



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:33 AM UTC

PDB ID : 6V8S / pdb_00006v8s
Title : Crystal structure of Ara h 8.0201
Authors : Pote, S.; Offermann, L.R.; Hurlburt, B.K.; McBride, J.K.; Chruszcz, M.
Deposited on : 2019-12-12
Resolution : 2.10 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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

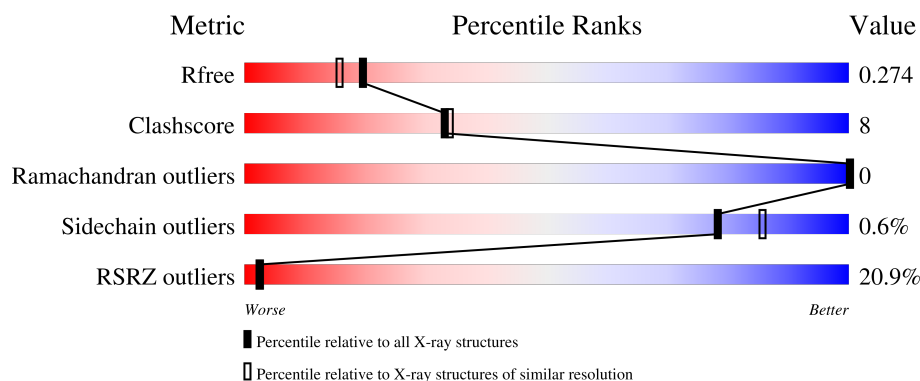
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	153	7% 92% 8%
1	B	153	8% 94% 5%
1	C	153	24% 92% 8%
1	D	153	25% 93% 7%
1	E	153	20% 93% 7%

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Mol	Chain	Length	Quality of chain
1	F	153	
1	G	153	
1	H	153	
1	I	153	
1	J	153	
1	K	153	
1	L	153	
1	M	153	
1	N	153	
1	O	153	
1	P	153	

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	P	508	-	-	X	-

2 Entry composition

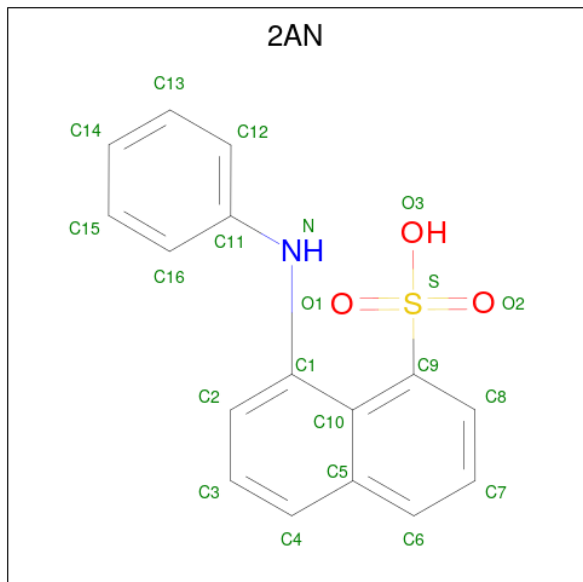
There are 4 unique types of molecules in this entry. The entry contains 21480 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Ara h 8 allergen isoform.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	152	Total	C	N	O	0	0	0
			1146	729	182	235			
1	B	152	Total	C	N	O	0	0	0
			1143	728	182	233			
1	C	152	Total	C	N	O	0	0	0
			1138	723	180	235			
1	D	152	Total	C	N	O	0	1	0
			1145	729	182	234			
1	E	152	Total	C	N	O	0	0	0
			1138	725	182	231			
1	F	152	Total	C	N	O	0	0	0
			1146	729	182	235			
1	G	152	Total	C	N	O	0	2	0
			1155	734	184	237			
1	H	152	Total	C	N	O	0	1	0
			1155	734	184	237			
1	I	152	Total	C	N	O	0	0	0
			1143	728	182	233			
1	J	151	Total	C	N	O	0	0	0
			1136	725	181	230			
1	K	151	Total	C	N	O	0	0	0
			1118	713	179	226			
1	L	152	Total	C	N	O	0	0	0
			1139	726	182	231			
1	M	152	Total	C	N	O	0	0	0
			1142	726	181	235			
1	N	152	Total	C	N	O	0	0	0
			1135	723	181	231			
1	O	152	Total	C	N	O	0	0	0
			1146	729	182	235			
1	P	152	Total	C	N	O	0	0	0
			1142	727	182	233			

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



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

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

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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	J	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	J	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	J	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	J	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	J	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	K	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	K	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	K	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	K	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	K	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	K	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	L	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	L	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	L	1	Total	C	N	O	S	0	0
			21	16	1	3	1		

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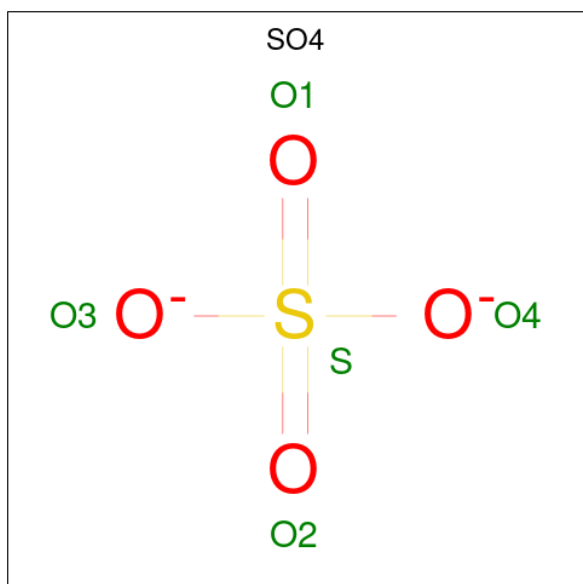
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	L	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	M	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	M	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	M	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	M	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	M	1	Total	C	N	O	S	0	0
			21	16	1	3	1		
2	M	1	Total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

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

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	H	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	83	Total	O	0	0
			83	83		
4	B	88	Total	O	0	0
			88	88		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	63	Total 63	O 63	0	0
4	D	61	Total 61	O 61	0	0
4	E	67	Total 67	O 67	0	0
4	F	58	Total 58	O 58	0	0
4	G	60	Total 60	O 60	0	0
4	H	63	Total 63	O 63	0	0
4	I	79	Total 79	O 79	0	0
4	J	62	Total 62	O 62	0	0
4	K	57	Total 57	O 57	0	0
4	L	90	Total 90	O 90	0	0
4	M	71	Total 71	O 71	0	0
4	N	63	Total 63	O 63	0	0
4	O	51	Total 51	O 51	0	0
4	P	50	Total 50	O 50	0	0

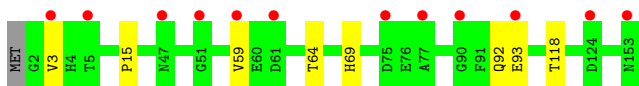
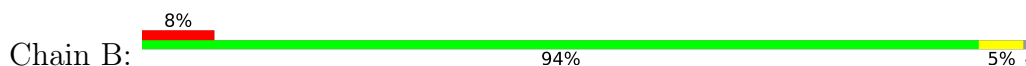
3 Residue-property plots [i](#)

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

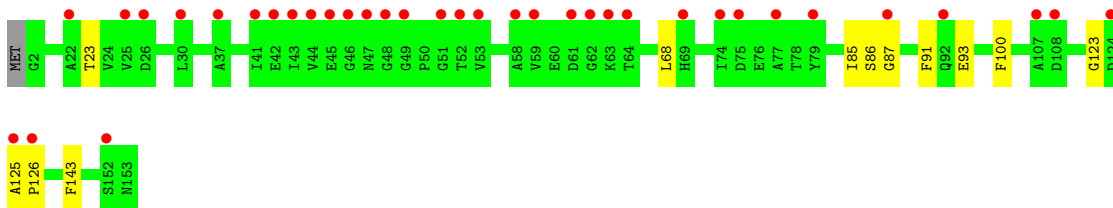
- Molecule 1: Ara h 8 allergen isoform



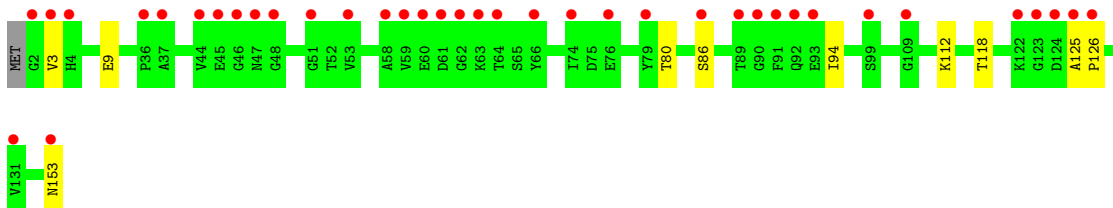
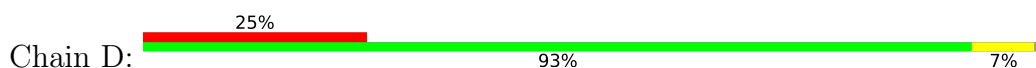
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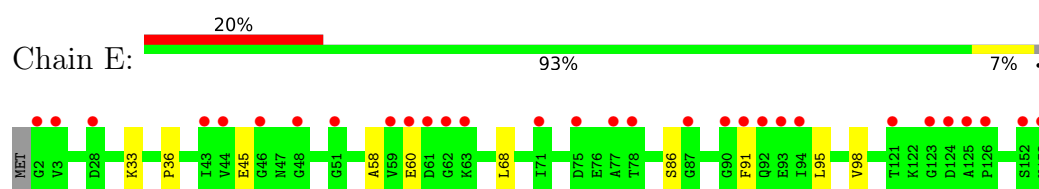
- Molecule 1: Ara h 8 allergen isoform



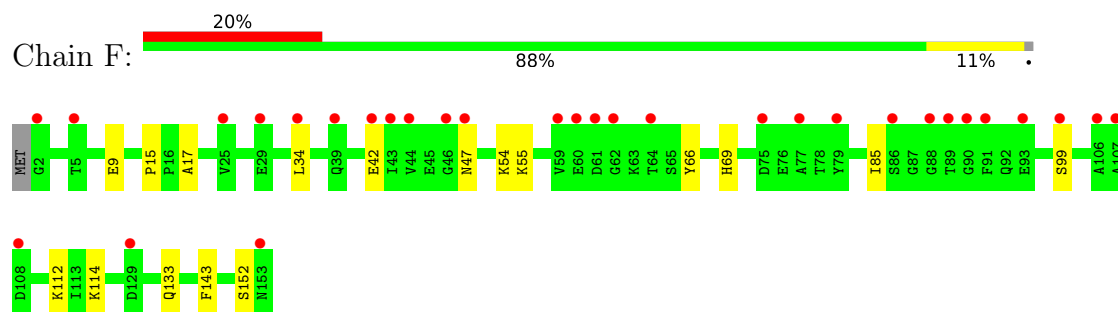
- Molecule 1: Ara h 8 allergen isoform



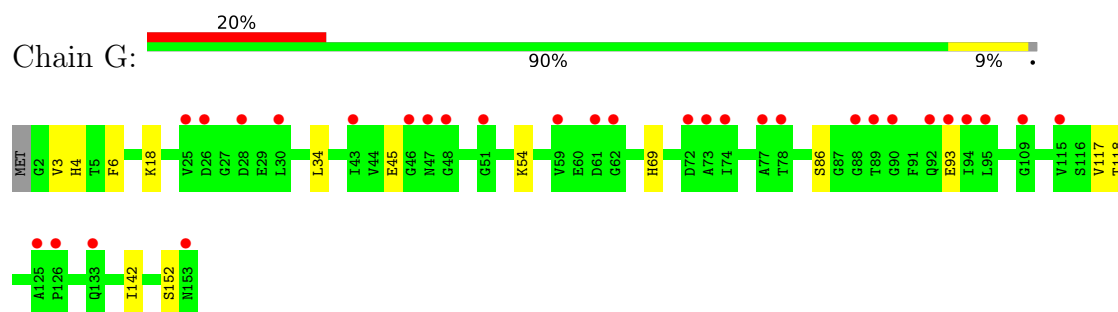
- Molecule 1: Ara h 8 allergen isoform



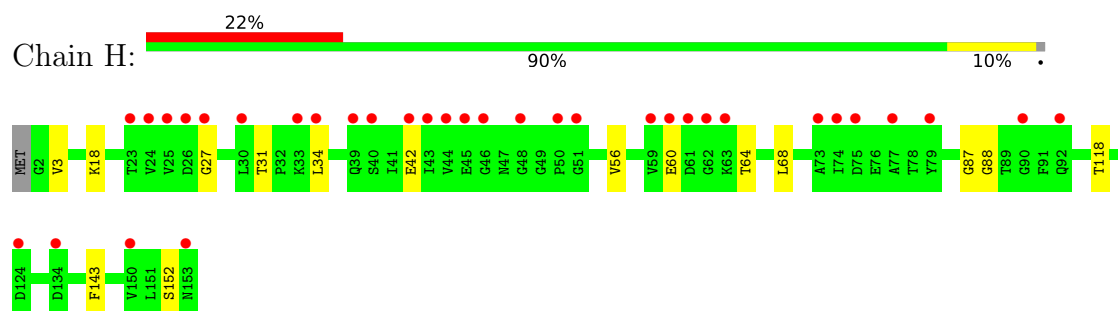
- Molecule 1: Ara h 8 allergen isoform



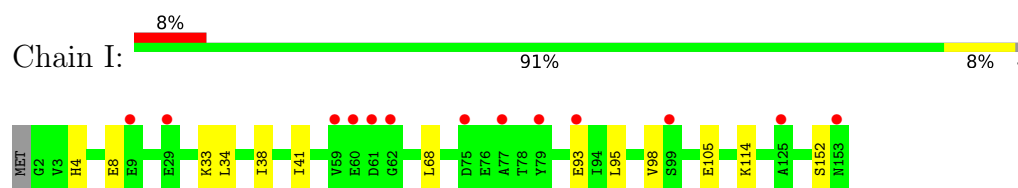
- Molecule 1: Ara h 8 allergen isoform



- Molecule 1: Ara h 8 allergen isoform

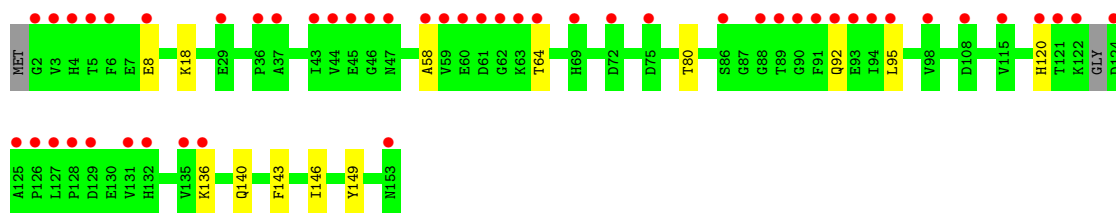


- Molecule 1: Ara h 8 allergen isoform

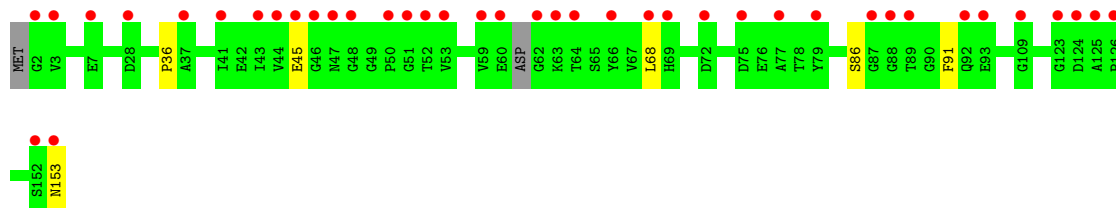


- Molecule 1: Ara h 8 allergen isoform

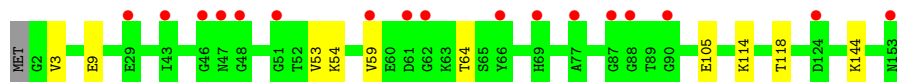




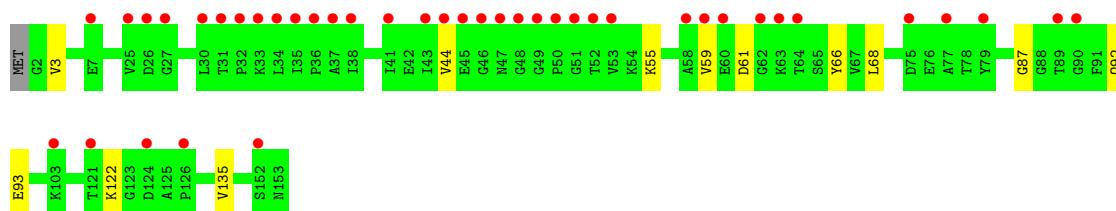
- Molecule 1: Ara h 8 allergen isoform



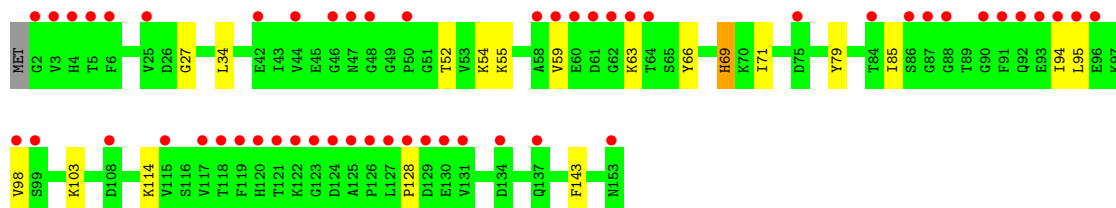
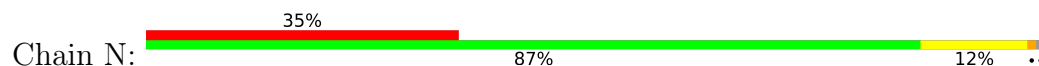
- Molecule 1: Ara h 8 allergen isoform



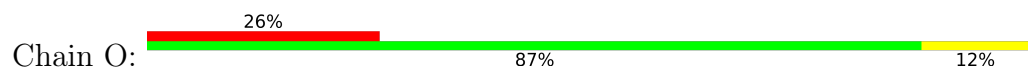
- Molecule 1: Ara h 8 allergen isoform

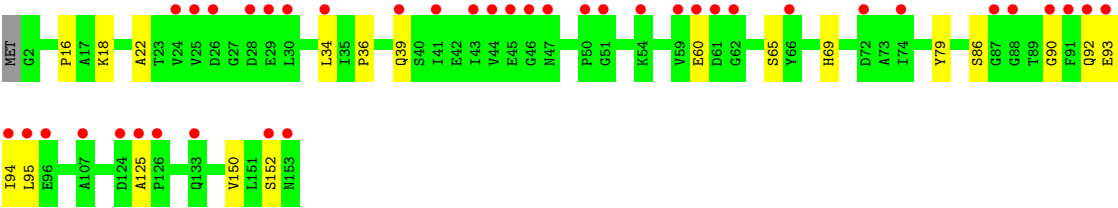


- Molecule 1: Ara h 8 allergen isoform

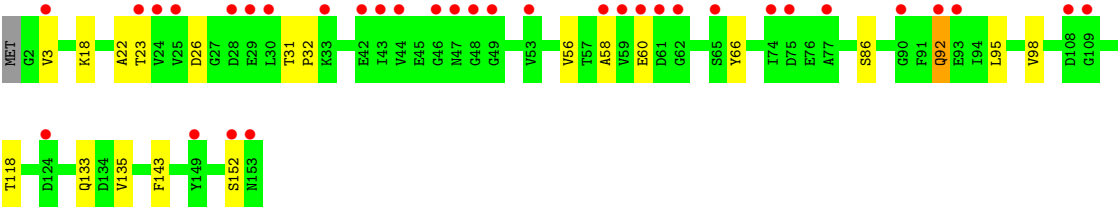
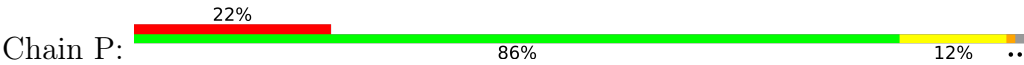


- Molecule 1: Ara h 8 allergen isoform





● Molecule 1: Ara h 8 allergen isoform



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	78.16Å 90.03Å 94.25Å 94.13° 106.91° 97.23°	Depositor
Resolution (Å)	38.09 – 2.10 38.09 – 2.10	Depositor EDS
% Data completeness (in resolution range)	91.5 (38.09-2.10) 91.5 (38.09-2.10)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.92 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.232 , 0.266 0.239 , 0.274	Depositor DCC
R_{free} test set	6331 reflections (4.48%)	wwPDB-VP
Wilson B-factor (Å ²)	19.6	Xtriage
Anisotropy	0.092	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 38.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	21480	wwPDB-VP
Average B, all atoms (Å ²)	41.0	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 77.19 % 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 8.9513e-07. 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: SO4, 2AN

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	1.16	0/1168	1.32	0/1583
1	B	1.13	2/1165 (0.2%)	1.30	0/1579
1	C	1.16	0/1160	1.33	0/1575
1	D	1.13	0/1167	1.29	0/1584
1	E	1.16	1/1160 (0.1%)	1.34	0/1573
1	F	1.23	4/1168 (0.3%)	1.37	1/1583 (0.1%)
1	G	1.11	0/1177	1.31	0/1595
1	H	1.23	1/1177 (0.1%)	1.41	3/1595 (0.2%)
1	I	1.15	2/1165 (0.2%)	1.33	0/1579
1	J	1.12	1/1157 (0.1%)	1.31	0/1567
1	K	1.10	1/1139 (0.1%)	1.28	0/1546
1	L	1.13	0/1161	1.29	0/1574
1	M	1.15	0/1164	1.35	1/1579 (0.1%)
1	N	1.17	0/1157	1.31	1/1570 (0.1%)
1	O	1.10	1/1168 (0.1%)	1.34	0/1583
1	P	1.17	0/1164	1.33	0/1578
All	All	1.15	13/18617 (0.1%)	1.33	6/25243 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1
1	E	0	1
1	G	0	1
1	K	0	1
1	O	0	1
1	P	0	1
All	All	0	6

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	15	PRO	C-O	-9.01	1.17	1.25
1	E	36	PRO	C-O	-6.50	1.15	1.24
1	F	85	ILE	C-O	6.01	1.31	1.24
1	B	15	PRO	C-O	-5.96	1.20	1.25
1	F	99	SER	C-O	5.75	1.30	1.24
1	I	41	ILE	C-O	-5.70	1.17	1.24
1	O	36	PRO	C-O	-5.66	1.16	1.24
1	B	92	GLN	C-O	5.63	1.30	1.23
1	H	27	GLY	CA-C	5.42	1.58	1.52
1	K	36	PRO	C-O	-5.37	1.17	1.24
1	F	17	ALA	C-O	-5.19	1.18	1.24
1	I	38	ILE	C-O	-5.15	1.18	1.24
1	J	120	HIS	C-O	5.14	1.30	1.24

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	87	GLY	CA-C-O	-7.34	113.19	120.75
1	H	88	GLY	CA-C-O	-6.14	113.40	121.51
1	F	15	PRO	CB-CA-C	6.10	117.12	111.39
1	N	27	GLY	CA-C-O	-5.58	115.01	120.75
1	M	87	GLY	N-CA-C	5.11	118.87	112.73
1	H	87	GLY	O-C-N	5.05	127.04	122.19

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	86	SER	Peptide
1	E	86	SER	Peptide
1	G	86	SER	Peptide
1	K	86	SER	Peptide
1	O	86	SER	Peptide
1	P	86	SER	Peptide

5.2 Too-close contacts

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

the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1146	0	1136	10	0
1	B	1143	0	1134	5	0
1	C	1138	0	1114	13	0
1	D	1145	0	1129	9	0
1	E	1138	0	1128	10	0
1	F	1146	0	1136	12	0
1	G	1155	0	1142	14	0
1	H	1155	0	1143	16	0
1	I	1143	0	1134	10	0
1	J	1136	0	1128	8	0
1	K	1118	0	1097	4	0
1	L	1139	0	1130	7	0
1	M	1142	0	1125	8	0
1	N	1135	0	1119	12	0
1	O	1146	0	1136	15	0
1	P	1142	0	1132	16	0
2	A	105	0	61	10	0
2	B	84	0	48	4	0
2	C	189	0	110	20	0
2	D	126	0	73	12	0
2	E	147	0	85	18	0
2	F	168	0	99	16	0
2	G	126	0	73	9	0
2	H	189	0	109	22	0
2	I	105	0	61	10	0
2	J	126	0	73	9	0
2	K	147	0	85	17	0
2	L	84	0	49	6	0
2	M	189	0	110	17	0
2	N	84	0	50	13	0
2	O	84	0	49	7	0
2	P	189	0	112	25	0
3	H	5	0	0	0	0
4	A	83	0	0	2	0
4	B	88	0	0	0	0
4	C	63	0	0	1	0
4	D	61	0	0	2	0
4	E	67	0	0	0	0
4	F	58	0	0	0	0
4	G	60	0	0	0	0
4	H	63	0	0	2	0
4	I	79	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	J	62	0	0	4	0
4	K	57	0	0	2	0
4	L	90	0	0	3	0
4	M	71	0	0	1	0
4	N	63	0	0	2	0
4	O	51	0	0	0	0
4	P	50	0	0	0	0
All	All	21480	0	19310	311	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (311) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:503:2AN:N	2:P:503:2AN:O1	2.07	0.88
2:K:205:2AN:O3	2:K:205:2AN:N	2.06	0.87
2:I:205:2AN:H13	1:O:18:LYS:HD3	1.58	0.86
2:J:202:2AN:N	2:J:202:2AN:O1	2.13	0.82
1:L:59:VAL:HG22	1:L:64:THR:HG22	1.65	0.78
1:O:60:GLU:HG2	2:O:202:2AN:H8	1.66	0.75
1:P:56:VAL:HG11	2:P:508:2AN:H3	1.67	0.75
1:M:93:GLU:O	1:M:122:LYS:HE3	1.86	0.75
1:J:18:LYS:HD2	4:J:310:HOH:O	1.86	0.73
1:H:56:VAL:HG11	2:H:1107:2AN:H3	1.72	0.72
1:O:93:GLU:HA	1:O:93:GLU:OE1	1.89	0.71
2:N:201:2AN:O3	2:N:201:2AN:N	2.24	0.70
2:E:507:2AN:H16	2:E:507:2AN:H2	1.73	0.69
1:A:153:ASN:HD21	1:E:33:LYS:HE2	1.58	0.69
1:P:56:VAL:HG12	2:P:508:2AN:H4	1.75	0.69
2:P:508:2AN:H2	2:P:508:2AN:C16	2.24	0.68
2:M:505:2AN:N	2:M:505:2AN:O1	2.27	0.67
2:C:306:2AN:O2	2:C:306:2AN:N	2.28	0.67
2:K:205:2AN:H2	2:K:205:2AN:C16	2.24	0.67
1:G:93:GLU:CD	1:G:93:GLU:H	2.04	0.66
1:E:91:PHE:HZ	1:E:98:VAL:HG23	1.60	0.65
1:D:9:GLU:OE1	1:D:112:LYS:CE	2.45	0.65
2:H:1103:2AN:N	2:H:1103:2AN:O1	2.29	0.65
2:C:307:2AN:H14	1:D:86:SER:OG	1.97	0.65
2:N:201:2AN:N	2:N:201:2AN:S	2.69	0.65
1:H:56:VAL:HG12	2:H:1107:2AN:H4	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:42:GLU:HG2	2:F:207:2AN:H13	1.81	0.63
1:P:135:VAL:HG13	2:P:508:2AN:H13	1.81	0.62
2:G:304:2AN:N	2:G:304:2AN:O1	2.32	0.62
2:D:706:2AN:O1	2:D:706:2AN:N	2.26	0.62
1:J:92:GLN:HG3	1:J:95:LEU:HD12	1.80	0.62
1:C:123:GLY:HA3	2:C:303:2AN:O2	1.99	0.62
1:I:34:LEU:O	1:O:152:SER:HA	2.00	0.61
2:O:204:2AN:S	2:O:204:2AN:N	2.73	0.61
1:A:4:HIS:CE1	4:A:307:HOH:O	2.52	0.61
1:H:60:GLU:HG2	2:H:1108:2AN:H8	1.82	0.60
2:P:508:2AN:H2	2:P:508:2AN:H16	1.83	0.59
1:L:54:LYS:NZ	4:L:302:HOH:O	2.36	0.59
2:J:205:2AN:N	2:J:205:2AN:S	2.76	0.59
1:C:126:PRO:HG3	4:C:462:HOH:O	2.03	0.58
1:D:126:PRO:HG2	2:E:507:2AN:O1	2.03	0.58
1:A:57:THR:HG23	4:A:324:HOH:O	2.04	0.58
2:M:505:2AN:H2	2:M:505:2AN:H16	1.85	0.58
2:N:202:2AN:C12	2:N:202:2AN:H2	2.33	0.58
2:I:203:2AN:H2	2:I:203:2AN:C16	2.34	0.58
2:D:705:2AN:S	2:D:705:2AN:N	2.77	0.57
1:G:54:LYS:HE2	1:G:69:HIS:CD2	2.39	0.57
2:I:205:2AN:C2	2:I:205:2AN:H16	2.34	0.57
2:A:202:2AN:H15	1:G:18:LYS:CD	2.34	0.57
1:P:60:GLU:HG3	2:P:507:2AN:H8	1.87	0.57
1:M:68:LEU:HD22	1:M:68:LEU:N	2.20	0.57
2:D:704:2AN:O1	2:D:704:2AN:N	2.36	0.57
2:I:205:2AN:H13	1:O:18:LYS:CD	2.32	0.57
2:J:204:2AN:S	2:J:204:2AN:N	2.78	0.57
2:P:501:2AN:N	2:P:501:2AN:S	2.78	0.57
2:K:206:2AN:H12	2:K:206:2AN:H2	1.85	0.56
1:N:59:VAL:HA	1:N:63:LYS:O	2.06	0.56
2:C:304:2AN:S	2:C:304:2AN:N	2.78	0.56
2:C:305:2AN:H16	2:C:305:2AN:C2	2.36	0.56
1:N:94:ILE:CD1	1:N:128:PRO:HG2	2.35	0.56
1:A:34:LEU:O	1:G:152:SER:HA	2.06	0.56
2:D:706:2AN:C2	2:D:706:2AN:H16	2.35	0.56
2:A:201:2AN:H2	2:A:201:2AN:C16	2.36	0.56
2:G:302:2AN:N	2:G:302:2AN:S	2.71	0.56
1:H:60:GLU:CG	2:H:1108:2AN:H8	2.34	0.56
1:H:42:GLU:HG2	2:H:1109:2AN:H13	1.87	0.56
2:H:1107:2AN:H2	2:H:1107:2AN:C16	2.34	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:203:2AN:H2	2:I:203:2AN:H16	1.88	0.56
2:N:203:2AN:S	2:N:203:2AN:N	2.75	0.55
2:C:304:2AN:N	2:C:304:2AN:O3	2.33	0.55
2:E:506:2AN:H2	2:E:506:2AN:C16	2.35	0.55
1:C:85:ILE:HD12	1:C:100:PHE:CE1	2.42	0.55
2:C:308:2AN:C9	2:D:702:2AN:H16	2.37	0.55
2:P:507:2AN:S	2:P:507:2AN:N	2.80	0.55
2:G:305:2AN:S	2:G:305:2AN:N	2.81	0.54
2:E:505:2AN:N	2:E:505:2AN:S	2.81	0.54
2:C:308:2AN:H12	2:D:702:2AN:C9	2.38	0.54
1:J:64:THR:HG22	4:J:353:HOH:O	2.08	0.53
2:D:706:2AN:H16	2:D:706:2AN:H2	1.90	0.53
2:K:204:2AN:H16	2:K:204:2AN:C2	2.38	0.53
2:P:508:2AN:O3	2:P:508:2AN:N	2.41	0.53
2:M:507:2AN:S	2:M:507:2AN:N	2.82	0.53
2:A:201:2AN:H2	2:A:201:2AN:H16	1.91	0.52
1:E:58:ALA:HB3	2:E:502:2AN:C14	2.40	0.52
2:F:201:2AN:S	2:F:201:2AN:N	2.81	0.52
2:H:1105:2AN:S	2:H:1105:2AN:N	2.81	0.52
1:H:18:LYS:HG3	2:H:1101:2AN:H13	1.92	0.52
2:C:306:2AN:H16	2:C:306:2AN:H2	1.91	0.52
2:L:203:2AN:N	2:L:203:2AN:S	2.82	0.52
2:P:509:2AN:S	2:P:509:2AN:N	2.82	0.52
2:H:1101:2AN:C2	2:H:1101:2AN:H16	2.38	0.52
2:H:1109:2AN:O3	2:H:1109:2AN:N	2.42	0.52
2:K:205:2AN:C16	2:K:205:2AN:C2	2.85	0.52
2:F:202:2AN:H2	2:F:202:2AN:C16	2.40	0.52
1:B:93:GLU:HG2	1:C:93:GLU:CG	2.39	0.52
2:D:702:2AN:N	2:D:702:2AN:S	2.82	0.52
2:A:204:2AN:N	2:A:204:2AN:S	2.83	0.51
1:E:45:GLU:HB2	2:E:506:2AN:C7	2.40	0.51
2:I:202:2AN:N	2:I:202:2AN:S	2.84	0.51
2:F:204:2AN:N	2:F:204:2AN:S	2.83	0.51
2:F:206:2AN:H16	2:F:206:2AN:H2	1.91	0.51
2:F:208:2AN:N	2:F:208:2AN:O1	2.43	0.51
2:O:202:2AN:S	2:O:202:2AN:N	2.83	0.51
1:D:153:ASN:O	1:D:153:ASN:ND2	2.43	0.51
2:B:203:2AN:S	2:B:203:2AN:N	2.83	0.51
1:C:87:GLY:HA2	1:C:91:PHE:CD2	2.46	0.51
2:H:1107:2AN:O3	2:H:1107:2AN:N	2.38	0.51
1:I:105:GLU:OE1	1:I:114:LYS:HE2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:3:VAL:HG13	1:L:118:THR:CG2	2.41	0.51
1:B:3:VAL:HG13	1:B:118:THR:CG2	2.41	0.51
1:G:3:VAL:HG13	1:G:118:THR:CG2	2.41	0.51
1:D:80:THR:HG23	4:D:803:HOH:O	2.11	0.50
2:A:202:2AN:H15	1:G:18:LYS:HD3	1.92	0.50
1:H:42:GLU:CD	2:H:1109:2AN:H13	2.35	0.50
2:L:204:2AN:S	2:L:204:2AN:N	2.84	0.50
1:O:94:ILE:HD11	1:O:125:ALA:HB1	1.93	0.50
1:I:8:GLU:OE1	1:I:8:GLU:HA	2.11	0.50
1:I:95:LEU:HD13	1:I:98:VAL:CG2	2.41	0.50
2:K:204:2AN:N	2:K:204:2AN:S	2.84	0.50
1:N:52:THR:HB	1:N:71:ILE:HD12	1.93	0.50
1:F:42:GLU:CG	2:F:207:2AN:H13	2.41	0.50
1:O:65:SER:HB3	1:O:90:GLY:CA	2.41	0.50
1:B:59:VAL:HG22	1:B:64:THR:HG22	1.94	0.50
1:P:23:THR:HG21	1:P:143:PHE:CE1	2.47	0.50
1:G:117:VAL:HG11	2:G:303:2AN:C14	2.41	0.50
2:P:502:2AN:S	2:P:502:2AN:N	2.85	0.50
1:A:153:ASN:HD21	1:E:33:LYS:CE	2.23	0.49
2:C:308:2AN:N	2:C:308:2AN:S	2.84	0.49
2:D:706:2AN:N	2:D:706:2AN:S	2.85	0.49
1:F:34:LEU:O	1:H:152:SER:HA	2.12	0.49
2:P:508:2AN:N	2:P:508:2AN:S	2.79	0.49
2:J:205:2AN:H12	4:J:320:HOH:O	2.12	0.49
1:L:105:GLU:HG2	4:L:360:HOH:O	2.10	0.49
2:C:307:2AN:S	2:C:307:2AN:N	2.86	0.49
1:F:152:SER:HA	1:H:34:LEU:O	2.12	0.49
2:K:204:2AN:H16	2:K:204:2AN:H2	1.95	0.49
1:H:64:THR:OG1	4:H:1201:HOH:O	2.20	0.49
1:K:153:ASN:O	4:K:301:HOH:O	2.20	0.49
2:I:205:2AN:S	2:I:205:2AN:N	2.86	0.49
2:G:301:2AN:S	2:G:301:2AN:N	2.86	0.48
2:A:202:2AN:H12	2:A:202:2AN:C2	2.43	0.48
2:H:1109:2AN:N	2:H:1109:2AN:S	2.77	0.48
1:J:136:LYS:HE2	1:J:140:GLN:NE2	2.27	0.48
2:K:203:2AN:S	2:K:203:2AN:N	2.87	0.48
1:P:95:LEU:HD21	1:P:98:VAL:CG2	2.43	0.48
1:M:92:GLN:HG2	4:M:652:HOH:O	2.14	0.48
2:F:202:2AN:N	2:F:202:2AN:O3	2.47	0.48
2:I:203:2AN:H16	2:I:203:2AN:C2	2.44	0.48
2:M:507:2AN:N	2:M:507:2AN:O3	2.39	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1108:2AN:N	2:H:1108:2AN:S	2.87	0.48
1:K:91:PHE:HB3	4:K:322:HOH:O	2.14	0.47
1:P:22:ALA:HA	1:P:26:ASP:HB2	1.96	0.47
2:A:202:2AN:H15	1:G:18:LYS:HD2	1.95	0.47
1:I:68:LEU:N	1:I:68:LEU:HD22	2.29	0.47
1:E:91:PHE:HE2	1:E:95:LEU:HB3	1.79	0.47
2:L:201:2AN:C2	2:L:201:2AN:H12	2.45	0.47
2:N:201:2AN:H2	2:N:201:2AN:C12	2.45	0.47
2:M:508:2AN:S	2:M:508:2AN:N	2.88	0.47
1:P:56:VAL:CG1	2:P:508:2AN:H3	2.39	0.47
2:P:503:2AN:O1	2:P:503:2AN:C11	2.63	0.47
2:N:202:2AN:O3	2:N:202:2AN:N	2.46	0.47
1:E:68:LEU:HD13	2:E:506:2AN:H2	1.96	0.47
2:E:503:2AN:C2	2:E:503:2AN:H16	2.45	0.47
2:M:506:2AN:N	2:M:506:2AN:O3	2.38	0.47
1:P:18:LYS:HG2	2:P:503:2AN:C15	2.45	0.47
2:O:203:2AN:O1	2:O:203:2AN:N	2.48	0.47
1:A:95:LEU:HD13	1:A:98:VAL:CG2	2.45	0.47
2:M:505:2AN:N	2:M:505:2AN:S	2.70	0.47
1:P:66:TYR:OH	2:P:509:2AN:H6	2.15	0.47
1:M:59:VAL:HG21	1:O:39:GLN:O	2.14	0.47
1:K:68:LEU:HD13	2:K:205:2AN:H2	1.96	0.46
2:N:202:2AN:H2	2:N:202:2AN:H12	1.97	0.46
1:M:135:VAL:HG13	2:M:505:2AN:H7	1.98	0.46
1:N:95:LEU:HD13	1:N:98:VAL:CG2	2.45	0.46
1:H:56:VAL:CG1	2:H:1107:2AN:H3	2.41	0.46
2:J:205:2AN:H16	2:J:205:2AN:H2	1.98	0.46
2:P:508:2AN:C16	2:P:508:2AN:C2	2.93	0.46
1:D:94:ILE:HD11	1:D:125:ALA:HB1	1.97	0.46
2:M:506:2AN:N	2:M:506:2AN:S	2.88	0.46
2:M:506:2AN:H16	2:M:506:2AN:C2	2.45	0.46
1:P:31:THR:N	1:P:32:PRO:CD	2.79	0.46
1:A:152:SER:HA	1:G:34:LEU:O	2.16	0.46
1:N:94:ILE:HD13	1:N:128:PRO:HG2	1.96	0.46
1:B:59:VAL:CG2	1:B:64:THR:HG22	2.45	0.46
2:G:305:2AN:N	2:G:305:2AN:O3	2.48	0.46
2:K:202:2AN:S	2:K:202:2AN:N	2.83	0.46
1:M:55:LYS:HE2	1:M:66:TYR:CG	2.50	0.46
1:O:92:GLN:HB2	1:O:95:LEU:HD12	1.98	0.46
2:P:504:2AN:S	2:P:504:2AN:N	2.88	0.46
2:C:305:2AN:N	2:C:305:2AN:S	2.88	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:702:2AN:N	2:D:702:2AN:O3	2.33	0.46
2:N:202:2AN:C12	2:N:202:2AN:C2	2.94	0.46
2:J:201:2AN:N	2:J:201:2AN:S	2.88	0.46
1:G:93:GLU:CD	1:G:93:GLU:N	2.72	0.45
2:N:203:2AN:H2	2:N:203:2AN:H12	1.98	0.45
2:B:204:2AN:N	2:B:204:2AN:S	2.89	0.45
1:C:68:LEU:HD13	2:D:701:2AN:H2	1.98	0.45
1:J:143:PHE:CG	2:J:201:2AN:H6	2.51	0.45
1:K:45:GLU:HB2	2:K:205:2AN:C7	2.47	0.45
2:G:303:2AN:S	2:G:303:2AN:N	2.90	0.45
2:E:506:2AN:S	2:E:506:2AN:N	2.88	0.45
2:B:202:2AN:S	2:B:202:2AN:N	2.90	0.45
1:H:31:THR:OG1	4:H:1202:HOH:O	2.20	0.45
1:I:152:SER:HA	1:O:34:LEU:O	2.16	0.45
2:F:203:2AN:S	2:F:203:2AN:N	2.90	0.45
1:G:142:ILE:CD1	2:G:304:2AN:H4	2.47	0.45
1:H:3:VAL:HG13	1:H:118:THR:CG2	2.48	0.45
1:P:18:LYS:HG2	2:P:503:2AN:H15	1.99	0.45
2:H:1102:2AN:N	2:H:1102:2AN:S	2.90	0.44
1:N:54:LYS:HE2	4:N:301:HOH:O	2.17	0.44
2:A:202:2AN:N	2:A:202:2AN:S	2.91	0.44
1:H:42:GLU:CG	2:H:1109:2AN:H13	2.47	0.44
2:I:205:2AN:N	2:I:205:2AN:O1	2.45	0.44
2:J:202:2AN:H2	2:J:202:2AN:H16	2.00	0.44
2:K:202:2AN:N	2:K:202:2AN:O1	2.49	0.44
2:M:504:2AN:N	2:M:504:2AN:S	2.91	0.44
1:P:3:VAL:HG13	1:P:118:THR:CG2	2.47	0.44
1:A:61:ASP:HB3	1:F:47:ASN:OD1	2.17	0.44
2:F:206:2AN:S	2:F:206:2AN:N	2.88	0.44
1:C:85:ILE:HD12	1:C:100:PHE:HE1	1.81	0.44
2:N:204:2AN:N	2:N:204:2AN:S	2.90	0.44
1:C:85:ILE:HG22	1:C:91:PHE:CZ	2.53	0.44
1:F:143:PHE:CG	2:F:201:2AN:H6	2.52	0.44
2:H:1101:2AN:C2	2:H:1101:2AN:C16	2.94	0.44
2:K:201:2AN:C2	2:K:201:2AN:H16	2.47	0.44
2:C:309:2AN:H6	1:F:34:LEU:CD2	2.48	0.44
2:E:507:2AN:H2	2:E:507:2AN:C16	2.46	0.44
2:N:202:2AN:H12	2:N:202:2AN:C2	2.48	0.44
1:O:65:SER:HB3	1:O:90:GLY:HA2	2.00	0.44
1:C:143:PHE:CG	2:C:302:2AN:H6	2.53	0.44
1:I:33:LYS:NZ	2:M:501:2AN:O3	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:9:GLU:OE1	1:D:112:LYS:HE3	2.18	0.43
2:F:204:2AN:H16	2:F:204:2AN:C2	2.47	0.43
1:G:45:GLU:HB2	2:G:305:2AN:C7	2.48	0.43
2:C:309:2AN:H2	2:C:309:2AN:C16	2.48	0.43
2:E:502:2AN:H16	2:E:502:2AN:H2	2.00	0.43
1:G:4:HIS:HA	1:M:3:VAL:O	2.17	0.43
2:H:1107:2AN:H2	2:H:1107:2AN:H16	2.00	0.43
2:L:201:2AN:C2	2:L:201:2AN:C12	2.96	0.43
1:N:55:LYS:HE2	1:N:66:TYR:CG	2.54	0.43
2:N:203:2AN:N	2:N:203:2AN:O1	2.52	0.43
2:O:203:2AN:H16	2:O:203:2AN:H2	2.00	0.43
2:L:201:2AN:N	2:L:201:2AN:S	2.92	0.43
2:C:308:2AN:N	2:C:308:2AN:O3	2.52	0.43
2:E:504:2AN:C2	2:E:504:2AN:H16	2.49	0.43
1:L:9:GLU:HG2	1:L:114:LYS:HG2	2.01	0.43
2:M:509:2AN:S	2:M:509:2AN:N	2.90	0.42
1:N:143:PHE:CG	2:N:201:2AN:H6	2.54	0.42
1:E:91:PHE:CE2	1:E:95:LEU:HB3	2.54	0.42
1:F:9:GLU:OE2	1:F:114:LYS:HE3	2.19	0.42
2:L:201:2AN:C12	2:L:201:2AN:H2	2.49	0.42
1:N:103:LYS:HE3	1:N:114:LYS:HE2	2.01	0.42
2:O:204:2AN:N	2:O:204:2AN:O3	2.51	0.42
2:C:302:2AN:S	2:C:302:2AN:N	2.93	0.42
1:D:9:GLU:OE1	1:D:112:LYS:HE2	2.19	0.42
2:E:505:2AN:C2	2:E:505:2AN:H16	2.48	0.42
1:F:54:LYS:HB2	1:F:69:HIS:HB3	2.00	0.42
2:P:501:2AN:N	2:P:501:2AN:O2	2.53	0.42
1:A:153:ASN:ND2	1:E:33:LYS:HE2	2.29	0.42
1:E:60:GLU:HG3	2:E:505:2AN:H8	2.01	0.42
2:E:502:2AN:O1	2:E:502:2AN:N	2.52	0.42
1:H:68:LEU:HD22	1:H:68:LEU:N	2.34	0.42
1:L:144:LYS:NZ	4:L:310:HOH:O	2.52	0.42
1:N:69:HIS:CE1	1:N:85:ILE:HG12	2.55	0.42
2:C:309:2AN:H6	1:F:34:LEU:HD23	2.01	0.42
1:C:125:ALA:HB2	2:C:303:2AN:C3	2.50	0.42
2:P:506:2AN:N	2:P:506:2AN:S	2.93	0.42
1:B:93:GLU:HG2	1:C:93:GLU:HG2	2.00	0.42
1:D:3:VAL:HG13	1:D:118:THR:CG2	2.50	0.42
2:E:504:2AN:S	2:E:504:2AN:N	2.92	0.42
2:H:1103:2AN:N	2:H:1103:2AN:S	2.93	0.42
2:I:201:2AN:S	2:I:201:2AN:N	2.93	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:58:ALA:HB3	2:P:508:2AN:C6	2.50	0.42
4:N:313:HOH:O	1:O:16:PRO:HG2	2.19	0.41
1:O:22:ALA:CB	1:O:150:VAL:HG21	2.50	0.41
2:O:201:2AN:N	2:O:201:2AN:S	2.93	0.41
1:A:8:GLU:OE2	1:A:8:GLU:HA	2.18	0.41
1:G:6:PHE:HB2	1:G:117:VAL:HG12	2.02	0.41
1:H:143:PHE:CG	2:H:1102:2AN:H6	2.55	0.41
1:O:92:GLN:CB	1:O:95:LEU:HD12	2.50	0.41
2:M:504:2AN:C2	2:M:504:2AN:H12	2.49	0.41
1:C:23:THR:HG21	1:C:143:PHE:CE2	2.56	0.41
2:F:203:2AN:N	2:F:203:2AN:O1	2.44	0.41
1:J:80:THR:HG23	4:J:303:HOH:O	2.20	0.41
1:N:79:TYR:HH	1:O:79:TYR:HH	1.65	0.41
1:C:125:ALA:HB2	2:C:303:2AN:C4	2.50	0.41
1:I:34:LEU:CD2	2:M:501:2AN:H6	2.51	0.41
1:I:93:GLU:CD	1:I:93:GLU:H	2.27	0.41
1:N:34:LEU:O	1:P:152:SER:HA	2.20	0.41
2:F:206:2AN:H2	2:F:206:2AN:C16	2.50	0.41
1:I:4:HIS:CE1	4:I:337:HOH:O	2.74	0.41
1:M:44:VAL:HG12	2:M:509:2AN:C13	2.51	0.41
2:P:501:2AN:H16	2:P:501:2AN:C2	2.50	0.41
2:K:201:2AN:C2	2:K:201:2AN:C16	2.99	0.41
2:K:205:2AN:H16	1:L:53:VAL:HG21	2.03	0.41
2:A:205:2AN:S	2:A:205:2AN:N	2.92	0.41
2:B:204:2AN:N	2:B:204:2AN:O1	2.47	0.41
1:F:55:LYS:HE2	1:F:66:TYR:CG	2.56	0.41
1:J:146:ILE:O	1:J:149:TYR:HB3	2.21	0.41
1:P:92:GLN:H	1:P:92:GLN:HG2	1.68	0.41
2:P:503:2AN:C2	2:P:503:2AN:H12	2.51	0.41
2:K:203:2AN:C2	2:K:203:2AN:H16	2.51	0.40
2:M:504:2AN:C2	2:M:504:2AN:C12	2.97	0.40
2:A:201:2AN:H16	2:A:201:2AN:C2	2.51	0.40
1:F:42:GLU:HG2	2:F:207:2AN:C13	2.51	0.40
2:E:506:2AN:C16	2:E:506:2AN:C2	3.00	0.40
2:D:706:2AN:H12	4:D:806:HOH:O	2.21	0.40
2:E:503:2AN:C2	2:E:503:2AN:C16	2.99	0.40
2:F:202:2AN:H2	2:F:202:2AN:H16	2.03	0.40
1:J:58:ALA:HB3	2:J:202:2AN:C14	2.52	0.40
2:K:201:2AN:C16	2:K:201:2AN:H2	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	150/153 (98%)	150 (100%)	0	0	100	100
1	B	150/153 (98%)	149 (99%)	1 (1%)	0	100	100
1	C	150/153 (98%)	150 (100%)	0	0	100	100
1	D	151/153 (99%)	150 (99%)	1 (1%)	0	100	100
1	E	150/153 (98%)	150 (100%)	0	0	100	100
1	F	150/153 (98%)	149 (99%)	1 (1%)	0	100	100
1	G	152/153 (99%)	152 (100%)	0	0	100	100
1	H	151/153 (99%)	150 (99%)	1 (1%)	0	100	100
1	I	150/153 (98%)	149 (99%)	1 (1%)	0	100	100
1	J	147/153 (96%)	147 (100%)	0	0	100	100
1	K	147/153 (96%)	147 (100%)	0	0	100	100
1	L	150/153 (98%)	150 (100%)	0	0	100	100
1	M	150/153 (98%)	150 (100%)	0	0	100	100
1	N	150/153 (98%)	150 (100%)	0	0	100	100
1	O	150/153 (98%)	149 (99%)	1 (1%)	0	100	100
1	P	150/153 (98%)	150 (100%)	0	0	100	100
All	All	2398/2448 (98%)	2392 (100%)	6 (0%)	0	100	100

There are no Ramachandran outliers to report.

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	126/128 (98%)	123 (98%)	3 (2%)	43	49
1	B	125/128 (98%)	124 (99%)	1 (1%)	73	81
1	C	124/128 (97%)	124 (100%)	0	100	100
1	D	125/128 (98%)	125 (100%)	0	100	100
1	E	124/128 (97%)	124 (100%)	0	100	100
1	F	126/128 (98%)	124 (98%)	2 (2%)	55	64
1	G	127/128 (99%)	127 (100%)	0	100	100
1	H	127/128 (99%)	127 (100%)	0	100	100
1	I	125/128 (98%)	125 (100%)	0	100	100
1	J	124/128 (97%)	123 (99%)	1 (1%)	73	81
1	K	120/128 (94%)	120 (100%)	0	100	100
1	L	124/128 (97%)	124 (100%)	0	100	100
1	M	125/128 (98%)	124 (99%)	1 (1%)	73	81
1	N	123/128 (96%)	122 (99%)	1 (1%)	73	81
1	O	126/128 (98%)	125 (99%)	1 (1%)	73	81
1	P	125/128 (98%)	123 (98%)	2 (2%)	55	64
All	All	1996/2048 (98%)	1984 (99%)	12 (1%)	78	86

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	60	GLU
1	A	69	HIS
1	A	112	LYS
1	B	69	HIS
1	F	112	LYS
1	F	133	GLN
1	J	8	GLU
1	M	61	ASP
1	N	69	HIS
1	O	69	HIS
1	P	92	GLN
1	P	133	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	153	ASN
1	C	120	HIS
1	E	120	HIS
1	E	153	ASN
1	F	153	ASN
1	H	120	HIS
1	I	133	GLN
1	I	137	GLN
1	J	120	HIS
1	K	153	ASN
1	M	153	ASN
1	N	69	HIS
1	N	153	ASN
1	O	153	ASN
1	P	120	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

103 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	M	504	-	22,23,23	0.91	2 (9%)	29,33,33	0.81	1 (3%)
2	2AN	A	203	-	22,23,23	0.80	1 (4%)	29,33,33	0.94	1 (3%)
2	2AN	B	204	-	22,23,23	0.81	1 (4%)	29,33,33	0.87	0
2	2AN	L	201	-	22,23,23	0.74	1 (4%)	29,33,33	0.95	2 (6%)
2	2AN	M	501	-	22,23,23	0.80	1 (4%)	29,33,33	0.80	0
2	2AN	M	505	-	22,23,23	0.84	1 (4%)	29,33,33	1.18	2 (6%)
2	2AN	L	202	-	22,23,23	0.86	1 (4%)	29,33,33	0.91	1 (3%)
2	2AN	H	1107	-	22,23,23	0.78	1 (4%)	29,33,33	0.76	0
2	2AN	K	202	-	22,23,23	0.79	1 (4%)	29,33,33	1.07	1 (3%)
2	2AN	H	1103	-	22,23,23	0.85	0	29,33,33	0.73	0
2	2AN	K	205	-	22,23,23	0.73	1 (4%)	29,33,33	1.24	2 (6%)
2	2AN	I	204	-	22,23,23	0.79	1 (4%)	29,33,33	0.90	2 (6%)
2	2AN	N	203	-	22,23,23	0.85	1 (4%)	29,33,33	0.85	1 (3%)
2	2AN	A	205	-	22,23,23	0.68	0	29,33,33	0.84	1 (3%)
2	2AN	P	503	-	22,23,23	0.79	1 (4%)	29,33,33	0.92	2 (6%)
2	2AN	D	705	-	22,23,23	0.83	1 (4%)	29,33,33	0.75	0
2	2AN	J	205	-	22,23,23	0.84	1 (4%)	29,33,33	0.90	1 (3%)
2	2AN	P	504	-	22,23,23	0.80	1 (4%)	29,33,33	0.80	0
2	2AN	J	204	-	22,23,23	0.87	1 (4%)	29,33,33	0.76	1 (3%)
2	2AN	P	501	-	22,23,23	0.76	1 (4%)	29,33,33	0.83	0
2	2AN	E	505	-	22,23,23	0.81	1 (4%)	29,33,33	0.70	0
2	2AN	E	507	-	22,23,23	1.13	3 (13%)	29,33,33	1.21	1 (3%)
2	2AN	K	207	-	22,23,23	0.76	1 (4%)	29,33,33	0.74	0
2	2AN	E	504	-	22,23,23	0.87	1 (4%)	29,33,33	0.78	0
2	2AN	F	207	-	22,23,23	0.78	1 (4%)	29,33,33	0.75	0
2	2AN	N	204	-	22,23,23	0.98	1 (4%)	29,33,33	0.83	0
2	2AN	O	203	-	22,23,23	0.77	1 (4%)	29,33,33	1.08	2 (6%)
2	2AN	C	306	-	22,23,23	0.68	1 (4%)	29,33,33	1.15	2 (6%)
2	2AN	G	302	-	22,23,23	0.78	1 (4%)	29,33,33	0.84	1 (3%)
2	2AN	G	305	-	22,23,23	0.83	1 (4%)	29,33,33	0.86	1 (3%)
2	2AN	D	701	-	22,23,23	1.01	1 (4%)	29,33,33	0.86	0
2	2AN	D	704	-	22,23,23	0.80	1 (4%)	29,33,33	0.83	1 (3%)
2	2AN	L	204	-	22,23,23	0.71	1 (4%)	29,33,33	0.78	0
2	2AN	M	509	-	22,23,23	0.68	0	29,33,33	0.84	0
2	2AN	A	201	-	22,23,23	0.91	1 (4%)	29,33,33	0.88	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	2AN	M	507	-	22,23,23	0.94	1 (4%)	29,33,33	0.72	0
2	2AN	N	201	-	22,23,23	0.62	0	29,33,33	0.61	0
2	2AN	J	206	-	22,23,23	0.71	1 (4%)	29,33,33	0.82	2 (6%)
2	2AN	F	203	-	22,23,23	0.85	1 (4%)	29,33,33	0.74	0
2	2AN	F	205	-	22,23,23	0.80	1 (4%)	29,33,33	0.86	1 (3%)
2	2AN	H	1109	-	22,23,23	0.97	2 (9%)	29,33,33	0.94	1 (3%)
2	2AN	J	203	-	22,23,23	1.00	2 (9%)	29,33,33	0.85	1 (3%)
2	2AN	K	203	-	22,23,23	0.82	1 (4%)	29,33,33	0.76	1 (3%)
2	2AN	G	303	-	22,23,23	0.80	0	29,33,33	0.76	0
2	2AN	I	201	-	22,23,23	0.53	0	29,33,33	0.94	1 (3%)
2	2AN	O	201	-	22,23,23	0.90	1 (4%)	29,33,33	0.91	0
2	2AN	P	506	-	22,23,23	0.83	1 (4%)	29,33,33	0.87	0
2	2AN	F	202	-	22,23,23	0.72	1 (4%)	29,33,33	0.81	0
2	2AN	O	204	-	22,23,23	0.86	1 (4%)	29,33,33	0.90	1 (3%)
2	2AN	C	304	-	22,23,23	0.75	1 (4%)	29,33,33	0.64	0
2	2AN	G	304	-	22,23,23	0.72	1 (4%)	29,33,33	0.94	1 (3%)
2	2AN	B	202	-	22,23,23	0.78	1 (4%)	29,33,33	0.82	0
2	2AN	G	301	-	22,23,23	0.69	1 (4%)	29,33,33	0.82	0
2	2AN	M	508	-	22,23,23	0.74	1 (4%)	29,33,33	0.85	0
2	2AN	K	201	-	22,23,23	1.00	1 (4%)	29,33,33	0.84	0
2	2AN	B	201	-	22,23,23	0.90	1 (4%)	29,33,33	0.97	1 (3%)
2	2AN	M	506	-	22,23,23	0.79	1 (4%)	29,33,33	0.80	0
2	2AN	P	505	-	22,23,23	0.77	0	29,33,33	1.01	2 (6%)
2	2AN	G	306	-	22,23,23	0.82	1 (4%)	29,33,33	0.77	1 (3%)
2	2AN	H	1101	-	22,23,23	0.78	1 (4%)	29,33,33	1.03	1 (3%)
2	2AN	N	202	-	22,23,23	1.00	1 (4%)	29,33,33	0.93	2 (6%)
2	2AN	A	204	-	22,23,23	0.73	1 (4%)	29,33,33	0.79	0
2	2AN	I	203	-	22,23,23	0.89	1 (4%)	29,33,33	0.98	1 (3%)
2	2AN	F	208	-	22,23,23	1.02	3 (13%)	29,33,33	0.89	1 (3%)
2	2AN	M	502	-	22,23,23	0.93	1 (4%)	29,33,33	1.11	3 (10%)
2	2AN	A	202	-	22,23,23	0.82	1 (4%)	29,33,33	0.79	0
2	2AN	K	206	-	22,23,23	1.20	3 (13%)	29,33,33	1.00	1 (3%)
2	2AN	C	302	-	22,23,23	0.83	1 (4%)	29,33,33	0.80	0
2	2AN	I	202	-	22,23,23	0.76	1 (4%)	29,33,33	0.88	0
2	2AN	P	502	-	22,23,23	0.70	1 (4%)	29,33,33	0.77	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	2AN	J	201	-	22,23,23	0.79	1 (4%)	29,33,33	0.88	0
2	2AN	E	506	-	22,23,23	0.88	1 (4%)	29,33,33	0.90	1 (3%)
2	2AN	C	305	-	22,23,23	0.83	1 (4%)	29,33,33	0.85	0
2	2AN	J	202	-	22,23,23	0.89	1 (4%)	29,33,33	0.98	1 (3%)
2	2AN	C	309	-	22,23,23	0.80	0	29,33,33	0.86	0
2	2AN	P	508	-	22,23,23	0.71	1 (4%)	29,33,33	0.75	0
2	2AN	O	202	-	22,23,23	0.77	1 (4%)	29,33,33	0.74	0
2	2AN	D	706	-	22,23,23	0.86	1 (4%)	29,33,33	0.77	0
2	2AN	D	703	-	22,23,23	0.77	0	29,33,33	1.06	2 (6%)
2	2AN	C	307	-	22,23,23	0.75	1 (4%)	29,33,33	0.83	0
2	2AN	E	501	-	22,23,23	0.70	0	29,33,33	0.80	0
3	SO4	H	1110	-	4,4,4	0.32	0	6,6,6	0.10	0
2	2AN	H	1108	-	22,23,23	0.87	1 (4%)	29,33,33	0.83	0
2	2AN	C	301	-	22,23,23	0.99	1 (4%)	29,33,33	0.97	1 (3%)
2	2AN	B	203	-	22,23,23	0.77	1 (4%)	29,33,33	0.82	0
2	2AN	E	503	-	22,23,23	0.94	2 (9%)	29,33,33	0.98	2 (6%)
2	2AN	H	1106	-	22,23,23	0.82	1 (4%)	29,33,33	1.01	2 (6%)
2	2AN	H	1102	-	22,23,23	0.72	0	29,33,33	0.91	0
2	2AN	F	204	-	22,23,23	0.82	1 (4%)	29,33,33	0.85	0
2	2AN	C	308	-	22,23,23	1.03	3 (13%)	29,33,33	0.96	1 (3%)
2	2AN	L	203	-	22,23,23	0.86	1 (4%)	29,33,33	0.79	0
2	2AN	K	204	-	22,23,23	0.88	1 (4%)	29,33,33	0.77	0
2	2AN	C	303	-	22,23,23	0.92	1 (4%)	29,33,33	0.96	1 (3%)
2	2AN	H	1105	-	22,23,23	0.72	1 (4%)	29,33,33	0.82	1 (3%)
2	2AN	F	201	-	22,23,23	0.65	0	29,33,33	0.72	0
2	2AN	E	502	-	22,23,23	0.85	1 (4%)	29,33,33	1.00	2 (6%)
2	2AN	I	205	-	22,23,23	0.76	1 (4%)	29,33,33	0.79	1 (3%)
2	2AN	H	1104	-	22,23,23	0.74	0	29,33,33	0.93	1 (3%)
2	2AN	M	503	-	22,23,23	0.89	1 (4%)	29,33,33	0.88	0
2	2AN	P	509	-	22,23,23	0.93	1 (4%)	29,33,33	0.72	0
2	2AN	D	702	-	22,23,23	0.87	2 (9%)	29,33,33	0.79	1 (3%)
2	2AN	F	206	-	22,23,23	0.79	1 (4%)	29,33,33	1.01	1 (3%)
2	2AN	P	507	-	22,23,23	0.74	1 (4%)	29,33,33	0.71	0

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	M	504	-	-	0/10/10/10	0/3/3/3
2	2AN	A	203	-	-	0/10/10/10	0/3/3/3
2	2AN	B	204	-	-	2/10/10/10	0/3/3/3
2	2AN	L	201	-	-	0/10/10/10	0/3/3/3
2	2AN	M	501	-	-	2/10/10/10	0/3/3/3
2	2AN	M	505	-	-	0/10/10/10	0/3/3/3
2	2AN	L	202	-	-	0/10/10/10	0/3/3/3
2	2AN	H	1107	-	-	0/10/10/10	0/3/3/3
2	2AN	K	202	-	-	0/10/10/10	0/3/3/3
2	2AN	H	1103	-	-	6/10/10/10	0/3/3/3
2	2AN	K	205	-	-	8/10/10/10	0/3/3/3
2	2AN	I	204	-	-	0/10/10/10	0/3/3/3
2	2AN	N	203	-	-	0/10/10/10	0/3/3/3
2	2AN	A	205	-	-	0/10/10/10	0/3/3/3
2	2AN	P	503	-	-	8/10/10/10	0/3/3/3
2	2AN	D	705	-	-	0/10/10/10	0/3/3/3
2	2AN	J	205	-	-	0/10/10/10	0/3/3/3
2	2AN	P	504	-	-	0/10/10/10	0/3/3/3
2	2AN	J	204	-	-	0/10/10/10	0/3/3/3
2	2AN	P	501	-	-	0/10/10/10	0/3/3/3
2	2AN	E	505	-	-	0/10/10/10	0/3/3/3
2	2AN	E	507	-	-	6/10/10/10	0/3/3/3
2	2AN	K	207	-	-	2/10/10/10	0/3/3/3
2	2AN	E	504	-	-	2/10/10/10	0/3/3/3
2	2AN	F	207	-	-	2/10/10/10	0/3/3/3
2	2AN	N	204	-	-	2/10/10/10	0/3/3/3
2	2AN	O	203	-	-	0/10/10/10	0/3/3/3
2	2AN	C	306	-	-	1/10/10/10	0/3/3/3
2	2AN	G	302	-	-	0/10/10/10	0/3/3/3
2	2AN	G	305	-	-	0/10/10/10	0/3/3/3
2	2AN	D	701	-	-	2/10/10/10	0/3/3/3
2	2AN	D	704	-	-	0/10/10/10	0/3/3/3
2	2AN	L	204	-	-	2/10/10/10	0/3/3/3
2	2AN	M	509	-	-	5/10/10/10	0/3/3/3
2	2AN	A	201	-	-	0/10/10/10	0/3/3/3
2	2AN	M	507	-	-	0/10/10/10	0/3/3/3
2	2AN	N	201	-	-	0/10/10/10	0/3/3/3
2	2AN	J	206	-	-	7/10/10/10	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	2AN	F	203	-	-	1/10/10/10	0/3/3/3
2	2AN	F	205	-	-	0/10/10/10	0/3/3/3
2	2AN	H	1109	-	-	2/10/10/10	0/3/3/3
2	2AN	J	203	-	-	2/10/10/10	0/3/3/3
2	2AN	K	203	-	-	0/10/10/10	0/3/3/3
2	2AN	G	303	-	-	0/10/10/10	0/3/3/3
2	2AN	I	201	-	-	0/10/10/10	0/3/3/3
2	2AN	O	201	-	-	0/10/10/10	0/3/3/3
2	2AN	P	506	-	-	0/10/10/10	0/3/3/3
2	2AN	F	202	-	-	1/10/10/10	0/3/3/3
2	2AN	O	204	-	-	0/10/10/10	0/3/3/3
2	2AN	C	304	-	-	0/10/10/10	0/3/3/3
2	2AN	G	304	-	-	1/10/10/10	0/3/3/3
2	2AN	B	202	-	-	0/10/10/10	0/3/3/3
2	2AN	G	301	-	-	2/10/10/10	0/3/3/3
2	2AN	M	508	-	-	2/10/10/10	0/3/3/3
2	2AN	K	201	-	-	0/10/10/10	0/3/3/3
2	2AN	B	201	-	-	0/10/10/10	0/3/3/3
2	2AN	M	506	-	-	2/10/10/10	0/3/3/3
2	2AN	P	505	-	-	0/10/10/10	0/3/3/3
2	2AN	G	306	-	-	0/10/10/10	0/3/3/3
2	2AN	H	1101	-	-	2/10/10/10	0/3/3/3
2	2AN	N	202	-	-	0/10/10/10	0/3/3/3
2	2AN	A	204	-	-	0/10/10/10	0/3/3/3
2	2AN	I	203	-	-	0/10/10/10	0/3/3/3
2	2AN	F	208	-	-	1/10/10/10	0/3/3/3
2	2AN	M	502	-	-	0/10/10/10	0/3/3/3
2	2AN	A	202	-	-	2/10/10/10	0/3/3/3
2	2AN	K	206	-	-	0/10/10/10	0/3/3/3
2	2AN	C	302	-	-	0/10/10/10	0/3/3/3
2	2AN	I	202	-	-	2/10/10/10	0/3/3/3
2	2AN	P	502	-	-	0/10/10/10	0/3/3/3
2	2AN	J	201	-	-	0/10/10/10	0/3/3/3
2	2AN	E	506	-	-	1/10/10/10	0/3/3/3
2	2AN	C	305	-	-	2/10/10/10	0/3/3/3
2	2AN	J	202	-	-	4/10/10/10	0/3/3/3
2	2AN	C	309	-	-	2/10/10/10	0/3/3/3
2	2AN	P	508	-	-	0/10/10/10	0/3/3/3
2	2AN	O	202	-	-	0/10/10/10	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	2AN	D	706	-	-	2/10/10/10	0/3/3/3
2	2AN	D	703	-	-	0/10/10/10	0/3/3/3
2	2AN	C	307	-	-	0/10/10/10	0/3/3/3
2	2AN	E	501	-	-	2/10/10/10	0/3/3/3
2	2AN	H	1108	-	-	0/10/10/10	0/3/3/3
2	2AN	C	301	-	-	0/10/10/10	0/3/3/3
2	2AN	B	203	-	-	1/10/10/10	0/3/3/3
2	2AN	E	503	-	-	0/10/10/10	0/3/3/3
2	2AN	H	1106	-	-	0/10/10/10	0/3/3/3
2	2AN	H	1102	-	-	0/10/10/10	0/3/3/3
2	2AN	F	204	-	-	0/10/10/10	0/3/3/3
2	2AN	C	308	-	-	2/10/10/10	0/3/3/3
2	2AN	L	203	-	-	0/10/10/10	0/3/3/3
2	2AN	K	204	-	-	2/10/10/10	0/3/3/3
2	2AN	C	303	-	-	0/10/10/10	0/3/3/3
2	2AN	H	1105	-	-	0/10/10/10	0/3/3/3
2	2AN	F	201	-	-	0/10/10/10	0/3/3/3
2	2AN	E	502	-	-	0/10/10/10	0/3/3/3
2	2AN	I	205	-	-	2/10/10/10	0/3/3/3
2	2AN	H	1104	-	-	2/10/10/10	0/3/3/3
2	2AN	M	503	-	-	0/10/10/10	0/3/3/3
2	2AN	P	509	-	-	2/10/10/10	0/3/3/3
2	2AN	D	702	-	-	2/10/10/10	0/3/3/3
2	2AN	F	206	-	-	0/10/10/10	0/3/3/3
2	2AN	P	507	-	-	0/10/10/10	0/3/3/3

All (102) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	203	2AN	O1-S	3.48	1.60	1.43
2	N	202	2AN	O1-S	3.34	1.59	1.43
2	M	507	2AN	O1-S	3.25	1.59	1.43
2	K	206	2AN	C1-N	3.22	1.47	1.38
2	B	201	2AN	O2-S	3.20	1.59	1.43
2	J	202	2AN	O2-S	3.20	1.59	1.43
2	E	502	2AN	O2-S	3.19	1.59	1.43
2	F	204	2AN	O2-S	3.17	1.59	1.43
2	D	706	2AN	O2-S	3.17	1.59	1.43
2	B	203	2AN	O1-S	3.10	1.58	1.43
2	M	505	2AN	O2-S	3.02	1.58	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	P	509	2AN	O1-S	3.01	1.58	1.43
2	D	701	2AN	O1-S	3.01	1.58	1.43
2	J	204	2AN	O1-S	3.01	1.58	1.43
2	C	301	2AN	O2-S	2.97	1.58	1.43
2	A	201	2AN	O1-S	2.96	1.58	1.43
2	H	1109	2AN	O1-S	2.94	1.57	1.43
2	F	207	2AN	O2-S	2.93	1.57	1.43
2	P	501	2AN	O2-S	2.89	1.57	1.43
2	E	506	2AN	O1-S	2.89	1.57	1.43
2	N	204	2AN	O2-S	2.88	1.57	1.43
2	H	1108	2AN	O1-S	2.87	1.57	1.43
2	K	203	2AN	O1-S	2.86	1.57	1.43
2	J	205	2AN	O2-S	2.86	1.57	1.43
2	D	705	2AN	O2-S	2.86	1.57	1.43
2	L	202	2AN	O2-S	2.85	1.57	1.43
2	I	202	2AN	O2-S	2.84	1.57	1.43
2	E	505	2AN	O1-S	2.84	1.57	1.43
2	F	208	2AN	O2-S	2.83	1.57	1.43
2	E	504	2AN	O1-S	2.82	1.57	1.43
2	K	206	2AN	O2-S	2.82	1.57	1.43
2	J	203	2AN	O1-S	2.81	1.57	1.43
2	M	506	2AN	O1-S	2.78	1.57	1.43
2	H	1106	2AN	O2-S	2.78	1.57	1.43
2	C	308	2AN	O1-S	2.77	1.57	1.43
2	M	503	2AN	O2-S	2.75	1.57	1.43
2	C	303	2AN	O2-S	2.74	1.57	1.43
2	E	507	2AN	O1-S	2.73	1.56	1.43
2	O	204	2AN	O1-S	2.72	1.56	1.43
2	H	1107	2AN	O1-S	2.70	1.56	1.43
2	C	304	2AN	O1-S	2.70	1.56	1.43
2	I	203	2AN	O1-S	2.70	1.56	1.43
2	M	502	2AN	O2-S	2.69	1.56	1.43
2	G	302	2AN	O1-S	2.67	1.56	1.43
2	B	204	2AN	O2-S	2.66	1.56	1.43
2	D	704	2AN	O2-S	2.65	1.56	1.43
2	K	201	2AN	O2-S	2.64	1.56	1.43
2	A	204	2AN	O1-S	2.64	1.56	1.43
2	G	306	2AN	O2-S	2.63	1.56	1.43
2	K	202	2AN	O2-S	2.63	1.56	1.43
2	E	507	2AN	C1-N	2.62	1.45	1.38
2	C	305	2AN	O1-S	2.58	1.56	1.43
2	H	1105	2AN	O1-S	2.56	1.56	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	205	2AN	O2-S	2.53	1.56	1.43
2	C	307	2AN	O3-S	2.52	1.58	1.45
2	F	205	2AN	O2-S	2.51	1.55	1.43
2	H	1101	2AN	O2-S	2.50	1.55	1.43
2	C	306	2AN	O2-S	2.50	1.55	1.43
2	F	203	2AN	O1-S	2.49	1.55	1.43
2	O	203	2AN	O1-S	2.48	1.55	1.43
2	E	507	2AN	C1-C10	2.43	1.46	1.43
2	K	205	2AN	O1-S	2.43	1.55	1.43
2	O	202	2AN	O3-S	2.41	1.58	1.45
2	G	305	2AN	O1-S	2.40	1.55	1.43
2	P	503	2AN	O3-S	2.39	1.57	1.45
2	K	204	2AN	O1-S	2.38	1.55	1.43
2	M	501	2AN	O3-S	2.37	1.57	1.45
2	I	204	2AN	O2-S	2.36	1.55	1.43
2	A	202	2AN	O2-S	2.35	1.55	1.43
2	O	201	2AN	O2-S	2.33	1.55	1.43
2	E	503	2AN	C1-C10	2.33	1.46	1.43
2	K	206	2AN	C1-C10	2.33	1.46	1.43
2	J	203	2AN	C1-C10	2.32	1.46	1.43
2	C	308	2AN	C1-C10	2.32	1.46	1.43
2	H	1109	2AN	C1-N	2.30	1.44	1.38
2	L	201	2AN	O1-S	2.29	1.54	1.43
2	A	203	2AN	O3-S	2.28	1.57	1.45
2	D	702	2AN	O3-S	2.25	1.57	1.45
2	J	206	2AN	O3-S	2.24	1.57	1.45
2	F	202	2AN	O3-S	2.23	1.57	1.45
2	B	202	2AN	O1-S	2.23	1.54	1.43
2	F	208	2AN	C1-C10	2.23	1.45	1.43
2	N	203	2AN	O3-S	2.19	1.56	1.45
2	G	301	2AN	O2-S	2.19	1.54	1.43
2	P	506	2AN	O3-S	2.17	1.56	1.45
2	E	503	2AN	O2-S	2.17	1.54	1.43
2	P	508	2AN	O3-S	2.17	1.56	1.45
2	P	507	2AN	O3-S	2.11	1.56	1.45
2	C	308	2AN	C1-N	2.10	1.44	1.38
2	M	508	2AN	O3-S	2.10	1.56	1.45
2	G	304	2AN	O3-S	2.09	1.56	1.45
2	D	702	2AN	C1-N	2.08	1.44	1.38
2	F	208	2AN	C1-N	2.07	1.44	1.38
2	J	201	2AN	O2-S	2.06	1.53	1.43
2	M	504	2AN	C1-C10	2.05	1.45	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	302	2AN	O2-S	2.05	1.53	1.43
2	L	204	2AN	O3-S	2.04	1.56	1.45
2	P	504	2AN	O2-S	2.04	1.53	1.43
2	K	207	2AN	O3-S	2.04	1.56	1.45
2	F	206	2AN	O3-S	2.03	1.56	1.45
2	P	502	2AN	O2-S	2.02	1.53	1.43
2	M	504	2AN	O2-S	2.00	1.53	1.43

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	205	2AN	C11-N-C1	-4.63	116.25	126.36
2	E	507	2AN	C11-N-C1	3.61	134.24	126.36
2	M	505	2AN	C10-C1-N	-3.41	115.41	120.39
2	K	202	2AN	C11-N-C1	3.38	133.74	126.36
2	C	306	2AN	C10-C1-N	-3.34	115.52	120.39
2	C	308	2AN	C11-N-C1	3.33	133.62	126.36
2	M	505	2AN	C11-N-C1	3.30	133.56	126.36
2	H	1109	2AN	C11-N-C1	3.26	133.47	126.36
2	O	203	2AN	C11-N-C1	3.17	133.28	126.36
2	K	206	2AN	C11-N-C1	3.02	132.96	126.36
2	F	206	2AN	C11-N-C1	2.97	132.85	126.36
2	B	201	2AN	C11-N-C1	2.82	132.51	126.36
2	O	204	2AN	C11-N-C1	2.79	132.45	126.36
2	D	703	2AN	O2-S-O1	-2.74	99.11	112.88
2	J	202	2AN	C11-N-C1	2.73	132.33	126.36
2	G	304	2AN	C11-N-C1	2.70	132.26	126.36
2	N	203	2AN	C11-N-C1	2.69	132.24	126.36
2	G	302	2AN	C11-N-C1	2.69	132.23	126.36
2	E	502	2AN	C11-N-C1	2.67	132.18	126.36
2	C	306	2AN	C11-N-C1	2.65	132.14	126.36
2	A	203	2AN	C11-N-C1	2.63	132.09	126.36
2	G	305	2AN	C11-N-C1	2.59	132.01	126.36
2	D	703	2AN	C1-C10-C5	-2.56	115.49	118.91
2	J	205	2AN	C11-N-C1	2.52	131.85	126.36
2	L	202	2AN	C11-N-C1	2.51	131.84	126.36
2	E	503	2AN	C2-C1-N	-2.48	117.20	123.47
2	J	206	2AN	C11-N-C1	2.47	131.75	126.36
2	M	502	2AN	C11-N-C1	2.45	131.70	126.36
2	H	1104	2AN	C11-N-C1	2.30	131.37	126.36
2	E	503	2AN	C1-C10-C5	-2.29	115.85	118.91
2	D	704	2AN	C11-N-C1	2.28	131.33	126.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	502	2AN	C10-C1-N	-2.28	117.07	120.39
2	M	502	2AN	O3-S-O2	-2.28	100.99	111.55
2	N	202	2AN	C1-C10-C5	-2.27	115.88	118.91
2	L	201	2AN	C1-C10-C5	-2.25	115.90	118.91
2	H	1101	2AN	C2-C1-N	-2.23	117.81	123.47
2	P	503	2AN	C2-C1-N	-2.22	117.86	123.47
2	O	203	2AN	C10-C1-N	-2.20	117.18	120.39
2	H	1106	2AN	O2-S-O1	-2.20	101.81	112.88
2	M	502	2AN	C1-C10-C5	-2.18	115.99	118.91
2	C	303	2AN	C1-C10-C5	-2.18	115.99	118.91
2	A	205	2AN	C1-C10-C5	-2.17	116.00	118.91
2	P	505	2AN	C1-C10-C5	-2.17	116.00	118.91
2	F	208	2AN	C2-C1-N	-2.15	118.03	123.47
2	K	205	2AN	C2-C1-N	-2.14	118.05	123.47
2	F	205	2AN	O3-S-O2	-2.14	101.63	111.55
2	H	1105	2AN	C11-N-C1	2.14	131.02	126.36
2	I	201	2AN	C1-C10-C5	-2.13	116.06	118.91
2	L	201	2AN	O2-S-O1	-2.12	102.23	112.88
2	I	204	2AN	C2-C1-N	-2.11	118.13	123.47
2	D	702	2AN	C11-N-C1	2.10	130.95	126.36
2	I	203	2AN	C1-C10-C5	-2.10	116.10	118.91
2	J	206	2AN	C10-C1-N	-2.09	117.34	120.39
2	N	202	2AN	C2-C1-N	-2.09	118.19	123.47
2	J	203	2AN	C2-C1-N	-2.08	118.20	123.47
2	P	503	2AN	C1-C10-C5	-2.06	116.16	118.91
2	H	1106	2AN	O2-S-C9	2.06	112.33	106.37
2	K	203	2AN	C2-C1-N	-2.05	118.27	123.47
2	E	506	2AN	C2-C1-N	-2.05	118.28	123.47
2	G	306	2AN	C11-N-C1	2.04	130.82	126.36
2	I	205	2AN	C2-C1-N	-2.03	118.33	123.47
2	P	505	2AN	C2-C1-N	-2.02	118.35	123.47
2	I	204	2AN	C1-C10-C5	-2.02	116.20	118.91
2	J	204	2AN	C11-N-C1	2.02	130.77	126.36
2	C	301	2AN	C1-C10-C5	-2.02	116.21	118.91
2	M	504	2AN	C2-C1-N	-2.00	118.40	123.47

There are no chirality outliers.

All (103) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	507	2AN	C10-C9-S-O1
2	E	507	2AN	C8-C9-S-O2

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Mol	Chain	Res	Type	Atoms
2	E	507	2AN	C10-C9-S-O2
2	E	507	2AN	C8-C9-S-O3
2	E	507	2AN	C10-C9-S-O3
2	J	206	2AN	C10-C9-S-O2
2	K	205	2AN	C8-C9-S-O1
2	K	205	2AN	C10-C9-S-O1
2	K	205	2AN	C8-C9-S-O3
2	M	509	2AN	C8-C9-S-O3
2	M	509	2AN	C10-C9-S-O3
2	P	503	2AN	C8-C9-S-O1
2	P	503	2AN	C10-C9-S-O1
2	P	503	2AN	C10-C9-S-O2
2	P	503	2AN	C8-C9-S-O3
2	P	503	2AN	C10-C9-S-O3
2	G	304	2AN	C10-C9-S-O1
2	H	1103	2AN	C10-C9-S-O1
2	J	202	2AN	C10-C9-S-O1
2	J	202	2AN	C10-C9-S-O2
2	K	205	2AN	C10-C9-S-O2
2	J	206	2AN	C12-C11-N-C1
2	P	509	2AN	C16-C11-N-C1
2	J	206	2AN	C16-C11-N-C1
2	H	1103	2AN	C8-C9-S-O1
2	J	202	2AN	C8-C9-S-O1
2	P	503	2AN	C8-C9-S-O2
2	P	509	2AN	C12-C11-N-C1
2	F	207	2AN	C16-C11-N-C1
2	F	207	2AN	C12-C11-N-C1
2	H	1109	2AN	C12-C11-N-C1
2	H	1109	2AN	C16-C11-N-C1
2	N	204	2AN	C16-C11-N-C1
2	D	702	2AN	C12-C11-N-C1
2	D	706	2AN	C10-C9-S-O1
2	F	202	2AN	C10-C9-S-O1
2	J	206	2AN	C10-C9-S-O1
2	M	509	2AN	C10-C9-S-O2
2	D	702	2AN	C16-C11-N-C1
2	N	204	2AN	C12-C11-N-C1
2	C	305	2AN	C2-C1-N-C11
2	D	701	2AN	C2-C1-N-C11
2	I	202	2AN	C2-C1-N-C11
2	P	503	2AN	C2-C1-N-C11

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Mol	Chain	Res	Type	Atoms
2	E	501	2AN	C12-C11-N-C1
2	H	1103	2AN	C8-C9-S-O3
2	J	206	2AN	C8-C9-S-O3
2	C	306	2AN	C10-C9-S-O3
2	H	1103	2AN	C10-C9-S-O3
2	J	202	2AN	C10-C9-S-O3
2	K	205	2AN	C10-C9-S-O3
2	D	706	2AN	C8-C9-S-O1
2	E	507	2AN	C8-C9-S-O1
2	J	206	2AN	C8-C9-S-O2
2	K	205	2AN	C8-C9-S-O2
2	H	1101	2AN	C10-C1-N-C11
2	P	503	2AN	C10-C1-N-C11
2	E	501	2AN	C16-C11-N-C1
2	E	506	2AN	C12-C11-N-C1
2	G	301	2AN	C2-C1-N-C11
2	H	1101	2AN	C2-C1-N-C11
2	K	205	2AN	C12-C11-N-C1
2	F	208	2AN	C10-C9-S-O1
2	M	509	2AN	C10-C9-S-O1
2	C	308	2AN	C12-C11-N-C1
2	C	308	2AN	C16-C11-N-C1
2	A	202	2AN	C2-C1-N-C11
2	E	504	2AN	C2-C1-N-C11
2	H	1103	2AN	C2-C1-N-C11
2	H	1104	2AN	C2-C1-N-C11
2	L	204	2AN	C2-C1-N-C11
2	M	506	2AN	C2-C1-N-C11
2	A	202	2AN	C10-C1-N-C11
2	C	305	2AN	C10-C1-N-C11
2	D	701	2AN	C10-C1-N-C11
2	H	1103	2AN	C10-C1-N-C11
2	H	1104	2AN	C10-C1-N-C11
2	J	203	2AN	C10-C1-N-C11
2	L	204	2AN	C10-C1-N-C11
2	M	506	2AN	C10-C1-N-C11
2	C	309	2AN	C12-C11-N-C1
2	J	206	2AN	C8-C9-S-O1
2	K	207	2AN	C12-C11-N-C1
2	J	203	2AN	C2-C1-N-C11
2	K	205	2AN	C16-C11-N-C1
2	M	501	2AN	C16-C11-N-C1

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Mol	Chain	Res	Type	Atoms
2	M	501	2AN	C12-C11-N-C1
2	C	309	2AN	C16-C11-N-C1
2	B	204	2AN	C10-C1-N-C11
2	E	504	2AN	C10-C1-N-C11
2	F	203	2AN	C10-C1-N-C11
2	G	301	2AN	C10-C1-N-C11
2	I	202	2AN	C10-C1-N-C11
2	I	205	2AN	C10-C1-N-C11
2	K	204	2AN	C10-C1-N-C11
2	M	508	2AN	C10-C1-N-C11
2	B	203	2AN	C2-C1-N-C11
2	B	204	2AN	C2-C1-N-C11
2	I	205	2AN	C2-C1-N-C11
2	K	204	2AN	C2-C1-N-C11
2	M	508	2AN	C2-C1-N-C11
2	M	509	2AN	C16-C11-N-C1
2	K	207	2AN	C16-C11-N-C1

There are no ring outliers.

