# wwPDB NMR Structure Validation Summary Report

Jun 17, 2020 – 04:45 am BST

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|---|---|---|
| PDB ID | : | 2V93 |
| Title | : | EQUILLIBRIUM MIXTURE OF OPEN AND PARTIALLY-CLOSED SPECIES IN THE APO STATE OF MALTODEXTRIN-BINDING PROTEIN BY PARAMAGNETIC RELAXATION ENHANCEMENT NMR |
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| Deposited on | : | 2007-08-21 |

This is a wwPDB NMR Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/NMRValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

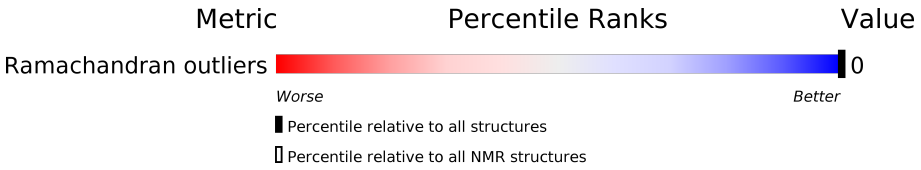
| | | |
|---|---|---|
| Cyrange | : | Kirchner and Güntert (2011) |
| NmrClust | : | Kelley et al. (1996) |
| MolProbity | : | 4.02b-467 |
| Mogul | : | 1.8.5 (274361), CSD as541be (2020) |
| buster-report | : | 1.1.7 (2018) |
| Percentile statistics | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| RCI | : | v_1n_11_5_13_A (Berjanski et al., 2005) |
| PANAV | : | Wang et al. (2010) |
| ShiftChecker | : | 2.11 |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | 2.11 |

# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
*SOLUTION NMR*

The overall completeness of chemical shifts assignment was not calculated.

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) | NMR archive (#Entries) |
|---|---|---|
| Ramachandran outliers | 154571 | 11451 |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and 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 <=5%

| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | A | 370 | 95% |

## 2 Ensemble composition and analysis

This entry contains 50 models. The atoms present in the NMR models are not consistent. Some calculations may have failed as a result. All residues are included in the validation scores. Model 39 is the overall representative, medoid model (most similar to other models).

The following residues are included in the computation of the global validation metrics.

| Well-defined (core) protein residues | | | |
|---|---|---|---|
| **Well-defined core** | **Residue range (total)** | **Backbone RMSD (Å)** | **Medoid model** |
| 1 | A:81-A:87, A:103-A:105, A:266-A:268, A:311-A:313 (16) | -0.00 | 39 |

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

NmrClust was unable to cluster the ensemble.

Error message: No clusters in NmrClust output

# 3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3792 atoms, of which 1003 are hydrogens and 0 are deuteriums.

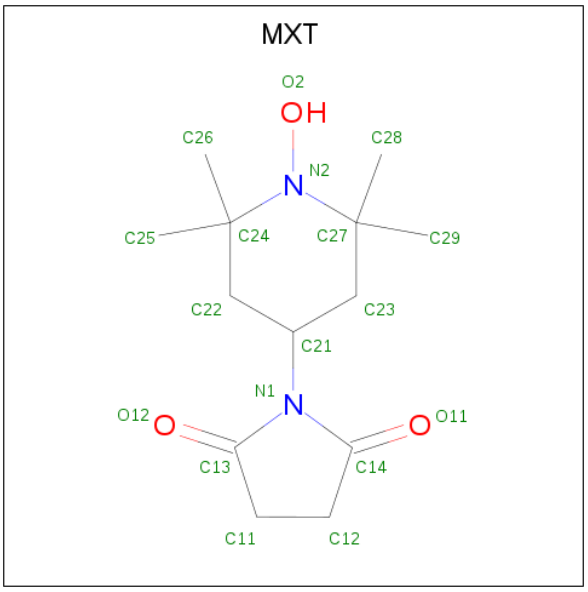
- Molecule 1 is a protein called MALTOSE-BINDING PERIPLASMIC PROTEIN.

| Mol | Chain | Residues | Atoms | | | | | | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 1 | A | 366 | Total | C | H | N | O | S | 0 |
| | | | 2904 | 1169 | 547 | 583 | 581 | 24 | |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| A | 41 | CYS | ASP | engineered mutation | UNP P0AEY0 |
| A | 211 | CYS | SER | engineered mutation | UNP P0AEY0 |

- Molecule 2 is 1-(1-HYDROXY-2,2,6,6-TETRAMETHYLPIPERIDIN-4-YL)PYRROLIDIN E-2,5-DIONE (three-letter code: MXT) (formula: $C_{13}H_{22}N_2O_3$).




| Mol | Chain | Residues | Atoms | | | | |
|---|---|---|---|---|---|---|---|
| 2 | A | 1 | Total | C | H | N | O |
| | | | 444 | 156 | 228 | 24 | 36 |
| 2 | A | 1 | Total | C | H | N | O |
| | | | 444 | 156 | 228 | 24 | 36 |

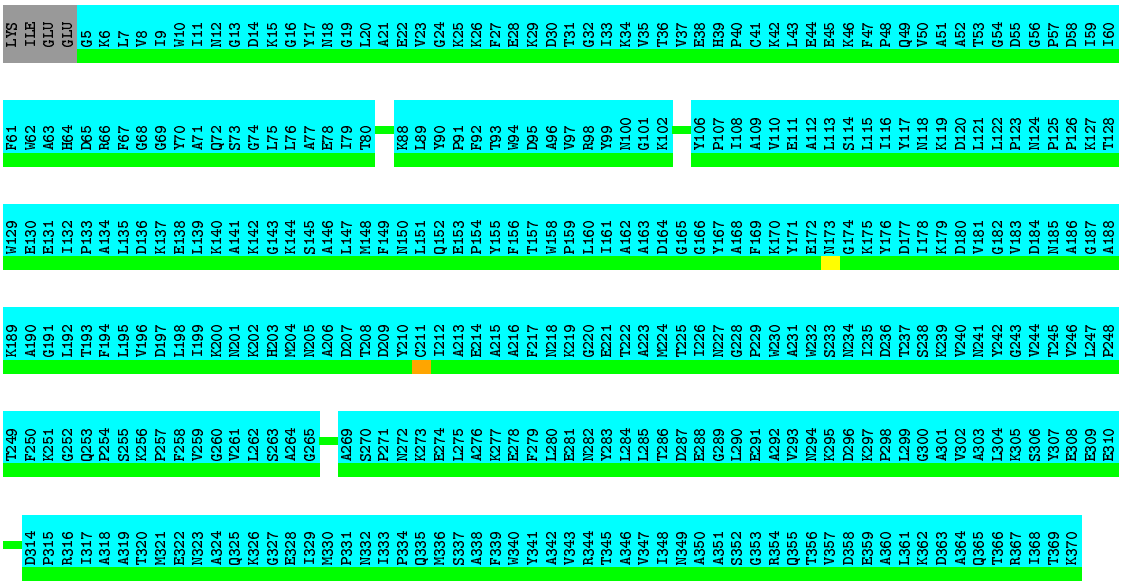
# 4 Residue-property plots

## 4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA and DNA chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-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. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

- Molecule 1: MALTOSE-BINDING PERIPLASMIC PROTEIN

Chain A:

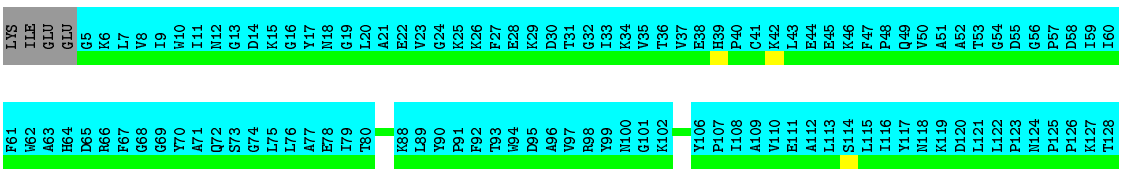



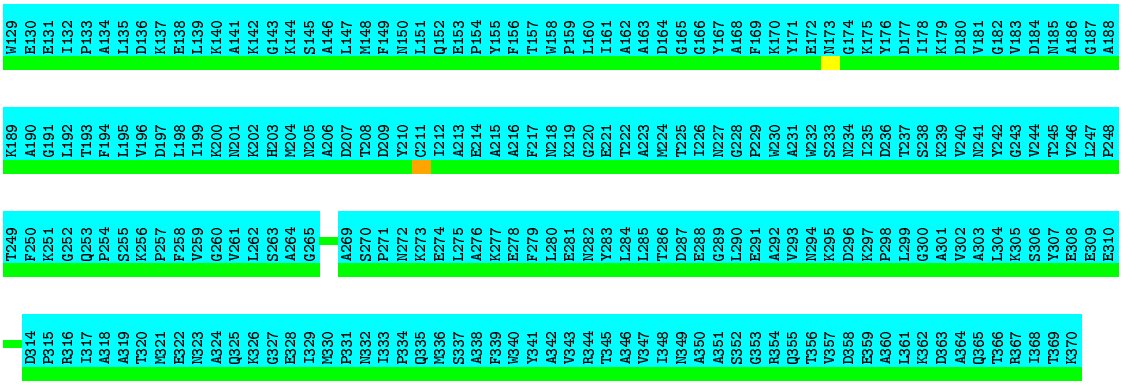
## 4.2 Residue scores for the representative (medoid) model from the NMR ensemble

The representative model is number 39. Colouring as in section 4.1 above.

- Molecule 1: MALTOSE-BINDING PERIPLASMIC PROTEIN

Chain A:


W129 E130 E131 I132 P133 A134 L135 D136 K137 E138 L139 K140 A141 K142 G143 K144 S145 A146 L147 M148 F149 N150 L151 Q152 E153 P154 Y155 F156 T157 W158 P159 L160 I161 A162 A163 D164 G165 G166 Y167 A168 F169 K170 Y171 E172 N173 G174 K175 Y176 D177 I178 K179 D180 V181 G182 V183 D184 N185 A186 G187 A188
K189 A190 G191 L192 T193 F194 L195 V196 D197 L198 I199 K200 N201 K202 E203 M204 N205 A206 D207 T208 D209 Y210 C211 I212 A213 E214 A215 A216 F217 N218 K219 G220 E221 T222 A223 M224 T225 I226 N227 G228 P229 W230 A231 W232 S233 N234 I235 D236 T237 S238 K239 V240 N241 Y242 G243 V244 T245 V246 L247 P248
T249 F250 K251 G252 Q253 P254 S255 K256 P257 F258 V259 G260 V261 L262 S263 A264 G265
A269 S270 P271 N272 K273 E274 L275 A276 K277 E278 F279 L280 E281 N282 Y283 L284 L285 T286 D287 E288 G289 L290 E291 A292 V293 N294 K295 D296 K297 P298 L299 G300 A301 V302 A303 L304 K305 S306 Y307 E308 E309 E310
D314 P315 R316 I317 A318 A319 T320 M321 E322 N323 A324 Q325 K326 G327 E328 I329 M330 P331 N332 I333 P334 Q335 M336 S337 A338 F339 W340 Y341 A342 V343 R344 T345 A346 V347 I348 N349 A350 A351 S352 G353 R354 Q355 T356 V357 D358 E359 A360 L361 K362 D363 A364 Q365 T366 R367 I368 T369 K370

# 5 Refinement protocol and experimental data overview

The models were refined using the following method: *CONJOINED RIGID BODY/TORSION ANGLE SIMULATED ANNEALING DYNAMICS*.

Of the 100 calculated structures, 50 were deposited, based on the following criterion: *PRE AND VDW ENERGIES*.

The following table shows the software used for structure solution, optimisation and refinement.

| Software name | Classification | Version |
|---|---|---|
| NIH | refinement | |
| XPLOR-NIH | structure solution | |

No chemical shift data was provided. No validations of the models with respect to experimental NMR restraints is performed at this time.

# 6 Model quality

## 6.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MXT

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 (average) root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | #Z>5 | RMSZ | #Z>5 |
| 1 | A | 1.00±0.01 | 0±0/64 ( 0.0± 0.0%) | 1.17±0.04 | 0±0/80 ( 0.1± 0.2%) |
| All | All | 1.00 | 0/3200 ( 0.0%) | 1.17 | 2/4000 ( 0.1%) |

There are no bond-length outliers.

All unique angle outliers are listed below.

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) | Models | |
|---|---|---|---|---|---|---|---|---|---|
| | | | | | | | | Worst | Total |
| 1 | A | 313 | LYS | O-C-N | -5.74 | 113.51 | 122.70 | 48 | 2 |

There are no chirality outliers.

There are no planarity outliers.

## 6.2 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 each 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 averaged over the ensemble.

| Mol | Chain | Non-H | H(model) | H(added) | Clashes |
|---|---|---|---|---|---|
| 1 | A | -2113 | -424 | 14 | 0±0 |
| 2 | A | 432 | 456 | 500 | 14±4 |
| All | All | -84050 | 1600 | 25660 | 695 |

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 0.

5 of 169 unique clashes are listed below, sorted by their clash magnitude.

| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) | Models | |
|---|---|---|---|---|---|
| | | | | Worst | Total |
| 2:A:600[A]:MXT:O11 | 2:A:600[A]:MXT:H231 | 0.83 | 1.73 | 29 | 3 |
| 2:A:500[F]:MXT:O11 | 2:A:500[F]:MXT:H231 | 0.83 | 1.73 | 24 | 7 |
| 2:A:600[B]:MXT:O11 | 2:A:600[B]:MXT:H231 | 0.83 | 1.73 | 46 | 4 |
| 2:A:500[D]:MXT:H231 | 2:A:500[D]:MXT:O11 | 0.83 | 1.73 | 10 | 5 |
| 2:A:500[A]:MXT:H231 | 2:A:500[A]:MXT:O11 | 0.82 | 1.75 | 24 | 3 |

## 6.3 Torsion angles

### 6.3.1 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 PDB entries followed by that with respect to all NMR entries. 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 | 16/370 (4%) | 15±0 (94±0%) | 1±0 (6±0%) | 0±0 (0±0%) | 100 | 100 |
| All | All | 800/18500 (4%) | 750 (94%) | 50 (6%) | 0 (0%) | 100 | 100 |

There are no Ramachandran outliers.

