



Full wwPDB EM Validation Report ⓘ

Mar 17, 2025 – 07:10 PM EDT

PDB ID : 9E78
EMDB ID : EMD-47661
Title : 48-nm repeat of the Leishmania tarentolae doublet microtubule
Authors : Doran, M.H.; Ren, P.; Hoog, J.L.; Brown, A.
Deposited on : 2024-11-01
Resolution : 2.90 Å(reported)
Based on initial model : .

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev117
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.41.4

1 Overall quality at a glance

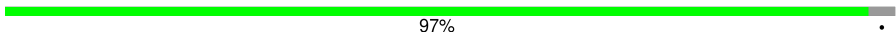

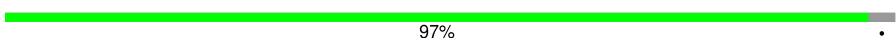
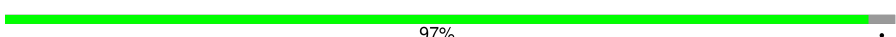









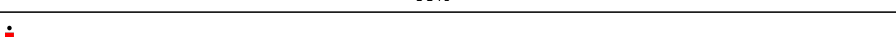
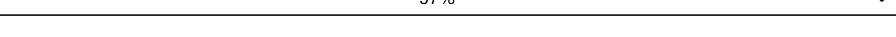
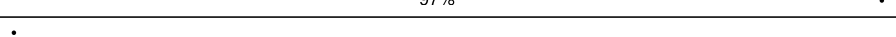
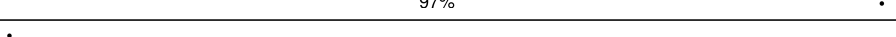
The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.90 Å.

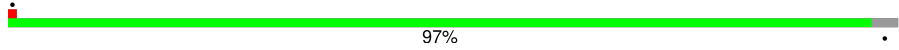
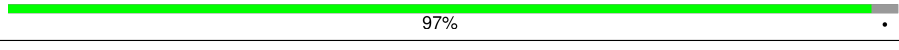
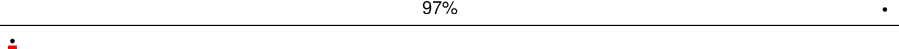
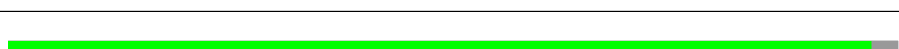

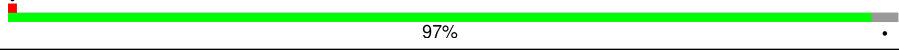
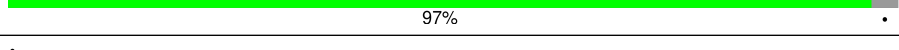
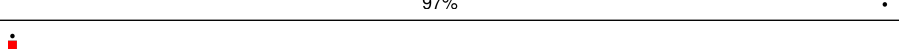
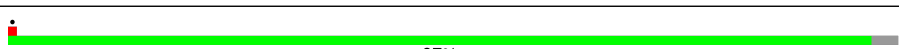
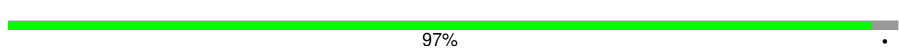
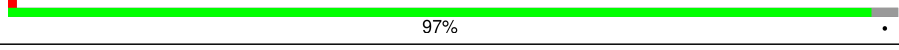
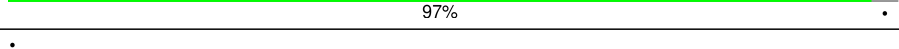
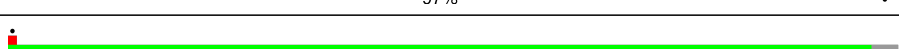
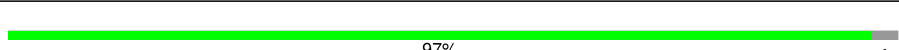
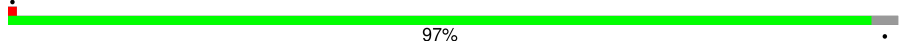
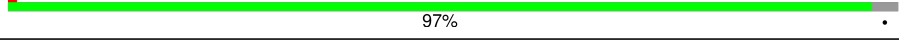
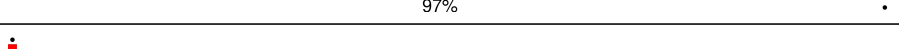


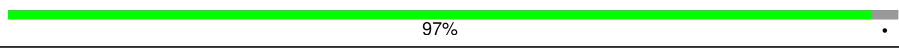
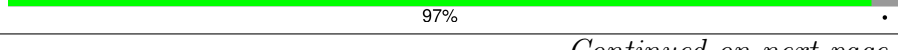



There are no overall percentile quality scores available for this entry.

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|-----------------------------------------------------------------------------------------------|
| 1 | A | 443 |  97% . |
| 1 | AB | 443 |  94% 5% . |
| 1 | AD | 443 |  97% . |
| 1 | AF | 443 |  97% . |
| 1 | AH | 443 |  97% . |
| 1 | AJ | 443 |  97% . |
| 1 | AL | 443 |  97% . |
| 1 | AN | 443 |  95% 5% . |
| 1 | B | 443 |  94% 6% . |
| 1 | BB | 443 |  97% . |
| 1 | BD | 443 |  97% . |
| 1 | BF | 443 |  97% . |
| 1 | BH | 443 |  96% . |
| 1 | BJ | 443 |  97% . |
| 1 | BL | 443 |  97% . |
| 1 | BN | 443 |  97% . |
| 1 | CA | 443 |  96% . |

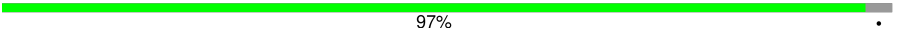
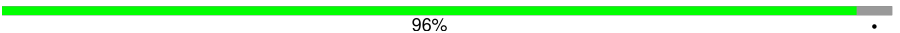
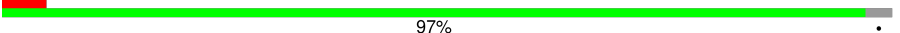
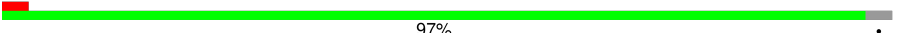

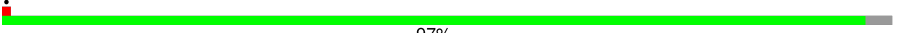









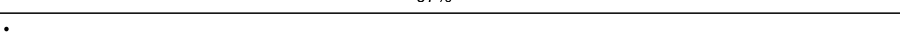
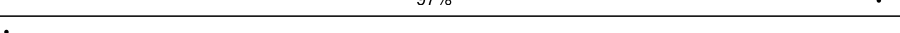
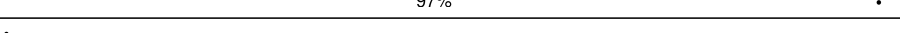
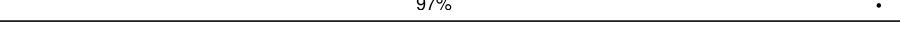
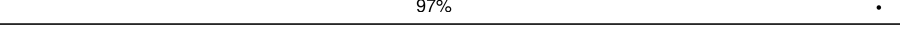
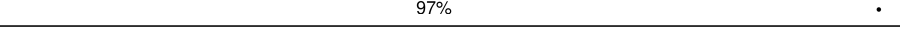
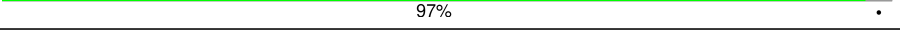
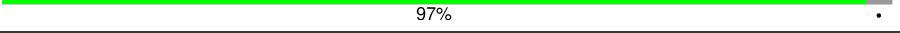
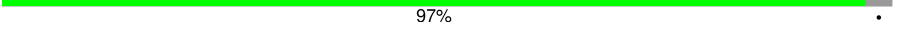
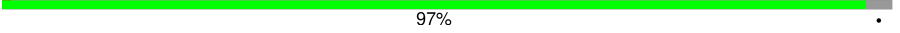
Continued on next page...

Continued from previous page...

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 1 | CC | 443 |  |
| 1 | CE | 443 |  |
| 1 | CG | 443 |  |
| 1 | CI | 443 |  |
| 1 | CK | 443 |  |
| 1 | CM | 443 |  |
| 1 | DA | 443 |  |
| 1 | DC | 443 |  |
| 1 | DE | 443 |  |
| 1 | DG | 443 |  |
| 1 | DI | 443 |  |
| 1 | DK | 443 |  |
| 1 | DM | 443 |  |
| 1 | E | 443 |  |
| 1 | EB | 443 |  |
| 1 | ED | 443 |  |
| 1 | EF | 443 |  |
| 1 | EH | 443 |  |
| 1 | EJ | 443 |  |
| 1 | EL | 443 |  |
| 1 | F | 443 |  |
| 1 | FB | 443 |  |
| 1 | FD | 443 |  |
| 1 | FF | 443 |  |
| 1 | FH | 443 | |

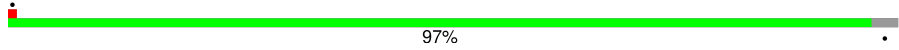
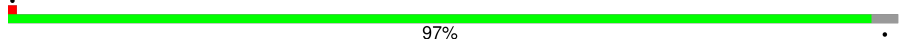
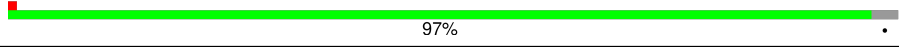
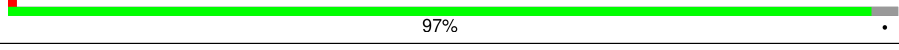
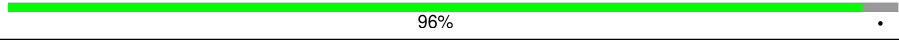
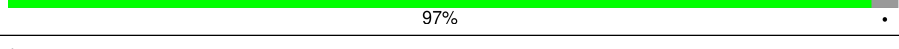
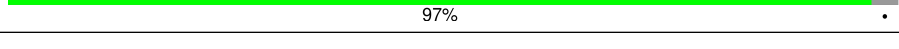
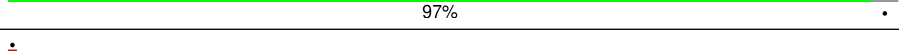
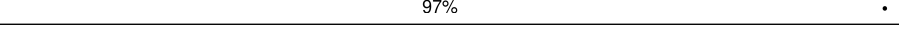
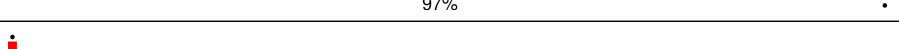
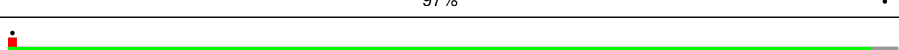
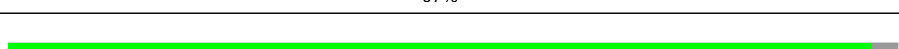
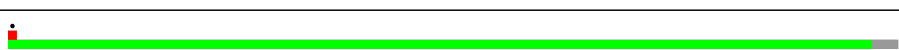
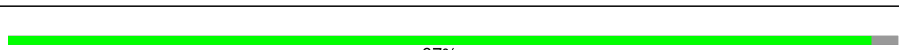
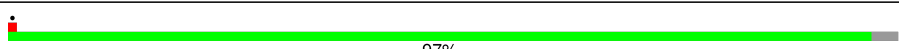
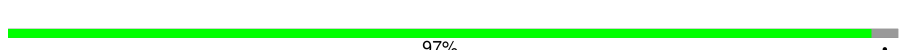

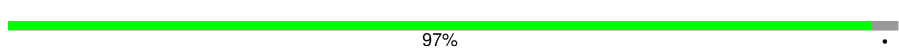
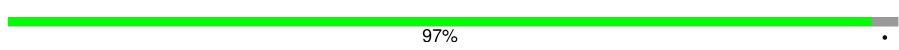
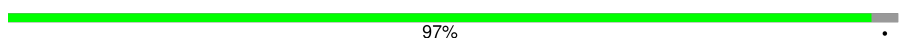
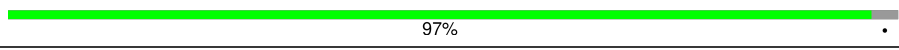
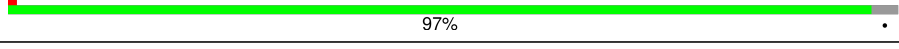
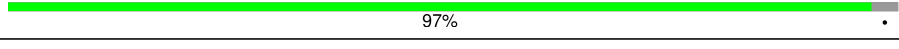
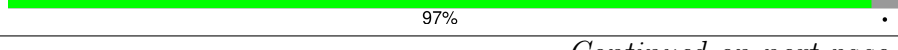

Continued on next page...

Continued from previous page...

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|-------------------------------------------------------------------------------------------|
| 1 | FJ | 443 |  97% |
| 1 | FL | 443 |  96% |
| 1 | G | 443 |  5% 97% |
| 1 | GB | 443 |  97% |
| 1 | GD | 443 |  96% |
| 1 | GF | 443 |  97% |
| 1 | GH | 443 |  97% |
| 1 | GJ | 443 |  96% |
| 1 | GL | 443 |  97% |
| 1 | H | 443 |  5% 97% |
| 1 | HB | 443 |  97% |
| 1 | HD | 443 |  97% |
| 1 | HF | 443 |  97% |
| 1 | HH | 443 |  97% |
| 1 | HJ | 443 |  97% |
| 1 | HL | 443 |  97% |
| 1 | I | 443 |  97% |
| 1 | IB | 443 |  97% |
| 1 | ID | 443 |  97% |
| 1 | IF | 443 |  97% |
| 1 | IH | 443 |  97% |
| 1 | IJ | 443 |  97% |
| 1 | IL | 443 |  97% |
| 1 | JA | 443 |  97% |
| 1 | JC | 443 |  97% |

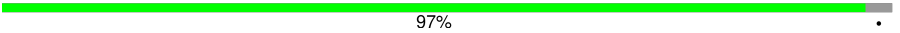
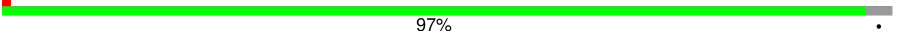
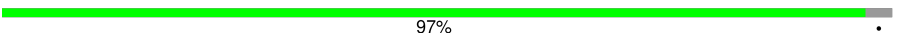
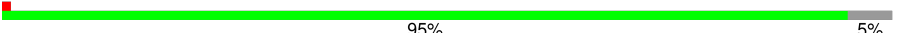

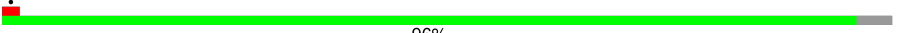









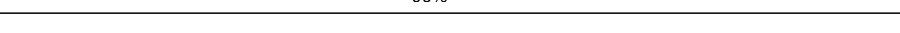
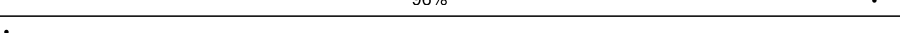
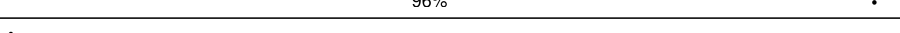

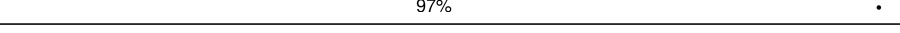
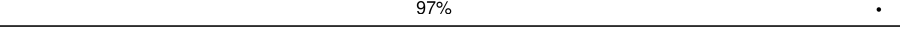
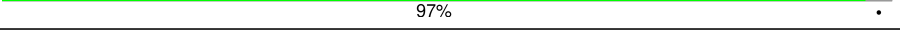
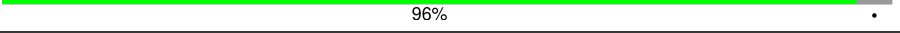
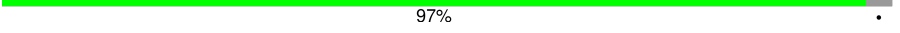
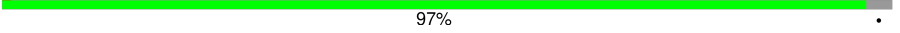
Continued on next page...

Continued from previous page...

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 1 | JE | 443 |  |
| 1 | JG | 443 |  |
| 1 | JI | 443 |  |
| 1 | JK | 443 |  |
| 1 | JM | 443 |  |
| 1 | KA | 443 |  |
| 1 | KC | 443 |  |
| 1 | KE | 443 |  |
| 1 | KG | 443 |  |
| 1 | KI | 443 |  |
| 1 | KK | 443 |  |
| 1 | KM | 443 |  |
| 1 | LA | 443 |  |
| 1 | LC | 443 |  |
| 1 | LE | 443 |  |
| 1 | LG | 443 |  |
| 1 | LI | 443 |  |
| 1 | LK | 443 |  |
| 1 | LM | 443 |  |
| 1 | LO | 443 |  |
| 1 | M | 443 |  |
| 1 | MB | 443 |  |
| 1 | MD | 443 |  |
| 1 | MF | 443 |  |
| 1 | MH | 443 |  |

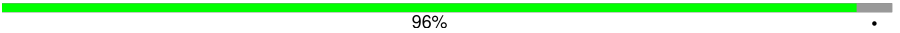
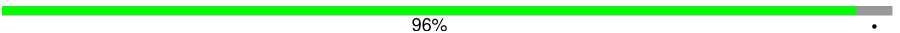
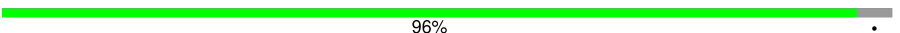
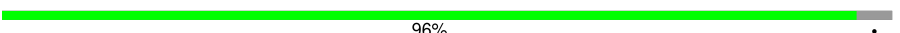

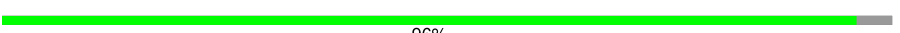









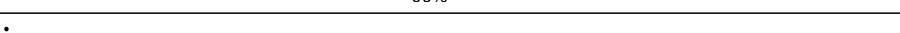
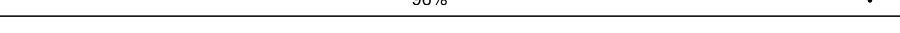
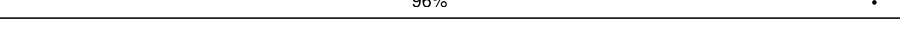
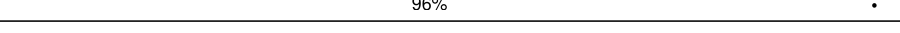
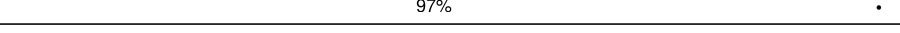
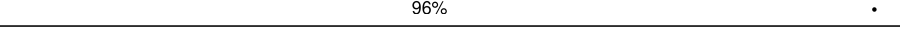
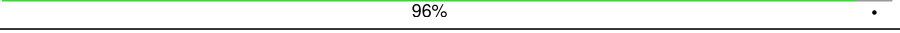
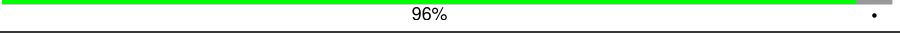
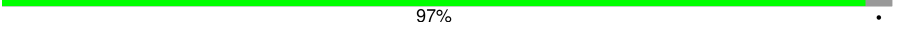
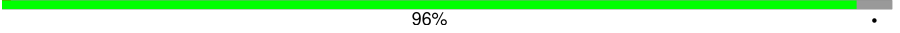
Continued on next page...

Continued from previous page...

