



# wwPDB X-ray Structure Validation Summary Report ⓘ

Dec 8, 2020 – 02:41 AM EST

PDB ID : 6V8S  
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 wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.15.1  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.15.1

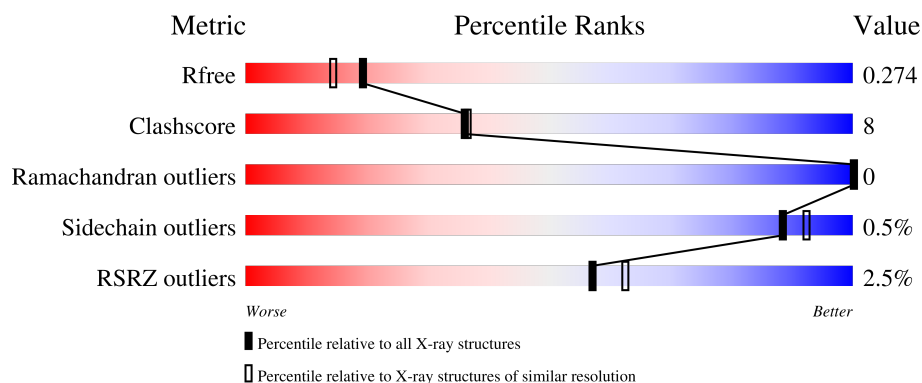
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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))
$R_{free}$	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	153	<div> <div>91%</div> <div>8% ..</div> </div>
1	B	153	<div> <div>95%</div> <div>5% .</div> </div>
1	C	153	<div> <div>92%</div> <div>8% .</div> </div>
1	D	153	<div> <div>4%</div> <div>92%</div> <div>7% .</div> </div>
1	E	153	<div> <div>3%</div> <div>93%</div> <div>7% .</div> </div>

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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	D	702	-	-	-	X
2	2AN	F	207	-	-	X	-
2	2AN	G	306	-	-	-	X
2	2AN	P	508	-	-	X	-

## 2 Entry composition [i](#)

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

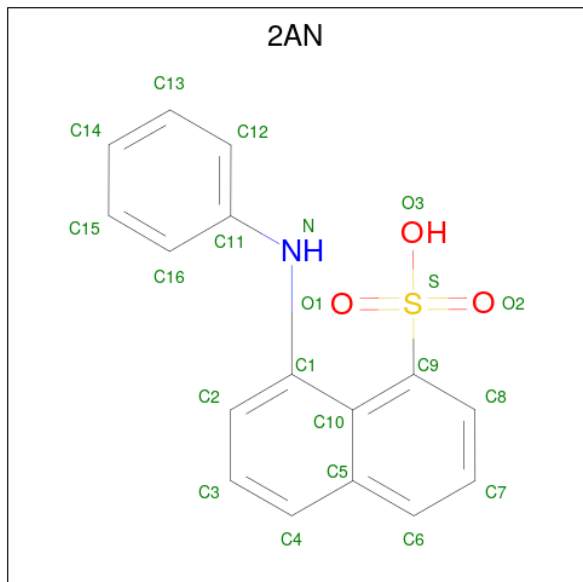
In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

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



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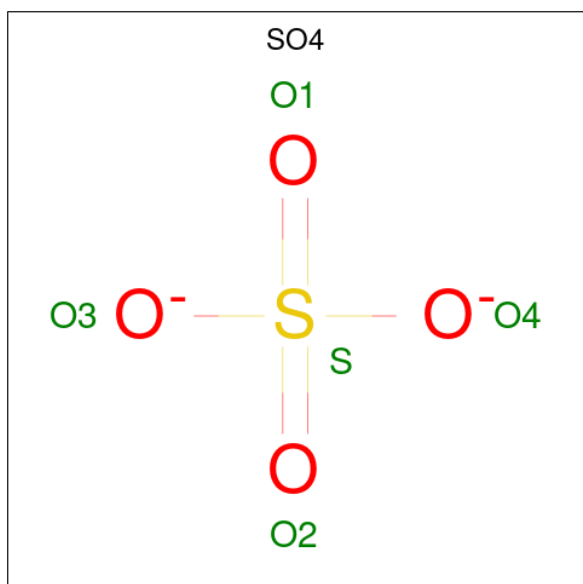
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	L	1	Total 21	C 16	N 1	O 3	S 1	0	0
2	M	1	Total 21	C 16	N 1	O 3	S 1	0	0
2	M	1	Total 21	C 16	N 1	O 3	S 1	0	0
2	M	1	Total 21	C 16	N 1	O 3	S 1	0	0
2	M	1	Total 21	C 16	N 1	O 3	S 1	0	0
2	M	1	Total 21	C 16	N 1	O 3	S 1	0	0
2	M	1	Total 21	C 16	N 1	O 3	S 1	0	0
2	M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

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



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

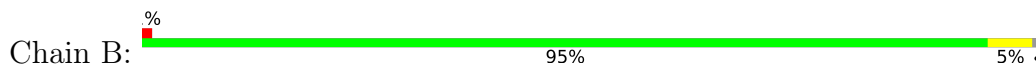
### 3 Residue-property plots [i](#)

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.

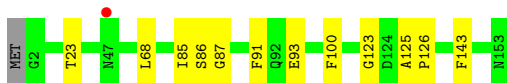
- Molecule 1: Ara h 8 allergen isoform



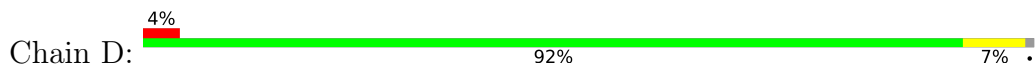
- Molecule 1: Ara h 8 allergen isoform



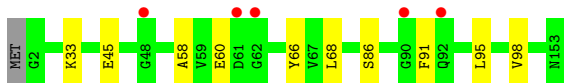
- Molecule 1: Ara h 8 allergen isoform



- Molecule 1: Ara h 8 allergen isoform

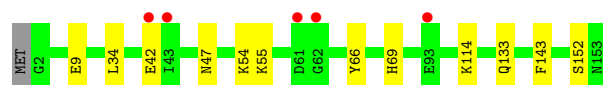
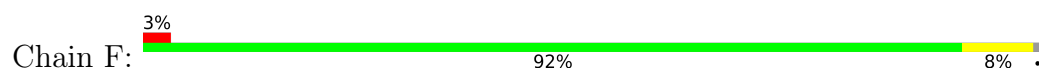


- Molecule 1: Ara h 8 allergen isoform

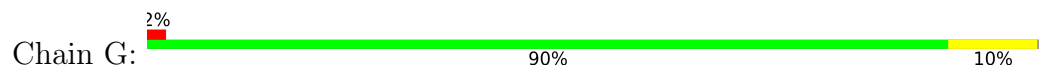


- Molecule 1: Ara h 8 allergen isoform

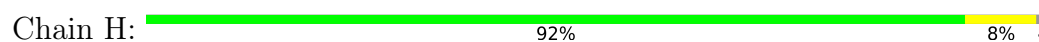




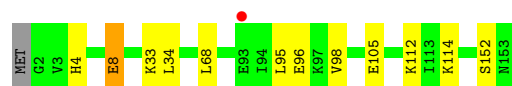
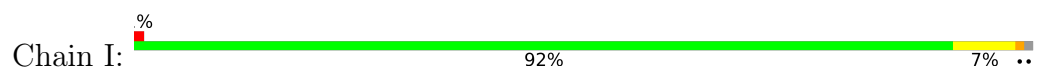
- Molecule 1: Ara h 8 allergen isoform



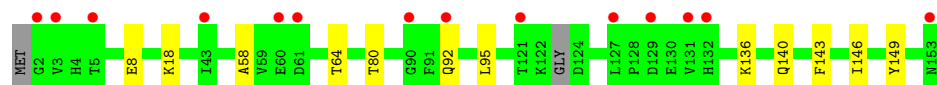
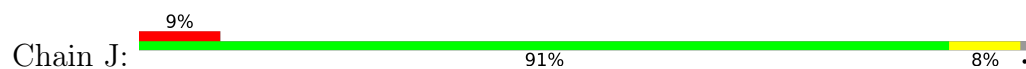
- Molecule 1: Ara h 8 allergen isoform



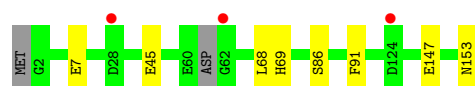
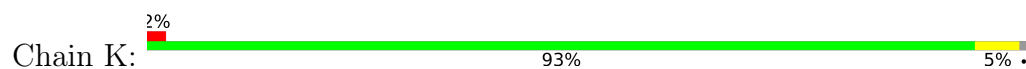
- Molecule 1: Ara h 8 allergen isoform



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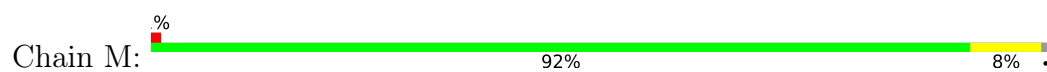
- Molecule 1: Ara h 8 allergen isoform



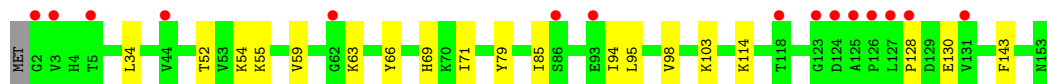
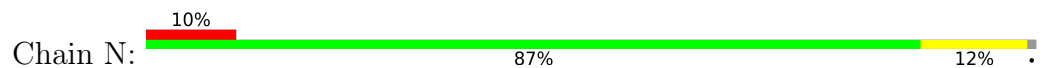
- Molecule 1: Ara h 8 allergen isoform



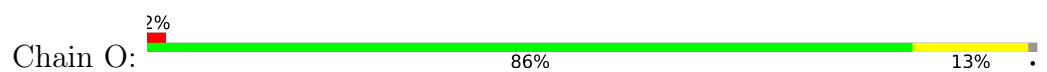
- Molecule 1: Ara h 8 allergen isoform



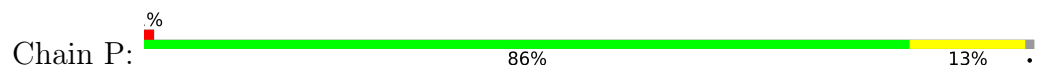
- Molecule 1: Ara h 8 allergen isoform



- Molecule 1: Ara h 8 allergen isoform



- Molecule 1: Ara h 8 allergen isoform



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	78.16Å 90.03Å 94.25Å 94.13° 106.91° 97.23°	Depositor
Resolution (Å)	38.09 – 2.10 38.06 – 2.10	Depositor EDS
% Data completeness (in resolution range)	91.5 (38.09-2.10) 91.5 (38.06-2.10)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	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 (4.89%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	19.6	Xtriage
Anisotropy	0.092	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 42.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.29$	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 <sup>2</sup> )	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.*

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

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.83	0/1168	0.85	0/1583
1	B	0.81	0/1165	0.85	0/1579
1	C	0.89	0/1160	0.89	0/1575
1	D	0.83	1/1167 (0.1%)	0.83	0/1584
1	E	0.84	0/1160	0.87	2/1573 (0.1%)
1	F	0.85	0/1168	0.88	0/1583
1	G	0.82	0/1177	0.87	2/1595 (0.1%)
1	H	0.88	0/1177	0.93	0/1595
1	I	0.83	2/1165 (0.2%)	0.86	0/1579
1	J	0.78	0/1157	0.86	0/1567
1	K	0.80	2/1139 (0.2%)	0.82	0/1546
1	L	0.79	0/1161	0.82	0/1574
1	M	0.86	1/1164 (0.1%)	0.90	0/1579
1	N	0.82	1/1157 (0.1%)	0.85	0/1570
1	O	0.82	2/1168 (0.2%)	0.87	0/1583
1	P	0.85	1/1164 (0.1%)	0.86	0/1578
All	All	0.83	10/18617 (0.1%)	0.86	4/25243 (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

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	76	GLU	CD-OE2	5.98	1.32	1.25
1	I	96	GLU	CD-OE2	5.80	1.32	1.25
1	M	8	GLU	CD-OE2	5.35	1.31	1.25
1	K	147	GLU	CD-OE1	5.32	1.31	1.25
1	O	96	GLU	CD-OE2	5.29	1.31	1.25

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	66	TYR	CB-CG-CD2	-5.50	117.70	121.00
1	G	66	TYR	CB-CG-CD1	5.46	124.28	121.00
1	E	66	TYR	CB-CG-CD1	5.12	124.07	121.00
1	E	66	TYR	CB-CG-CD2	-5.02	117.99	121.00

There are no chirality outliers.

5 of 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

## 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	11	0
1	B	1143	0	1134	6	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	I	1143	0	1134	9	0
1	J	1136	0	1128	8	0
1	K	1118	0	1097	4	0
1	L	1139	0	1130	6	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	20	0
2	G	126	0	73	11	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	1	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
4	J	62	0	0	4	0
4	K	57	0	0	2	0
4	L	90	0	0	2	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	317	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.

The worst 5 of 317 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:O1	2:P:503:2AN:N	2.07	0.88
2:K:205:2AN:N	2:K:205:2AN:O3	2.06	0.87
2:I:205:2AN:H13	1:O:18:LYS:HD3	1.58	0.86
2:J:202:2AN:O1	2:J:202:2AN:N	2.13	0.82
1:L:59:VAL:HG22	1:L:64:THR:HG22	1.65	0.78

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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	49	53
1	B	125/128 (98%)	124 (99%)	1 (1%)	81	86
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%)	125 (99%)	1 (1%)	81	86
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%)	124 (99%)	1 (1%)	81	86
1	J	124/128 (97%)	123 (99%)	1 (1%)	81	86
1	K	120/128 (94%)	119 (99%)	1 (1%)	81	86
1	L	124/128 (97%)	124 (100%)	0	100	100
1	M	125/128 (98%)	124 (99%)	1 (1%)	81	86
1	N	123/128 (96%)	123 (100%)	0	100	100
1	O	126/128 (98%)	125 (99%)	1 (1%)	81	86
1	P	125/128 (98%)	125 (100%)	0	100	100
All	All	1996/2048 (98%)	1986 (100%)	10 (0%)	88	92



5 of 10 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	133	GLN
1	I	112	LYS
1	K	69	HIS
1	B	69	HIS
1	J	8	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	153	ASN
1	N	69	HIS
1	N	153	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

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	P	508	-	22,23,23	0.68	1 (4%)	29,33,33	0.74	0
2	2AN	K	207	-	22,23,23	0.71	1 (4%)	29,33,33	0.73	0
2	2AN	H	1107	-	22,23,23	0.72	1 (4%)	29,33,33	0.74	0
2	2AN	B	203	-	22,23,23	0.73	1 (4%)	29,33,33	0.80	0
2	2AN	E	506	-	22,23,23	0.83	1 (4%)	29,33,33	0.88	1 (3%)
2	2AN	H	1104	-	22,23,23	0.68	0	29,33,33	0.88	0
2	2AN	F	202	-	22,23,23	0.70	1 (4%)	29,33,33	0.80	0
2	2AN	E	502	-	22,23,23	0.80	1 (4%)	29,33,33	1.00	2 (6%)
2	2AN	G	303	-	22,23,23	0.75	0	29,33,33	0.75	0
2	2AN	M	505	-	22,23,23	0.77	1 (4%)	29,33,33	1.16	2 (6%)
2	2AN	L	201	-	22,23,23	0.68	1 (4%)	29,33,33	0.95	2 (6%)
2	2AN	F	204	-	22,23,23	0.76	1 (4%)	29,33,33	0.83	0
2	2AN	I	201	-	22,23,23	0.49	0	29,33,33	0.90	1 (3%)
2	2AN	E	504	-	22,23,23	0.81	1 (4%)	29,33,33	0.77	0
2	2AN	N	203	-	22,23,23	0.83	1 (4%)	29,33,33	0.81	1 (3%)
2	2AN	I	203	-	22,23,23	0.84	1 (4%)	29,33,33	0.95	1 (3%)
2	2AN	P	501	-	22,23,23	0.71	1 (4%)	29,33,33	0.81	0
2	2AN	C	308	-	22,23,23	0.99	3 (13%)	29,33,33	0.89	1 (3%)
2	2AN	B	201	-	22,23,23	0.85	1 (4%)	29,33,33	0.93	1 (3%)
2	2AN	G	302	-	22,23,23	0.72	1 (4%)	29,33,33	0.81	1 (3%)
2	2AN	G	306	-	22,23,23	0.77	1 (4%)	29,33,33	0.77	0
2	2AN	J	204	-	22,23,23	0.82	1 (4%)	29,33,33	0.74	0
2	2AN	M	502	-	22,23,23	0.89	1 (4%)	29,33,33	1.06	3 (10%)
2	2AN	F	207	-	22,23,23	0.72	1 (4%)	29,33,33	0.77	1 (3%)
2	2AN	J	203	-	22,23,23	0.95	2 (9%)	29,33,33	0.83	1 (3%)
2	2AN	F	208	-	22,23,23	0.97	3 (13%)	29,33,33	0.85	1 (3%)
2	2AN	P	503	-	22,23,23	0.78	1 (4%)	29,33,33	0.89	1 (3%)
2	2AN	D	701	-	22,23,23	0.97	1 (4%)	29,33,33	0.84	0
2	2AN	K	204	-	22,23,23	0.83	1 (4%)	29,33,33	0.76	0
2	2AN	P	505	-	22,23,23	0.73	0	29,33,33	0.97	2 (6%)
2	2AN	E	505	-	22,23,23	0.75	1 (4%)	29,33,33	0.72	0
2	2AN	P	507	-	22,23,23	0.72	1 (4%)	29,33,33	0.70	0
2	2AN	N	202	-	22,23,23	0.96	1 (4%)	29,33,33	0.91	2 (6%)
2	2AN	A	203	-	22,23,23	0.79	1 (4%)	29,33,33	0.90	1 (3%)
2	2AN	I	202	-	22,23,23	0.71	1 (4%)	29,33,33	0.84	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	2AN	L	203	-	22,23,23	0.80	1 (4%)	29,33,33	0.78	0
2	2AN	M	506	-	22,23,23	0.75	1 (4%)	29,33,33	0.81	0
2	2AN	A	202	-	22,23,23	0.78	1 (4%)	29,33,33	0.77	0
2	2AN	D	705	-	22,23,23	0.78	1 (4%)	29,33,33	0.73	0
2	2AN	E	501	-	22,23,23	0.66	0	29,33,33	0.79	0
2	2AN	G	304	-	22,23,23	0.69	1 (4%)	29,33,33	0.92	1 (3%)
2	2AN	P	504	-	22,23,23	0.74	0	29,33,33	0.80	0
2	2AN	C	306	-	22,23,23	0.63	1 (4%)	29,33,33	1.16	3 (10%)
2	2AN	J	201	-	22,23,23	0.73	0	29,33,33	0.88	0
2	2AN	H	1105	-	22,23,23	0.68	1 (4%)	29,33,33	0.80	0
2	2AN	B	202	-	22,23,23	0.72	1 (4%)	29,33,33	0.82	0
2	2AN	I	204	-	22,23,23	0.73	1 (4%)	29,33,33	0.87	1 (3%)
2	2AN	K	201	-	22,23,23	0.94	1 (4%)	29,33,33	0.82	0
2	2AN	H	1106	-	22,23,23	0.77	1 (4%)	29,33,33	0.99	1 (3%)
2	2AN	P	509	-	22,23,23	0.89	1 (4%)	29,33,33	0.71	0
2	2AN	E	507	-	22,23,23	1.09	3 (13%)	29,33,33	1.14	1 (3%)
2	2AN	L	202	-	22,23,23	0.81	1 (4%)	29,33,33	0.87	1 (3%)
2	2AN	H	1108	-	22,23,23	0.81	1 (4%)	29,33,33	0.81	1 (3%)
2	2AN	F	205	-	22,23,23	0.76	1 (4%)	29,33,33	0.84	1 (3%)
2	2AN	J	205	-	22,23,23	0.80	1 (4%)	29,33,33	0.88	1 (3%)
2	2AN	I	205	-	22,23,23	0.71	1 (4%)	29,33,33	0.77	1 (3%)
2	2AN	D	704	-	22,23,23	0.75	1 (4%)	29,33,33	0.80	0
2	2AN	A	204	-	22,23,23	0.68	1 (4%)	29,33,33	0.78	0
2	2AN	D	702	-	22,23,23	0.86	2 (9%)	29,33,33	0.76	0
2	2AN	G	305	-	22,23,23	0.76	1 (4%)	29,33,33	0.84	1 (3%)
2	2AN	M	504	-	22,23,23	0.84	0	29,33,33	0.80	1 (3%)
2	2AN	E	503	-	22,23,23	0.89	2 (9%)	29,33,33	0.95	2 (6%)
2	2AN	F	206	-	22,23,23	0.77	1 (4%)	29,33,33	0.96	1 (3%)
2	2AN	J	202	-	22,23,23	0.84	1 (4%)	29,33,33	0.95	1 (3%)
2	2AN	K	205	-	22,23,23	0.67	1 (4%)	29,33,33	1.17	2 (6%)
2	2AN	M	503	-	22,23,23	0.86	1 (4%)	29,33,33	0.86	0
2	2AN	O	202	-	22,23,23	0.74	1 (4%)	29,33,33	0.72	0
2	2AN	C	301	-	22,23,23	0.98	1 (4%)	29,33,33	0.94	0
2	2AN	L	204	-	22,23,23	0.69	1 (4%)	29,33,33	0.76	0
2	2AN	C	303	-	22,23,23	0.90	1 (4%)	29,33,33	0.91	1 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	2AN	H	1102	-	22,23,23	0.66	0	29,33,33	0.91	0
2	2AN	M	509	-	22,23,23	0.62	0	29,33,33	0.80	0
2	2AN	H	1109	-	22,23,23	0.92	2 (9%)	29,33,33	0.90	1 (3%)
2	2AN	N	201	-	22,23,23	0.57	0	29,33,33	0.66	0
2	2AN	M	508	-	22,23,23	0.73	1 (4%)	29,33,33	0.85	0
2	2AN	K	206	-	22,23,23	1.17	3 (13%)	29,33,33	0.95	1 (3%)
2	2AN	C	309	-	22,23,23	0.75	1 (4%)	29,33,33	0.85	0
2	2AN	F	201	-	22,23,23	0.62	0	29,33,33	0.73	0
2	2AN	A	205	-	22,23,23	0.63	0	29,33,33	0.82	1 (3%)
2	2AN	B	204	-	22,23,23	0.77	1 (4%)	29,33,33	0.85	0
2	2AN	C	305	-	22,23,23	0.78	1 (4%)	29,33,33	0.84	0
2	2AN	G	301	-	22,23,23	0.63	1 (4%)	29,33,33	0.79	0
2	2AN	F	203	-	22,23,23	0.80	1 (4%)	29,33,33	0.74	0
2	2AN	N	204	-	22,23,23	0.95	1 (4%)	29,33,33	0.81	0
2	2AN	D	706	-	22,23,23	0.81	1 (4%)	29,33,33	0.76	0
2	2AN	K	203	-	22,23,23	0.76	1 (4%)	29,33,33	0.75	1 (3%)
2	2AN	J	206	-	22,23,23	0.68	1 (4%)	29,33,33	0.83	2 (6%)
2	2AN	C	307	-	22,23,23	0.74	1 (4%)	29,33,33	0.80	0
2	2AN	A	201	-	22,23,23	0.86	1 (4%)	29,33,33	0.86	0
2	2AN	K	202	-	22,23,23	0.74	1 (4%)	29,33,33	1.02	2 (6%)
2	2AN	O	201	-	22,23,23	0.85	1 (4%)	29,33,33	0.88	0
2	2AN	P	502	-	22,23,23	0.63	0	29,33,33	0.77	0
2	2AN	C	304	-	22,23,23	0.70	1 (4%)	29,33,33	0.63	0
2	2AN	O	203	-	22,23,23	0.74	1 (4%)	29,33,33	1.04	2 (6%)
2	2AN	M	507	-	22,23,23	0.89	1 (4%)	29,33,33	0.71	0
2	2AN	P	506	-	22,23,23	0.80	1 (4%)	29,33,33	0.84	0
3	SO4	H	1110	-	4,4,4	0.34	0	6,6,6	0.08	0
2	2AN	H	1103	-	22,23,23	0.83	1 (4%)	29,33,33	0.72	0
2	2AN	D	703	-	22,23,23	0.72	0	29,33,33	1.05	2 (6%)
2	2AN	O	204	-	22,23,23	0.79	1 (4%)	29,33,33	0.89	2 (6%)
2	2AN	M	501	-	22,23,23	0.77	1 (4%)	29,33,33	0.79	0
2	2AN	C	302	-	22,23,23	0.76	0	29,33,33	0.80	0
2	2AN	H	1101	-	22,23,23	0.73	1 (4%)	29,33,33	0.99	1 (3%)

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	P	508	-	-	0/10/10/10	0/3/3/3
2	2AN	K	207	-	-	2/10/10/10	0/3/3/3
2	2AN	H	1107	-	-	0/10/10/10	0/3/3/3
2	2AN	B	203	-	-	0/10/10/10	0/3/3/3
2	2AN	E	506	-	-	2/10/10/10	0/3/3/3
2	2AN	H	1104	-	-	2/10/10/10	0/3/3/3
2	2AN	F	202	-	-	1/10/10/10	0/3/3/3
2	2AN	E	502	-	-	0/10/10/10	0/3/3/3
2	2AN	G	303	-	-	0/10/10/10	0/3/3/3
2	2AN	M	505	-	-	1/10/10/10	0/3/3/3
2	2AN	L	201	-	-	0/10/10/10	0/3/3/3
2	2AN	F	204	-	-	0/10/10/10	0/3/3/3
2	2AN	I	201	-	-	0/10/10/10	0/3/3/3
2	2AN	E	504	-	-	1/10/10/10	0/3/3/3
2	2AN	N	203	-	-	0/10/10/10	0/3/3/3
2	2AN	I	203	-	-	0/10/10/10	0/3/3/3
2	2AN	P	501	-	-	0/10/10/10	0/3/3/3
2	2AN	C	308	-	-	2/10/10/10	0/3/3/3
2	2AN	B	201	-	-	0/10/10/10	0/3/3/3
2	2AN	G	302	-	-	0/10/10/10	0/3/3/3
2	2AN	G	306	-	-	0/10/10/10	0/3/3/3
2	2AN	J	204	-	-	0/10/10/10	0/3/3/3
2	2AN	M	502	-	-	0/10/10/10	0/3/3/3
2	2AN	F	207	-	-	2/10/10/10	0/3/3/3
2	2AN	J	203	-	-	1/10/10/10	0/3/3/3
2	2AN	F	208	-	-	1/10/10/10	0/3/3/3
2	2AN	P	503	-	-	8/10/10/10	0/3/3/3
2	2AN	D	701	-	-	2/10/10/10	0/3/3/3
2	2AN	K	204	-	-	0/10/10/10	0/3/3/3
2	2AN	P	505	-	-	0/10/10/10	0/3/3/3
2	2AN	E	505	-	-	0/10/10/10	0/3/3/3
2	2AN	P	507	-	-	0/10/10/10	0/3/3/3
2	2AN	N	202	-	-	0/10/10/10	0/3/3/3
2	2AN	A	203	-	-	0/10/10/10	0/3/3/3
2	2AN	I	202	-	-	1/10/10/10	0/3/3/3
2	2AN	L	203	-	-	0/10/10/10	0/3/3/3
2	2AN	M	506	-	-	2/10/10/10	0/3/3/3
2	2AN	A	202	-	-	2/10/10/10	0/3/3/3
2	2AN	D	705	-	-	0/10/10/10	0/3/3/3
2	2AN	E	501	-	-	2/10/10/10	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	2AN	G	304	-	-	1/10/10/10	0/3/3/3
2	2AN	P	504	-	-	0/10/10/10	0/3/3/3
2	2AN	C	306	-	-	0/10/10/10	0/3/3/3
2	2AN	J	201	-	-	0/10/10/10	0/3/3/3
2	2AN	H	1105	-	-	0/10/10/10	0/3/3/3
2	2AN	B	202	-	-	0/10/10/10	0/3/3/3
2	2AN	I	204	-	-	0/10/10/10	0/3/3/3
2	2AN	K	201	-	-	0/10/10/10	0/3/3/3
2	2AN	H	1106	-	-	0/10/10/10	0/3/3/3
2	2AN	P	509	-	-	2/10/10/10	0/3/3/3
2	2AN	E	507	-	-	6/10/10/10	0/3/3/3
2	2AN	L	202	-	-	0/10/10/10	0/3/3/3
2	2AN	H	1108	-	-	0/10/10/10	0/3/3/3
2	2AN	F	205	-	-	0/10/10/10	0/3/3/3
2	2AN	J	205	-	-	0/10/10/10	0/3/3/3
2	2AN	I	205	-	-	0/10/10/10	0/3/3/3
2	2AN	D	704	-	-	0/10/10/10	0/3/3/3
2	2AN	A	204	-	-	0/10/10/10	0/3/3/3
2	2AN	D	702	-	-	2/10/10/10	0/3/3/3
2	2AN	G	305	-	-	0/10/10/10	0/3/3/3
2	2AN	M	504	-	-	0/10/10/10	0/3/3/3
2	2AN	E	503	-	-	0/10/10/10	0/3/3/3
2	2AN	F	206	-	-	0/10/10/10	0/3/3/3
2	2AN	J	202	-	-	3/10/10/10	0/3/3/3
2	2AN	K	205	-	-	8/10/10/10	0/3/3/3
2	2AN	M	503	-	-	0/10/10/10	0/3/3/3
2	2AN	O	202	-	-	0/10/10/10	0/3/3/3
2	2AN	C	301	-	-	0/10/10/10	0/3/3/3
2	2AN	L	204	-	-	2/10/10/10	0/3/3/3
2	2AN	C	303	-	-	0/10/10/10	0/3/3/3
2	2AN	H	1102	-	-	0/10/10/10	0/3/3/3
2	2AN	M	509	-	-	5/10/10/10	0/3/3/3
2	2AN	H	1109	-	-	2/10/10/10	0/3/3/3
2	2AN	N	201	-	-	0/10/10/10	0/3/3/3
2	2AN	M	508	-	-	0/10/10/10	0/3/3/3
2	2AN	K	206	-	-	0/10/10/10	0/3/3/3
2	2AN	C	309	-	-	2/10/10/10	0/3/3/3
2	2AN	F	201	-	-	0/10/10/10	0/3/3/3
2	2AN	A	205	-	-	0/10/10/10	0/3/3/3
2	2AN	B	204	-	-	0/10/10/10	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	2AN	C	305	-	-	2/10/10/10	0/3/3/3
2	2AN	G	301	-	-	1/10/10/10	0/3/3/3
2	2AN	F	203	-	-	0/10/10/10	0/3/3/3
2	2AN	N	204	-	-	2/10/10/10	0/3/3/3
2	2AN	D	706	-	-	2/10/10/10	0/3/3/3
2	2AN	K	203	-	-	0/10/10/10	0/3/3/3
2	2AN	J	206	-	-	7/10/10/10	0/3/3/3
2	2AN	C	307	-	-	0/10/10/10	0/3/3/3
2	2AN	A	201	-	-	0/10/10/10	0/3/3/3
2	2AN	K	202	-	-	0/10/10/10	0/3/3/3
2	2AN	O	201	-	-	0/10/10/10	0/3/3/3
2	2AN	P	502	-	-	0/10/10/10	0/3/3/3
2	2AN	C	304	-	-	0/10/10/10	0/3/3/3
2	2AN	O	203	-	-	0/10/10/10	0/3/3/3
2	2AN	M	507	-	-	0/10/10/10	0/3/3/3
2	2AN	P	506	-	-	0/10/10/10	0/3/3/3
2	2AN	H	1103	-	-	5/10/10/10	0/3/3/3
2	2AN	D	703	-	-	0/10/10/10	0/3/3/3
2	2AN	O	204	-	-	0/10/10/10	0/3/3/3
2	2AN	M	501	-	-	2/10/10/10	0/3/3/3
2	2AN	C	302	-	-	0/10/10/10	0/3/3/3
2	2AN	H	1101	-	-	2/10/10/10	0/3/3/3

The worst 5 of 98 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	203	2AN	O1-S	3.34	1.60	1.43
2	K	206	2AN	C1-N	3.30	1.47	1.38
2	N	202	2AN	O1-S	3.21	1.59	1.43
2	M	507	2AN	O1-S	3.13	1.59	1.43
2	B	201	2AN	O2-S	3.07	1.59	1.43

The worst 5 of 61 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	205	2AN	C11-N-C1	-4.21	116.25	126.71
2	M	505	2AN	C10-C1-N	-3.55	115.41	120.71
2	C	306	2AN	C10-C1-N	-3.48	115.52	120.71
2	E	507	2AN	C11-N-C1	3.03	134.24	126.71
2	K	202	2AN	C11-N-C1	2.83	133.74	126.71

There are no chirality outliers.

5 of 88 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	P	503	2AN	C8-C9-S-O1
2	P	503	2AN	C10-C9-S-O1
2	P	503	2AN	C8-C9-S-O2
2	P	503	2AN	C10-C9-S-O2
2	P	503	2AN	C8-C9-S-O3

There are no ring outliers.

86 monomers are involved in 219 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	P	508	2AN	10	0
2	H	1107	2AN	6	0
2	B	203	2AN	1	0
2	E	506	2AN	5	0
2	F	202	2AN	3	0
2	E	502	2AN	3	0
2	G	303	2AN	2	0
2	M	505	2AN	4	0
2	L	201	2AN	4	0
2	F	204	2AN	2	0
2	I	201	2AN	1	0
2	E	504	2AN	2	0
2	N	203	2AN	3	0
2	I	203	2AN	3	0
2	P	501	2AN	3	0
2	C	308	2AN	4	0
2	G	302	2AN	1	0
2	G	306	2AN	2	0
2	J	204	2AN	1	0
2	F	207	2AN	7	0
2	F	208	2AN	1	0
2	P	503	2AN	5	0
2	D	701	2AN	1	0
2	K	204	2AN	3	0
2	E	505	2AN	3	0
2	P	507	2AN	2	0
2	N	202	2AN	5	0
2	I	202	2AN	1	0
2	L	203	2AN	1	0
2	M	506	2AN	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	202	2AN	5	0
2	D	705	2AN	1	0
2	G	304	2AN	2	0
2	P	504	2AN	1	0
2	C	306	2AN	2	0
2	J	201	2AN	2	0
2	H	1105	2AN	1	0
2	B	202	2AN	1	0
2	K	201	2AN	3	0
2	P	509	2AN	2	0
2	E	507	2AN	3	0
2	H	1108	2AN	3	0
2	J	205	2AN	3	0
2	I	205	2AN	5	0
2	D	704	2AN	1	0
2	A	204	2AN	1	0
2	D	702	2AN	4	0
2	G	305	2AN	3	0
2	M	504	2AN	3	0
2	E	503	2AN	2	0
2	F	206	2AN	3	0
2	J	202	2AN	3	0
2	K	205	2AN	6	0
2	O	202	2AN	2	0
2	L	204	2AN	1	0
2	C	303	2AN	3	0
2	H	1102	2AN	2	0
2	M	509	2AN	2	0
2	H	1109	2AN	5	0
2	N	201	2AN	4	0
2	M	508	2AN	1	0
2	K	206	2AN	1	0
2	C	309	2AN	3	0
2	F	201	2AN	2	0
2	A	205	2AN	1	0
2	B	204	2AN	2	0
2	C	305	2AN	2	0
2	G	301	2AN	1	0
2	F	203	2AN	2	0
2	N	204	2AN	1	0
2	D	706	2AN	5	0
2	K	203	2AN	2	0

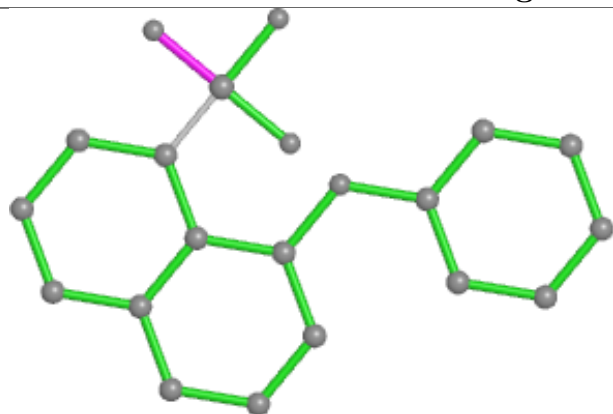
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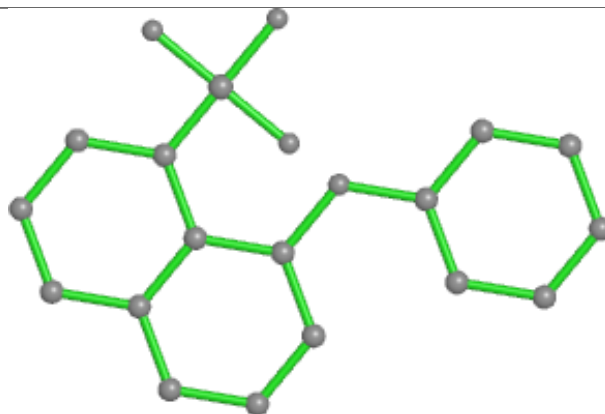
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	307	2AN	2	0
2	A	201	2AN	3	0
2	K	202	2AN	2	0
2	O	201	2AN	1	0
2	P	502	2AN	1	0
2	C	304	2AN	2	0
2	O	203	2AN	2	0
2	M	507	2AN	2	0
2	P	506	2AN	1	0
2	H	1103	2AN	2	0
2	O	204	2AN	2	0
2	M	501	2AN	2	0
2	C	302	2AN	2	0
2	H	1101	2AN	3	0