### 6.3.2 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 PDB entries followed by that with respect to all NMR entries. 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 | 0 | - | - | - |
| All | All | 0 | - | - | - |

There are no protein residues with a non-rotameric sidechain to report.

### 6.3.3 RNA

There are no RNA molecules in this entry.

## 6.4 Non-standard residues in protein, DNA, RNA chains (i)

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

## 6.5 Carbohydrates (i)

There are no carbohydrates in this entry.

## 6.6 Ligand geometry (i)

24 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds for which Mogul statistics could be retrieved, the number of bonds that are observed in the model and the number of bonds 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 is the number of standard deviations the observed value is removed from the expected value. A bond length with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond lengths.

| Mol | Type | Chain | Res | Link | Bond lengths | | |
|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | #Z>2 |
| 2 | MXT | A | 600[F] | 1 | 19,19,19 | 1.94±0.00 | 0±0 (0±0%) |
| 2 | MXT | A | 600[Z] | 1 | 19,19,19 | 1.94±0.00 | 0±0 (0±0%) |
| 2 | MXT | A | 600[X] | 1 | 19,19,19 | 1.94±0.00 | 0±0 (0±0%) |
| 2 | MXT | A | 600[C] | 1 | 19,19,19 | 1.95±0.00 | 0±0 (0±0%) |
| 2 | MXT | A | 600[V] | 1 | 19,19,19 | 1.94±0.00 | 0±0 (0±0%) |
| 2 | MXT | A | 600[U] | 1 | 19,19,19 | 1.94±0.00 | 0±0 (0±0%) |
| 2 | MXT | A | 500[U] | 1 | 19,19,19 | 1.94±0.00 | 0±0 (0±0%) |
| 2 | MXT | A | 600[A] | 1 | 19,19,19 | 1.94±0.00 | 0±0 (0±0%) |
| 2 | MXT | A | 600[W] | 1 | 19,19,19 | 1.95±0.00 | 0±0 (0±0%) |
| 2 | MXT | A | 500[B] | 1 | 19,19,19 | 1.94±0.00 | 0±0 (0±0%) |
| 2 | MXT | A | 600[D] | 1 | 19,19,19 | 1.94±0.00 | 0±0 (0±0%) |
| 2 | MXT | A | 500[Y] | 1 | 19,19,19 | 1.94±0.00 | 0±0 (0±0%) |
| 2 | MXT | A | 600[Y] | 1 | 19,19,19 | 1.95±0.00 | 0±0 (0±0%) |
| 2 | MXT | A | 500[Z] | 1 | 19,19,19 | 1.96±0.00 | 0±0 (0±0%) |
| 2 | MXT | A | 500[A] | 1 | 19,19,19 | 1.95±0.00 | 0±0 (0±0%) |
| 2 | MXT | A | 500[X] | 1 | 19,19,19 | 1.93±0.00 | 0±0 (0±0%) |
| 2 | MXT | A | 500[W] | 1 | 19,19,19 | 1.94±0.01 | 0±0 (0±0%) |
| 2 | MXT | A | 500[V] | 1 | 19,19,19 | 1.95±0.00 | 0±0 (0±0%) |
| 2 | MXT | A | 500[E] | 1 | 19,19,19 | 1.94±0.00 | 0±0 (0±0%) |
| 2 | MXT | A | 600[E] | 1 | 19,19,19 | 1.95±0.00 | 0±0 (0±0%) |
| 2 | MXT | A | 500[F] | 1 | 19,19,19 | 1.96±0.00 | 0±0 (0±0%) |
| 2 | MXT | A | 600[B] | 1 | 19,19,19 | 1.94±0.00 | 0±0 (0±0%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | |
|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | #Z>2 |
| 2 | MXT | A | 500[C] | 1 | 19,19,19 | 1.94±0.00 | 0±0 (0±0%) |
| 2 | MXT | A | 500[D] | 1 | 19,19,19 | 1.93±0.00 | 0±0 (0±0%) |

In the following table, the Counts columns list the number of angles for which Mogul statistics could be retrieved, the number of angles that are observed in the model and the number of 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 angle is the number of standard deviations the observed value is removed from the expected value. A bond angle with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond angles.

| Mol | Type | Chain | Res | Link | Bond angles | | |
|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | #Z>2 |
| 2 | MXT | A | 600[F] | 1 | 27,31,31 | 1.31±0.01 | 0±0 (0±0%) |
| 2 | MXT | A | 600[Z] | 1 | 27,31,31 | 1.31±0.01 | 0±0 (0±0%) |
| 2 | MXT | A | 600[X] | 1 | 27,31,31 | 1.36±0.01 | 0±0 (0±0%) |
| 2 | MXT | A | 600[C] | 1 | 27,31,31 | 1.34±0.01 | 0±0 (0±0%) |
| 2 | MXT | A | 600[V] | 1 | 27,31,31 | 1.31±0.01 | 0±0 (0±0%) |
| 2 | MXT | A | 600[U] | 1 | 27,31,31 | 1.33±0.01 | 0±0 (0±0%) |
| 2 | MXT | A | 500[U] | 1 | 27,31,31 | 1.33±0.01 | 0±0 (0±0%) |
| 2 | MXT | A | 600[A] | 1 | 27,31,31 | 1.33±0.01 | 0±0 (0±0%) |
| 2 | MXT | A | 600[W] | 1 | 27,31,31 | 1.34±0.01 | 0±0 (0±0%) |
| 2 | MXT | A | 500[B] | 1 | 27,31,31 | 1.34±0.01 | 0±0 (0±0%) |
| 2 | MXT | A | 600[D] | 1 | 27,31,31 | 1.36±0.01 | 0±0 (0±0%) |
| 2 | MXT | A | 500[Y] | 1 | 27,31,31 | 1.32±0.01 | 0±0 (0±0%) |
| 2 | MXT | A | 600[Y] | 1 | 27,31,31 | 1.35±0.01 | 0±0 (0±0%) |
| 2 | MXT | A | 500[Z] | 1 | 27,31,31 | 1.35±0.01 | 0±0 (0±0%) |
| 2 | MXT | A | 500[A] | 1 | 27,31,31 | 1.33±0.01 | 0±0 (0±0%) |
| 2 | MXT | A | 500[X] | 1 | 27,31,31 | 1.32±0.01 | 0±0 (0±0%) |
| 2 | MXT | A | 500[W] | 1 | 27,31,31 | 1.33±0.01 | 0±0 (0±0%) |
| 2 | MXT | A | 500[V] | 1 | 27,31,31 | 1.34±0.01 | 0±0 (0±0%) |
| 2 | MXT | A | 500[E] | 1 | 27,31,31 | 1.32±0.01 | 0±0 (0±0%) |
| 2 | MXT | A | 600[E] | 1 | 27,31,31 | 1.35±0.01 | 0±0 (0±0%) |
| 2 | MXT | A | 500[F] | 1 | 27,31,31 | 1.35±0.01 | 0±0 (0±0%) |
| 2 | MXT | A | 600[B] | 1 | 27,31,31 | 1.31±0.01 | 0±0 (0±0%) |
| 2 | MXT | A | 500[C] | 1 | 27,31,31 | 1.33±0.01 | 0±0 (0±0%) |
| 2 | MXT | A | 500[D] | 1 | 27,31,31 | 1.32±0.01 | 0±0 (0±0%) |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 2 | MXT | A | 600[Z] | 1 | - | 0±0,4,39,39 | 0±0,2,2,2 |
| 2 | MXT | A | 600[X] | 1 | - | 0±0,4,39,39 | 0±0,2,2,2 |
| 2 | MXT | A | 600[V] | 1 | - | 0±0,4,39,39 | 0±0,2,2,2 |
| 2 | MXT | A | 600[F] | 1 | - | 0±0,4,39,39 | 0±0,2,2,2 |
| 2 | MXT | A | 600[D] | 1 | - | 0±0,4,39,39 | 0±0,2,2,2 |
| 2 | MXT | A | 600[B] | 1 | - | 0±0,4,39,39 | 0±0,2,2,2 |
| 2 | MXT | A | 500[D] | 1 | - | 0±0,4,39,39 | 0±0,2,2,2 |
| 2 | MXT | A | 500[A] | 1 | - | 0±0,4,39,39 | 0±0,2,2,2 |
| 2 | MXT | A | 500[C] | 1 | - | 0±0,4,39,39 | 0±0,2,2,2 |
| 2 | MXT | A | 500[Y] | 1 | - | 0±0,4,39,39 | 0±0,2,2,2 |
| 2 | MXT | A | 500[V] | 1 | - | 0±0,4,39,39 | 0±0,2,2,2 |
| 2 | MXT | A | 600[Y] | 1 | - | 0±0,4,39,39 | 0±0,2,2,2 |
| 2 | MXT | A | 600[W] | 1 | - | 0±0,4,39,39 | 0±0,2,2,2 |
| 2 | MXT | A | 600[U] | 1 | - | 0±0,4,39,39 | 0±0,2,2,2 |
| 2 | MXT | A | 600[E] | 1 | - | 0±0,4,39,39 | 0±0,2,2,2 |
| 2 | MXT | A | 600[C] | 1 | - | 0±0,4,39,39 | 0±0,2,2,2 |
| 2 | MXT | A | 600[A] | 1 | - | 0±0,4,39,39 | 0±0,2,2,2 |
| 2 | MXT | A | 500[X] | 1 | - | 0±0,4,39,39 | 0±0,2,2,2 |
| 2 | MXT | A | 500[Z] | 1 | - | 0±0,4,39,39 | 0±0,2,2,2 |
| 2 | MXT | A | 500[F] | 1 | - | 0±0,4,39,39 | 0±0,2,2,2 |
| 2 | MXT | A | 500[E] | 1 | - | 0±0,4,39,39 | 0±0,2,2,2 |
| 2 | MXT | A | 500[B] | 1 | - | 0±0,4,39,39 | 0±0,2,2,2 |
| 2 | MXT | A | 500[U] | 1 | - | 0±0,4,39,39 | 0±0,2,2,2 |
| 2 | MXT | A | 500[W] | 1 | - | 0±0,4,39,39 | 0±0,2,2,2 |

There are no bond-length outliers.

There are no bond-angle outliers.

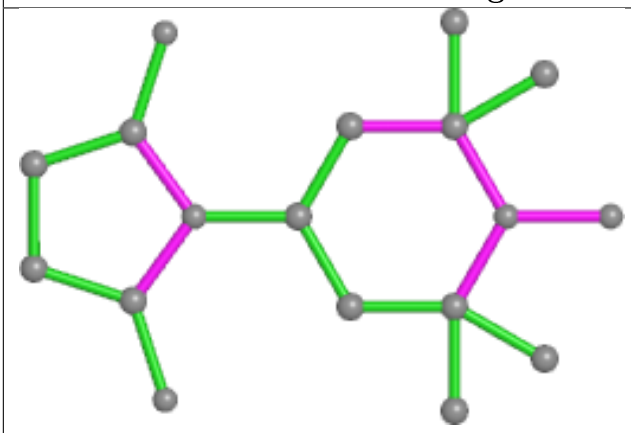
There are no chirality outliers.

There are no torsion outliers.

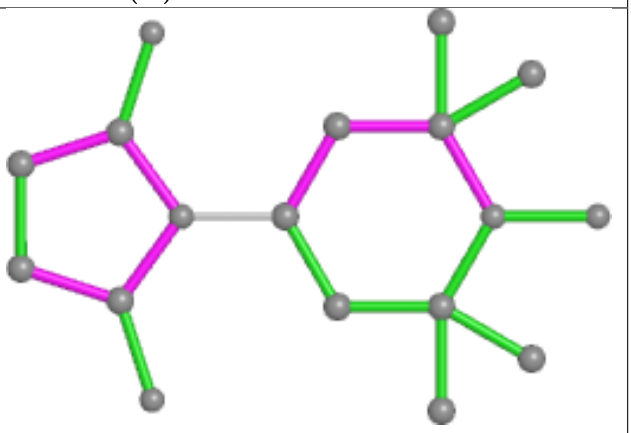
There are no ring outliers.

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 then 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.