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|-----------------------------------------------------------------------------------------------|
| 1 | MJ | 443 |  97% . |
| 1 | ML | 443 |  97% . |
| 1 | MN | 443 |  97% . |
| 1 | N | 443 |  95% 5% . |
| 1 | NB | 443 |  95% 5% . |
| 1 | ND | 443 |  96% . |
| 1 | NF | 443 |  96% . |
| 1 | NH | 443 |  96% . |
| 1 | NJ | 443 |  97% . |
| 1 | NL | 443 |  96% . |
| 1 | O | 443 |  96% . |
| 1 | OB | 443 |  96% . |
| 1 | OD | 443 |  96% . |
| 1 | OF | 443 |  96% . |
| 1 | OH | 443 |  96% . |
| 1 | OJ | 443 |  96% . |
| 1 | OL | 443 |  96% . |
| 1 | P | 443 |  90% 9% . |
| 1 | PB | 443 |  97% . |
| 1 | PD | 443 |  97% . |
| 1 | PF | 443 |  97% . |
| 1 | PH | 443 |  96% . |
| 1 | PJ | 443 |  97% . |
| 1 | PL | 443 |  97% . |
| 1 | QA | 443 |  96% . |

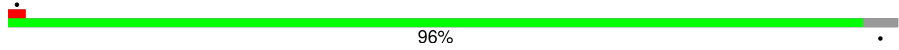
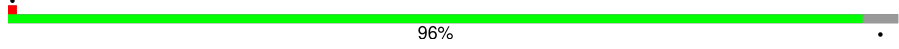
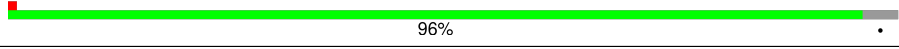
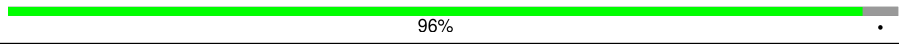
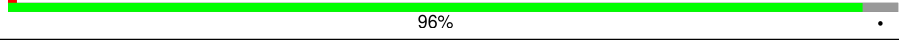
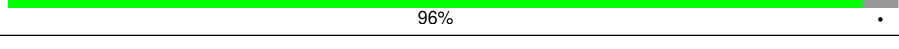
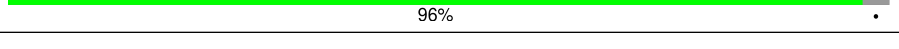
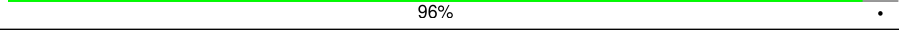
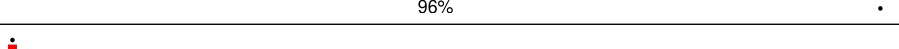
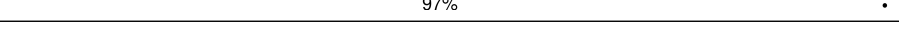
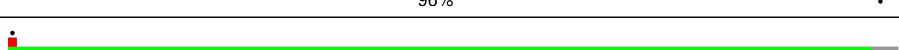
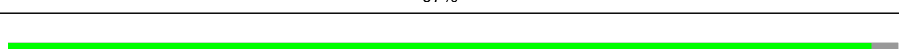
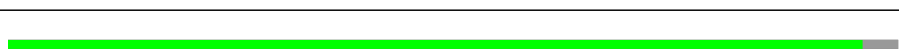
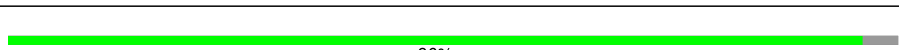
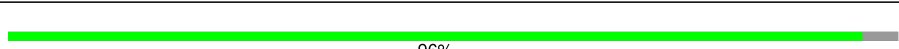
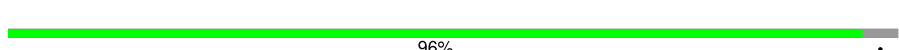

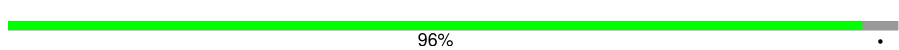
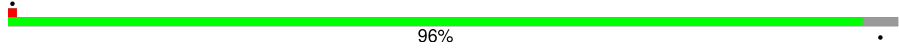
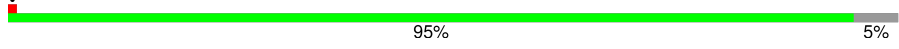
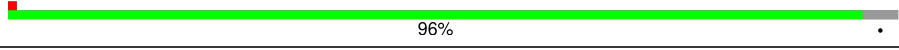
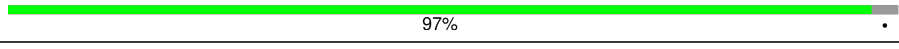
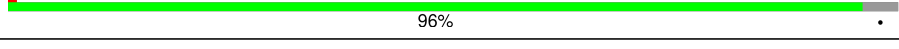
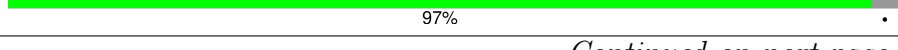

Continued on next page...

Continued from previous page...

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--------------------------------------------------------------------------------------------|
| 1 | QC | 443 |  96% . |
| 1 | QE | 443 |  96% . |
| 1 | QG | 443 |  96% . |
| 1 | QI | 443 |  96% . |
| 1 | QK | 443 |  96% . |
| 1 | RA | 443 |  96% . |
| 1 | RC | 443 |  97% . |
| 1 | RE | 443 |  96% . |
| 1 | RG | 443 |  96% . |
| 1 | RI | 443 |  96% . |
| 1 | RK | 443 |  97% . |
| 1 | S | 443 |  96% . |
| 1 | SB | 443 |  96% . |
| 1 | SD | 443 |  96% . |
| 1 | SF | 443 |  96% . |
| 1 | SH | 443 |  96% . |
| 1 | SJ | 443 |  96% . |
| 1 | T | 443 |  96% . |
| 1 | TB | 443 |  97% . |
| 1 | TD | 443 |  96% . |
| 1 | TF | 443 |  96% . |
| 1 | TH | 443 |  96% . |
| 1 | TJ | 443 |  97% . |
| 1 | TL | 443 |  96% . |
| 1 | U | 443 |  96% . |

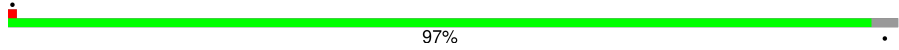
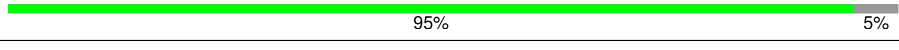
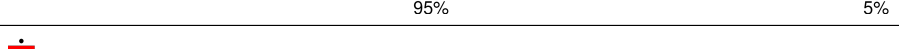
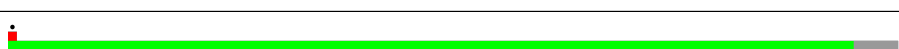
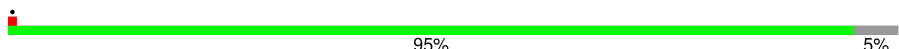
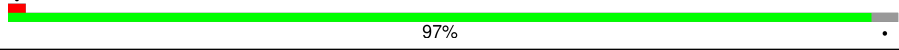
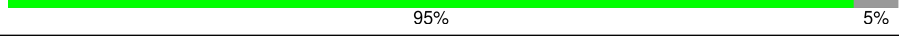
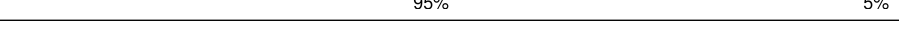
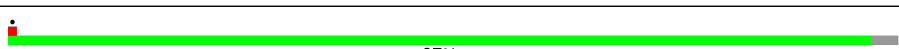
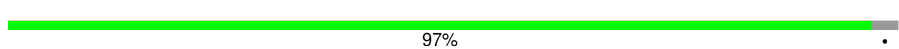
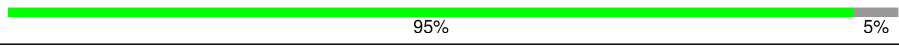
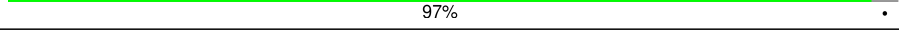
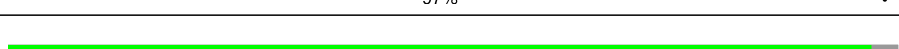
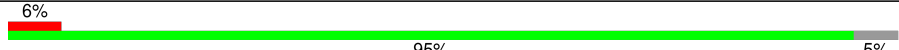
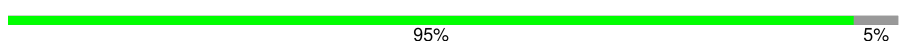
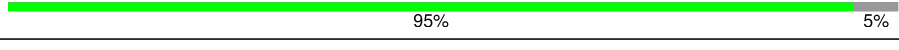
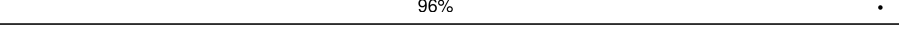


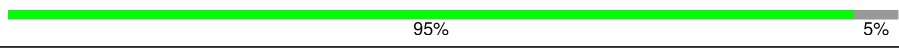
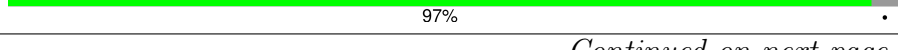



Continued on next page...

Continued from previous page...

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|----------------------------------------------------------------------------------------------|
| 1 | UB | 443 |  96%. |
| 1 | UD | 443 |  96%. |
| 1 | UF | 443 |  96%. |
| 1 | UH | 443 |  96%. |
| 1 | UJ | 443 |  96%. |
| 1 | UL | 443 |  96%. |
| 1 | V | 443 |  96%. |
| 1 | VB | 443 |  96%. |
| 1 | VD | 443 |  96%. |
| 1 | VF | 443 |  97%. |
| 1 | VH | 443 |  96%. |
| 1 | VJ | 443 |  97%. |
| 1 | VL | 443 |  97%. |
| 1 | W | 443 |  96%. |
| 1 | WB | 443 |  96%. |
| 1 | WD | 443 |  96%. |
| 1 | WF | 443 |  96%. |
| 1 | WH | 443 |  96%. |
| 1 | WJ | 443 |  96%. |
| 1 | WL | 443 |  96%. |
| 2 | AA | 451 |  95% 5%. |
| 2 | AC | 451 |  96%. |
| 2 | AE | 451 |  97%. |
| 2 | AG | 451 |  96%. |
| 2 | AI | 451 |  97%. |

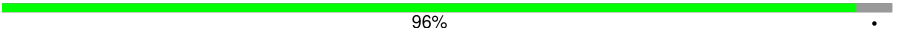
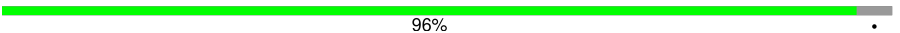
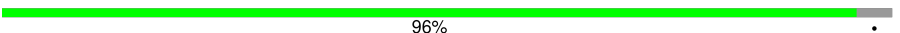
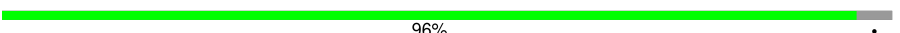

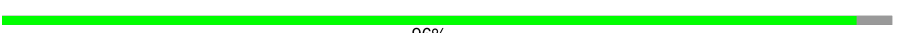









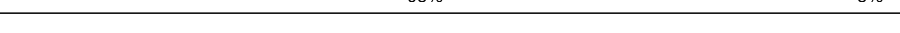
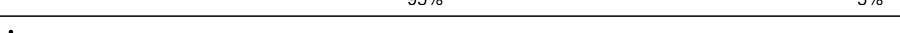
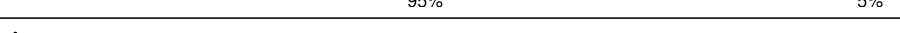
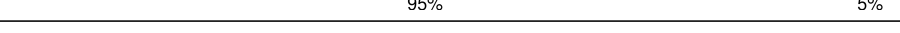
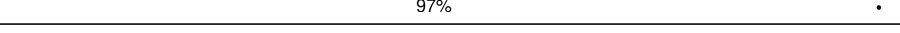
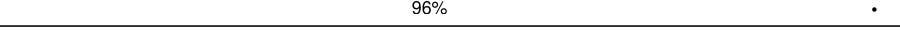
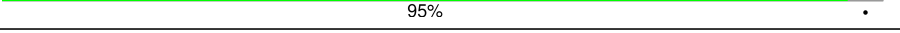
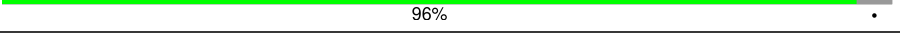
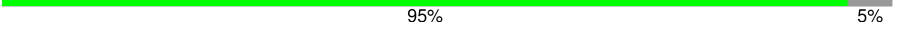
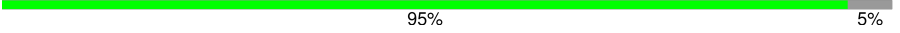
Continued on next page...

Continued from previous page...

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 2 | AK | 451 |  |
| 2 | AM | 451 |  |
| 2 | BA | 451 |  |
| 2 | BC | 451 |  |
| 2 | BE | 451 |  |
| 2 | BG | 451 |  |
| 2 | BI | 451 |  |
| 2 | BK | 451 |  |
| 2 | BM | 451 |  |
| 2 | C | 451 |  |
| 2 | CB | 451 |  |
| 2 | CD | 451 |  |
| 2 | CF | 451 |  |
| 2 | CH | 451 |  |
| 2 | CJ | 451 |  |
| 2 | CL | 451 |  |
| 2 | D | 451 |  |
| 2 | DB | 451 |  |
| 2 | DD | 451 |  |
| 2 | DF | 451 |  |
| 2 | DH | 451 |  |
| 2 | DJ | 451 |  |
| 2 | DL | 451 |  |
| 2 | EA | 451 |  |
| 2 | EC | 451 | |

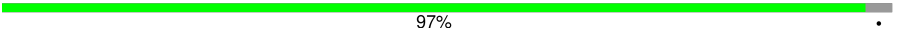
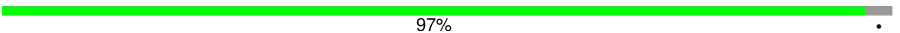
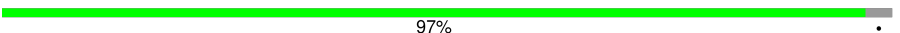
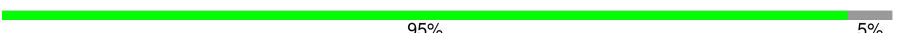

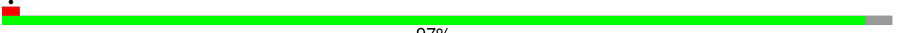









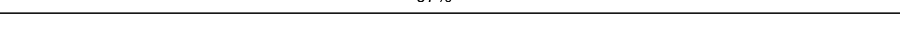
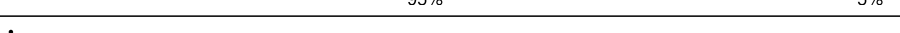
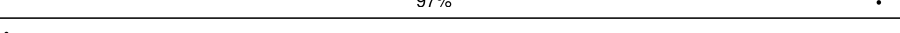
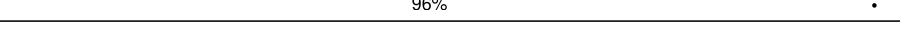
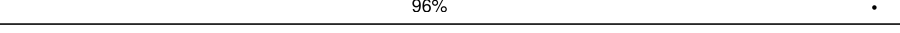
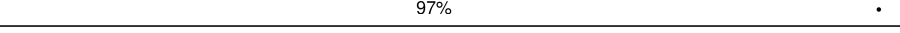
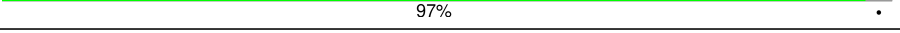
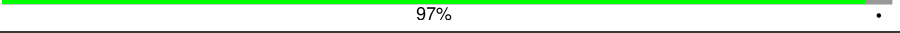
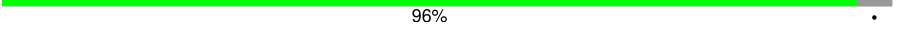
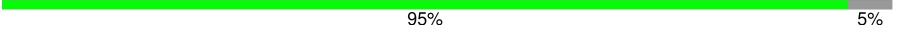
Continued on next page...

Continued from previous page...

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|---------------------------------------------------------------------------------------------|
| 2 | EE | 451 |  96% . |
| 2 | EG | 451 |  96% . |
| 2 | EI | 451 |  96% . |
| 2 | EK | 451 |  96% . |
| 2 | FA | 451 |  97% . |
| 2 | FC | 451 |  96% . |
| 2 | FE | 451 |  96% . |
| 2 | FG | 451 |  96% . |
| 2 | FI | 451 |  95% 5% |
| 2 | FK | 451 |  96% . |
| 2 | GA | 451 |  95% 5% |
| 2 | GC | 451 |  95% 5% |
| 2 | GE | 451 |  96% . |
| 2 | GG | 451 |  95% 5% |
| 2 | GI | 451 |  95% 5% |
| 2 | GK | 451 |  95% 5% |
| 2 | HA | 451 |  95% 5% |
| 2 | HC | 451 |  95% 5% |
| 2 | HE | 451 |  97% . |
| 2 | HG | 451 |  96% . |
| 2 | HI | 451 |  95% . |
| 2 | HK | 451 |  96% . |
| 2 | HM | 451 |  95% 5% |
| 2 | IA | 451 |  95% 5% |
| 2 | IC | 451 |  96% . |

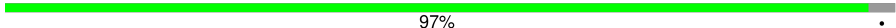
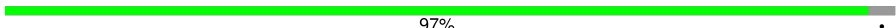
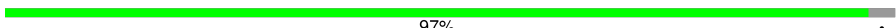
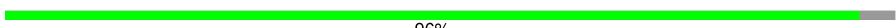









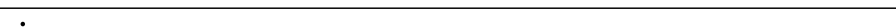

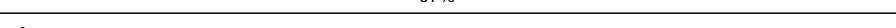
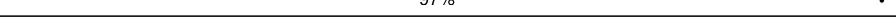
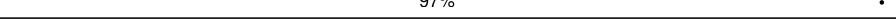
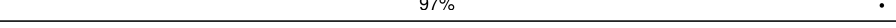
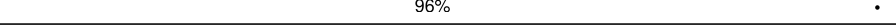
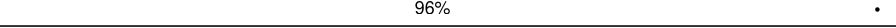
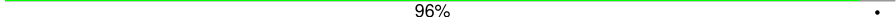
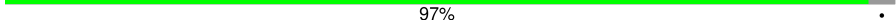
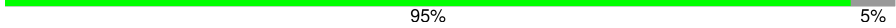
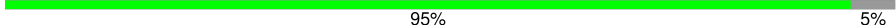
Continued on next page...

Continued from previous page...

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|---------------------------------------------------------------------------------------------|
| 2 | IE | 451 |  97% . |
| 2 | IG | 451 |  97% . |
| 2 | II | 451 |  97% . |
| 2 | IK | 451 |  95% 5% |
| 2 | IM | 451 |  95% 5% |
| 2 | J | 451 |  97% . |
| 2 | JB | 451 |  97% . |
| 2 | JD | 451 |  95% 5% |
| 2 | JF | 451 |  95% 5% |
| 2 | JH | 451 |  96% . |
| 2 | JJ | 451 |  96% . |
| 2 | JL | 451 |  96% . |
| 2 | JN | 451 |  97% . |
| 2 | K | 451 |  96% . |
| 2 | KB | 451 |  97% . |
| 2 | KD | 451 |  95% 5% |
| 2 | KF | 451 |  97% . |
| 2 | KH | 451 |  96% . |
| 2 | KJ | 451 |  96% . |
| 2 | KL | 451 |  97% . |
| 2 | KN | 451 |  97% . |
| 2 | L | 451 |  97% . |
| 2 | LB | 451 |  96% . |
| 2 | LD | 451 |  95% 5% |
| 2 | LF | 451 |  97% . |

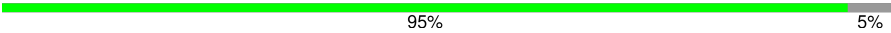
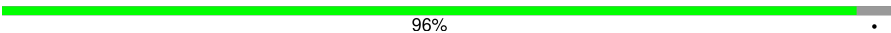
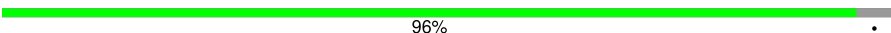
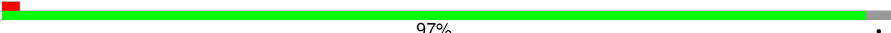
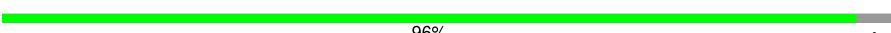
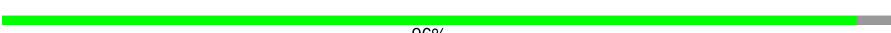









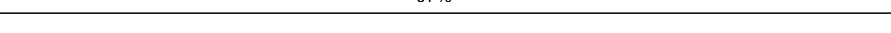
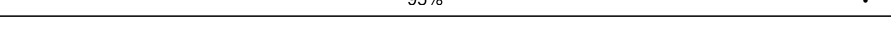
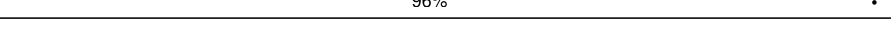
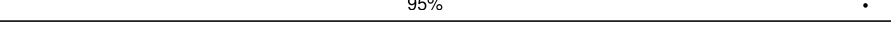
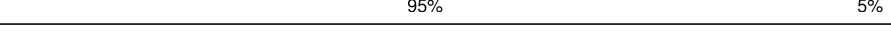
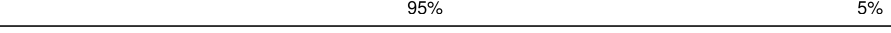
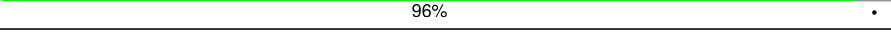
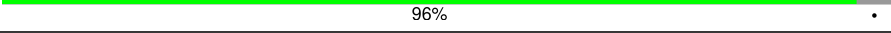
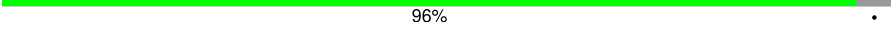
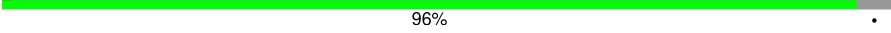
Continued on next page...

Continued from previous page...