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

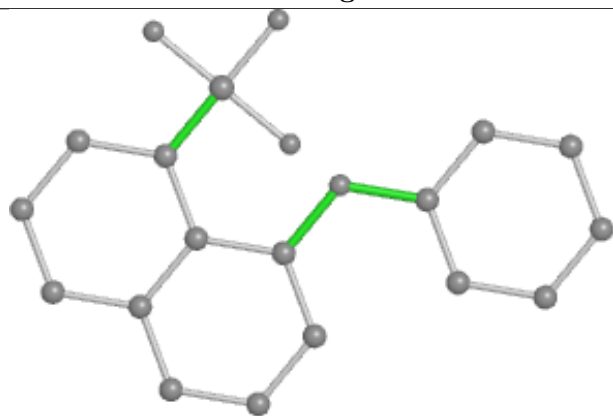
## Ligand 2AN P 508



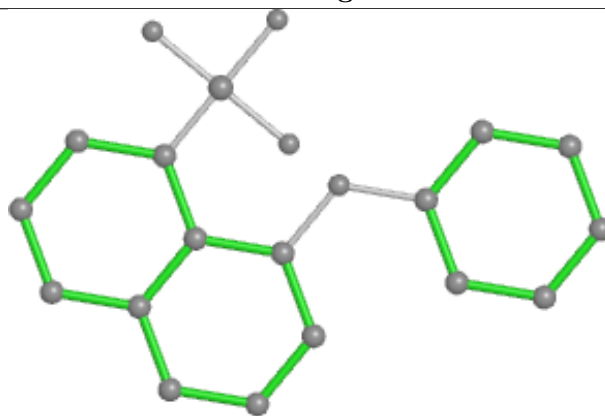
Bond lengths



Bond angles

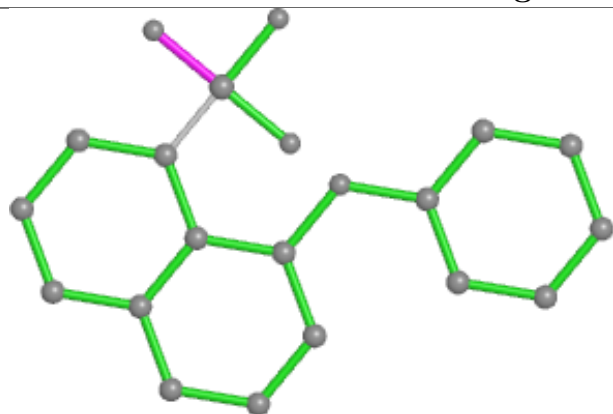


Torsions

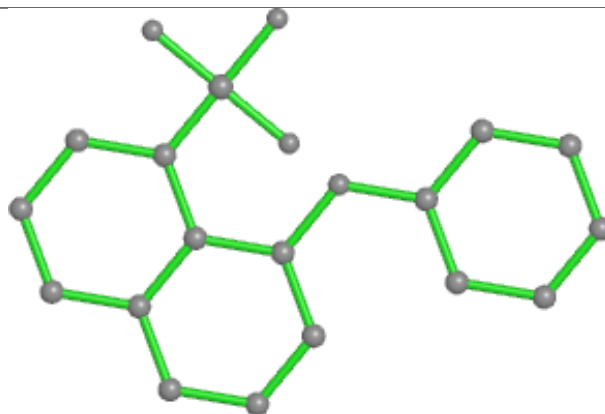


Rings

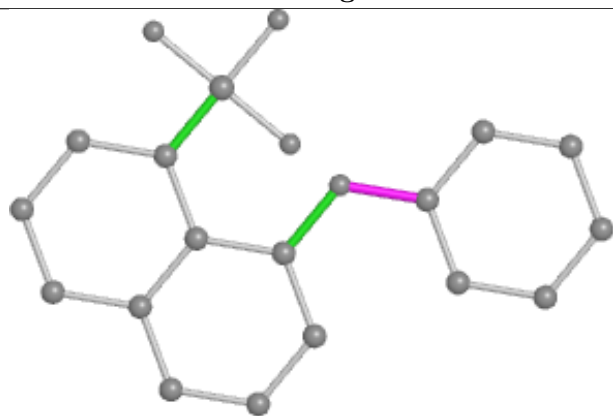
## Ligand 2AN K 207



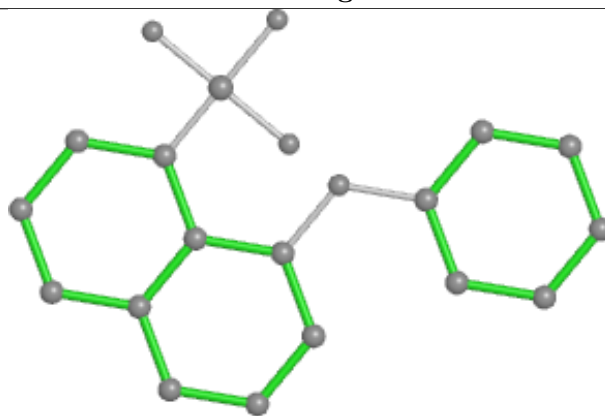
Bond lengths



Bond angles

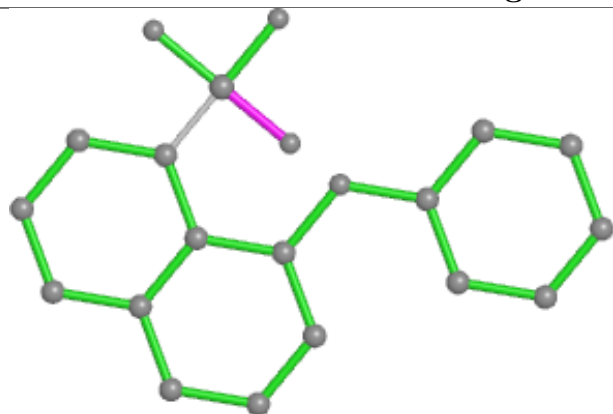


Torsions

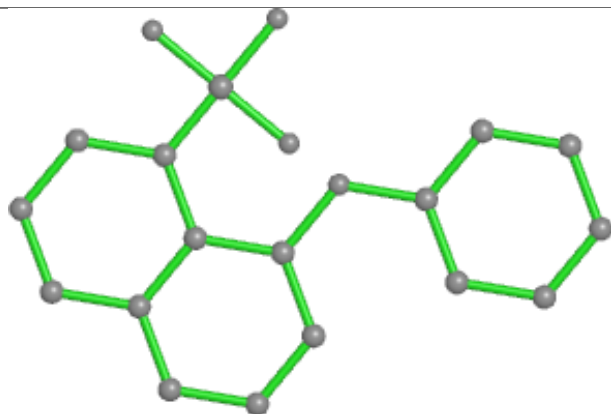


Rings

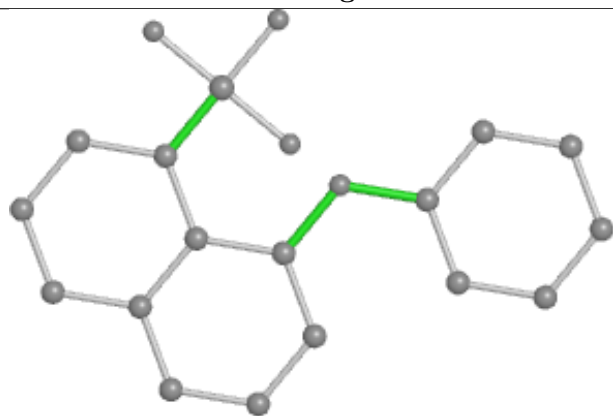
## Ligand 2AN H 1107



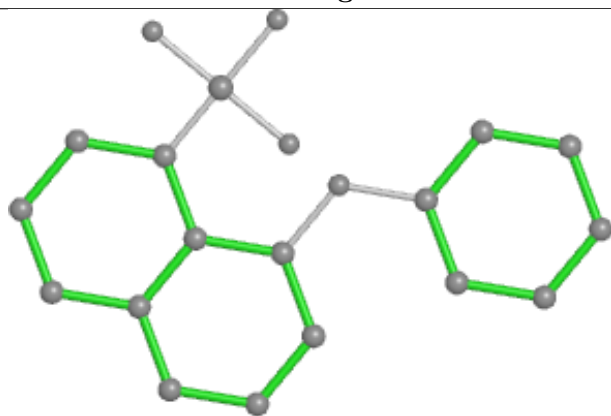
Bond lengths



Bond angles

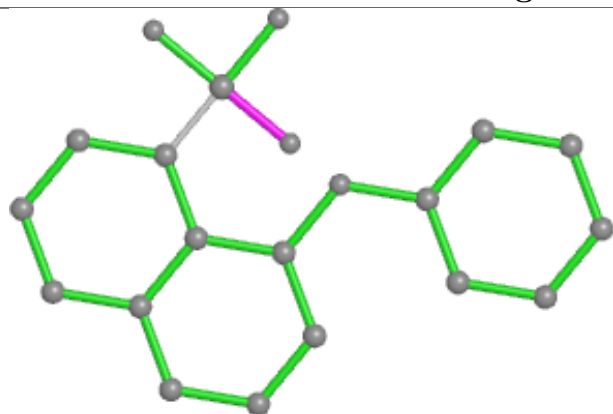


Torsions

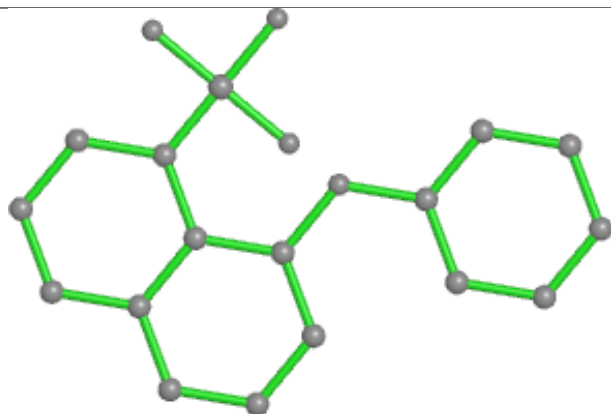


Rings

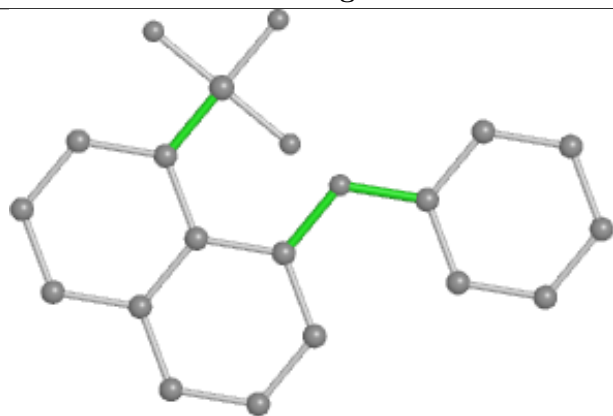
## Ligand 2AN B 203



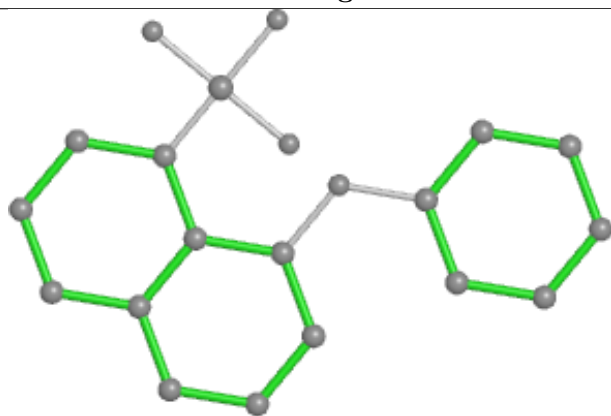
Bond lengths



Bond angles

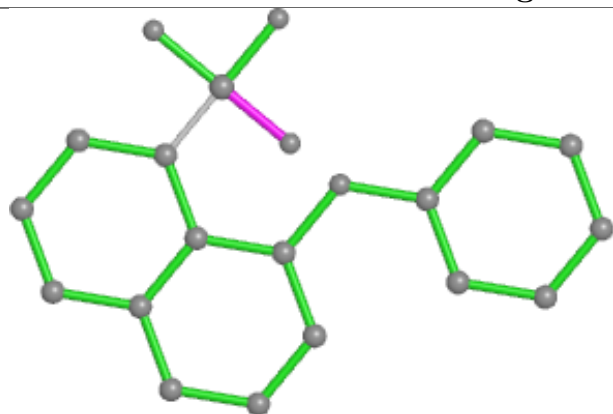


Torsions

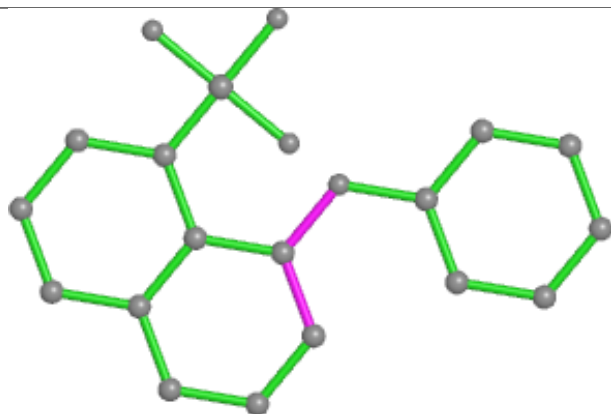


Rings

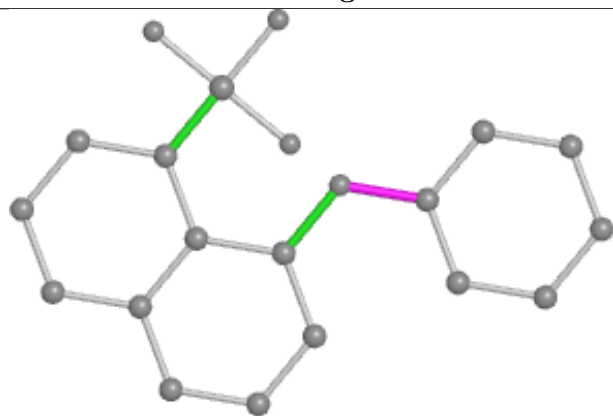
## Ligand 2AN E 506



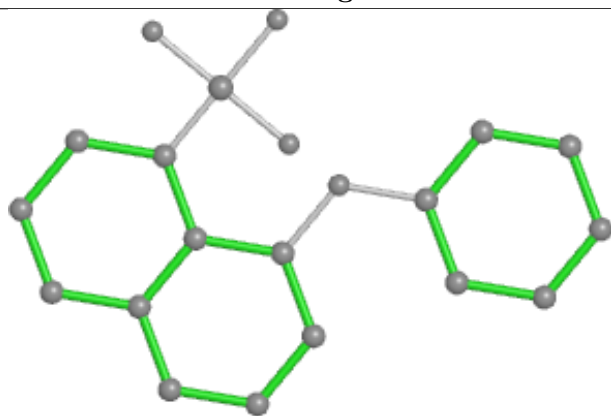
Bond lengths



Bond angles

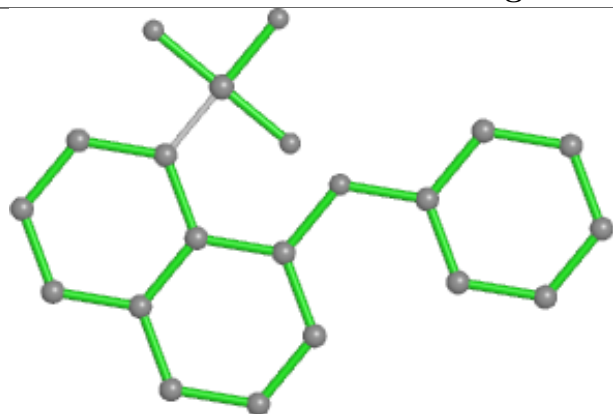


Torsions

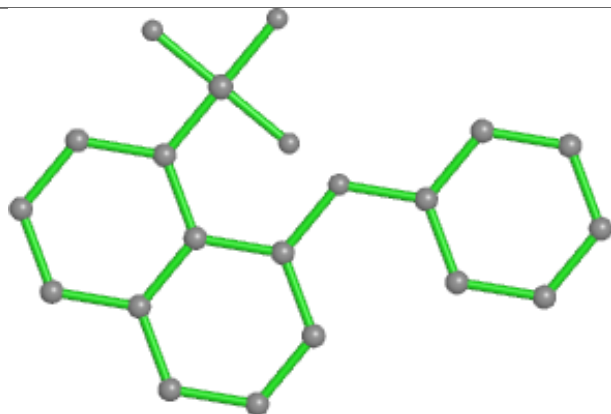


Rings

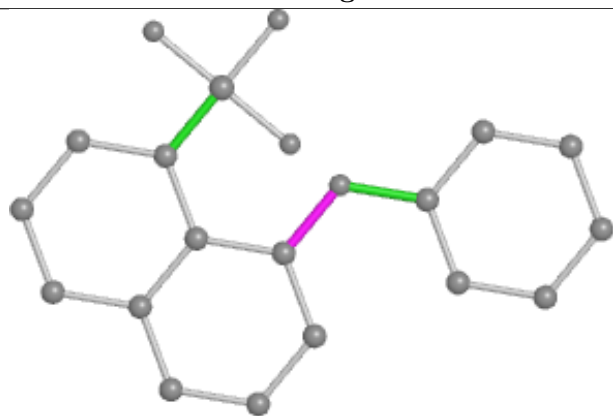
## Ligand 2AN H 1104



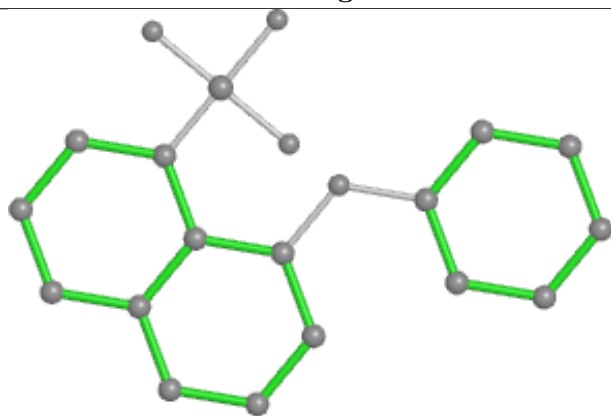
Bond lengths



Bond angles



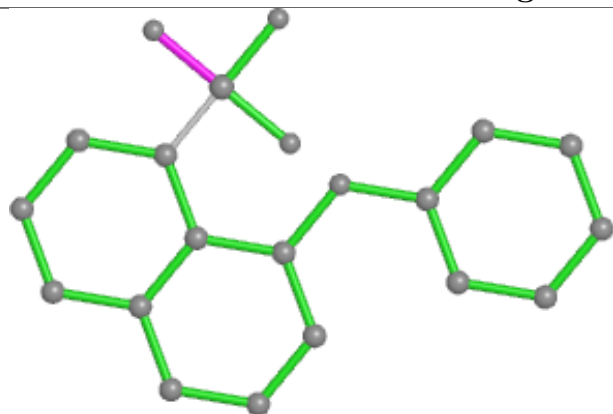
Torsions



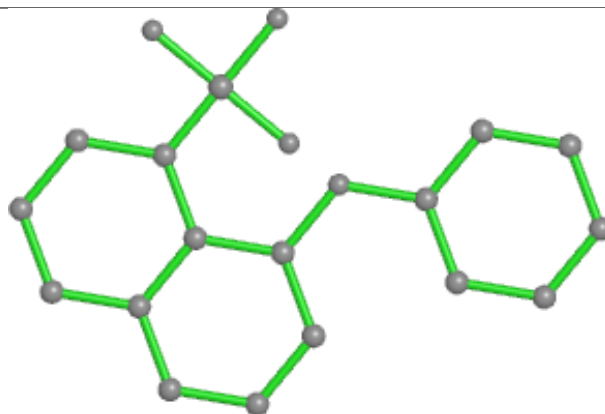
Rings



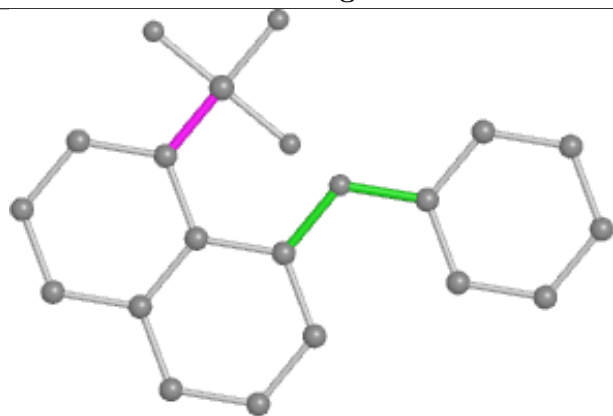
## Ligand 2AN F 202



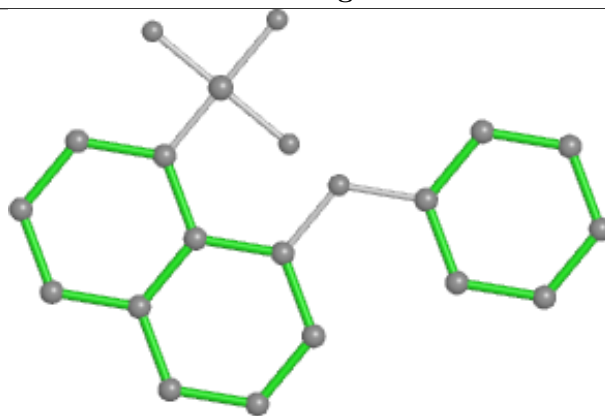
Bond lengths



Bond angles

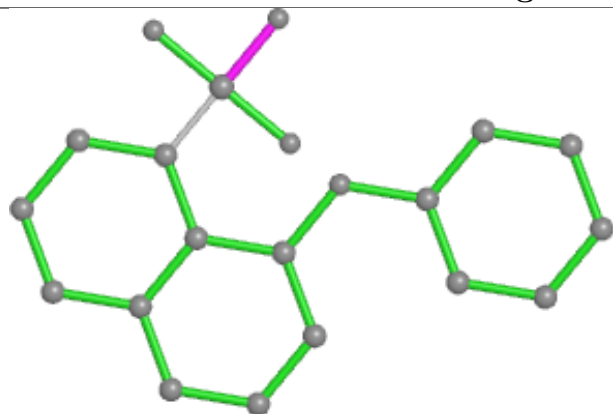


Torsions

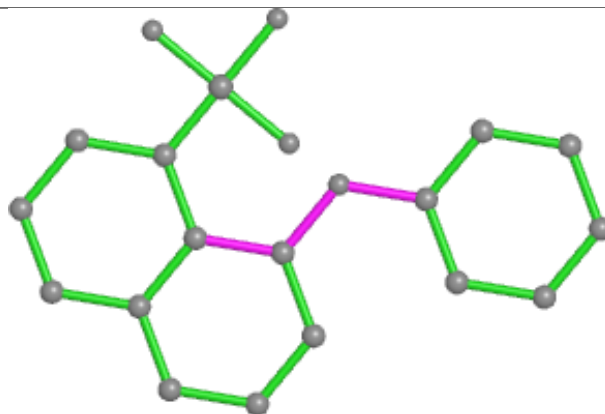


Rings

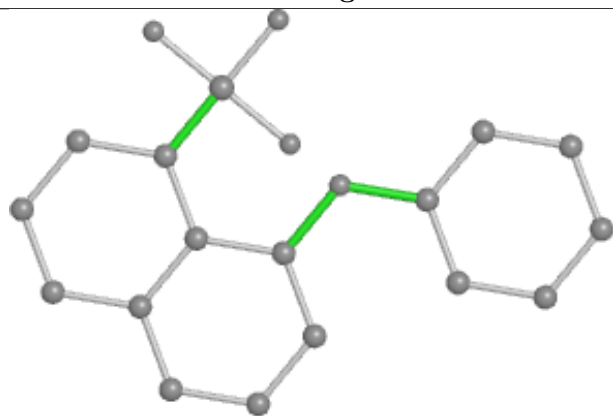
## Ligand 2AN E 502



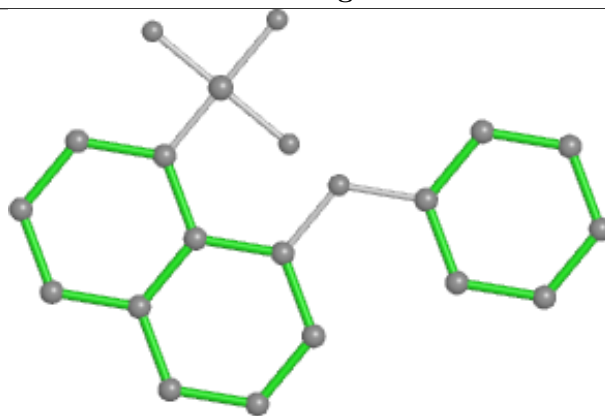
Bond lengths



Bond angles

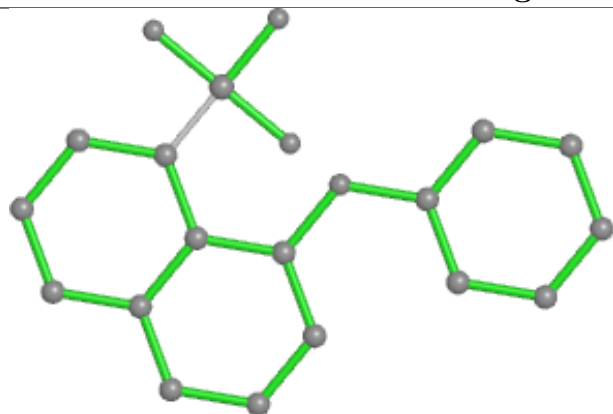


Torsions

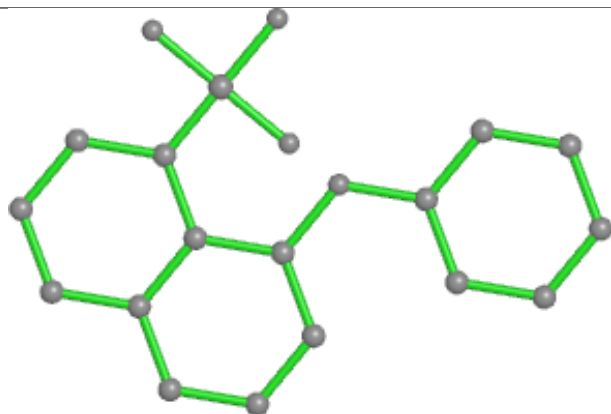


Rings

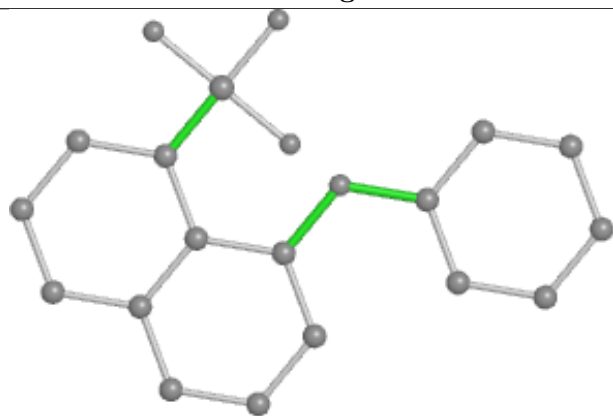
## Ligand 2AN G 303



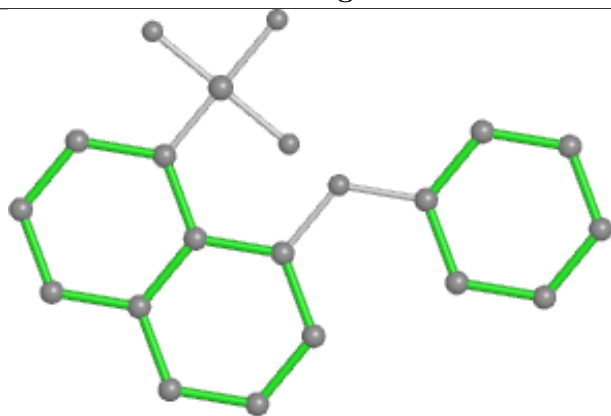
Bond lengths



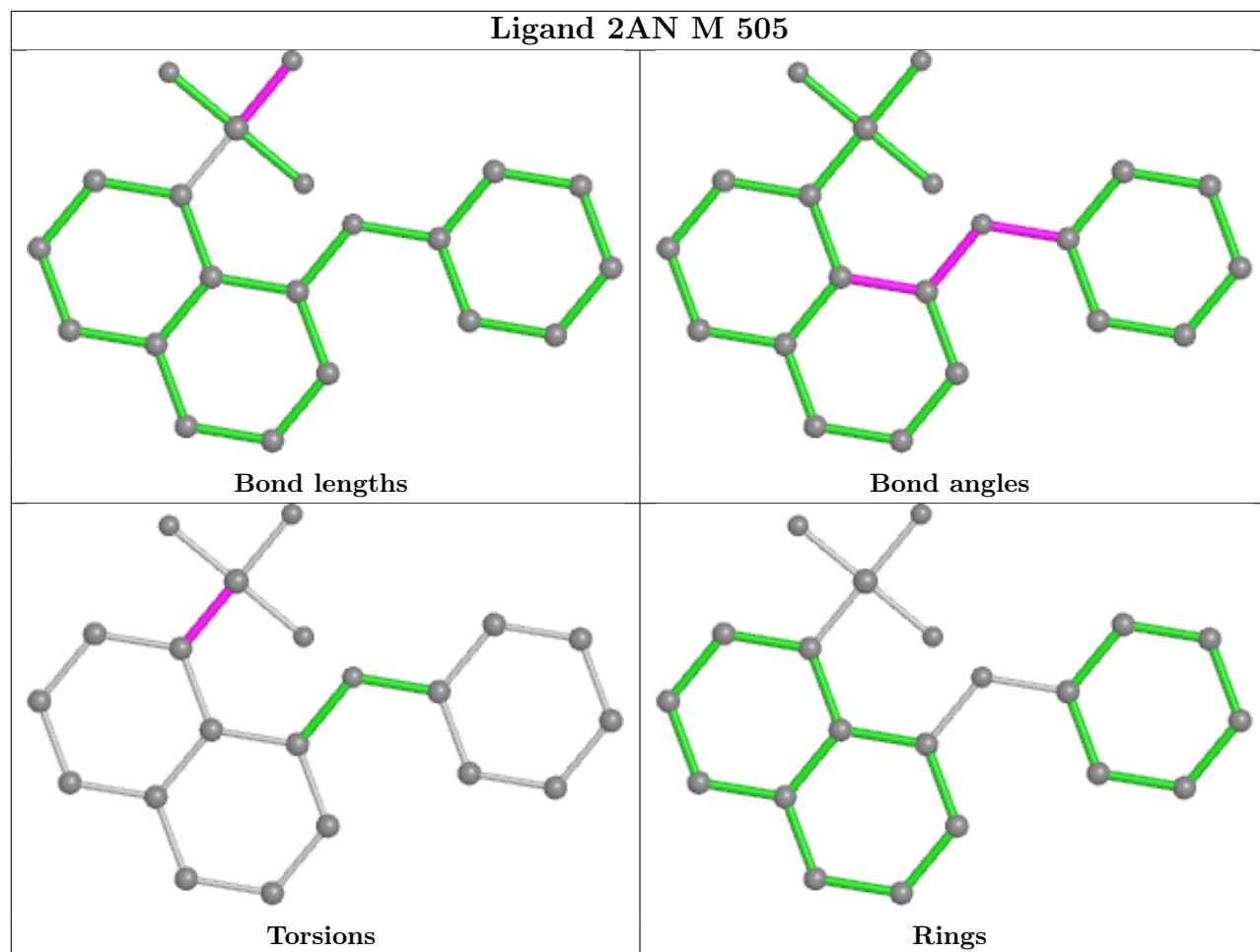
Bond angles



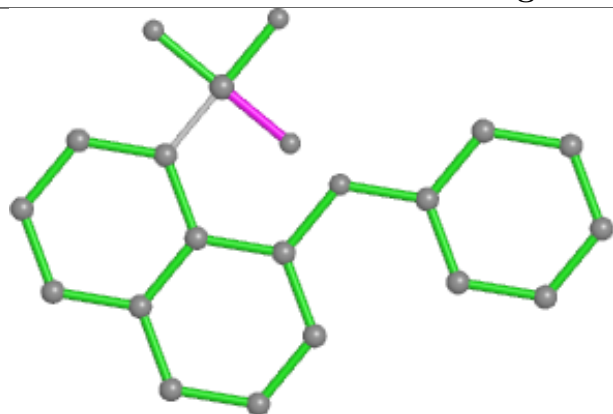
Torsions



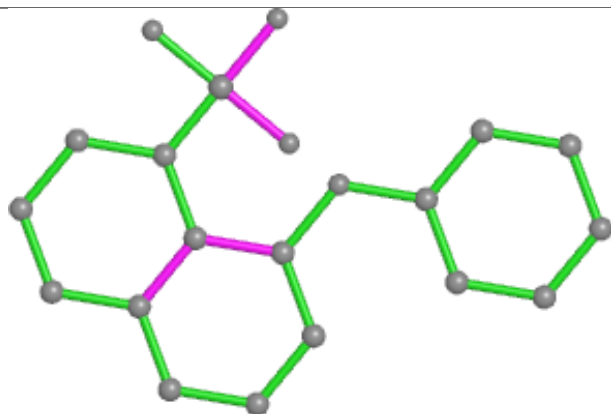
Rings



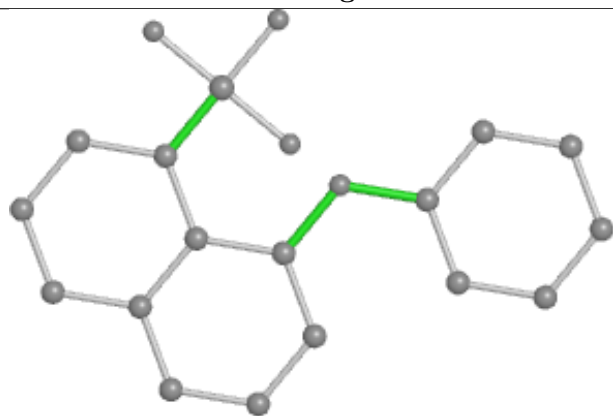
## Ligand 2AN L 201



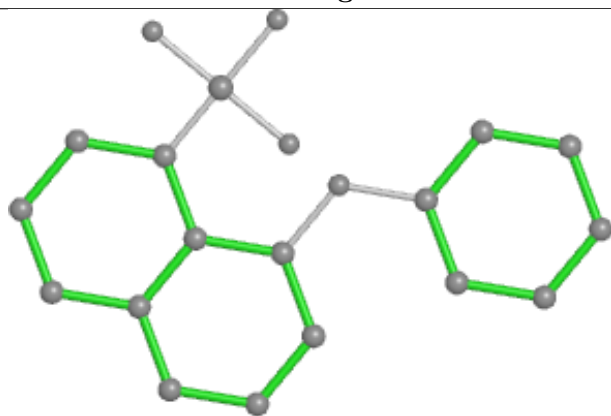
Bond lengths



Bond angles

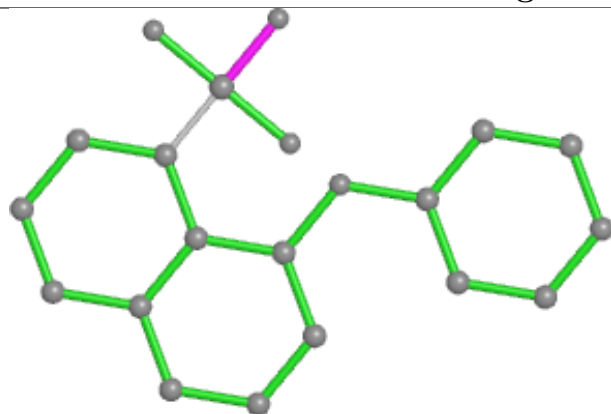


Torsions

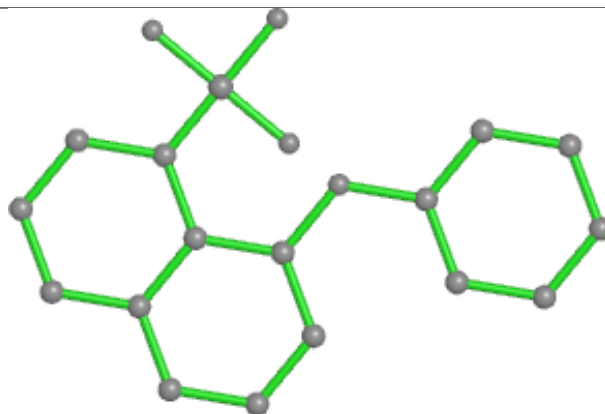


Rings

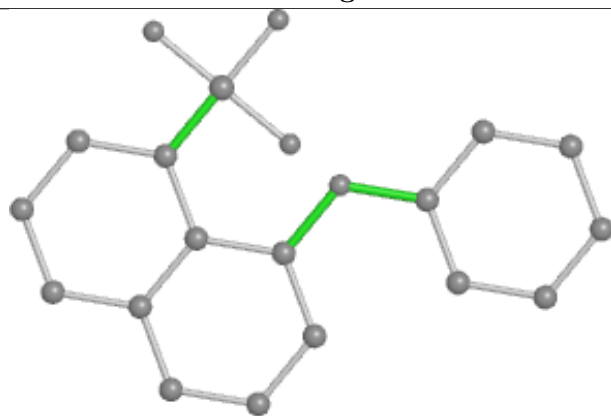
## Ligand 2AN F 204



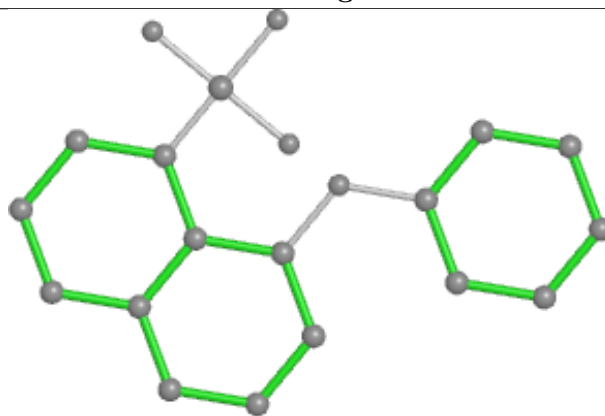
Bond lengths



Bond angles

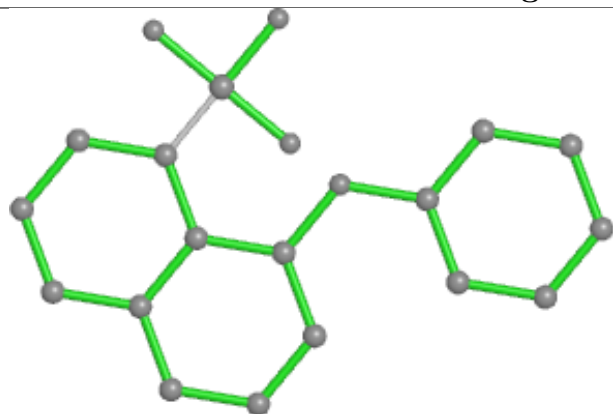


Torsions

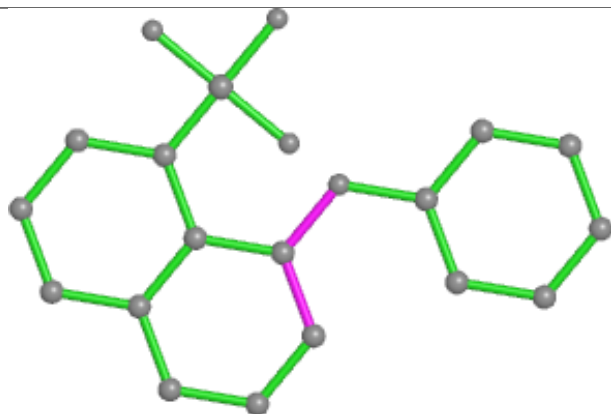


Rings

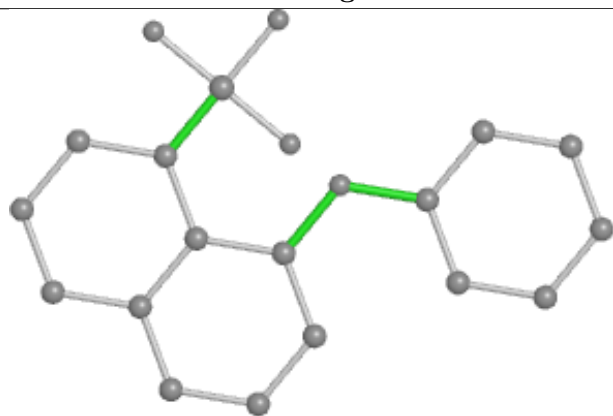
## Ligand 2AN I 201



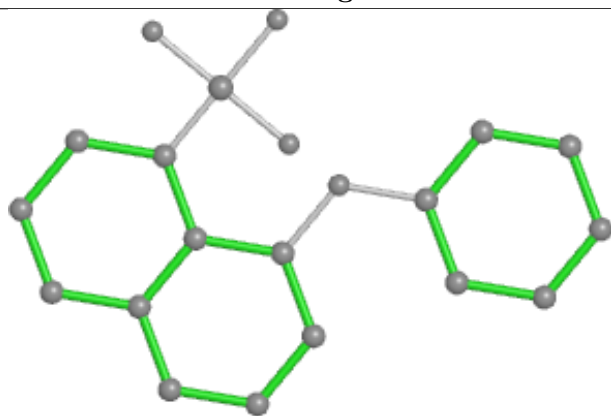
Bond lengths



Bond angles

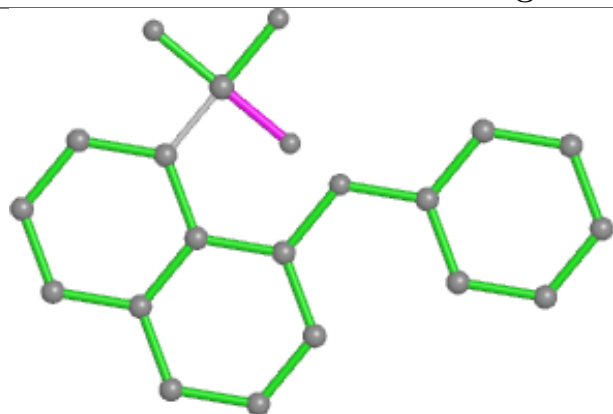


Torsions

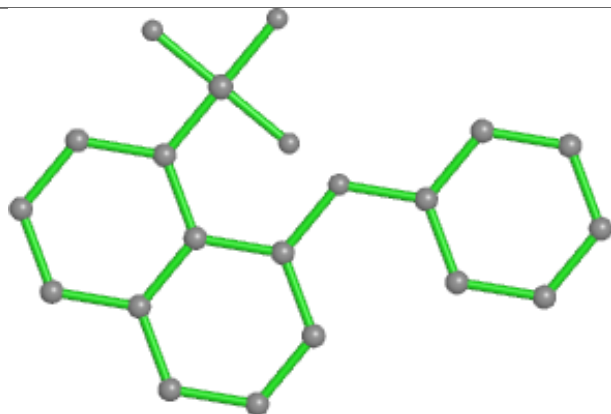


Rings

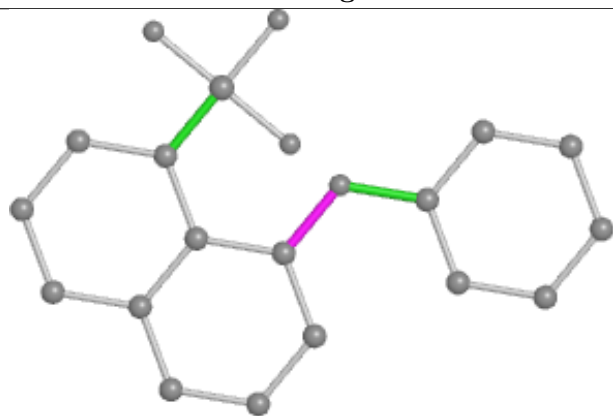
## Ligand 2AN E 504



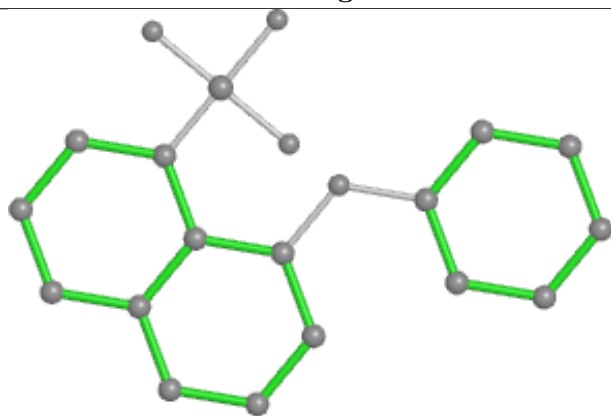
Bond lengths



Bond angles



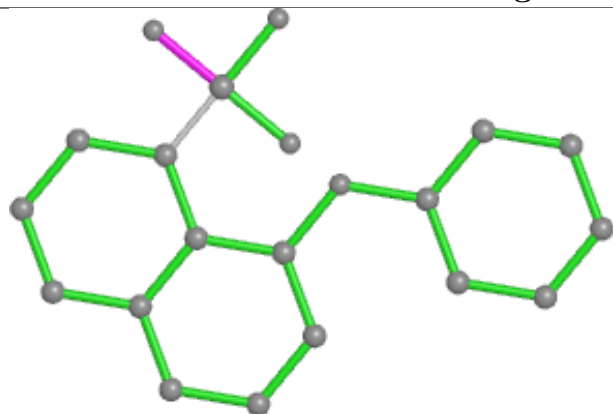
Torsions



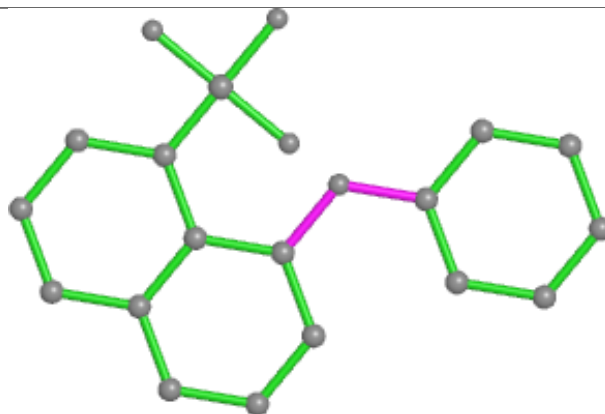
Rings



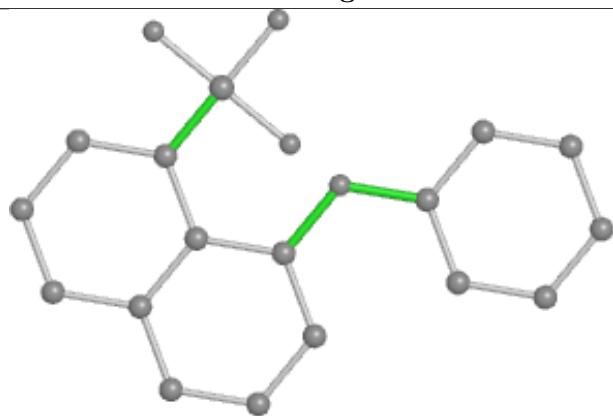
## Ligand 2AN N 203



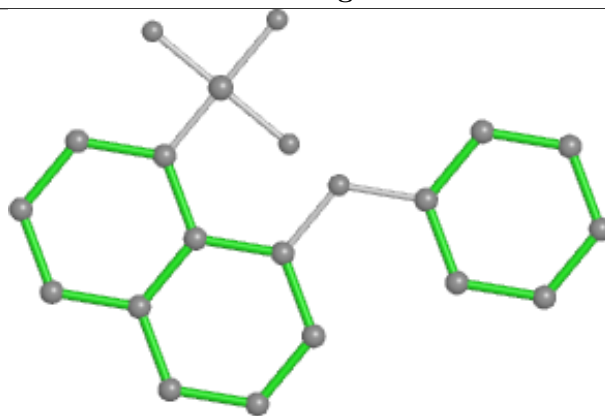
Bond lengths



Bond angles

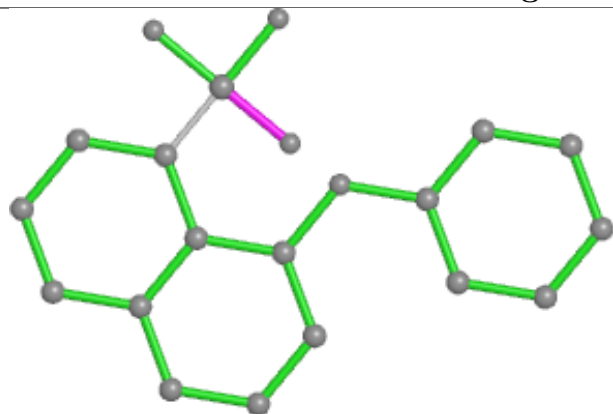


Torsions

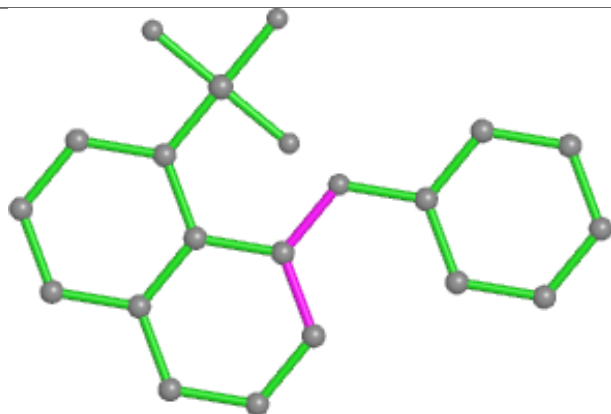


Rings

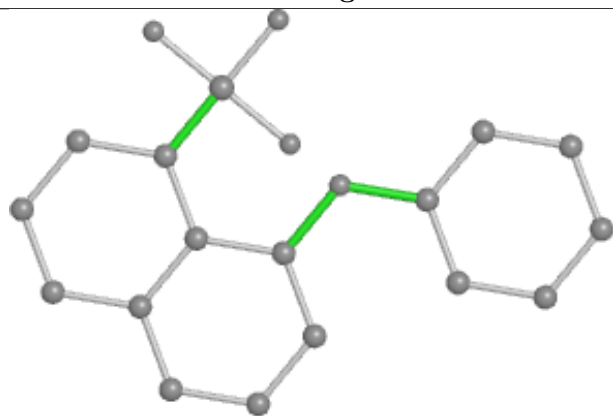
## Ligand 2AN I 203



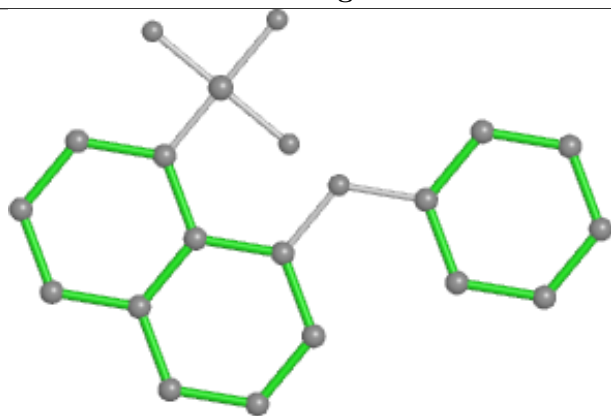
Bond lengths



Bond angles

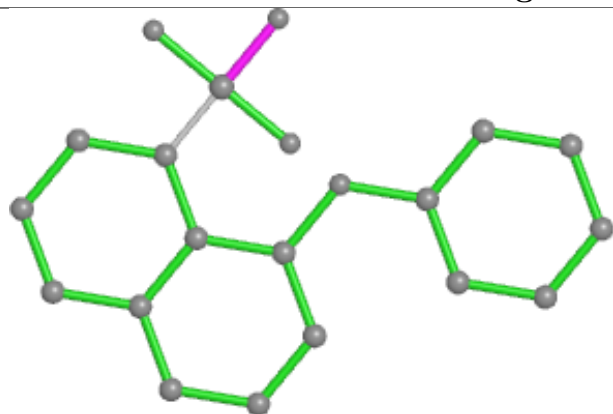


Torsions

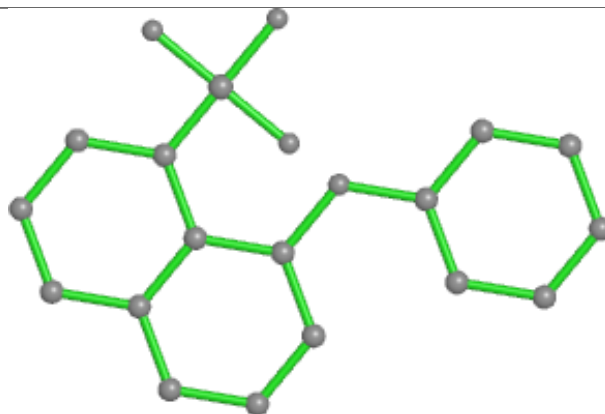


Rings

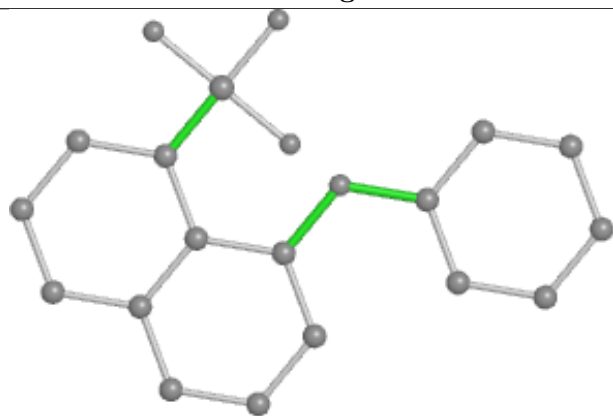
## Ligand 2AN P 501



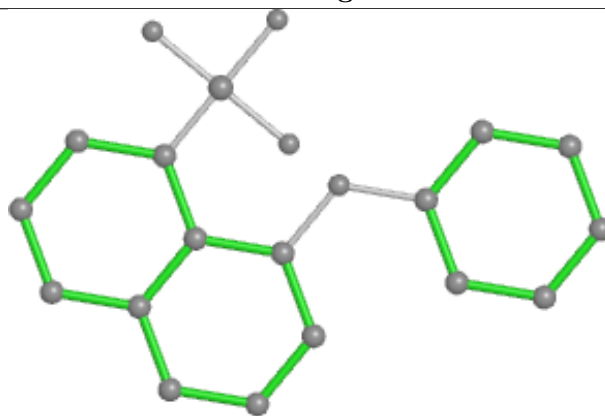
Bond lengths



Bond angles

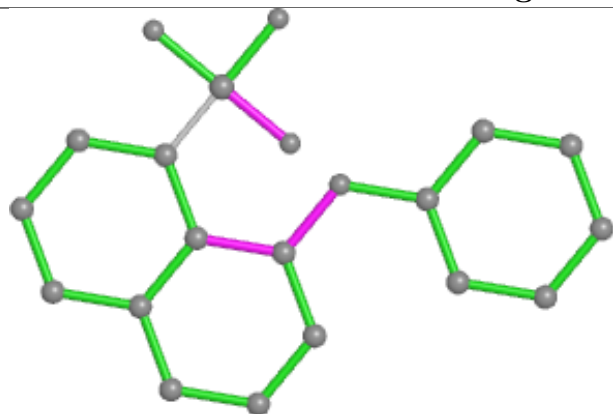


Torsions

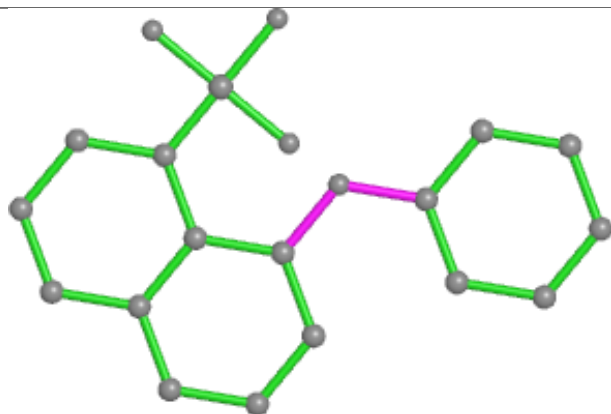


Rings

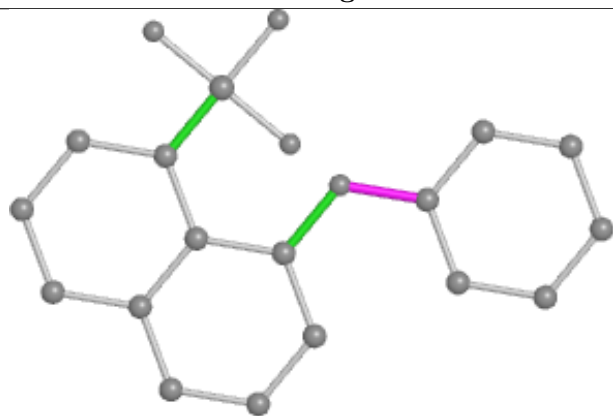
## Ligand 2AN C 308



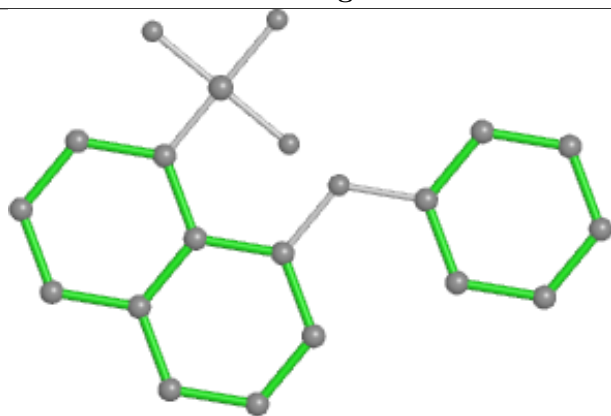
Bond lengths



Bond angles

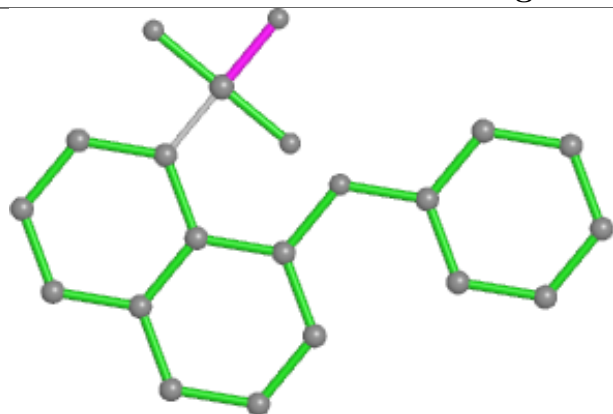


Torsions

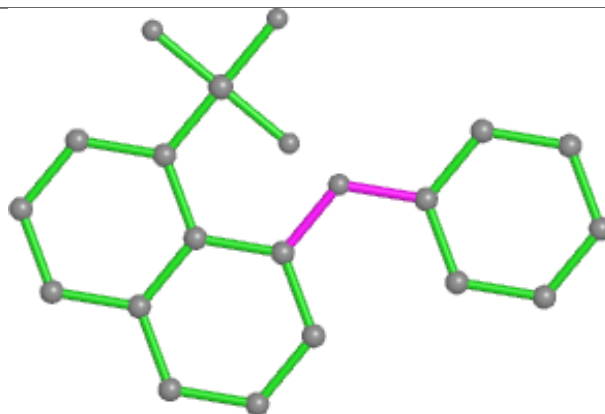


Rings

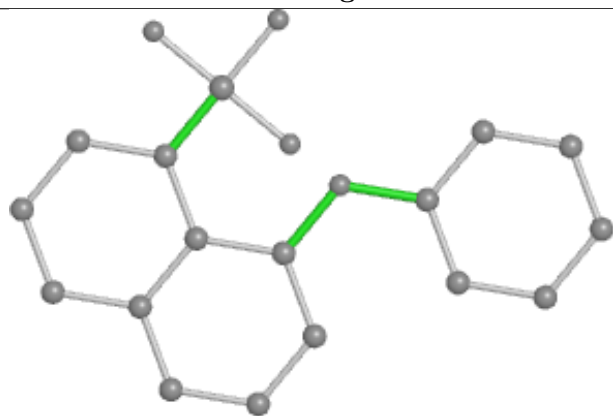
## Ligand 2AN B 201



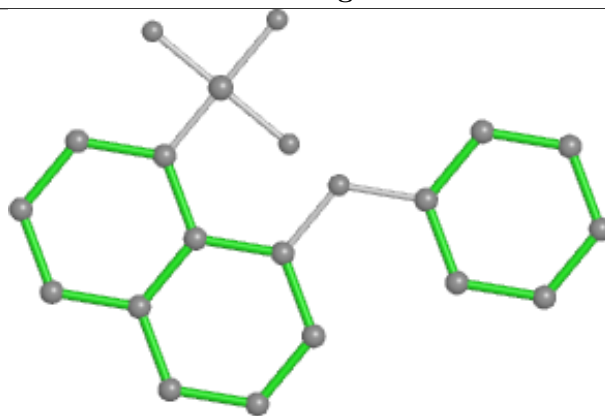
Bond lengths



Bond angles

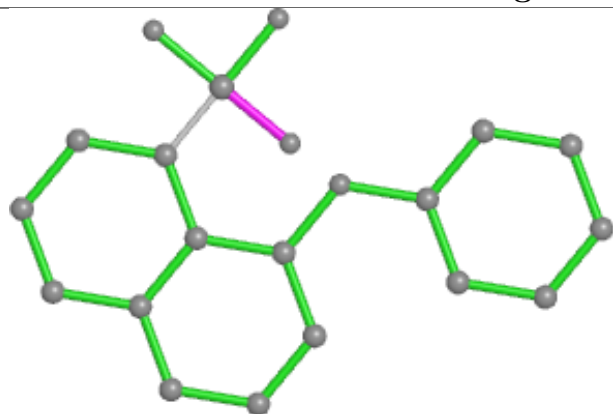


Torsions

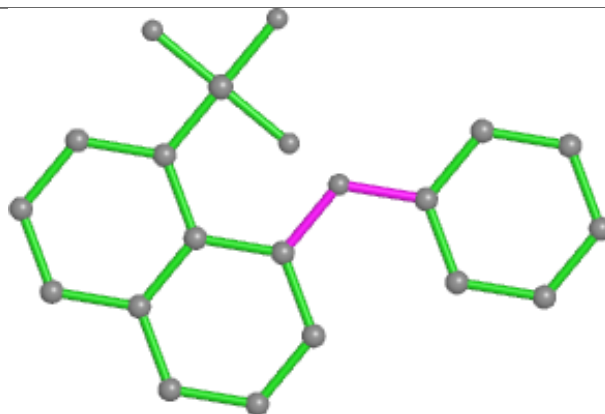


Rings

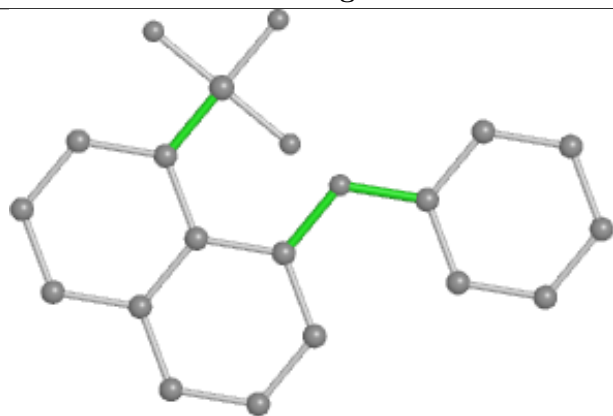
## Ligand 2AN G 302



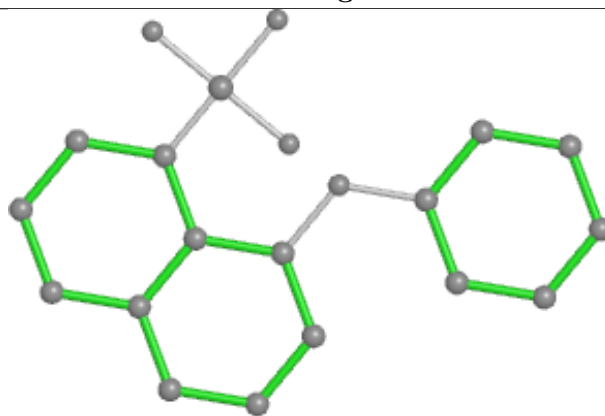
Bond lengths



Bond angles

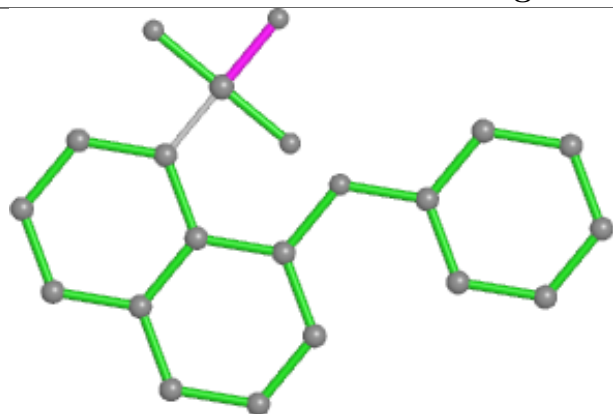


Torsions

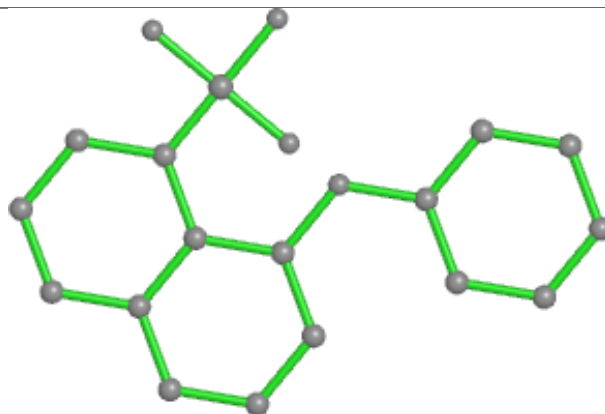


Rings

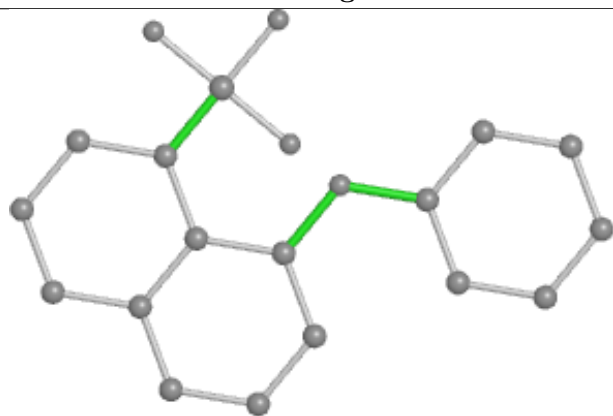
## Ligand 2AN G 306



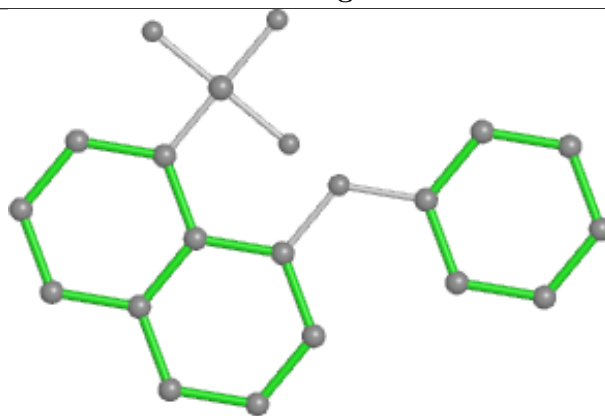
Bond lengths



Bond angles

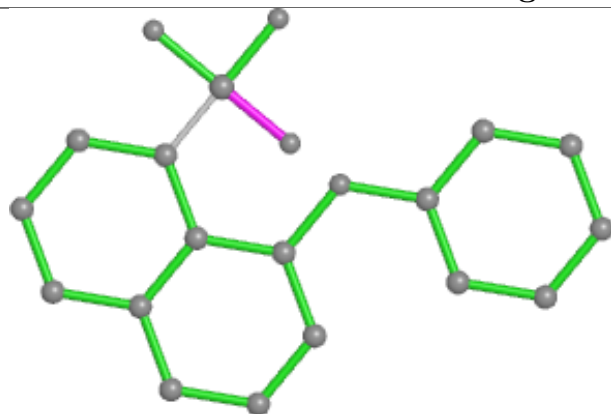


Torsions

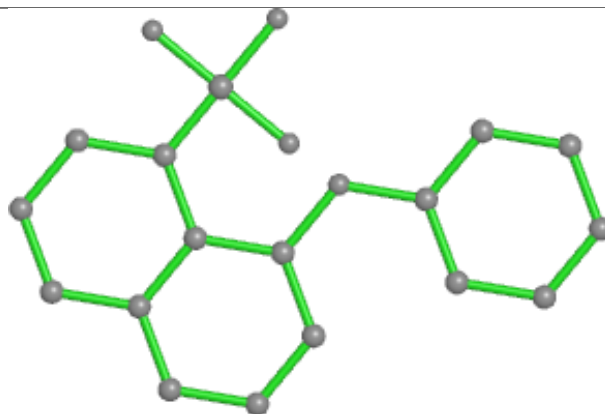


Rings

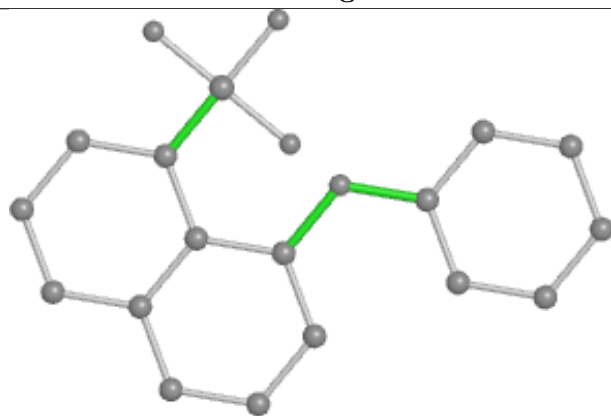
## Ligand 2AN J 204



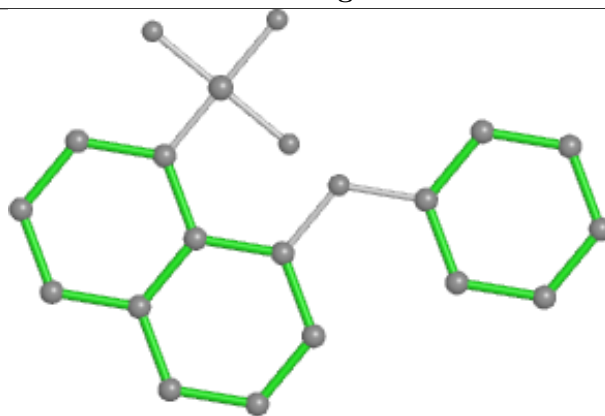
Bond lengths



Bond angles

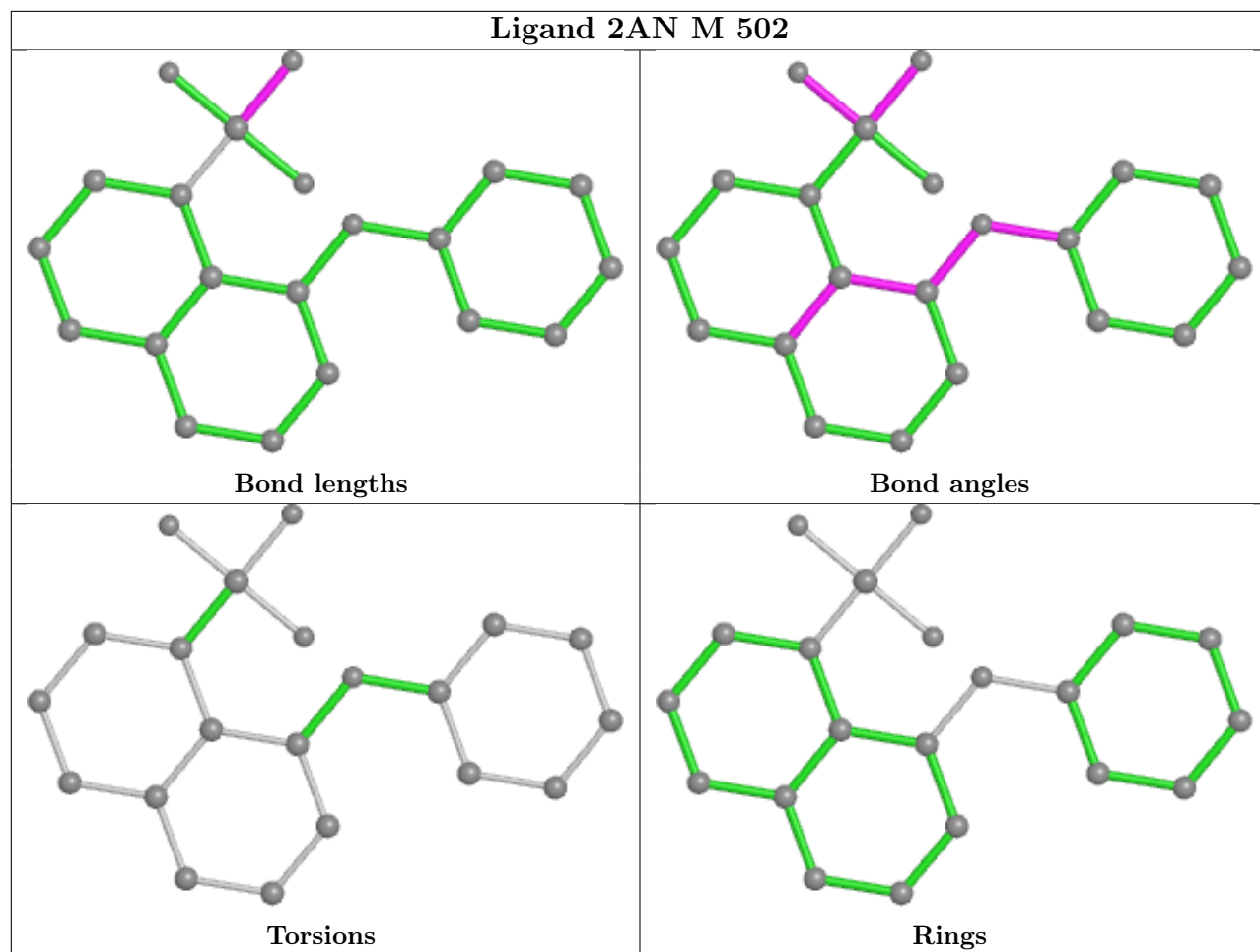


Torsions

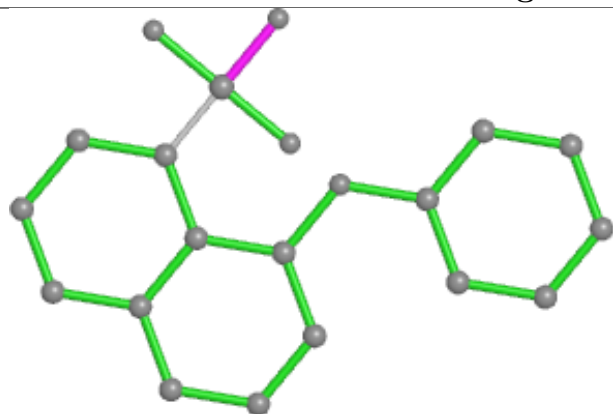


Rings

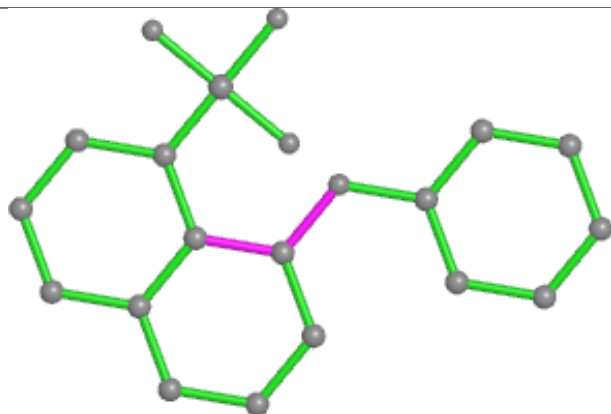




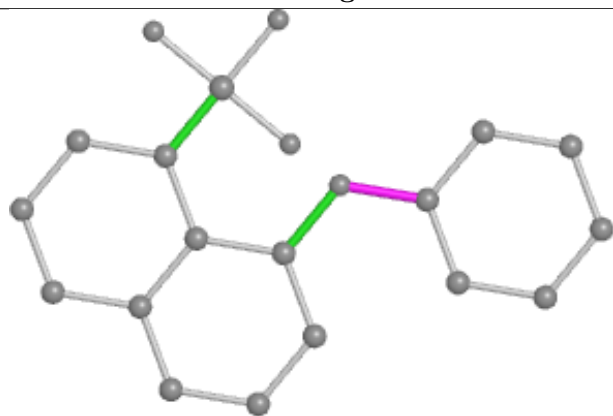
## Ligand 2AN F 207



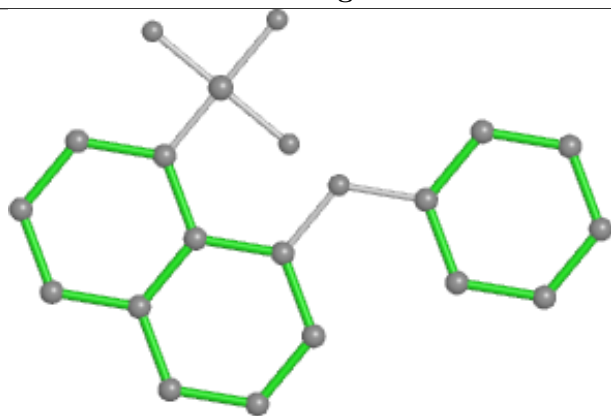
Bond lengths



Bond angles

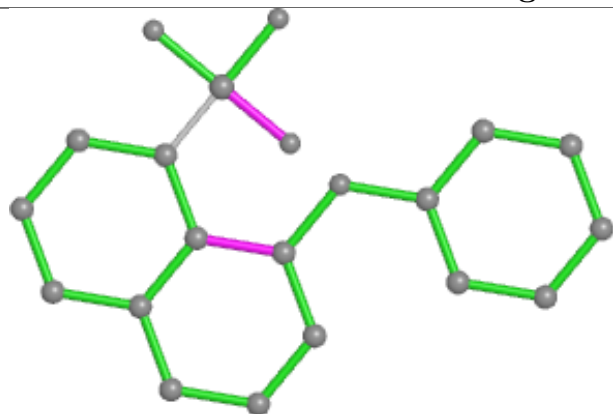


Torsions

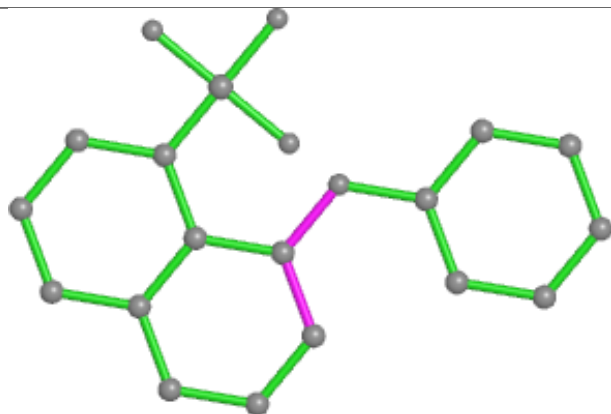


Rings

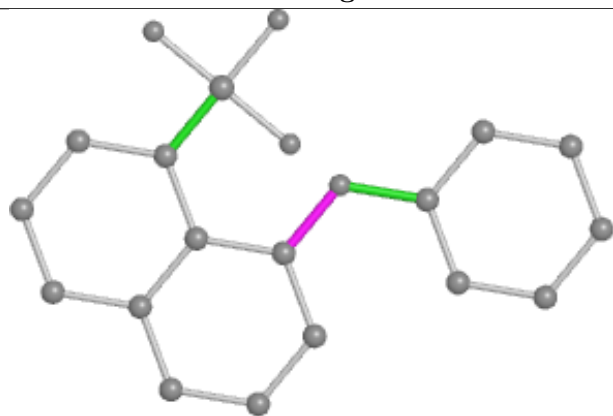
## Ligand 2AN J 203



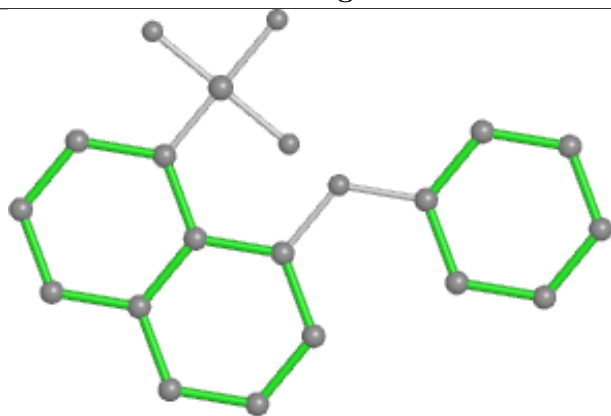
Bond lengths



Bond angles

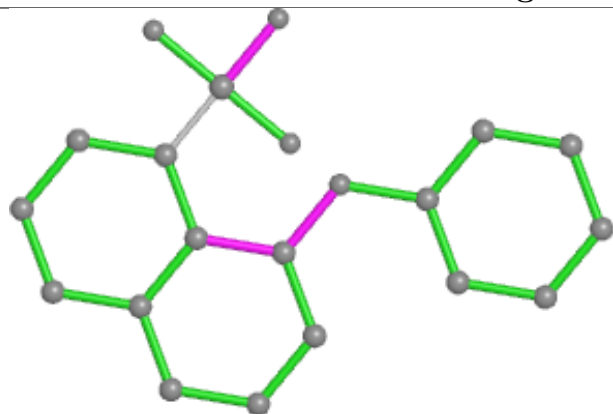


Torsions

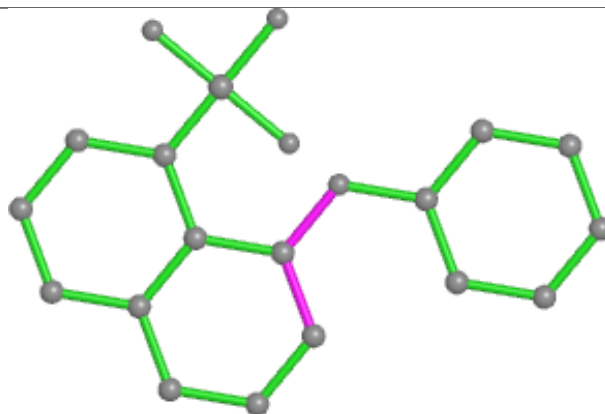


Rings

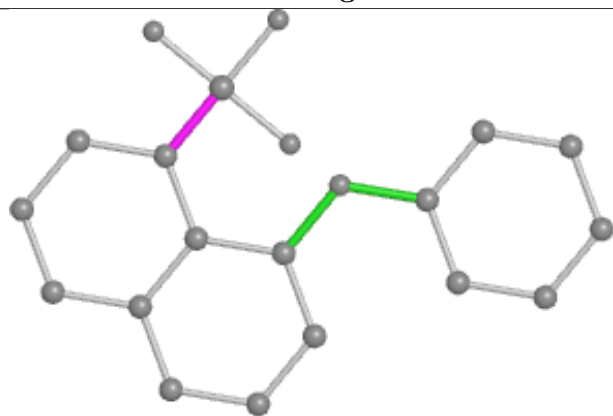
## Ligand 2AN F 208



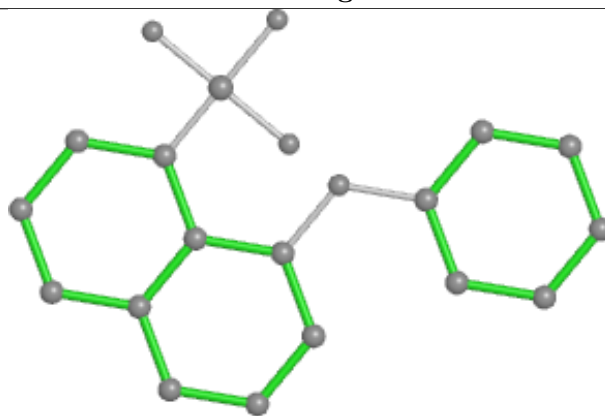
Bond lengths



Bond angles

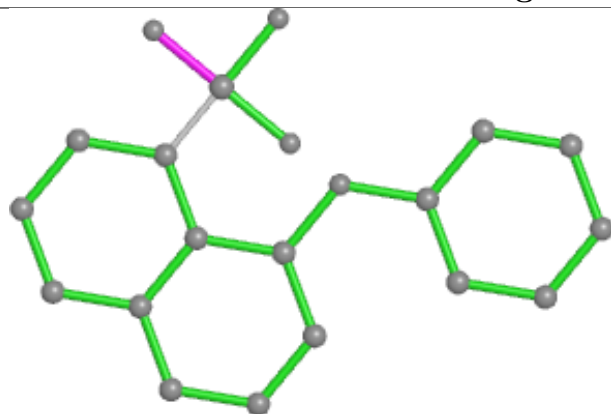


Torsions

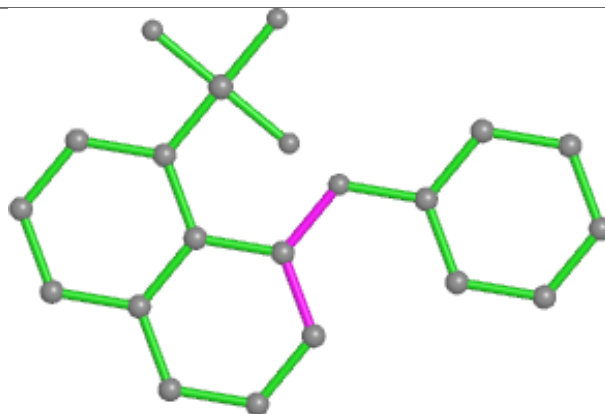


Rings

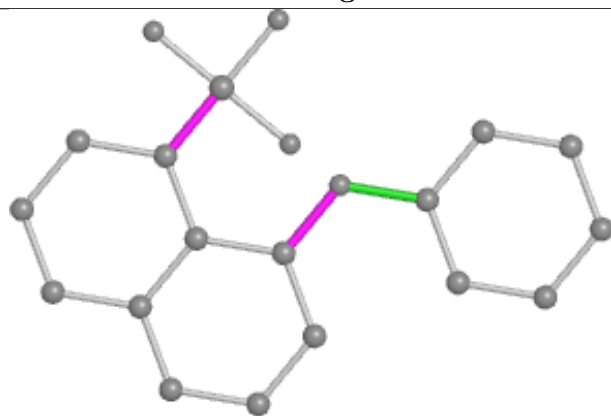
## Ligand 2AN P 503



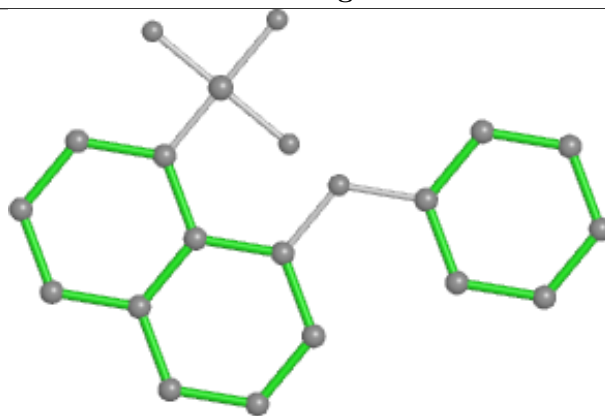
Bond lengths



Bond angles

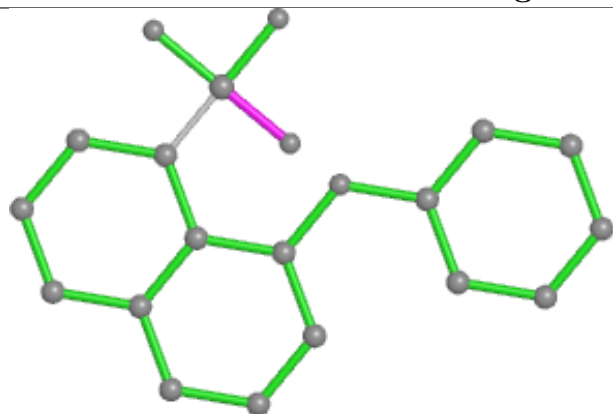


Torsions

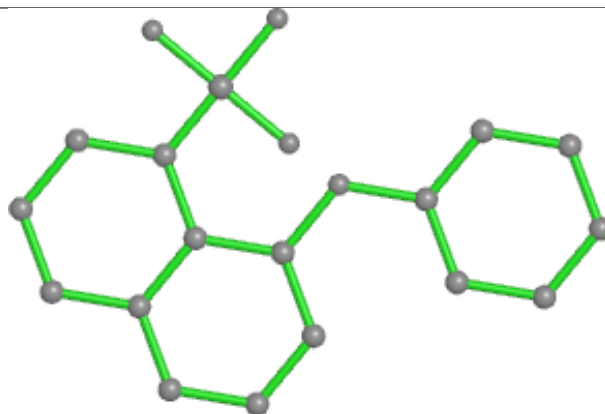


Rings

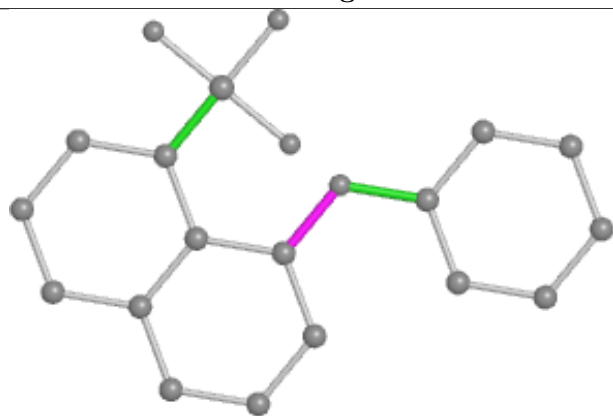
## Ligand 2AN D 701



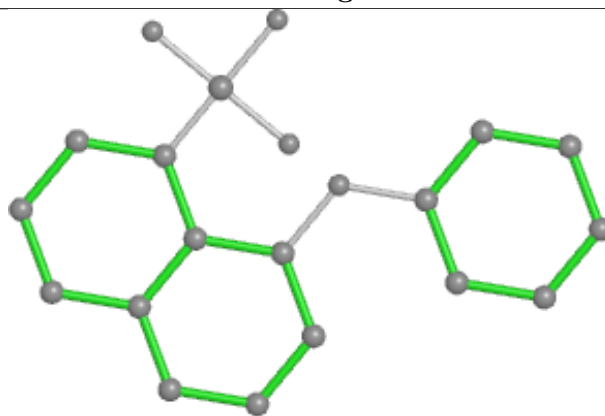