85 monomers are involved in 213 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	M	504	2AN	3	0
2	B	204	2AN	2	0
2	L	201	2AN	4	0
2	M	501	2AN	2	0
2	M	505	2AN	4	0
2	H	1107	2AN	6	0
2	K	202	2AN	2	0
2	H	1103	2AN	2	0
2	K	205	2AN	6	0
2	N	203	2AN	3	0
2	A	205	2AN	1	0
2	P	503	2AN	5	0
2	D	705	2AN	1	0
2	J	205	2AN	3	0
2	P	504	2AN	1	0
2	J	204	2AN	1	0
2	P	501	2AN	3	0
2	E	505	2AN	3	0
2	E	507	2AN	3	0
2	E	504	2AN	2	0

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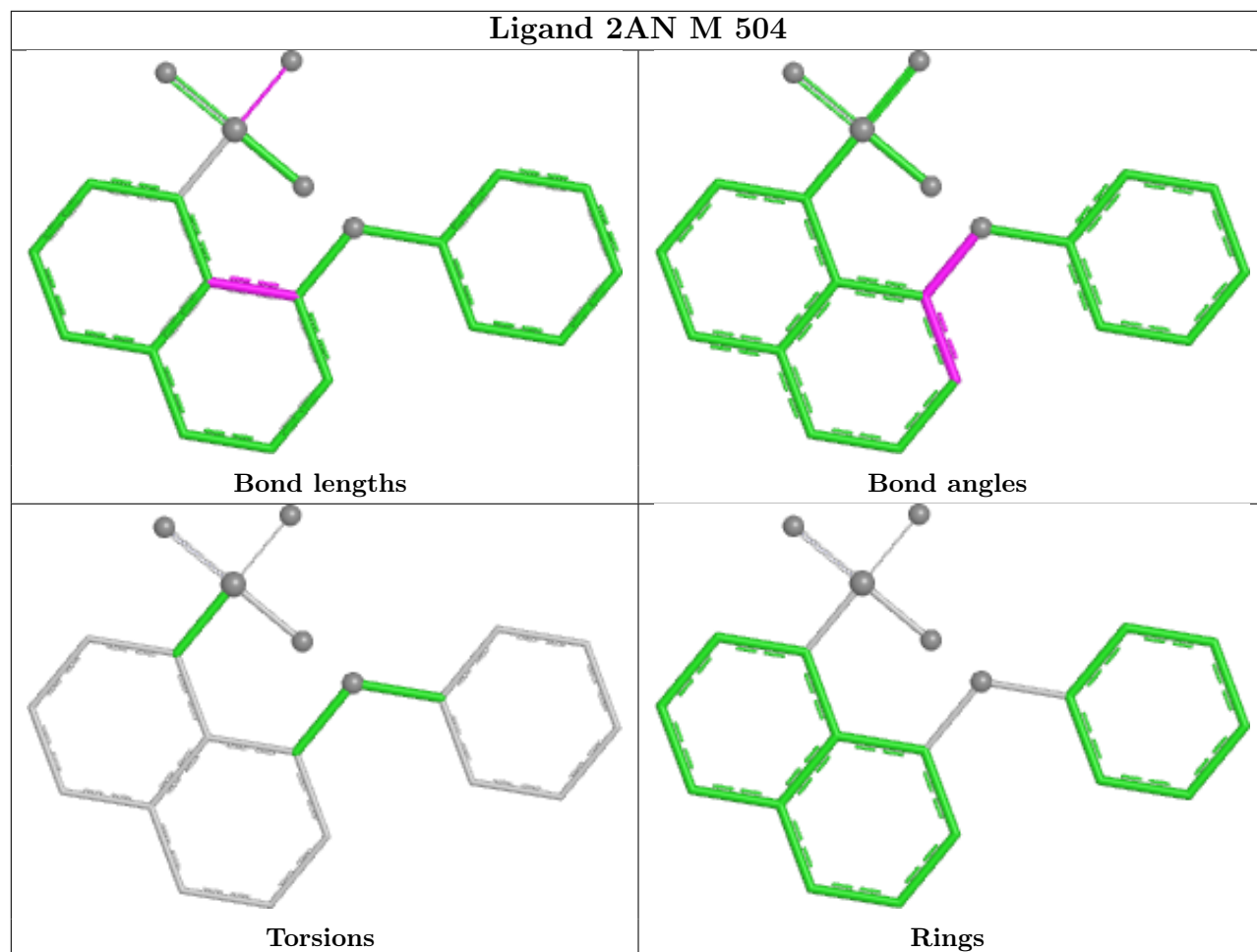
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	207	2AN	3	0
2	N	204	2AN	1	0
2	O	203	2AN	2	0
2	C	306	2AN	2	0
2	G	302	2AN	1	0
2	G	305	2AN	3	0
2	D	701	2AN	1	0
2	D	704	2AN	1	0
2	L	204	2AN	1	0
2	M	509	2AN	2	0
2	A	201	2AN	3	0
2	M	507	2AN	2	0
2	N	201	2AN	4	0
2	F	203	2AN	2	0
2	H	1109	2AN	5	0
2	K	203	2AN	2	0
2	G	303	2AN	2	0
2	I	201	2AN	1	0
2	O	201	2AN	1	0
2	P	506	2AN	1	0
2	F	202	2AN	3	0
2	O	204	2AN	2	0
2	C	304	2AN	2	0
2	G	304	2AN	2	0
2	B	202	2AN	1	0
2	G	301	2AN	1	0
2	M	508	2AN	1	0
2	K	201	2AN	3	0
2	M	506	2AN	3	0
2	H	1101	2AN	3	0
2	N	202	2AN	5	0
2	A	204	2AN	1	0
2	I	203	2AN	3	0
2	F	208	2AN	1	0
2	A	202	2AN	5	0
2	K	206	2AN	1	0
2	C	302	2AN	2	0
2	I	202	2AN	1	0
2	P	502	2AN	1	0
2	J	201	2AN	2	0
2	E	506	2AN	5	0
2	C	305	2AN	2	0

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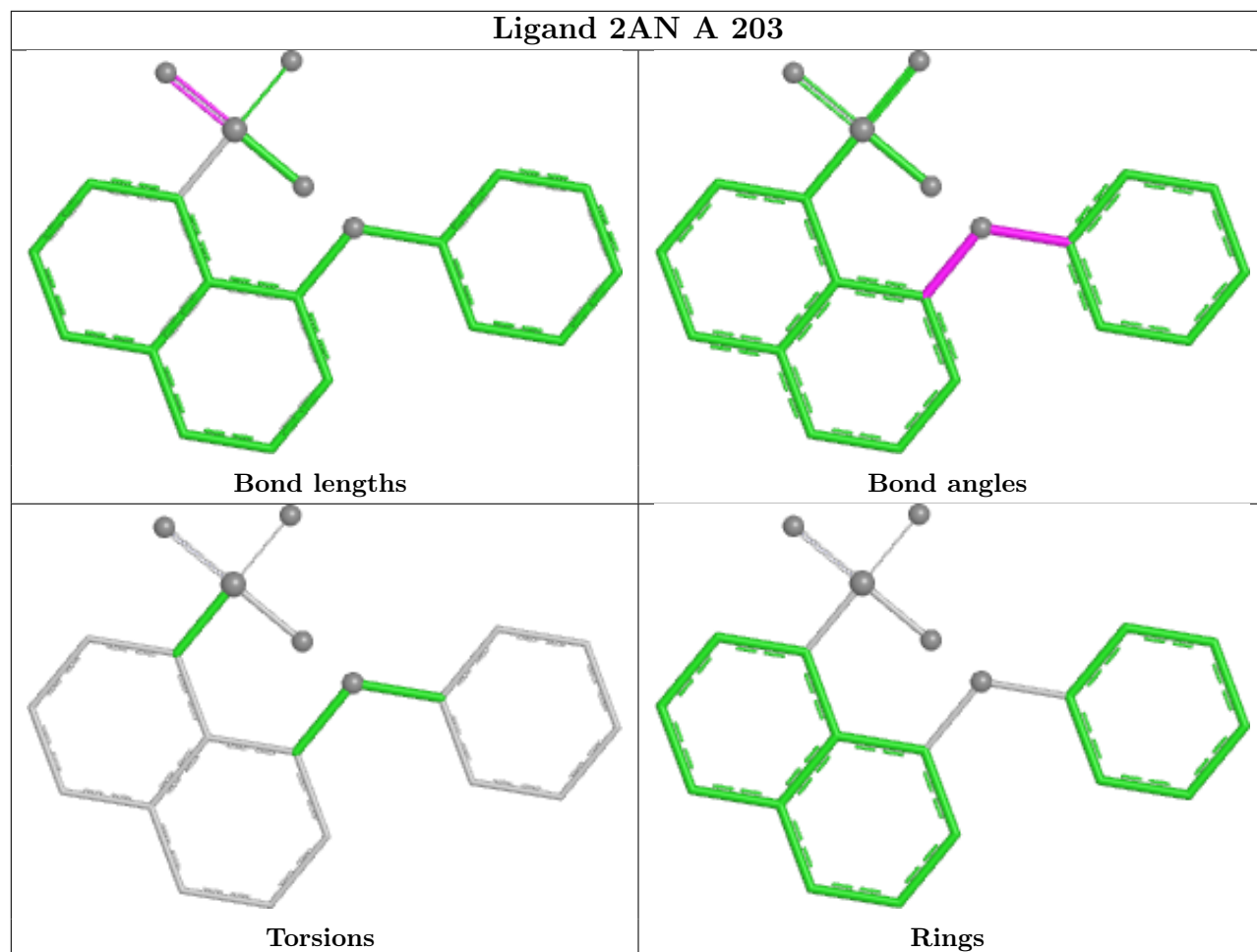
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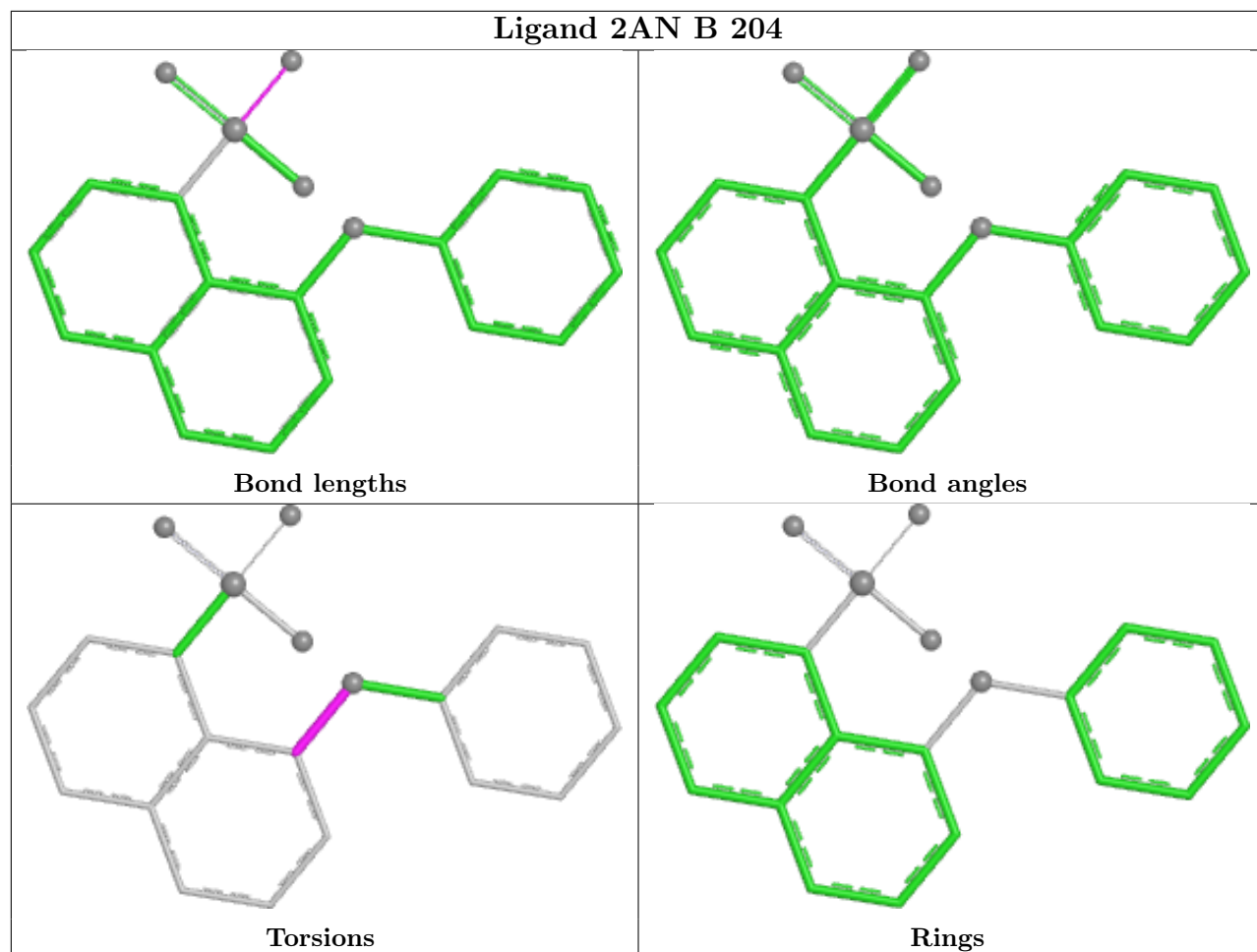
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	J	202	2AN	3	0
2	C	309	2AN	3	0
2	P	508	2AN	10	0
2	O	202	2AN	2	0
2	D	706	2AN	5	0
2	C	307	2AN	2	0
2	H	1108	2AN	3	0
2	B	203	2AN	1	0
2	E	503	2AN	2	0
2	H	1102	2AN	2	0
2	F	204	2AN	2	0
2	C	308	2AN	4	0
2	L	203	2AN	1	0
2	K	204	2AN	3	0
2	C	303	2AN	3	0
2	H	1105	2AN	1	0
2	F	201	2AN	2	0
2	E	502	2AN	3	0
2	I	205	2AN	5	0
2	P	509	2AN	2	0
2	D	702	2AN	4	0
2	F	206	2AN	3	0
2	P	507	2AN	2	0

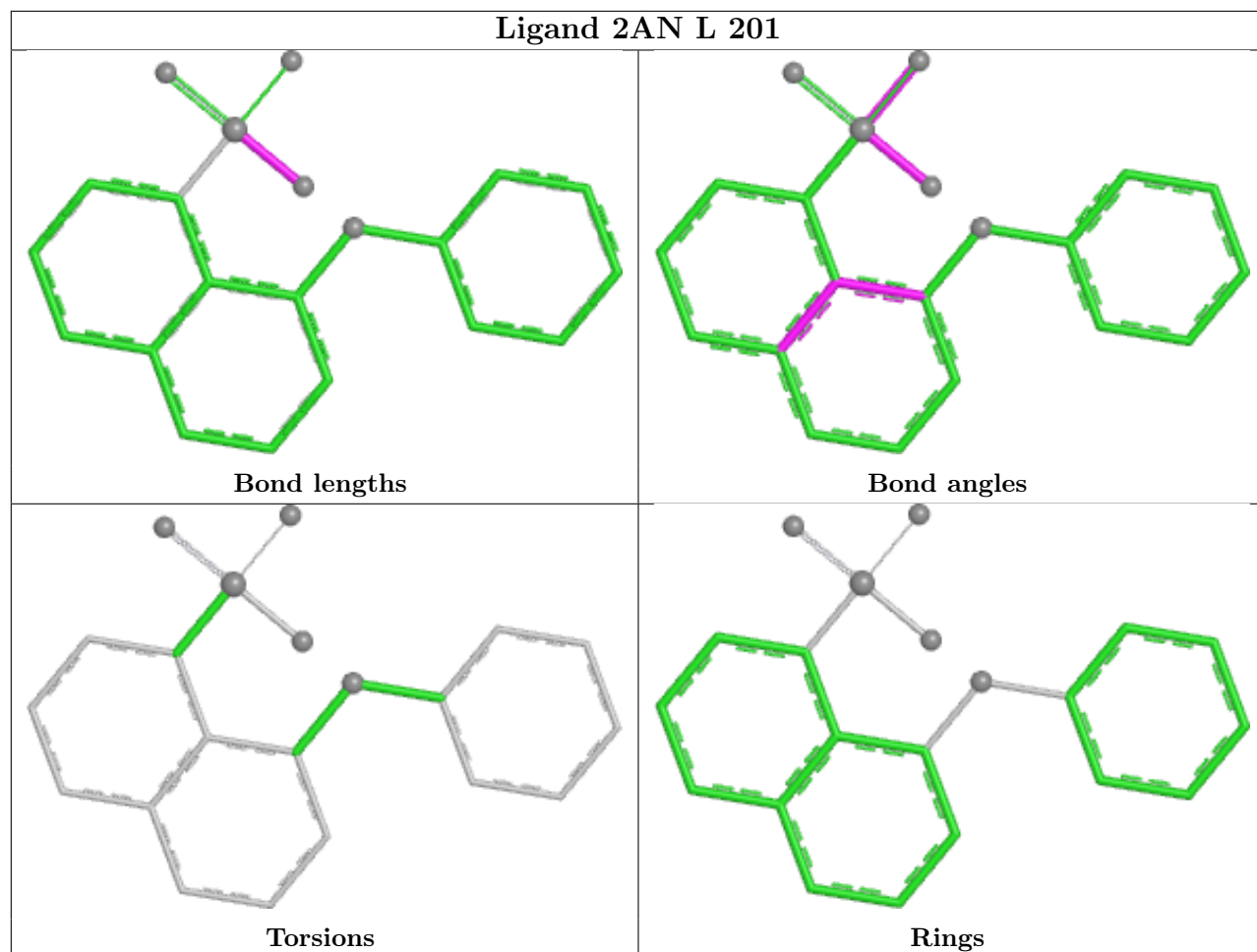
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

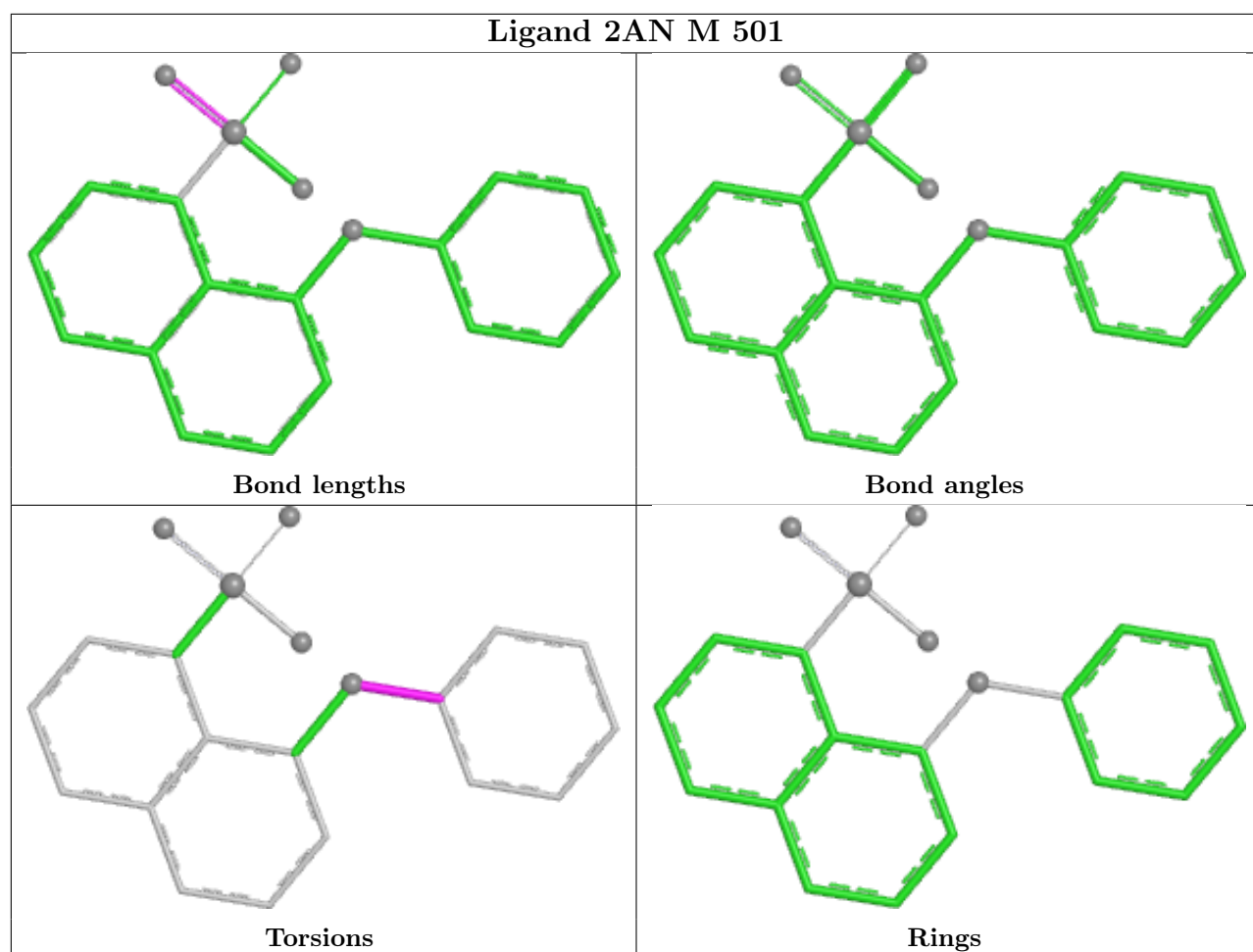


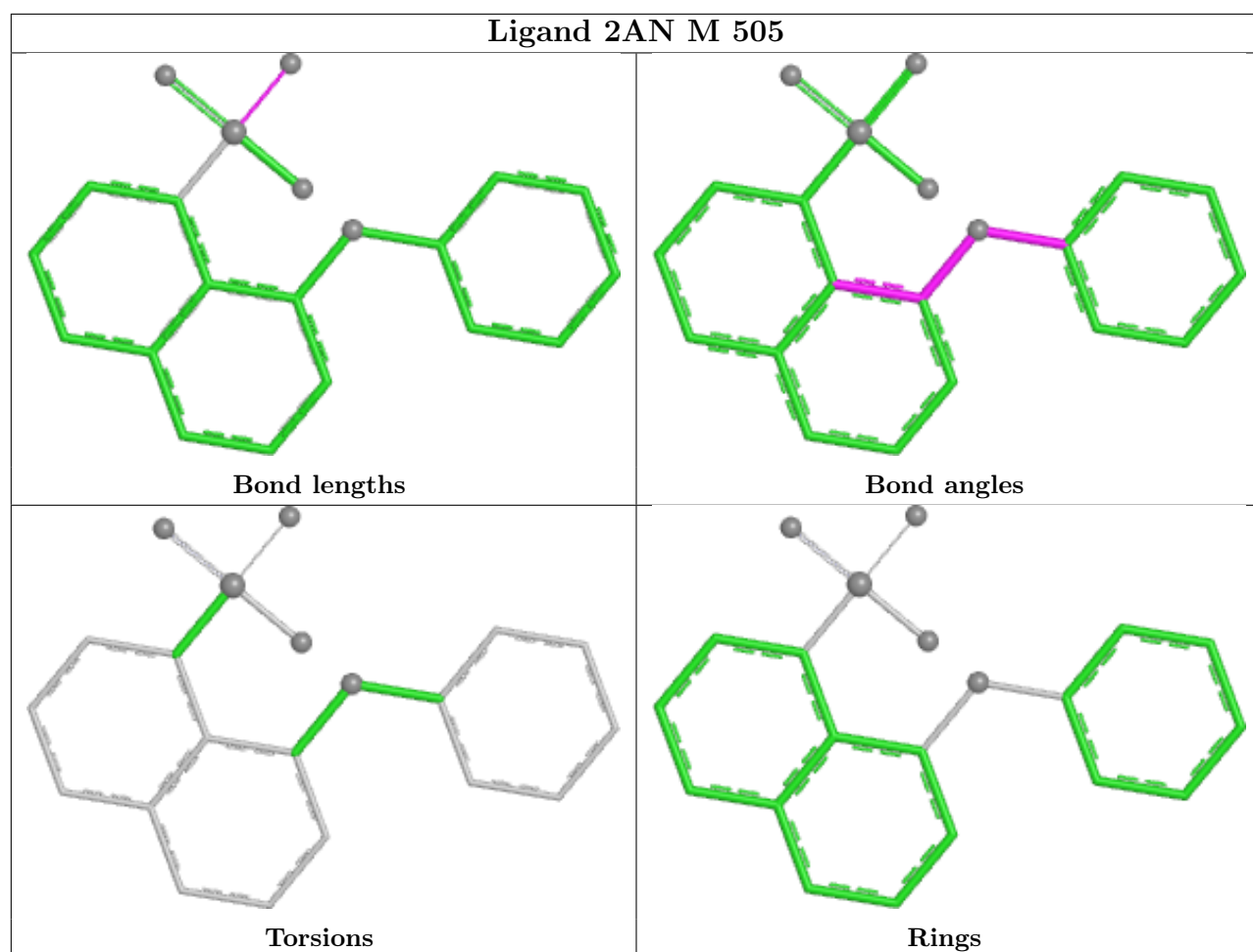
Ligand 2AN A 203



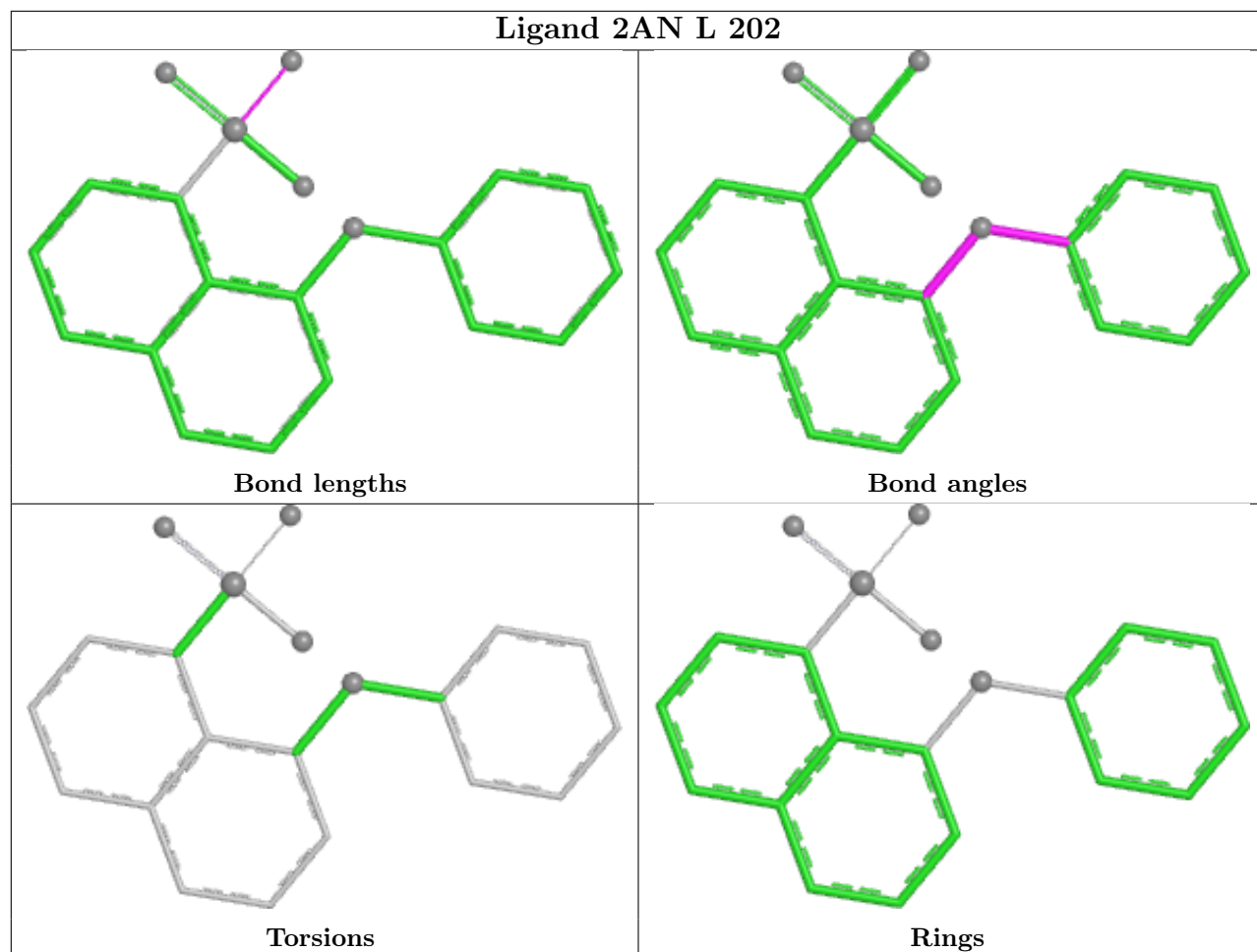


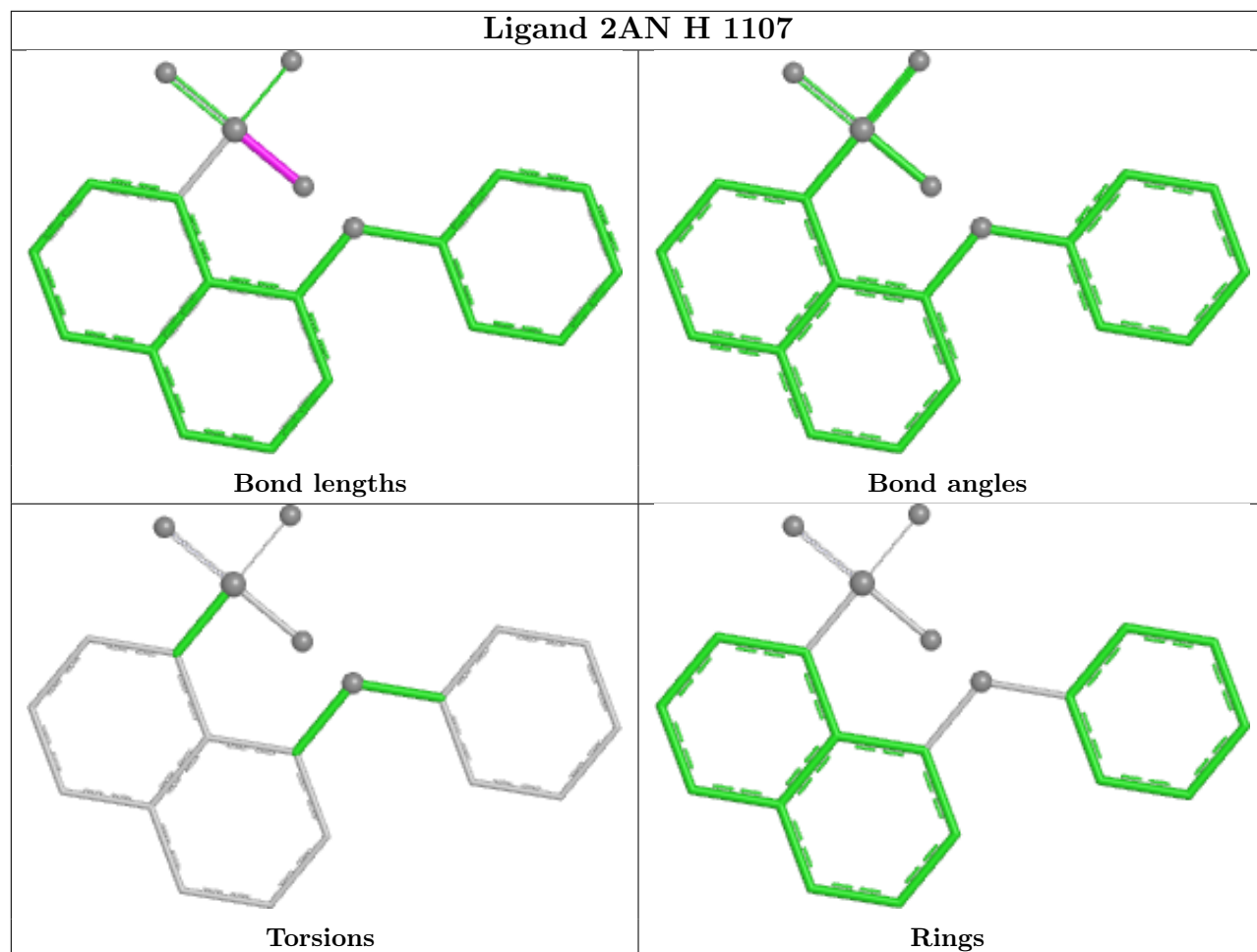


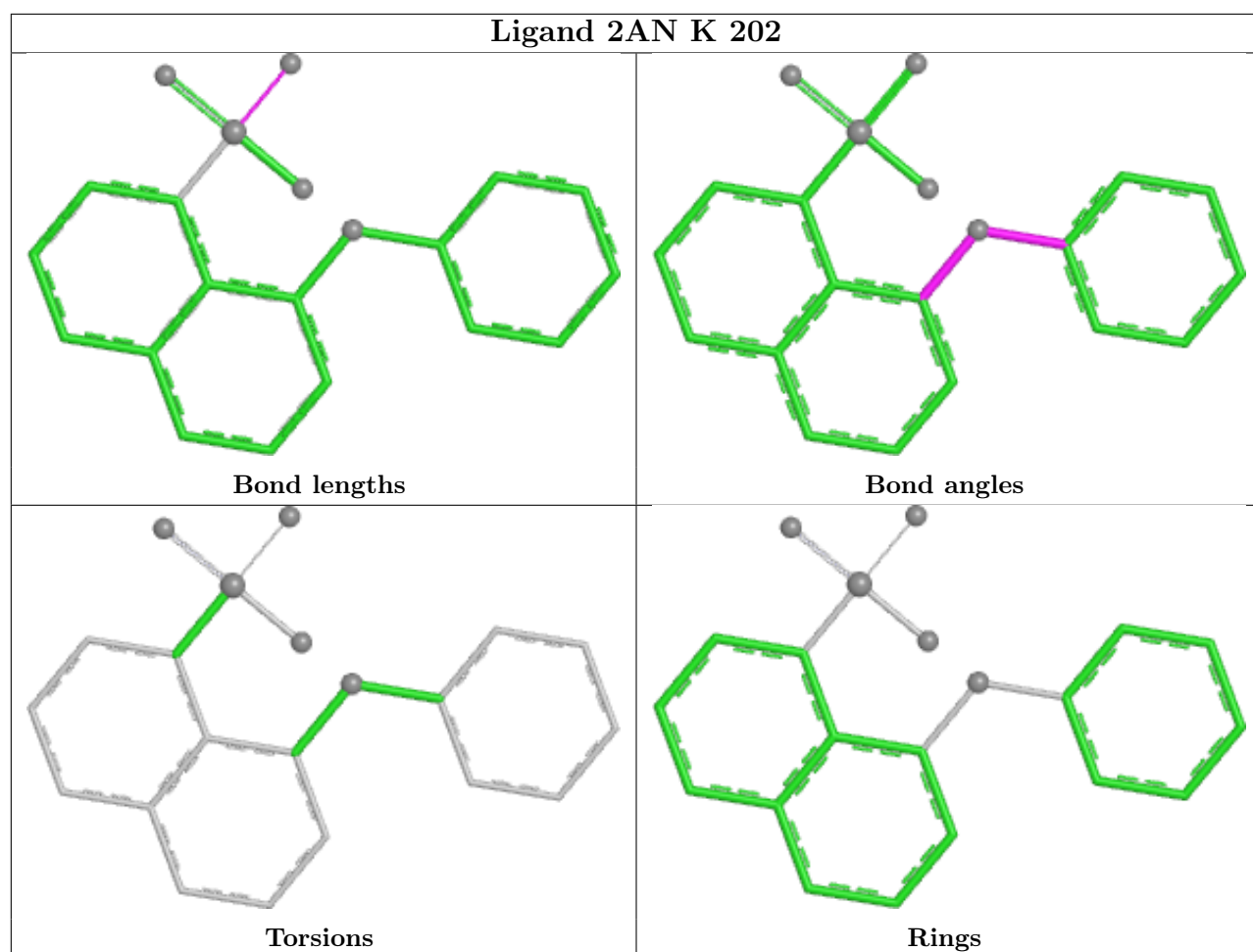


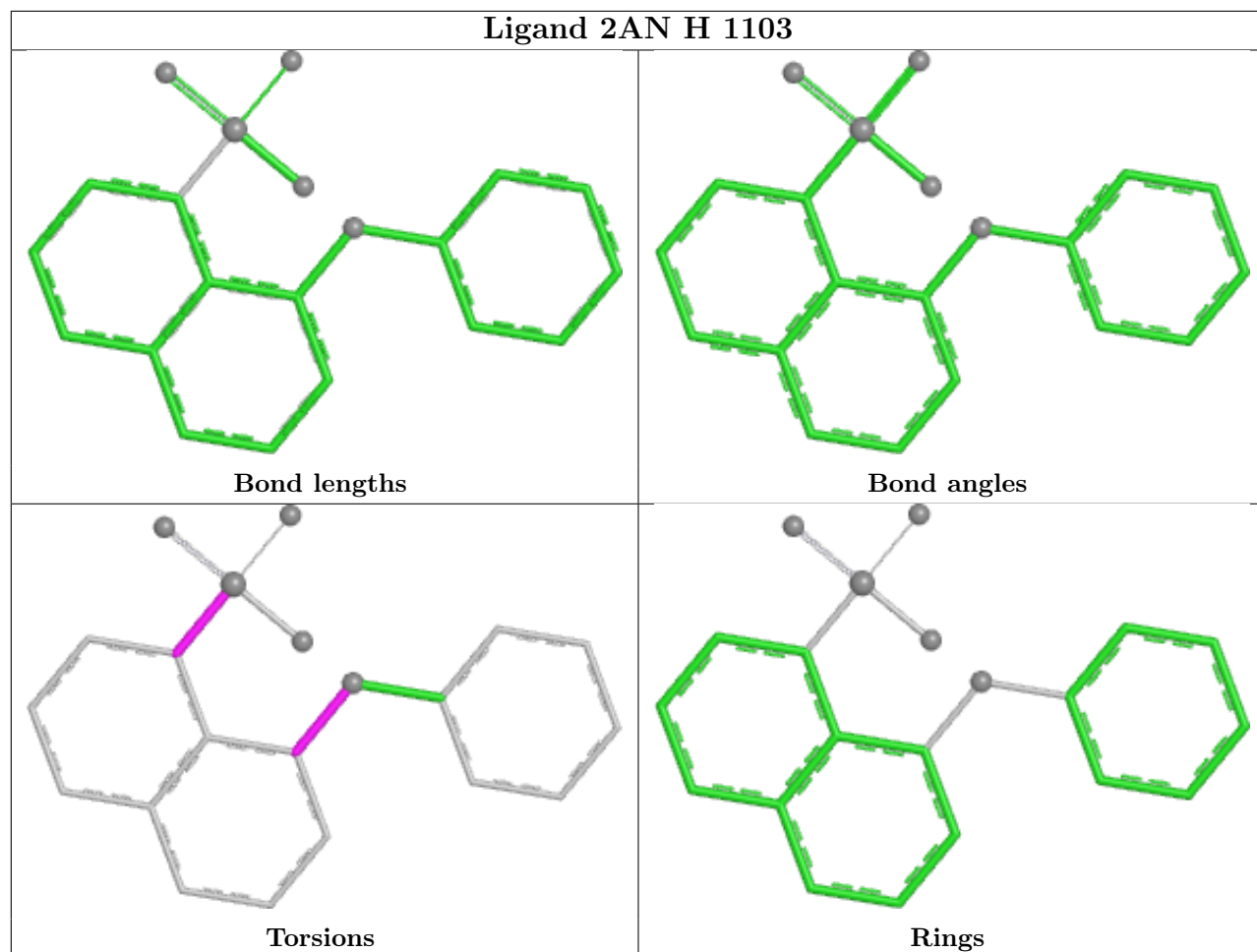


Ligand 2AN L 202

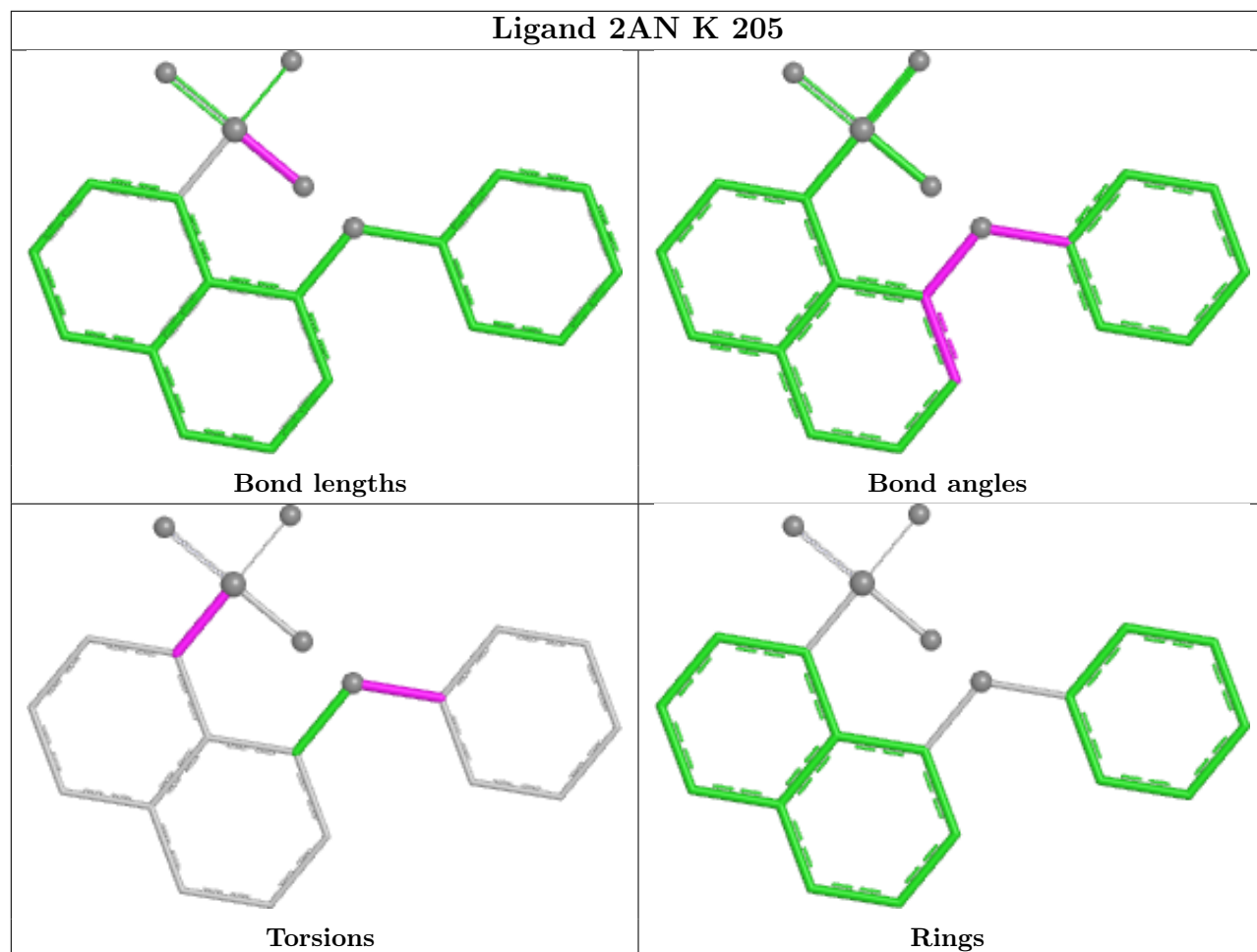




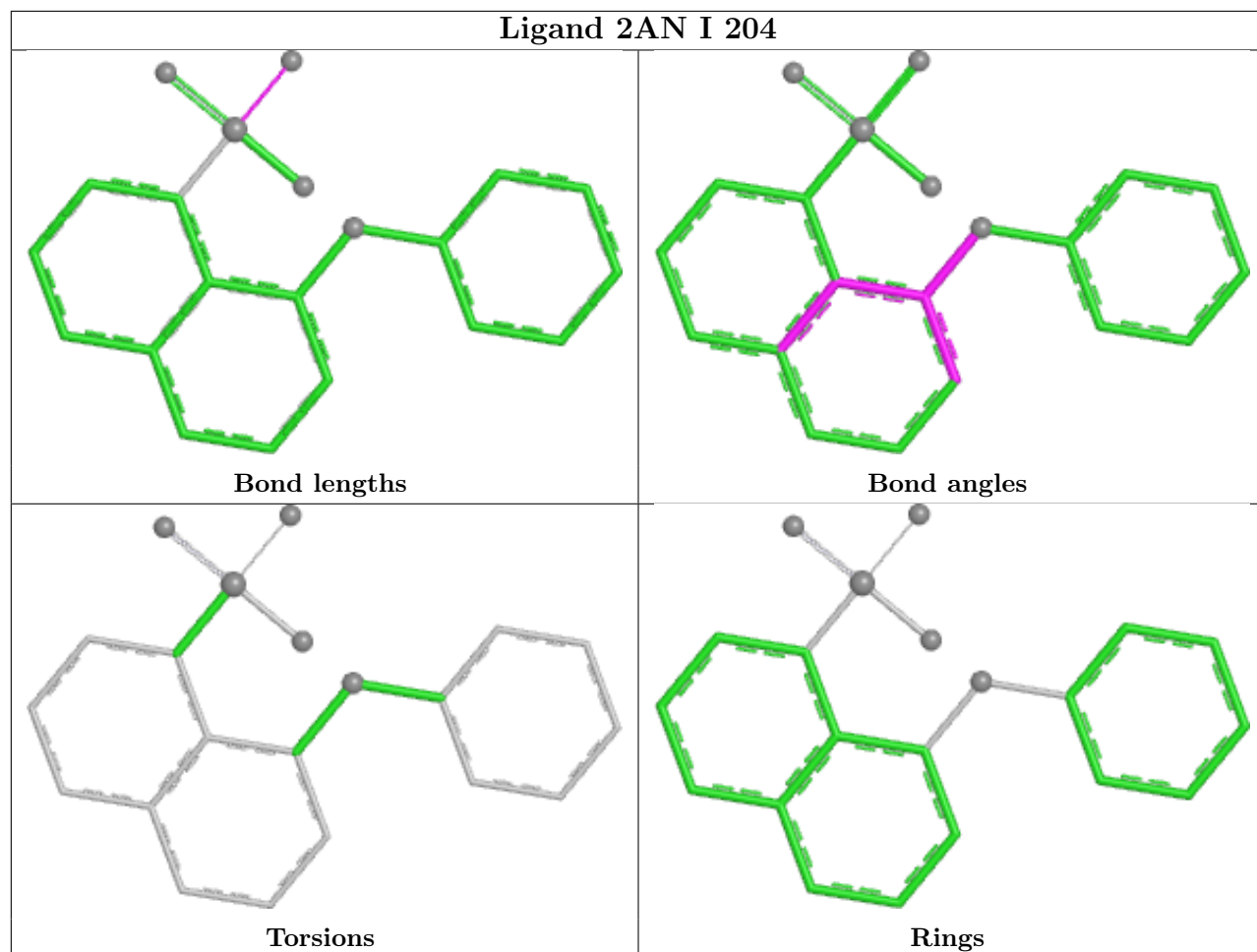


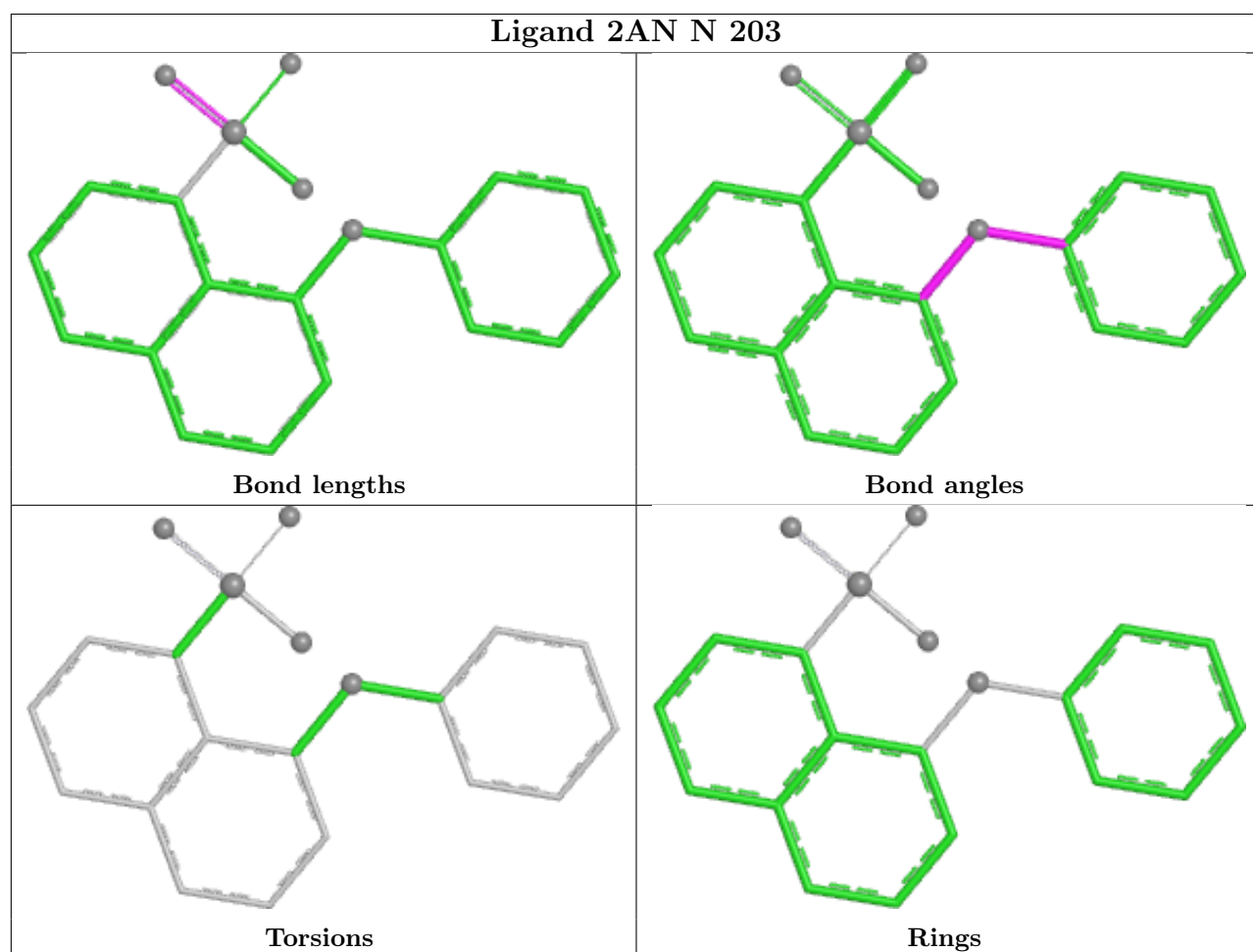


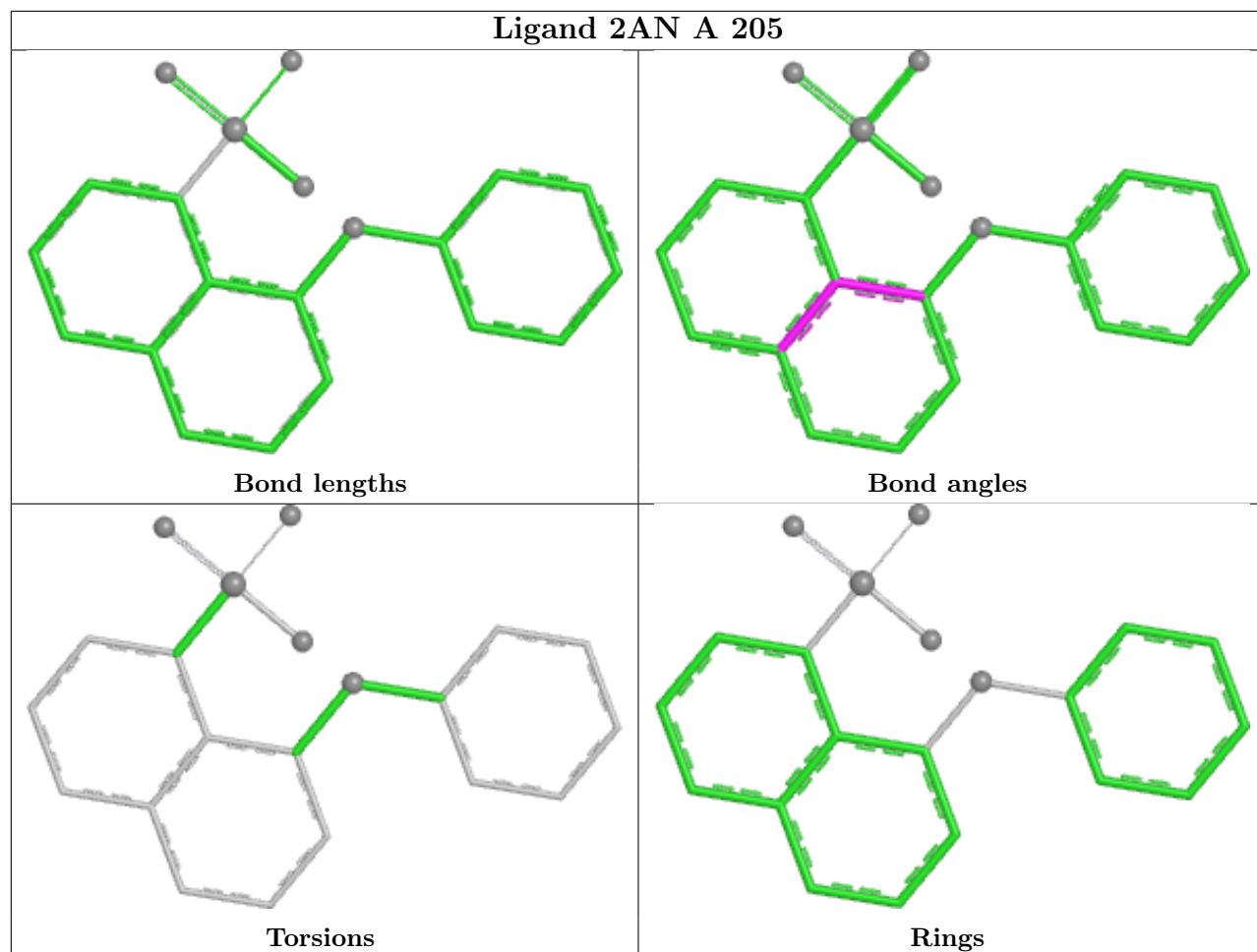
Ligand 2AN K 205



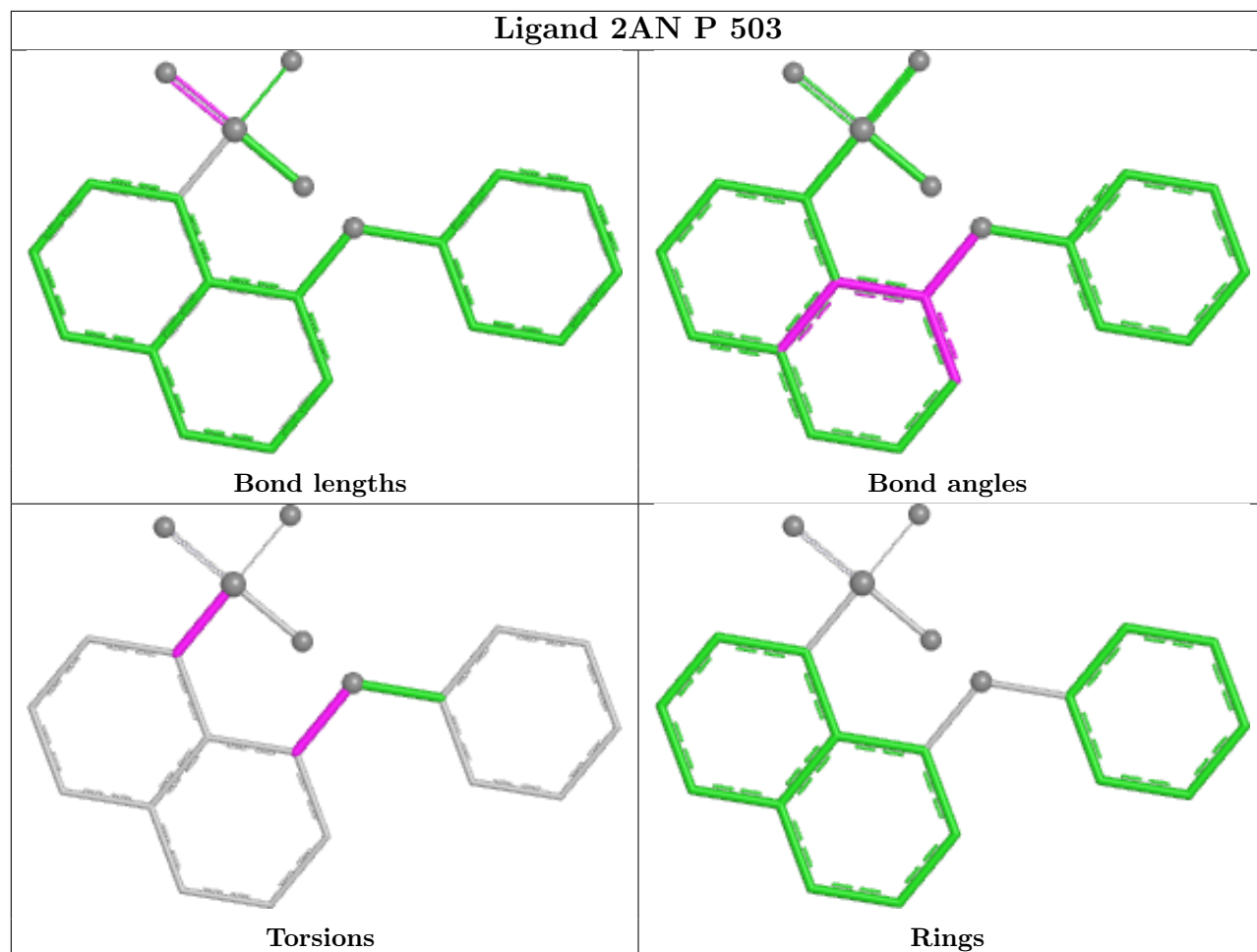
Ligand 2AN I 204

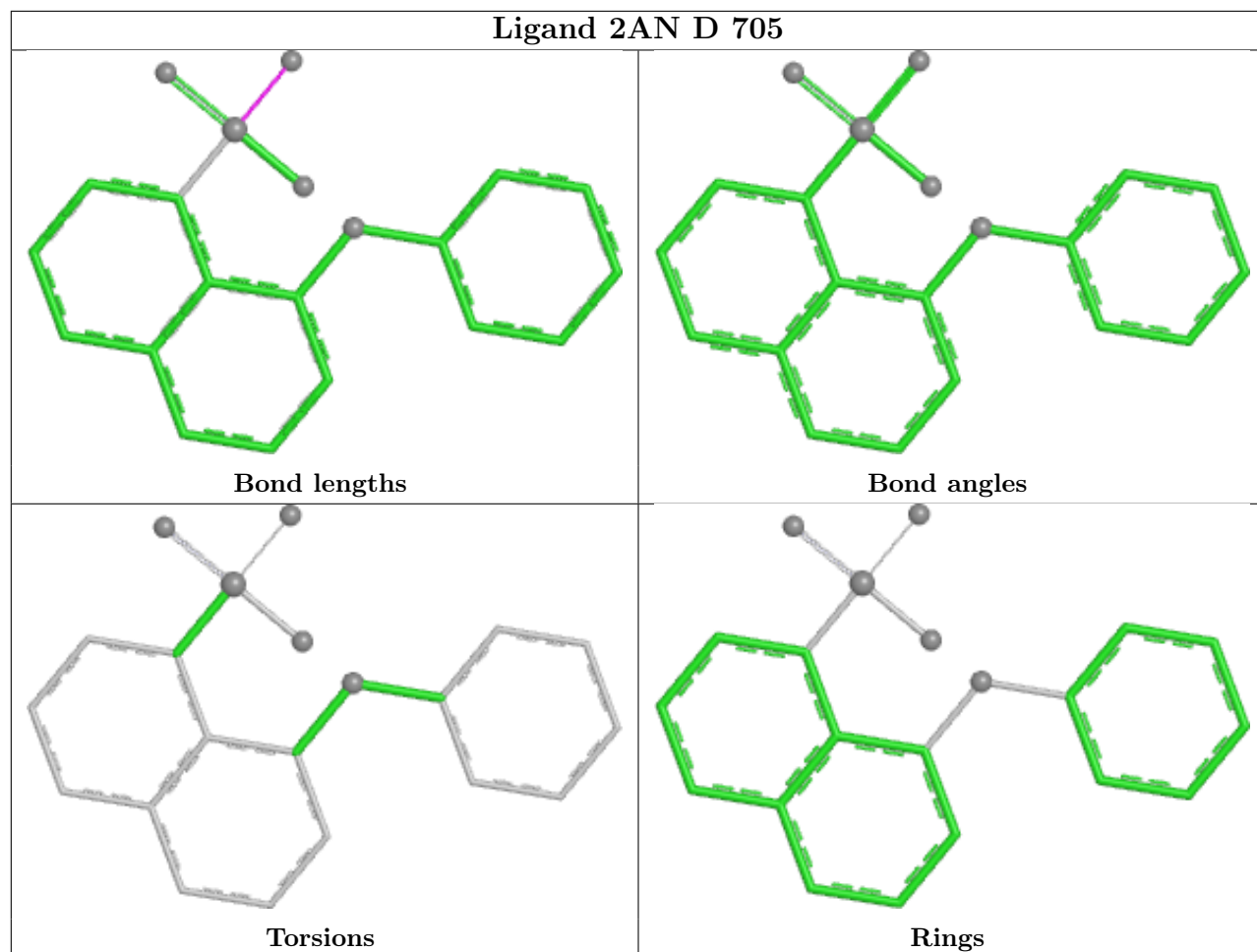




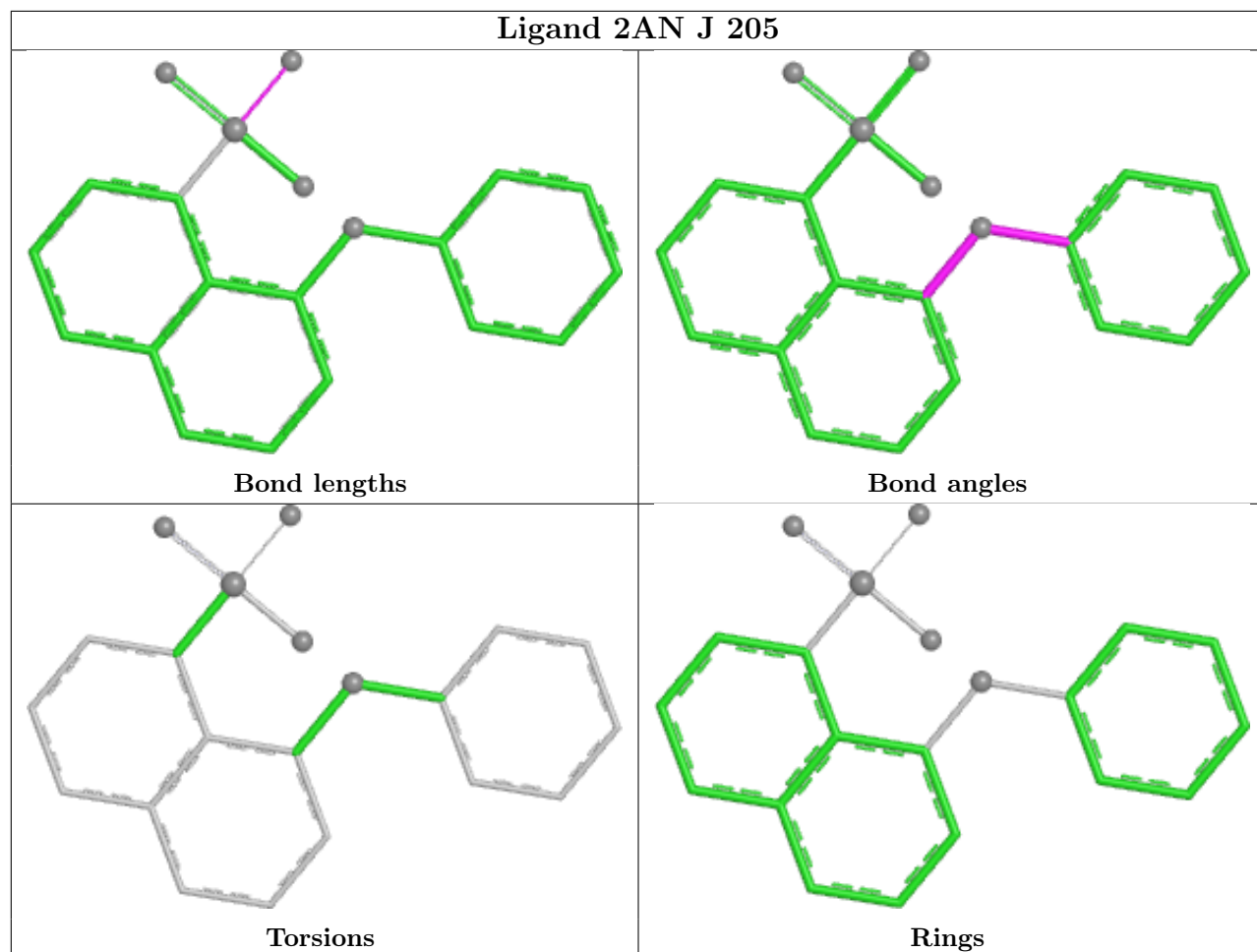


Ligand 2AN P 503

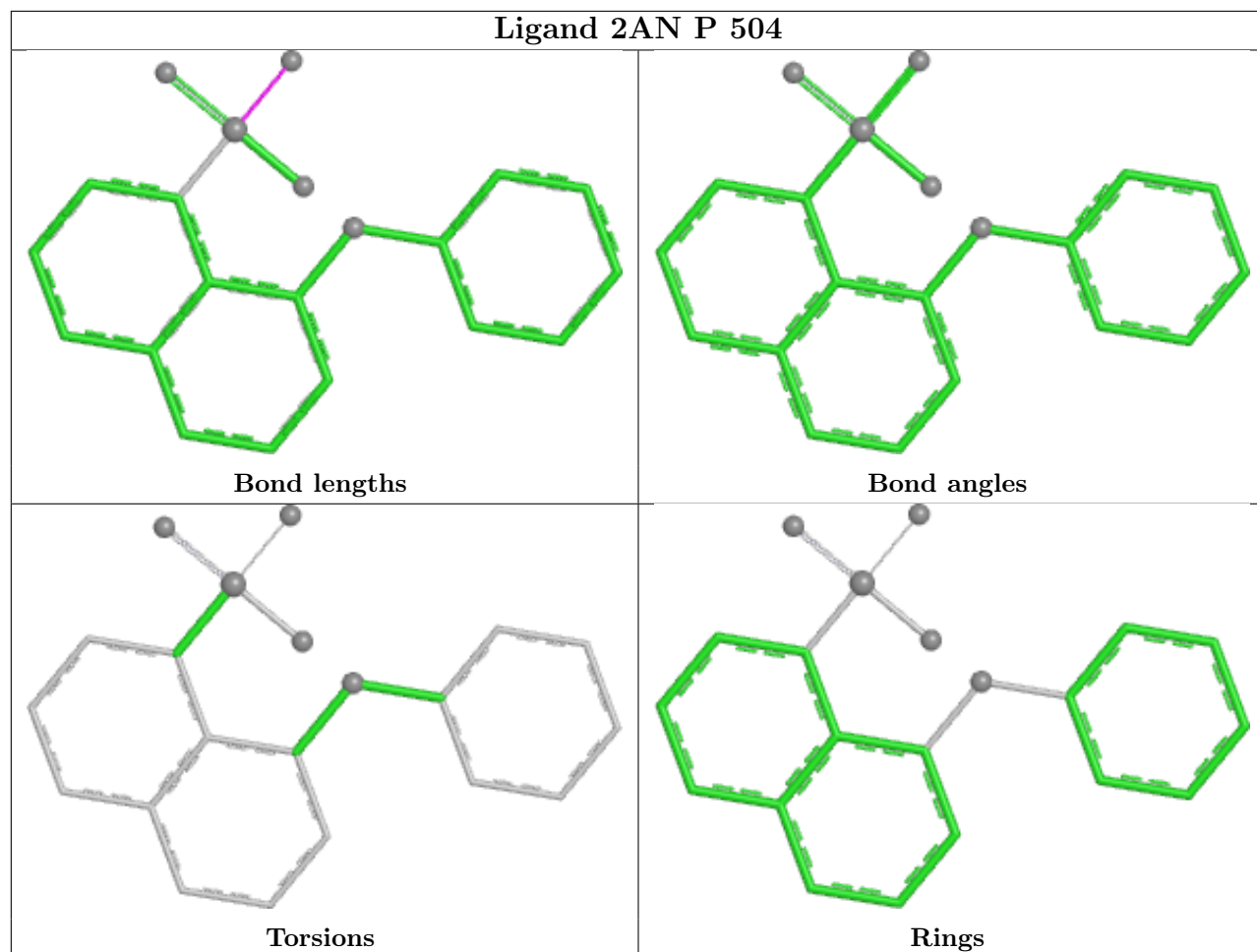




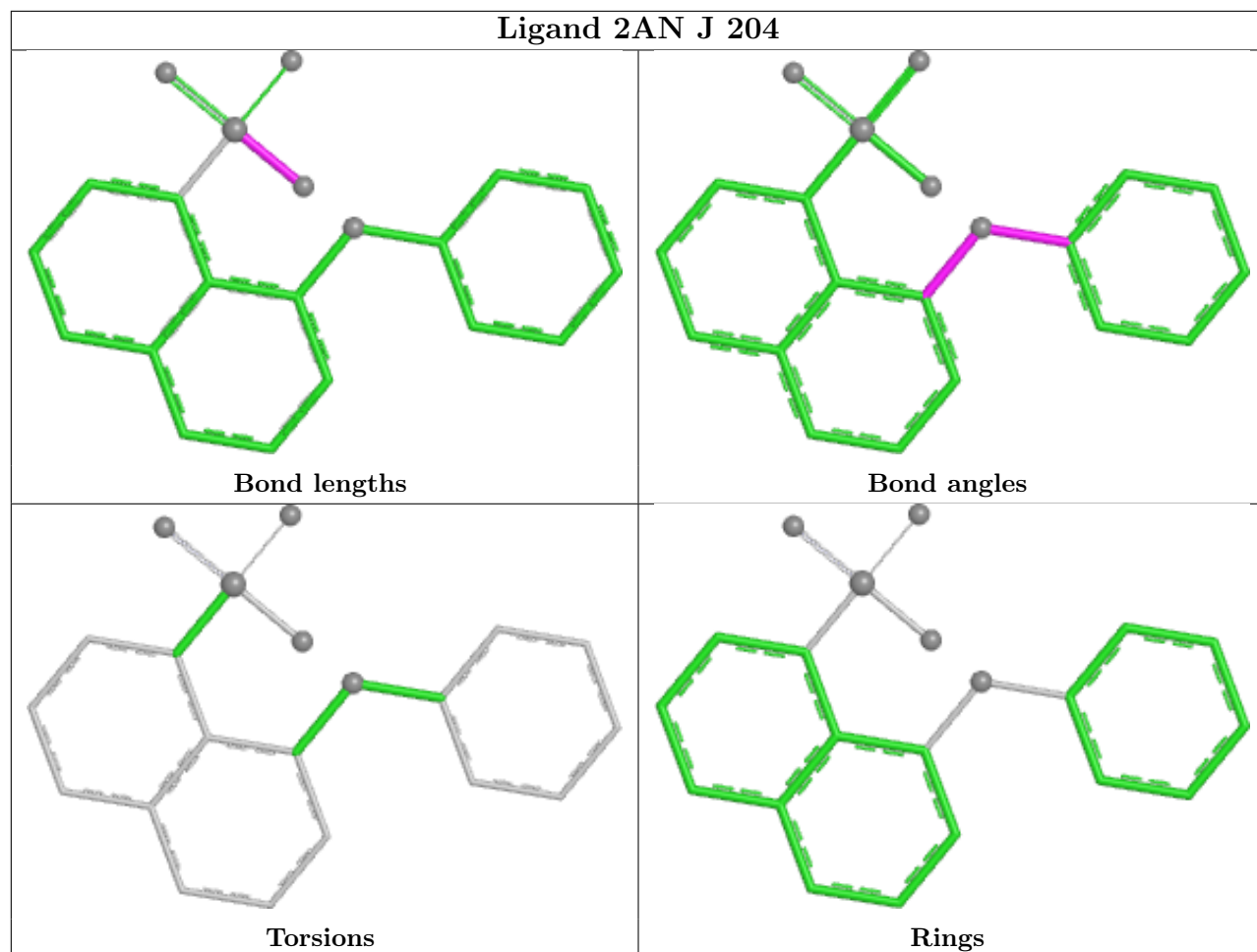
Ligand 2AN J 205



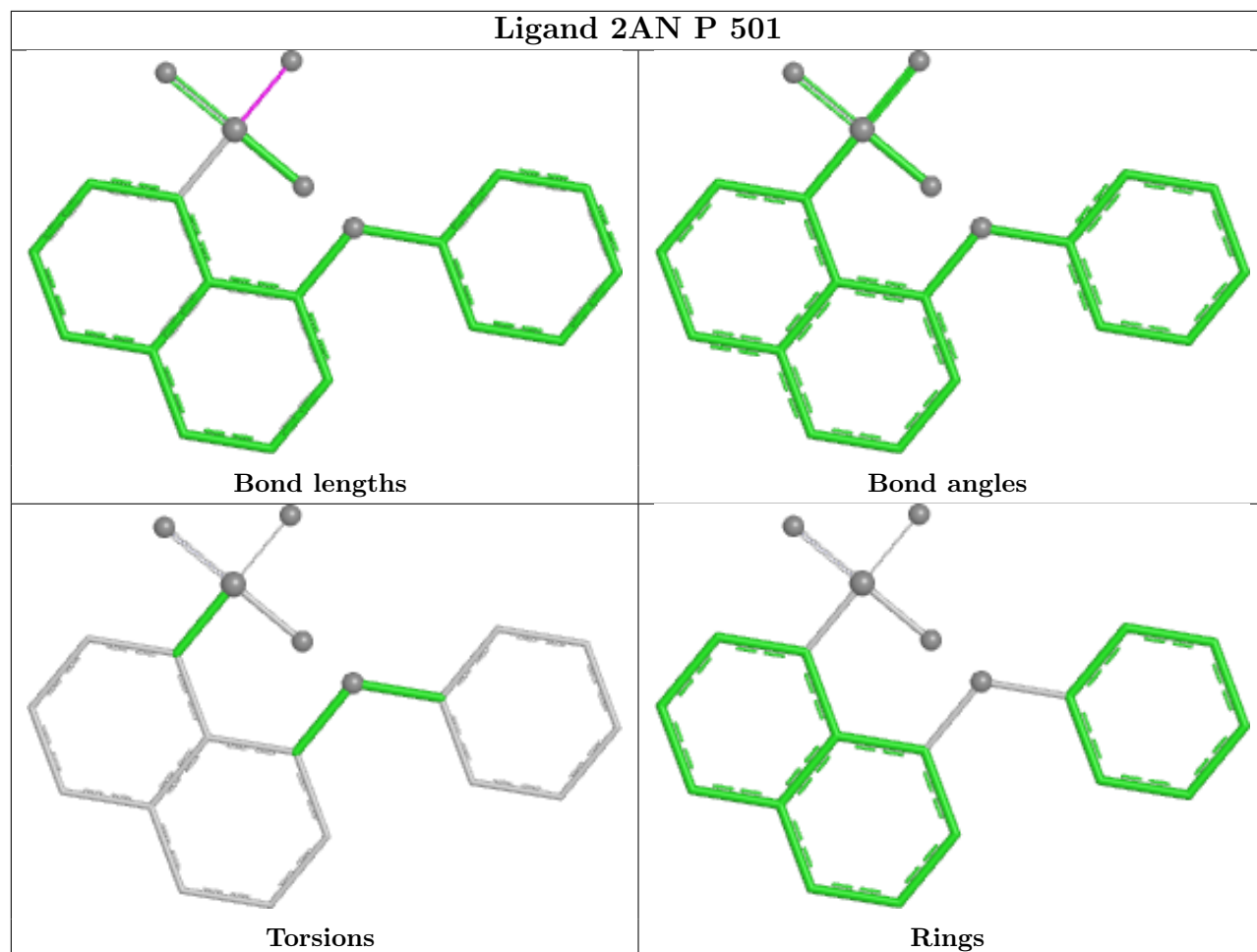
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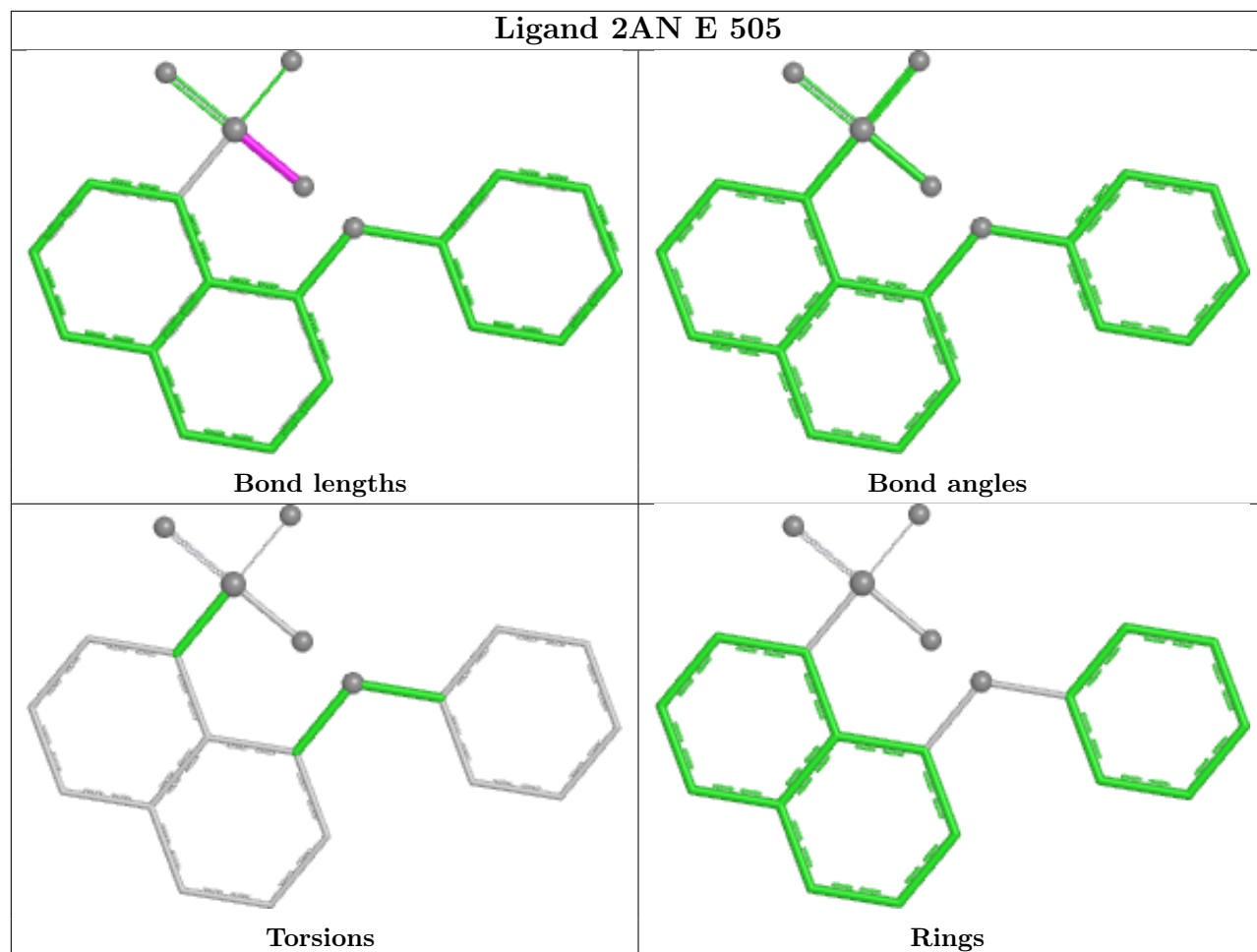
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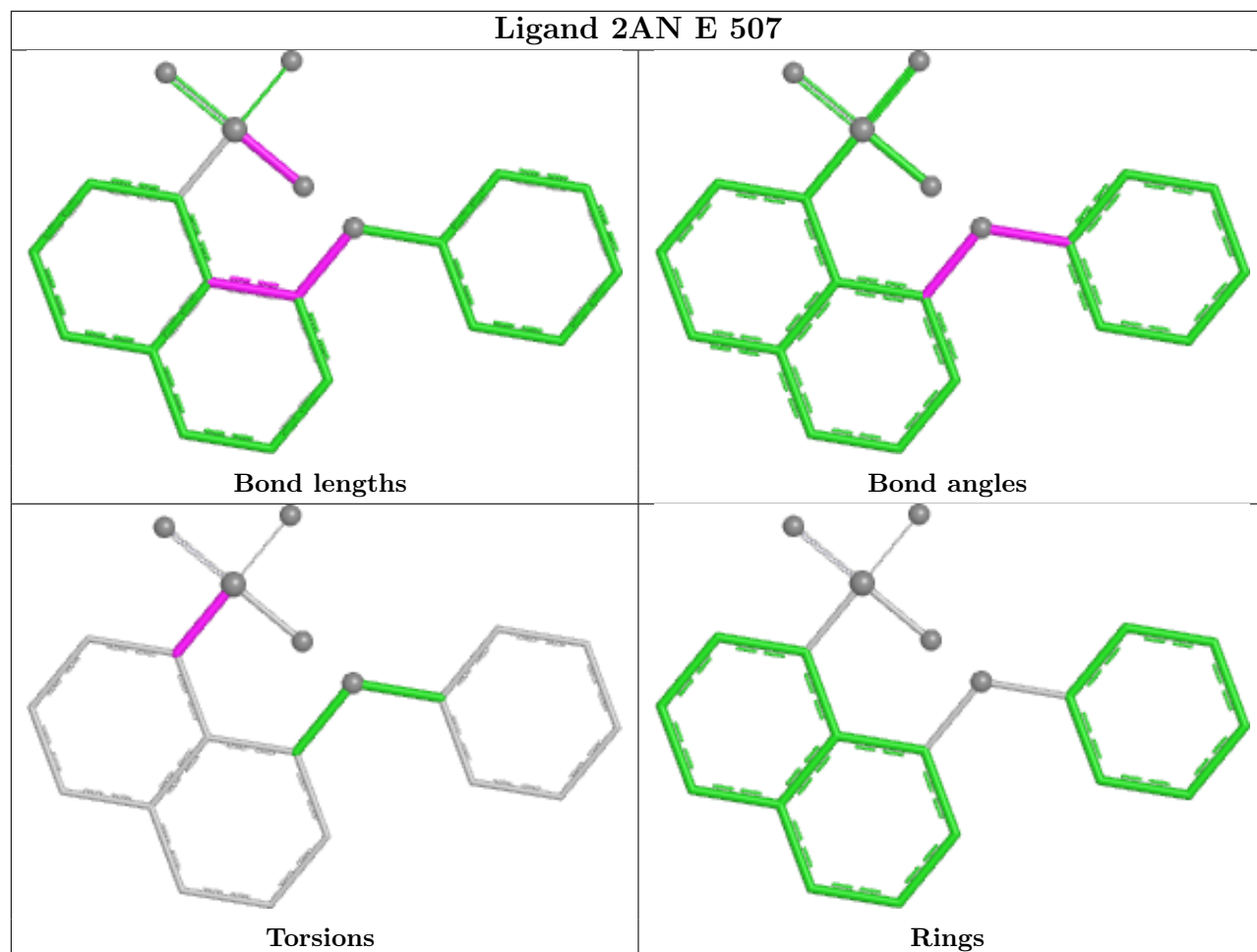
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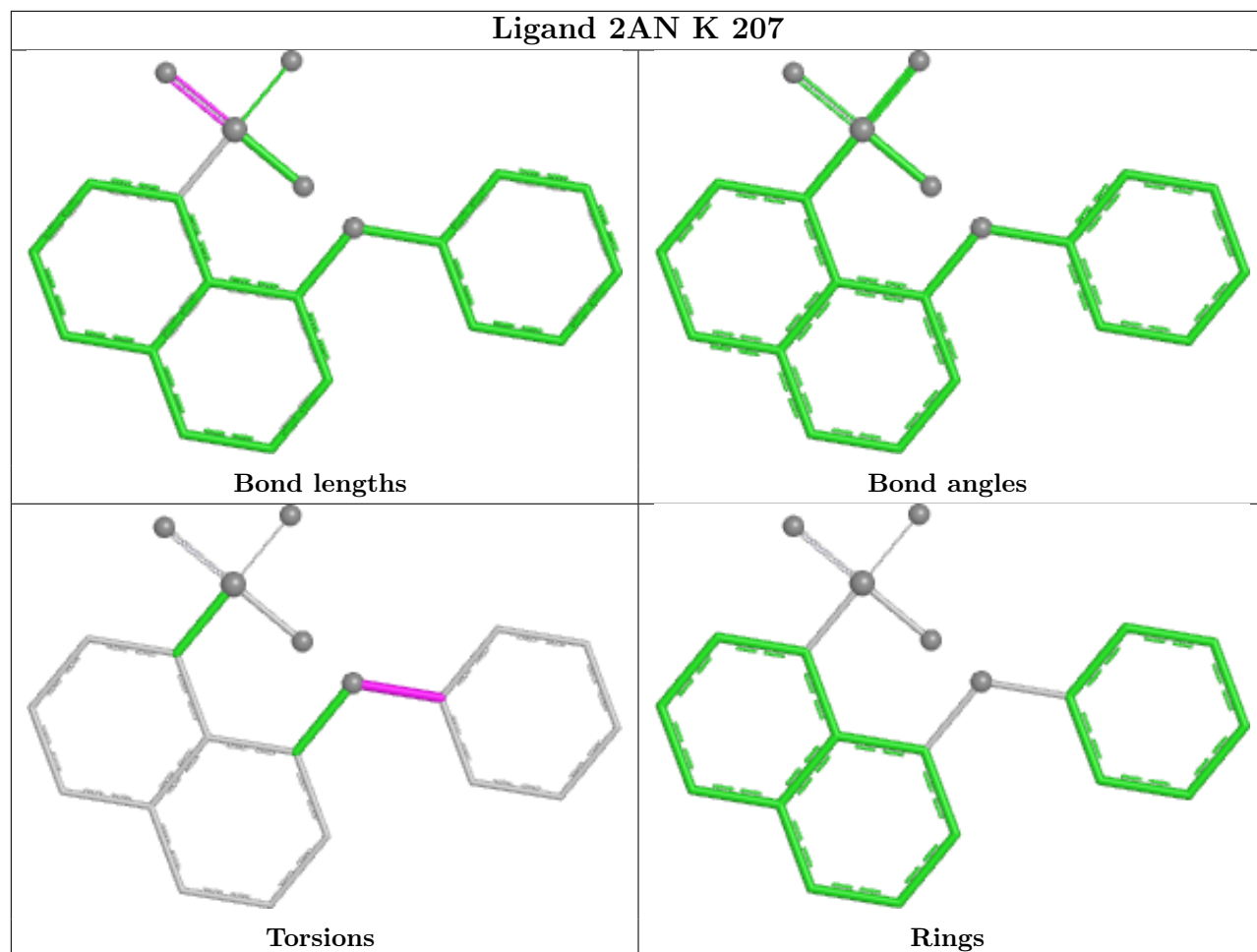