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|-----------------------------------------------------------------------------------------------|
| 2 | LH | 451 |  97% . |
| 2 | LJ | 451 |  97% . |
| 2 | LL | 451 |  97% . |
| 2 | LN | 451 |  96% . |
| 2 | MA | 451 |  96% . |
| 2 | MC | 451 |  97% . |
| 2 | ME | 451 |  97% . |
| 2 | MG | 451 |  97% . |
| 2 | MI | 451 |  97% . |
| 2 | MK | 451 |  97% . |
| 2 | MM | 451 |  96% . |
| 2 | NA | 451 |  97% . |
| 2 | NC | 451 |  5% 97% . |
| 2 | NE | 451 |  97% . |
| 2 | NG | 451 |  97% . |
| 2 | NI | 451 |  97% . |
| 2 | NK | 451 |  97% . |
| 2 | NM | 451 |  97% . |
| 2 | OA | 451 |  96% . |
| 2 | OC | 451 |  96% . |
| 2 | OE | 451 |  96% . |
| 2 | OG | 451 |  97% . |
| 2 | OI | 451 |  95% 5% . |
| 2 | OK | 451 |  95% 5% . |
| 2 | OM | 451 |  96% . |

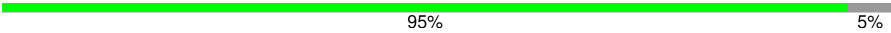
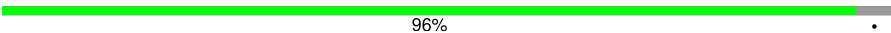
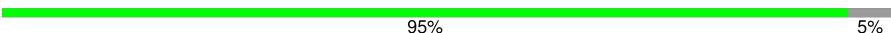
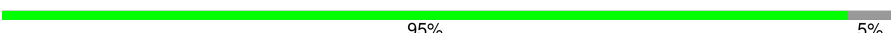

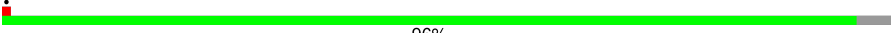









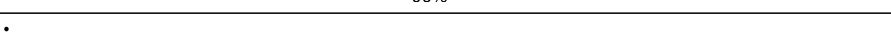
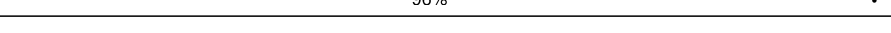
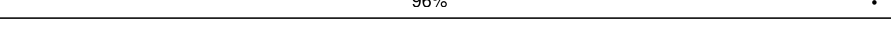
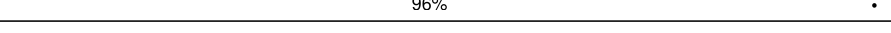
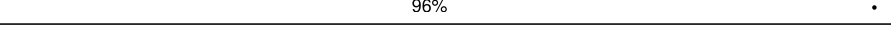
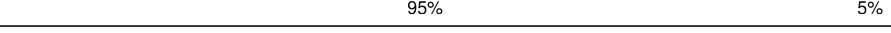
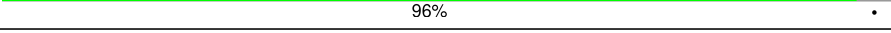
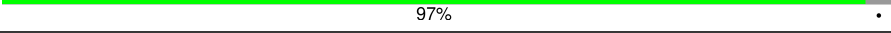
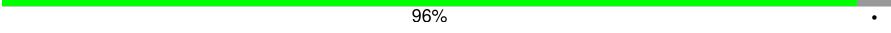
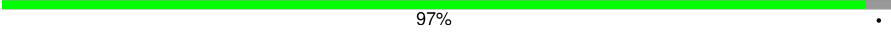
Continued on next page...

Continued from previous page...

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|---------------------------------------------------------------------------------------------|
| 2 | PA | 451 |  95% 5% |
| 2 | PC | 451 |  96% . |
| 2 | PE | 451 |  96% . |
| 2 | PG | 451 |  97% . |
| 2 | PI | 451 |  96% . |
| 2 | PK | 451 |  96% . |
| 2 | PM | 451 |  96% . |
| 2 | Q | 451 |  97% . |
| 2 | QB | 451 |  95% 5% |
| 2 | QD | 451 |  95% 5% |
| 2 | QF | 451 |  95% 5% |
| 2 | QH | 451 |  97% . |
| 2 | QJ | 451 |  96% . |
| 2 | QL | 451 |  96% . |
| 2 | R | 451 |  97% . |
| 2 | RB | 451 |  95% . |
| 2 | RD | 451 |  96% . |
| 2 | RF | 451 |  95% . |
| 2 | RH | 451 |  95% 5% |
| 2 | RJ | 451 |  95% 5% |
| 2 | RL | 451 |  96% . |
| 2 | SA | 451 |  96% . |
| 2 | SC | 451 |  96% . |
| 2 | SE | 451 |  96% . |
| 2 | SG | 451 |  96% . |

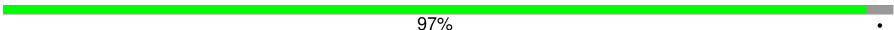
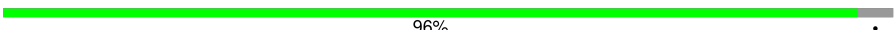
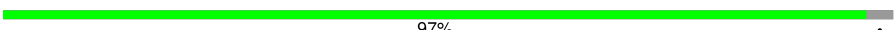







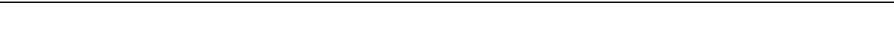

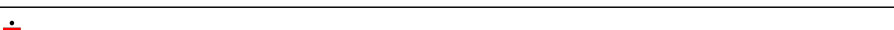
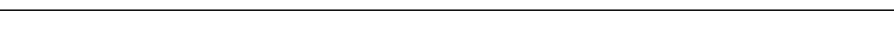



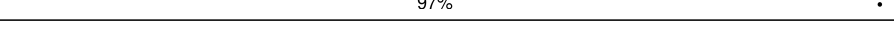
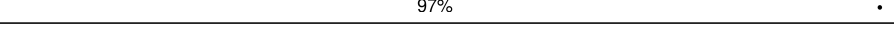






Continued on next page...

Continued from previous page...

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|---------------------------------------------------------------------------------------------|
| 2 | SI | 451 |  95% 5% |
| 2 | SK | 451 |  96% . |
| 2 | TA | 451 |  95% 5% |
| 2 | TC | 451 |  95% 5% |
| 2 | TE | 451 |  95% 5% |
| 2 | TG | 451 |  96% . |
| 2 | TI | 451 |  95% 5% |
| 2 | TK | 451 |  96% . |
| 2 | UA | 451 |  95% 5% |
| 2 | UC | 451 |  95% 5% |
| 2 | UE | 451 |  95% 5% |
| 2 | UG | 451 |  96% . |
| 2 | UI | 451 |  95% 5% |
| 2 | UK | 451 |  95% 5% |
| 2 | VA | 451 |  96% . |
| 2 | VC | 451 |  96% . |
| 2 | VE | 451 |  96% . |
| 2 | VG | 451 |  96% . |
| 2 | VI | 451 |  96% . |
| 2 | VK | 451 |  95% 5% |
| 2 | VM | 451 |  96% . |
| 2 | WA | 451 |  97% . |
| 2 | WC | 451 |  96% . |
| 2 | WE | 451 |  97% . |
| 2 | WG | 451 |  95% . |

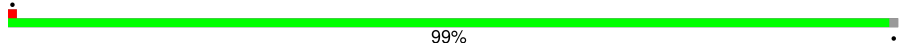
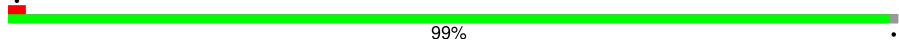
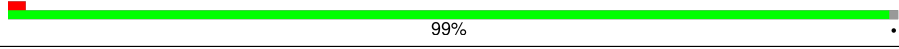
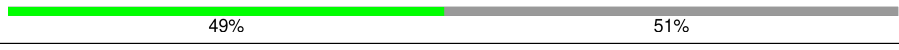

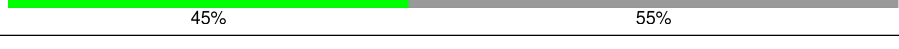
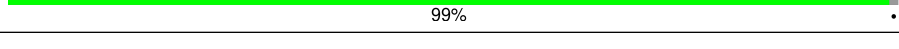
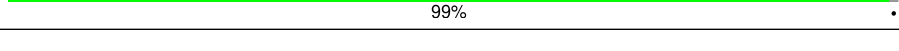
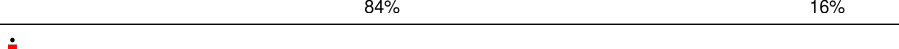
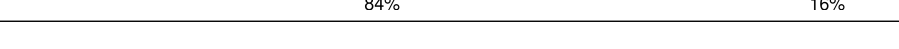
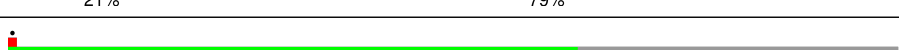

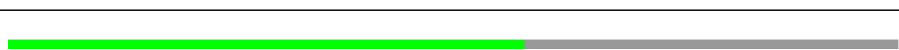

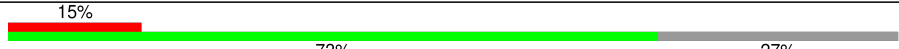



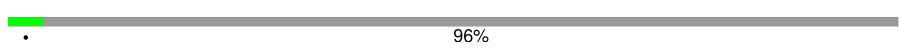

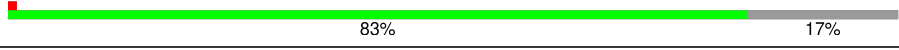
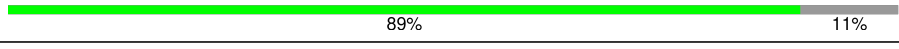



Continued on next page...

Continued from previous page...

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|----------------------------------------------------------------------------------------------|
| 2 | WI | 451 |  97% . |
| 2 | WK | 451 |  96% . |
| 2 | WM | 451 |  97% . |
| 3 | X | 214 |  86% 14% |
| 3 | XA | 214 |  85% 14% |
| 3 | XB | 214 |  86% 14% |
| 3 | XC | 214 |  86% 14% |
| 3 | XD | 214 |  86% 14% |
| 3 | XE | 214 |  86% 14% |
| 3 | XF | 214 |  86% 14% |
| 4 | XM | 310 |  84% 16% |
| 4 | XO | 310 |  84% 16% |
| 4 | XQ | 310 |  84% 16% |
| 4 | XR | 310 |  84% 16% |
| 5 | XN | 314 |  86% 14% |
| 5 | XP | 314 |  86% 14% |
| 6 | 0 | 264 |  97% . |
| 6 | 0A | 264 |  97% . |
| 7 | 0C | 408 |  30% 70% |
| 7 | 0D | 408 |  86% 13% |
| 8 | 0F | 480 |  37% 63% |
| 8 | 0G | 480 |  73% 27% |
| 8 | 0H | 480 |  6% 94% |
| 8 | 0I | 480 |  59% 41% |
| 8 | 0J | 480 |  47% 53% |


























Continued on next page...

Continued from previous page...

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 9 | 0L | 629 |  |
| 9 | 0M | 629 |  |
| 9 | 0N | 629 |  |
| 9 | 0O | 629 |  |
| 10 | 0R | 490 |  |
| 10 | 0S | 490 |  |
| 11 | 0U | 337 |  |
| 12 | 0W | 343 |  |
| 13 | 0Y | 279 |  |
| 13 | 0Z | 279 |  |
| 13 | 0a | 279 |  |
| 14 | 0c | 370 |  |
| 14 | 0d | 370 |  |
| 15 | 0f | 277 |  |
| 15 | 0g | 277 |  |
| 16 | 0k | 979 |  |
| 16 | 0l | 979 |  |
| 17 | 0m | 446 |  |
| 17 | 0n | 446 |  |
| 17 | 0o | 446 |  |
| 18 | 0p | 305 |  |
| 19 | 0r | 306 |  |
| 20 | 0t | 295 |  |
| 20 | 0u | 295 |  |
| 21 | 0v | 533 |  |














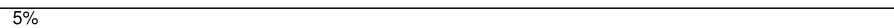











Continued on next page...

Continued from previous page...

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 21 | 0w | 533 |  |
| 21 | 0x | 533 |  |
| 22 | 0z | 282 |  |
| 22 | 1w | 282 |  |
| 22 | 1x | 282 |  |
| 22 | 1y | 282 |  |
| 23 | 1A | 397 |  |
| 23 | 1B | 397 |  |
| 23 | 1D | 397 |  |
| 23 | 1E | 397 |  |
| 23 | 1F | 397 |  |
| 24 | 1H | 756 |  |
| 24 | 1I | 756 |  |
| 24 | 1J | 756 |  |
| 24 | 1K | 756 |  |
| 25 | 1O | 774 |  |
| 26 | 1Q | 741 |  |
| 27 | 1S | 861 |  |
| 27 | 1T | 861 |  |
| 28 | 1U | 266 |  |
| 28 | 1V | 266 |  |
| 28 | 1X | 266 |  |
| 28 | 1Y | 266 |  |
| 28 | 1a | 266 |  |
| 28 | 1b | 266 |  |



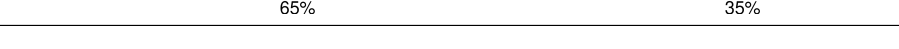
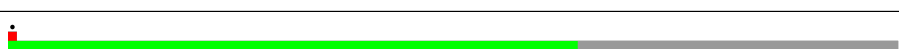



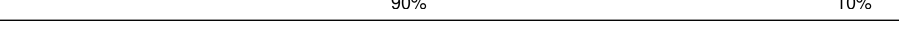



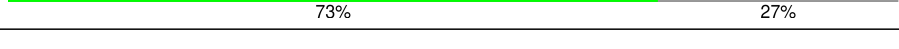




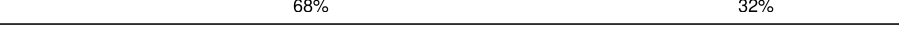


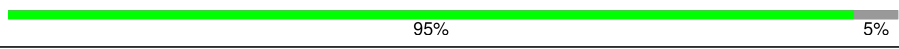




Continued on next page...

Continued from previous page...

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 28 | 1c | 266 |  |
| 28 | 1d | 266 |  |
| 28 | 1e | 266 |  |
| 28 | 1g | 266 |  |
| 28 | 1h | 266 |  |
| 28 | 4V | 266 |  |
| 28 | 4W | 266 |  |
| 29 | 1j | 226 |  |
| 29 | 1k | 226 |  |
| 29 | 1l | 226 |  |
| 29 | 1m | 226 |  |
| 30 | 1o | 236 |  |
| 31 | 1q | 275 |  |
| 31 | 1r | 275 |  |
| 31 | 1s | 275 |  |
| 31 | 1t | 275 |  |
| 32 | 2B | 289 |  |
| 32 | 2C | 289 |  |
| 33 | 2F | 312 |  |
| 33 | 2G | 312 |  |
| 33 | 2H | 312 |  |
| 33 | 2I | 312 |  |
| 34 | 2L | 311 |  |
| 35 | 2N | 314 |  |
| 35 | 2O | 314 |  |




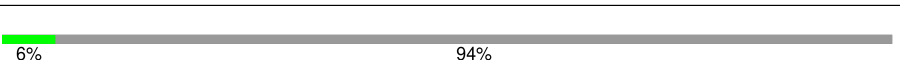
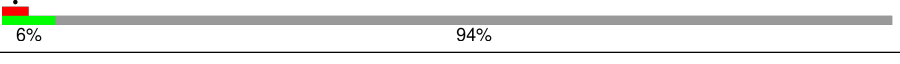

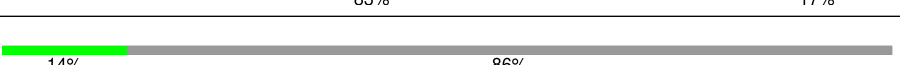



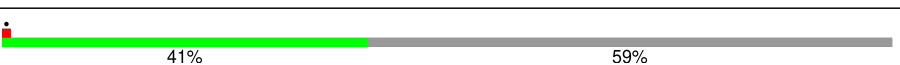
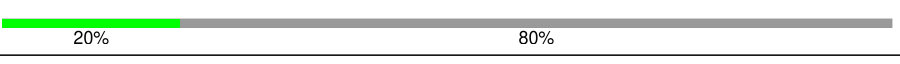
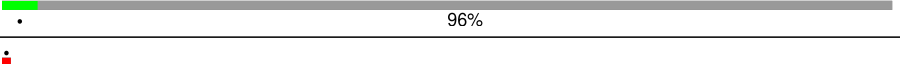
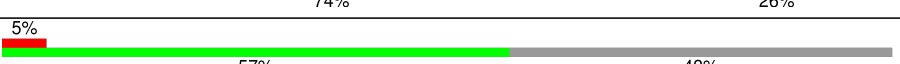

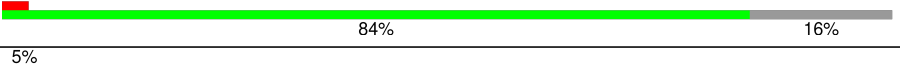

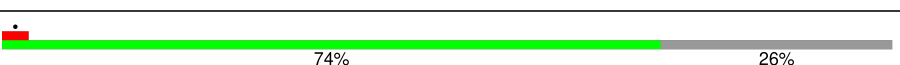

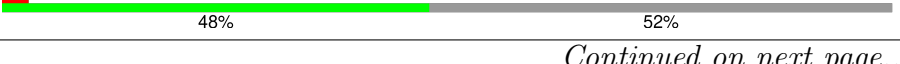



Continued on next page...

Continued from previous page...

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 36 | 2Q | 338 |  |
| 37 | 2S | 358 |  |
| 38 | 2U | 352 |  |
| 38 | 2V | 352 |  |
| 39 | 2X | 352 |  |
| 40 | 2Z | 371 |  |
| 41 | 2b | 360 |  |
| 41 | 2c | 360 |  |
| 41 | 2e | 360 |  |
| 41 | 2f | 360 |  |
| 41 | 2h | 360 |  |
| 41 | 2i | 360 |  |
| 41 | 2k | 360 |  |
| 41 | 2l | 360 |  |
| 41 | 2n | 360 |  |
| 41 | 2o | 360 |  |
| 41 | 2p | 360 |  |
| 42 | 2r | 410 |  |
| 43 | 2t | 343 |  |
| 44 | 2v | 413 |  |
| 44 | 2w | 413 |  |
| 45 | 2y | 430 |  |
| 45 | 2z | 430 |  |
| 46 | 3B | 439 |  |
| 47 | 3D | 457 | |



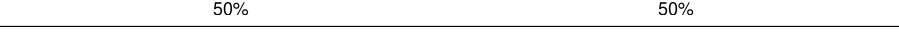




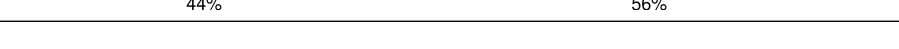




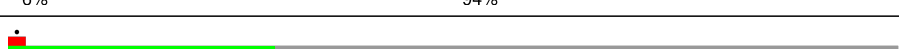



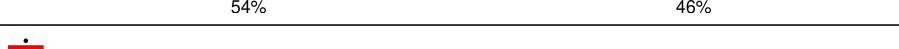


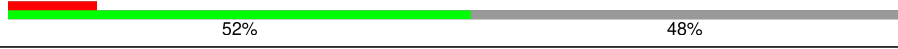




Continued on next page...

Continued from previous page...

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 48 | 3F | 468 |  |
| 48 | 3G | 468 |  |
| 48 | 3H | 468 |  |
| 48 | 3I | 468 |  |
| 48 | 3L | 468 |  |
| 48 | 3M | 468 |  |
| 49 | 3P | 588 |  |
| 49 | 3Q | 588 |  |
| 50 | 3S | 176 |  |
| 51 | X1 | 308 |  |
| 52 | 3U | 409 |  |
| 53 | 3W | 373 |  |
| 53 | 3X | 373 |  |
| 54 | 3Z | 443 |  |
| 54 | 3a | 443 |  |
| 54 | 4Y | 443 |  |
| 55 | 3b | 183 |  |
| 56 | 3d | 261 |  |
| 57 | 3f | 197 |  |
| 57 | 3g | 197 |  |
| 57 | 3h | 197 |  |
| 57 | 3i | 197 |  |
| 58 | 3m | 195 |  |
| 59 | 3o | 306 | |
| 59 | 3p | 306 | |

Continued on next page...

Continued from previous page...

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 59 | 4O | 306 |  |
| 59 | 4P | 306 |  |
| 59 | 4a | 306 |  |
| 59 | 4b | 306 |  |
| 60 | 3r | 158 |  |
| 60 | 3s | 158 |  |
| 60 | 3t | 158 |  |
| 61 | 3w | 288 |  |
| 61 | 3x | 288 |  |
| 62 | 4A | 480 |  |
| 62 | 4B | 480 |  |
| 63 | 4I | 590 |  |
| 64 | 5B | 675 |  |
| 64 | 5C | 675 |  |
| 64 | 5D | 675 |  |
| 65 | 5G | 617 |  |
| 65 | 5H | 617 |  |
| 65 | 5I | 617 |  |
| 66 | 5K | 492 |  |
| 66 | 5L | 492 |  |
| 67 | 5O | 111 |  |
| 67 | 5P | 111 |  |
| 68 | 5S | 176 |  |
| 68 | 5T | 176 |  |

2 Entry composition

There are 74 unique types of molecules in this entry. The entry contains 1371722 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Tubulin beta chain.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 1 | A | 429 | Total | C | N | O | S | 0 | 0 |
| | | | 3362 | 2101 | 578 | 652 | 31 | | |
| 1 | AB | 419 | Total | C | N | O | S | 0 | 0 |
| | | | 3283 | 2056 | 560 | 636 | 31 | | |
| 1 | AD | 429 | Total | C | N | O | S | 0 | 0 |
| | | | 3362 | 2101 | 578 | 652 | 31 | | |
| 1 | AF | 429 | Total | C | N | O | S | 0 | 0 |
| | | | 3362 | 2101 | 578 | 652 | 31 | | |
| 1 | AH | 429 | Total | C | N | O | S | 0 | 0 |
| | | | 3362 | 2101 | 578 | 652 | 31 | | |
| 1 | AJ | 429 | Total | C | N | O | S | 0 | 0 |
| | | | 3362 | 2101 | 578 | 652 | 31 | | |
| 1 | AL | 429 | Total | C | N | O | S | 0 | 0 |
| | | | 3362 | 2101 | 578 | 652 | 31 | | |
| 1 | AN | 419 | Total | C | N | O | S | 0 | 0 |
| | | | 3283 | 2056 | 560 | 636 | 31 | | |
| 1 | B | 418 | Total | C | N | O | S | 0 | 0 |
| | | | 3270 | 2039 | 564 | 637 | 30 | | |
| 1 | BB | 429 | Total | C | N | O | S | 0 | 0 |
| | | | 3362 | 2101 | 578 | 652 | 31 | | |
| 1 | BD | 430 | Total | C | N | O | S | 0 | 0 |
| | | | 3370 | 2106 | 579 | 653 | 32 | | |
| 1 | BF | 429 | Total | C | N | O | S | 0 | 0 |
| | | | 3362 | 2101 | 578 | 652 | 31 | | |
| 1 | BH | 429 | Total | C | N | O | S | 0 | 0 |
| | | | 3362 | 2101 | 578 | 652 | 31 | | |
| 1 | BJ | 429 | Total | C | N | O | S | 0 | 0 |
| | | | 3362 | 2101 | 578 | 652 | 31 | | |
| 1 | BL | 429 | Total | C | N | O | S | 0 | 0 |
| | | | 3362 | 2101 | 578 | 652 | 31 | | |
| 1 | BN | 429 | Total | C | N | O | S | 0 | 0 |
| | | | 3362 | 2101 | 578 | 652 | 31 | | |
| 1 | CA | 424 | Total | C | N | O | S | 0 | 0 |
| | | | 3319 | 2076 | 568 | 643 | 32 | | |

Continued on next page...