Bond lengths



Bond angles

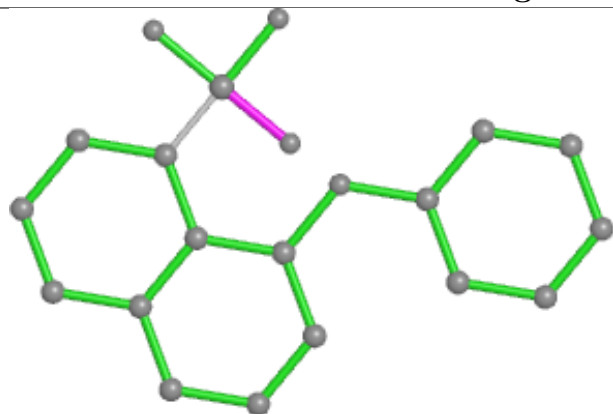


Torsions

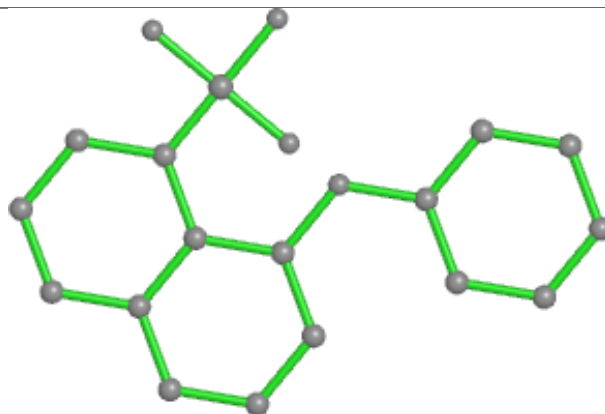


Rings

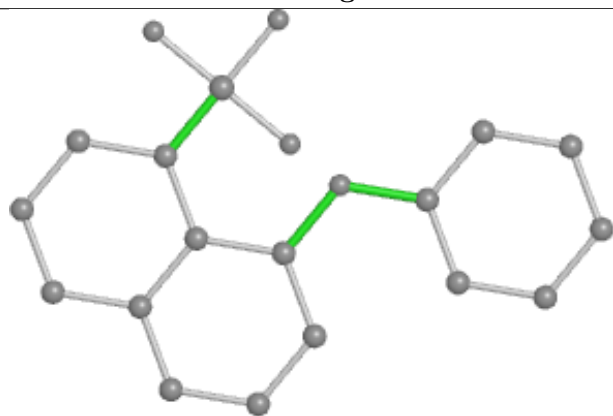
## Ligand 2AN K 204



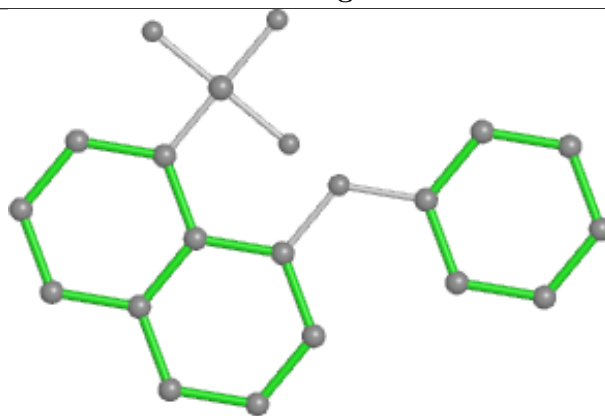
Bond lengths



Bond angles

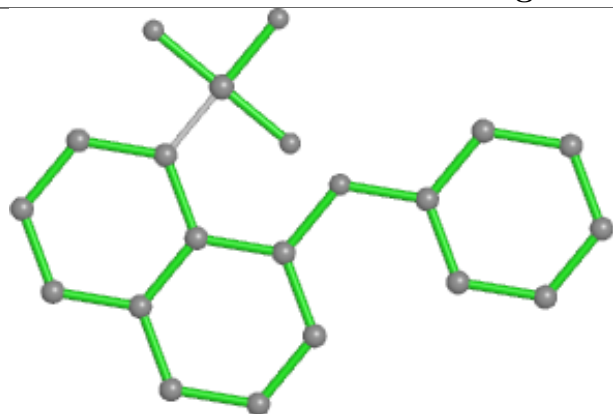


Torsions

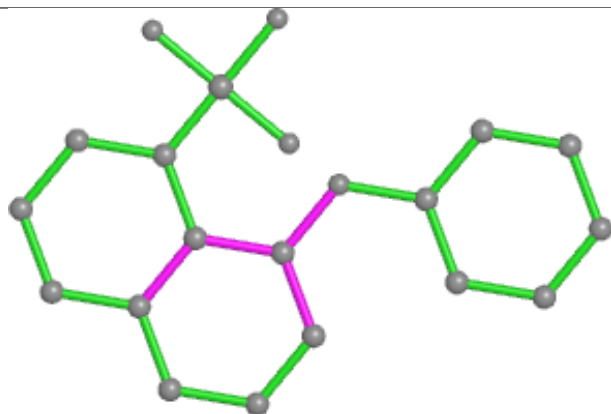


Rings

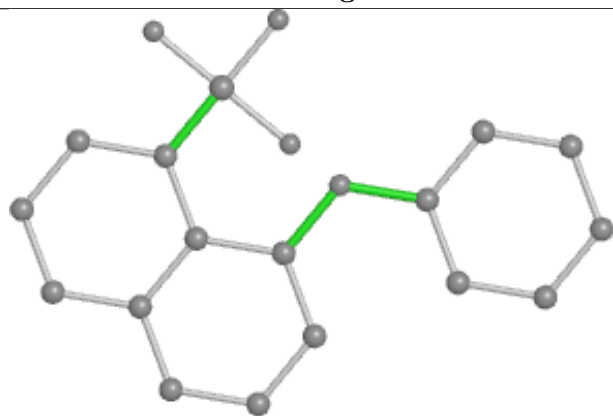
## Ligand 2AN P 505



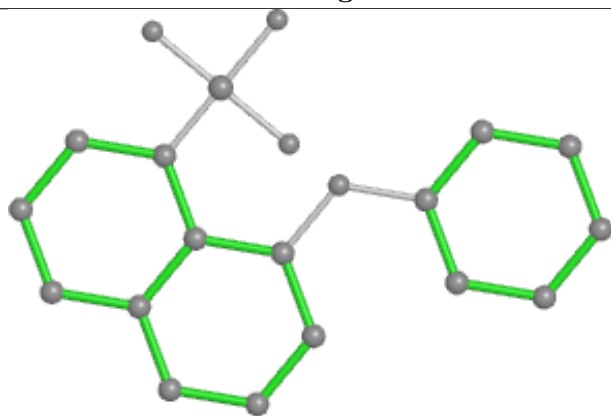
Bond lengths



Bond angles



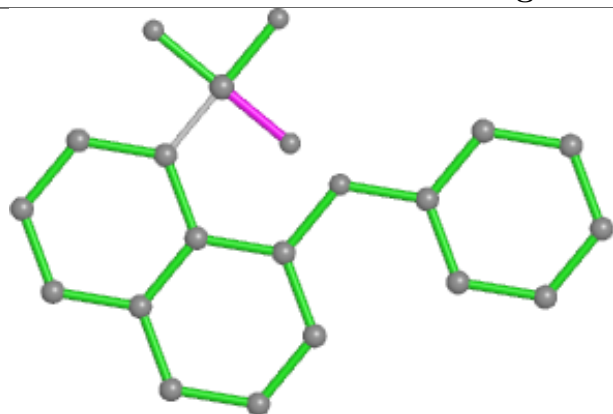
Torsions



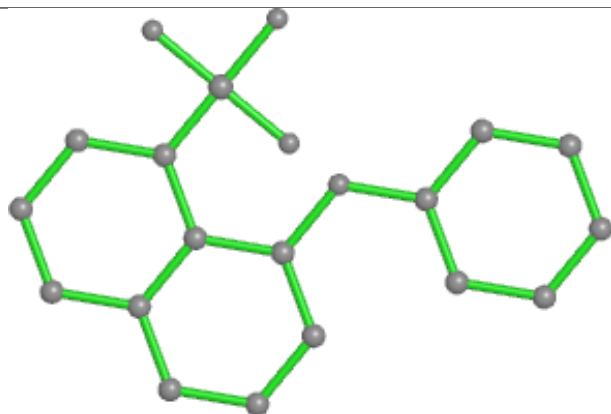
Rings



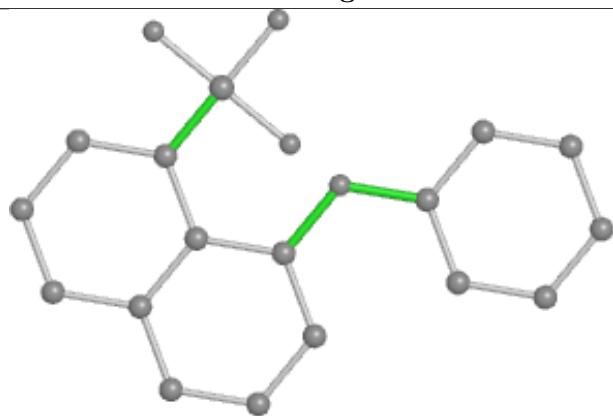
## Ligand 2AN E 505



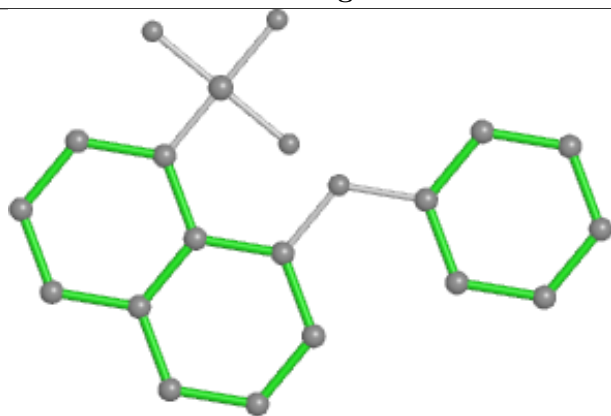
Bond lengths



Bond angles

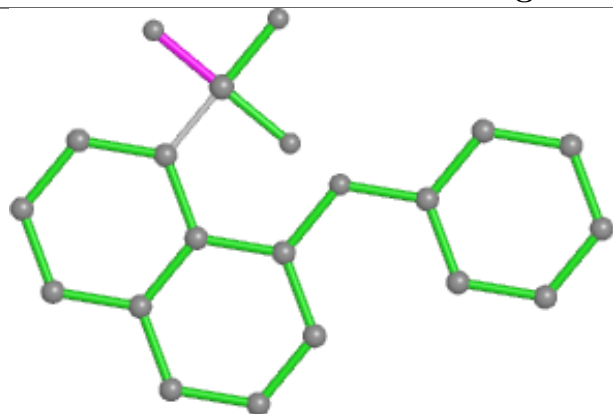


Torsions

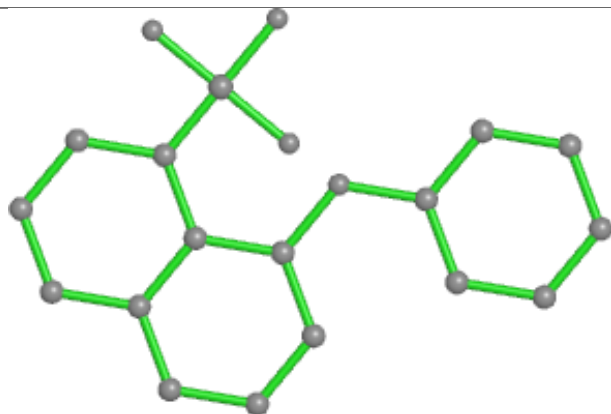


Rings

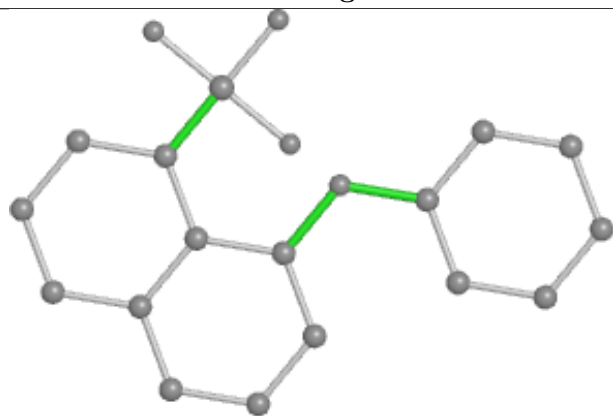
## Ligand 2AN P 507



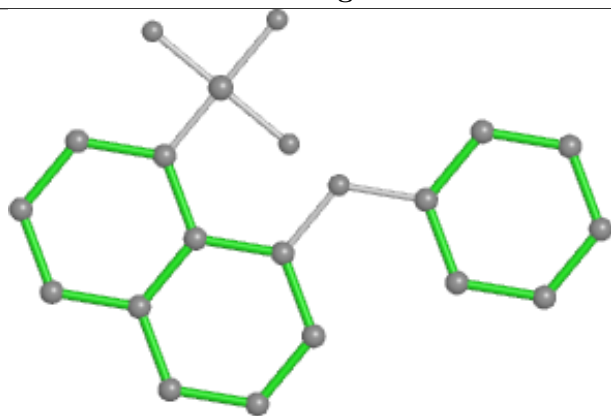
Bond lengths



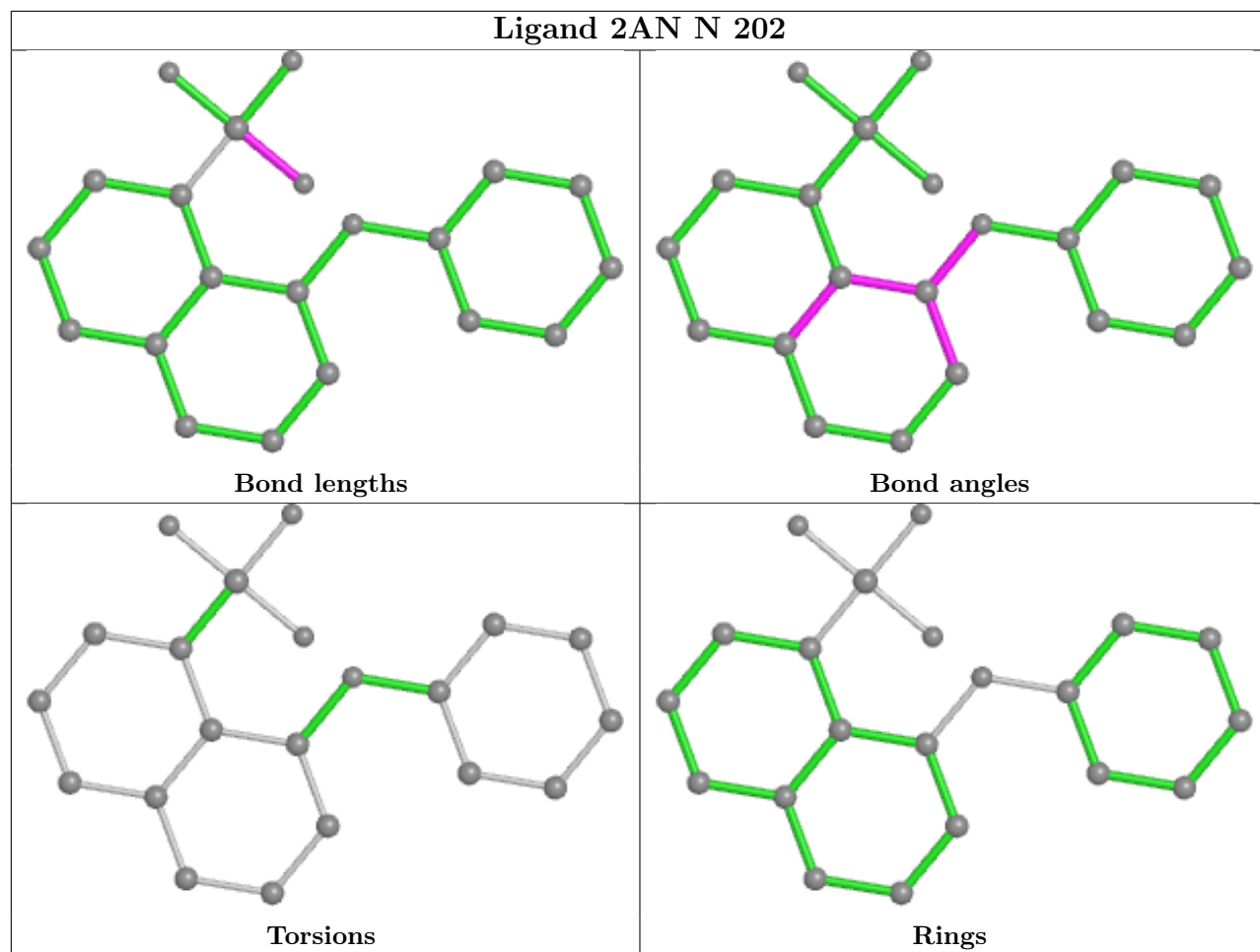
Bond angles



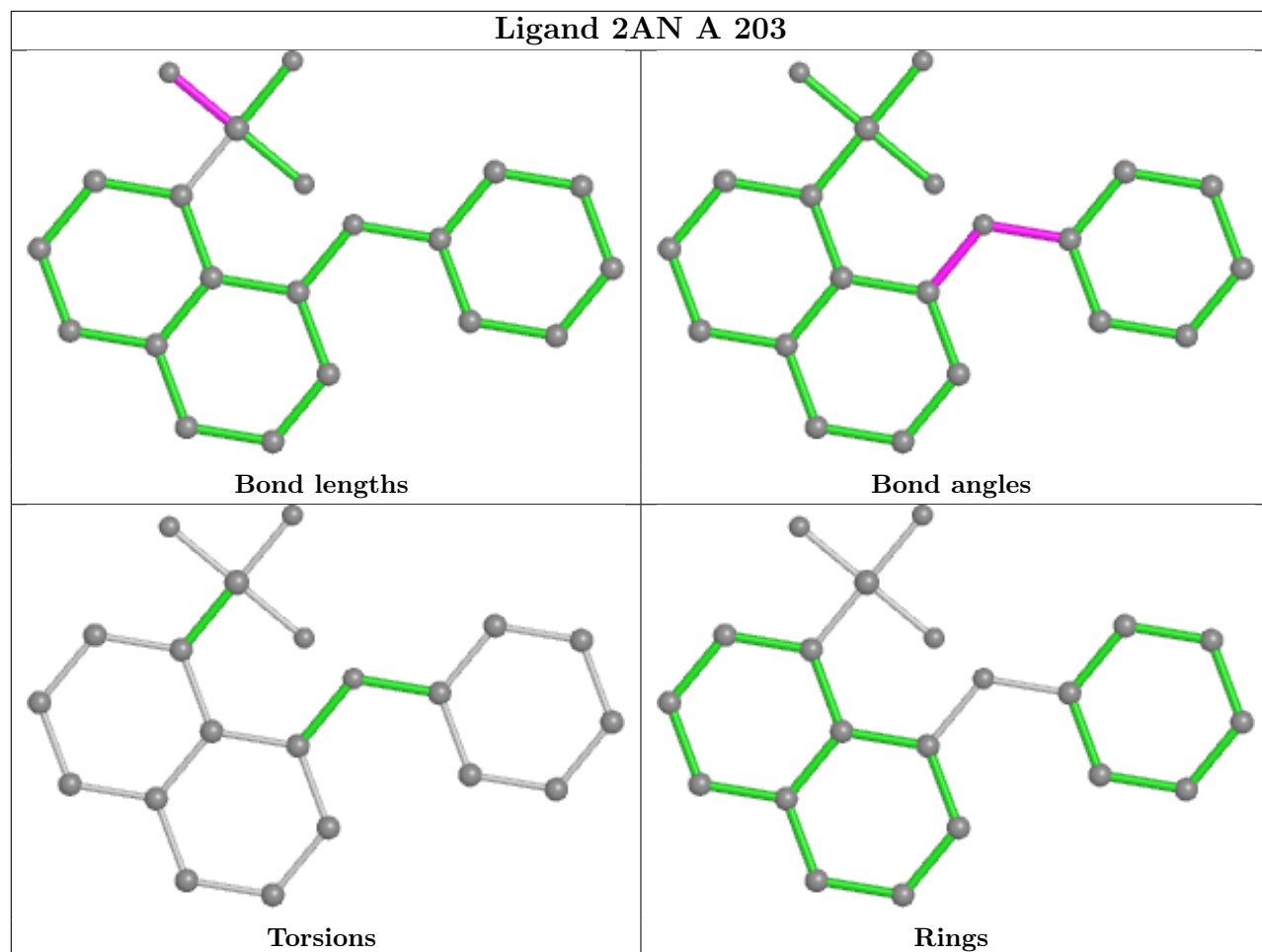
Torsions



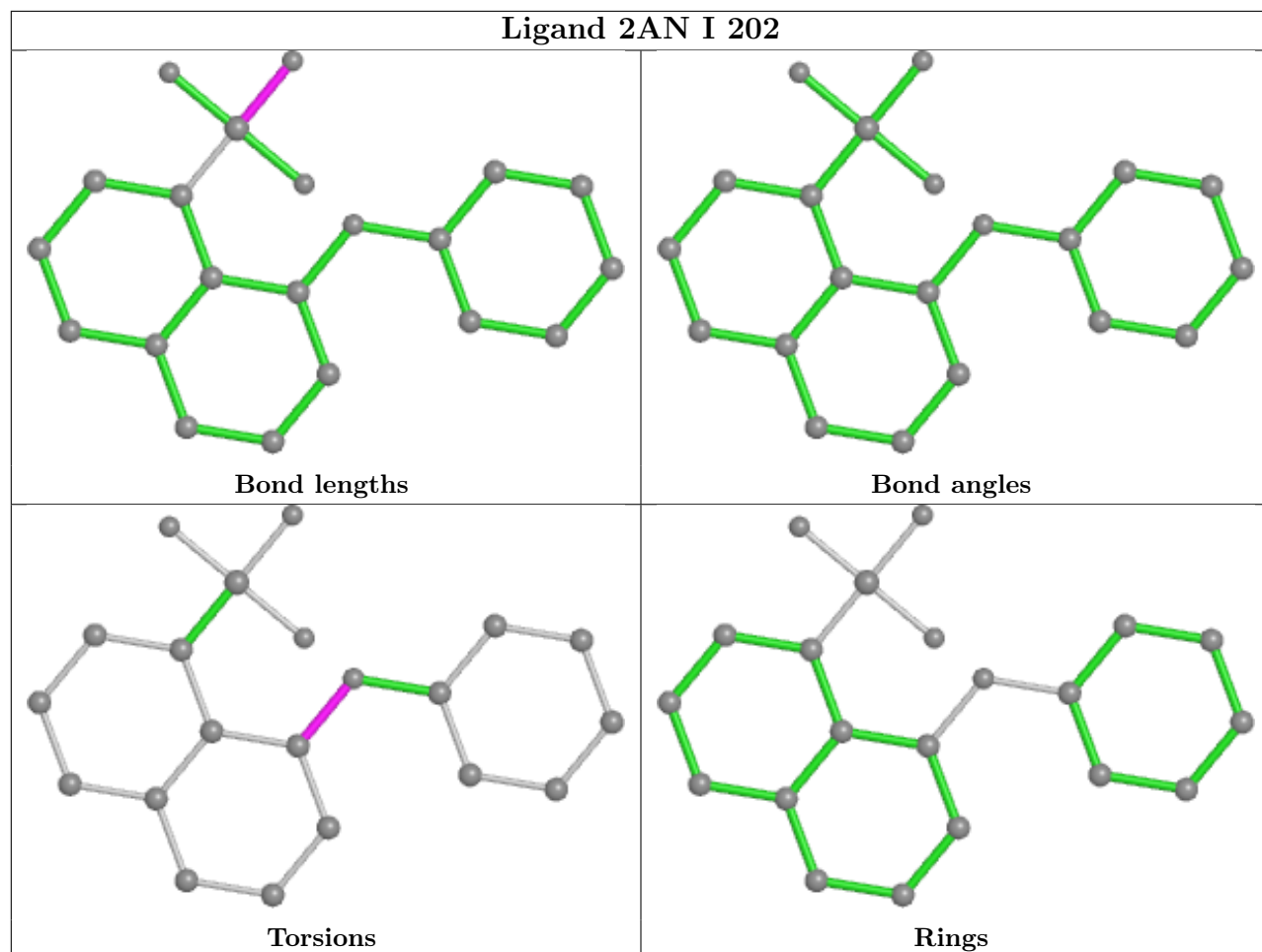
Rings



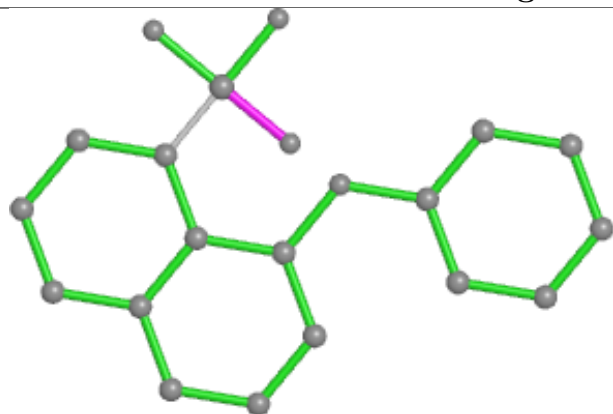
## Ligand 2AN A 203



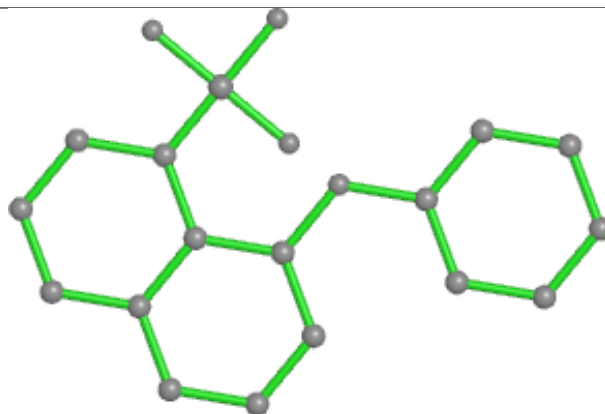
## Ligand 2AN I 202



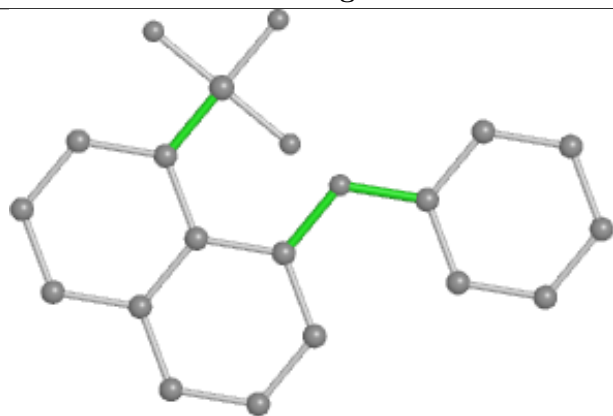
## Ligand 2AN L 203



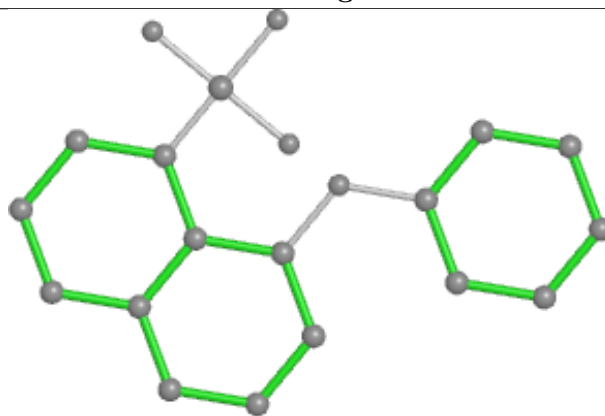
Bond lengths



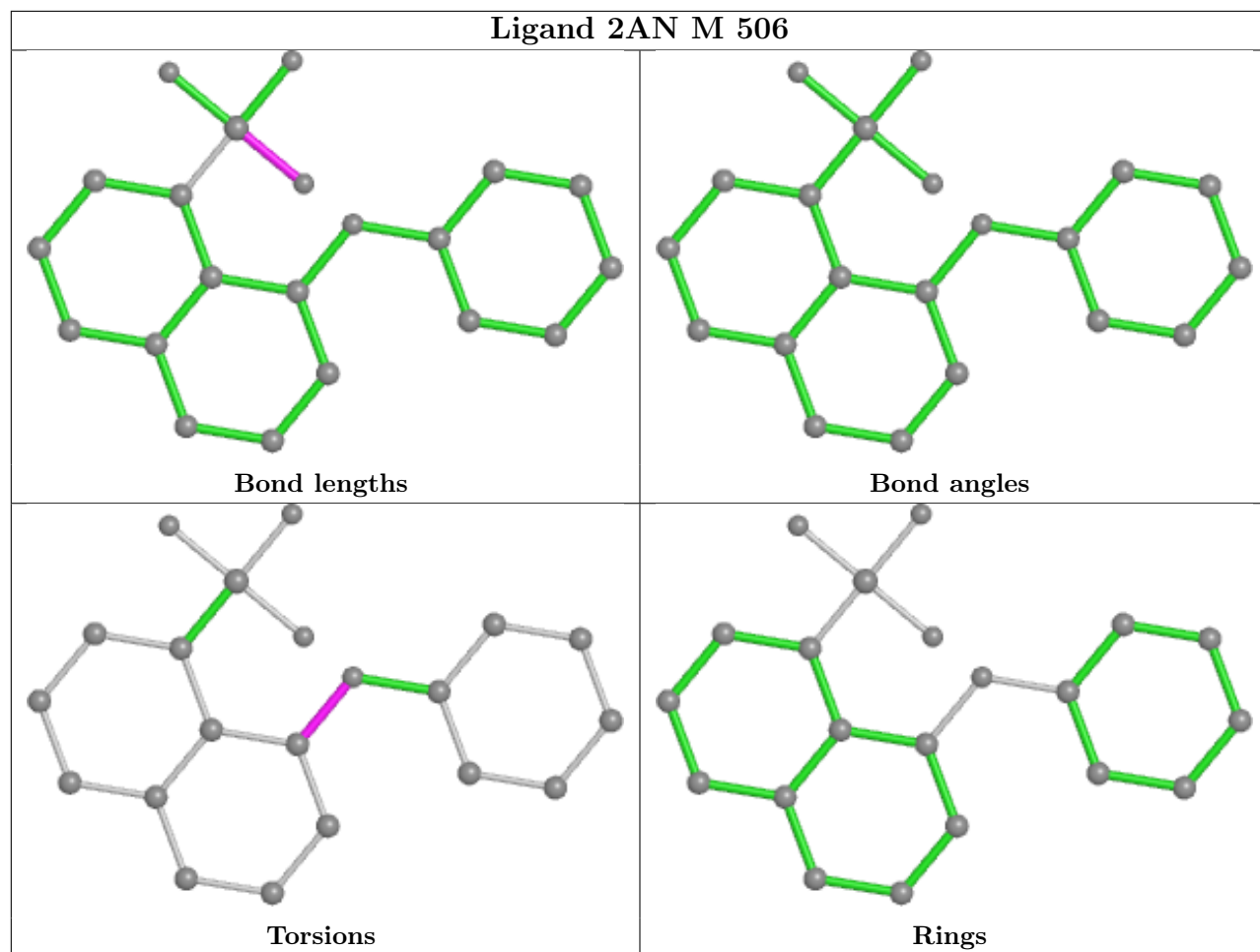
Bond angles

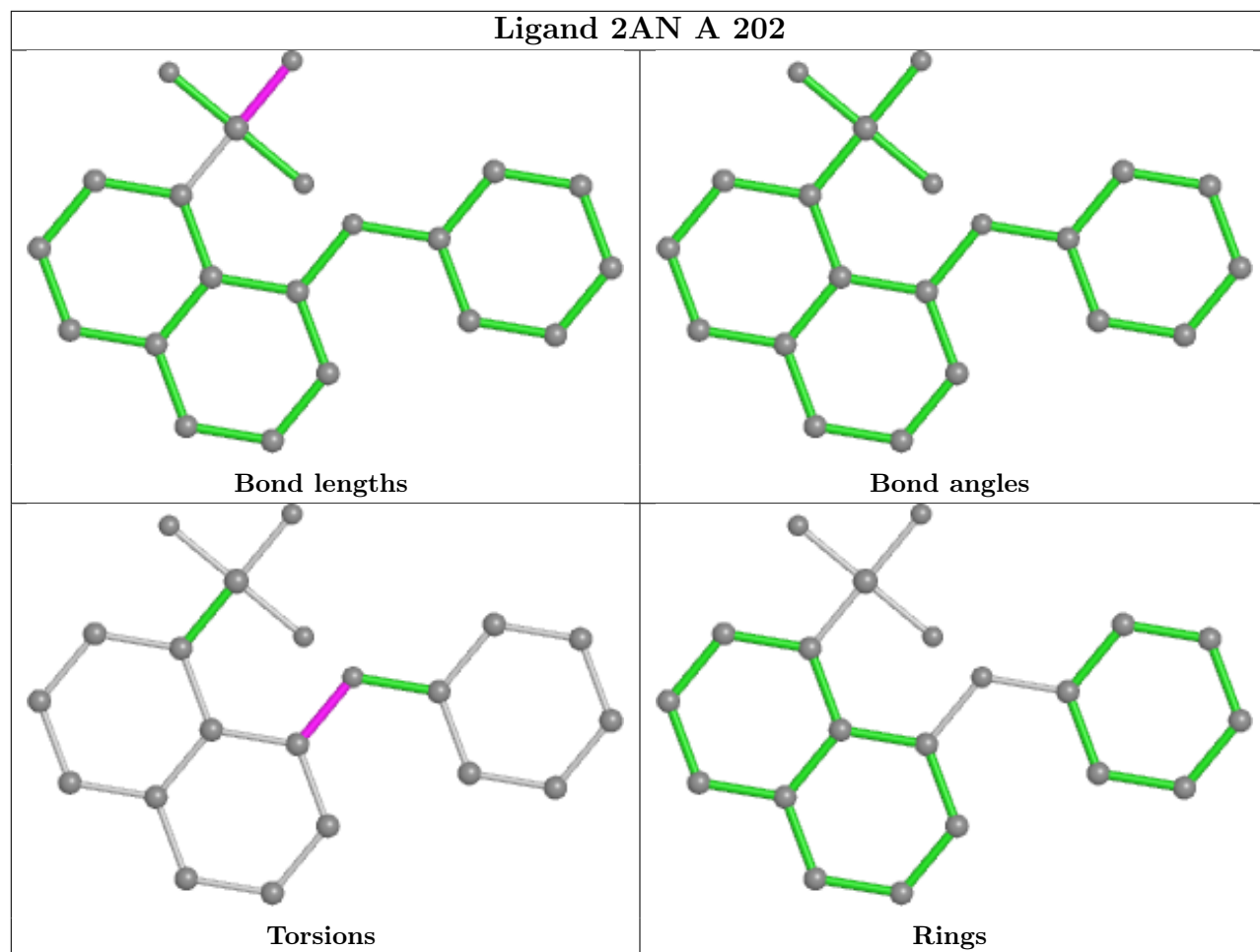


Torsions



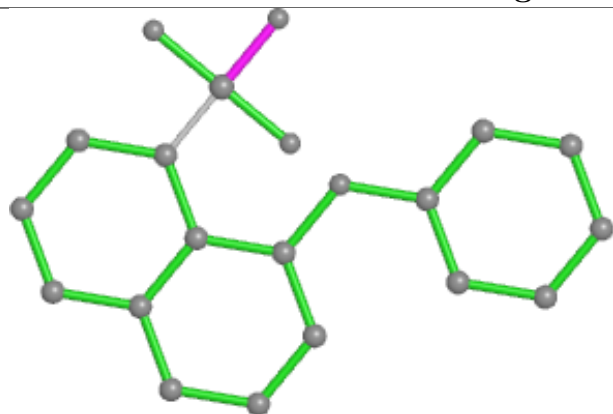
Rings



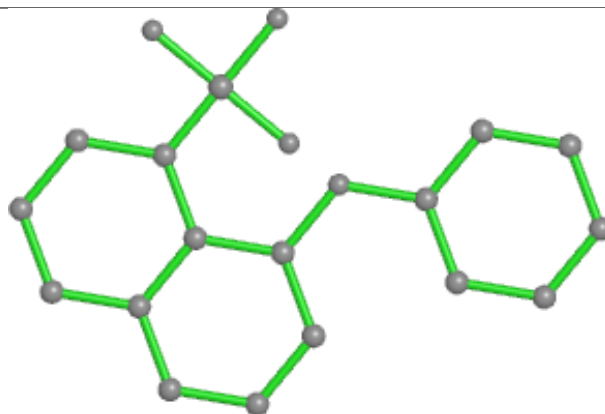




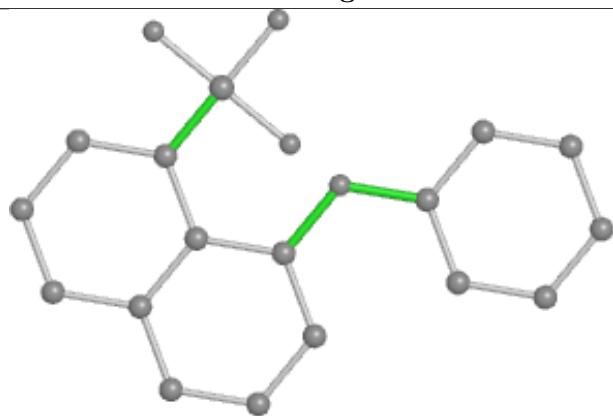
## Ligand 2AN D 705



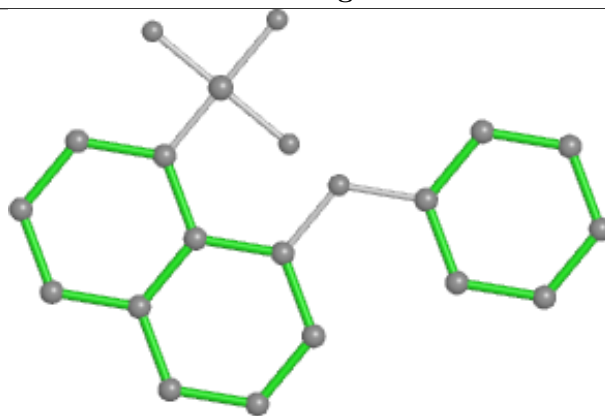
Bond lengths



Bond angles

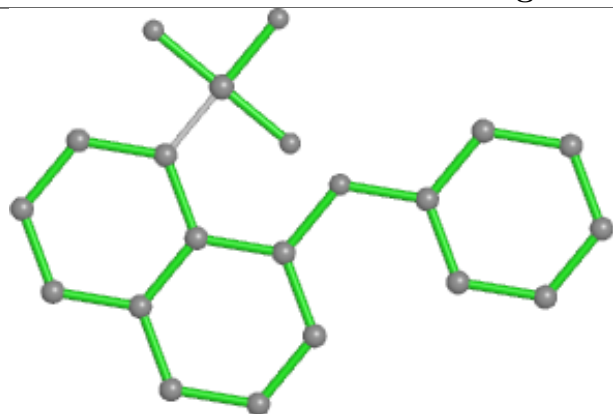


Torsions

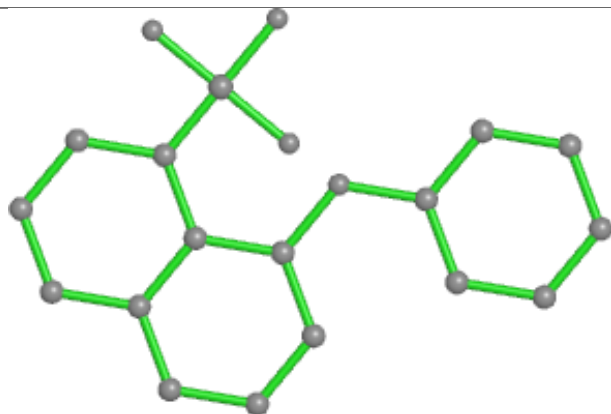


Rings

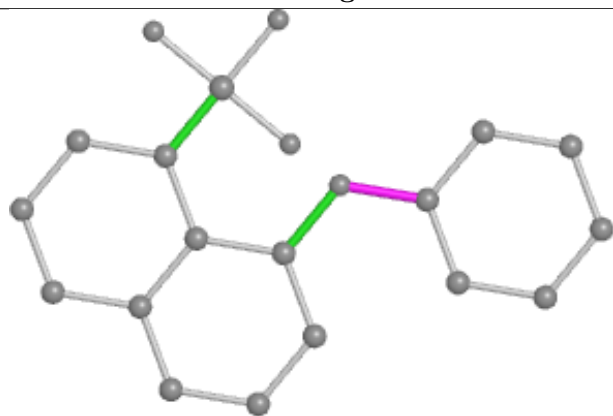
## Ligand 2AN E 501



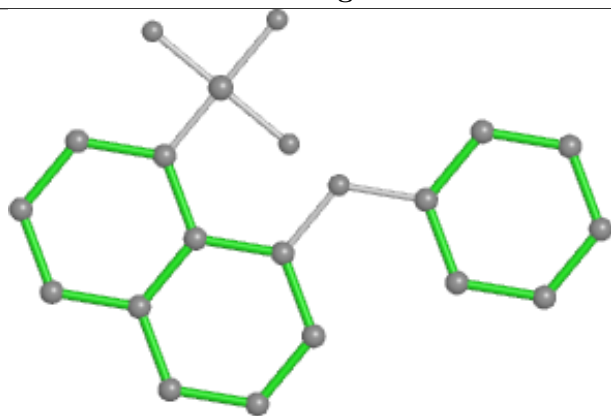
Bond lengths



Bond angles

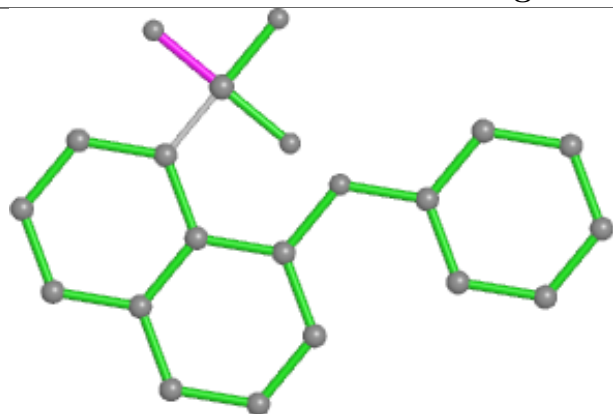


Torsions

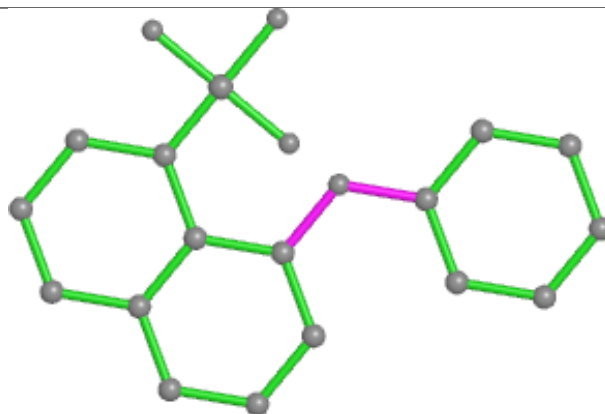


Rings

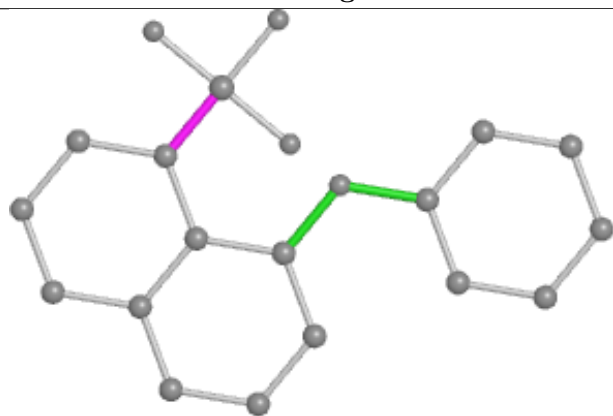
## Ligand 2AN G 304



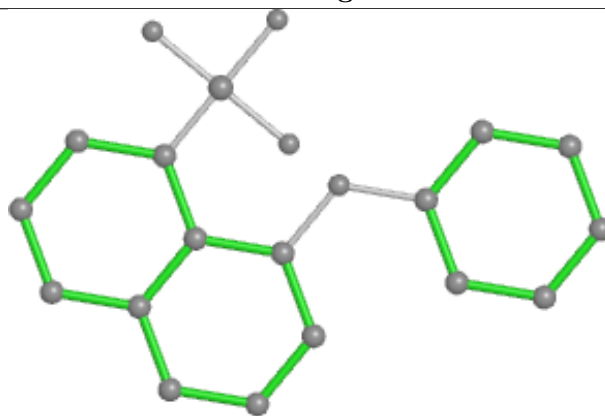
Bond lengths



Bond angles

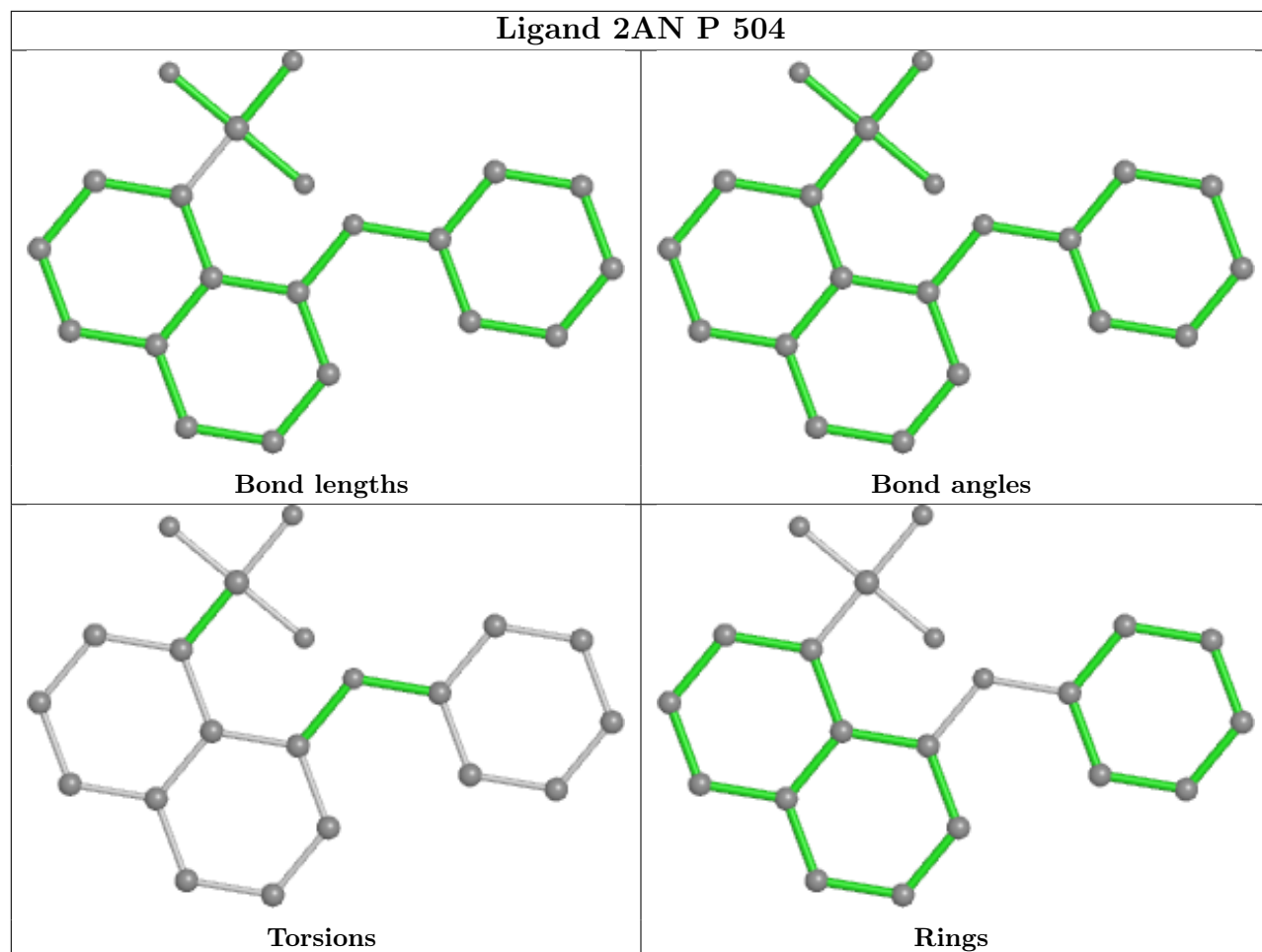


Torsions

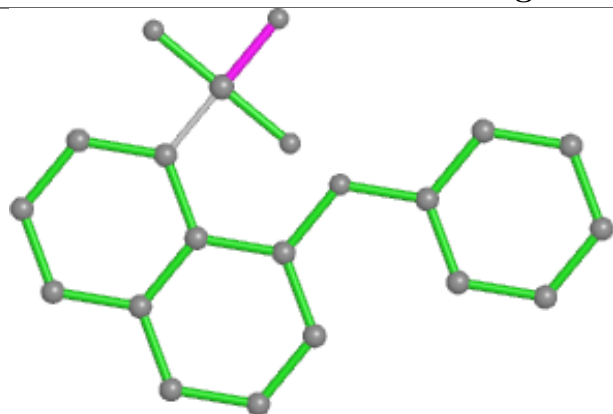


Rings

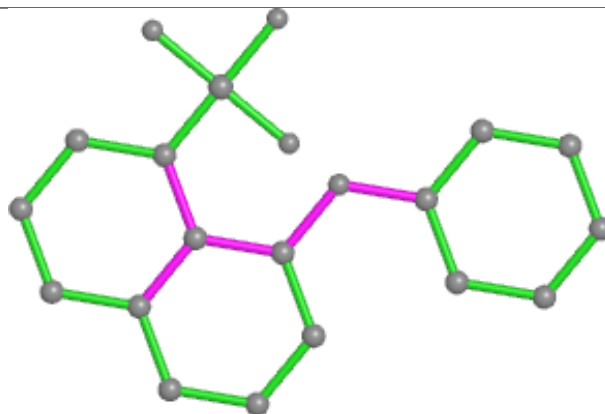
## Ligand 2AN P 504



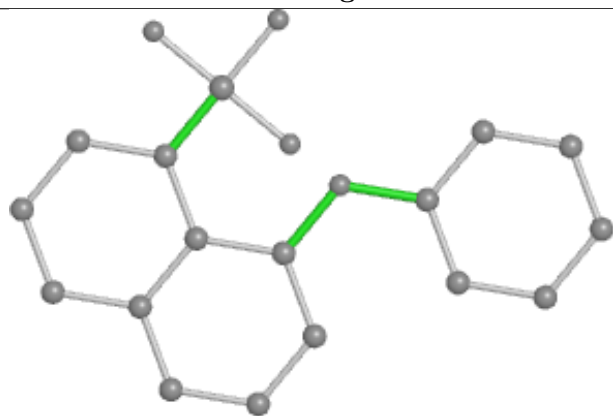
## Ligand 2AN C 306



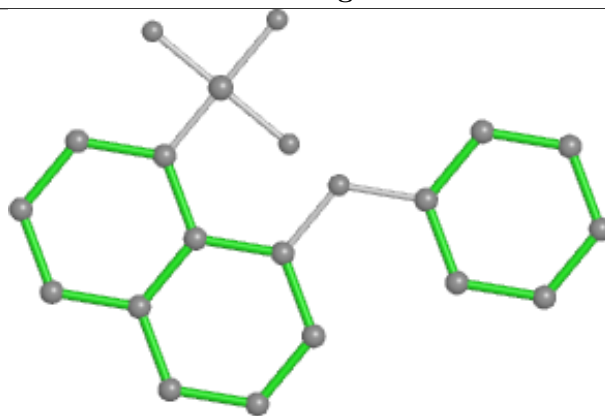
Bond lengths



Bond angles

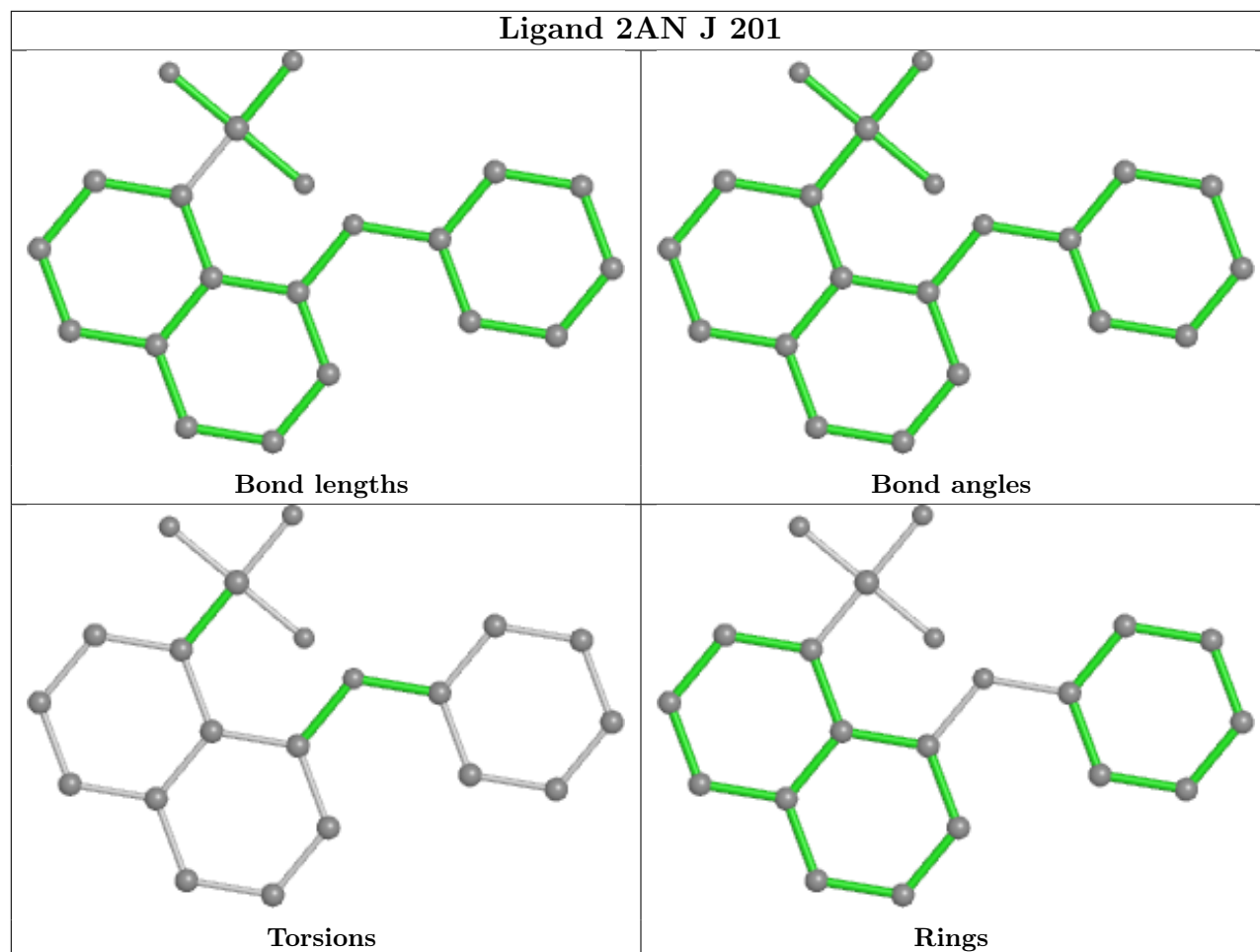


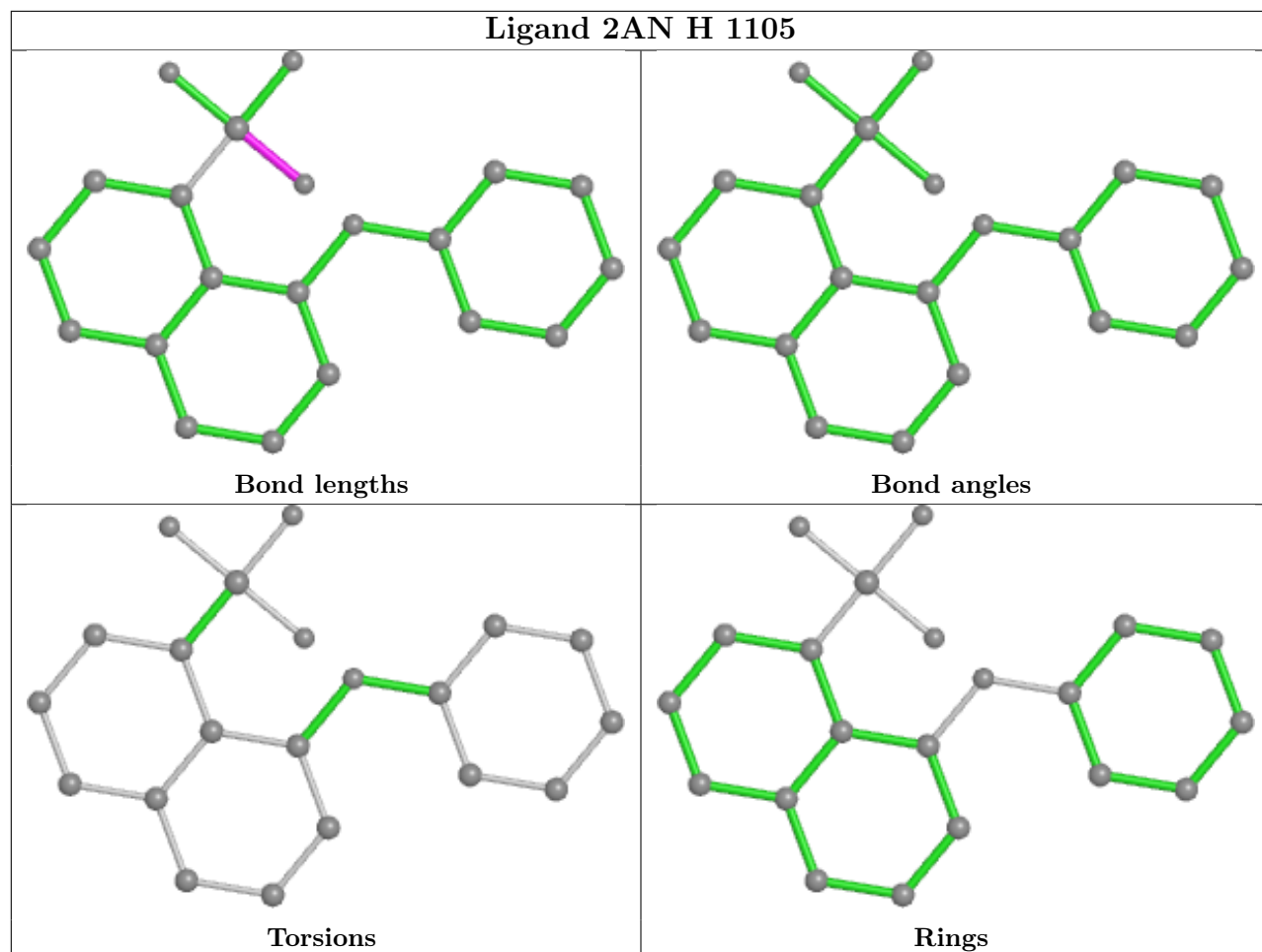
Torsions



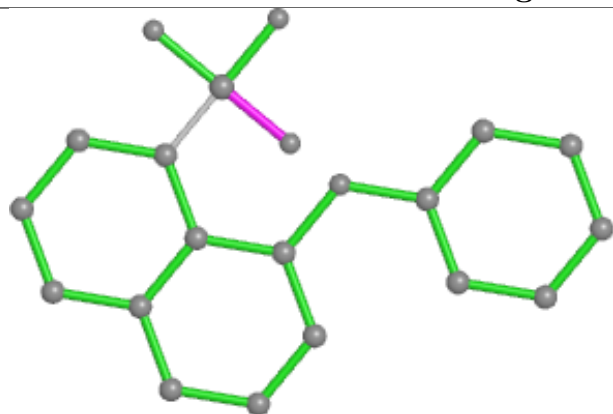
Rings

## Ligand 2AN J 201

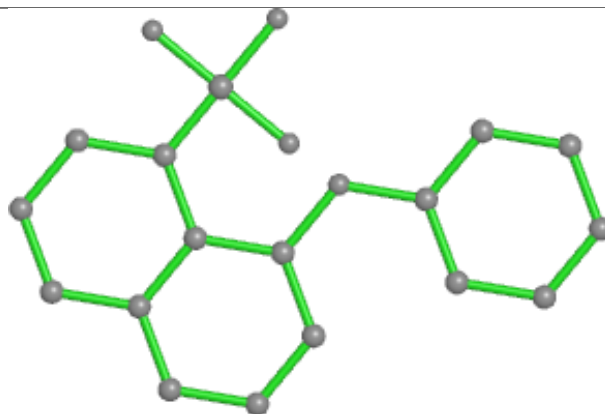




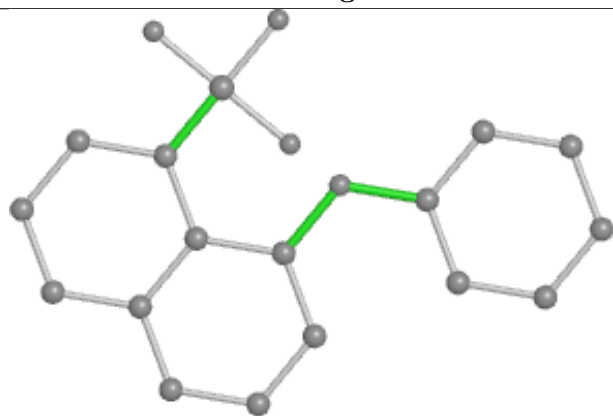
## Ligand 2AN B 202



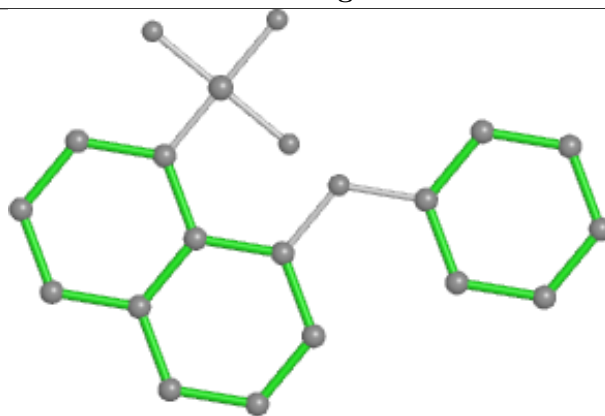
Bond lengths



Bond angles



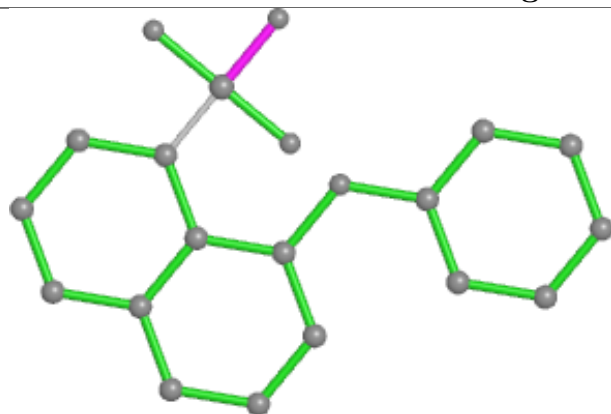
Torsions



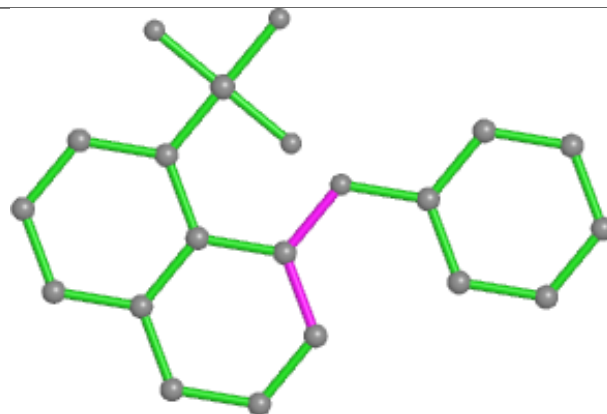
Rings



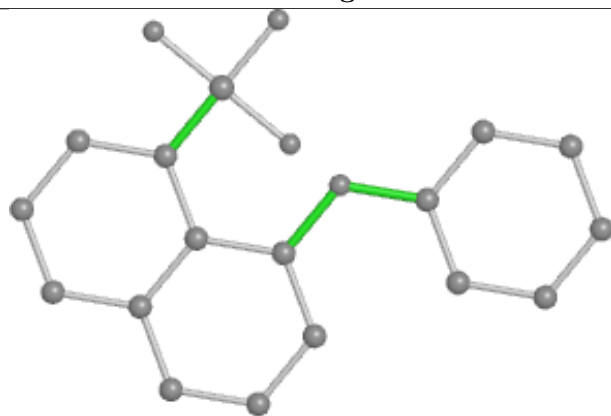
## Ligand 2AN I 204



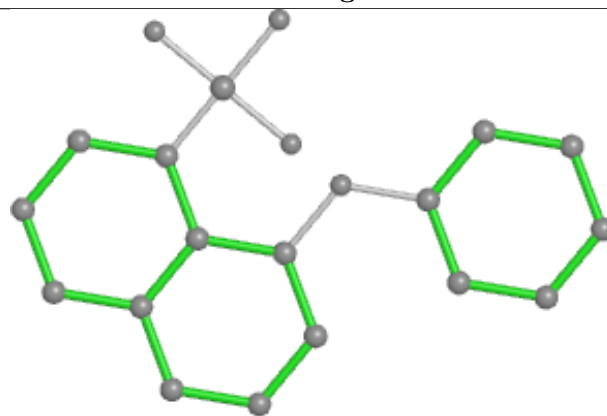
Bond lengths



Bond angles

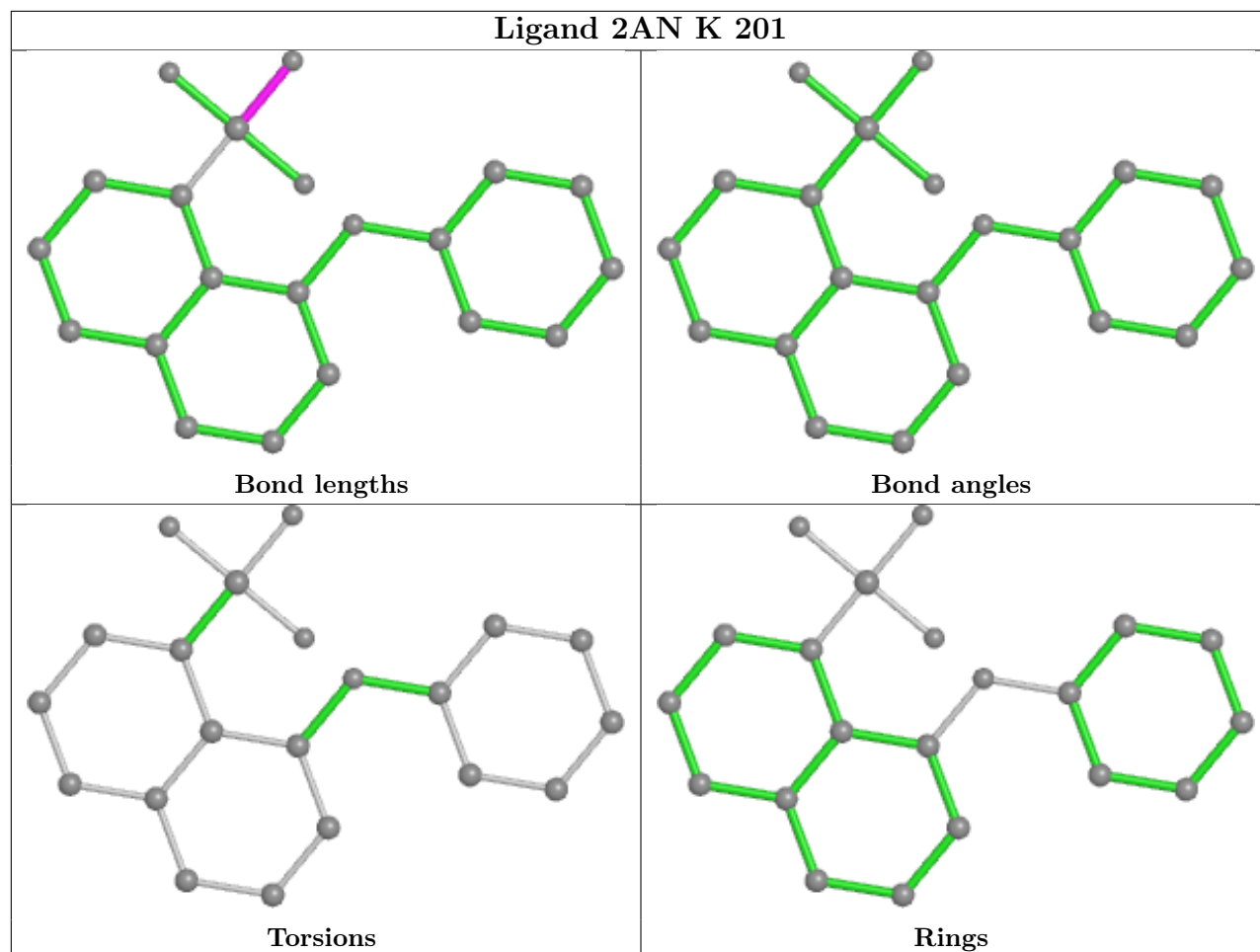


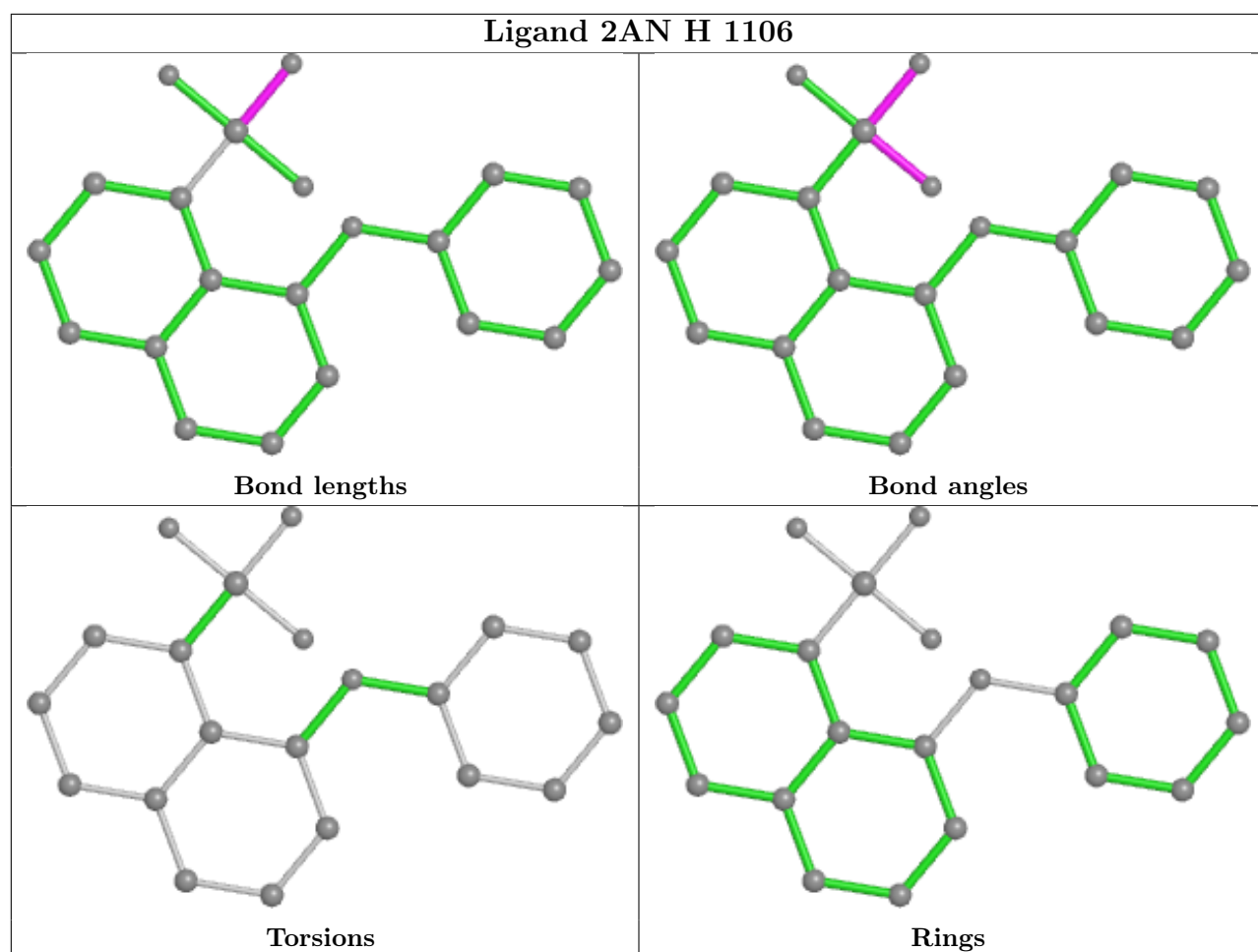
Torsions



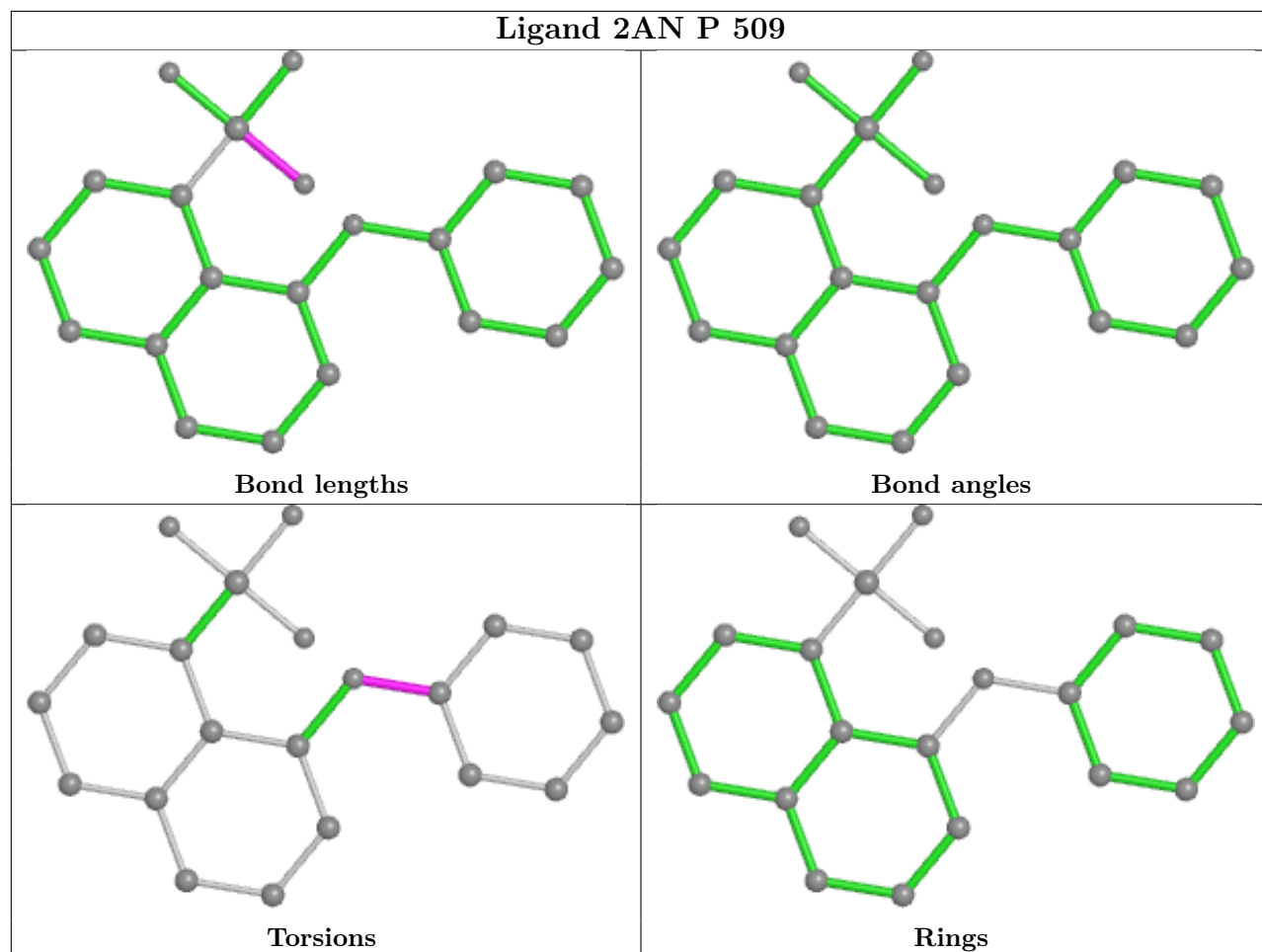
Rings

## Ligand 2AN K 201

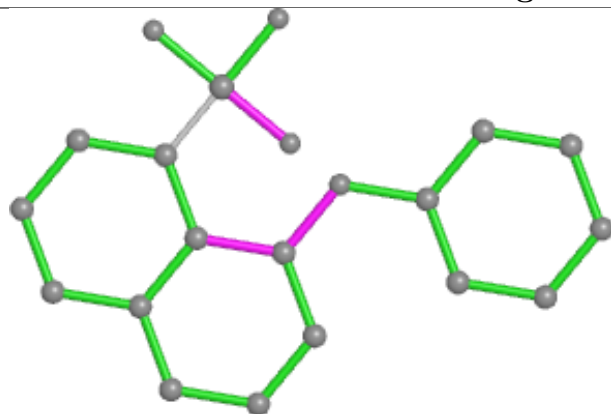




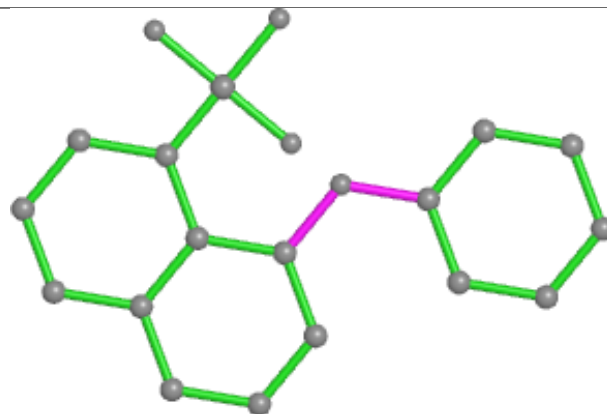
## Ligand 2AN P 509



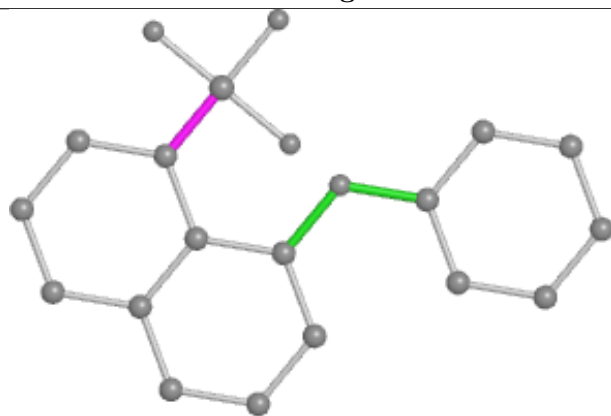
## Ligand 2AN E 507



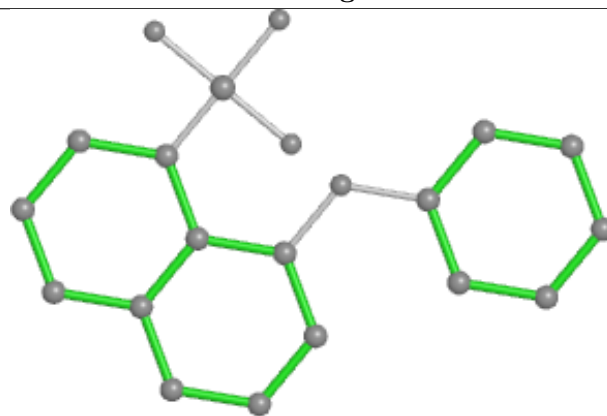
Bond lengths



Bond angles

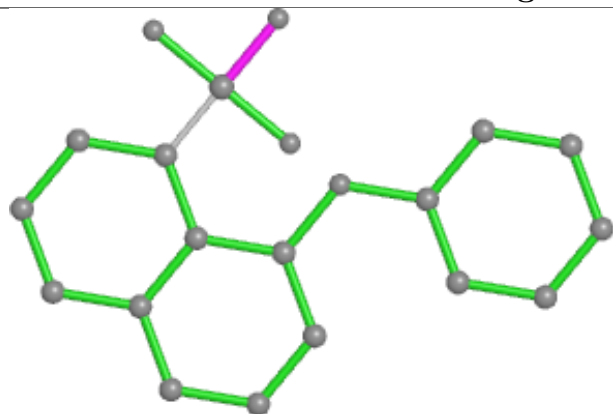


Torsions

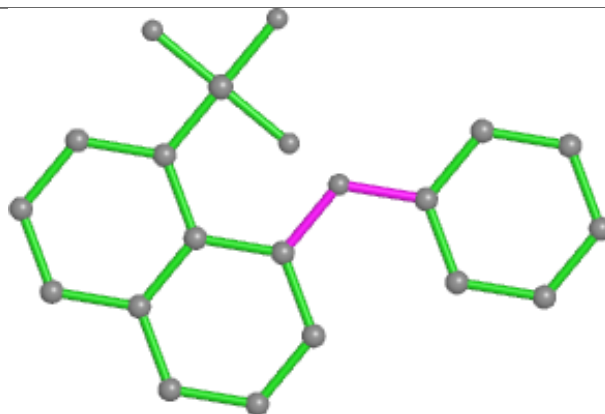


Rings

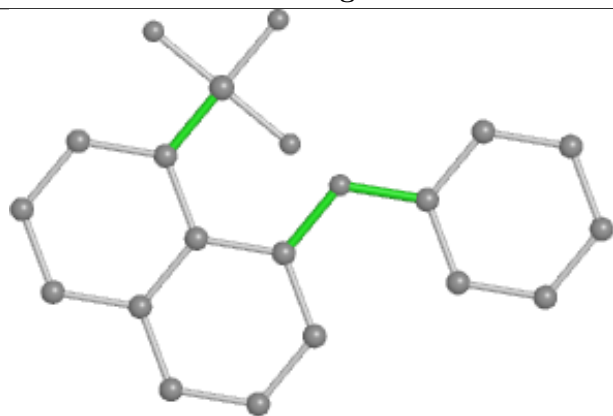
## Ligand 2AN L 202



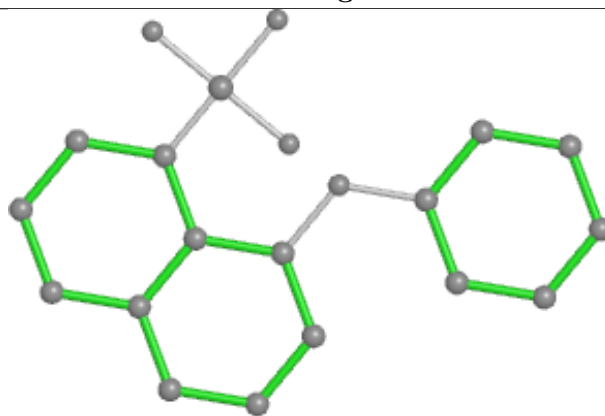
Bond lengths



Bond angles

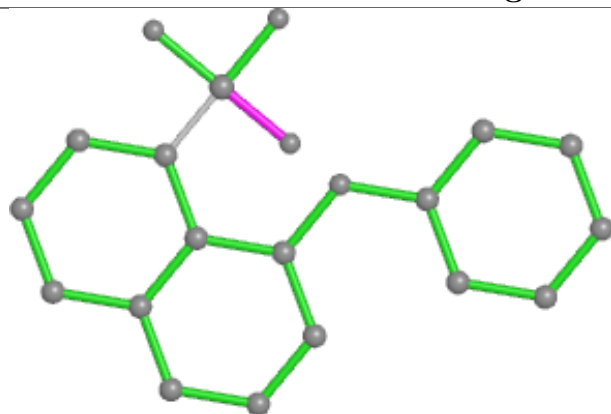


Torsions

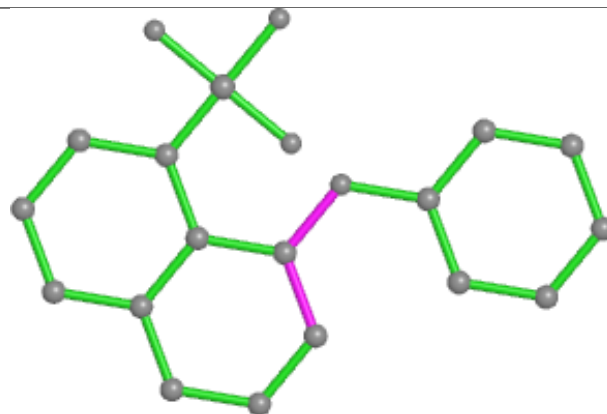


Rings

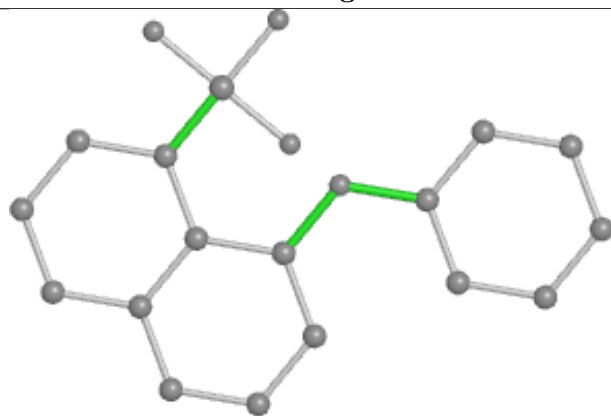
## Ligand 2AN H 1108



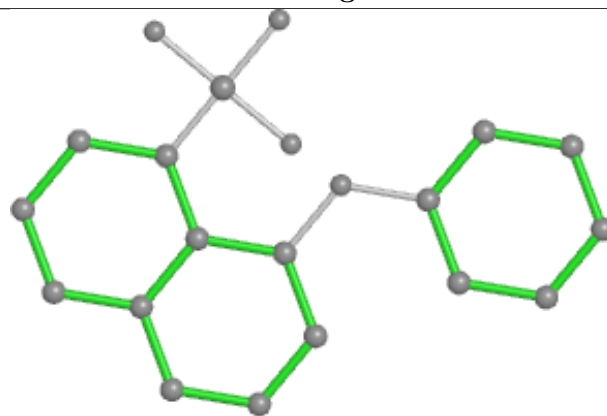
Bond lengths



Bond angles

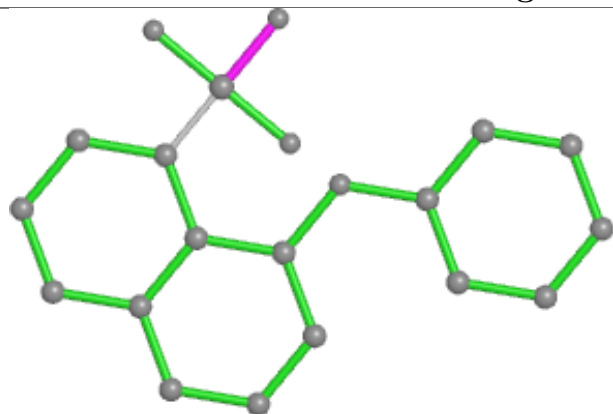


Torsions

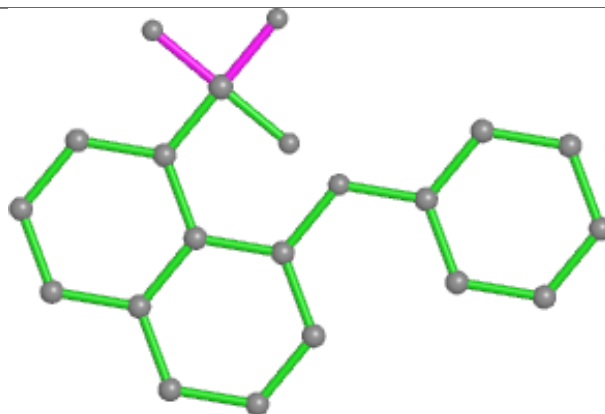


Rings

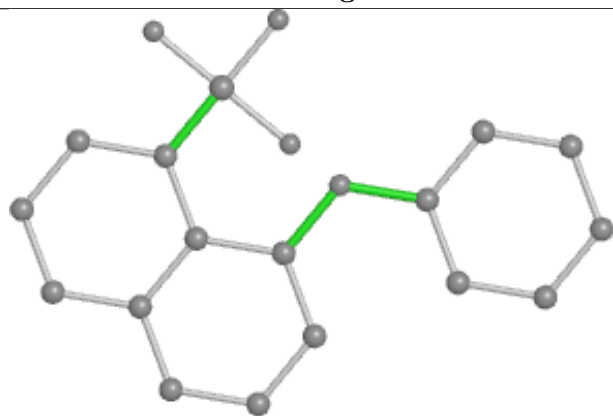
## Ligand 2AN F 205



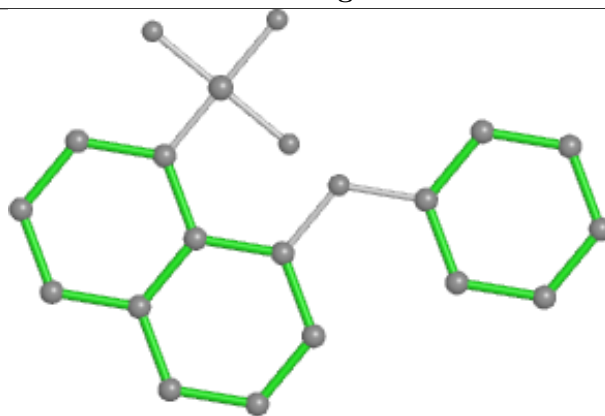
Bond lengths



Bond angles



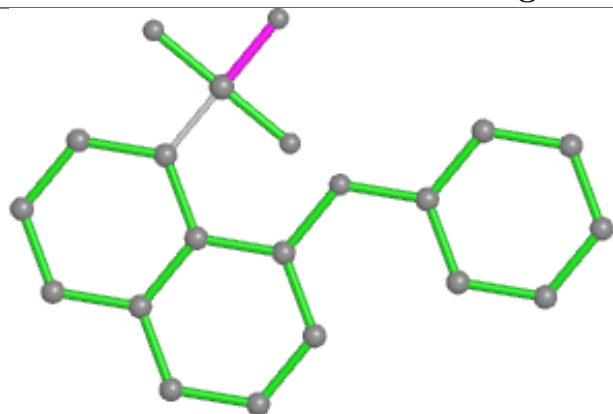
Torsions



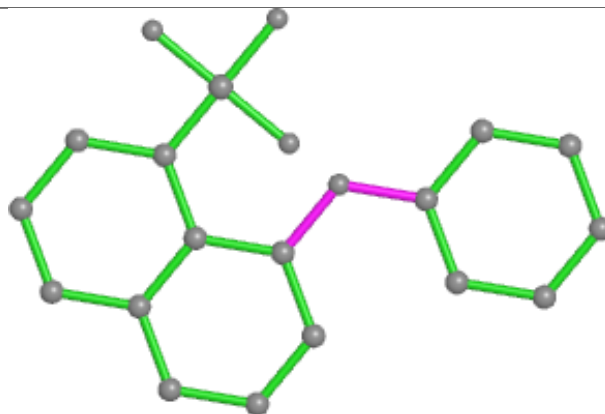
Rings



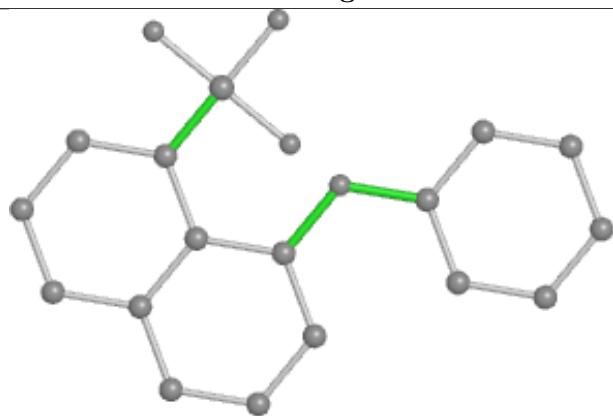
## Ligand 2AN J 205



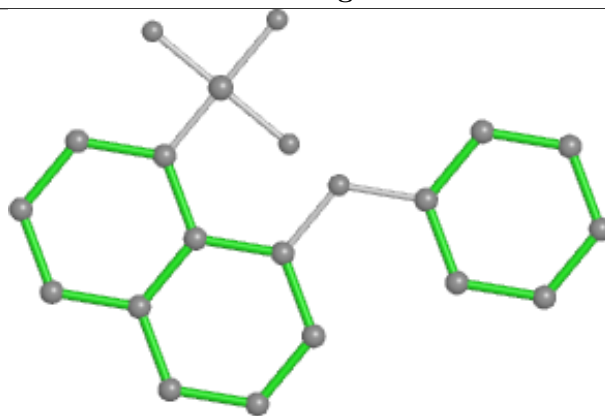
Bond lengths



Bond angles

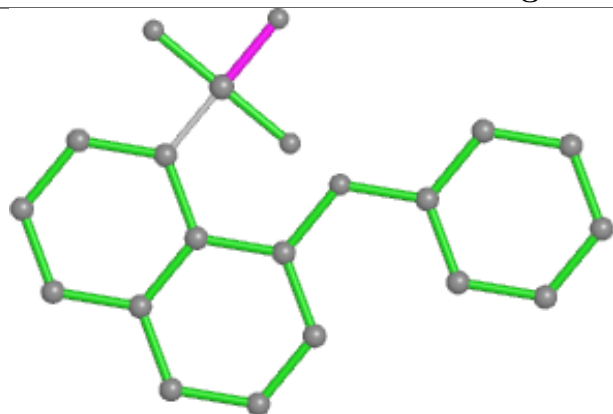


Torsions

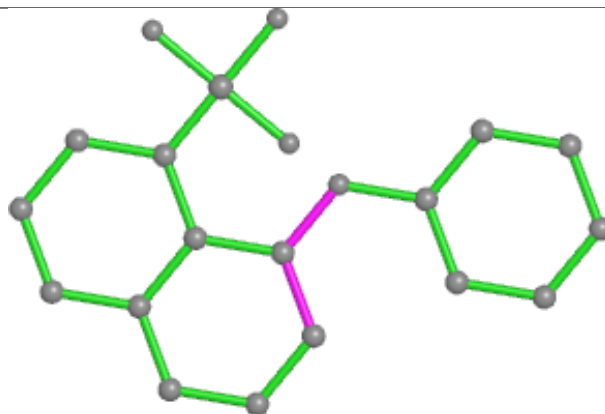


Rings

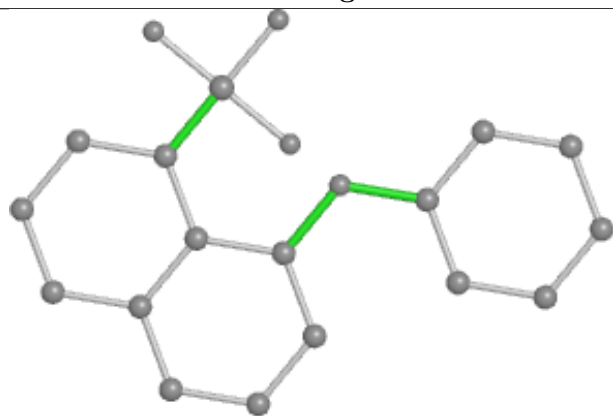
## Ligand 2AN I 205



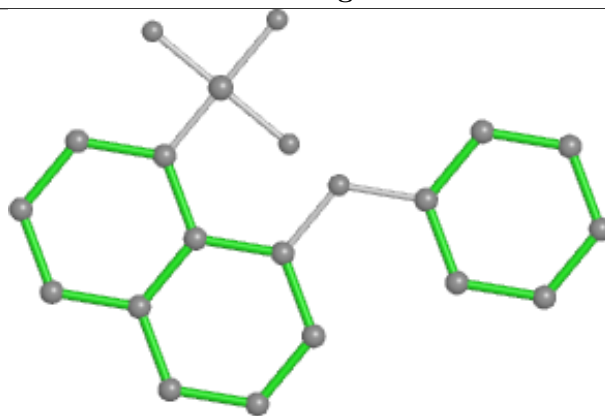
Bond lengths



Bond angles

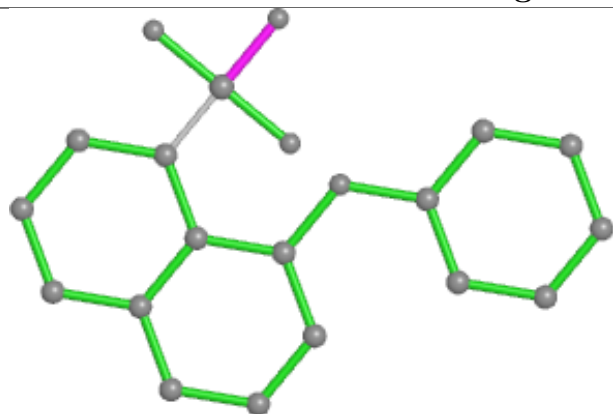


Torsions

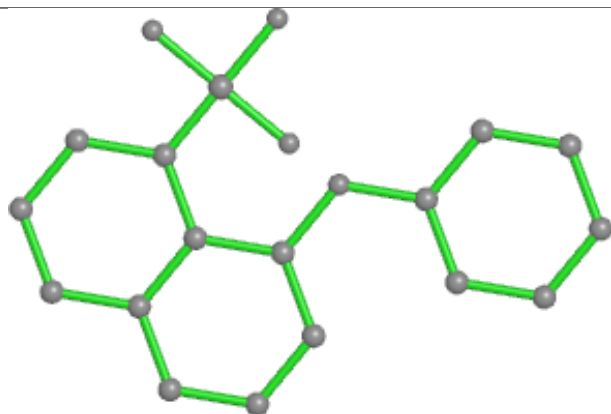


Rings

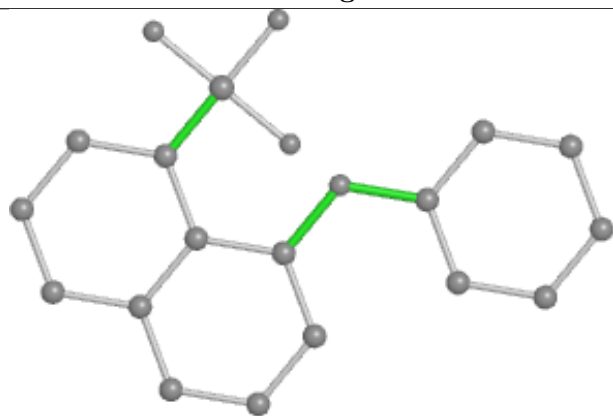
## Ligand 2AN D 704



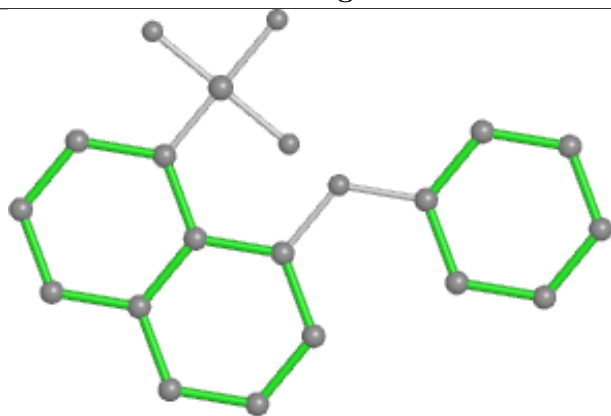
Bond lengths



Bond angles

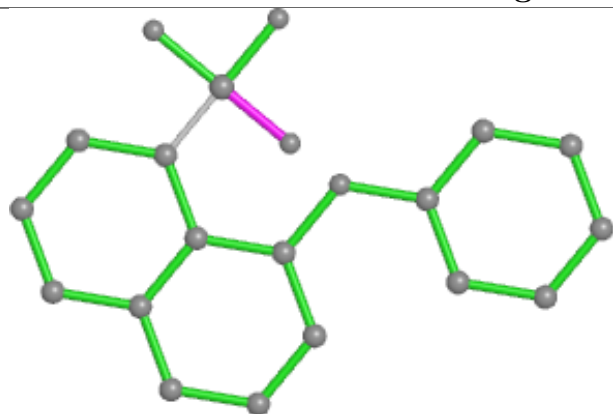


Torsions

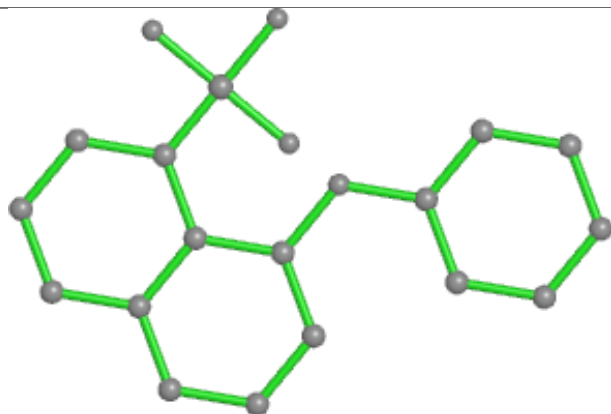


Rings

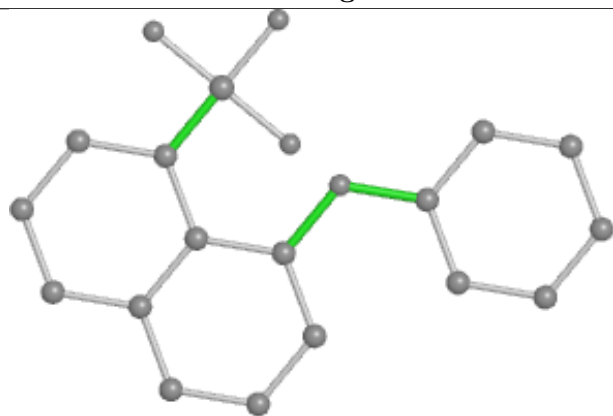
## Ligand 2AN A 204



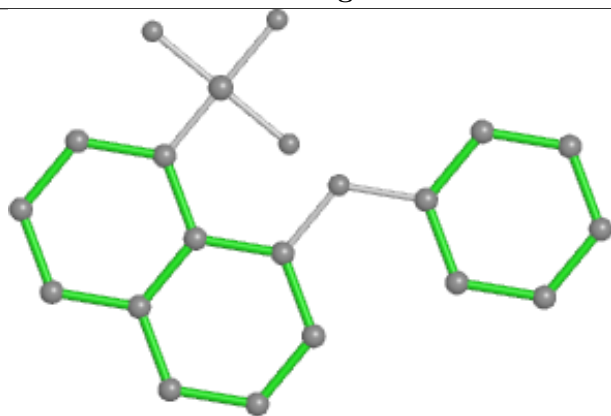
Bond lengths



Bond angles

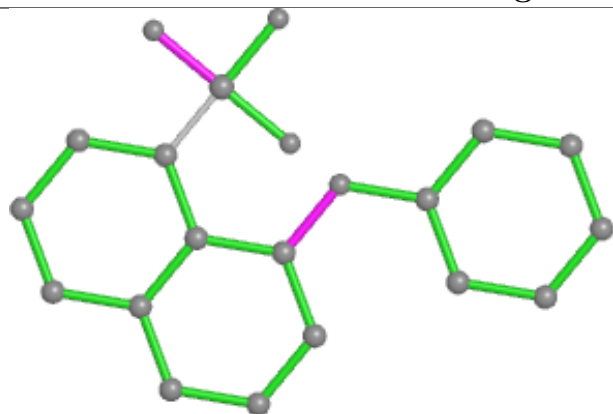


Torsions

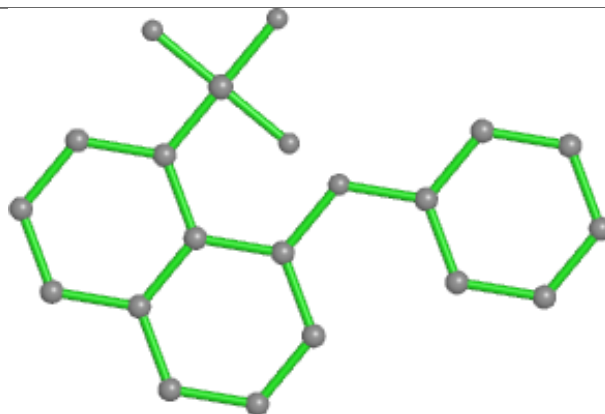


Rings

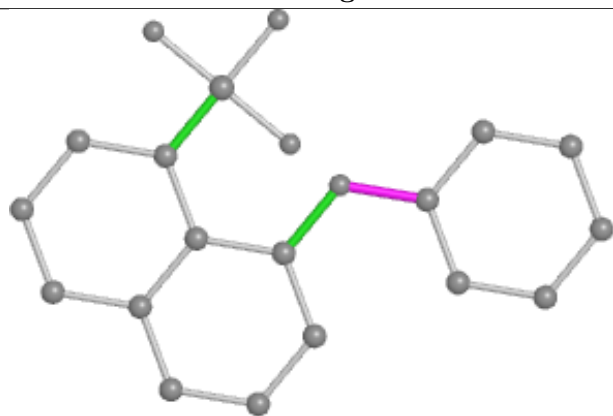
## Ligand 2AN D 702



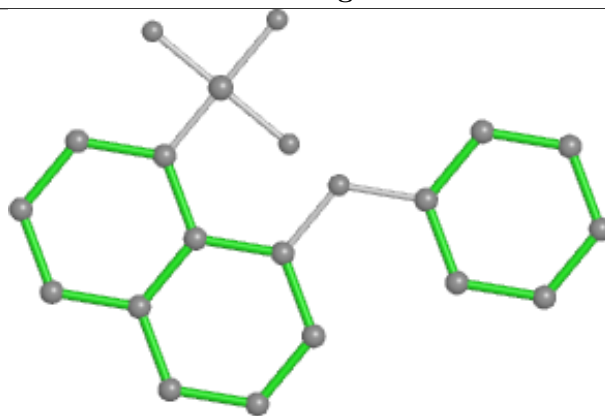
Bond lengths



Bond angles

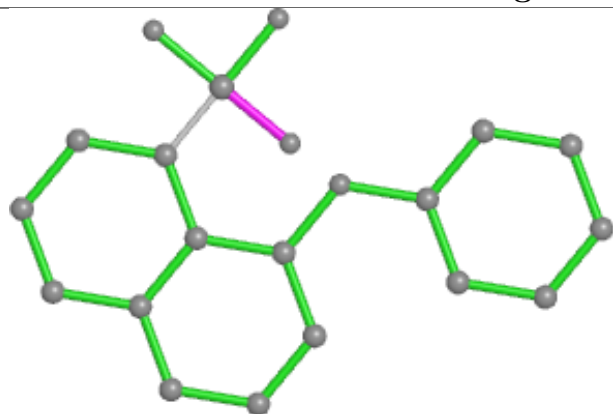


Torsions

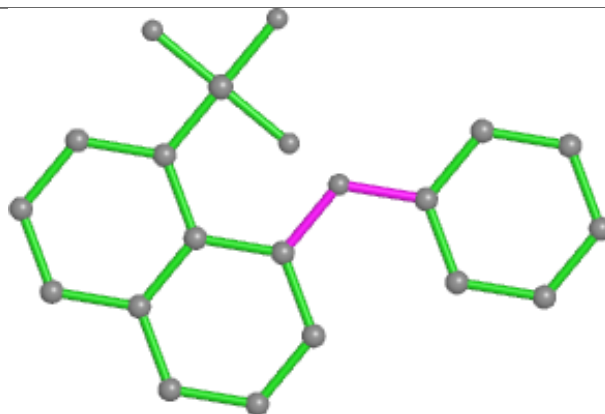


Rings

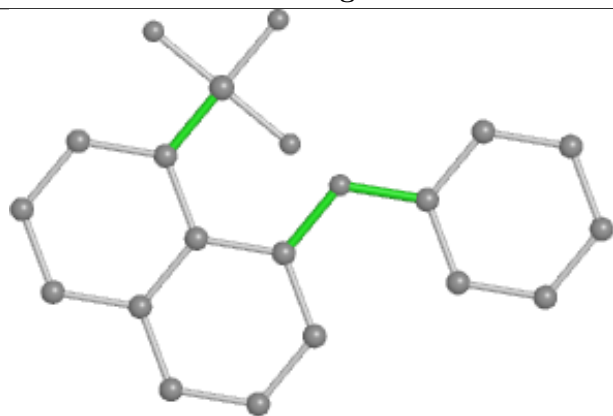
## Ligand 2AN G 305



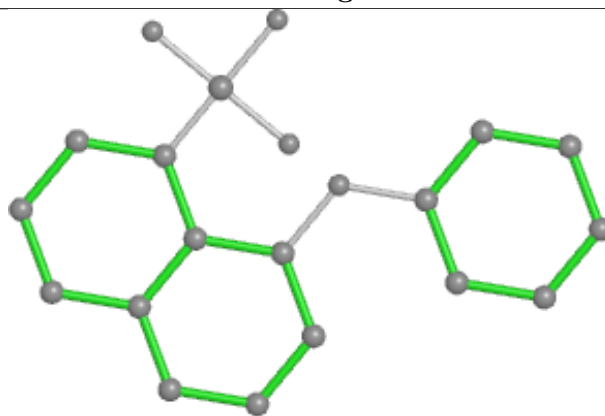
Bond lengths



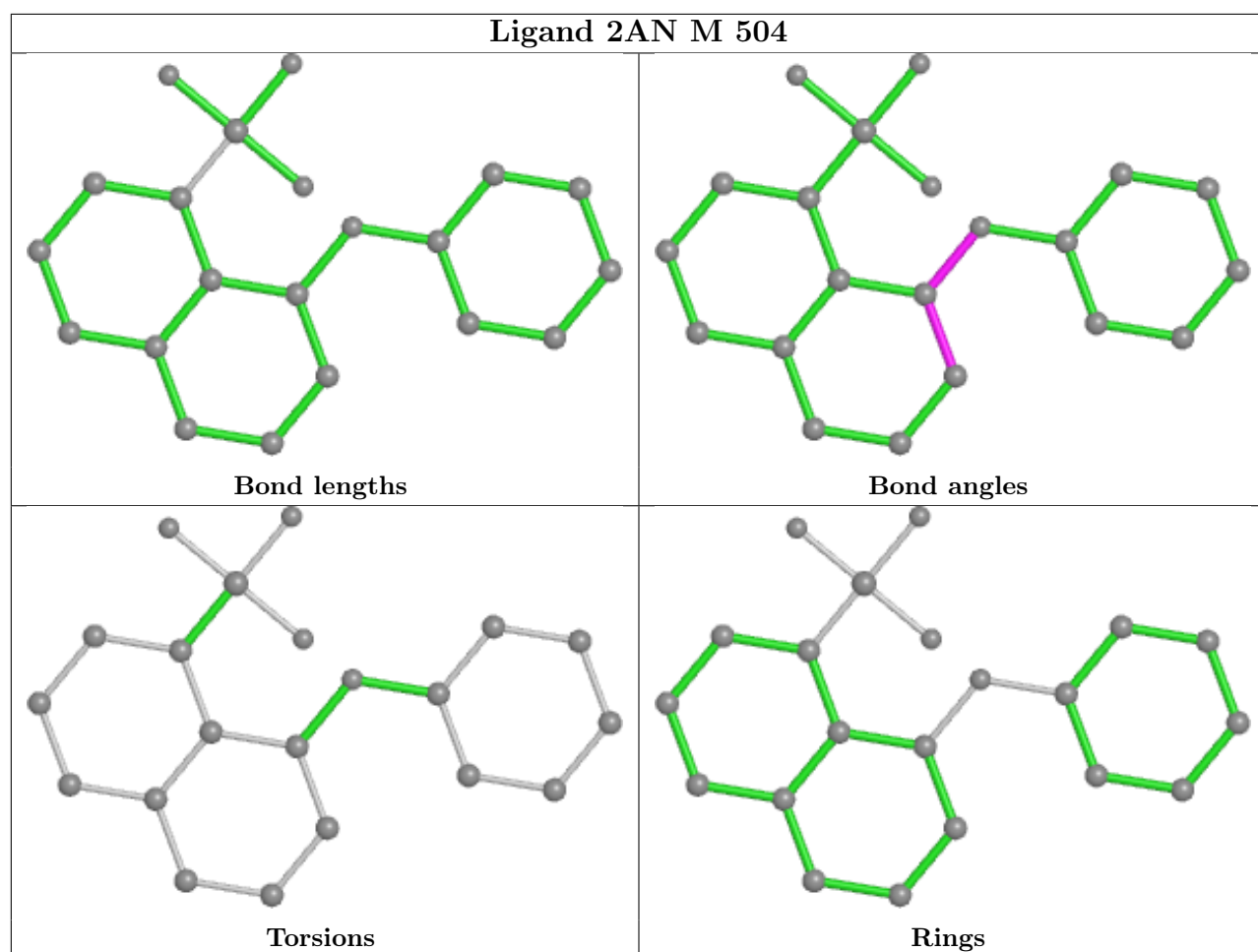
Bond angles



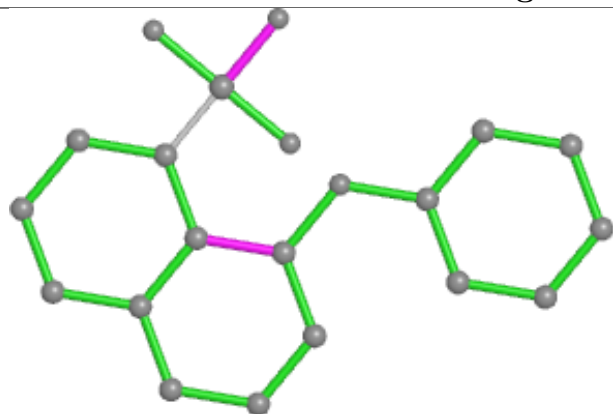
Torsions



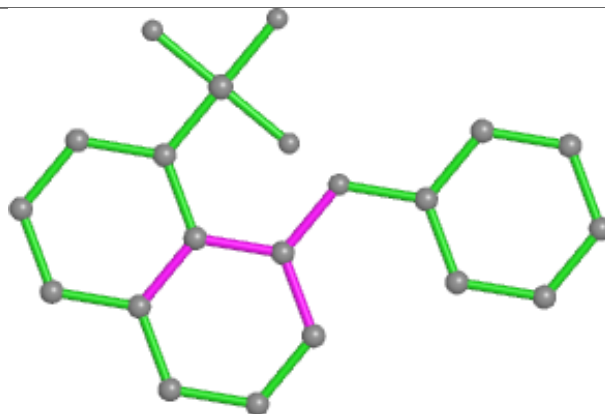
Rings



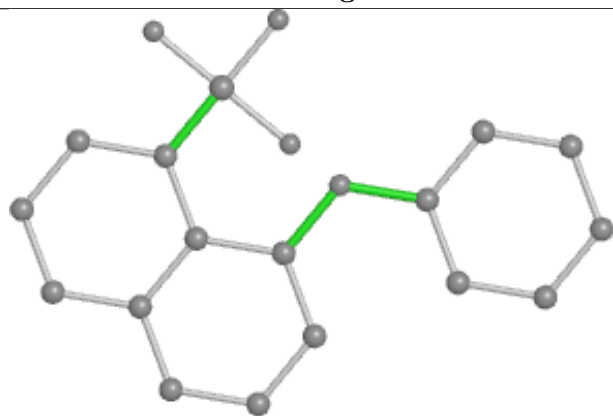
## Ligand 2AN E 503



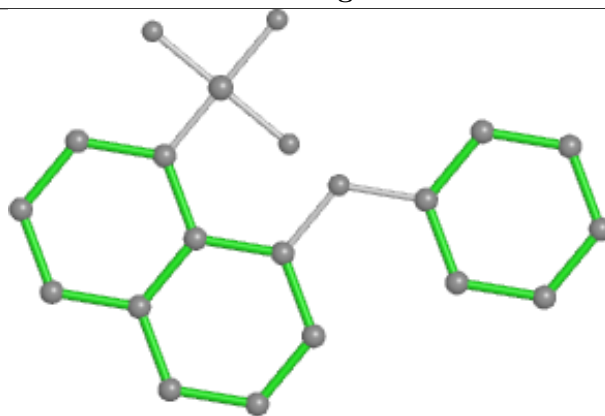
Bond lengths



Bond angles



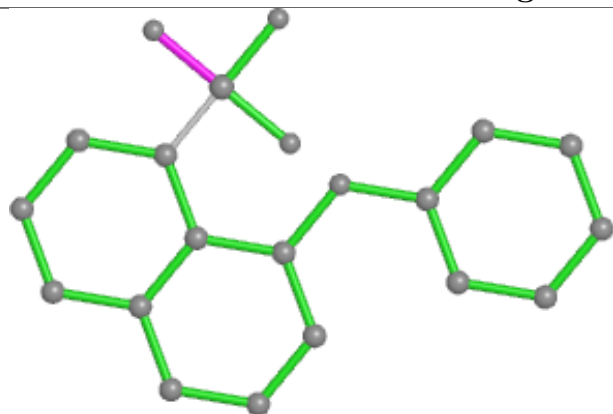
Torsions



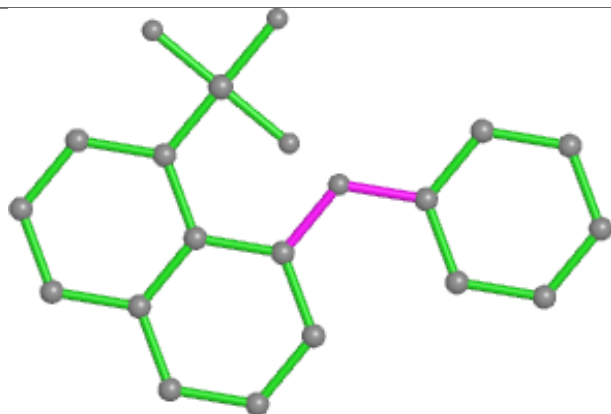
Rings



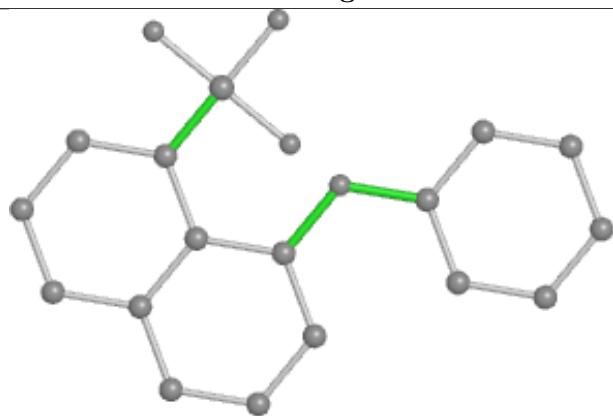
## Ligand 2AN F 206



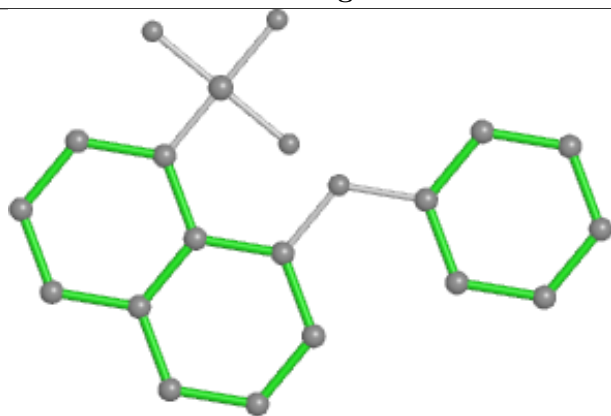
Bond lengths



Bond angles