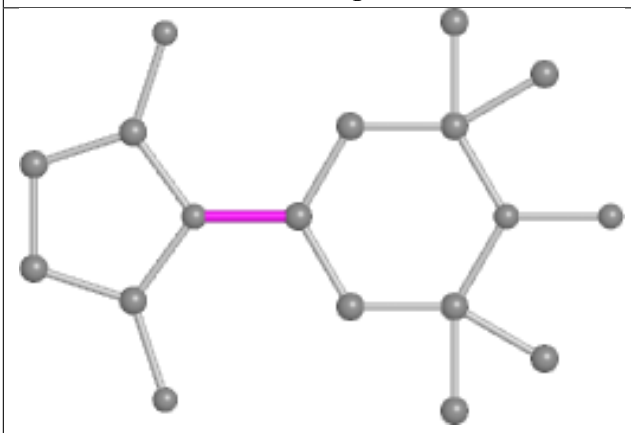
**Ligand MXT A 600 (Z)**



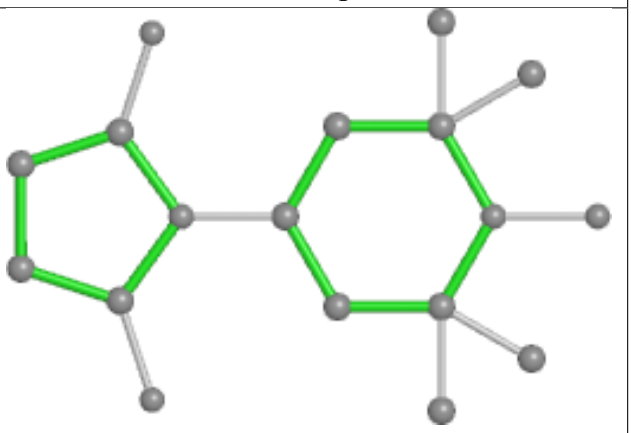
Bond lengths



Bond angles

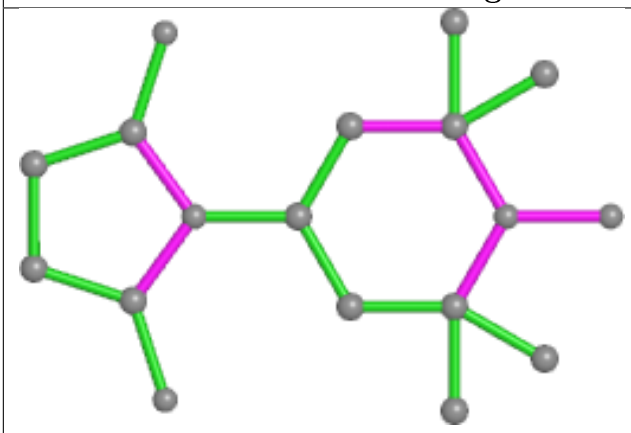


Torsions

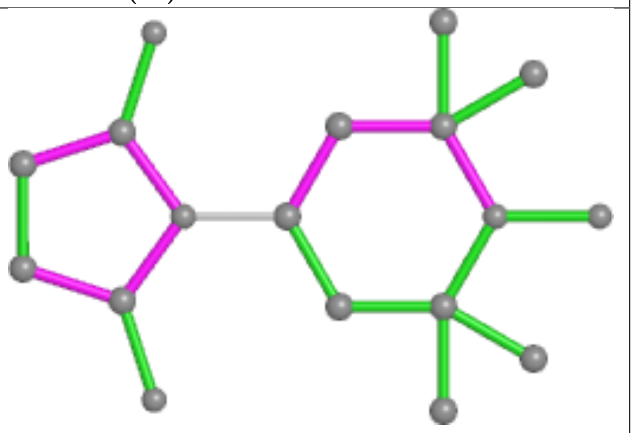


Rings

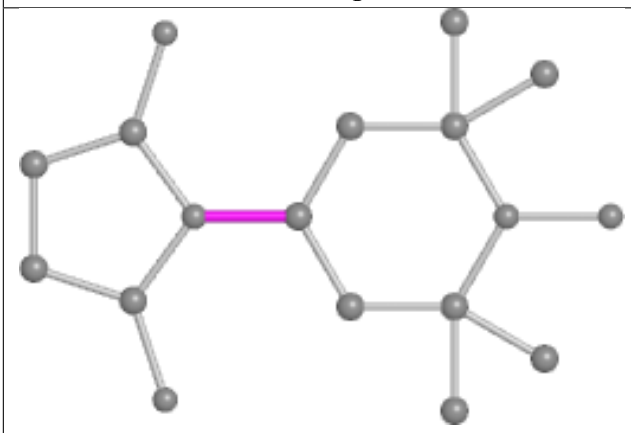
**Ligand MXT A 600 (X)**



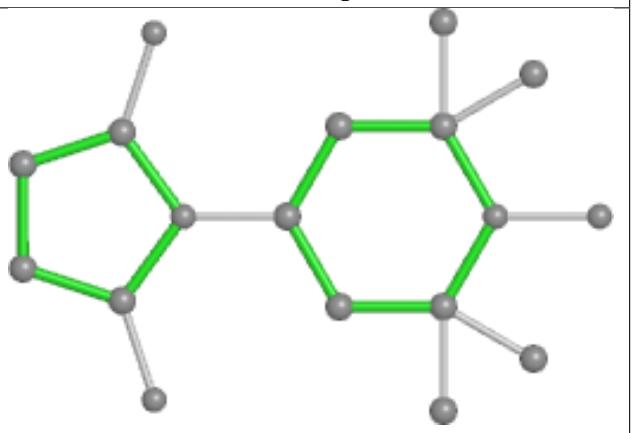
Bond lengths



Bond angles

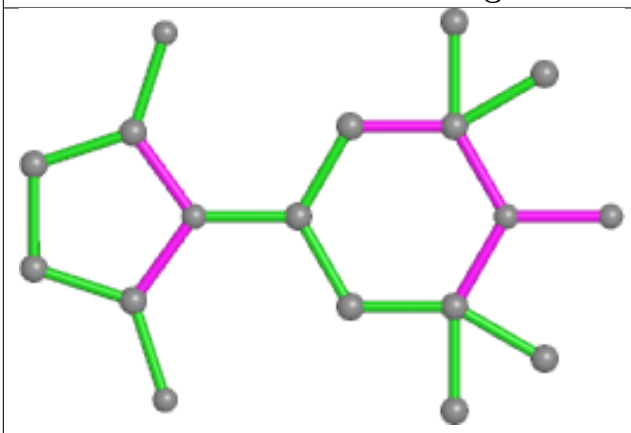


Torsions



Rings

**Ligand MXT A 600 (V)**



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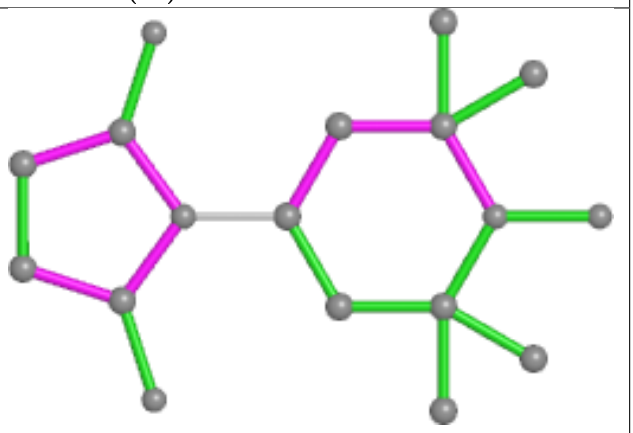
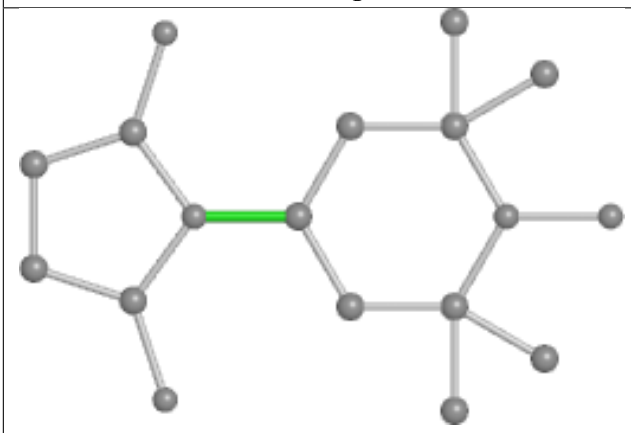
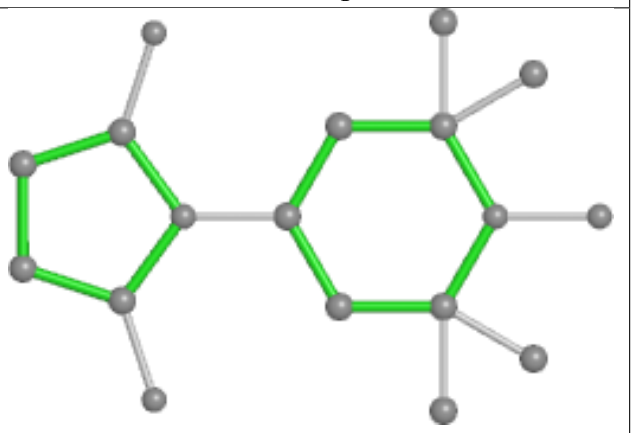


Bond angles

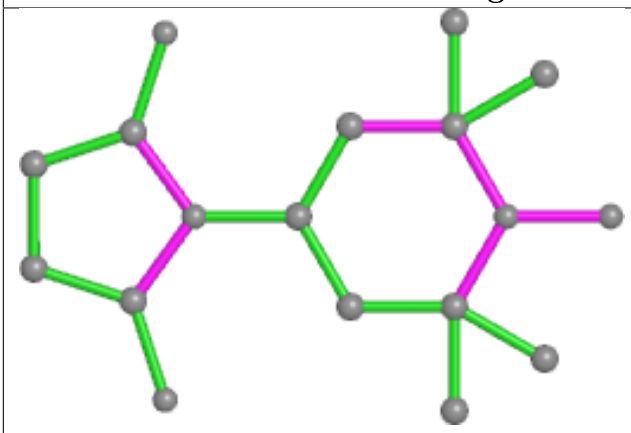


Torsions



Rings

**Ligand MXT A 600 (F)**



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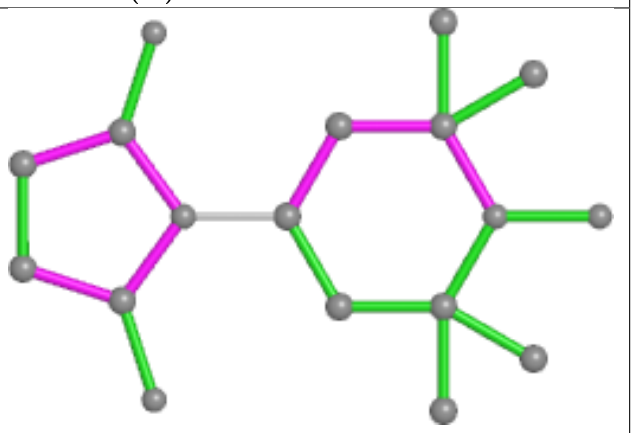
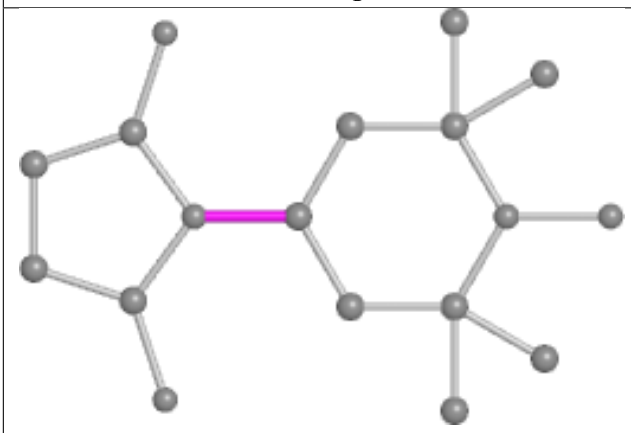
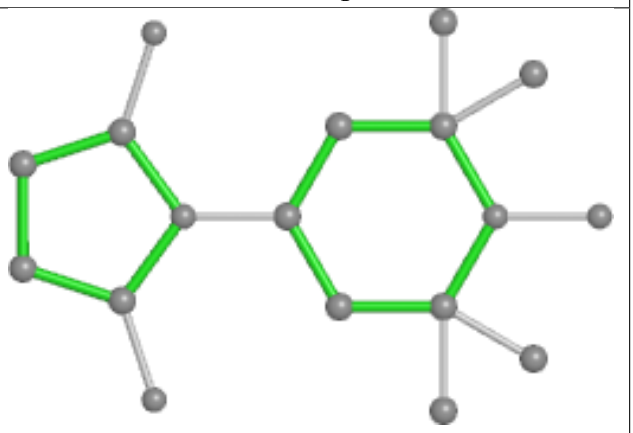