Continued from previous page...

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 1 | CC | 430 | Total | C | N | O | S | 0 | 0 |
| | | | 3370 | 2106 | 579 | 653 | 32 | | |
| 1 | CE | 430 | Total | C | N | O | S | 0 | 0 |
| | | | 3370 | 2106 | 579 | 653 | 32 | | |
| 1 | CG | 430 | Total | C | N | O | S | 0 | 0 |
| | | | 3370 | 2106 | 579 | 653 | 32 | | |
| 1 | CI | 429 | Total | C | N | O | S | 0 | 0 |
| | | | 3362 | 2101 | 578 | 652 | 31 | | |
| 1 | CK | 429 | Total | C | N | O | S | 0 | 0 |
| | | | 3362 | 2101 | 578 | 652 | 31 | | |
| 1 | CM | 429 | Total | C | N | O | S | 0 | 0 |
| | | | 3362 | 2101 | 578 | 652 | 31 | | |
| 1 | DA | 429 | Total | C | N | O | S | 0 | 0 |
| | | | 3362 | 2101 | 578 | 652 | 31 | | |
| 1 | DC | 429 | Total | C | N | O | S | 0 | 0 |
| | | | 3362 | 2101 | 578 | 652 | 31 | | |
| 1 | DE | 429 | Total | C | N | O | S | 0 | 0 |
| | | | 3362 | 2101 | 578 | 652 | 31 | | |
| 1 | DG | 429 | Total | C | N | O | S | 0 | 0 |
| | | | 3362 | 2101 | 578 | 652 | 31 | | |
| 1 | DI | 429 | Total | C | N | O | S | 0 | 0 |
| | | | 3362 | 2101 | 578 | 652 | 31 | | |
| 1 | DK | 429 | Total | C | N | O | S | 0 | 0 |
| | | | 3362 | 2101 | 578 | 652 | 31 | | |
| 1 | DM | 429 | Total | C | N | O | S | 0 | 0 |
| | | | 3362 | 2101 | 578 | 652 | 31 | | |
| 1 | E | 430 | Total | C | N | O | S | 0 | 0 |
| | | | 3370 | 2106 | 579 | 653 | 32 | | |
| 1 | EB | 430 | Total | C | N | O | S | 0 | 0 |
| | | | 3370 | 2106 | 579 | 653 | 32 | | |
| 1 | ED | 430 | Total | C | N | O | S | 0 | 0 |
| | | | 3370 | 2106 | 579 | 653 | 32 | | |
| 1 | EF | 430 | Total | C | N | O | S | 0 | 0 |
| | | | 3370 | 2106 | 579 | 653 | 32 | | |
| 1 | EH | 430 | Total | C | N | O | S | 0 | 0 |
| | | | 3370 | 2106 | 579 | 653 | 32 | | |
| 1 | EJ | 430 | Total | C | N | O | S | 0 | 0 |
| | | | 3370 | 2106 | 579 | 653 | 32 | | |
| 1 | EL | 429 | Total | C | N | O | S | 0 | 0 |
| | | | 3362 | 2101 | 578 | 652 | 31 | | |
| 1 | F | 429 | Total | C | N | O | S | 0 | 0 |
| | | | 3362 | 2101 | 578 | 652 | 31 | | |

Continued on next page...

Continued from previous page...

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 1 | FB | 429 | Total | C | N | O | S | 0 | 0 |
| | | | 3362 | 2101 | 578 | 652 | 31 | | |
| 1 | FD | 429 | Total | C | N | O | S | 0 | 0 |
| | | | 3362 | 2101 | 578 | 652 | 31 | | |
| 1 | FF | 429 | Total | C | N | O | S | 0 | 0 |
| | | | 3362 | 2101 | 578 | 652 | 31 | | |
| 1 | FH | 429 | Total | C | N | O | S | 0 | 0 |
| | | | 3362 | 2101 | 578 | 652 | 31 | | |
| 1 | FJ | 429 | Total | C | N | O | S | 0 | 0 |
| | | | 3361 | 2100 | 578 | 652 | 31 | | |
| 1 | FL | 426 | Total | C | N | O | S | 0 | 0 |
| | | | 3343 | 2089 | 575 | 648 | 31 | | |
| 1 | G | 429 | Total | C | N | O | S | 0 | 0 |
| | | | 3362 | 2101 | 578 | 652 | 31 | | |
| 1 | GB | 429 | Total | C | N | O | S | 0 | 0 |
| | | | 3362 | 2101 | 578 | 652 | 31 | | |
| 1 | GD | 426 | Total | C | N | O | S | 0 | 0 |
| | | | 3343 | 2089 | 575 | 648 | 31 | | |
| 1 | GF | 429 | Total | C | N | O | S | 0 | 0 |
| | | | 3362 | 2101 | 578 | 652 | 31 | | |
| 1 | GH | 429 | Total | C | N | O | S | 0 | 0 |
| | | | 3362 | 2101 | 578 | 652 | 31 | | |
| 1 | GJ | 425 | Total | C | N | O | S | 0 | 0 |
| | | | 3335 | 2085 | 574 | 645 | 31 | | |
| 1 | GL | 429 | Total | C | N | O | S | 0 | 0 |
| | | | 3362 | 2101 | 578 | 652 | 31 | | |
| 1 | H | 429 | Total | C | N | O | S | 0 | 0 |
| | | | 3362 | 2101 | 578 | 652 | 31 | | |
| 1 | HB | 429 | Total | C | N | O | S | 0 | 0 |
| | | | 3362 | 2101 | 578 | 652 | 31 | | |
| 1 | HD | 429 | Total | C | N | O | S | 0 | 0 |
| | | | 3362 | 2101 | 578 | 652 | 31 | | |
| 1 | HF | 429 | Total | C | N | O | S | 0 | 0 |
| | | | 3362 | 2101 | 578 | 652 | 31 | | |
| 1 | HH | 429 | Total | C | N | O | S | 0 | 0 |
| | | | 3362 | 2101 | 578 | 652 | 31 | | |
| 1 | HJ | 429 | Total | C | N | O | S | 0 | 0 |
| | | | 3362 | 2101 | 578 | 652 | 31 | | |
| 1 | HL | 429 | Total | C | N | O | S | 0 | 0 |
| | | | 3362 | 2101 | 578 | 652 | 31 | | |
| 1 | I | 430 | Total | C | N | O | S | 0 | 0 |
| | | | 3370 | 2106 | 579 | 653 | 32 | | |

Continued on next page...

Continued from previous page...

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 1 | IB | 429 | Total | C | N | O | S | 0 | 0 |
| | | | 3362 | 2101 | 578 | 652 | 31 | | |
| 1 | ID | 429 | Total | C | N | O | S | 0 | 0 |
| | | | 3362 | 2101 | 578 | 652 | 31 | | |
| 1 | IF | 429 | Total | C | N | O | S | 0 | 0 |
| | | | 3362 | 2101 | 578 | 652 | 31 | | |
| 1 | IH | 429 | Total | C | N | O | S | 0 | 0 |
| | | | 3362 | 2101 | 578 | 652 | 31 | | |
| 1 | IJ | 429 | Total | C | N | O | S | 0 | 0 |
| | | | 3362 | 2101 | 578 | 652 | 31 | | |
| 1 | IL | 429 | Total | C | N | O | S | 0 | 0 |
| | | | 3362 | 2101 | 578 | 652 | 31 | | |
| 1 | JA | 429 | Total | C | N | O | S | 0 | 0 |
| | | | 3362 | 2101 | 578 | 652 | 31 | | |
| 1 | JC | 429 | Total | C | N | O | S | 0 | 0 |
| | | | 3362 | 2101 | 578 | 652 | 31 | | |
| 1 | JE | 429 | Total | C | N | O | S | 0 | 0 |
| | | | 3362 | 2101 | 578 | 652 | 31 | | |
| 1 | JG | 429 | Total | C | N | O | S | 0 | 0 |
| | | | 3362 | 2101 | 578 | 652 | 31 | | |
| 1 | JI | 429 | Total | C | N | O | S | 0 | 0 |
| | | | 3362 | 2101 | 578 | 652 | 31 | | |
| 1 | JK | 429 | Total | C | N | O | S | 0 | 0 |
| | | | 3362 | 2101 | 578 | 652 | 31 | | |
| 1 | JM | 426 | Total | C | N | O | S | 0 | 0 |
| | | | 3343 | 2089 | 575 | 648 | 31 | | |
| 1 | KA | 430 | Total | C | N | O | S | 0 | 0 |
| | | | 3370 | 2106 | 579 | 653 | 32 | | |
| 1 | KC | 429 | Total | C | N | O | S | 0 | 0 |
| | | | 3362 | 2101 | 578 | 652 | 31 | | |
| 1 | KE | 429 | Total | C | N | O | S | 0 | 0 |
| | | | 3362 | 2101 | 578 | 652 | 31 | | |
| 1 | KG | 429 | Total | C | N | O | S | 0 | 0 |
| | | | 3362 | 2101 | 578 | 652 | 31 | | |
| 1 | KI | 429 | Total | C | N | O | S | 0 | 0 |
| | | | 3362 | 2101 | 578 | 652 | 31 | | |
| 1 | KK | 429 | Total | C | N | O | S | 0 | 0 |
| | | | 3362 | 2101 | 578 | 652 | 31 | | |
| 1 | KM | 429 | Total | C | N | O | S | 0 | 0 |
| | | | 3362 | 2101 | 578 | 652 | 31 | | |
| 1 | LA | 429 | Total | C | N | O | S | 0 | 0 |
| | | | 3362 | 2101 | 578 | 652 | 31 | | |

Continued on next page...

Continued from previous page...

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 1 | LC | 429 | Total | C | N | O | S | 0 | 0 |
| | | | 3362 | 2101 | 578 | 652 | 31 | | |
| 1 | LE | 429 | Total | C | N | O | S | 0 | 0 |
| | | | 3362 | 2101 | 578 | 652 | 31 | | |
| 1 | LG | 429 | Total | C | N | O | S | 0 | 0 |
| | | | 3362 | 2101 | 578 | 652 | 31 | | |
| 1 | LI | 429 | Total | C | N | O | S | 0 | 0 |
| | | | 3362 | 2101 | 578 | 652 | 31 | | |
| 1 | LK | 429 | Total | C | N | O | S | 0 | 0 |
| | | | 3362 | 2101 | 578 | 652 | 31 | | |
| 1 | LM | 429 | Total | C | N | O | S | 0 | 0 |
| | | | 3362 | 2101 | 578 | 652 | 31 | | |
| 1 | LO | 429 | Total | C | N | O | S | 0 | 0 |
| | | | 3362 | 2101 | 578 | 652 | 31 | | |
| 1 | M | 429 | Total | C | N | O | S | 0 | 0 |
| | | | 3362 | 2101 | 578 | 652 | 31 | | |
| 1 | MB | 429 | Total | C | N | O | S | 0 | 0 |
| | | | 3362 | 2101 | 578 | 652 | 31 | | |
| 1 | MD | 429 | Total | C | N | O | S | 0 | 0 |
| | | | 3362 | 2101 | 578 | 652 | 31 | | |
| 1 | MF | 429 | Total | C | N | O | S | 0 | 0 |
| | | | 3362 | 2101 | 578 | 652 | 31 | | |
| 1 | MH | 429 | Total | C | N | O | S | 0 | 0 |
| | | | 3362 | 2101 | 578 | 652 | 31 | | |
| 1 | MJ | 429 | Total | C | N | O | S | 0 | 0 |
| | | | 3362 | 2101 | 578 | 652 | 31 | | |
| 1 | ML | 429 | Total | C | N | O | S | 0 | 0 |
| | | | 3362 | 2101 | 578 | 652 | 31 | | |
| 1 | MN | 429 | Total | C | N | O | S | 0 | 0 |
| | | | 3362 | 2101 | 578 | 652 | 31 | | |
| 1 | N | 420 | Total | C | N | O | S | 0 | 0 |
| | | | 3290 | 2060 | 561 | 638 | 31 | | |
| 1 | NB | 420 | Total | C | N | O | S | 0 | 0 |
| | | | 3290 | 2060 | 561 | 638 | 31 | | |
| 1 | ND | 427 | Total | C | N | O | S | 0 | 0 |
| | | | 3348 | 2092 | 576 | 649 | 31 | | |
| 1 | NF | 427 | Total | C | N | O | S | 0 | 0 |
| | | | 3348 | 2092 | 576 | 649 | 31 | | |
| 1 | NH | 426 | Total | C | N | O | S | 0 | 0 |
| | | | 3343 | 2089 | 575 | 648 | 31 | | |
| 1 | NJ | 429 | Total | C | N | O | S | 0 | 0 |
| | | | 3362 | 2101 | 578 | 652 | 31 | | |

Continued on next page...

Continued from previous page...

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|---------------|-----------|----------|----------|---------|---------|-------|
| 1 | NL | 426 | Total 3343 | C 2089 | N 575 | O 648 | S 31 | 0 | 0 |
| 1 | O | 426 | Total 3343 | C 2089 | N 575 | O 648 | S 31 | 0 | 0 |
| 1 | OB | 425 | Total 3335 | C 2085 | N 574 | O 645 | S 31 | 0 | 0 |
| 1 | OD | 426 | Total 3343 | C 2089 | N 575 | O 648 | S 31 | 0 | 0 |
| 1 | OF | 426 | Total 3343 | C 2089 | N 575 | O 648 | S 31 | 0 | 0 |
| 1 | OH | 426 | Total 3343 | C 2089 | N 575 | O 648 | S 31 | 0 | 0 |
| 1 | OJ | 426 | Total 3343 | C 2089 | N 575 | O 648 | S 31 | 0 | 0 |
| 1 | OL | 426 | Total 3343 | C 2089 | N 575 | O 648 | S 31 | 0 | 0 |
| 1 | P | 401 | Total 3123 | C 1946 | N 540 | O 609 | S 28 | 0 | 0 |
| 1 | PB | 429 | Total 3362 | C 2101 | N 578 | O 652 | S 31 | 0 | 0 |
| 1 | PD | 429 | Total 3362 | C 2101 | N 578 | O 652 | S 31 | 0 | 0 |
| 1 | PF | 429 | Total 3362 | C 2101 | N 578 | O 652 | S 31 | 0 | 0 |
| 1 | PH | 426 | Total 3342 | C 2089 | N 575 | O 647 | S 31 | 0 | 0 |
| 1 | PJ | 429 | Total 3362 | C 2101 | N 578 | O 652 | S 31 | 0 | 0 |
| 1 | PL | 429 | Total 3362 | C 2101 | N 578 | O 652 | S 31 | 0 | 0 |
| 1 | QA | 427 | Total 3348 | C 2092 | N 576 | O 649 | S 31 | 0 | 0 |
| 1 | QC | 427 | Total 3348 | C 2092 | N 576 | O 649 | S 31 | 0 | 0 |
| 1 | QE | 426 | Total 3343 | C 2089 | N 575 | O 648 | S 31 | 0 | 0 |
| 1 | QG | 427 | Total 3348 | C 2092 | N 576 | O 649 | S 31 | 0 | 0 |
| 1 | QI | 427 | Total 3348 | C 2092 | N 576 | O 649 | S 31 | 0 | 0 |
| 1 | QK | 427 | Total 3348 | C 2092 | N 576 | O 649 | S 31 | 0 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 1 | RA | 426 | Total | C | N | O | S | 0 | 0 |
| | | | 3343 | 2089 | 575 | 648 | 31 | | |
| 1 | RC | 429 | Total | C | N | O | S | 0 | 0 |
| | | | 3362 | 2101 | 578 | 652 | 31 | | |
| 1 | RE | 426 | Total | C | N | O | S | 0 | 0 |
| | | | 3343 | 2089 | 575 | 648 | 31 | | |
| 1 | RG | 426 | Total | C | N | O | S | 0 | 0 |
| | | | 3343 | 2089 | 575 | 648 | 31 | | |
| 1 | RI | 426 | Total | C | N | O | S | 0 | 0 |
| | | | 3342 | 2088 | 575 | 648 | 31 | | |
| 1 | RK | 428 | Total | C | N | O | S | 0 | 0 |
| | | | 3355 | 2096 | 577 | 651 | 31 | | |
| 1 | S | 425 | Total | C | N | O | S | 0 | 0 |
| | | | 3335 | 2085 | 574 | 645 | 31 | | |
| 1 | SB | 425 | Total | C | N | O | S | 0 | 0 |
| | | | 3335 | 2085 | 574 | 645 | 31 | | |
| 1 | SD | 425 | Total | C | N | O | S | 0 | 0 |
| | | | 3335 | 2085 | 574 | 645 | 31 | | |
| 1 | SF | 425 | Total | C | N | O | S | 0 | 0 |
| | | | 3335 | 2085 | 574 | 645 | 31 | | |
| 1 | SH | 428 | Total | C | N | O | S | 0 | 0 |
| | | | 3355 | 2096 | 577 | 651 | 31 | | |
| 1 | SJ | 427 | Total | C | N | O | S | 0 | 0 |
| | | | 3348 | 2092 | 576 | 649 | 31 | | |
| 1 | T | 427 | Total | C | N | O | S | 0 | 0 |
| | | | 3348 | 2092 | 576 | 649 | 31 | | |
| 1 | TB | 428 | Total | C | N | O | S | 0 | 0 |
| | | | 3355 | 2096 | 577 | 651 | 31 | | |
| 1 | TD | 426 | Total | C | N | O | S | 0 | 0 |
| | | | 3343 | 2089 | 575 | 648 | 31 | | |
| 1 | TF | 427 | Total | C | N | O | S | 0 | 0 |
| | | | 3348 | 2092 | 576 | 649 | 31 | | |
| 1 | TH | 426 | Total | C | N | O | S | 0 | 0 |
| | | | 3343 | 2089 | 575 | 648 | 31 | | |
| 1 | TJ | 429 | Total | C | N | O | S | 0 | 0 |
| | | | 3362 | 2101 | 578 | 652 | 31 | | |
| 1 | TL | 427 | Total | C | N | O | S | 0 | 0 |
| | | | 3348 | 2092 | 576 | 649 | 31 | | |
| 1 | U | 425 | Total | C | N | O | S | 0 | 0 |
| | | | 3335 | 2085 | 574 | 645 | 31 | | |
| 1 | UB | 425 | Total | C | N | O | S | 0 | 0 |
| | | | 3335 | 2085 | 574 | 645 | 31 | | |

Continued on next page...

Continued from previous page...