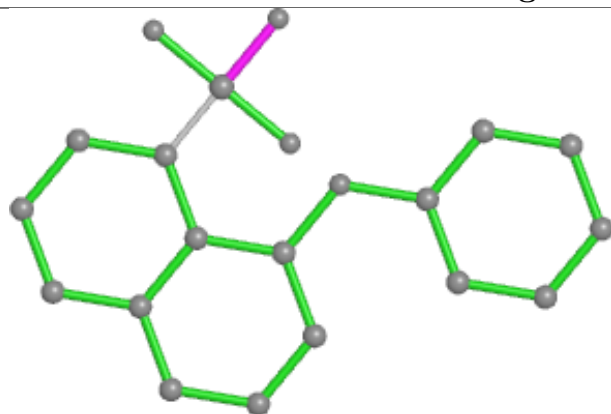


Torsions

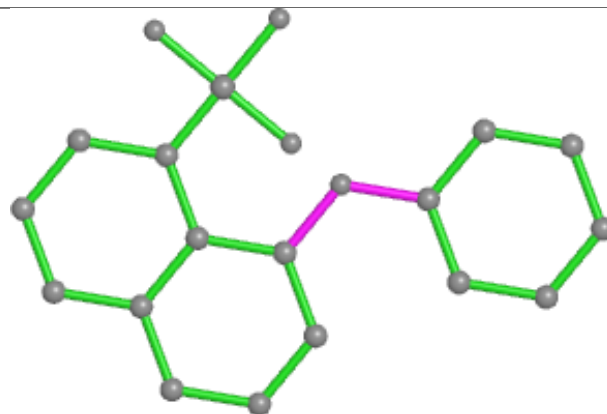


Rings

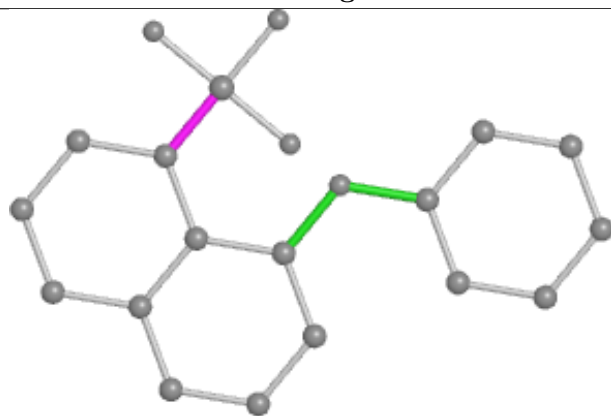
## Ligand 2AN J 202



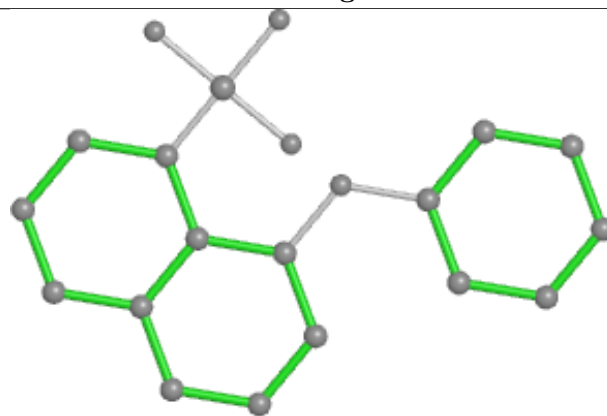
Bond lengths



Bond angles

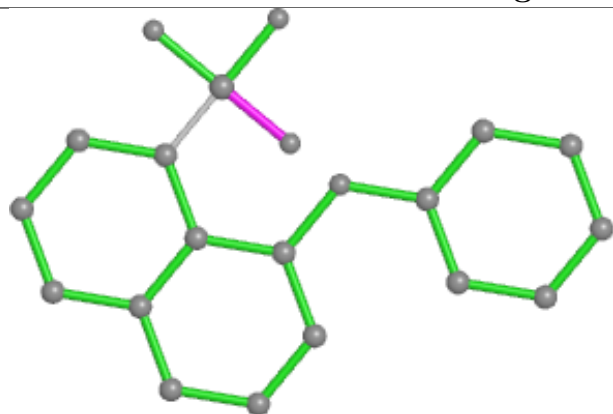


Torsions

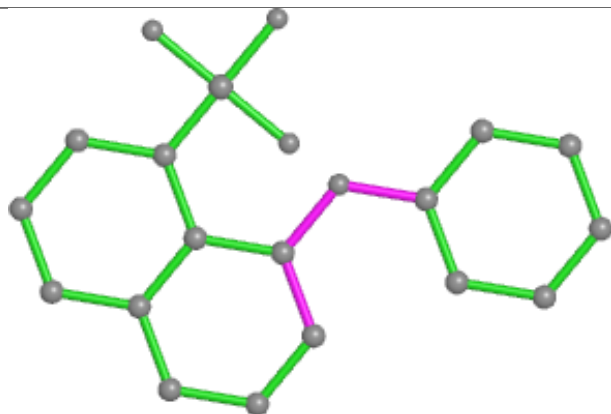


Rings

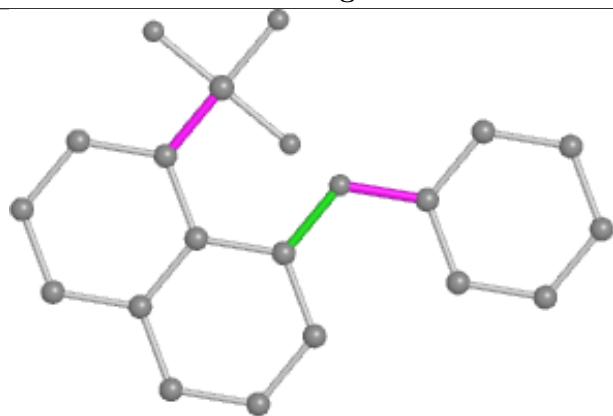
## Ligand 2AN K 205



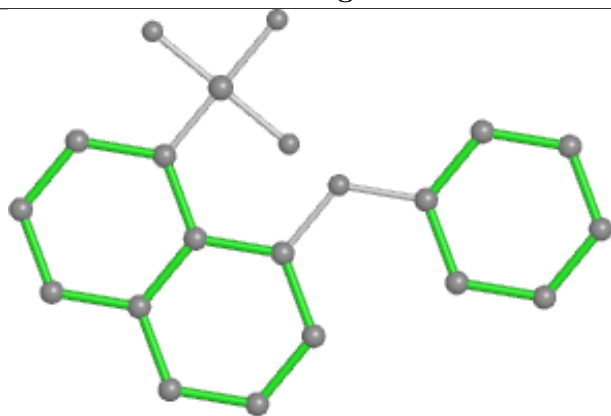
Bond lengths



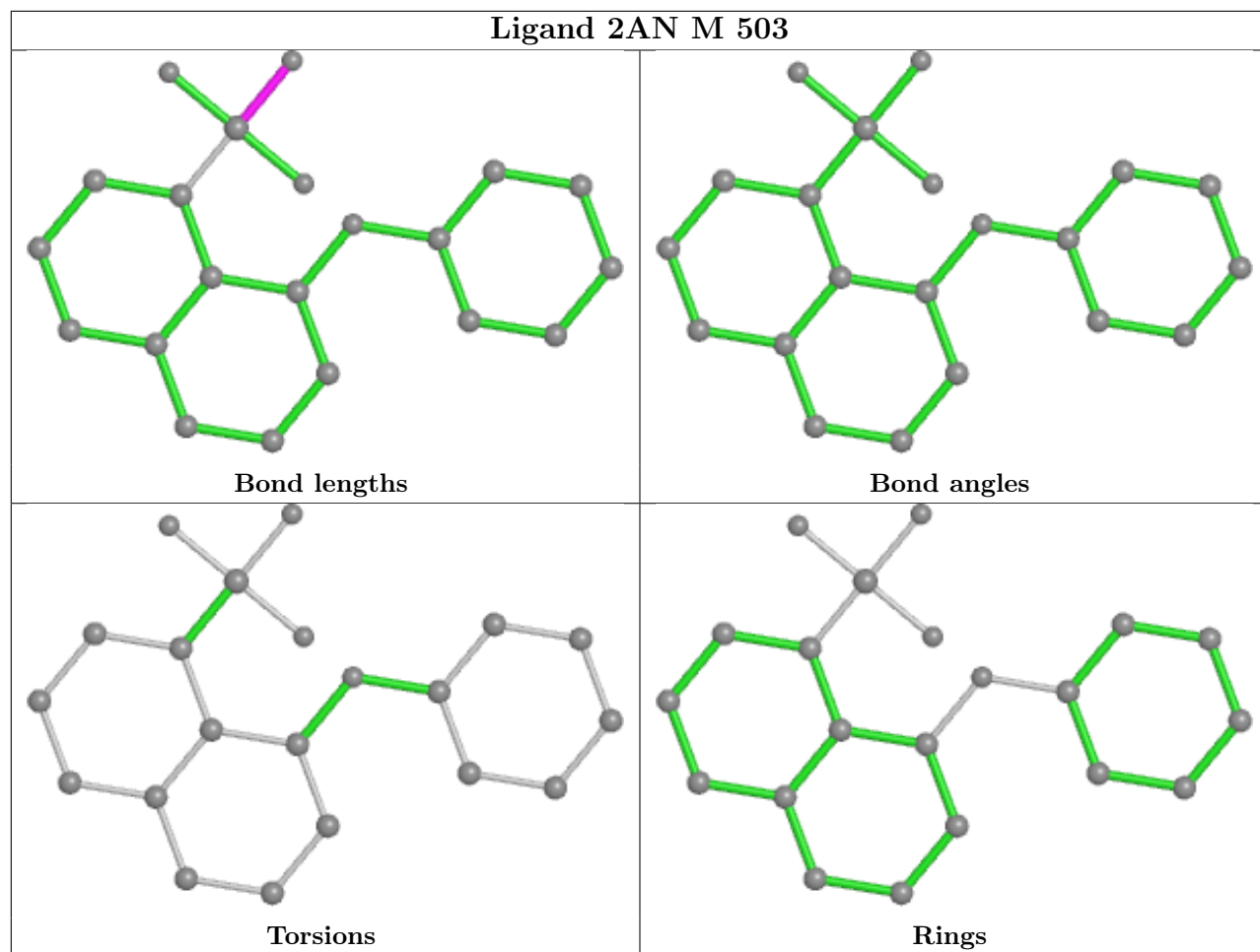
Bond angles



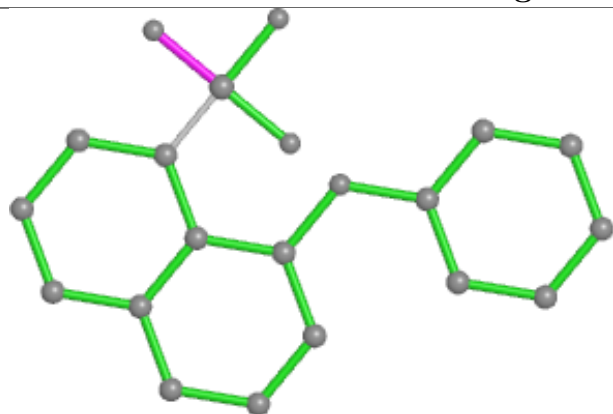
Torsions



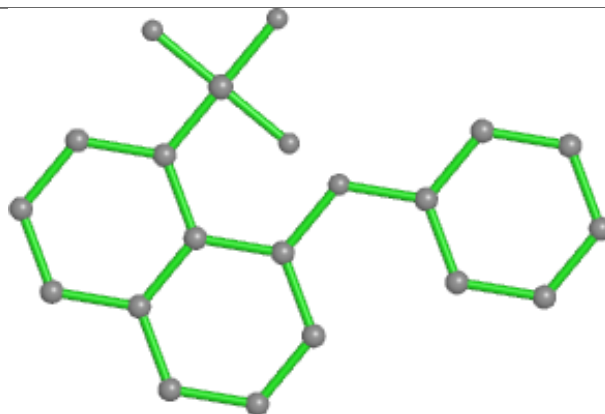
Rings



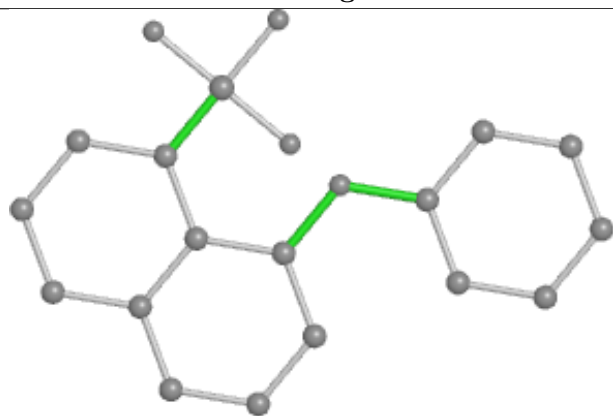
## Ligand 2AN O 202



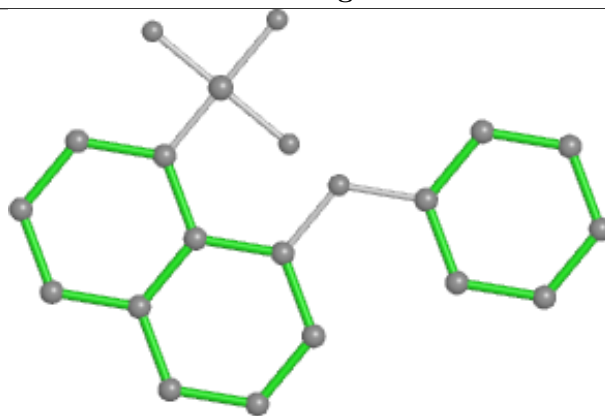
Bond lengths



Bond angles

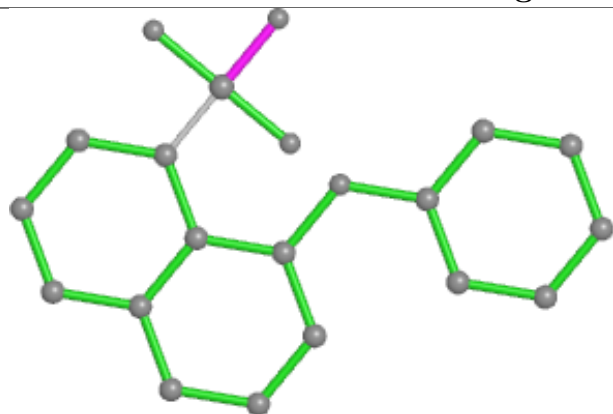


Torsions

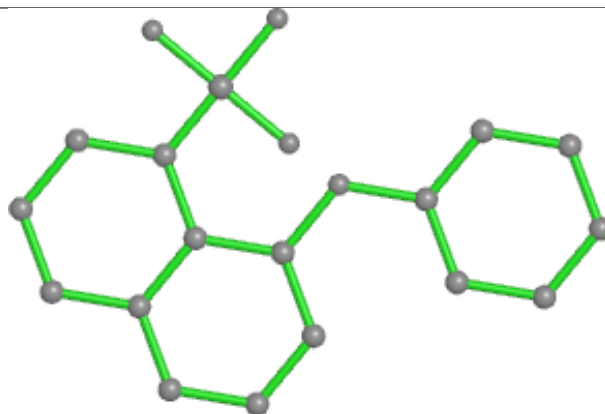


Rings

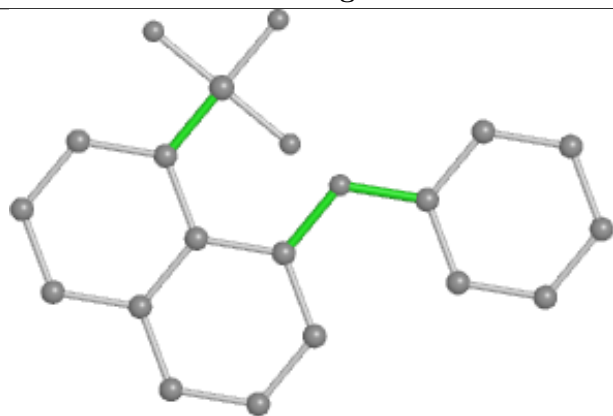
## Ligand 2AN C 301



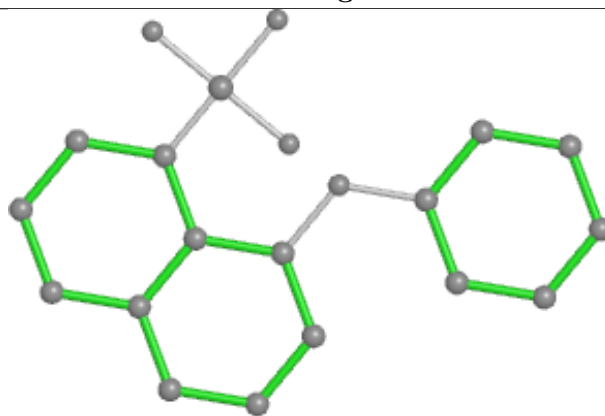
Bond lengths



Bond angles

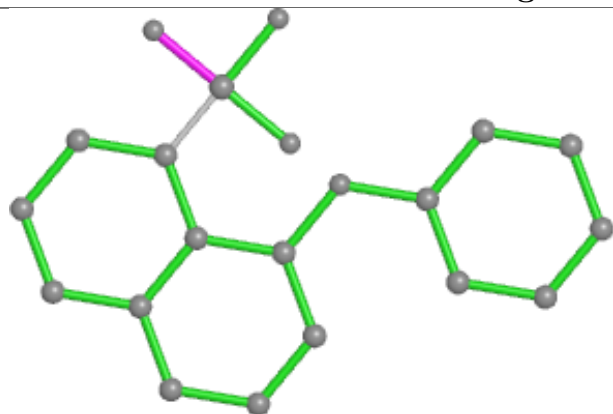


Torsions

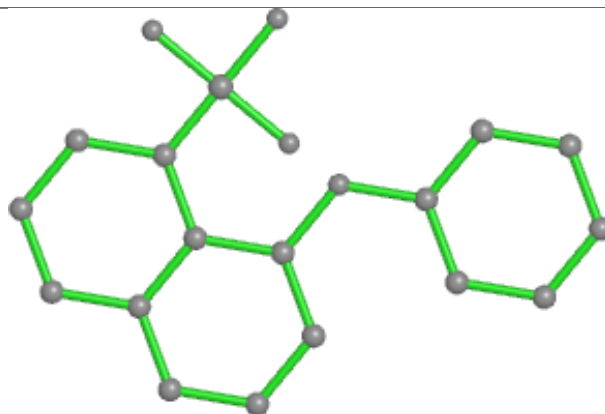


Rings

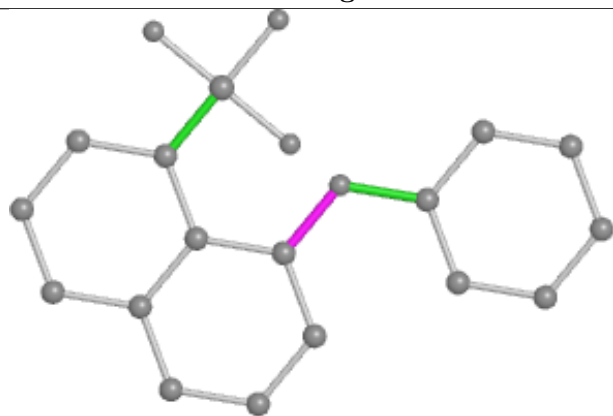
## Ligand 2AN L 204



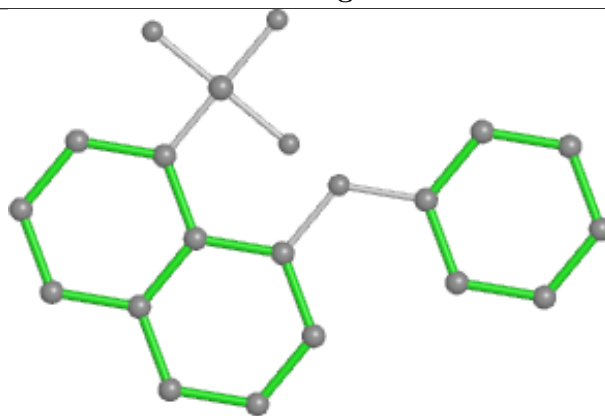
Bond lengths



Bond angles

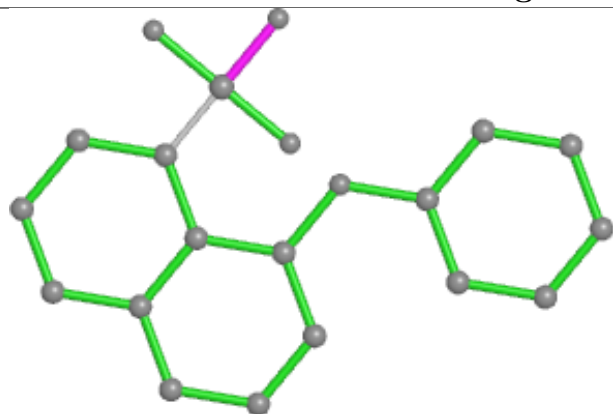


Torsions

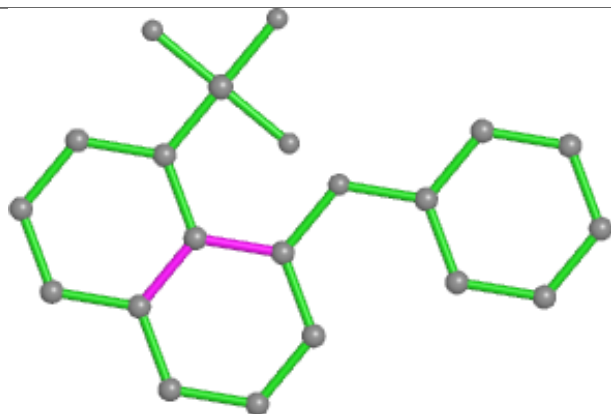


Rings

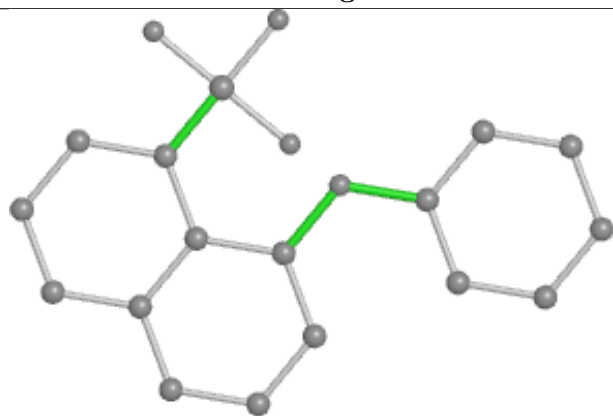
## Ligand 2AN C 303



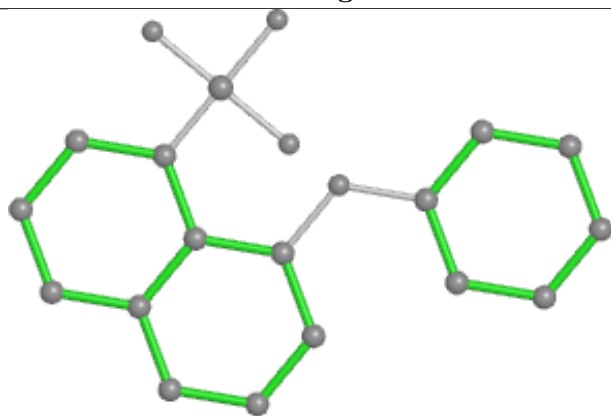
Bond lengths



Bond angles

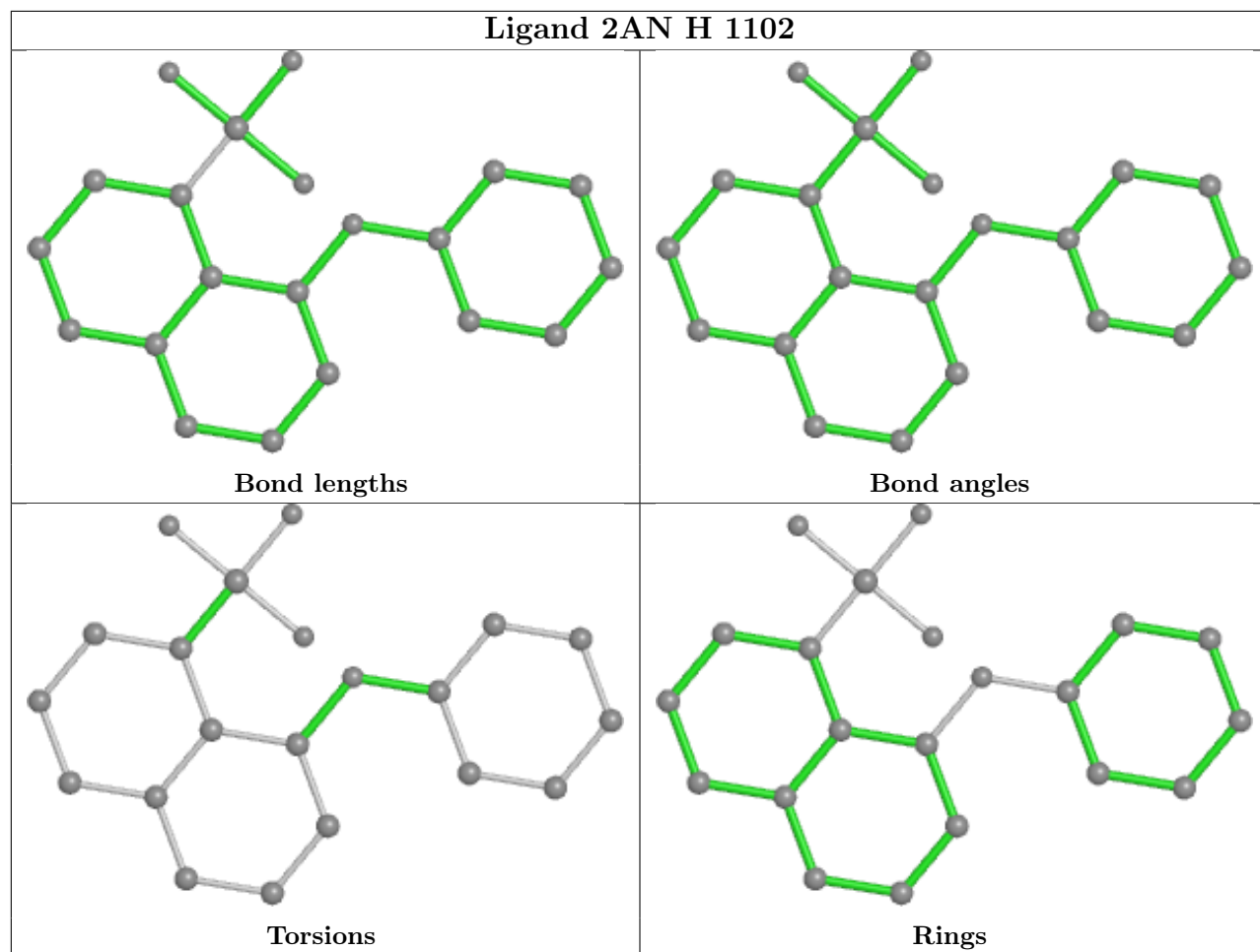


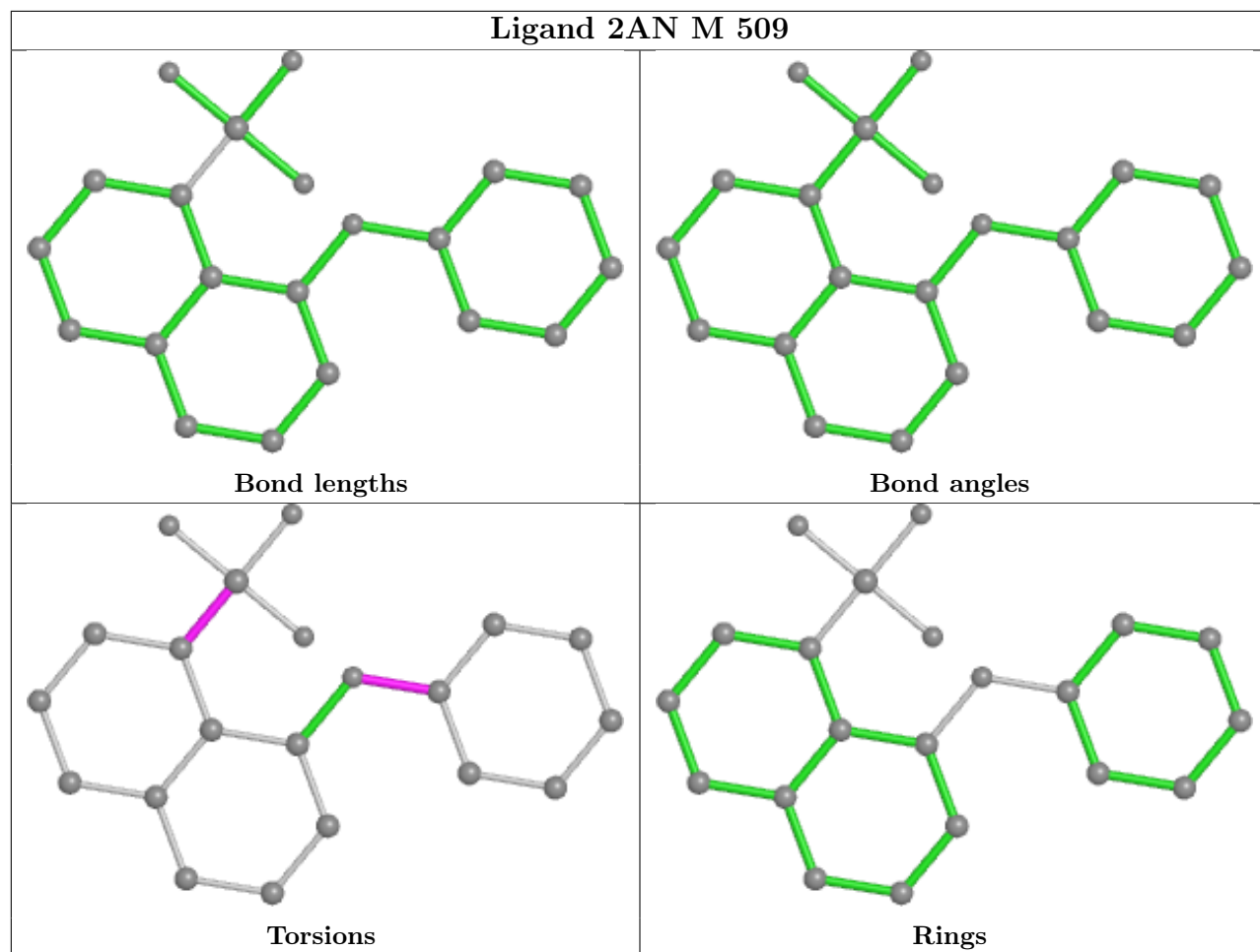
Torsions



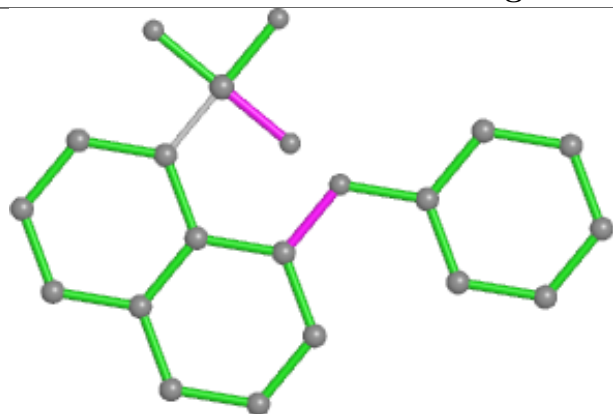
Rings



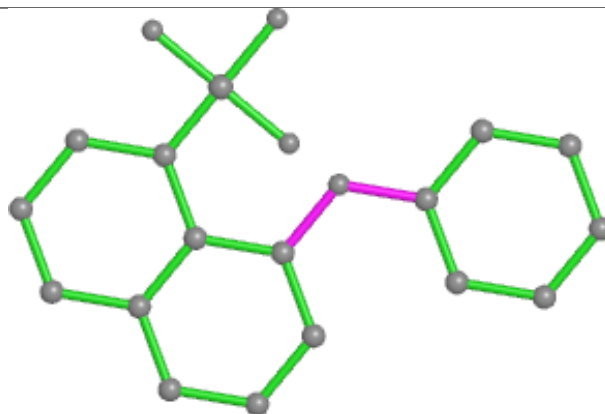




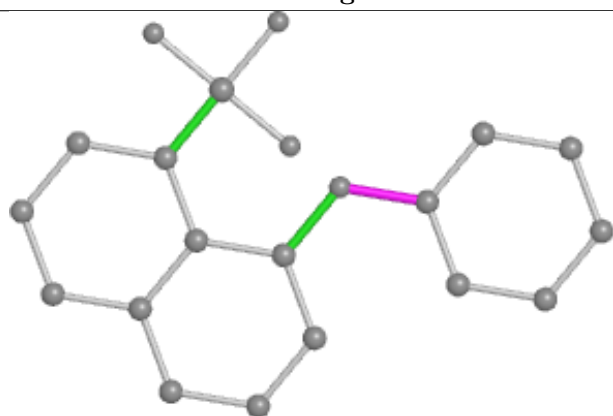
## Ligand 2AN H 1109



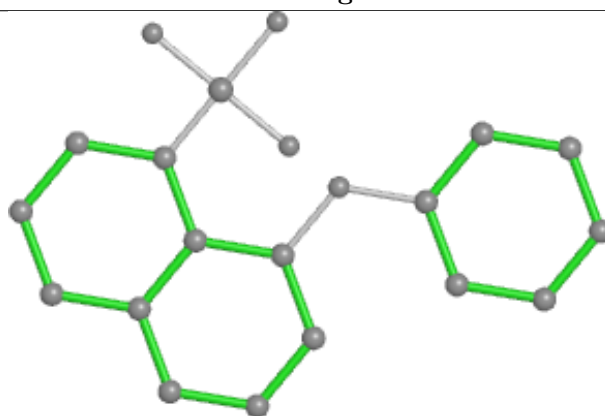
Bond lengths



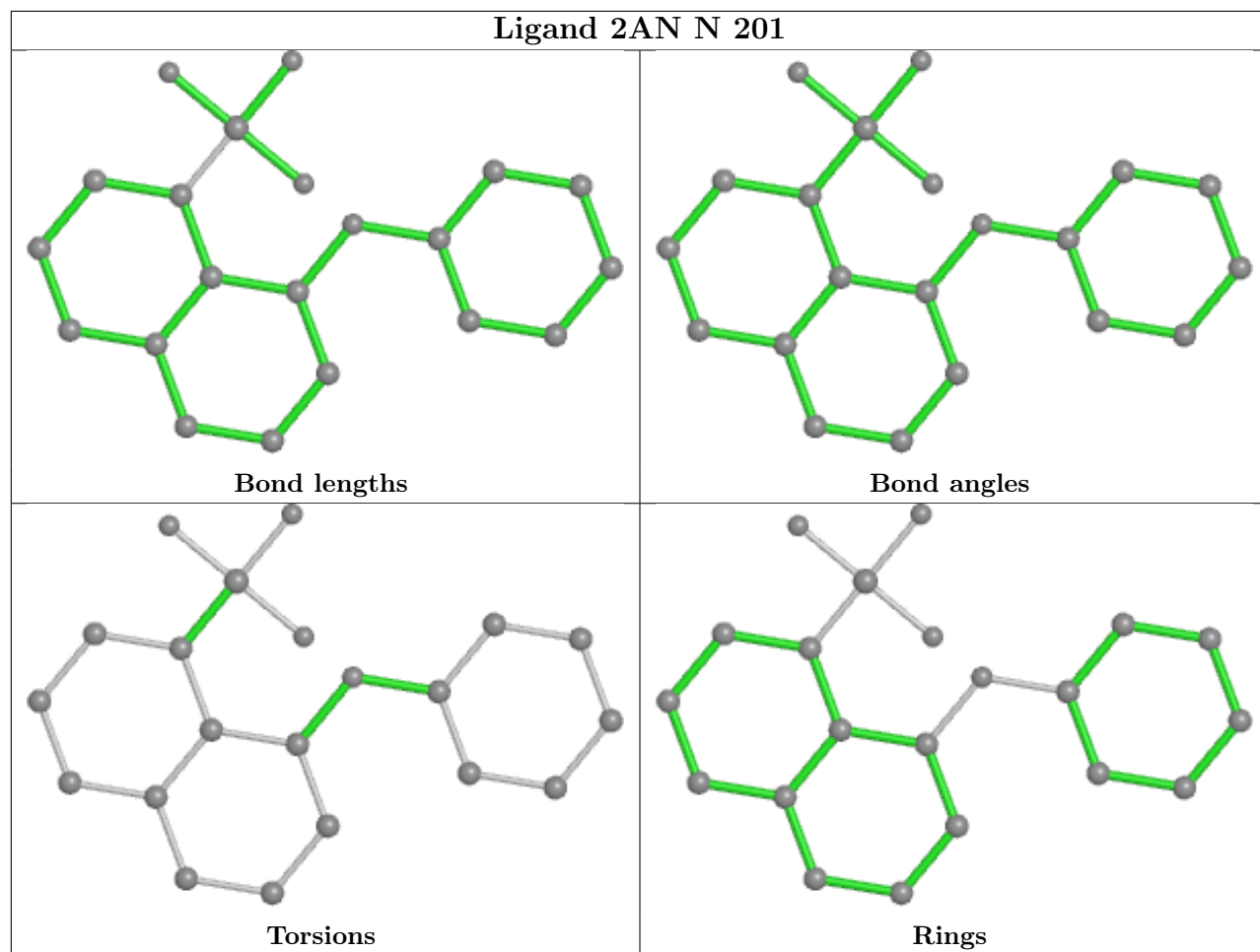
Bond angles

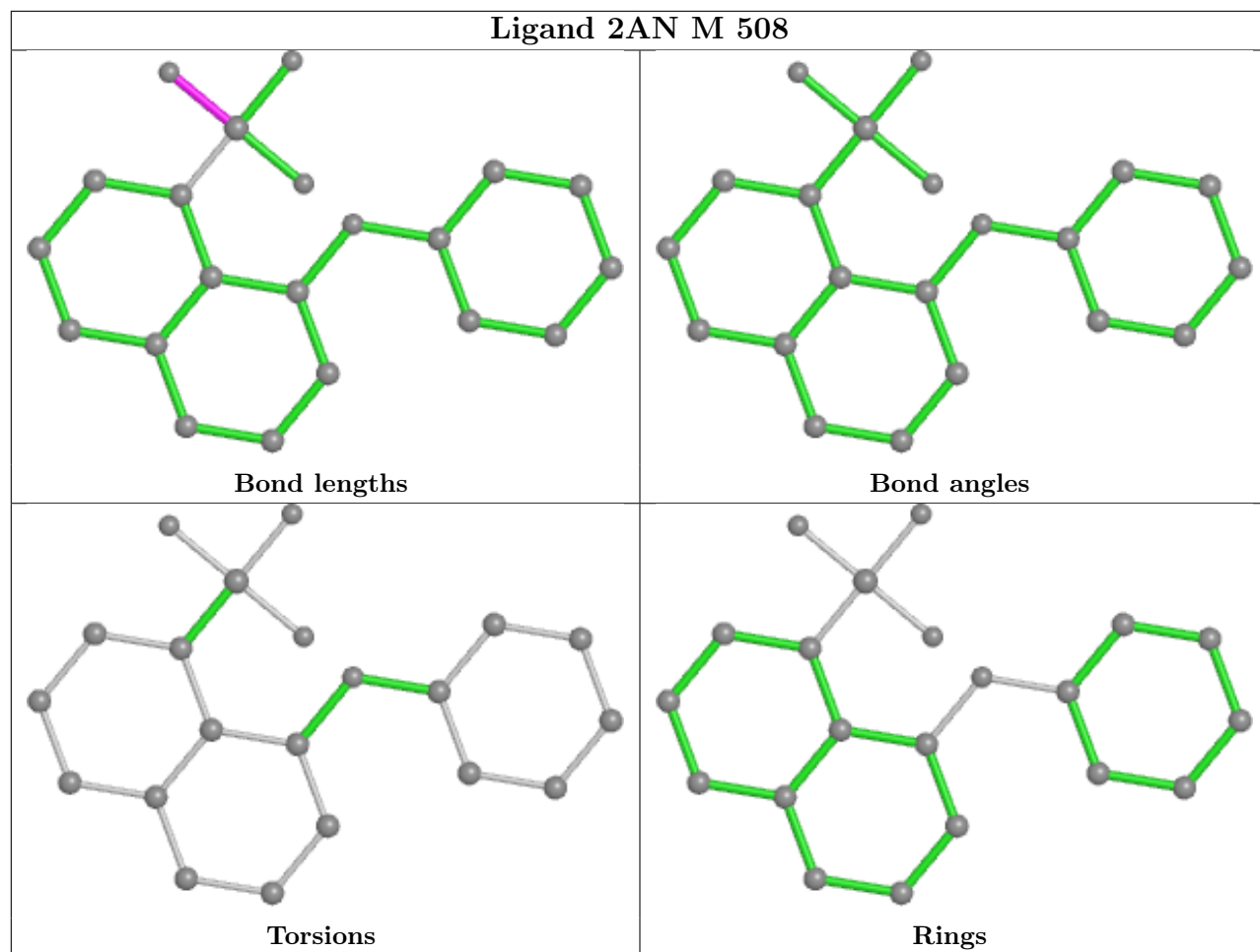


Torsions

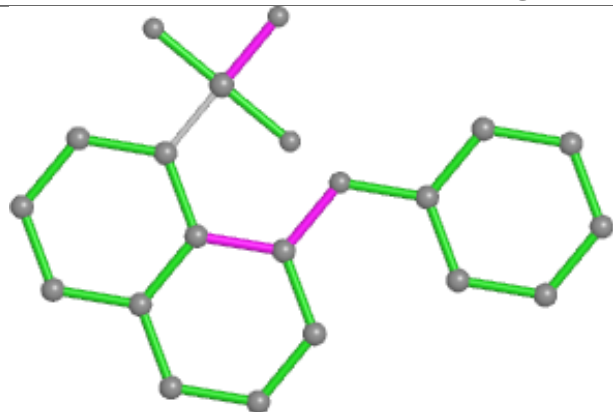


Rings

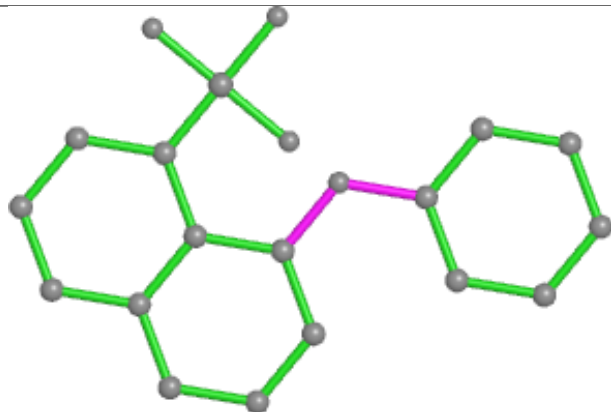




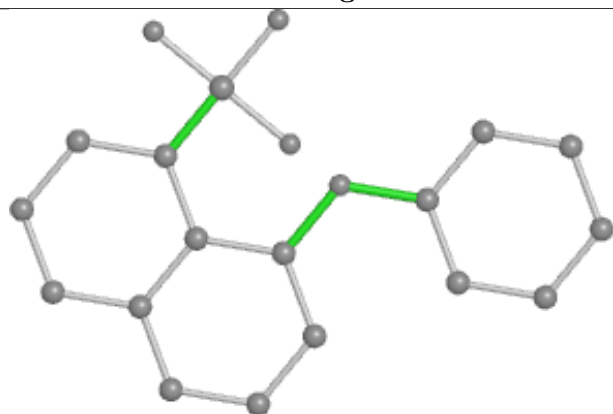
## Ligand 2AN K 206



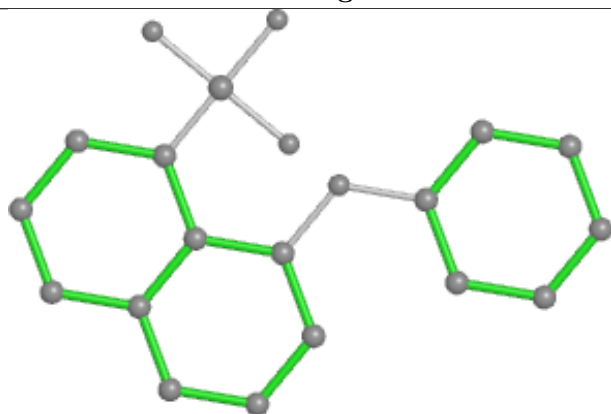
Bond lengths



Bond angles

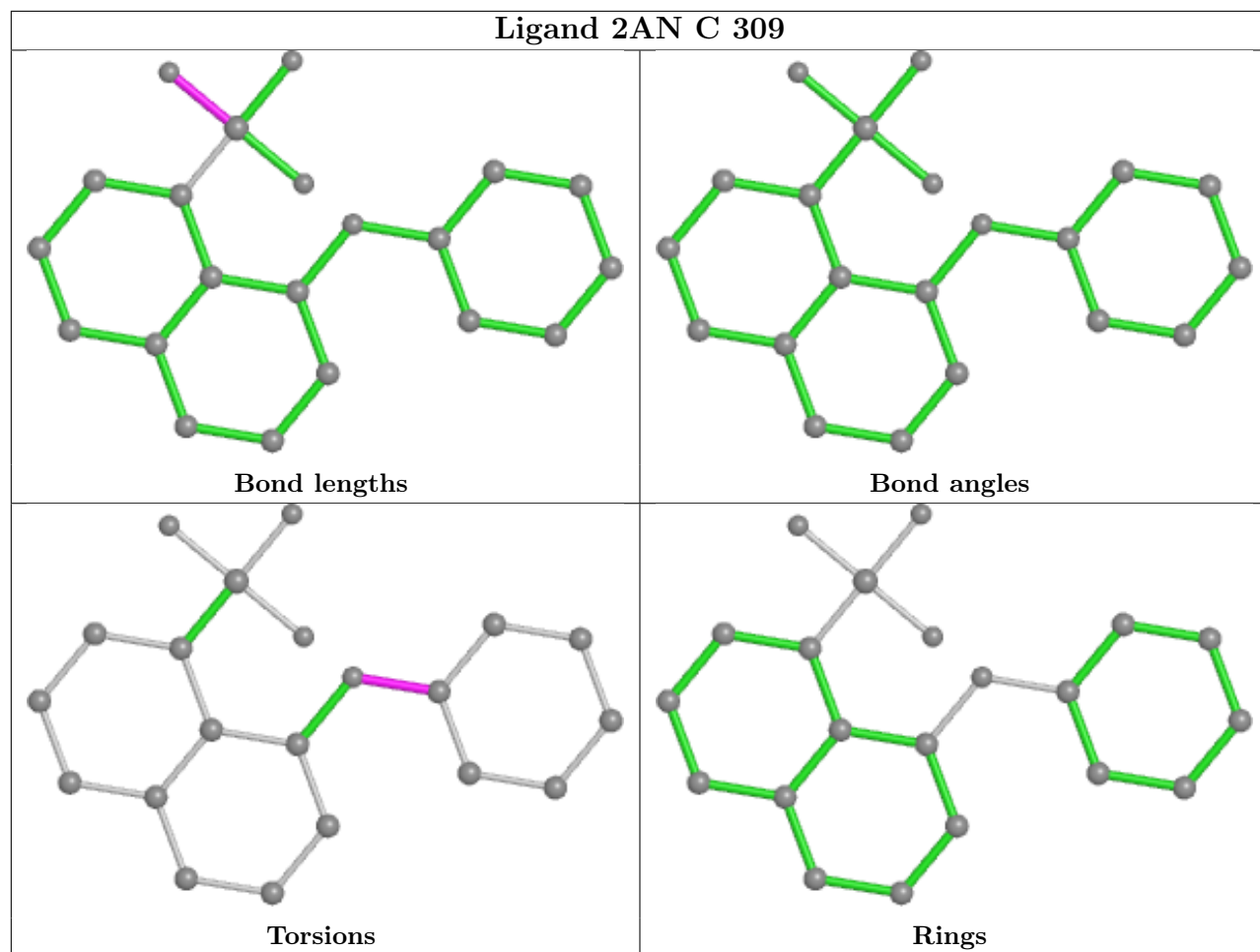


Torsions

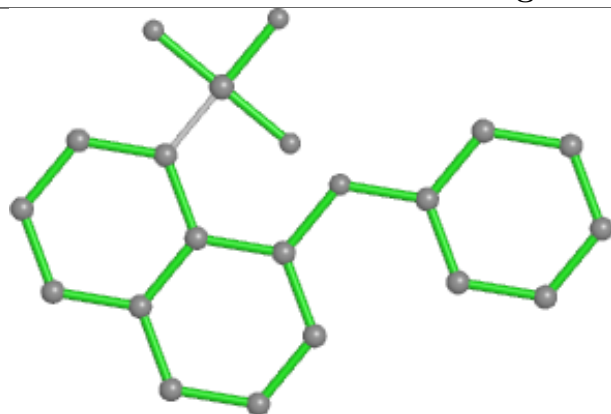


Rings

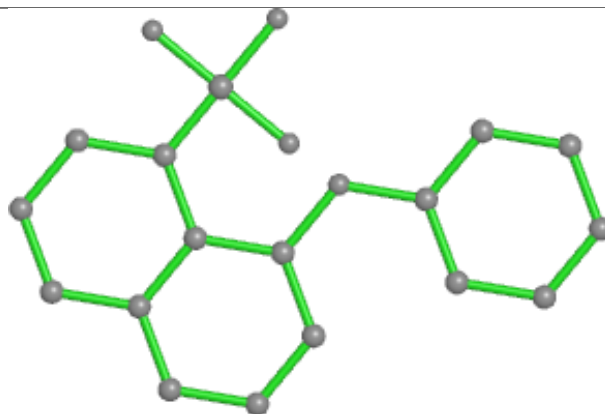
## Ligand 2AN C 309



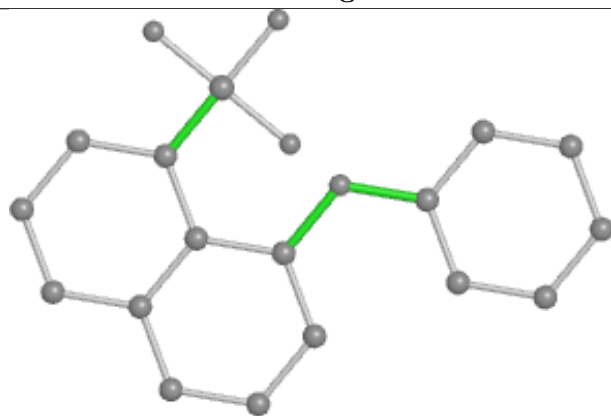
## Ligand 2AN F 201



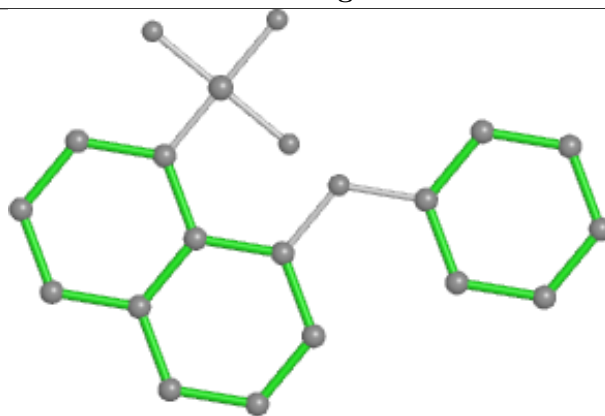
Bond lengths



Bond angles



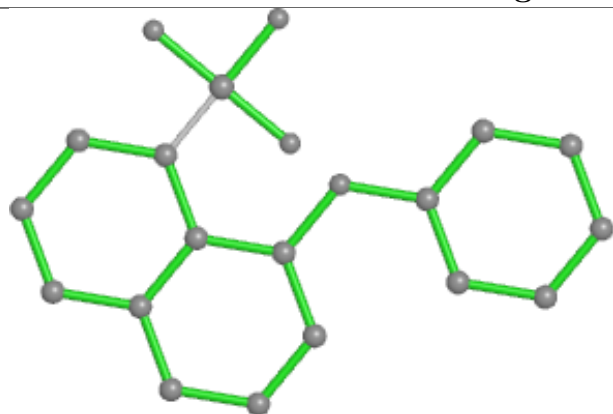
Torsions



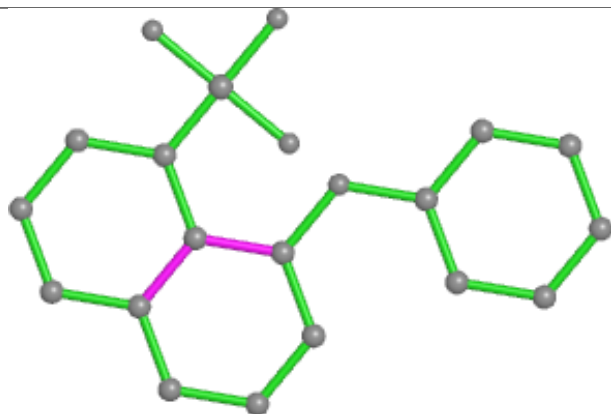
Rings



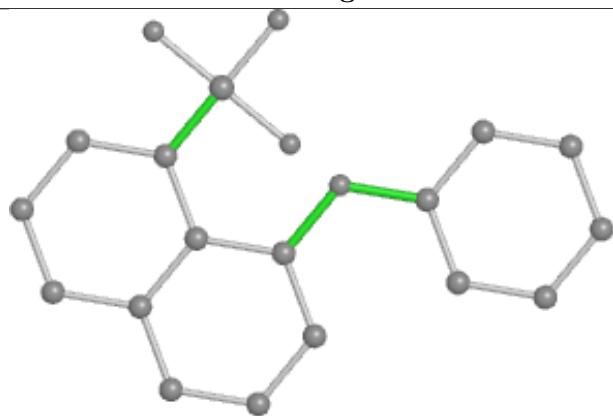
## Ligand 2AN A 205



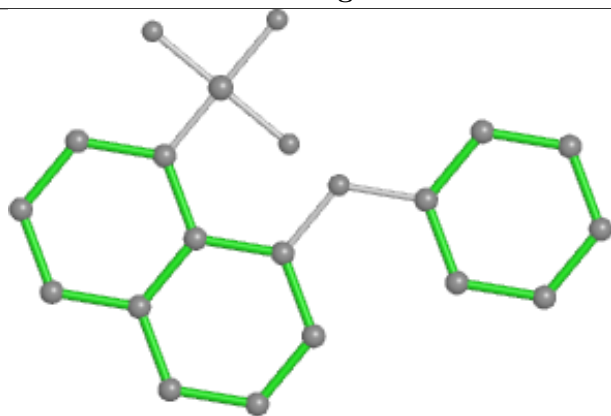
Bond lengths



Bond angles

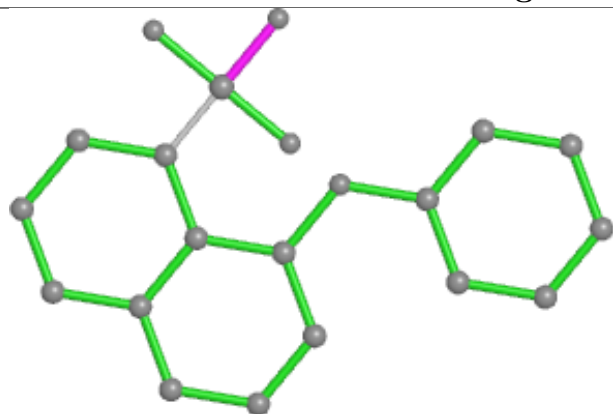


Torsions

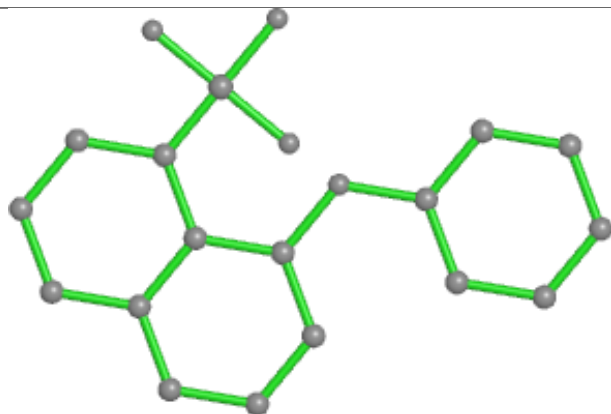


Rings

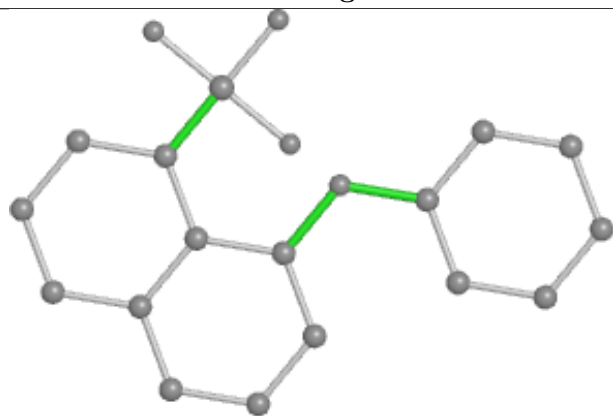
## Ligand 2AN B 204



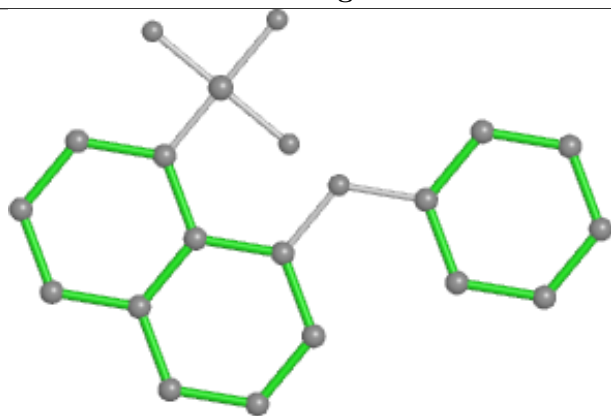
Bond lengths



Bond angles

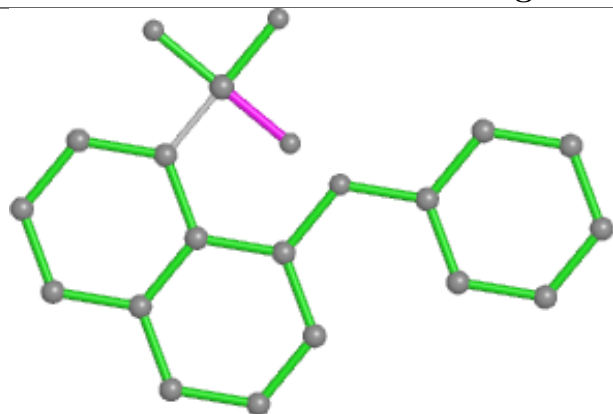


Torsions

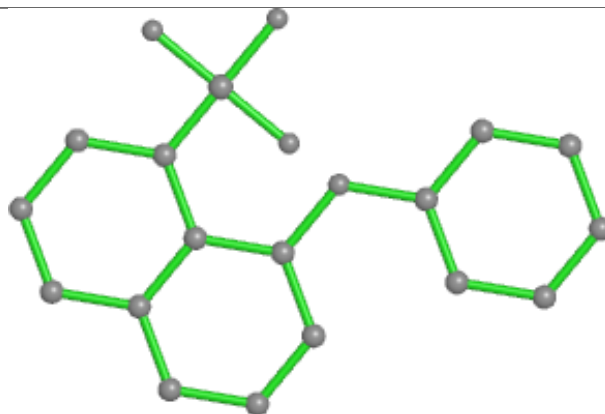


Rings

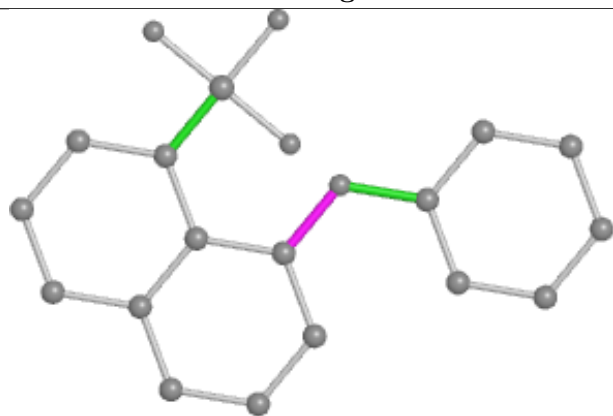
## Ligand 2AN C 305



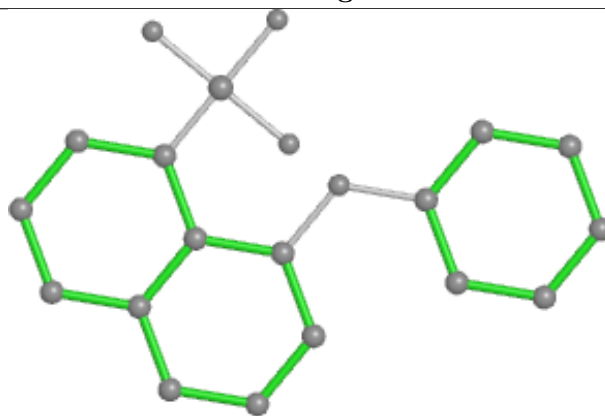
Bond lengths



Bond angles

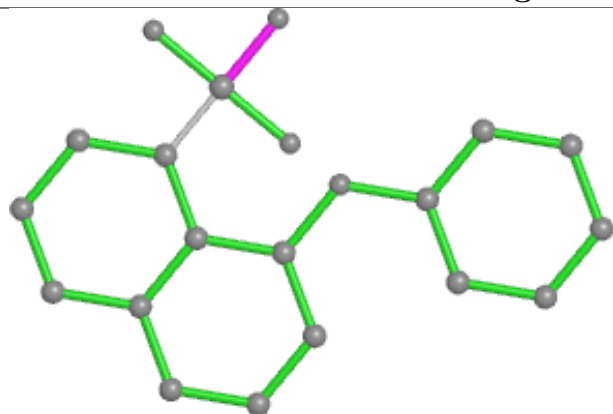


Torsions

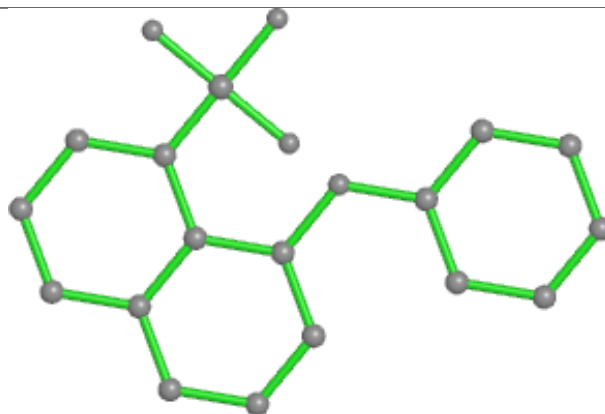


Rings

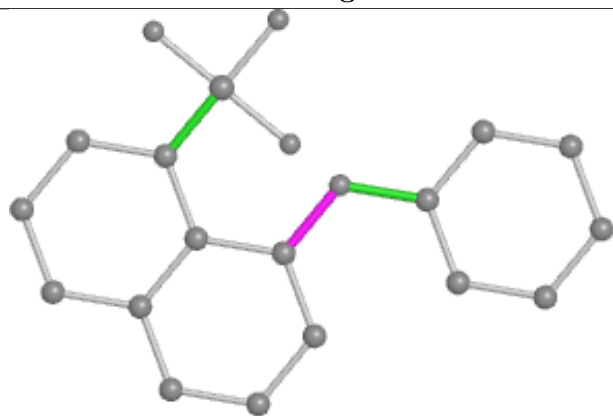
## Ligand 2AN G 301



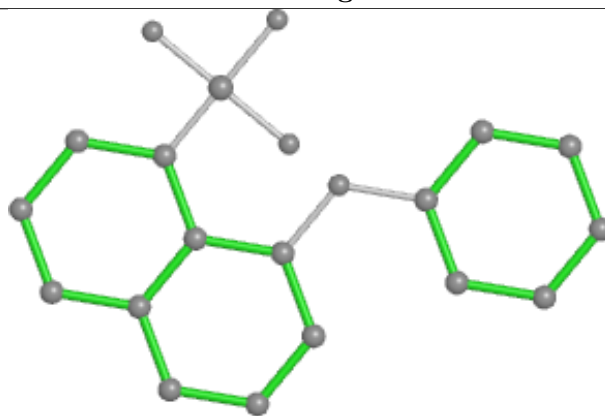
Bond lengths



Bond angles

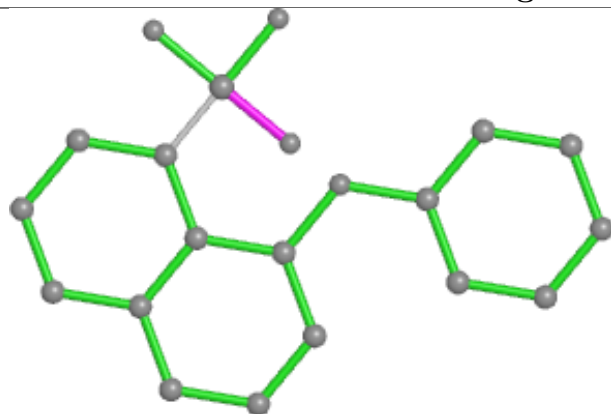


Torsions

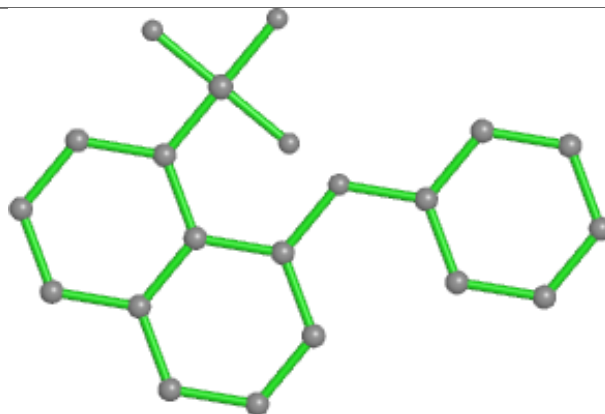


Rings

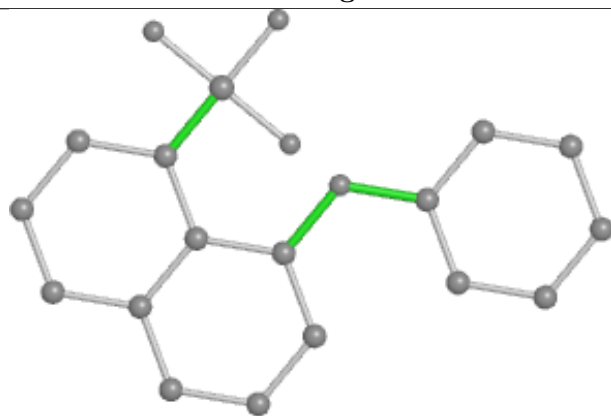
## Ligand 2AN F 203



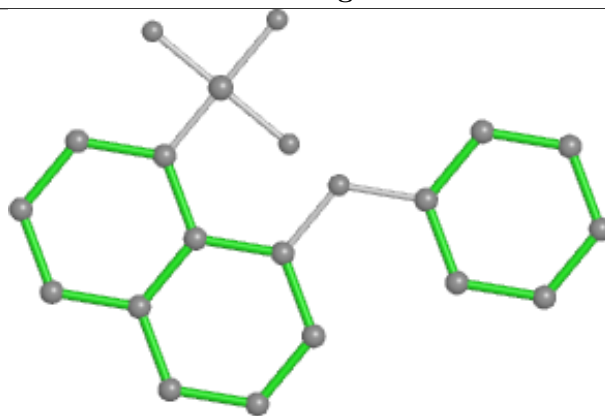
Bond lengths



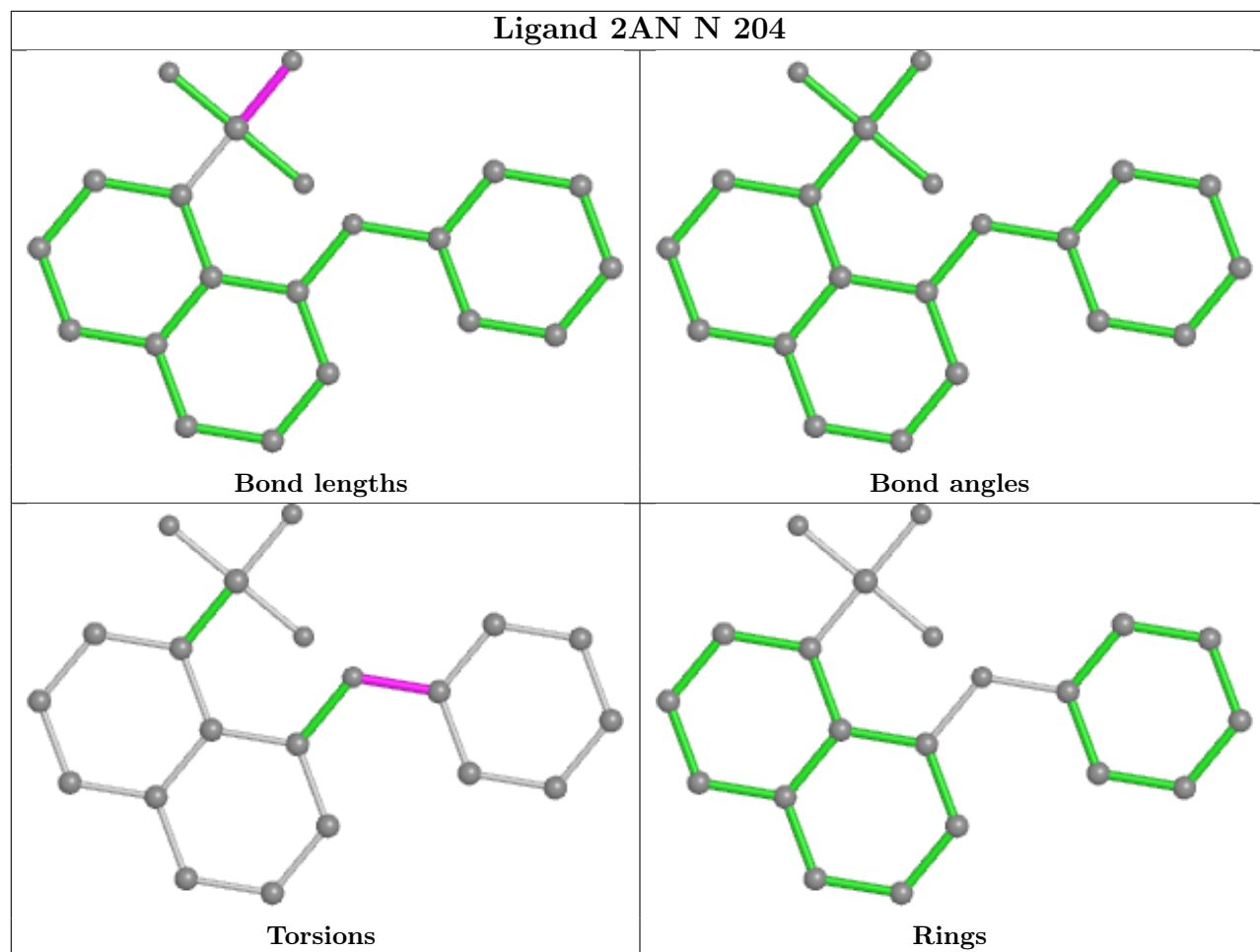
Bond angles



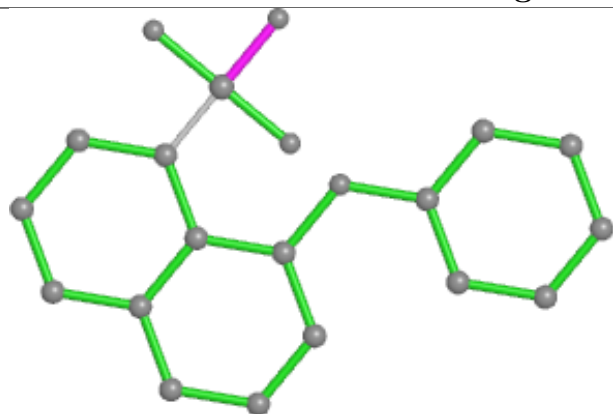
Torsions



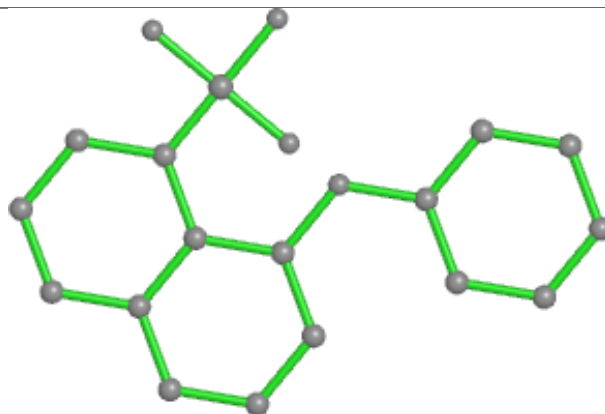
Rings



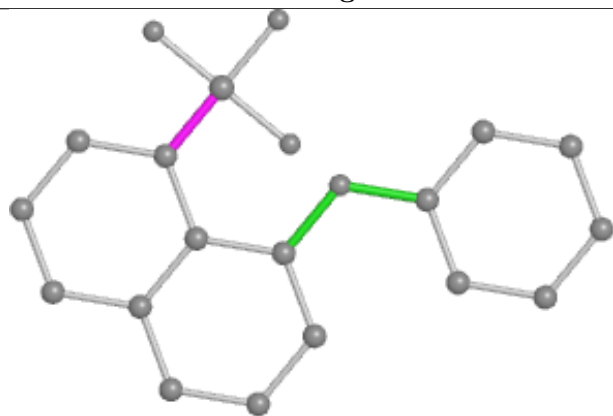
## Ligand 2AN D 706



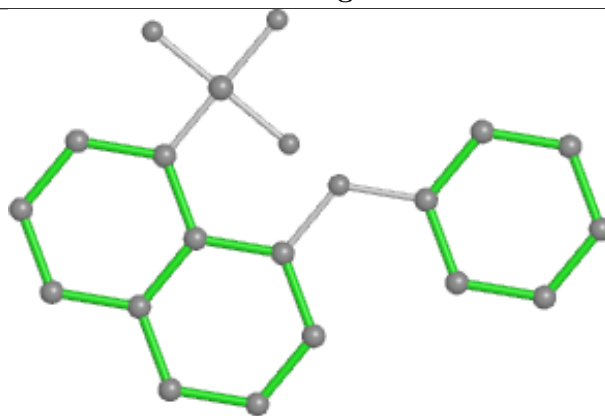
Bond lengths



Bond angles

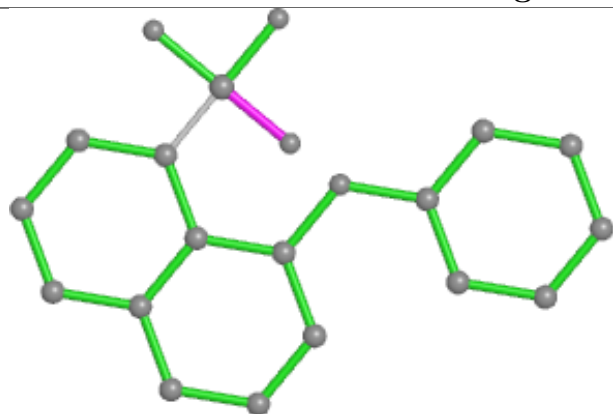


Torsions

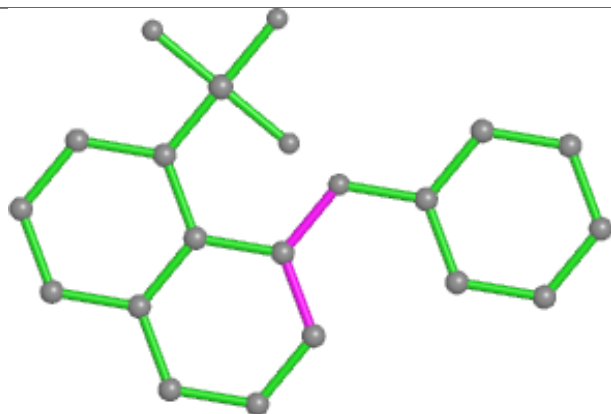


Rings

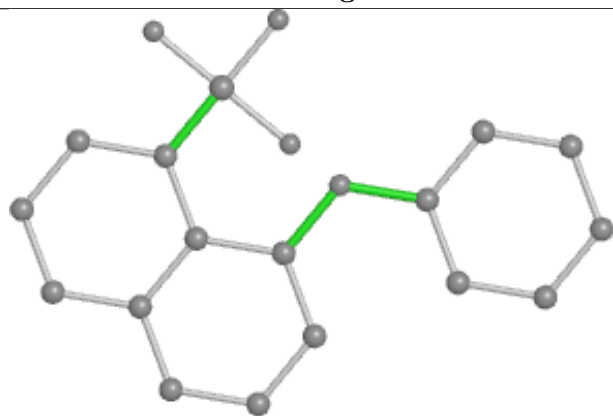
## Ligand 2AN K 203



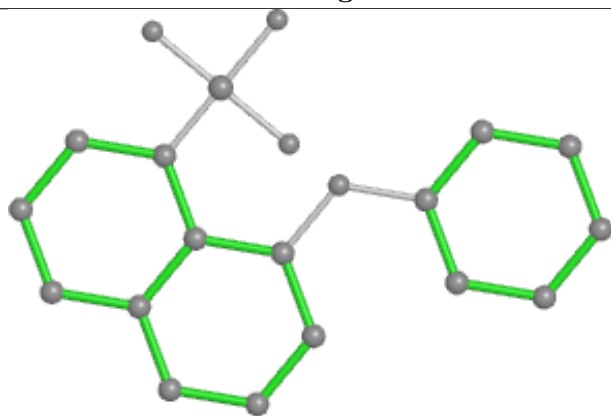
Bond lengths



Bond angles



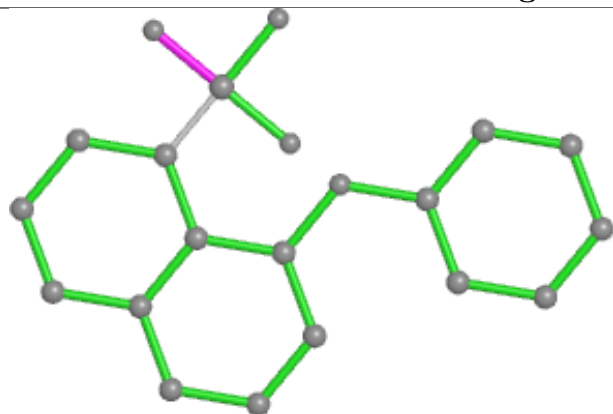
Torsions



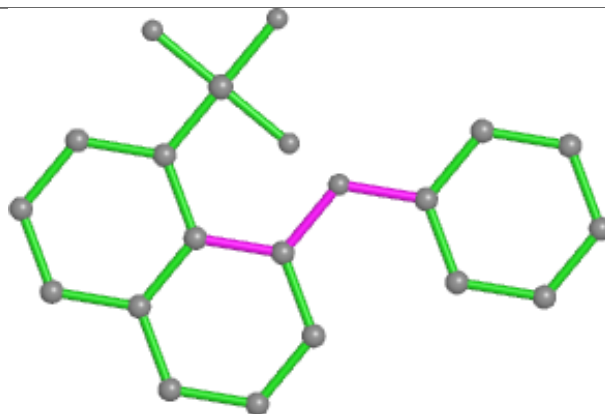
Rings



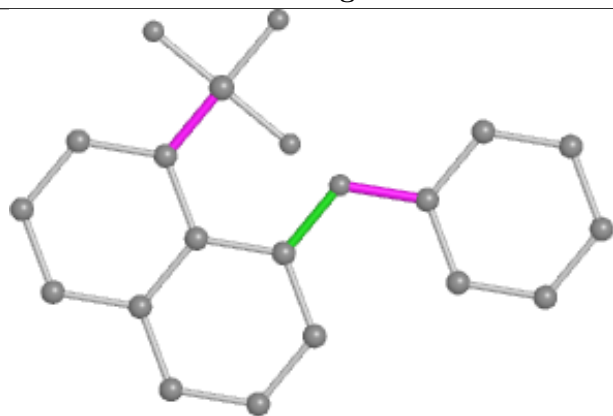
## Ligand 2AN J 206



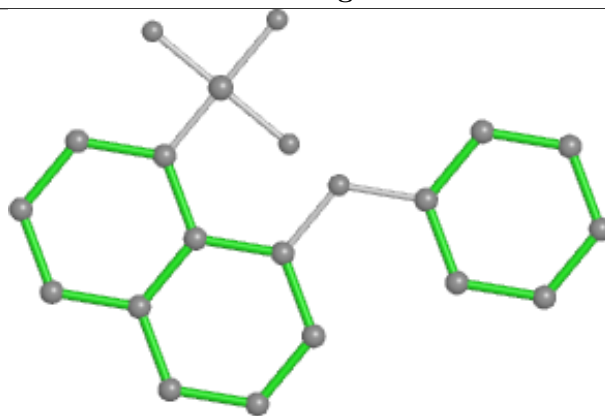
Bond lengths



Bond angles

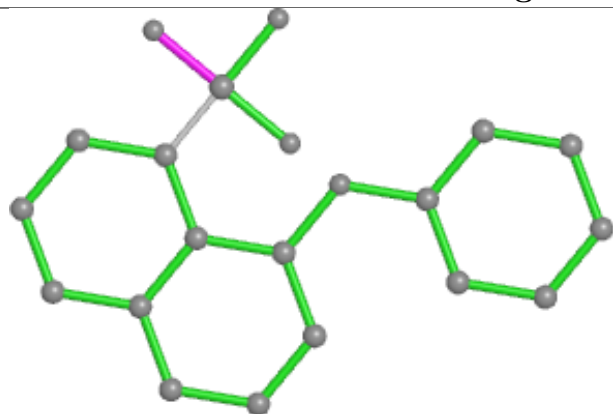


Torsions

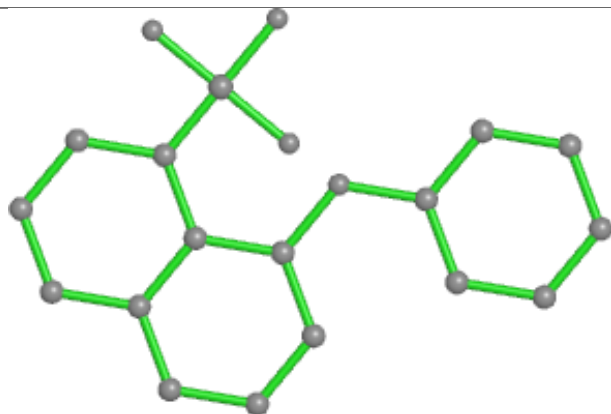


Rings

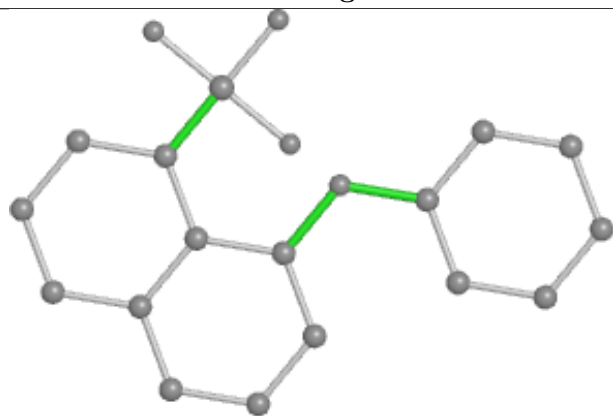
## Ligand 2AN C 307



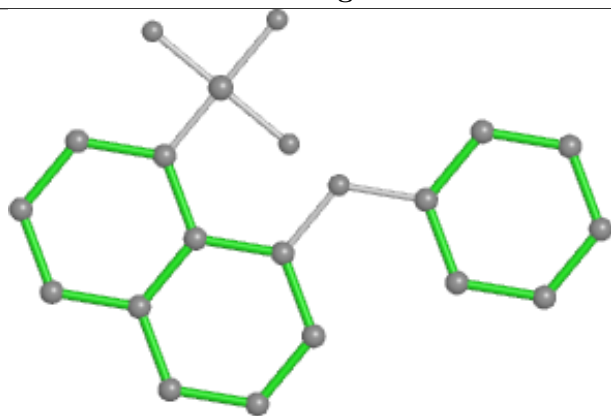
Bond lengths



Bond angles

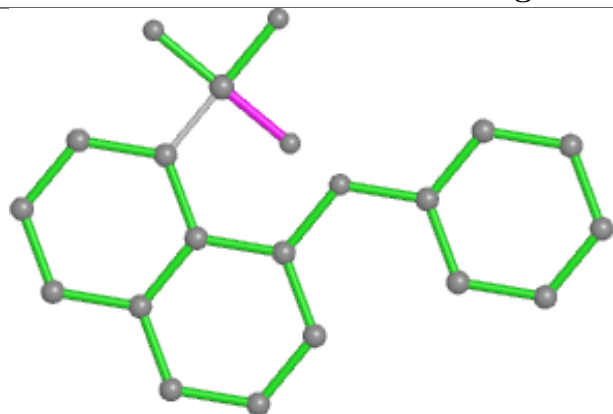


Torsions

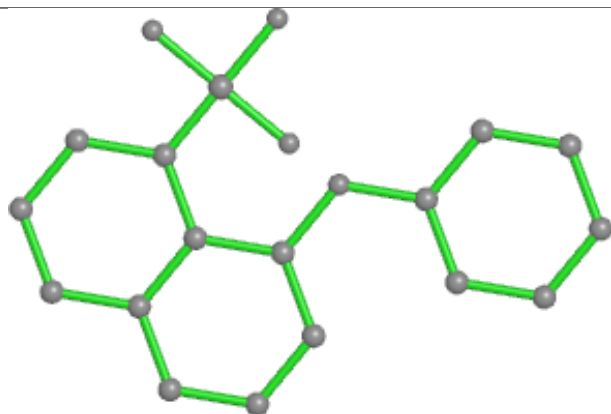


Rings

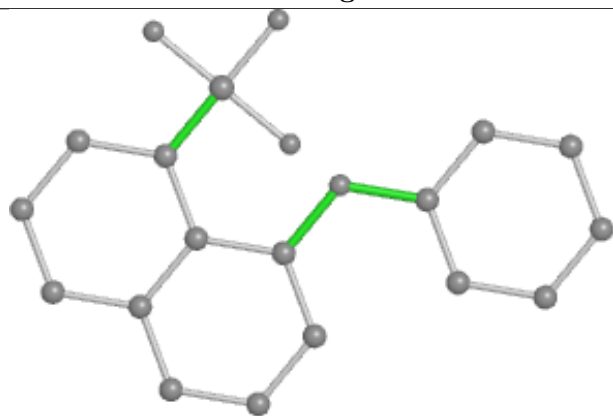
## Ligand 2AN A 201



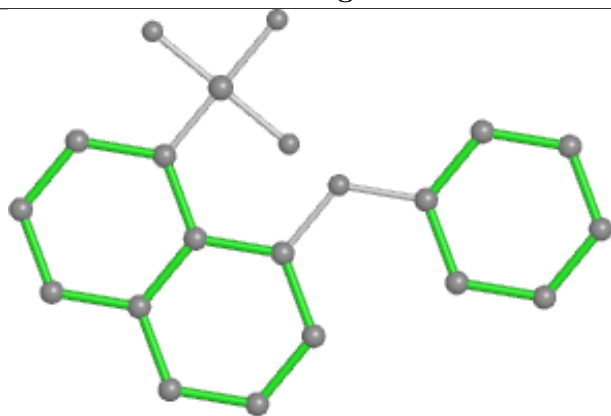
Bond lengths



Bond angles

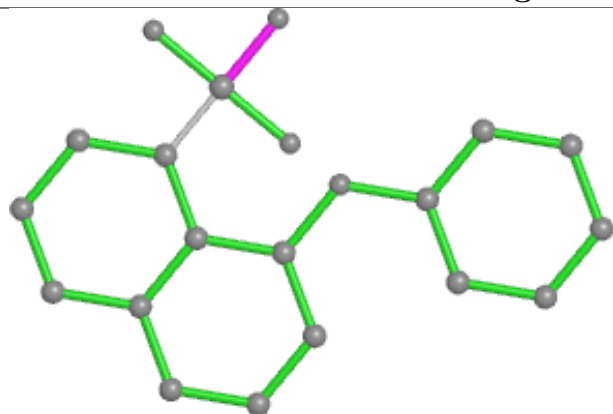


Torsions

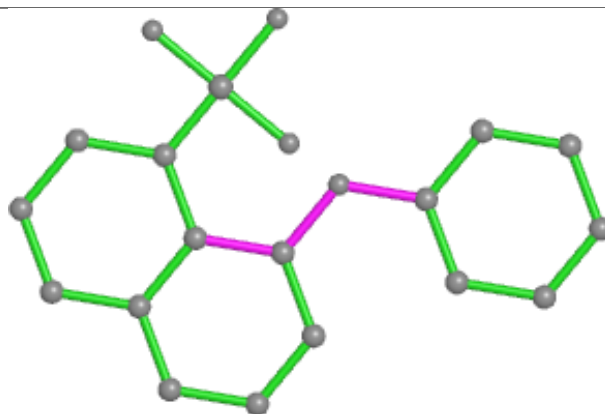


Rings

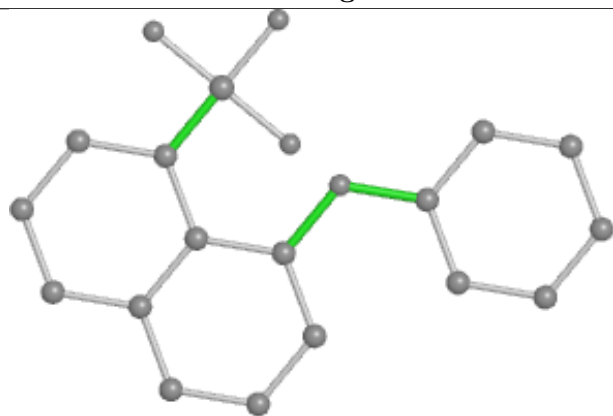
## Ligand 2AN K 202



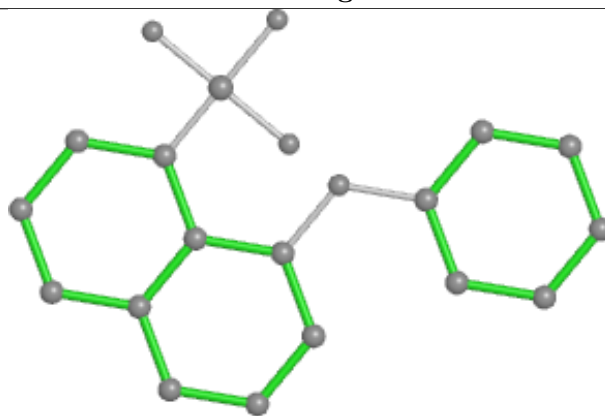
Bond lengths



Bond angles

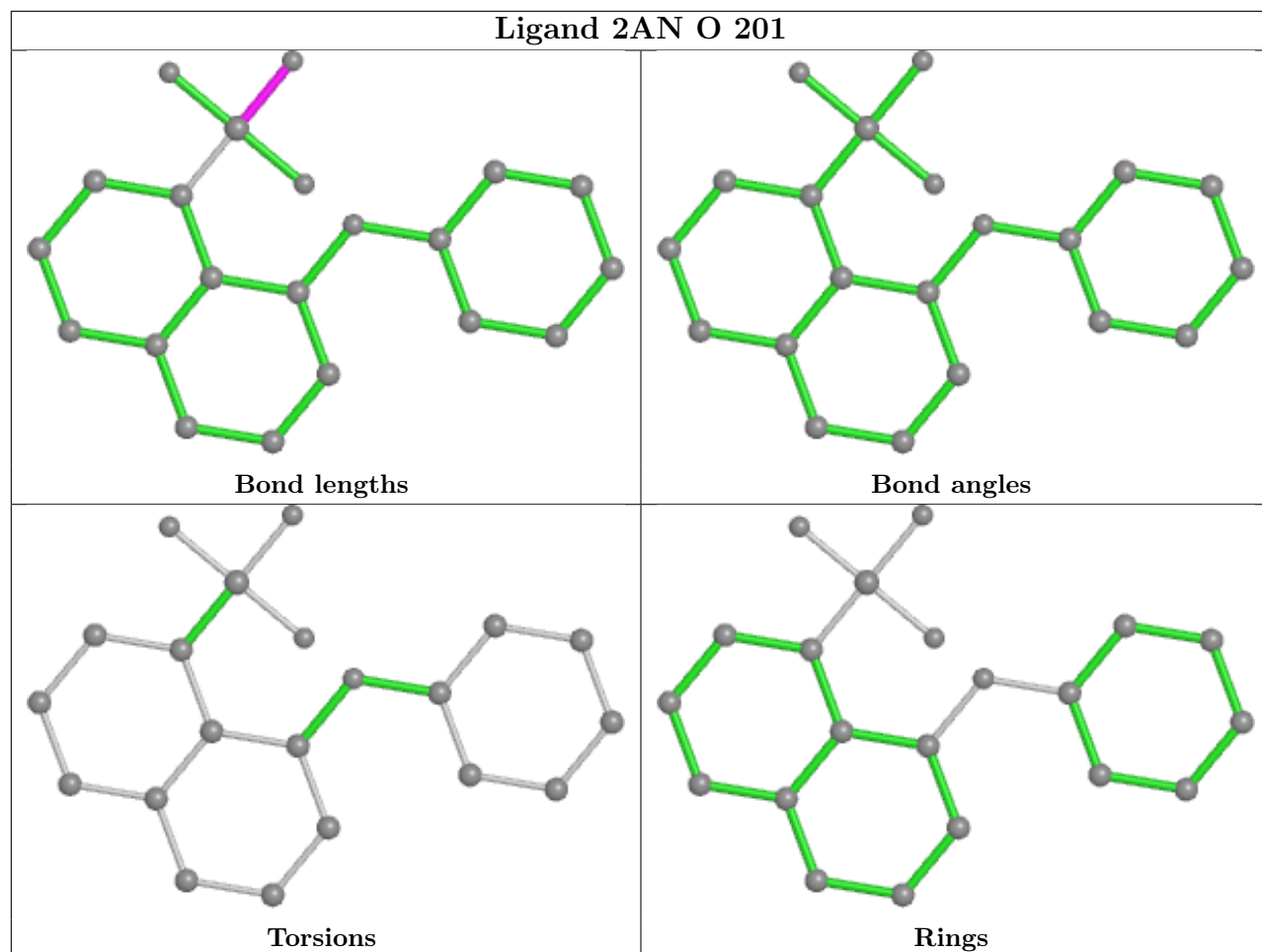


Torsions

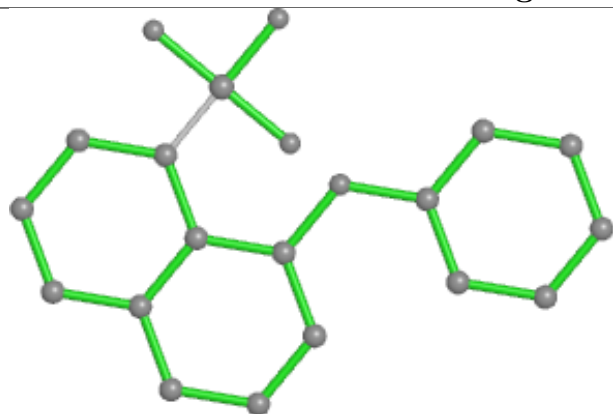


Rings

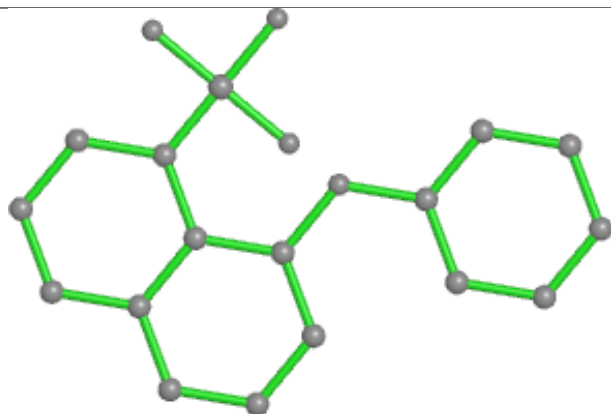
## Ligand 2AN O 201



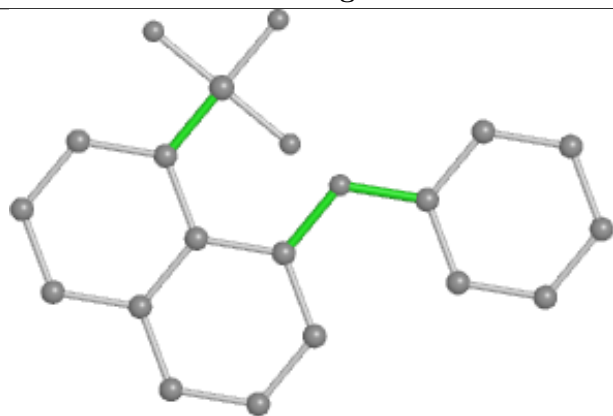
## Ligand 2AN P 502



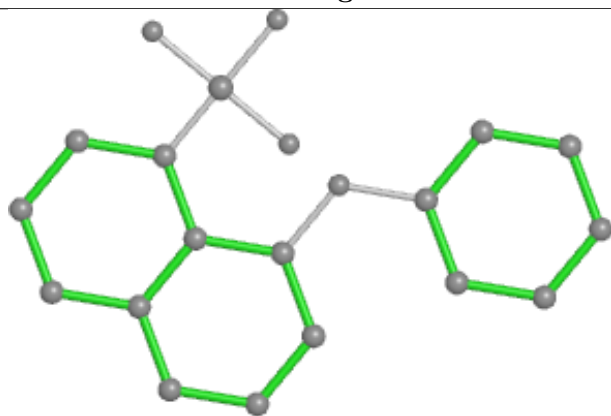
Bond lengths



Bond angles

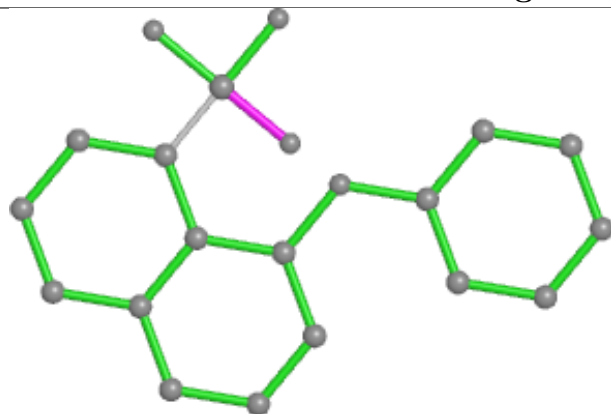


Torsions

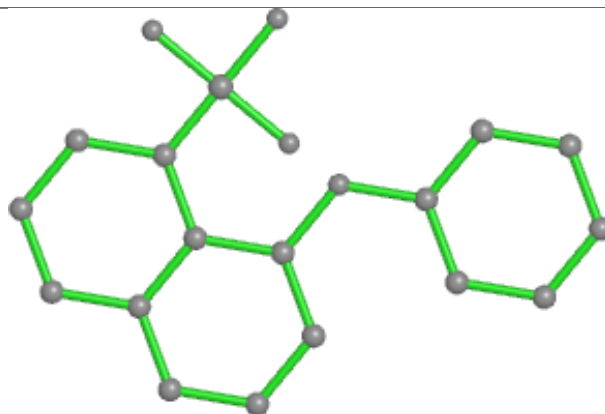


Rings

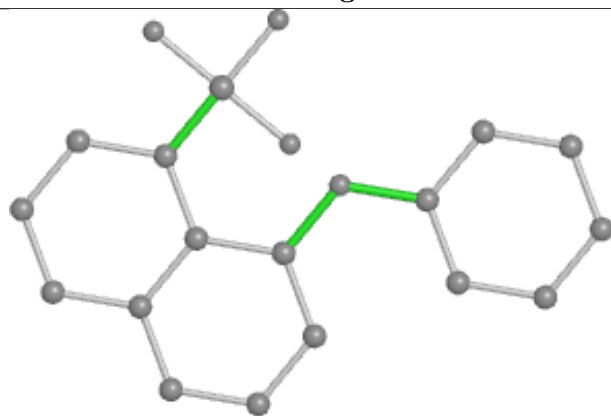
## Ligand 2AN C 304



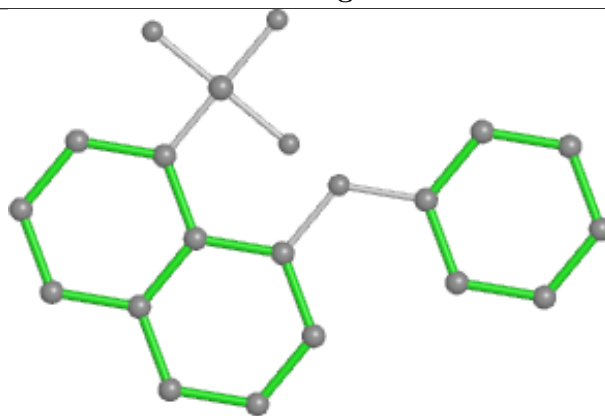
Bond lengths



Bond angles

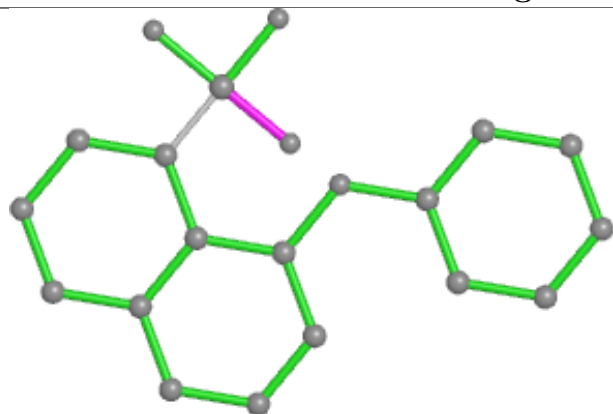


Torsions

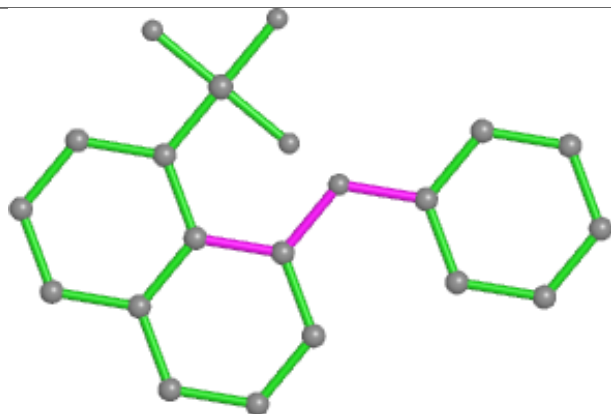


Rings

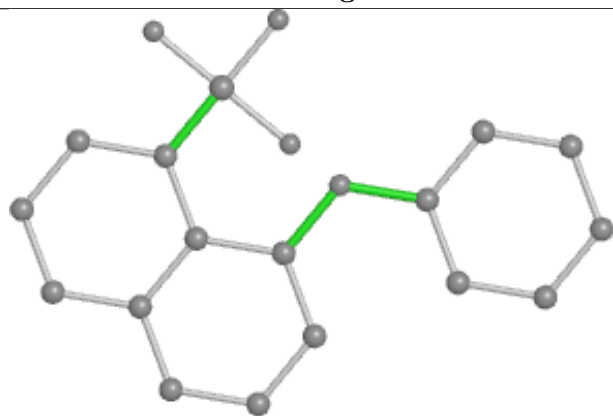
## Ligand 2AN O 203



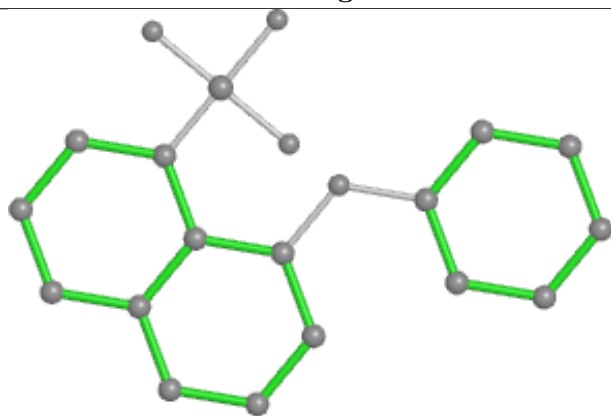
Bond lengths



Bond angles

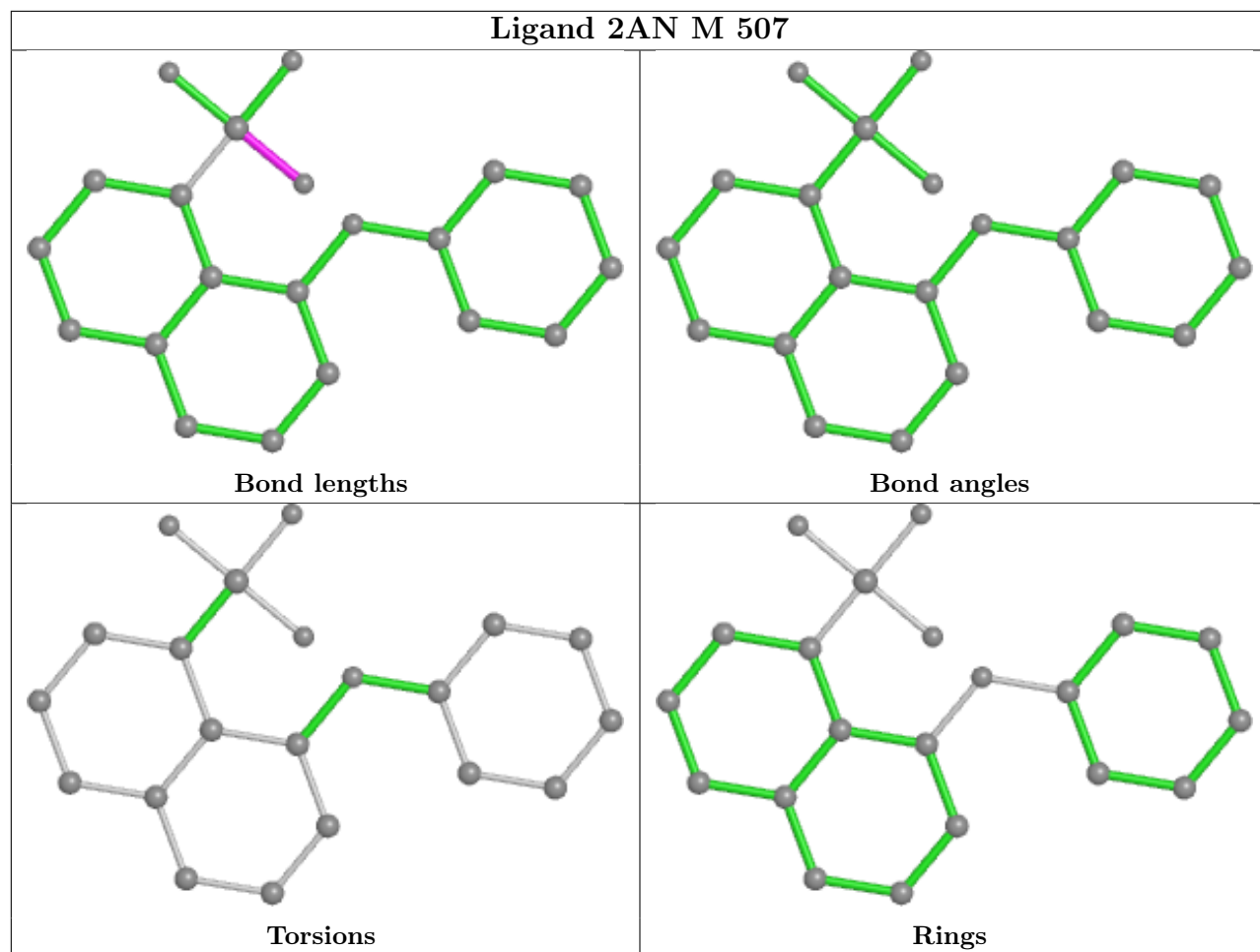


Torsions

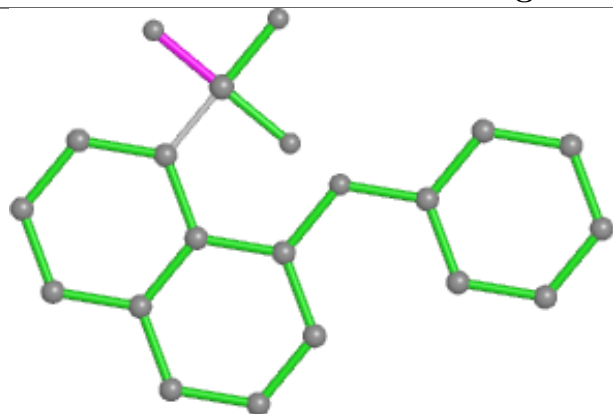


Rings

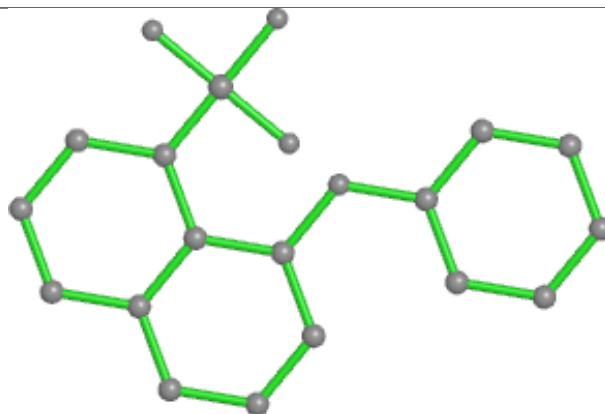




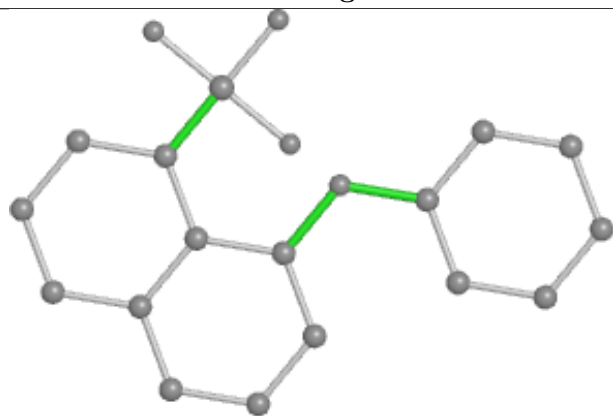
## Ligand 2AN P 506



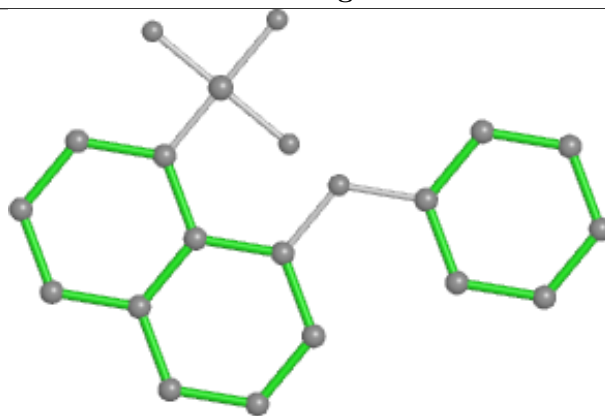
Bond lengths



Bond angles

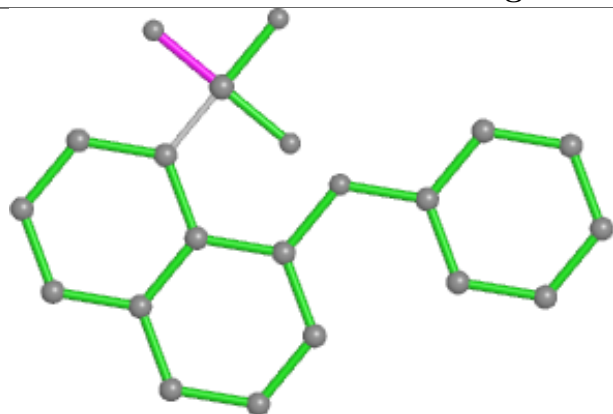