Bond angles

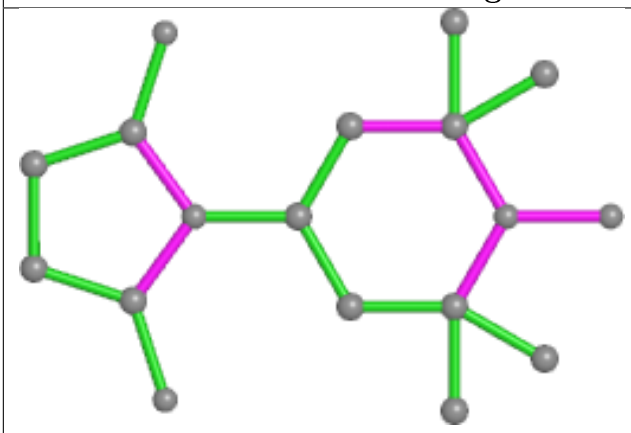


Torsions

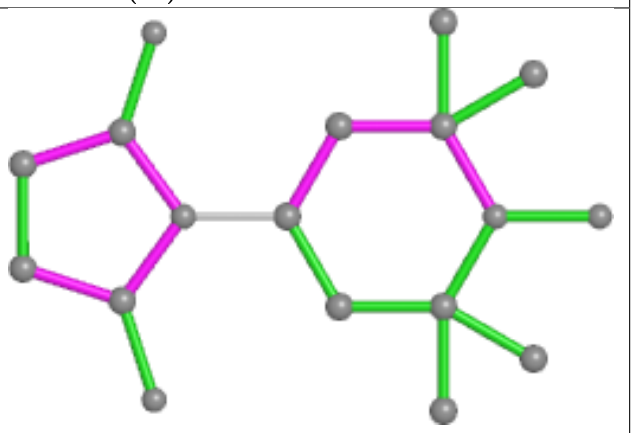


Rings

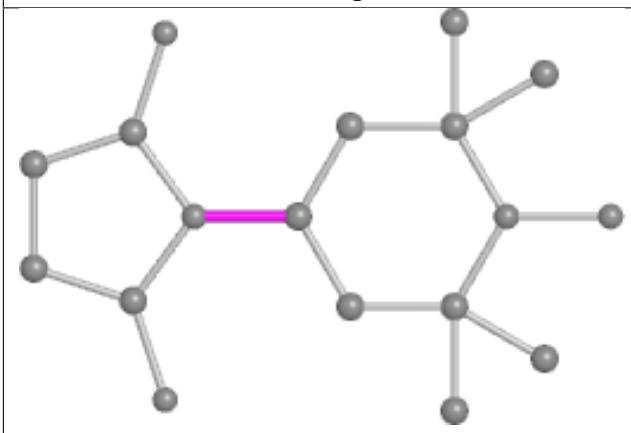
**Ligand MXT A 600 (D)**



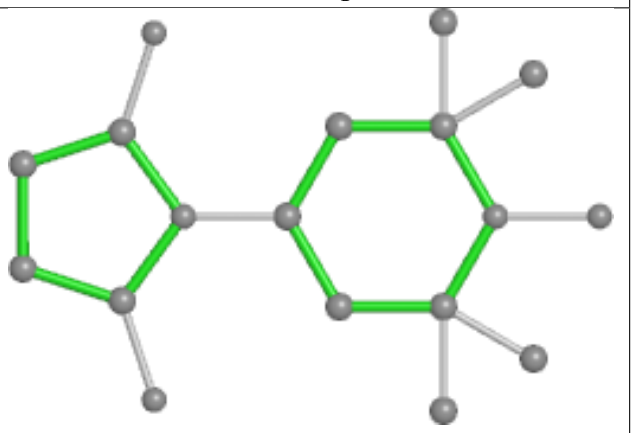
Bond lengths



Bond angles

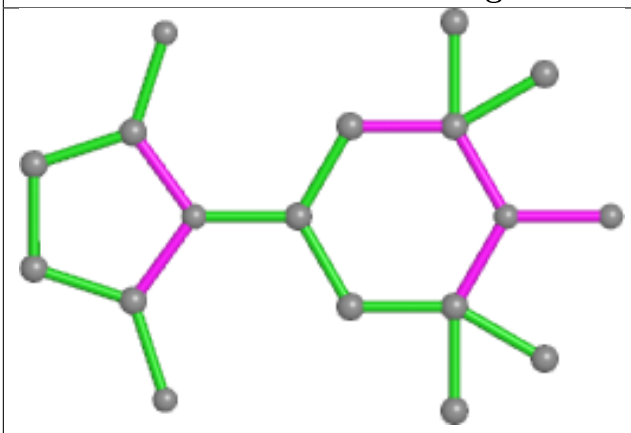


Torsions

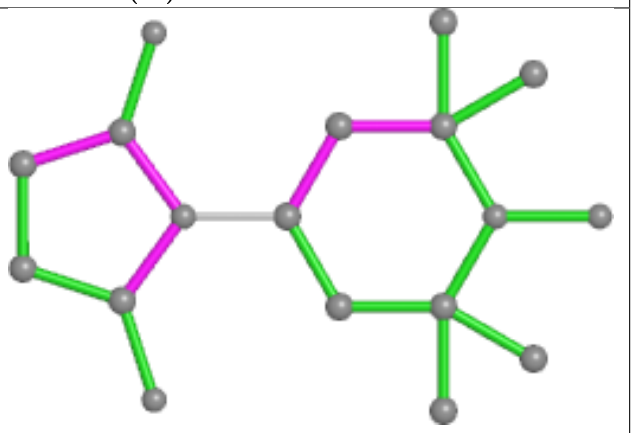


Rings

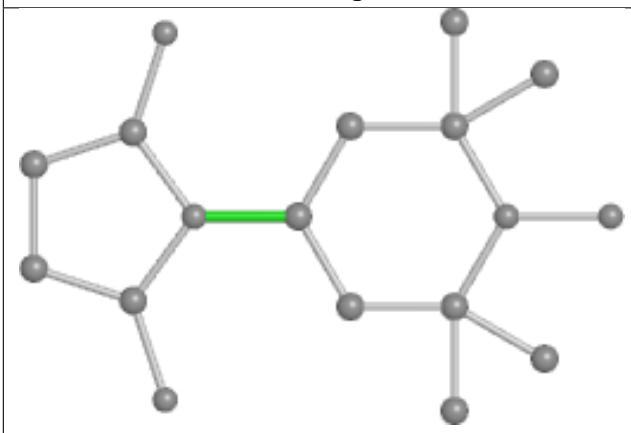
**Ligand MXT A 600 (B)**



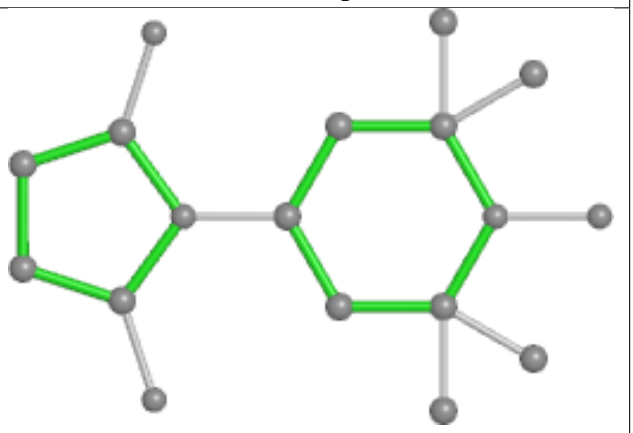
Bond lengths



Bond angles

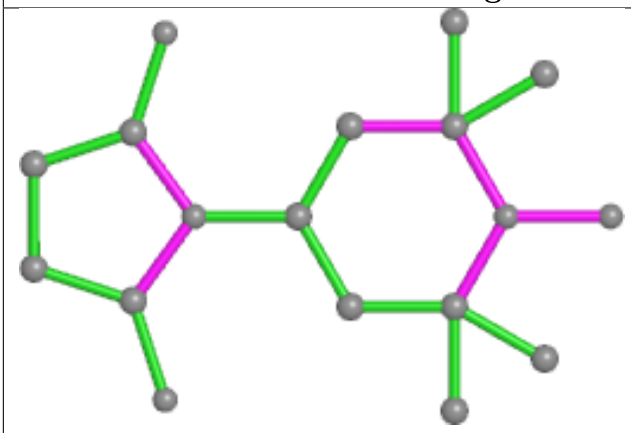


Torsions

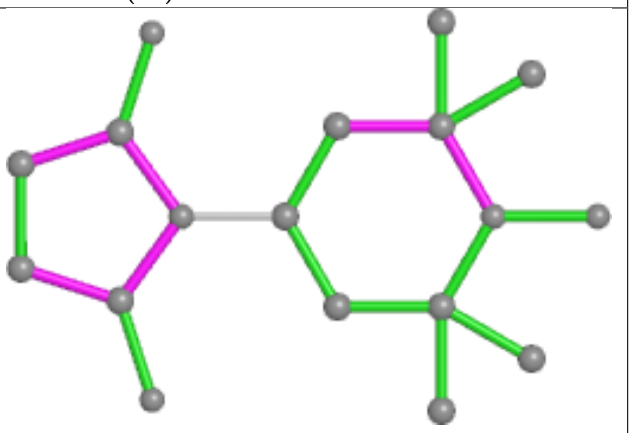


Rings

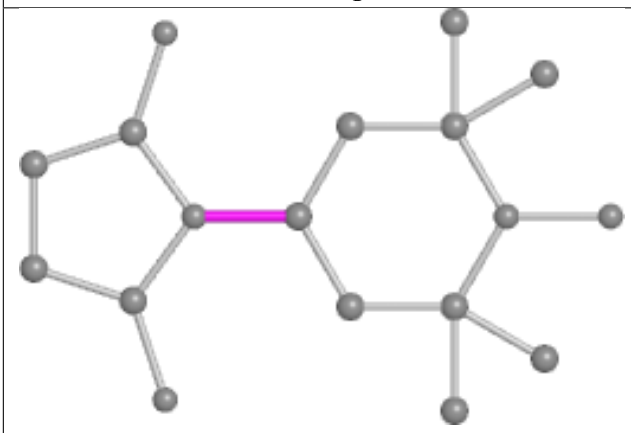
**Ligand MXT A 500 (D)**



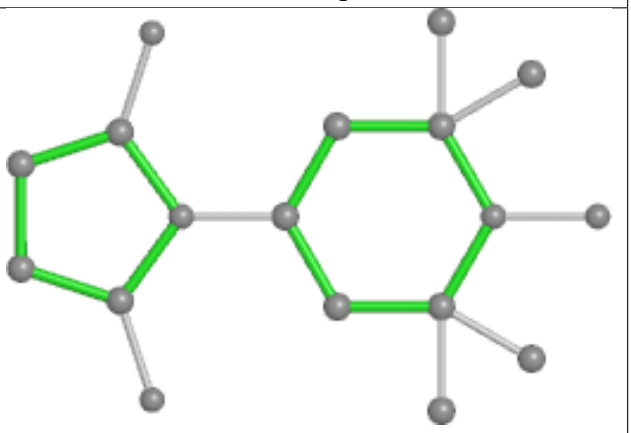
Bond lengths



Bond angles

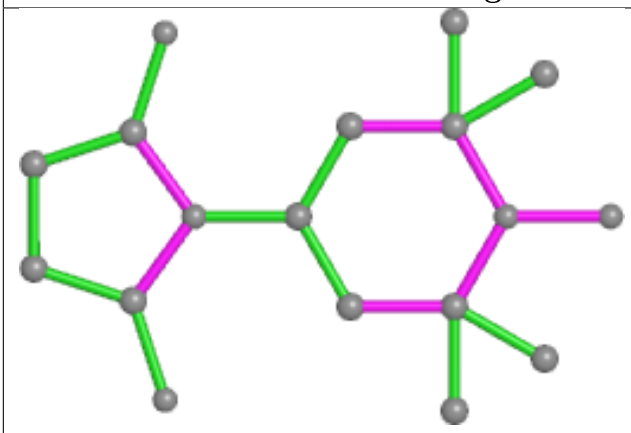


Torsions

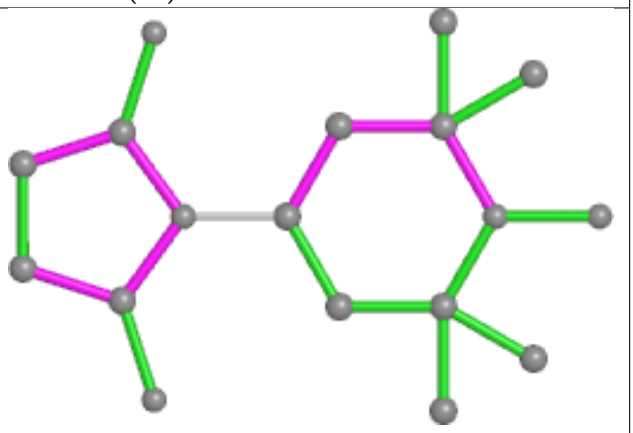


Rings

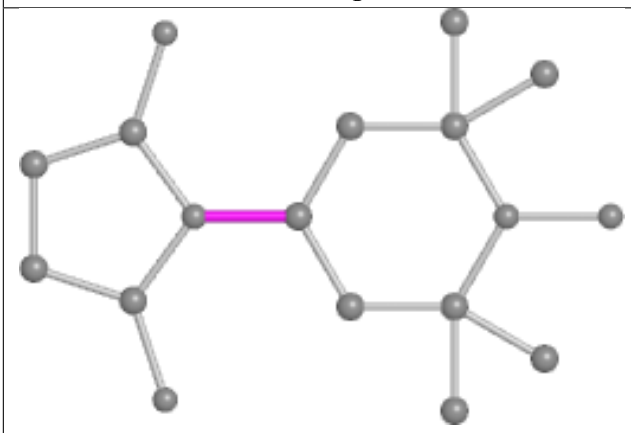
**Ligand MXT A 500 (A)**



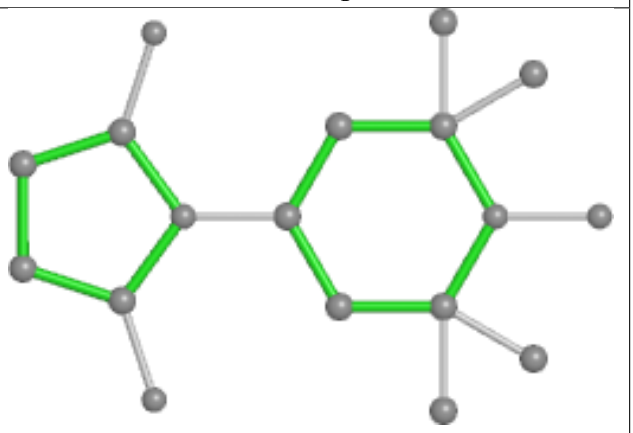
Bond lengths



Bond angles