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|---------------|-----------|----------|----------|---------|---------|-------|
| 1 | UD | 425 | Total 3335 | C 2085 | N 574 | O 645 | S 31 | 0 | 0 |
| 1 | UF | 425 | Total 3335 | C 2085 | N 574 | O 645 | S 31 | 0 | 0 |
| 1 | UH | 425 | Total 3335 | C 2085 | N 574 | O 645 | S 31 | 0 | 0 |
| 1 | UJ | 427 | Total 3348 | C 2092 | N 576 | O 649 | S 31 | 0 | 0 |
| 1 | UL | 426 | Total 3343 | C 2089 | N 575 | O 648 | S 31 | 0 | 0 |
| 1 | V | 428 | Total 3355 | C 2096 | N 577 | O 651 | S 31 | 0 | 0 |
| 1 | VB | 426 | Total 3343 | C 2089 | N 575 | O 648 | S 31 | 0 | 0 |
| 1 | VD | 427 | Total 3348 | C 2092 | N 576 | O 649 | S 31 | 0 | 0 |
| 1 | VF | 428 | Total 3355 | C 2096 | N 577 | O 651 | S 31 | 0 | 0 |
| 1 | VH | 425 | Total 3335 | C 2085 | N 574 | O 645 | S 31 | 0 | 0 |
| 1 | VJ | 429 | Total 3362 | C 2101 | N 578 | O 652 | S 31 | 0 | 0 |
| 1 | VL | 429 | Total 3362 | C 2101 | N 578 | O 652 | S 31 | 0 | 0 |
| 1 | W | 425 | Total 3335 | C 2085 | N 574 | O 645 | S 31 | 0 | 0 |
| 1 | WB | 425 | Total 3335 | C 2085 | N 574 | O 645 | S 31 | 0 | 0 |
| 1 | WD | 425 | Total 3335 | C 2085 | N 574 | O 645 | S 31 | 0 | 0 |
| 1 | WF | 427 | Total 3348 | C 2092 | N 576 | O 649 | S 31 | 0 | 0 |
| 1 | WH | 425 | Total 3335 | C 2085 | N 574 | O 645 | S 31 | 0 | 0 |
| 1 | WJ | 425 | Total 3335 | C 2085 | N 574 | O 645 | S 31 | 0 | 0 |
| 1 | WL | 426 | Total 3343 | C 2089 | N 575 | O 648 | S 31 | 0 | 0 |

- Molecule 2 is a protein called Tubulin alpha chain.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 2 | AA | 430 | Total | C | N | O | S | 0 | 0 |
| | | | 3329 | 2103 | 567 | 636 | 23 | | |
| 2 | AC | 433 | Total | C | N | O | S | 0 | 0 |
| | | | 3353 | 2117 | 570 | 643 | 23 | | |
| 2 | AE | 439 | Total | C | N | O | S | 0 | 0 |
| | | | 3394 | 2141 | 577 | 652 | 24 | | |
| 2 | AG | 433 | Total | C | N | O | S | 0 | 0 |
| | | | 3352 | 2116 | 571 | 642 | 23 | | |
| 2 | AI | 439 | Total | C | N | O | S | 0 | 0 |
| | | | 3394 | 2141 | 577 | 652 | 24 | | |
| 2 | AK | 439 | Total | C | N | O | S | 0 | 0 |
| | | | 3394 | 2141 | 577 | 652 | 24 | | |
| 2 | AM | 430 | Total | C | N | O | S | 0 | 0 |
| | | | 3329 | 2103 | 567 | 636 | 23 | | |
| 2 | BA | 429 | Total | C | N | O | S | 0 | 0 |
| | | | 3322 | 2098 | 566 | 635 | 23 | | |
| 2 | BC | 430 | Total | C | N | O | S | 0 | 0 |
| | | | 3329 | 2103 | 567 | 636 | 23 | | |
| 2 | BE | 429 | Total | C | N | O | S | 0 | 0 |
| | | | 3322 | 2098 | 566 | 635 | 23 | | |
| 2 | BG | 430 | Total | C | N | O | S | 0 | 0 |
| | | | 3329 | 2103 | 567 | 636 | 23 | | |
| 2 | BI | 439 | Total | C | N | O | S | 0 | 0 |
| | | | 3394 | 2141 | 577 | 652 | 24 | | |
| 2 | BK | 429 | Total | C | N | O | S | 0 | 0 |
| | | | 3322 | 2098 | 566 | 635 | 23 | | |
| 2 | BM | 430 | Total | C | N | O | S | 0 | 0 |
| | | | 3329 | 2103 | 567 | 636 | 23 | | |
| 2 | C | 439 | Total | C | N | O | S | 0 | 0 |
| | | | 3394 | 2141 | 577 | 652 | 24 | | |
| 2 | CB | 439 | Total | C | N | O | S | 0 | 0 |
| | | | 3394 | 2141 | 577 | 652 | 24 | | |
| 2 | CD | 439 | Total | C | N | O | S | 0 | 0 |
| | | | 3394 | 2141 | 577 | 652 | 24 | | |
| 2 | CF | 430 | Total | C | N | O | S | 0 | 0 |
| | | | 3329 | 2103 | 567 | 636 | 23 | | |
| 2 | CH | 439 | Total | C | N | O | S | 0 | 0 |
| | | | 3394 | 2141 | 577 | 652 | 24 | | |
| 2 | CJ | 439 | Total | C | N | O | S | 0 | 0 |
| | | | 3394 | 2141 | 577 | 652 | 24 | | |
| 2 | CL | 439 | Total | C | N | O | S | 0 | 0 |
| | | | 3394 | 2141 | 577 | 652 | 24 | | |
| 2 | D | 430 | Total | C | N | O | S | 0 | 0 |
| | | | 3329 | 2103 | 567 | 636 | 23 | | |

Continued on next page...

Continued from previous page...

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 2 | DB | 430 | Total | C | N | O | S | 0 | 0 |
| | | | 3329 | 2103 | 567 | 636 | 23 | | |
| 2 | DD | 430 | Total | C | N | O | S | 0 | 0 |
| | | | 3329 | 2103 | 567 | 636 | 23 | | |
| 2 | DF | 431 | Total | C | N | O | S | 0 | 0 |
| | | | 3337 | 2107 | 568 | 639 | 23 | | |
| 2 | DH | 430 | Total | C | N | O | S | 0 | 0 |
| | | | 3328 | 2102 | 567 | 636 | 23 | | |
| 2 | DJ | 430 | Total | C | N | O | S | 0 | 0 |
| | | | 3329 | 2103 | 567 | 636 | 23 | | |
| 2 | DL | 430 | Total | C | N | O | S | 0 | 0 |
| | | | 3329 | 2103 | 567 | 636 | 23 | | |
| 2 | EA | 430 | Total | C | N | O | S | 0 | 0 |
| | | | 3329 | 2103 | 567 | 636 | 23 | | |
| 2 | EC | 439 | Total | C | N | O | S | 0 | 0 |
| | | | 3394 | 2141 | 577 | 652 | 24 | | |
| 2 | EE | 432 | Total | C | N | O | S | 0 | 0 |
| | | | 3346 | 2112 | 569 | 642 | 23 | | |
| 2 | EG | 433 | Total | C | N | O | S | 0 | 0 |
| | | | 3351 | 2114 | 570 | 644 | 23 | | |
| 2 | EI | 431 | Total | C | N | O | S | 0 | 0 |
| | | | 3337 | 2107 | 568 | 639 | 23 | | |
| 2 | EK | 431 | Total | C | N | O | S | 0 | 0 |
| | | | 3337 | 2107 | 568 | 639 | 23 | | |
| 2 | FA | 439 | Total | C | N | O | S | 0 | 0 |
| | | | 3394 | 2141 | 577 | 652 | 24 | | |
| 2 | FC | 434 | Total | C | N | O | S | 0 | 0 |
| | | | 3360 | 2119 | 571 | 647 | 23 | | |
| 2 | FE | 432 | Total | C | N | O | S | 0 | 0 |
| | | | 3343 | 2110 | 569 | 641 | 23 | | |
| 2 | FG | 431 | Total | C | N | O | S | 0 | 0 |
| | | | 3337 | 2107 | 568 | 639 | 23 | | |
| 2 | FI | 429 | Total | C | N | O | S | 0 | 0 |
| | | | 3322 | 2098 | 566 | 635 | 23 | | |
| 2 | FK | 431 | Total | C | N | O | S | 0 | 0 |
| | | | 3337 | 2107 | 568 | 639 | 23 | | |
| 2 | GA | 430 | Total | C | N | O | S | 0 | 0 |
| | | | 3329 | 2103 | 567 | 636 | 23 | | |
| 2 | GC | 430 | Total | C | N | O | S | 0 | 0 |
| | | | 3329 | 2103 | 567 | 636 | 23 | | |
| 2 | GE | 431 | Total | C | N | O | S | 0 | 0 |
| | | | 3337 | 2107 | 568 | 639 | 23 | | |

Continued on next page...

Continued from previous page...

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 2 | GG | 430 | Total | C | N | O | S | 0 | 0 |
| | | | 3329 | 2103 | 567 | 636 | 23 | | |
| 2 | GI | 430 | Total | C | N | O | S | 0 | 0 |
| | | | 3329 | 2103 | 567 | 636 | 23 | | |
| 2 | GK | 430 | Total | C | N | O | S | 0 | 0 |
| | | | 3329 | 2103 | 567 | 636 | 23 | | |
| 2 | HA | 430 | Total | C | N | O | S | 0 | 0 |
| | | | 3329 | 2103 | 567 | 636 | 23 | | |
| 2 | HC | 430 | Total | C | N | O | S | 0 | 0 |
| | | | 3329 | 2103 | 567 | 636 | 23 | | |
| 2 | HE | 439 | Total | C | N | O | S | 0 | 0 |
| | | | 3394 | 2141 | 577 | 652 | 24 | | |
| 2 | HG | 432 | Total | C | N | O | S | 0 | 0 |
| | | | 3343 | 2110 | 569 | 641 | 23 | | |
| 2 | HI | 431 | Total | C | N | O | S | 0 | 0 |
| | | | 3336 | 2106 | 568 | 639 | 23 | | |
| 2 | HK | 432 | Total | C | N | O | S | 0 | 0 |
| | | | 3343 | 2110 | 569 | 641 | 23 | | |
| 2 | HM | 430 | Total | C | N | O | S | 0 | 0 |
| | | | 3329 | 2103 | 567 | 636 | 23 | | |
| 2 | IA | 430 | Total | C | N | O | S | 0 | 0 |
| | | | 3329 | 2103 | 567 | 636 | 23 | | |
| 2 | IC | 432 | Total | C | N | O | S | 0 | 0 |
| | | | 3343 | 2110 | 569 | 641 | 23 | | |
| 2 | IE | 439 | Total | C | N | O | S | 0 | 0 |
| | | | 3394 | 2141 | 577 | 652 | 24 | | |
| 2 | IG | 439 | Total | C | N | O | S | 0 | 0 |
| | | | 3394 | 2141 | 577 | 652 | 24 | | |
| 2 | II | 439 | Total | C | N | O | S | 0 | 0 |
| | | | 3394 | 2141 | 577 | 652 | 24 | | |
| 2 | IK | 430 | Total | C | N | O | S | 0 | 0 |
| | | | 3329 | 2103 | 567 | 636 | 23 | | |
| 2 | IM | 430 | Total | C | N | O | S | 0 | 0 |
| | | | 3329 | 2103 | 567 | 636 | 23 | | |
| 2 | J | 439 | Total | C | N | O | S | 0 | 0 |
| | | | 3394 | 2141 | 577 | 652 | 24 | | |
| 2 | JB | 439 | Total | C | N | O | S | 0 | 0 |
| | | | 3394 | 2141 | 577 | 652 | 24 | | |
| 2 | JD | 430 | Total | C | N | O | S | 0 | 0 |
| | | | 3329 | 2103 | 567 | 636 | 23 | | |
| 2 | JF | 430 | Total | C | N | O | S | 0 | 0 |
| | | | 3329 | 2103 | 567 | 636 | 23 | | |

Continued on next page...

Continued from previous page...

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 2 | JH | 432 | Total | C | N | O | S | 0 | 0 |
| | | | 3342 | 2110 | 569 | 640 | 23 | | |
| 2 | JJ | 432 | Total | C | N | O | S | 0 | 0 |
| | | | 3343 | 2110 | 569 | 641 | 23 | | |
| 2 | JL | 432 | Total | C | N | O | S | 0 | 0 |
| | | | 3343 | 2110 | 569 | 641 | 23 | | |
| 2 | JN | 439 | Total | C | N | O | S | 0 | 0 |
| | | | 3394 | 2141 | 577 | 652 | 24 | | |
| 2 | K | 434 | Total | C | N | O | S | 0 | 0 |
| | | | 3358 | 2119 | 572 | 643 | 24 | | |
| 2 | KB | 439 | Total | C | N | O | S | 0 | 0 |
| | | | 3394 | 2141 | 577 | 652 | 24 | | |
| 2 | KD | 430 | Total | C | N | O | S | 0 | 0 |
| | | | 3329 | 2103 | 567 | 636 | 23 | | |
| 2 | KF | 439 | Total | C | N | O | S | 0 | 0 |
| | | | 3394 | 2141 | 577 | 652 | 24 | | |
| 2 | KH | 431 | Total | C | N | O | S | 0 | 0 |
| | | | 3335 | 2106 | 568 | 638 | 23 | | |
| 2 | KJ | 432 | Total | C | N | O | S | 0 | 0 |
| | | | 3346 | 2112 | 569 | 642 | 23 | | |
| 2 | KL | 439 | Total | C | N | O | S | 0 | 0 |
| | | | 3394 | 2141 | 577 | 652 | 24 | | |
| 2 | KN | 439 | Total | C | N | O | S | 0 | 0 |
| | | | 3394 | 2141 | 577 | 652 | 24 | | |
| 2 | L | 439 | Total | C | N | O | S | 0 | 0 |
| | | | 3394 | 2141 | 577 | 652 | 24 | | |
| 2 | LB | 432 | Total | C | N | O | S | 0 | 0 |
| | | | 3346 | 2112 | 569 | 642 | 23 | | |
| 2 | LD | 429 | Total | C | N | O | S | 0 | 0 |
| | | | 3322 | 2097 | 566 | 637 | 22 | | |
| 2 | LF | 439 | Total | C | N | O | S | 0 | 0 |
| | | | 3394 | 2141 | 577 | 652 | 24 | | |
| 2 | LH | 439 | Total | C | N | O | S | 0 | 0 |
| | | | 3394 | 2141 | 577 | 652 | 24 | | |
| 2 | LJ | 439 | Total | C | N | O | S | 0 | 0 |
| | | | 3394 | 2141 | 577 | 652 | 24 | | |
| 2 | LL | 439 | Total | C | N | O | S | 0 | 0 |
| | | | 3394 | 2141 | 577 | 652 | 24 | | |
| 2 | LN | 432 | Total | C | N | O | S | 0 | 0 |
| | | | 3346 | 2112 | 569 | 642 | 23 | | |
| 2 | MA | 431 | Total | C | N | O | S | 0 | 0 |
| | | | 3335 | 2106 | 568 | 638 | 23 | | |

Continued on next page...

Continued from previous page...

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 2 | MC | 437 | Total | C | N | O | S | 0 | 0 |
| | | | 3379 | 2133 | 575 | 647 | 24 | | |
| 2 | ME | 436 | Total | C | N | O | S | 0 | 0 |
| | | | 3368 | 2124 | 573 | 647 | 24 | | |
| 2 | MG | 439 | Total | C | N | O | S | 0 | 0 |
| | | | 3394 | 2141 | 577 | 652 | 24 | | |
| 2 | MI | 439 | Total | C | N | O | S | 0 | 0 |
| | | | 3394 | 2141 | 577 | 652 | 24 | | |
| 2 | MK | 439 | Total | C | N | O | S | 0 | 0 |
| | | | 3394 | 2141 | 577 | 652 | 24 | | |
| 2 | MM | 431 | Total | C | N | O | S | 0 | 0 |
| | | | 3335 | 2106 | 568 | 638 | 23 | | |
| 2 | NA | 439 | Total | C | N | O | S | 0 | 0 |
| | | | 3394 | 2141 | 577 | 652 | 24 | | |
| 2 | NC | 439 | Total | C | N | O | S | 0 | 0 |
| | | | 3394 | 2141 | 577 | 652 | 24 | | |
| 2 | NE | 439 | Total | C | N | O | S | 0 | 0 |
| | | | 3394 | 2141 | 577 | 652 | 24 | | |
| 2 | NG | 439 | Total | C | N | O | S | 0 | 0 |
| | | | 3394 | 2141 | 577 | 652 | 24 | | |
| 2 | NI | 439 | Total | C | N | O | S | 0 | 0 |
| | | | 3394 | 2141 | 577 | 652 | 24 | | |
| 2 | NK | 439 | Total | C | N | O | S | 0 | 0 |
| | | | 3394 | 2141 | 577 | 652 | 24 | | |
| 2 | NM | 439 | Total | C | N | O | S | 0 | 0 |
| | | | 3394 | 2141 | 577 | 652 | 24 | | |
| 2 | OA | 432 | Total | C | N | O | S | 0 | 0 |
| | | | 3343 | 2110 | 569 | 641 | 23 | | |
| 2 | OC | 431 | Total | C | N | O | S | 0 | 0 |
| | | | 3337 | 2107 | 568 | 639 | 23 | | |
| 2 | OE | 431 | Total | C | N | O | S | 0 | 0 |
| | | | 3337 | 2107 | 568 | 639 | 23 | | |
| 2 | OG | 439 | Total | C | N | O | S | 0 | 0 |
| | | | 3394 | 2141 | 577 | 652 | 24 | | |
| 2 | OI | 430 | Total | C | N | O | S | 0 | 0 |
| | | | 3329 | 2103 | 567 | 636 | 23 | | |
| 2 | OK | 430 | Total | C | N | O | S | 0 | 0 |
| | | | 3329 | 2103 | 567 | 636 | 23 | | |
| 2 | OM | 433 | Total | C | N | O | S | 0 | 0 |
| | | | 3352 | 2115 | 570 | 644 | 23 | | |
| 2 | PA | 430 | Total | C | N | O | S | 0 | 0 |
| | | | 3329 | 2103 | 567 | 636 | 23 | | |

Continued on next page...

Continued from previous page...

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|---------------|-----------|----------|----------|---------|---------|-------|
| 2 | PC | 431 | Total 3337 | C 2107 | N 568 | O 639 | S 23 | 0 | 0 |
| 2 | PE | 431 | Total 3337 | C 2107 | N 568 | O 639 | S 23 | 0 | 0 |
| 2 | PG | 439 | Total 3394 | C 2141 | N 577 | O 652 | S 24 | 0 | 0 |
| 2 | PI | 431 | Total 3337 | C 2107 | N 568 | O 639 | S 23 | 0 | 0 |
| 2 | PK | 432 | Total 3343 | C 2110 | N 569 | O 641 | S 23 | 0 | 0 |
| 2 | PM | 432 | Total 3343 | C 2110 | N 569 | O 641 | S 23 | 0 | 0 |
| 2 | Q | 439 | Total 3394 | C 2141 | N 577 | O 652 | S 24 | 0 | 0 |
| 2 | QB | 429 | Total 3323 | C 2100 | N 566 | O 634 | S 23 | 0 | 0 |
| 2 | QD | 430 | Total 3329 | C 2103 | N 567 | O 636 | S 23 | 0 | 0 |
| 2 | QF | 430 | Total 3329 | C 2103 | N 567 | O 636 | S 23 | 0 | 0 |
| 2 | QH | 439 | Total 3394 | C 2141 | N 577 | O 652 | S 24 | 0 | 0 |
| 2 | QJ | 431 | Total 3337 | C 2107 | N 568 | O 639 | S 23 | 0 | 0 |
| 2 | QL | 432 | Total 3343 | C 2110 | N 569 | O 641 | S 23 | 0 | 0 |
| 2 | R | 439 | Total 3394 | C 2141 | N 577 | O 652 | S 24 | 0 | 0 |
| 2 | RB | 431 | Total 3337 | C 2107 | N 568 | O 639 | S 23 | 0 | 0 |
| 2 | RD | 431 | Total 3337 | C 2107 | N 568 | O 639 | S 23 | 0 | 0 |
| 2 | RF | 431 | Total 3337 | C 2107 | N 568 | O 639 | S 23 | 0 | 0 |
| 2 | RH | 430 | Total 3329 | C 2103 | N 567 | O 636 | S 23 | 0 | 0 |
| 2 | RJ | 430 | Total 3329 | C 2103 | N 567 | O 636 | S 23 | 0 | 0 |
| 2 | RL | 431 | Total 3335 | C 2106 | N 568 | O 638 | S 23 | 0 | 0 |
| 2 | SA | 431 | Total 3337 | C 2107 | N 568 | O 639 | S 23 | 0 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 2 | SC | 431 | Total | C | N | O | S | 0 | 0 |
| | | | 3335 | 2106 | 568 | 638 | 23 | | |
| 2 | SE | 431 | Total | C | N | O | S | 0 | 0 |
| | | | 3335 | 2106 | 568 | 638 | 23 | | |
| 2 | SG | 431 | Total | C | N | O | S | 0 | 0 |
| | | | 3337 | 2107 | 568 | 639 | 23 | | |
| 2 | SI | 430 | Total | C | N | O | S | 0 | 0 |
| | | | 3329 | 2103 | 567 | 636 | 23 | | |
| 2 | SK | 432 | Total | C | N | O | S | 0 | 0 |
| | | | 3343 | 2110 | 569 | 641 | 23 | | |
| 2 | TA | 430 | Total | C | N | O | S | 0 | 0 |
| | | | 3329 | 2103 | 567 | 636 | 23 | | |
| 2 | TC | 428 | Total | C | N | O | S | 0 | 0 |
| | | | 3314 | 2093 | 565 | 634 | 22 | | |
| 2 | TE | 430 | Total | C | N | O | S | 0 | 0 |
| | | | 3329 | 2103 | 567 | 636 | 23 | | |
| 2 | TG | 431 | Total | C | N | O | S | 0 | 0 |
| | | | 3337 | 2107 | 568 | 639 | 23 | | |
| 2 | TI | 430 | Total | C | N | O | S | 0 | 0 |
| | | | 3329 | 2103 | 567 | 636 | 23 | | |
| 2 | TK | 433 | Total | C | N | O | S | 0 | 0 |
| | | | 3353 | 2117 | 570 | 643 | 23 | | |
| 2 | UA | 430 | Total | C | N | O | S | 0 | 0 |
| | | | 3329 | 2103 | 567 | 636 | 23 | | |
| 2 | UC | 429 | Total | C | N | O | S | 0 | 0 |
| | | | 3322 | 2097 | 566 | 637 | 22 | | |
| 2 | UE | 430 | Total | C | N | O | S | 0 | 0 |
| | | | 3329 | 2103 | 567 | 636 | 23 | | |
| 2 | UG | 431 | Total | C | N | O | S | 0 | 0 |
| | | | 3337 | 2107 | 568 | 639 | 23 | | |
| 2 | UI | 430 | Total | C | N | O | S | 0 | 0 |
| | | | 3329 | 2103 | 567 | 636 | 23 | | |
| 2 | UK | 430 | Total | C | N | O | S | 0 | 0 |
| | | | 3329 | 2103 | 567 | 636 | 23 | | |
| 2 | VA | 431 | Total | C | N | O | S | 0 | 0 |
| | | | 3337 | 2107 | 568 | 639 | 23 | | |
| 2 | VC | 431 | Total | C | N | O | S | 0 | 0 |
| | | | 3337 | 2107 | 568 | 639 | 23 | | |
| 2 | VE | 431 | Total | C | N | O | S | 0 | 0 |
| | | | 3337 | 2107 | 568 | 639 | 23 | | |
| 2 | VG | 431 | Total | C | N | O | S | 0 | 0 |
| | | | 3337 | 2107 | 568 | 639 | 23 | | |

Continued on next page...