Torsions

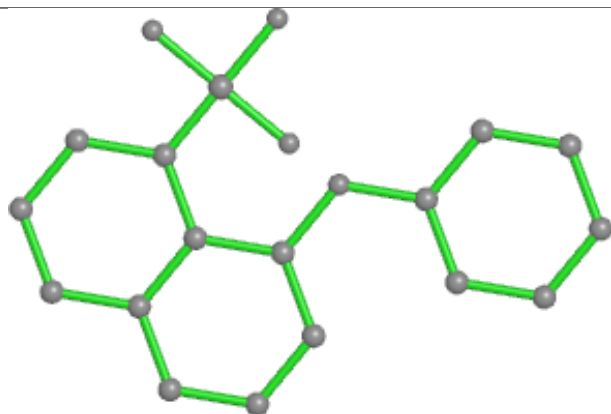


Rings

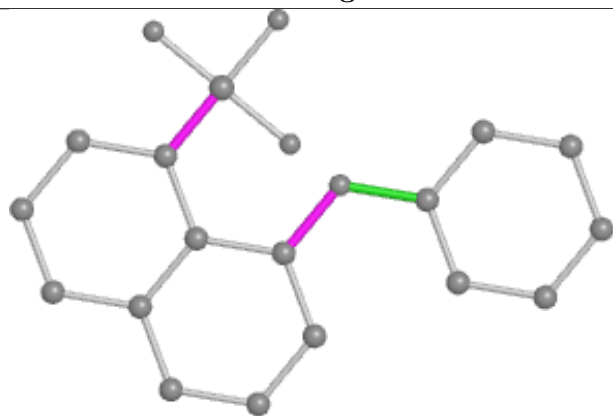
## Ligand 2AN H 1103



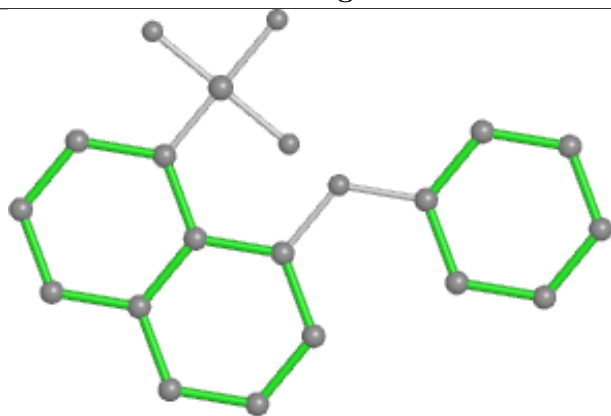
Bond lengths



Bond angles

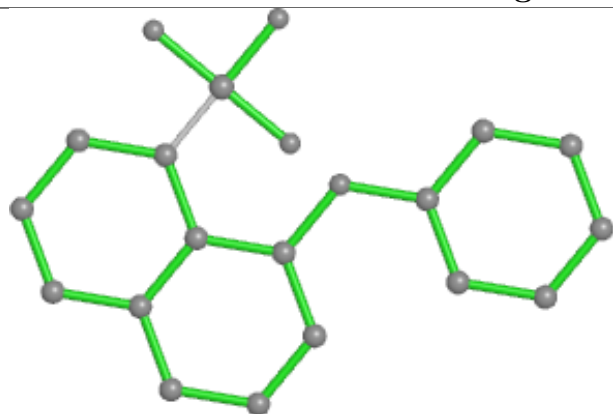


Torsions

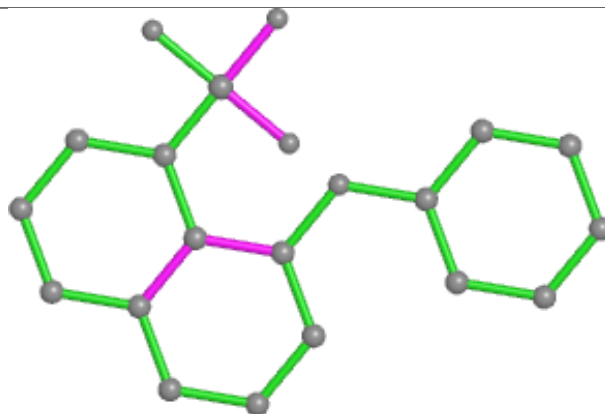


Rings

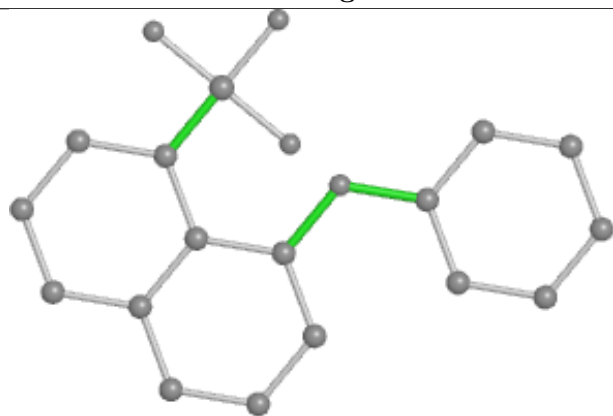
## Ligand 2AN D 703



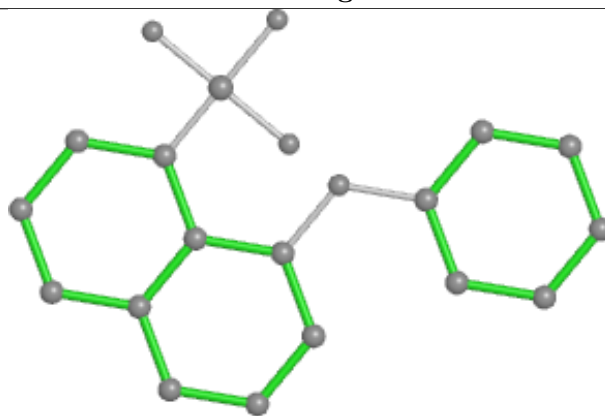
Bond lengths



Bond angles

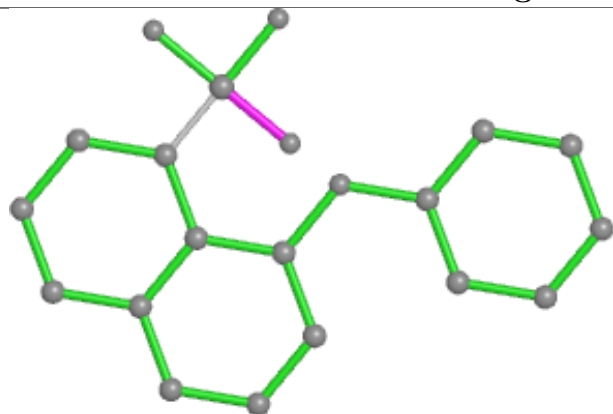


Torsions

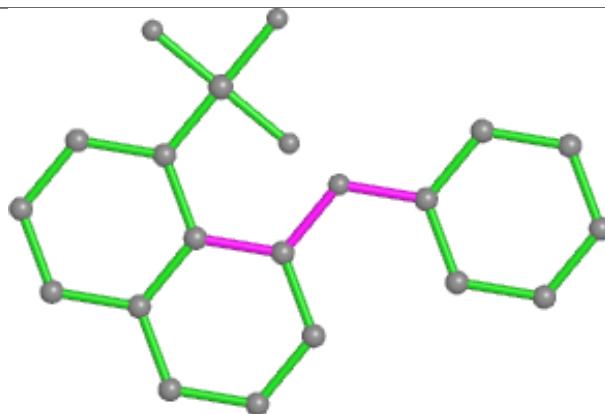


Rings

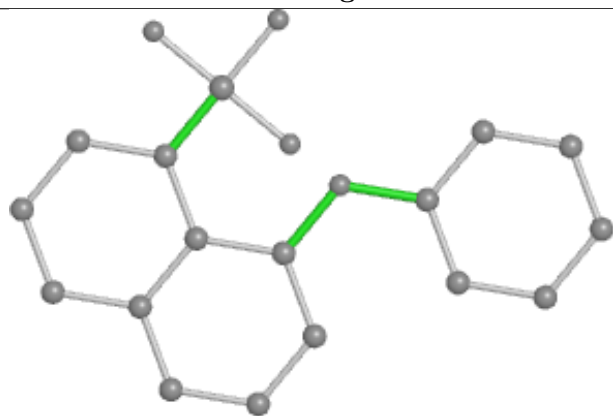
## Ligand 2AN O 204



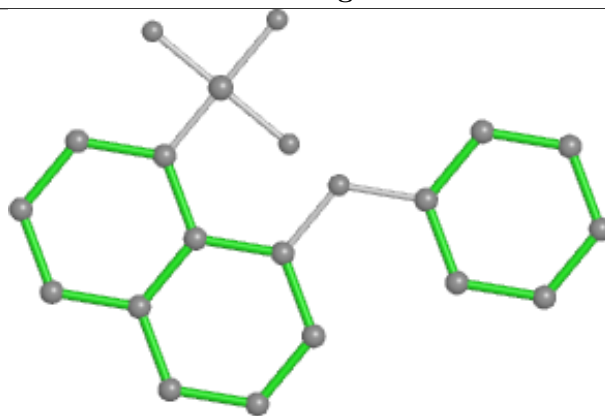
Bond lengths



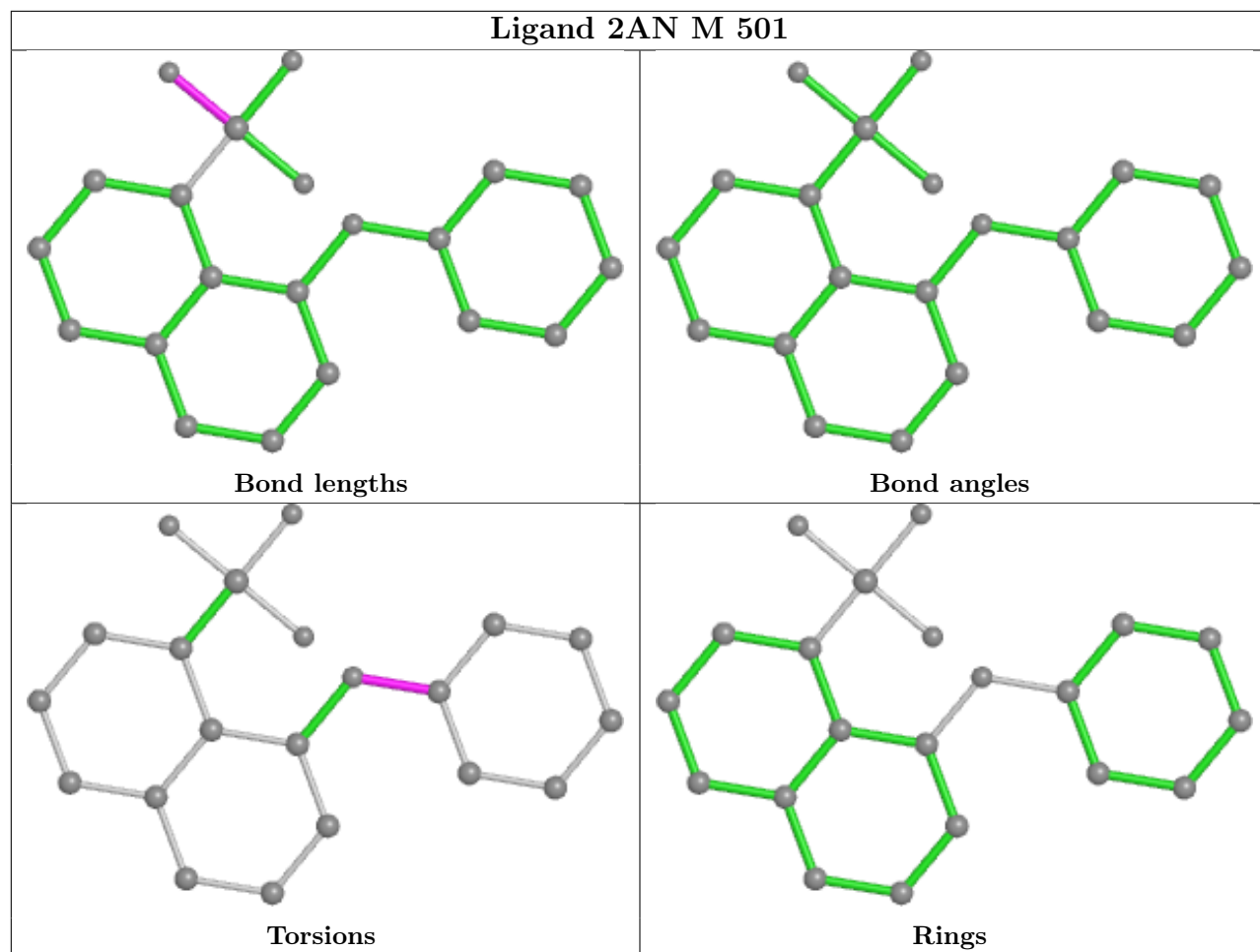
Bond angles



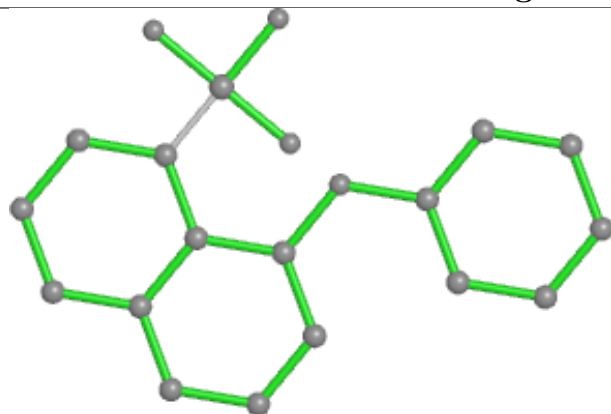
Torsions



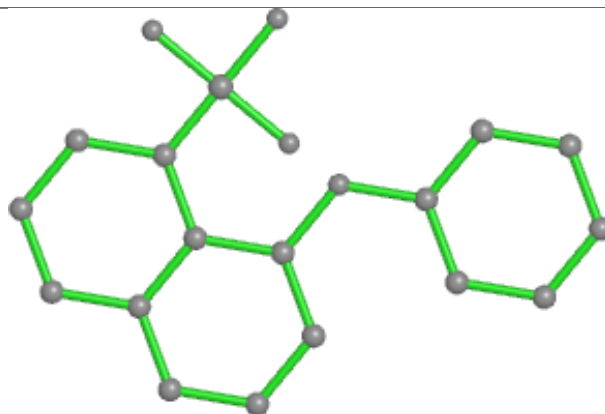
Rings



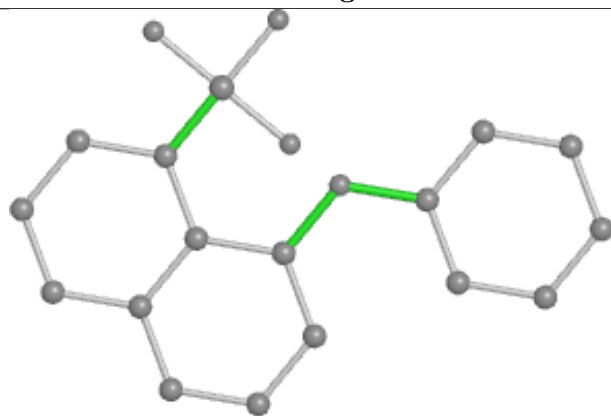
## Ligand 2AN C 302



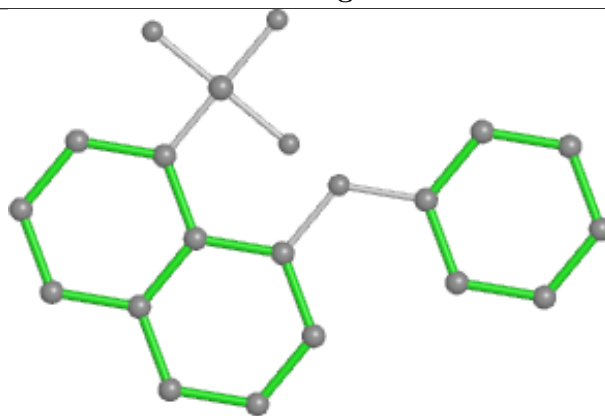
Bond lengths



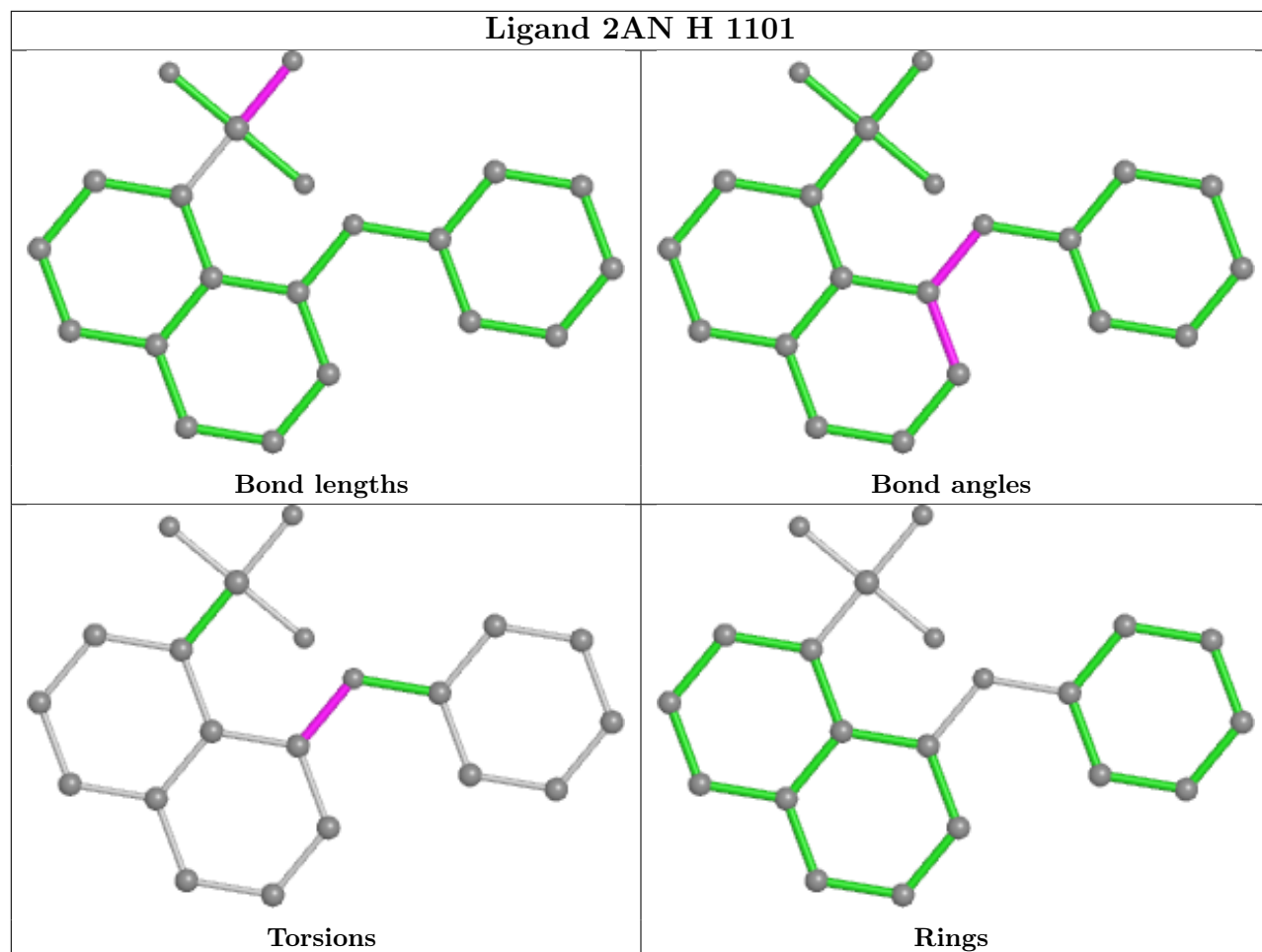
Bond angles



Torsions



Rings



## 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, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	152/153 (99%)	0.14	1 (0%) 87 89	24, 35, 55, 79	0
1	B	152/153 (99%)	0.10	2 (1%) 77 80	22, 33, 49, 68	0
1	C	152/153 (99%)	0.22	1 (0%) 87 89	23, 40, 62, 81	0
1	D	152/153 (99%)	0.26	6 (3%) 39 45	24, 40, 66, 111	0
1	E	152/153 (99%)	0.24	5 (3%) 46 53	22, 38, 62, 99	0
1	F	152/153 (99%)	0.22	5 (3%) 46 53	23, 39, 56, 94	0
1	G	152/153 (99%)	0.19	3 (1%) 65 69	24, 39, 57, 84	0
1	H	152/153 (99%)	0.15	0 100 100	24, 40, 66, 90	0
1	I	152/153 (99%)	0.03	1 (0%) 87 89	22, 34, 56, 83	0
1	J	151/153 (98%)	0.50	14 (9%) 8 11	22, 41, 75, 100	0
1	K	151/153 (98%)	0.24	3 (1%) 65 69	24, 40, 63, 90	0
1	L	152/153 (99%)	0.08	0 100 100	23, 35, 55, 75	0
1	M	152/153 (99%)	0.29	1 (0%) 87 89	22, 39, 66, 89	0
1	N	152/153 (99%)	0.70	15 (9%) 7 9	28, 43, 79, 103	0
1	O	152/153 (99%)	0.27	3 (1%) 65 69	24, 40, 65, 85	0
1	P	152/153 (99%)	0.21	1 (0%) 87 89	24, 41, 62, 110	0
All	All	2430/2448 (99%)	0.24	61 (2%) 57 62	22, 39, 65, 111	0

The worst 5 of 61 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	N	123	GLY	8.1
1	N	2	GLY	6.5
1	N	131	VAL	5.8
1	N	3	VAL	4.7
1	J	2	GLY	4.6

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	2AN	G	306	21/21	0.62	0.42	61,64,70,71	21
2	2AN	D	702	21/21	0.66	0.51	74,80,93,97	0
2	2AN	J	206	21/21	0.67	0.31	41,46,55,57	21
2	2AN	K	206	21/21	0.68	0.25	67,76,106,113	0
2	2AN	K	205	21/21	0.68	0.26	62,69,86,91	0
2	2AN	P	509	21/21	0.69	0.30	73,84,92,96	0
2	2AN	C	308	21/21	0.74	0.26	58,62,73,77	0
2	2AN	F	207	21/21	0.77	0.30	38,40,42,43	21
2	2AN	E	506	21/21	0.77	0.24	49,60,78,82	0
2	2AN	N	203	21/21	0.77	0.22	71,83,97,99	0
2	2AN	E	507	21/21	0.78	0.23	64,72,78,82	0
2	2AN	M	508	21/21	0.79	0.26	45,50,54,57	0
2	2AN	M	509	21/21	0.79	0.22	67,81,91,94	0
2	2AN	H	1109	21/21	0.79	0.23	53,60,66,66	0
2	2AN	C	307	21/21	0.79	0.26	51,56,68,73	0
2	2AN	F	208	21/21	0.80	0.24	53,64,78,85	0
2	2AN	P	503	21/21	0.80	0.19	48,52,68,69	0
2	2AN	J	205	21/21	0.81	0.21	64,69,91,93	0
2	2AN	J	202	21/21	0.83	0.23	50,55,58,64	0
2	2AN	C	306	21/21	0.83	0.17	47,52,78,86	0
2	2AN	M	505	21/21	0.84	0.15	49,55,79,81	0
2	2AN	H	1101	21/21	0.84	0.16	47,50,56,59	0
2	2AN	G	304	21/21	0.85	0.14	41,45,58,60	0
2	2AN	J	204	21/21	0.85	0.18	60,68,72,73	0
2	2AN	P	508	21/21	0.85	0.19	47,54,61,62	0
2	2AN	P	501	21/21	0.86	0.19	42,46,54,60	0
2	2AN	N	204	21/21	0.86	0.26	41,45,48,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	2AN	D	706	21/21	0.86	0.19	51,56,65,65	0
2	2AN	N	202	21/21	0.86	0.20	44,48,54,57	0
2	2AN	F	206	21/21	0.86	0.16	50,55,66,69	0
2	2AN	O	203	21/21	0.86	0.14	41,46,54,58	0
2	2AN	F	204	21/21	0.86	0.16	40,45,57,61	0
2	2AN	D	705	21/21	0.87	0.18	53,56,62,64	0
3	SO4	H	1110	5/5	0.87	0.39	80,84,85,88	0
2	2AN	D	701	21/21	0.87	0.18	44,51,58,60	0
2	2AN	K	202	21/21	0.88	0.13	40,42,48,50	0
2	2AN	M	503	21/21	0.88	0.16	44,47,52,57	0
2	2AN	P	506	21/21	0.88	0.20	46,50,59,61	0
2	2AN	H	1107	21/21	0.88	0.17	43,50,53,54	0
2	2AN	D	704	21/21	0.88	0.18	46,53,56,59	0
2	2AN	A	202	21/21	0.89	0.14	37,40,52,56	0
2	2AN	H	1105	21/21	0.89	0.15	38,44,57,68	0
2	2AN	B	203	21/21	0.89	0.15	44,49,56,61	0
2	2AN	L	204	21/21	0.89	0.14	37,44,53,55	0
2	2AN	C	303	21/21	0.89	0.17	39,42,47,50	0
2	2AN	F	202	21/21	0.89	0.16	44,49,55,58	0
2	2AN	E	504	21/21	0.90	0.14	36,42,47,51	0
2	2AN	J	203	21/21	0.90	0.15	43,45,52,54	0
2	2AN	B	204	21/21	0.90	0.15	44,48,52,53	0
2	2AN	H	1104	21/21	0.90	0.16	38,41,46,48	0
2	2AN	A	203	21/21	0.90	0.15	37,42,53,56	0
2	2AN	I	205	21/21	0.90	0.14	40,43,46,52	0
2	2AN	L	202	21/21	0.91	0.15	38,41,44,45	0
2	2AN	I	202	21/21	0.91	0.14	41,44,49,52	0
2	2AN	B	201	21/21	0.91	0.14	35,41,42,44	0
2	2AN	M	502	21/21	0.91	0.17	38,40,43,44	0
2	2AN	E	502	21/21	0.91	0.15	43,47,53,55	0
2	2AN	L	203	21/21	0.92	0.12	38,41,46,47	0
2	2AN	M	506	21/21	0.92	0.16	40,43,55,59	0
2	2AN	F	203	21/21	0.92	0.16	43,47,51,54	0
2	2AN	G	305	21/21	0.92	0.17	40,42,50,53	0
2	2AN	N	201	21/21	0.92	0.16	38,42,49,53	0
2	2AN	K	204	21/21	0.92	0.12	36,41,50,54	0
2	2AN	H	1108	21/21	0.93	0.15	41,45,59,64	0
2	2AN	C	305	21/21	0.93	0.12	43,48,54,59	0
2	2AN	P	505	21/21	0.93	0.12	33,36,39,40	0
2	2AN	C	301	21/21	0.93	0.18	38,39,42,45	0
2	2AN	P	507	21/21	0.93	0.15	42,45,59,62	0
2	2AN	O	204	21/21	0.93	0.15	44,48,56,57	0

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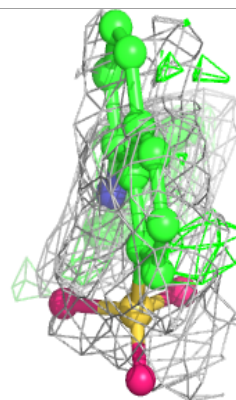
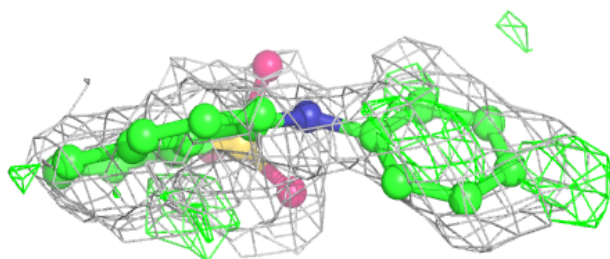
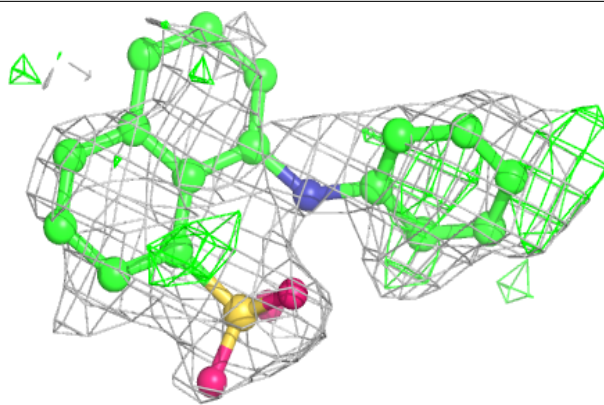
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	2AN	H	1106	21/21	0.93	0.11	34,36,38,39	0
2	2AN	A	201	21/21	0.94	0.13	37,40,41,45	0
2	2AN	I	203	21/21	0.94	0.14	37,39,42,44	0
2	2AN	P	502	21/21	0.94	0.13	40,44,47,54	0
2	2AN	G	302	21/21	0.94	0.12	36,41,56,59	0
2	2AN	M	507	21/21	0.94	0.14	41,43,50,51	0
2	2AN	J	201	21/21	0.94	0.14	38,43,48,49	0
2	2AN	K	203	21/21	0.94	0.13	37,40,48,50	0
2	2AN	A	204	21/21	0.94	0.12	36,38,39,40	0
2	2AN	G	301	21/21	0.94	0.12	39,41,45,45	0
2	2AN	E	505	21/21	0.95	0.11	39,41,46,47	0
2	2AN	O	202	21/21	0.95	0.11	38,43,56,59	0
2	2AN	M	504	21/21	0.95	0.13	31,33,34,37	0
2	2AN	E	501	21/21	0.95	0.14	29,32,37,39	0
2	2AN	F	201	21/21	0.95	0.12	36,38,41,42	0
2	2AN	A	205	21/21	0.95	0.12	34,39,42,44	0
2	2AN	H	1103	21/21	0.95	0.14	40,43,45,46	0