Ligand 2AN E 505

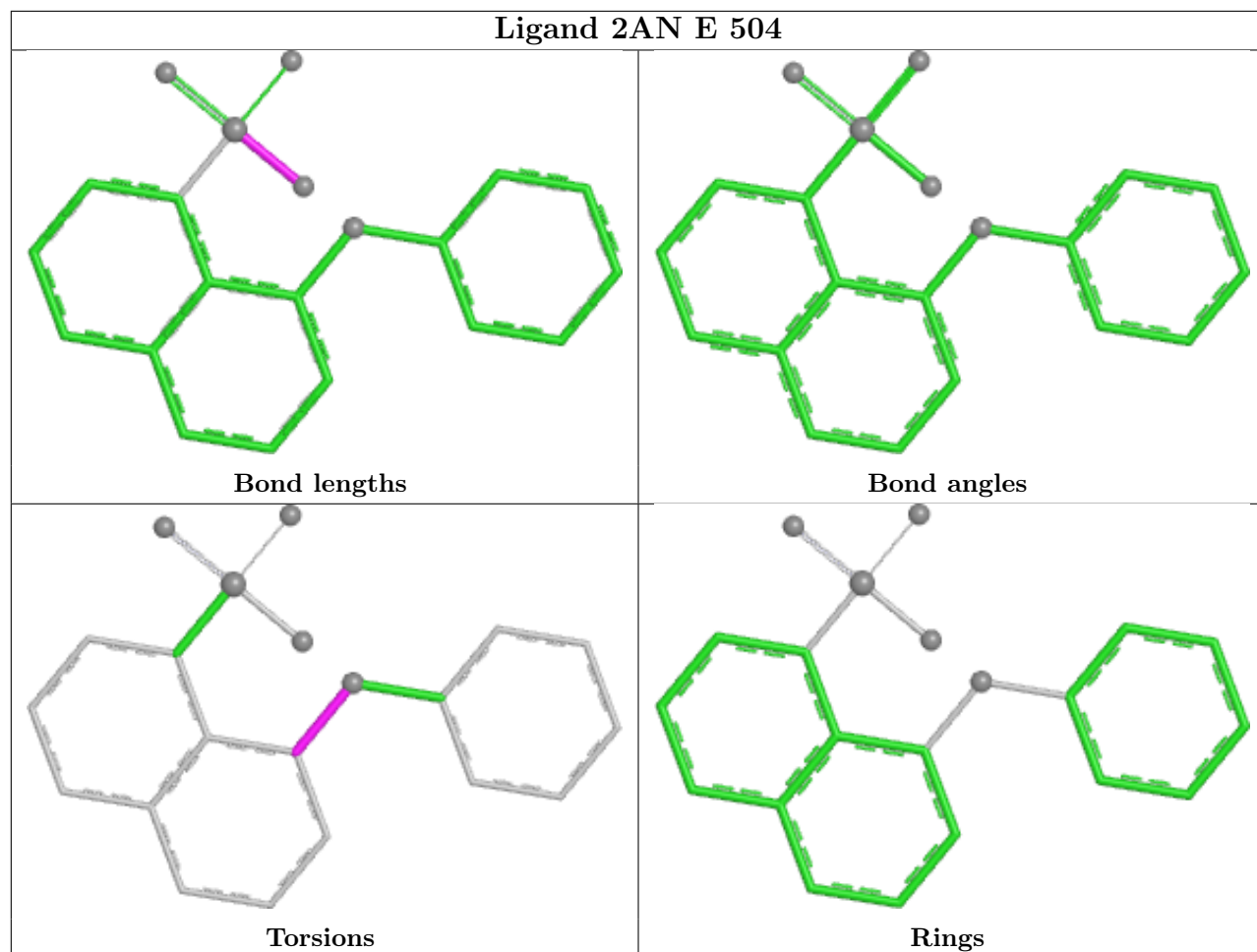


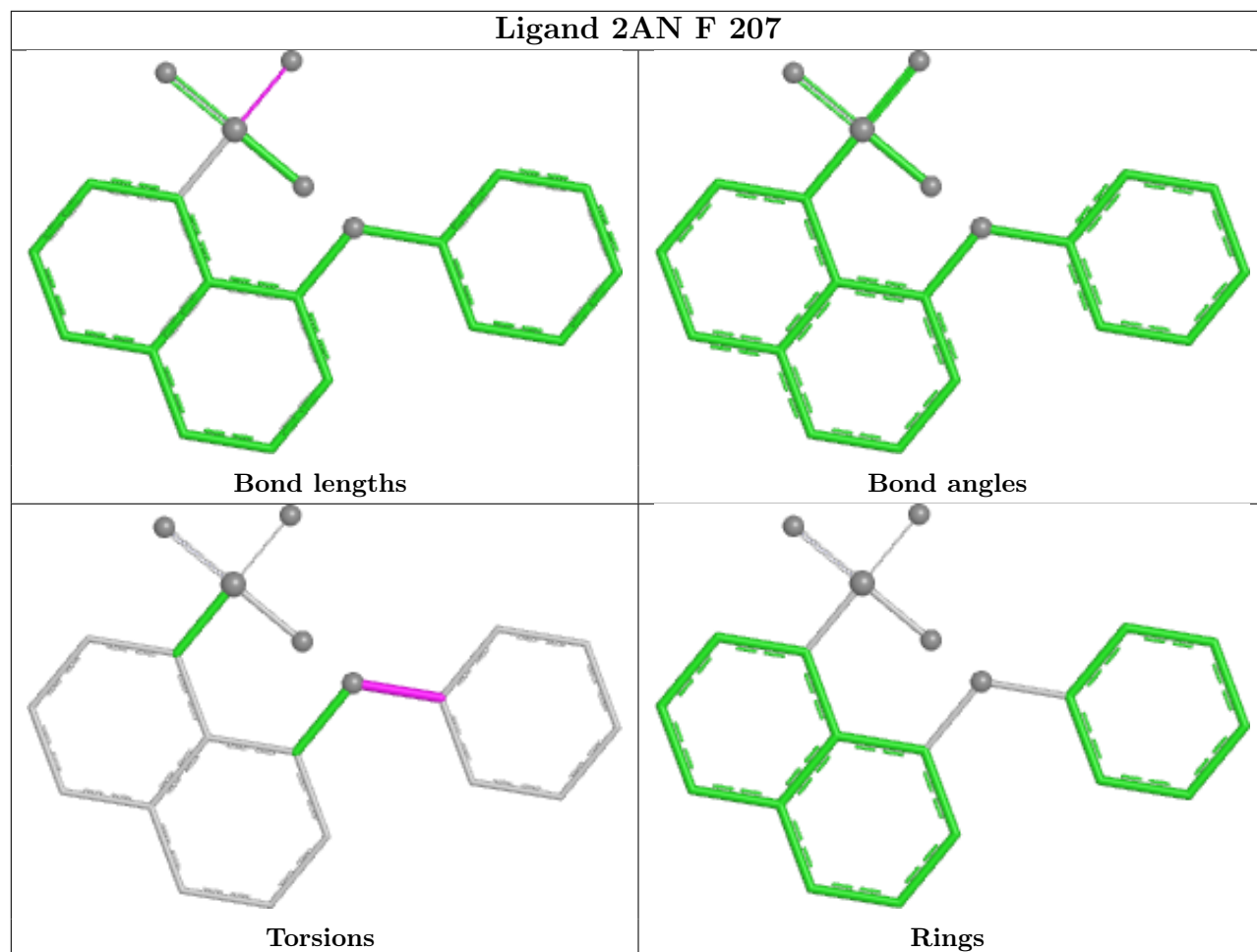
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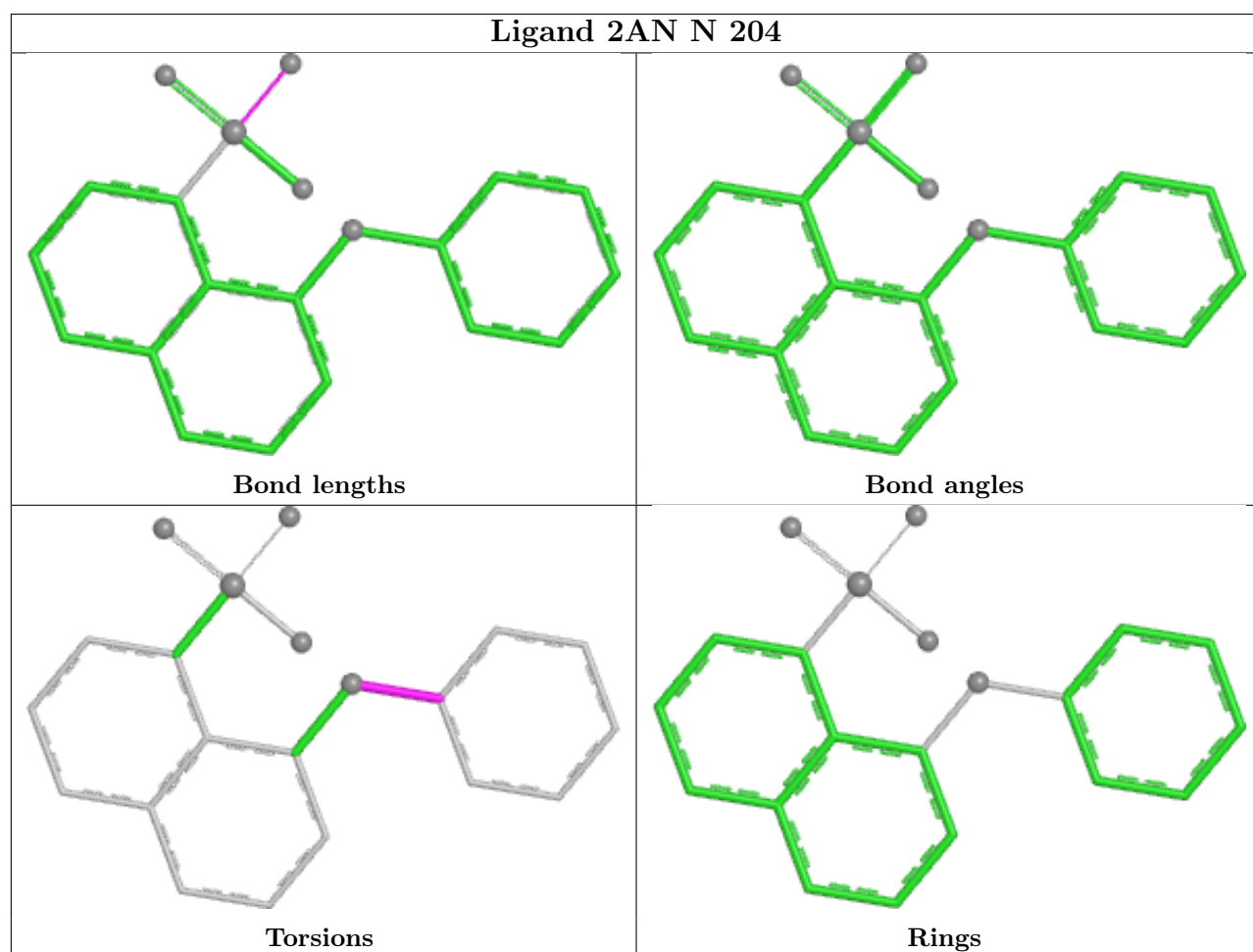


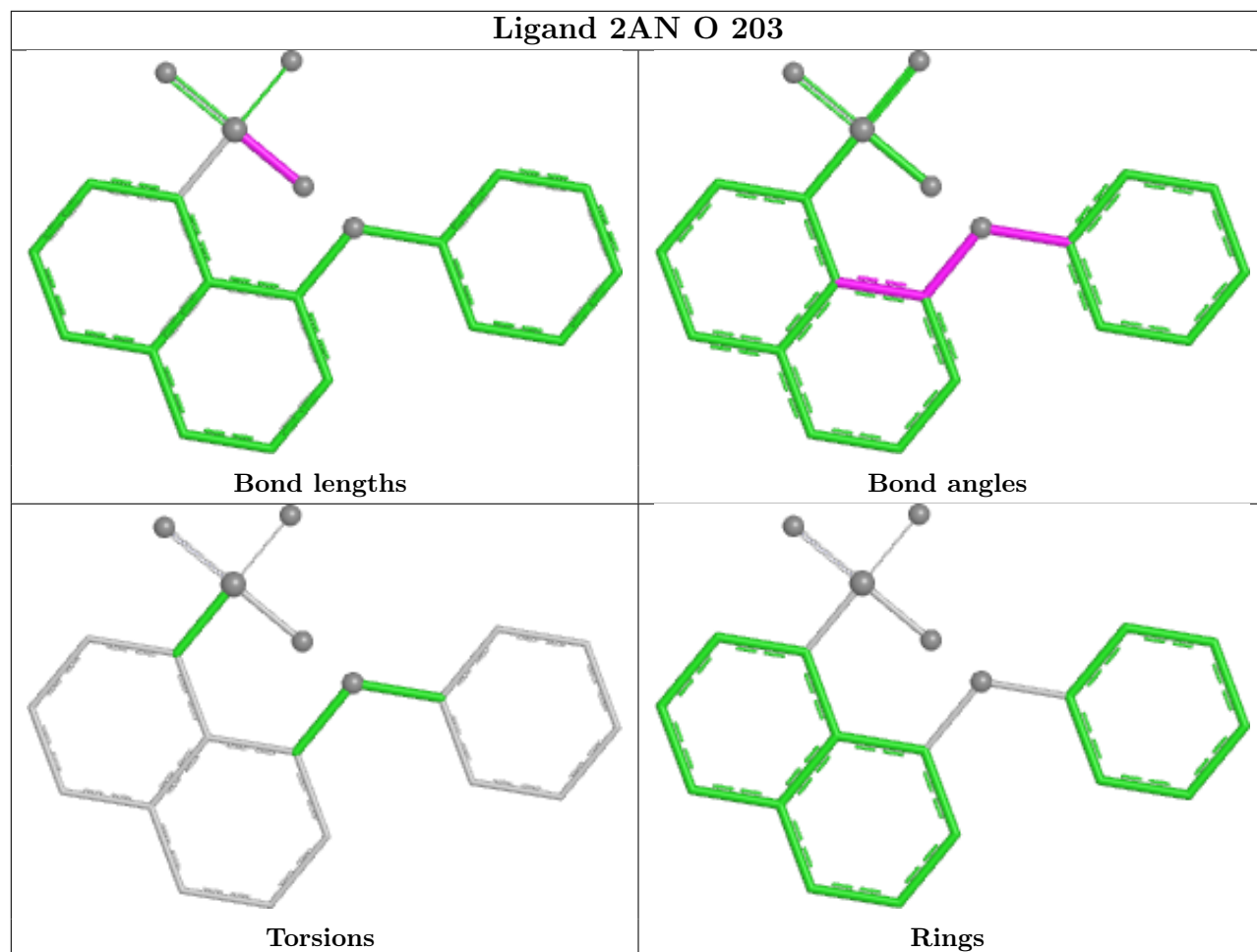


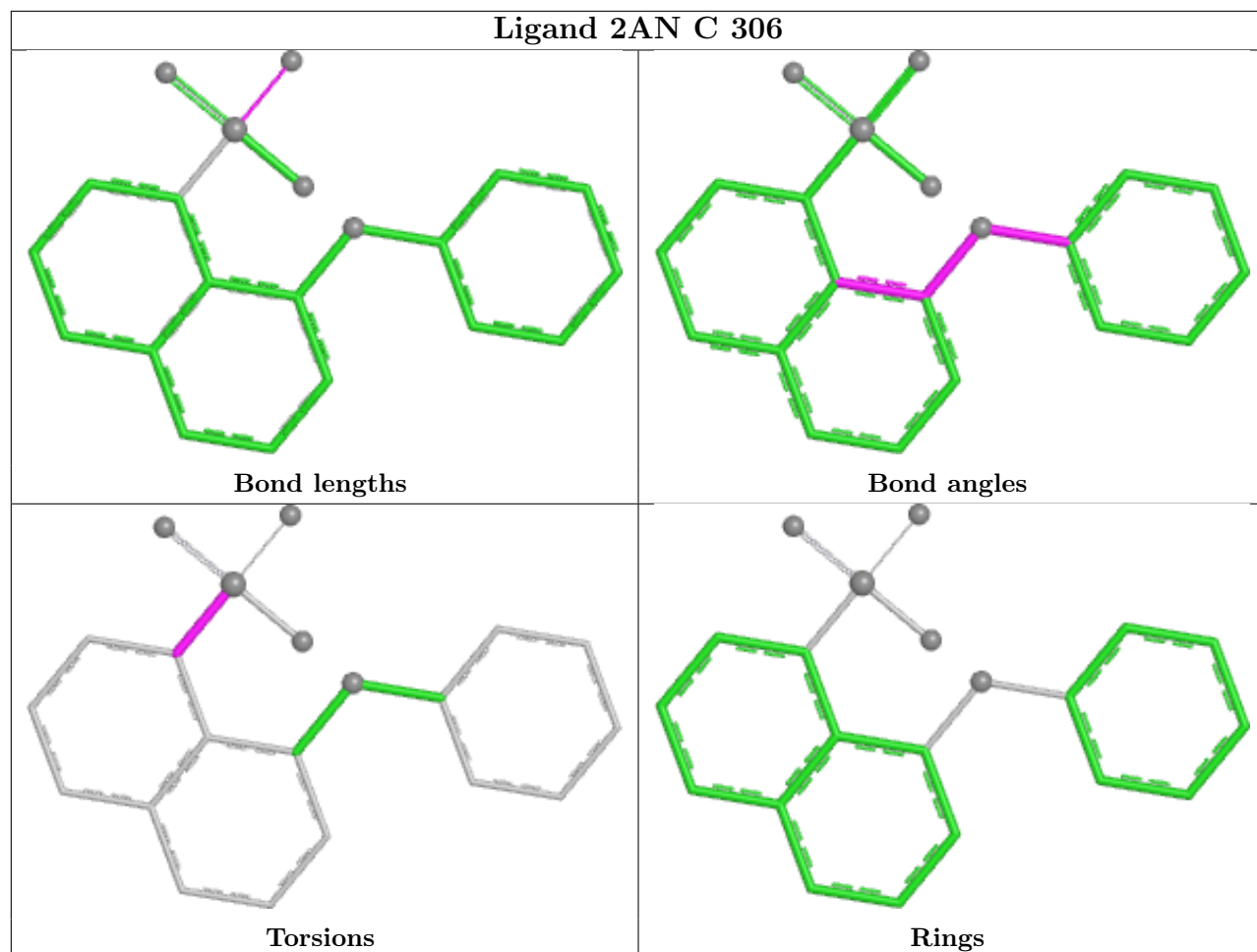
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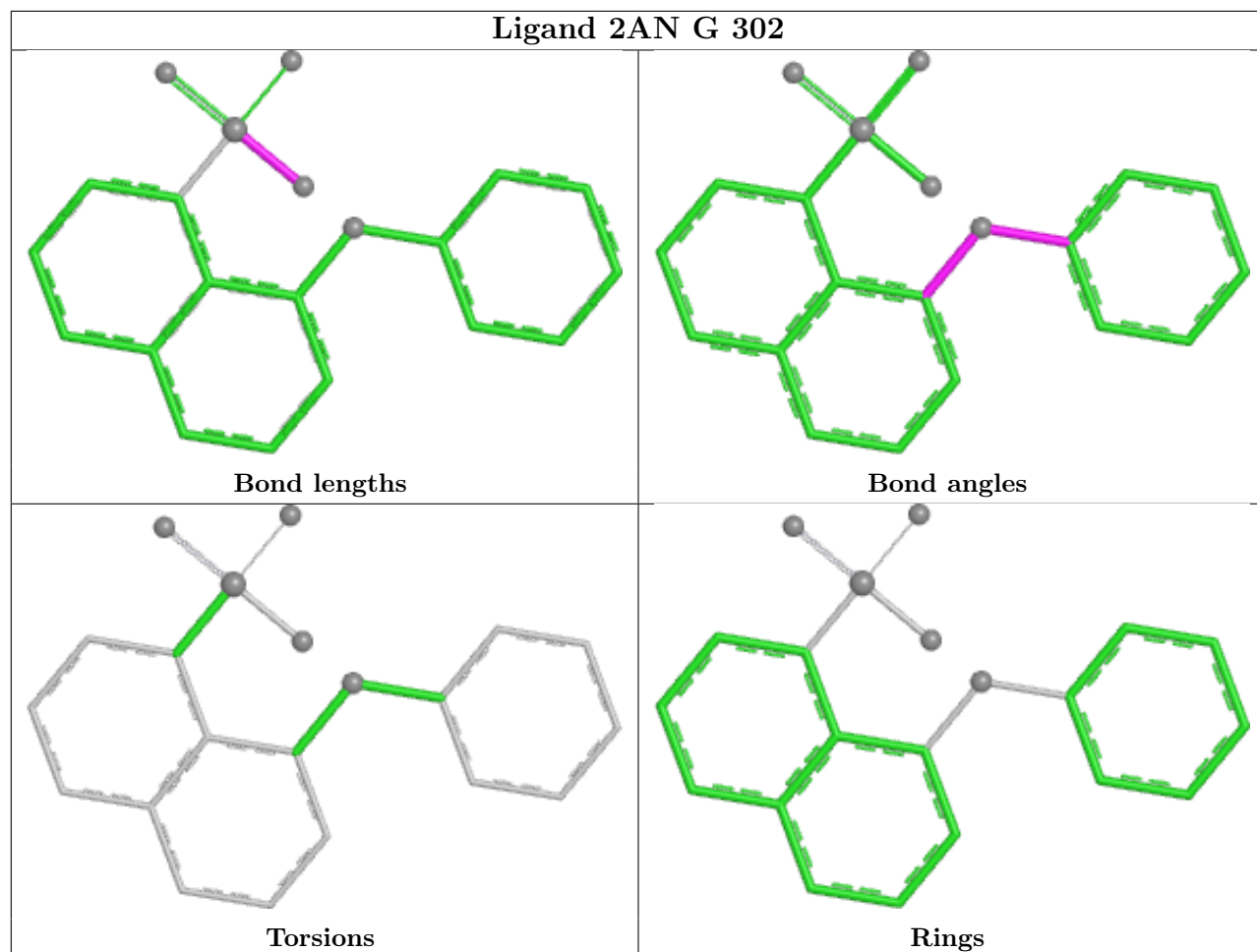


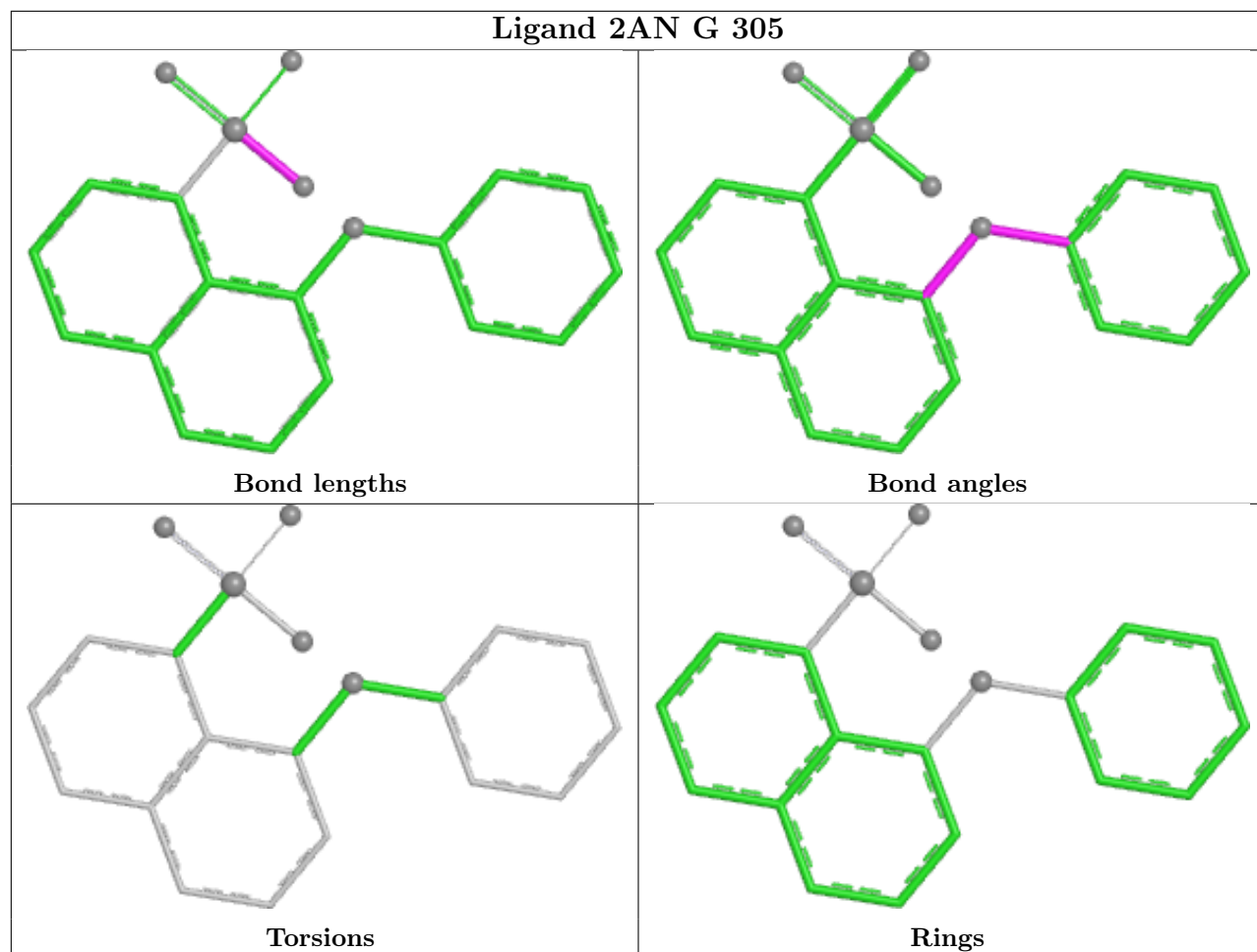


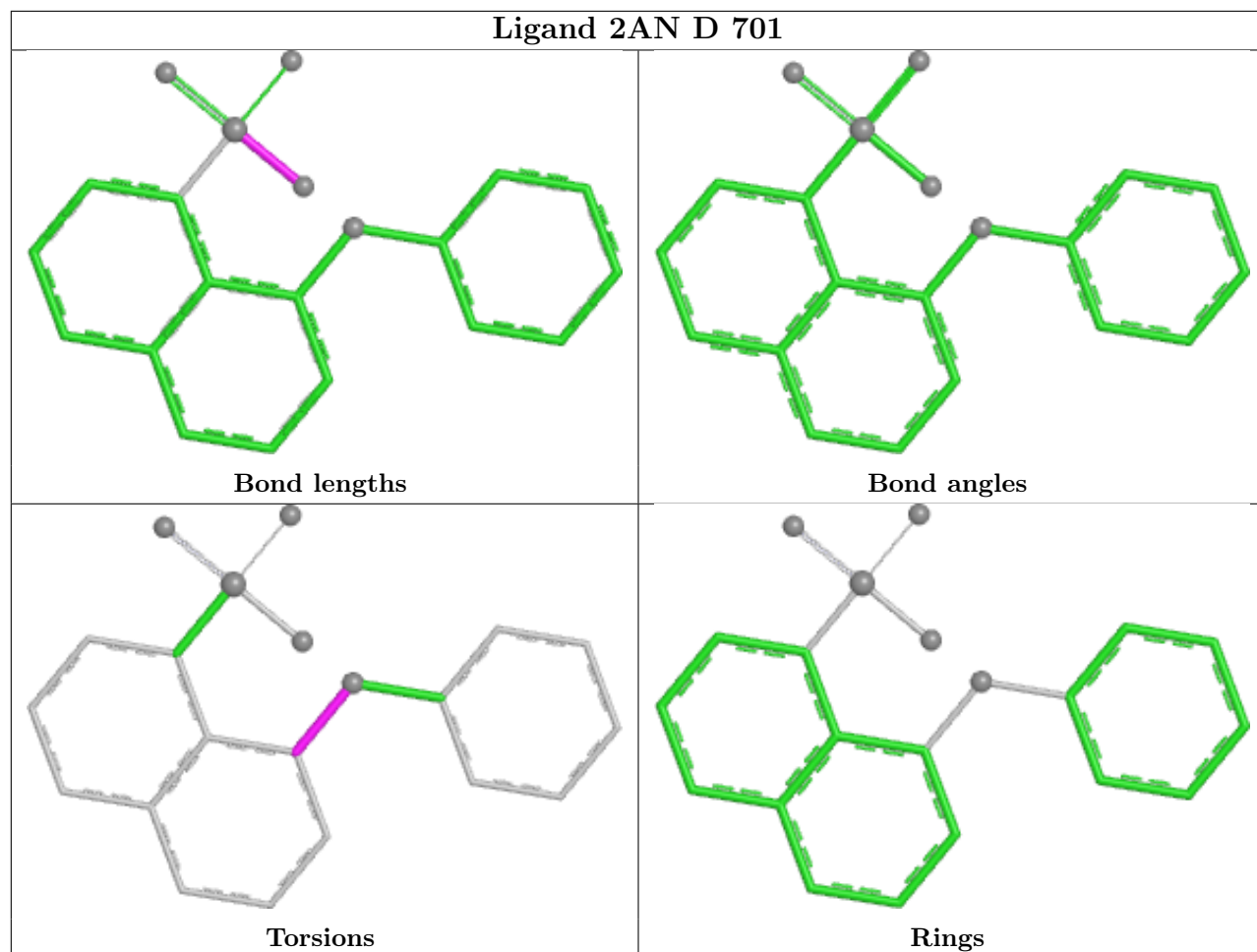




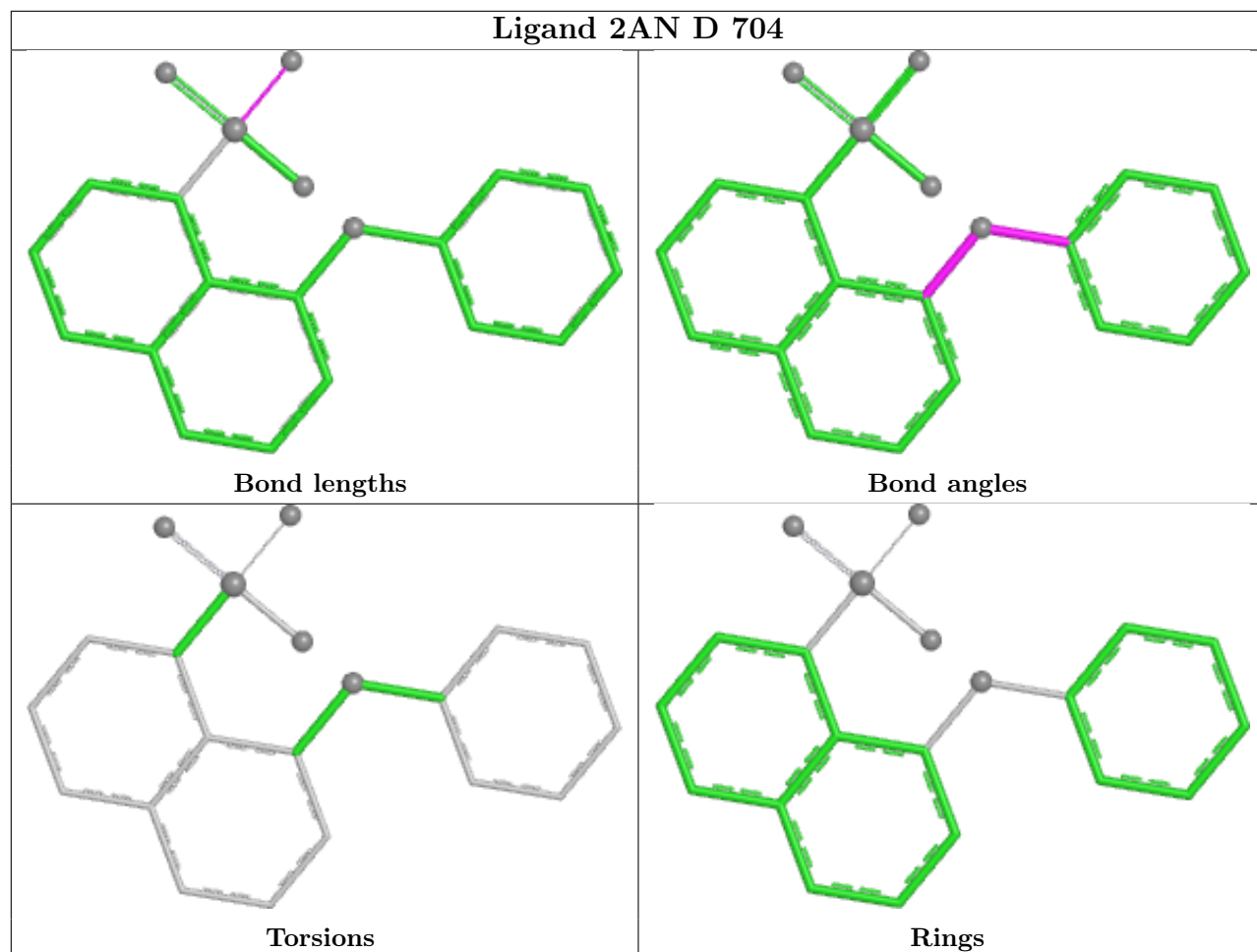




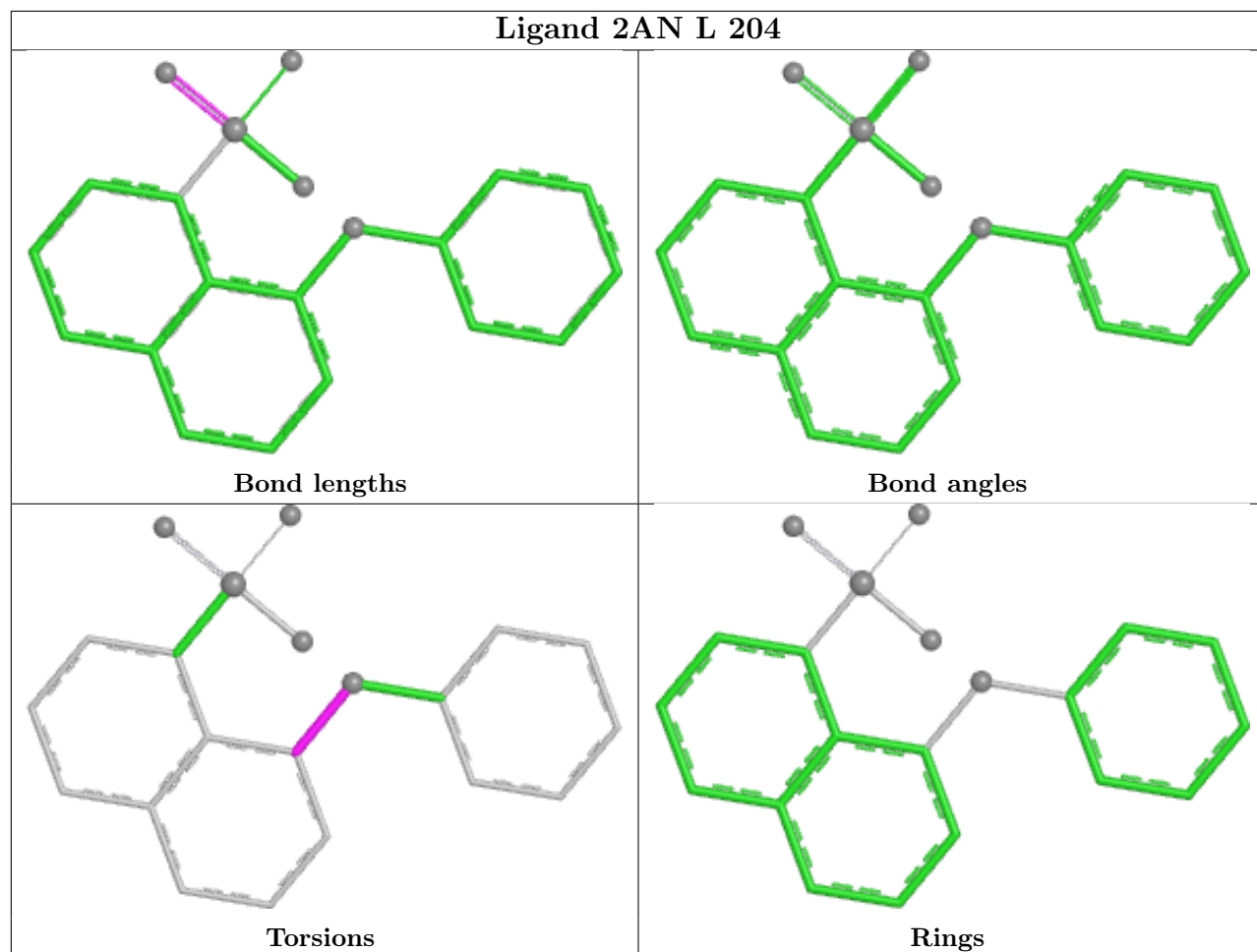


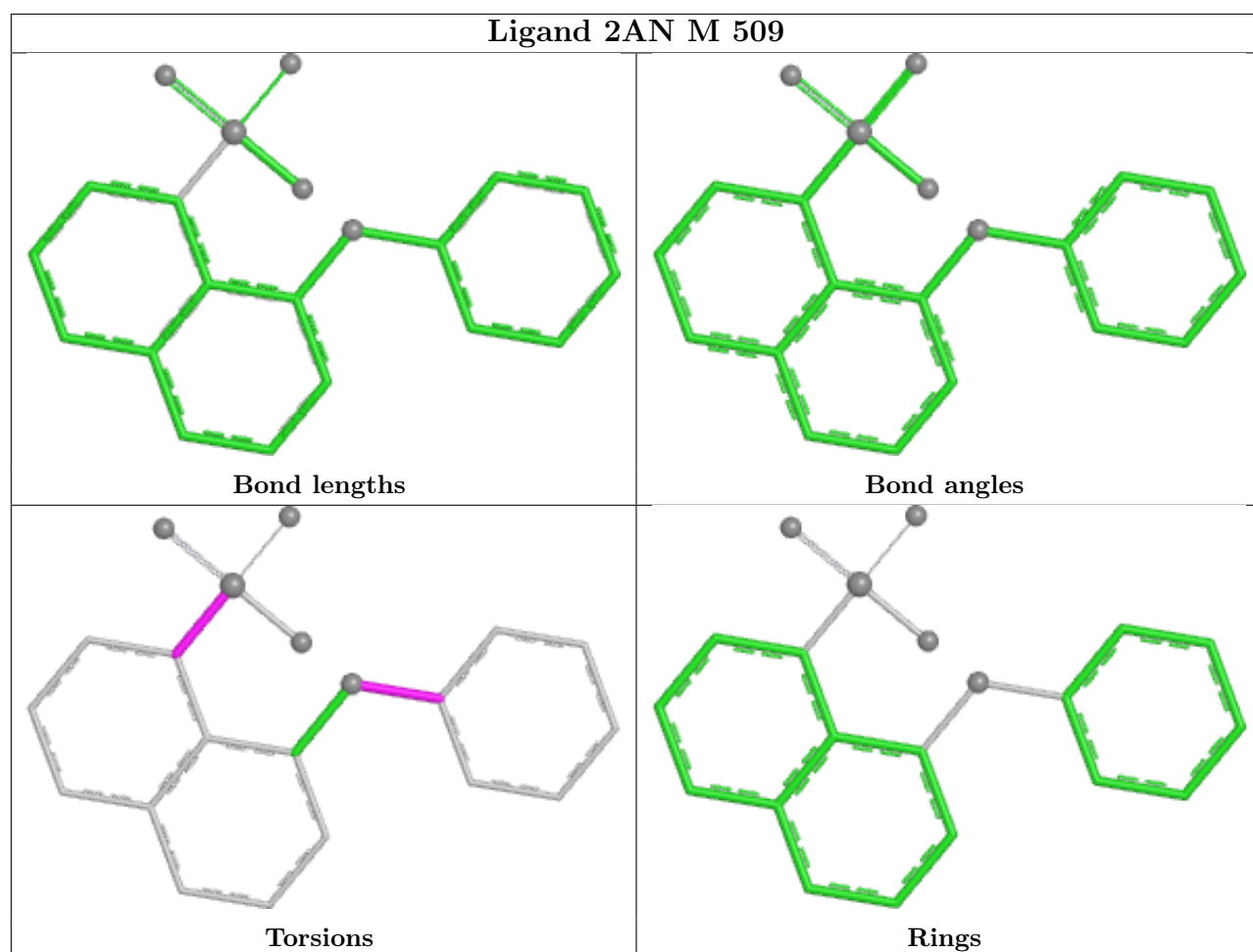


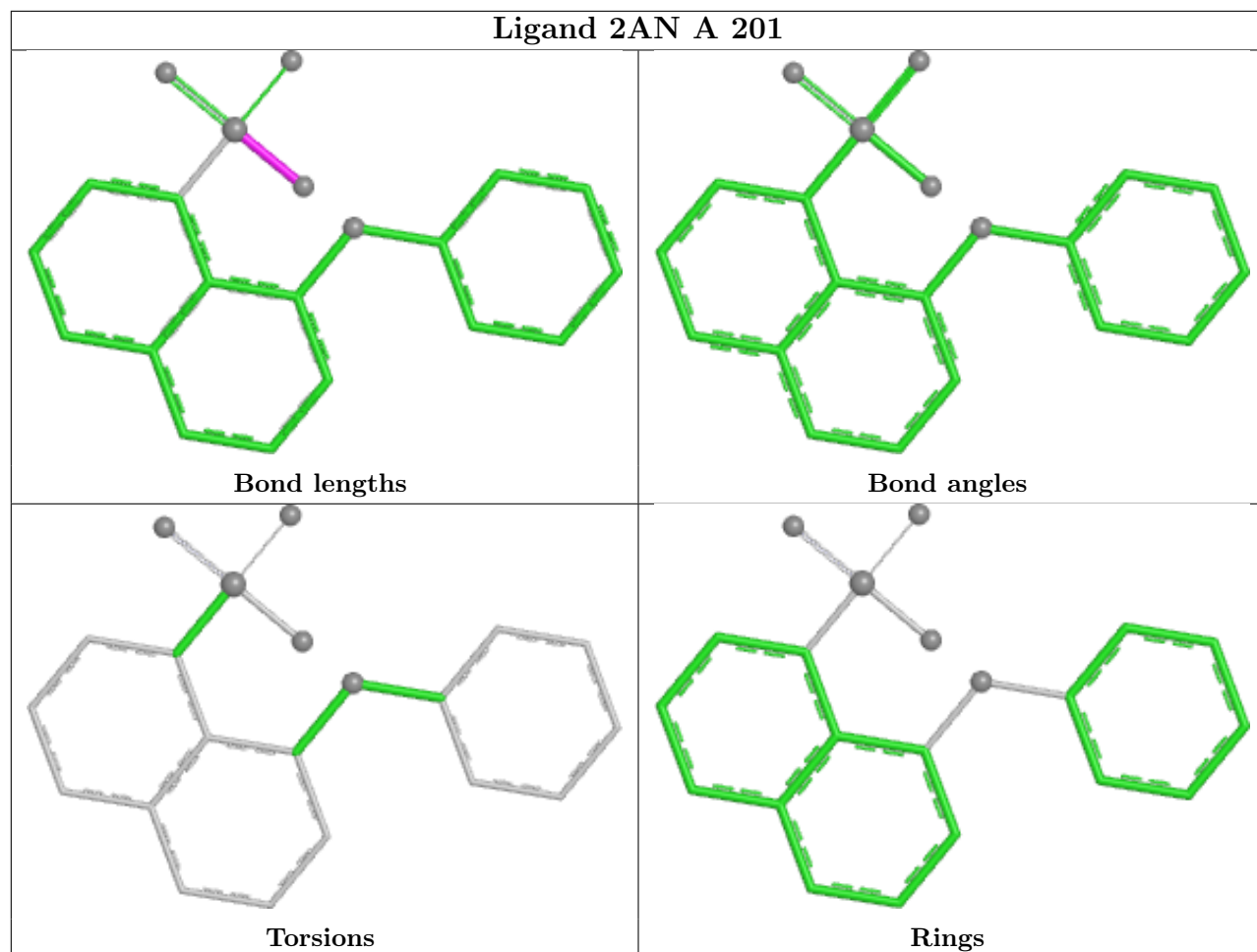
Ligand 2AN D 704

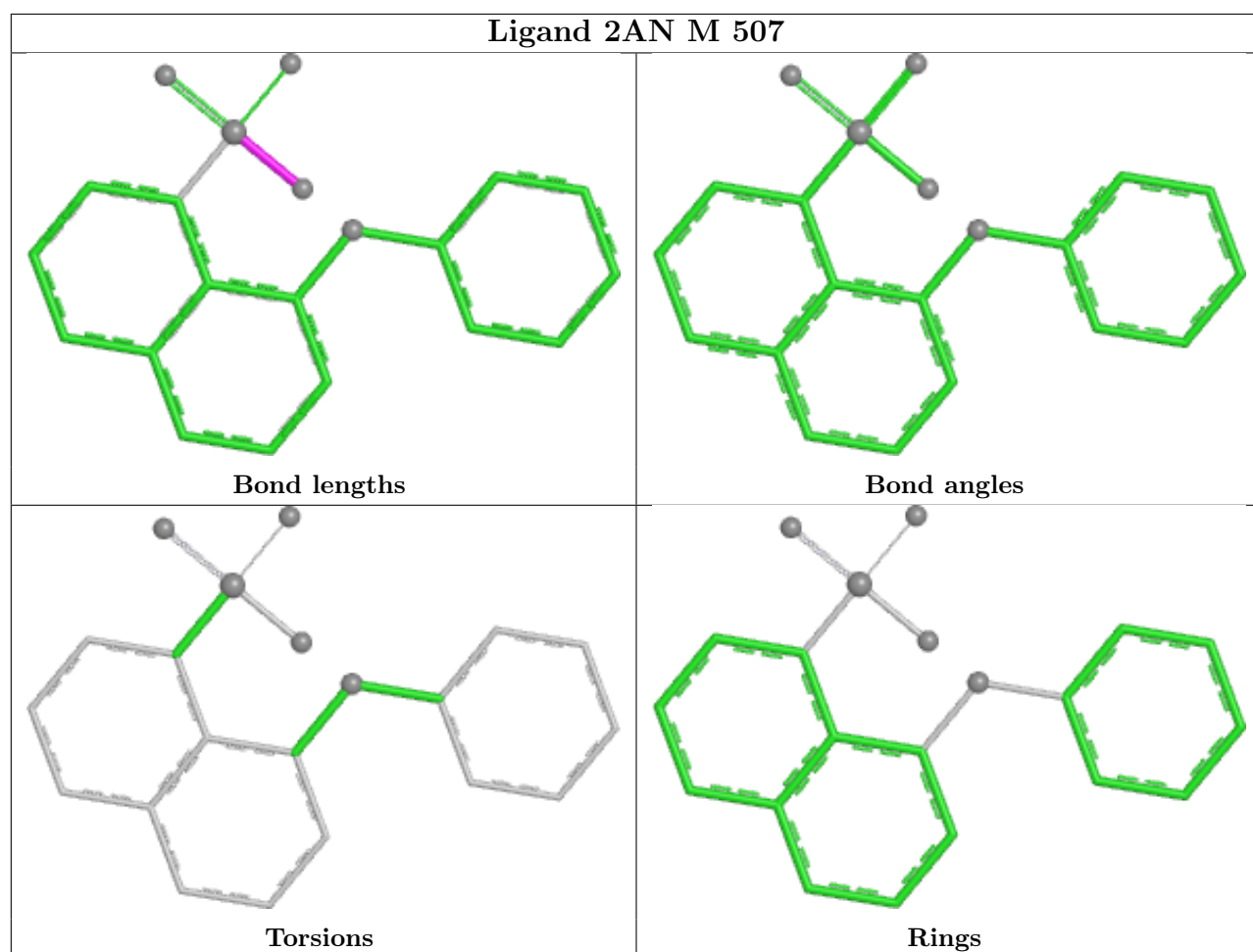


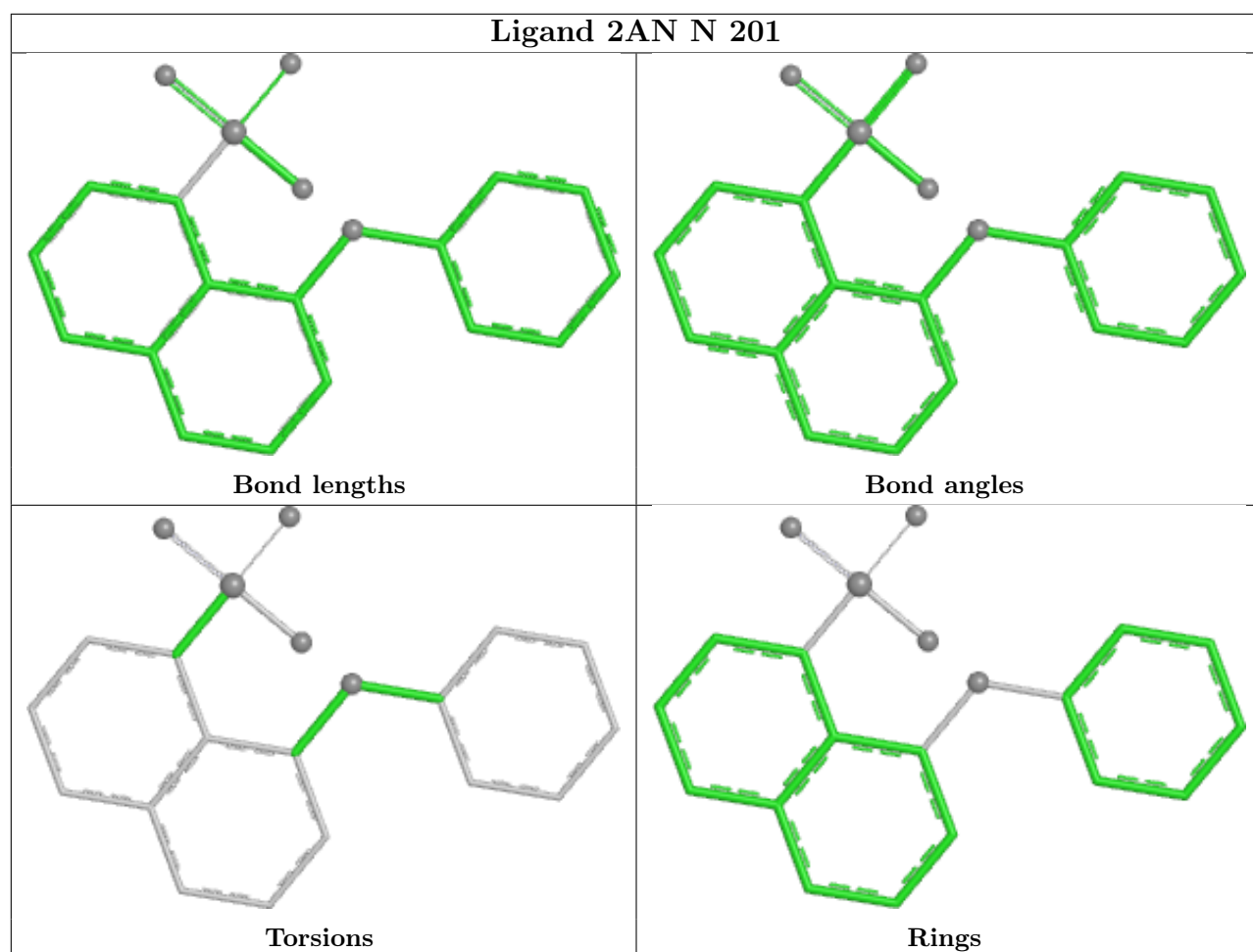
Ligand 2AN L 204



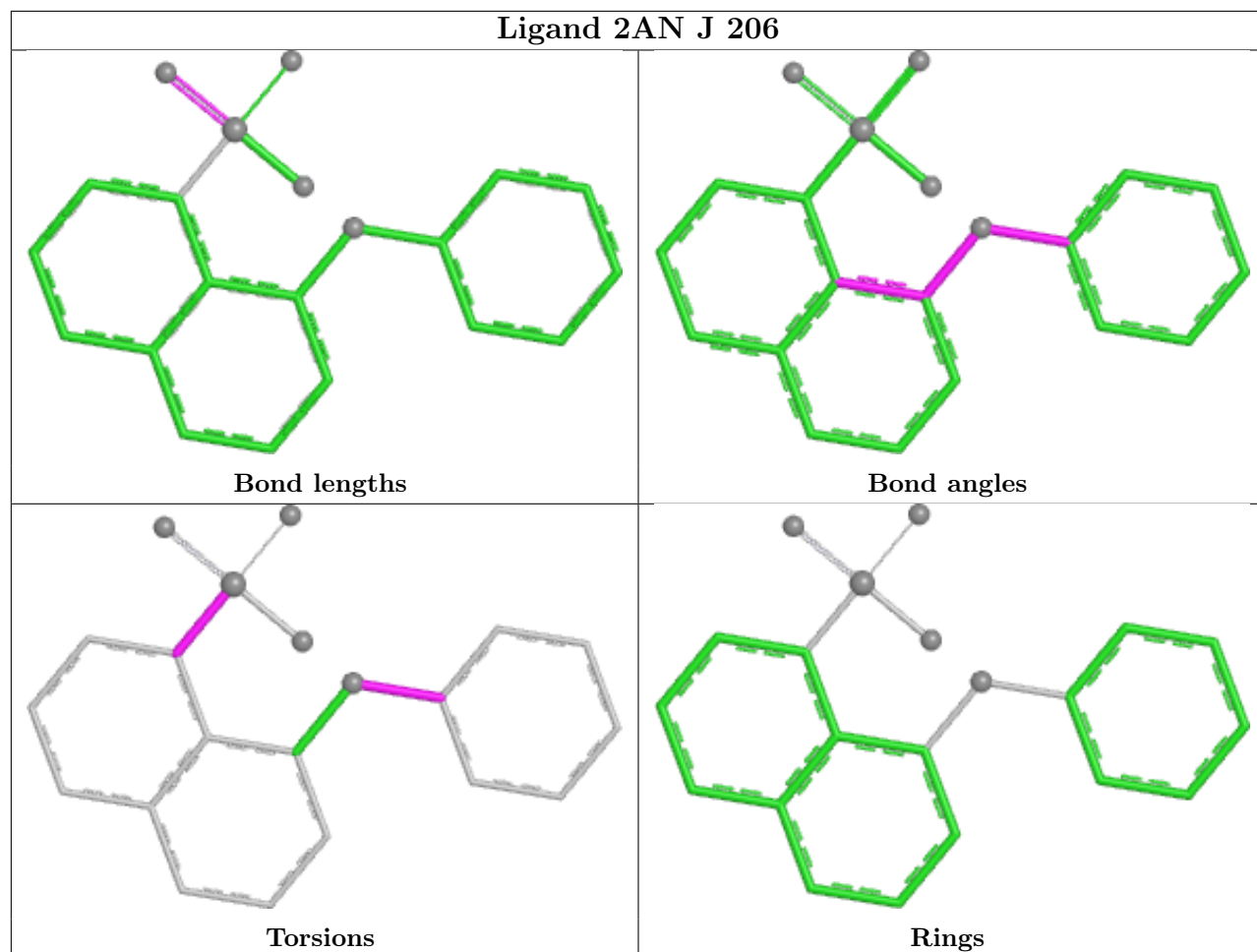




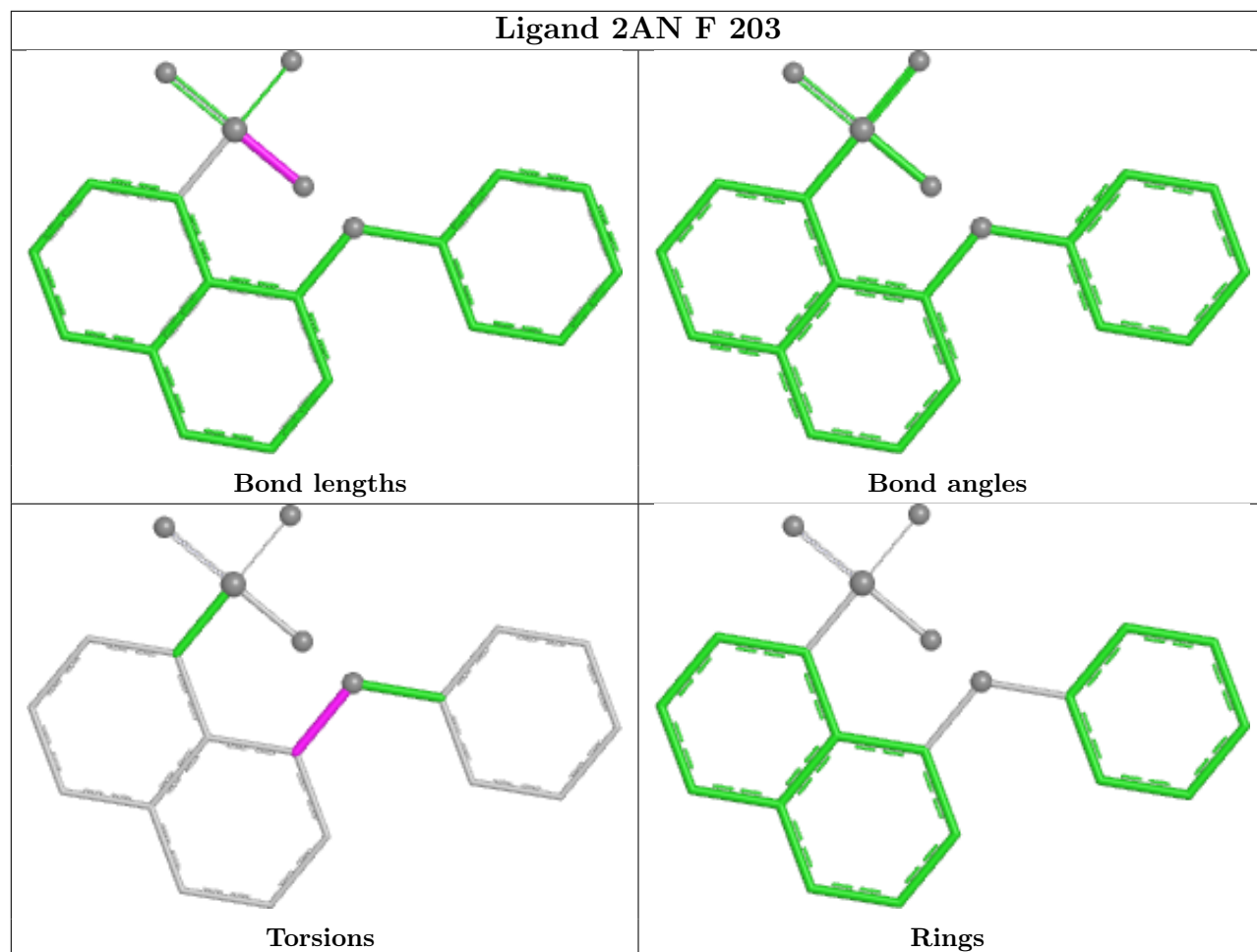




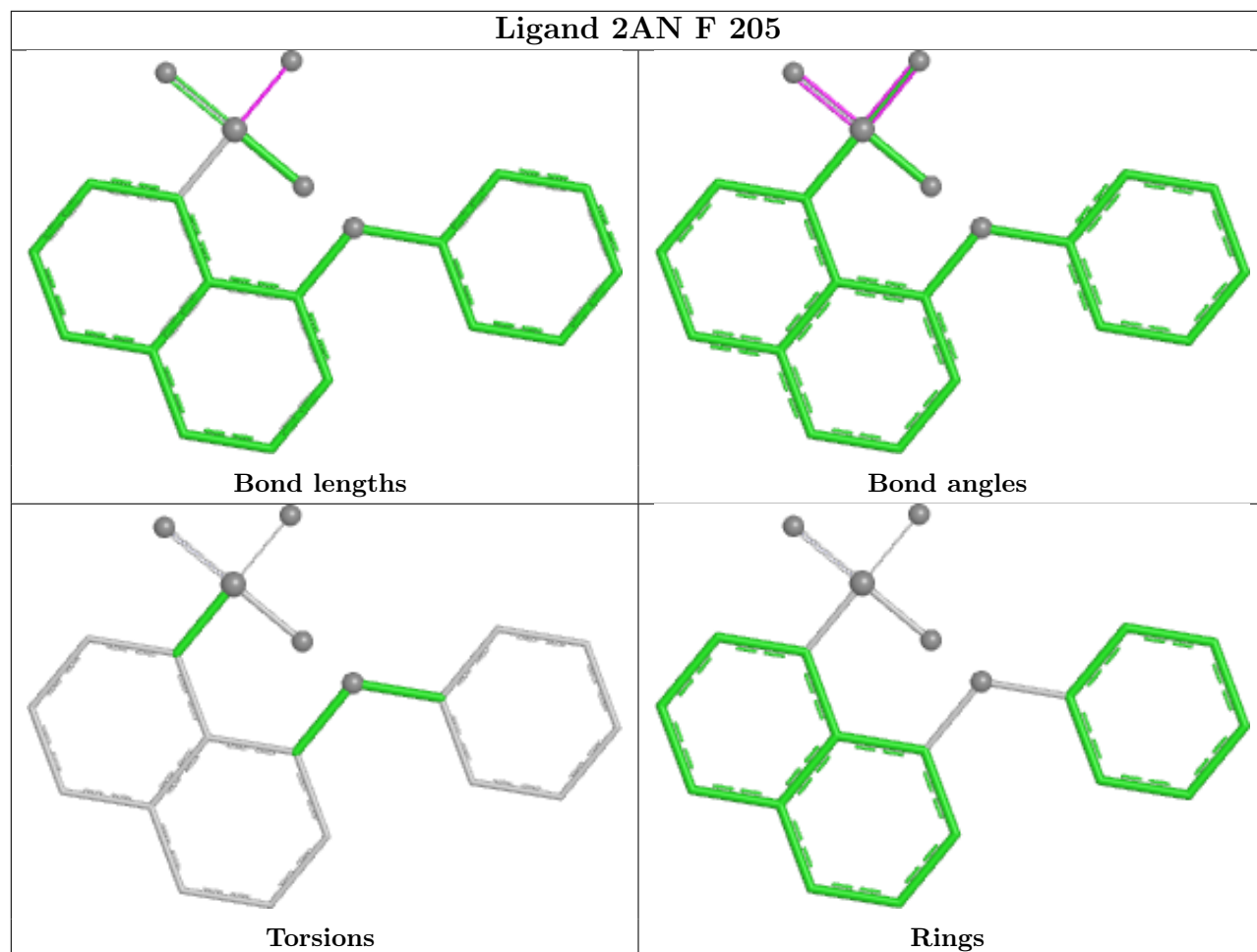
Ligand 2AN J 206

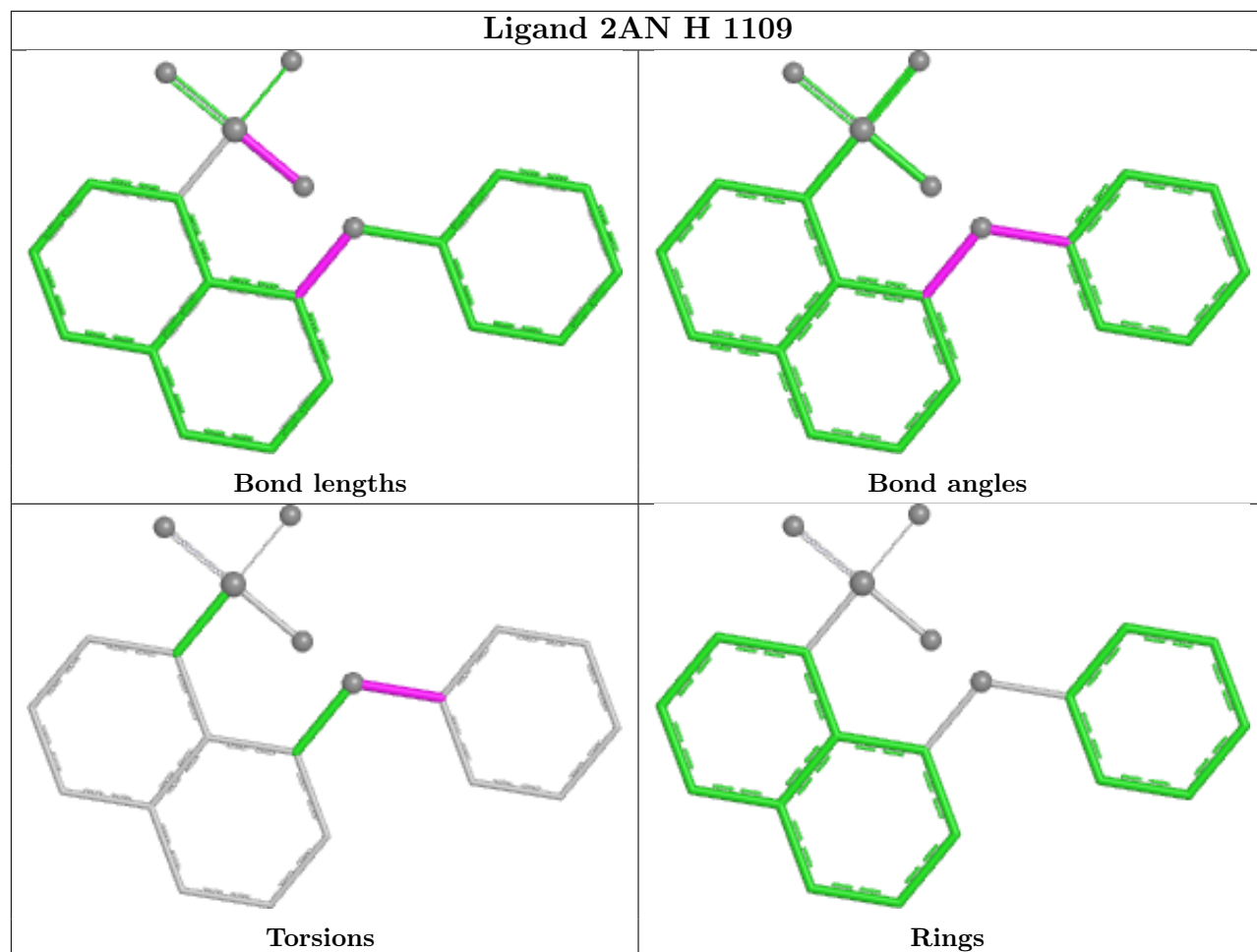


Ligand 2AN F 203

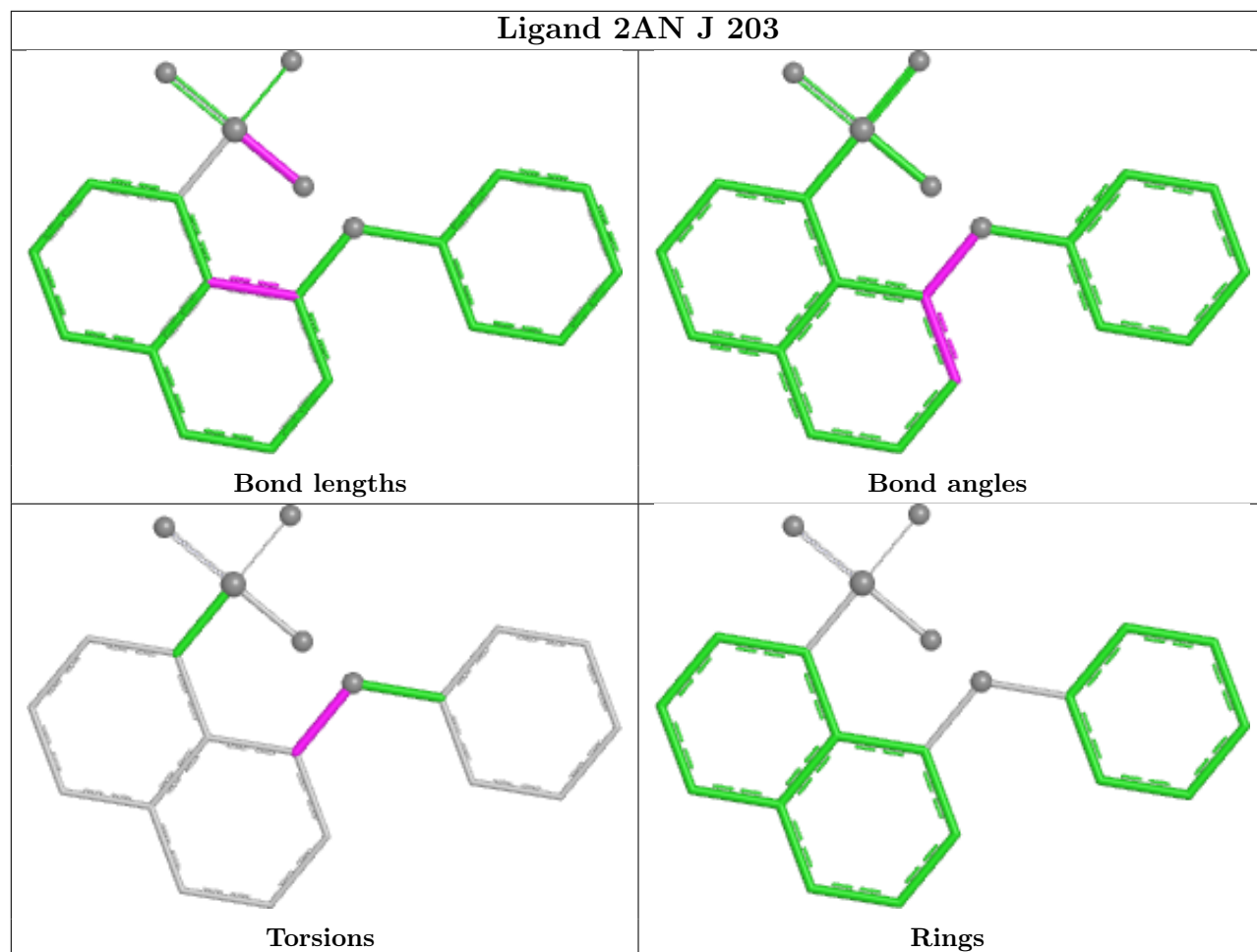


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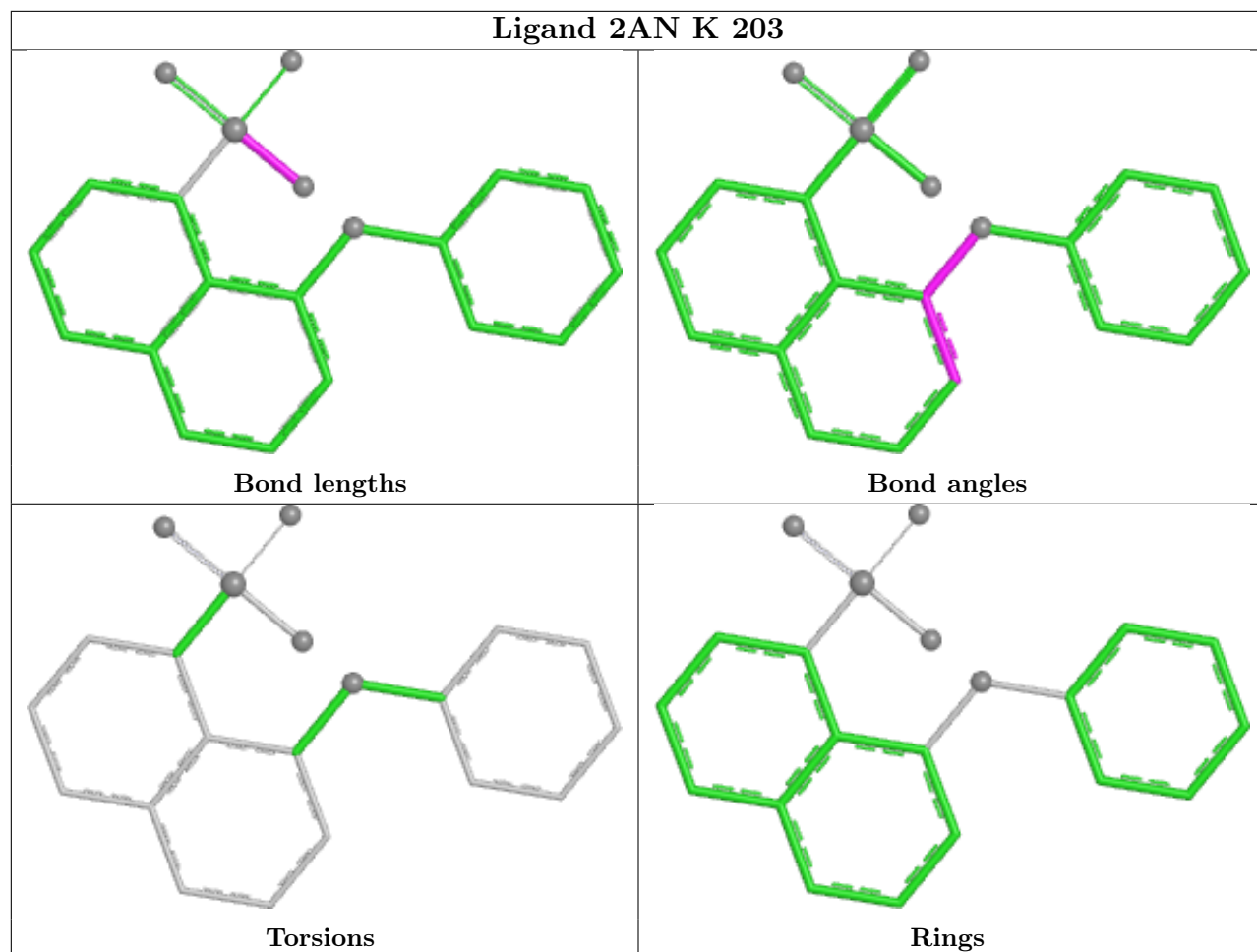


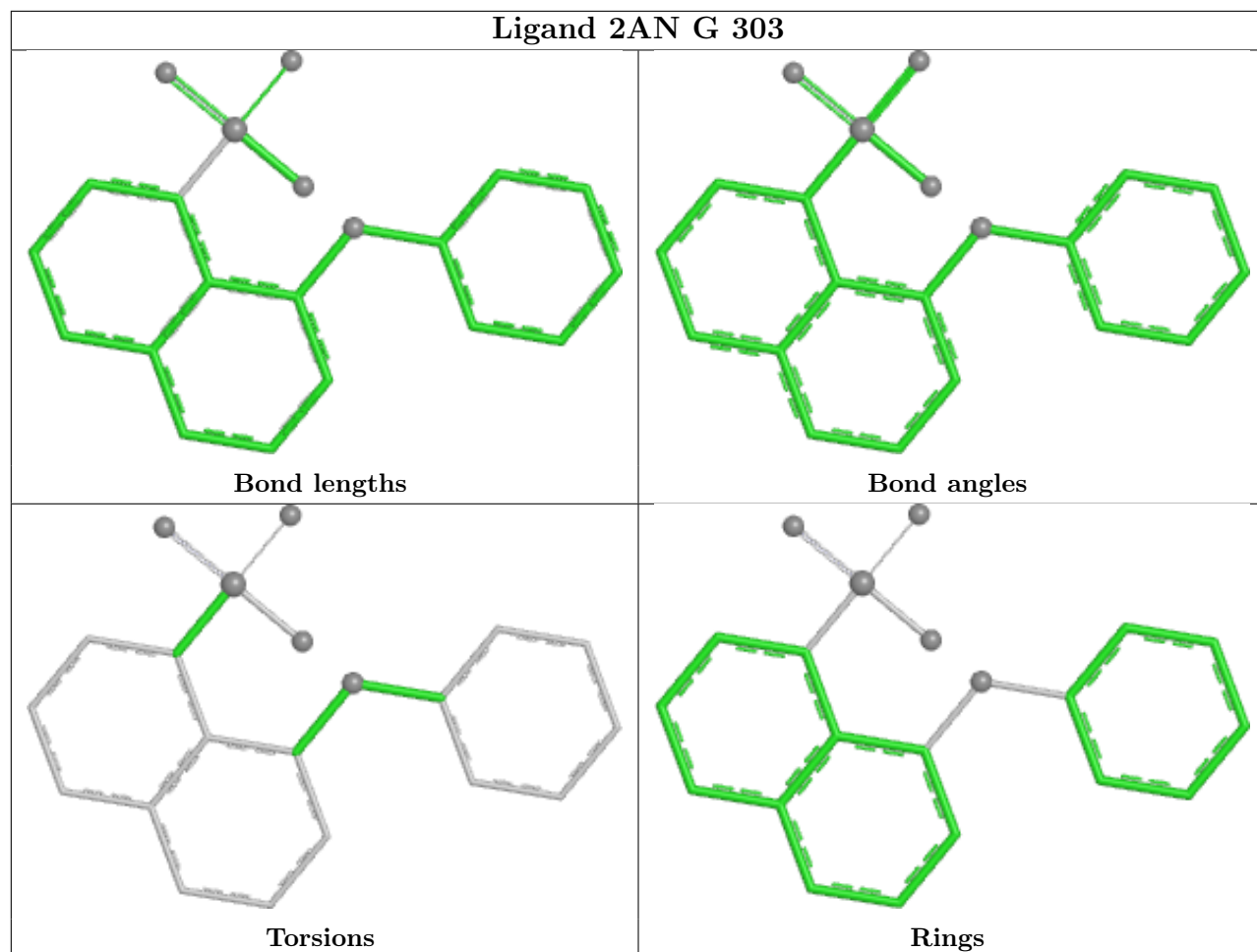


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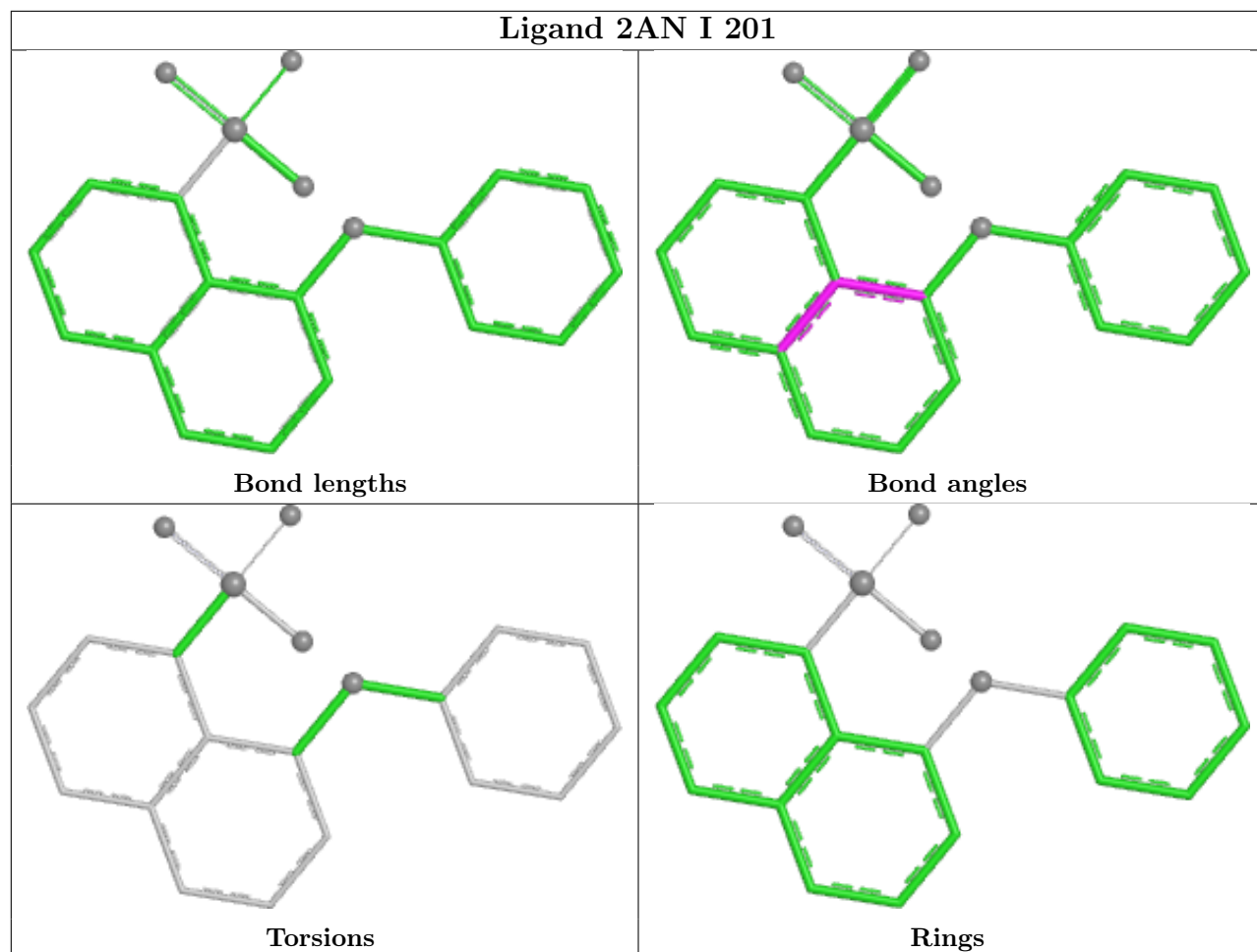


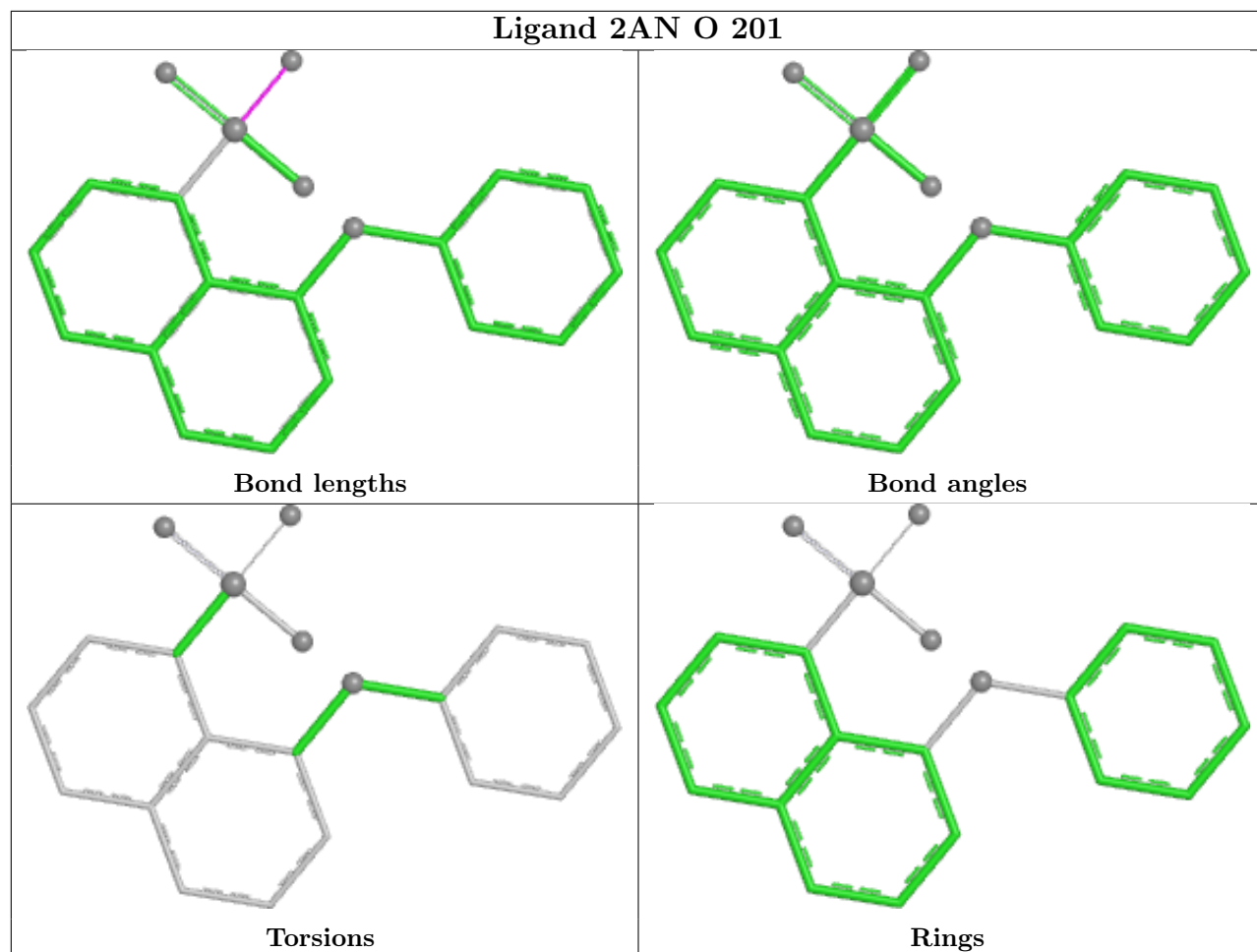
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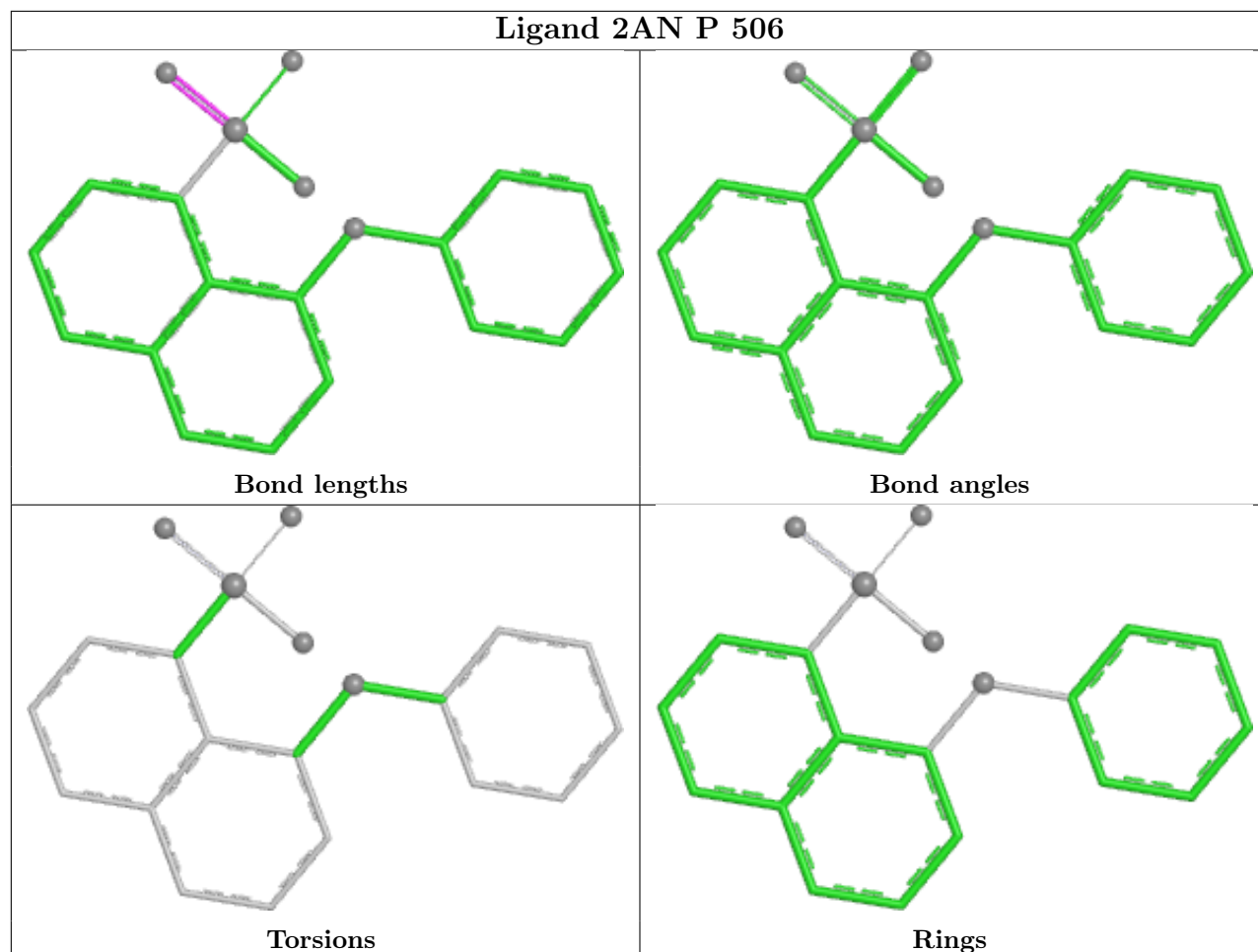


