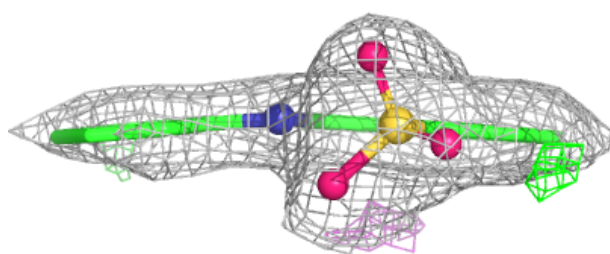
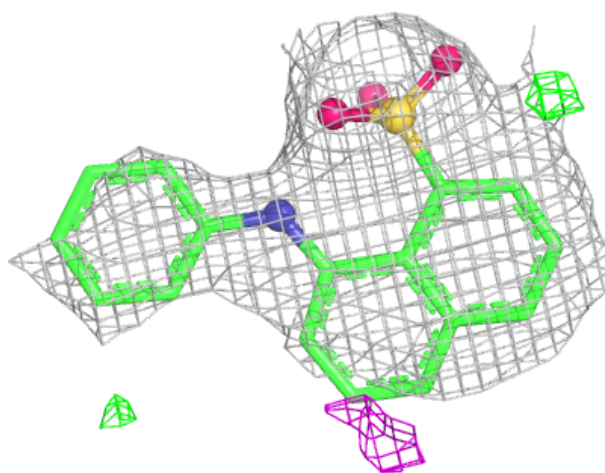
Electron density around 2AN G 201:

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



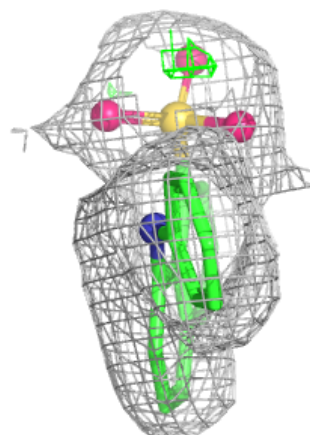
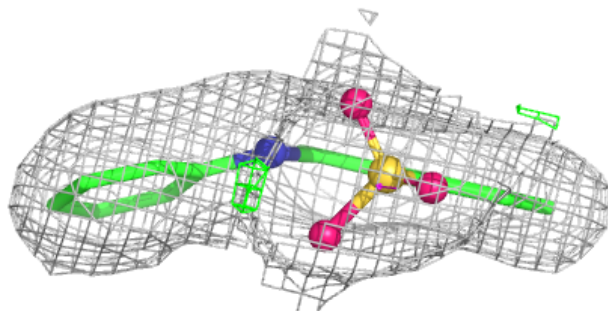
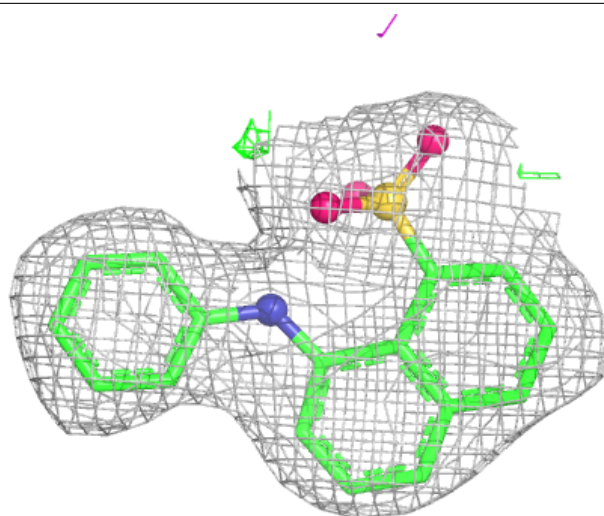
Electron density around 2AN g 201:

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



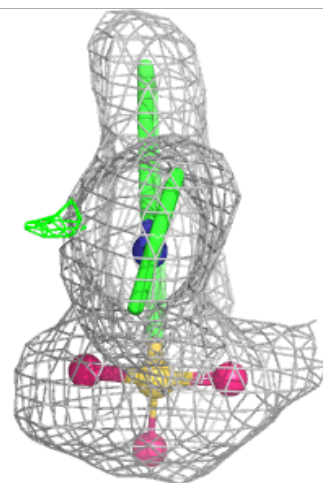
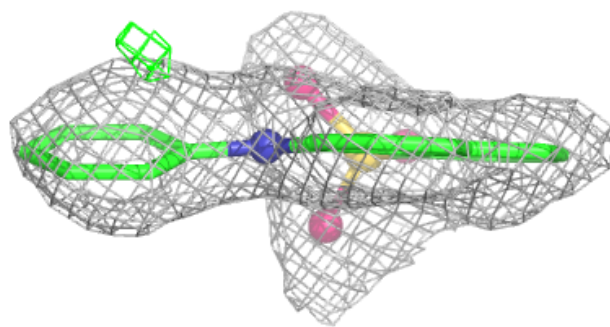
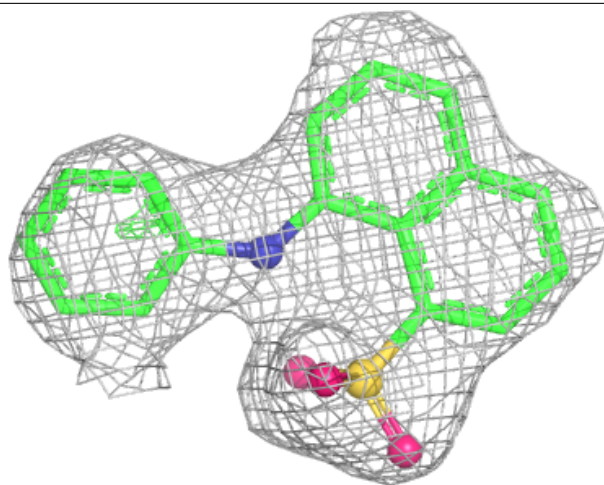
Electron density around 2AN X 205:

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



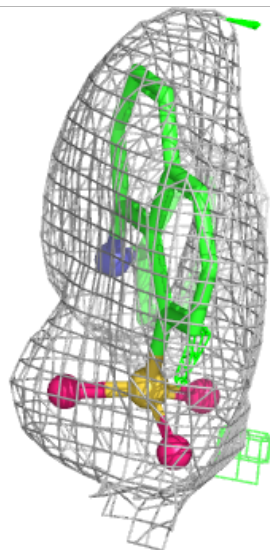
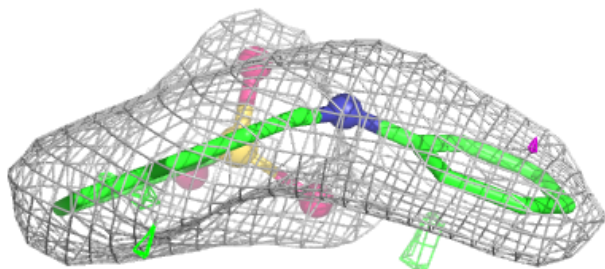
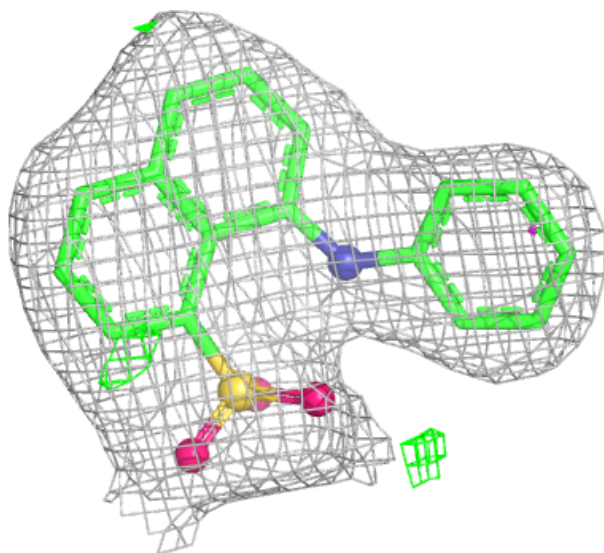
Electron density around 2AN B 204:

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



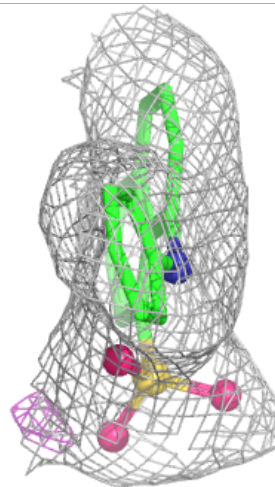
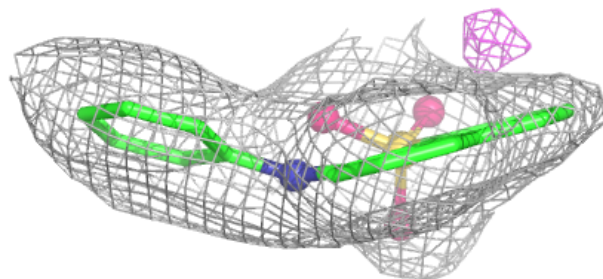
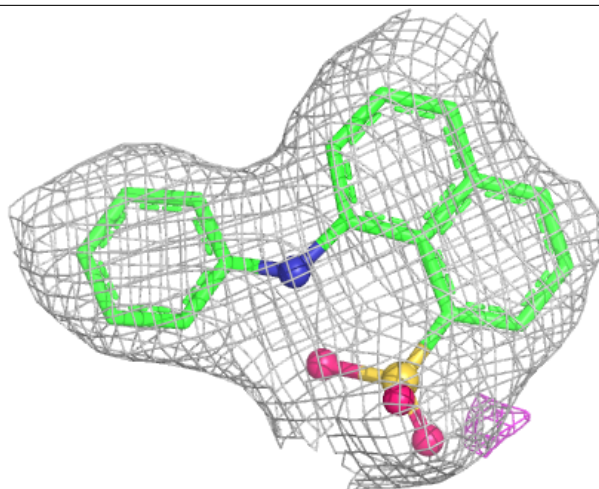
Electron density around 2AN D 202:

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



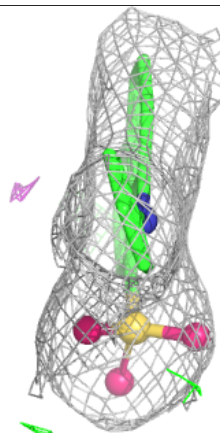
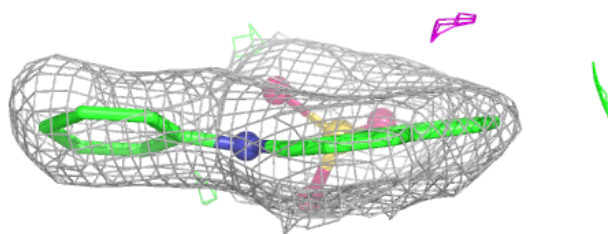
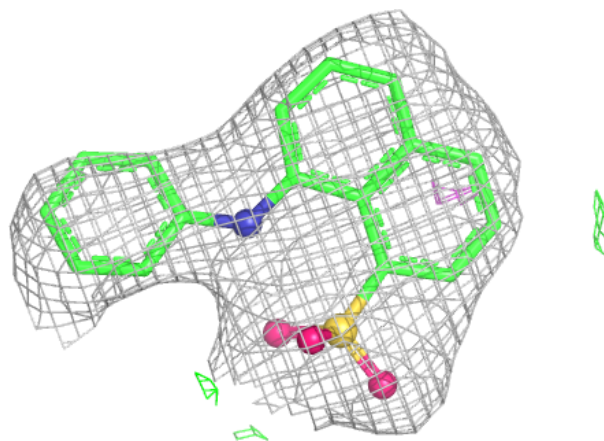
Electron density around 2AN d 202:

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



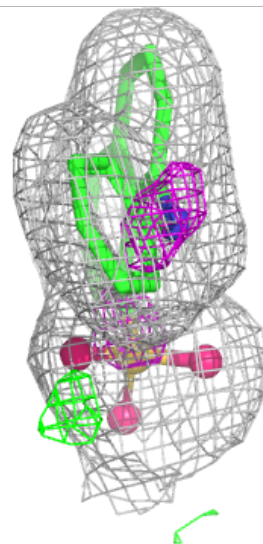
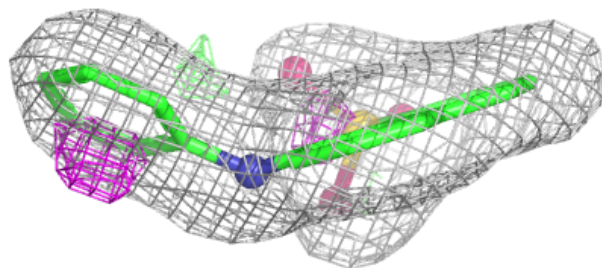
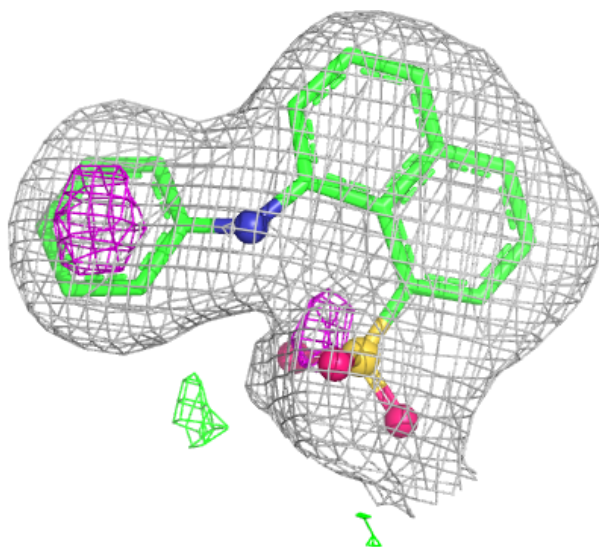
Electron density around 2AN Z 203:

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



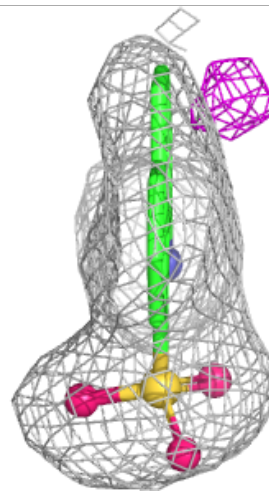
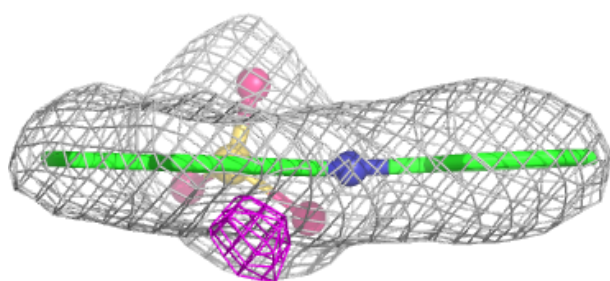
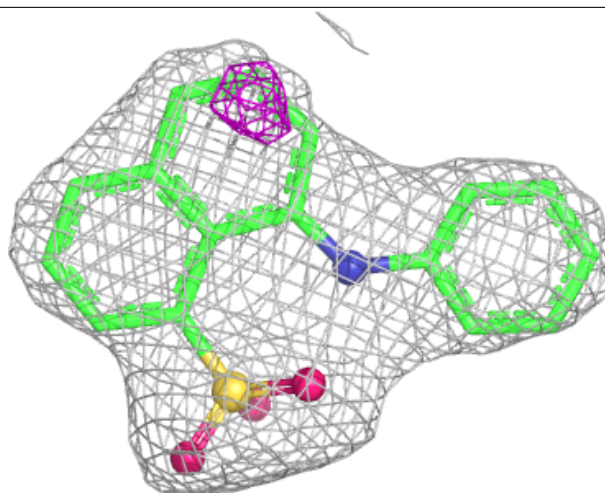
Electron density around 2AN R 202:

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



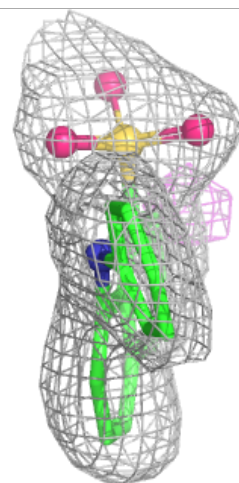
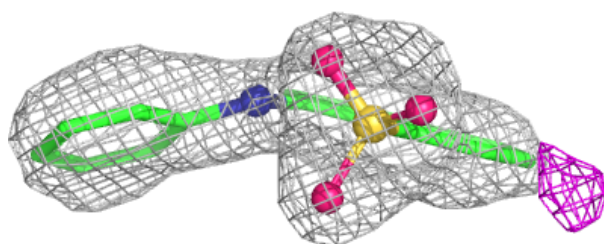
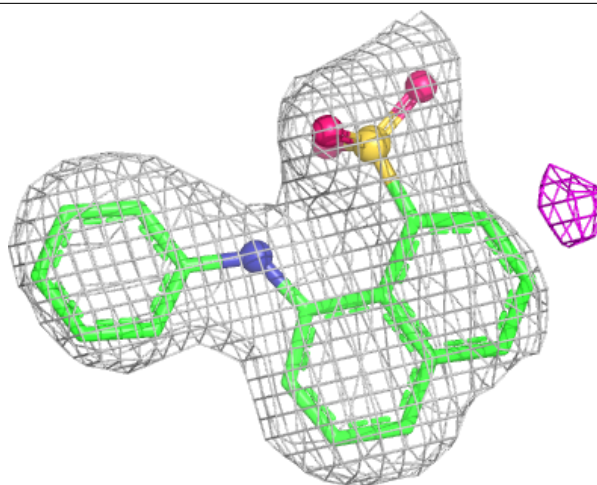
Electron density around 2AN L 204:

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



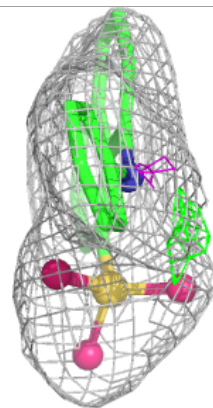
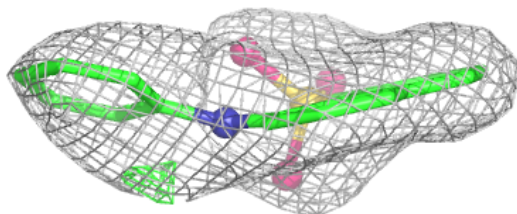
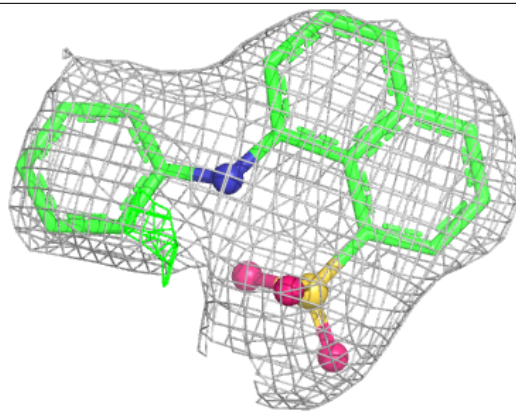
Electron density around 2AN i 201:

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



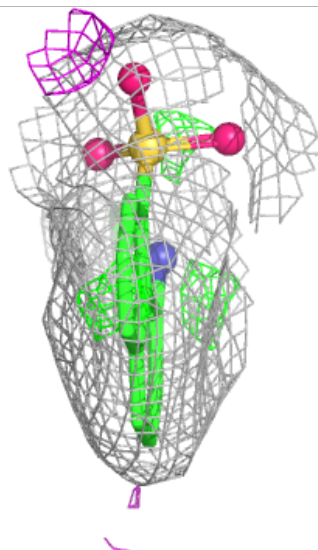
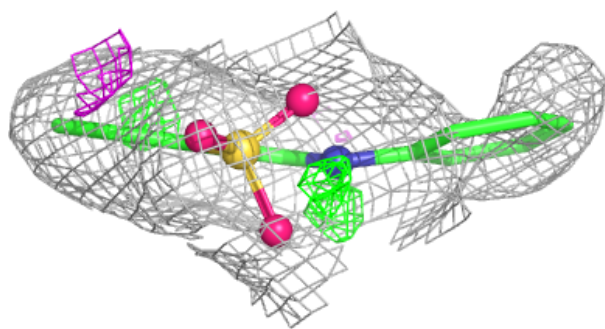
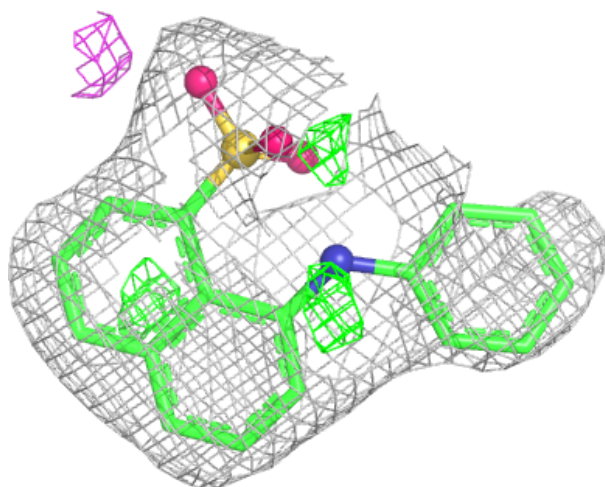
Electron density around 2AN b 202:

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



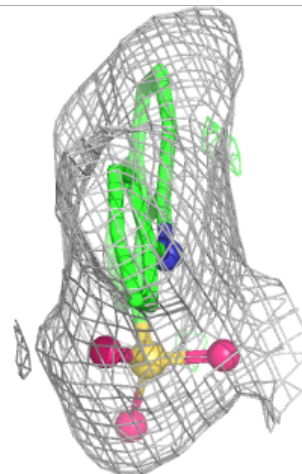
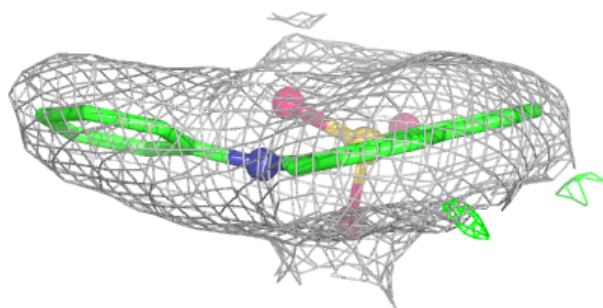
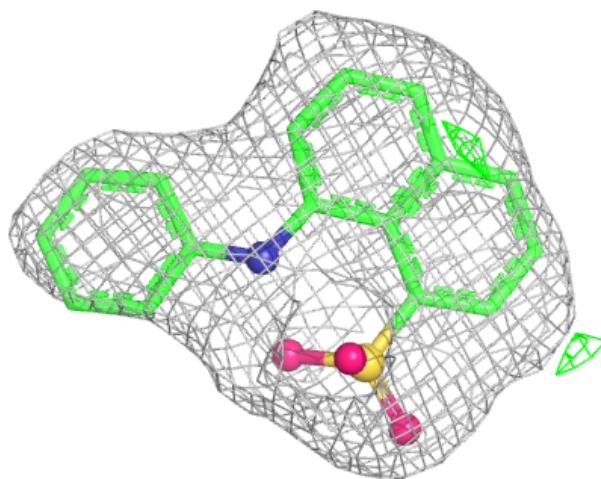
Electron density around 2AN h 204:

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



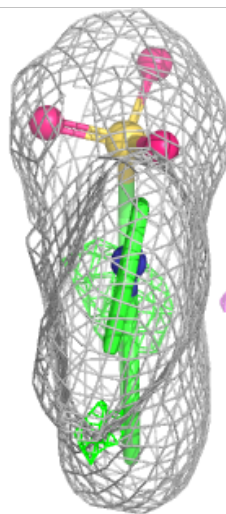
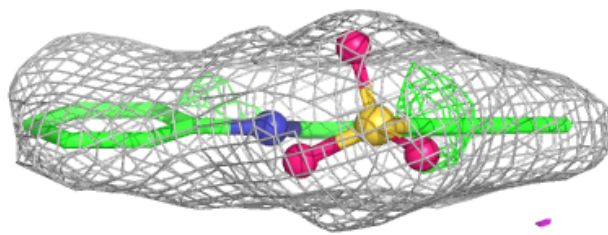
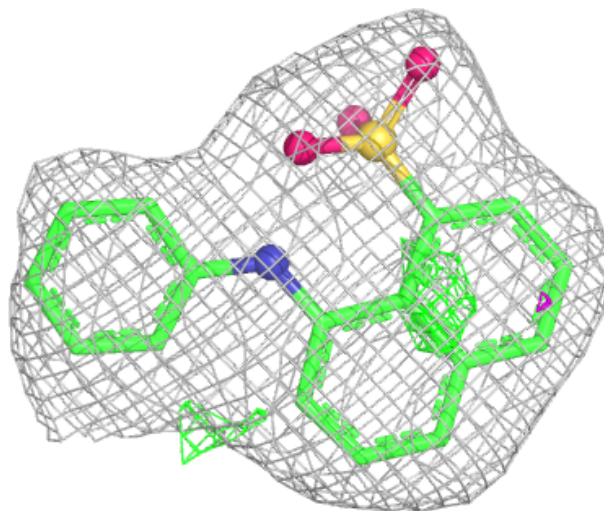
Electron density around 2AN b 204:

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



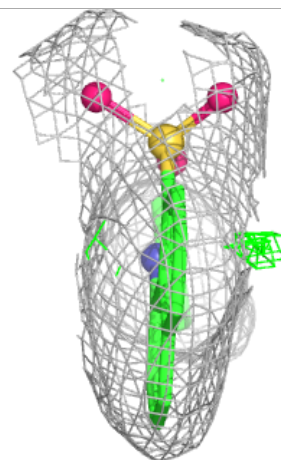
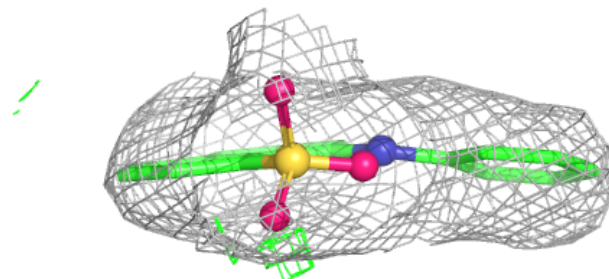
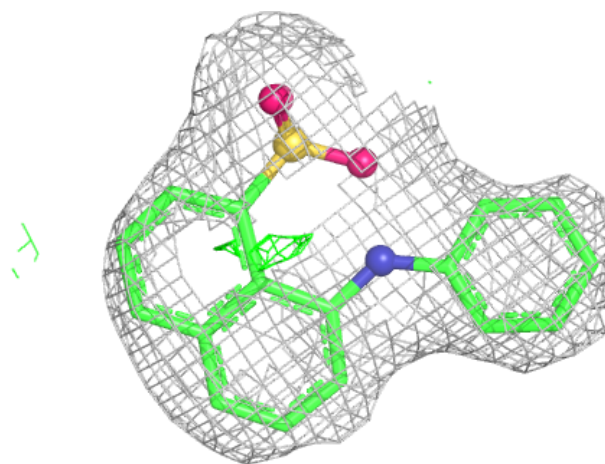
Electron density around 2AN P 203:

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



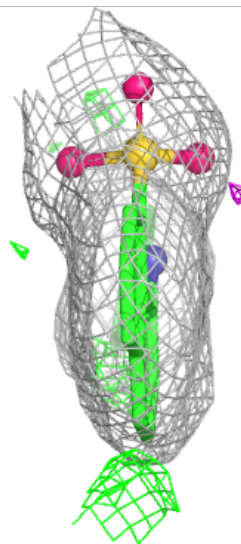
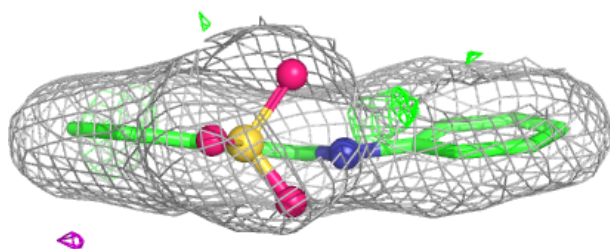
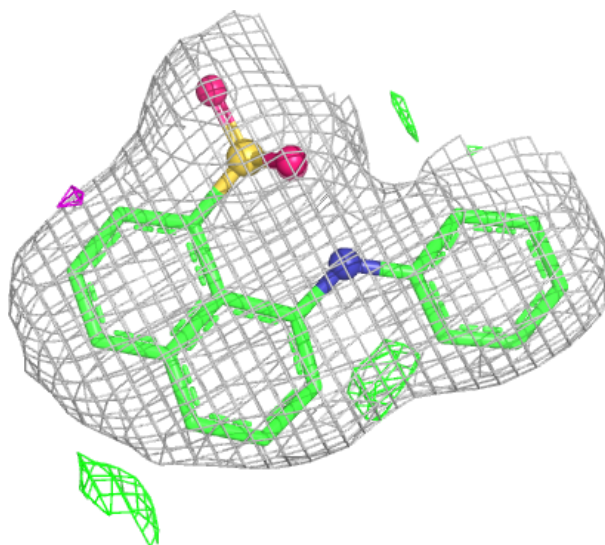
Electron density around 2AN R 203:

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



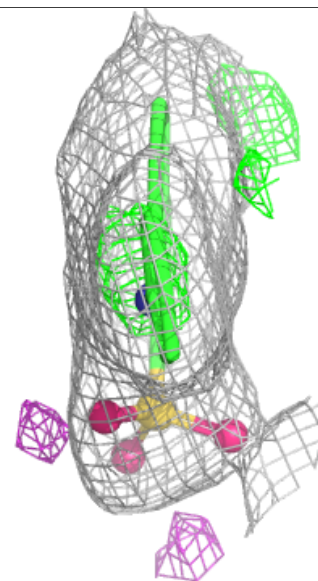
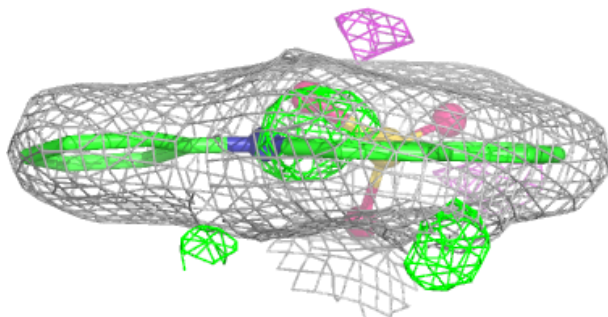
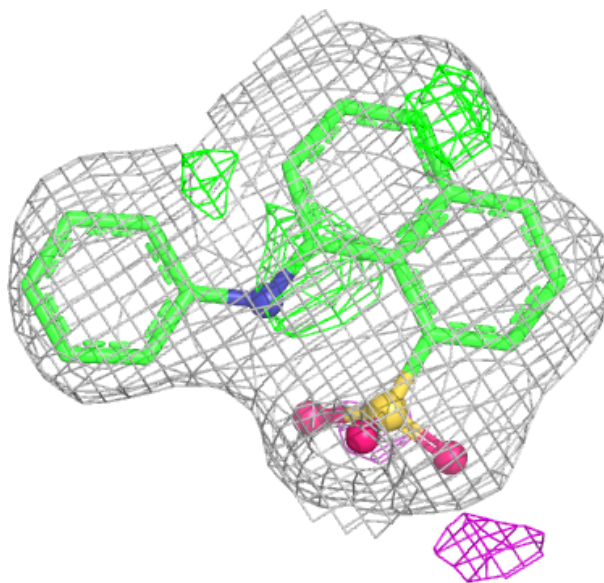
Electron density around 2AN b 201:

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



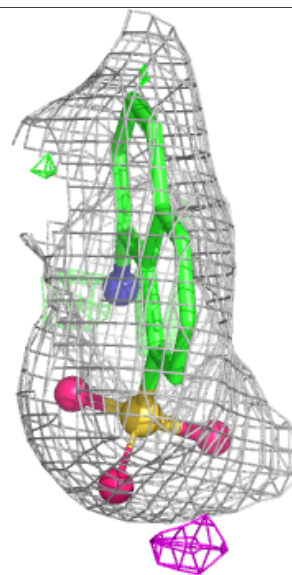
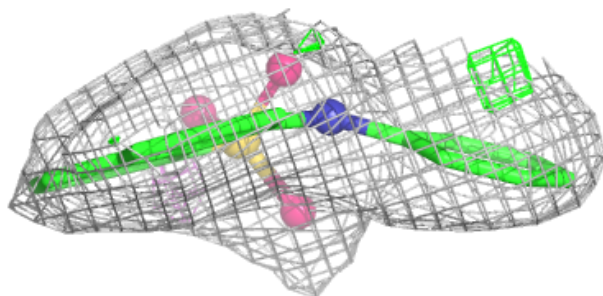
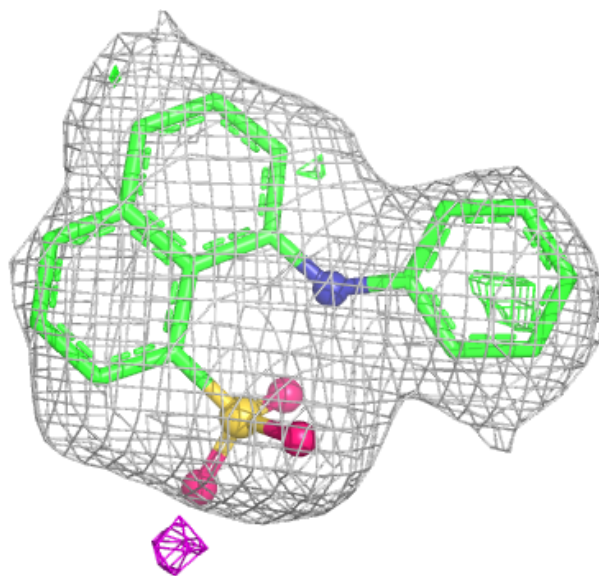
Electron density around 2AN j 204:

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



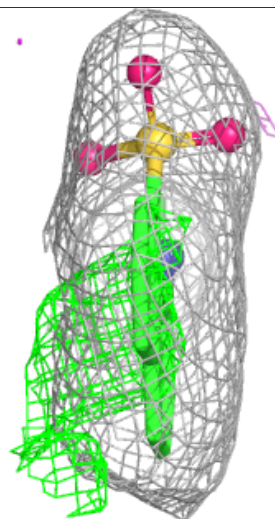
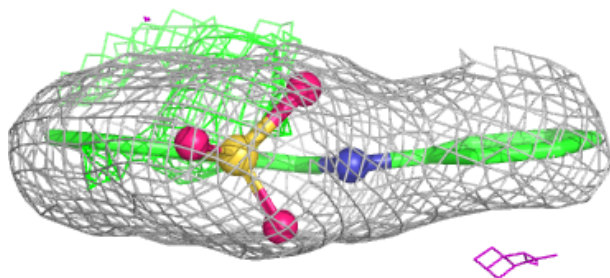
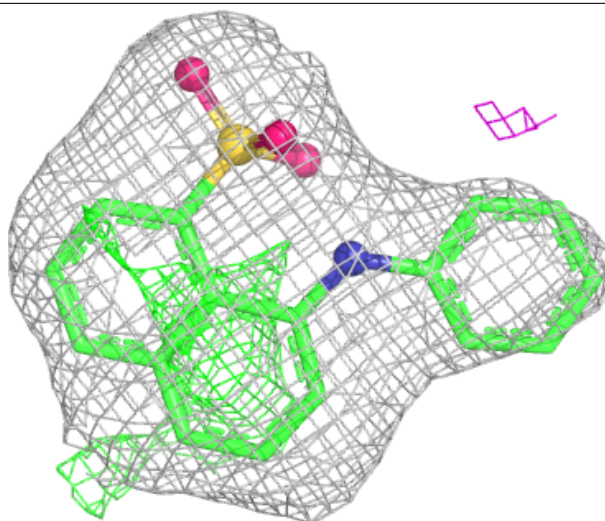
Electron density around 2AN F 205:

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



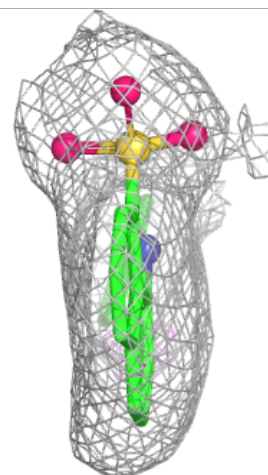
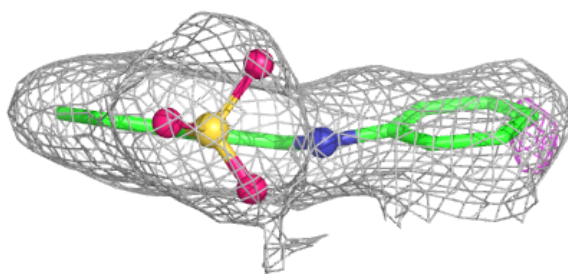
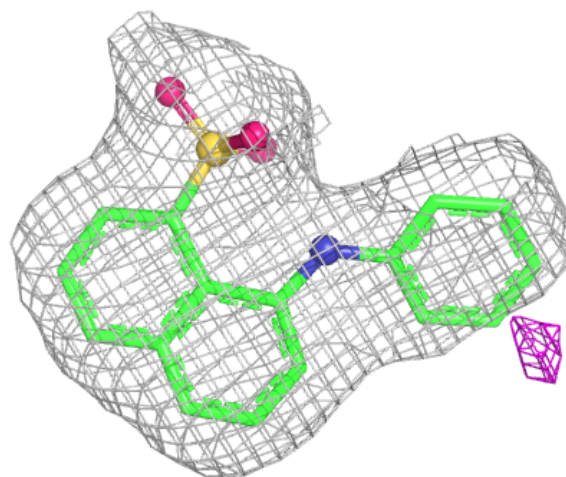
Electron density around 2AN J 201:

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



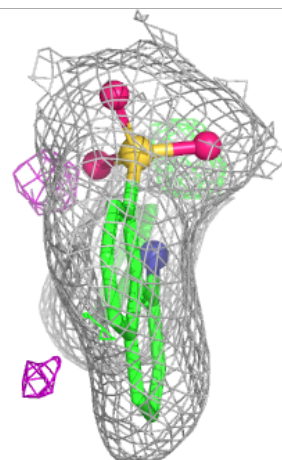
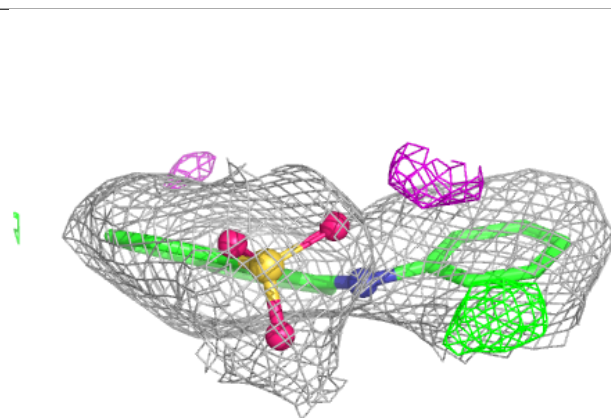
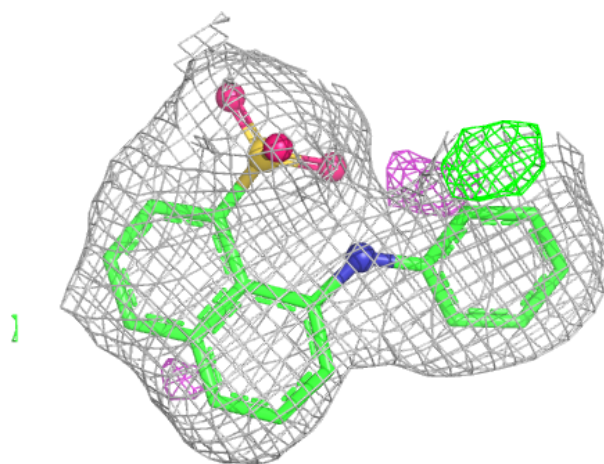
Electron density around 2AN E 201:

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



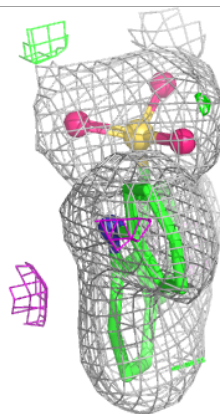
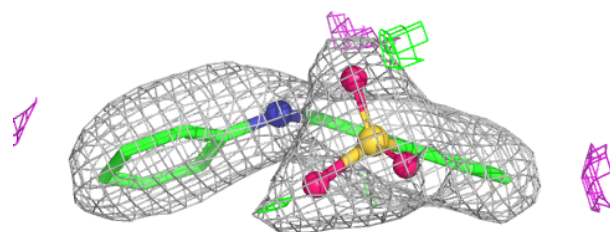
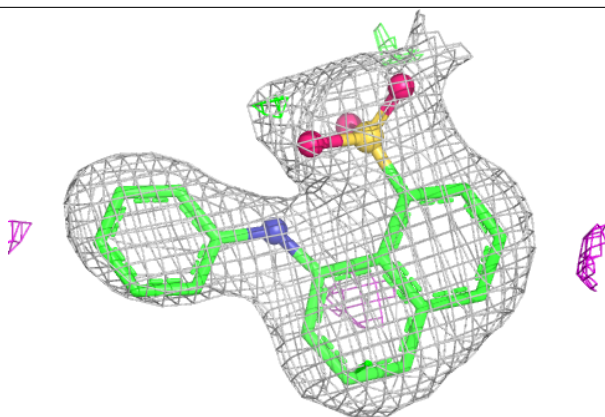
Electron density around 2AN B 202:

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



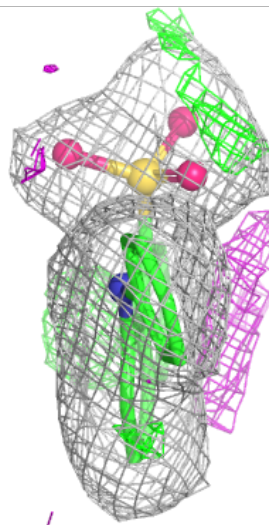
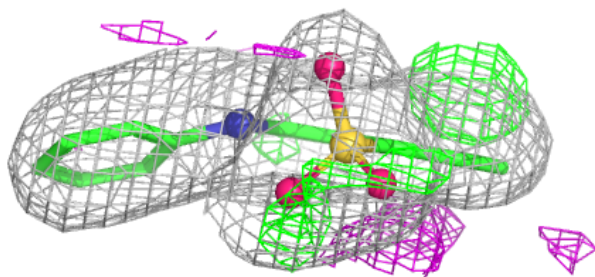
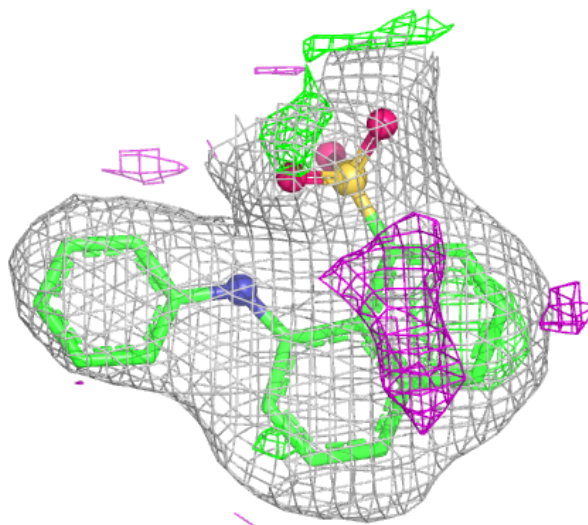
Electron density around 2AN T 202:

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



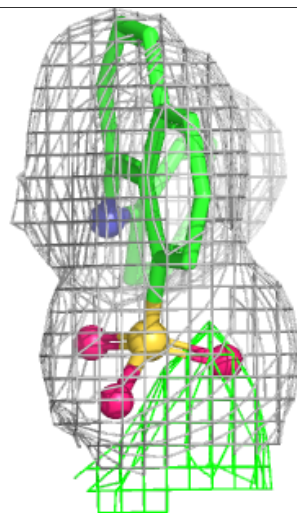
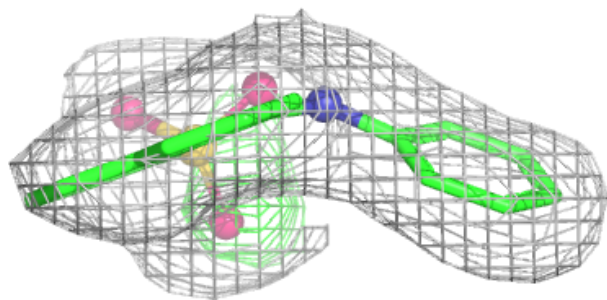
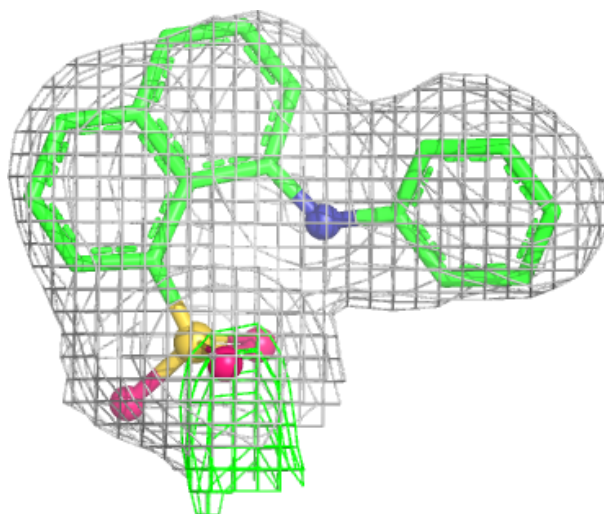
Electron density around 2AN h 203:

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



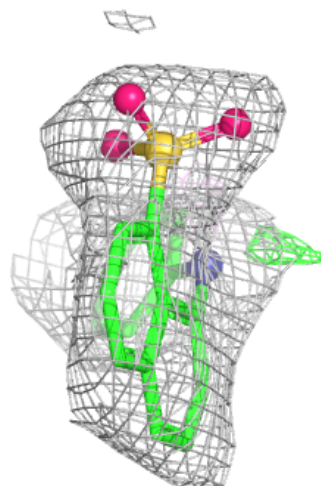
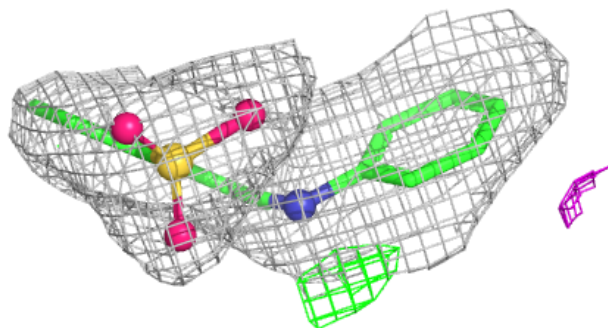
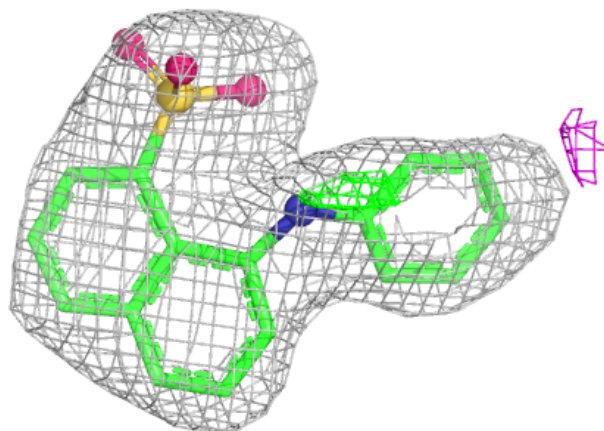
Electron density around 2AN B 205:

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



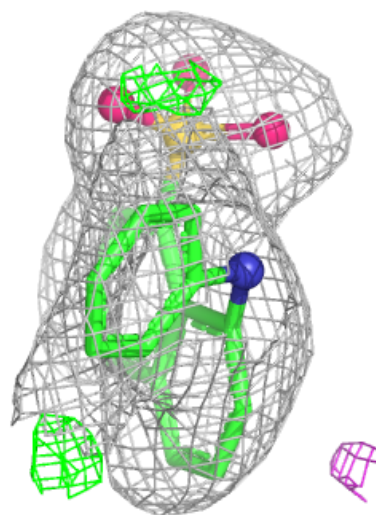
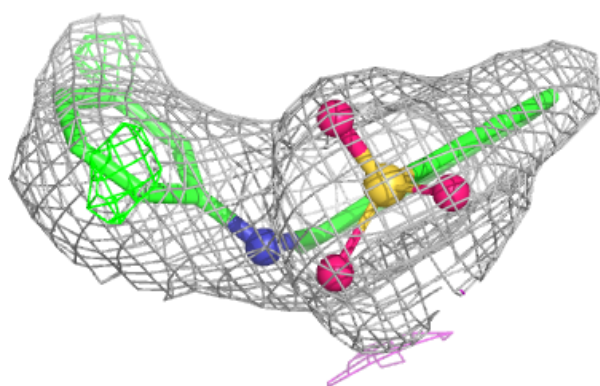
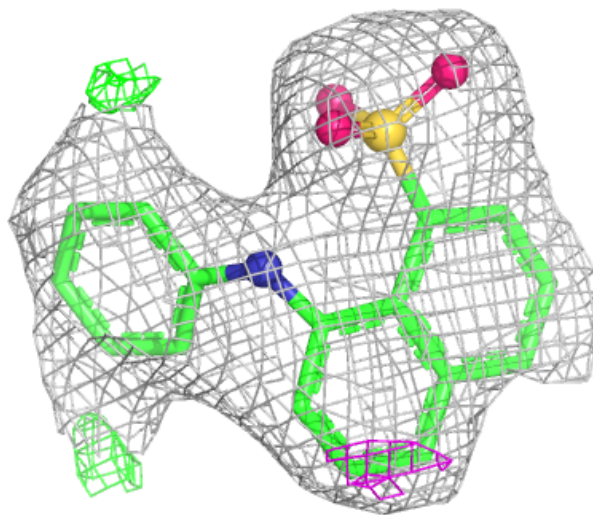
Electron density around 2AN A 202:

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



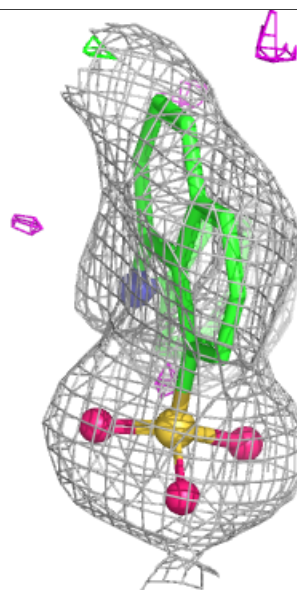
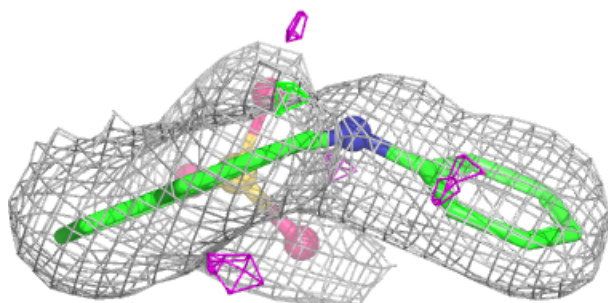
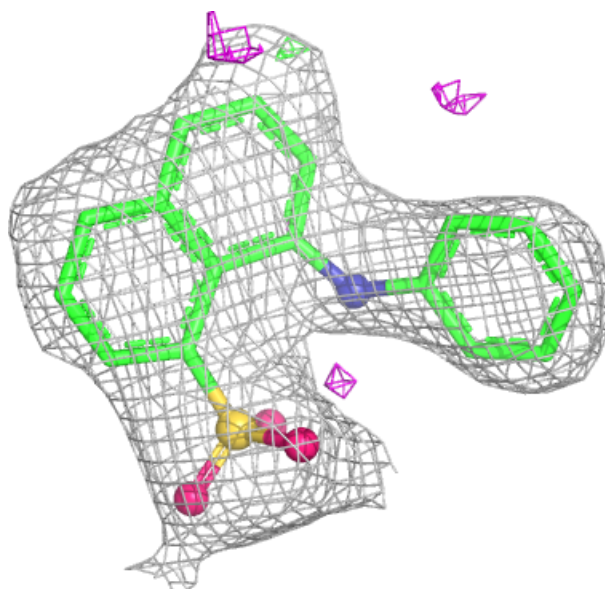
Electron density around 2AN M 203:

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



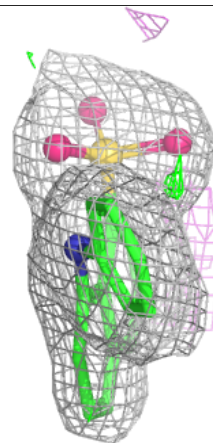
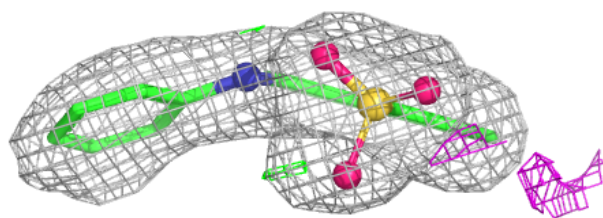
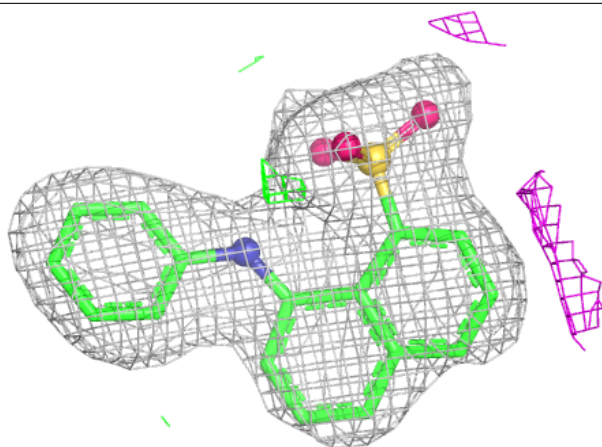
Electron density around 2AN Z 201:

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



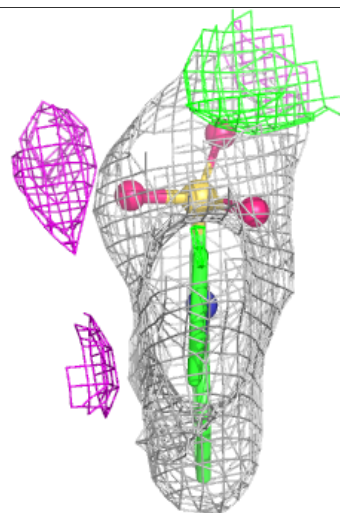
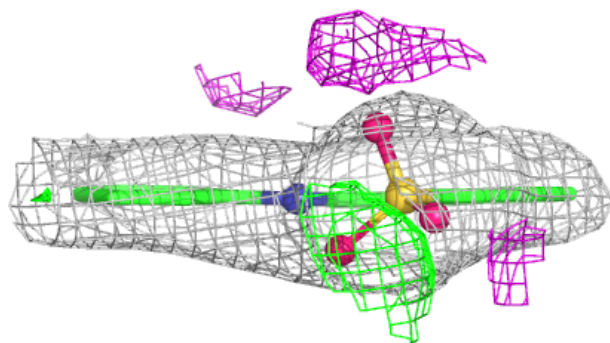
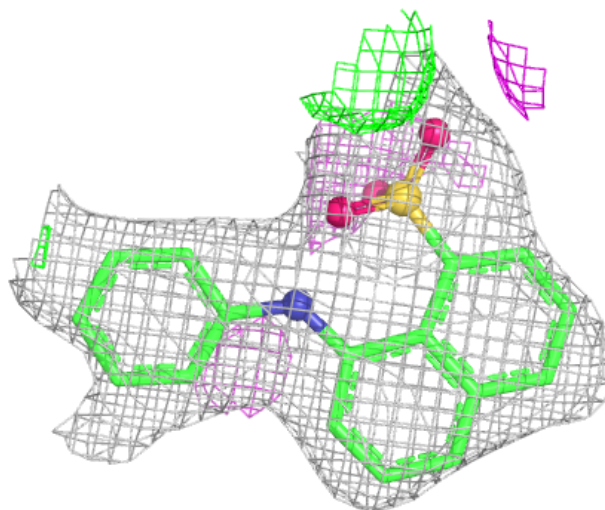
Electron density around 2AN S 202:

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



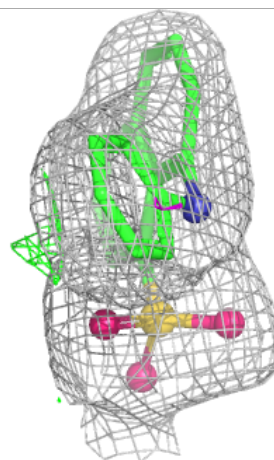
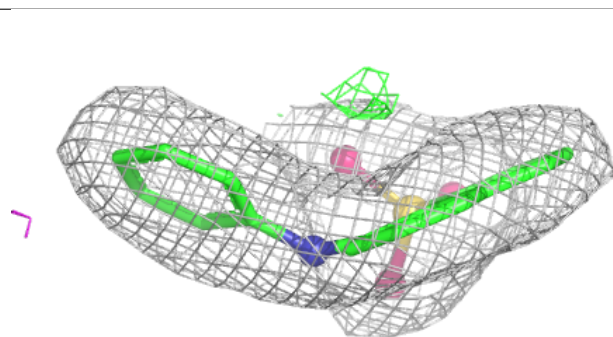
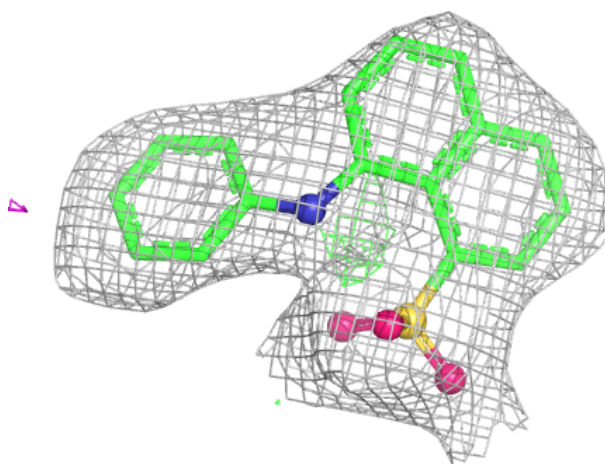
Electron density around 2AN X 204:

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



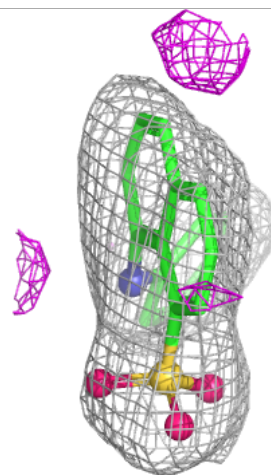
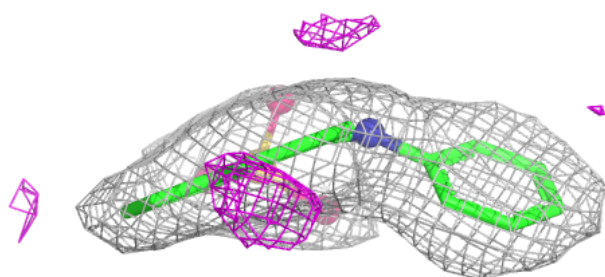
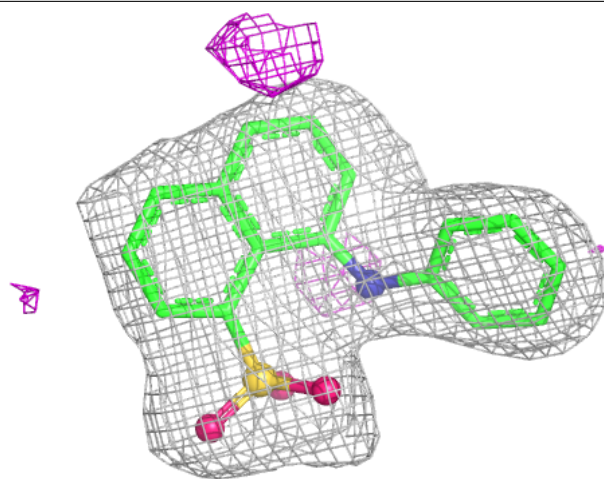
Electron density around 2AN H 202:

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



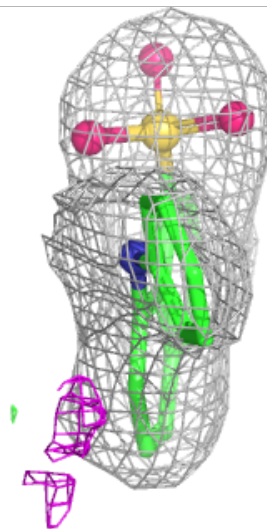
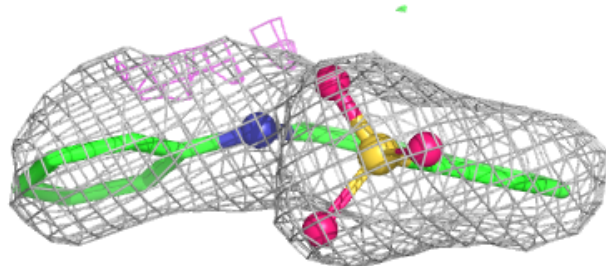
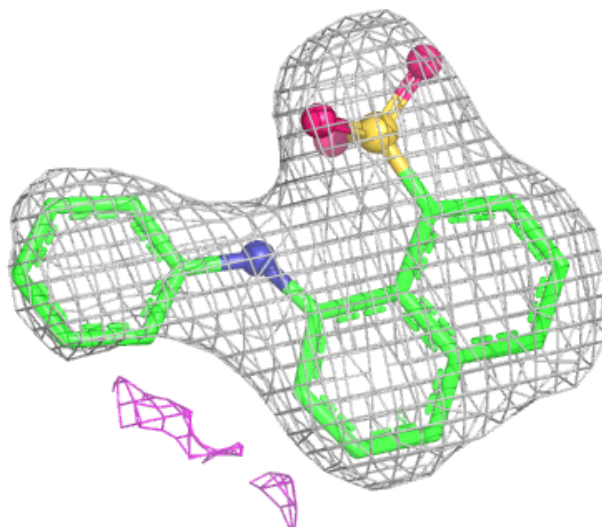
Electron density around 2AN C 201:

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



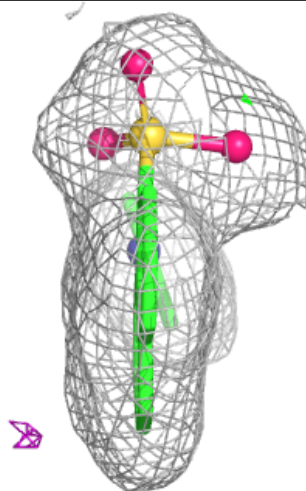
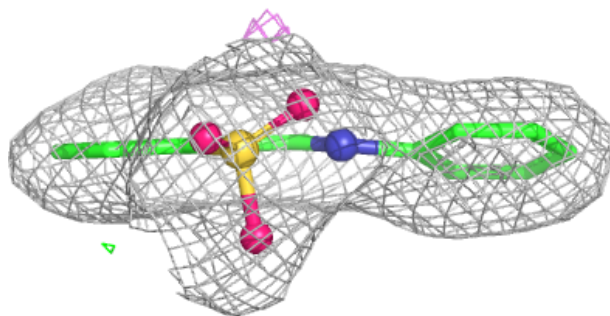
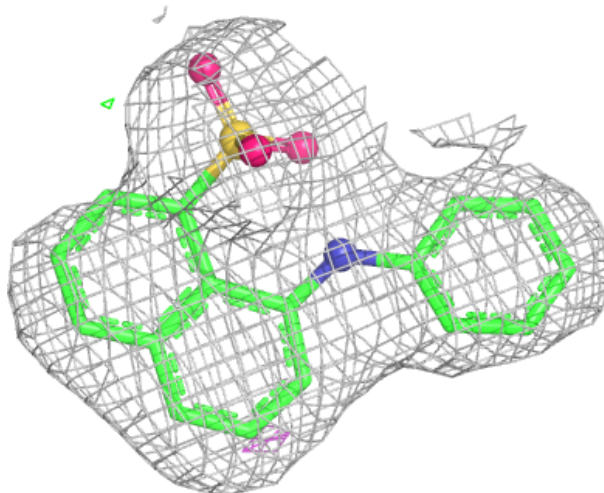
Electron density around 2AN Y 203:

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



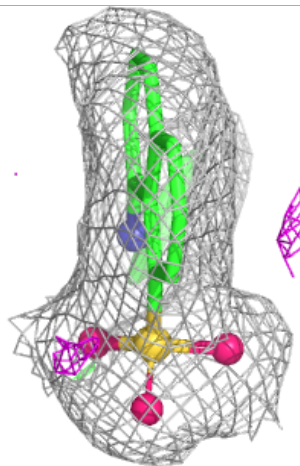
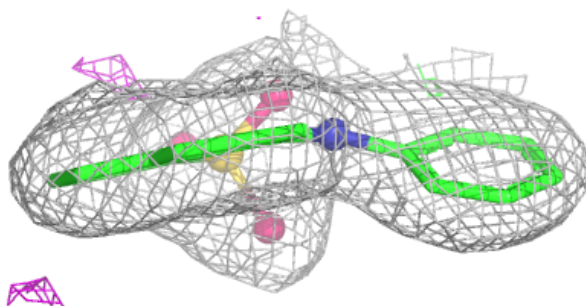
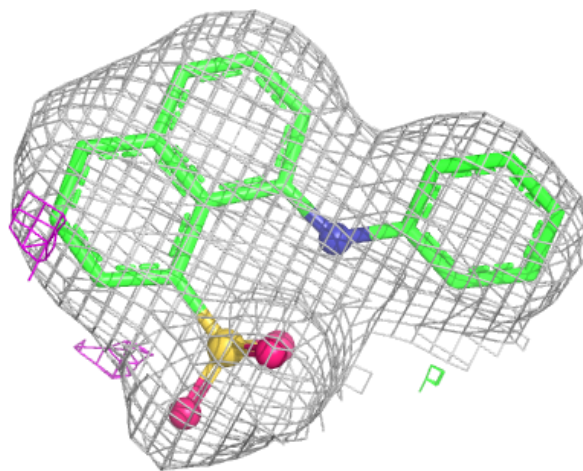
Electron density around 2AN V 201:

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



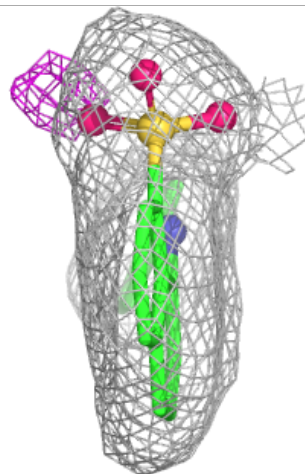
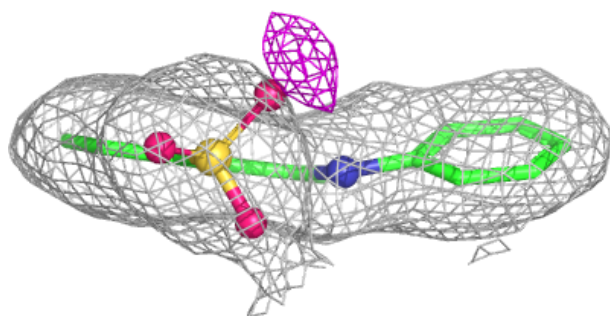
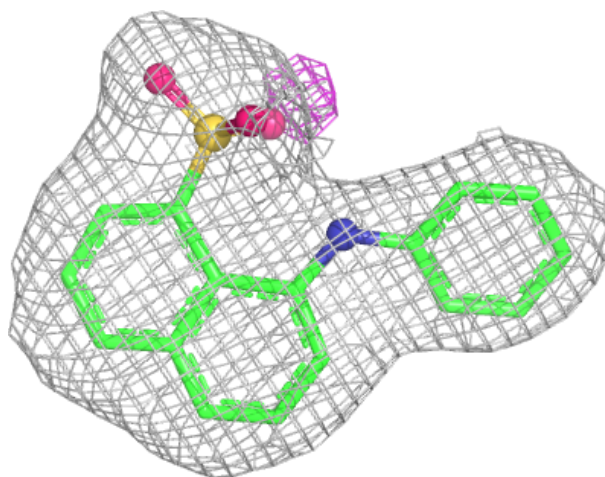
Electron density around 2AN V 203:

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



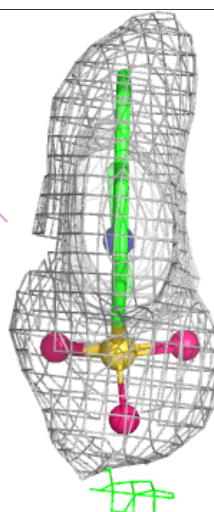
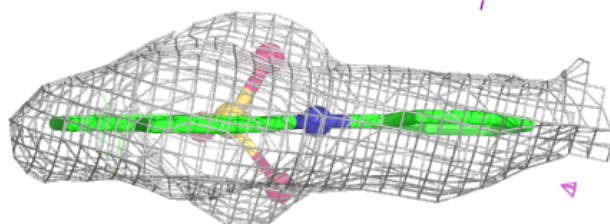
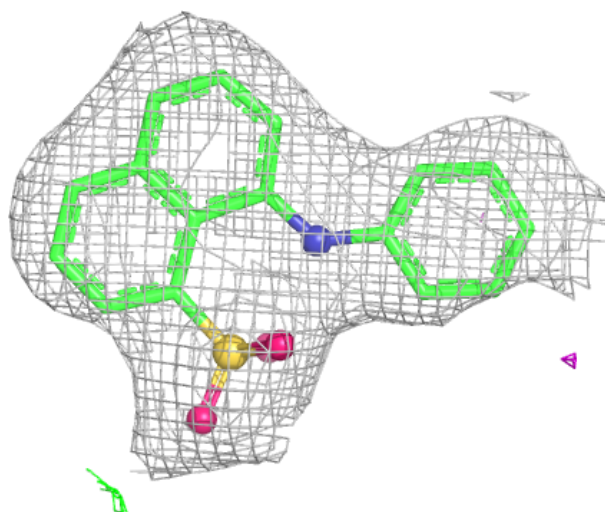
Electron density around 2AN I 202:

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



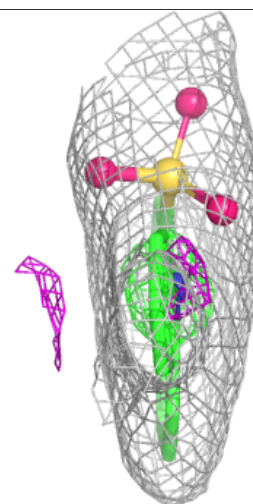
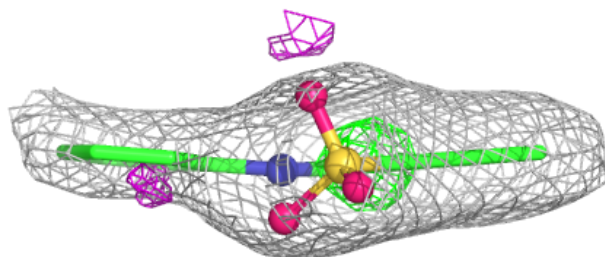
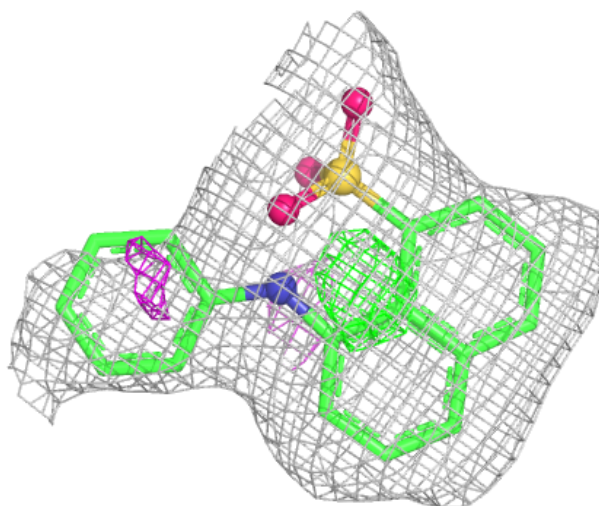
Electron density around 2AN Z 204:

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



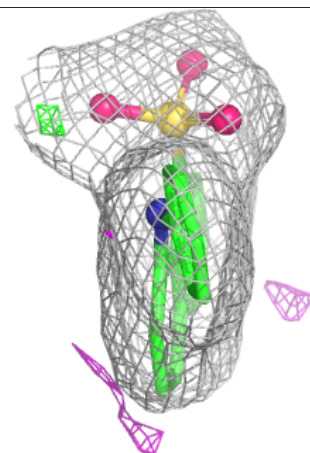
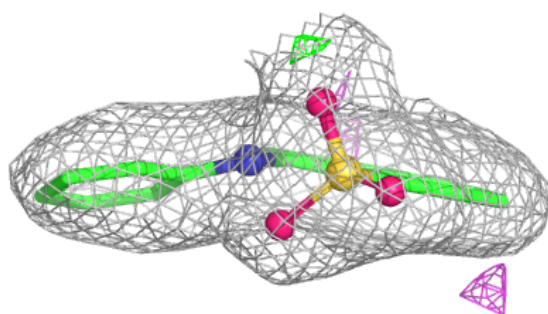
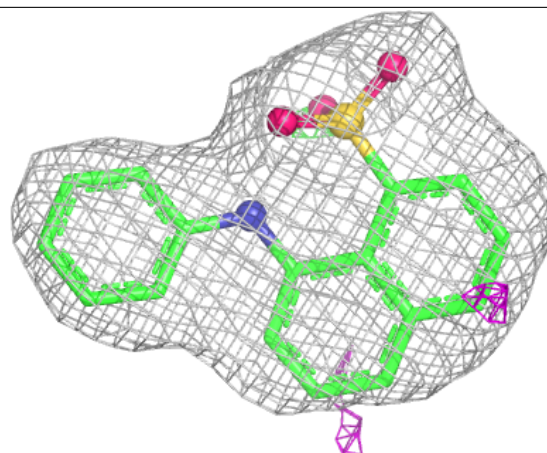
Electron density around 2AN O 201:

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



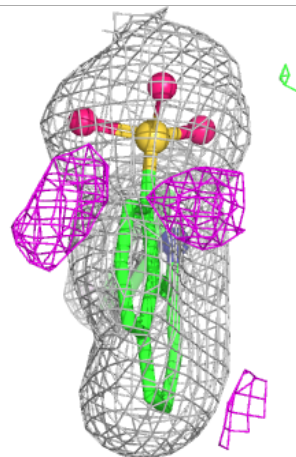
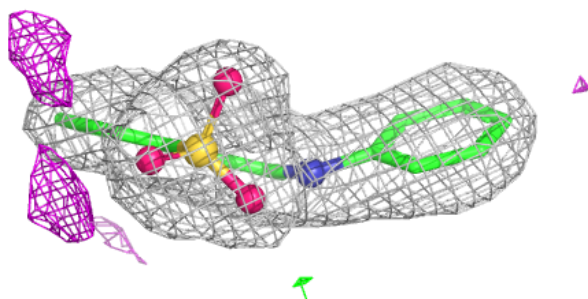
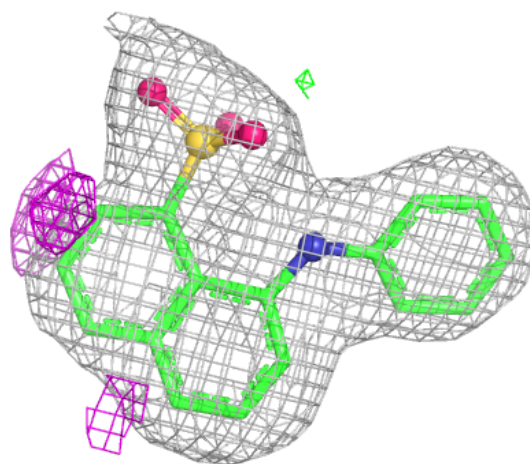
Electron density around 2AN N 201:

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



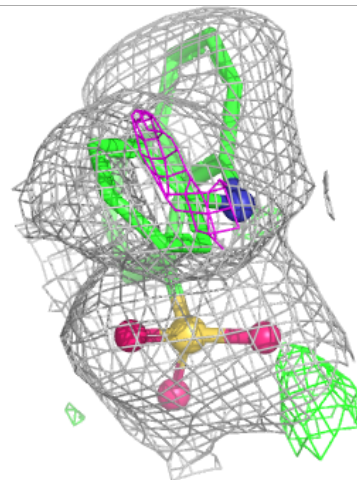
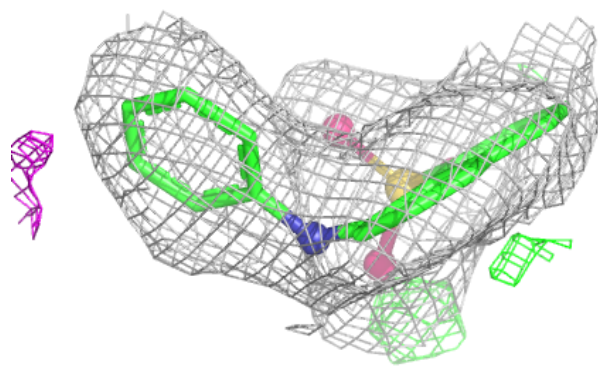
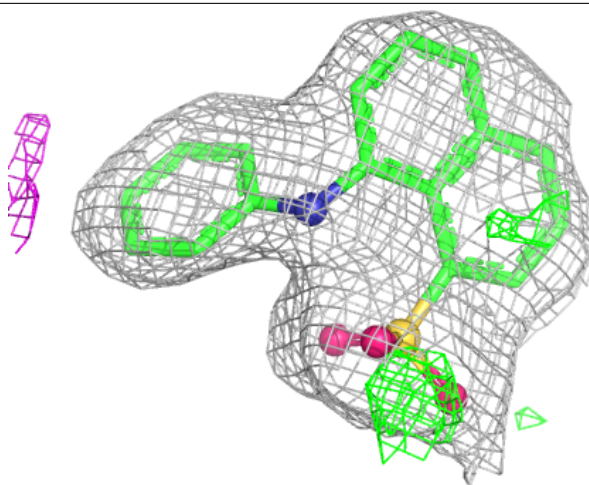
Electron density around 2AN e 201:

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



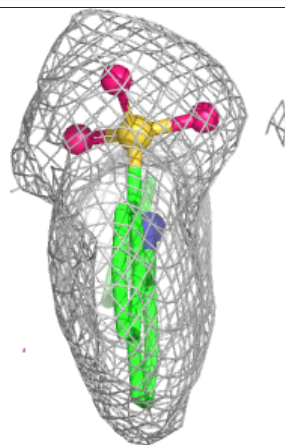
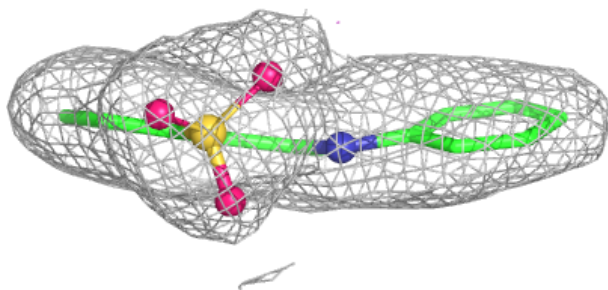
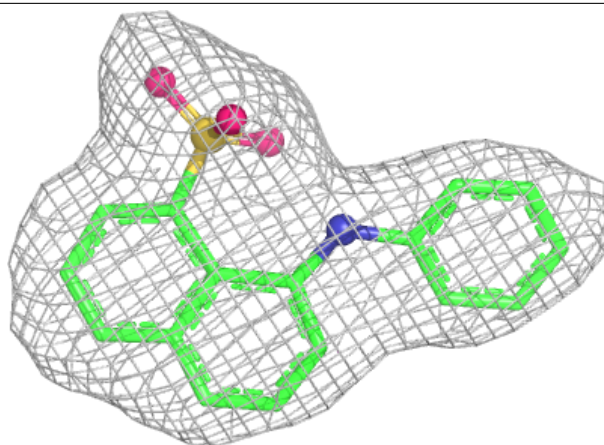
Electron density around 2AN J 203:

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



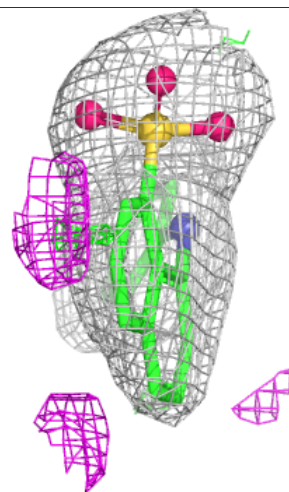
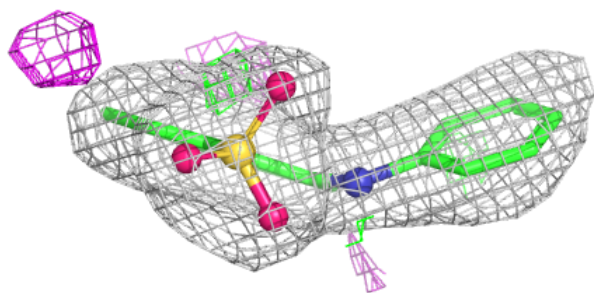
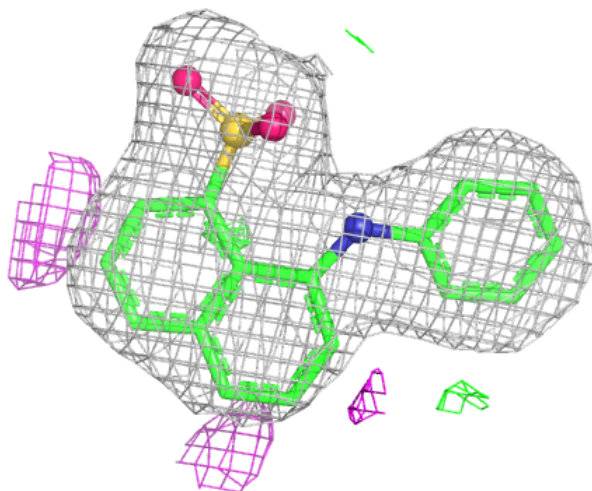
Electron density around 2AN M 201:

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



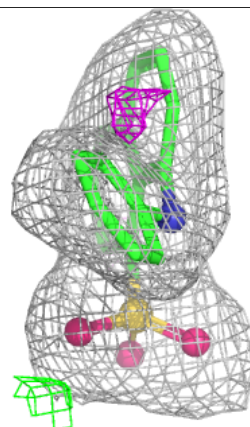
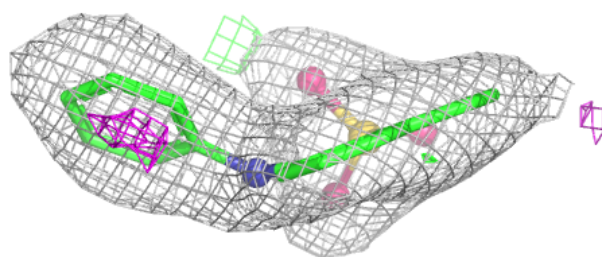
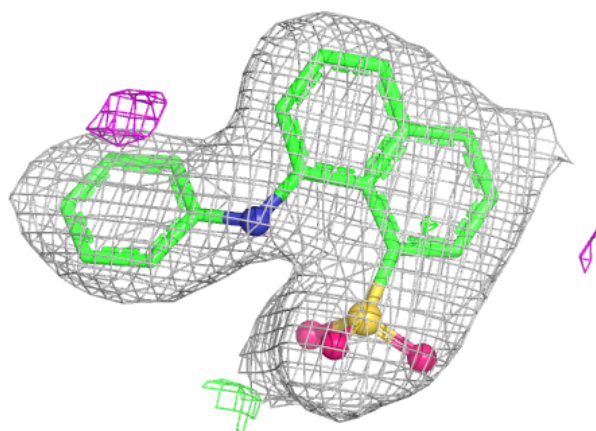
Electron density around 2AN g 202:

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



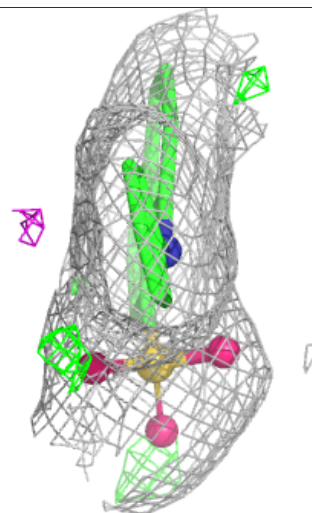
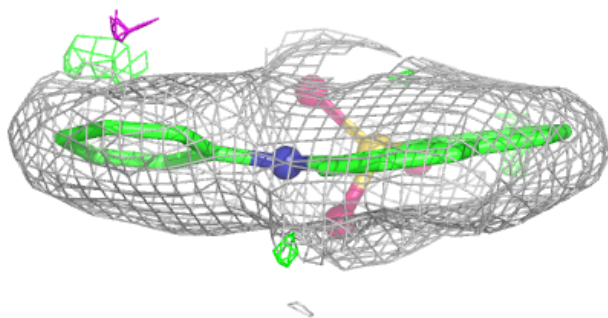
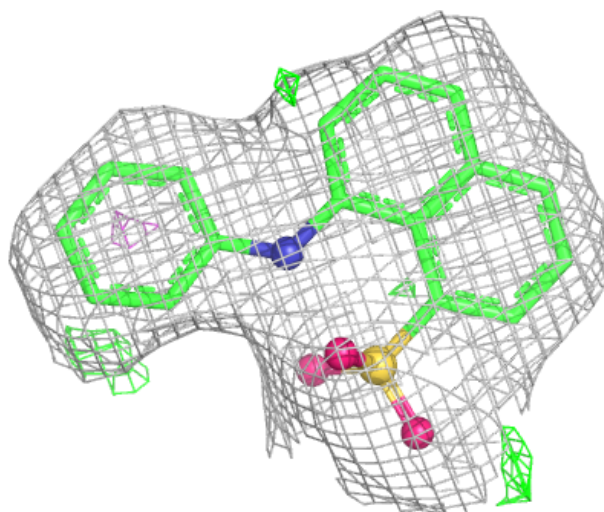
Electron density around 2AN E 202:

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



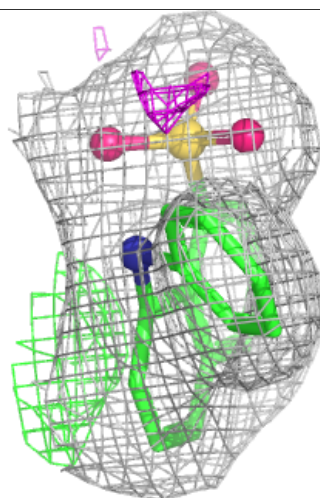
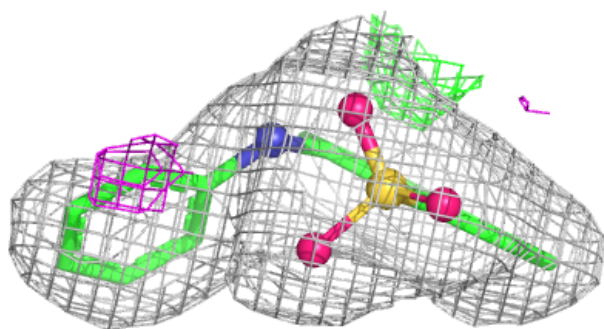
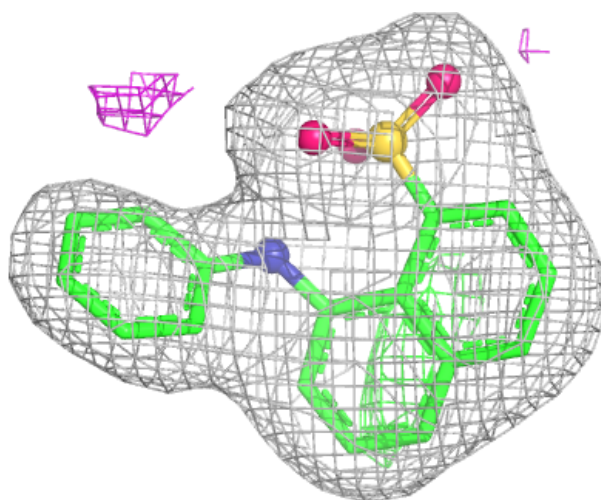
Electron density around 2AN T 201:

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



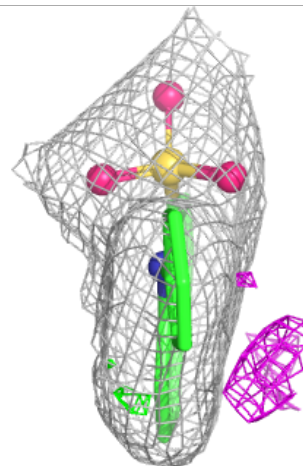
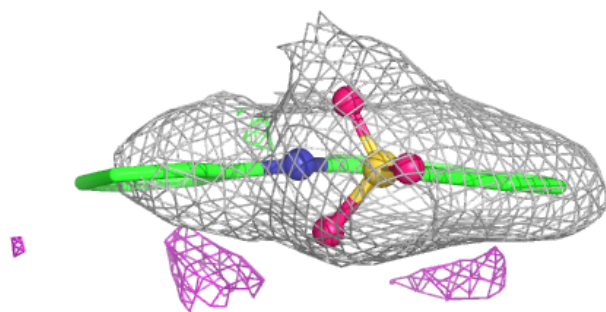
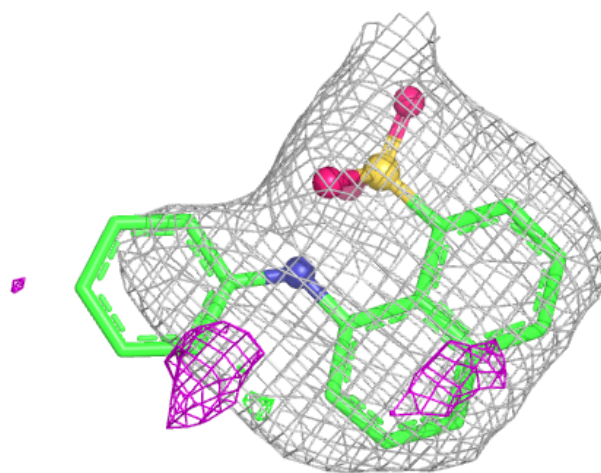
Electron density around 2AN G 202:

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



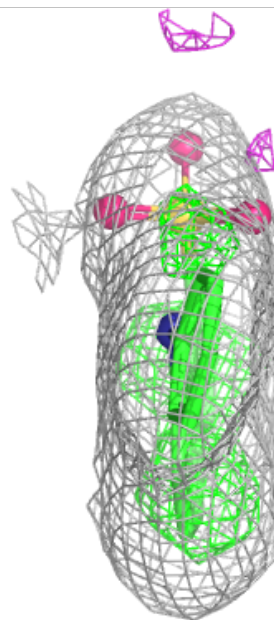
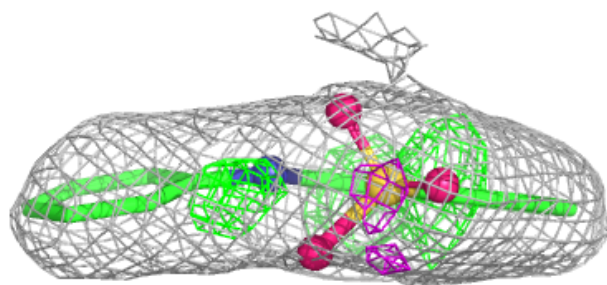
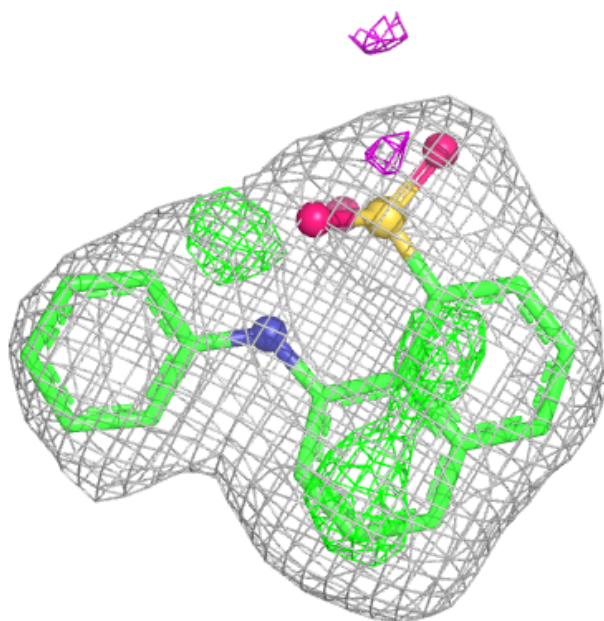
Electron density around 2AN G 203:

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



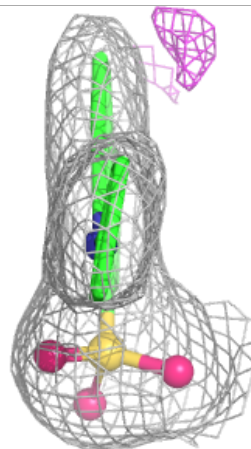
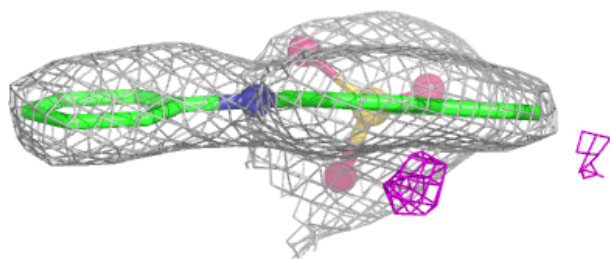
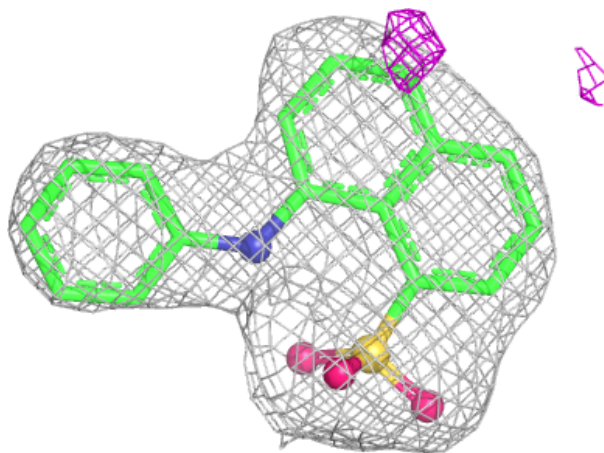
Electron density around 2AN B 203:

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



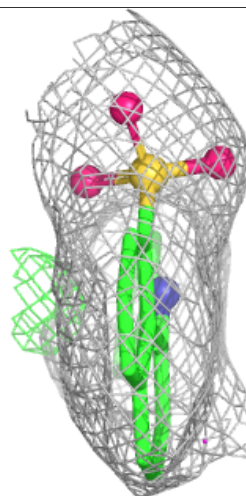
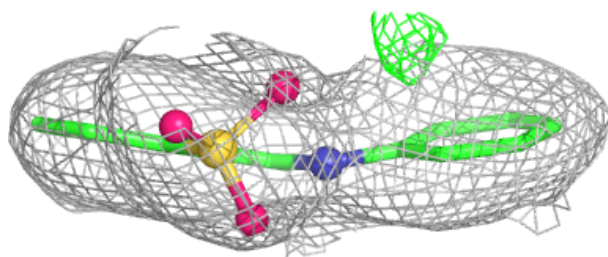
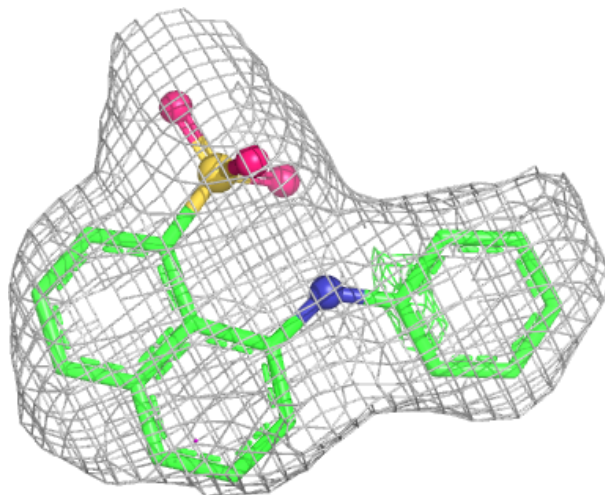
Electron density around 2AN c 204:

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



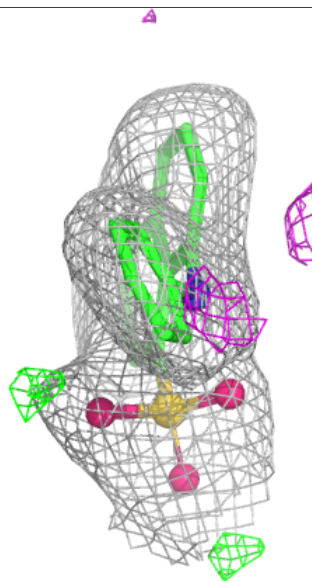
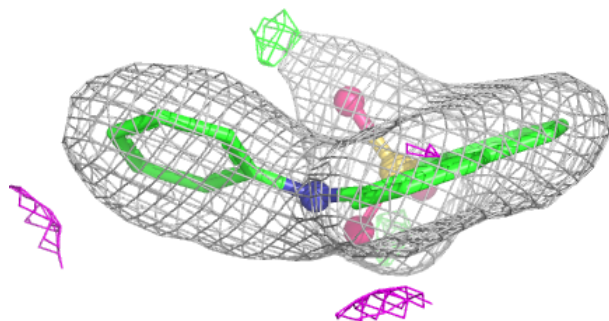
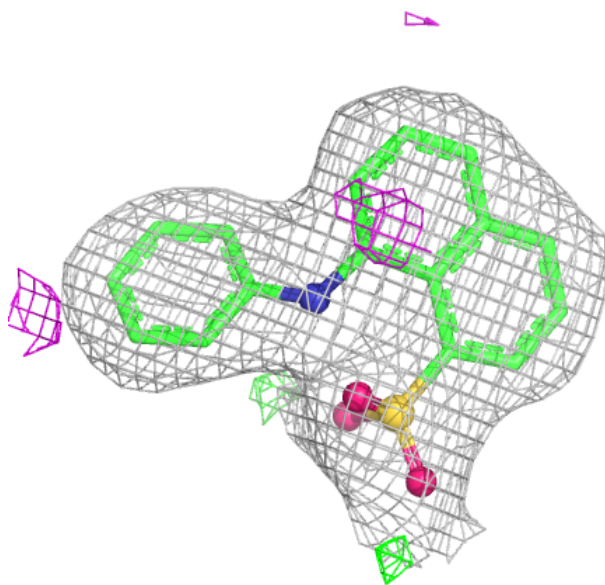
Electron density around 2AN Q 202:

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



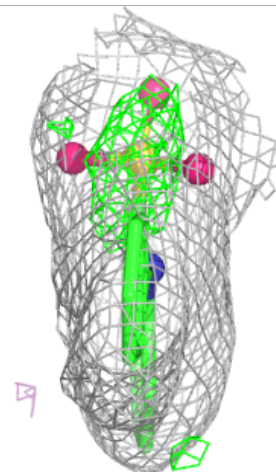
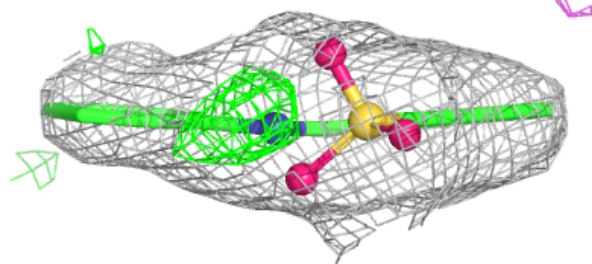
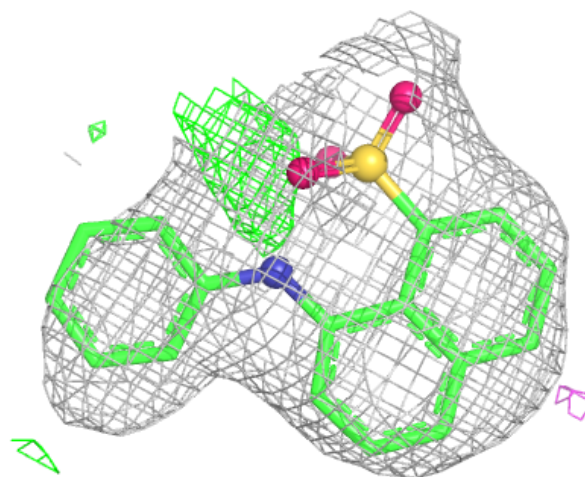
Electron density around 2AN K 201:

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



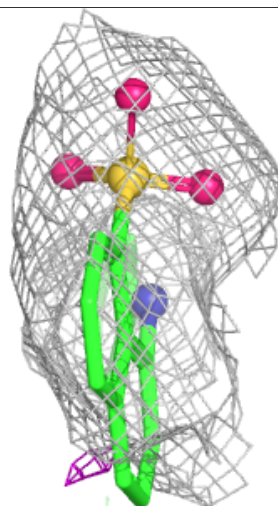
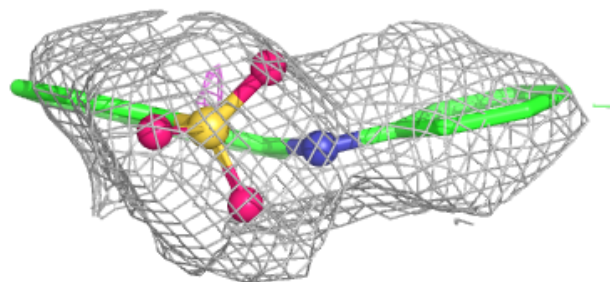
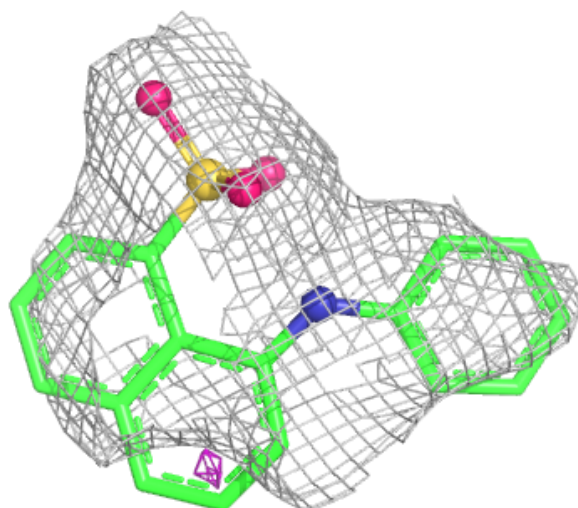
Electron density around 2AN N 204:

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



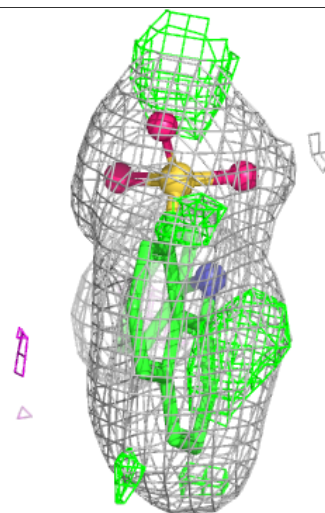
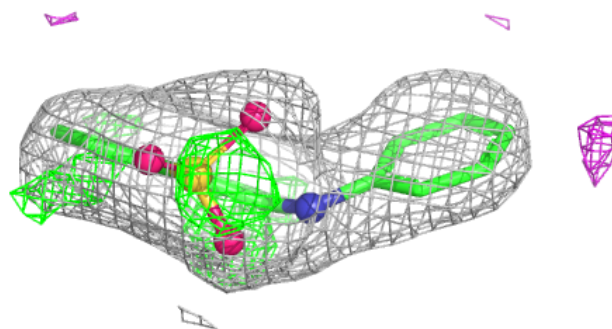
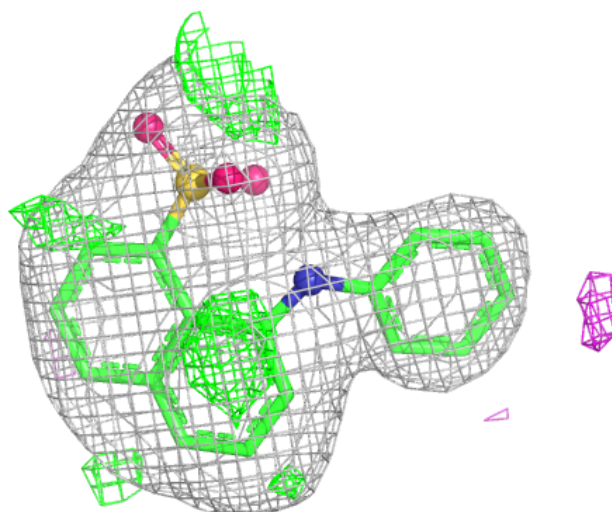
Electron density around 2AN C 202:

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



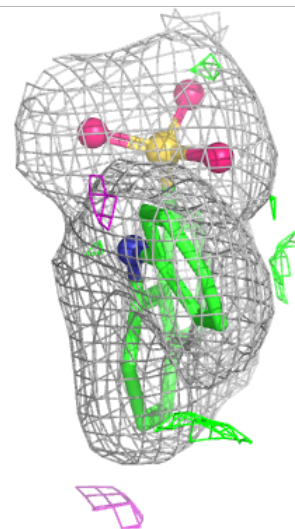
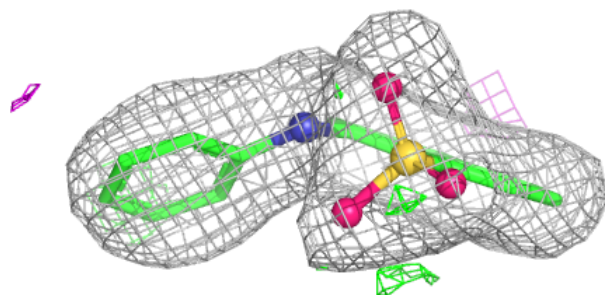
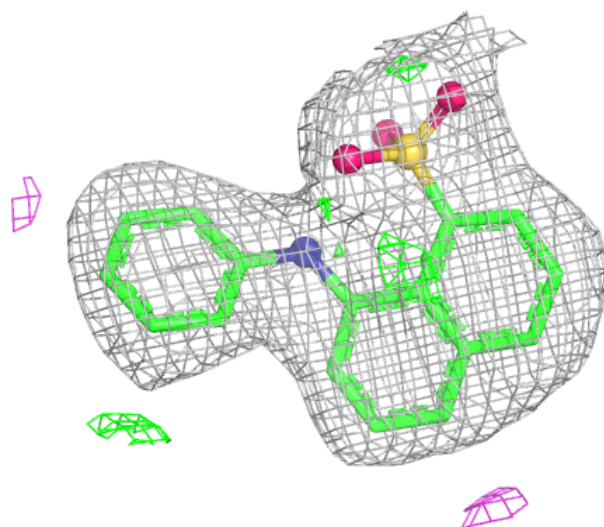
Electron density around 2AN P 204:

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



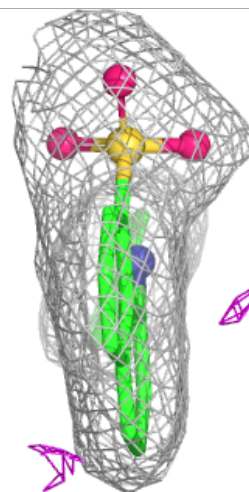
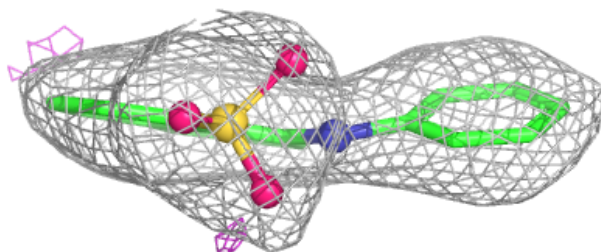
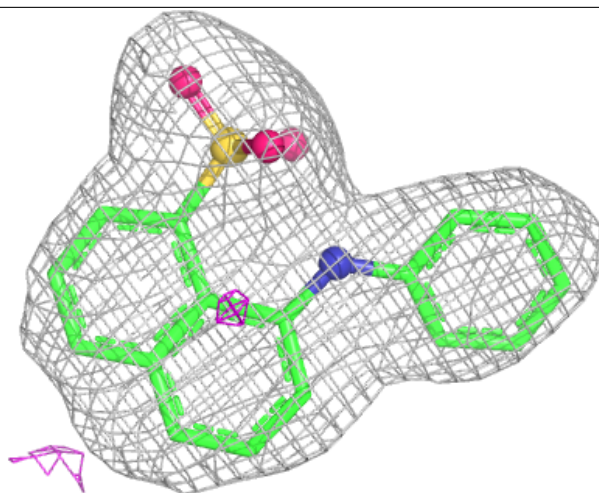
Electron density around 2AN f 202:

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



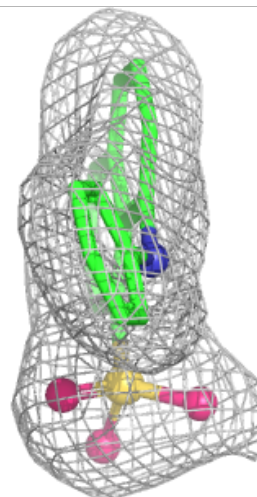
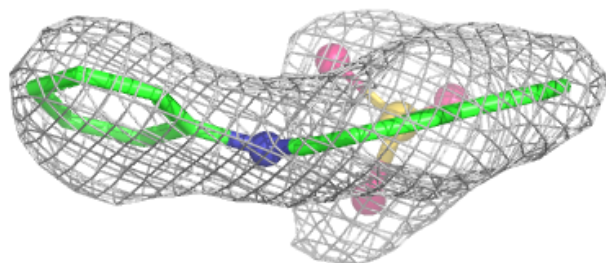
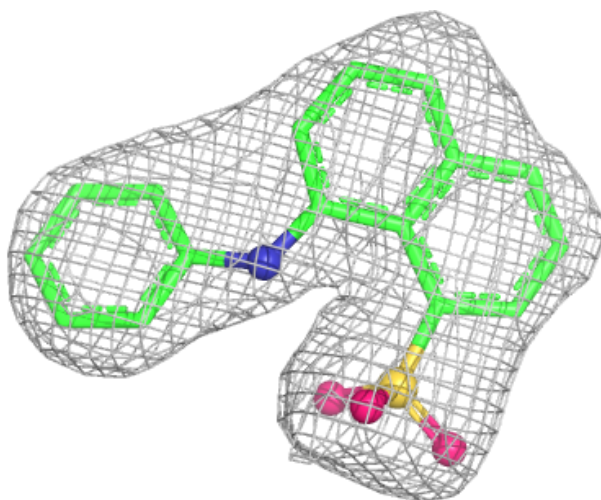
Electron density around 2AN H 201:

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



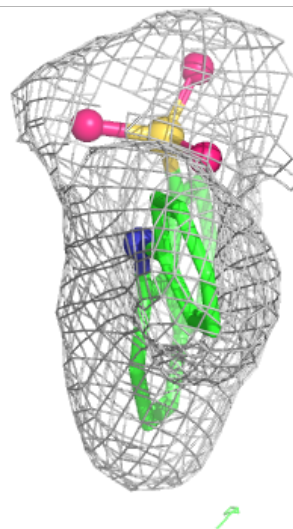
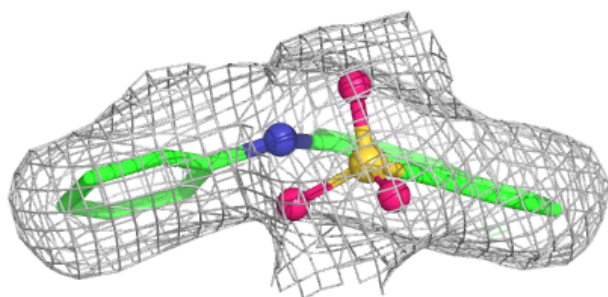
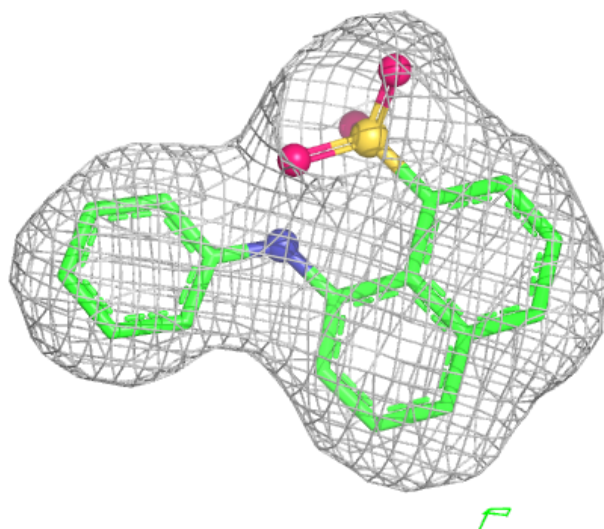
Electron density around 2AN a 202:

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



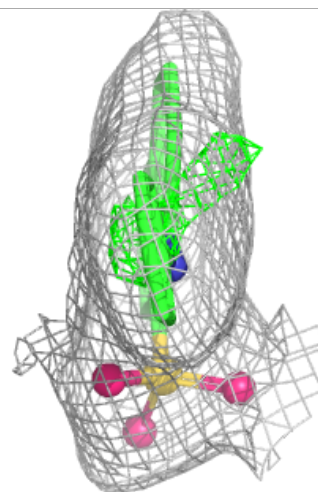
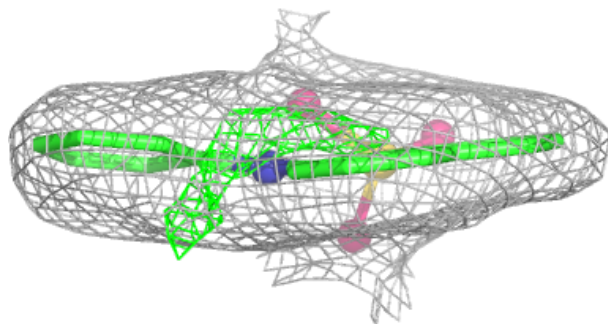
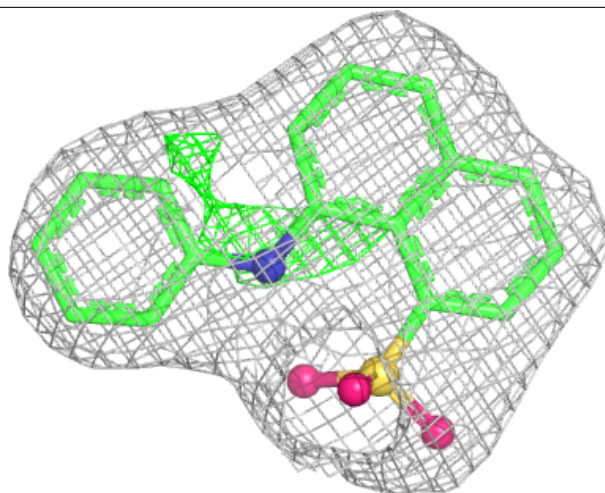
Electron density around 2AN f 204:

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



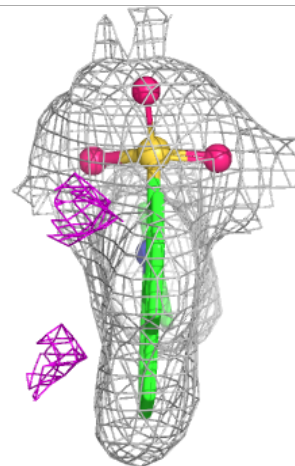
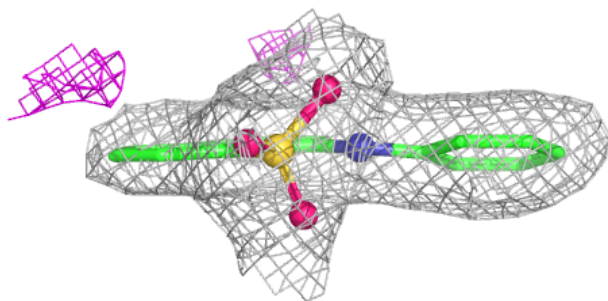
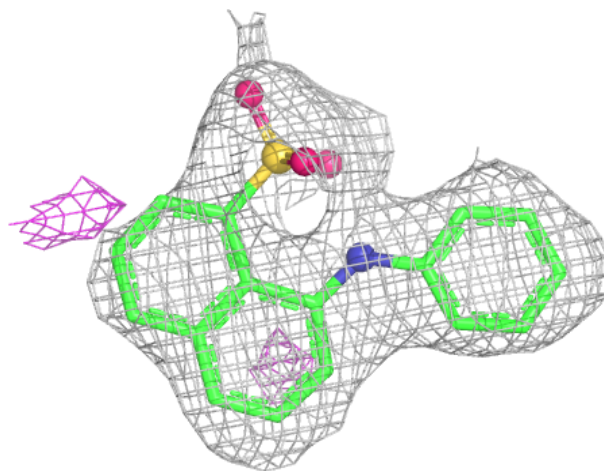
Electron density around 2AN f 205:

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



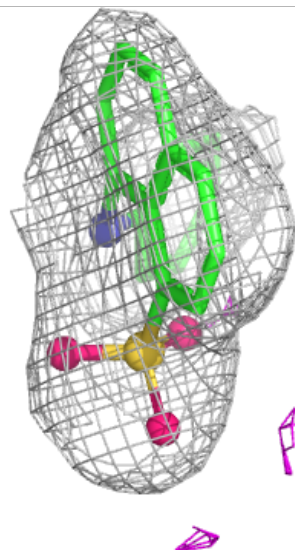
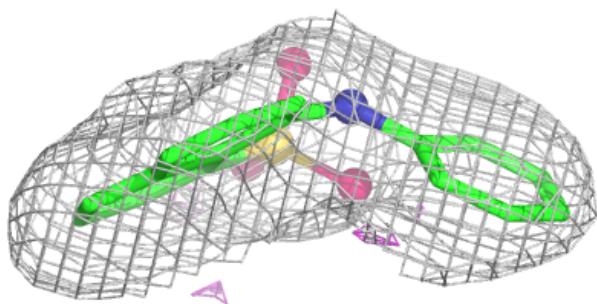
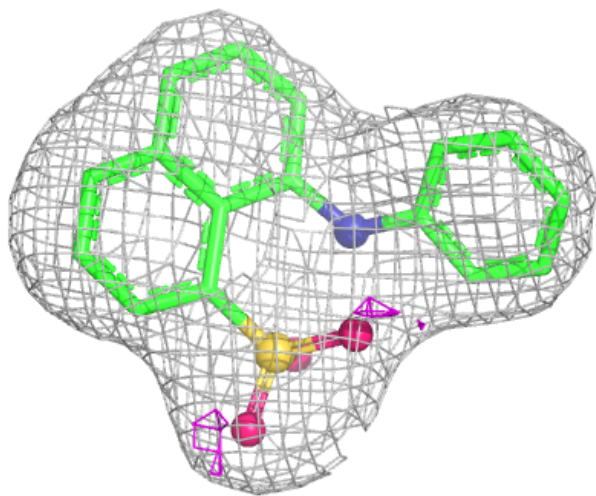
Electron density around 2AN V 204:

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



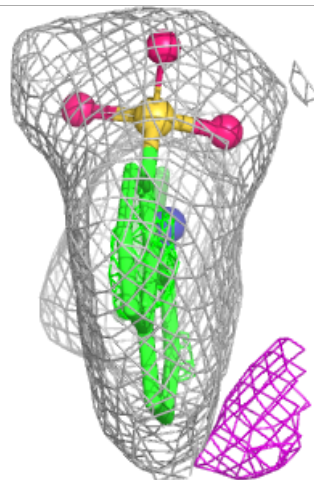
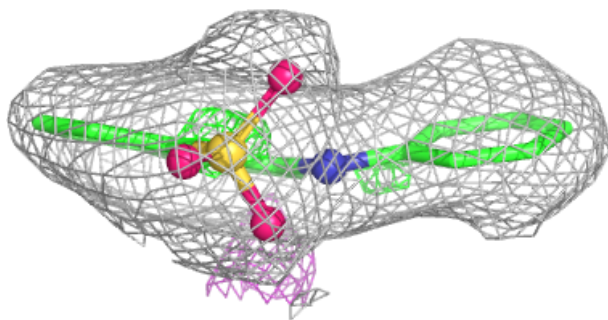
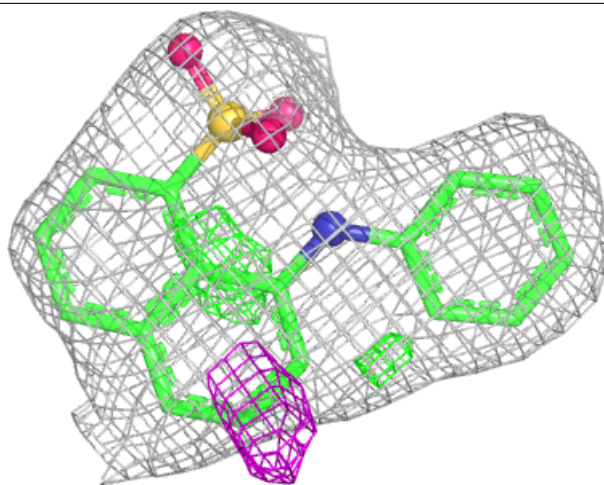
Electron density around 2AN V 205:

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



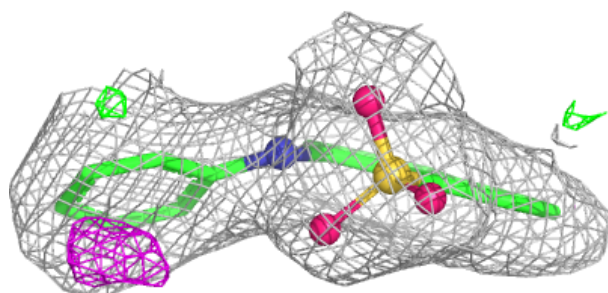
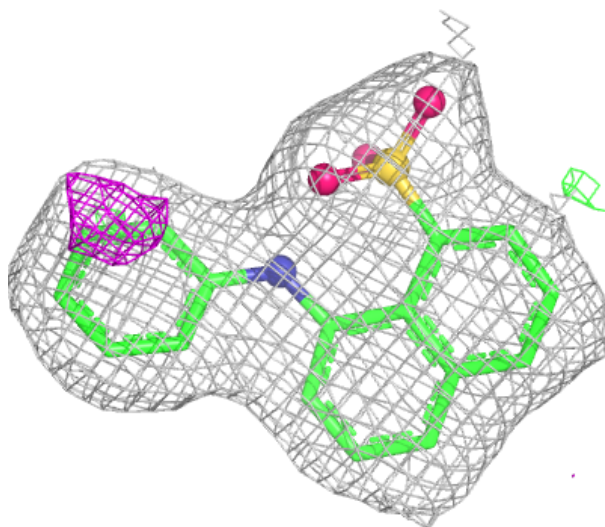
Electron density around 2AN J 202:

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



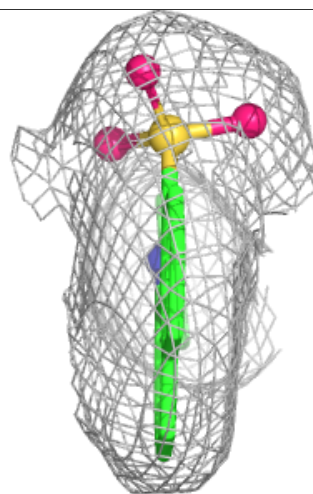
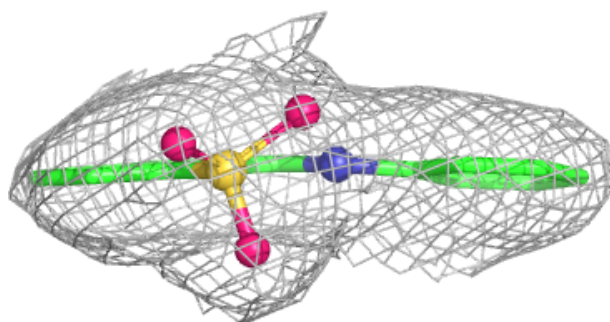
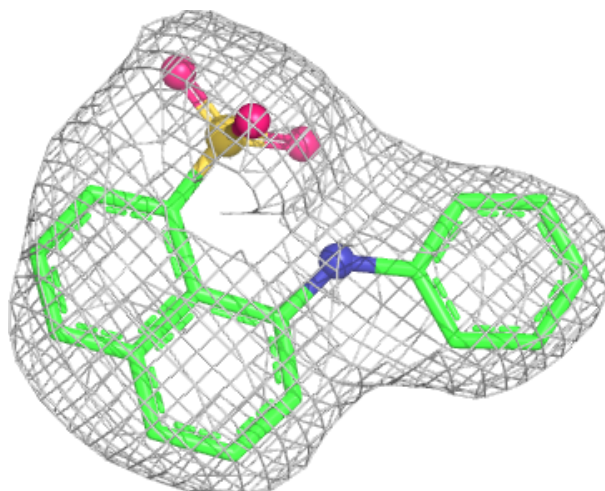
Electron density around 2AN P 201:

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



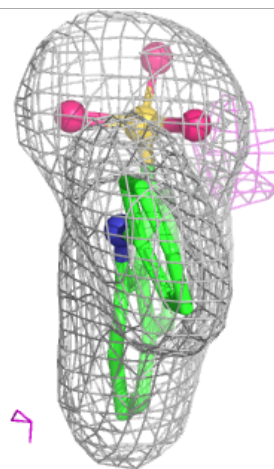
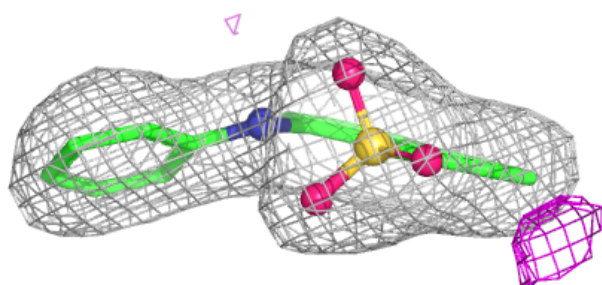
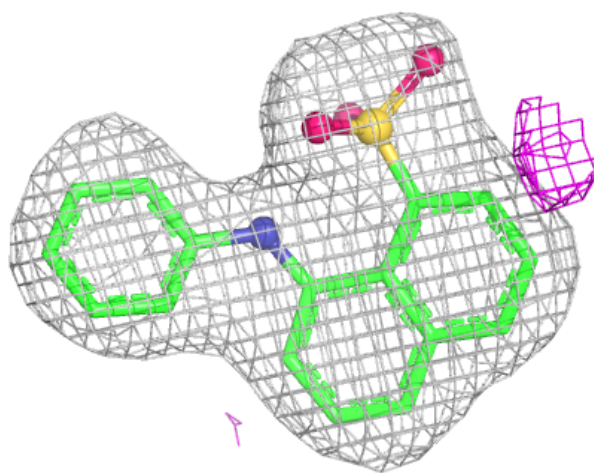
Electron density around 2AN H 203:

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



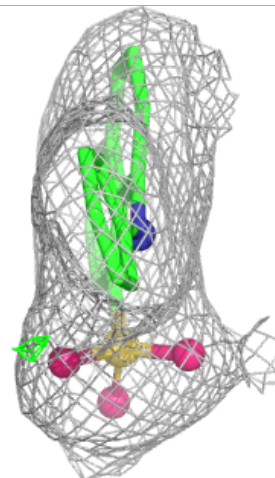
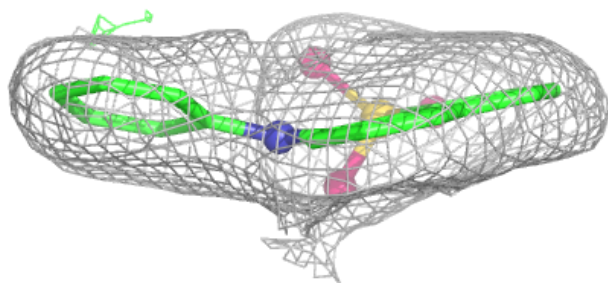
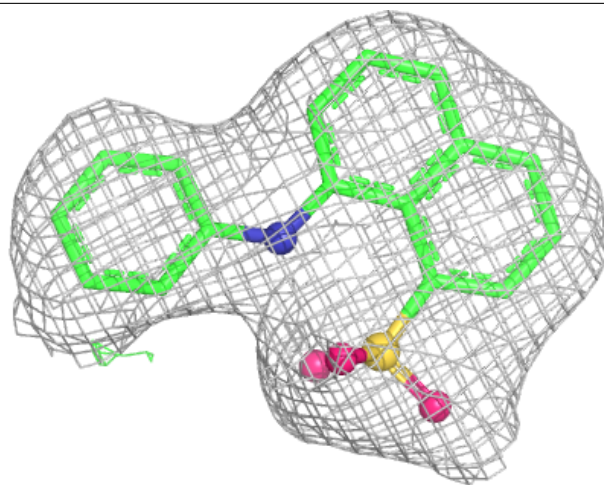
Electron density around 2AN c 206:

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



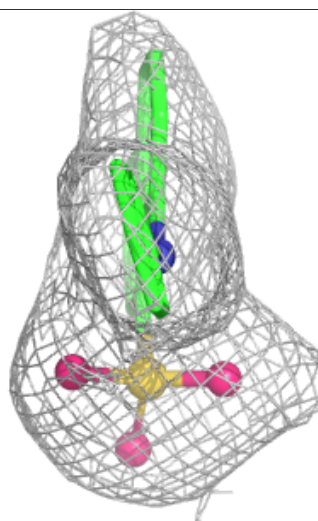
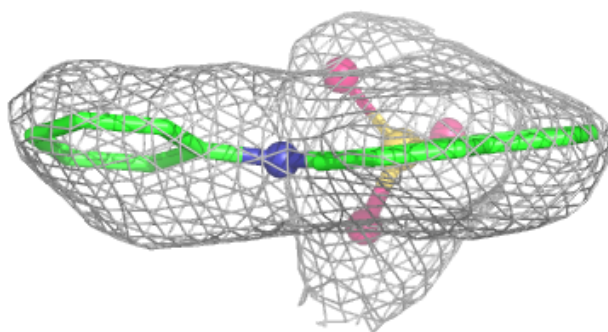
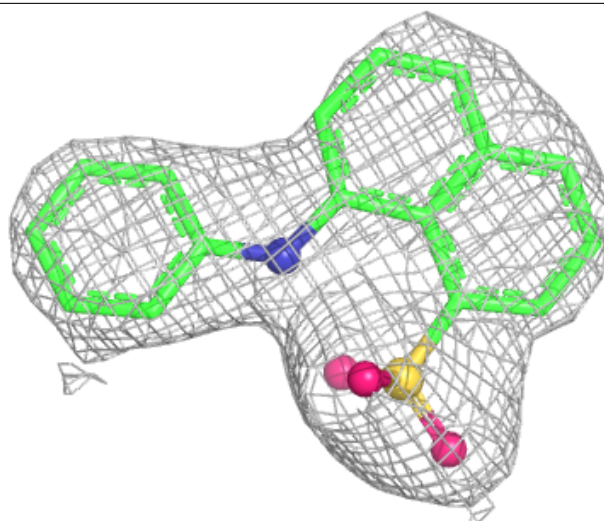
Electron density around 2AN h 202:

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



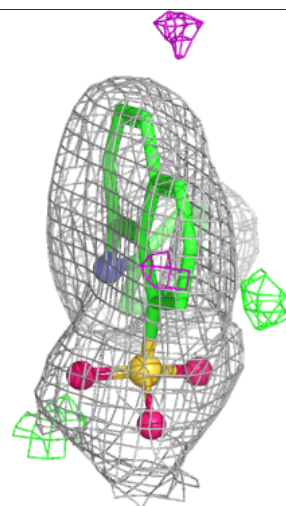
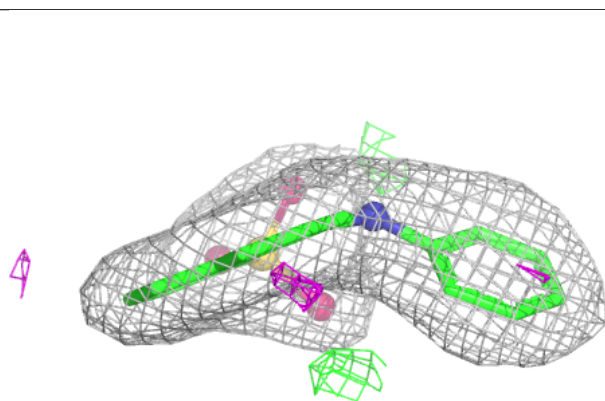
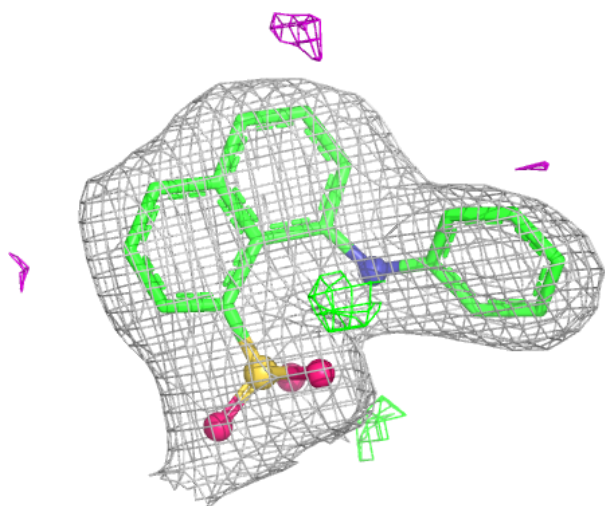
Electron density around 2AN D 201:

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



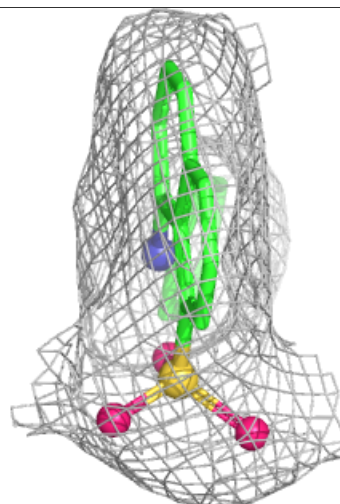
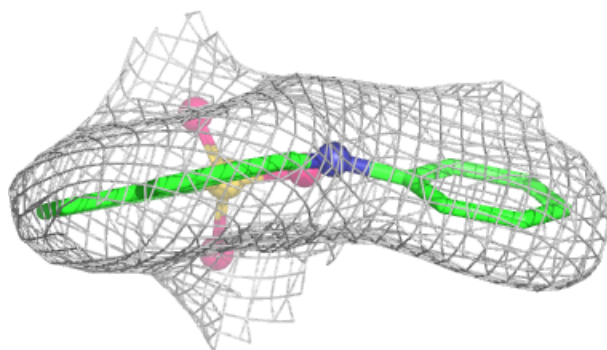
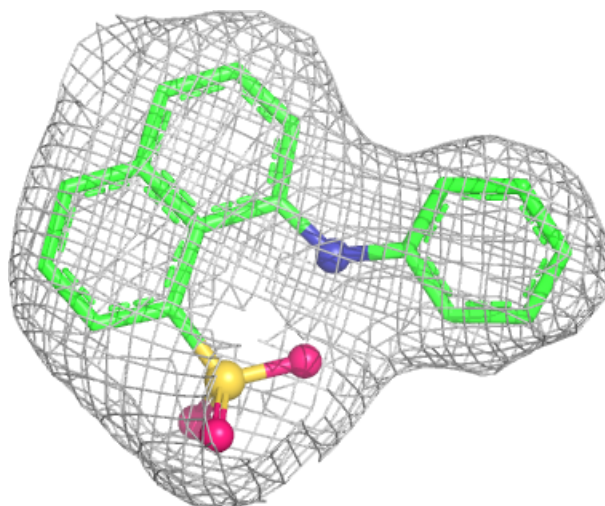
Electron density around 2AN Q 201:

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



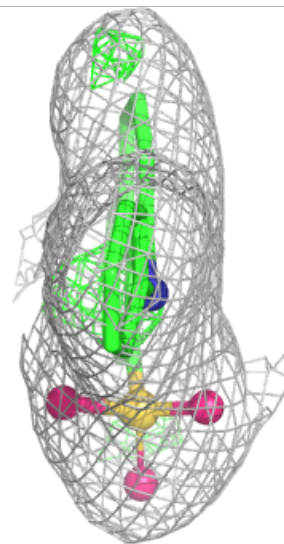
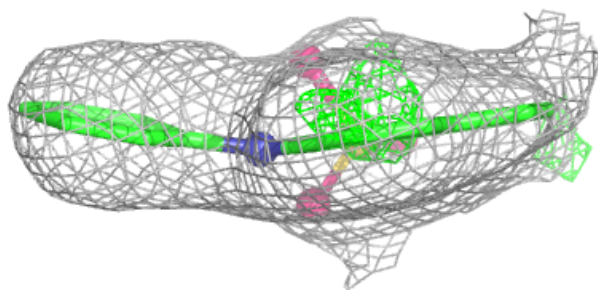
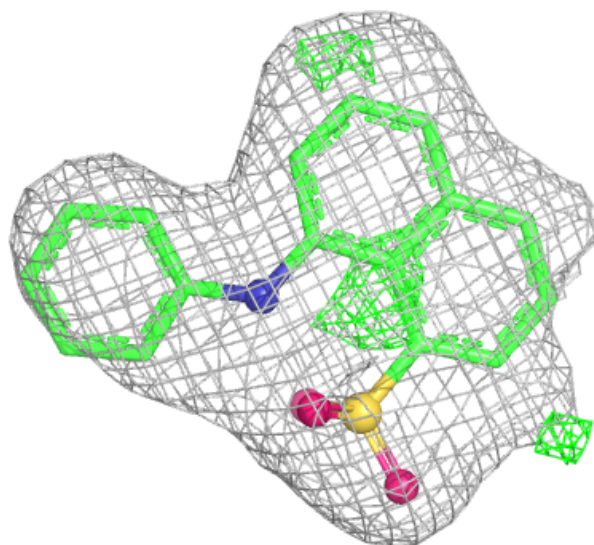
Electron density around 2AN b 203:

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



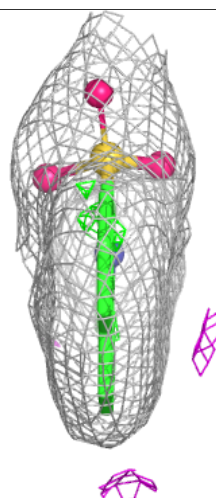
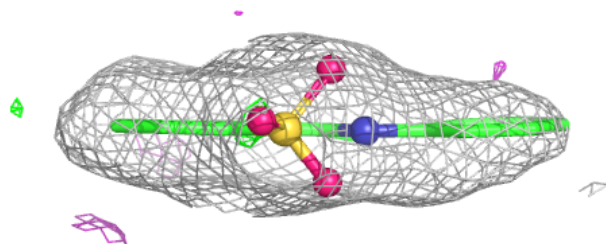
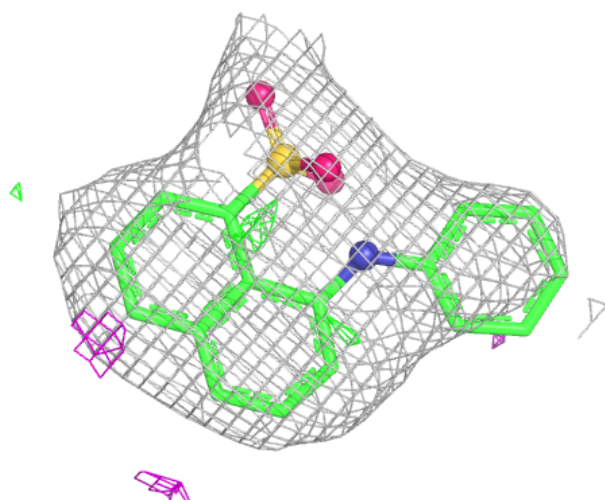
Electron density around 2AN F 203:

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



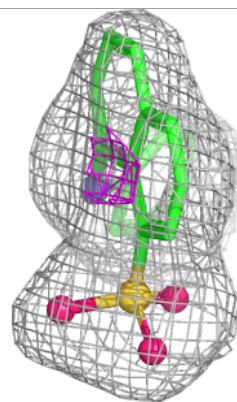
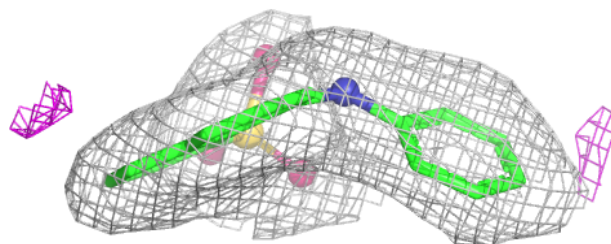
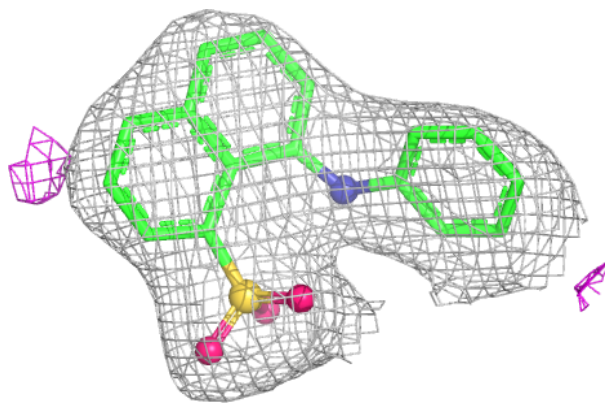
Electron density around 2AN K 202:

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



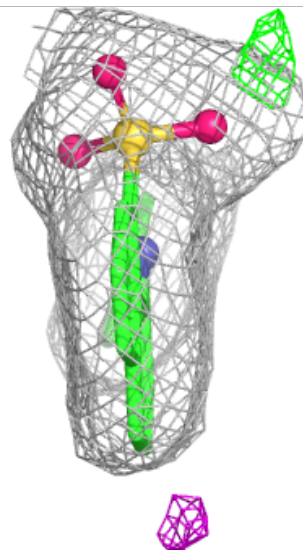
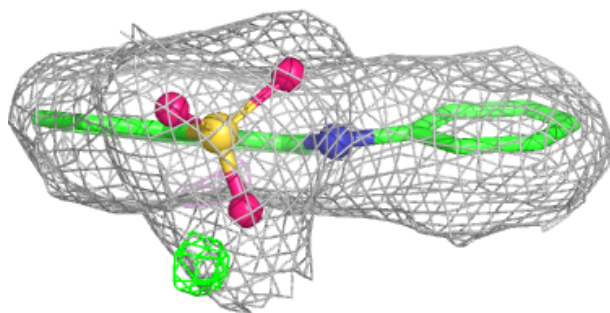
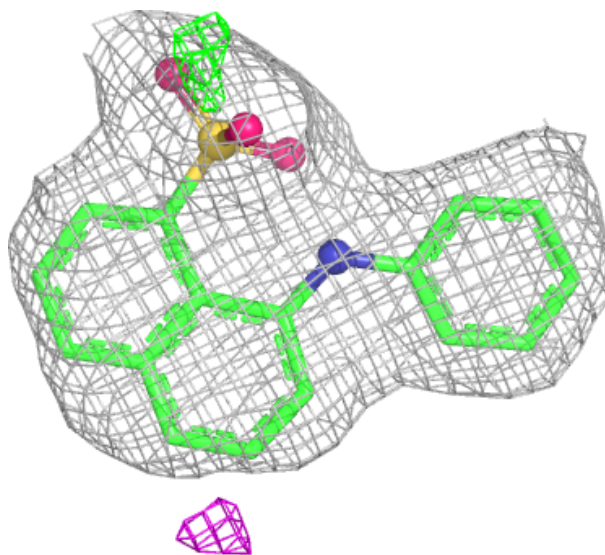
Electron density around 2AN B 201:

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



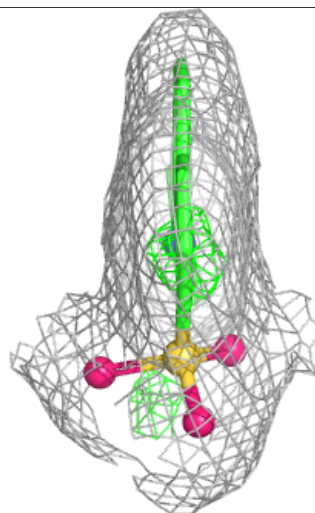
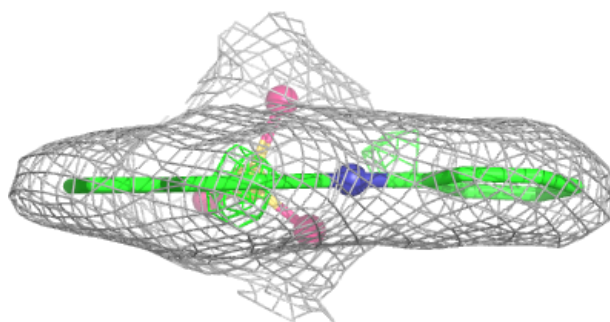
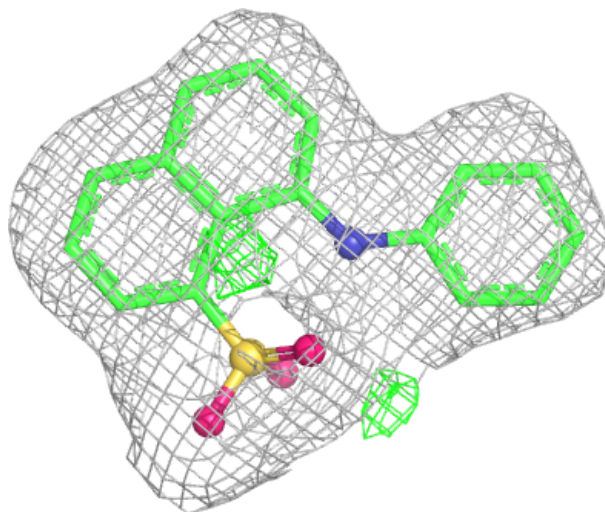
Electron density around 2AN R 201:

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



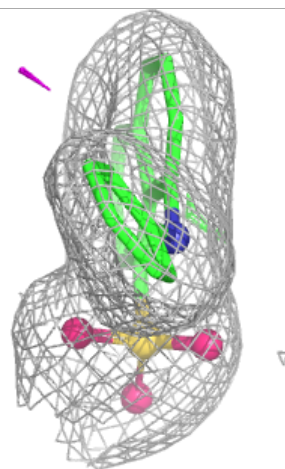
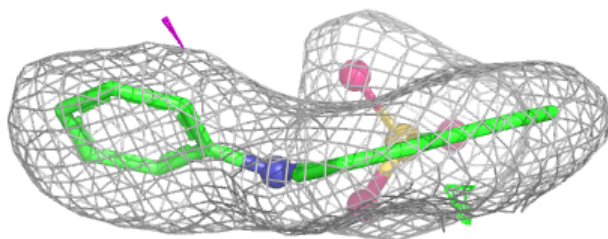
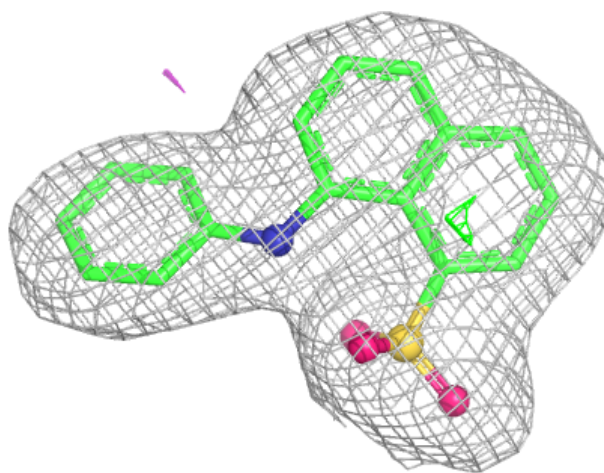
Electron density around 2AN L 202:

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



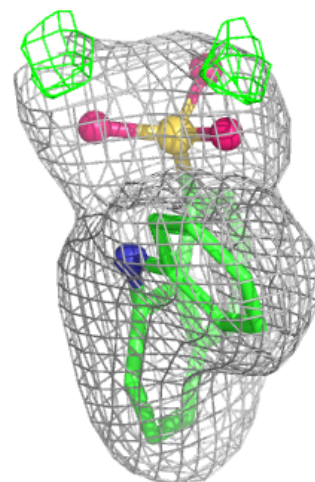
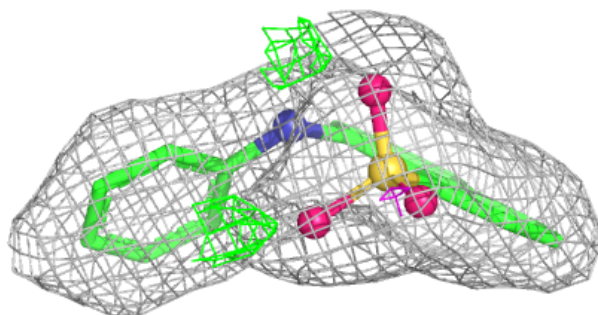
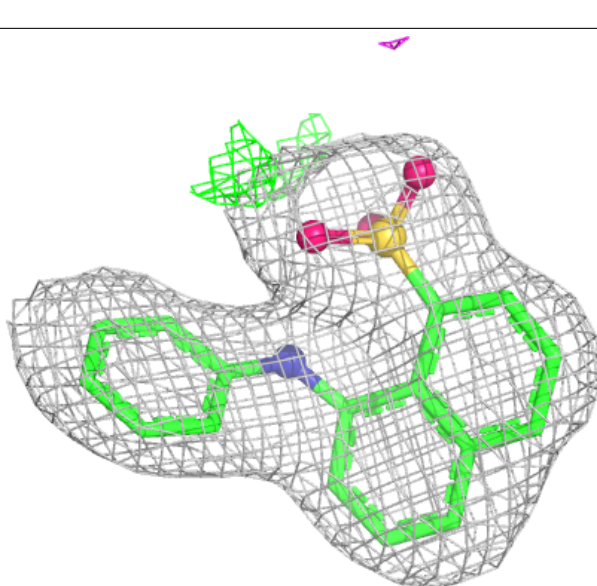
Electron density around 2AN f 201:

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



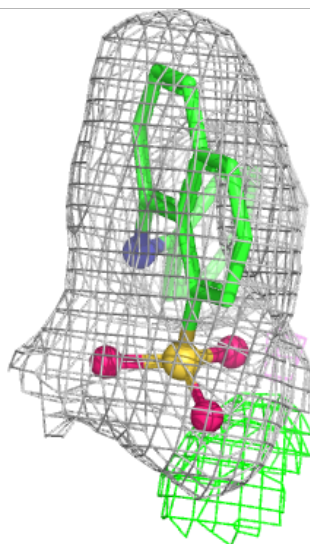
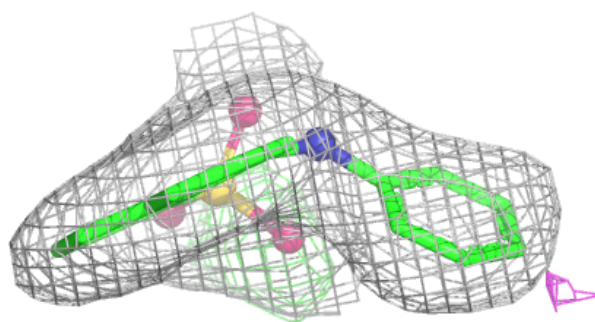
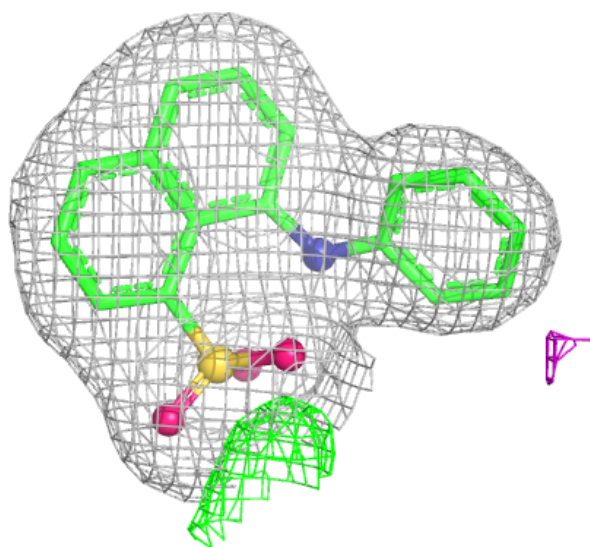
Electron density around 2AN L 203:

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



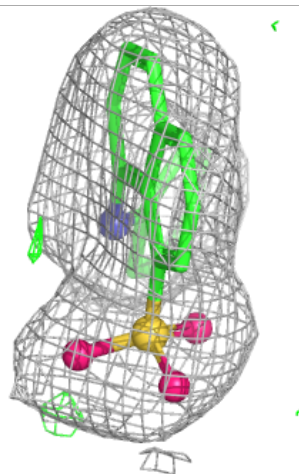
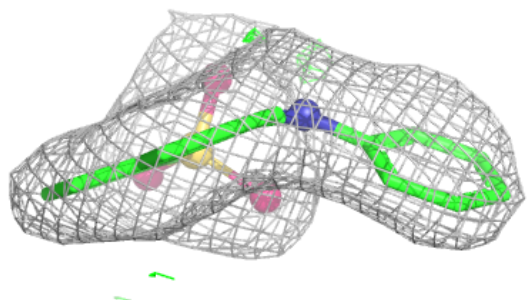
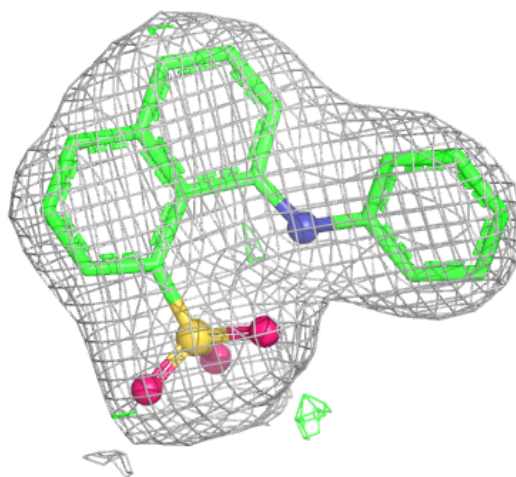
Electron density around 2AN c 201:

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



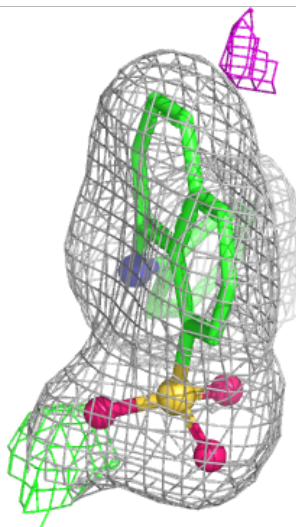
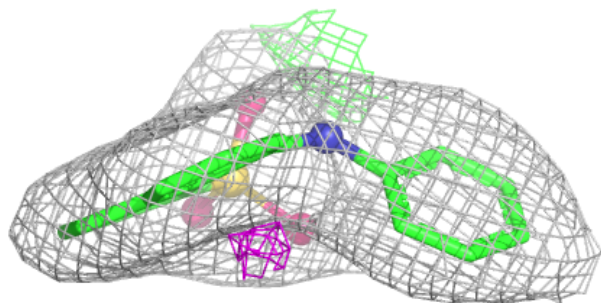
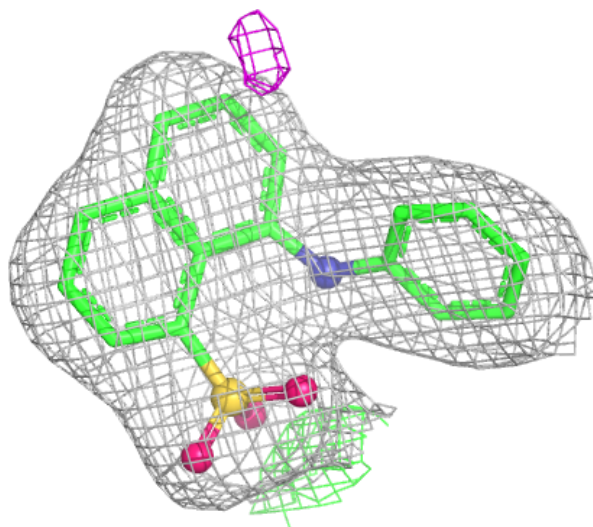
Electron density around 2AN N 202:

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



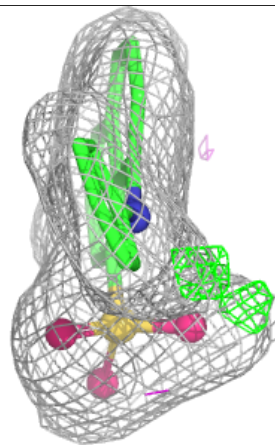
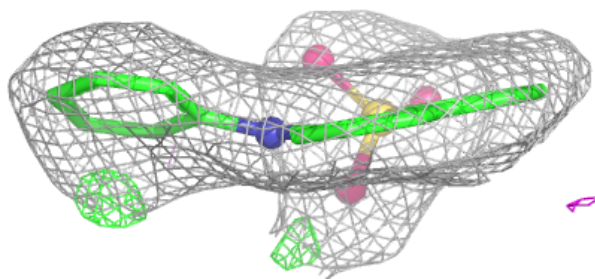
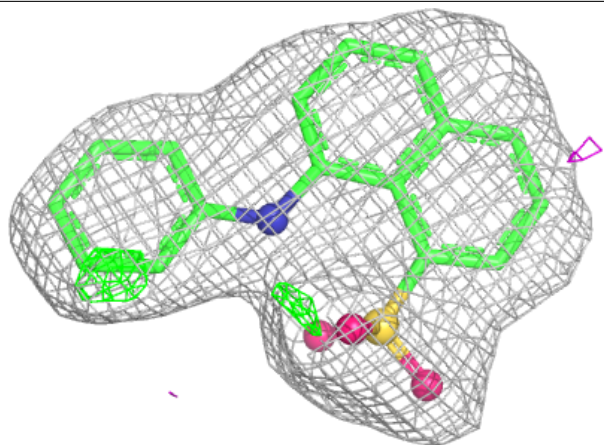
Electron density around 2AN P 202:

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



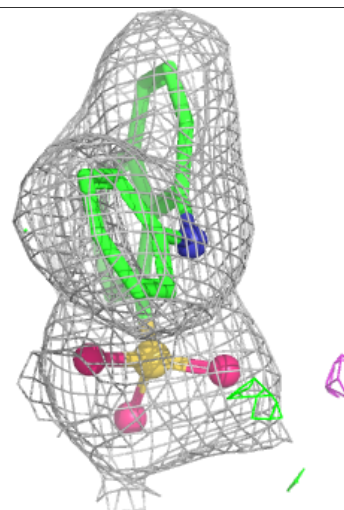
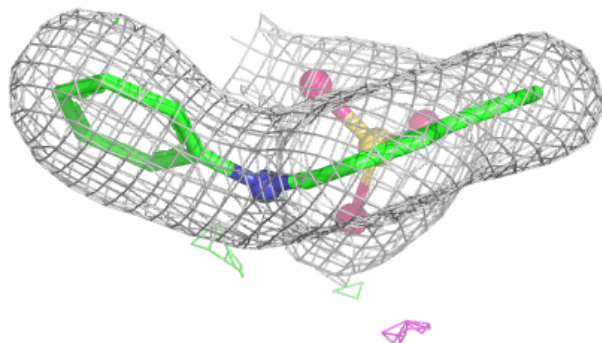
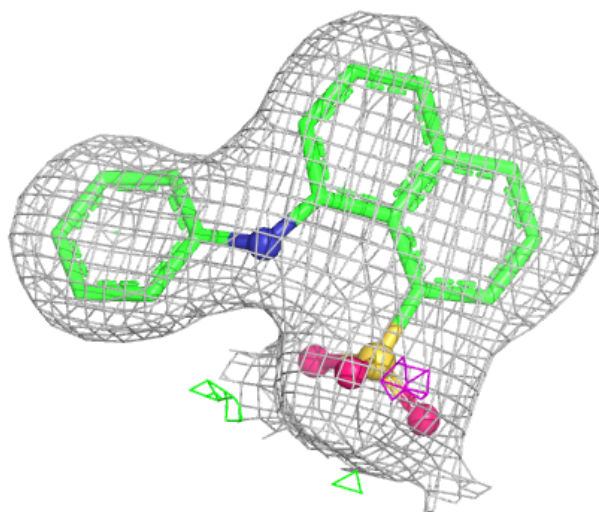
Electron density around 2AN L 201:

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



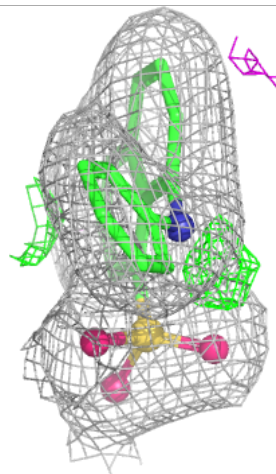
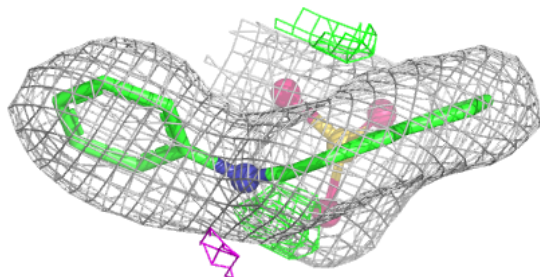
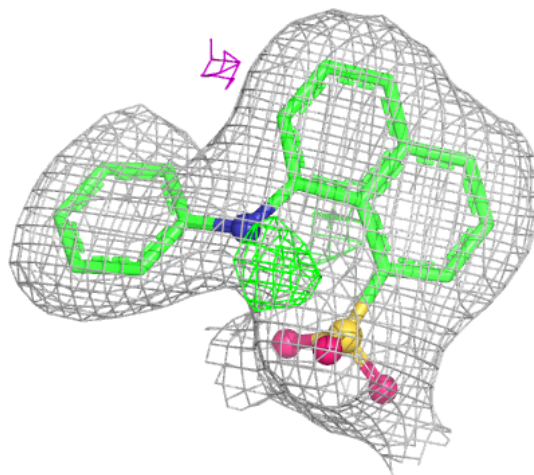
Electron density around 2AN V 202:

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



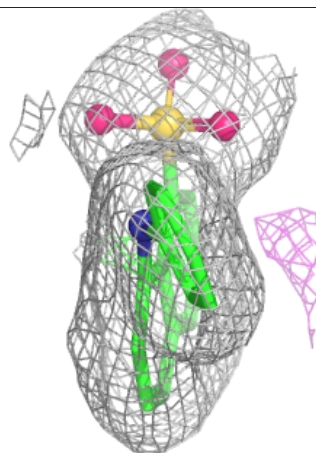
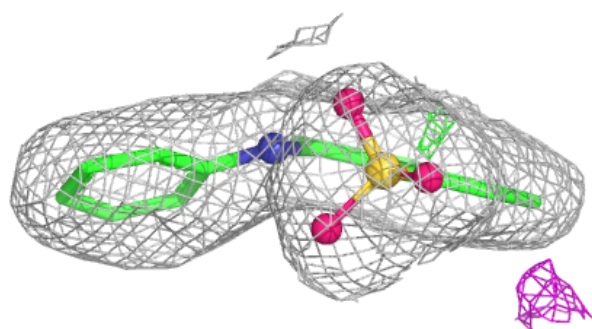
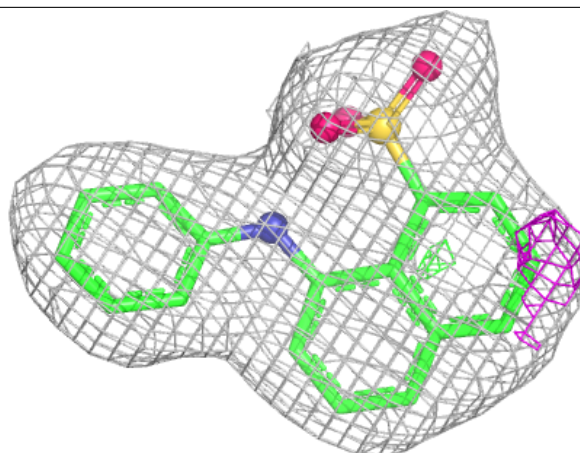
Electron density around 2AN j 202:

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



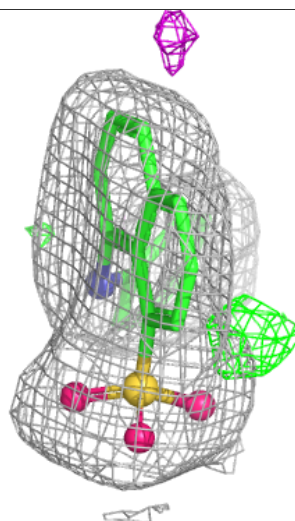
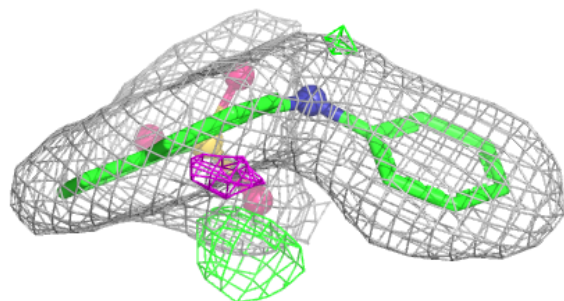
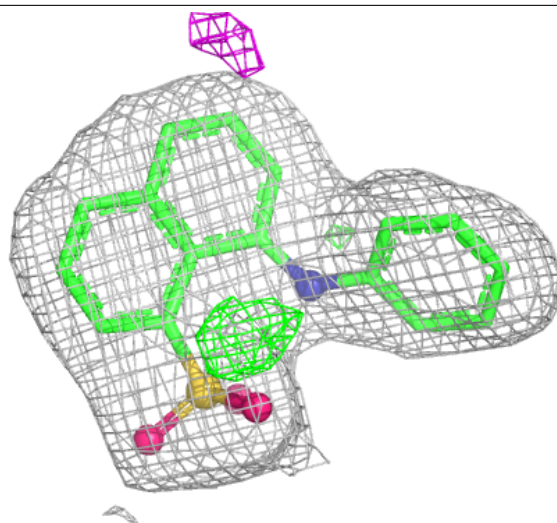
Electron density around 2AN j 203:

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



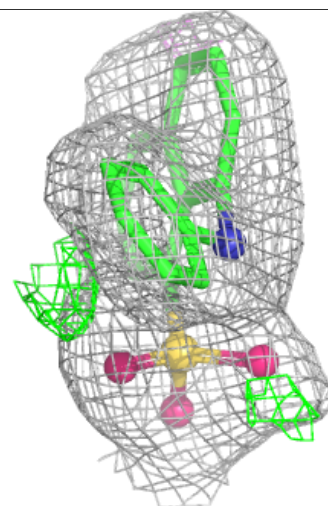
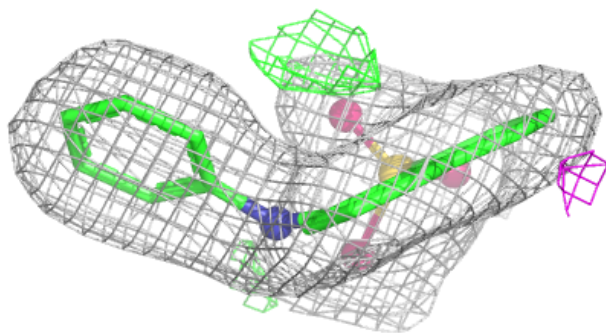
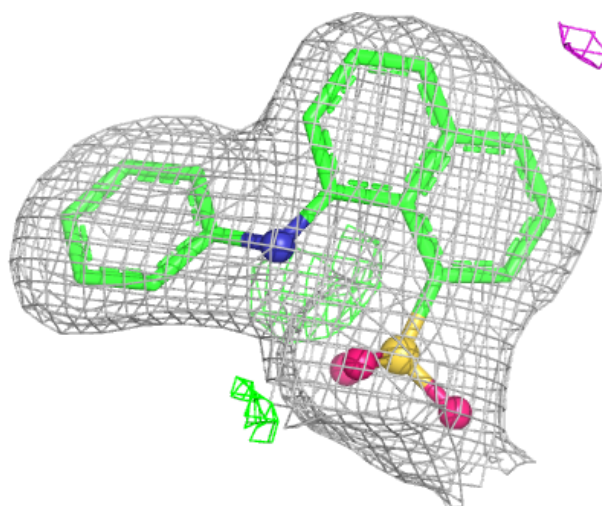
Electron density around 2AN I 201:

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



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)



6.5 Other polymers [i](#)

There are no such residues in this entry.