2	2AN	F	205	21/21	0.95	0.12	43,47,50,53	0
2	2AN	B	202	21/21	0.95	0.13	33,35,39,40	0
2	2AN	C	309	21/21	0.96	0.13	30,38,40,42	0
2	2AN	K	207	21/21	0.96	0.12	31,35,39,42	0
2	2AN	O	201	21/21	0.96	0.12	30,32,35,36	0
2	2AN	E	503	21/21	0.96	0.11	32,34,37,38	0
2	2AN	D	703	21/21	0.96	0.13	34,35,38,38	0
2	2AN	C	304	21/21	0.96	0.12	44,46,51,55	0
2	2AN	M	501	21/21	0.96	0.12	28,34,39,40	0
2	2AN	C	302	21/21	0.96	0.12	30,34,36,37	0
2	2AN	I	204	21/21	0.96	0.11	37,42,44,47	0
2	2AN	K	201	21/21	0.97	0.10	32,34,37,38	0
2	2AN	I	201	21/21	0.97	0.11	31,33,34,36	0
2	2AN	L	201	21/21	0.97	0.11	31,33,36,37	0
2	2AN	H	1102	21/21	0.97	0.11	31,32,35,37	0
2	2AN	P	504	21/21	0.97	0.10	30,34,37,38	0
2	2AN	G	303	21/21	0.97	0.12	33,34,36,39	0

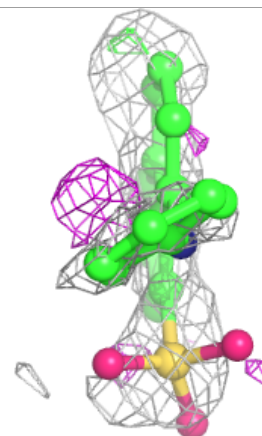
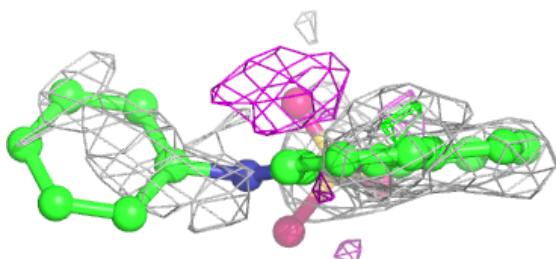
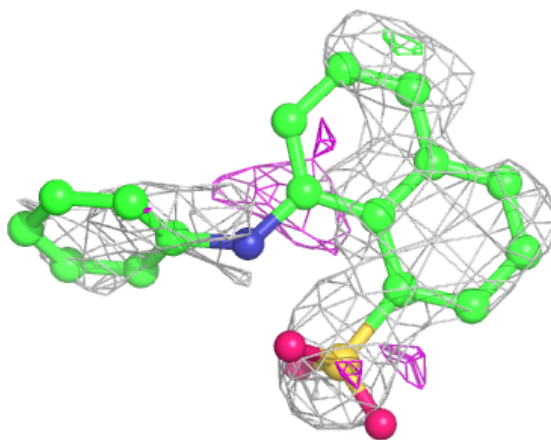
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around 2AN 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)

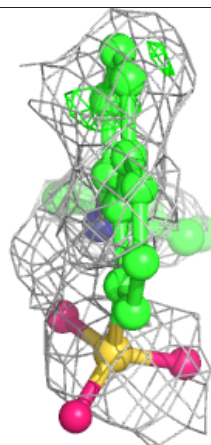
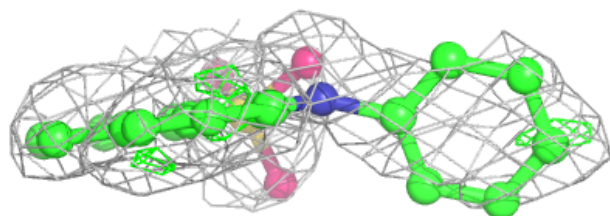
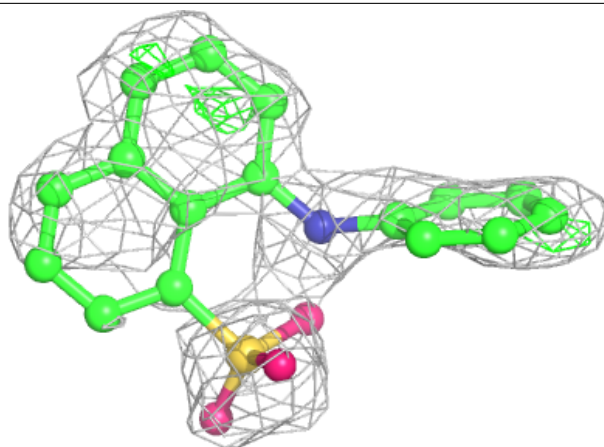
**Electron density around 2AN D 702:**

$2mF_o-DF_c$  (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:**

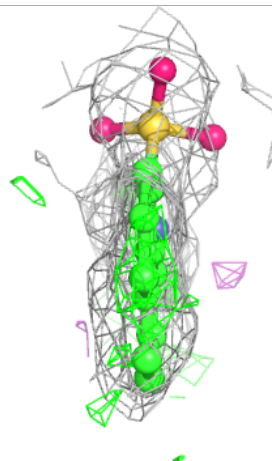
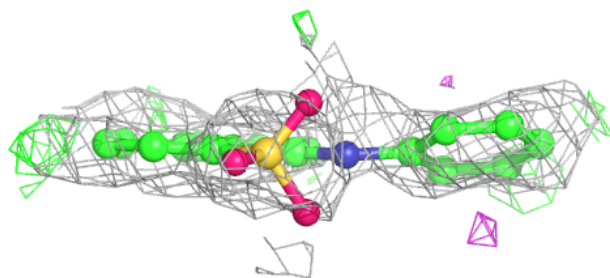
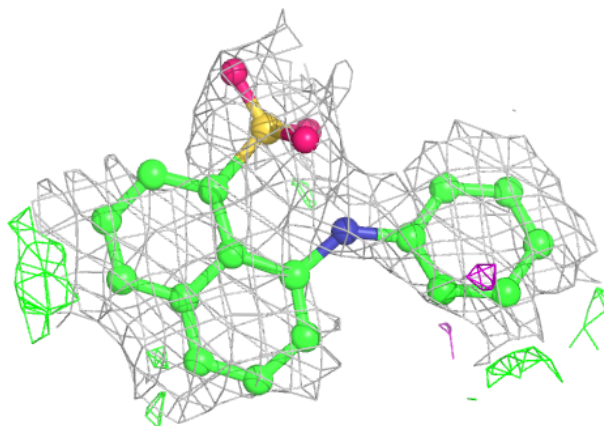
$2mF_o - DF_c$  (at 0.7 rmsd) in gray  
 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





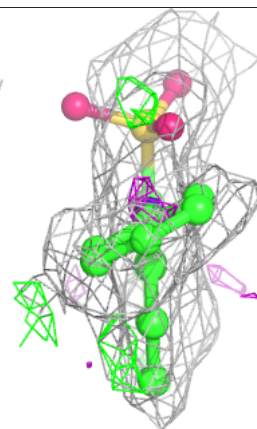
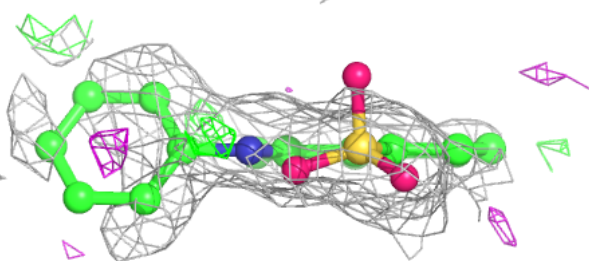
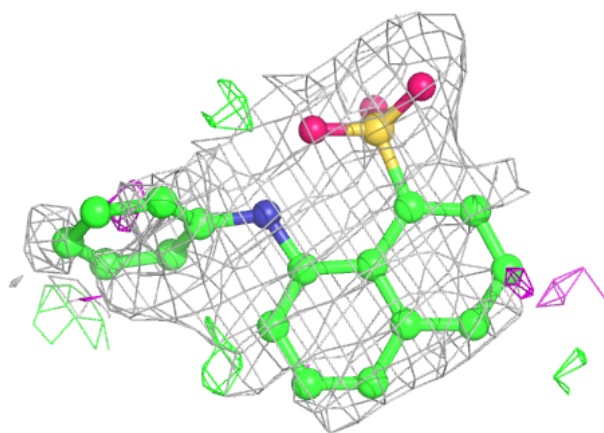
**Electron density around 2AN K 206:**

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



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

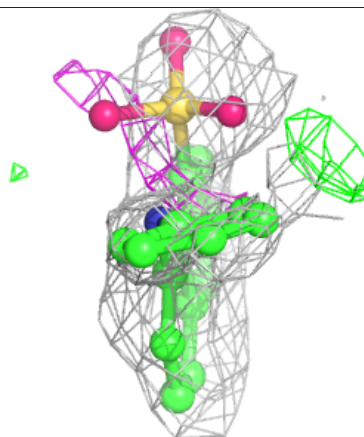
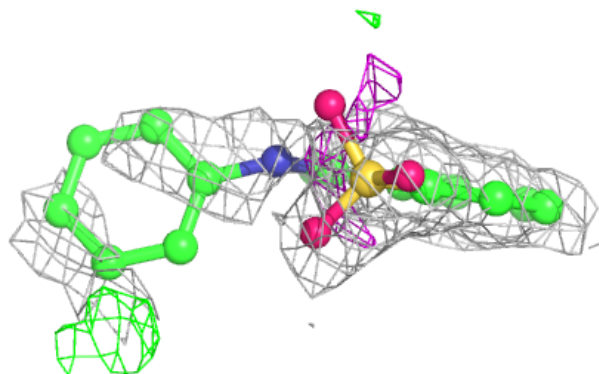
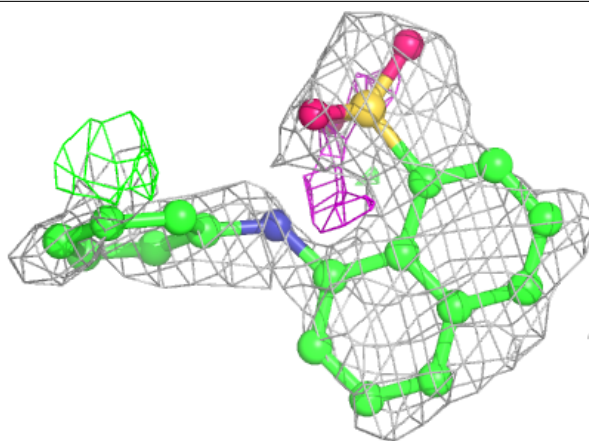
$2mF_o - DF_c$  (at 0.7 rmsd) in gray  
 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





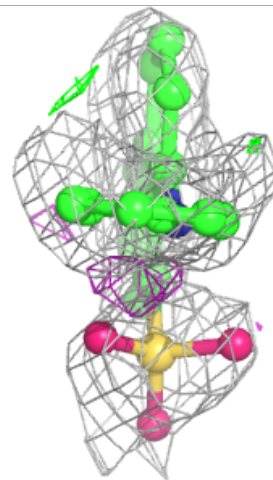
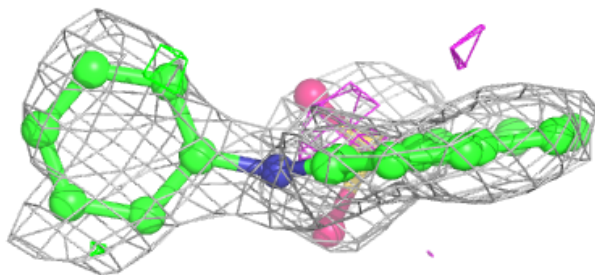
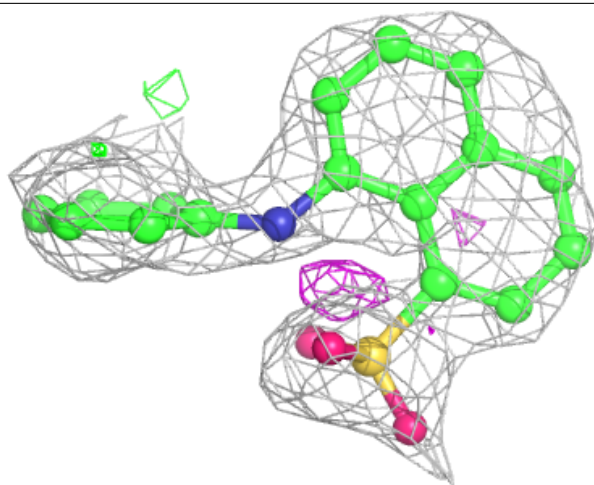
**Electron density around 2AN P 509:**

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



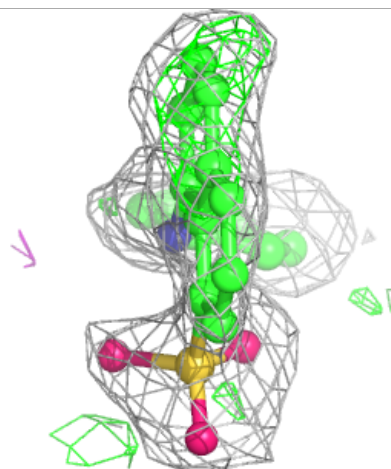
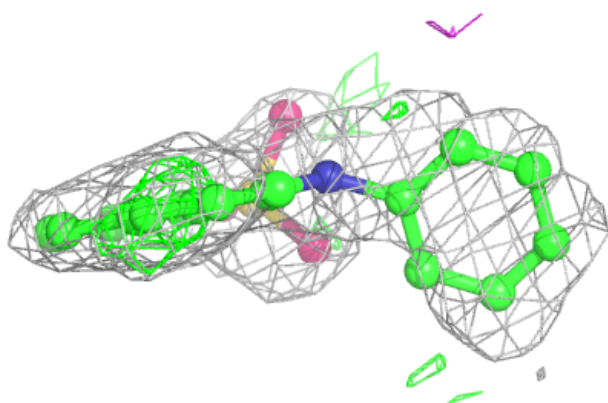
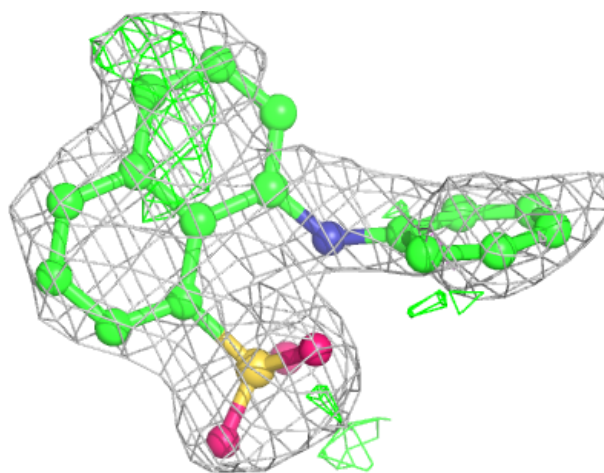
**Electron density around 2AN C 308:**

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



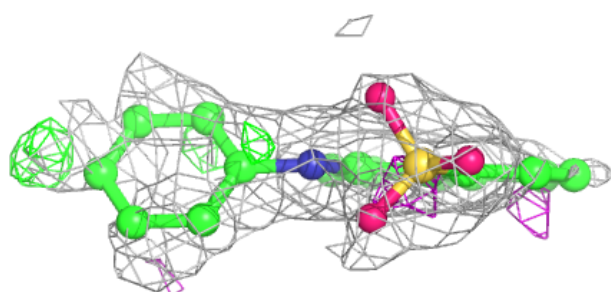
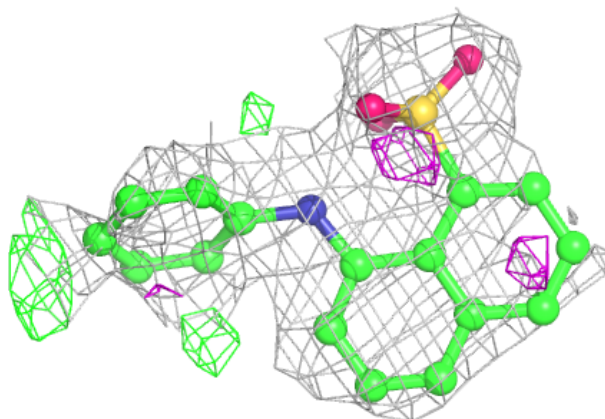
**Electron density around 2AN F 207:**

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

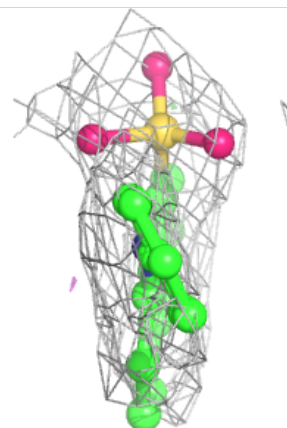
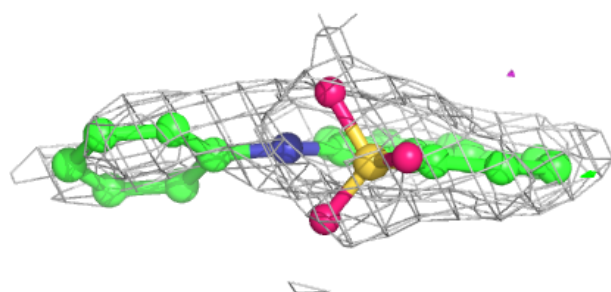
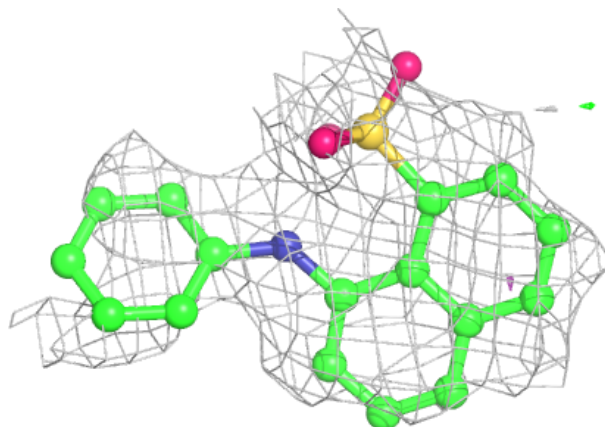


**Electron density around 2AN E 506:**

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

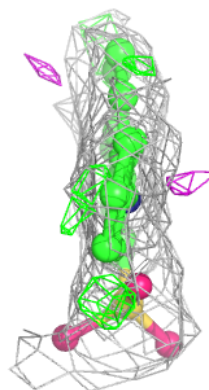
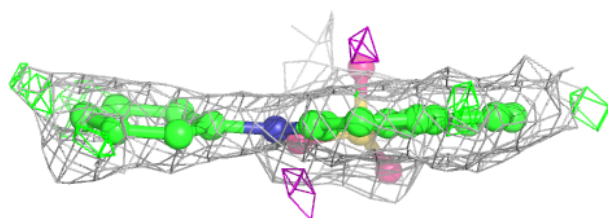
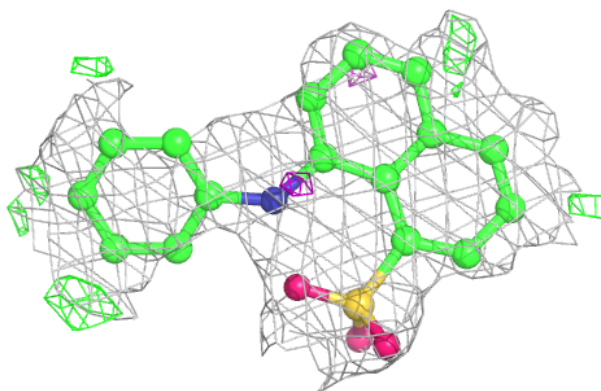
**Electron density around 2AN N 203:**

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



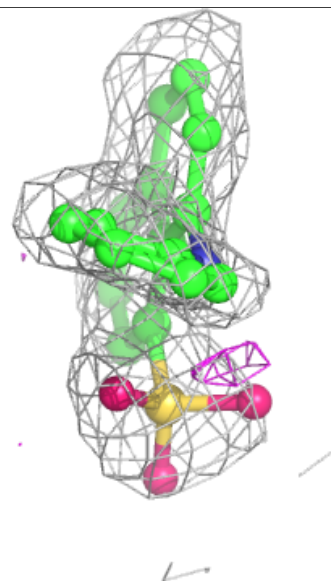
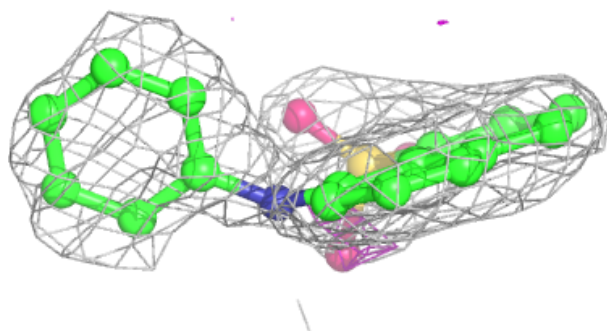
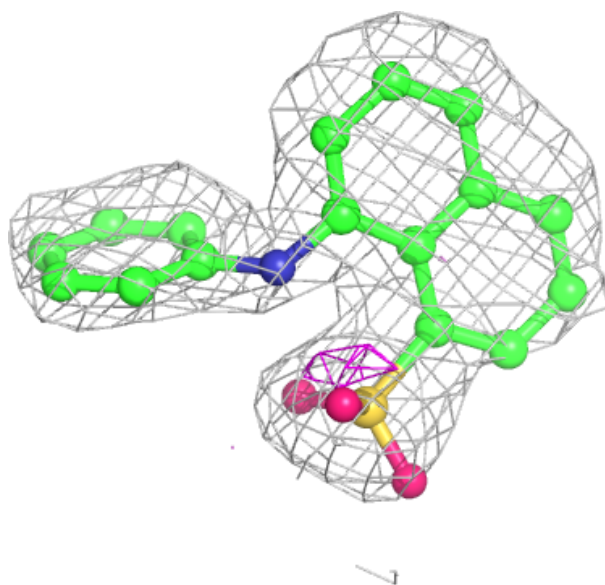
**Electron density around 2AN E 507:**

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



**Electron density around 2AN M 508:**

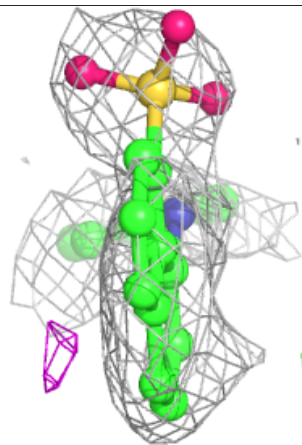
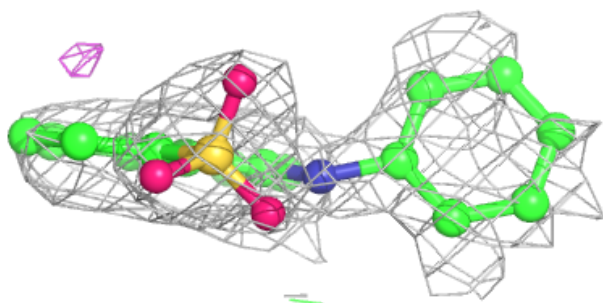
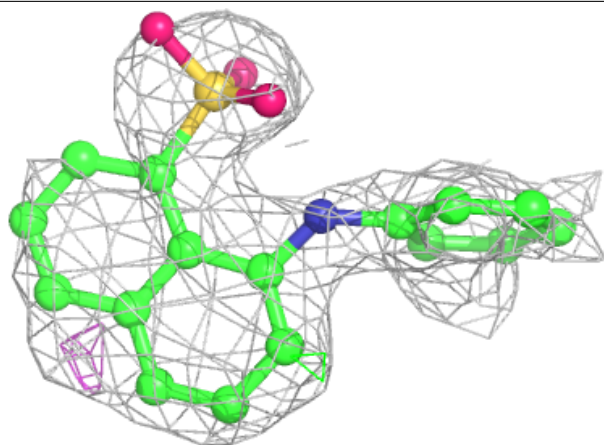
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





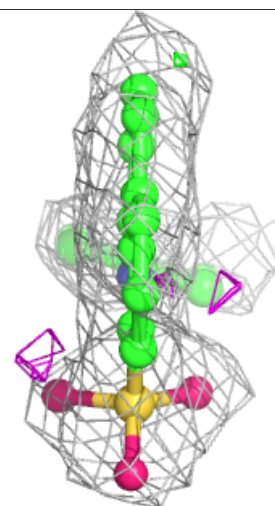
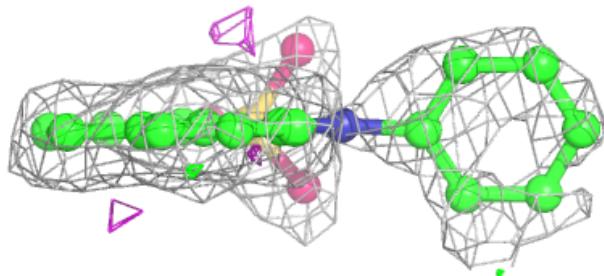
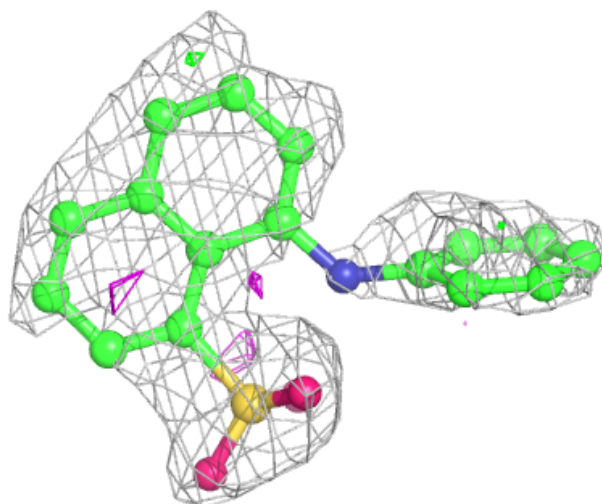
**Electron density around 2AN M 509:**

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



**Electron density around 2AN H 1109:**

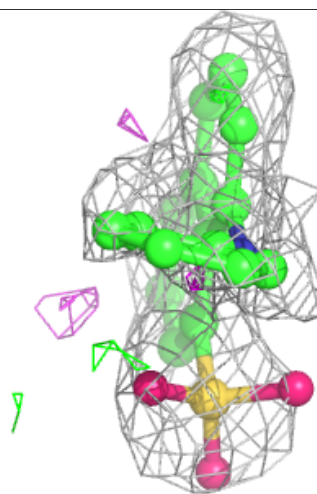
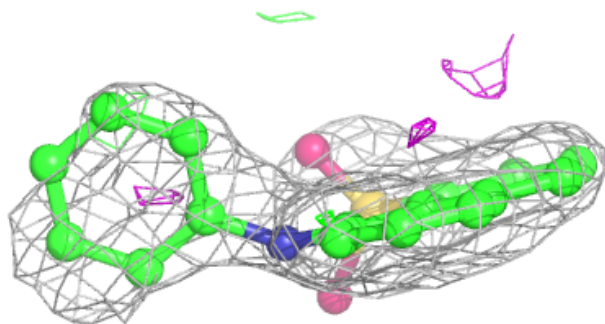
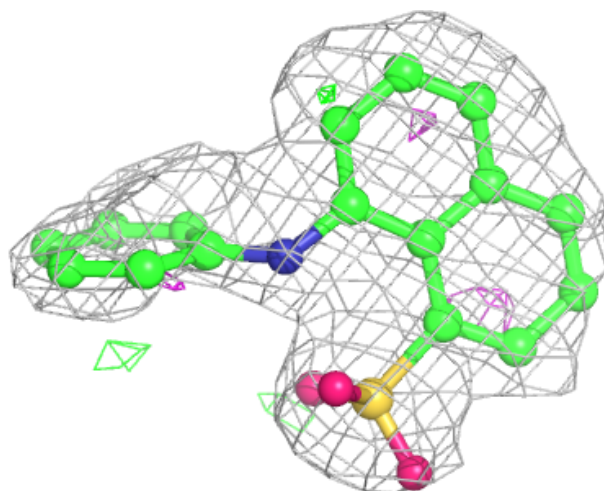
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





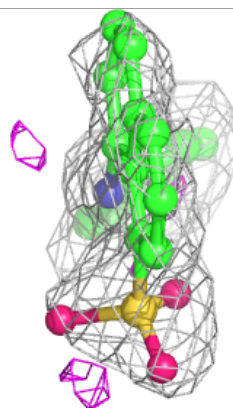
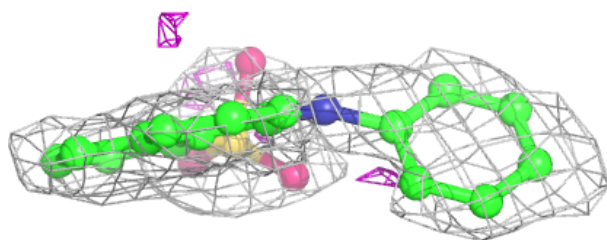
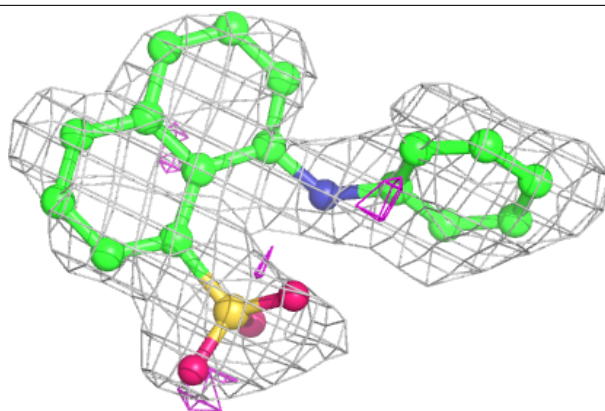
**Electron density around 2AN C 307:**

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



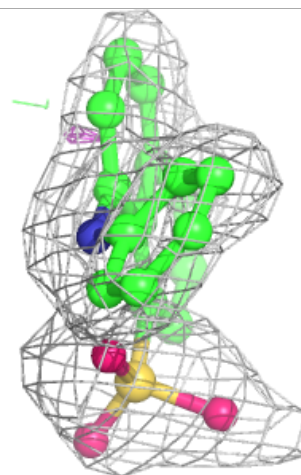
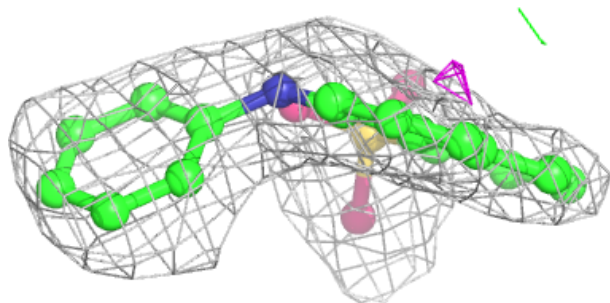
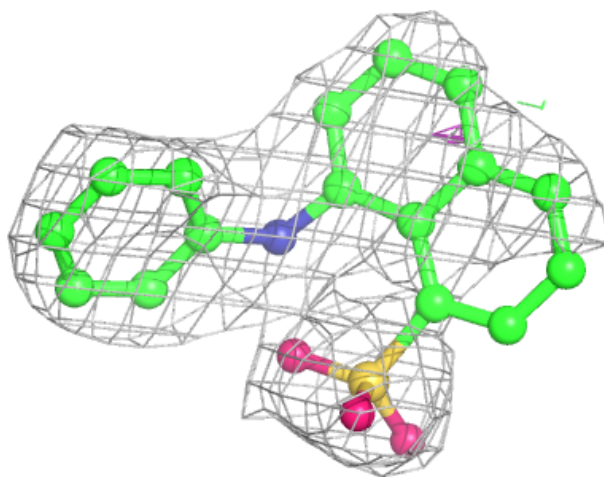
**Electron density around 2AN F 208:**

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



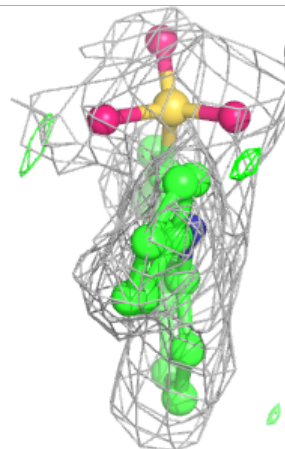
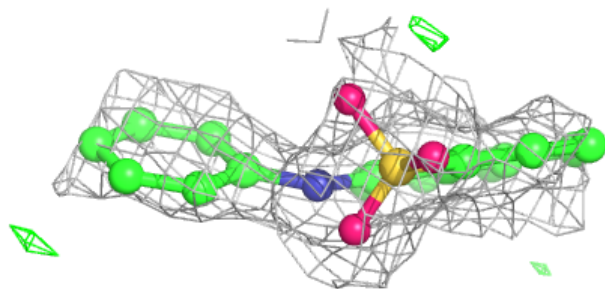
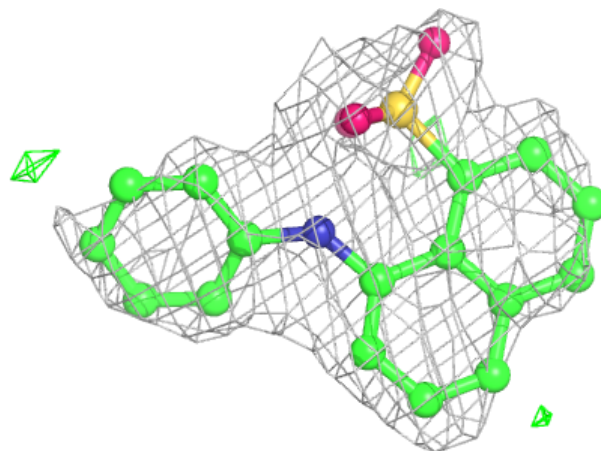
**Electron density around 2AN P 503:**

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



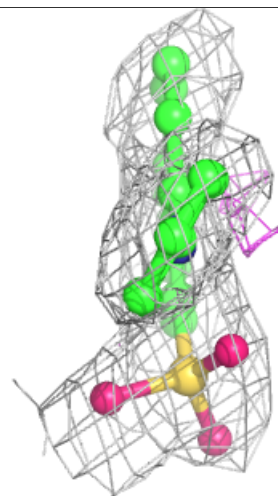
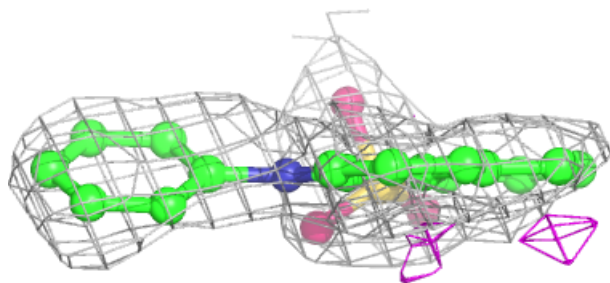
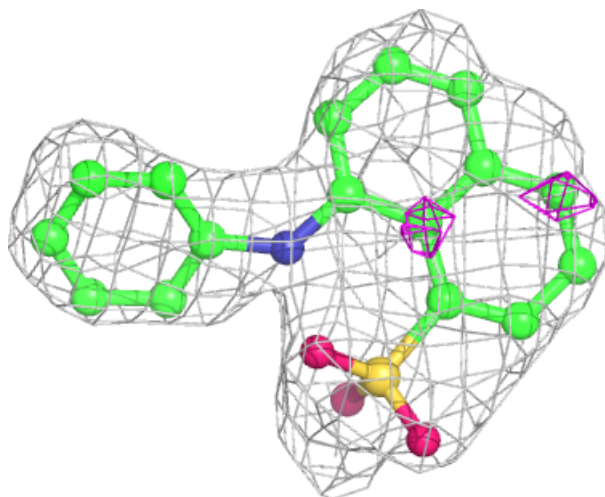
**Electron density around 2AN J 205:**

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



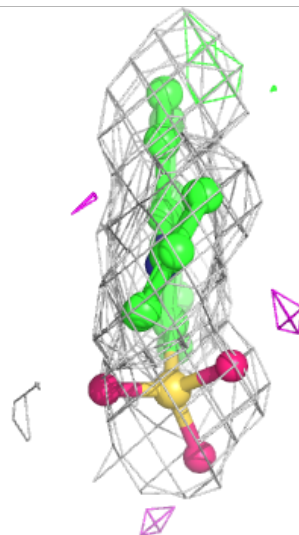
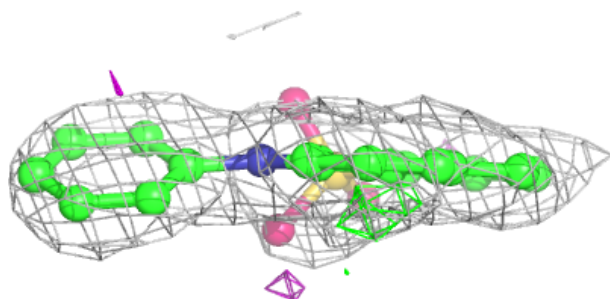
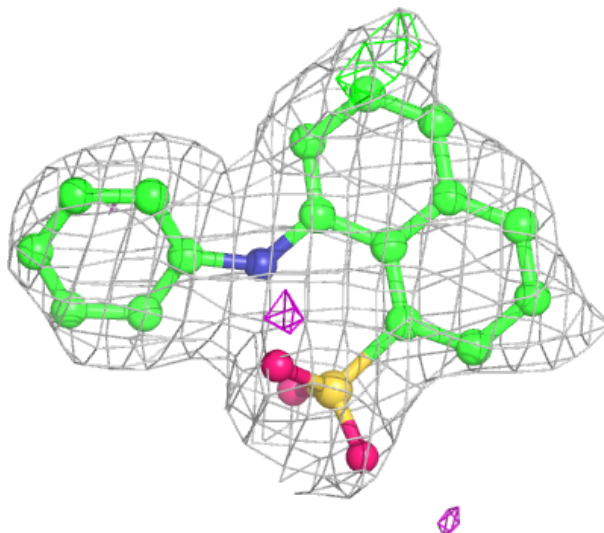
**Electron density around 2AN J 202:**

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



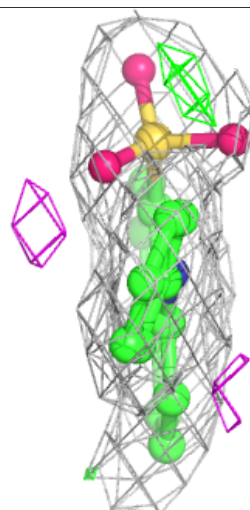
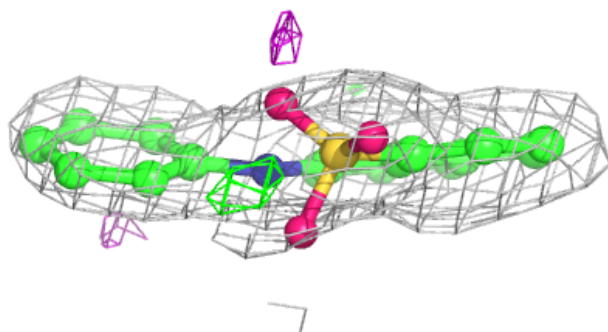
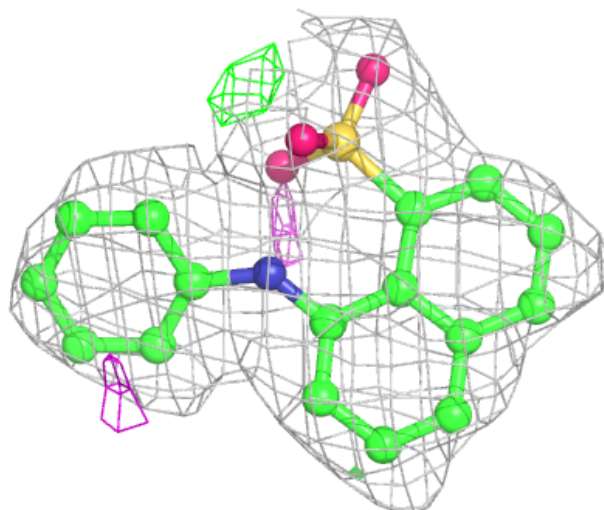
**Electron density around 2AN C 306:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around 2AN M 505:**

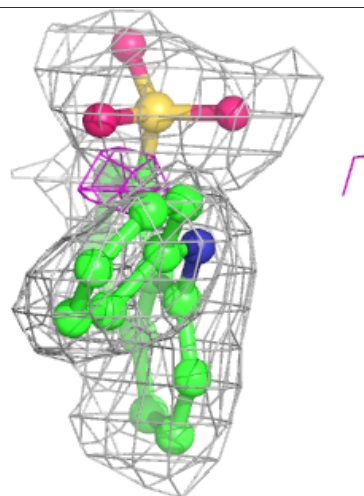
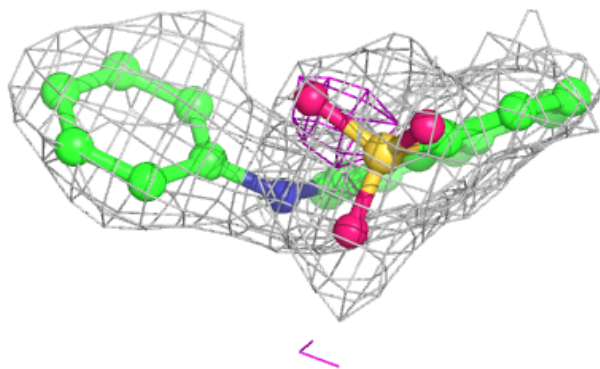
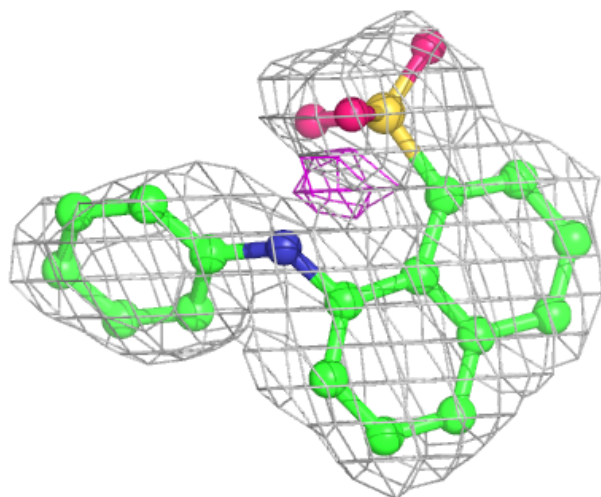
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around 2AN H 1101:**

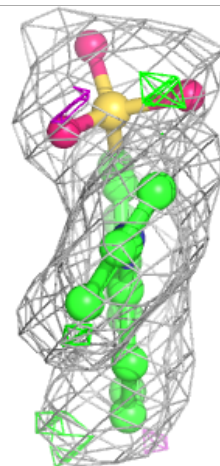
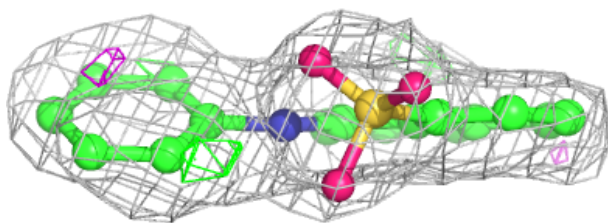
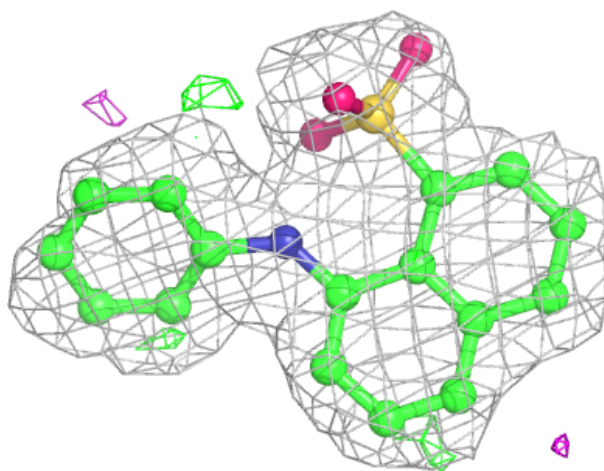
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





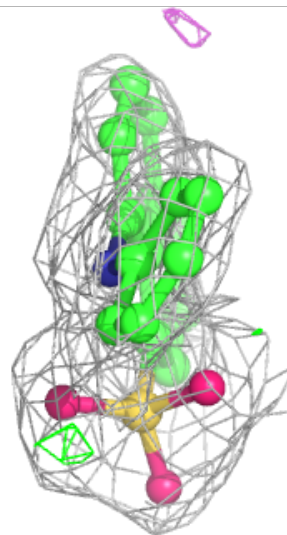
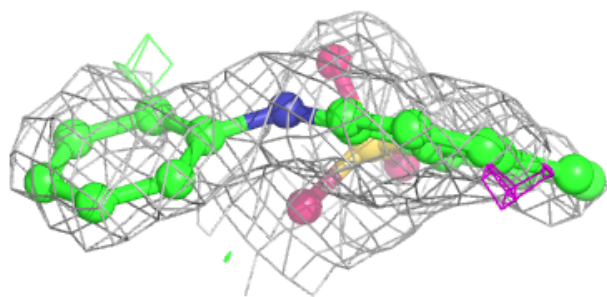
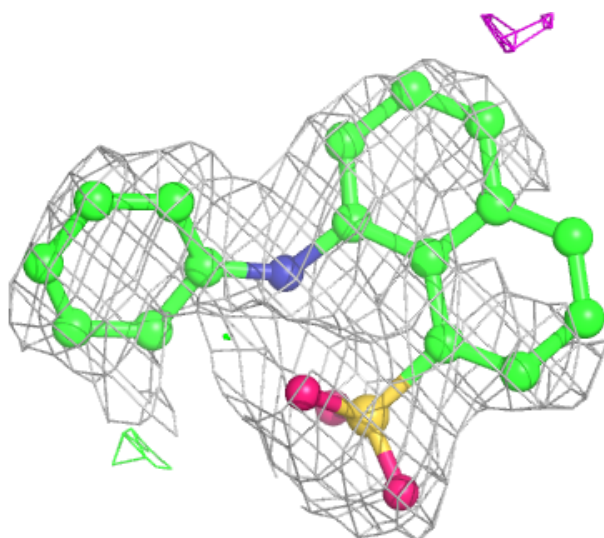
**Electron density around 2AN G 304:**

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



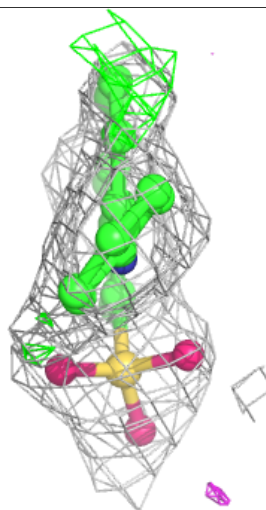
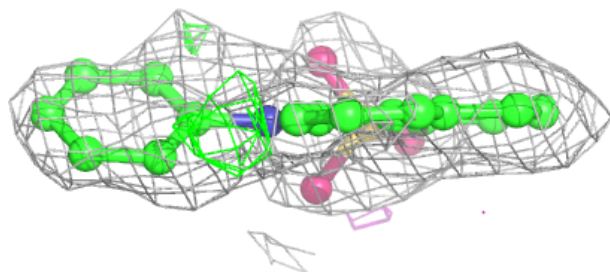
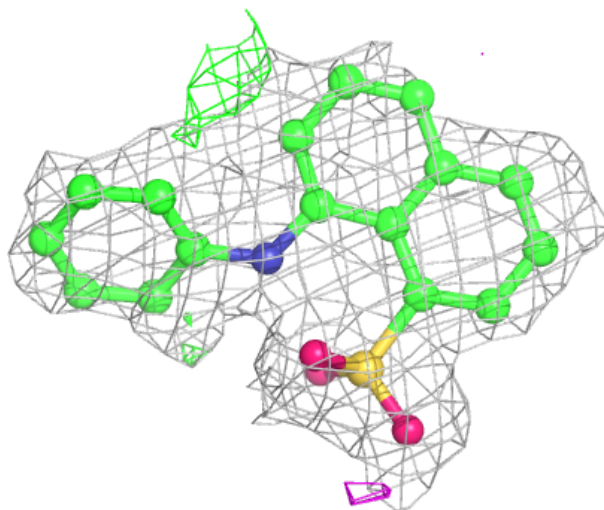
**Electron density around 2AN J 204:**

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



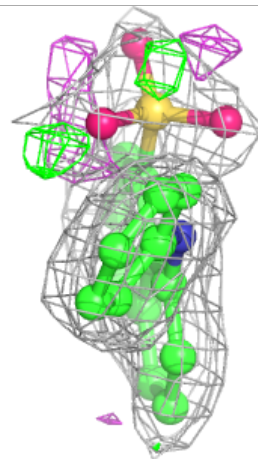
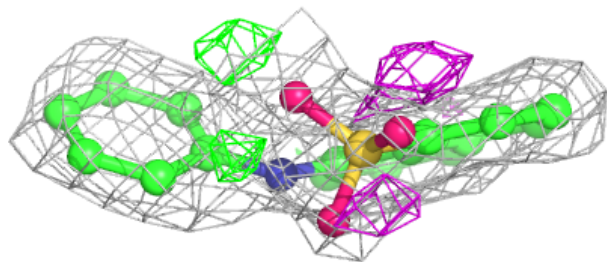
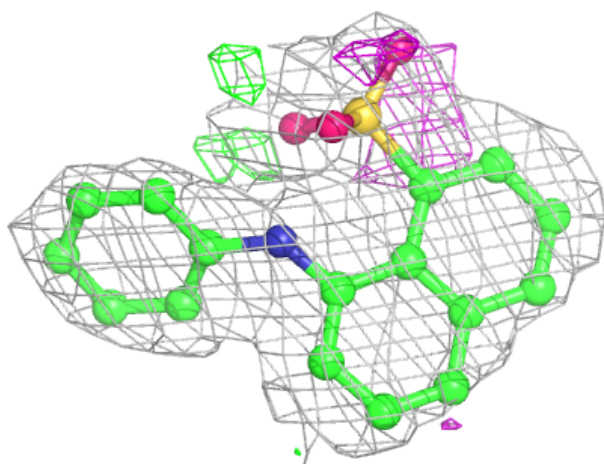
**Electron density around 2AN P 508:**