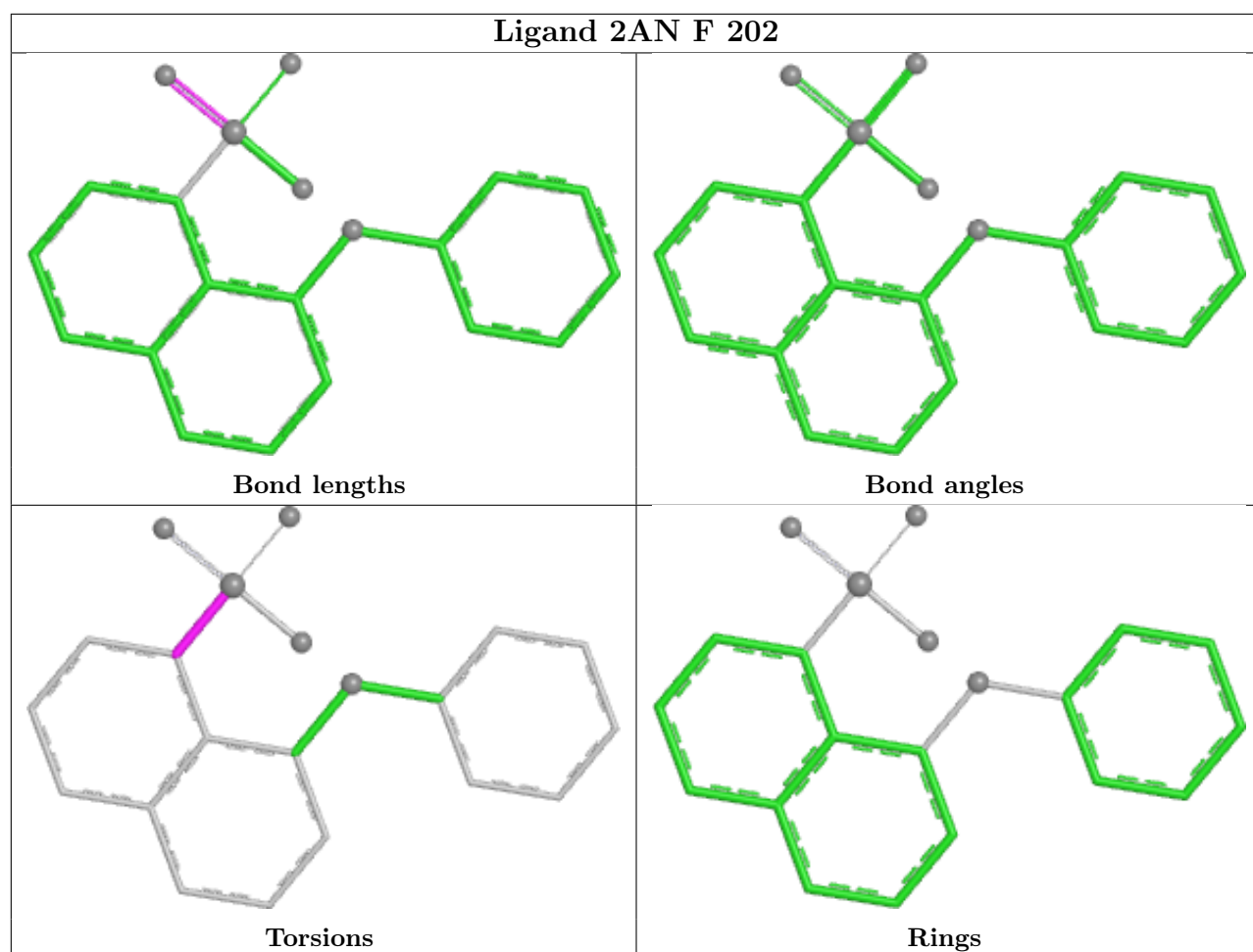
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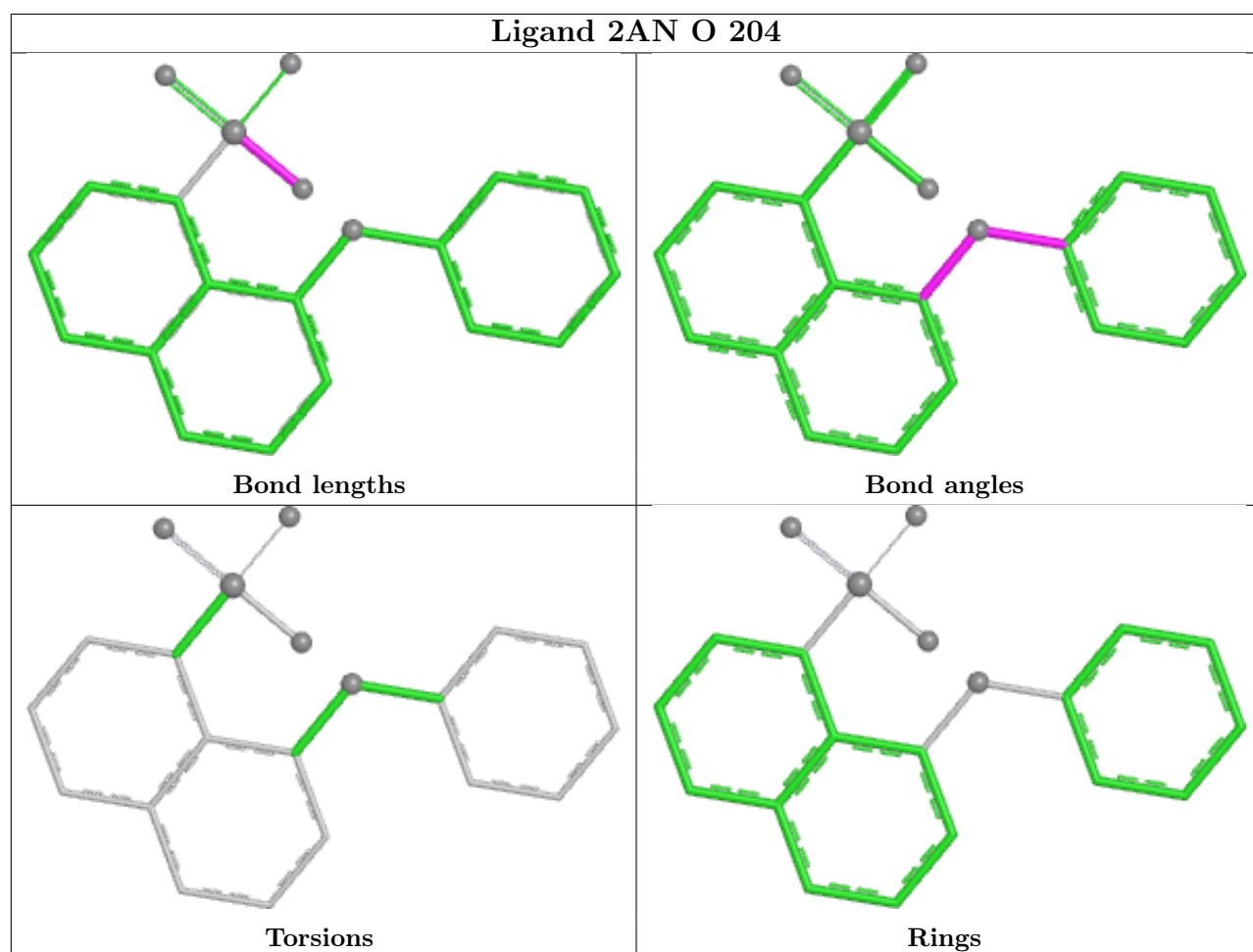




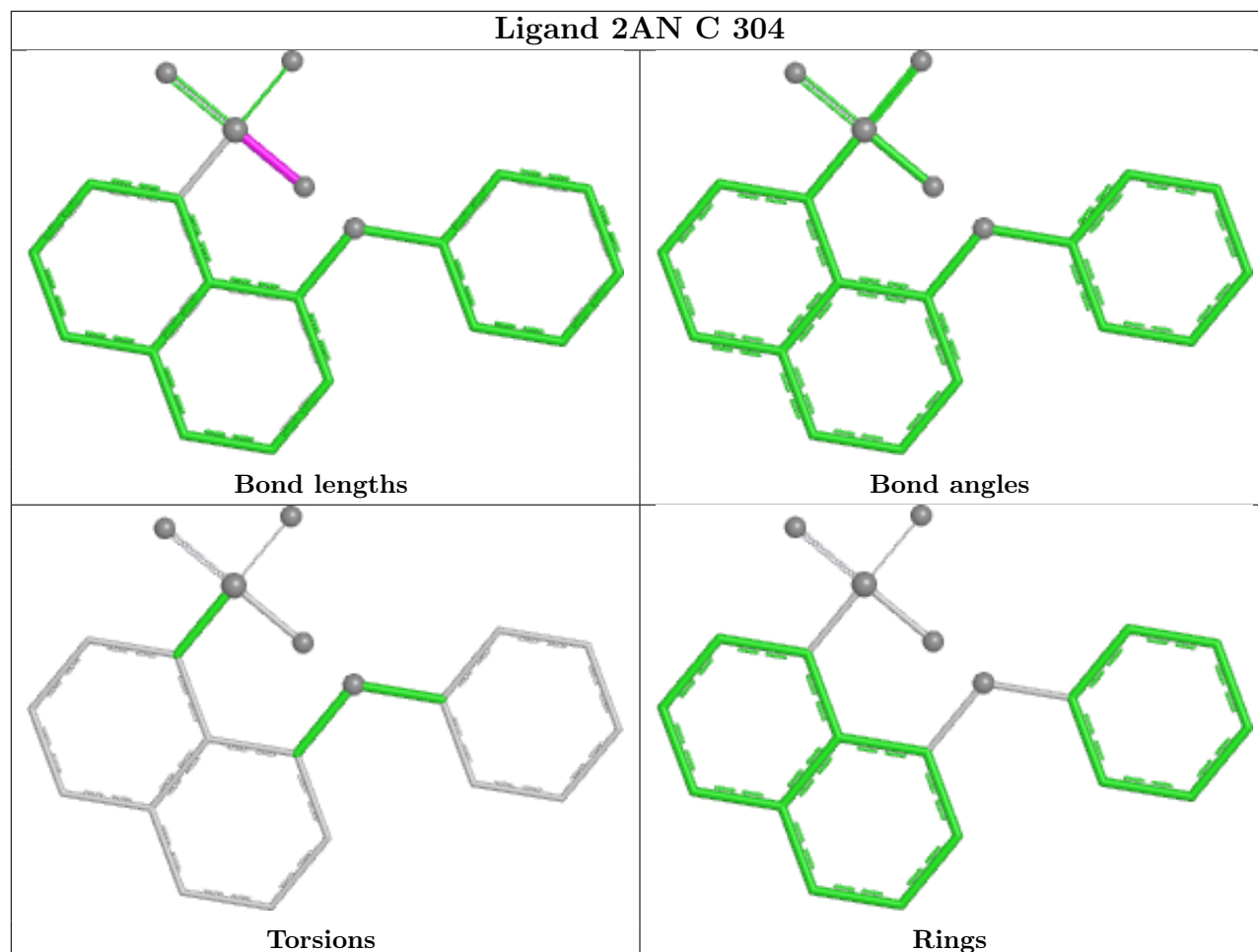
Ligand 2AN P 506

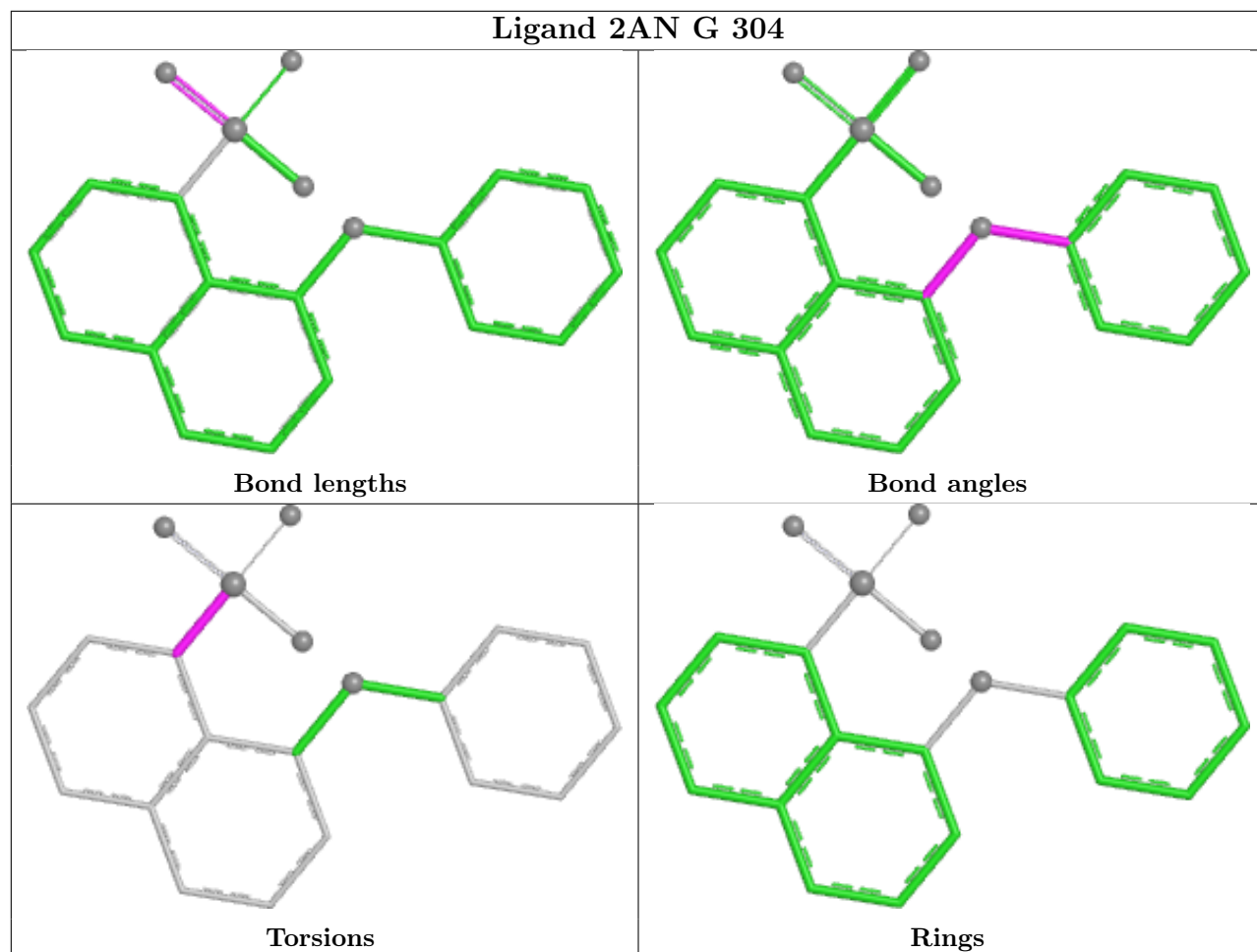




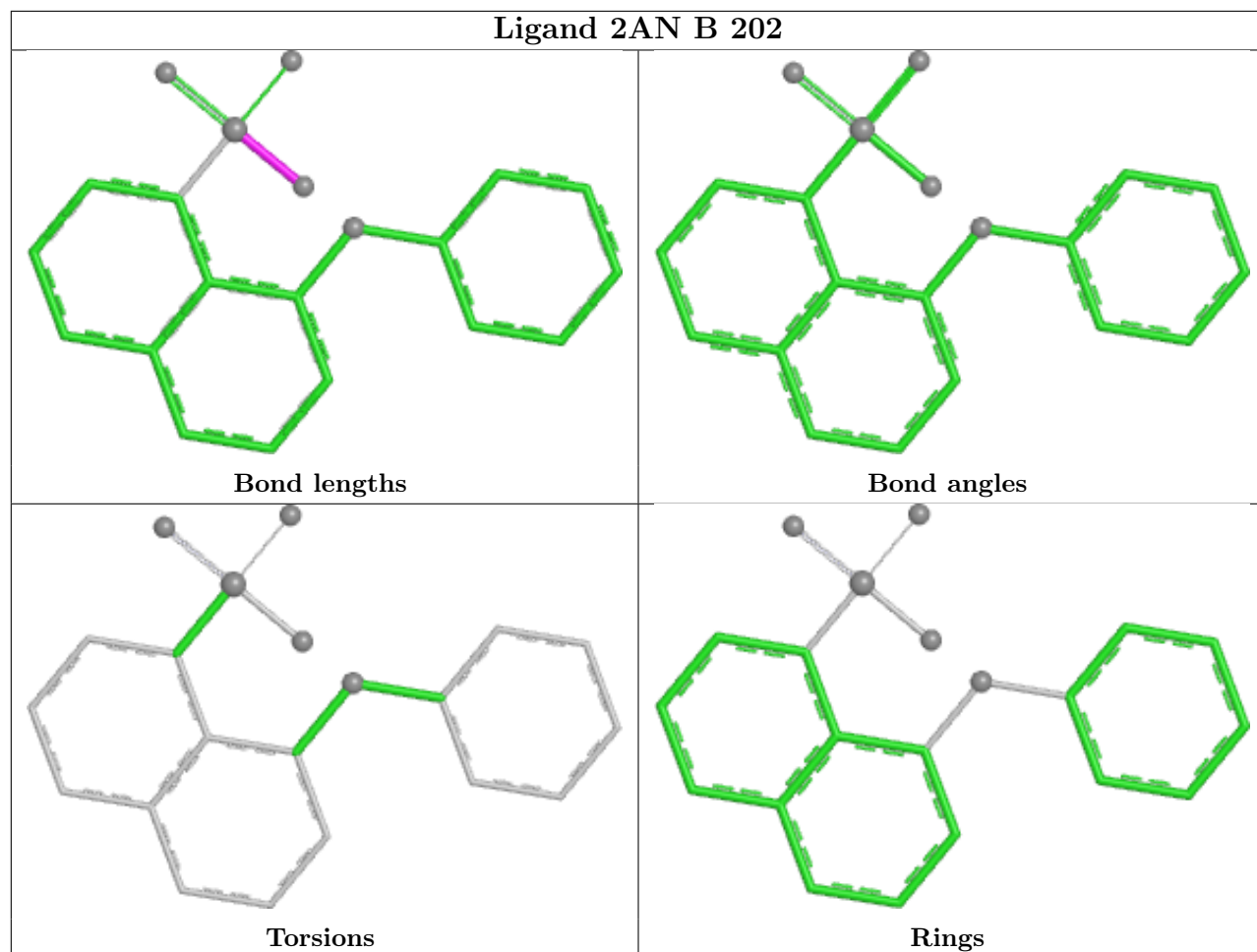


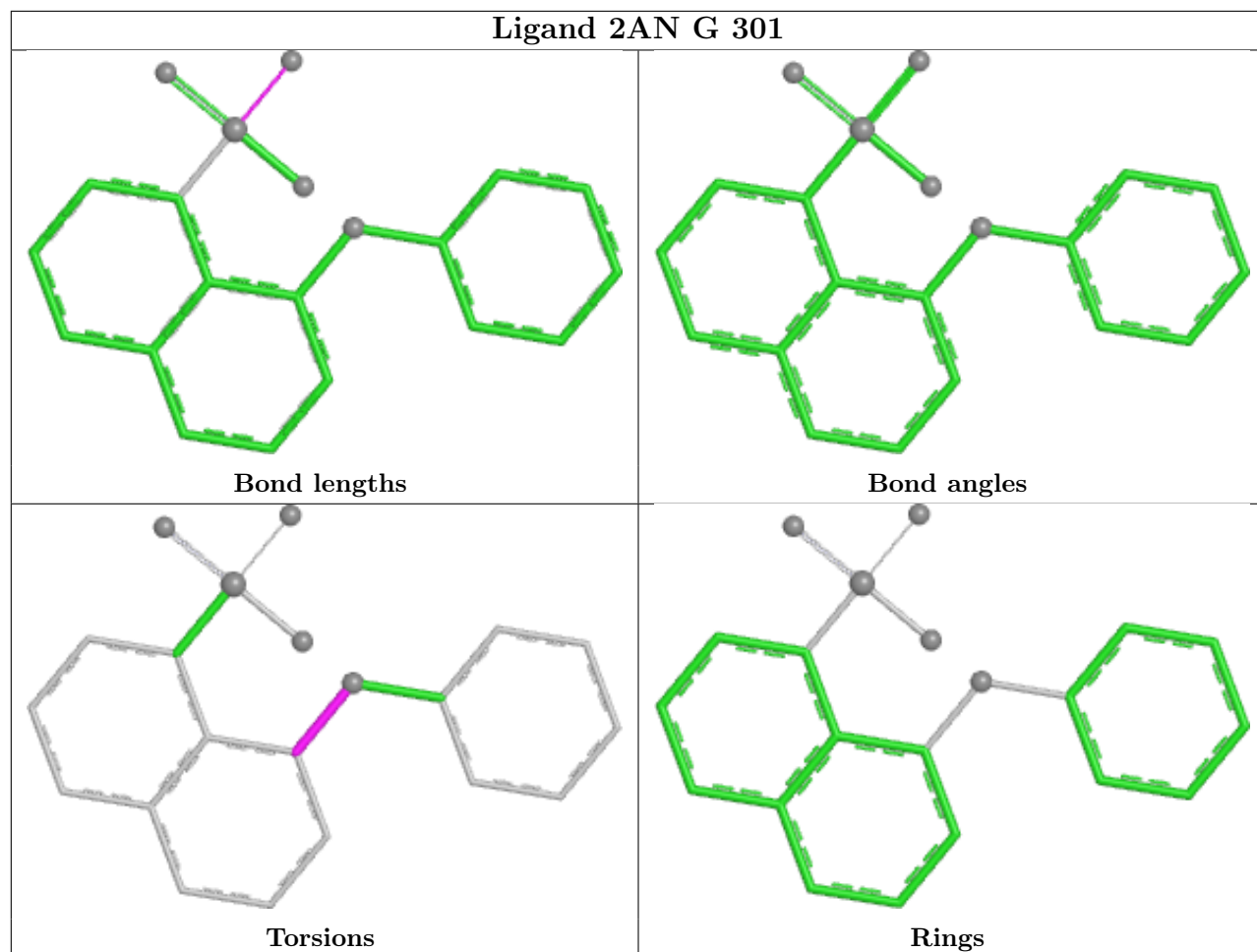
Ligand 2AN C 304

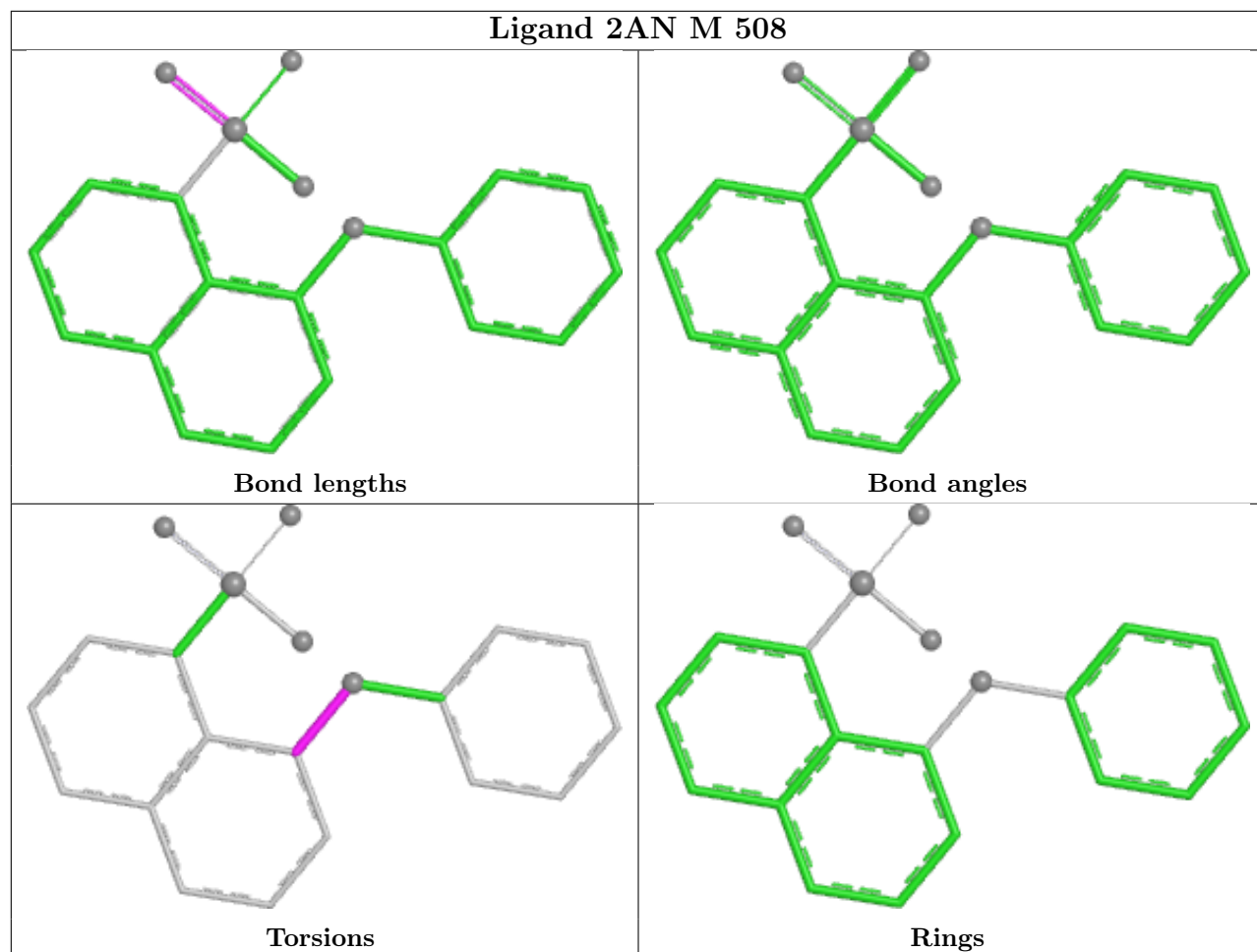


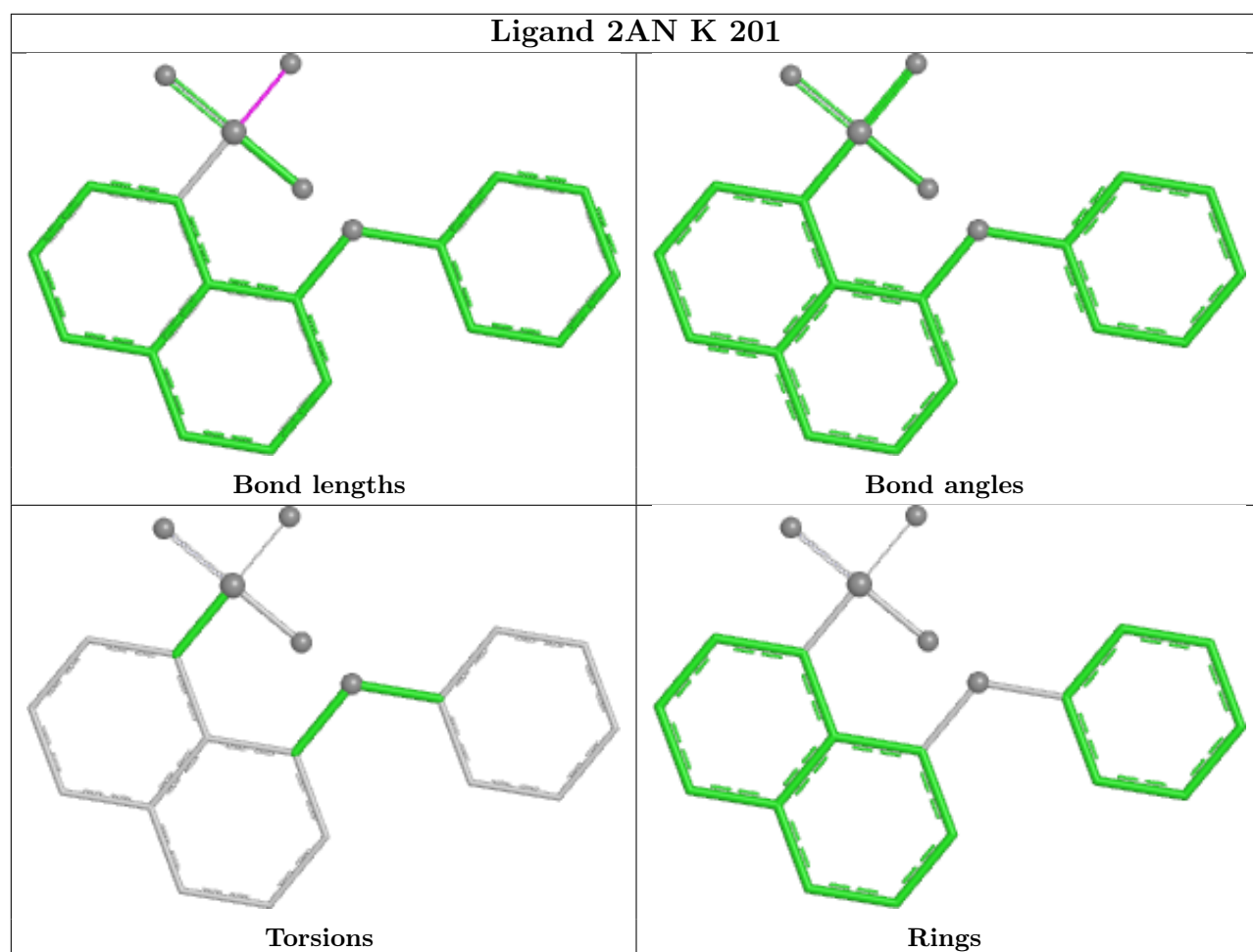


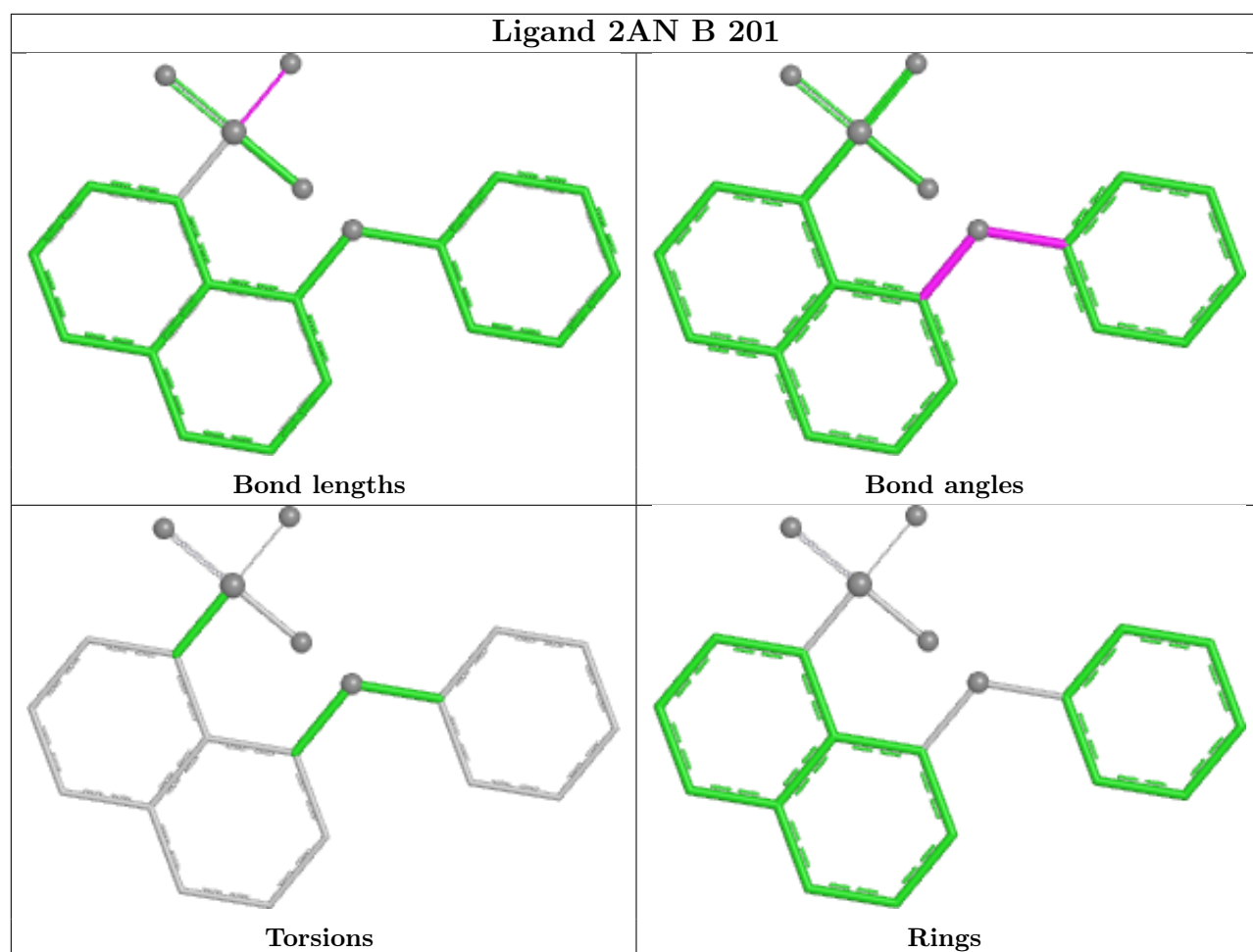
Ligand 2AN B 202

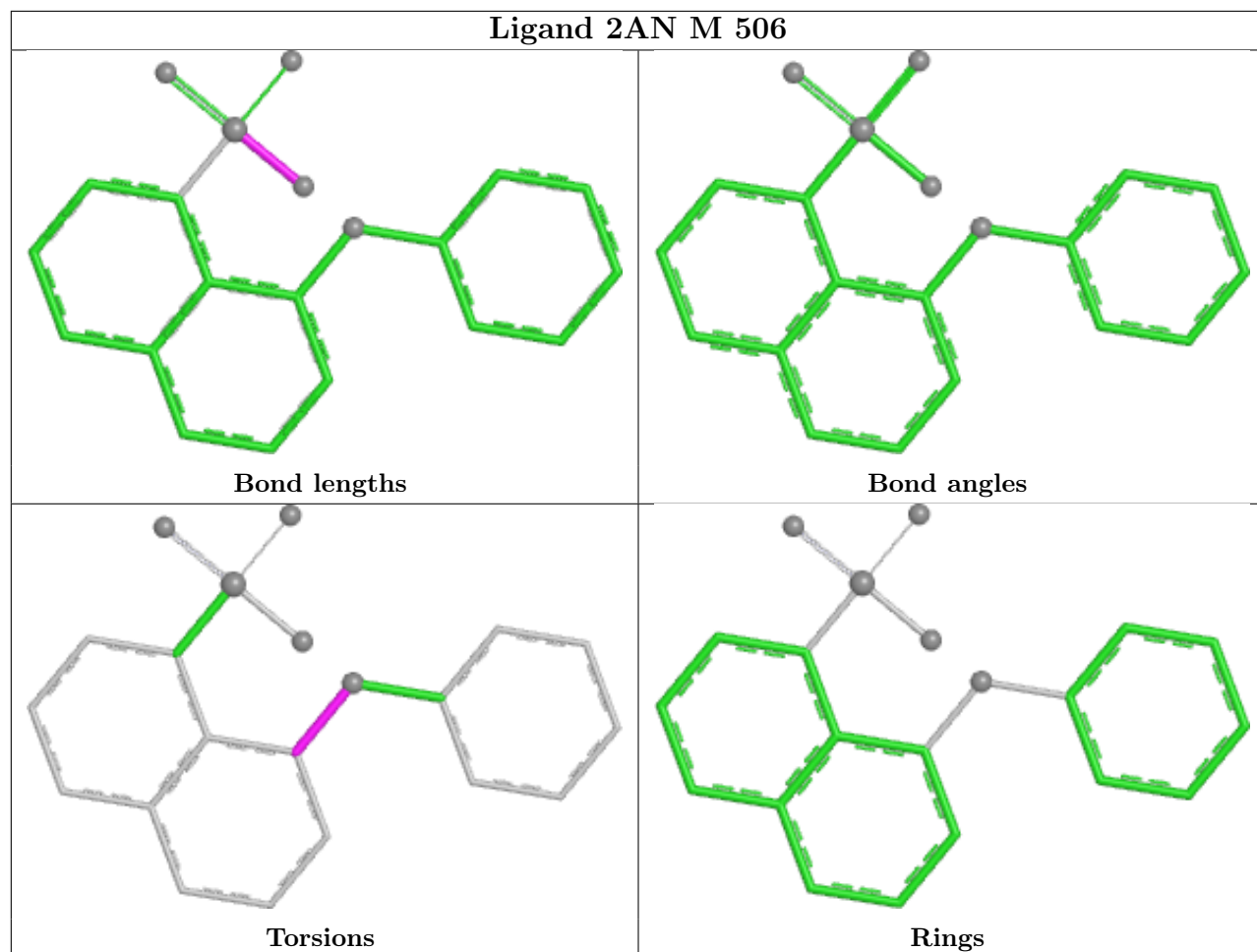




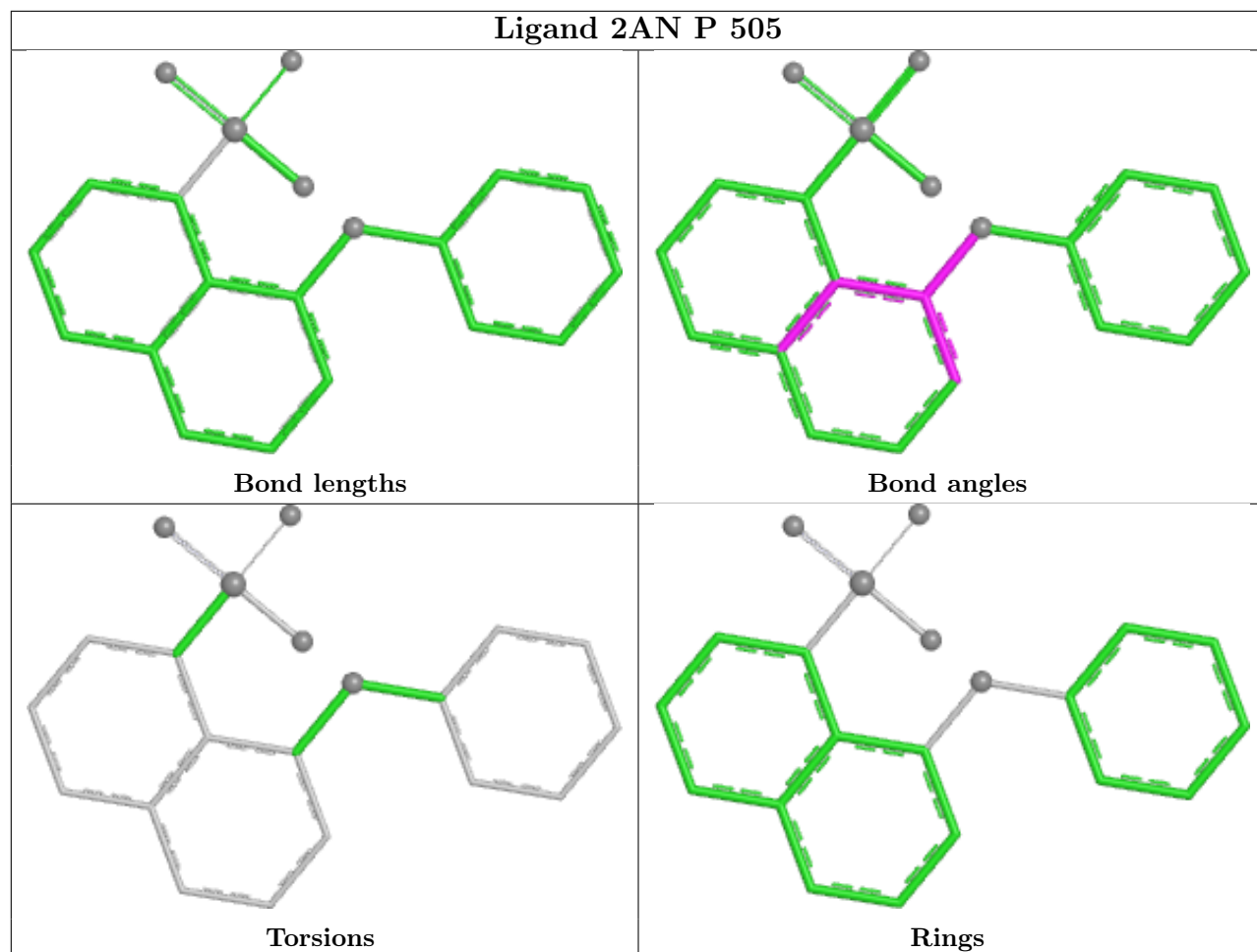


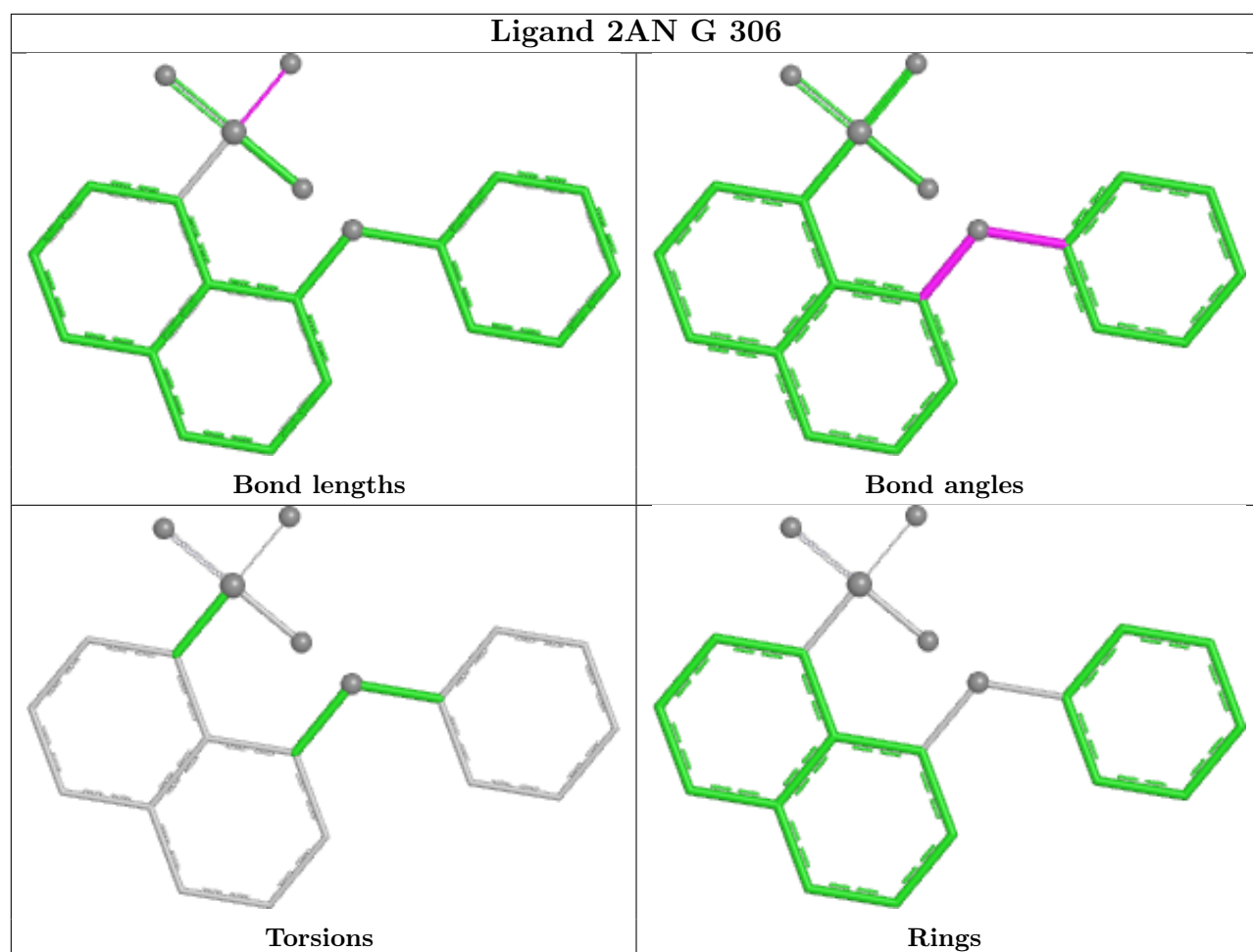


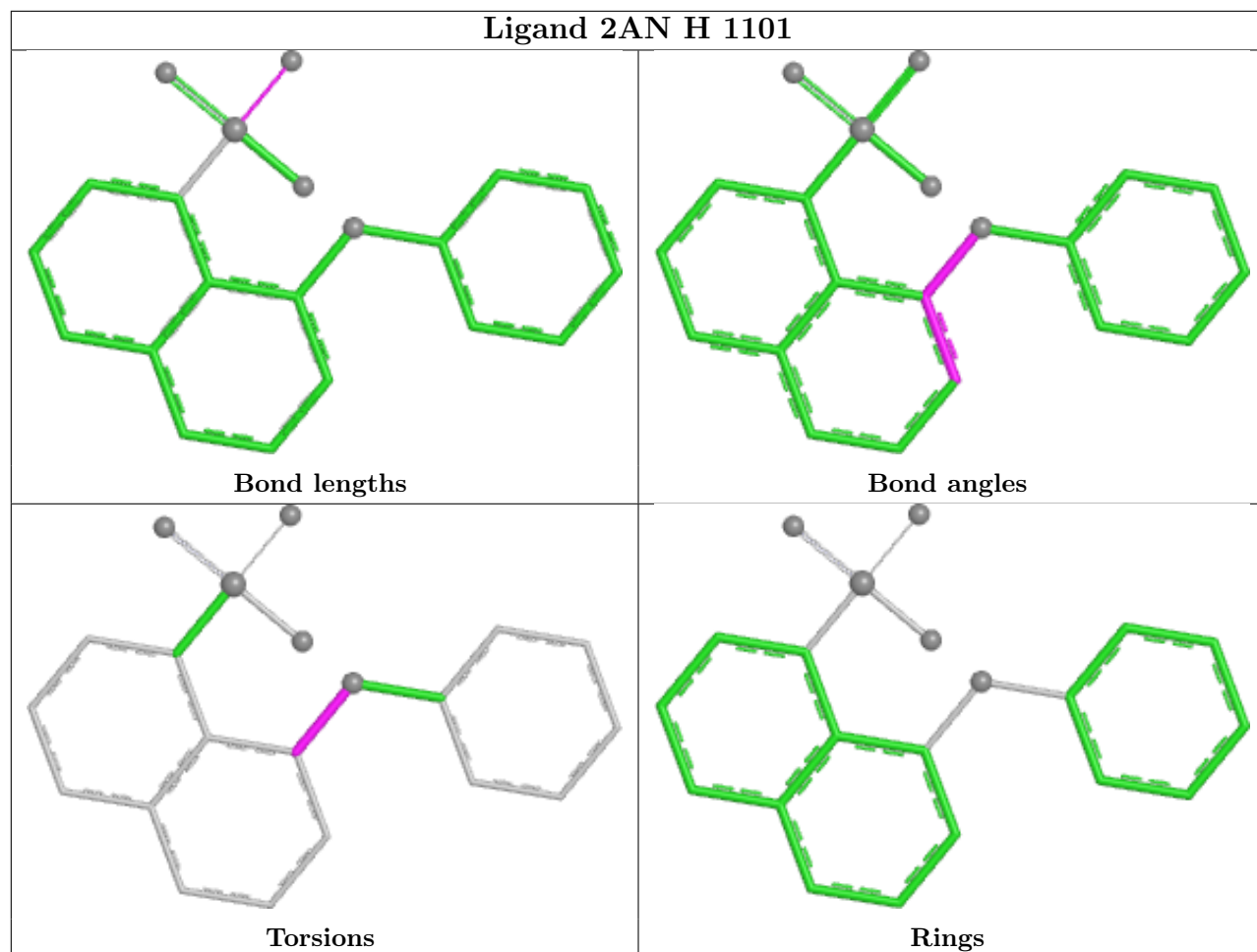


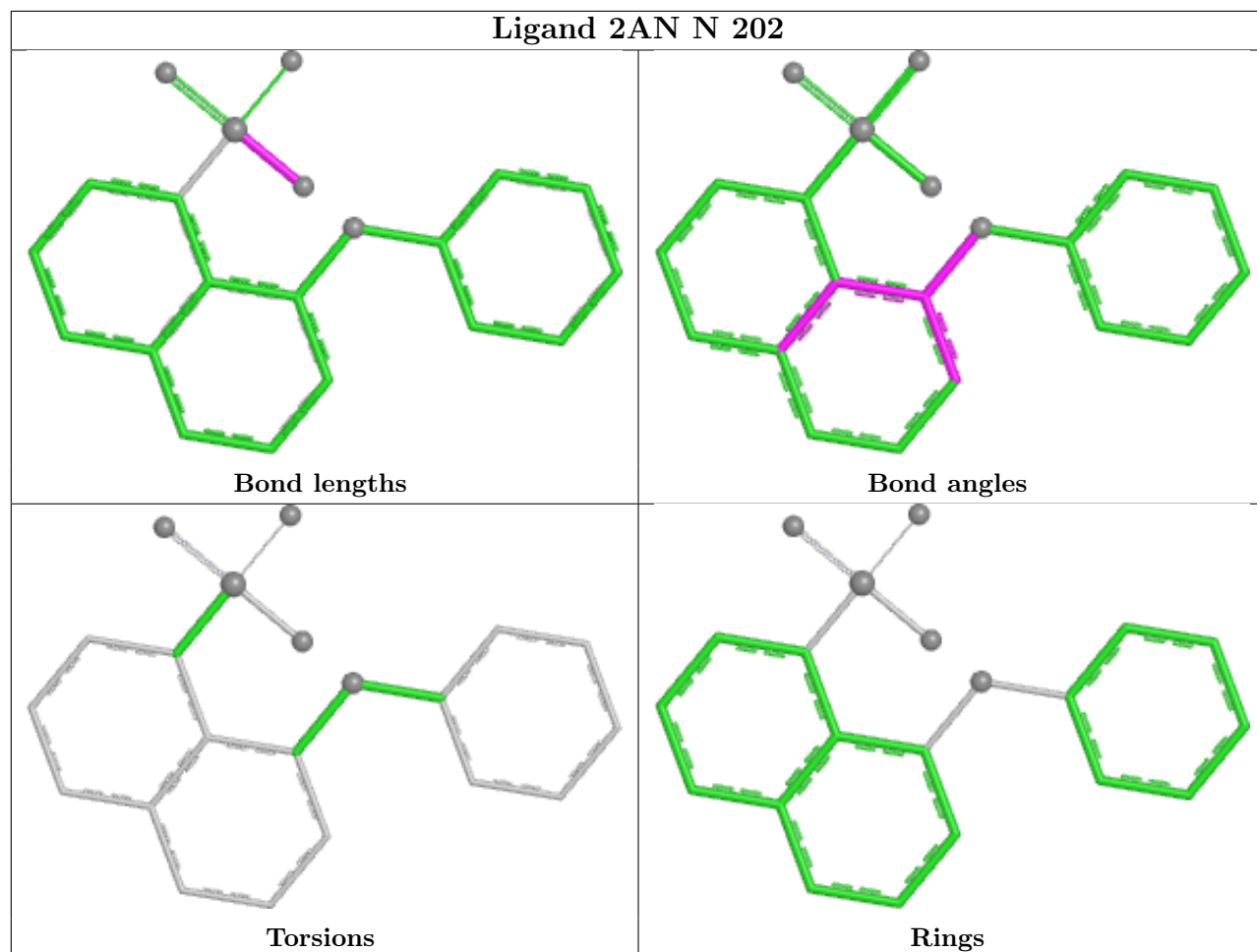


Ligand 2AN P 505

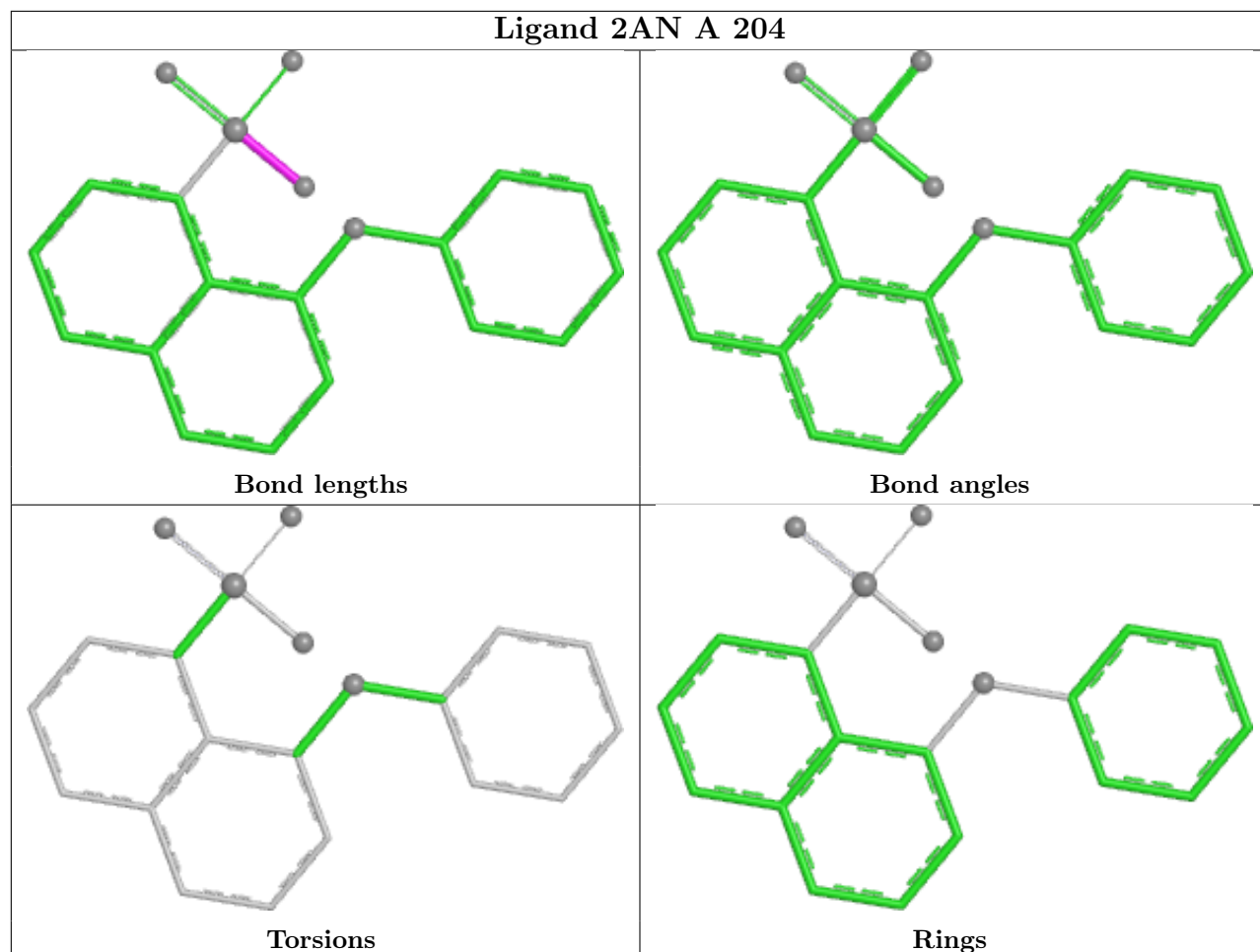




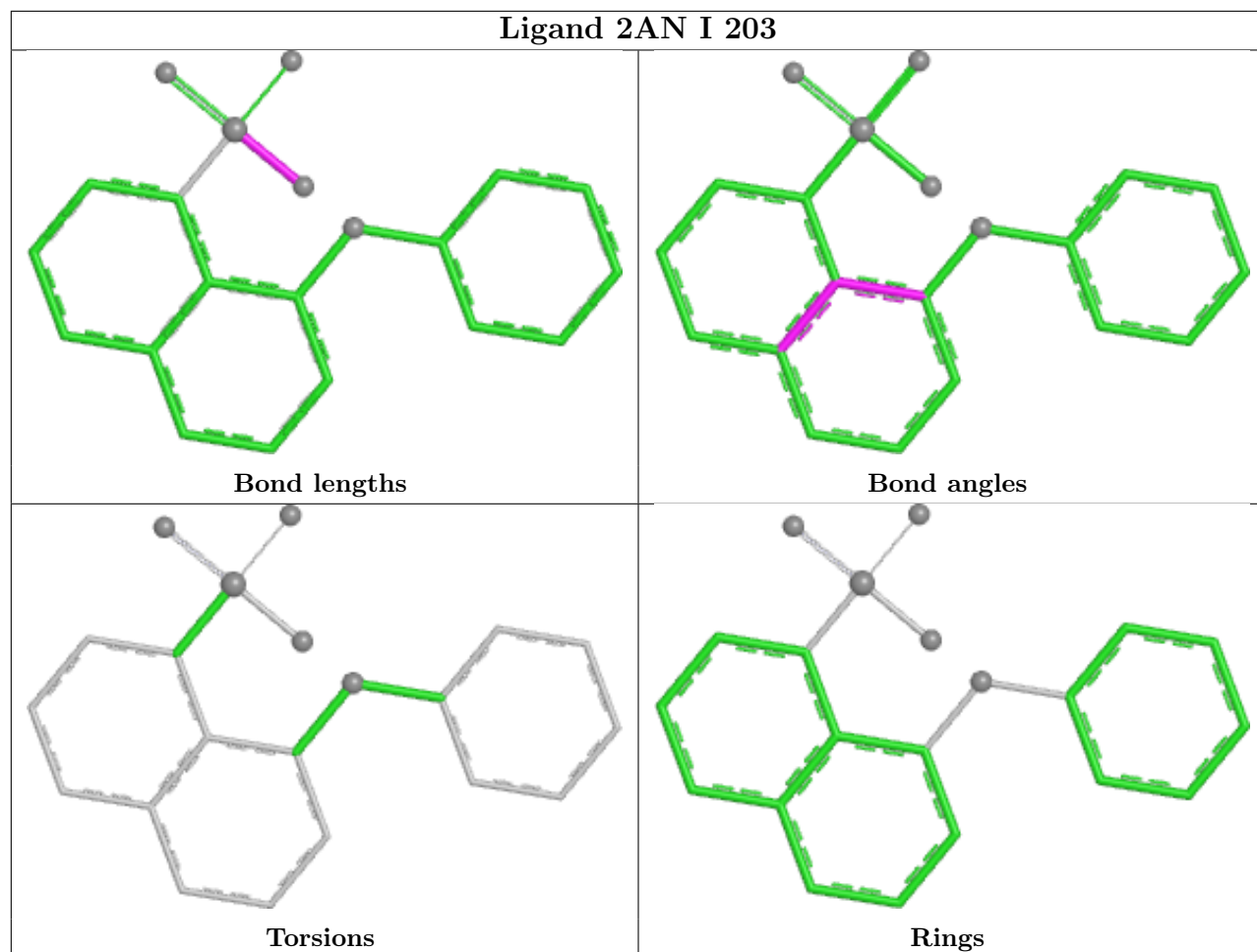




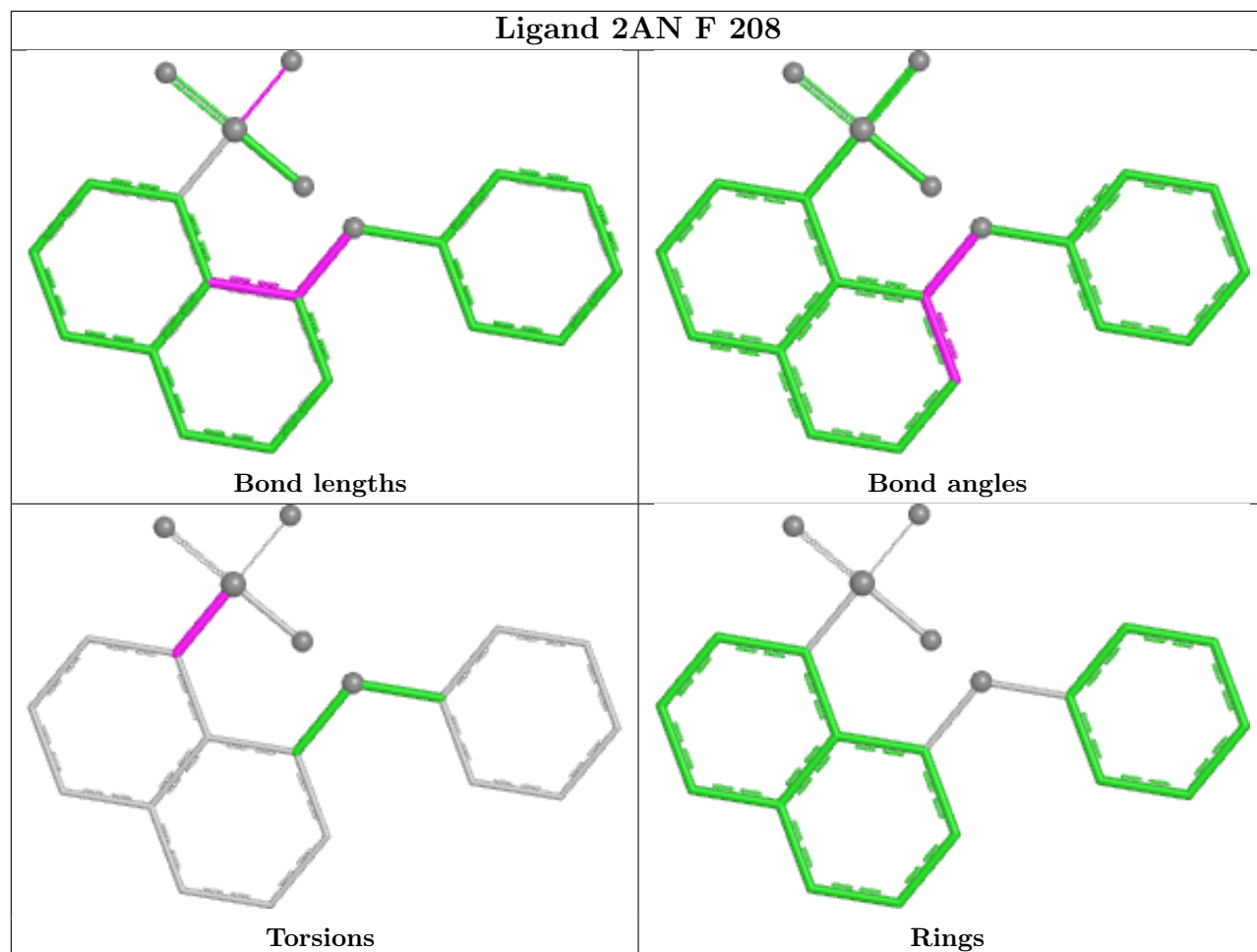
Ligand 2AN A 204

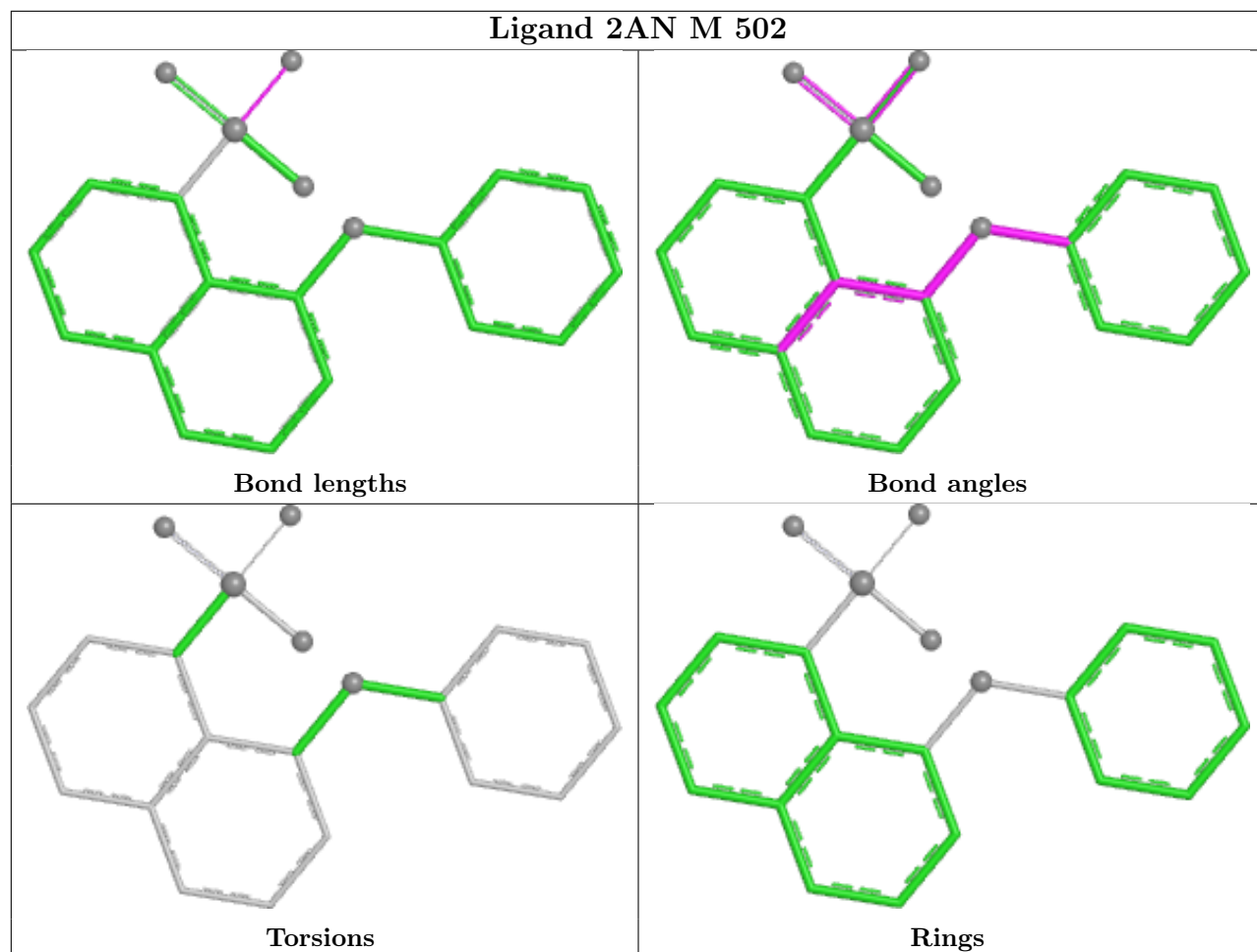


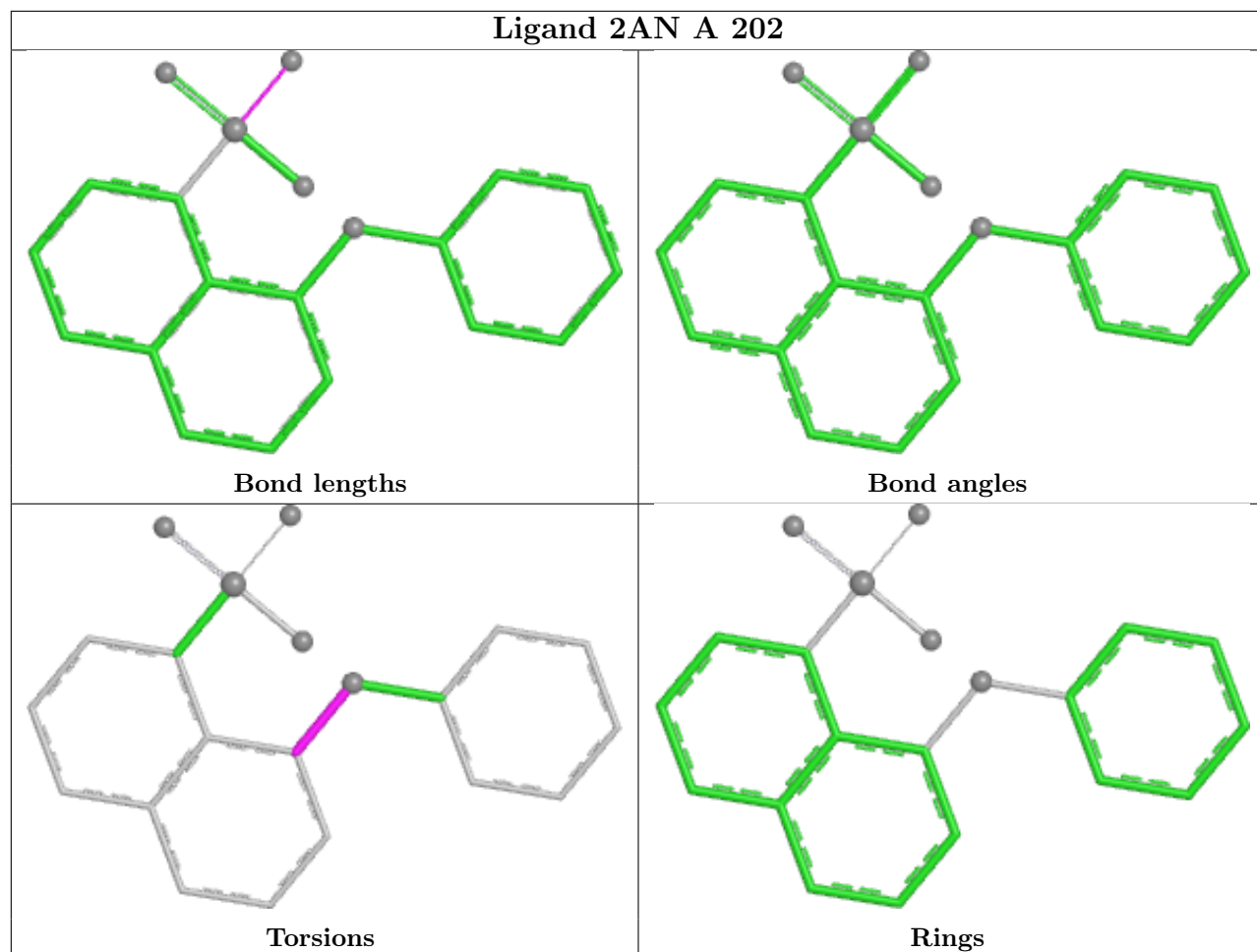
Ligand 2AN I 203

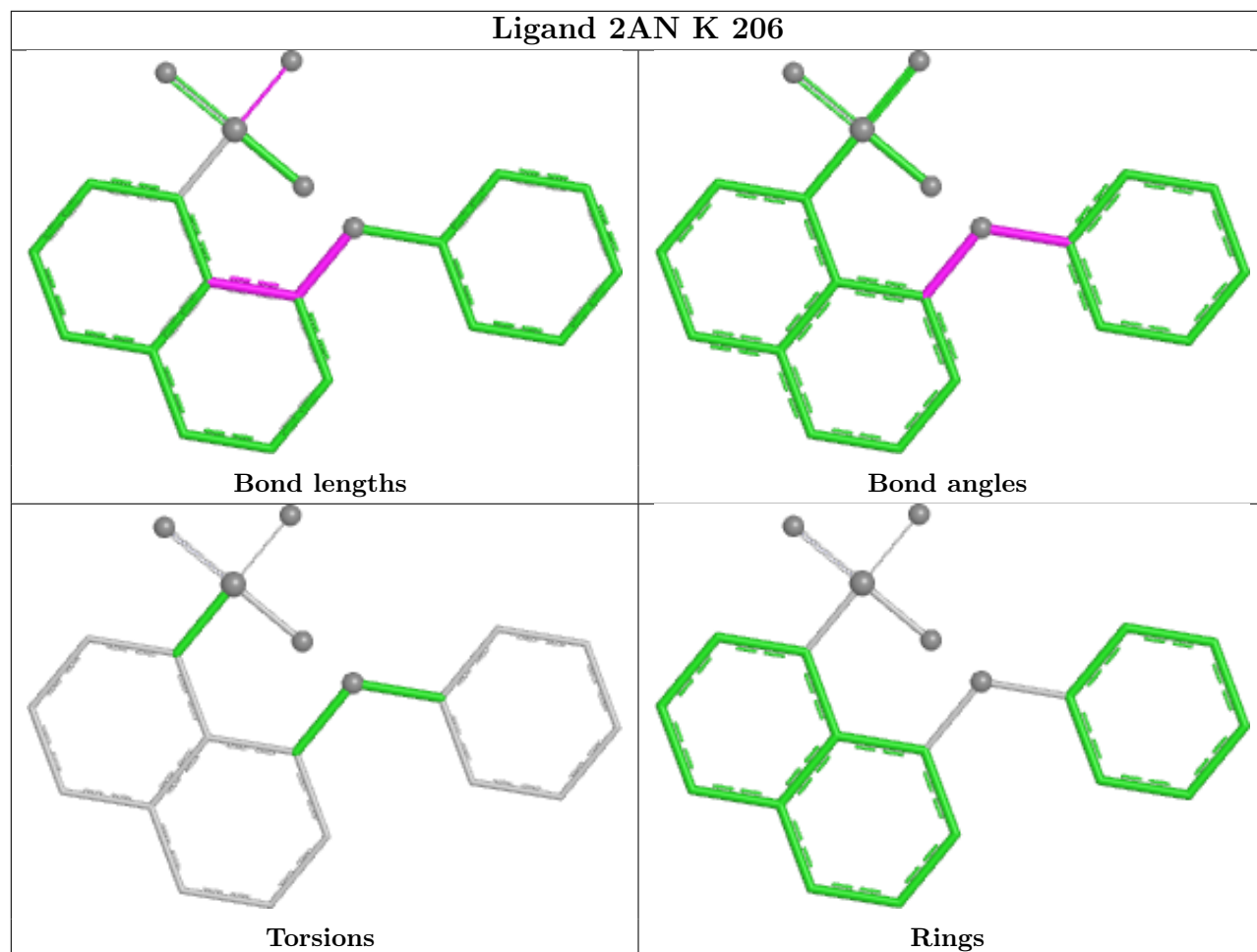


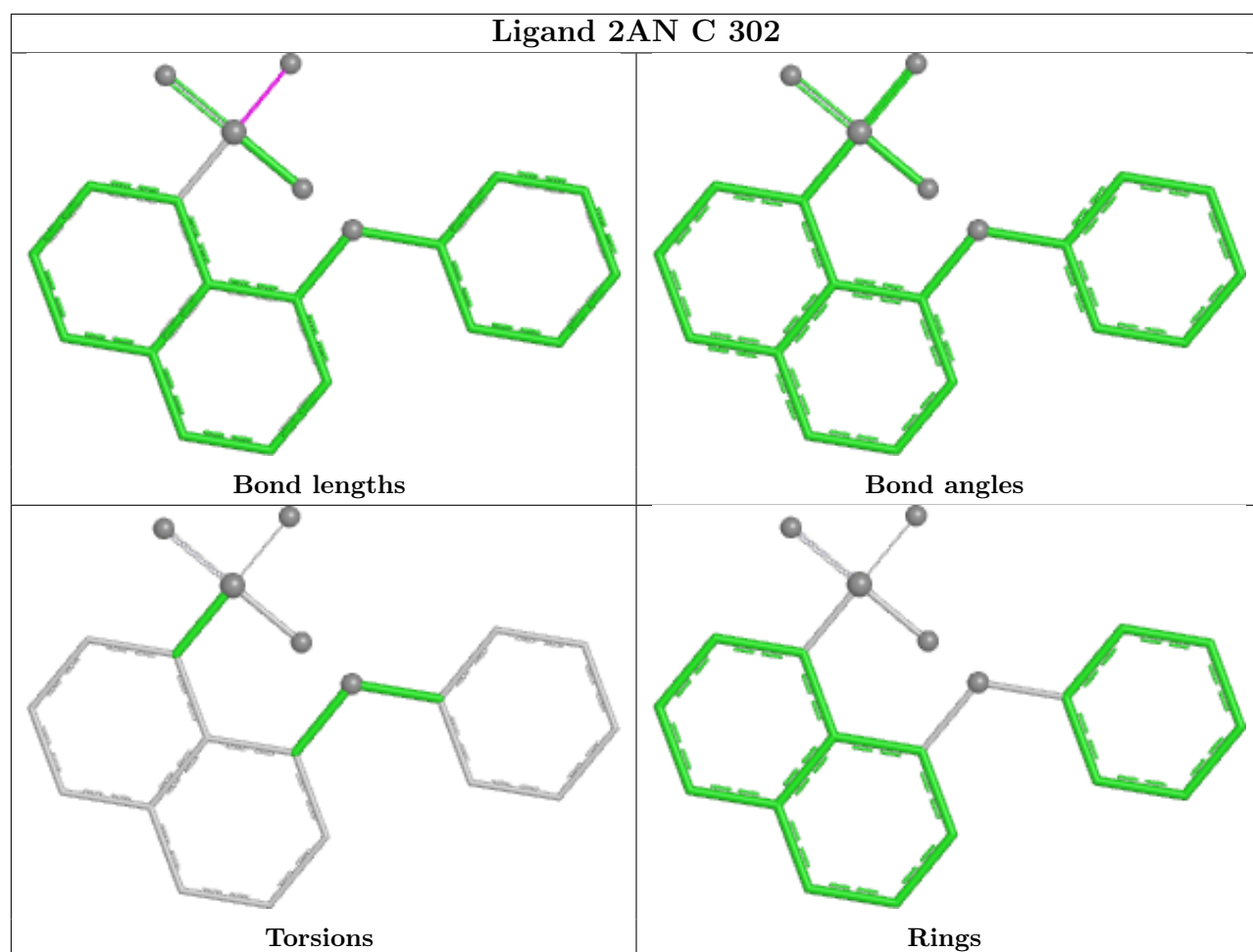
Ligand 2AN F 208



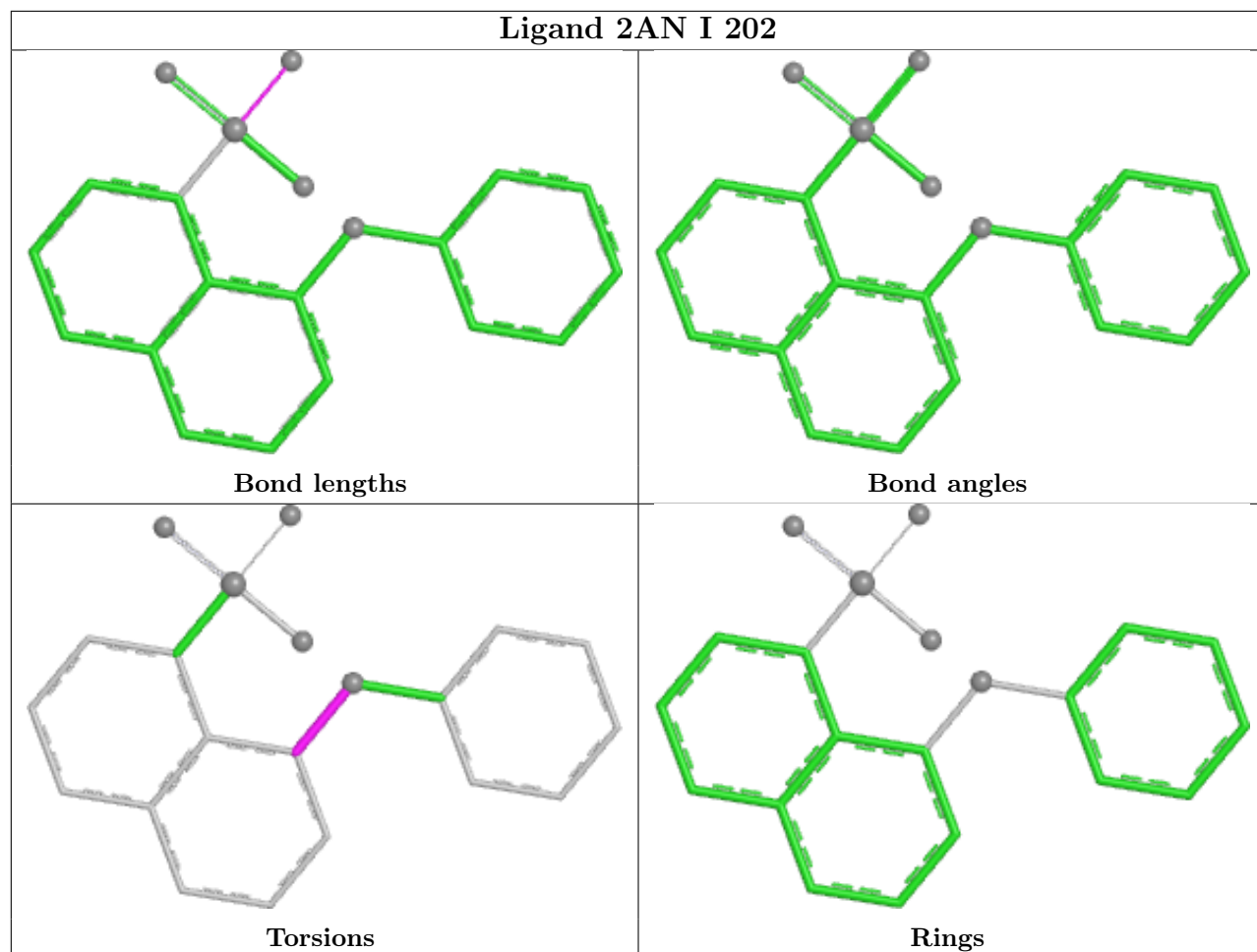




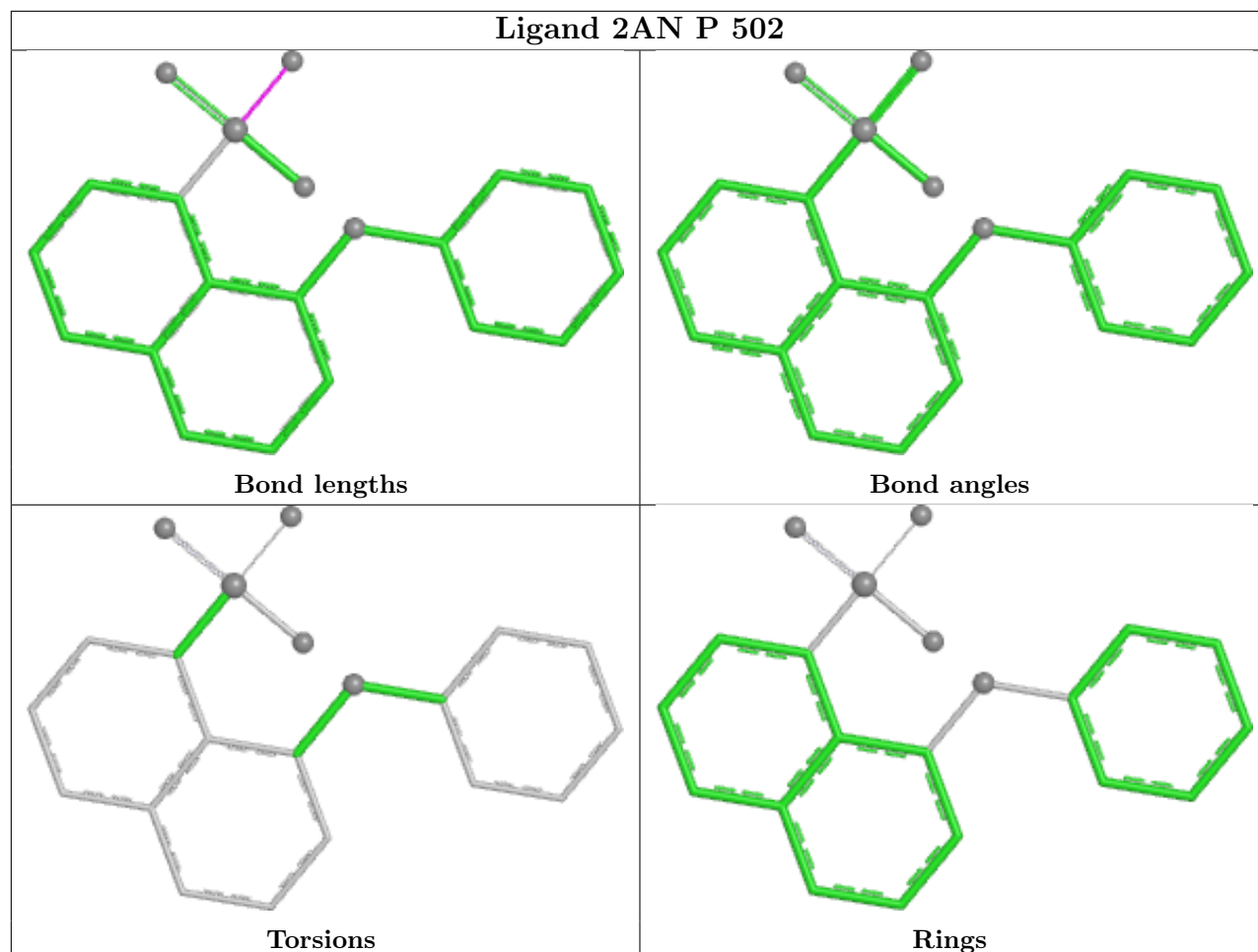




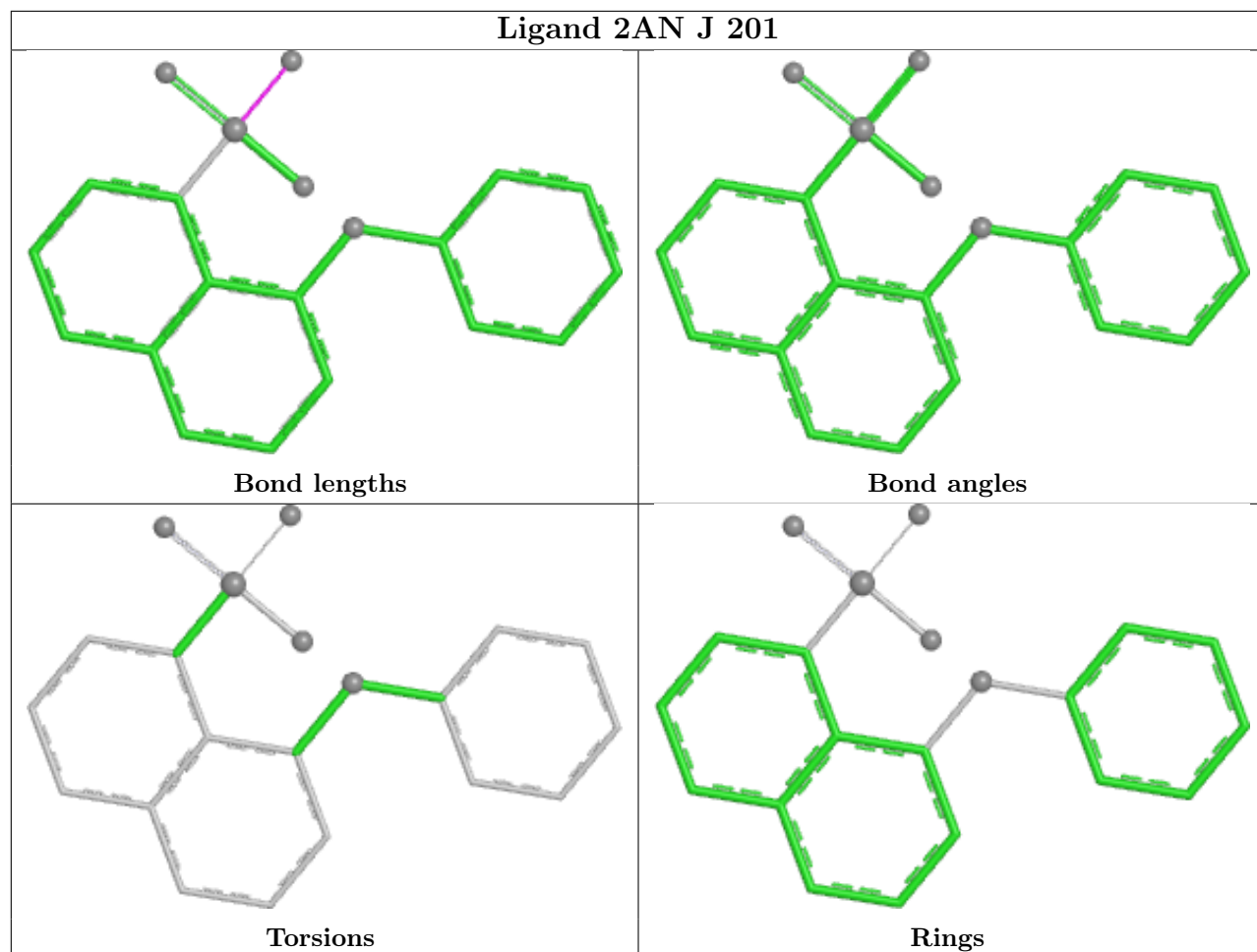
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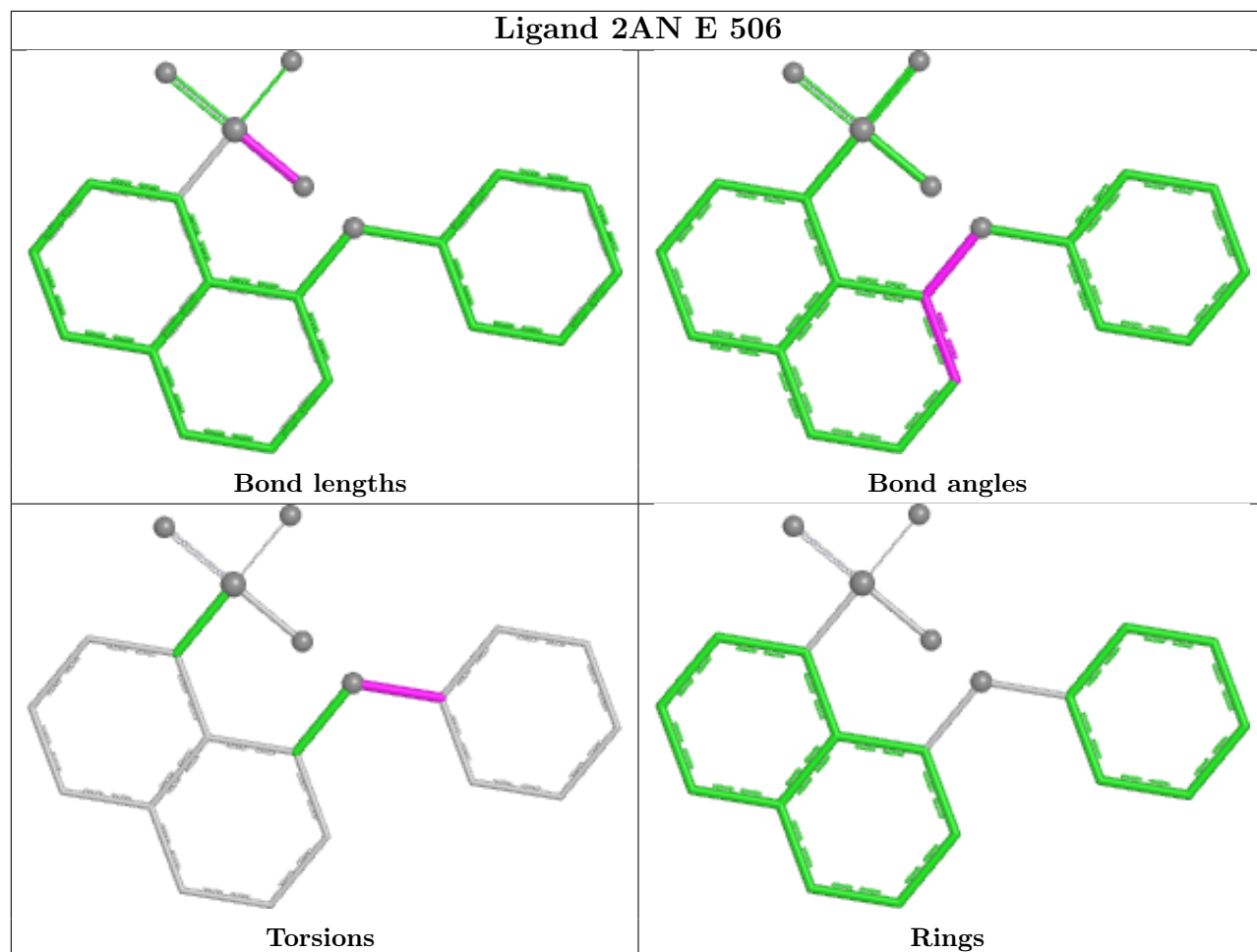
Ligand 2AN P 502