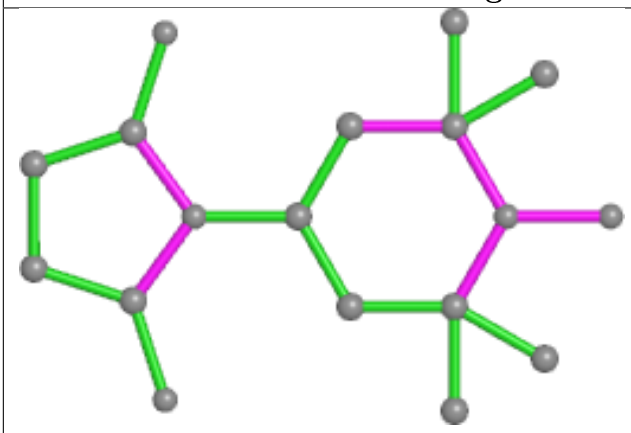


Torsions

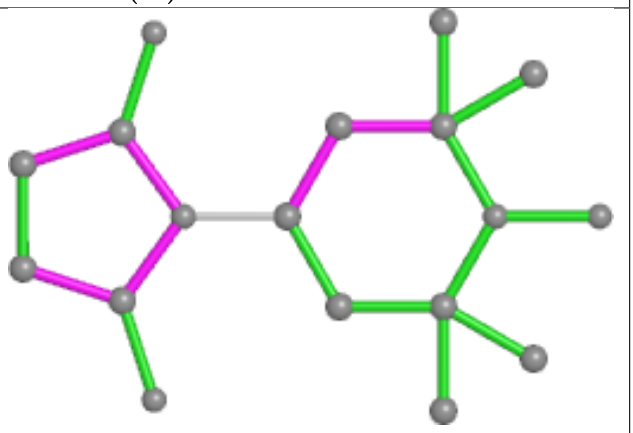


Rings

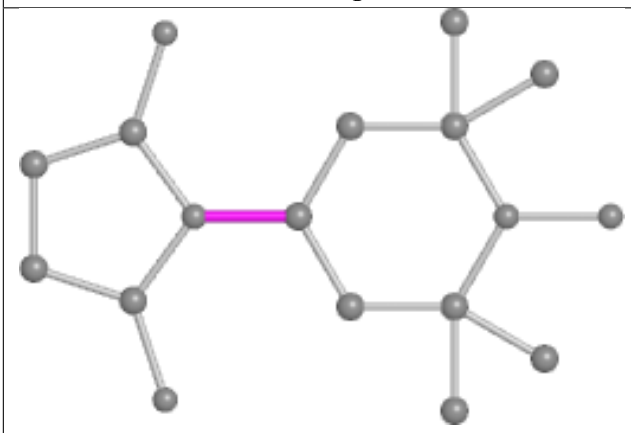
**Ligand MXT A 500 (C)**



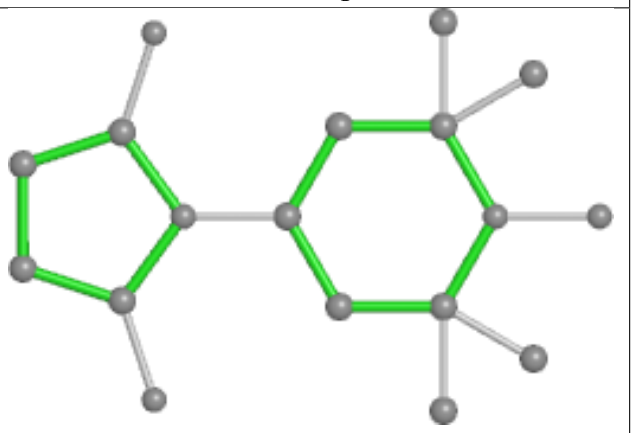
Bond lengths



Bond angles

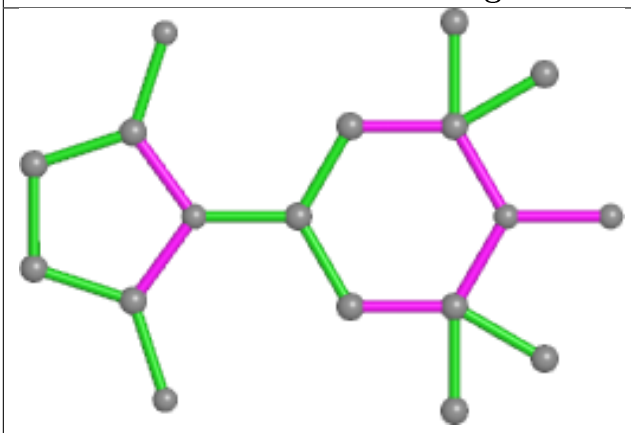


Torsions

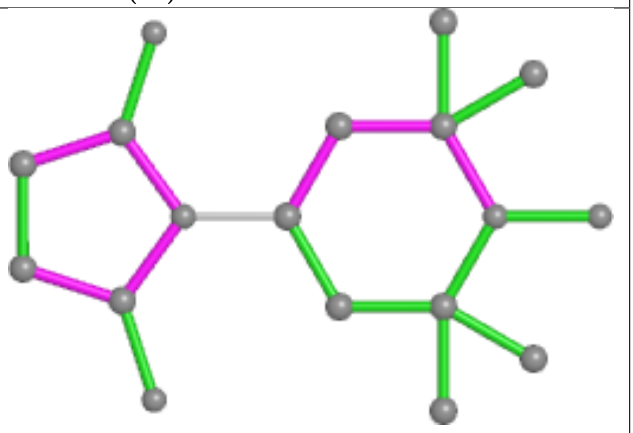


Rings

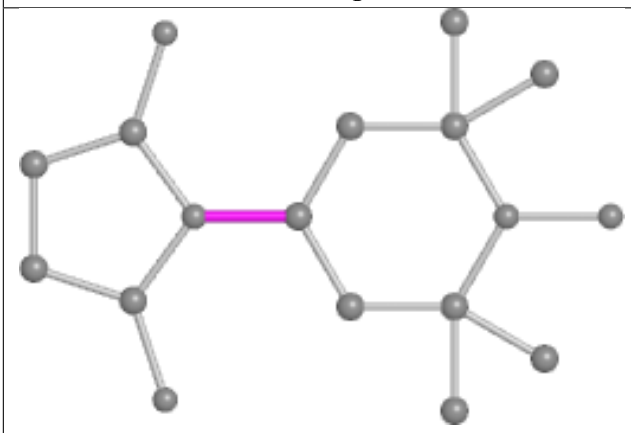
**Ligand MXT A 500 (Y)**



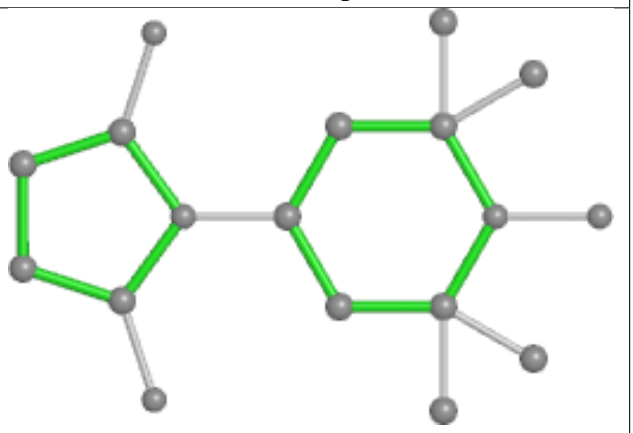
Bond lengths



Bond angles

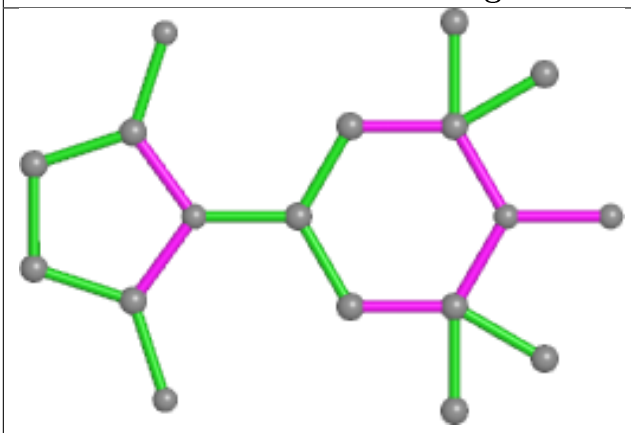


Torsions

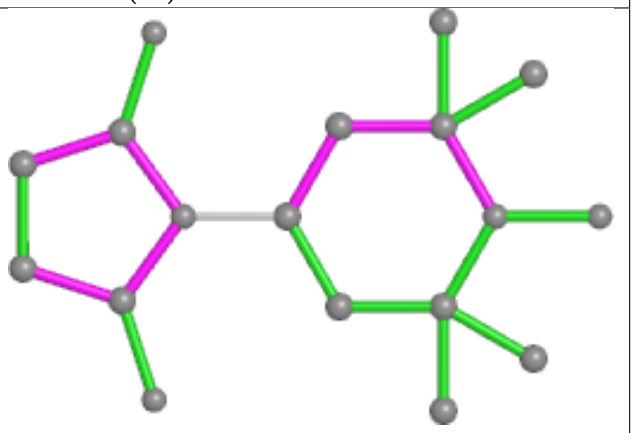


Rings

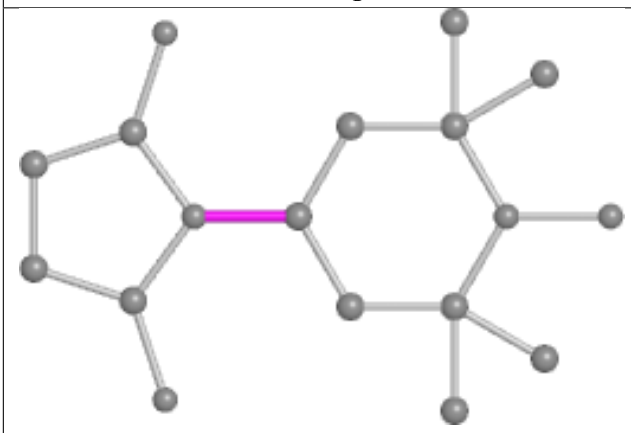
**Ligand MXT A 500 (V)**



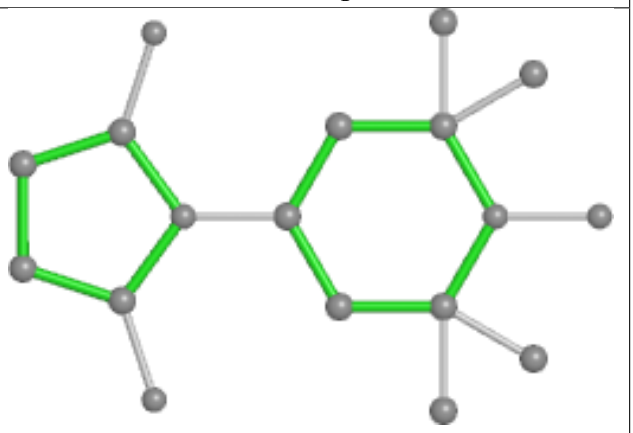
Bond lengths



Bond angles

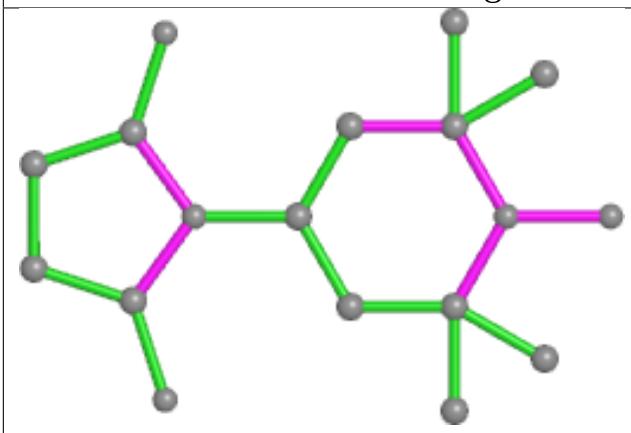


Torsions

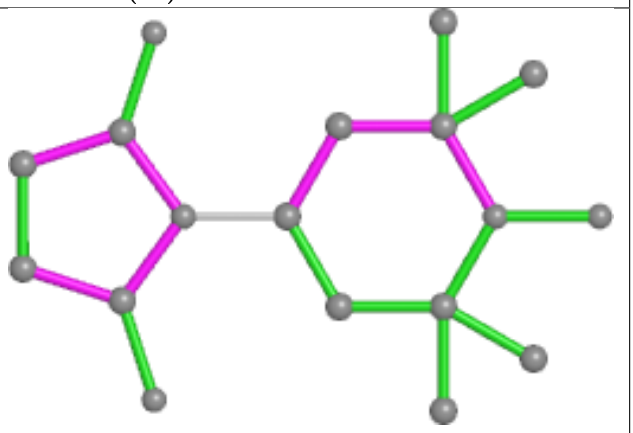


Rings

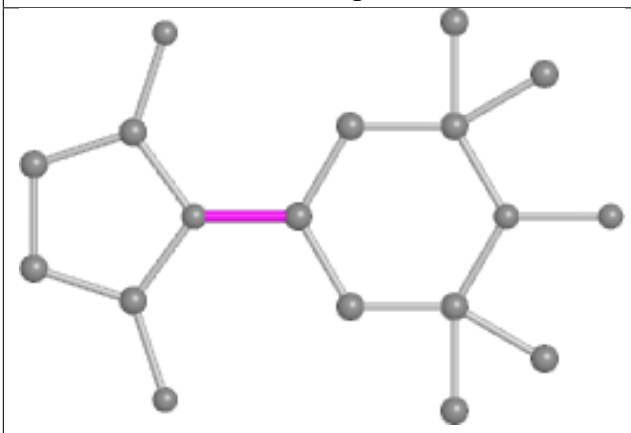
**Ligand MXT A 600 (Y)**



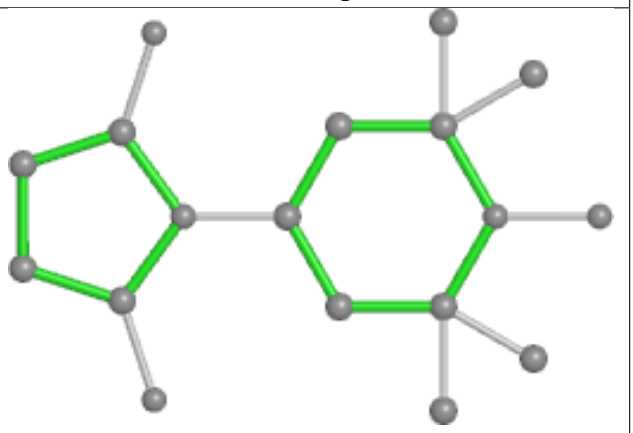
Bond lengths



Bond angles