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



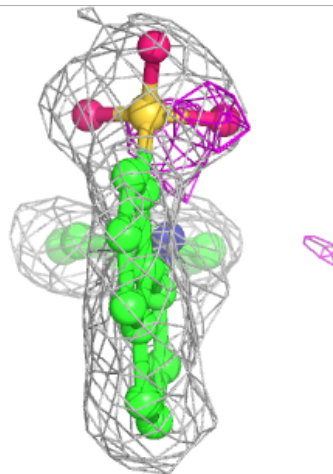
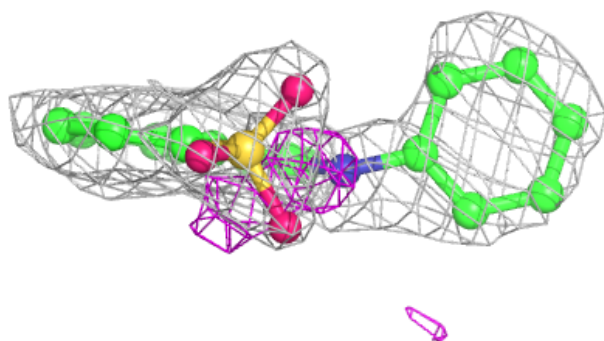
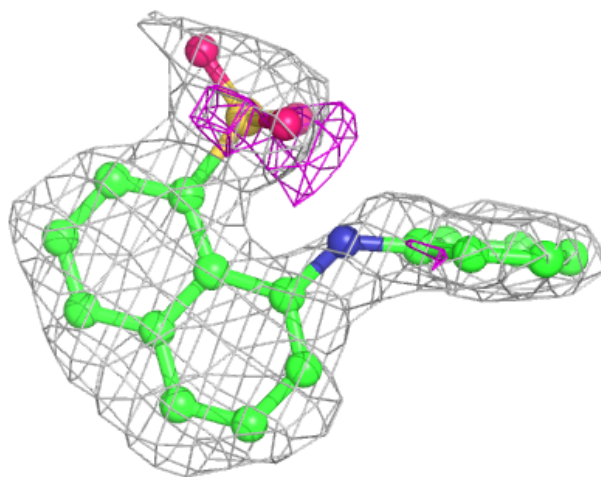
**Electron density around 2AN P 501:**

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



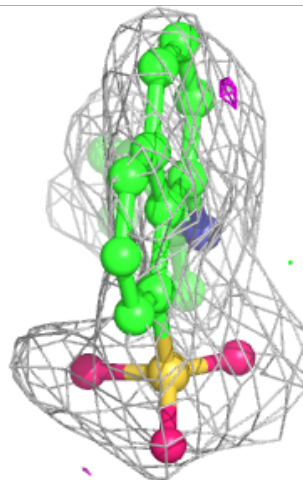
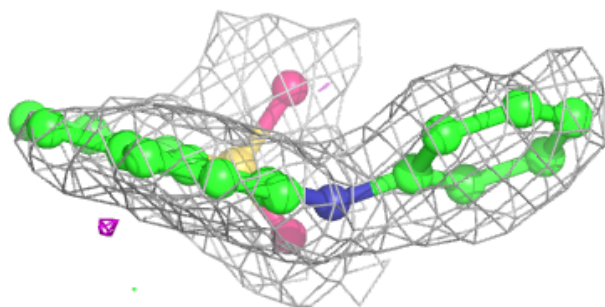
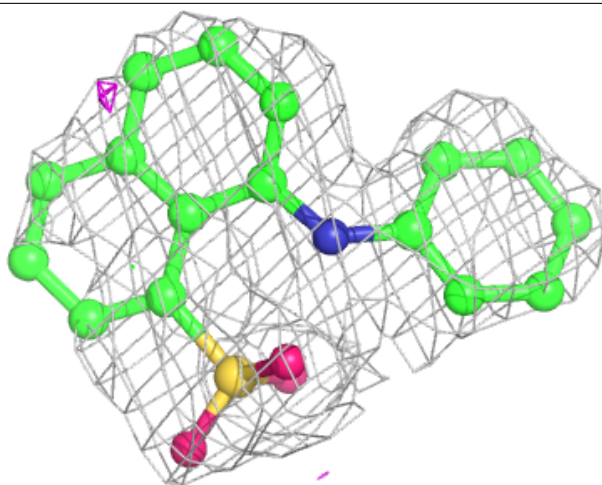
**Electron density around 2AN N 204:**

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



**Electron density around 2AN D 706:**

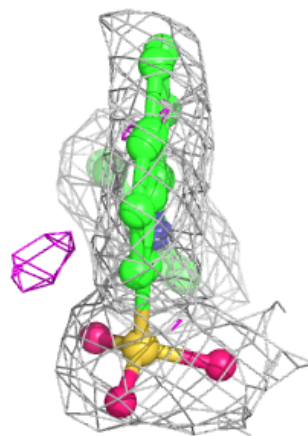
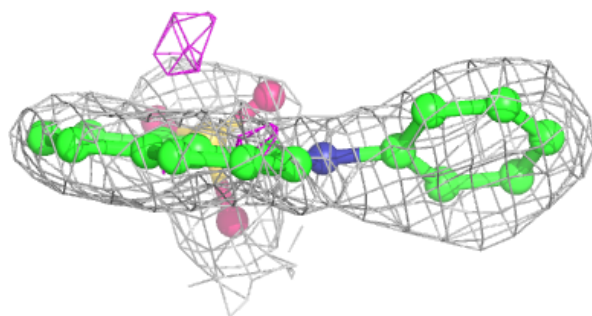
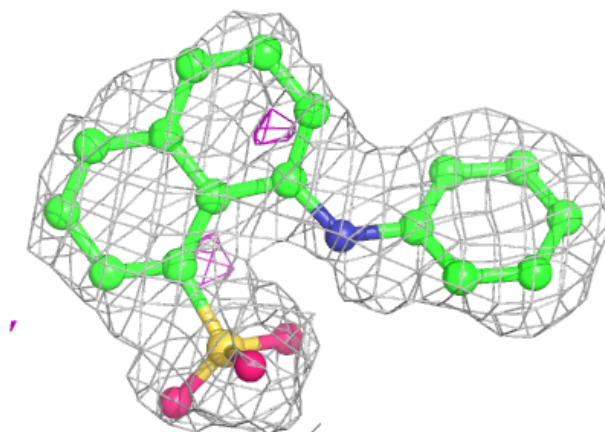
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





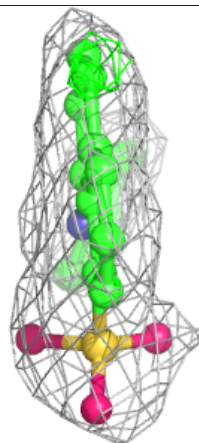
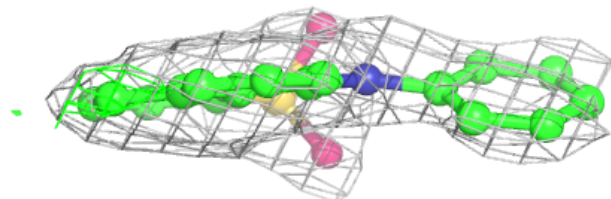
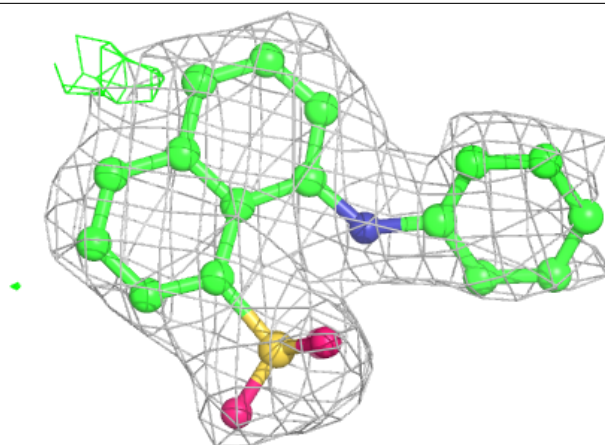
**Electron density around 2AN N 202:**

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



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

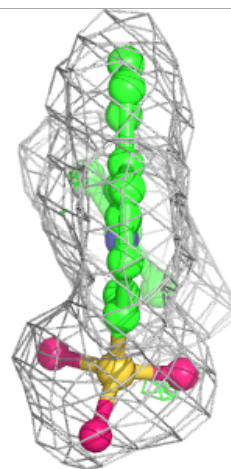
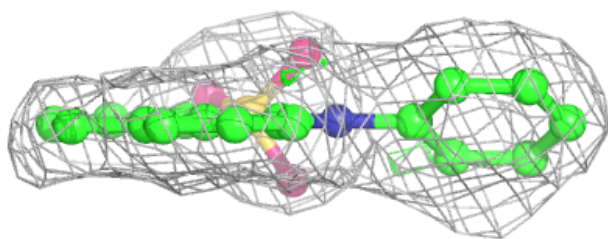
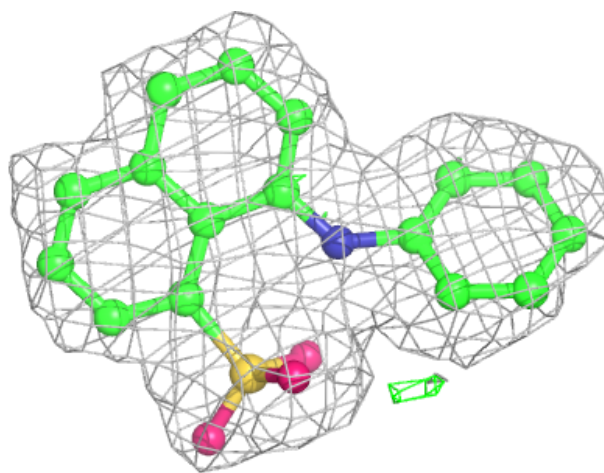
$2mF_o - DF_c$  (at 0.7 rmsd) in gray  
 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





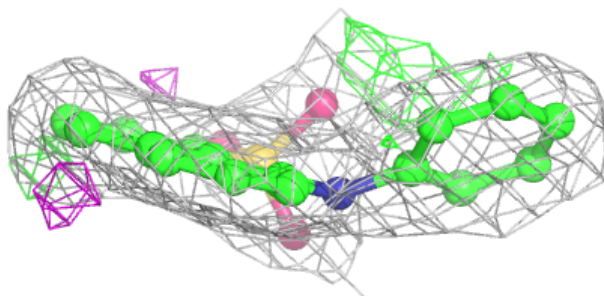
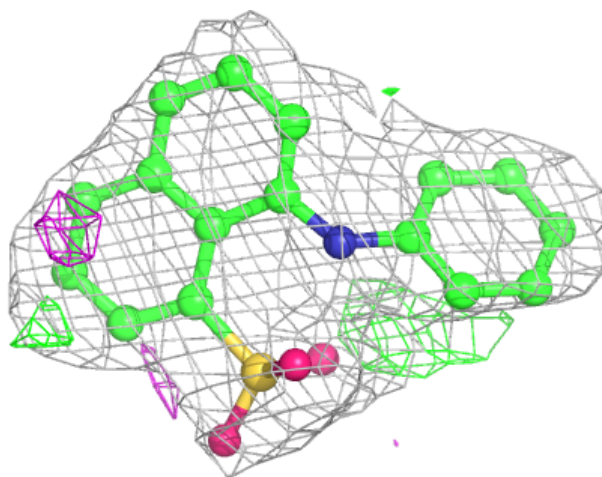
**Electron density around 2AN O 203:**

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



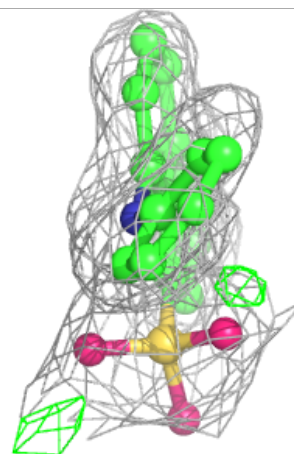
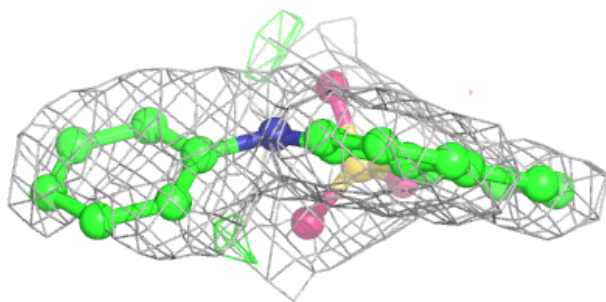
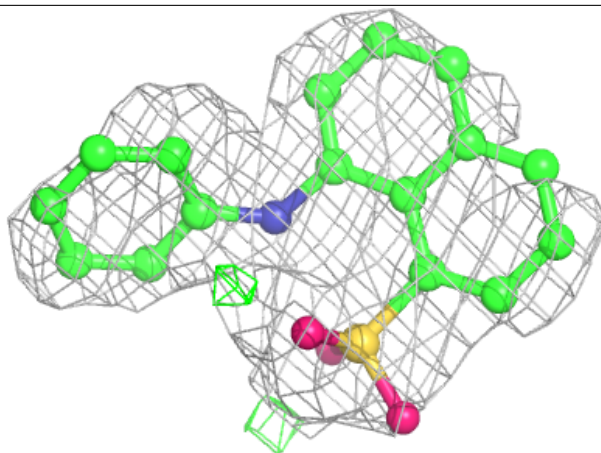
**Electron density around 2AN F 204:**

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



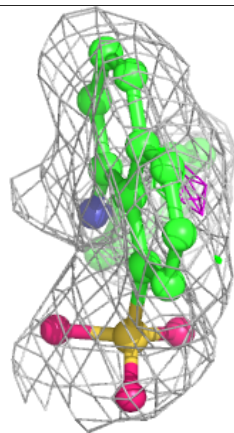
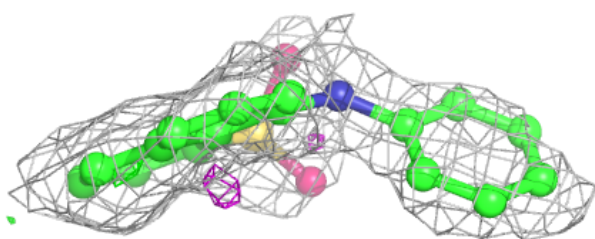
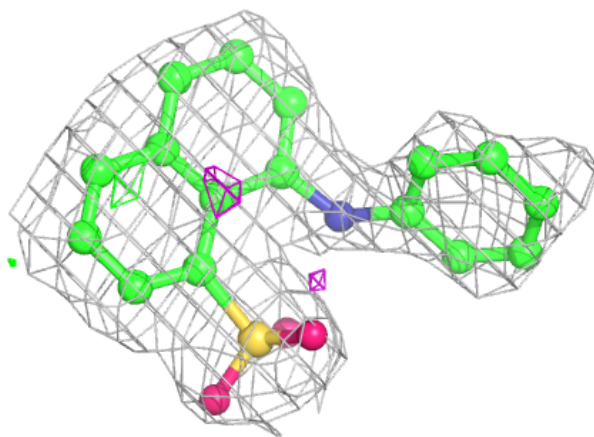
**Electron density around 2AN D 705:**

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



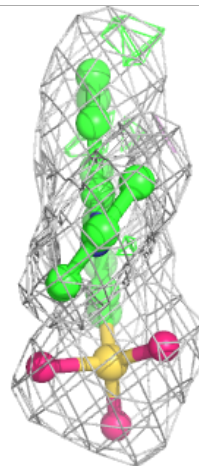
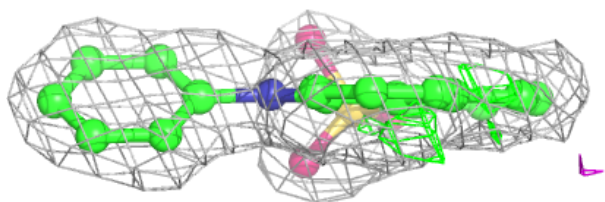
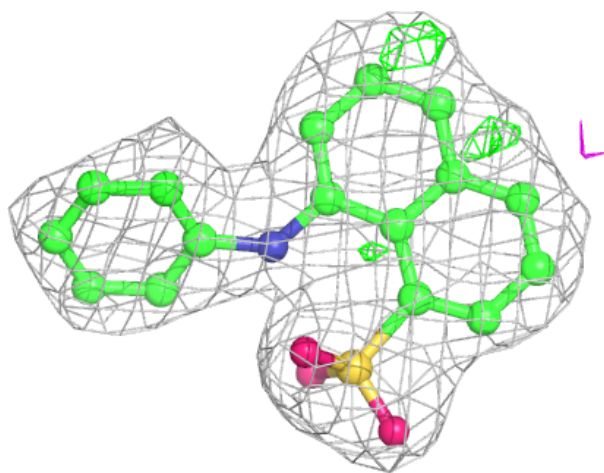
**Electron density around 2AN D 701:**

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



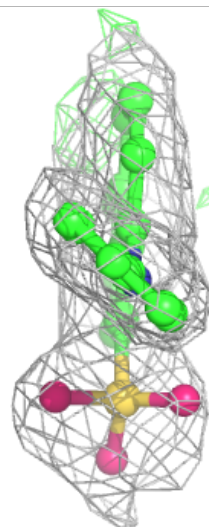
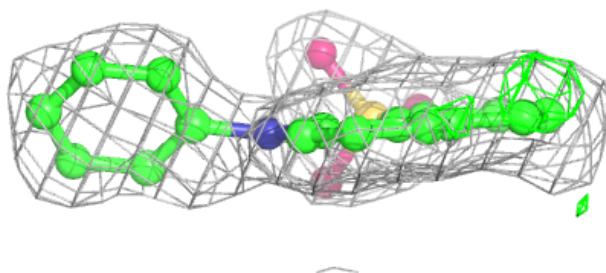
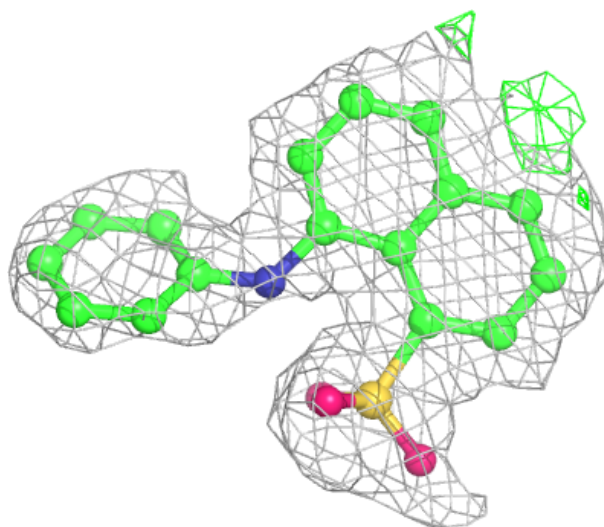
**Electron density around 2AN K 202:**

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



**Electron density around 2AN M 503:**

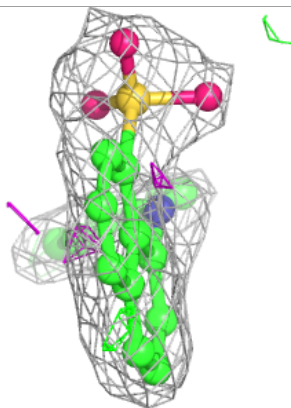
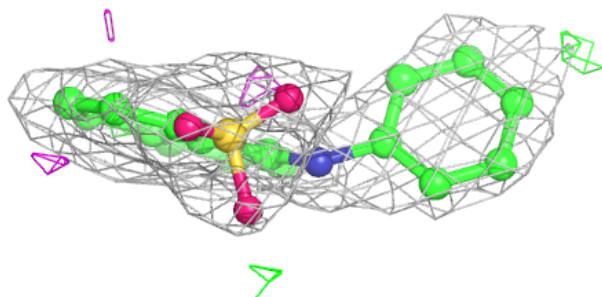
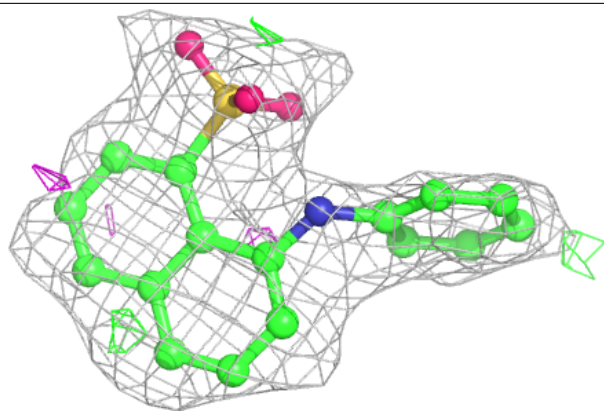
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



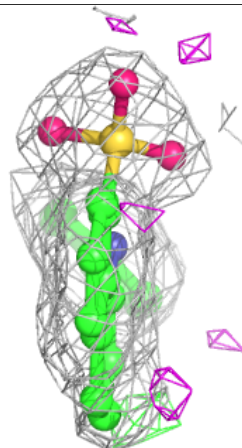
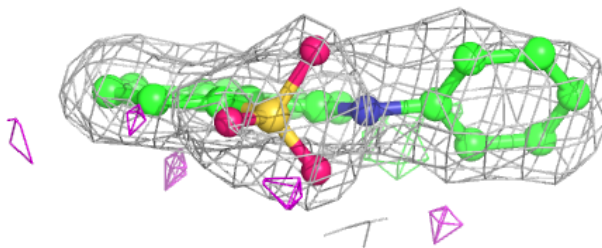
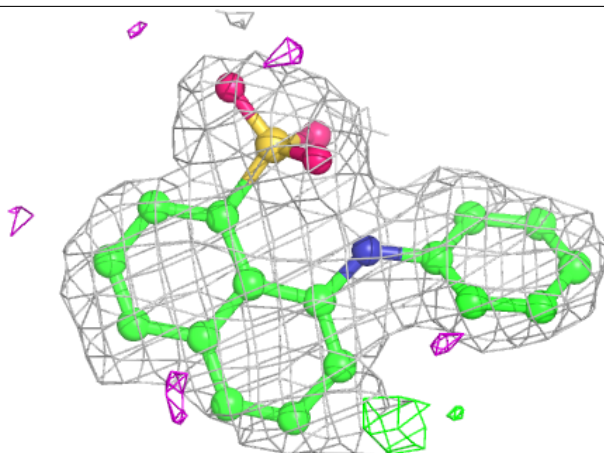


**Electron density around 2AN P 506:**

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

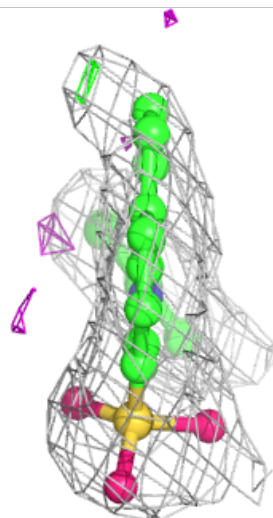
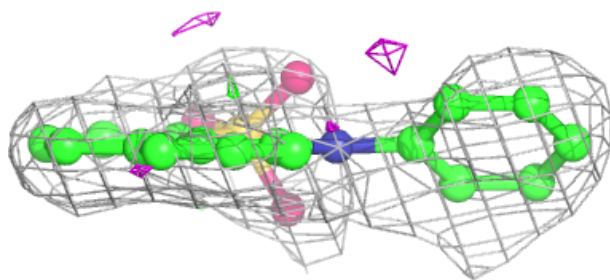
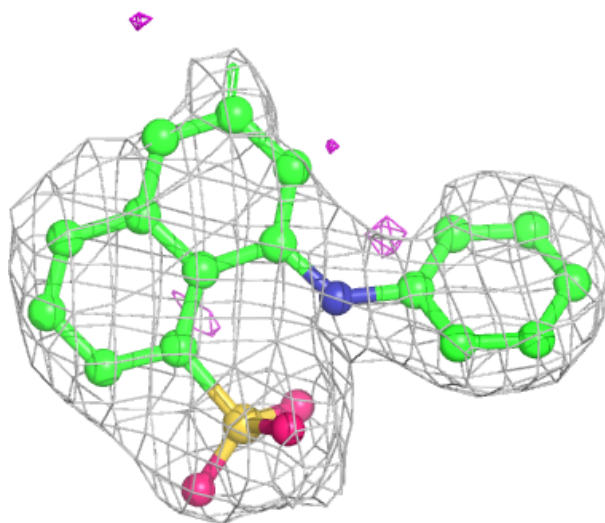
**Electron density around 2AN H 1107:**

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



**Electron density around 2AN D 704:**

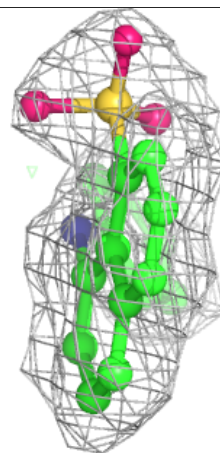
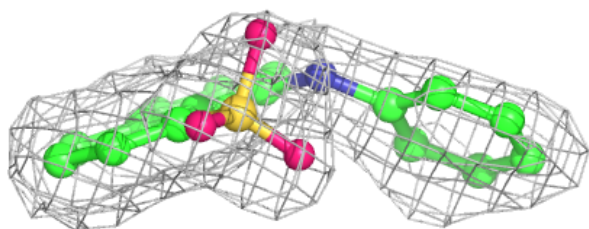
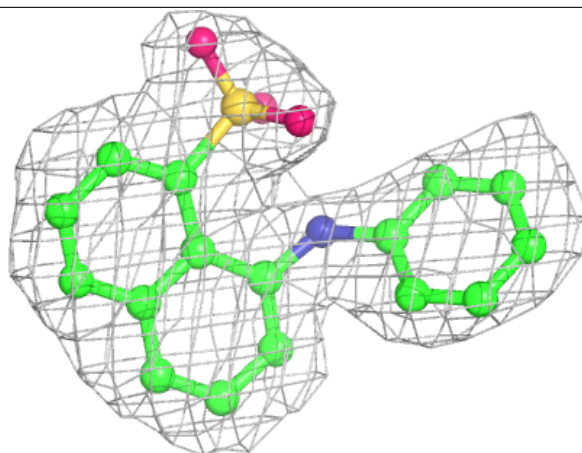
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





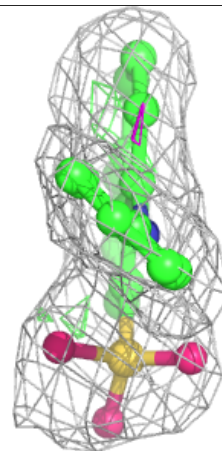
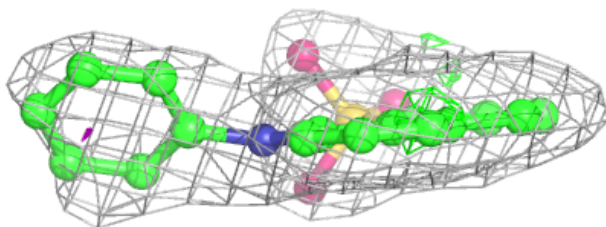
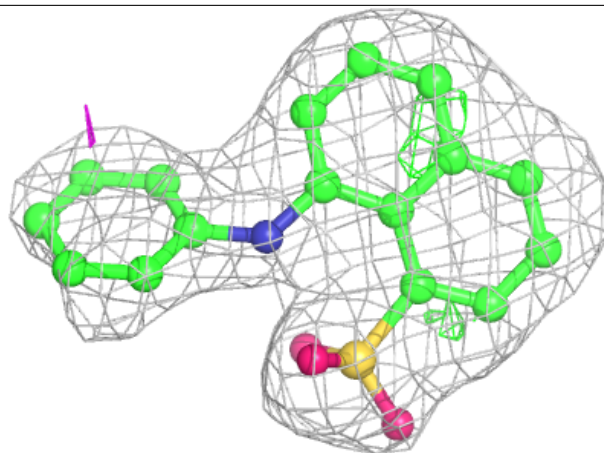
**Electron density around 2AN A 202:**

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



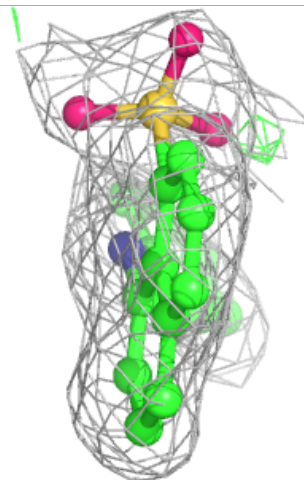
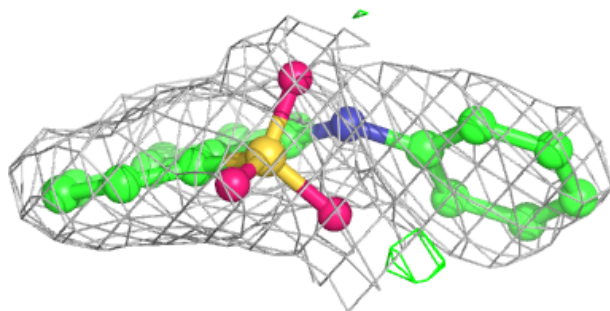
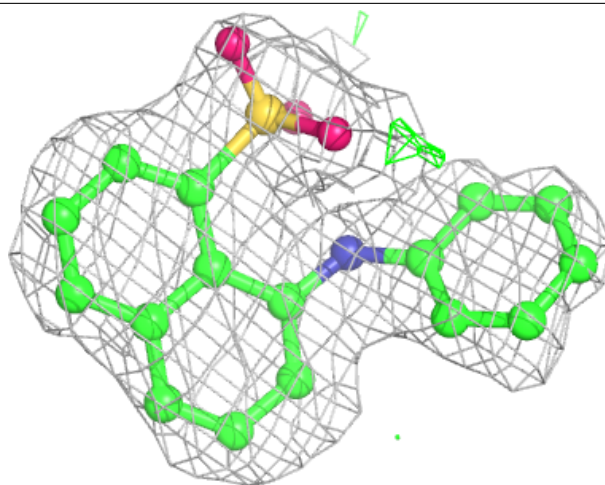
**Electron density around 2AN H 1105:**

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



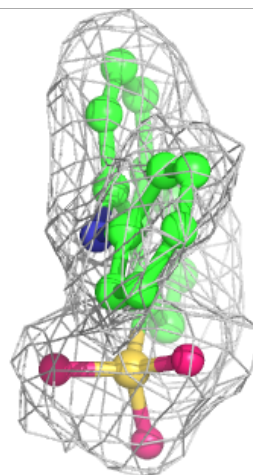
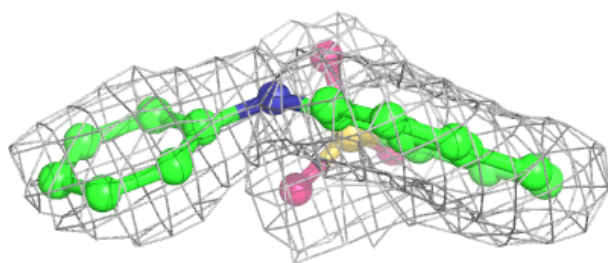
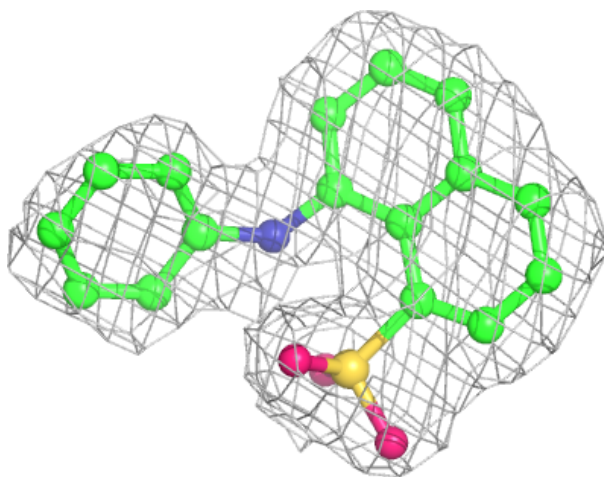
**Electron density around 2AN B 203:**

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



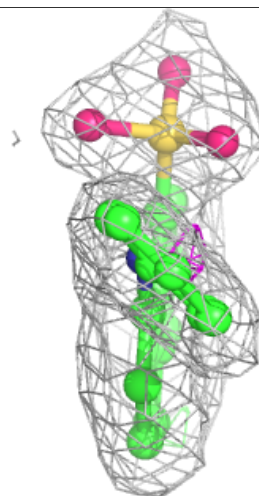
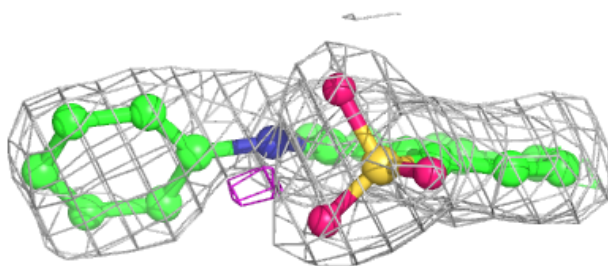
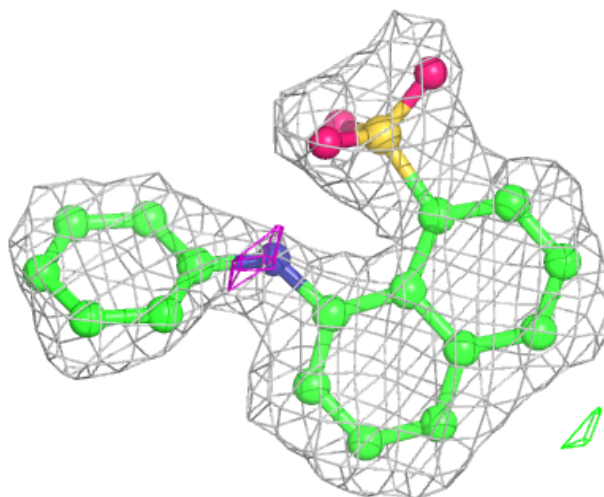
**Electron density around 2AN L 204:**

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



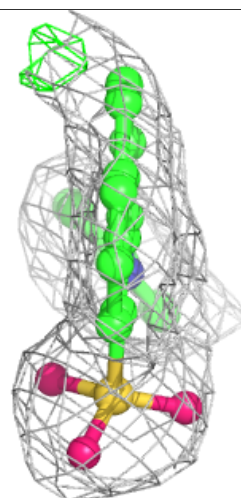
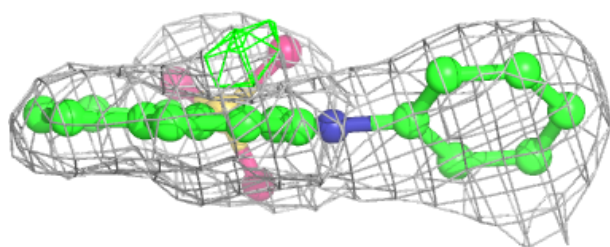
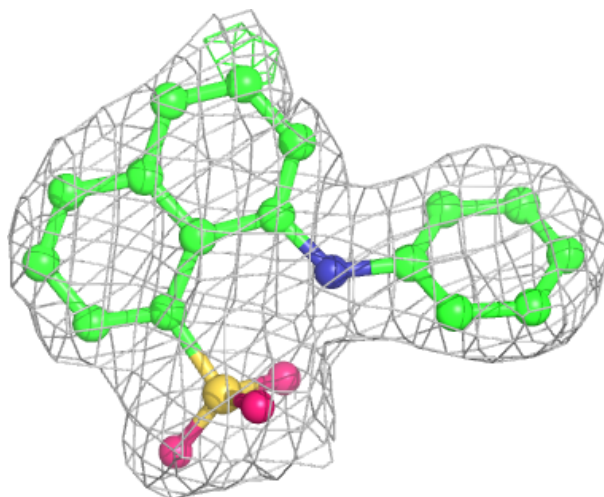
**Electron density around 2AN C 303:**

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



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

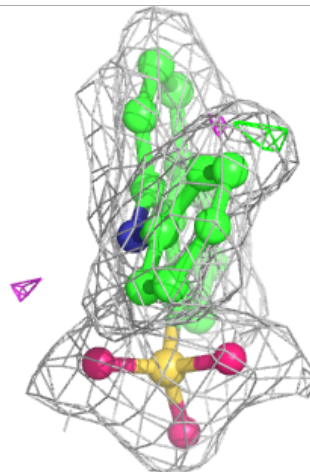
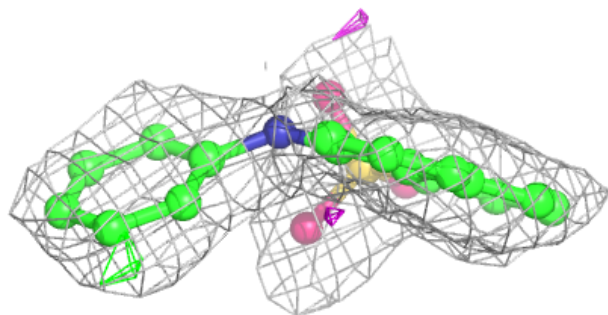
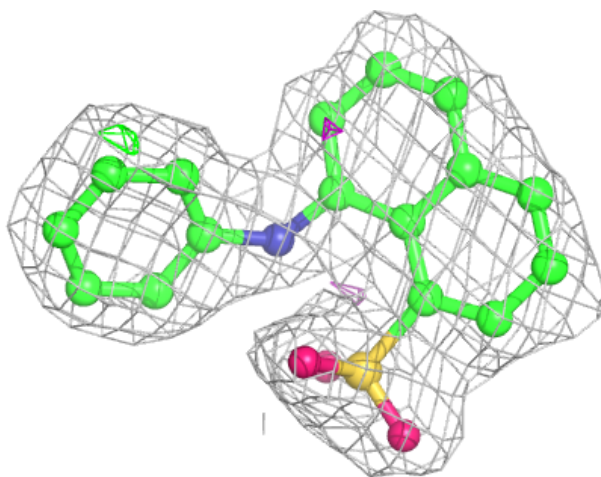
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





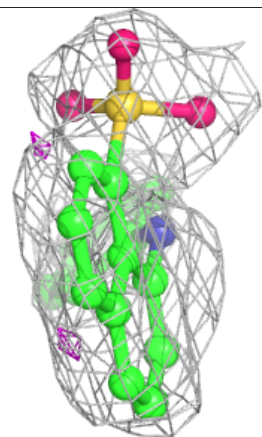
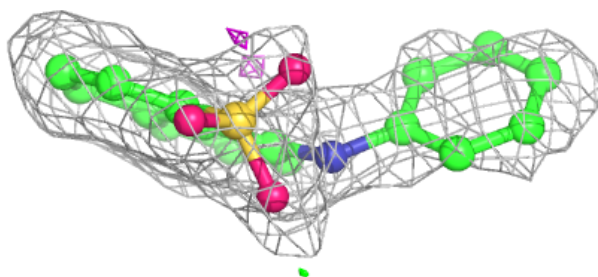
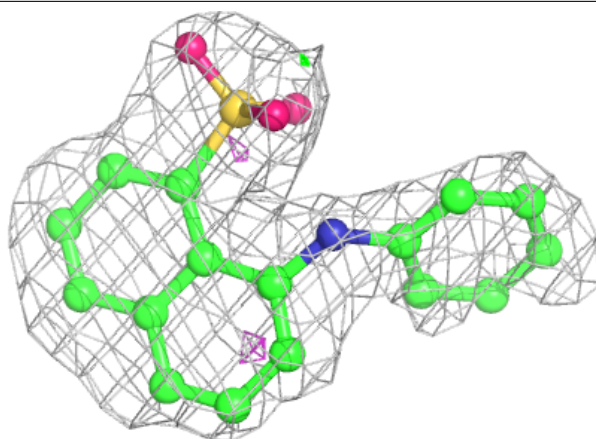
**Electron density around 2AN E 504:**

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



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

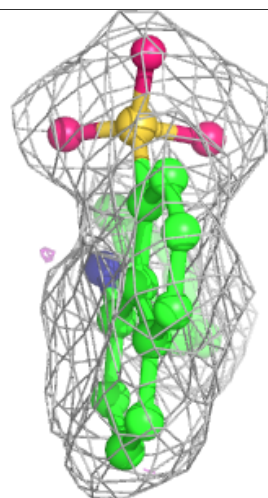
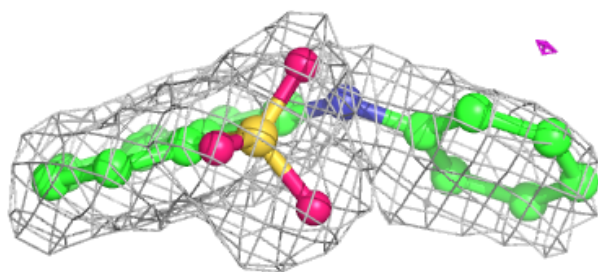
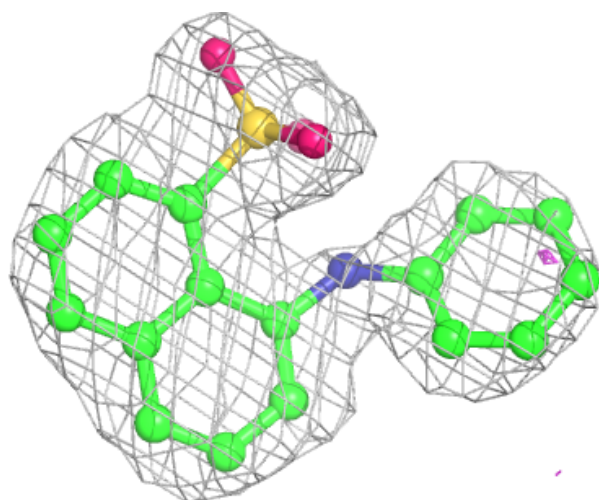
$2mF_o - DF_c$  (at 0.7 rmsd) in gray  
 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





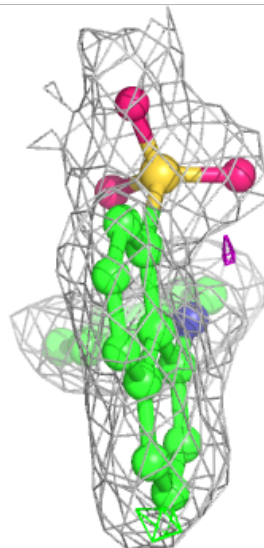
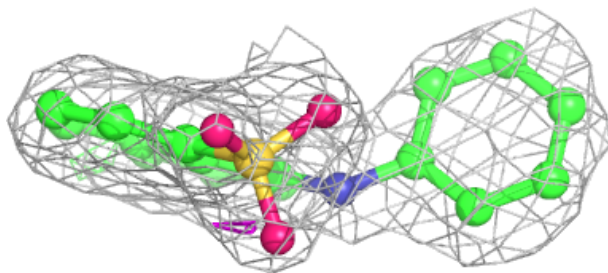
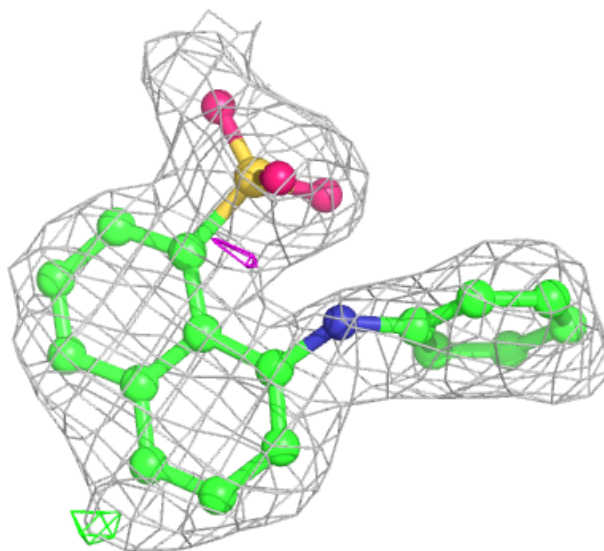
**Electron density around 2AN B 204:**

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



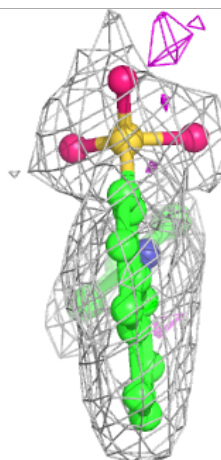
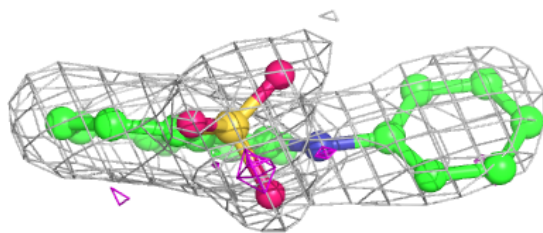
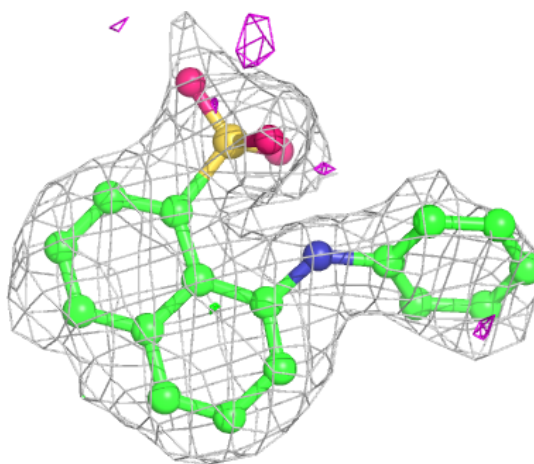
**Electron density around 2AN H 1104:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)



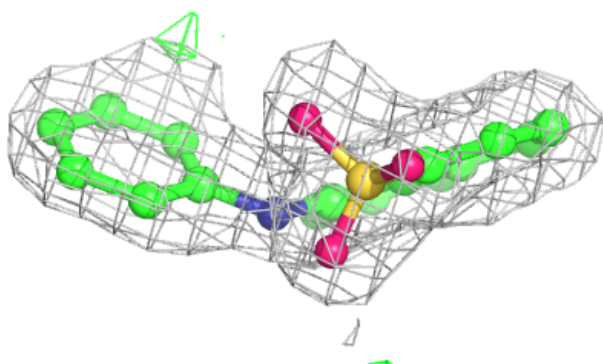
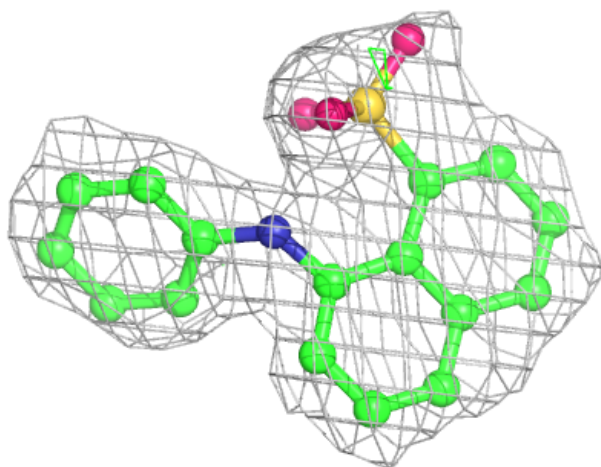
**Electron density around 2AN A 203:**

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



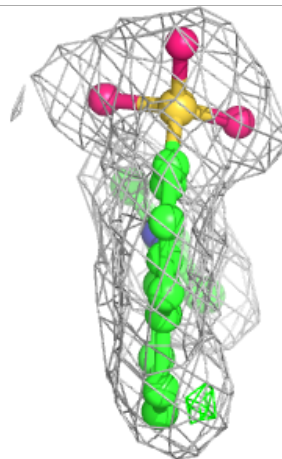
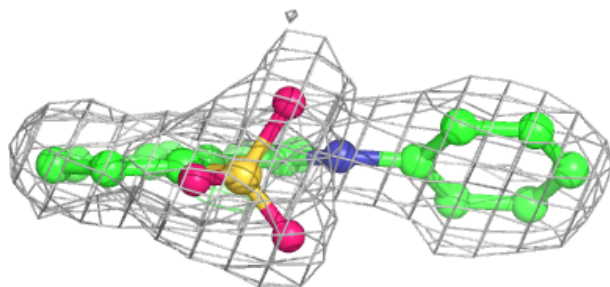
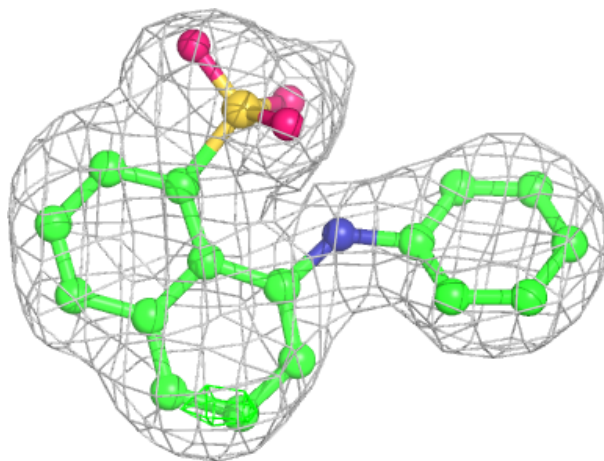
**Electron density around 2AN I 205:**

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



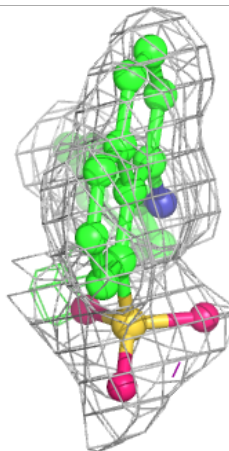
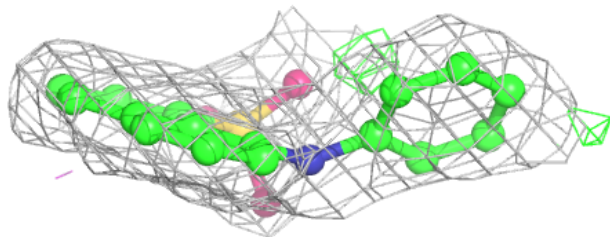
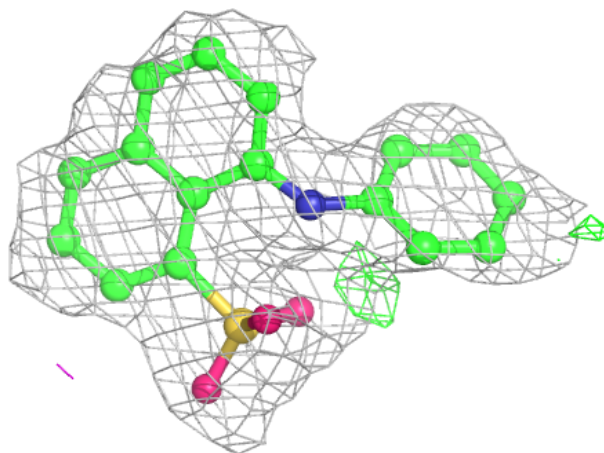
**Electron density around 2AN L 202:**

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



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

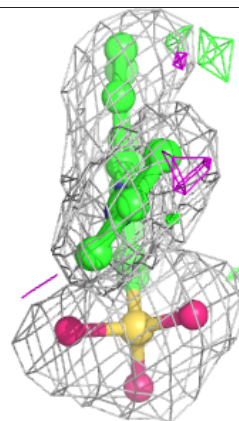
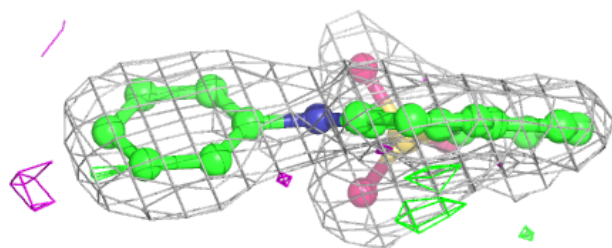
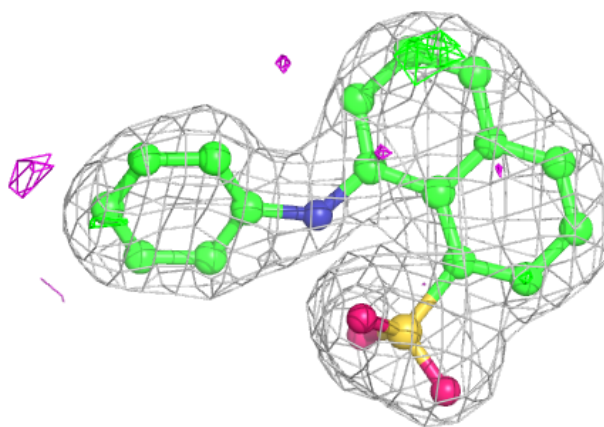
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





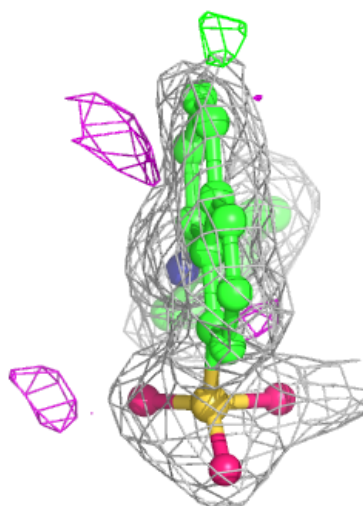
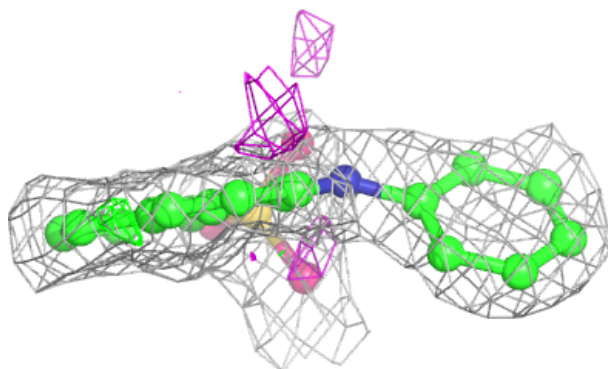
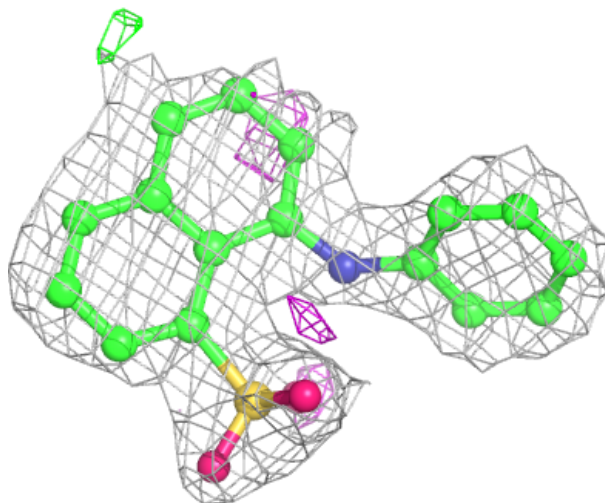
**Electron density around 2AN B 201:**

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



**Electron density around 2AN M 502:**

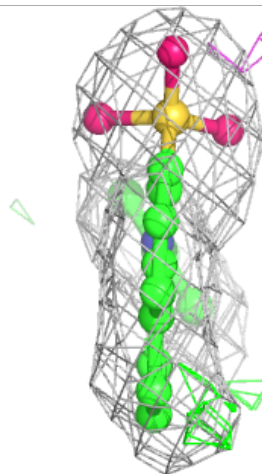
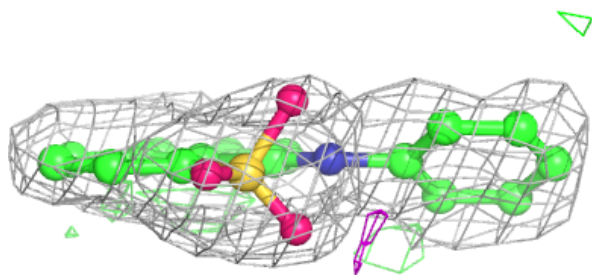
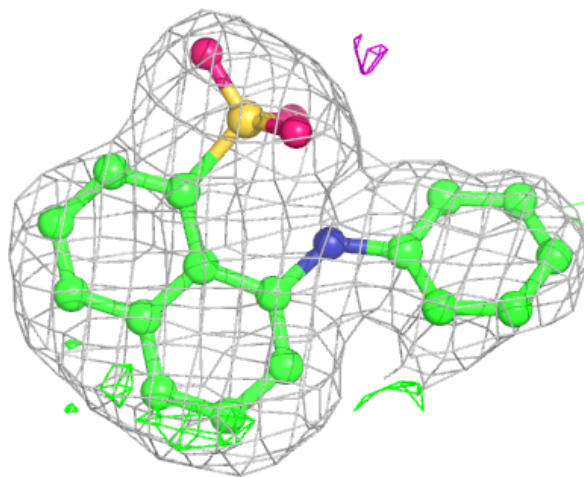
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





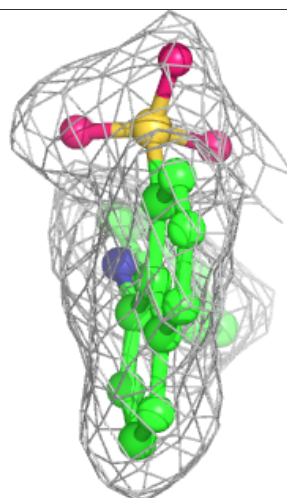
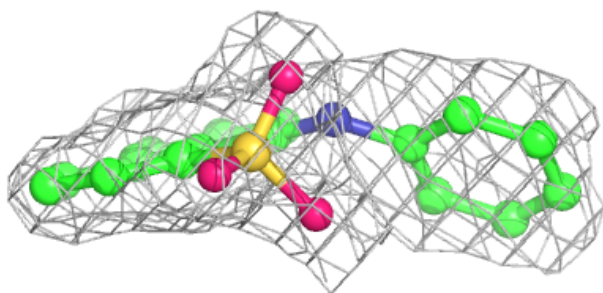
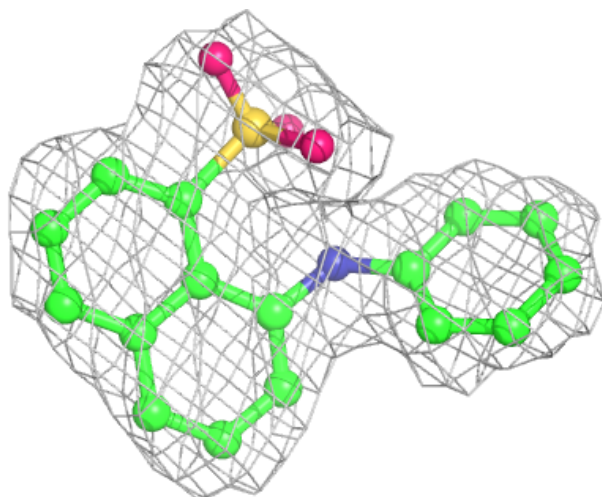
**Electron density around 2AN E 502:**

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



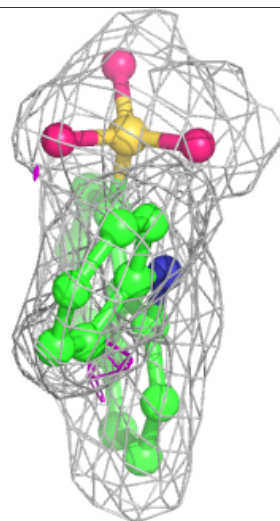
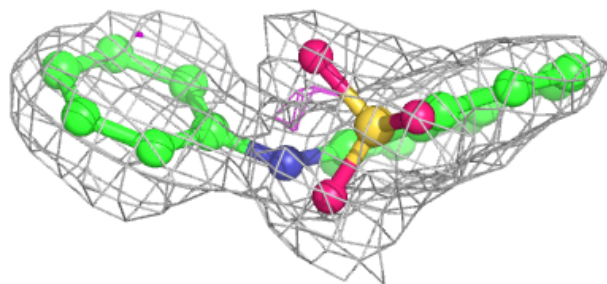
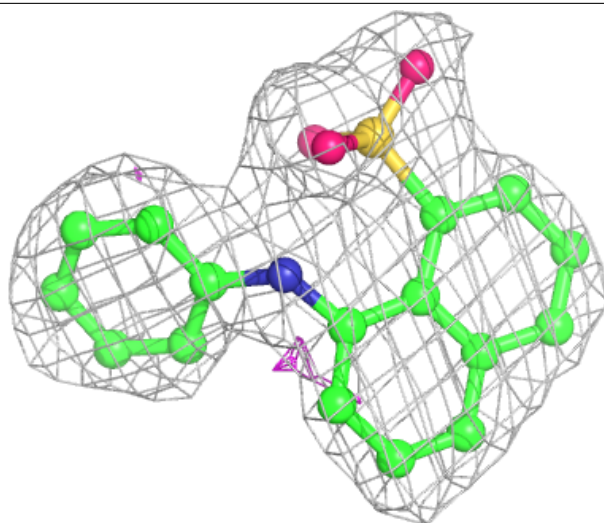
**Electron density around 2AN L 203:**

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



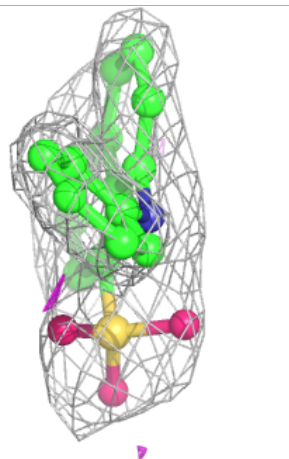
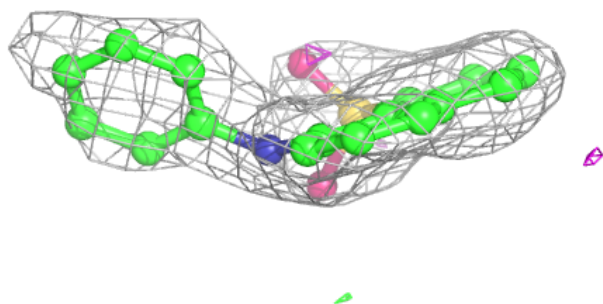
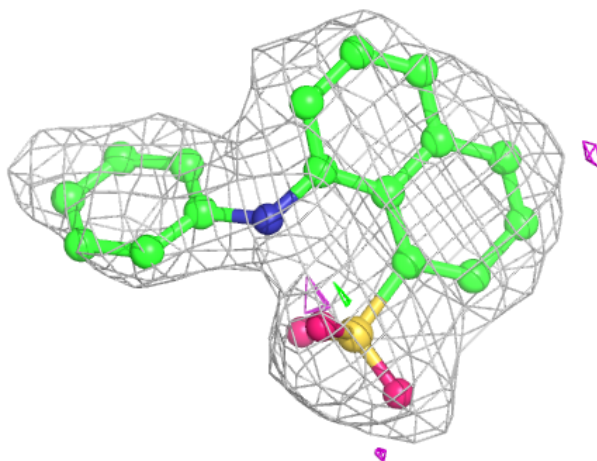
**Electron density around 2AN M 506:**

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



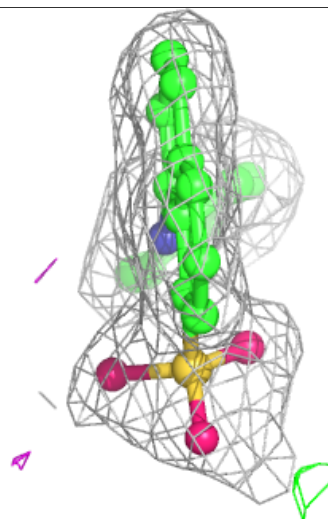
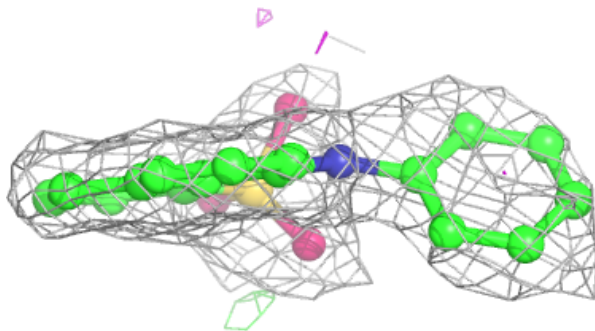
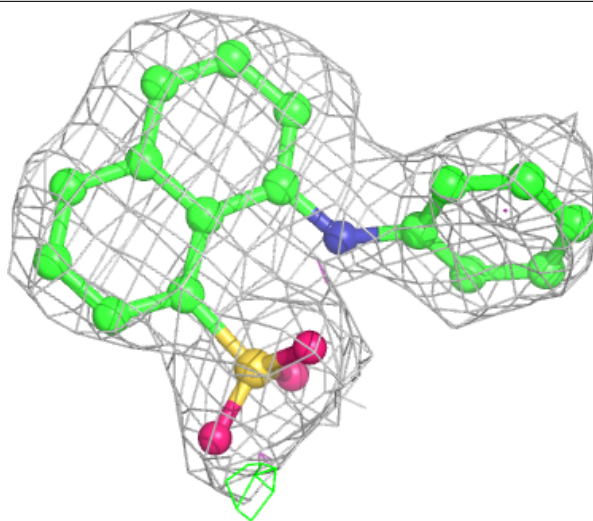
**Electron density around 2AN F 203:**

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



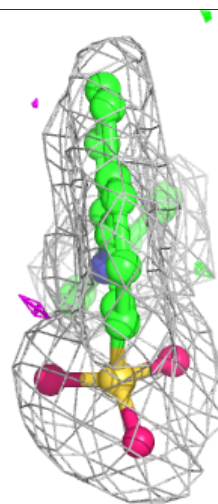
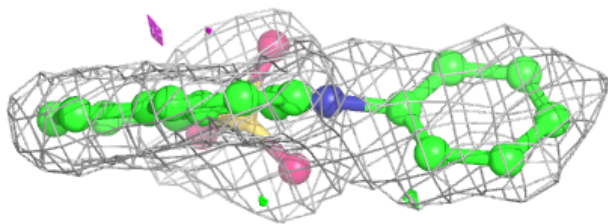
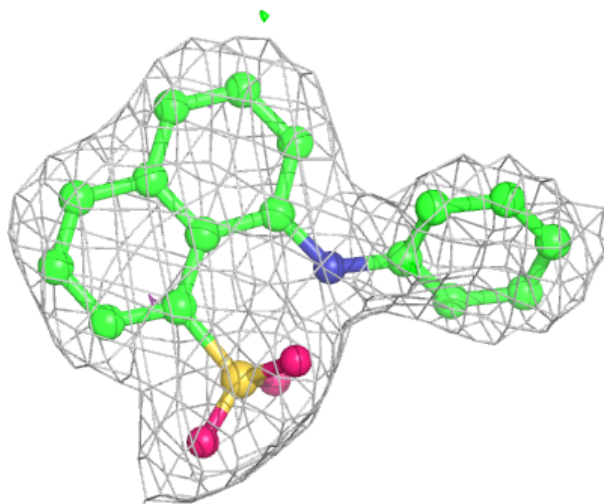
**Electron density around 2AN G 305:**

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



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

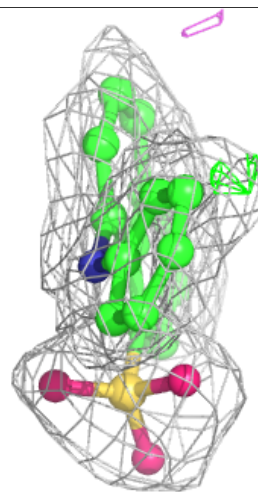
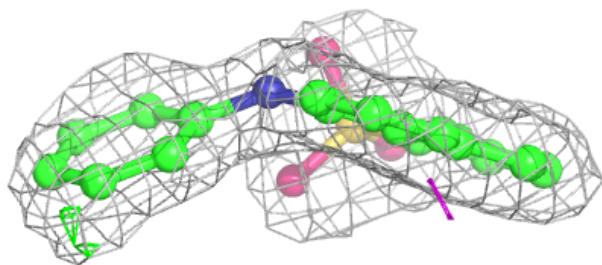
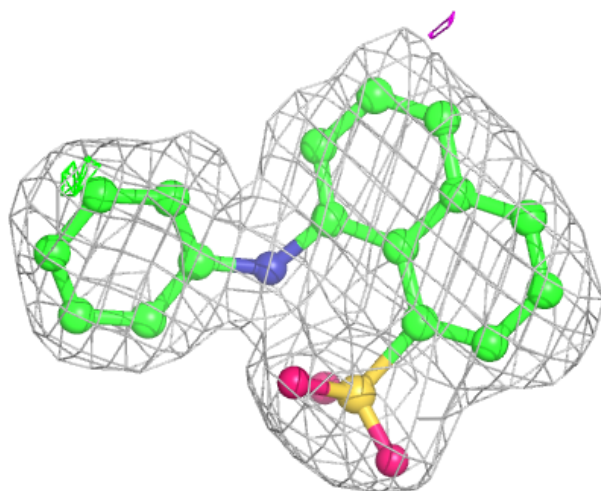
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





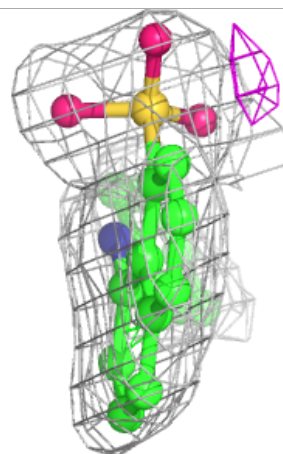
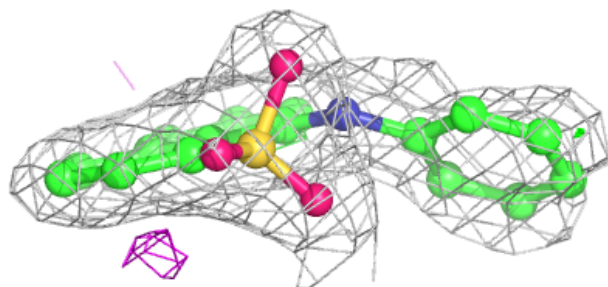
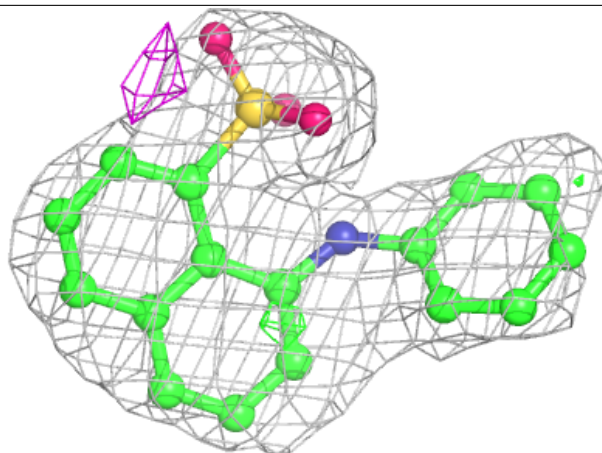
**Electron density around 2AN K 204:**

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



**Electron density around 2AN H 1108:**

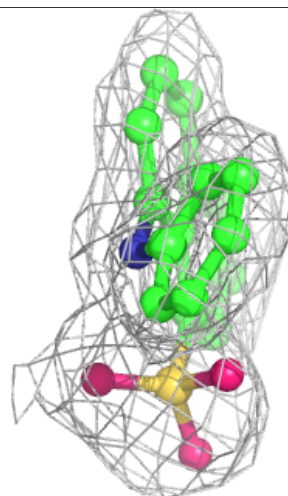
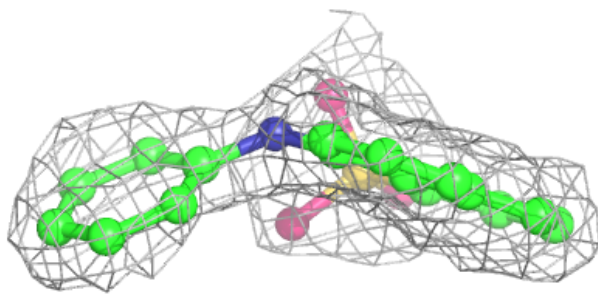
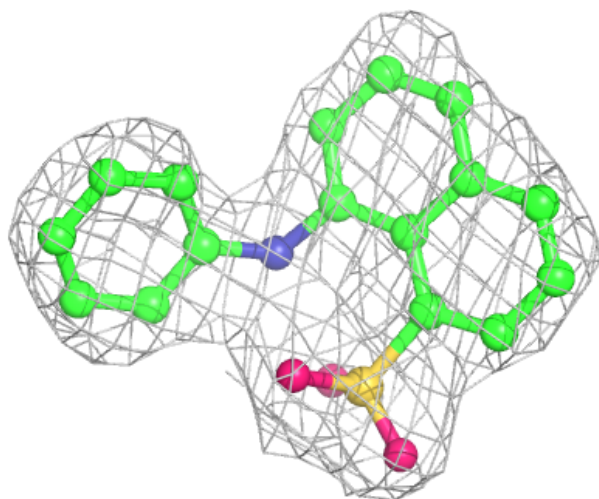
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





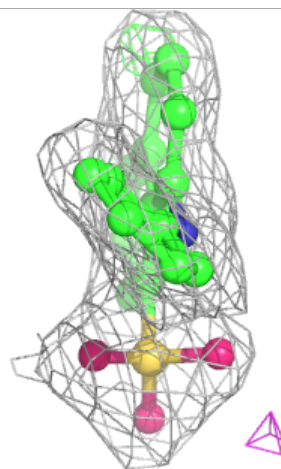
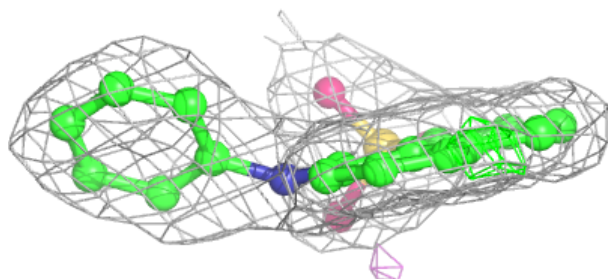
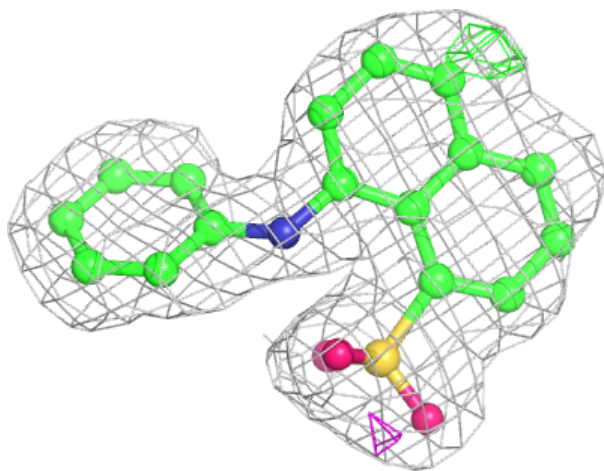
**Electron density around 2AN C 305:**