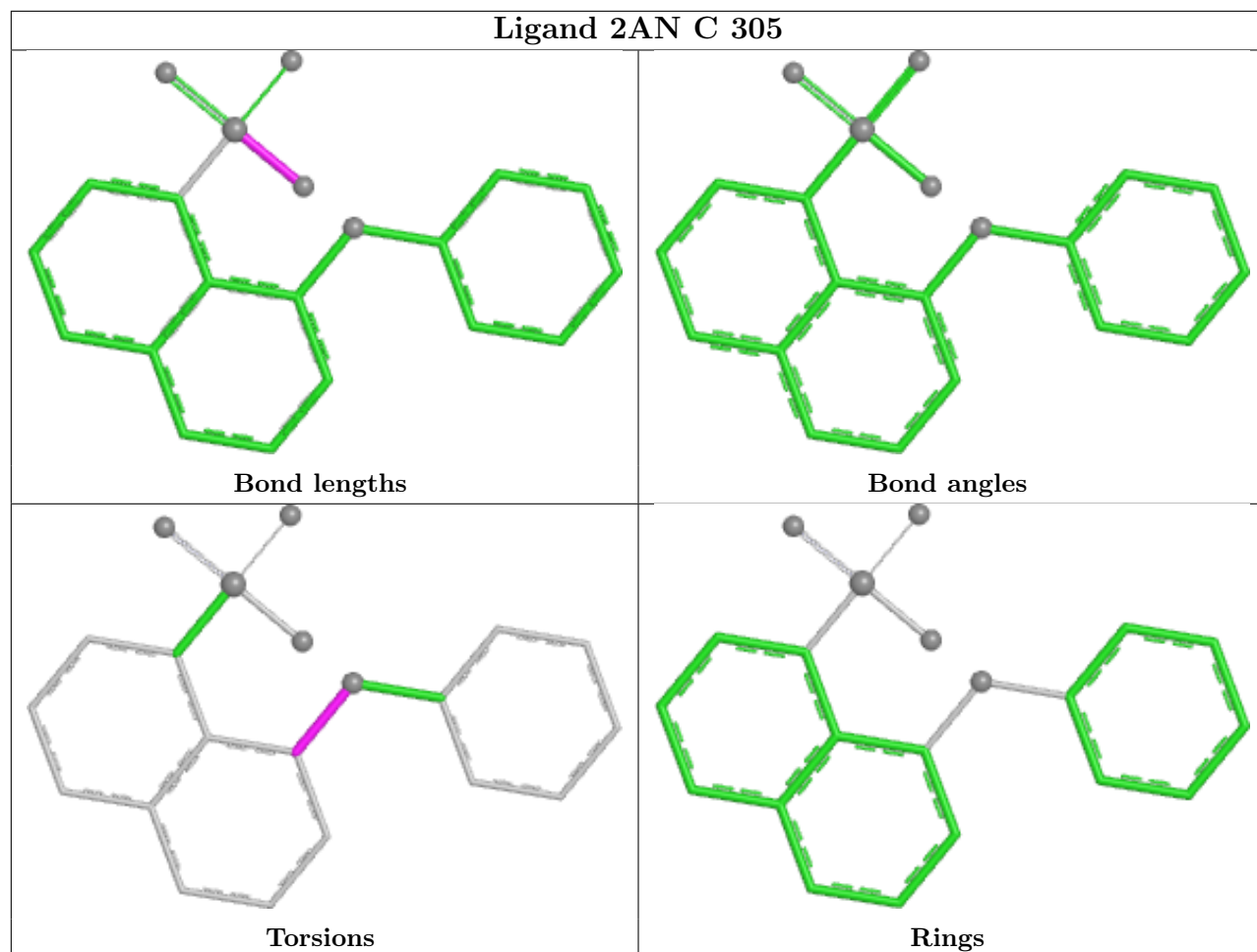
Ligand 2AN J 201



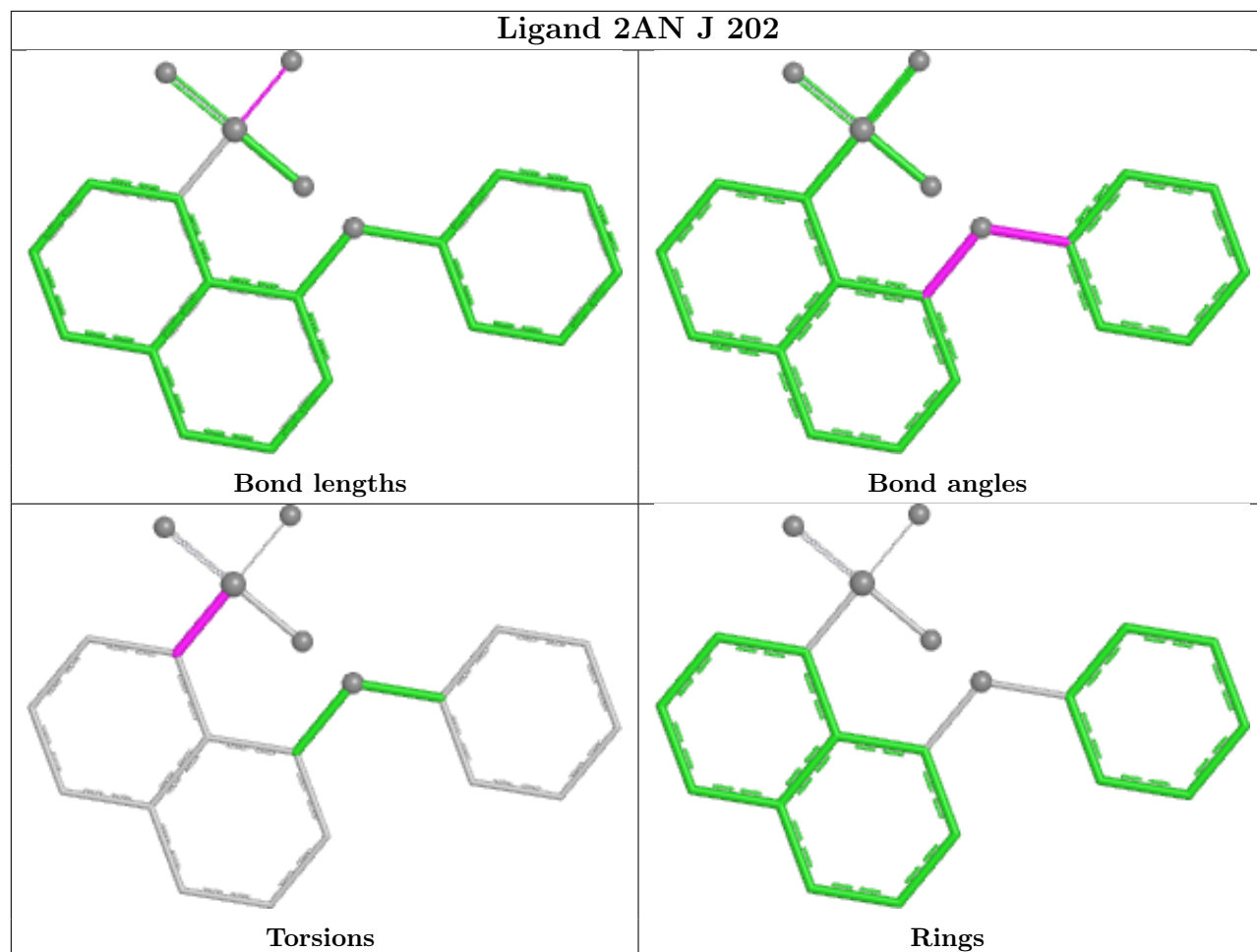
Ligand 2AN E 506

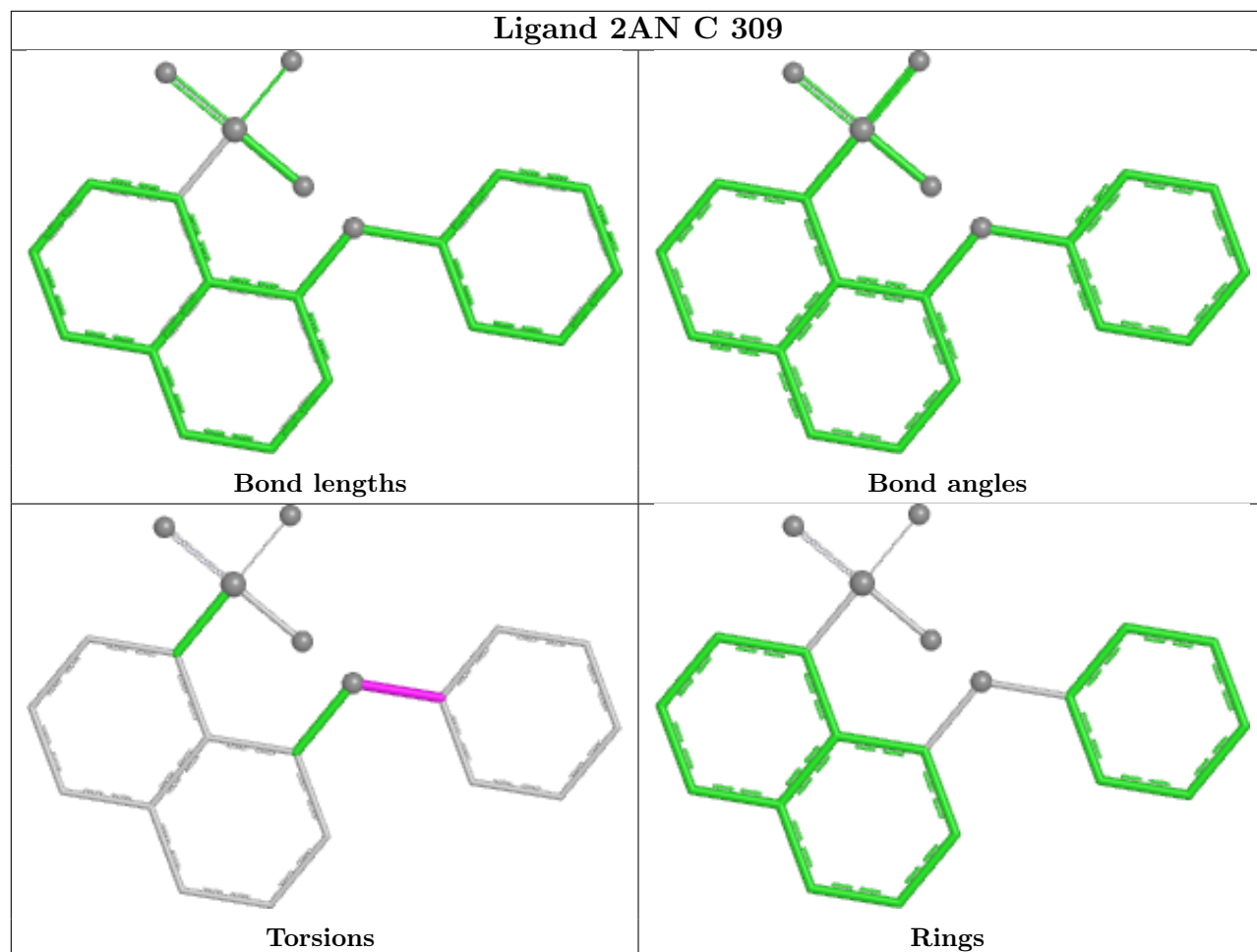


Ligand 2AN C 305

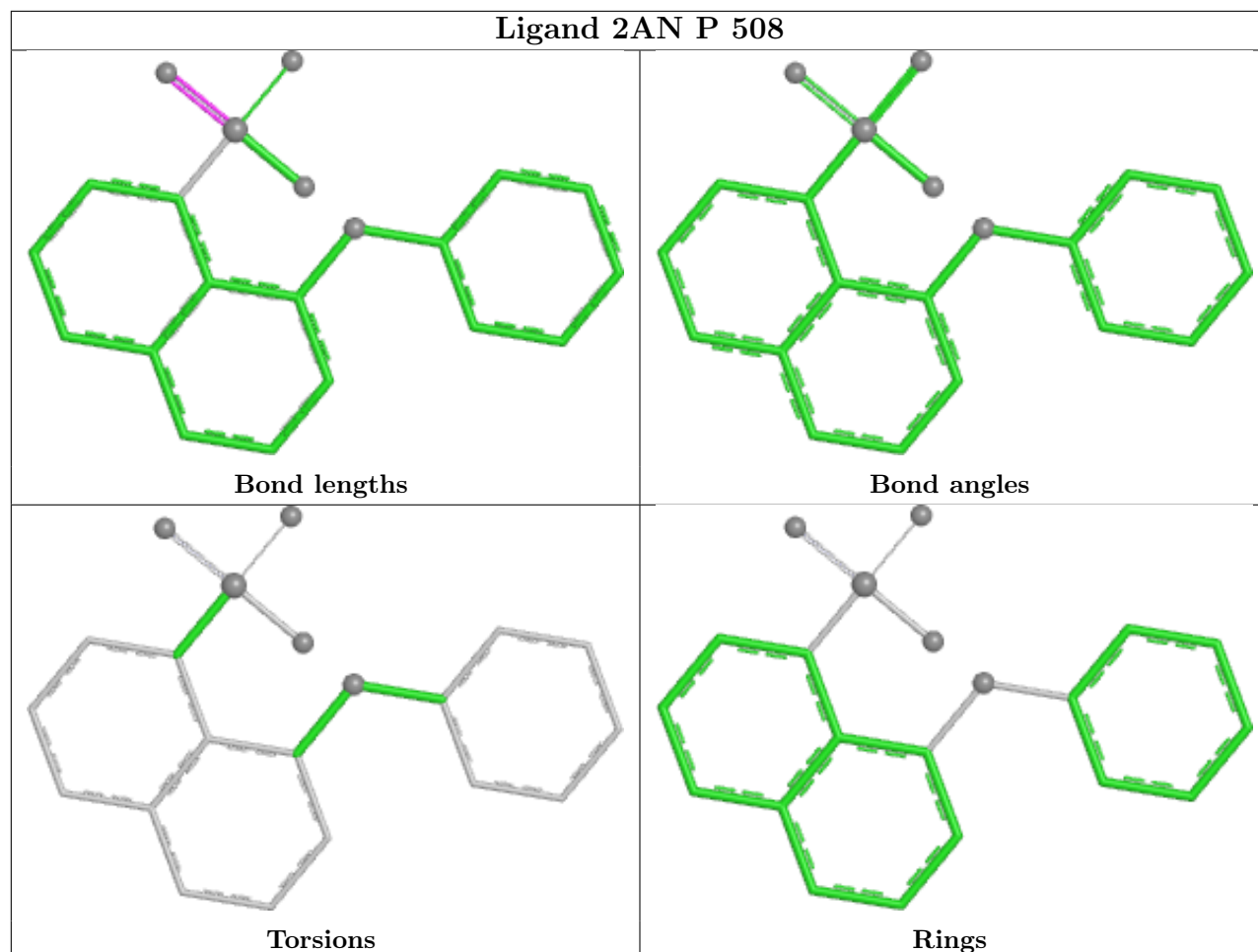


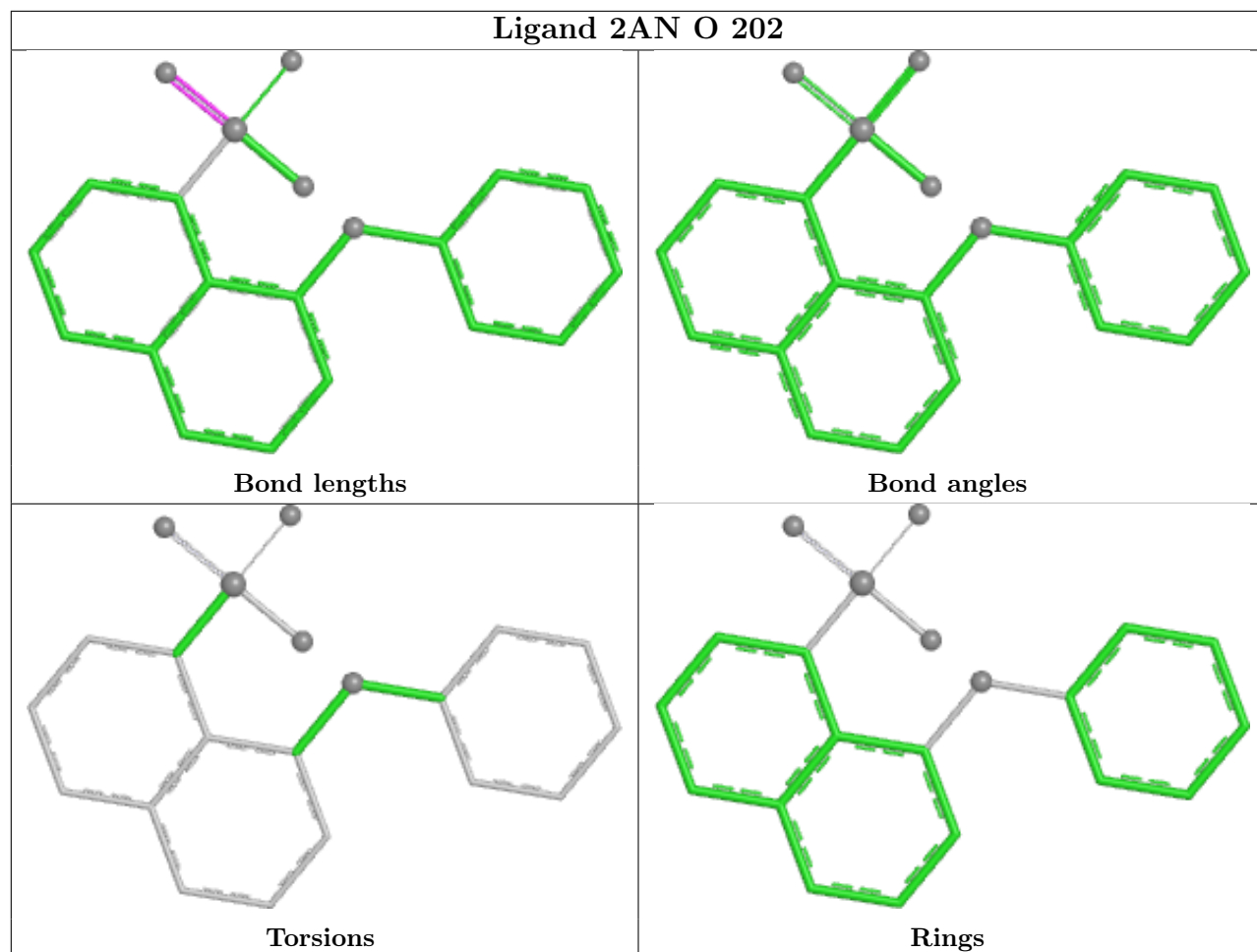
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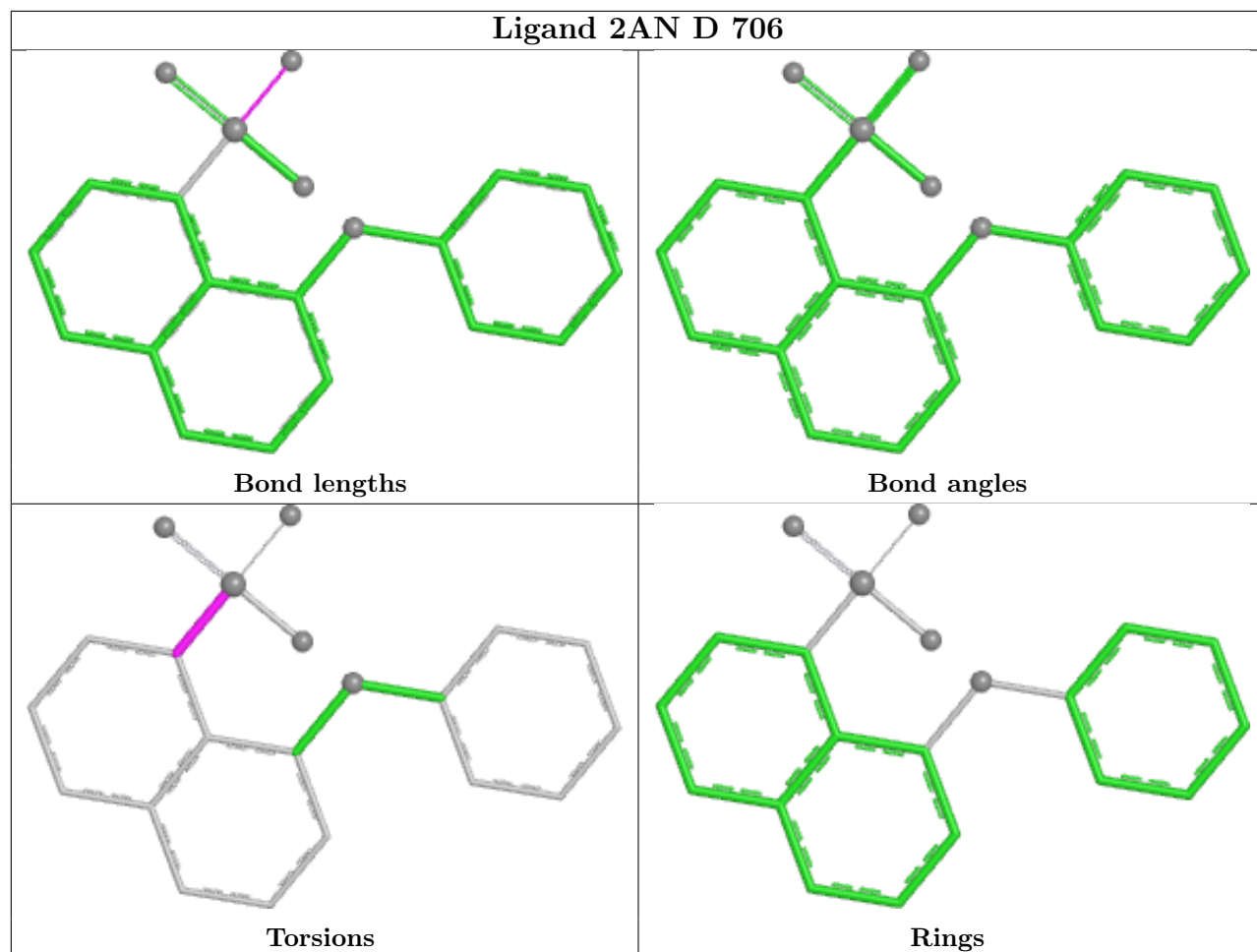


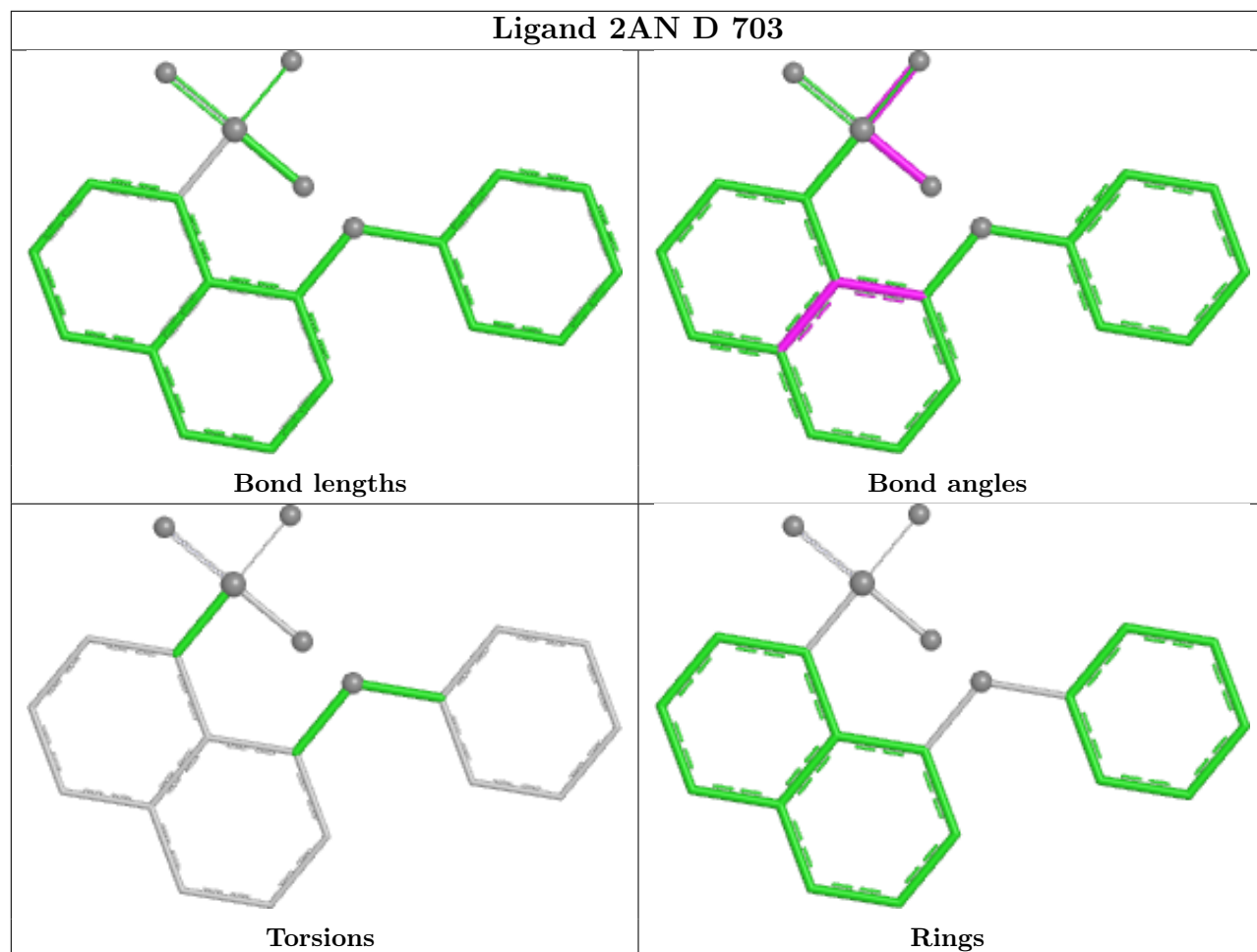


Ligand 2AN P 508

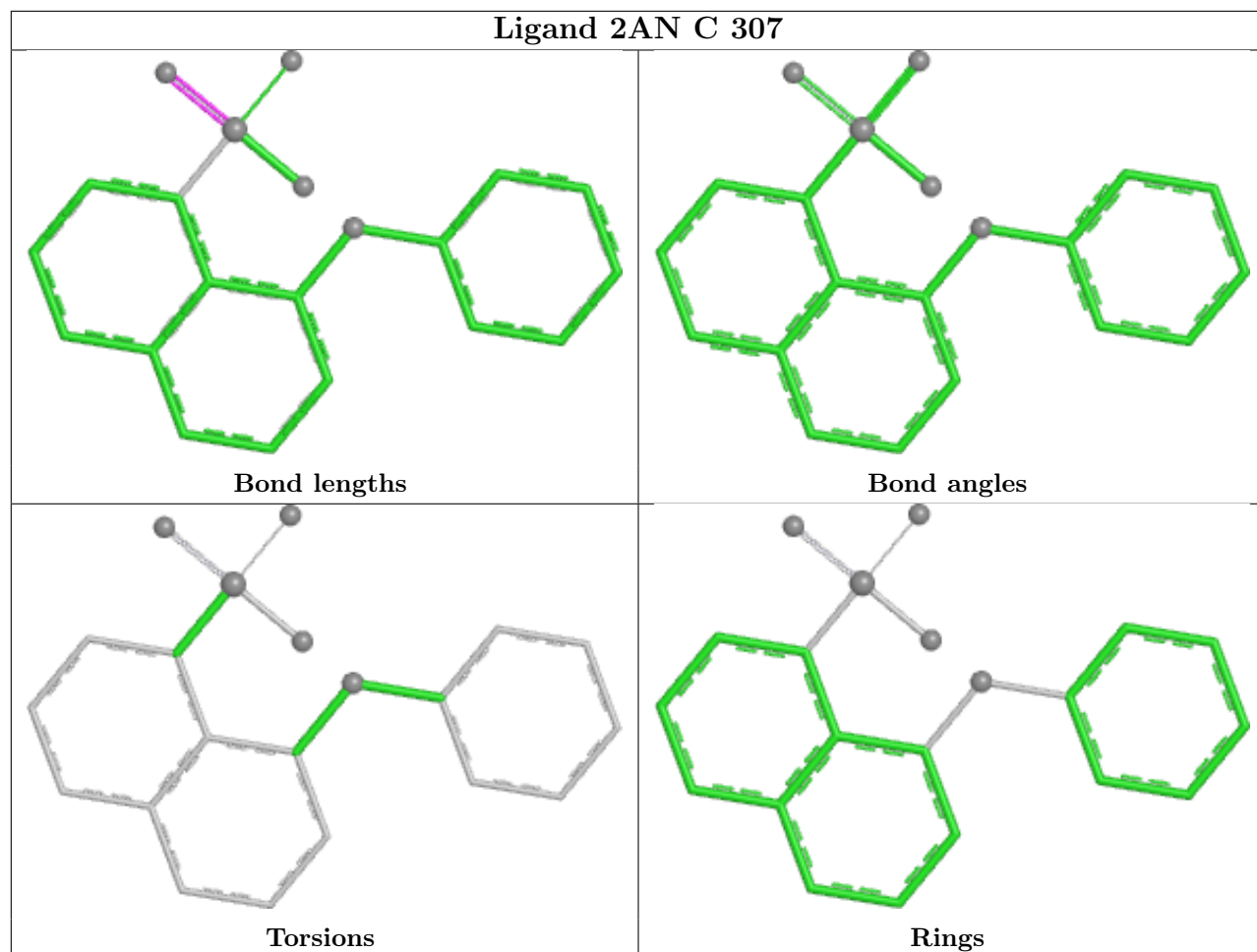


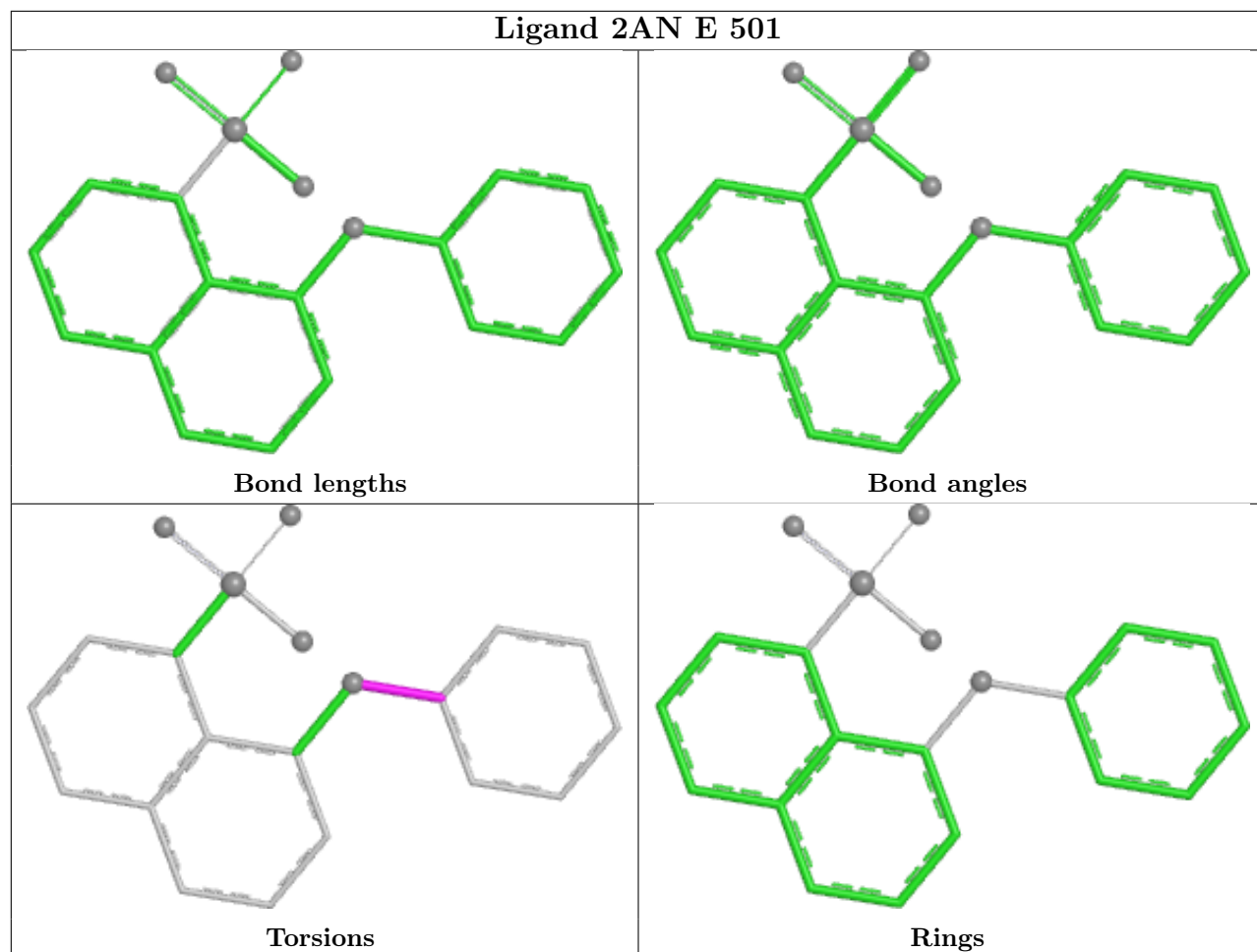


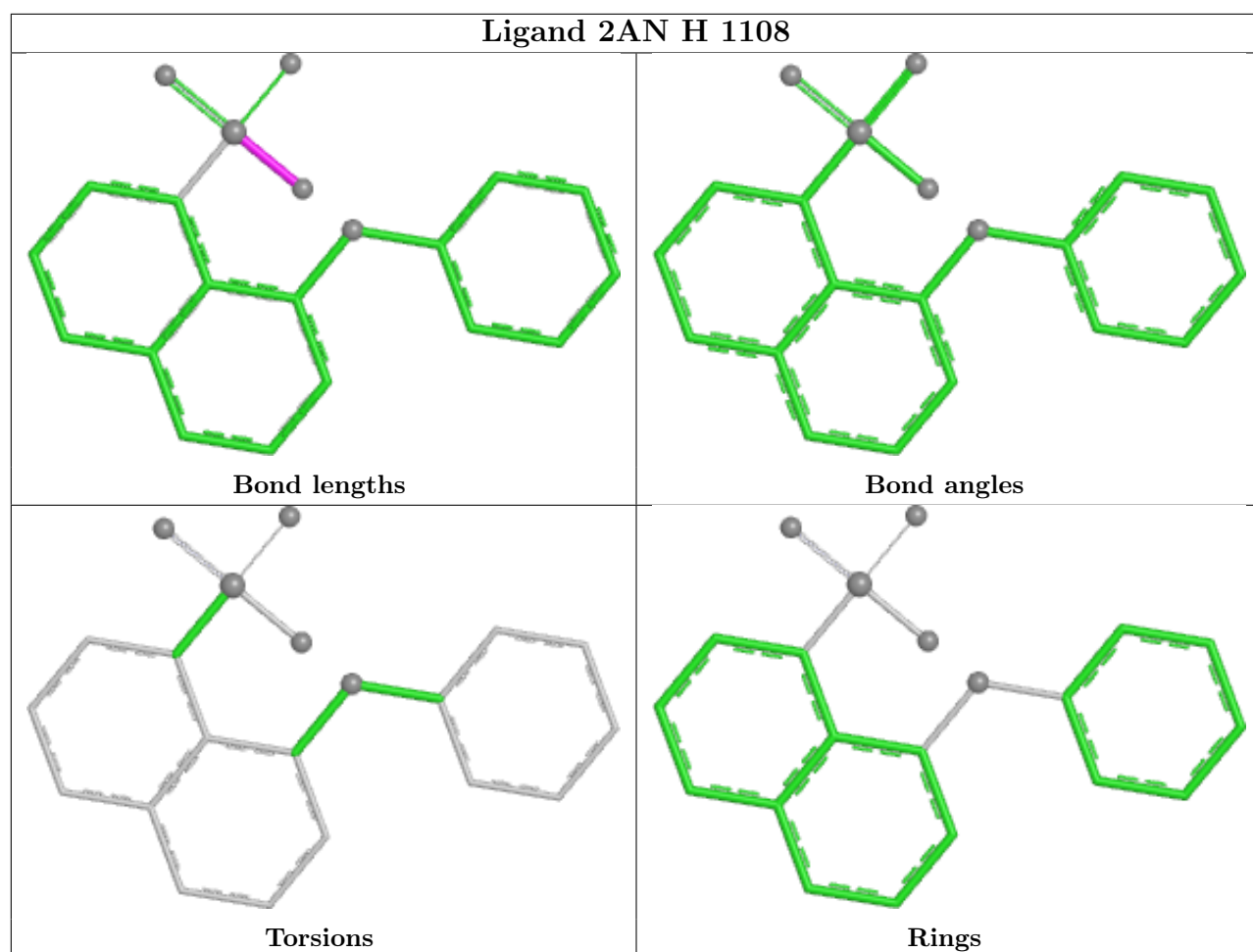


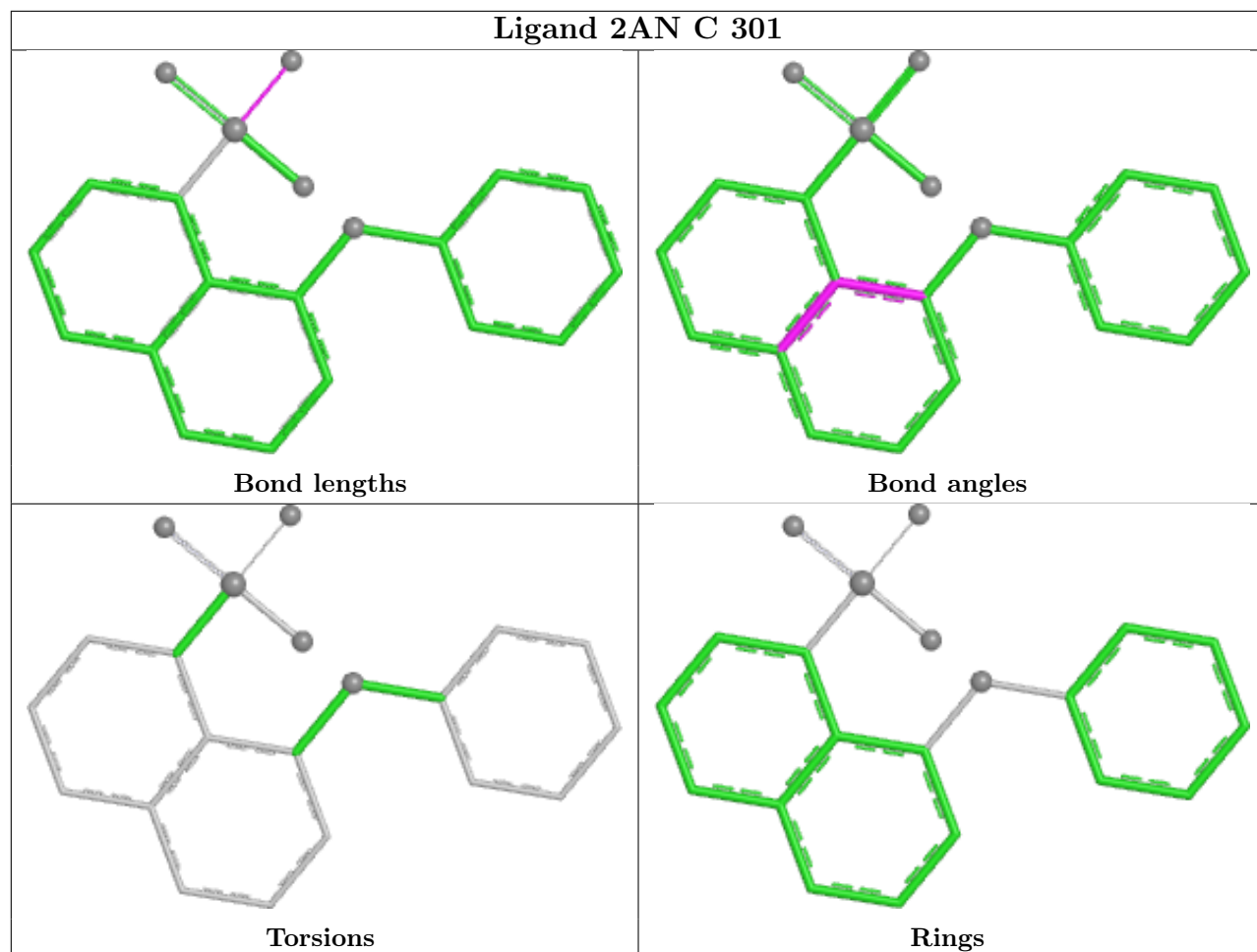


Ligand 2AN C 307

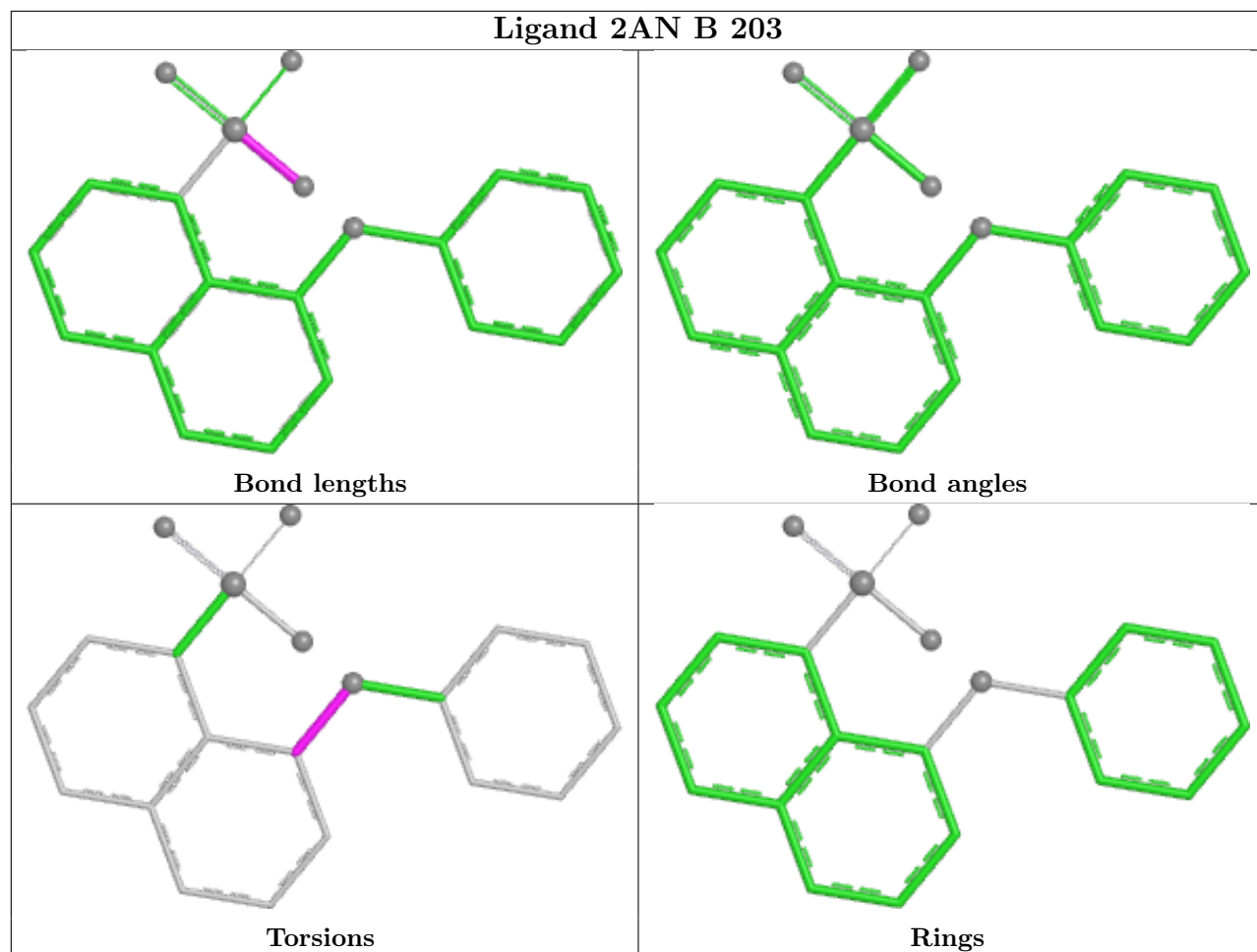




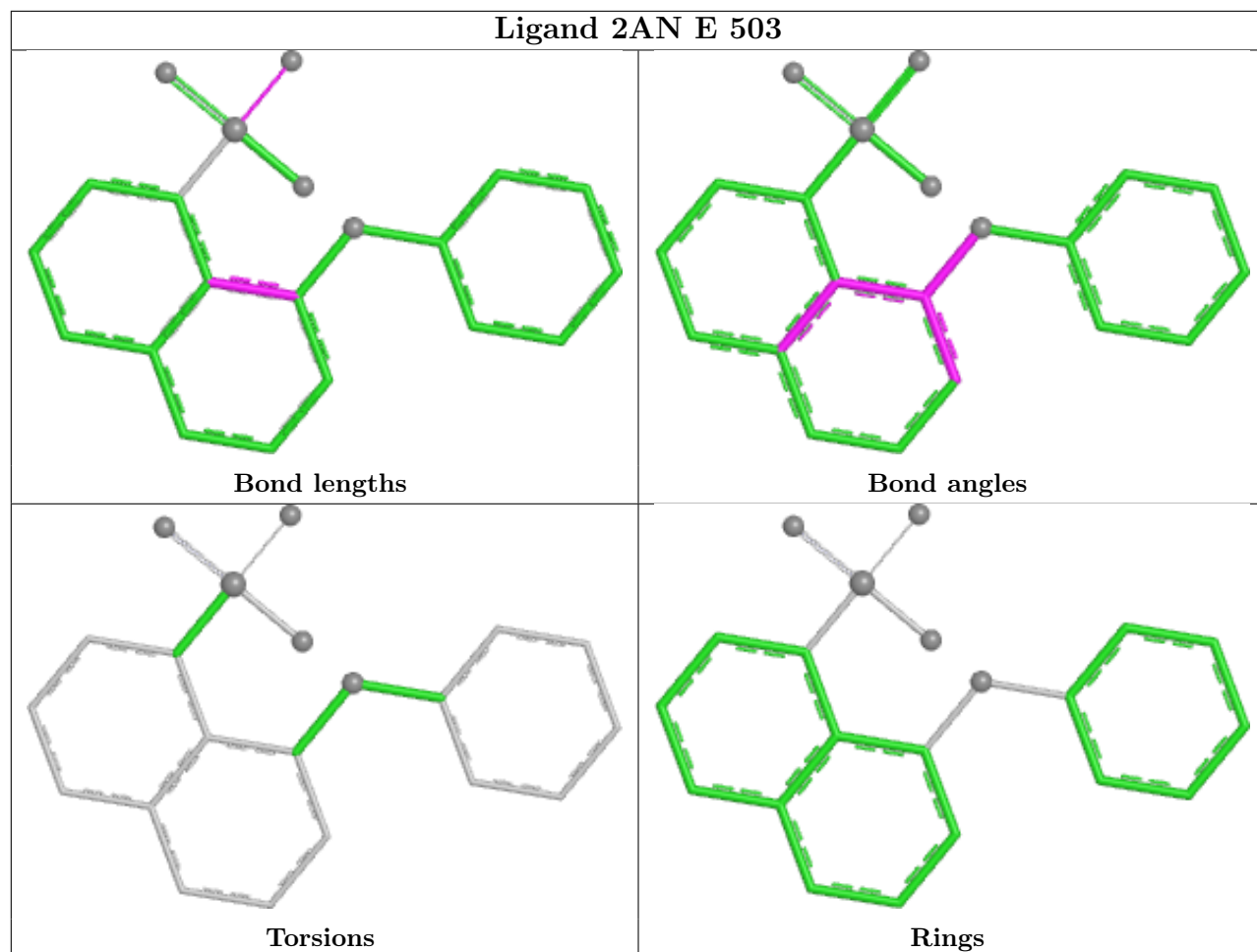


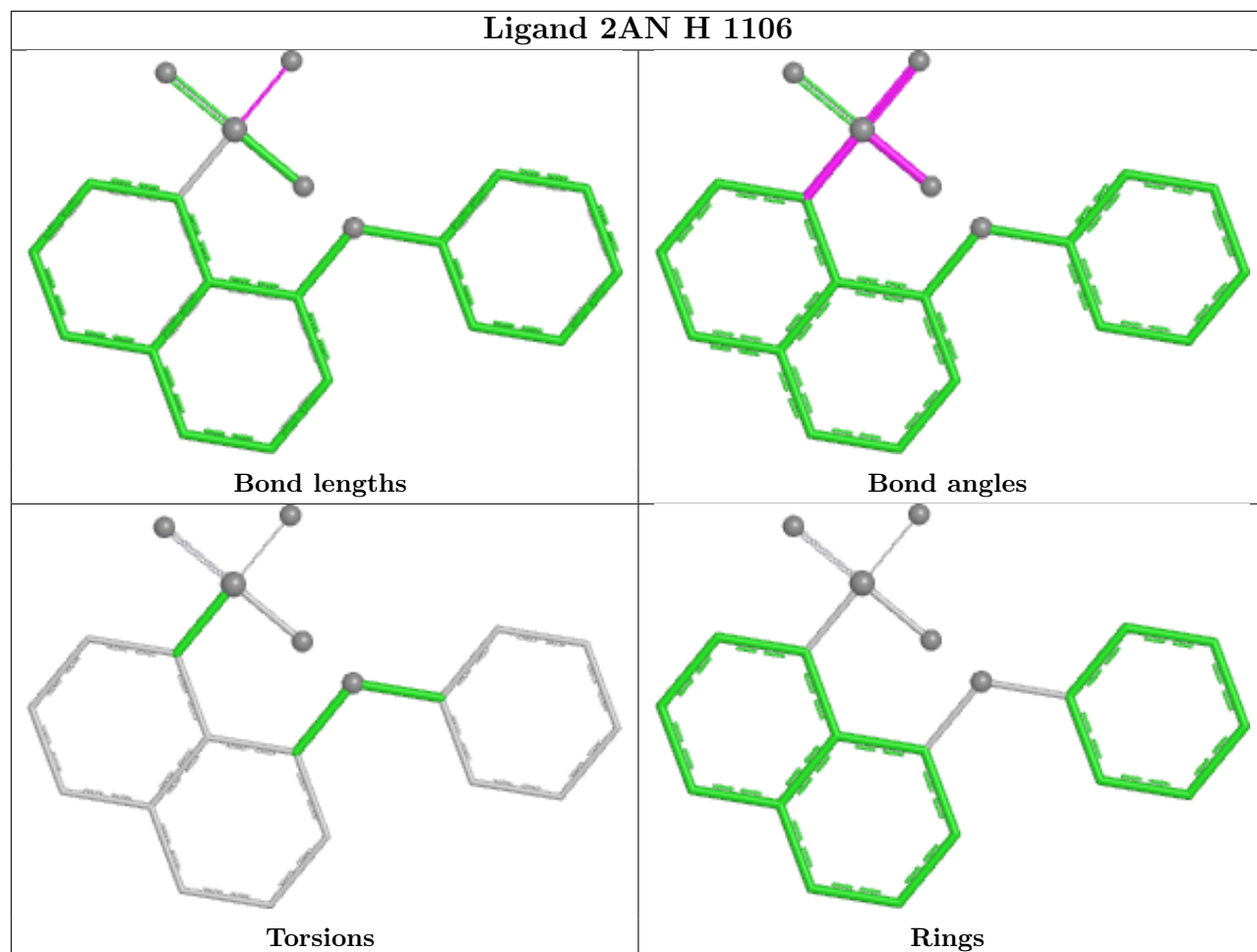


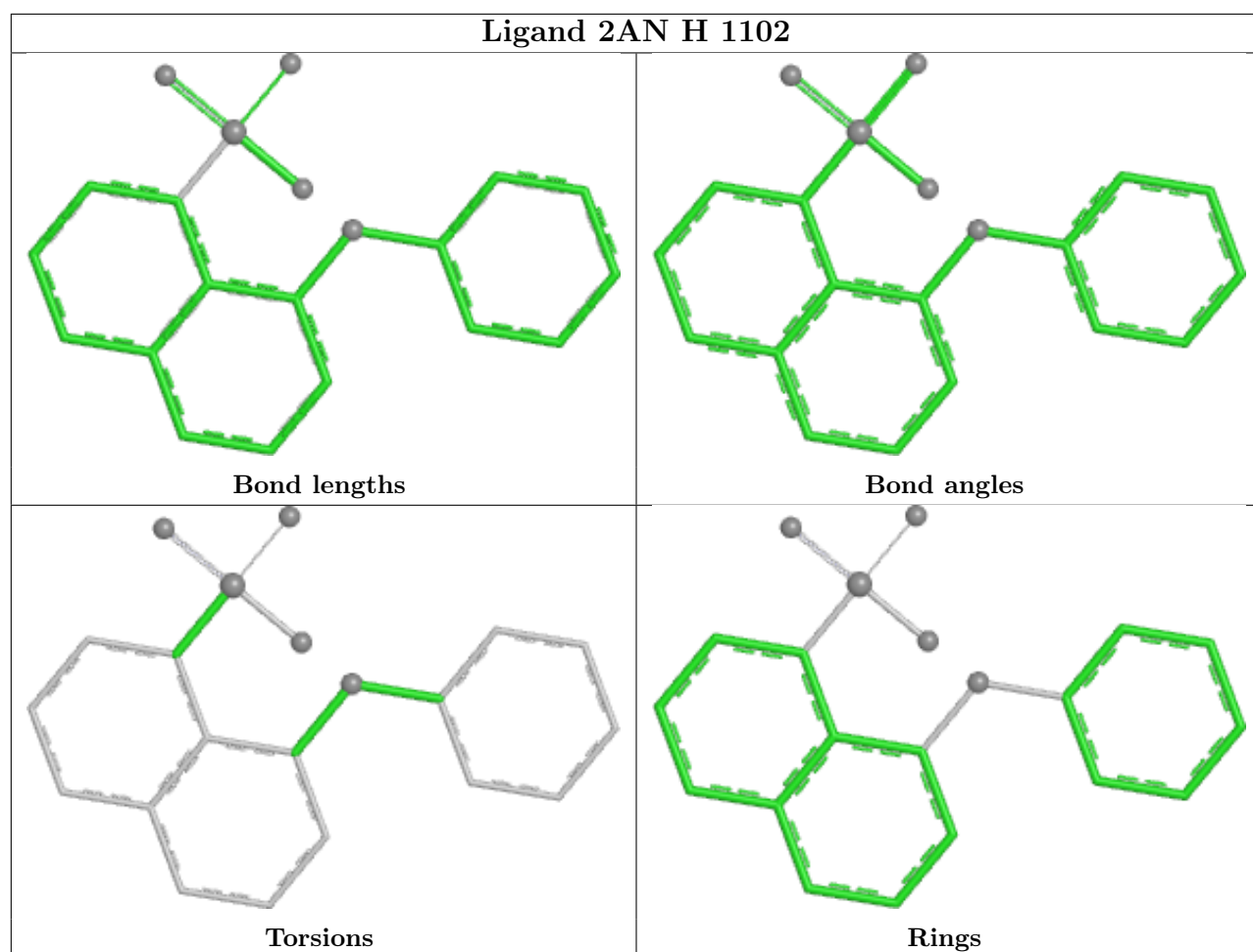
Ligand 2AN B 203



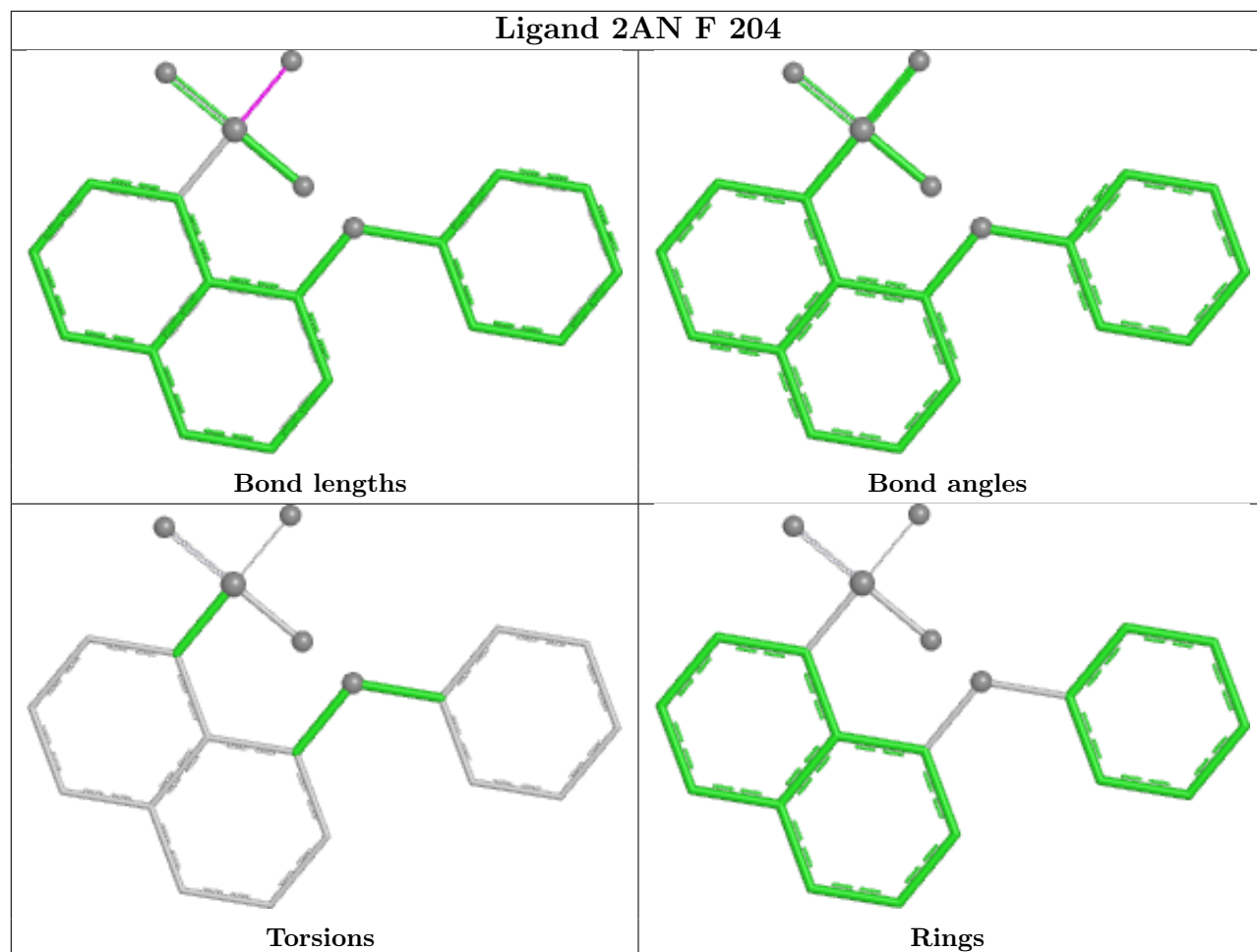
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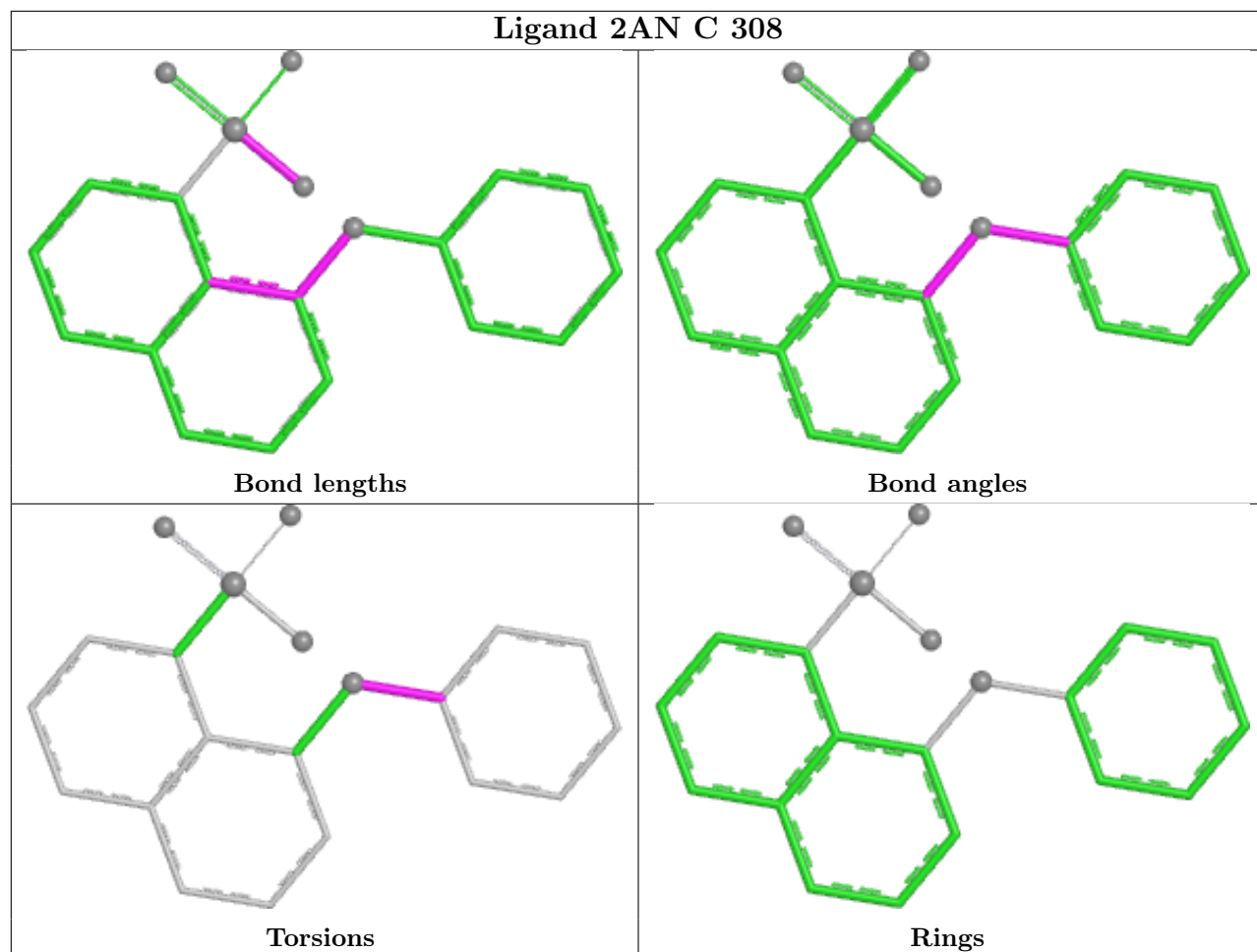




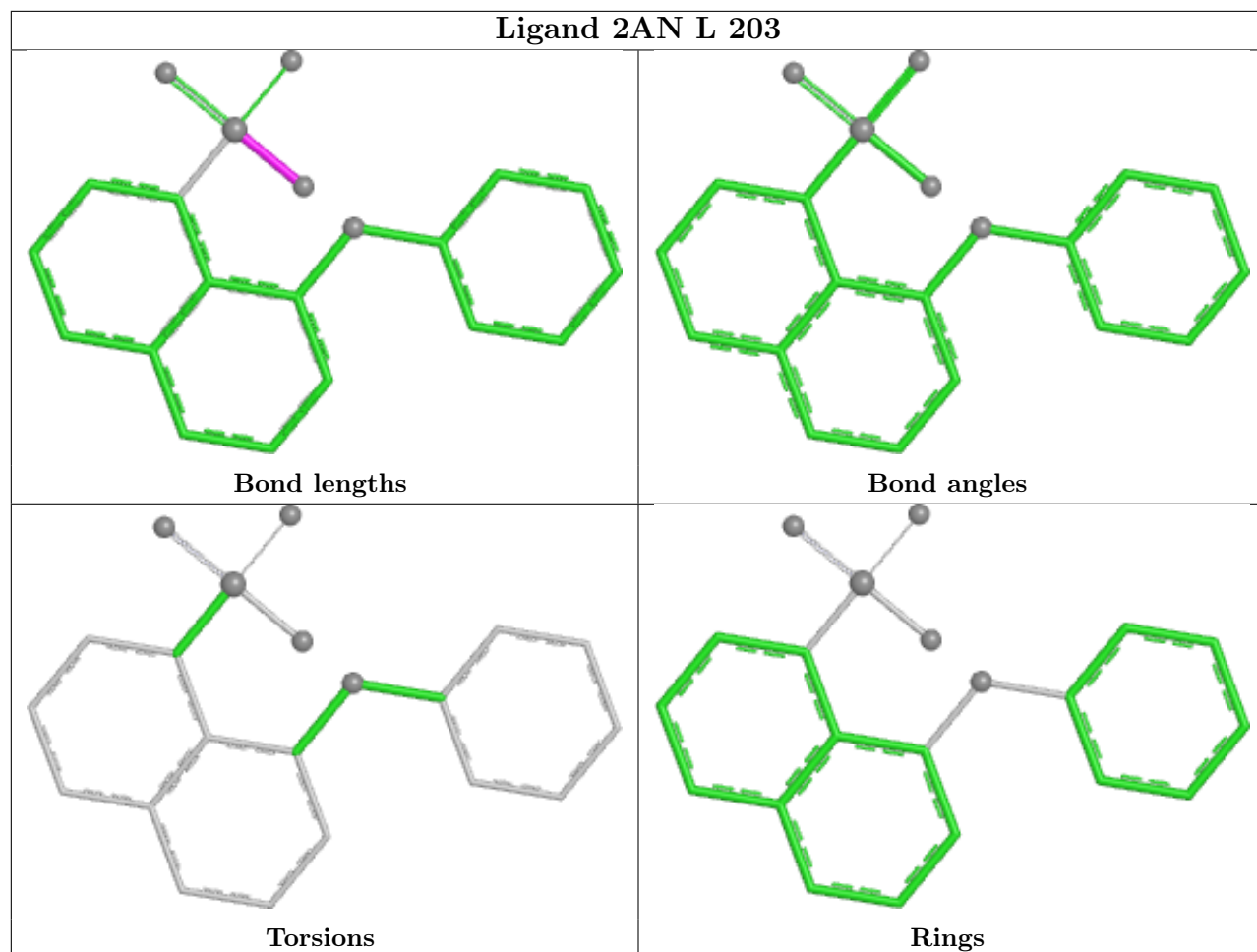
Ligand 2AN F 204



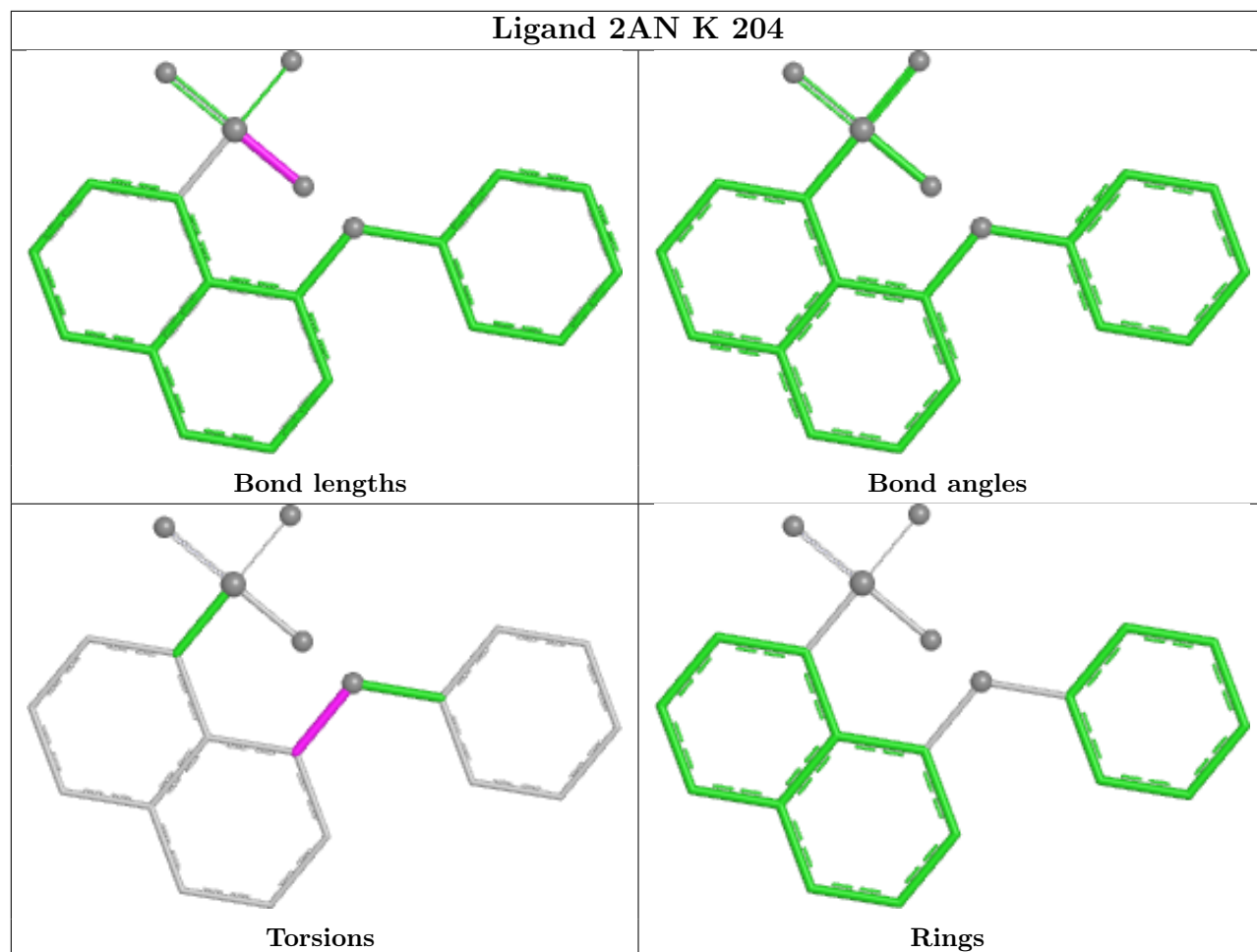
Ligand 2AN C 308



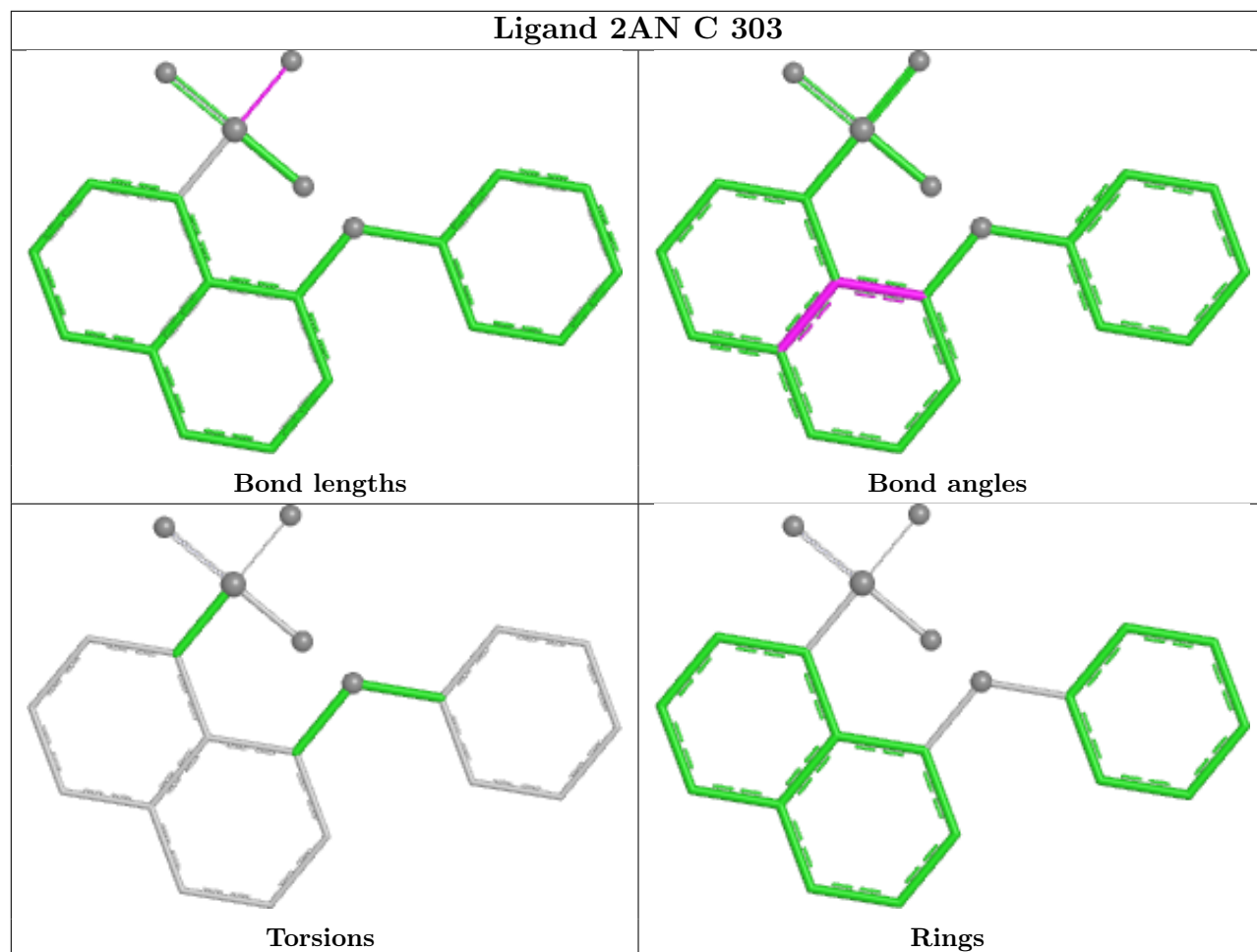
Ligand 2AN L 203

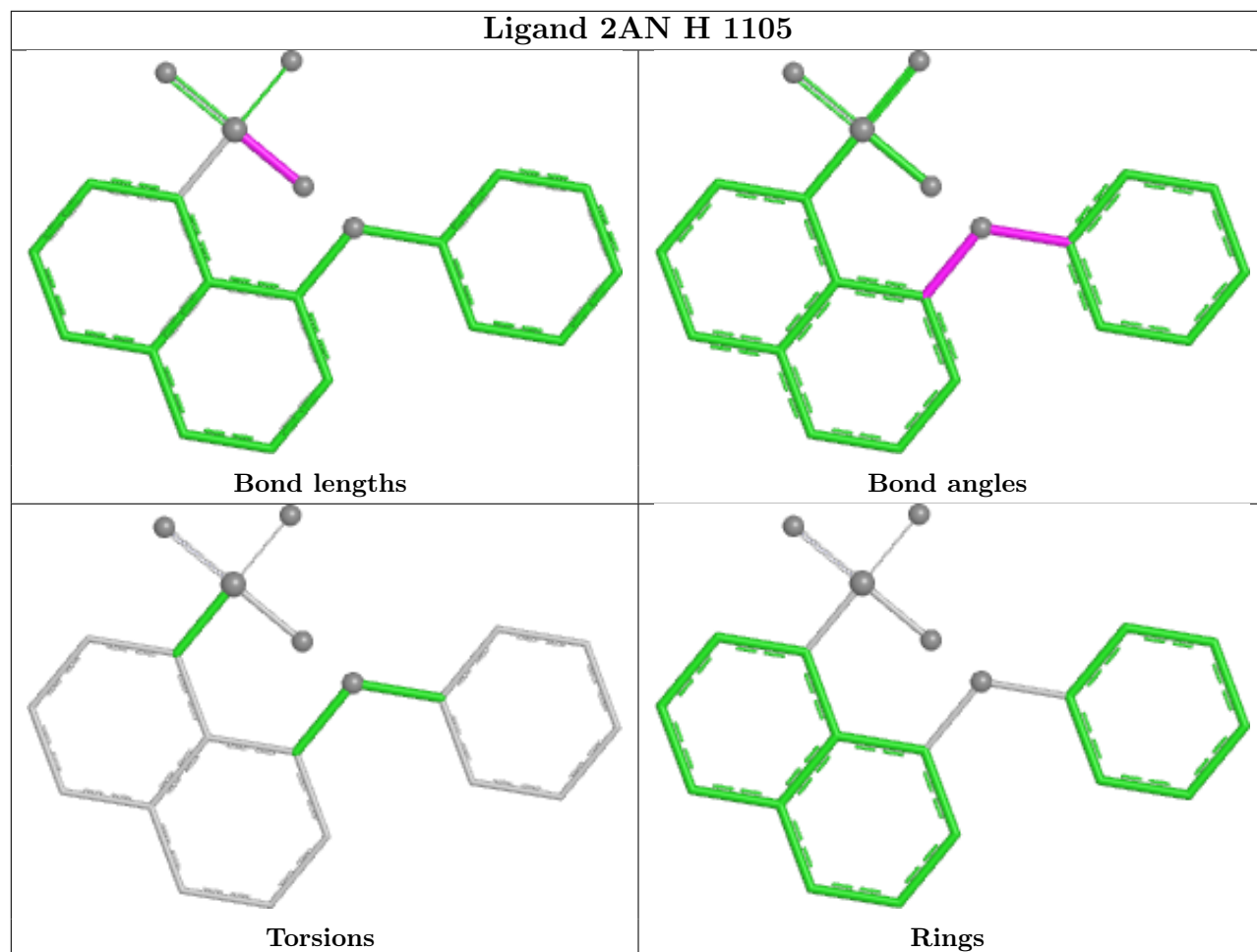


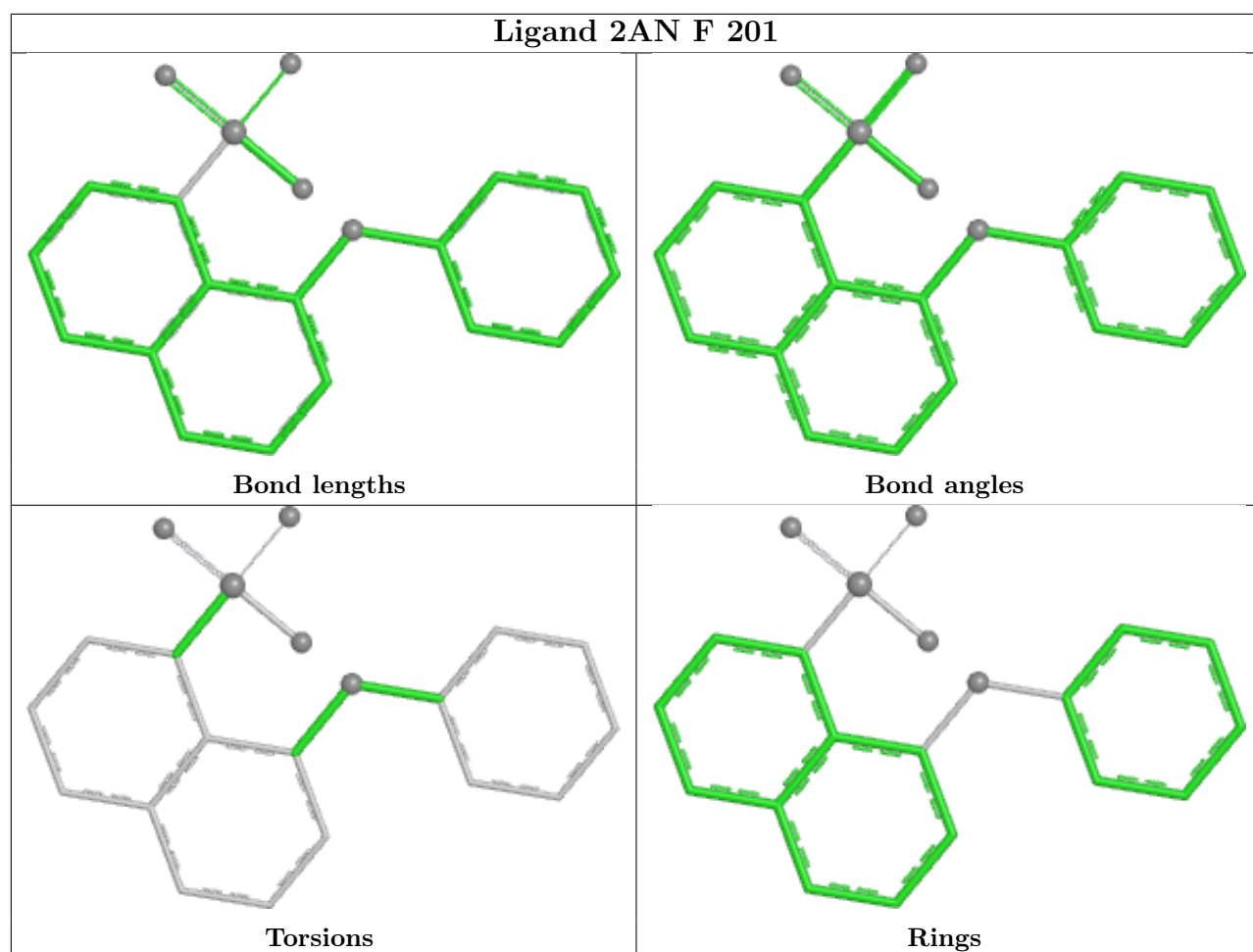
Ligand 2AN K 204



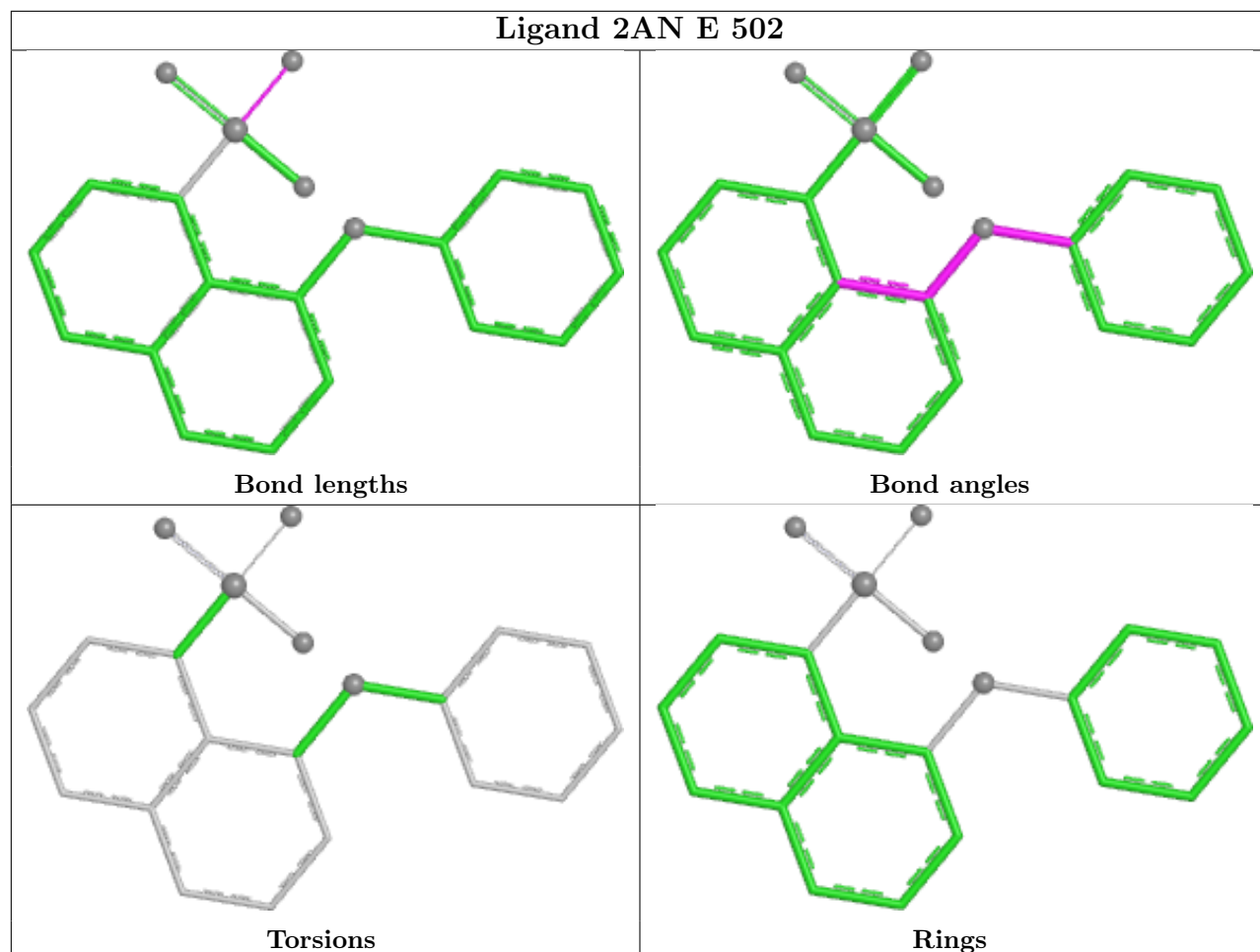
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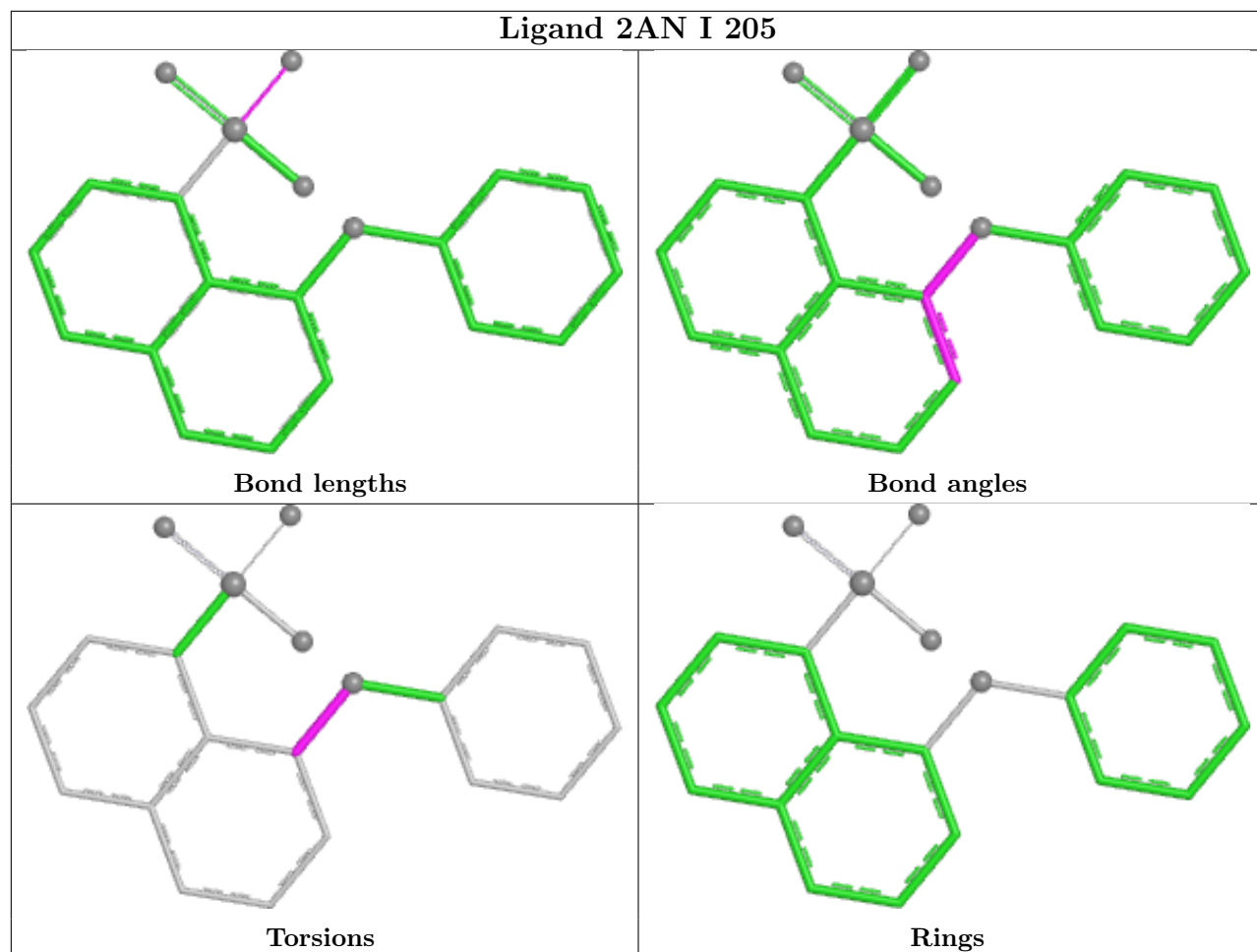