Continued from previous page...

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 2 | VI | 432 | Total | C | N | O | S | 0 | 0 |
| | | | 3342 | 2109 | 569 | 641 | 23 | | |
| 2 | VK | 430 | Total | C | N | O | S | 0 | 0 |
| | | | 3329 | 2103 | 567 | 636 | 23 | | |
| 2 | VM | 434 | Total | C | N | O | S | 0 | 0 |
| | | | 3360 | 2119 | 571 | 647 | 23 | | |
| 2 | WA | 439 | Total | C | N | O | S | 0 | 0 |
| | | | 3394 | 2141 | 577 | 652 | 24 | | |
| 2 | WC | 431 | Total | C | N | O | S | 0 | 0 |
| | | | 3337 | 2107 | 568 | 639 | 23 | | |
| 2 | WE | 439 | Total | C | N | O | S | 0 | 0 |
| | | | 3394 | 2141 | 577 | 652 | 24 | | |
| 2 | WG | 431 | Total | C | N | O | S | 0 | 0 |
| | | | 3337 | 2107 | 568 | 639 | 23 | | |
| 2 | WI | 439 | Total | C | N | O | S | 0 | 0 |
| | | | 3394 | 2141 | 577 | 652 | 24 | | |
| 2 | WK | 431 | Total | C | N | O | S | 0 | 0 |
| | | | 3337 | 2107 | 568 | 639 | 23 | | |
| 2 | WM | 439 | Total | C | N | O | S | 0 | 0 |
| | | | 3394 | 2141 | 577 | 652 | 24 | | |

- Molecule 3 is a protein called CFAP20.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 3 | X | 183 | Total | C | N | O | S | 0 | 0 |
| | | | 1510 | 965 | 264 | 270 | 11 | | |
| 3 | XA | 183 | Total | C | N | O | S | 0 | 0 |
| | | | 1510 | 965 | 264 | 270 | 11 | | |
| 3 | XB | 183 | Total | C | N | O | S | 0 | 0 |
| | | | 1510 | 965 | 264 | 270 | 11 | | |
| 3 | XC | 183 | Total | C | N | O | S | 0 | 0 |
| | | | 1510 | 965 | 264 | 270 | 11 | | |
| 3 | XD | 183 | Total | C | N | O | S | 0 | 0 |
| | | | 1510 | 965 | 264 | 270 | 11 | | |
| 3 | XE | 183 | Total | C | N | O | S | 0 | 0 |
| | | | 1510 | 965 | 264 | 270 | 11 | | |
| 3 | XF | 183 | Total | C | N | O | S | 0 | 0 |
| | | | 1510 | 965 | 264 | 270 | 11 | | |

- Molecule 4 is a protein called PACRGA.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 4 | XM | 259 | Total | C | N | O | S | 0 | 0 |
| | | | 2045 | 1307 | 360 | 370 | 8 | | |
| 4 | XO | 260 | Total | C | N | O | S | 0 | 0 |
| | | | 2053 | 1311 | 361 | 373 | 8 | | |
| 4 | XQ | 260 | Total | C | N | O | S | 0 | 0 |
| | | | 2053 | 1311 | 361 | 373 | 8 | | |
| 4 | XR | 260 | Total | C | N | O | S | 0 | 0 |
| | | | 2056 | 1313 | 364 | 371 | 8 | | |

- Molecule 5 is a protein called PACRGB.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 5 | XN | 269 | Total | C | N | O | S | 0 | 0 |
| | | | 2116 | 1359 | 366 | 384 | 7 | | |
| 5 | XP | 269 | Total | C | N | O | S | 0 | 0 |
| | | | 2116 | 1359 | 366 | 384 | 7 | | |

- Molecule 6 is a protein called CCDC81.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 6 | 0A | 257 | Total | C | N | O | S | 0 | 0 |
| | | | 2004 | 1261 | 359 | 371 | 13 | | |
| 6 | 0 | 257 | Total | C | N | O | S | 0 | 0 |
| | | | 2004 | 1261 | 359 | 371 | 13 | | |

- Molecule 7 is a protein called CFAP21.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 7 | 0C | 121 | Total | C | N | O | S | 0 | 0 |
| | | | 935 | 584 | 159 | 188 | 4 | | |
| 7 | 0D | 354 | Total | C | N | O | S | 0 | 0 |
| | | | 2723 | 1683 | 492 | 537 | 11 | | |

- Molecule 8 is a protein called CFAP45.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 8 | 0F | 176 | Total | C | N | O | S | 0 | 0 |
| | | | 1439 | 859 | 288 | 280 | 12 | | |
| 8 | 0G | 349 | Total | C | N | O | S | 0 | 0 |
| | | | 2955 | 1772 | 596 | 570 | 17 | | |
| 8 | 0H | 28 | Total | C | N | O | | 0 | 0 |
| | | | 229 | 146 | 41 | 42 | | | |

Continued on next page...

Continued from previous page...

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 8 | 0I | 285 | Total | C | N | O | S | 0 | 0 |
| | | | 2369 | 1421 | 471 | 459 | 18 | | |
| 8 | 0J | 226 | Total | C | N | O | S | 0 | 0 |
| | | | 1906 | 1147 | 379 | 373 | 7 | | |

- Molecule 9 is a protein called CFAP52.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 9 | 0L | 624 | Total | C | N | O | S | 0 | 0 |
| | | | 4757 | 2973 | 844 | 908 | 32 | | |
| 9 | 0M | 624 | Total | C | N | O | S | 0 | 0 |
| | | | 4757 | 2973 | 844 | 908 | 32 | | |
| 9 | 0N | 624 | Total | C | N | O | S | 0 | 0 |
| | | | 4757 | 2973 | 844 | 908 | 32 | | |
| 9 | 0O | 310 | Total | C | N | O | S | 0 | 0 |
| | | | 2357 | 1482 | 416 | 445 | 14 | | |

- Molecule 10 is a protein called CFAP53.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 10 | 0R | 309 | Total | C | N | O | S | 0 | 0 |
| | | | 2628 | 1579 | 535 | 501 | 13 | | |
| 10 | 0S | 221 | Total | C | N | O | S | 0 | 0 |
| | | | 1874 | 1148 | 360 | 359 | 7 | | |

- Molecule 11 is a protein called CFAP67A.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 11 | 0U | 333 | Total | C | N | O | S | 0 | 0 |
| | | | 2570 | 1621 | 437 | 495 | 17 | | |

- Molecule 12 is a protein called CFAP67B.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 12 | 0W | 339 | Total | C | N | O | S | 0 | 0 |
| | | | 2595 | 1647 | 427 | 501 | 20 | | |

- Molecule 13 is a protein called CFAP106A.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 13 | 0Y | 233 | Total | C | N | O | S | 0 | 0 |
| | | | 1836 | 1152 | 334 | 345 | 5 | | |

Continued on next page...

Continued from previous page...

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 13 | 0Z | 235 | Total | C | N | O | S | 0 | 0 |
| | | | 1849 | 1160 | 337 | 347 | 5 | | |
| 13 | 0a | 58 | Total | C | N | O | | 0 | 0 |
| | | | 422 | 263 | 78 | 81 | | | |

- Molecule 14 is a protein called CFAP106B.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 14 | 0c | 237 | Total | C | N | O | S | 0 | 0 |
| | | | 1929 | 1221 | 337 | 362 | 9 | | |
| 14 | 0d | 265 | Total | C | N | O | S | 0 | 0 |
| | | | 2150 | 1359 | 378 | 404 | 9 | | |

- Molecule 15 is a protein called CFAP107.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 15 | 0f | 160 | Total | C | N | O | S | 0 | 0 |
| | | | 1257 | 783 | 222 | 241 | 11 | | |
| 15 | 0g | 30 | Total | C | N | O | S | 0 | 0 |
| | | | 218 | 137 | 34 | 46 | 1 | | |

- Molecule 16 is a protein called CFAP115.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|-------|
| 16 | 0l | 640 | Total | C | N | O | S | 0 | 0 |
| | | | 5045 | 3192 | 918 | 914 | 21 | | |
| 16 | 0k | 710 | Total | C | N | O | S | 0 | 0 |
| | | | 5599 | 3537 | 1026 | 1009 | 27 | | |

- Molecule 17 is a protein called CFAP127.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 17 | 0m | 142 | Total | C | N | O | S | 0 | 0 |
| | | | 1155 | 704 | 220 | 227 | 4 | | |
| 17 | 0n | 406 | Total | C | N | O | S | 0 | 0 |
| | | | 3388 | 2054 | 668 | 654 | 12 | | |
| 17 | 0o | 20 | Total | C | N | O | | 0 | 0 |
| | | | 171 | 107 | 35 | 29 | | | |

- Molecule 18 is a protein called CFAP141.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 18 | 0p | 108 | Total | C | N | O | S | 0 | 0 |
| | | | 906 | 557 | 177 | 169 | 3 | | |

- Molecule 19 is a protein called CFAP143.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 19 | 0r | 254 | Total | C | N | O | S | 0 | 0 |
| | | | 2033 | 1246 | 376 | 396 | 15 | | |

- Molecule 20 is a protein called CFAP161.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 20 | 0t | 262 | Total | C | N | O | S | 0 | 0 |
| | | | 2062 | 1298 | 358 | 388 | 18 | | |
| 20 | 0u | 227 | Total | C | N | O | S | 0 | 0 |
| | | | 1769 | 1117 | 306 | 330 | 16 | | |

- Molecule 21 is a protein called CFAP210.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 21 | 0w | 449 | Total | C | N | O | S | 0 | 0 |
| | | | 3715 | 2242 | 741 | 724 | 8 | | |
| 21 | 0x | 111 | Total | C | N | O | S | 0 | 0 |
| | | | 906 | 556 | 175 | 172 | 3 | | |
| 21 | 0v | 73 | Total | C | N | O | | 0 | 0 |
| | | | 582 | 351 | 115 | 116 | | | |

- Molecule 22 is a protein called DMIP5.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 22 | 0z | 143 | Total | C | N | O | S | 0 | 0 |
| | | | 1160 | 716 | 220 | 219 | 5 | | |
| 22 | 1w | 180 | Total | C | N | O | S | 0 | 0 |
| | | | 1481 | 915 | 278 | 281 | 7 | | |
| 22 | 1x | 206 | Total | C | N | O | S | 0 | 0 |
| | | | 1680 | 1031 | 322 | 315 | 12 | | |
| 22 | 1y | 91 | Total | C | N | O | S | 0 | 0 |
| | | | 722 | 449 | 130 | 141 | 2 | | |

- Molecule 23 is a protein called RIB43.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 23 | 1A | 270 | Total | C | N | O | S | 0 | 0 |
| | | | 2286 | 1390 | 449 | 436 | 11 | | |
| 23 | 1B | 195 | Total | C | N | O | S | 0 | 0 |
| | | | 1667 | 1015 | 321 | 322 | 9 | | |
| 23 | 1D | 54 | Total | C | N | O | S | 0 | 0 |
| | | | 464 | 285 | 91 | 85 | 3 | | |
| 23 | 1E | 362 | Total | C | N | O | S | 0 | 0 |
| | | | 3050 | 1855 | 590 | 590 | 15 | | |
| 23 | 1F | 74 | Total | C | N | O | S | 0 | 0 |
| | | | 635 | 387 | 120 | 124 | 4 | | |

- Molecule 24 is a protein called RIB72A.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|------|----|---------|-------|
| 24 | 1H | 588 | Total | C | N | O | S | 0 | 0 |
| | | | 4698 | 2967 | 812 | 900 | 19 | | |
| 24 | 1I | 659 | Total | C | N | O | S | 0 | 0 |
| | | | 5276 | 3326 | 920 | 1003 | 27 | | |
| 24 | 1J | 670 | Total | C | N | O | S | 0 | 0 |
| | | | 5356 | 3372 | 940 | 1018 | 26 | | |
| 24 | 1K | 588 | Total | C | N | O | S | 0 | 0 |
| | | | 4697 | 2966 | 812 | 900 | 19 | | |

- Molecule 25 is a protein called RIB72B.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|-------|
| 25 | 1O | 710 | Total | C | N | O | S | 0 | 0 |
| | | | 5751 | 3614 | 1021 | 1096 | 20 | | |

- Molecule 26 is a protein called RIB72C.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 26 | 1Q | 655 | Total | C | N | O | S | 0 | 0 |
| | | | 5263 | 3323 | 927 | 988 | 25 | | |

- Molecule 27 is a protein called RIB72D.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|-------|
| 27 | 1S | 726 | Total | C | N | O | S | 0 | 0 |
| | | | 5834 | 3696 | 1029 | 1076 | 33 | | |
| 27 | 1T | 222 | Total | C | N | O | S | 0 | 0 |
| | | | 1787 | 1125 | 315 | 335 | 12 | | |

- Molecule 28 is a protein called DMIP1.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 28 | 1U | 120 | Total | C | N | O | S | 0 | 0 |
| | | | 942 | 594 | 162 | 181 | 5 | | |
| 28 | 1V | 48 | Total | C | N | O | S | 0 | 0 |
| | | | 371 | 229 | 68 | 69 | 5 | | |
| 28 | 1X | 120 | Total | C | N | O | S | 0 | 0 |
| | | | 942 | 594 | 162 | 181 | 5 | | |
| 28 | 1Y | 169 | Total | C | N | O | S | 0 | 0 |
| | | | 1325 | 829 | 237 | 252 | 7 | | |
| 28 | 1a | 57 | Total | C | N | O | S | 0 | 0 |
| | | | 446 | 279 | 80 | 84 | 3 | | |
| 28 | 1b | 168 | Total | C | N | O | S | 0 | 0 |
| | | | 1313 | 823 | 230 | 250 | 10 | | |
| 28 | 1c | 35 | Total | C | N | O | S | 0 | 0 |
| | | | 263 | 162 | 50 | 46 | 5 | | |
| 28 | 1d | 120 | Total | C | N | O | S | 0 | 0 |
| | | | 942 | 594 | 162 | 181 | 5 | | |
| 28 | 1e | 48 | Total | C | N | O | S | 0 | 0 |
| | | | 371 | 229 | 68 | 69 | 5 | | |
| 28 | 1g | 120 | Total | C | N | O | S | 0 | 0 |
| | | | 942 | 594 | 162 | 181 | 5 | | |
| 28 | 1h | 155 | Total | C | N | O | S | 0 | 0 |
| | | | 1218 | 767 | 214 | 230 | 7 | | |
| 28 | 4V | 62 | Total | C | N | O | S | 0 | 0 |
| | | | 486 | 305 | 86 | 91 | 4 | | |
| 28 | 4W | 188 | Total | C | N | O | S | 0 | 0 |
| | | | 1474 | 927 | 255 | 283 | 9 | | |

- Molecule 29 is a protein called DMIP2.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 29 | 1j | 113 | Total | C | N | O | S | 0 | 0 |
| | | | 909 | 584 | 153 | 168 | 4 | | |
| 29 | 1k | 103 | Total | C | N | O | S | 0 | 0 |
| | | | 801 | 502 | 140 | 157 | 2 | | |
| 29 | 1l | 113 | Total | C | N | O | S | 0 | 0 |
| | | | 909 | 584 | 153 | 168 | 4 | | |
| 29 | 1m | 53 | Total | C | N | O | S | 0 | 0 |
| | | | 420 | 268 | 72 | 78 | 2 | | |

- Molecule 30 is a protein called DMIP3.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 30 | 1o | 128 | Total | C | N | O | S | 0 | 0 |
| | | | 1035 | 645 | 193 | 192 | 5 | | |

- Molecule 31 is a protein called DMIP4.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 31 | 1q | 214 | Total | C | N | O | S | 0 | 0 |
| | | | 1679 | 1025 | 322 | 321 | 11 | | |
| 31 | 1r | 106 | Total | C | N | O | S | 0 | 0 |
| | | | 868 | 532 | 166 | 165 | 5 | | |
| 31 | 1s | 183 | Total | C | N | O | S | 0 | 0 |
| | | | 1446 | 884 | 273 | 277 | 12 | | |
| 31 | 1t | 75 | Total | C | N | O | S | 0 | 0 |
| | | | 618 | 372 | 125 | 116 | 5 | | |

- Molecule 32 is a protein called DMIP6.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 32 | 2B | 251 | Total | C | N | O | S | 0 | 0 |
| | | | 1977 | 1231 | 357 | 377 | 12 | | |
| 32 | 2C | 230 | Total | C | N | O | S | 0 | 0 |
| | | | 1814 | 1130 | 329 | 344 | 11 | | |

- Molecule 33 is a protein called DMIP7.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 33 | 2F | 284 | Total | C | N | O | S | 0 | 0 |
| | | | 2253 | 1411 | 411 | 418 | 13 | | |
| 33 | 2G | 283 | Total | C | N | O | S | 0 | 0 |
| | | | 2245 | 1407 | 409 | 416 | 13 | | |
| 33 | 2H | 288 | Total | C | N | O | S | 0 | 0 |
| | | | 2281 | 1428 | 416 | 424 | 13 | | |
| 33 | 2I | 243 | Total | C | N | O | S | 0 | 0 |
| | | | 1937 | 1208 | 355 | 363 | 11 | | |

- Molecule 34 is a protein called DMIP8.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 34 | 2L | 172 | Total | C | N | O | S | 0 | 0 |
| | | | 1433 | 904 | 254 | 269 | 6 | | |

- Molecule 35 is a protein called DMIP9.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 35 | 2N | 135 | Total | C | N | O | S | 0 | 0 |
| | | | 1103 | 698 | 208 | 194 | 3 | | |
| 35 | 2O | 161 | Total | C | N | O | S | 0 | 0 |
| | | | 1324 | 827 | 251 | 240 | 6 | | |

- Molecule 36 is a protein called DMIP10.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 36 | 2Q | 291 | Total | C | N | O | S | 0 | 0 |
| | | | 2320 | 1483 | 394 | 429 | 14 | | |

- Molecule 37 is a protein called DMIP11.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 37 | 2S | 237 | Total | C | N | O | S | 0 | 0 |
| | | | 1800 | 1127 | 317 | 341 | 15 | | |

- Molecule 38 is a protein called DMIP12.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 38 | 2U | 229 | Total | C | N | O | S | 0 | 0 |
| | | | 1807 | 1111 | 329 | 355 | 12 | | |
| 38 | 2V | 109 | Total | C | N | O | S | 0 | 0 |
| | | | 870 | 530 | 167 | 169 | 4 | | |

- Molecule 39 is a protein called DMIP13.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 39 | 2X | 227 | Total | C | N | O | S | 0 | 0 |
| | | | 1774 | 1081 | 355 | 328 | 10 | | |

- Molecule 40 is a protein called DMIP14.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 40 | 2Z | 283 | Total | C | N | O | S | 0 | 0 |
| | | | 2258 | 1427 | 412 | 414 | 5 | | |

- Molecule 41 is a protein called DMIP15.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 41 | 2b | 121 | Total | C | N | O | S | 0 | 0 |
| | | | 1006 | 613 | 195 | 194 | 4 | | |

Continued on next page...

Continued from previous page...