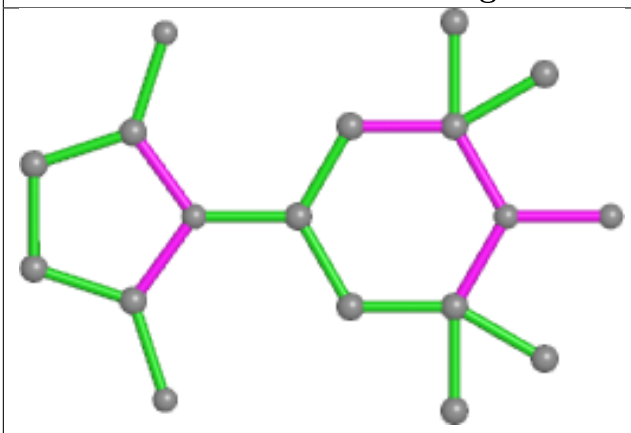


Torsions

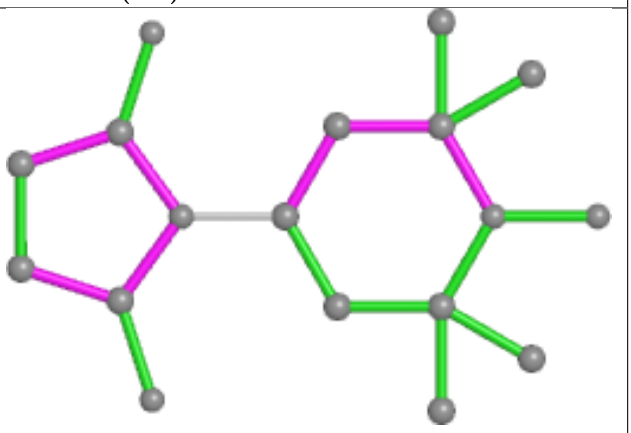


Rings

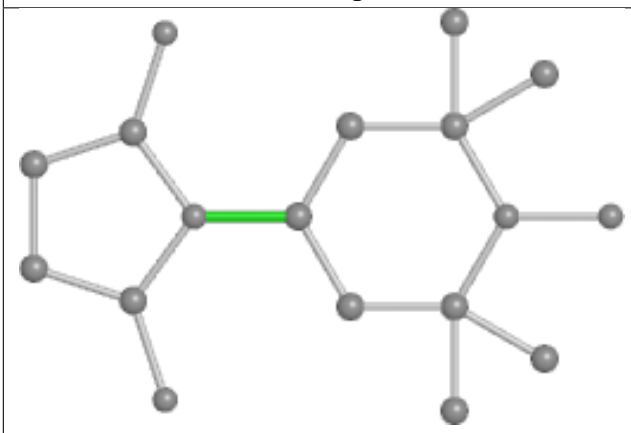
**Ligand MXT A 600 (W)**



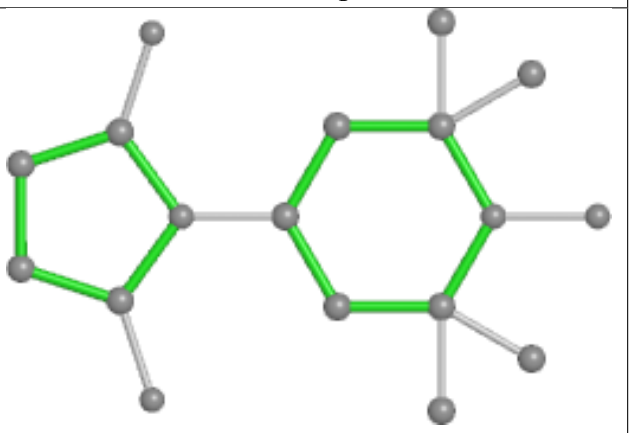
Bond lengths



Bond angles

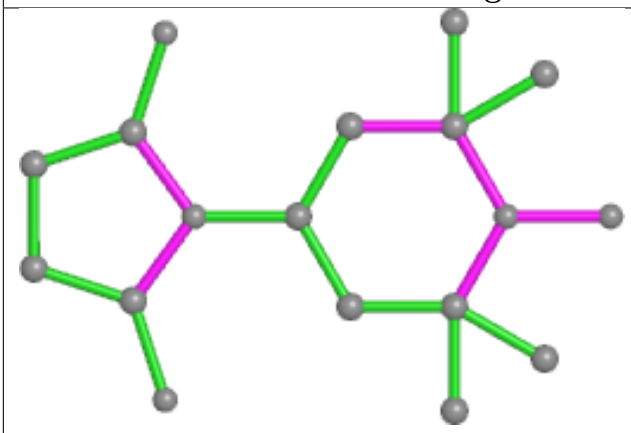


Torsions

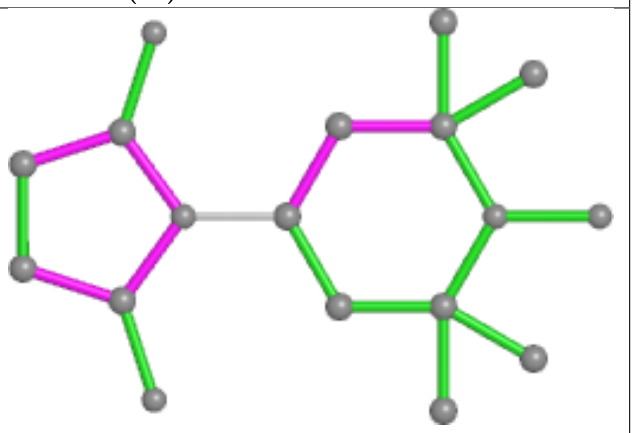


Rings

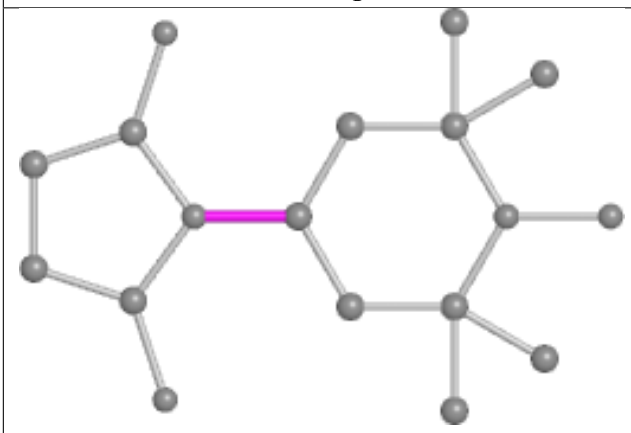
**Ligand MXT A 600 (U)**



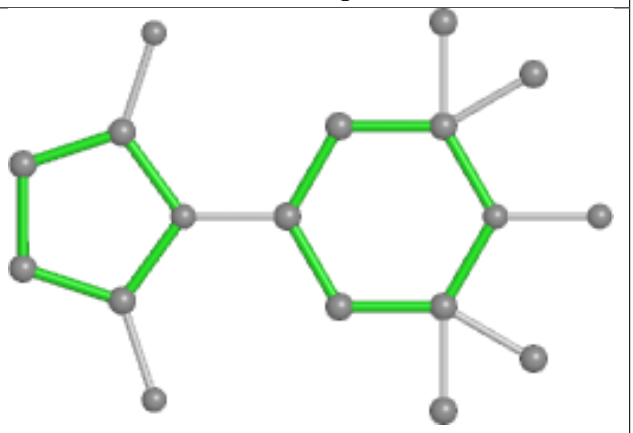
**Bond lengths**



**Bond angles**

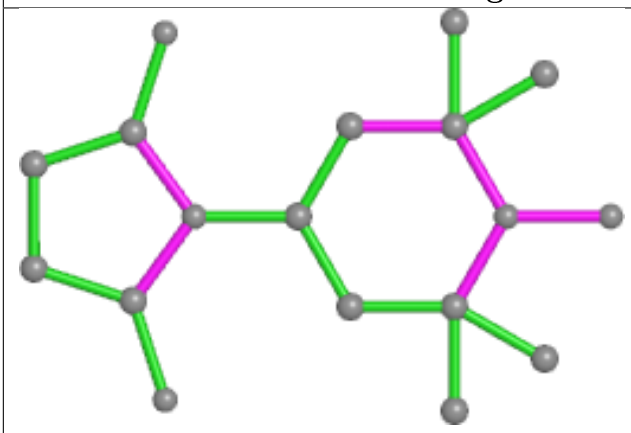


**Torsions**

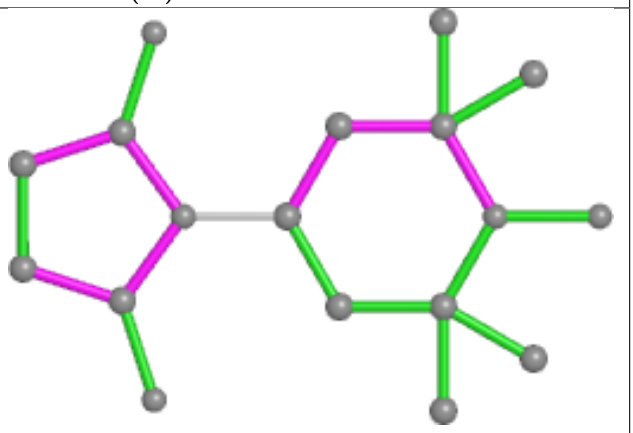


**Rings**

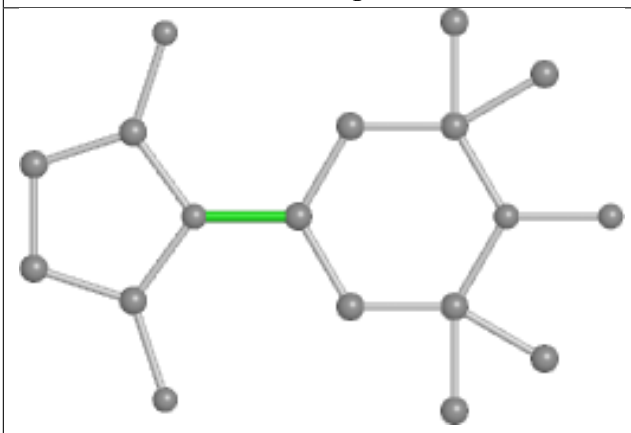
**Ligand MXT A 600 (E)**



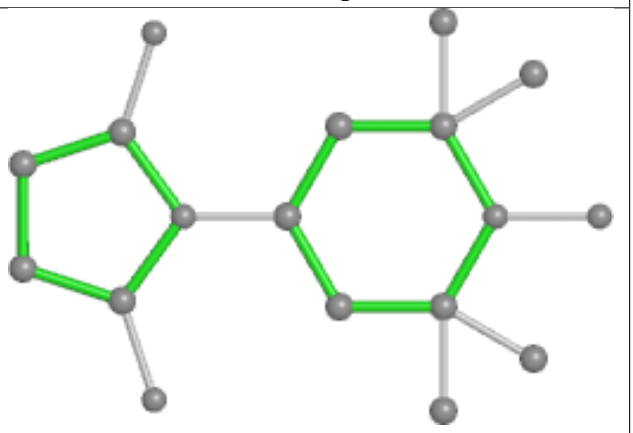
Bond lengths



Bond angles

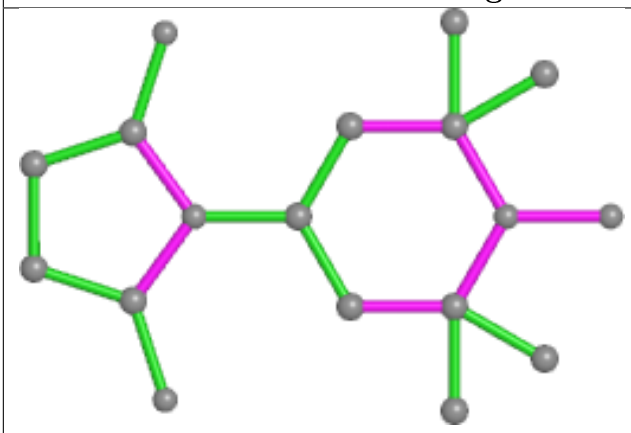


Torsions

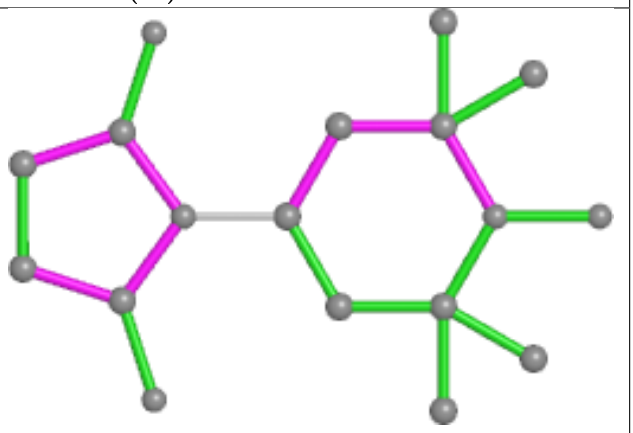


Rings

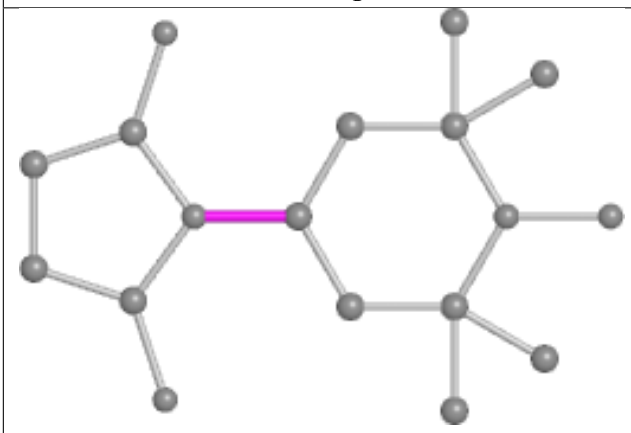
**Ligand MXT A 600 (C)**



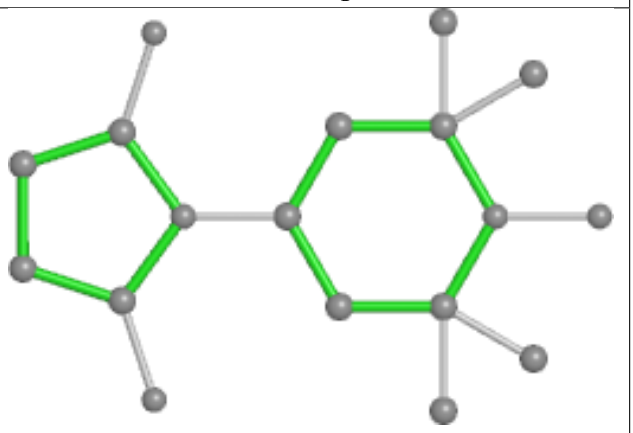
Bond lengths



Bond angles