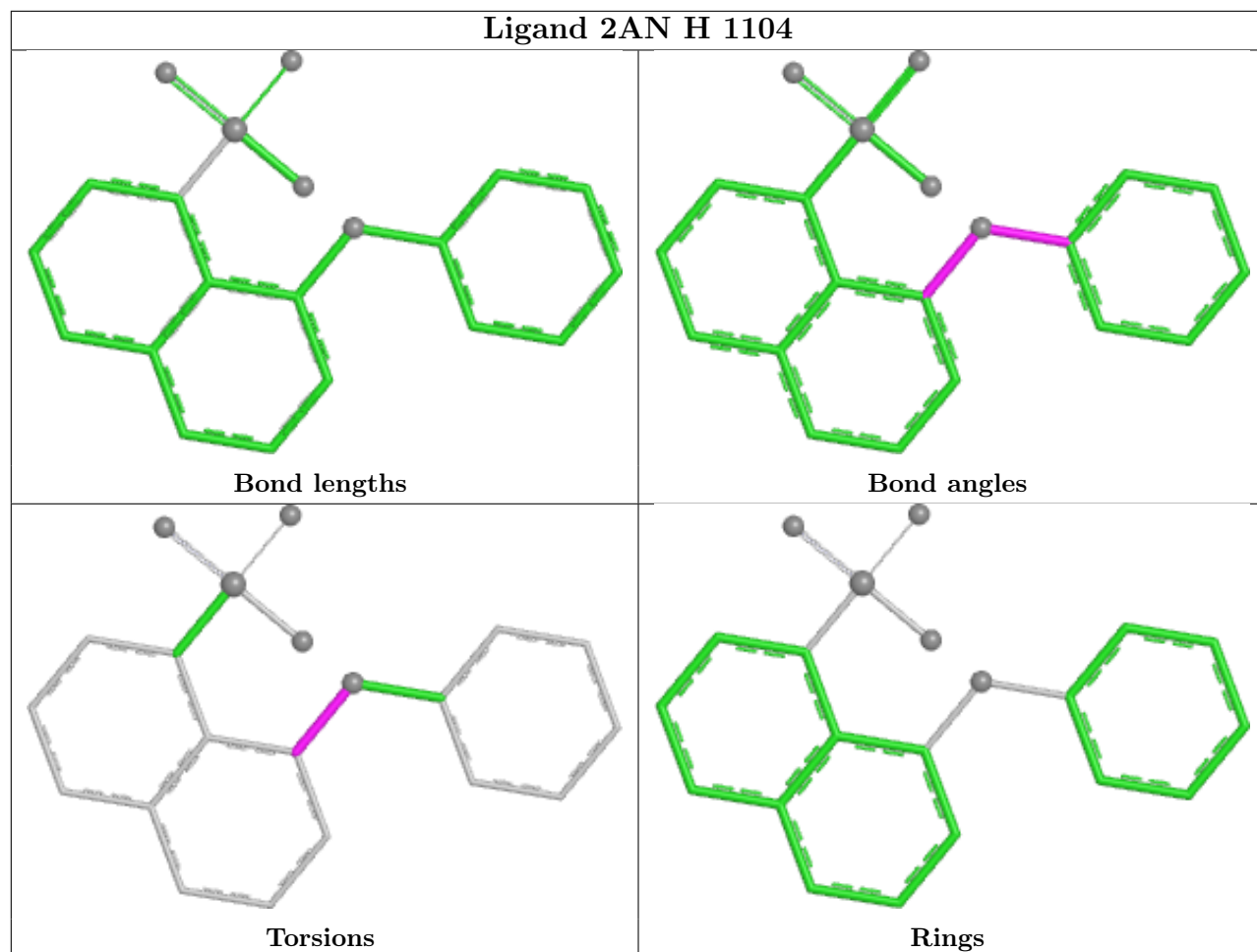


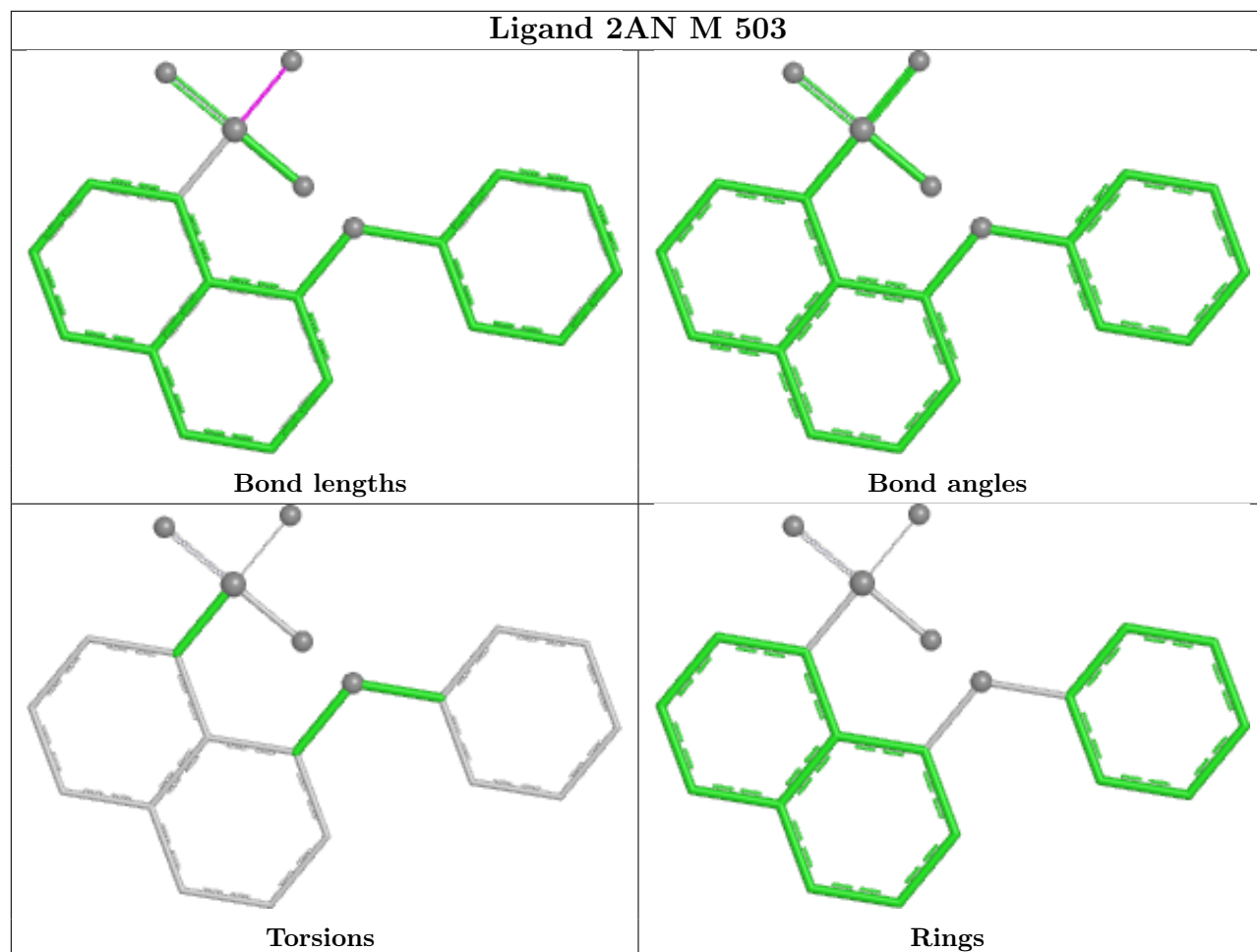
Ligand 2AN E 502



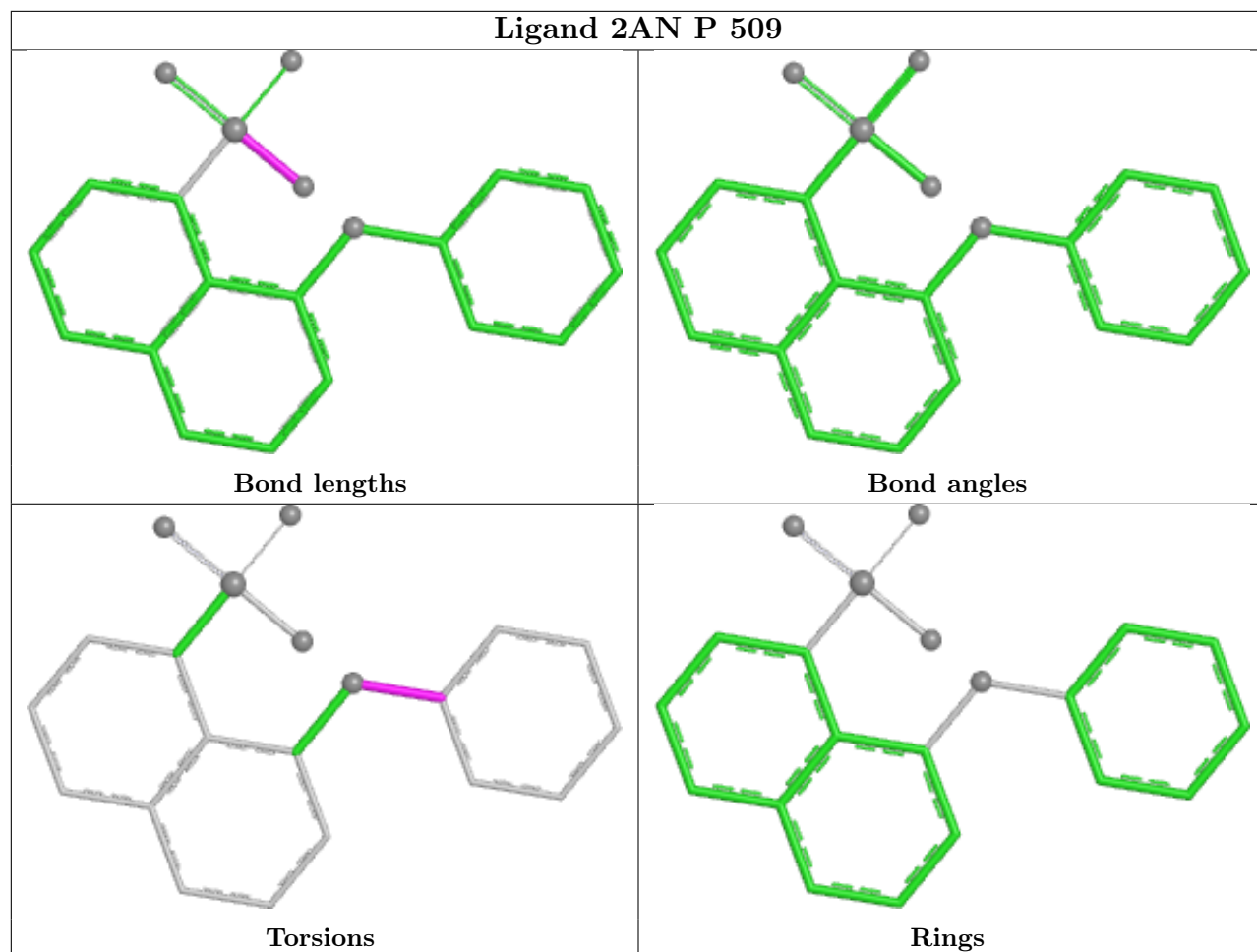
Ligand 2AN I 205

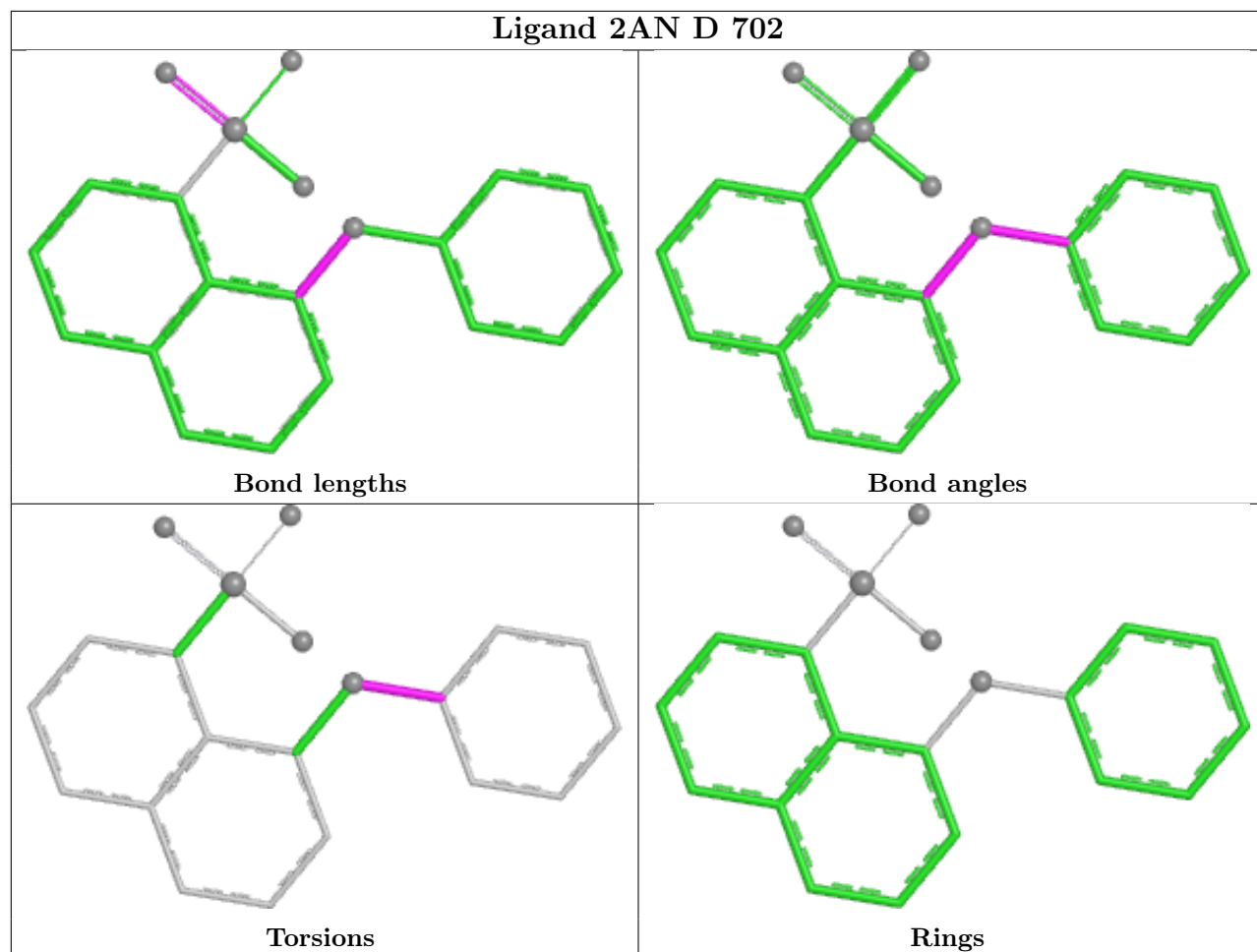




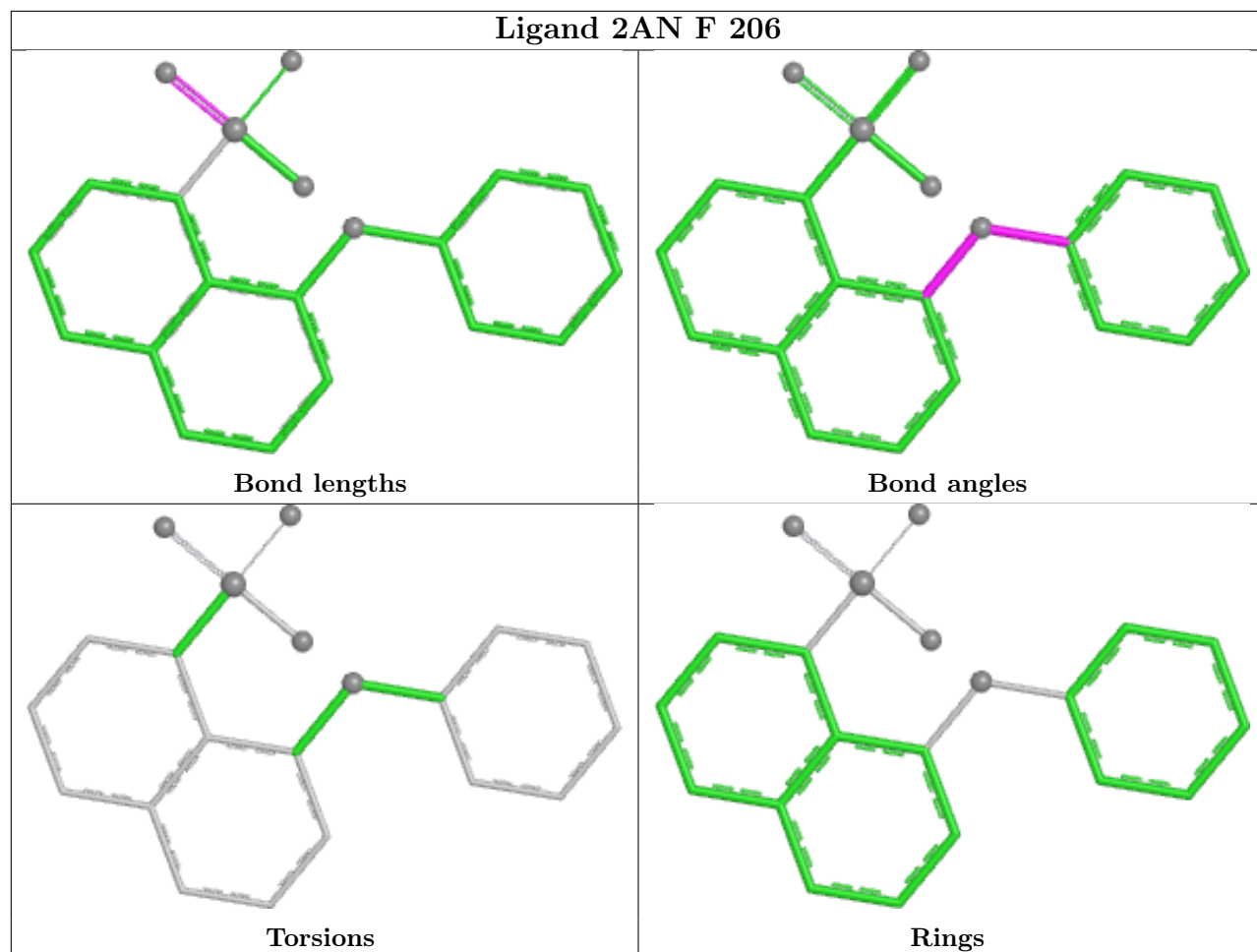


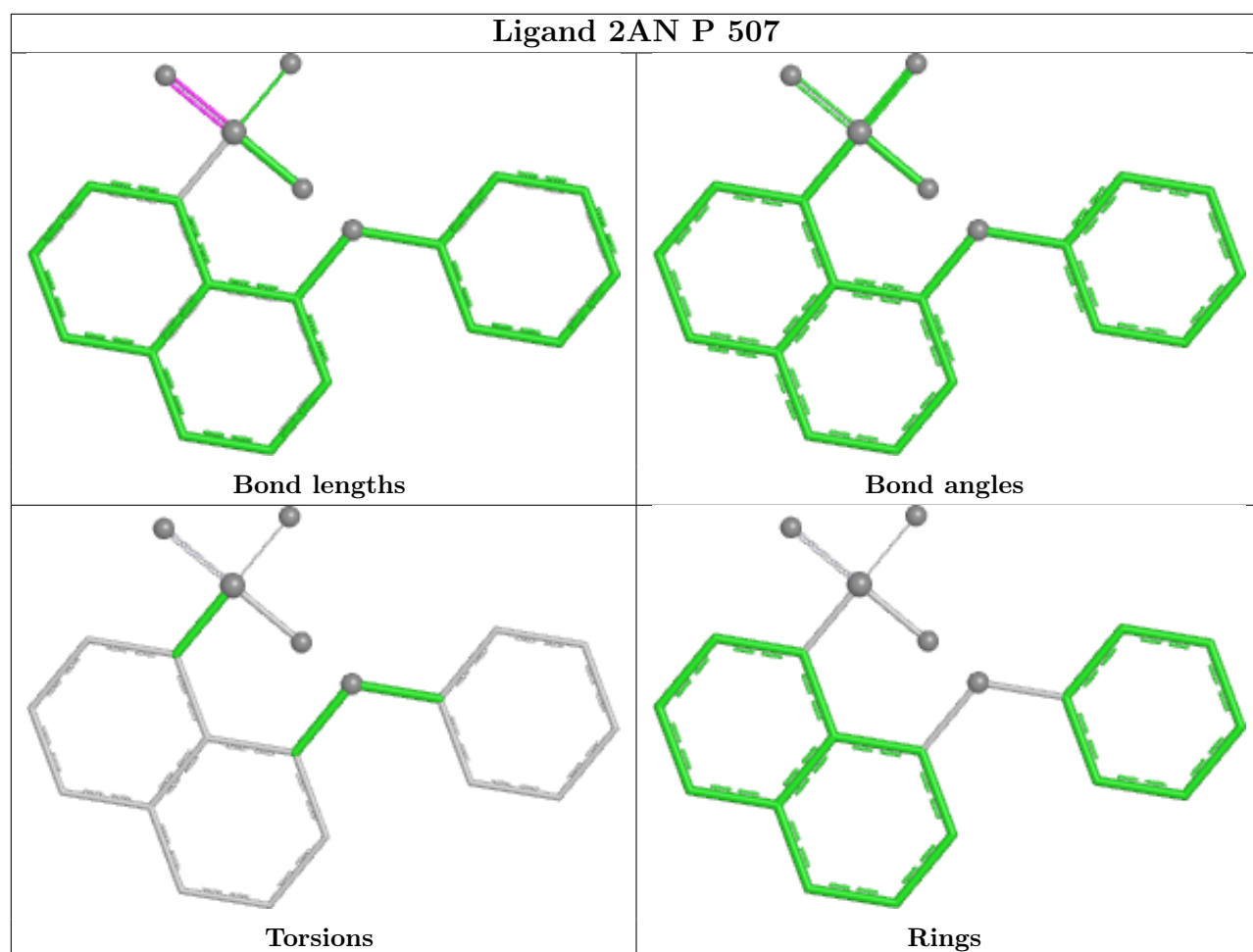
Ligand 2AN P 509





Ligand 2AN F 206





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	152/153 (99%)	0.98	10 (6%) 24 26	24, 35, 55, 79	0
1	B	152/153 (99%)	0.96	12 (7%) 18 20	22, 33, 49, 68	0
1	C	152/153 (99%)	1.36	36 (23%) 2 2	23, 40, 62, 81	0
1	D	152/153 (99%)	1.34	38 (25%) 2 2	16, 40, 66, 111	1 (0%)
1	E	152/153 (99%)	1.29	30 (19%) 3 3	22, 38, 62, 99	0
1	F	152/153 (99%)	1.25	31 (20%) 3 3	23, 39, 56, 94	0
1	G	152/153 (99%)	1.27	30 (19%) 3 3	15, 39, 57, 84	2 (1%)
1	H	152/153 (99%)	1.32	34 (22%) 2 2	23, 39, 66, 90	1 (0%)
1	I	152/153 (99%)	0.88	13 (8%) 16 17	22, 34, 56, 83	0
1	J	151/153 (98%)	1.62	50 (33%) 1 1	22, 41, 75, 100	0
1	K	151/153 (98%)	1.40	40 (26%) 1 1	24, 40, 63, 90	0
1	L	152/153 (99%)	1.04	17 (11%) 10 10	23, 35, 55, 75	0
1	M	152/153 (99%)	1.44	41 (26%) 1 1	22, 39, 66, 89	0
1	N	152/153 (99%)	1.73	53 (34%) 1 1	28, 43, 79, 103	0
1	O	152/153 (99%)	1.41	40 (26%) 1 1	24, 40, 65, 85	0
1	P	152/153 (99%)	1.41	34 (22%) 2 2	24, 41, 62, 110	0
All	All	2430/2448 (99%)	1.29	509 (20%) 2 2	15, 39, 65, 111	4 (0%)

All (509) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	62	GLY	6.7
1	G	90	GLY	5.6
1	D	59	VAL	5.4
1	N	123	GLY	5.3
1	D	63	LYS	5.2

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Mol	Chain	Res	Type	RSRZ
1	J	2	GLY	5.1
1	O	90	GLY	4.8
1	J	59	VAL	4.8
1	N	3	VAL	4.6
1	D	62	GLY	4.6
1	J	62	GLY	4.6
1	N	126	PRO	4.5
1	I	79	TYR	4.5
1	F	42	GLU	4.4
1	N	93	GLU	4.3
1	N	2	GLY	4.2
1	J	3	VAL	4.2
1	N	131	VAL	4.2
1	L	59	VAL	4.1
1	J	131	VAL	4.1
1	M	25	VAL	4.0
1	N	94	ILE	4.0
1	E	62	GLY	4.0
1	N	58	ALA	4.0
1	E	152	SER	3.9
1	L	47	ASN	3.9
1	J	91	PHE	3.9
1	N	124	ASP	3.9
1	J	5	THR	3.9
1	N	125	ALA	3.9
1	J	94	ILE	3.8
1	J	92	GLN	3.8
1	M	44	VAL	3.8
1	N	59	VAL	3.8
1	C	25	VAL	3.8
1	P	23	THR	3.8
1	J	124	ASP	3.7
1	E	87	GLY	3.7
1	N	118	THR	3.7
1	I	61	ASP	3.7
1	N	46	GLY	3.7
1	J	153	ASN	3.7
1	P	90	GLY	3.7
1	P	30	LEU	3.6
1	P	62	GLY	3.6
1	N	95	LEU	3.6
1	J	88	GLY	3.6

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Mol	Chain	Res	Type	RSRZ
1	O	44	VAL	3.6
1	C	44	VAL	3.6
1	O	59	VAL	3.6
1	H	62	GLY	3.6
1	N	5	THR	3.5
1	B	153	ASN	3.5
1	D	123	GLY	3.5
1	K	51	GLY	3.5
1	K	59	VAL	3.5
1	J	127	LEU	3.5
1	N	86	SER	3.4
1	P	48	GLY	3.4
1	H	23	THR	3.4
1	N	4	HIS	3.4
1	F	2	GLY	3.4
1	H	24	VAL	3.4
1	F	62	GLY	3.4
1	O	46	GLY	3.4
1	B	77	ALA	3.4
1	D	92	GLN	3.4
1	J	61	ASP	3.3
1	J	126	PRO	3.3
1	M	152	SER	3.3
1	N	75	ASP	3.3
1	H	51	GLY	3.3
1	I	153	ASN	3.3
1	D	60	GLU	3.3
1	E	92	GLN	3.3
1	J	121	THR	3.3
1	C	46	GLY	3.3
1	H	27	GLY	3.3
1	C	125	ALA	3.3
1	D	47	ASN	3.3
1	J	93	GLU	3.3
1	J	63	LYS	3.3
1	M	48	GLY	3.2
1	B	61	ASP	3.2
1	F	108	ASP	3.2
1	N	99	SER	3.2
1	K	46	GLY	3.2
1	N	127	LEU	3.2
1	N	64	THR	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	48	GLY	3.2
1	J	47	ASN	3.2
1	N	44	VAL	3.2
1	K	77	ALA	3.2
1	O	124	ASP	3.2
1	G	93	GLU	3.2
1	J	90	GLY	3.2
1	N	87	GLY	3.2
1	M	36	PRO	3.2
1	N	92	GLN	3.2
1	O	92	GLN	3.2
1	M	75	ASP	3.1
1	J	64	THR	3.1
1	N	88	GLY	3.1
1	O	62	GLY	3.1
1	G	47	ASN	3.1
1	J	132	HIS	3.1
1	E	91	PHE	3.1
1	G	46	GLY	3.1
1	E	61	ASP	3.1
1	H	25	VAL	3.1
1	J	120	HIS	3.1
1	G	51	GLY	3.1
1	M	46	GLY	3.1
1	N	6	PHE	3.1
1	C	75	ASP	3.1
1	C	108	ASP	3.1
1	H	26	ASP	3.1
1	J	125	ALA	3.1
1	J	43	ILE	3.1
1	J	6	PHE	3.0
1	H	75	ASP	3.0
1	H	124	ASP	3.0
1	P	77	ALA	3.0
1	H	30	LEU	3.0
1	J	98	VAL	3.0
1	D	153	ASN	3.0
1	F	47	ASN	3.0
1	N	62	GLY	3.0
1	N	130	GLU	3.0
1	N	91	PHE	3.0
1	N	129	ASP	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	3	VAL	3.0
1	M	59	VAL	3.0
1	K	43	ILE	3.0
1	L	51	GLY	3.0
1	O	61	ASP	3.0
1	I	77	ALA	3.0
1	M	37	ALA	3.0
1	B	51	GLY	3.0
1	I	62	GLY	3.0
1	M	41	ILE	3.0
1	K	28	ASP	3.0
1	E	125	ALA	2.9
1	D	51	GLY	2.9
1	M	33	LYS	2.9
1	A	75	ASP	2.9
1	N	121	THR	2.9
1	K	126	PRO	2.9
1	O	133	GLN	2.9
1	M	77	ALA	2.9
1	M	30	LEU	2.9
1	E	48	GLY	2.9
1	P	124	ASP	2.9
1	J	60	GLU	2.9
1	O	91	PHE	2.9
1	K	152	SER	2.9
1	J	122	LYS	2.9
1	D	44	VAL	2.9
1	I	59	VAL	2.9
1	P	59	VAL	2.9
1	G	92	GLN	2.9
1	E	126	PRO	2.9
1	N	47	ASN	2.9
1	H	77	ALA	2.9
1	L	29	GLU	2.8
1	P	60	GLU	2.8
1	J	86	SER	2.8
1	H	92	GLN	2.8
1	E	51	GLY	2.8
1	G	26	ASP	2.8
1	K	123	GLY	2.8
1	L	90	GLY	2.8
1	P	75	ASP	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	52	THR	2.8
1	A	4	HIS	2.8
1	C	59	VAL	2.8
1	J	115	VAL	2.8
1	C	47	ASN	2.8
1	G	61	ASP	2.8
1	P	108	ASP	2.8
1	K	2	GLY	2.8
1	O	125	ALA	2.8
1	G	95	LEU	2.8
1	H	63	LYS	2.8
1	J	89	THR	2.8
1	D	3	VAL	2.8
1	H	59	VAL	2.8
1	C	41	ILE	2.8
1	K	41	ILE	2.8
1	F	86	SER	2.7
1	P	29	GLU	2.7
1	L	77	ALA	2.7
1	C	79	TYR	2.7
1	M	34	LEU	2.7
1	M	31	THR	2.7
1	M	126	PRO	2.7
1	B	59	VAL	2.7
1	K	44	VAL	2.7
1	M	35	ILE	2.7
1	M	60	GLU	2.7
1	P	65	SER	2.7
1	K	124	ASP	2.7
1	L	88	GLY	2.7
1	E	77	ALA	2.7
1	K	92	GLN	2.7
1	O	126	PRO	2.7
1	E	93	GLU	2.7
1	J	4	HIS	2.7
1	P	44	VAL	2.7
1	E	43	ILE	2.7
1	E	28	ASP	2.7
1	D	90	GLY	2.7
1	N	48	GLY	2.7
1	O	96	GLU	2.7
1	D	79	TYR	2.7

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Mol	Chain	Res	Type	RSRZ
1	G	59	VAL	2.7
1	G	94	ILE	2.7
1	P	25	VAL	2.7
1	N	134	ASP	2.7
1	N	63	LYS	2.7
1	K	87	GLY	2.7
1	C	92	GLN	2.6
1	M	58	ALA	2.6
1	A	64	THR	2.6
1	O	47	ASN	2.6
1	E	124	ASP	2.6
1	F	129	ASP	2.6
1	N	61	ASP	2.6
1	P	3	VAL	2.6
1	H	46	GLY	2.6
1	M	90	GLY	2.6
1	P	92	GLN	2.6
1	F	64	THR	2.6
1	H	153	ASN	2.6
1	K	64	THR	2.6
1	L	153	ASN	2.6
1	J	95	LEU	2.6
1	K	68	LEU	2.6
1	N	50	PRO	2.6
1	F	75	ASP	2.6
1	N	108	ASP	2.6
1	O	28	ASP	2.6
1	M	79	TYR	2.6
1	C	43	ILE	2.6
1	N	98	VAL	2.6
1	P	74	ILE	2.6
1	C	62	GLY	2.6
1	L	62	GLY	2.6
1	I	93	GLU	2.6
1	H	73	ALA	2.6
1	M	26	ASP	2.6
1	D	99	SER	2.6
1	F	59	VAL	2.6
1	G	25	VAL	2.6
1	G	74	ILE	2.6
1	H	43	ILE	2.6
1	M	27	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
1	E	153	ASN	2.6
1	F	5	THR	2.6
1	G	125	ALA	2.6
1	F	93	GLU	2.5
1	M	45	GLU	2.5
1	C	51	GLY	2.5
1	D	46	GLY	2.5
1	B	47	ASN	2.5
1	G	153	ASN	2.5
1	J	136	LYS	2.5
1	C	61	ASP	2.5
1	C	64	THR	2.5
1	G	78	THR	2.5
1	J	36	PRO	2.5
1	C	87	GLY	2.5
1	F	43	ILE	2.5
1	C	63	LYS	2.5
1	F	107	ALA	2.5
1	I	99	SER	2.5
1	J	45	GLU	2.5
1	K	45	GLU	2.5
1	F	34	LEU	2.5
1	H	34	LEU	2.5
1	M	51	GLY	2.5
1	C	53	VAL	2.5
1	E	59	VAL	2.5
1	J	44	VAL	2.5
1	M	38	ILE	2.5
1	M	53	VAL	2.5
1	A	47	ASN	2.5
1	D	61	ASP	2.5
1	P	61	ASP	2.5
1	K	93	GLU	2.5
1	M	52	THR	2.5
1	P	58	ALA	2.5
1	O	30	LEU	2.5
1	O	95	LEU	2.5
1	G	62	GLY	2.5
1	J	46	GLY	2.5
1	M	47	ASN	2.5
1	A	43	ILE	2.5
1	M	43	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	N	115	VAL	2.4
1	O	94	ILE	2.5
1	H	60	GLU	2.4
1	J	129	ASP	2.4
1	O	72	ASP	2.4
1	P	28	ASP	2.4
1	L	66	TYR	2.4
1	C	49	GLY	2.4
1	E	123	GLY	2.4
1	N	90	GLY	2.4
1	O	88	GLY	2.4
1	E	94	ILE	2.4
1	O	25	VAL	2.4
1	D	4	HIS	2.4
1	E	90	GLY	2.4
1	D	91	PHE	2.4
1	F	44	VAL	2.4
1	D	86	SER	2.4
1	J	69	HIS	2.4
1	C	77	ALA	2.4
1	O	51	GLY	2.4
1	G	115	VAL	2.4
1	O	24	VAL	2.4
1	O	74	ILE	2.4
1	P	33	LYS	2.4
1	K	69	HIS	2.4
1	N	120	HIS	2.4
1	D	93	GLU	2.3
1	F	77	ALA	2.3
1	A	153	ASN	2.3
1	G	30	LEU	2.3
1	L	124	ASP	2.3
1	N	119	PHE	2.3
1	C	74	ILE	2.3
1	H	74	ILE	2.3
1	O	43	ILE	2.3
1	N	117	VAL	2.3
1	F	89	THR	2.3
1	D	45	GLU	2.3
1	J	128	PRO	2.3
1	M	32	PRO	2.3
1	P	46	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	P	49	GLY	2.3
1	C	26	ASP	2.3
1	E	44	VAL	2.3
1	O	45	GLU	2.3
1	D	89	THR	2.3
1	K	153	ASN	2.3
1	P	47	ASN	2.3
1	A	61	ASP	2.3
1	D	124	ASP	2.3
1	E	2	GLY	2.3
1	G	88	GLY	2.3
1	K	66	TYR	2.3
1	L	61	ASP	2.3
1	M	62	GLY	2.3
1	M	103	LYS	2.3
1	F	99	SER	2.3
1	N	96	GLU	2.3
1	L	43	ILE	2.3
1	N	137	GLN	2.3
1	O	41	ILE	2.3
1	N	128	PRO	2.3
1	K	47	ASN	2.3
1	D	58	ALA	2.3
1	F	88	GLY	2.3
1	H	33	LYS	2.3
1	J	75	ASP	2.3
1	K	37	ALA	2.3
1	K	109	GLY	2.3
1	F	79	TYR	2.3
1	P	149	TYR	2.3
1	F	29	GLU	2.2
1	K	7	GLU	2.2
1	M	7	GLU	2.2
1	N	60	GLU	2.2
1	P	42	GLU	2.2
1	O	152	SER	2.2
1	E	71	ILE	2.2
1	D	36	PRO	2.2
1	G	126	PRO	2.2
1	D	122	LYS	2.2
1	C	37	ALA	2.2
1	D	37	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	M	49	GLY	2.2
1	C	45	GLU	2.2
1	J	8	GLU	2.2
1	J	29	GLU	2.2
1	K	60	GLU	2.2
1	O	29	GLU	2.2
1	O	93	GLU	2.2
1	D	131	VAL	2.2
1	E	63	LYS	2.2
1	K	52	THR	2.2
1	F	25	VAL	2.2
1	J	135	VAL	2.2
1	M	50	PRO	2.2
1	G	28	ASP	2.2
1	H	90	GLY	2.2
1	K	88	GLY	2.2
1	C	58	ALA	2.2
1	D	76	GLU	2.2
1	I	60	GLU	2.2
1	H	79	TYR	2.2
1	M	63	LYS	2.2
1	B	5	THR	2.2
1	C	126	PRO	2.2
1	E	78	THR	2.2
1	M	64	THR	2.2
1	O	50	PRO	2.2
1	B	75	ASP	2.2
1	E	75	ASP	2.2
1	F	61	ASP	2.2
1	E	3	VAL	2.2
1	P	53	VAL	2.2
1	E	46	GLY	2.2
1	F	60	GLU	2.2
1	O	34	LEU	2.2
1	O	66	TYR	2.2
1	E	121	THR	2.2
1	G	72	ASP	2.2
1	K	89	THR	2.2
1	A	9	GLU	2.1
1	B	93	GLU	2.1
1	I	29	GLU	2.1
1	H	44	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	F	39	GLN	2.1
1	F	46	GLY	2.1
1	H	48	GLY	2.1
1	C	69	HIS	2.1
1	L	69	HIS	2.1
1	D	125	ALA	2.1
1	F	106	ALA	2.1
1	G	77	ALA	2.1
1	J	37	ALA	2.1
1	O	107	ALA	2.1
1	H	40	SER	2.1
1	P	152	SER	2.1
1	H	45	GLU	2.1
1	I	9	GLU	2.1
1	J	72	ASP	2.1
1	M	124	ASP	2.1
1	O	26	ASP	2.1
1	O	60	GLU	2.1
1	D	64	THR	2.1
1	D	126	PRO	2.1
1	H	50	PRO	2.1
1	D	74	ILE	2.1
1	H	39[A]	GLN	2.1
1	P	43	ILE	2.1
1	F	90	GLY	2.1
1	G	109	GLY	2.1
1	L	46	GLY	2.1
1	P	24	VAL	2.1
1	P	109	GLY	2.1
1	N	122	LYS	2.1
1	C	42	GLU	2.1
1	F	153	ASN	2.1
1	H	134	ASP	2.1
1	I	75	ASP	2.1
1	K	75	ASP	2.1
1	G	89	THR	2.1
1	M	89	THR	2.1
1	M	121	THR	2.1
1	D	48	GLY	2.1
1	K	48	GLY	2.1
1	L	48	GLY	2.1
1	F	91	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	59	VAL	2.1
1	D	53	VAL	2.1
1	I	125	ALA	2.1
1	K	125	ALA	2.1
1	A	99	SER	2.1
1	C	30	LEU	2.1
1	E	60	GLU	2.1
1	P	93	GLU	2.1
1	N	153	ASN	2.1
1	P	153	ASN	2.1
1	B	124	ASP	2.1
1	O	39	GLN	2.1
1	G	43	ILE	2.1
1	O	54	LYS	2.1
1	K	53	VAL	2.1
1	C	22	ALA	2.1
1	G	73	ALA	2.1
1	N	42	GLU	2.0
1	O	153	ASN	2.0
1	G	133	GLN	2.0
1	H	61	ASP	2.0
1	J	108	ASP	2.0
1	N	84	THR	2.0
1	H	42	GLU	2.0
1	H	150	VAL	2.0
1	K	3	VAL	2.0
1	N	25	VAL	2.0
1	C	152	SER	2.0
1	C	107	ALA	2.0
1	J	58	ALA	2.0
1	C	124	ASP	2.0
1	K	72	ASP	2.0
1	K	63	LYS	2.0
1	K	50	PRO	2.0
1	B	90	GLY	2.0
1	D	2	GLY	2.0
1	D	109	GLY	2.0
1	G	48	GLY	2.0
1	L	87	GLY	2.0
1	O	87	GLY	2.0
1	D	66	TYR	2.0
1	K	79	TYR	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	2AN	K	206	21/21	0.60	0.23	67,76,106,113	0
2	2AN	E	507	21/21	0.63	0.20	64,72,78,82	0
2	2AN	K	205	21/21	0.69	0.24	62,69,86,91	0
2	2AN	P	509	21/21	0.69	0.21	73,84,92,96	0
2	2AN	M	509	21/21	0.73	0.18	67,81,91,94	0
2	2AN	D	702	21/21	0.73	0.17	74,80,93,97	0
3	SO4	H	1110	5/5	0.73	0.19	80,84,85,88	0
2	2AN	J	206	21/21	0.74	0.26	41,46,55,57	21
2	2AN	C	308	21/21	0.75	0.15	58,62,73,77	0
2	2AN	N	203	21/21	0.76	0.19	71,83,97,99	0
2	2AN	G	306	21/21	0.77	0.30	61,64,70,71	21
2	2AN	J	205	21/21	0.77	0.18	64,69,91,93	0
2	2AN	F	204	21/21	0.77	0.16	40,45,57,61	0
2	2AN	D	705	21/21	0.79	0.16	53,56,62,64	0
2	2AN	E	506	21/21	0.80	0.18	49,60,78,82	0
2	2AN	P	501	21/21	0.81	0.17	42,46,54,60	0
2	2AN	P	508	21/21	0.81	0.17	47,54,61,62	0
2	2AN	F	208	21/21	0.81	0.17	53,64,78,85	0
2	2AN	C	306	21/21	0.81	0.16	47,52,78,86	0
2	2AN	J	204	21/21	0.82	0.17	60,68,72,73	0
2	2AN	D	706	21/21	0.83	0.14	51,56,65,65	0
2	2AN	M	505	21/21	0.83	0.17	49,55,79,81	0
2	2AN	C	307	21/21	0.84	0.17	51,56,68,73	0
2	2AN	F	207	21/21	0.84	0.25	38,40,42,43	21
2	2AN	H	1109	21/21	0.84	0.16	53,60,66,66	0
2	2AN	F	206	21/21	0.85	0.14	50,55,66,69	0
2	2AN	J	202	21/21	0.85	0.16	50,55,58,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	2AN	G	304	21/21	0.86	0.15	41,45,58,60	0
2	2AN	E	504	21/21	0.86	0.13	36,42,47,51	0
2	2AN	P	503	21/21	0.86	0.13	48,52,68,69	0
2	2AN	P	507	21/21	0.86	0.16	42,45,59,62	0
2	2AN	M	506	21/21	0.86	0.12	40,43,55,59	0
2	2AN	M	508	21/21	0.86	0.15	45,50,54,57	0
2	2AN	H	1107	21/21	0.86	0.15	43,50,53,54	0
2	2AN	A	202	21/21	0.87	0.13	37,40,52,56	0
2	2AN	N	204	21/21	0.87	0.14	41,45,48,51	0
2	2AN	I	202	21/21	0.87	0.14	41,44,49,52	0
2	2AN	M	503	21/21	0.87	0.13	44,47,52,57	0
2	2AN	P	506	21/21	0.87	0.15	46,50,59,61	0
2	2AN	D	701	21/21	0.87	0.15	44,51,58,60	0
2	2AN	C	305	21/21	0.87	0.13	43,48,54,59	0
2	2AN	H	1101	21/21	0.87	0.14	47,50,56,59	0
2	2AN	D	704	21/21	0.87	0.15	46,53,56,59	0
2	2AN	O	203	21/21	0.88	0.14	41,46,54,58	0
2	2AN	F	202	21/21	0.88	0.14	44,49,55,58	0
2	2AN	H	1108	21/21	0.88	0.15	41,45,59,64	0
2	2AN	B	204	21/21	0.88	0.14	44,48,52,53	0
2	2AN	B	203	21/21	0.88	0.14	44,49,56,61	0
2	2AN	E	502	21/21	0.88	0.14	43,47,53,55	0
2	2AN	L	204	21/21	0.88	0.13	37,44,53,55	0
2	2AN	M	502	21/21	0.88	0.13	38,40,43,44	0
2	2AN	K	204	21/21	0.89	0.12	36,41,50,54	0
2	2AN	J	203	21/21	0.89	0.14	43,45,52,54	0
2	2AN	H	1105	21/21	0.89	0.13	38,44,57,68	0
2	2AN	K	202	21/21	0.89	0.13	40,42,48,50	0
2	2AN	G	305	21/21	0.90	0.12	40,42,50,53	0
2	2AN	P	502	21/21	0.90	0.12	40,44,47,54	0
2	2AN	C	303	21/21	0.90	0.11	39,42,47,50	0
2	2AN	N	201	21/21	0.90	0.12	38,42,49,53	0
2	2AN	I	205	21/21	0.90	0.12	40,43,46,52	0
2	2AN	A	203	21/21	0.90	0.12	37,42,53,56	0
2	2AN	L	203	21/21	0.90	0.13	38,41,46,47	0
2	2AN	O	204	21/21	0.90	0.11	44,48,56,57	0
2	2AN	H	1106	21/21	0.91	0.11	34,36,38,39	0
2	2AN	N	202	21/21	0.91	0.12	44,48,54,57	0
2	2AN	P	505	21/21	0.91	0.11	33,36,39,40	0
2	2AN	L	202	21/21	0.91	0.12	38,41,44,45	0
2	2AN	G	302	21/21	0.91	0.13	36,41,56,59	0
2	2AN	M	507	21/21	0.91	0.12	41,43,50,51	0

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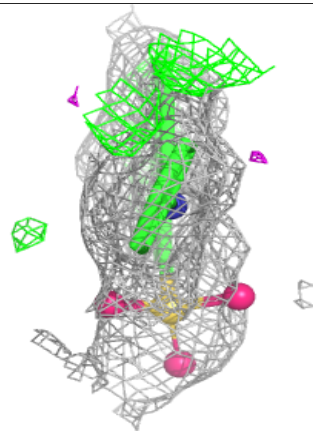
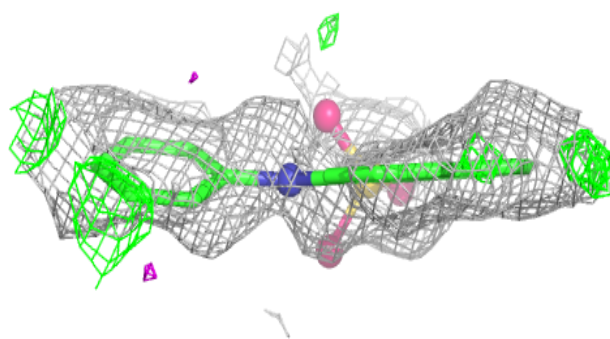
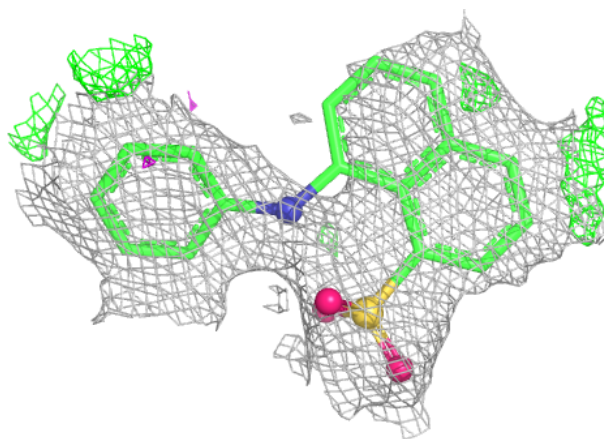
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	2AN	C	301	21/21	0.91	0.11	38,39,42,45	0
2	2AN	J	201	21/21	0.91	0.13	38,43,48,49	0
2	2AN	C	304	21/21	0.92	0.12	44,46,51,55	0
2	2AN	B	201	21/21	0.92	0.12	35,41,42,44	0
2	2AN	F	201	21/21	0.92	0.12	36,38,41,42	0
2	2AN	G	301	21/21	0.92	0.12	39,41,45,45	0
2	2AN	B	202	21/21	0.92	0.12	33,35,39,40	0
2	2AN	F	203	21/21	0.92	0.12	43,47,51,54	0
2	2AN	A	204	21/21	0.92	0.12	36,38,39,40	0
2	2AN	K	203	21/21	0.92	0.11	37,40,48,50	0
2	2AN	F	205	21/21	0.92	0.12	43,47,50,53	0
2	2AN	O	202	21/21	0.93	0.11	38,43,56,59	0
2	2AN	M	504	21/21	0.93	0.11	31,33,34,37	0
2	2AN	H	1104	21/21	0.93	0.12	38,41,46,48	0
2	2AN	A	205	21/21	0.93	0.11	34,39,42,44	0
2	2AN	E	505	21/21	0.93	0.10	39,41,46,47	0
2	2AN	A	201	21/21	0.93	0.11	37,40,41,45	0
2	2AN	E	503	21/21	0.94	0.10	32,34,37,38	0
2	2AN	C	309	21/21	0.94	0.11	30,38,40,42	0
2	2AN	D	703	21/21	0.94	0.11	34,35,38,38	0
2	2AN	E	501	21/21	0.94	0.11	29,32,37,39	0
2	2AN	K	207	21/21	0.94	0.11	31,35,39,42	0
2	2AN	P	504	21/21	0.94	0.10	30,34,37,38	0
2	2AN	H	1103	21/21	0.94	0.10	40,43,45,46	0
2	2AN	C	302	21/21	0.94	0.11	30,34,36,37	0
2	2AN	I	203	21/21	0.94	0.12	37,39,42,44	0
2	2AN	M	501	21/21	0.94	0.10	28,34,39,40	0
2	2AN	K	201	21/21	0.94	0.10	32,34,37,38	0
2	2AN	I	204	21/21	0.94	0.10	37,42,44,47	0
2	2AN	L	201	21/21	0.95	0.10	31,33,36,37	0
2	2AN	O	201	21/21	0.95	0.11	30,32,35,36	0
2	2AN	I	201	21/21	0.95	0.09	31,33,34,36	0
2	2AN	H	1102	21/21	0.95	0.10	31,32,35,37	0
2	2AN	G	303	21/21	0.95	0.10	33,34,36,39	0

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

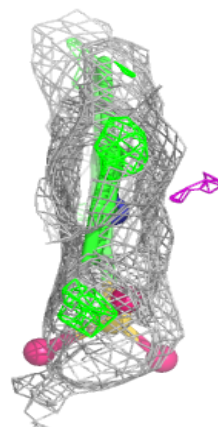
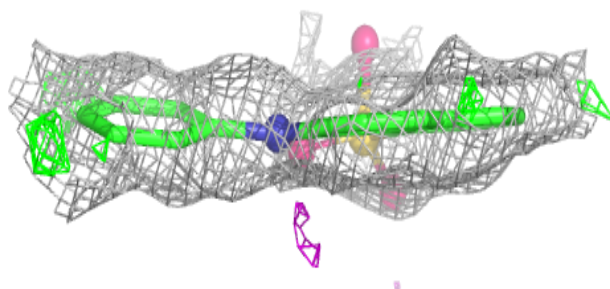
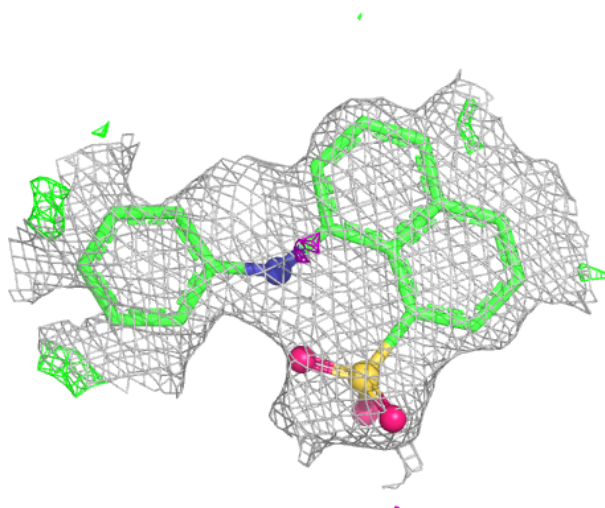
Electron density around 2AN K 206:

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



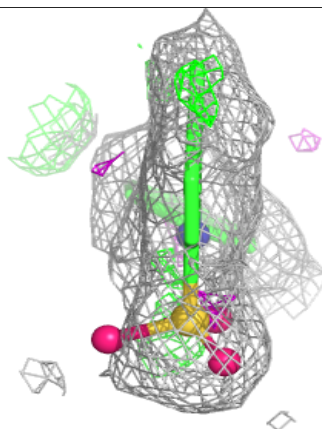
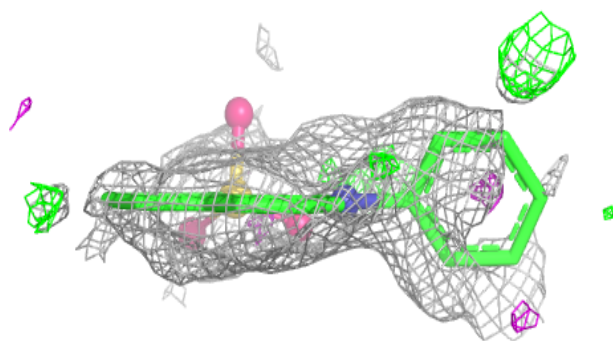
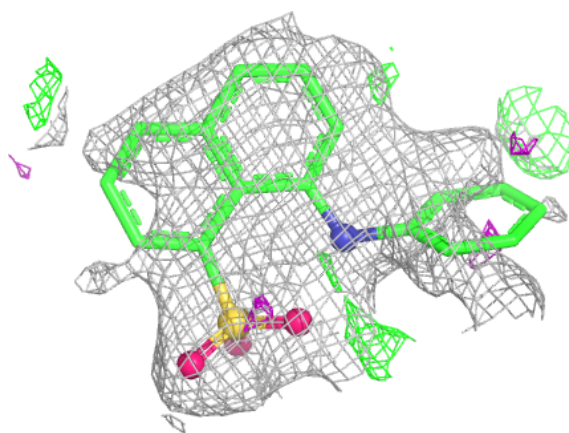
Electron density around 2AN E 507:

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



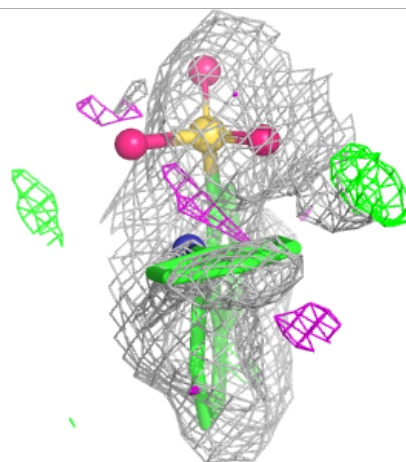
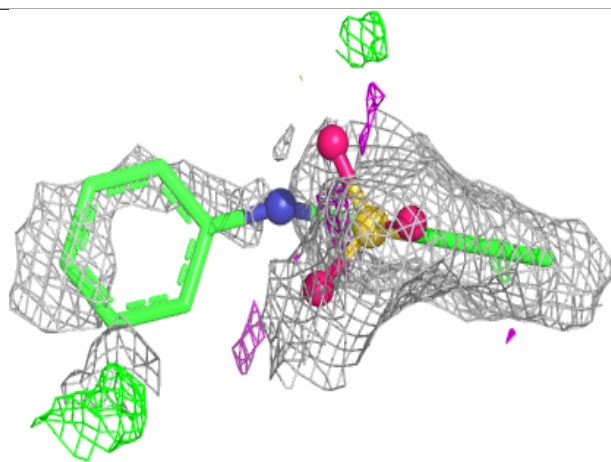
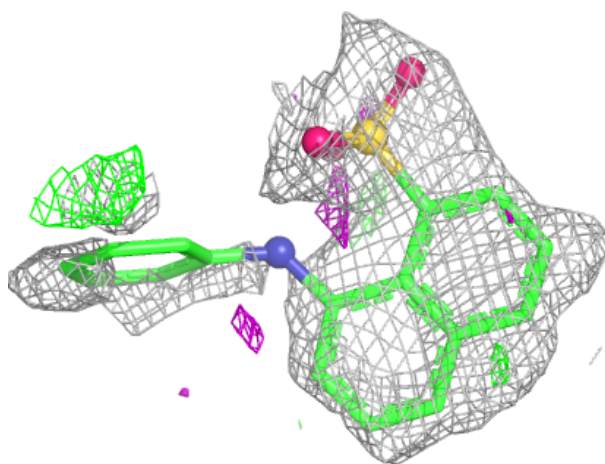
Electron density around 2AN K 205:

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



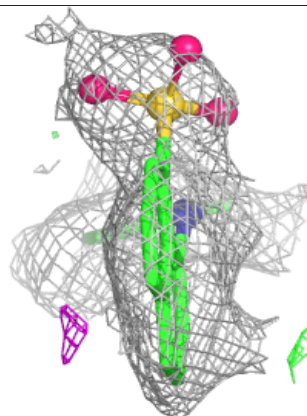
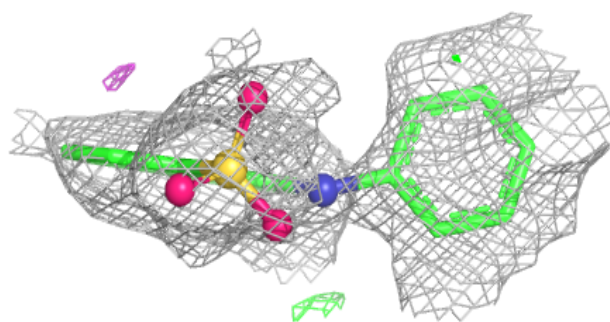
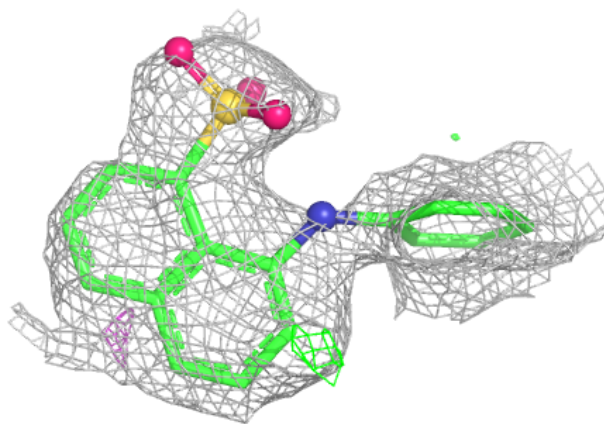
Electron density around 2AN P 509:

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



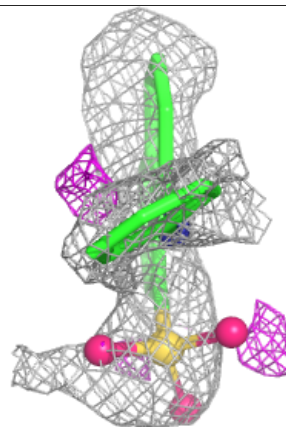
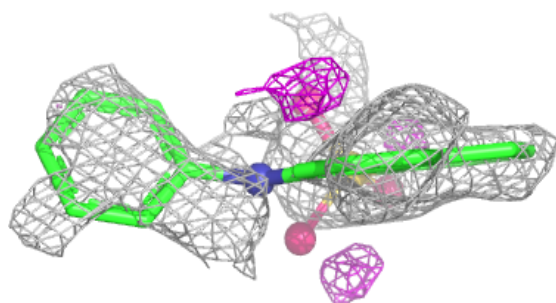
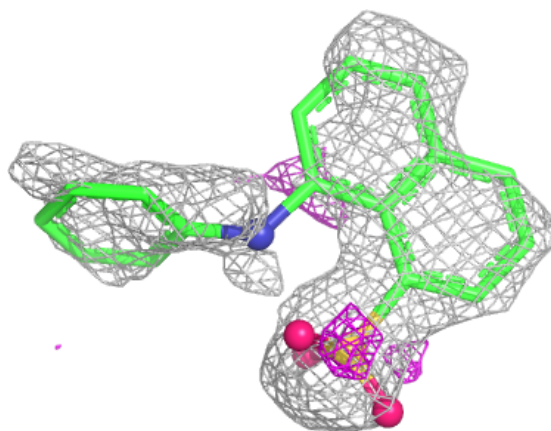
Electron density around 2AN M 509:

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



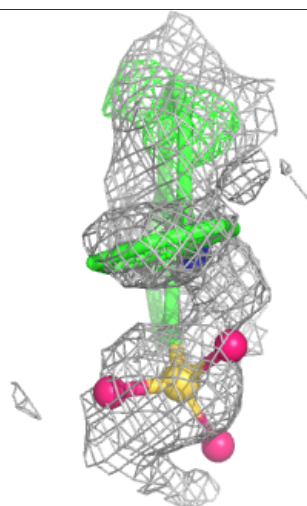
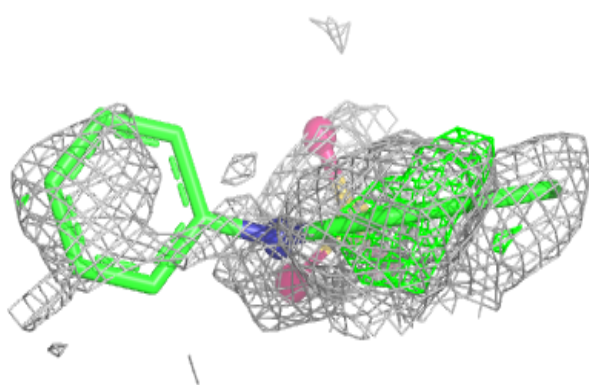
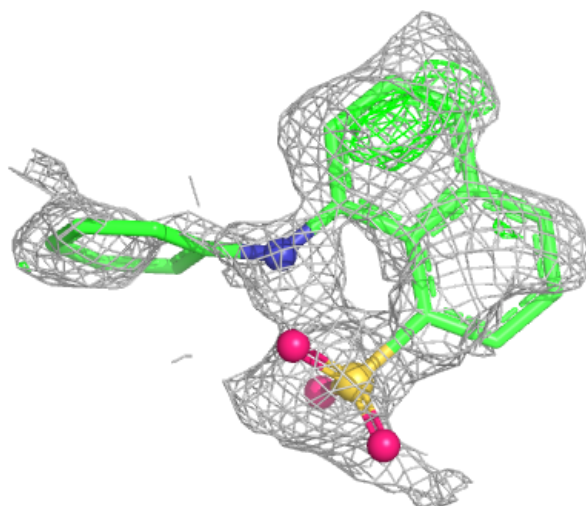
Electron density around 2AN D 702:

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



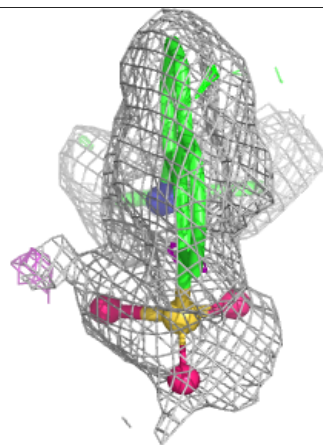
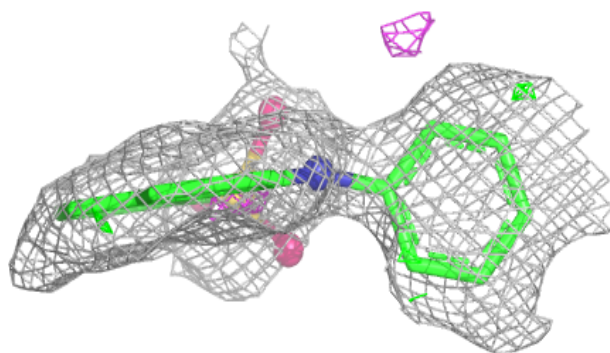
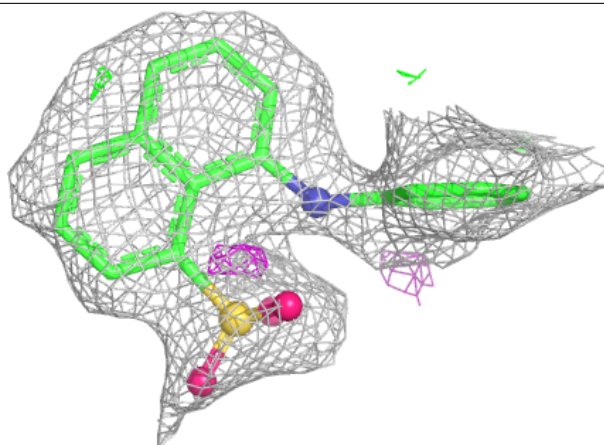
Electron density around 2AN J 206:

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



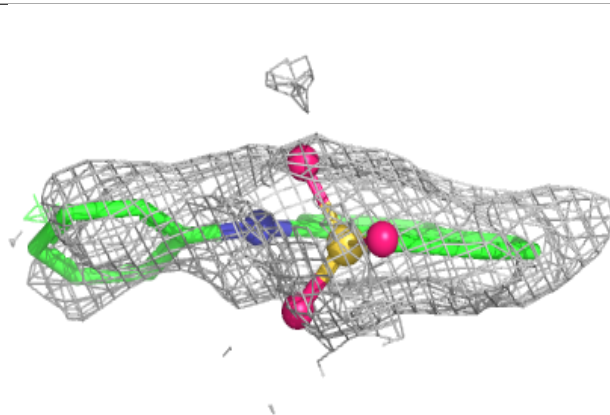
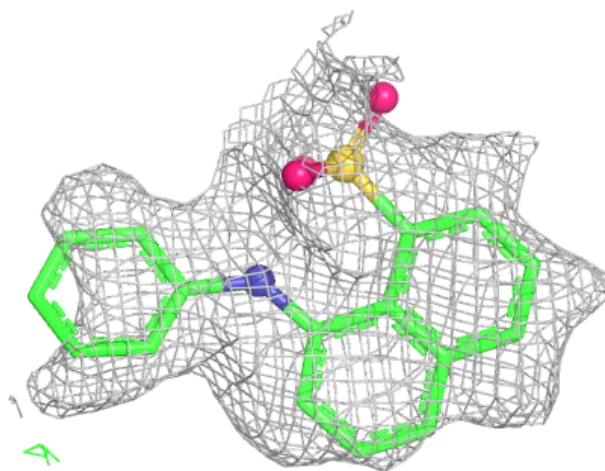
Electron density around 2AN C 308:

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



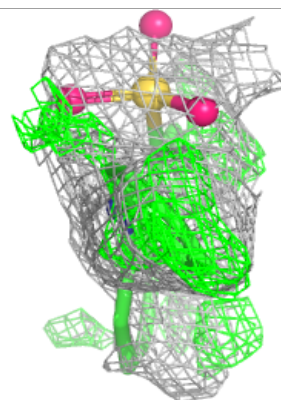
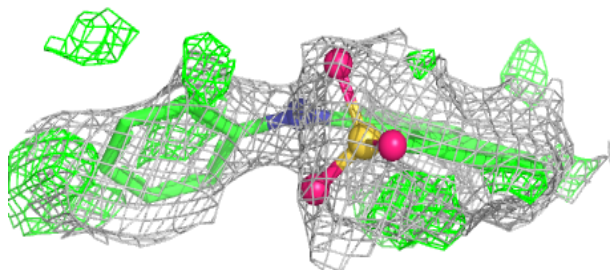
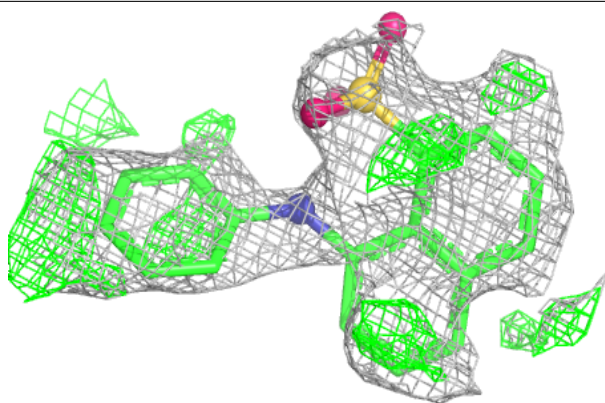
Electron density around 2AN N 203:

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

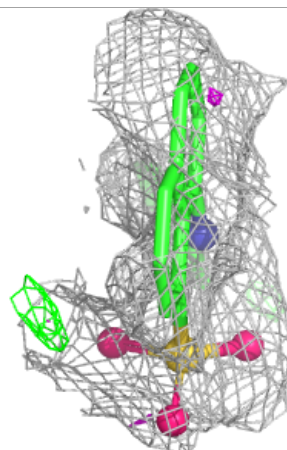
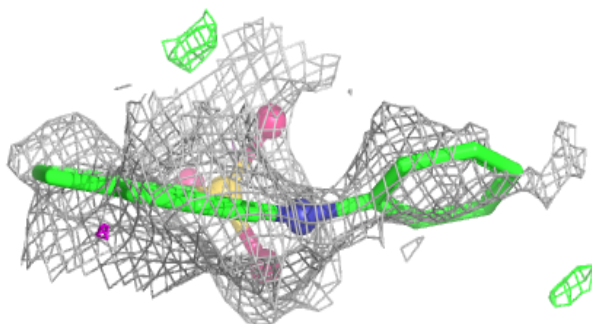
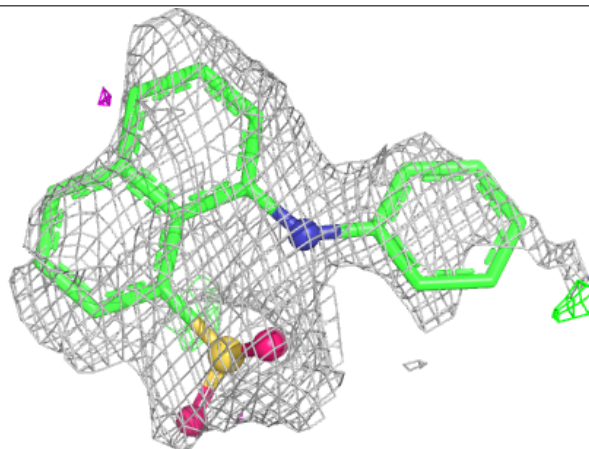


Electron density around 2AN G 306:

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

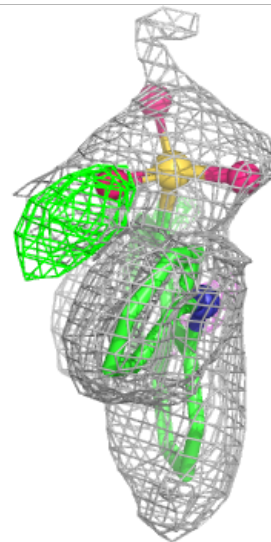
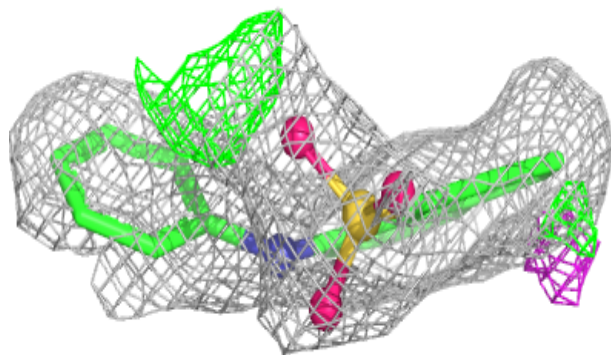
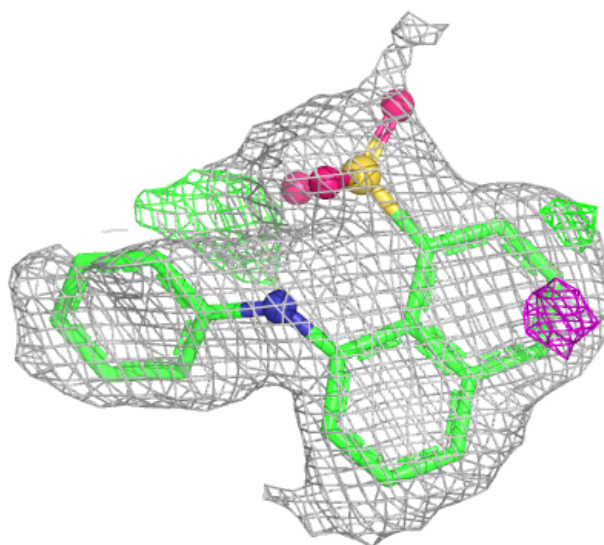
**Electron density around 2AN J 205:**

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



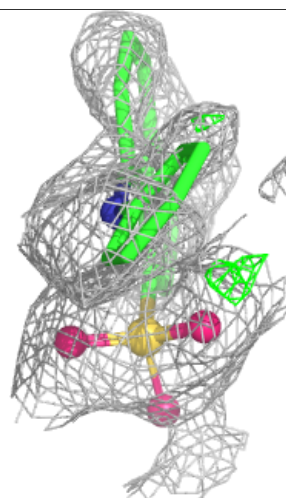
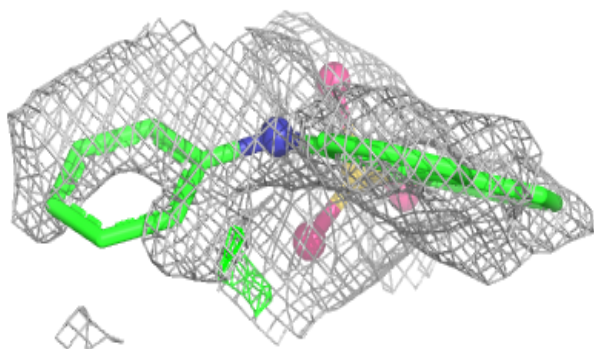
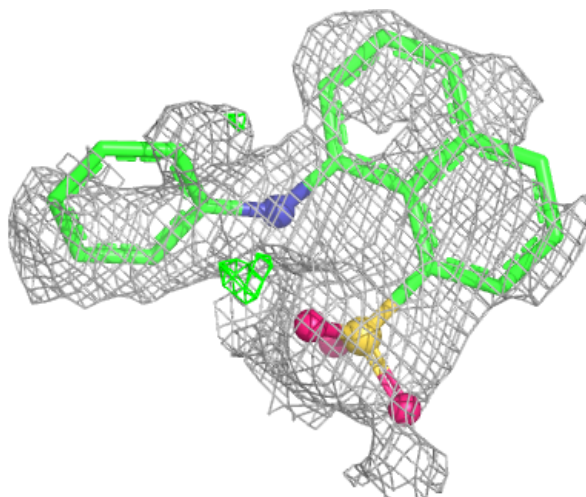
Electron density around 2AN F 204:

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



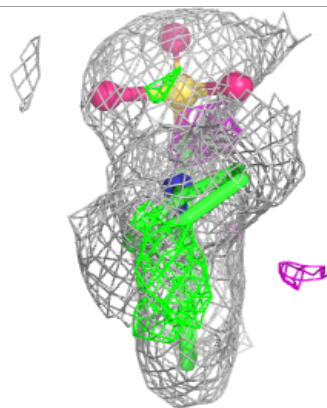
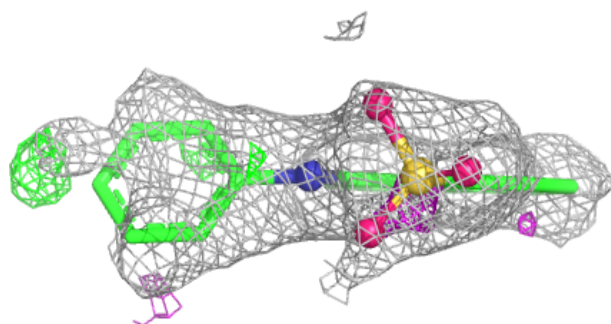
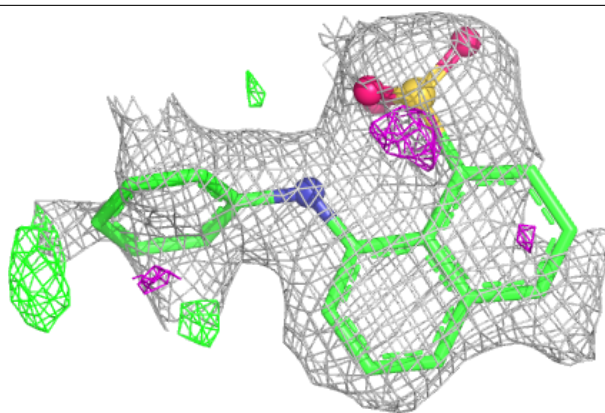
Electron density around 2AN D 705:

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



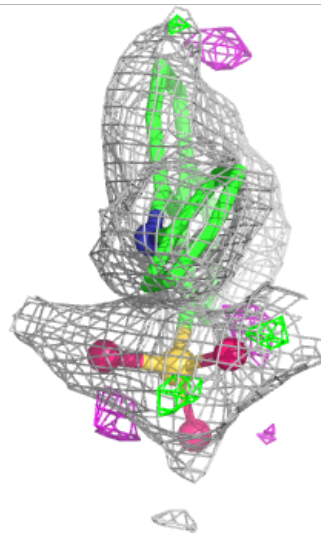
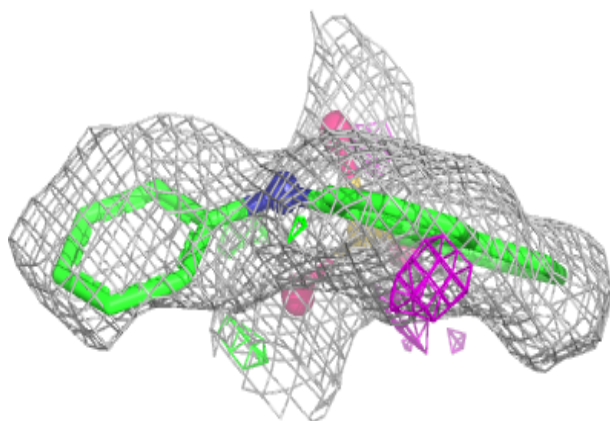
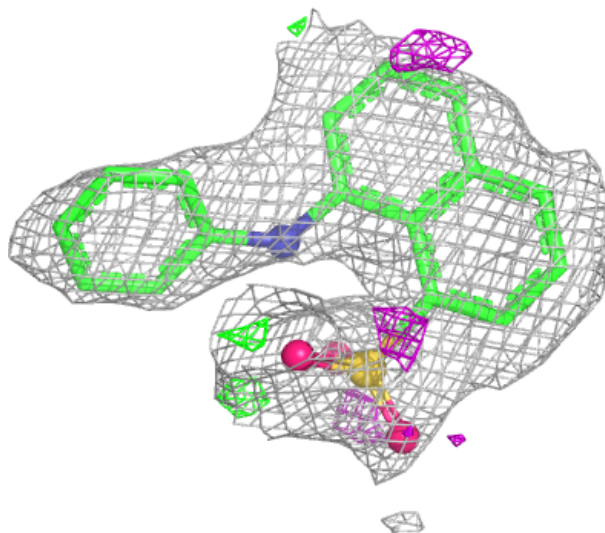
Electron density around 2AN E 506:

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



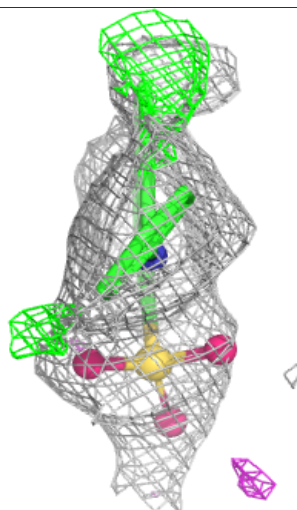
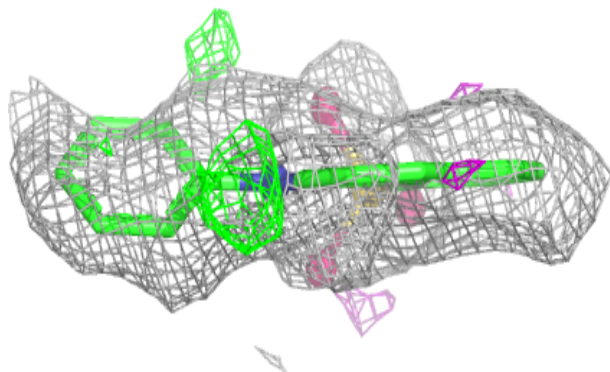
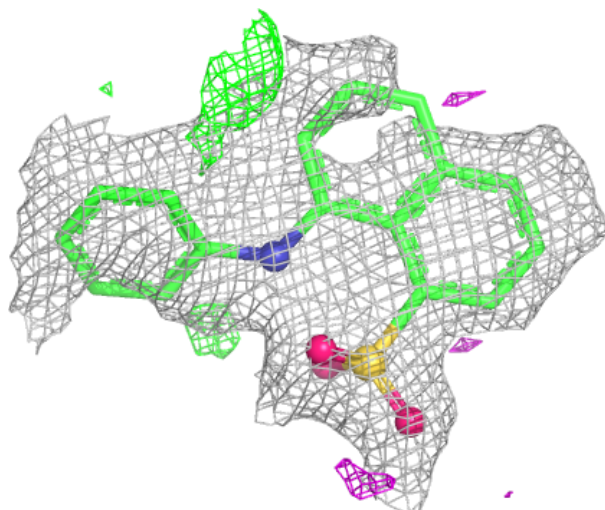
Electron density around 2AN P 501:

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



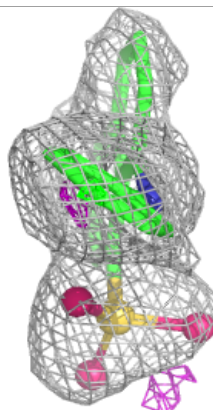
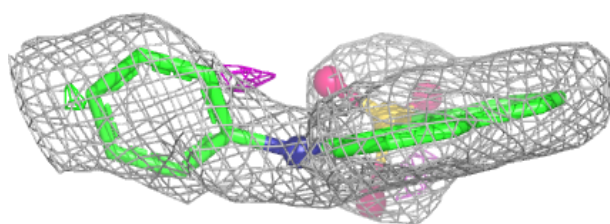
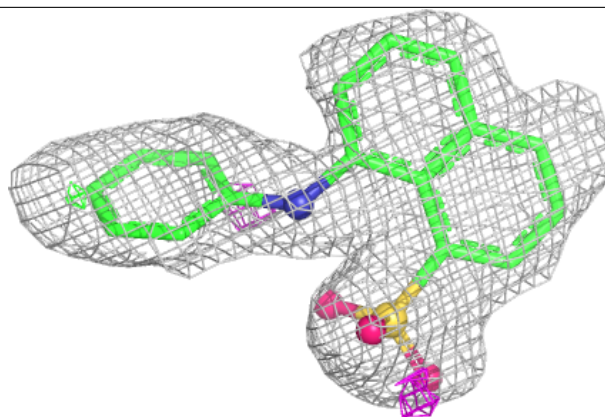
Electron density around 2AN P 508:

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



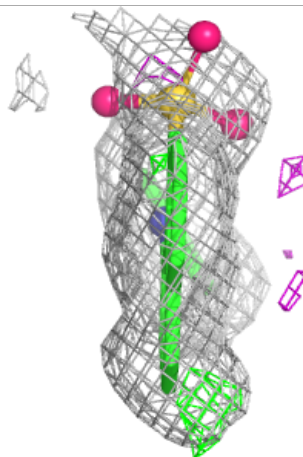
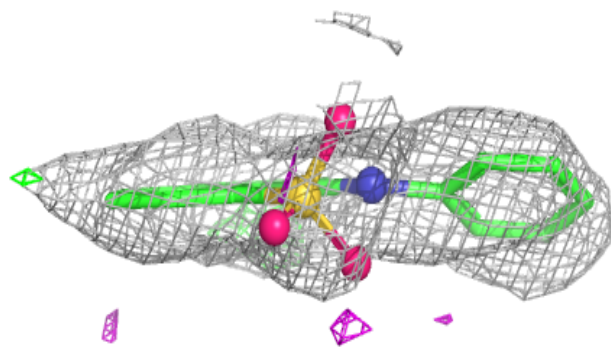
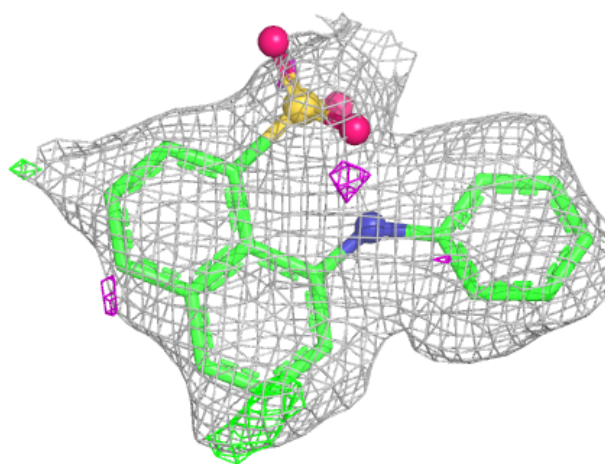
Electron density around 2AN F 208:

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



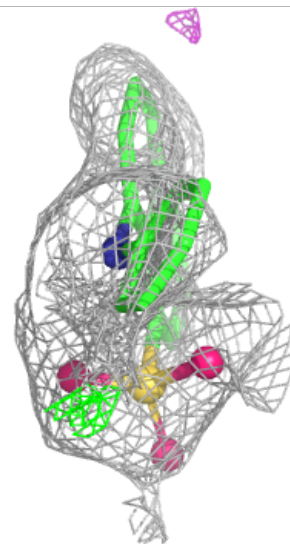
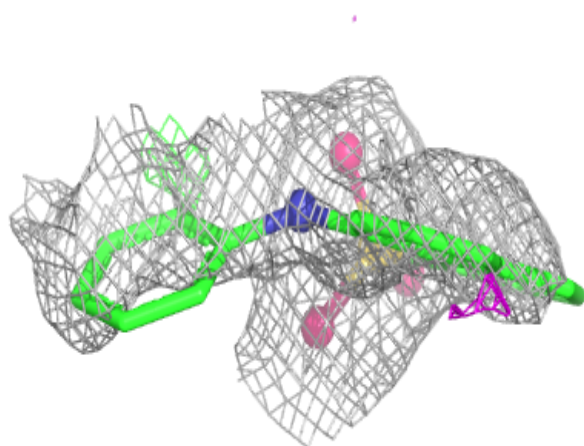
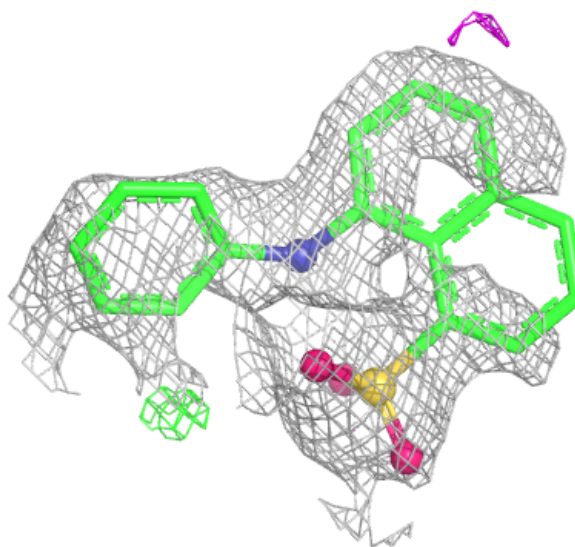
Electron density around 2AN C 306:

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



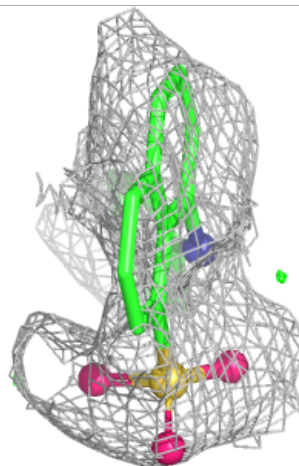
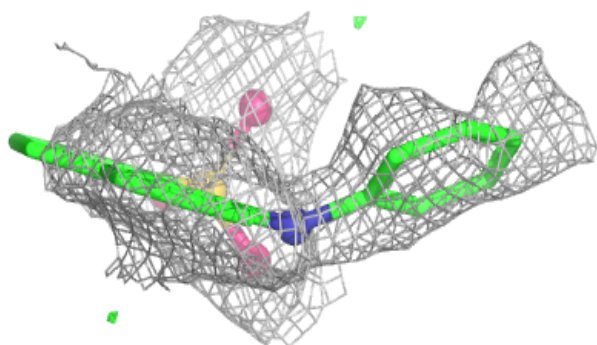
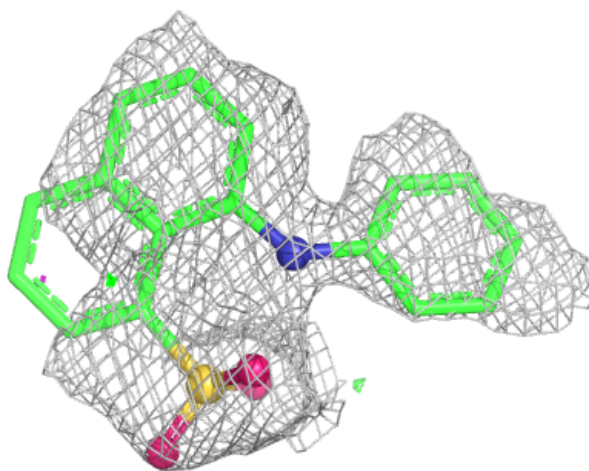
Electron density around 2AN J 204:

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



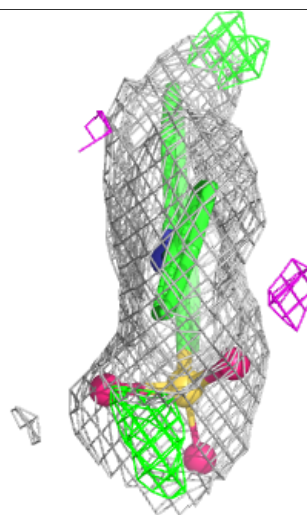
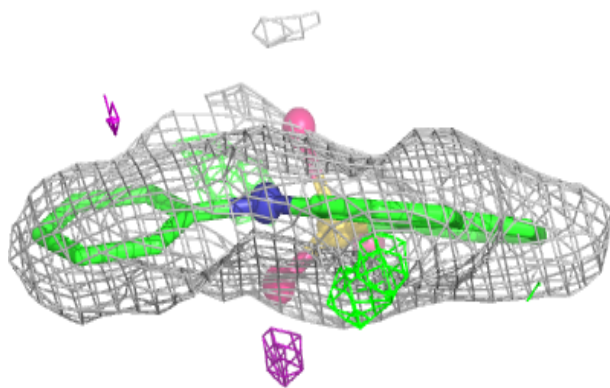
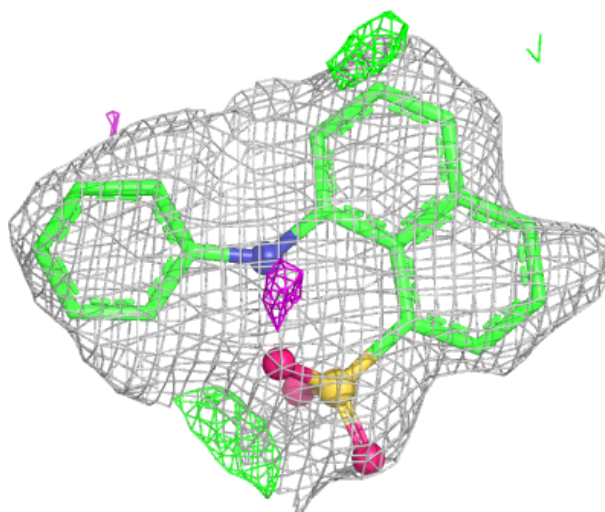
Electron density around 2AN D 706:

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



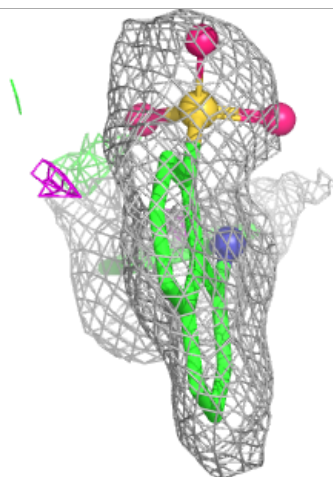
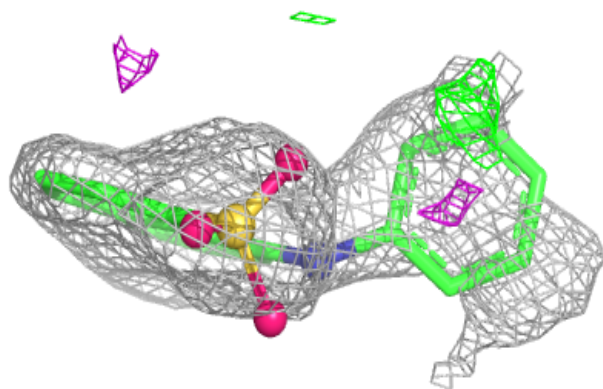
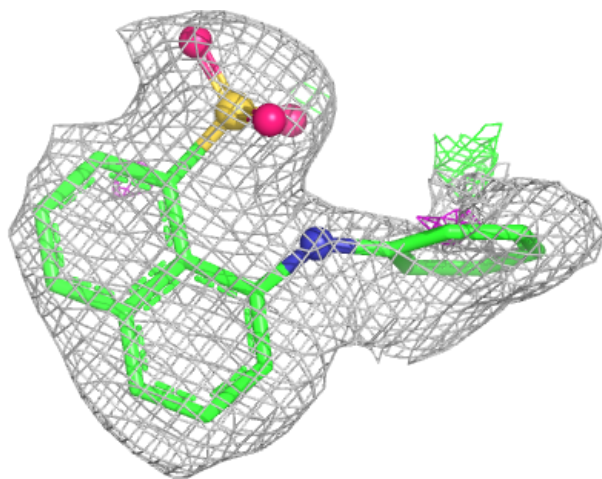
Electron density around 2AN M 505:

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



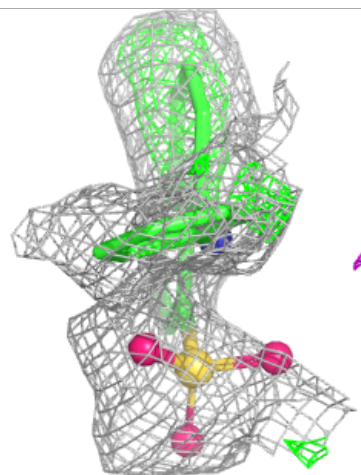
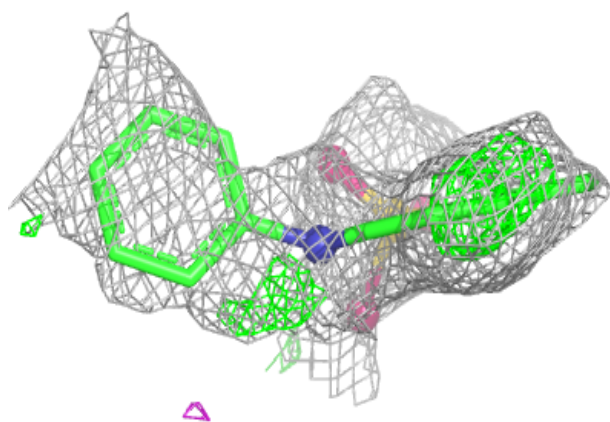
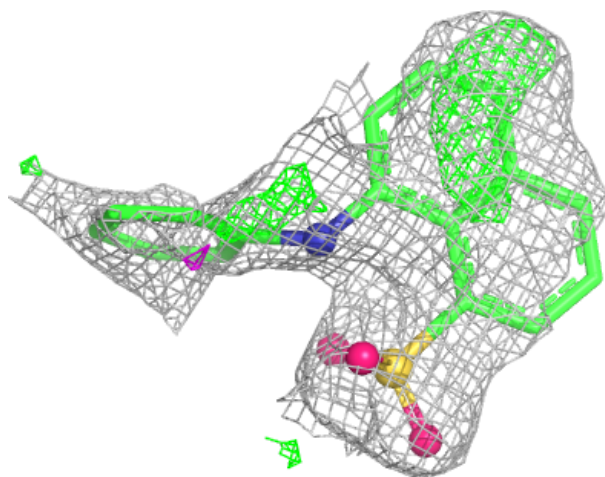
Electron density around 2AN C 307:

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



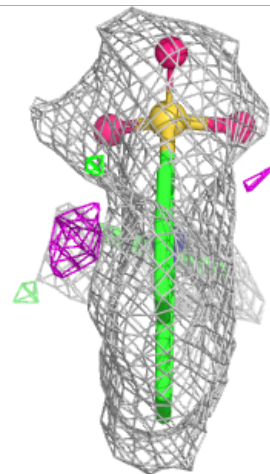
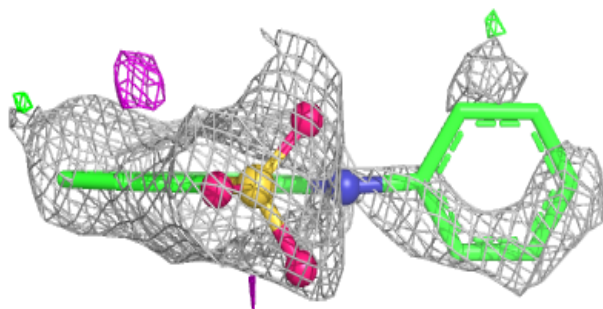
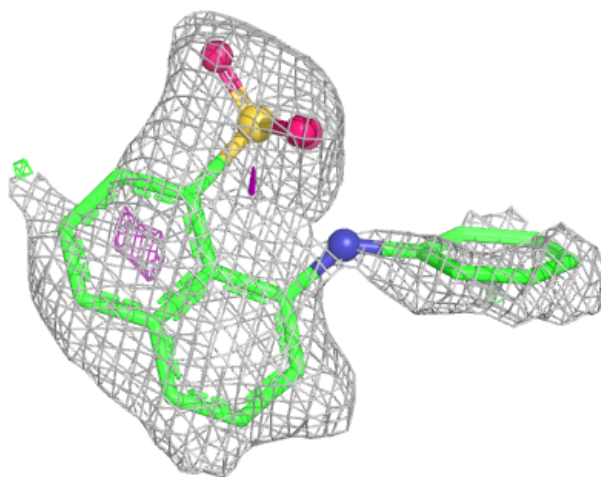
Electron density around 2AN F 207:

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



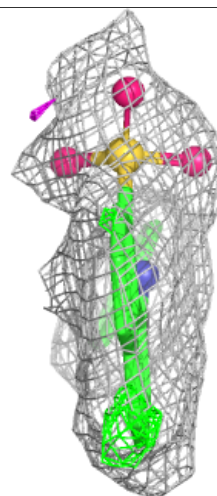
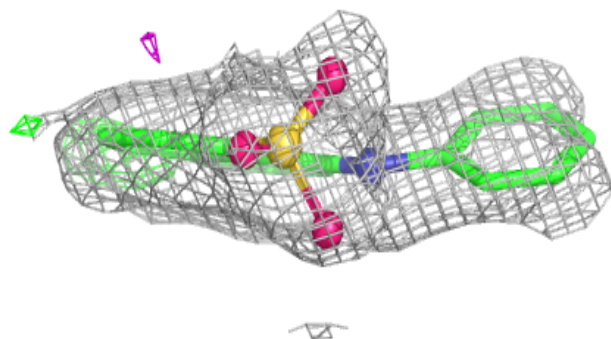
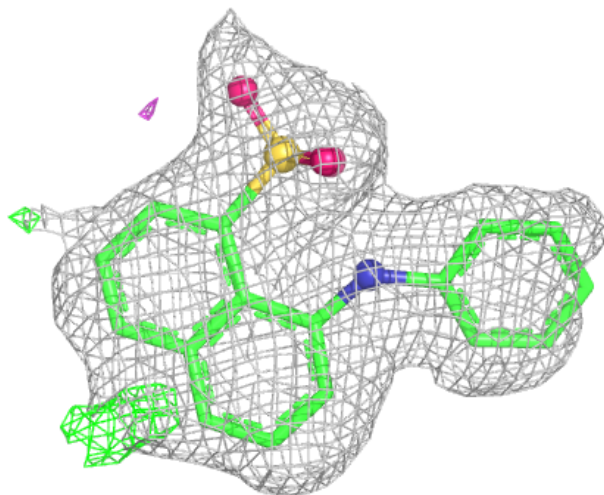
Electron density around 2AN H 1109:

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



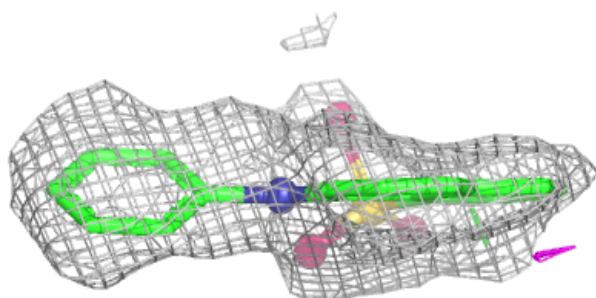
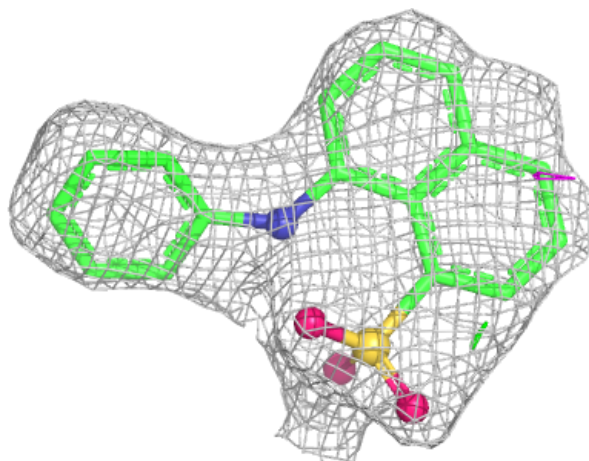
Electron density around 2AN F 206:

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



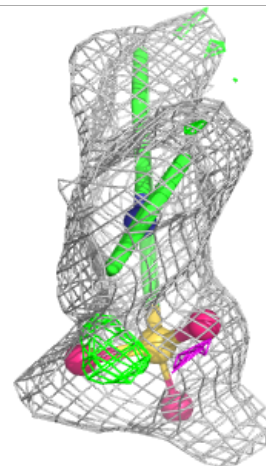
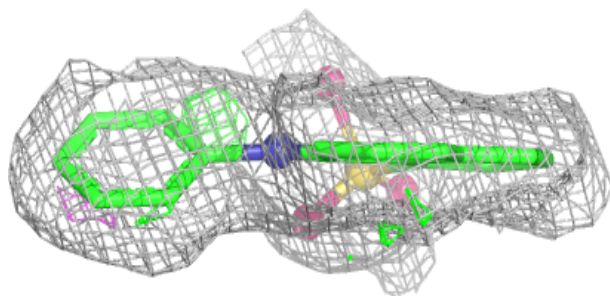
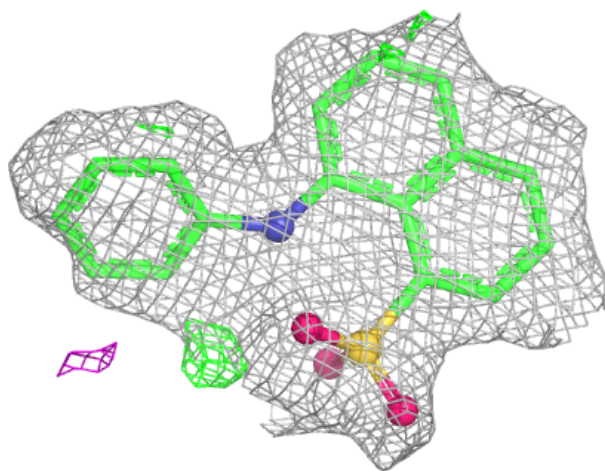
Electron density around 2AN J 202:

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



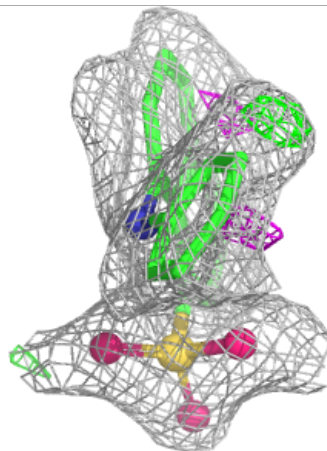
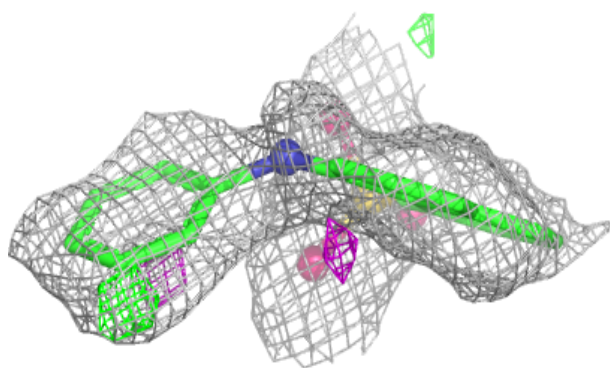
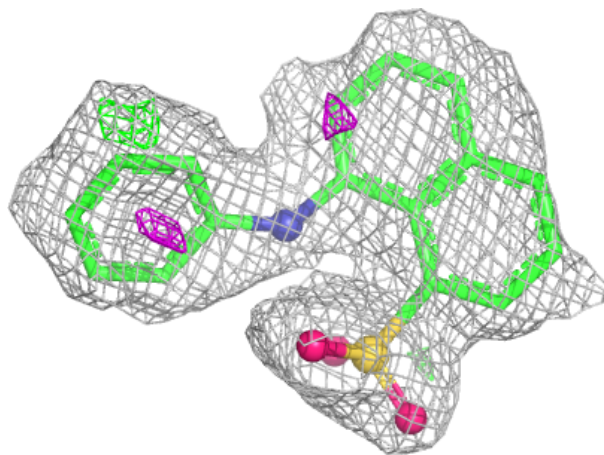
Electron density around 2AN G 304:

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



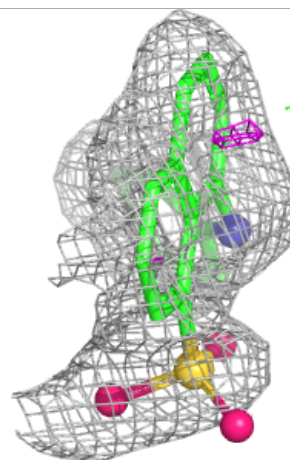
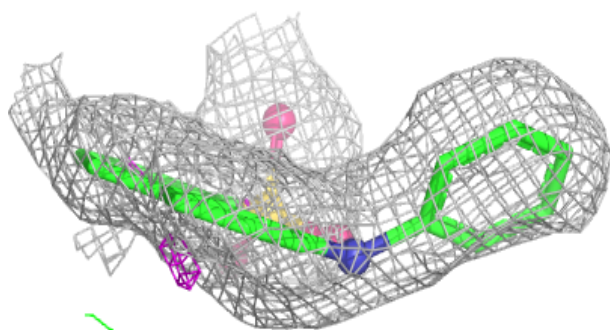
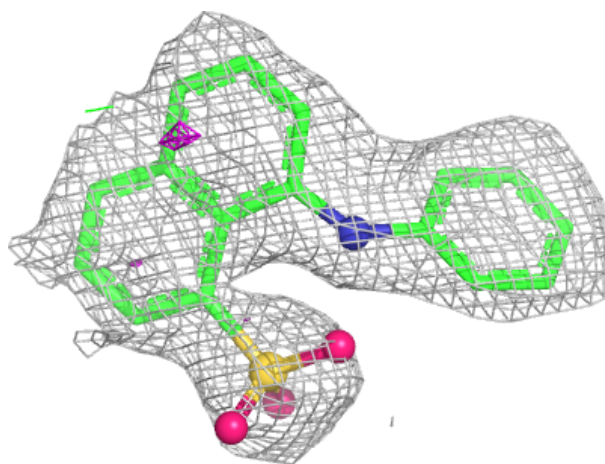
Electron density around 2AN E 504:

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



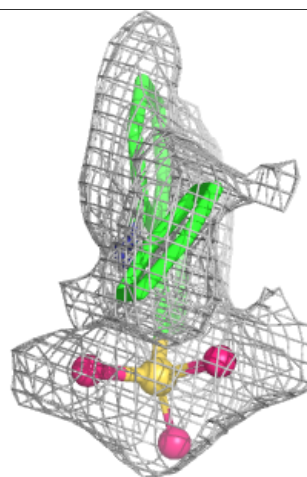
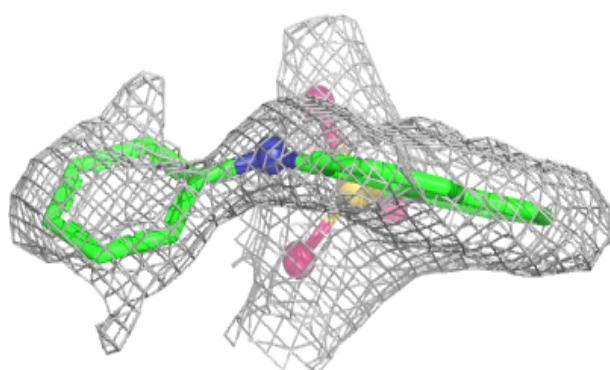
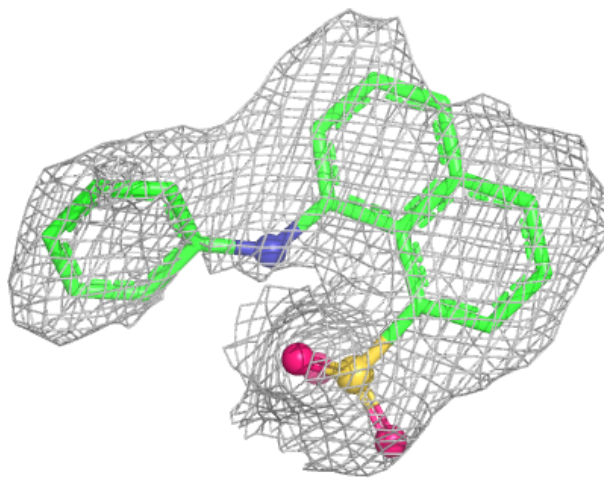
Electron density around 2AN P 503:

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



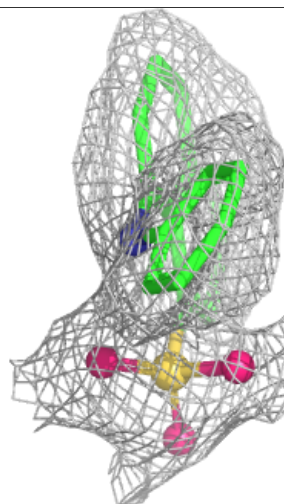
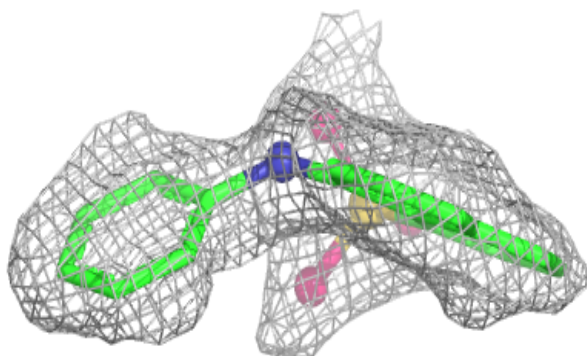
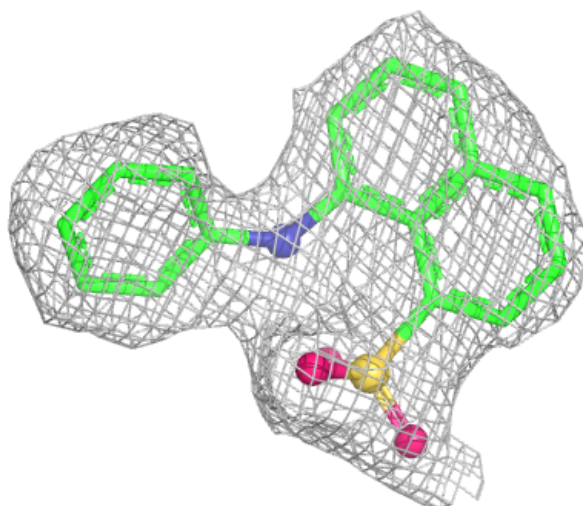
Electron density around 2AN P 507:

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



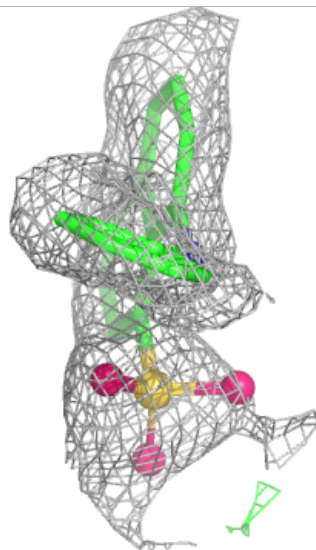
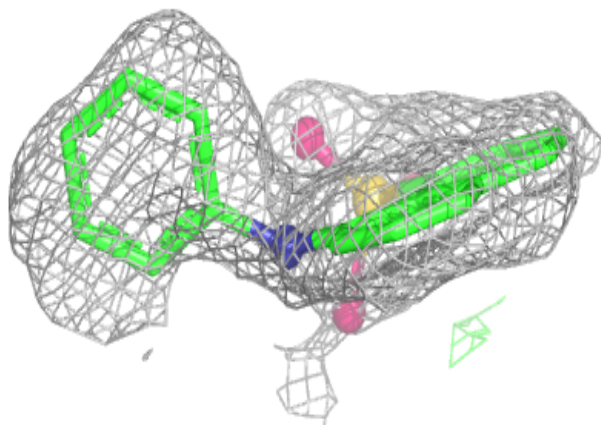
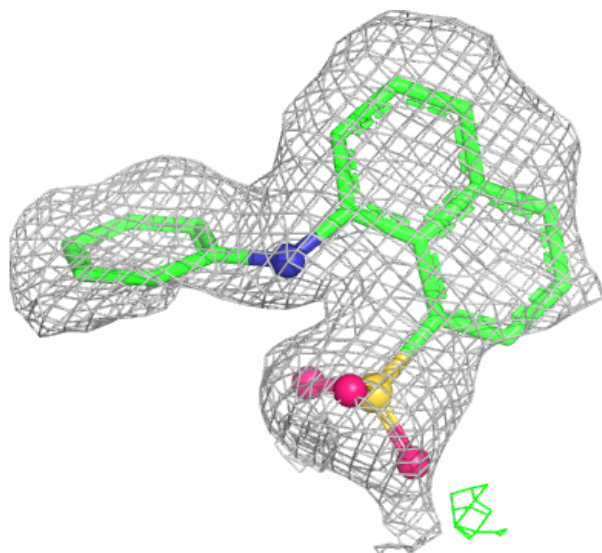
Electron density around 2AN M 506:

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



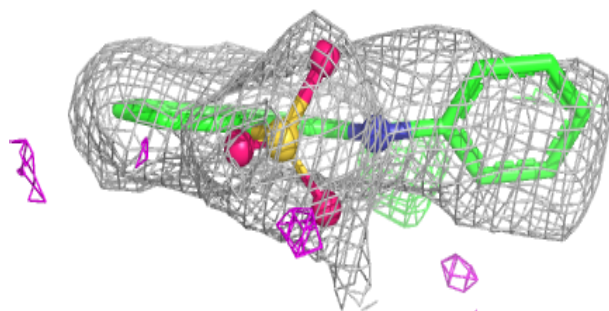
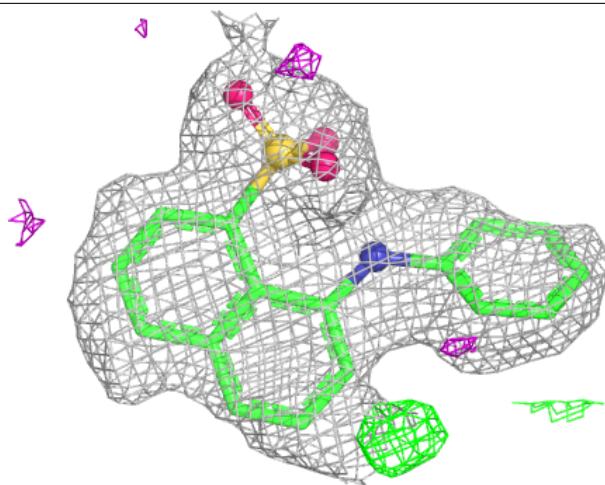
Electron density around 2AN M 508:

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



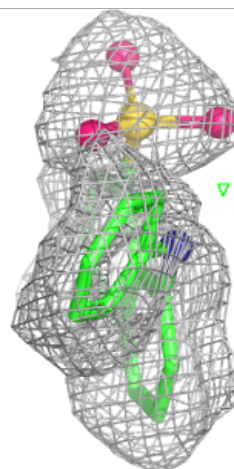
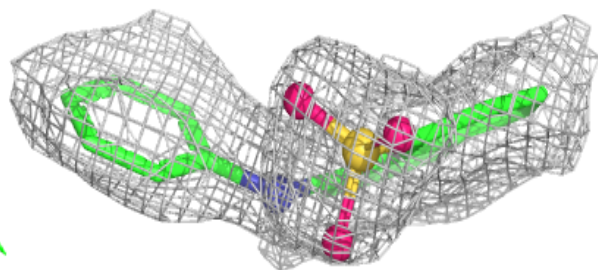
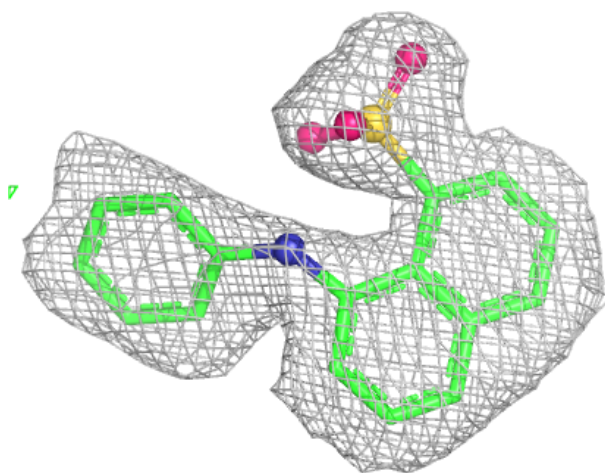
Electron density around 2AN H 1107:

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



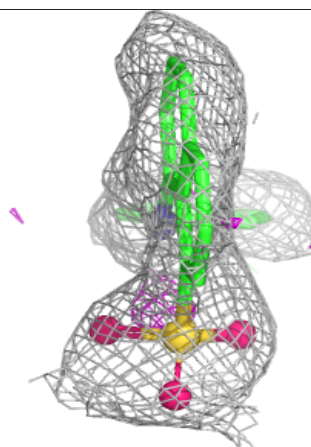
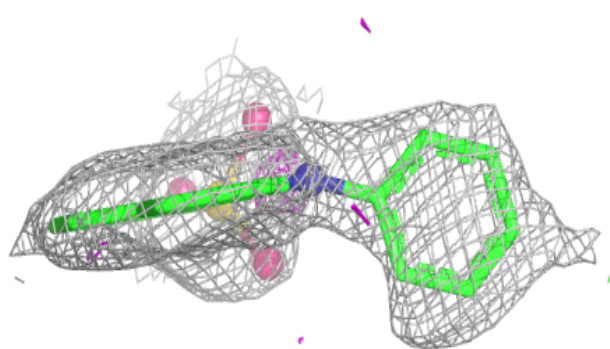
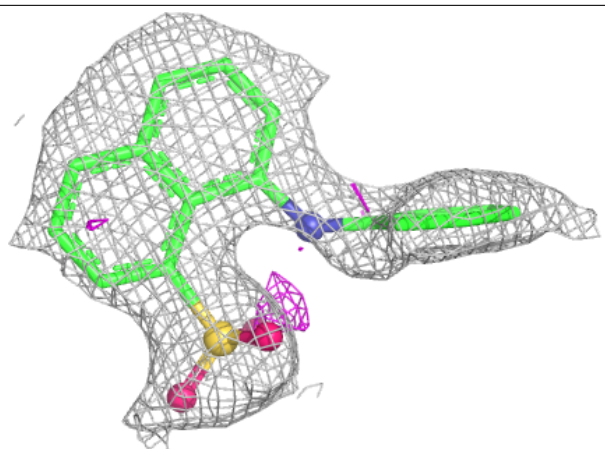
Electron density around 2AN A 202:

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



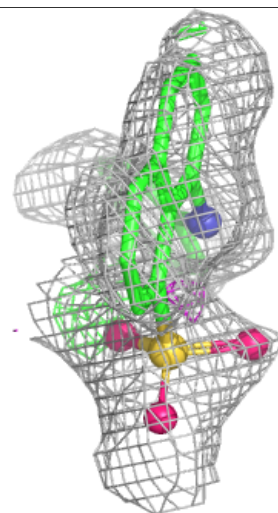
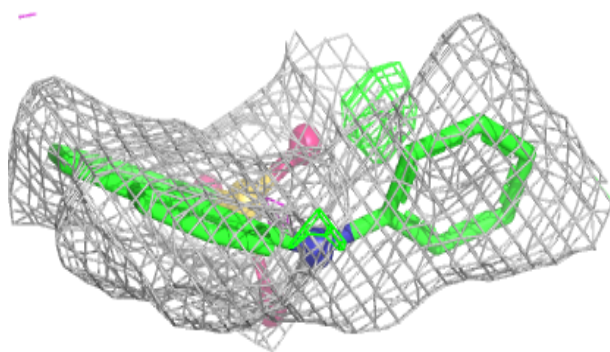
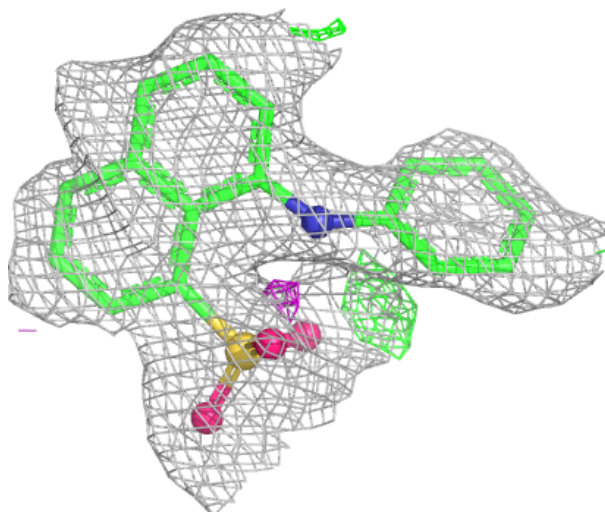
Electron density around 2AN N 204:

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



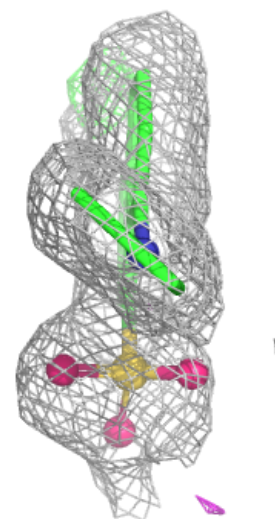
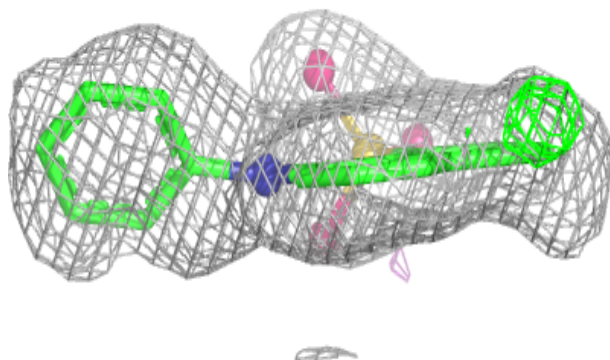
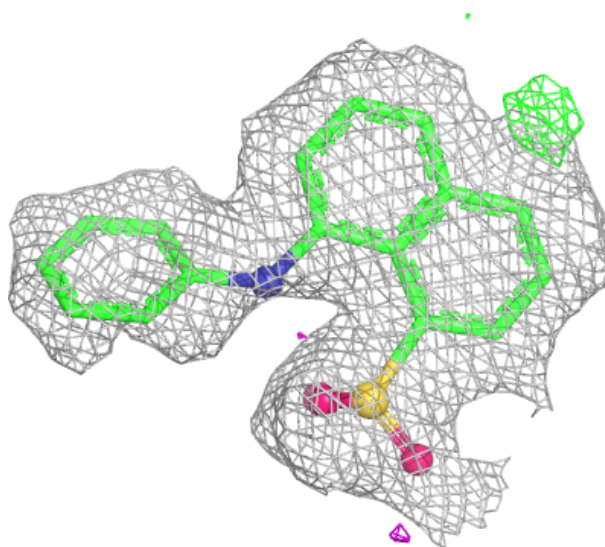
Electron density around 2AN I 202:

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



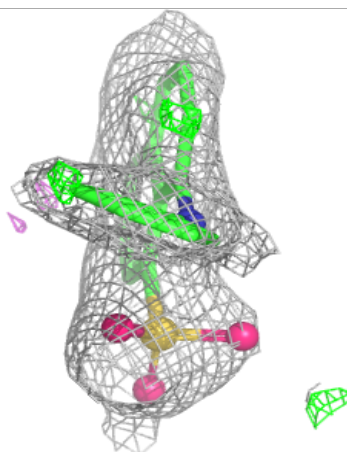
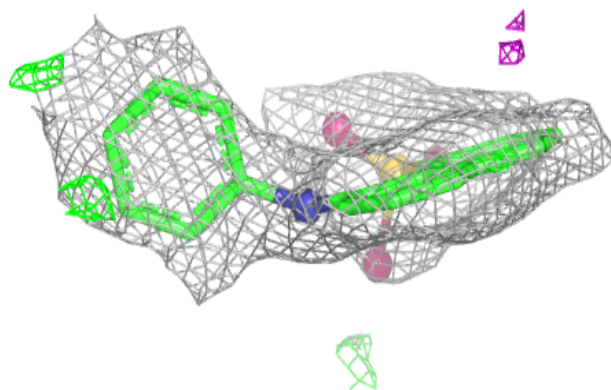
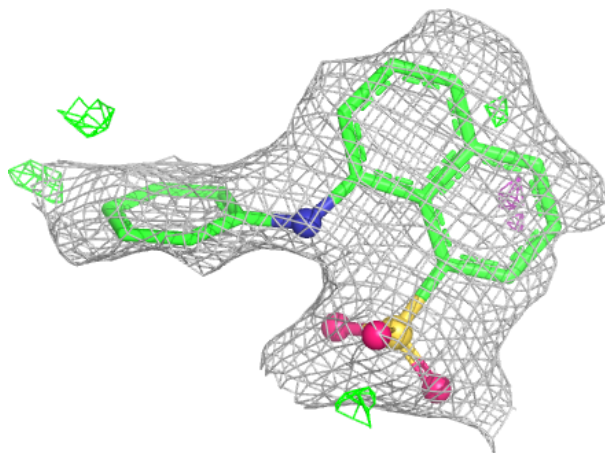
Electron density around 2AN M 503:

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



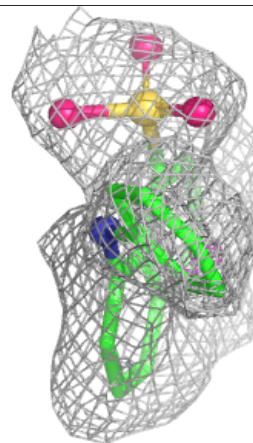
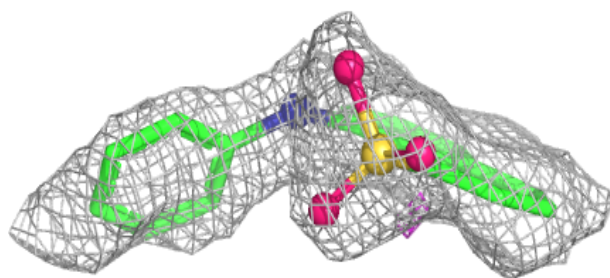
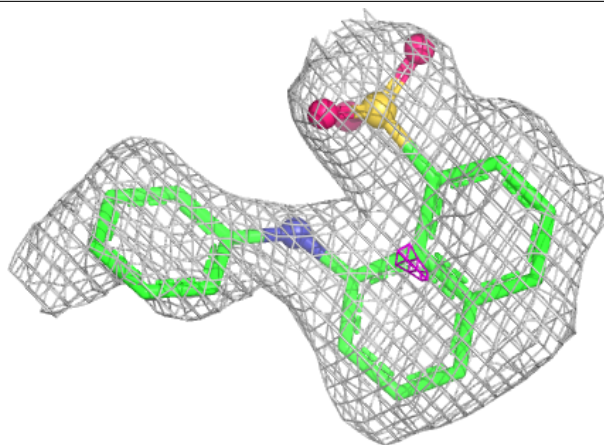
Electron density around 2AN P 506:

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



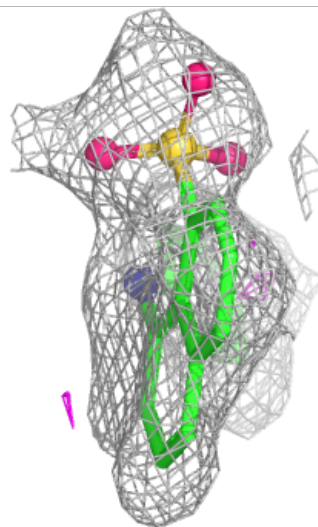
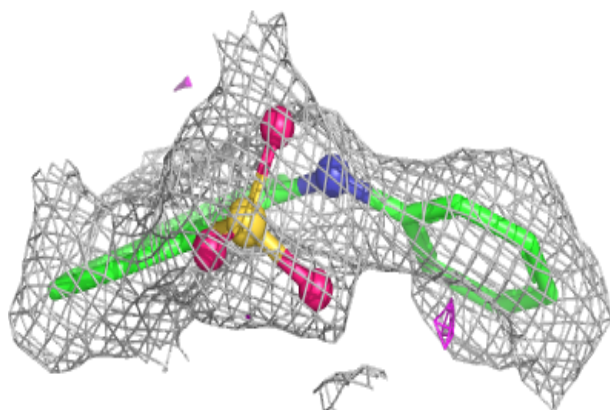
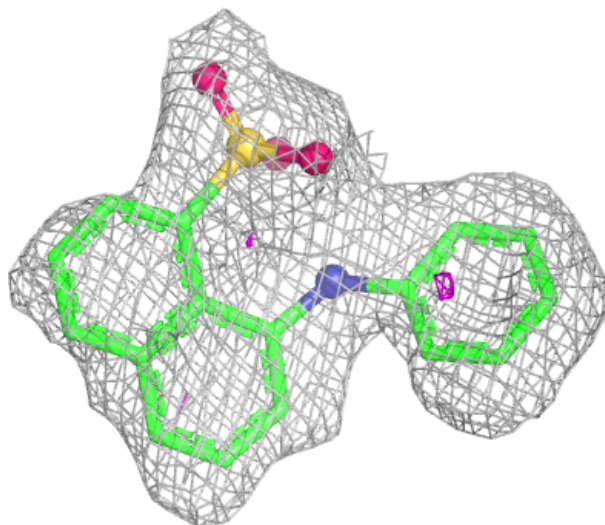
Electron density around 2AN D 701:

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



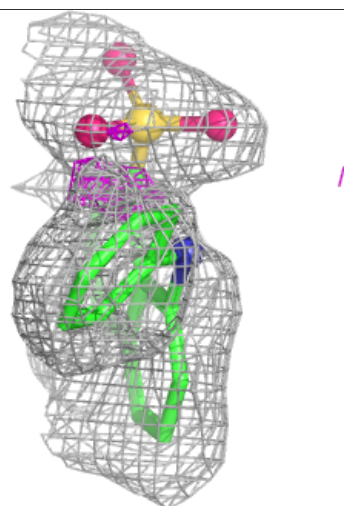
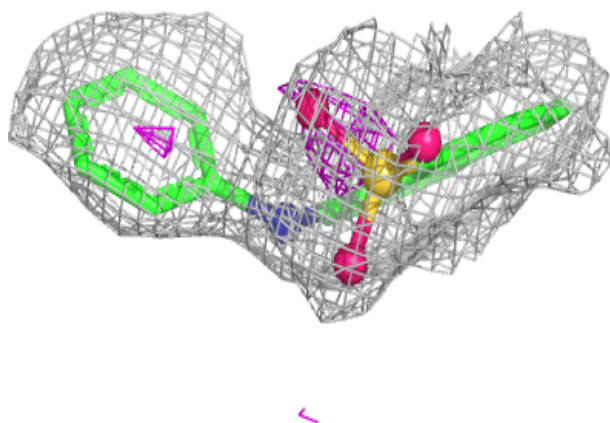
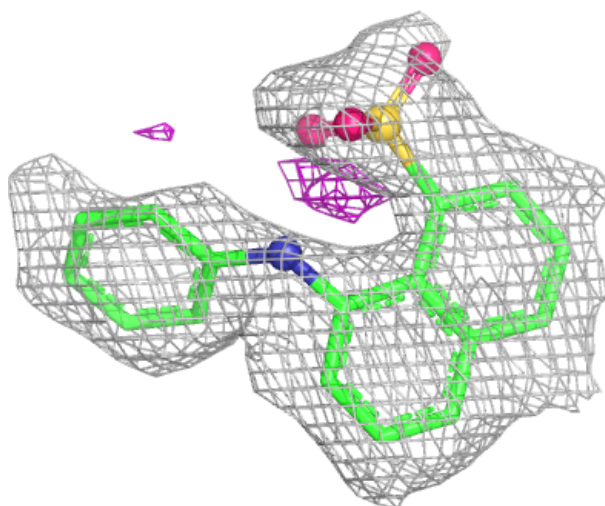
Electron density around 2AN C 305:

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



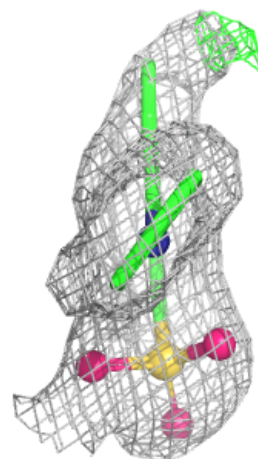
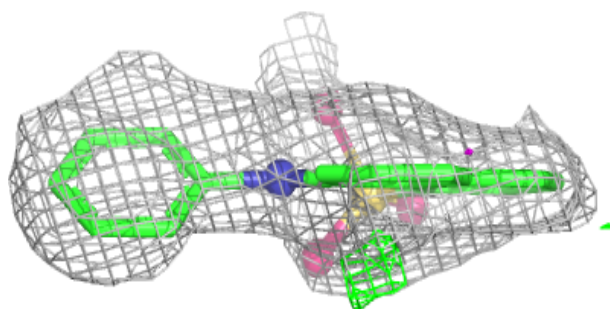
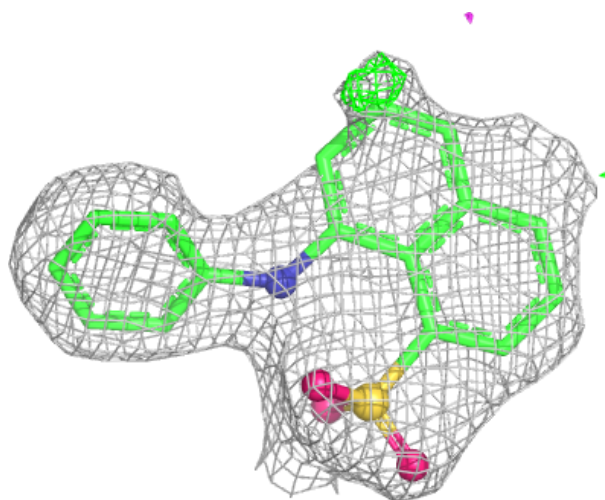
Electron density around 2AN H 1101:

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



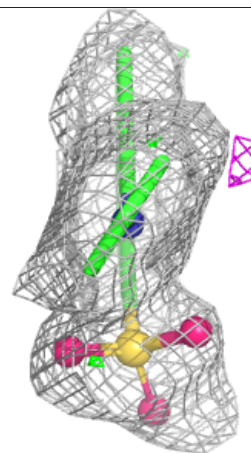
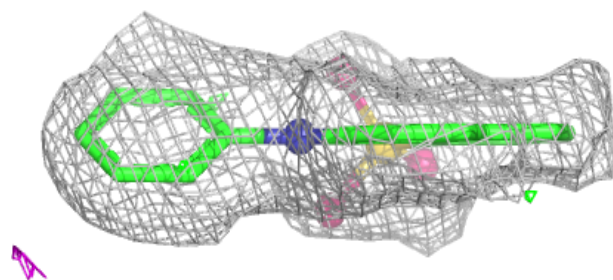
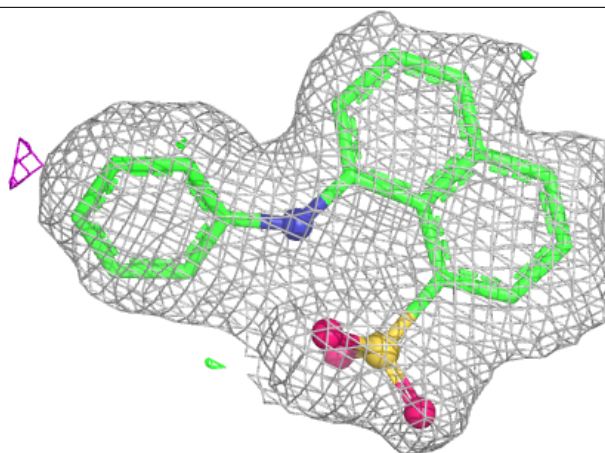
Electron density around 2AN D 704:

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



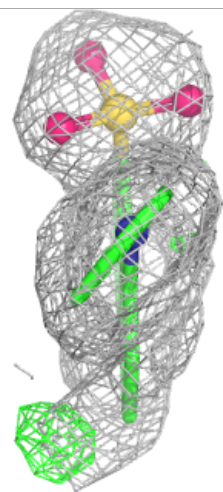
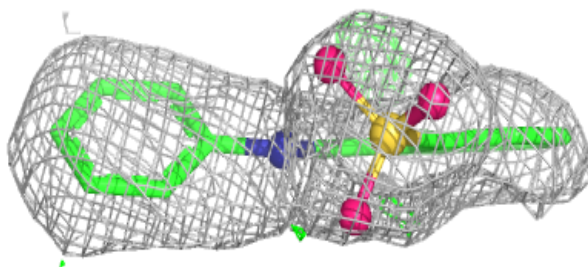
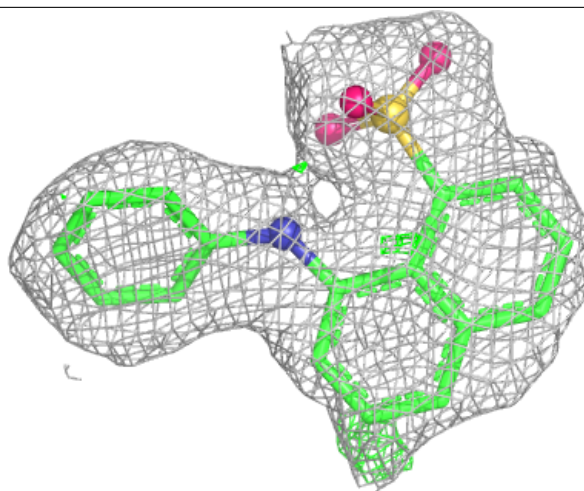
Electron density around 2AN O 203:

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



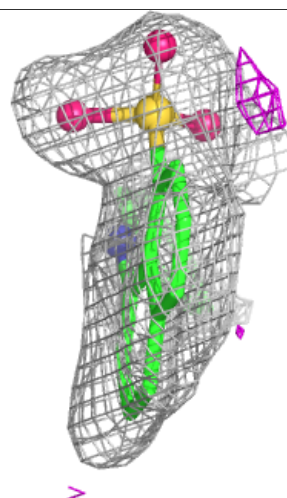
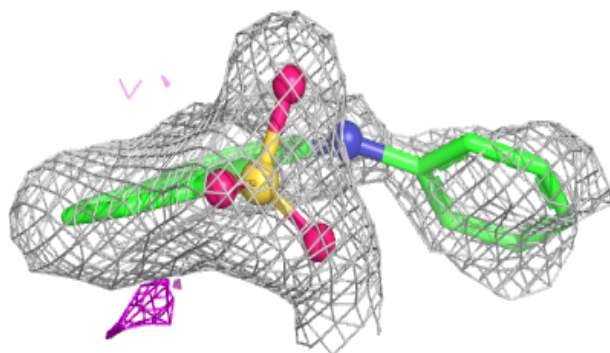
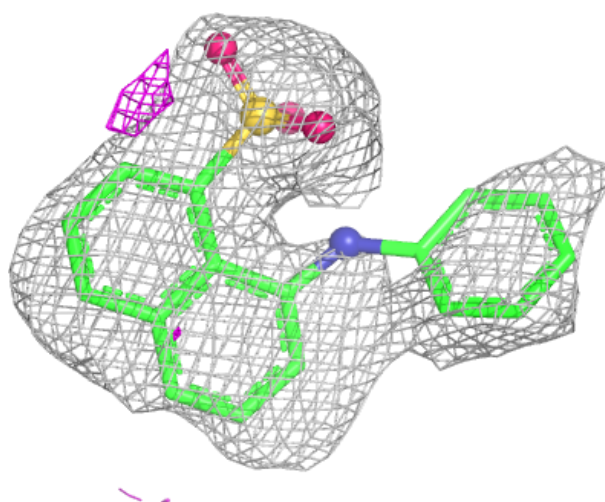
Electron density around 2AN F 202:

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



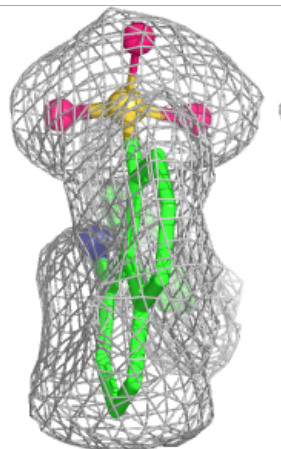
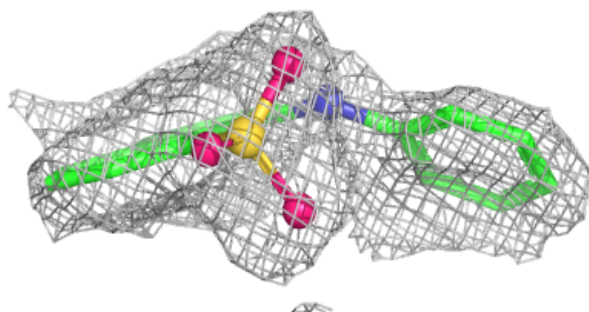
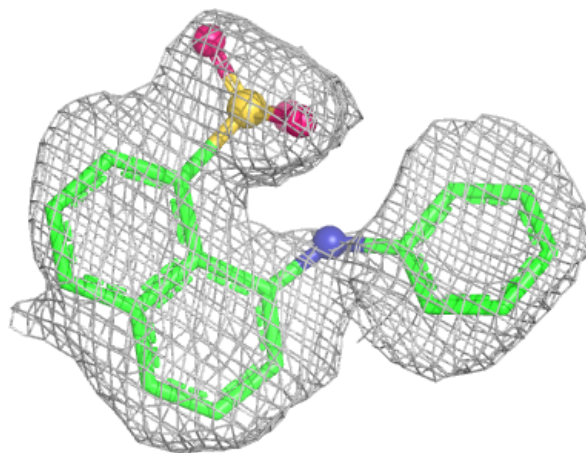
Electron density around 2AN H 1108:

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



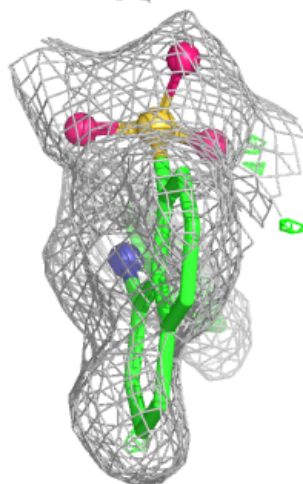
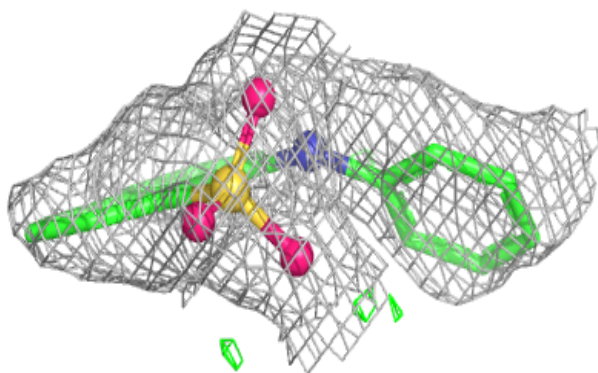
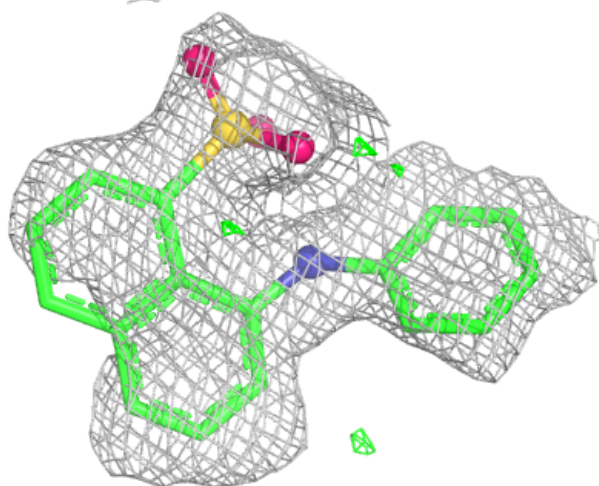
Electron density around 2AN B 204:

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



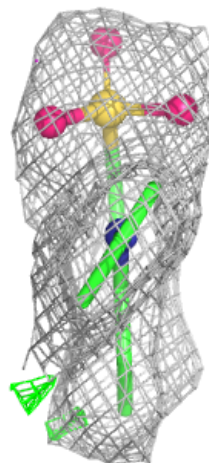
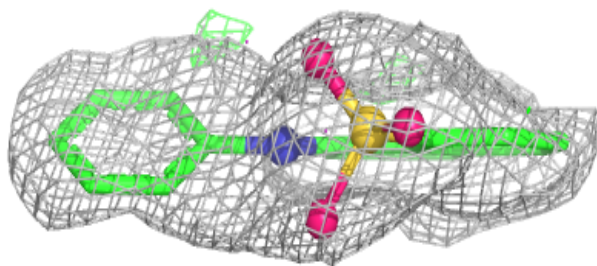
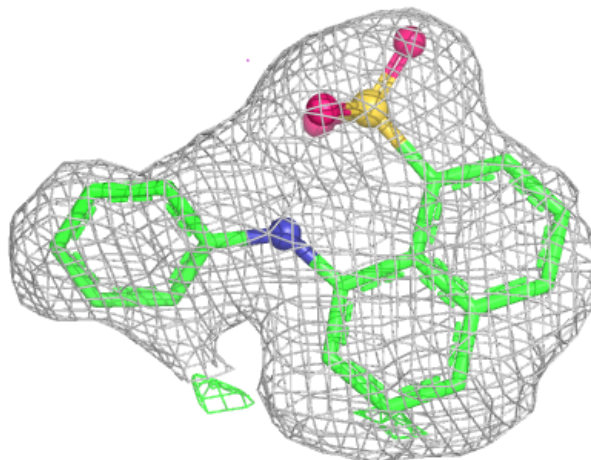
Electron density around 2AN B 203:

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



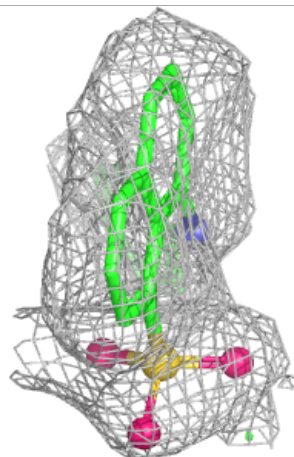
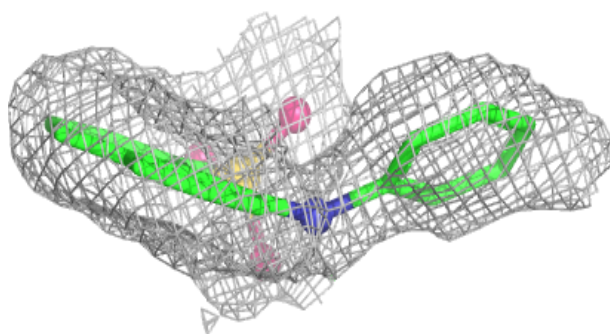
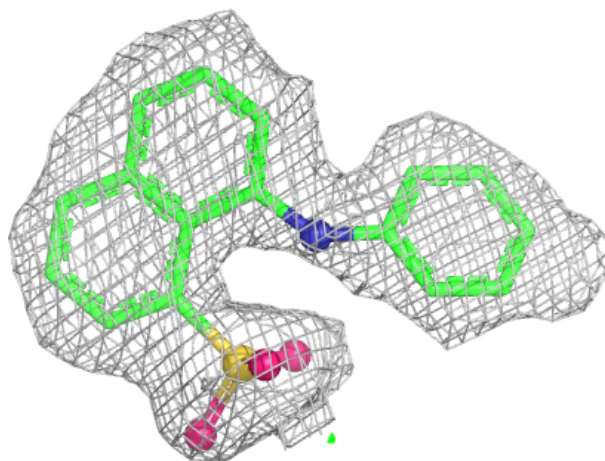
Electron density around 2AN E 502:

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



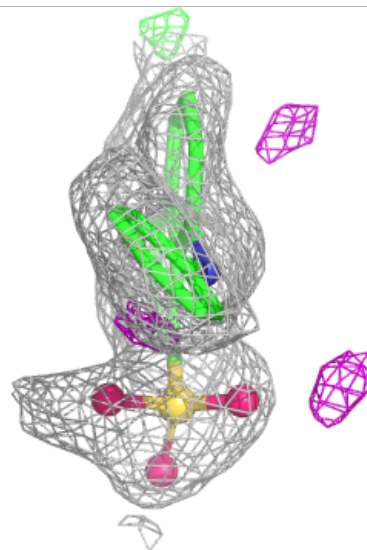
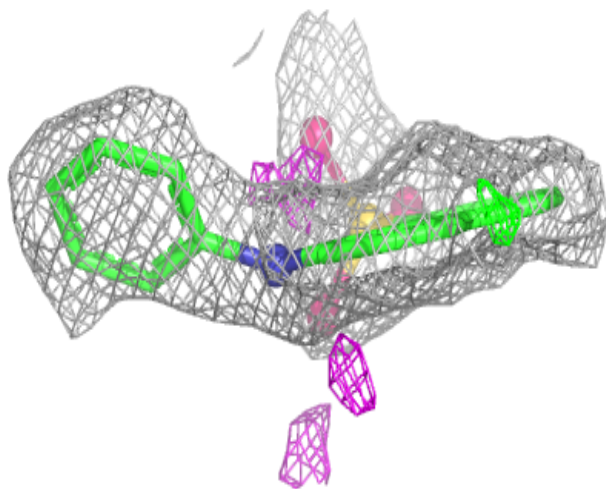
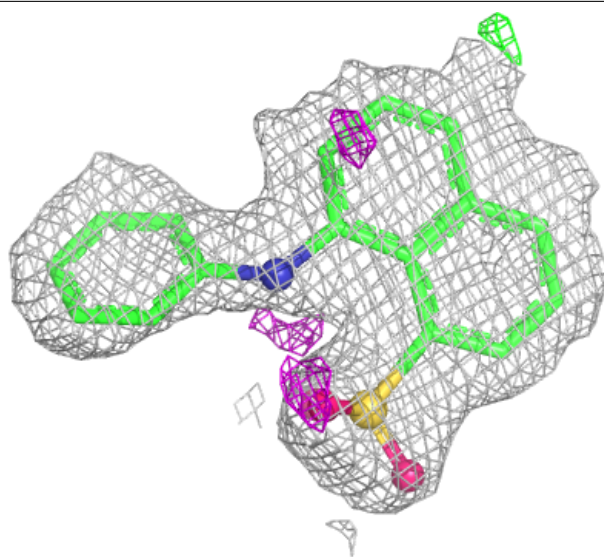
Electron density around 2AN L 204:

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



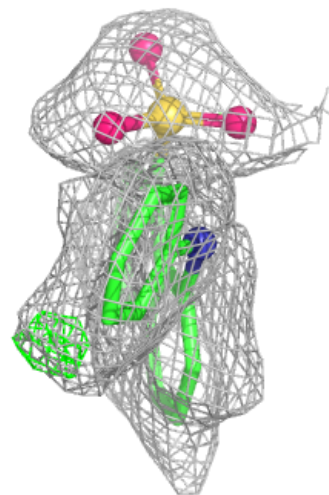
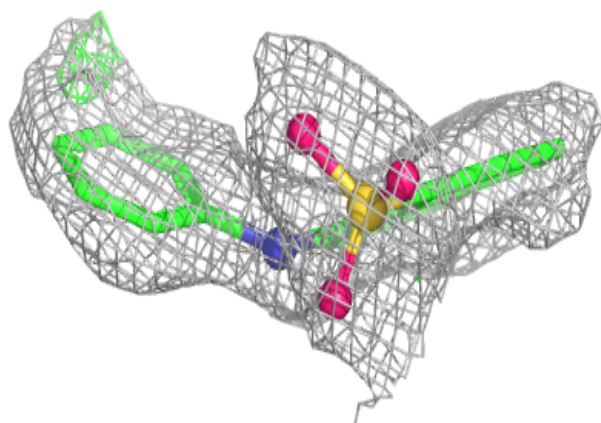
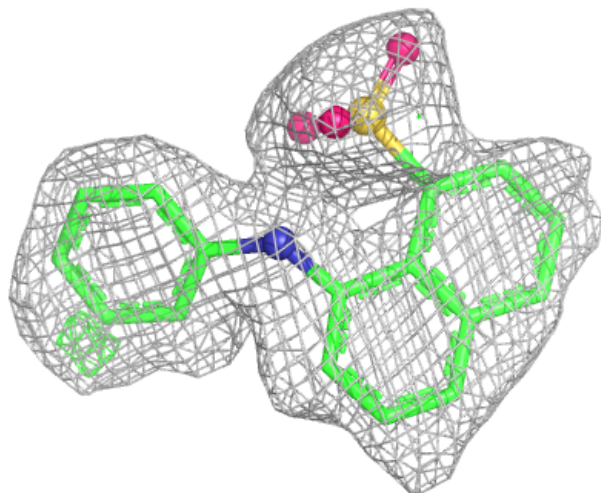
Electron density around 2AN M 502:

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



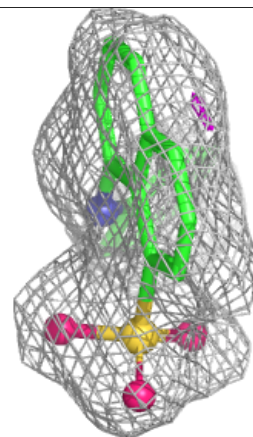
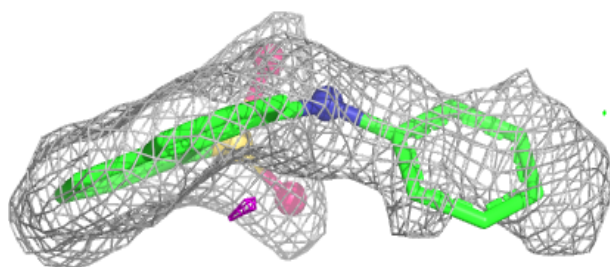
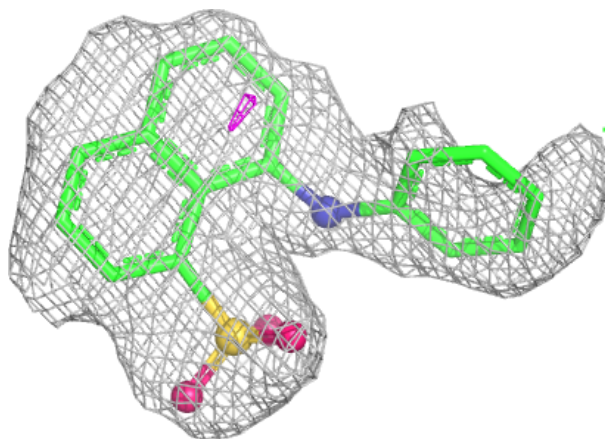
Electron density around 2AN K 204:

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



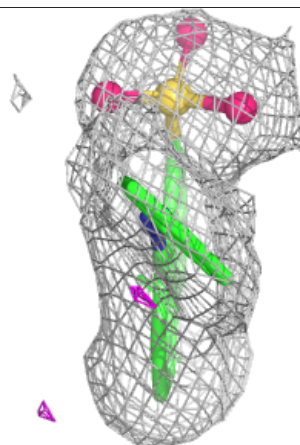
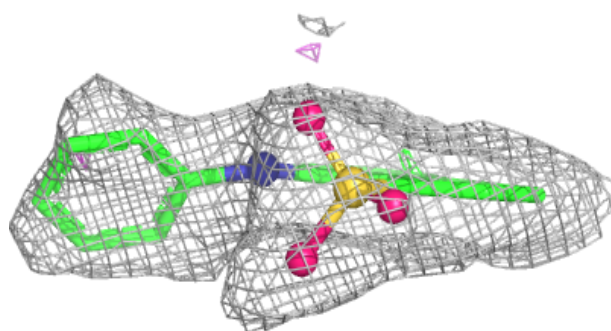
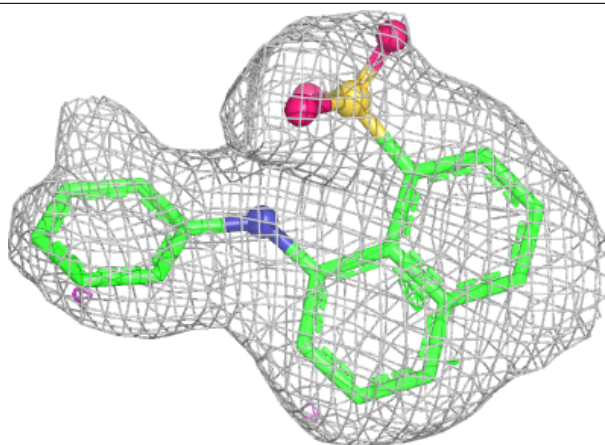
Electron density around 2AN J 203:

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



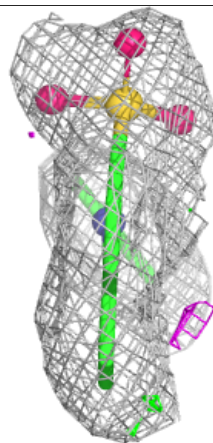
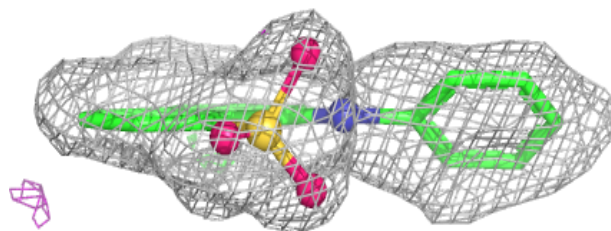
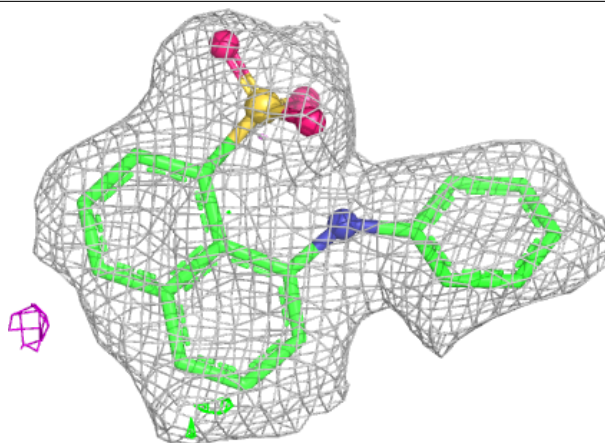
Electron density around 2AN H 1105:

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



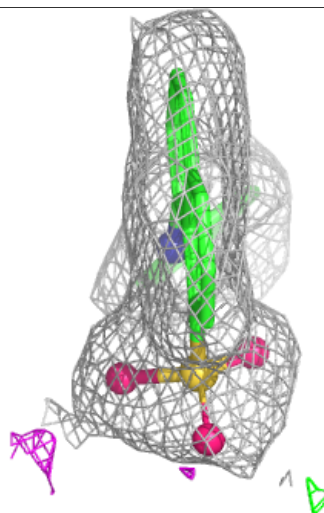
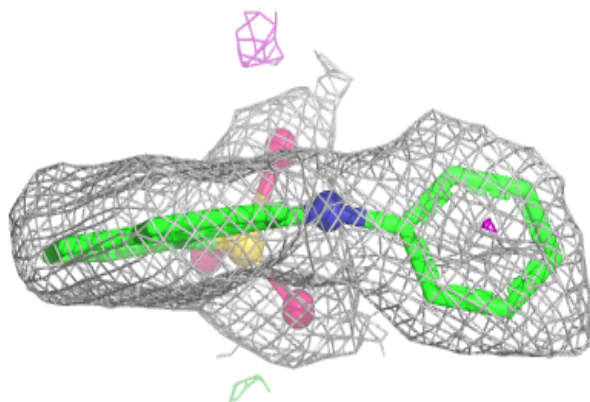
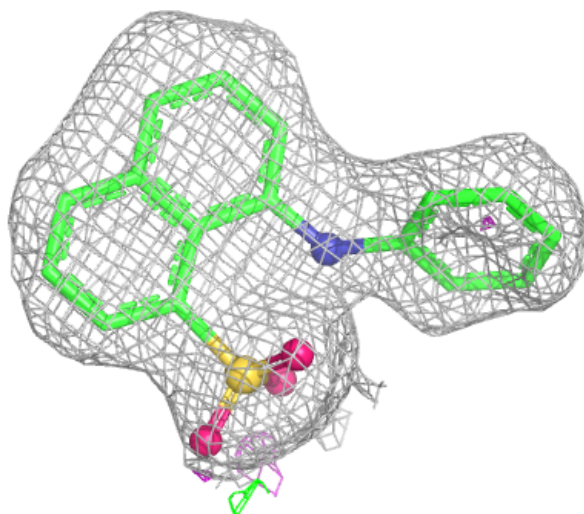
Electron density around 2AN K 202:

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



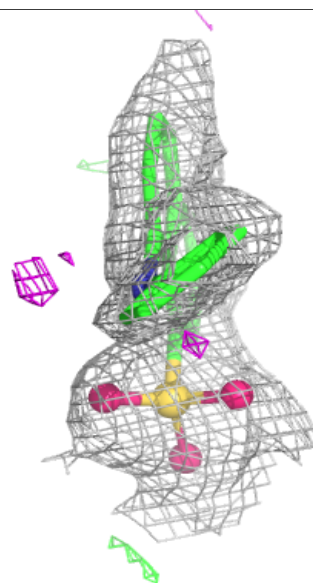
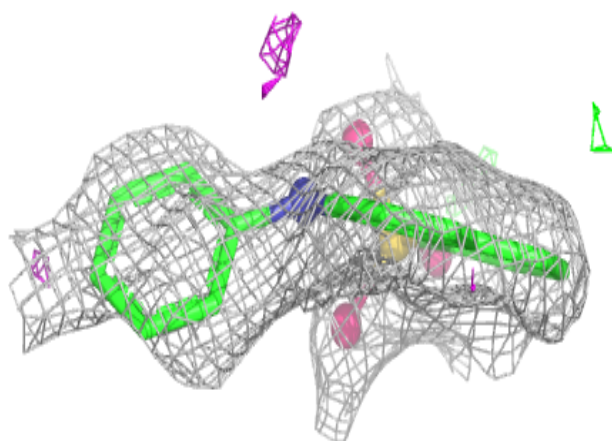
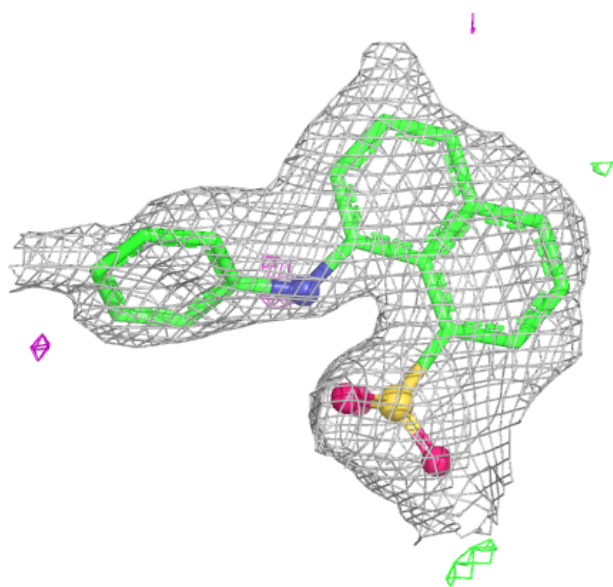
Electron density around 2AN G 305:

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



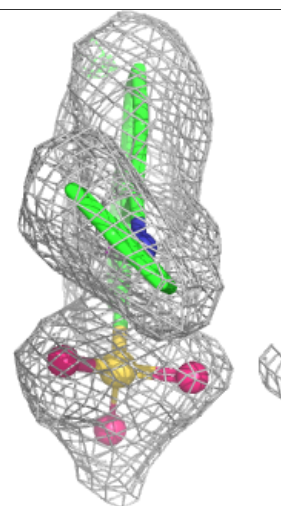
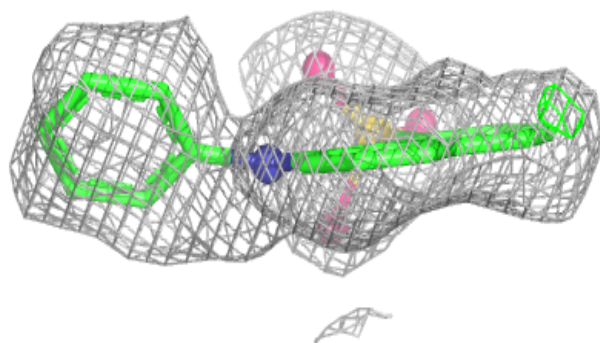
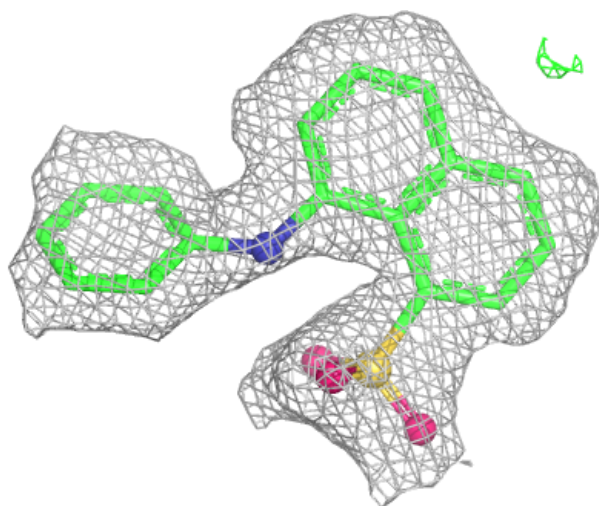
Electron density around 2AN P 502:

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



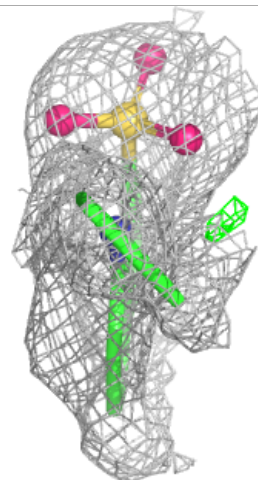
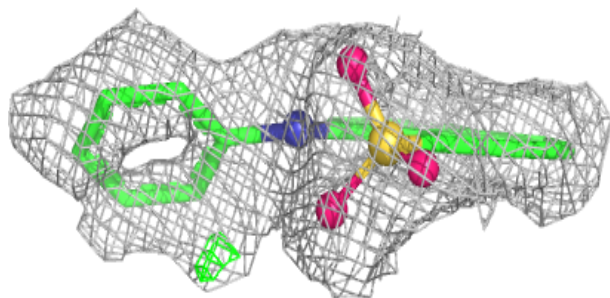
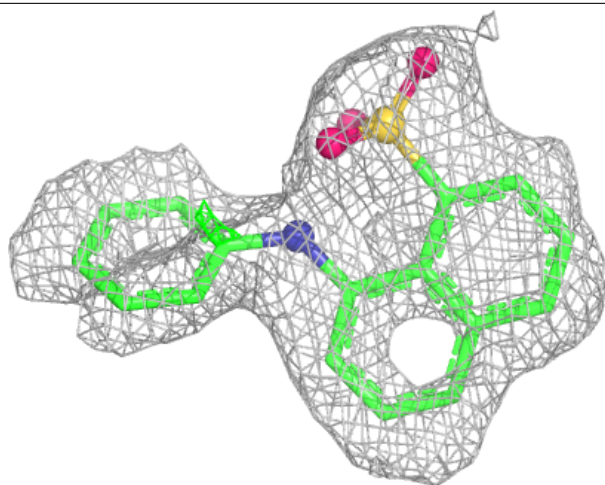
Electron density around 2AN C 303:

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



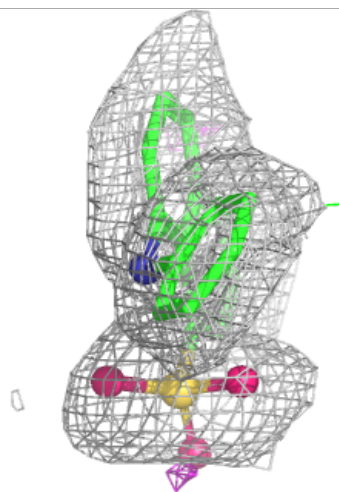
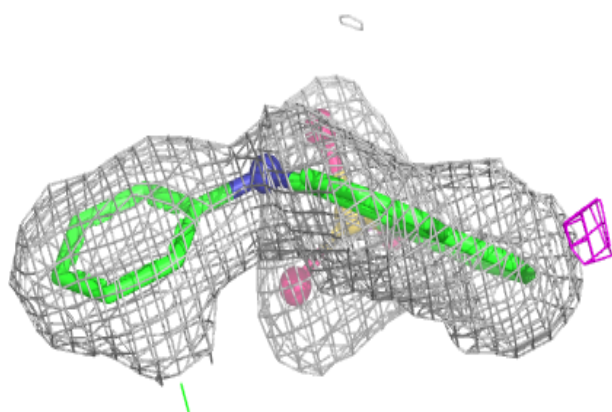
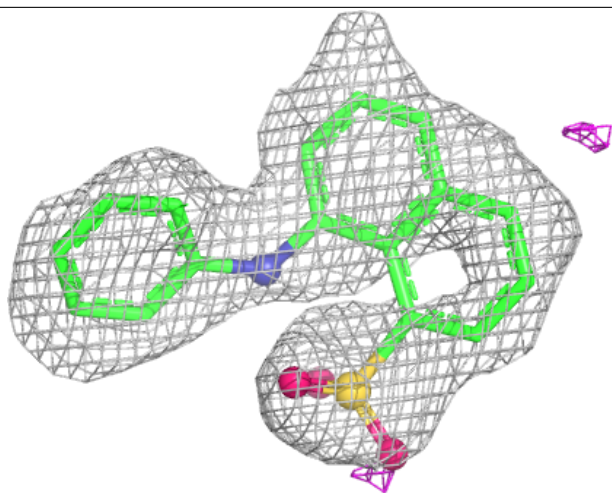
Electron density around 2AN N 201:

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



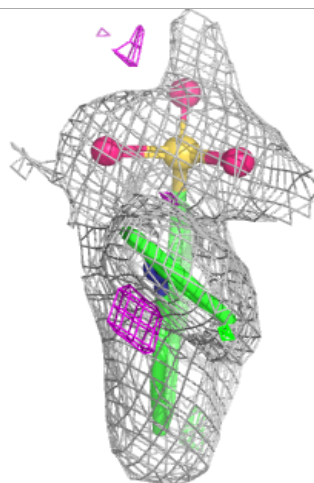
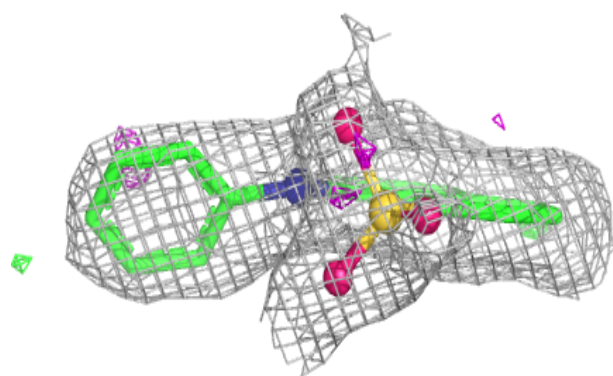
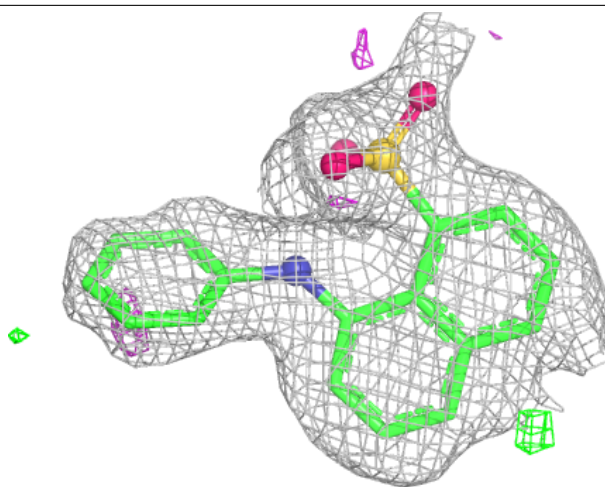
Electron density around 2AN I 205:

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



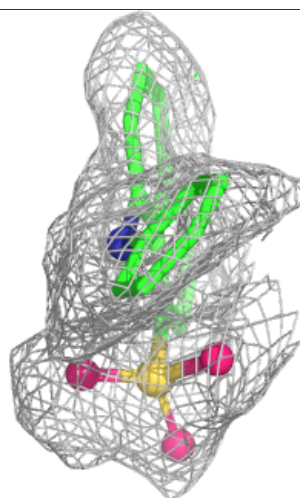
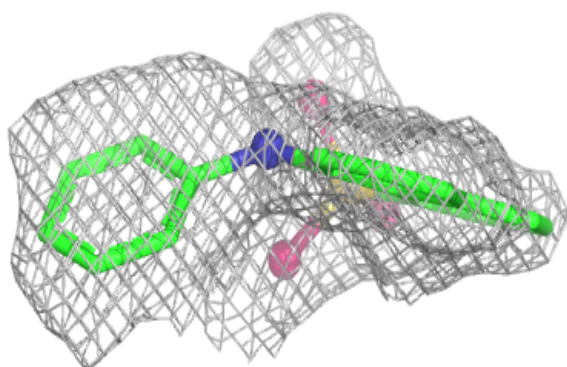
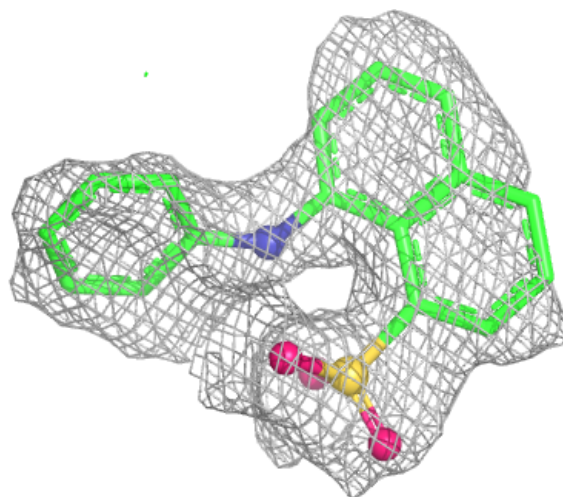
Electron density around 2AN A 203:

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



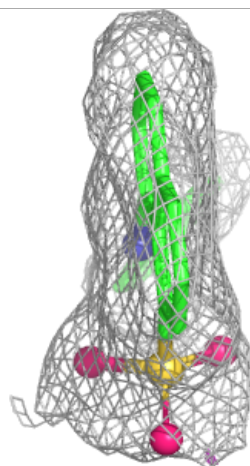
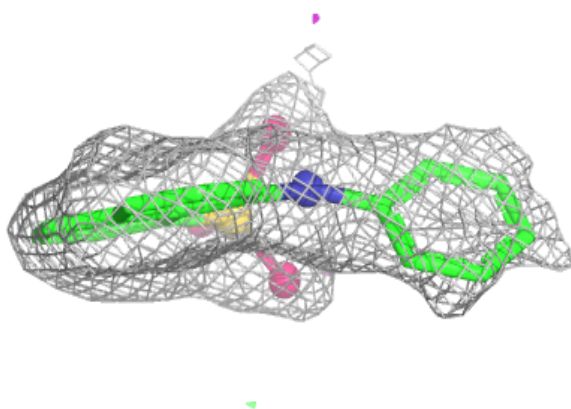
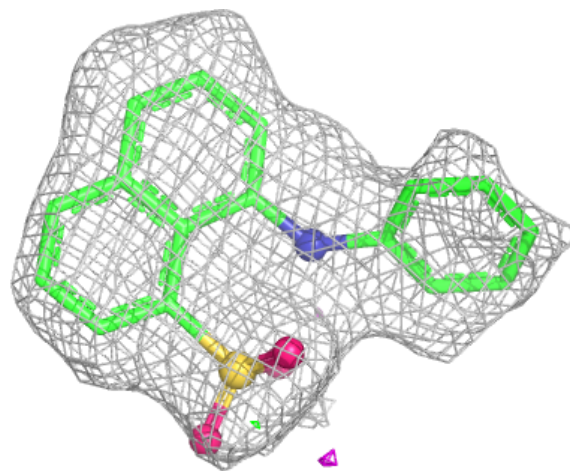
Electron density around 2AN L 203:

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



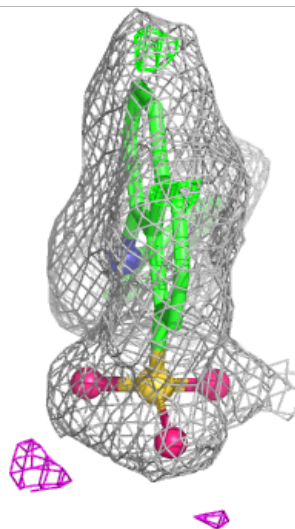
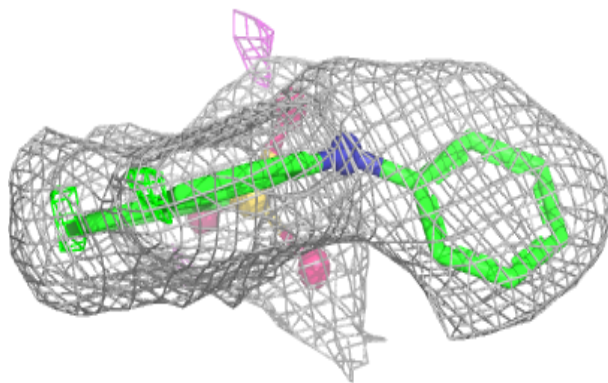
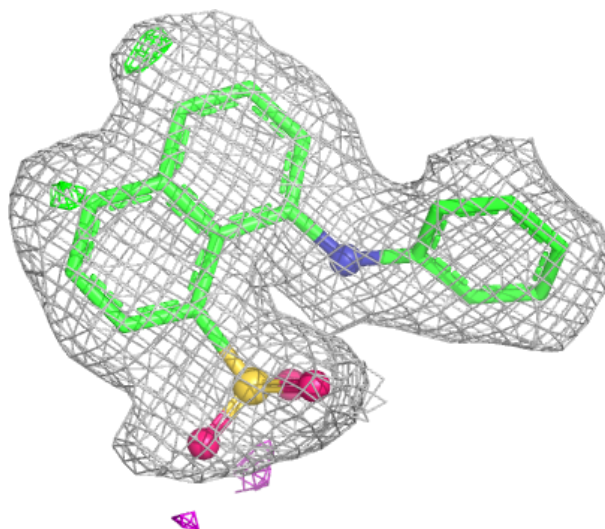
Electron density around 2AN O 204:

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



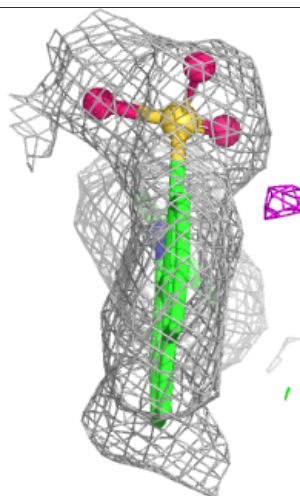
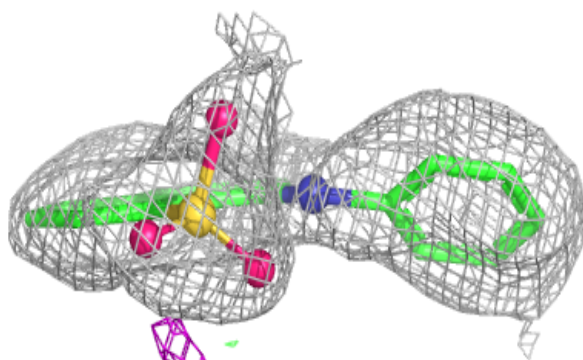
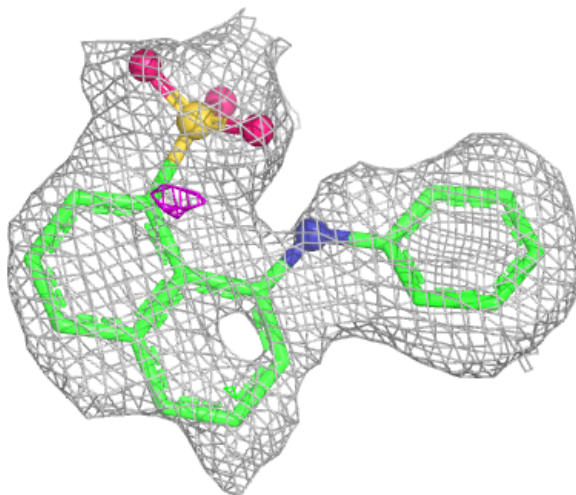
Electron density around 2AN H 1106:

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



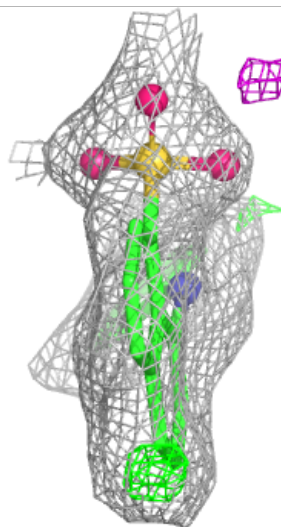
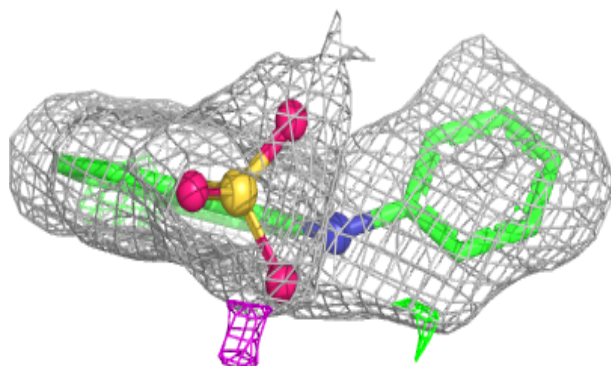
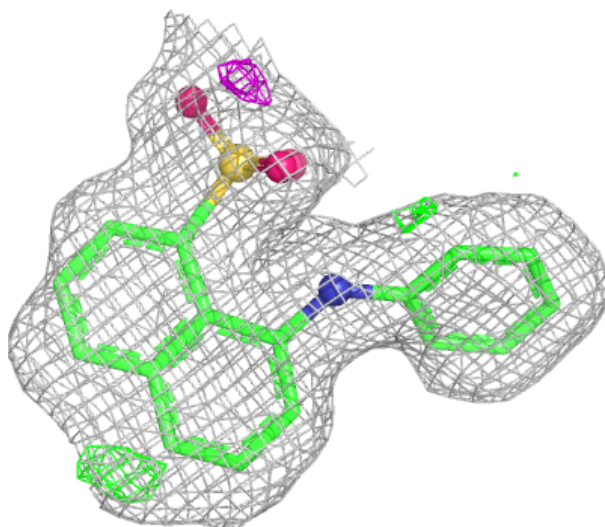
Electron density around 2AN N 202:

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



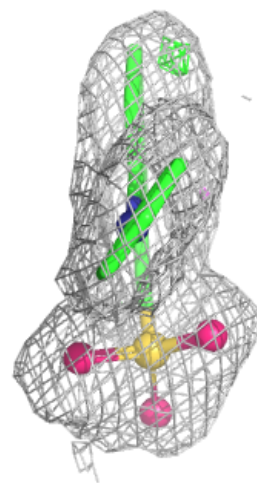
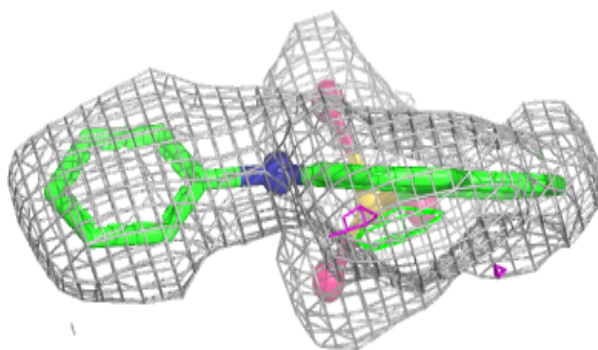
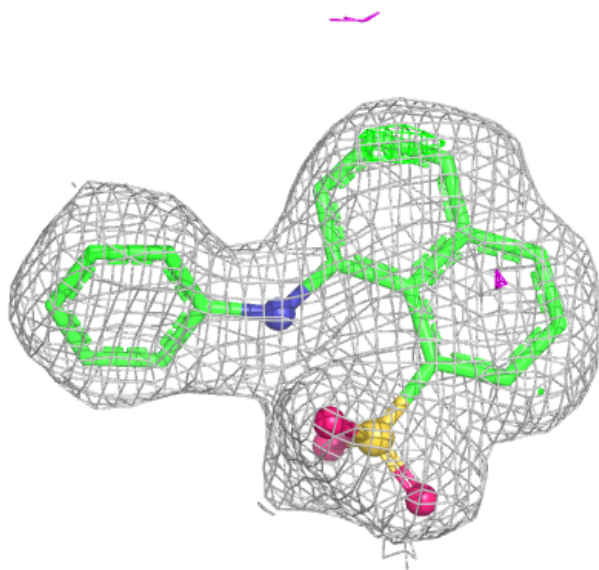
Electron density around 2AN P 505:

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



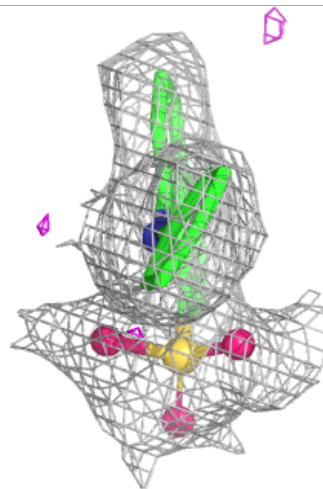
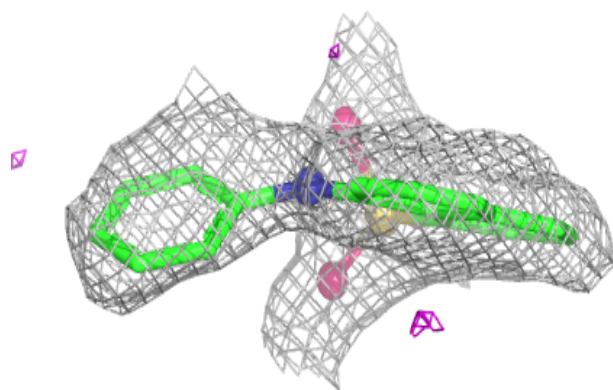
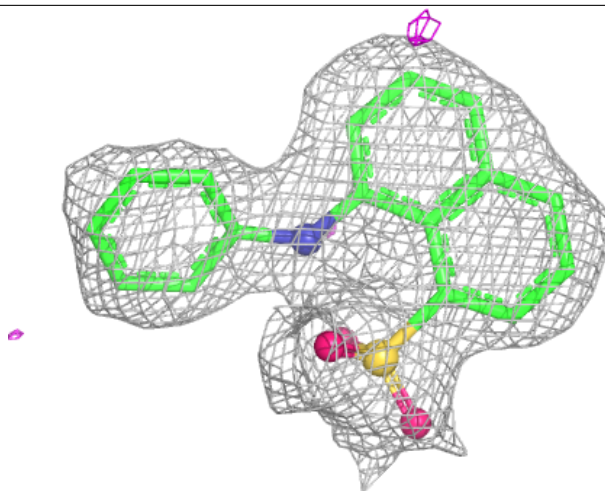
Electron density around 2AN L 202:

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



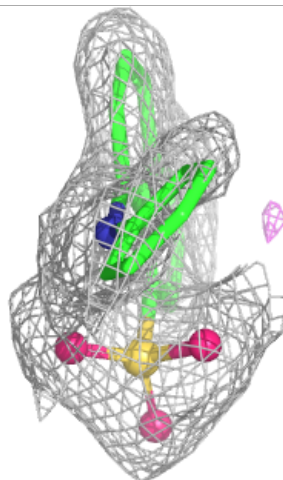
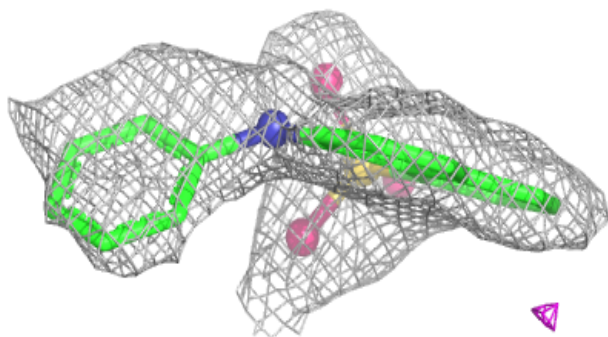
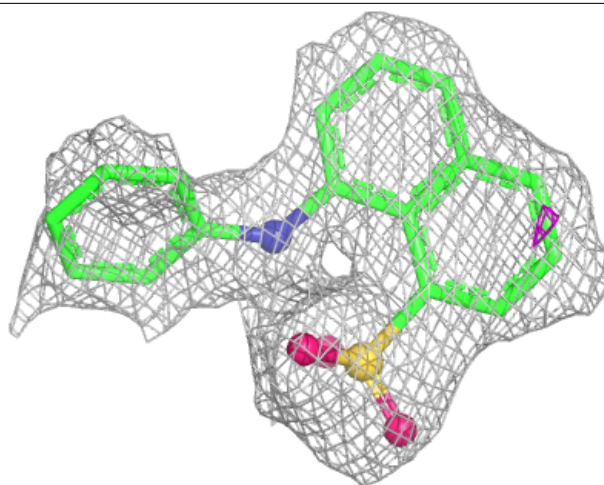
Electron density around 2AN G 302:

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



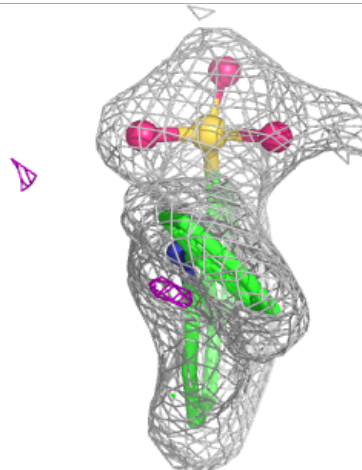
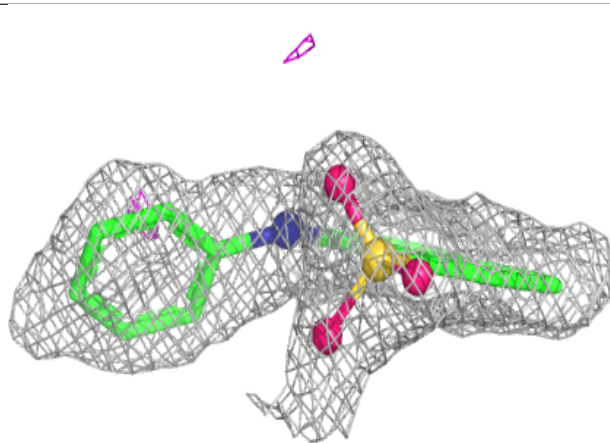
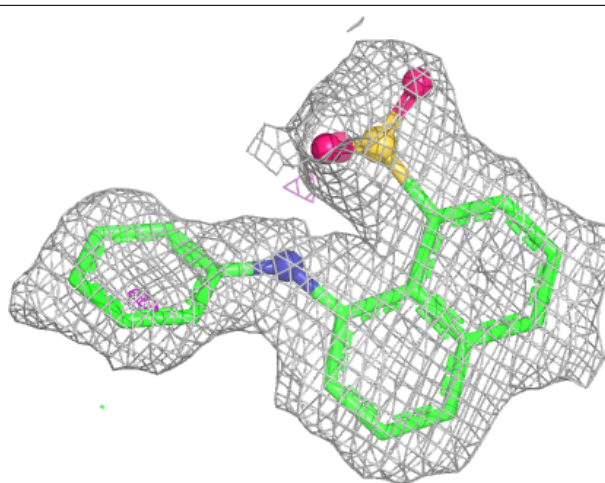
Electron density around 2AN M 507:

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



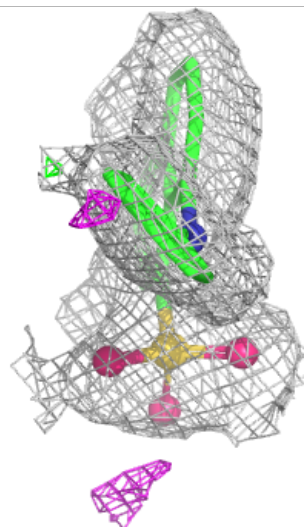
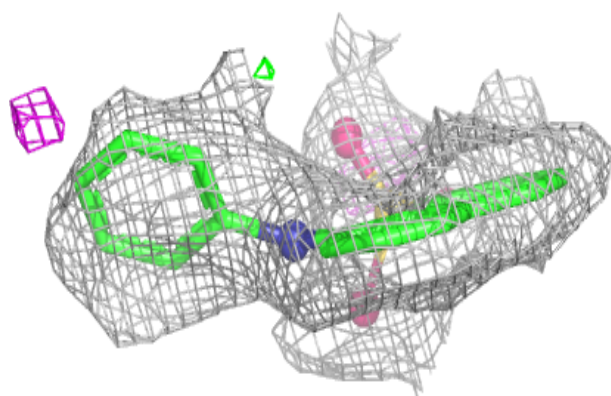
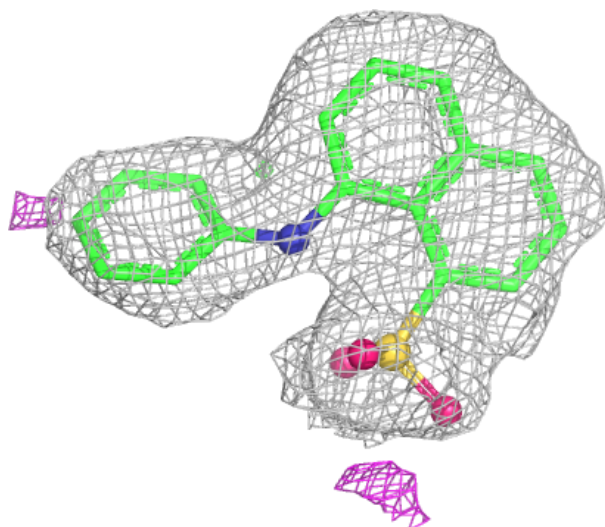
Electron density around 2AN C 301:

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



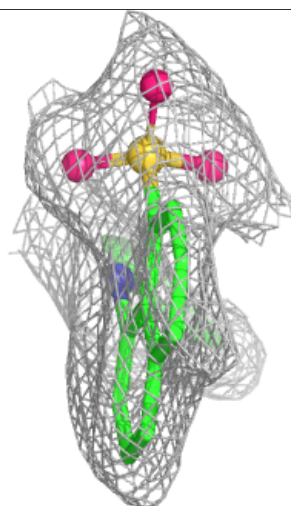
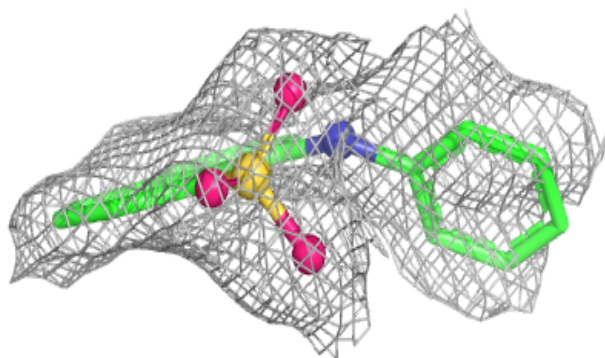
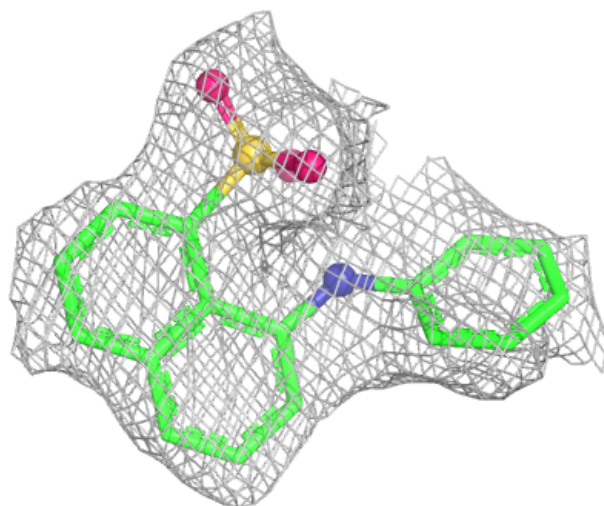
Electron density around 2AN J 201:

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



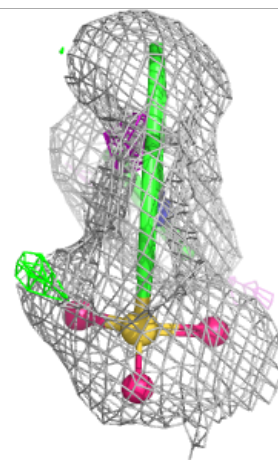
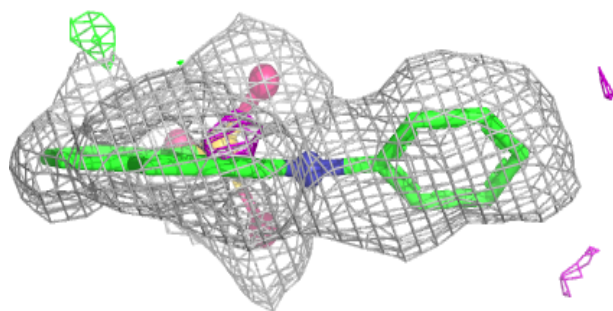
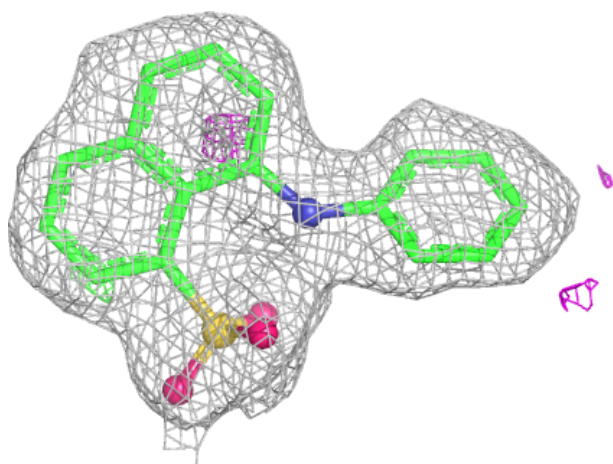
Electron density around 2AN C 304:

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



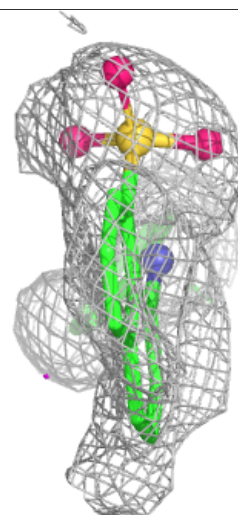
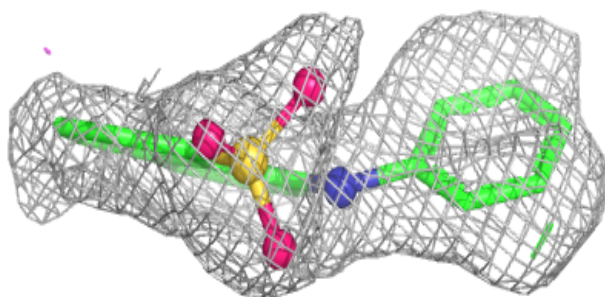
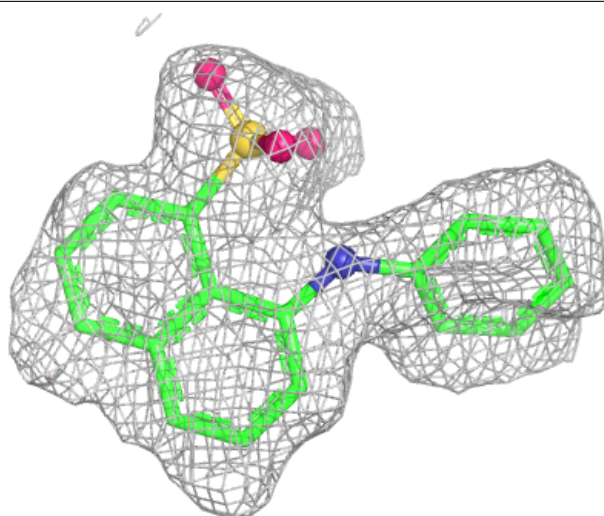
Electron density around 2AN B 201:

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



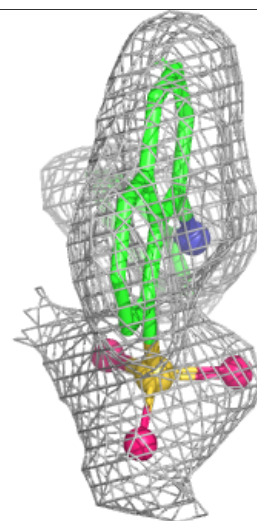
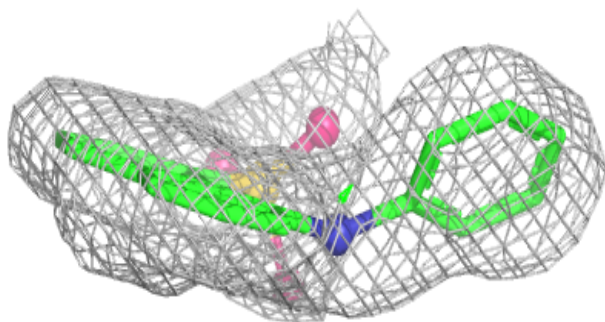
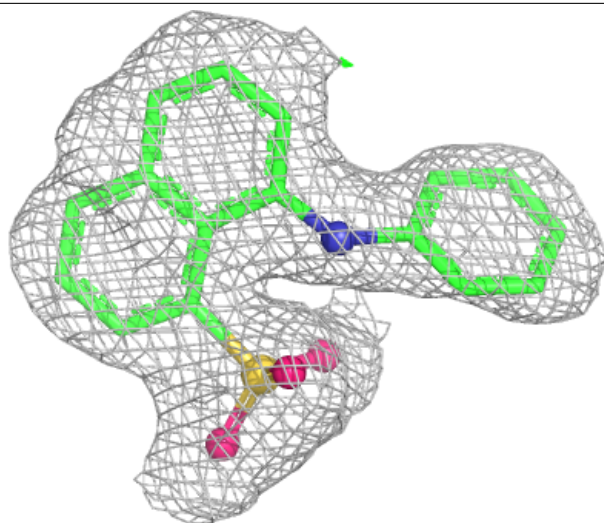
Electron density around 2AN F 201:

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



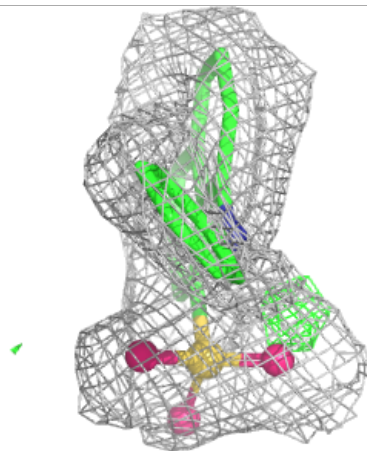
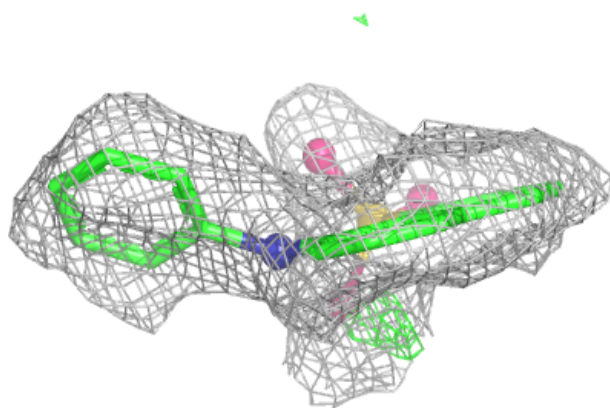
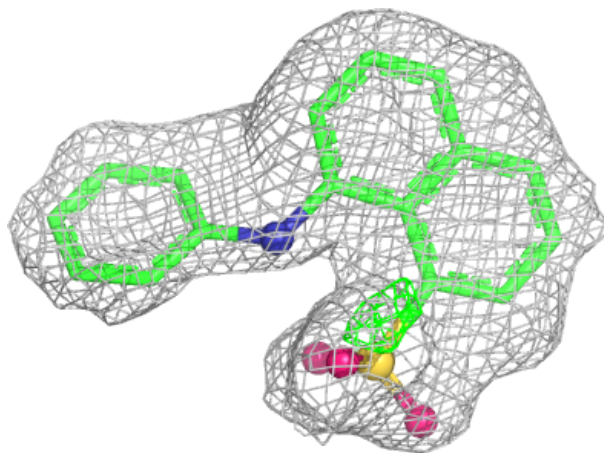
Electron density around 2AN G 301:

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



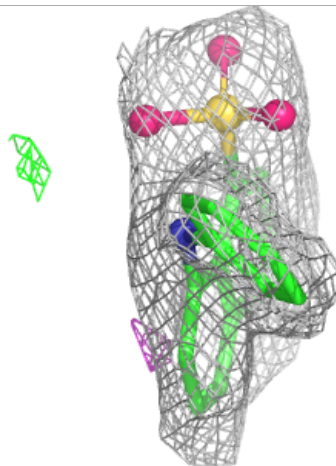
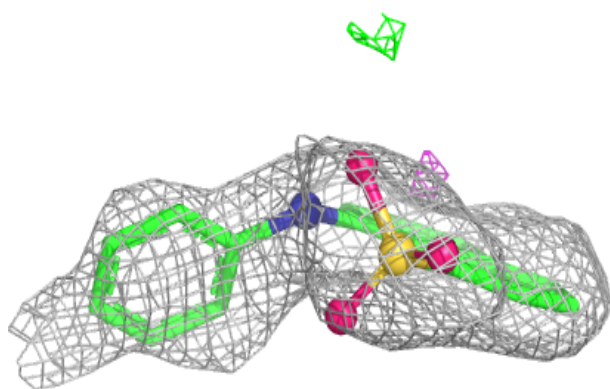
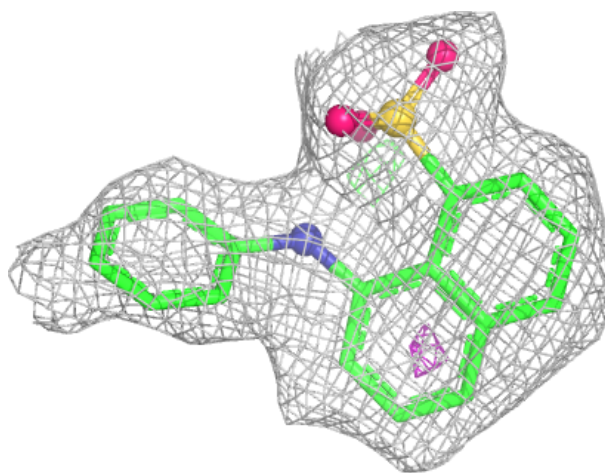
Electron density around 2AN B 202:

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



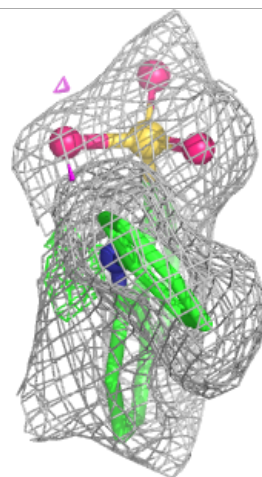
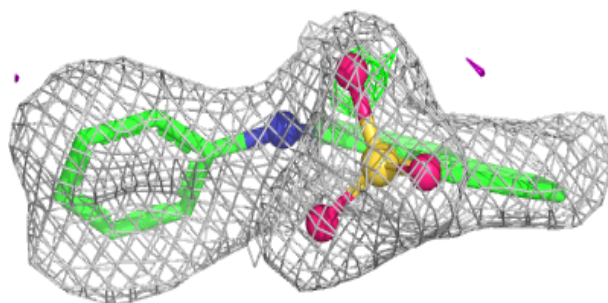
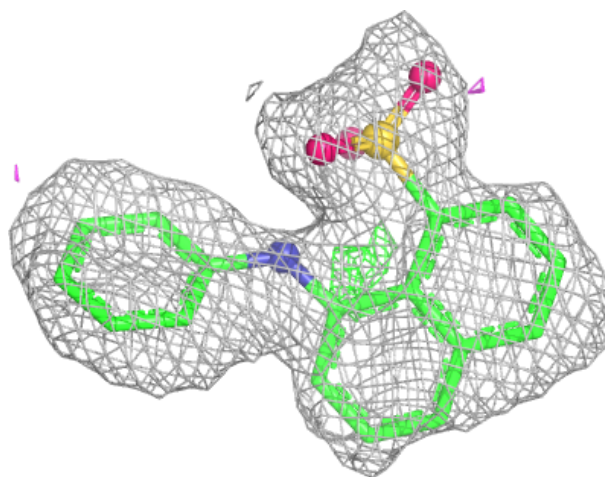
Electron density around 2AN F 203:

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



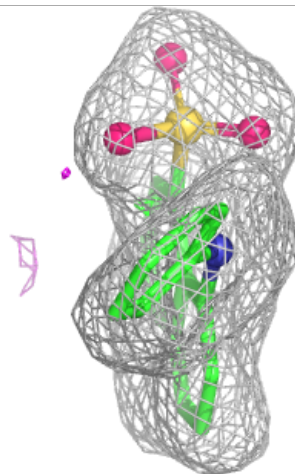
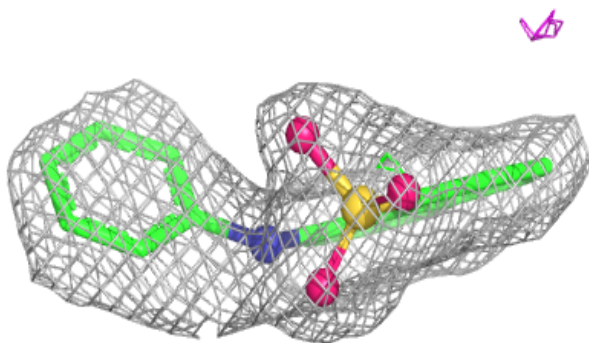
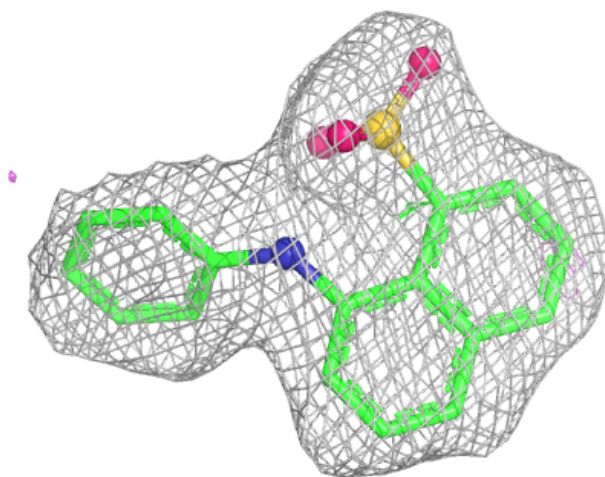
Electron density around 2AN A 204:

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



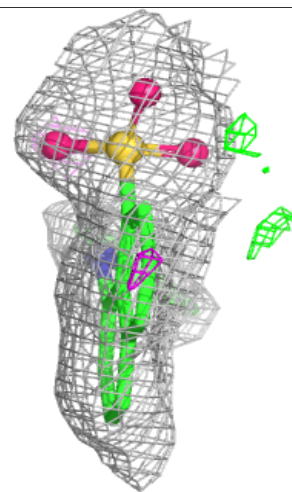
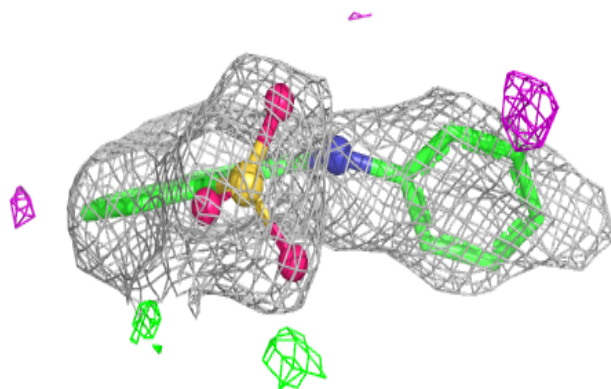
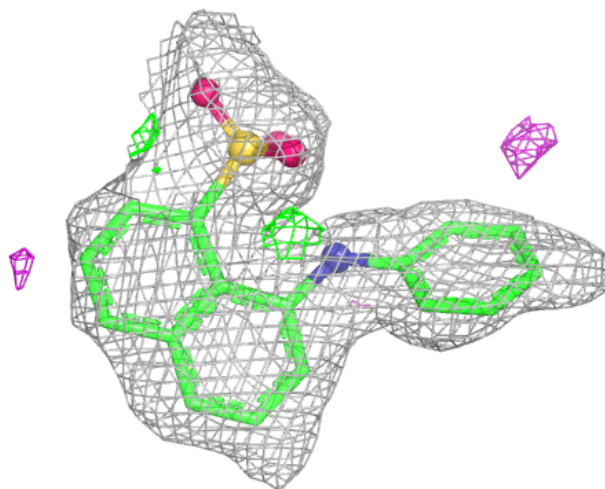
Electron density around 2AN K 203:

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



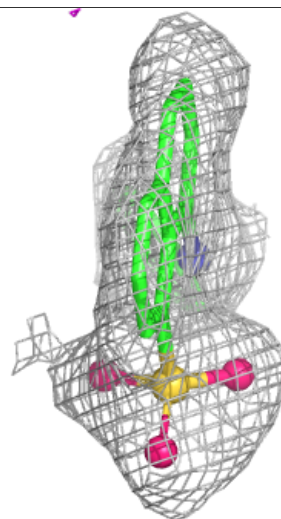
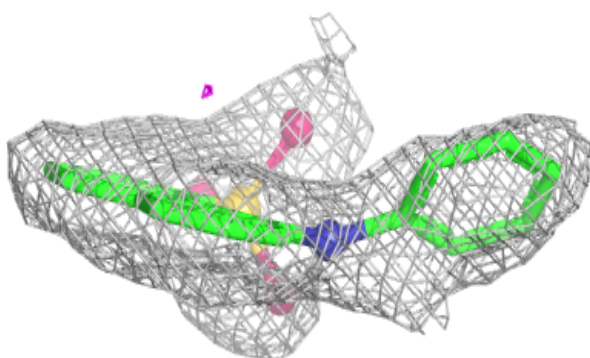
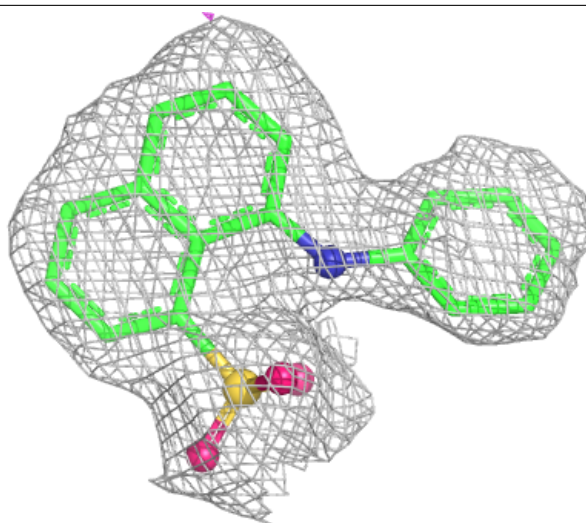
Electron density around 2AN F 205:

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



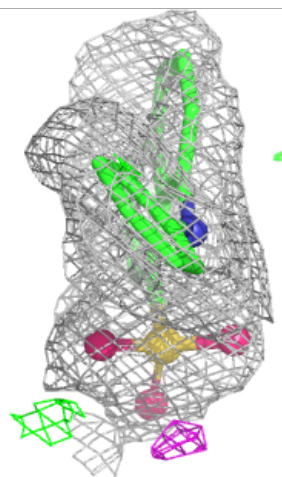
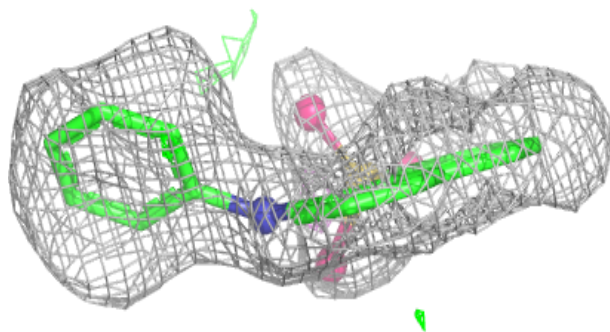
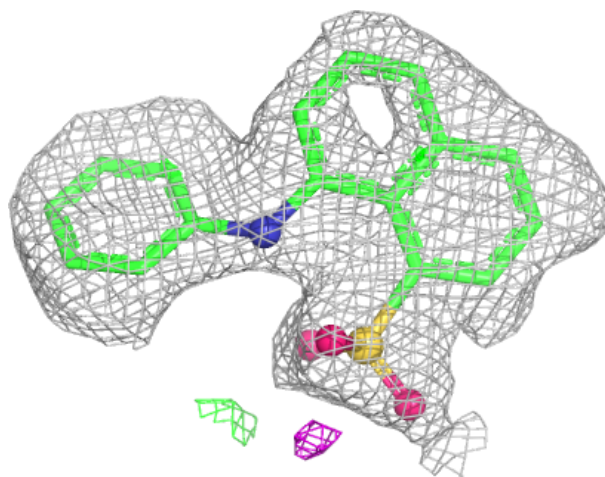
Electron density around 2AN O 202:

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



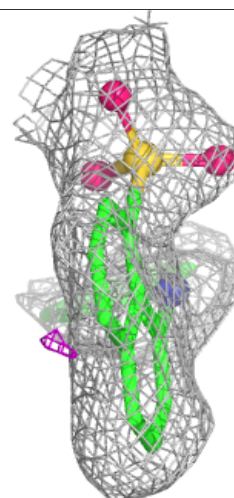
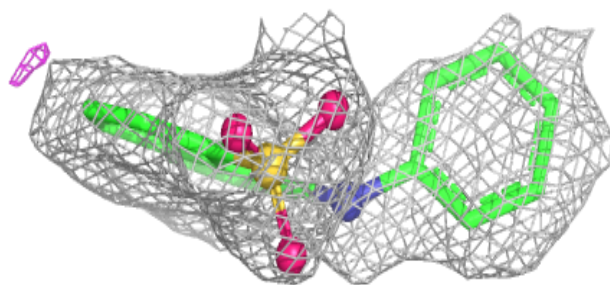
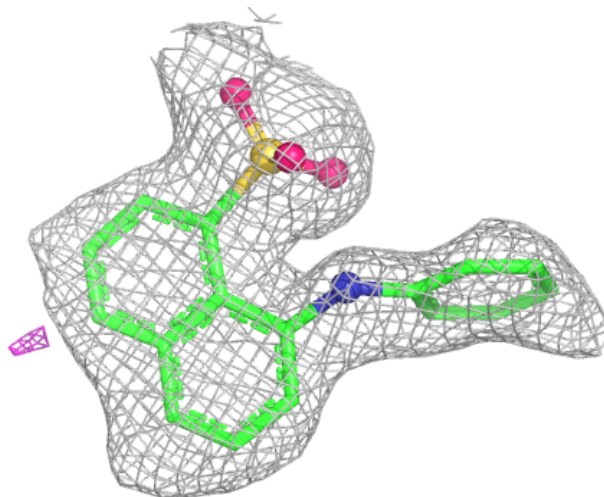
Electron density around 2AN M 504:

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



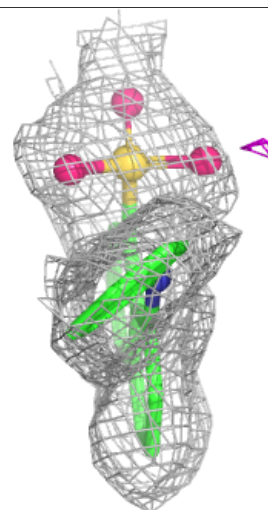
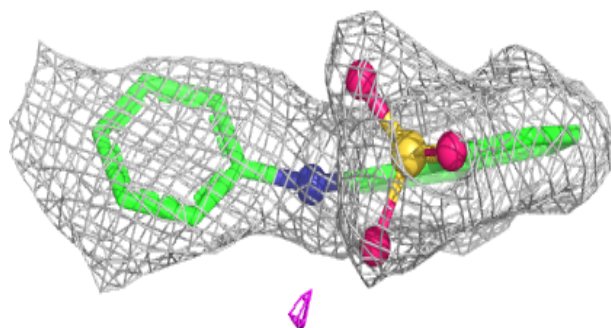
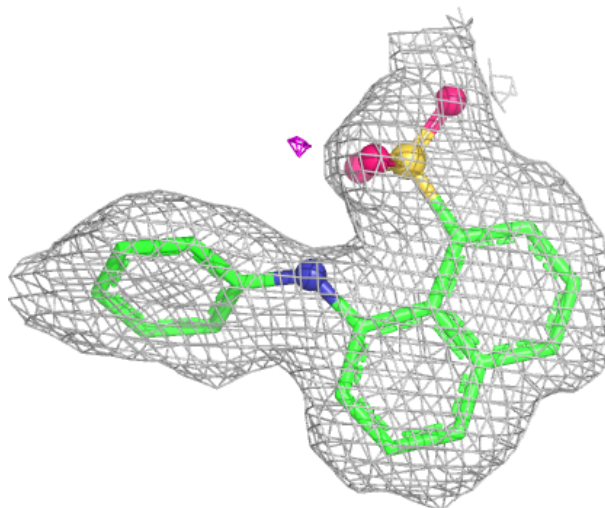
Electron density around 2AN H 1104:

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



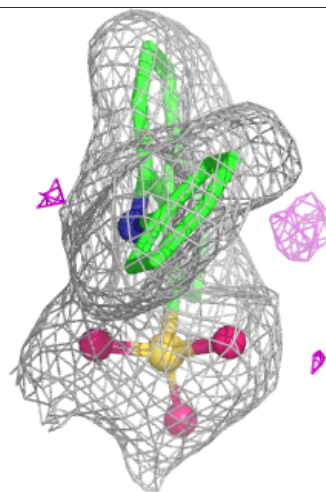
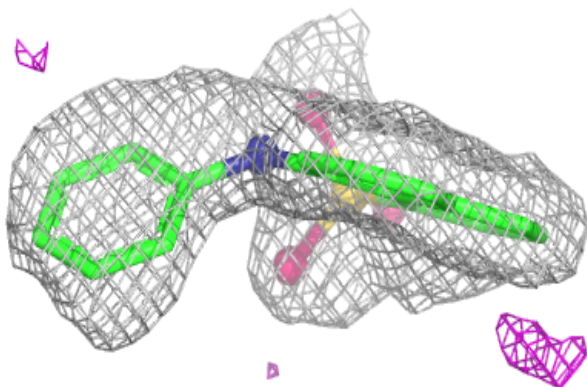
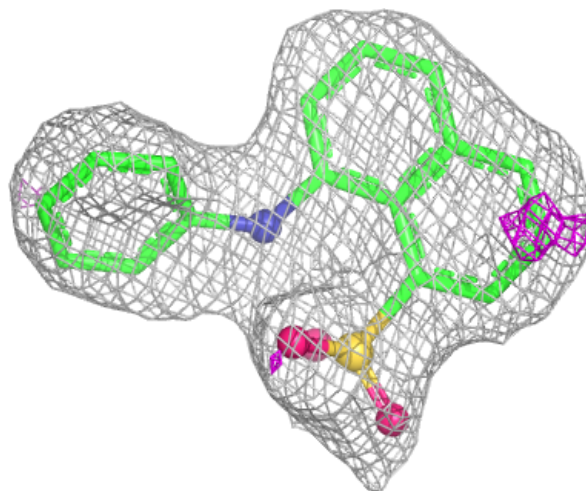
Electron density around 2AN A 205:

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



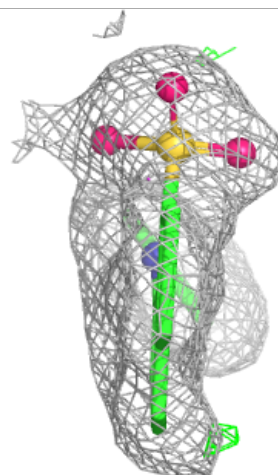
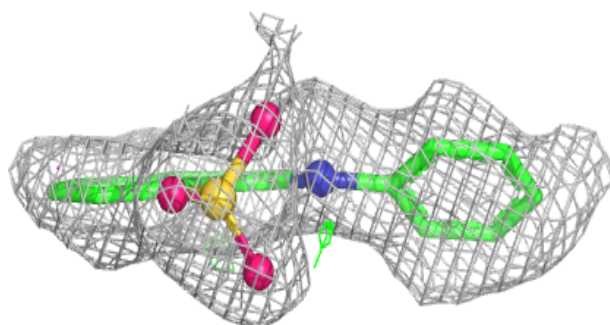
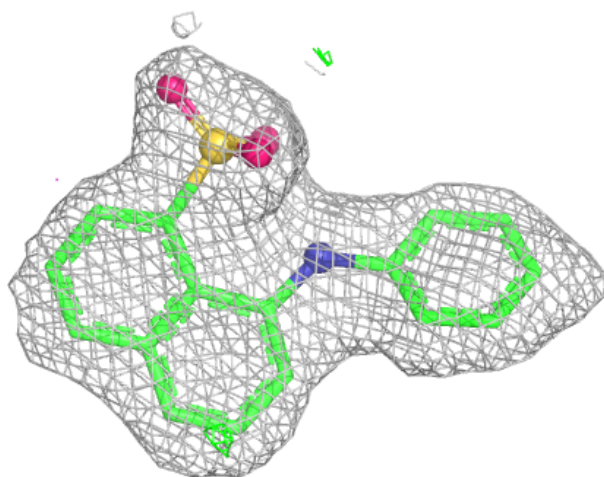
Electron density around 2AN E 505:

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



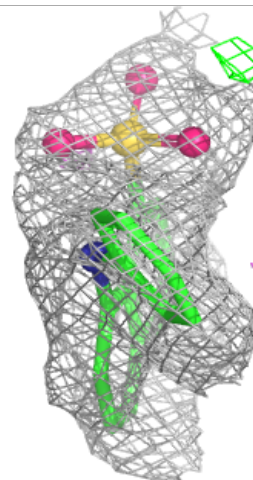
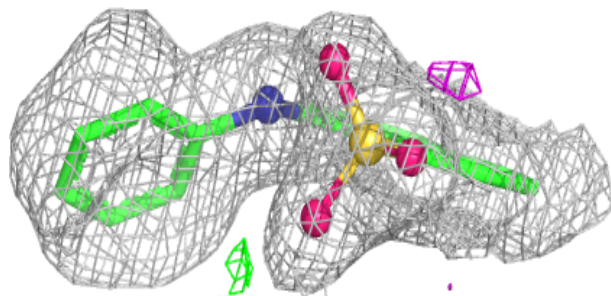
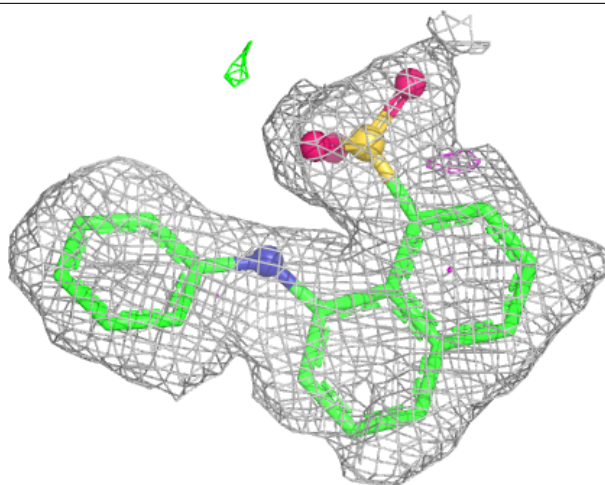
Electron density around 2AN A 201:

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



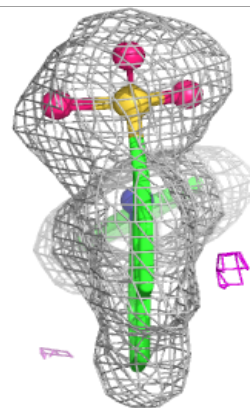
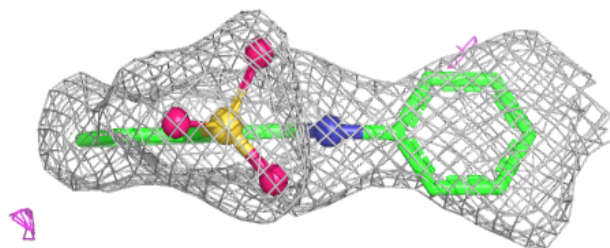
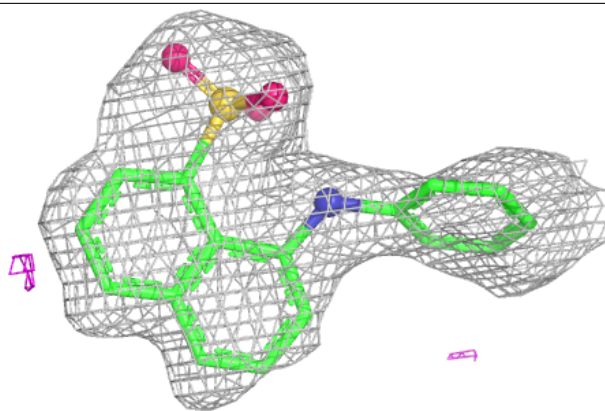
Electron density around 2AN E 503:

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



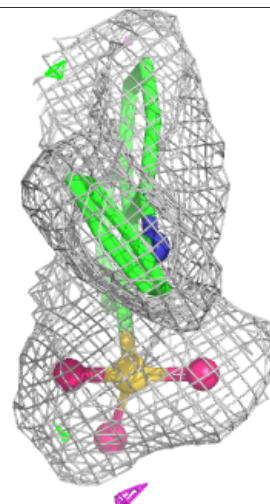
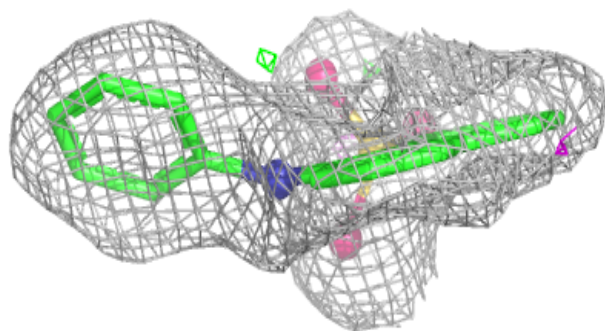
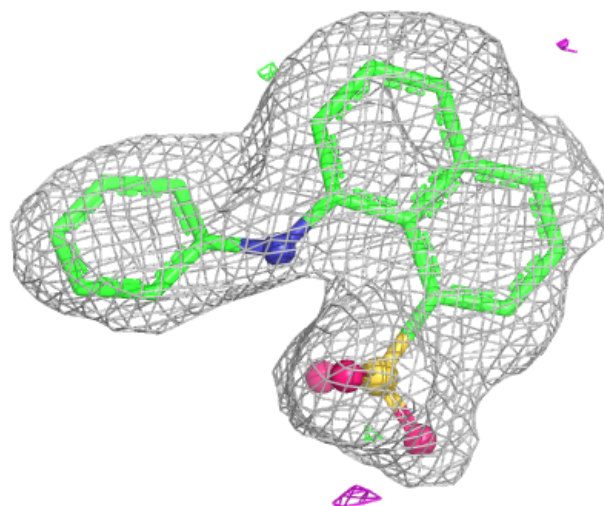
Electron density around 2AN C 309:

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



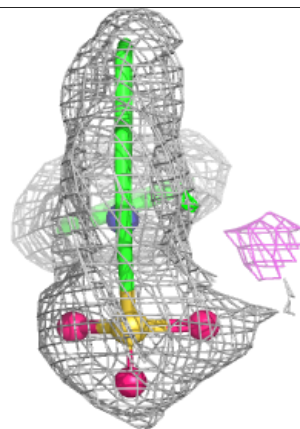
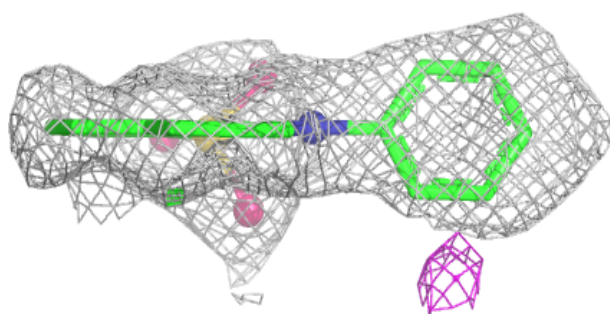
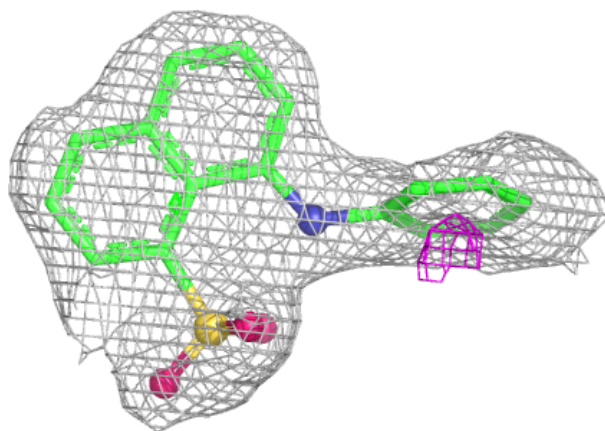
Electron density around 2AN D 703:

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



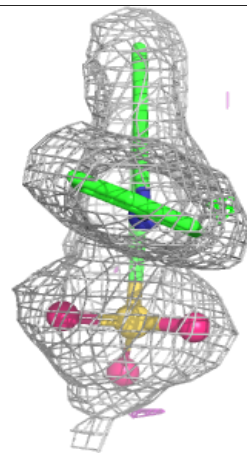
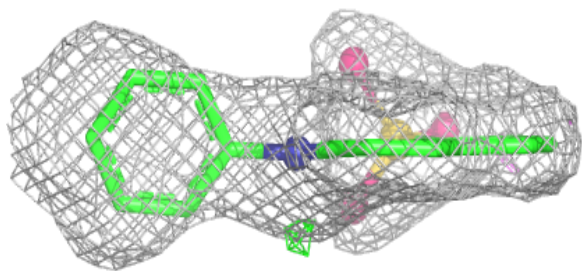
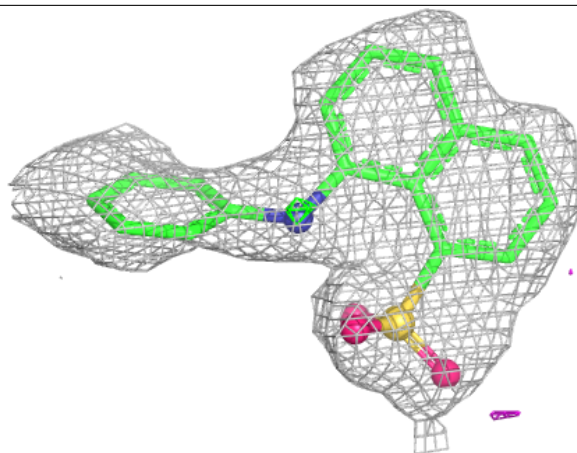
Electron density around 2AN E 501:

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



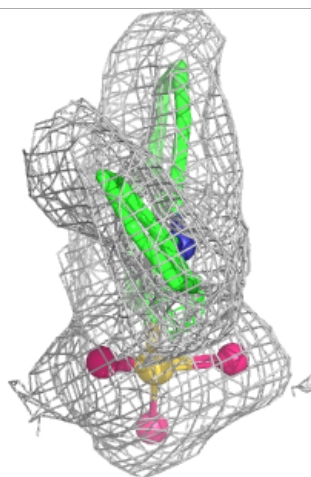
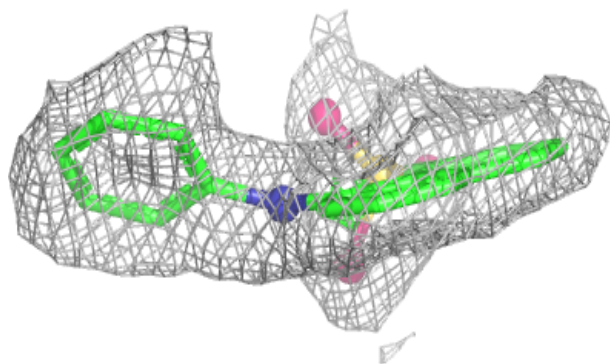
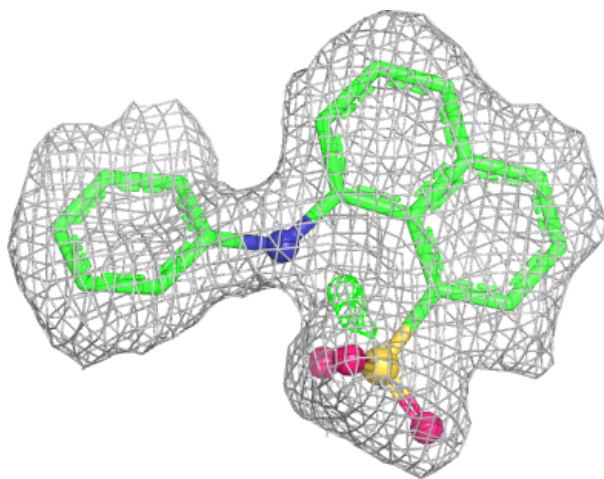
Electron density around 2AN K 207:

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



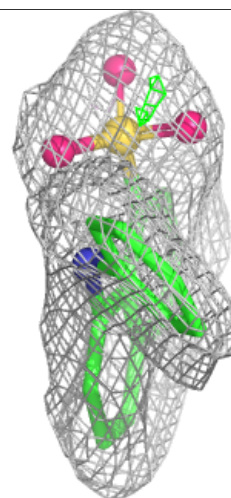
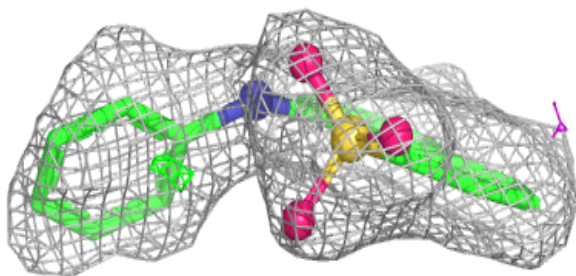
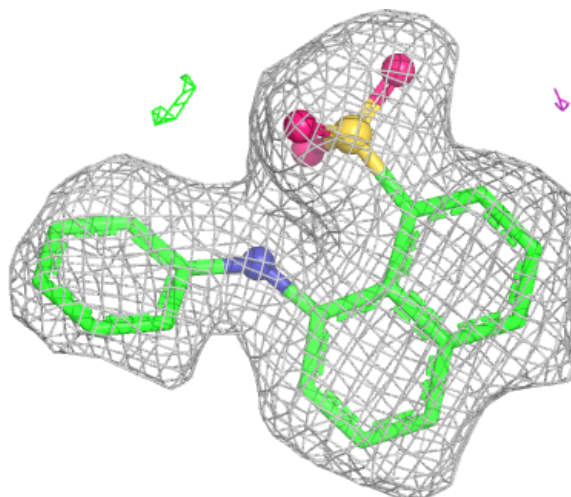
Electron density around 2AN P 504:

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



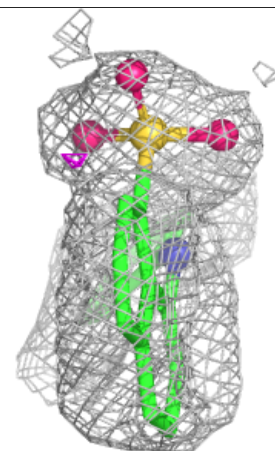
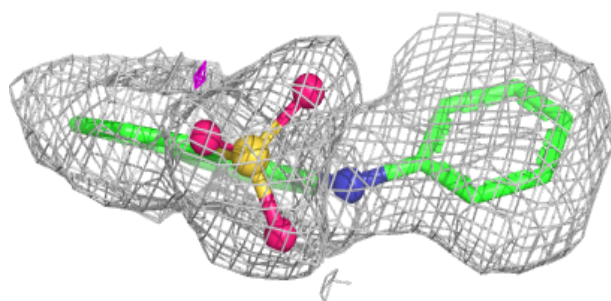
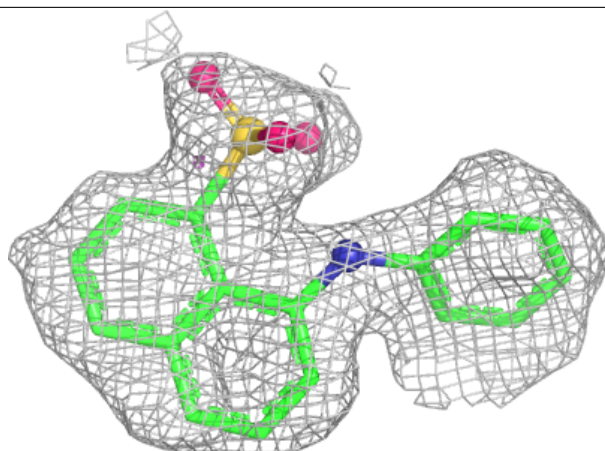
Electron density around 2AN H 1103:

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



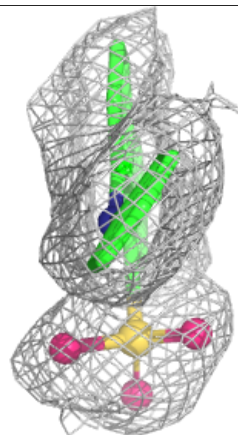
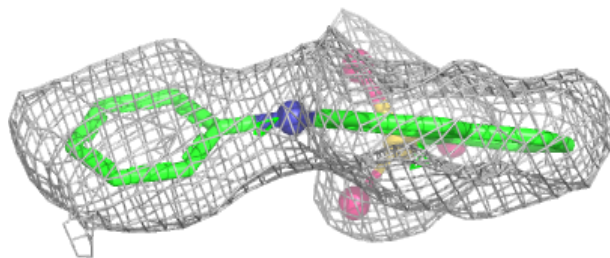
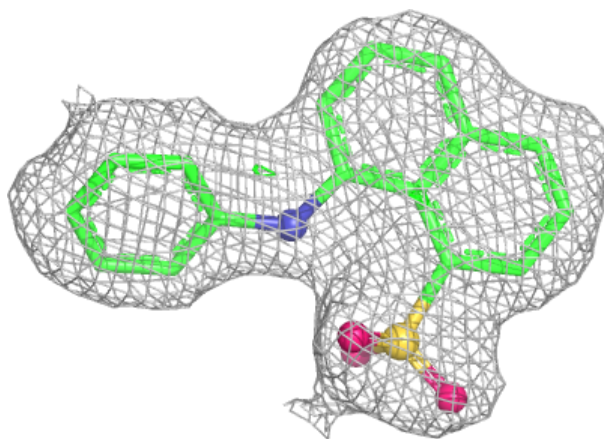
Electron density around 2AN C 302:

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



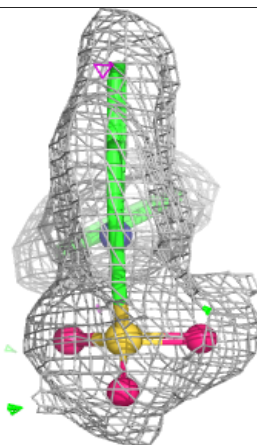
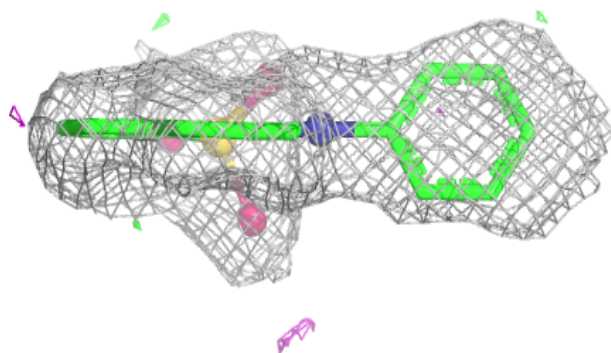
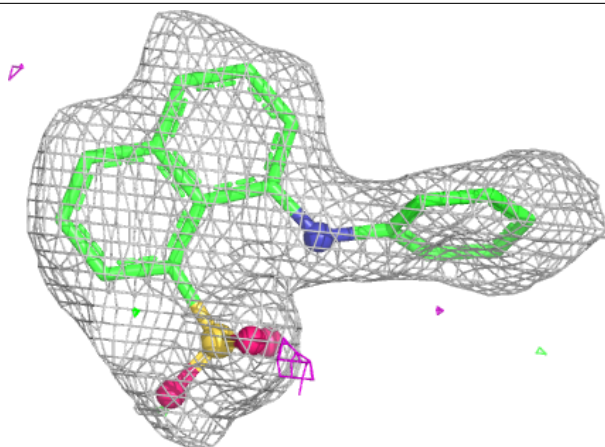
Electron density around 2AN I 203:

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



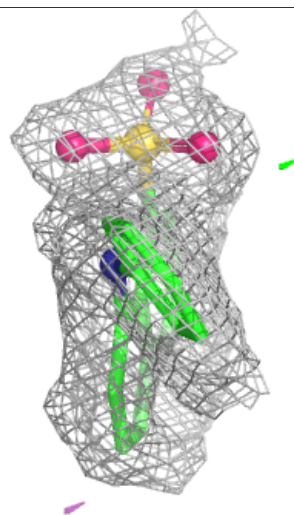
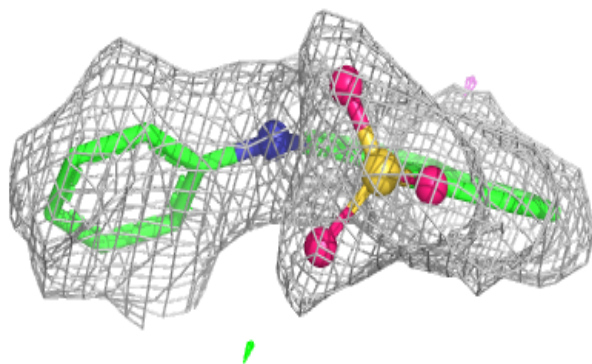
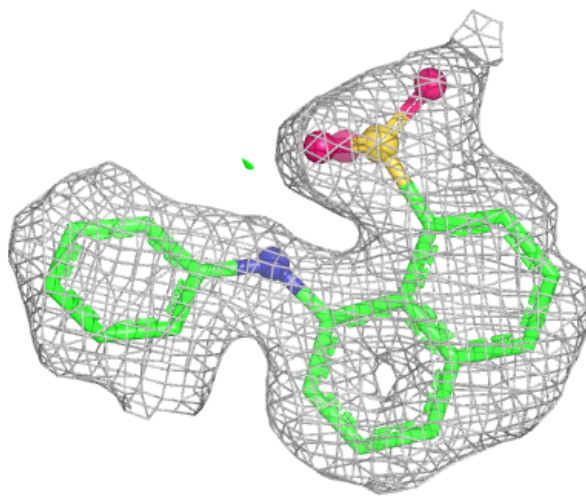
Electron density around 2AN M 501:

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



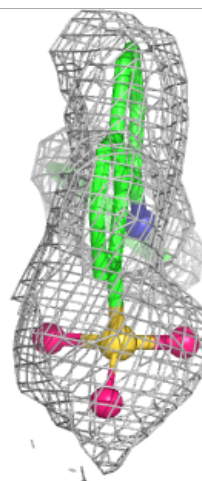
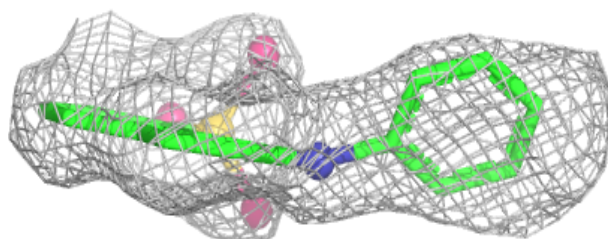
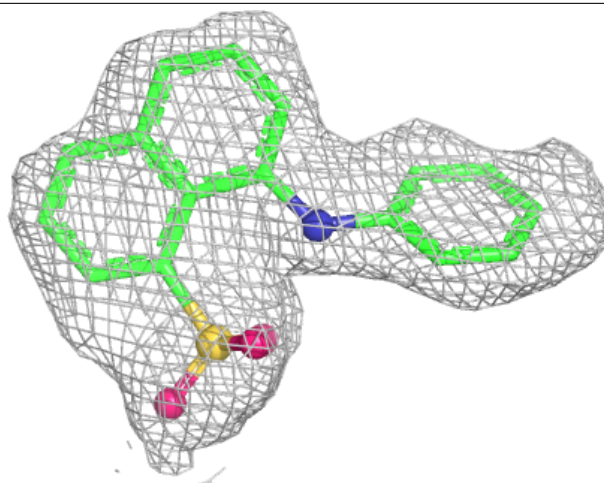
Electron density around 2AN K 201:

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



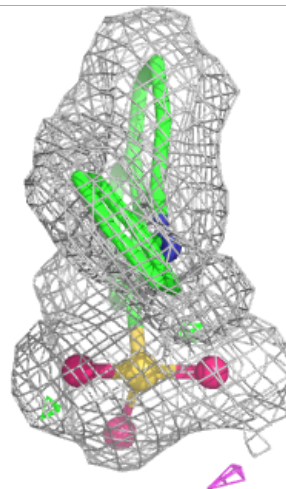
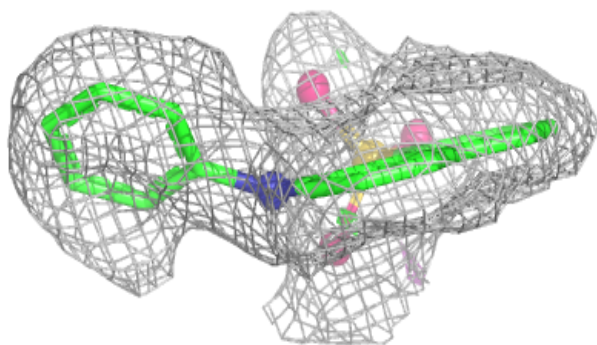
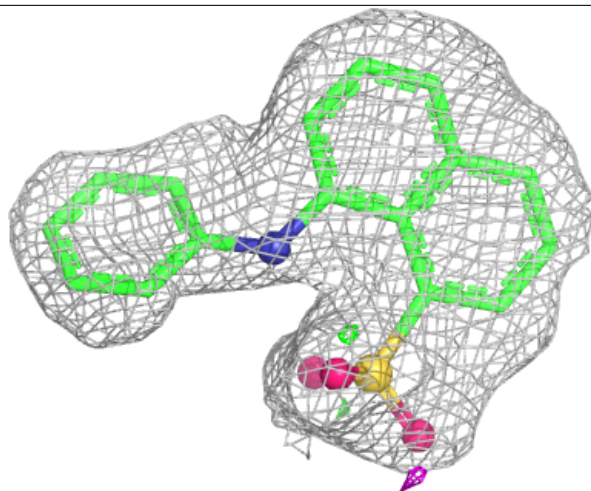
Electron density around 2AN I 204:

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



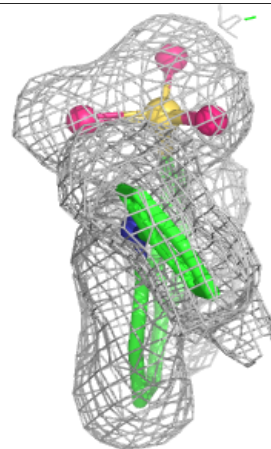
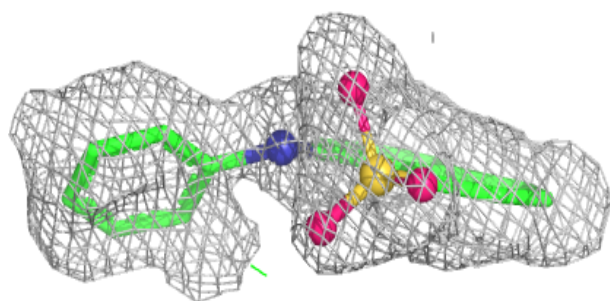
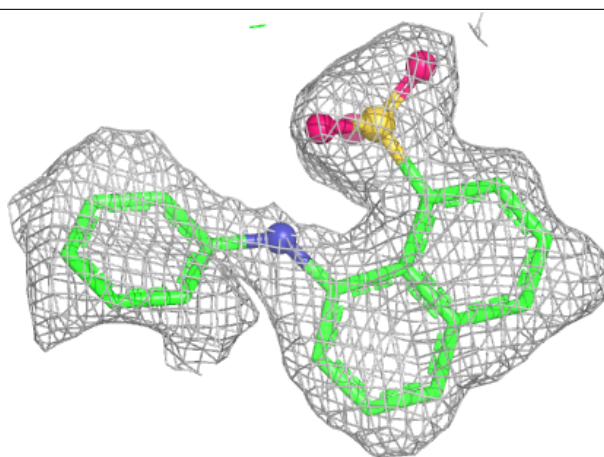
Electron density around 2AN L 201:

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



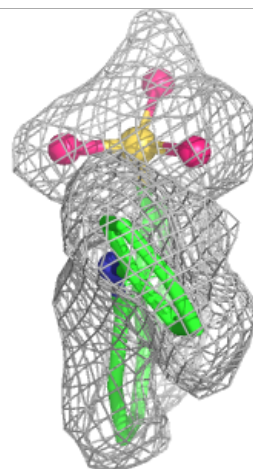
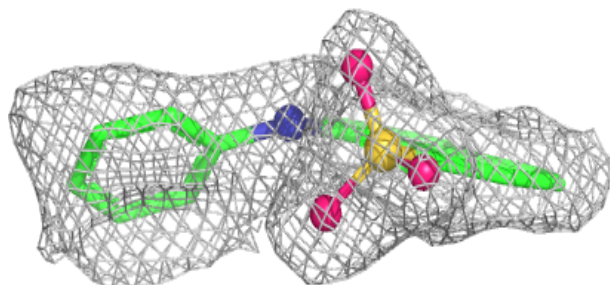
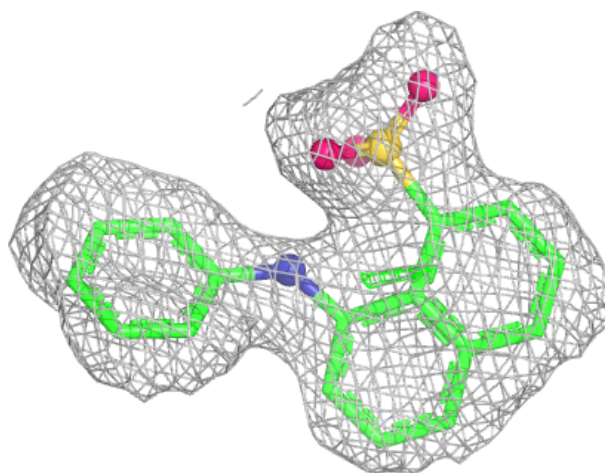
Electron density around 2AN O 201:

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



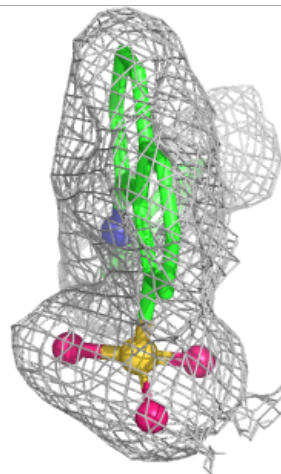
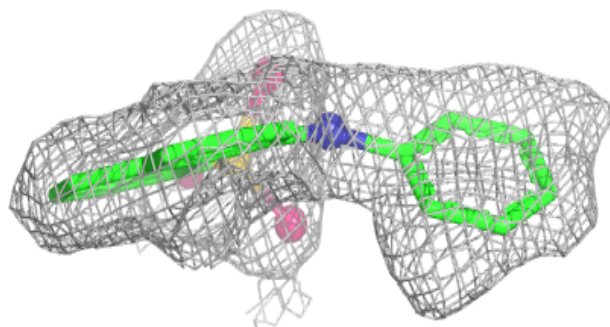
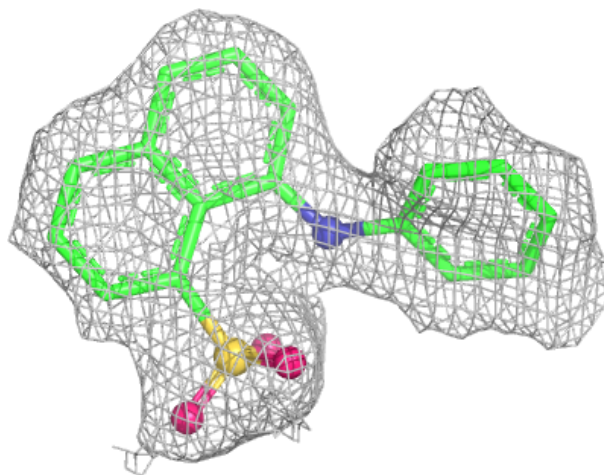
Electron density around 2AN I 201:

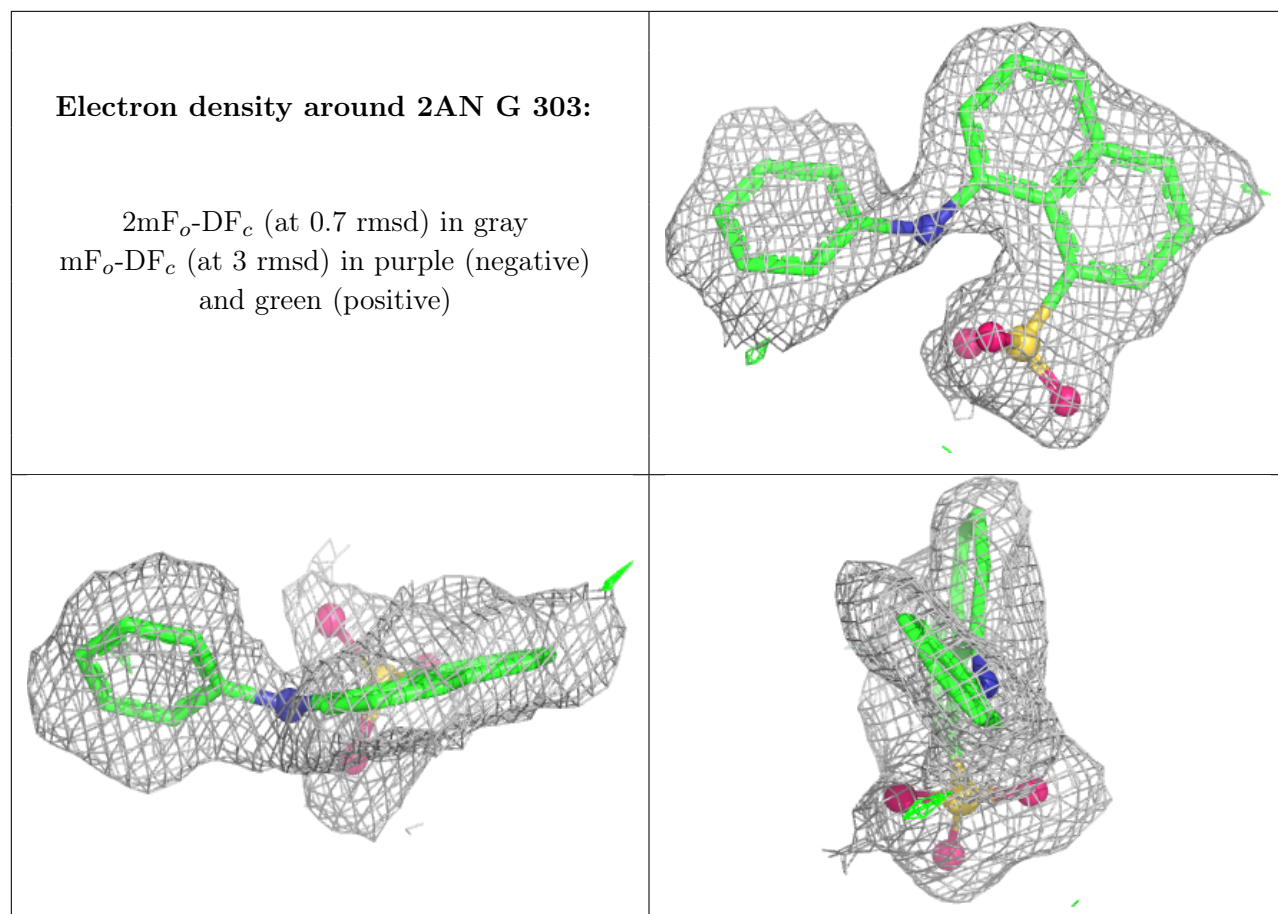
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around 2AN H 1102:

$2mF_o-DF_c$ (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.