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 41 | 2c | 245 | Total | C | N | O | S | 0 | 0 |
| | | | 2092 | 1254 | 418 | 408 | 12 | | |
| 41 | 2e | 325 | Total | C | N | O | S | 0 | 0 |
| | | | 2735 | 1649 | 546 | 526 | 14 | | |
| 41 | 2f | 52 | Total | C | N | O | S | 0 | 0 |
| | | | 454 | 275 | 89 | 88 | 2 | | |
| 41 | 2h | 237 | Total | C | N | O | S | 0 | 0 |
| | | | 1978 | 1187 | 396 | 385 | 10 | | |
| 41 | 2i | 149 | Total | C | N | O | S | 0 | 0 |
| | | | 1301 | 776 | 266 | 252 | 7 | | |
| 41 | 2k | 167 | Total | C | N | O | S | 0 | 0 |
| | | | 1369 | 834 | 266 | 262 | 7 | | |
| 41 | 2l | 264 | Total | C | N | O | S | 0 | 0 |
| | | | 2228 | 1338 | 445 | 432 | 13 | | |
| 41 | 2n | 42 | Total | C | N | O | | 0 | 0 |
| | | | 361 | 219 | 72 | 70 | | | |
| 41 | 2o | 287 | Total | C | N | O | S | 0 | 0 |
| | | | 2453 | 1473 | 490 | 478 | 12 | | |
| 41 | 2p | 49 | Total | C | N | O | S | 0 | 0 |
| | | | 425 | 257 | 86 | 80 | 2 | | |

- Molecule 42 is a protein called DMIP16.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 42 | 2r | 315 | Total | C | N | O | S | 0 | 0 |
| | | | 2473 | 1564 | 439 | 460 | 10 | | |

- Molecule 43 is a protein called DMIP17.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 43 | 2t | 214 | Total | C | N | O | S | 0 | 0 |
| | | | 1713 | 1075 | 302 | 324 | 12 | | |

- Molecule 44 is a protein called DMIP18.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 44 | 2v | 280 | Total | C | N | O | S | 0 | 0 |
| | | | 2264 | 1438 | 391 | 425 | 10 | | |
| 44 | 2w | 412 | Total | C | N | O | S | 0 | 0 |
| | | | 3291 | 2082 | 565 | 629 | 15 | | |

- Molecule 45 is a protein called DMIP19.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 45 | 2y | 287 | Total | C | N | O | S | 0 | 0 |
| | | | 2316 | 1424 | 424 | 460 | 8 | | |
| 45 | 2z | 187 | Total | C | N | O | S | 0 | 0 |
| | | | 1435 | 890 | 257 | 287 | 1 | | |

- Molecule 46 is a protein called DMIP20.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 46 | 3B | 418 | Total | C | N | O | S | 0 | 0 |
| | | | 3308 | 2069 | 596 | 631 | 12 | | |

- Molecule 47 is a protein called DMIP21.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 47 | 3D | 412 | Total | C | N | O | S | 0 | 0 |
| | | | 3212 | 1986 | 586 | 628 | 12 | | |

- Molecule 48 is a protein called DMIP22.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 48 | 3I | 80 | Total | C | N | O | S | 0 | 0 |
| | | | 640 | 400 | 114 | 122 | 4 | | |
| 48 | 3F | 155 | Total | C | N | O | S | 0 | 0 |
| | | | 1254 | 777 | 240 | 230 | 7 | | |
| 48 | 3G | 90 | Total | C | N | O | S | 0 | 0 |
| | | | 733 | 456 | 139 | 134 | 4 | | |
| 48 | 3H | 103 | Total | C | N | O | S | 0 | 0 |
| | | | 832 | 516 | 161 | 151 | 4 | | |
| 48 | 3M | 29 | Total | C | N | O | S | 0 | 0 |
| | | | 247 | 155 | 44 | 45 | 3 | | |
| 48 | 3L | 29 | Total | C | N | O | S | 0 | 0 |
| | | | 247 | 155 | 44 | 45 | 3 | | |

- Molecule 49 is a protein called DMIP23.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 49 | 3P | 256 | Total | C | N | O | S | 0 | 0 |
| | | | 2002 | 1260 | 351 | 380 | 11 | | |
| 49 | 3Q | 490 | Total | C | N | O | S | 0 | 0 |
| | | | 3825 | 2406 | 666 | 735 | 18 | | |

- Molecule 50 is a protein called DMIP24.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 50 | 3S | 25 | Total | C | N | O | S | 0 | 0 |
| | | | 182 | 109 | 36 | 33 | 4 | | |

- Molecule 51 is a protein called DMIP24.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|-------|
| 51 | X1 | 39 | Total | C | N | O | S | 0 | 0 |
| | | | 304 | 183 | 58 | 63 | | | |

- Molecule 52 is a protein called DMIP25.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 52 | 3U | 140 | Total | C | N | O | S | 0 | 0 |
| | | | 1074 | 681 | 186 | 203 | 4 | | |

- Molecule 53 is a protein called DMIP26.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 53 | 3X | 49 | Total | C | N | O | S | 0 | 0 |
| | | | 386 | 239 | 74 | 70 | 3 | | |
| 53 | 3W | 153 | Total | C | N | O | S | 0 | 0 |
| | | | 1264 | 786 | 231 | 239 | 8 | | |

- Molecule 54 is a protein called DMIP27.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 54 | 3Z | 181 | Total | C | N | O | S | 0 | 0 |
| | | | 1405 | 862 | 264 | 271 | 8 | | |
| 54 | 3a | 87 | Total | C | N | O | S | 0 | 0 |
| | | | 712 | 442 | 130 | 136 | 4 | | |
| 54 | 4Y | 16 | Total | C | N | O | S | 0 | 0 |
| | | | 122 | 75 | 18 | 28 | 1 | | |

- Molecule 55 is a protein called ArcMAP2.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 55 | 3b | 136 | Total | C | N | O | S | 0 | 0 |
| | | | 1126 | 695 | 204 | 223 | 4 | | |

- Molecule 56 is a protein called ArcMAP1.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 56 | 3d | 148 | Total | C | N | O | S | 0 | 0 |
| | | | 1240 | 765 | 229 | 240 | 6 | | |

- Molecule 57 is a protein called ArcMAP4.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 57 | 3f | 165 | Total | C | N | O | S | 0 | 0 |
| | | | 1408 | 857 | 263 | 280 | 8 | | |
| 57 | 3g | 165 | Total | C | N | O | S | 0 | 0 |
| | | | 1408 | 857 | 263 | 280 | 8 | | |
| 57 | 3h | 165 | Total | C | N | O | S | 0 | 0 |
| | | | 1408 | 857 | 263 | 280 | 8 | | |
| 57 | 3i | 165 | Total | C | N | O | S | 0 | 0 |
| | | | 1408 | 857 | 263 | 280 | 8 | | |

- Molecule 58 is a protein called ArcMAP3.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 58 | 3m | 144 | Total | C | N | O | S | 0 | 0 |
| | | | 1216 | 745 | 236 | 231 | 4 | | |

- Molecule 59 is a protein called CFAP96.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 59 | 3o | 55 | Total | C | N | O | S | 0 | 0 |
| | | | 459 | 293 | 79 | 85 | 2 | | |
| 59 | 3p | 148 | Total | C | N | O | S | 0 | 0 |
| | | | 1159 | 744 | 201 | 212 | 2 | | |
| 59 | 4O | 175 | Total | C | N | O | S | 0 | 0 |
| | | | 1399 | 899 | 245 | 253 | 2 | | |
| 59 | 4P | 69 | Total | C | N | O | S | 0 | 0 |
| | | | 529 | 346 | 84 | 98 | 1 | | |
| 59 | 4a | 154 | Total | C | N | O | S | 0 | 0 |
| | | | 1233 | 796 | 213 | 223 | 1 | | |
| 59 | 4b | 69 | Total | C | N | O | S | 0 | 0 |
| | | | 529 | 346 | 84 | 98 | 1 | | |

- Molecule 60 is a protein called CFAP97.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 60 | 3r | 130 | Total | C | N | O | S | 0 | 0 |
| | | | 1098 | 668 | 221 | 205 | 4 | | |

Continued on next page...

Continued from previous page...

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 60 | 3s | 130 | Total | C | N | O | S | 0 | 0 |
| | | | 1098 | 668 | 221 | 205 | 4 | | |
| 60 | 3t | 63 | Total | C | N | O | S | 0 | 0 |
| | | | 533 | 326 | 105 | 98 | 4 | | |

- Molecule 61 is a protein called DMAP1.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 61 | 3w | 166 | Total | C | N | O | S | 0 | 0 |
| | | | 1362 | 872 | 235 | 249 | 6 | | |
| 61 | 3x | 126 | Total | C | N | O | S | 0 | 0 |
| | | | 987 | 626 | 178 | 182 | 1 | | |

- Molecule 62 is a protein called DMAP2.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 62 | 4A | 29 | Total | C | N | O | S | 0 | 0 |
| | | | 229 | 142 | 43 | 43 | 1 | | |
| 62 | 4B | 201 | Total | C | N | O | S | 0 | 0 |
| | | | 1584 | 1003 | 275 | 302 | 4 | | |

- Molecule 63 is a protein called DMAP7.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 63 | 4I | 77 | Total | C | N | O | S | 0 | 0 |
| | | | 620 | 385 | 128 | 106 | 1 | | |

- Molecule 64 is a protein called distal DC1.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 64 | 5B | 168 | Total | C | N | O | S | 0 | 0 |
| | | | 1348 | 828 | 258 | 257 | 5 | | |
| 64 | 5C | 168 | Total | C | N | O | S | 0 | 0 |
| | | | 1348 | 828 | 258 | 257 | 5 | | |
| 64 | 5D | 40 | Total | C | N | O | S | 0 | 0 |
| | | | 321 | 196 | 61 | 61 | 3 | | |

- Molecule 65 is a protein called distal DC2.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 65 | 5G | 185 | Total | C | N | O | S | 0 | 0 |
| | | | 1541 | 942 | 295 | 296 | 8 | | |

Continued on next page...

Continued from previous page...

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 65 | 5H | 185 | Total | C | N | O | S | 0 | 0 |
| | | | 1541 | 942 | 295 | 296 | 8 | | |
| 65 | 5I | 47 | Total | C | N | O | S | 0 | 0 |
| | | | 401 | 251 | 77 | 72 | 1 | | |

- Molecule 66 is a protein called distal DC4.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 66 | 5K | 266 | Total | C | N | O | S | 0 | 0 |
| | | | 2155 | 1372 | 377 | 393 | 13 | | |
| 66 | 5L | 266 | Total | C | N | O | S | 0 | 0 |
| | | | 2155 | 1372 | 377 | 393 | 13 | | |

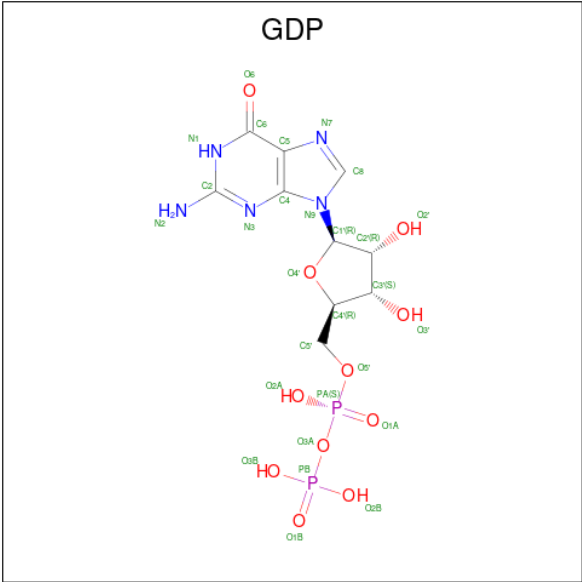
- Molecule 67 is a protein called DC5.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 67 | 5O | 107 | Total | C | N | O | S | 0 | 0 |
| | | | 809 | 523 | 130 | 152 | 4 | | |
| 67 | 5P | 107 | Total | C | N | O | S | 0 | 0 |
| | | | 809 | 523 | 130 | 152 | 4 | | |

- Molecule 68 is a protein called DC6.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 68 | 5S | 92 | Total | C | N | O | S | 0 | 0 |
| | | | 749 | 470 | 137 | 133 | 9 | | |
| 68 | 5T | 92 | Total | C | N | O | S | 0 | 0 |
| | | | 749 | 470 | 137 | 133 | 9 | | |

- Molecule 69 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).



| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|
| 69 | A | 1 | Total | C | N | O | P | 0 |
| | | | 28 | 10 | 5 | 11 | 2 | |
| 69 | AB | 1 | Total | C | N | O | P | 0 |
| | | | 28 | 10 | 5 | 11 | 2 | |
| 69 | AD | 1 | Total | C | N | O | P | 0 |
| | | | 28 | 10 | 5 | 11 | 2 | |
| 69 | AF | 1 | Total | C | N | O | P | 0 |
| | | | 28 | 10 | 5 | 11 | 2 | |
| 69 | AH | 1 | Total | C | N | O | P | 0 |
| | | | 28 | 10 | 5 | 11 | 2 | |
| 69 | AJ | 1 | Total | C | N | O | P | 0 |
| | | | 28 | 10 | 5 | 11 | 2 | |
| 69 | AL | 1 | Total | C | N | O | P | 0 |
| | | | 28 | 10 | 5 | 11 | 2 | |
| 69 | AN | 1 | Total | C | N | O | P | 0 |
| | | | 28 | 10 | 5 | 11 | 2 | |
| 69 | BB | 1 | Total | C | N | O | P | 0 |
| | | | 28 | 10 | 5 | 11 | 2 | |
| 69 | BD | 1 | Total | C | N | O | P | 0 |
| | | | 28 | 10 | 5 | 11 | 2 | |
| 69 | BF | 1 | Total | C | N | O | P | 0 |
| | | | 28 | 10 | 5 | 11 | 2 | |
| 69 | BH | 1 | Total | C | N | O | P | 0 |
| | | | 28 | 10 | 5 | 11 | 2 | |
| 69 | BJ | 1 | Total | C | N | O | P | 0 |
| | | | 28 | 10 | 5 | 11 | 2 | |
| 69 | BL | 1 | Total | C | N | O | P | 0 |
| | | | 28 | 10 | 5 | 11 | 2 | |

Continued on next page...

Continued from previous page...

| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|
| 69 | BN | 1 | Total | C | N | O | P | 0 |
| | | | 28 | 10 | 5 | 11 | 2 | |
| 69 | CA | 1 | Total | C | N | O | P | 0 |
| | | | 28 | 10 | 5 | 11 | 2 | |
| 69 | CC | 1 | Total | C | N | O | P | 0 |
| | | | 28 | 10 | 5 | 11 | 2 | |
| 69 | CE | 1 | Total | C | N | O | P | 0 |
| | | | 28 | 10 | 5 | 11 | 2 | |
| 69 | CG | 1 | Total | C | N | O | P | 0 |
| | | | 28 | 10 | 5 | 11 | 2 | |
| 69 | CI | 1 | Total | C | N | O | P | 0 |
| | | | 28 | 10 | 5 | 11 | 2 | |
| 69 | CK | 1 | Total | C | N | O | P | 0 |
| | | | 28 | 10 | 5 | 11 | 2 | |
| 69 | CM | 1 | Total | C | N | O | P | 0 |
| | | | 28 | 10 | 5 | 11 | 2 | |
| 69 | DA | 1 | Total | C | N | O | P | 0 |
| | | | 28 | 10 | 5 | 11 | 2 | |
| 69 | DC | 1 | Total | C | N | O | P | 0 |
| | | | 28 | 10 | 5 | 11 | 2 | |
| 69 | DE | 1 | Total | C | N | O | P | 0 |
| | | | 28 | 10 | 5 | 11 | 2 | |
| 69 | DG | 1 | Total | C | N | O | P | 0 |
| | | | 28 | 10 | 5 | 11 | 2 | |
| 69 | DI | 1 | Total | C | N | O | P | 0 |
| | | | 28 | 10 | 5 | 11 | 2 | |
| 69 | DK | 1 | Total | C | N | O | P | 0 |
| | | | 28 | 10 | 5 | 11 | 2 | |
| 69 | DM | 1 | Total | C | N | O | P | 0 |
| | | | 28 | 10 | 5 | 11 | 2 | |
| 69 | E | 1 | Total | C | N | O | P | 0 |
| | | | 28 | 10 | 5 | 11 | 2 | |
| 69 | EB | 1 | Total | C | N | O | P | 0 |
| | | | 28 | 10 | 5 | 11 | 2 | |
| 69 | ED | 1 | Total | C | N | O | P | 0 |
| | | | 28 | 10 | 5 | 11 | 2 | |
| 69 | EF | 1 | Total | C | N | O | P | 0 |
| | | | 28 | 10 | 5 | 11 | 2 | |
| 69 | EH | 1 | Total | C | N | O | P | 0 |
| | | | 28 | 10 | 5 | 11 | 2 | |
| 69 | EJ | 1 | Total | C | N | O | P | 0 |
| | | | 28 | 10 | 5 | 11 | 2 | |

Continued on next page...

Continued from previous page...

| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|
| 69 | EL | 1 | Total | C | N | O | P | 0 |
| | | | 28 | 10 | 5 | 11 | 2 | |
| 69 | F | 1 | Total | C | N | O | P | 0 |
| | | | 28 | 10 | 5 | 11 | 2 | |
| 69 | FB | 1 | Total | C | N | O | P | 0 |
| | | | 28 | 10 | 5 | 11 | 2 | |
| 69 | FD | 1 | Total | C | N | O | P | 0 |
| | | | 28 | 10 | 5 | 11 | 2 | |
| 69 | FF | 1 | Total | C | N | O | P | 0 |
| | | | 28 | 10 | 5 | 11 | 2 | |
| 69 | FH | 1 | Total | C | N | O | P | 0 |
| | | | 28 | 10 | 5 | 11 | 2 | |
| 69 | FJ | 1 | Total | C | N | O | P | 0 |
| | | | 28 | 10 | 5 | 11 | 2 | |
| 69 | FL | 1 | Total | C | N | O | P | 0 |
| | | | 28 | 10 | 5 | 11 | 2 | |
| 69 | G | 1 | Total | C | N | O | P | 0 |
| | | | 28 | 10 | 5 | 11 | 2 | |
| 69 | GB | 1 | Total | C | N | O | P | 0 |
| | | | 28 | 10 | 5 | 11 | 2 | |
| 69 | GD | 1 | Total | C | N | O | P | 0 |
| | | | 28 | 10 | 5 | 11 | 2 | |
| 69 | GF | 1 | Total | C | N | O | P | 0 |
| | | | 28 | 10 | 5 | 11 | 2 | |
| 69 | GH | 1 | Total | C | N | O | P | 0 |
| | | | 28 | 10 | 5 | 11 | 2 | |
| 69 | GJ | 1 | Total | C | N | O | P | 0 |
| | | | 28 | 10 | 5 | 11 | 2 | |
| 69 | GL | 1 | Total | C | N | O | P | 0 |
| | | | 28 | 10 | 5 | 11 | 2 | |
| 69 | H | 1 | Total | C | N | O | P | 0 |
| | | | 28 | 10 | 5 | 11 | 2 | |
| 69 | HB | 1 | Total | C | N | O | P | 0 |
| | | | 28 | 10 | 5 | 11 | 2 | |
| 69 | HD | 1 | Total | C | N | O | P | 0 |
| | | | 28 | 10 | 5 | 11 | 2 | |
| 69 | HF | 1 | Total | C | N | O | P | 0 |
| | | | 28 | 10 | 5 | 11 | 2 | |
| 69 | HH | 1 | Total | C | N | O | P | 0 |
| | | | 28 | 10 | 5 | 11 | 2 | |
| 69 | HJ | 1 | Total | C | N | O | P | 0 |
| | | | 28 | 10 | 5 | 11 | 2 | |

Continued on next page...

Continued from previous page...

| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|
| 69 | HL | 1 | Total | C | N | O | P | 0 |
| | | | 28 | 10 | 5 | 11 | 2 | |
| 69 | I | 1 | Total | C | N | O | P | 0 |
| | | | 28 | 10 | 5 | 11 | 2 | |
| 69 | IB | 1 | Total | C | N | O | P | 0 |
| | | | 28 | 10 | 5 | 11 | 2 | |
| 69 | ID | 1 | Total | C | N | O | P | 0 |
| | | | 28 | 10 | 5 | 11 | 2 | |
| 69 | IF | 1 | Total | C | N | O | P | 0 |
| | | | 28 | 10 | 5 | 11 | 2 | |
| 69 | IH | 1 | Total | C | N | O | P | 0 |
| | | | 28 | 10 | 5 | 11 | 2 | |
| 69 | IJ | 1 | Total | C | N | O | P | 0 |
| | | | 28 | 10 | 5 | 11 | 2 | |
| 69 | IL | 1 | Total | C | N | O | P | 0 |
| | | | 28 | 10 | 5 | 11 | 2 | |
| 69 | JA | 1 | Total | C | N | O | P | 0 |
| | | | 28 | 10 | 5 | 11 | 2 | |
| 69 | JC | 1 | Total | C | N | O | P | 0 |
| | | | 28 | 10 | 5 | 11 | 2 | |
| 69 | JE | 1 | Total | C | N | O | P | 0 |
| | | | 28 | 10 | 5 | 11 | 2 | |
| 69 | JG | 1 | Total | C | N | O | P | 0 |
| | | | 28 | 10 | 5 | 11 | 2 | |
| 69 | JI | 1 | Total | C | N | O | P | 0 |
| | | | 28 | 10 | 5 | 11 | 2 | |
| 69 | JK | 1 | Total | C | N | O | P | 0 |
| | | | 28 | 10 | 5 | 11 | 2 | |
| 69 | JM | 1 | Total | C | N | O | P | 0 |
| | | | 28 | 10 | 5 | 11 | 2 | |
| 69 | KA | 1 | Total | C | N | O | P | 0 |
| | | | 28 | 10 | 5 | 11 | 2 | |
| 69 | KC | 1 | Total | C | N | O | P | 0 |
| | | | 28 | 10 | 5 | 11 | 2 | |
| 69 | KE | 1 | Total | C | N | O | P | 0 |
| | | | 28 | 10 | 5 | 11 | 2 | |
| 69 | KG | 1 | Total | C | N | O | P | 0 |
| | | | 28 | 10 | 5 | 11 | 2 | |
| 69 | KI | 1 | Total | C | N | O | P | 0 |
| | | | 28 | 10 | 5 | 11 | 2 | |
| 69 | KK | 1 | Total | C | N | O | P | 0 |
| | | | 28 | 10 | 5 | 11 | 2 | |

Continued on next page...

Continued from previous page...

| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|
| 69 | KM | 1 | Total | C | N | O | P | 0 |
| | | | 28 | 10 | 5 | 11 | 2 | |
| 69 | LA | 1 | Total | C | N | O | P | 0 |
| | | | 28 | 10 | 5 | 11 | 2 | |
| 69 | LC | 1 | Total | C | N | O | P | 0 |
| | | | 28 | 10 | 5 | 11 | 2 | |
| 69 | LE | 1 | Total | C | N | O | P | 0 |
| | | | 28 | 10 | 5 | 11 | 2 | |
| 69 | LG | 1 | Total | C | N | O | P | 0 |
| | | | 28 | 10 | 5 | 11 | 2 | |
| 69 | LI | 1 | Total | C | N | O | P | 0 |
| | | | 28 | 10 | 5 | 11 | 2 | |
| 69 | LK | 1 | Total | C | N | O | P | 0 |
| | | | 28 | 10 | 5 | 11 | 2 | |
| 69 | LM | 1 | Total | C | N | O | P | 0 |
| | | | 28 | 10 | 5 | 11 | 2 | |
| 69 | LO | 1 | Total | C | N | O | P | 0 |
| | | | 28 | 10 | 5 | 11 | 2 | |
| 69 | M | 1 | Total | C | N | O | P | 0 |
| | | | 28 | 10 | 5 | 11 | 2 | |
| 69 | MB | 1 | Total | C | N | O | P | 0 |
| | | | 28 | 10 | 5 | 11 | 2 | |
| 69 | MD | 1 | Total | C | N | O | P | 0 |
| | | | 28 | 10 | 5 | 11 | 2 | |
| 69 | MF | 1 | Total | C | N | O | P | 0 |
| | | | 28 | 10 | 5 | 11 | 2 | |
| 69 | MH | 1 | Total | C | N | O | P | 0 |
| | | | 28 | 10 | 5 | 11 | 2 | |
| 69 | MJ | 1 | Total | C | N | O | P | 0 |
| | | | 28 | 10 | 5 | 11 | 2 | |
| 69 | ML | 1 | Total | C | N | O | P | 0 |
| | | | 28 | 10 | 5 | 11 | 2 | |
| 69 | MN | 1 | Total | C | N | O | P | 0 |
| | | | 28 | 10 | 5 | 11 | 2 | |
| 69 | N | 1 | Total | C | N | O | P | 0 |
| | | | 28 | 10 | 5 | 11 | 2 | |
| 69 | NB | 1 | Total | C | N | O | P | 0 |
| | | | 28 | 10 | 5 | 11 | 2 | |
| 69 | ND | 1 | Total | C | N | O | P | 0 |
| | | | 28 | 10 | 5 | 11 | 2 | |
| 69 | NF | 1 | Total | C | N | O | P | 0 |
| | | | 28 | 10 | 5 | 11 | 2 | |

Continued on next page...