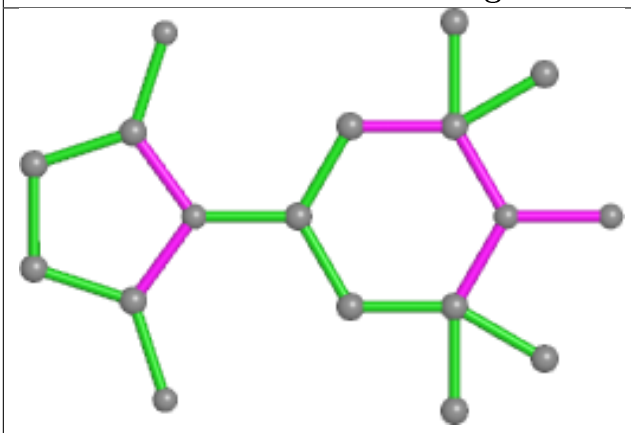


Torsions

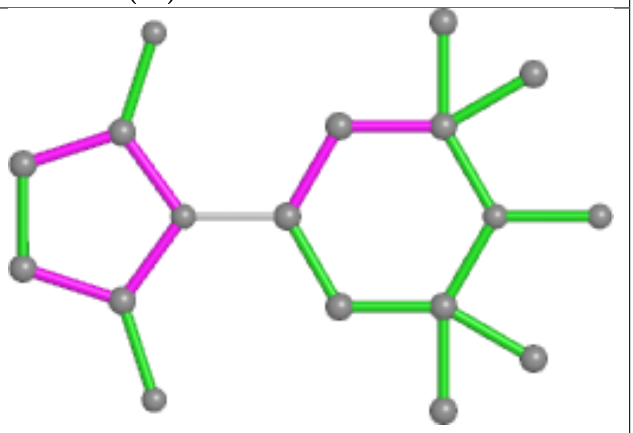


Rings

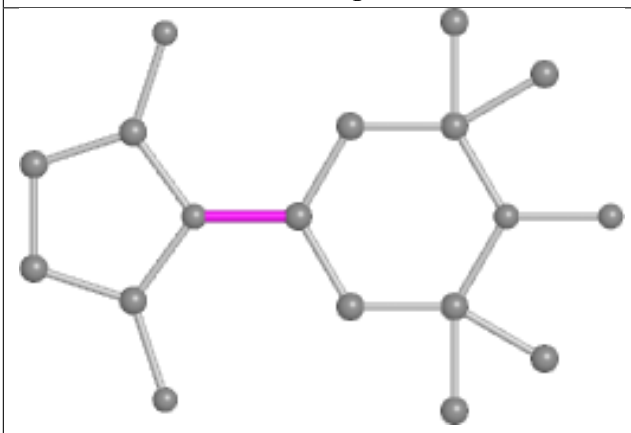
**Ligand MXT A 600 (A)**



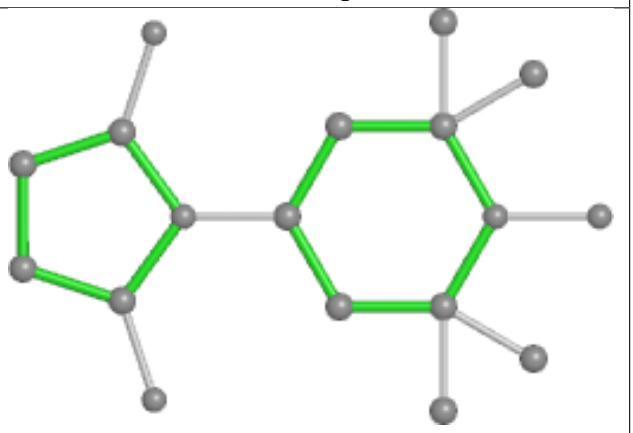
Bond lengths



Bond angles

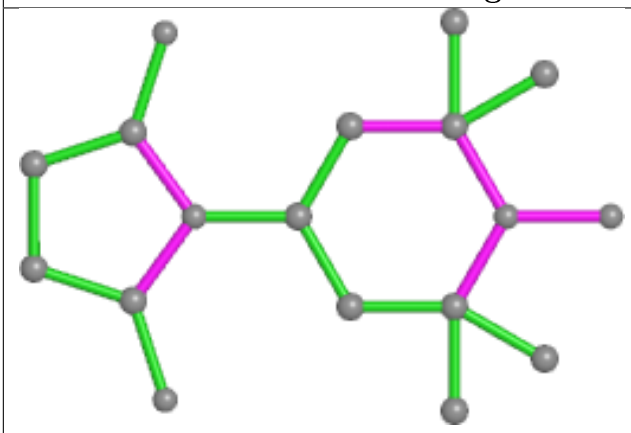


Torsions

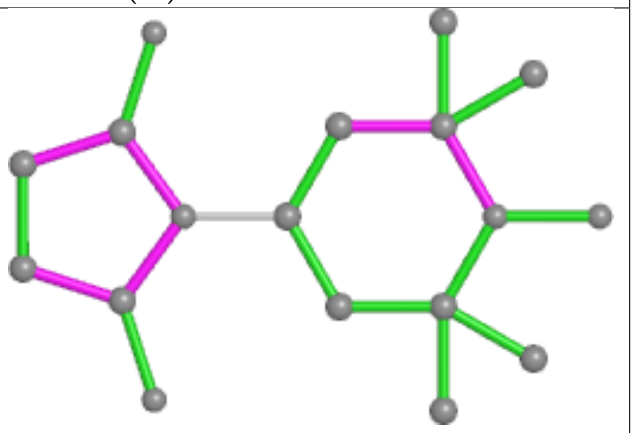


Rings

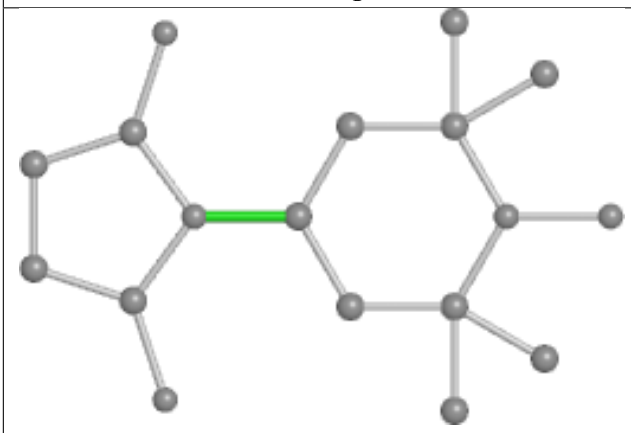
**Ligand MXT A 500 (X)**



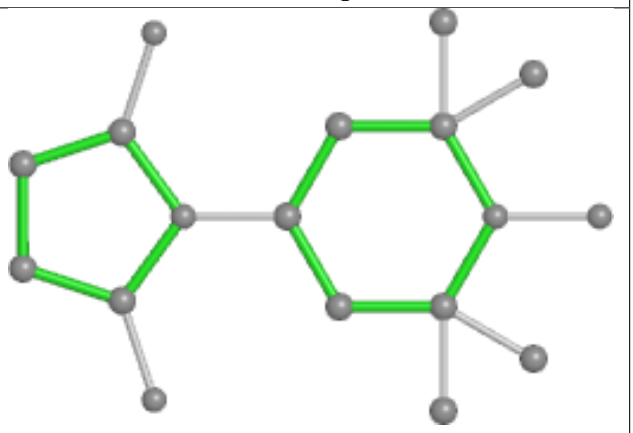
Bond lengths



Bond angles

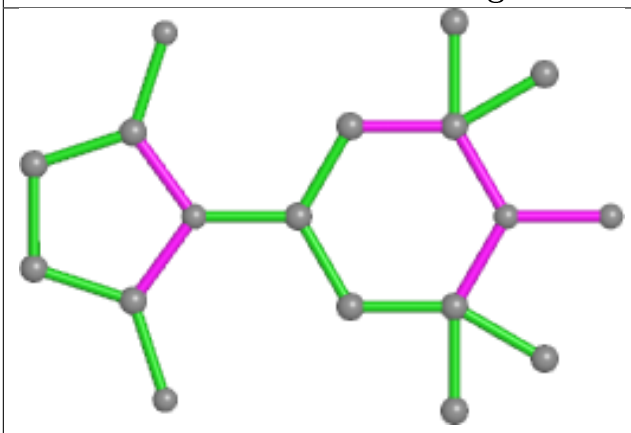


Torsions

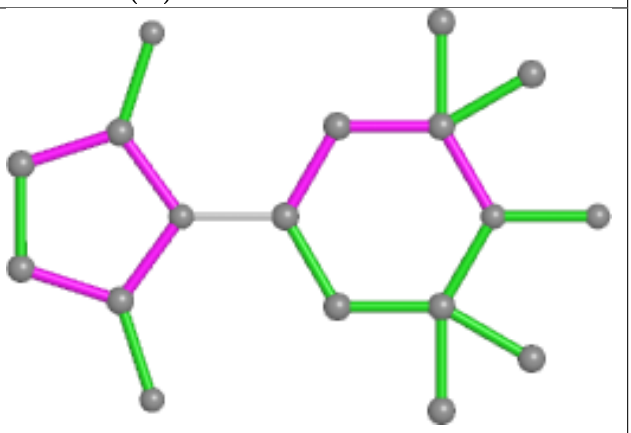


Rings

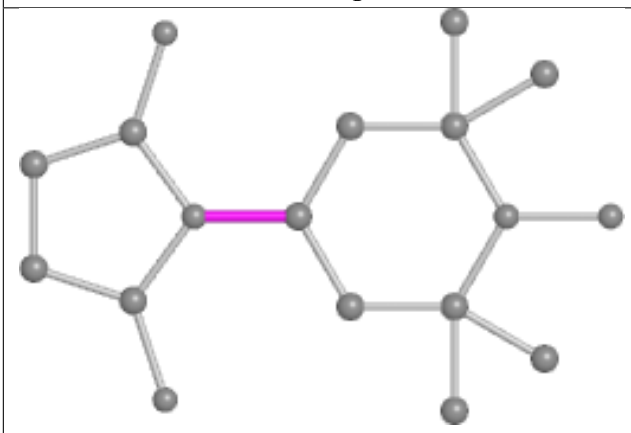
**Ligand MXT A 500 (Z)**



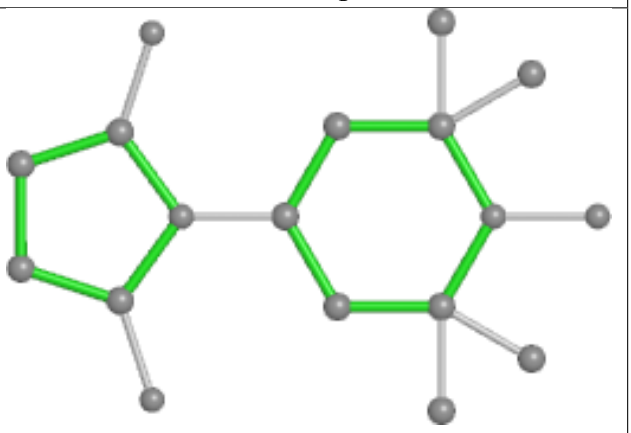
Bond lengths



Bond angles

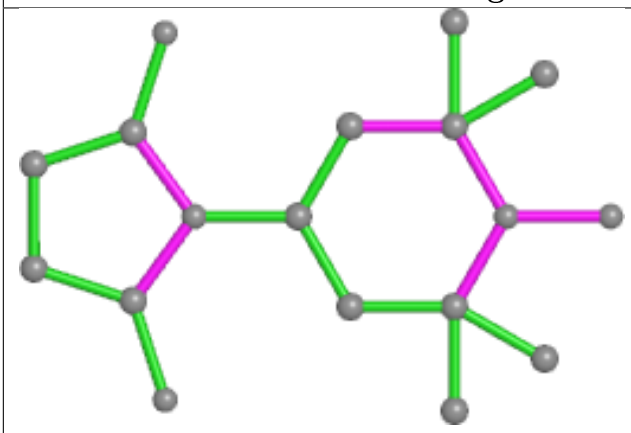


Torsions

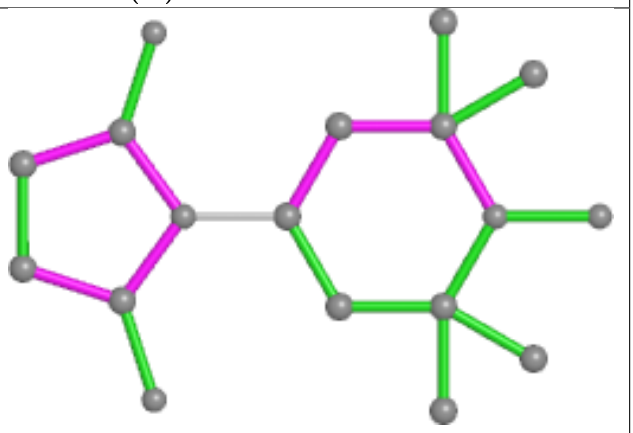


Rings

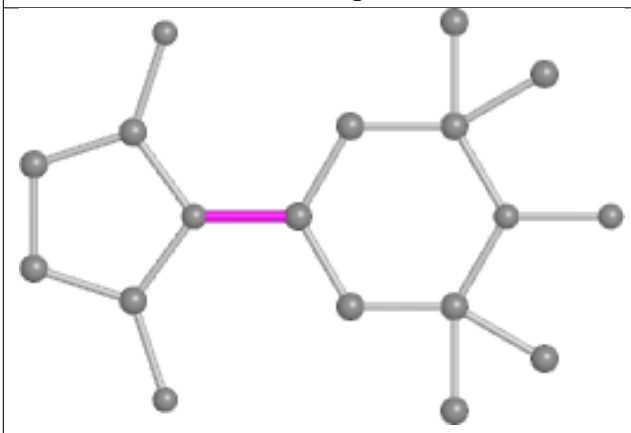
**Ligand MXT A 500 (F)**



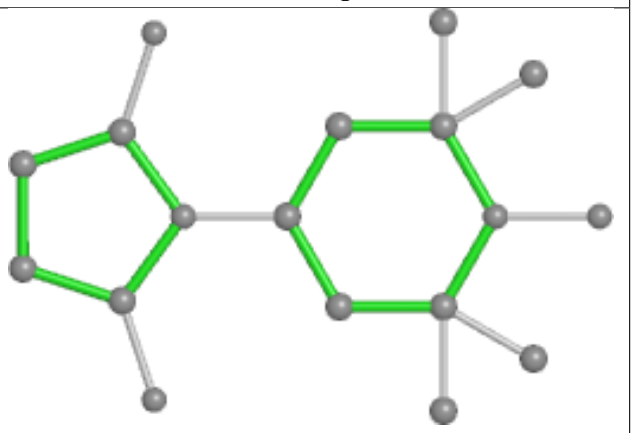
Bond lengths



Bond angles

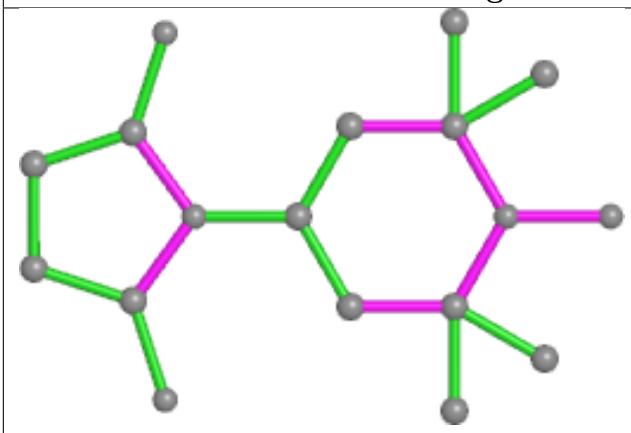