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



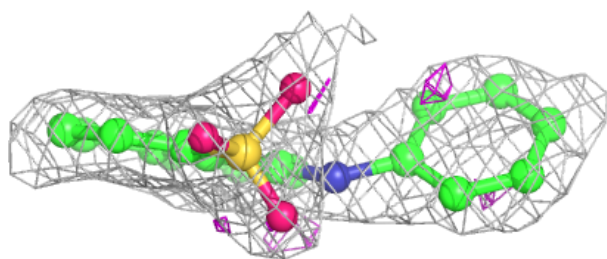
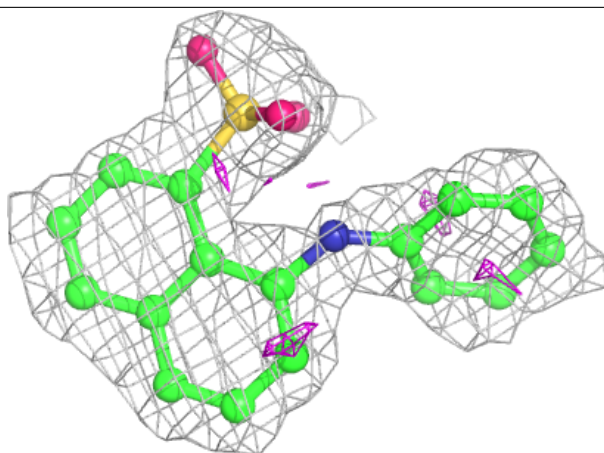
**Electron density around 2AN P 505:**

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



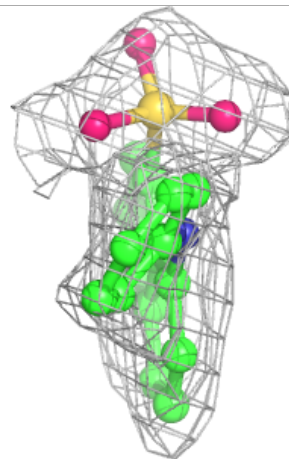
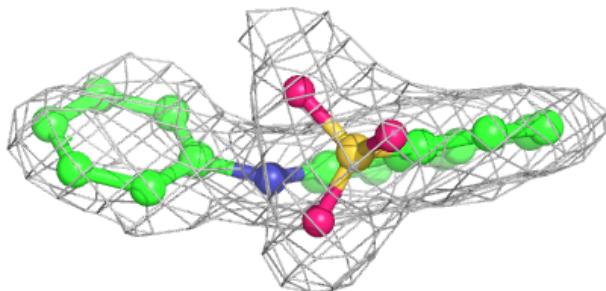
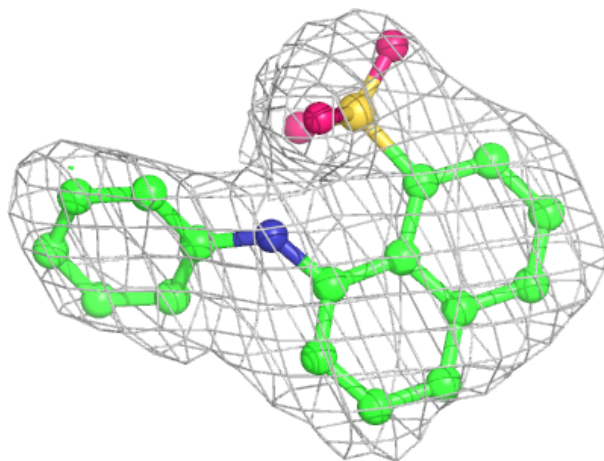
**Electron density around 2AN C 301:**

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



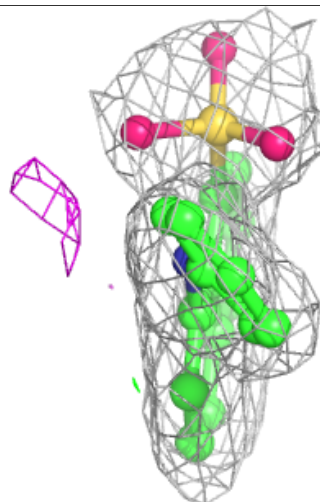
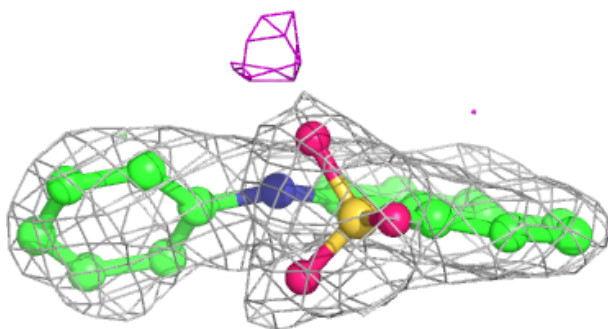
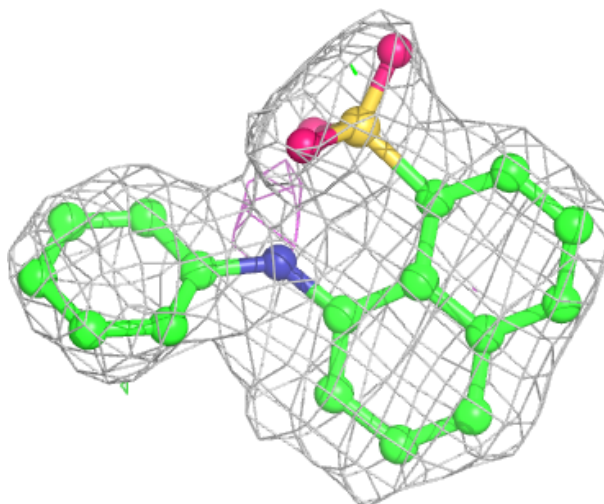
**Electron density around 2AN P 507:**

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



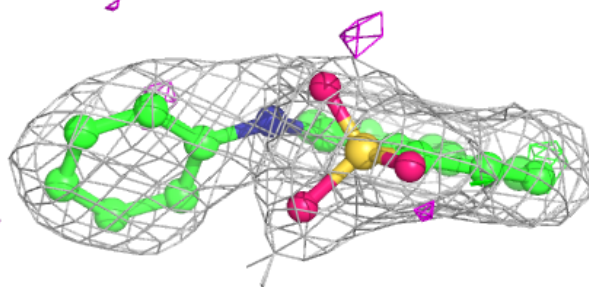
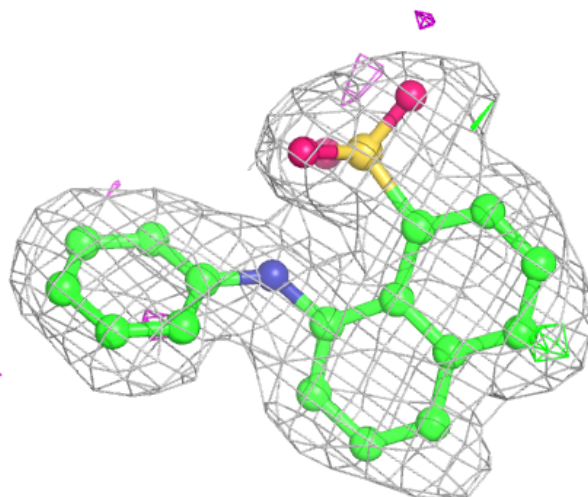
**Electron density around 2AN O 204:**

$2mF_o-DF_c$  (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:**

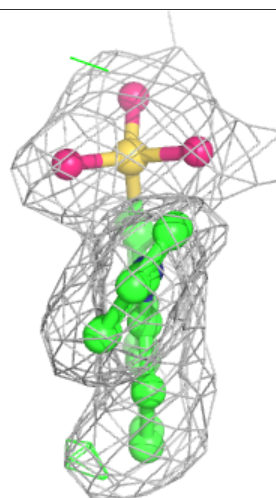
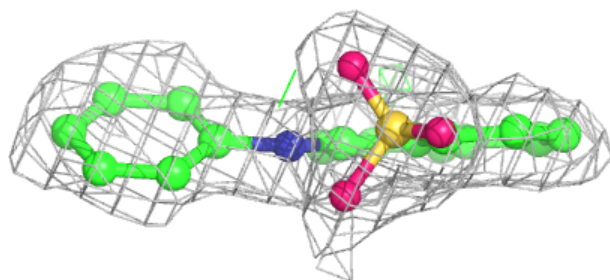
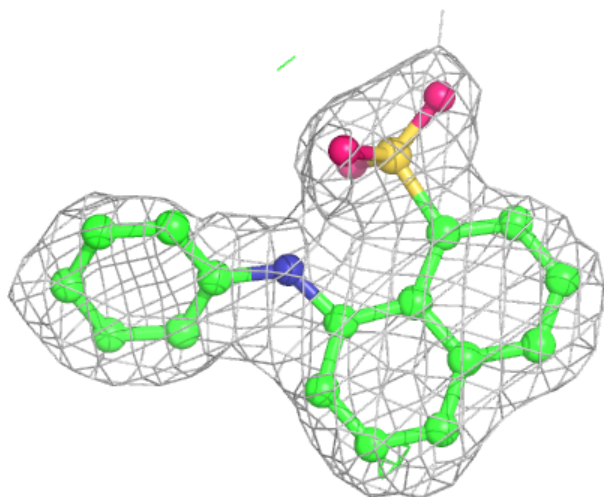
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





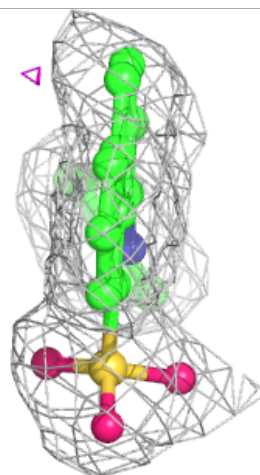
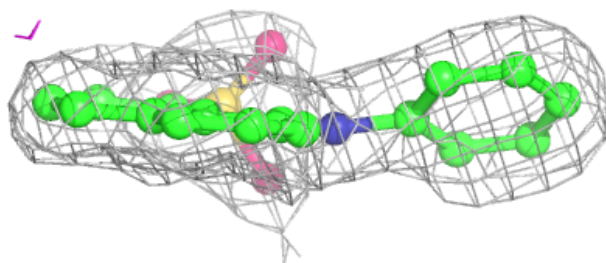
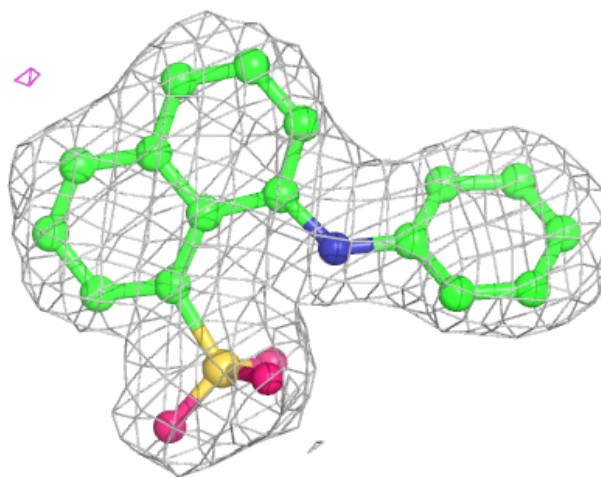
**Electron density around 2AN A 201:**

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



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

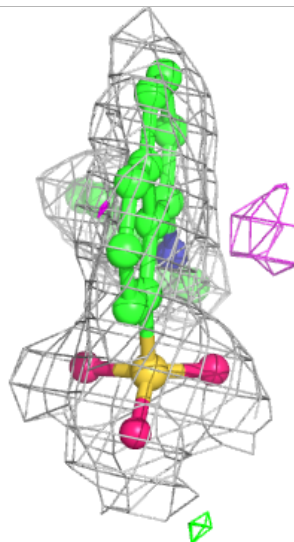
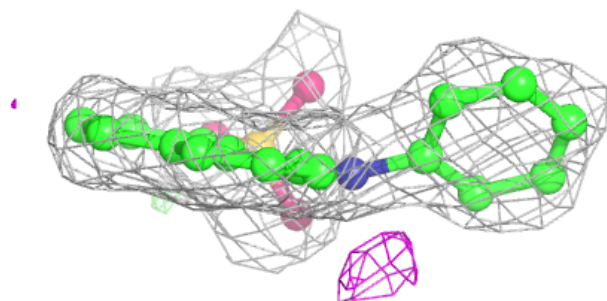
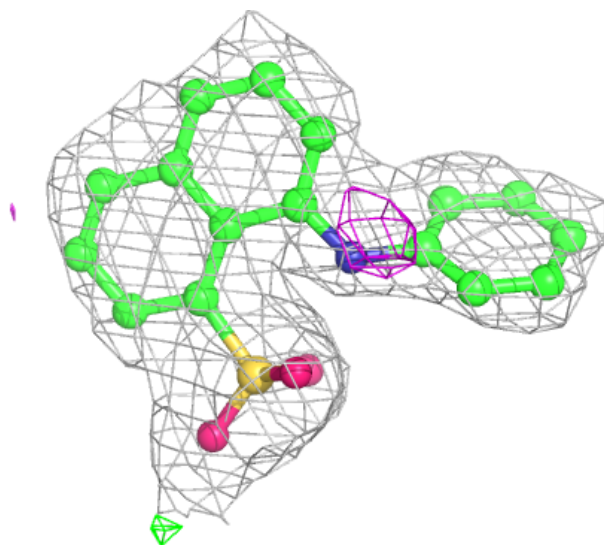
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





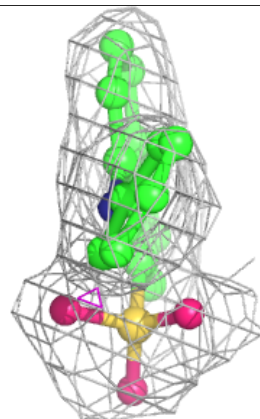
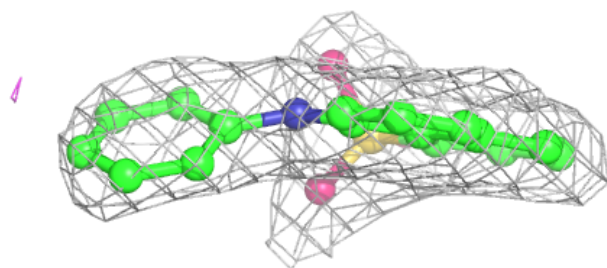
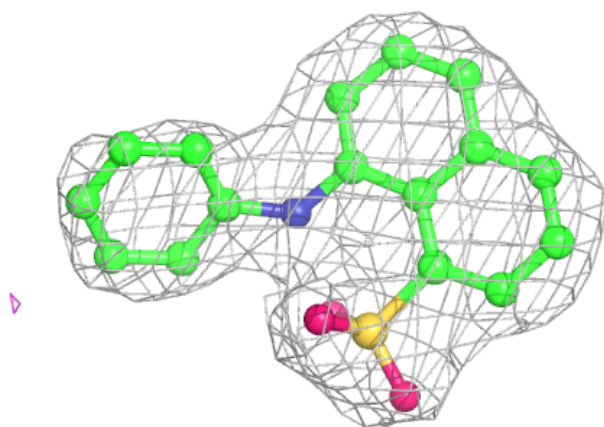
**Electron density around 2AN P 502:**

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



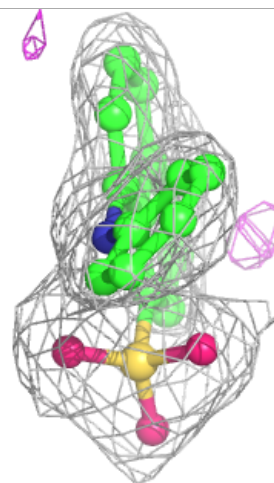
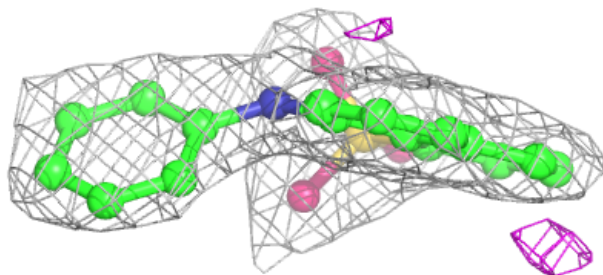
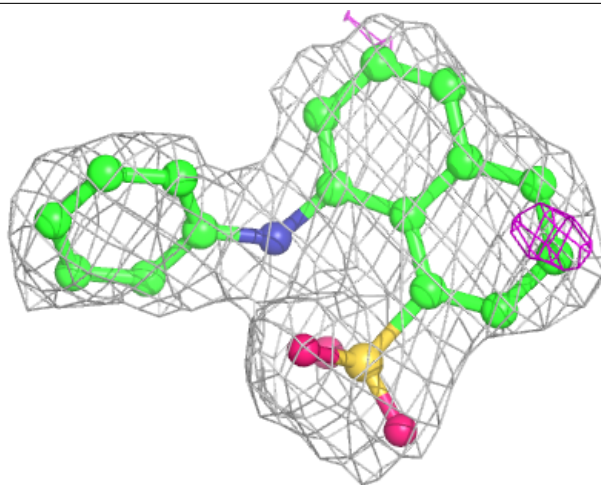
**Electron density around 2AN G 302:**

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



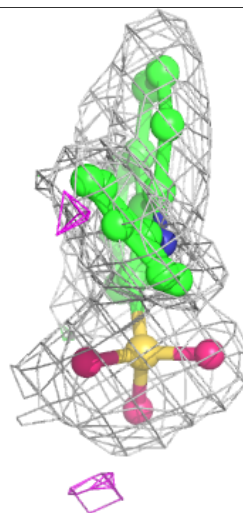
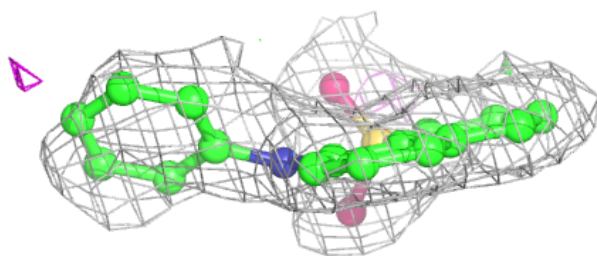
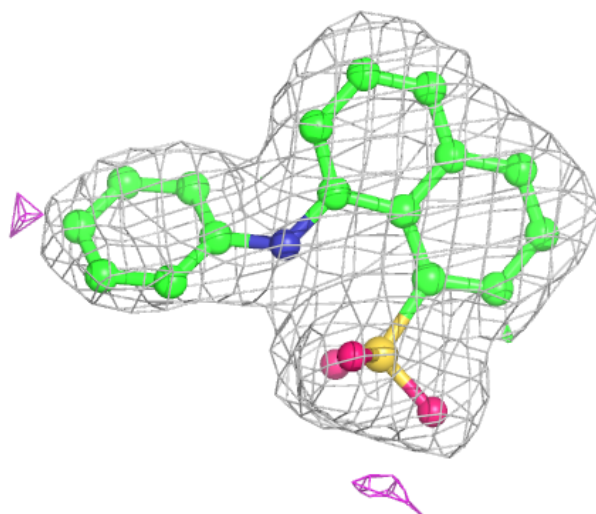
**Electron density around 2AN M 507:**

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



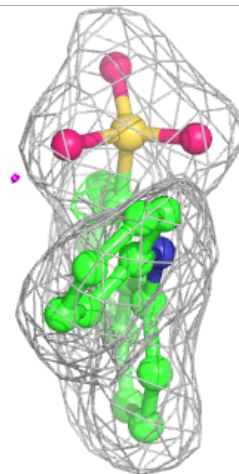
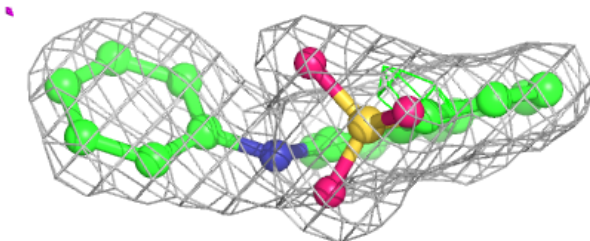
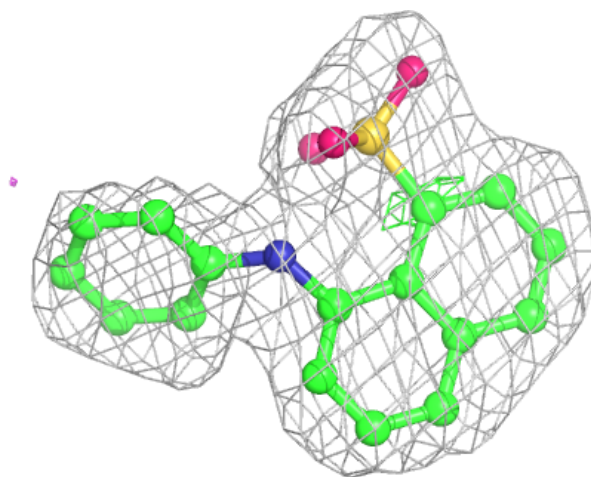
**Electron density around 2AN J 201:**

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



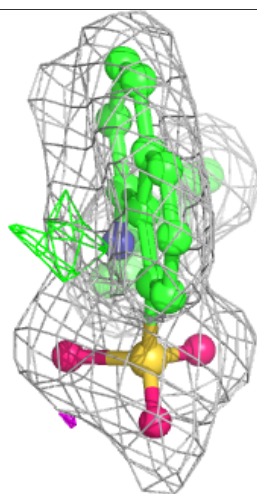
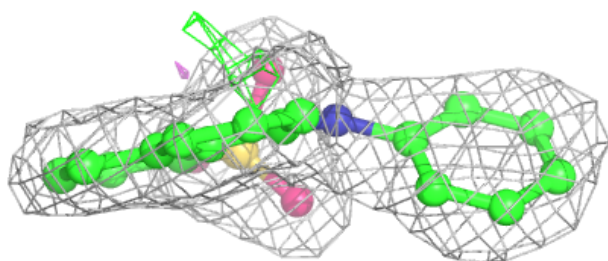
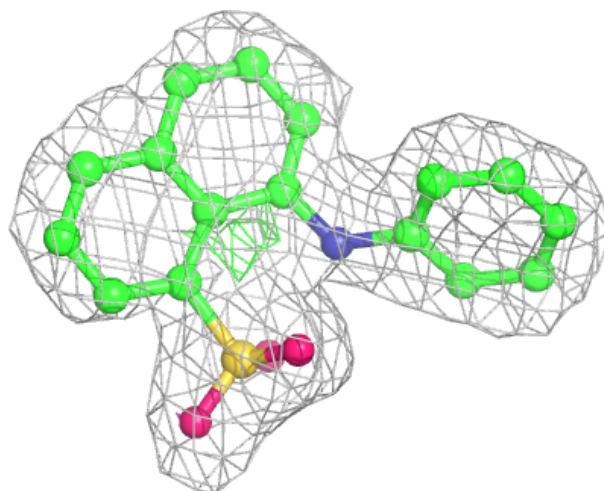
**Electron density around 2AN K 203:**

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



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

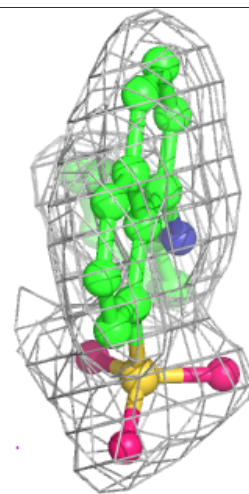
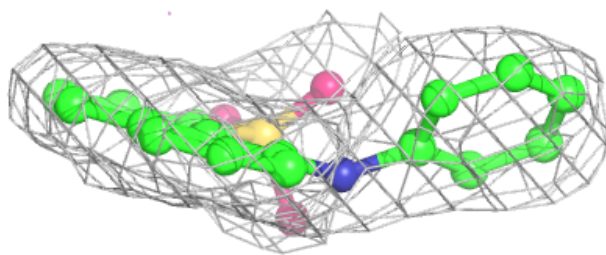
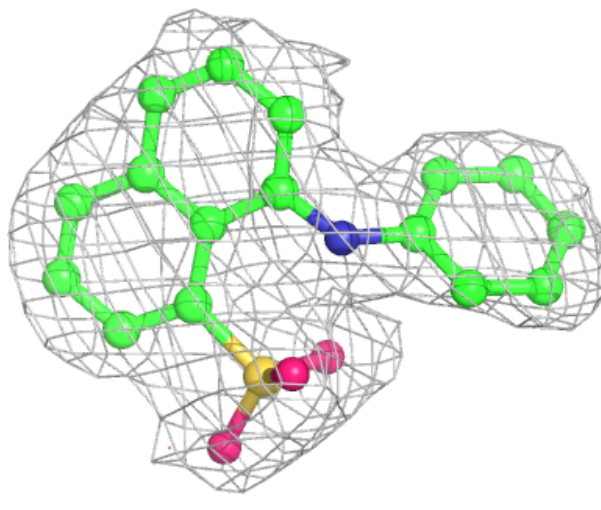
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





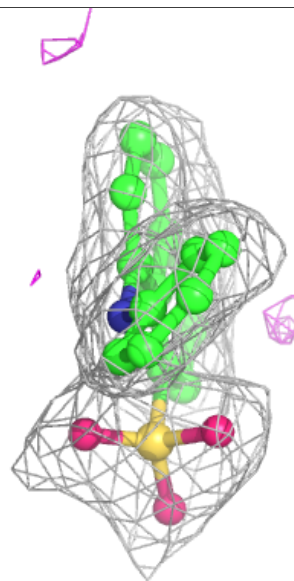
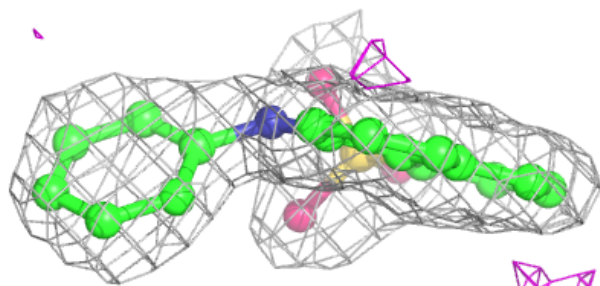
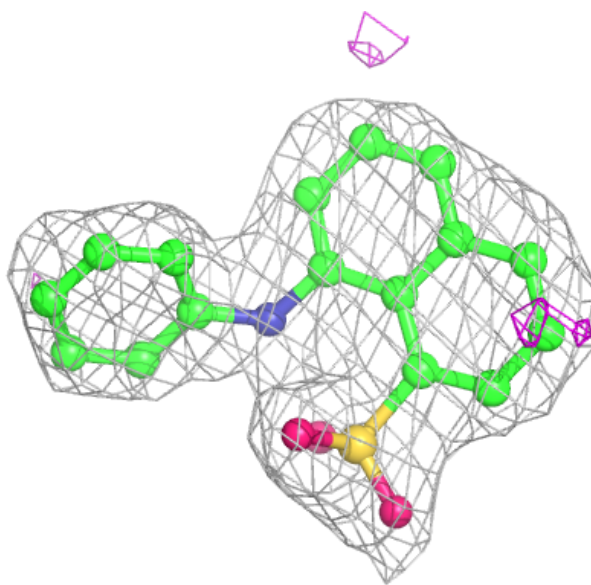
**Electron density around 2AN G 301:**

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



**Electron density around 2AN E 505:**

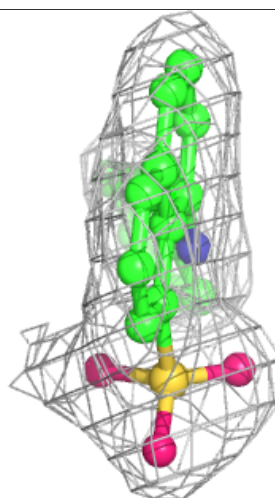
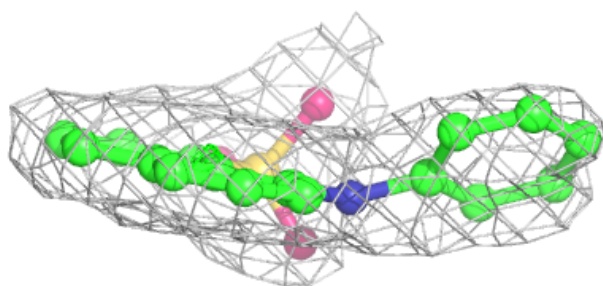
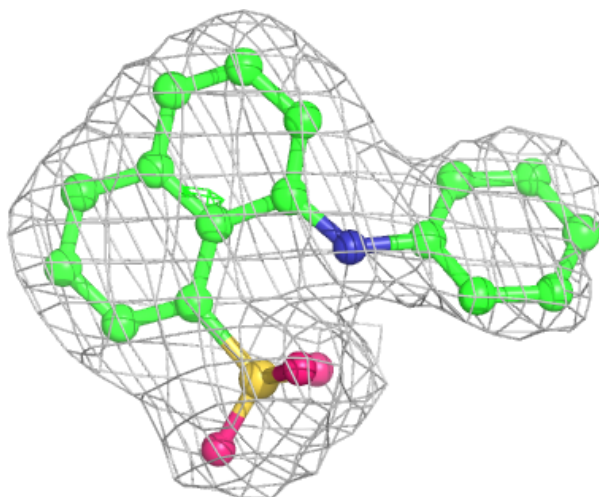
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





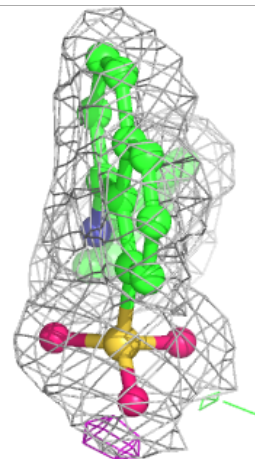
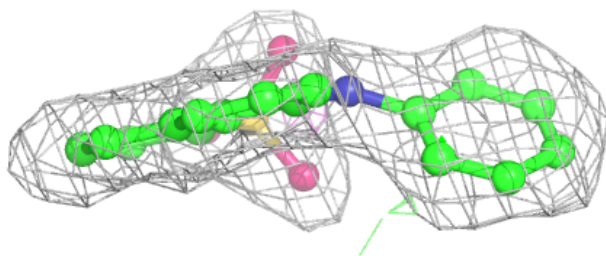
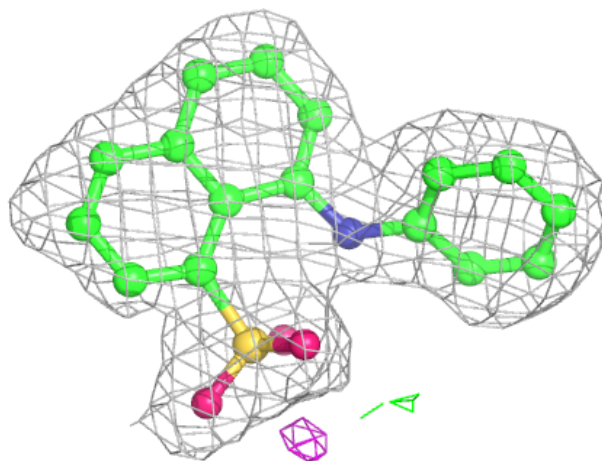
**Electron density around 2AN O 202:**

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



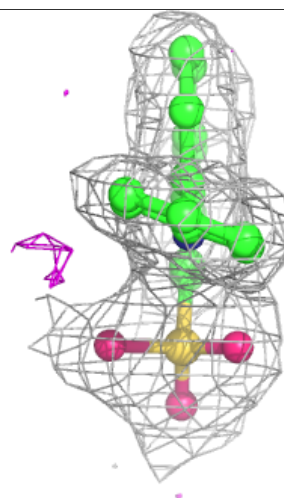
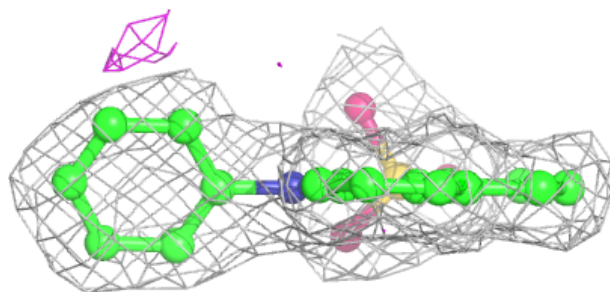
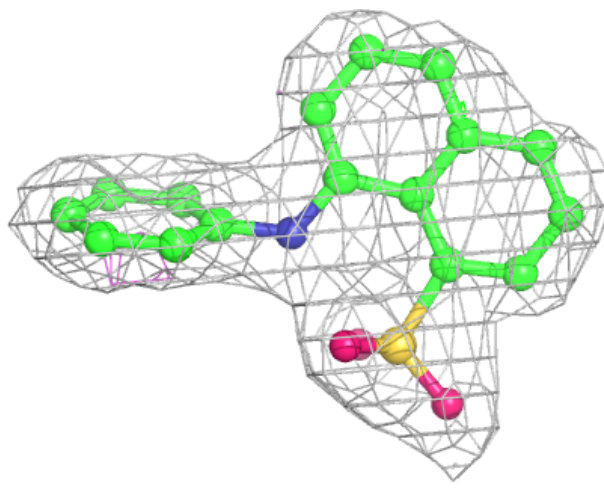
**Electron density around 2AN M 504:**

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



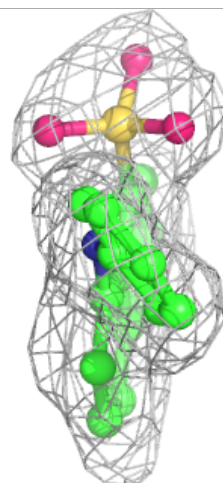
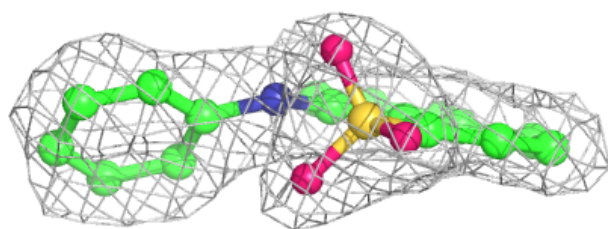
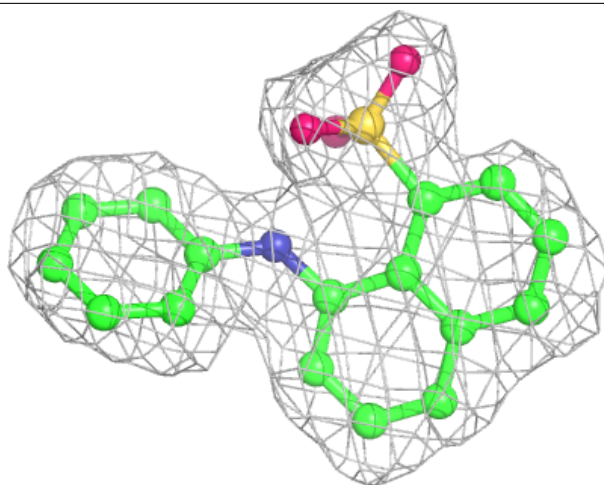
**Electron density around 2AN E 501:**

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



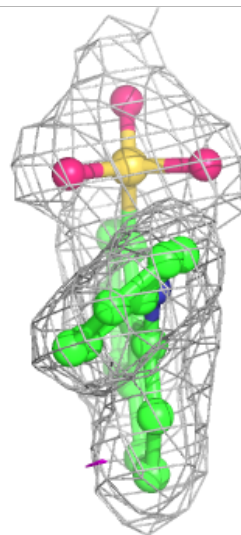
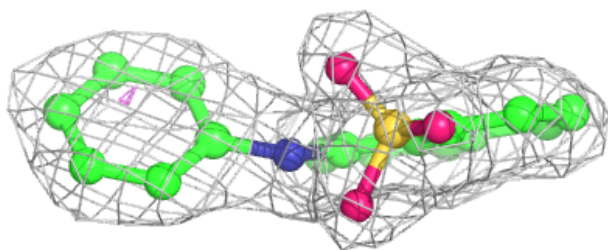
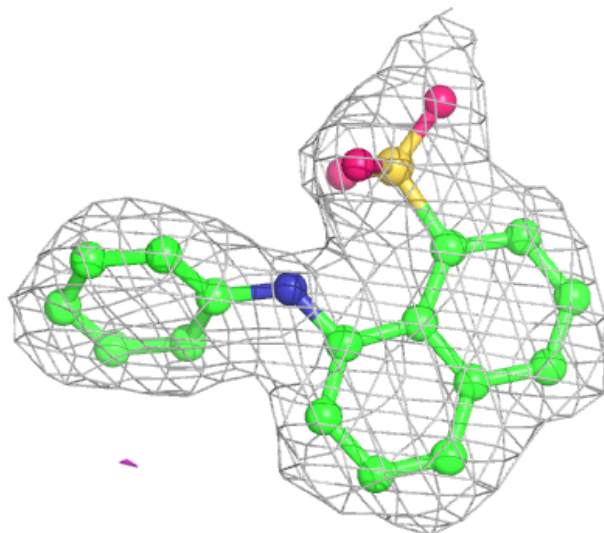
**Electron density around 2AN F 201:**

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



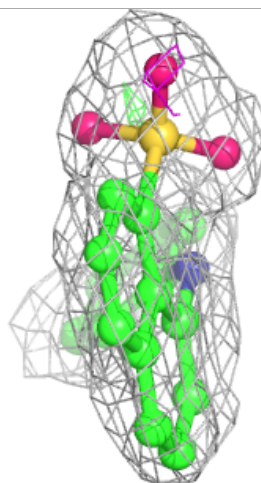
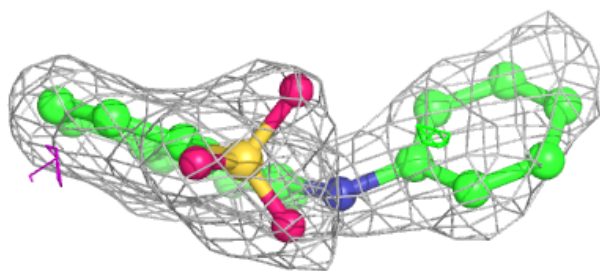
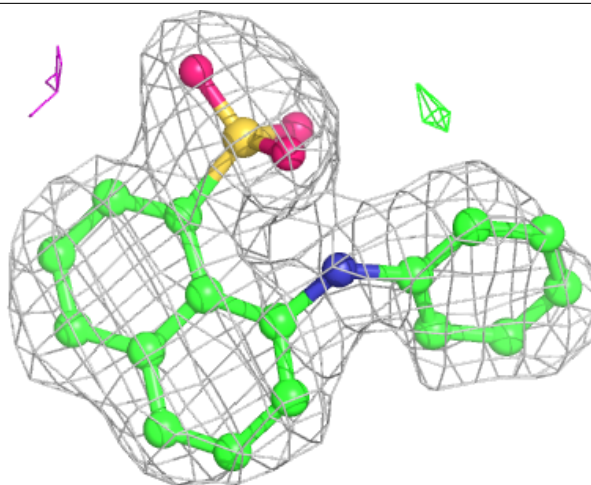
**Electron density around 2AN A 205:**

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



**Electron density around 2AN H 1103:**

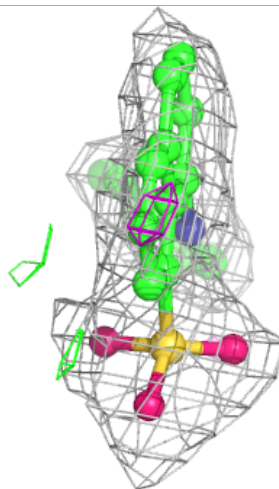
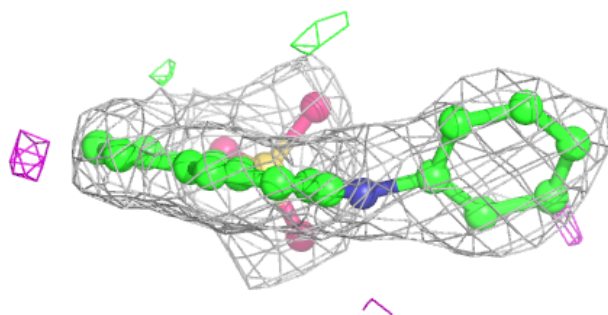
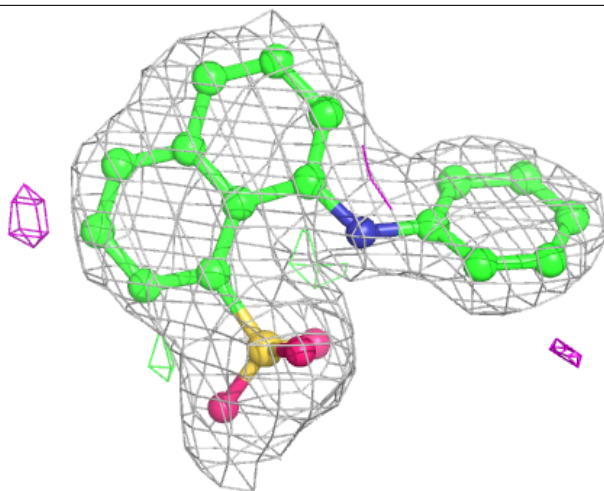
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





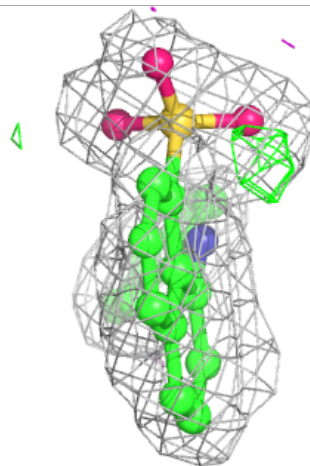
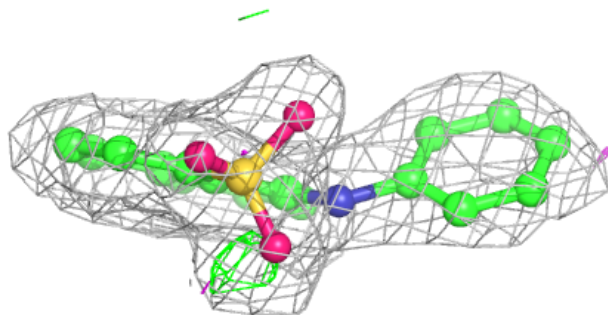
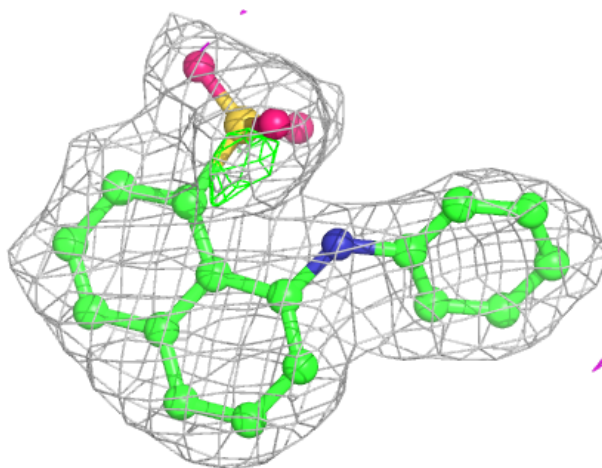
**Electron density around 2AN F 205:**

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



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

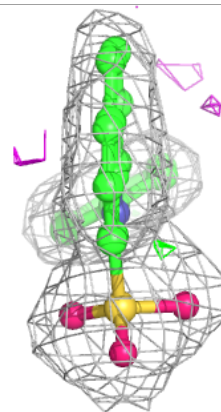
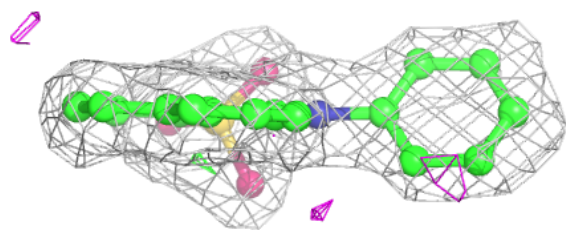
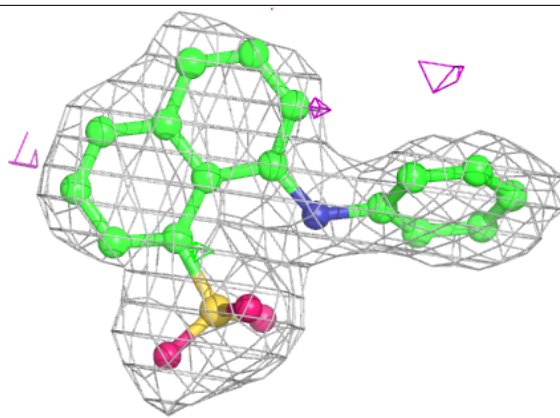
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





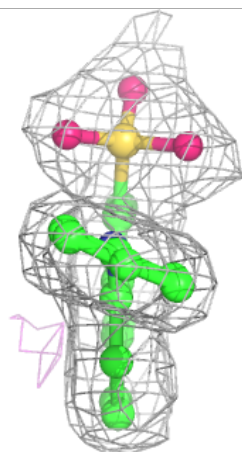
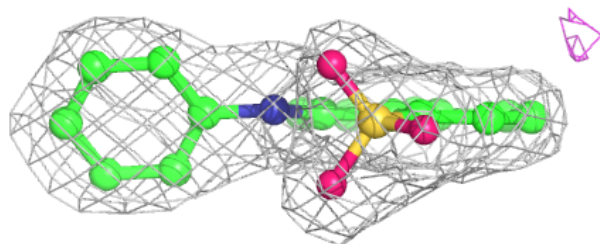
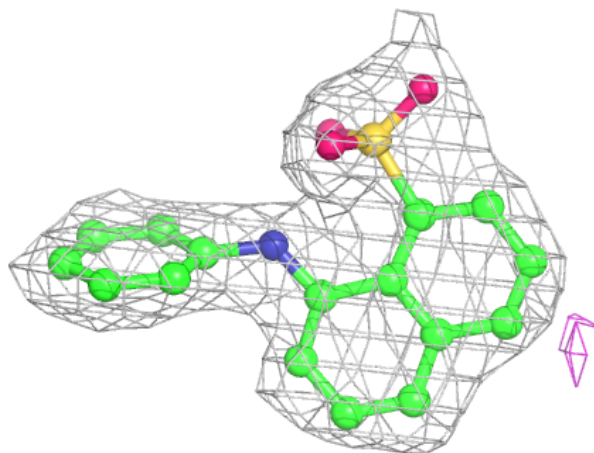
**Electron density around 2AN C 309:**

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



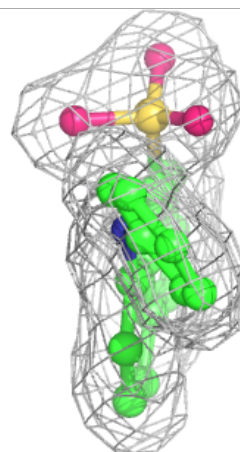
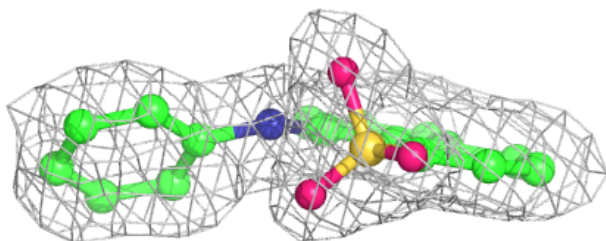
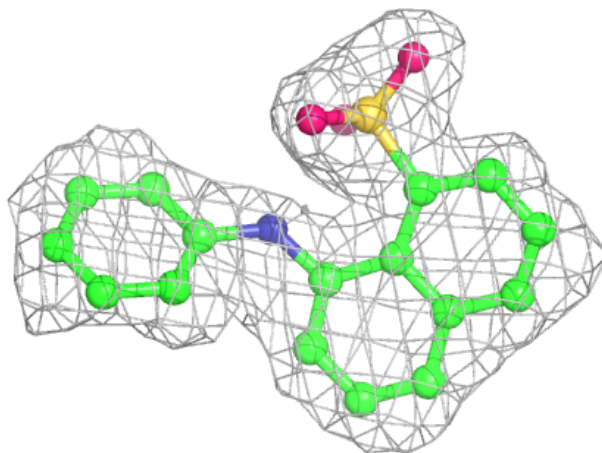
**Electron density around 2AN K 207:**

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



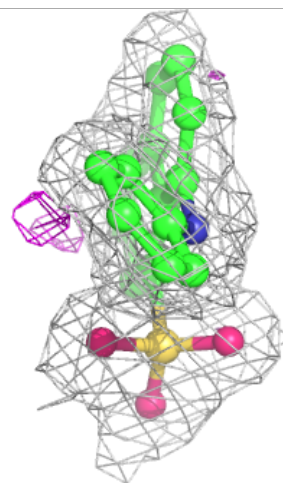
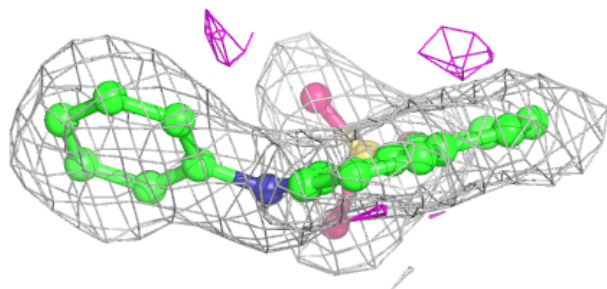
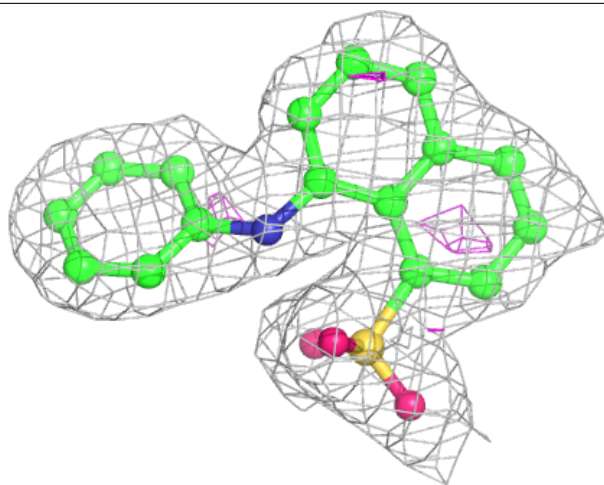
**Electron density around 2AN O 201:**

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



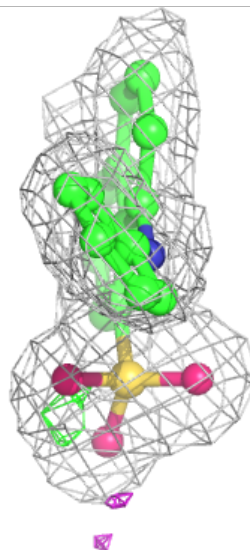
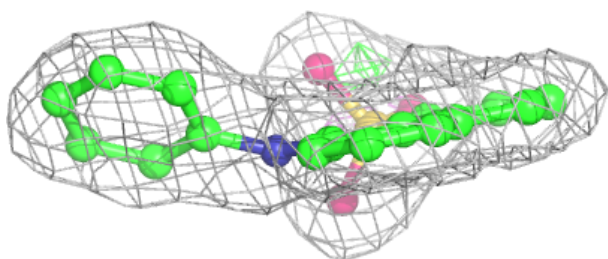
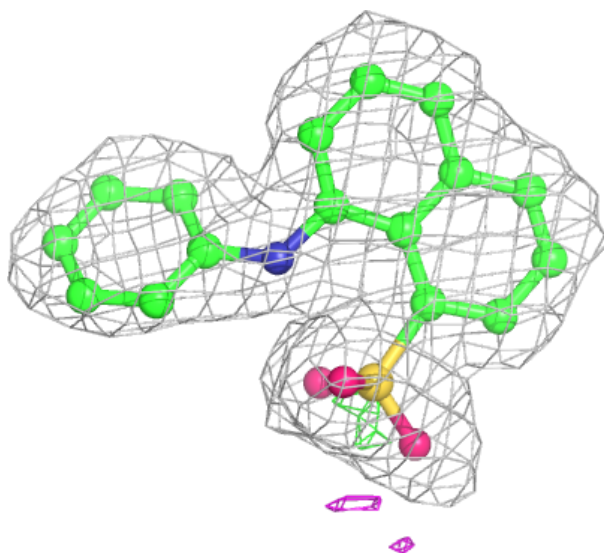
**Electron density around 2AN E 503:**

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



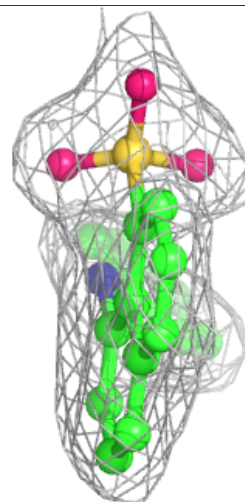
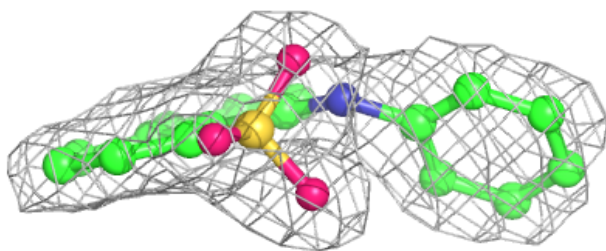
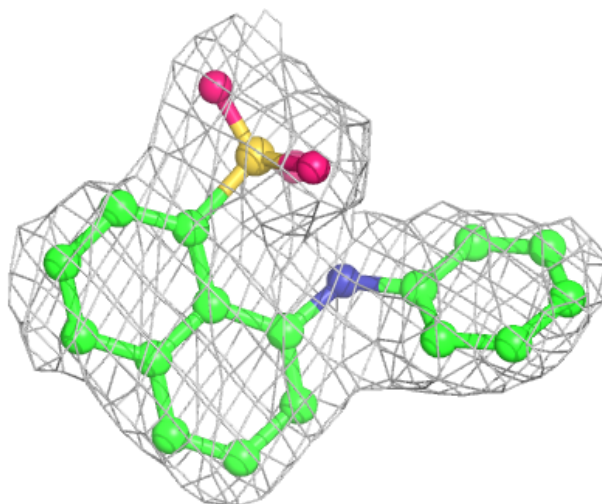
**Electron density around 2AN D 703:**

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



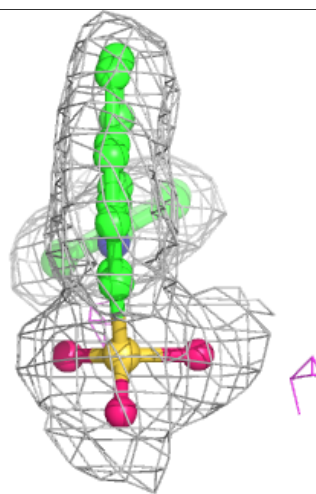
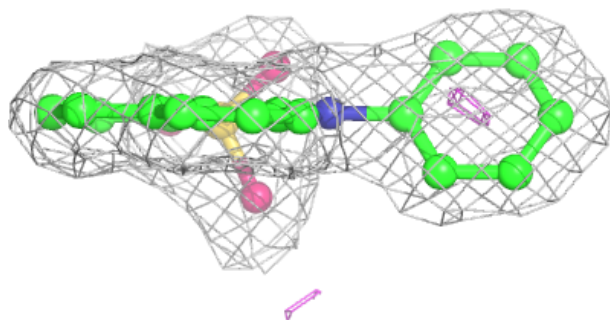
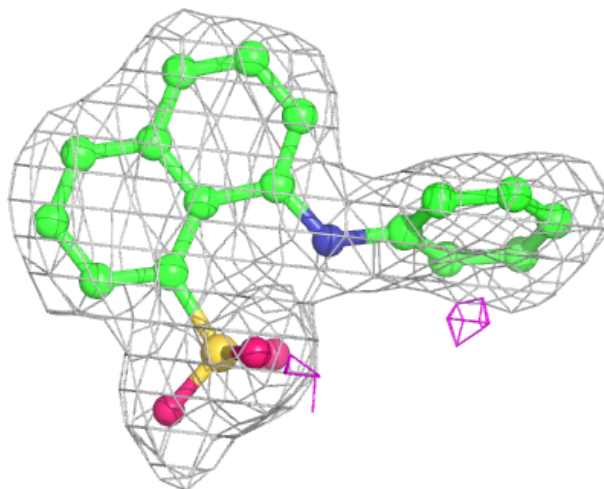
**Electron density around 2AN C 304:**

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



**Electron density around 2AN M 501:**

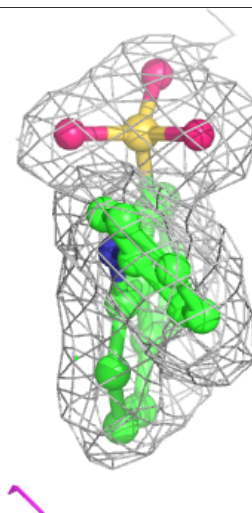
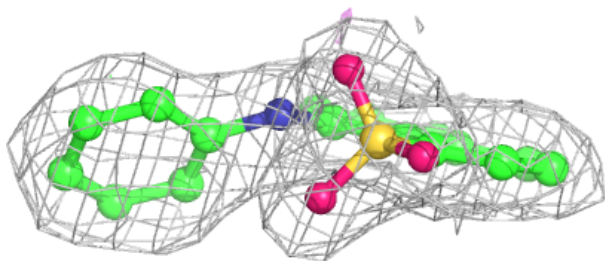
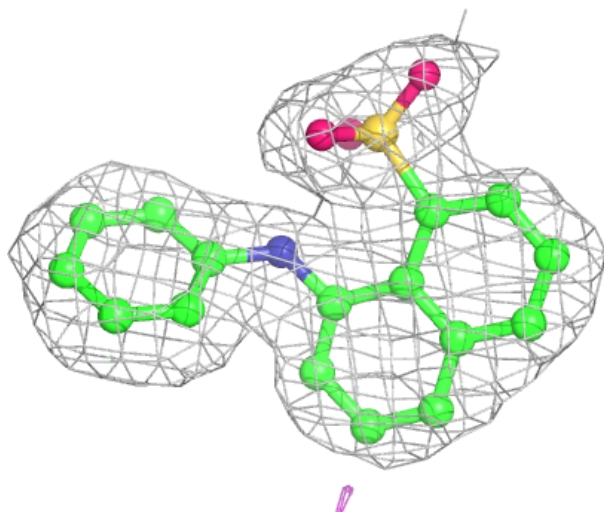
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around 2AN C 302:**

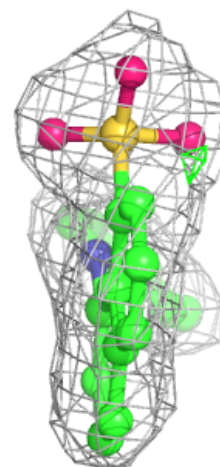
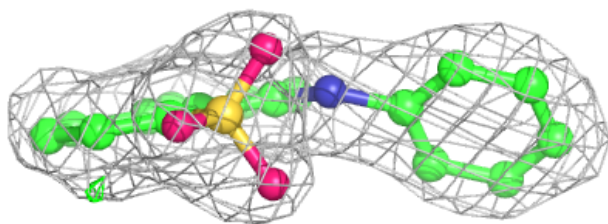
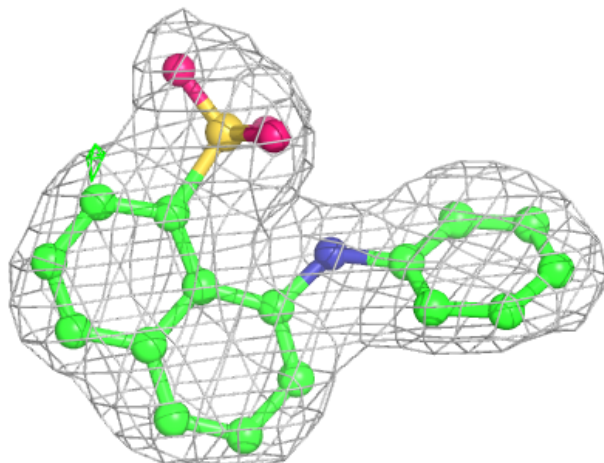
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





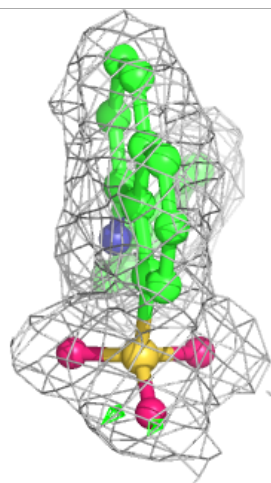
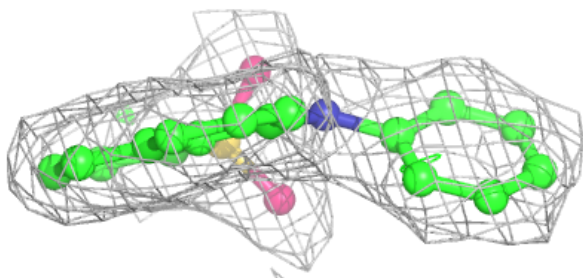
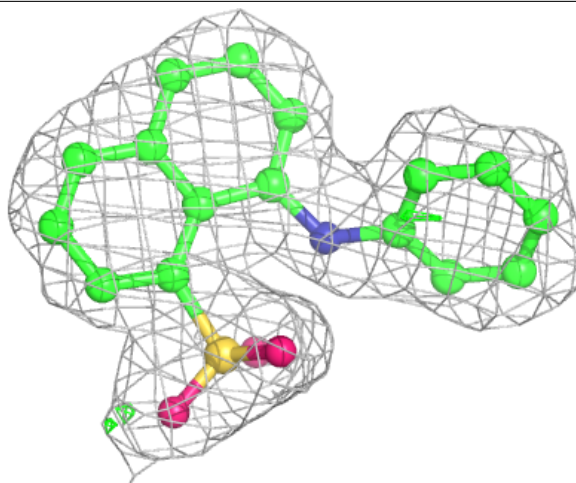
**Electron density around 2AN I 204:**

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



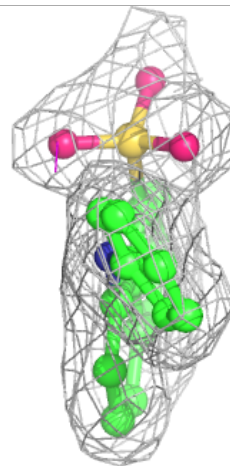
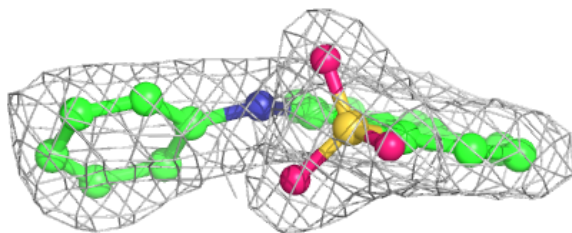
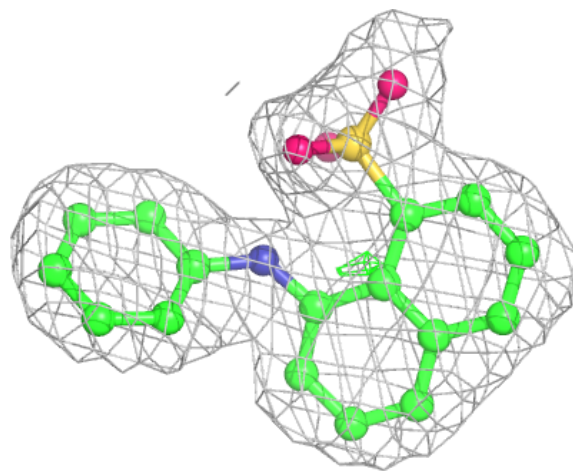
**Electron density around 2AN K 201:**

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



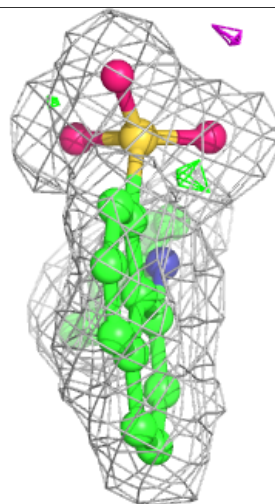
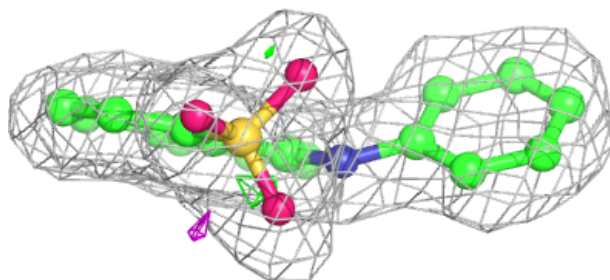
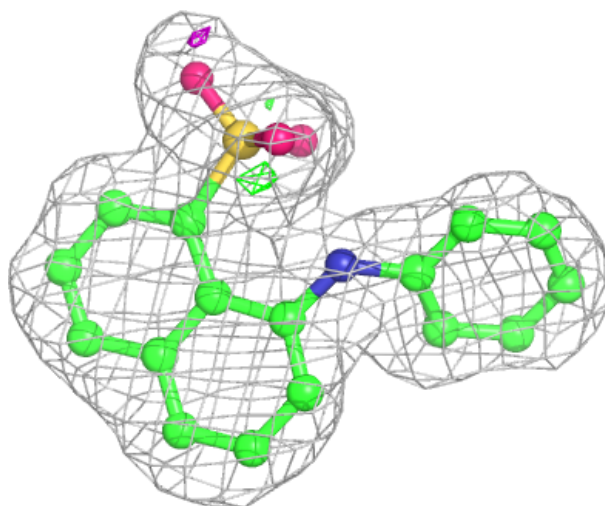
**Electron density around 2AN I 201:**

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



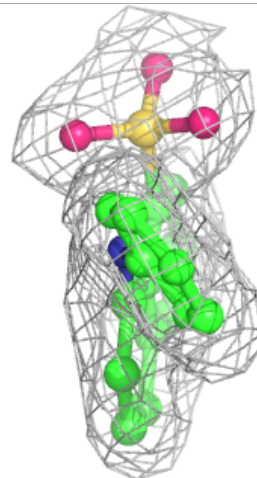
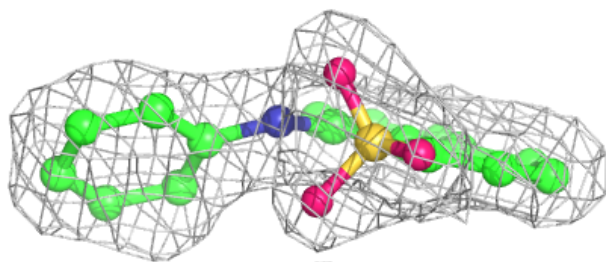
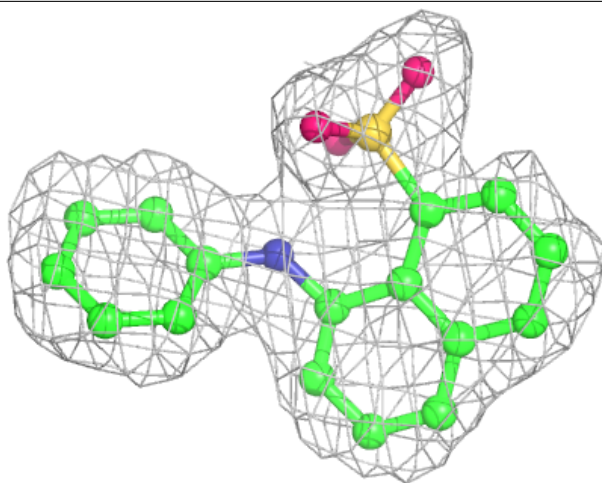
**Electron density around 2AN L 201:**

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



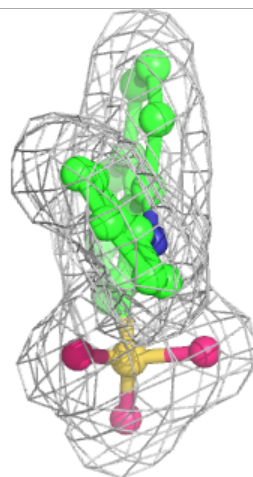
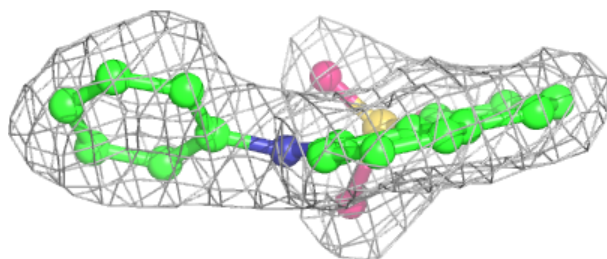
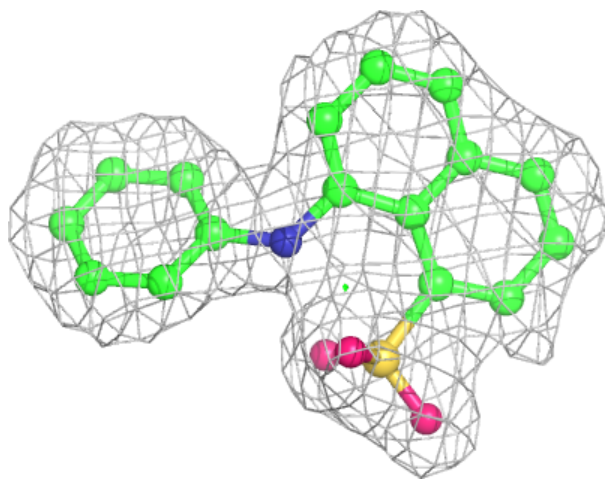
**Electron density around 2AN H 1102:**

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

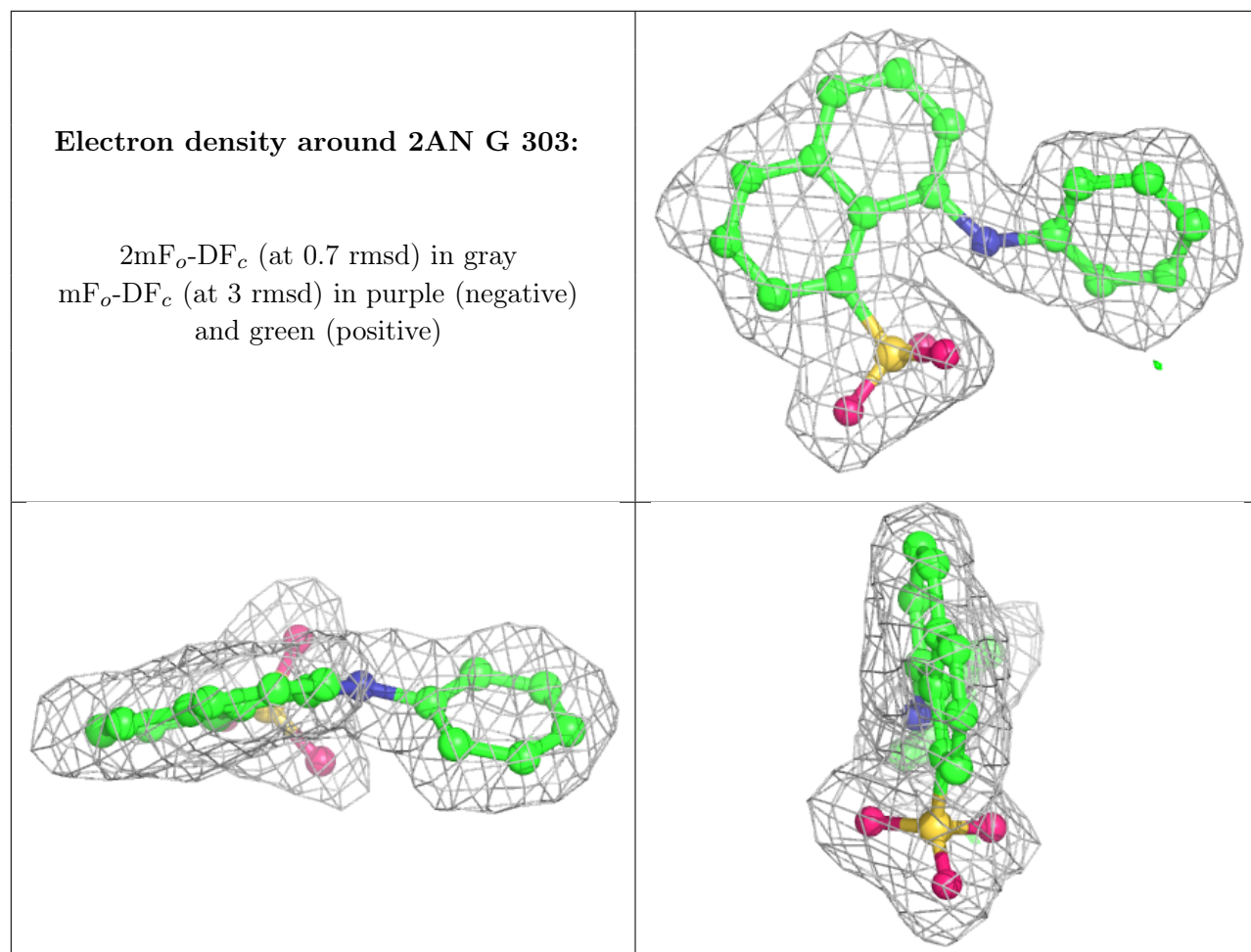


**Electron density around 2AN P 504:**

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







## 6.5 Other polymers [i](#)

There are no such residues in this entry.