Torsions

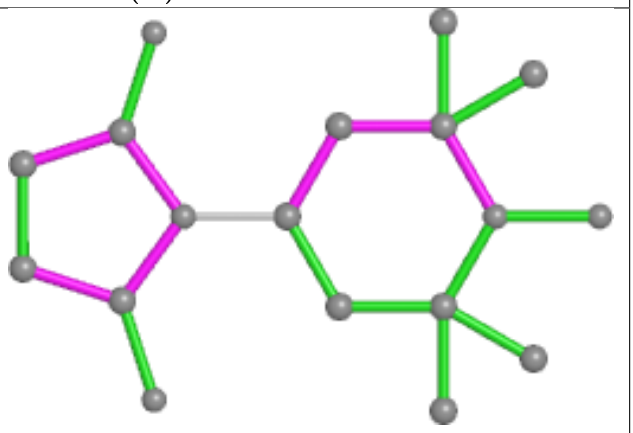


Rings

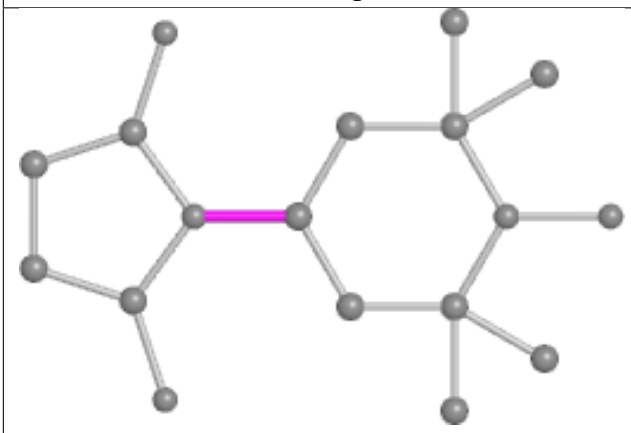
**Ligand MXT A 500 (E)**



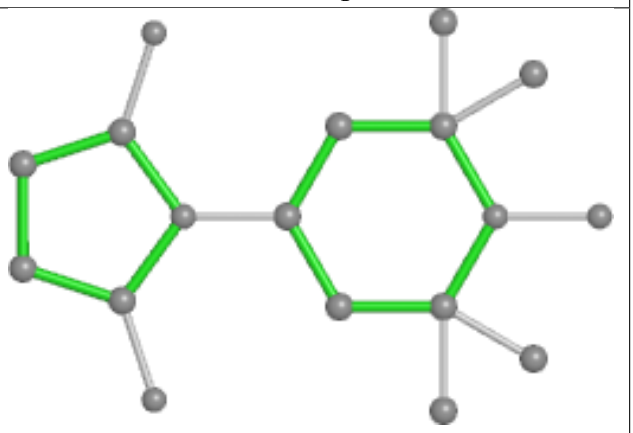
Bond lengths



Bond angles

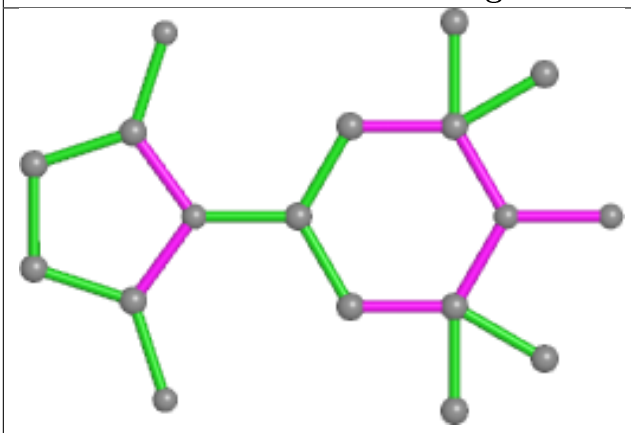


Torsions

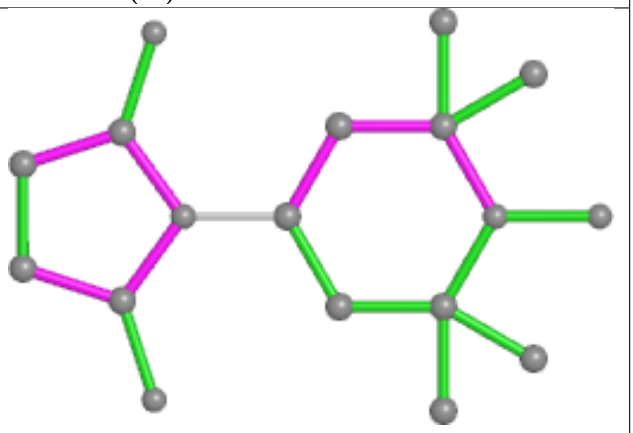


Rings

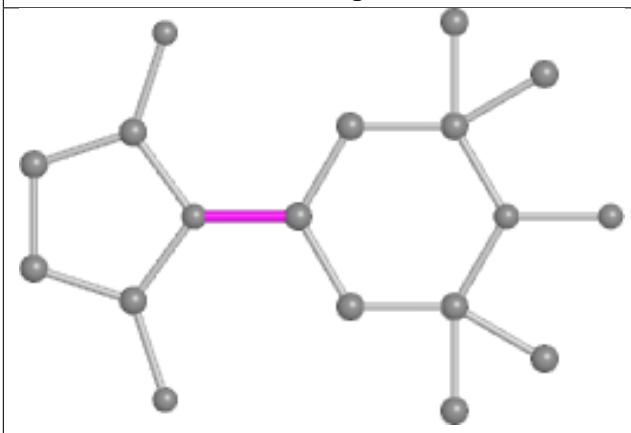
**Ligand MXT A 500 (B)**



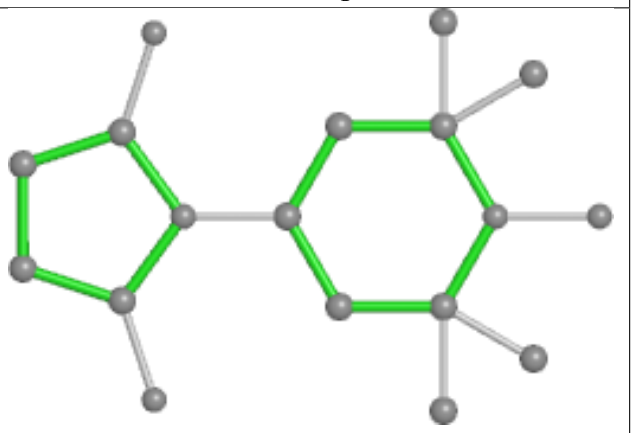
Bond lengths



Bond angles

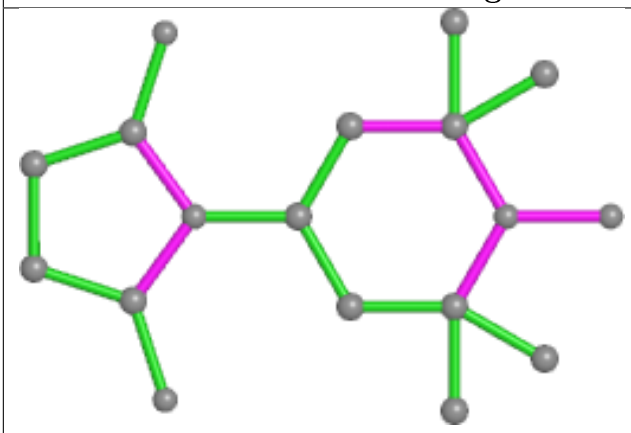


Torsions

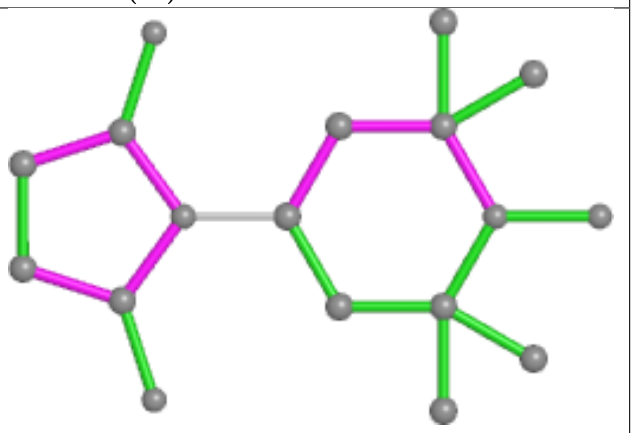


Rings

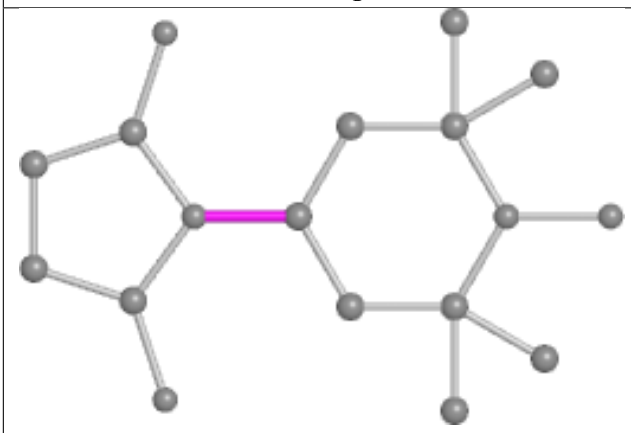
**Ligand MXT A 500 (U)**



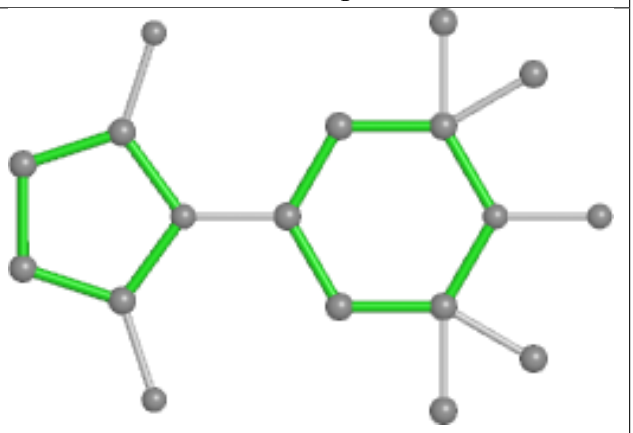
Bond lengths



Bond angles

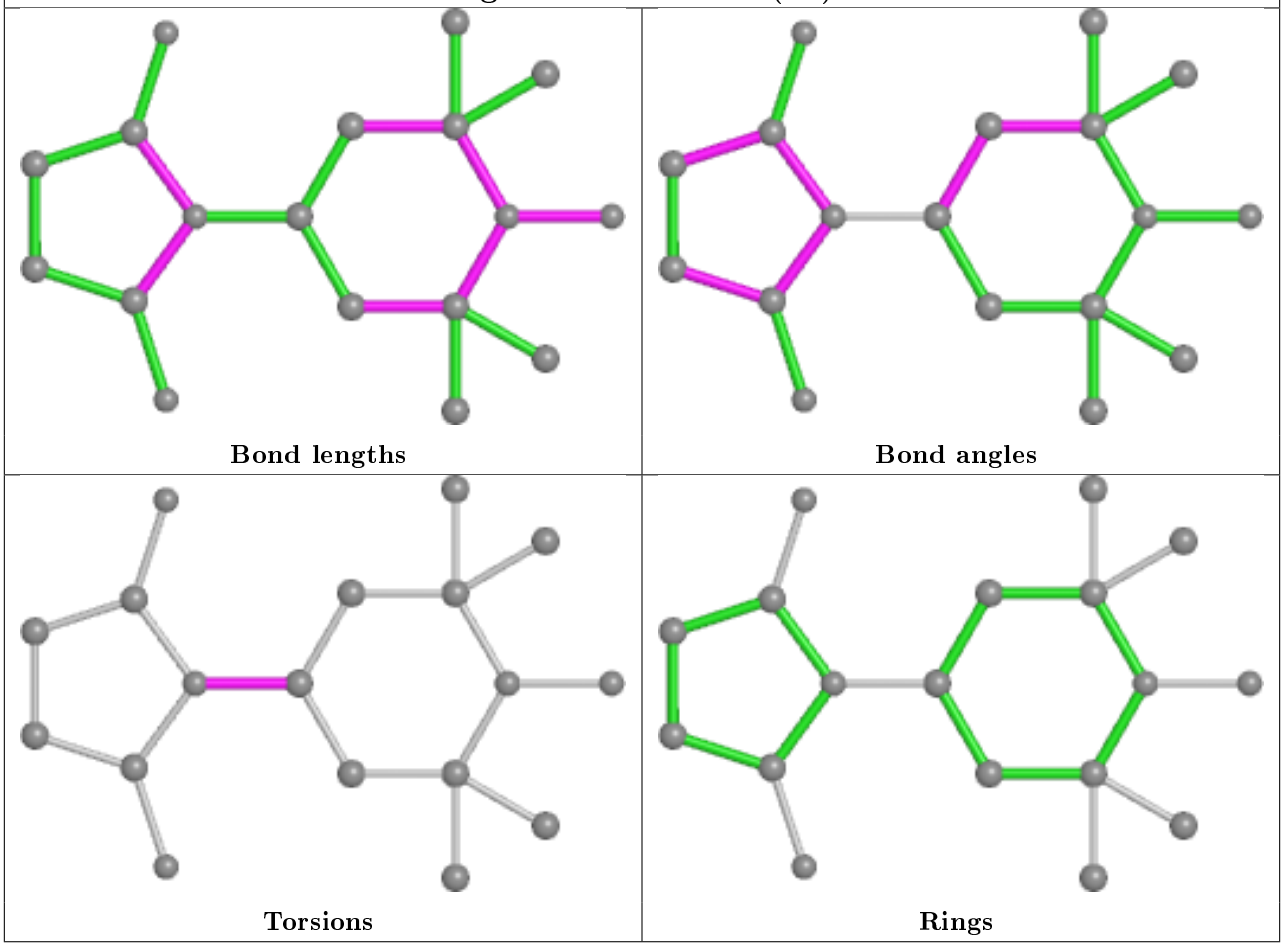


Torsions



Rings

**Ligand MXT A 500 (W)**




## 6.7 Other polymers (i)

There are no such molecules in this entry.

## 6.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

# 7 Chemical shift validation

No chemical shift data were provided