Continued from previous page...

| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|
| 69 | NH | 1 | Total | C | N | O | P | 0 |
| | | | 28 | 10 | 5 | 11 | 2 | |
| 69 | NJ | 1 | Total | C | N | O | P | 0 |
| | | | 28 | 10 | 5 | 11 | 2 | |
| 69 | NL | 1 | Total | C | N | O | P | 0 |
| | | | 28 | 10 | 5 | 11 | 2 | |
| 69 | O | 1 | Total | C | N | O | P | 0 |
| | | | 28 | 10 | 5 | 11 | 2 | |
| 69 | OB | 1 | Total | C | N | O | P | 0 |
| | | | 28 | 10 | 5 | 11 | 2 | |
| 69 | OD | 1 | Total | C | N | O | P | 0 |
| | | | 28 | 10 | 5 | 11 | 2 | |
| 69 | OF | 1 | Total | C | N | O | P | 0 |
| | | | 28 | 10 | 5 | 11 | 2 | |
| 69 | OH | 1 | Total | C | N | O | P | 0 |
| | | | 28 | 10 | 5 | 11 | 2 | |
| 69 | OJ | 1 | Total | C | N | O | P | 0 |
| | | | 28 | 10 | 5 | 11 | 2 | |
| 69 | OL | 1 | Total | C | N | O | P | 0 |
| | | | 28 | 10 | 5 | 11 | 2 | |
| 69 | P | 1 | Total | C | N | O | P | 0 |
| | | | 28 | 10 | 5 | 11 | 2 | |
| 69 | PB | 1 | Total | C | N | O | P | 0 |
| | | | 28 | 10 | 5 | 11 | 2 | |
| 69 | PD | 1 | Total | C | N | O | P | 0 |
| | | | 28 | 10 | 5 | 11 | 2 | |
| 69 | PF | 1 | Total | C | N | O | P | 0 |
| | | | 28 | 10 | 5 | 11 | 2 | |
| 69 | PH | 1 | Total | C | N | O | P | 0 |
| | | | 28 | 10 | 5 | 11 | 2 | |
| 69 | PJ | 1 | Total | C | N | O | P | 0 |
| | | | 28 | 10 | 5 | 11 | 2 | |
| 69 | PL | 1 | Total | C | N | O | P | 0 |
| | | | 28 | 10 | 5 | 11 | 2 | |
| 69 | QA | 1 | Total | C | N | O | P | 0 |
| | | | 28 | 10 | 5 | 11 | 2 | |
| 69 | QC | 1 | Total | C | N | O | P | 0 |
| | | | 28 | 10 | 5 | 11 | 2 | |
| 69 | QE | 1 | Total | C | N | O | P | 0 |
| | | | 28 | 10 | 5 | 11 | 2 | |
| 69 | QG | 1 | Total | C | N | O | P | 0 |
| | | | 28 | 10 | 5 | 11 | 2 | |

Continued on next page...

Continued from previous page...

| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------------|---------|--------|---------|--------|---------|
| 69 | QI | 1 | Total 28 | C 10 | N 5 | O 11 | P 2 | 0 |
| 69 | QK | 1 | Total 28 | C 10 | N 5 | O 11 | P 2 | 0 |
| 69 | RA | 1 | Total 28 | C 10 | N 5 | O 11 | P 2 | 0 |
| 69 | RC | 1 | Total 28 | C 10 | N 5 | O 11 | P 2 | 0 |
| 69 | RE | 1 | Total 28 | C 10 | N 5 | O 11 | P 2 | 0 |
| 69 | RG | 1 | Total 28 | C 10 | N 5 | O 11 | P 2 | 0 |
| 69 | RI | 1 | Total 28 | C 10 | N 5 | O 11 | P 2 | 0 |
| 69 | RK | 1 | Total 28 | C 10 | N 5 | O 11 | P 2 | 0 |
| 69 | S | 1 | Total 28 | C 10 | N 5 | O 11 | P 2 | 0 |
| 69 | SB | 1 | Total 28 | C 10 | N 5 | O 11 | P 2 | 0 |
| 69 | SD | 1 | Total 28 | C 10 | N 5 | O 11 | P 2 | 0 |
| 69 | SF | 1 | Total 28 | C 10 | N 5 | O 11 | P 2 | 0 |
| 69 | SH | 1 | Total 28 | C 10 | N 5 | O 11 | P 2 | 0 |
| 69 | SJ | 1 | Total 28 | C 10 | N 5 | O 11 | P 2 | 0 |
| 69 | T | 1 | Total 28 | C 10 | N 5 | O 11 | P 2 | 0 |
| 69 | TB | 1 | Total 28 | C 10 | N 5 | O 11 | P 2 | 0 |
| 69 | TD | 1 | Total 28 | C 10 | N 5 | O 11 | P 2 | 0 |
| 69 | TF | 1 | Total 28 | C 10 | N 5 | O 11 | P 2 | 0 |
| 69 | TH | 1 | Total 28 | C 10 | N 5 | O 11 | P 2 | 0 |
| 69 | TJ | 1 | Total 28 | C 10 | N 5 | O 11 | P 2 | 0 |
| 69 | TL | 1 | Total 28 | C 10 | N 5 | O 11 | P 2 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|
| 69 | U | 1 | Total | C | N | O | P | 0 |
| | | | 28 | 10 | 5 | 11 | 2 | |
| 69 | UB | 1 | Total | C | N | O | P | 0 |
| | | | 28 | 10 | 5 | 11 | 2 | |
| 69 | UD | 1 | Total | C | N | O | P | 0 |
| | | | 28 | 10 | 5 | 11 | 2 | |
| 69 | UF | 1 | Total | C | N | O | P | 0 |
| | | | 28 | 10 | 5 | 11 | 2 | |
| 69 | UH | 1 | Total | C | N | O | P | 0 |
| | | | 28 | 10 | 5 | 11 | 2 | |
| 69 | UJ | 1 | Total | C | N | O | P | 0 |
| | | | 28 | 10 | 5 | 11 | 2 | |
| 69 | UL | 1 | Total | C | N | O | P | 0 |
| | | | 28 | 10 | 5 | 11 | 2 | |
| 69 | V | 1 | Total | C | N | O | P | 0 |
| | | | 28 | 10 | 5 | 11 | 2 | |
| 69 | VB | 1 | Total | C | N | O | P | 0 |
| | | | 28 | 10 | 5 | 11 | 2 | |
| 69 | VD | 1 | Total | C | N | O | P | 0 |
| | | | 28 | 10 | 5 | 11 | 2 | |
| 69 | VF | 1 | Total | C | N | O | P | 0 |
| | | | 28 | 10 | 5 | 11 | 2 | |
| 69 | VH | 1 | Total | C | N | O | P | 0 |
| | | | 28 | 10 | 5 | 11 | 2 | |
| 69 | VJ | 1 | Total | C | N | O | P | 0 |
| | | | 28 | 10 | 5 | 11 | 2 | |
| 69 | VL | 1 | Total | C | N | O | P | 0 |
| | | | 28 | 10 | 5 | 11 | 2 | |
| 69 | W | 1 | Total | C | N | O | P | 0 |
| | | | 28 | 10 | 5 | 11 | 2 | |
| 69 | WB | 1 | Total | C | N | O | P | 0 |
| | | | 28 | 10 | 5 | 11 | 2 | |
| 69 | WD | 1 | Total | C | N | O | P | 0 |
| | | | 28 | 10 | 5 | 11 | 2 | |
| 69 | WF | 1 | Total | C | N | O | P | 0 |
| | | | 28 | 10 | 5 | 11 | 2 | |
| 69 | WH | 1 | Total | C | N | O | P | 0 |
| | | | 28 | 10 | 5 | 11 | 2 | |
| 69 | WJ | 1 | Total | C | N | O | P | 0 |
| | | | 28 | 10 | 5 | 11 | 2 | |
| 69 | WL | 1 | Total | C | N | O | P | 0 |
| | | | 28 | 10 | 5 | 11 | 2 | |

- Molecule 70 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms | | AltConf |
|-----|-------|----------|------------|---------|---------|
| 70 | AA | 1 | Total 1 | Mg 1 | 0 |
| 70 | AC | 1 | Total 1 | Mg 1 | 0 |
| 70 | AE | 1 | Total 1 | Mg 1 | 0 |
| 70 | AG | 1 | Total 1 | Mg 1 | 0 |
| 70 | AI | 1 | Total 1 | Mg 1 | 0 |
| 70 | AK | 1 | Total 1 | Mg 1 | 0 |
| 70 | AM | 1 | Total 1 | Mg 1 | 0 |
| 70 | BA | 1 | Total 1 | Mg 1 | 0 |
| 70 | BC | 1 | Total 1 | Mg 1 | 0 |
| 70 | BE | 1 | Total 1 | Mg 1 | 0 |
| 70 | BG | 1 | Total 1 | Mg 1 | 0 |
| 70 | BI | 1 | Total 1 | Mg 1 | 0 |
| 70 | BK | 1 | Total 1 | Mg 1 | 0 |
| 70 | BM | 1 | Total 1 | Mg 1 | 0 |
| 70 | C | 1 | Total 1 | Mg 1 | 0 |
| 70 | CB | 1 | Total 1 | Mg 1 | 0 |
| 70 | CD | 1 | Total 1 | Mg 1 | 0 |
| 70 | CF | 1 | Total 1 | Mg 1 | 0 |
| 70 | CH | 1 | Total 1 | Mg 1 | 0 |
| 70 | CJ | 1 | Total 1 | Mg 1 | 0 |
| 70 | CL | 1 | Total 1 | Mg 1 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Residues | Atoms | | AltConf |
|-----|-------|----------|------------|---------|---------|
| 70 | D | 1 | Total 1 | Mg 1 | 0 |
| 70 | DB | 1 | Total 1 | Mg 1 | 0 |
| 70 | DD | 1 | Total 1 | Mg 1 | 0 |
| 70 | DF | 1 | Total 1 | Mg 1 | 0 |
| 70 | DH | 1 | Total 1 | Mg 1 | 0 |
| 70 | DJ | 1 | Total 1 | Mg 1 | 0 |
| 70 | DL | 1 | Total 1 | Mg 1 | 0 |
| 70 | EA | 1 | Total 1 | Mg 1 | 0 |
| 70 | EC | 1 | Total 1 | Mg 1 | 0 |
| 70 | EE | 1 | Total 1 | Mg 1 | 0 |
| 70 | EG | 1 | Total 1 | Mg 1 | 0 |
| 70 | EI | 1 | Total 1 | Mg 1 | 0 |
| 70 | EK | 1 | Total 1 | Mg 1 | 0 |
| 70 | FA | 1 | Total 1 | Mg 1 | 0 |
| 70 | FC | 1 | Total 1 | Mg 1 | 0 |
| 70 | FE | 1 | Total 1 | Mg 1 | 0 |
| 70 | FG | 1 | Total 1 | Mg 1 | 0 |
| 70 | FI | 1 | Total 1 | Mg 1 | 0 |
| 70 | FK | 1 | Total 1 | Mg 1 | 0 |
| 70 | GA | 1 | Total 1 | Mg 1 | 0 |
| 70 | GC | 1 | Total 1 | Mg 1 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Residues | Atoms | | AltConf |
|-----|-------|----------|------------|---------|---------|
| 70 | GE | 1 | Total 1 | Mg 1 | 0 |
| 70 | GG | 1 | Total 1 | Mg 1 | 0 |
| 70 | GI | 1 | Total 1 | Mg 1 | 0 |
| 70 | GK | 1 | Total 1 | Mg 1 | 0 |
| 70 | HA | 1 | Total 1 | Mg 1 | 0 |
| 70 | HC | 1 | Total 1 | Mg 1 | 0 |
| 70 | HE | 1 | Total 1 | Mg 1 | 0 |
| 70 | HG | 1 | Total 1 | Mg 1 | 0 |
| 70 | HI | 1 | Total 1 | Mg 1 | 0 |
| 70 | HK | 1 | Total 1 | Mg 1 | 0 |
| 70 | HM | 1 | Total 1 | Mg 1 | 0 |
| 70 | IA | 1 | Total 1 | Mg 1 | 0 |
| 70 | IC | 1 | Total 1 | Mg 1 | 0 |
| 70 | IE | 1 | Total 1 | Mg 1 | 0 |
| 70 | IG | 1 | Total 1 | Mg 1 | 0 |
| 70 | II | 1 | Total 1 | Mg 1 | 0 |
| 70 | IK | 1 | Total 1 | Mg 1 | 0 |
| 70 | IM | 1 | Total 1 | Mg 1 | 0 |
| 70 | J | 1 | Total 1 | Mg 1 | 0 |
| 70 | JB | 1 | Total 1 | Mg 1 | 0 |
| 70 | JD | 1 | Total 1 | Mg 1 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Residues | Atoms | | AltConf |
|-----|-------|----------|------------|---------|---------|
| 70 | JF | 1 | Total 1 | Mg 1 | 0 |
| 70 | JH | 1 | Total 1 | Mg 1 | 0 |
| 70 | JJ | 1 | Total 1 | Mg 1 | 0 |
| 70 | JL | 1 | Total 1 | Mg 1 | 0 |
| 70 | JN | 1 | Total 1 | Mg 1 | 0 |
| 70 | K | 1 | Total 1 | Mg 1 | 0 |
| 70 | KB | 1 | Total 1 | Mg 1 | 0 |
| 70 | KD | 1 | Total 1 | Mg 1 | 0 |
| 70 | KF | 1 | Total 1 | Mg 1 | 0 |
| 70 | KH | 1 | Total 1 | Mg 1 | 0 |
| 70 | KJ | 1 | Total 1 | Mg 1 | 0 |
| 70 | KL | 1 | Total 1 | Mg 1 | 0 |
| 70 | KN | 1 | Total 1 | Mg 1 | 0 |
| 70 | L | 1 | Total 1 | Mg 1 | 0 |
| 70 | LB | 1 | Total 1 | Mg 1 | 0 |
| 70 | LD | 1 | Total 1 | Mg 1 | 0 |
| 70 | LF | 1 | Total 1 | Mg 1 | 0 |
| 70 | LH | 1 | Total 1 | Mg 1 | 0 |
| 70 | LJ | 1 | Total 1 | Mg 1 | 0 |
| 70 | LL | 1 | Total 1 | Mg 1 | 0 |
| 70 | LN | 1 | Total 1 | Mg 1 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Residues | Atoms | | AltConf |
|-----|-------|----------|------------|---------|---------|
| 70 | MA | 1 | Total 1 | Mg 1 | 0 |
| 70 | MC | 1 | Total 1 | Mg 1 | 0 |
| 70 | ME | 1 | Total 1 | Mg 1 | 0 |
| 70 | MG | 1 | Total 1 | Mg 1 | 0 |
| 70 | MI | 1 | Total 1 | Mg 1 | 0 |
| 70 | MK | 1 | Total 1 | Mg 1 | 0 |
| 70 | MM | 1 | Total 1 | Mg 1 | 0 |
| 70 | NA | 1 | Total 1 | Mg 1 | 0 |
| 70 | NC | 1 | Total 1 | Mg 1 | 0 |
| 70 | NE | 1 | Total 1 | Mg 1 | 0 |
| 70 | NG | 1 | Total 1 | Mg 1 | 0 |
| 70 | NI | 1 | Total 1 | Mg 1 | 0 |
| 70 | NK | 1 | Total 1 | Mg 1 | 0 |
| 70 | NM | 1 | Total 1 | Mg 1 | 0 |
| 70 | OA | 1 | Total 1 | Mg 1 | 0 |
| 70 | OC | 1 | Total 1 | Mg 1 | 0 |
| 70 | OE | 1 | Total 1 | Mg 1 | 0 |
| 70 | OG | 1 | Total 1 | Mg 1 | 0 |
| 70 | OI | 1 | Total 1 | Mg 1 | 0 |
| 70 | OK | 1 | Total 1 | Mg 1 | 0 |
| 70 | OM | 1 | Total 1 | Mg 1 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Residues | Atoms | | AltConf |
|-----|-------|----------|------------|---------|---------|
| 70 | PA | 1 | Total 1 | Mg 1 | 0 |
| 70 | PC | 1 | Total 1 | Mg 1 | 0 |
| 70 | PE | 1 | Total 1 | Mg 1 | 0 |
| 70 | PG | 1 | Total 1 | Mg 1 | 0 |
| 70 | PI | 1 | Total 1 | Mg 1 | 0 |
| 70 | PK | 1 | Total 1 | Mg 1 | 0 |
| 70 | PM | 1 | Total 1 | Mg 1 | 0 |
| 70 | Q | 1 | Total 1 | Mg 1 | 0 |
| 70 | QB | 1 | Total 1 | Mg 1 | 0 |
| 70 | QD | 1 | Total 1 | Mg 1 | 0 |
| 70 | QF | 1 | Total 1 | Mg 1 | 0 |
| 70 | QH | 1 | Total 1 | Mg 1 | 0 |
| 70 | QJ | 1 | Total 1 | Mg 1 | 0 |
| 70 | QL | 1 | Total 1 | Mg 1 | 0 |
| 70 | R | 1 | Total 1 | Mg 1 | 0 |
| 70 | RB | 1 | Total 1 | Mg 1 | 0 |
| 70 | RD | 1 | Total 1 | Mg 1 | 0 |
| 70 | RF | 1 | Total 1 | Mg 1 | 0 |
| 70 | RH | 1 | Total 1 | Mg 1 | 0 |
| 70 | RJ | 1 | Total 1 | Mg 1 | 0 |
| 70 | RL | 1 | Total 1 | Mg 1 | 0 |

Continued on next page...

Continued from previous page...

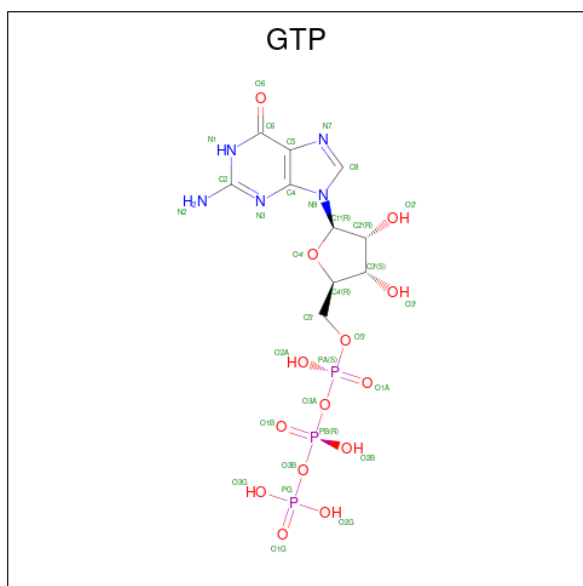
| Mol | Chain | Residues | Atoms | | AltConf |
|-----|-------|----------|------------|---------|---------|
| 70 | SA | 1 | Total 1 | Mg 1 | 0 |
| 70 | SC | 1 | Total 1 | Mg 1 | 0 |
| 70 | SE | 1 | Total 1 | Mg 1 | 0 |
| 70 | SG | 1 | Total 1 | Mg 1 | 0 |
| 70 | SI | 1 | Total 1 | Mg 1 | 0 |
| 70 | SK | 1 | Total 1 | Mg 1 | 0 |
| 70 | TA | 1 | Total 1 | Mg 1 | 0 |
| 70 | TC | 1 | Total 1 | Mg 1 | 0 |
| 70 | TE | 1 | Total 1 | Mg 1 | 0 |
| 70 | TG | 1 | Total 1 | Mg 1 | 0 |
| 70 | TI | 1 | Total 1 | Mg 1 | 0 |
| 70 | TK | 1 | Total 1 | Mg 1 | 0 |
| 70 | UA | 1 | Total 1 | Mg 1 | 0 |
| 70 | UC | 1 | Total 1 | Mg 1 | 0 |
| 70 | UE | 1 | Total 1 | Mg 1 | 0 |
| 70 | UG | 1 | Total 1 | Mg 1 | 0 |
| 70 | UI | 1 | Total 1 | Mg 1 | 0 |
| 70 | UK | 1 | Total 1 | Mg 1 | 0 |
| 70 | VA | 1 | Total 1 | Mg 1 | 0 |
| 70 | VC | 1 | Total 1 | Mg 1 | 0 |
| 70 | VE | 1 | Total 1 | Mg 1 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Residues | Atoms | | AltConf |
|-----|-------|----------|-------|----|---------|
| 70 | VG | 1 | Total | Mg | 0 |
| | | | 1 | 1 | |
| 70 | VI | 1 | Total | Mg | 0 |
| | | | 1 | 1 | |
| 70 | VK | 1 | Total | Mg | 0 |
| | | | 1 | 1 | |
| 70 | VM | 1 | Total | Mg | 0 |
| | | | 1 | 1 | |
| 70 | WA | 1 | Total | Mg | 0 |
| | | | 1 | 1 | |
| 70 | WC | 1 | Total | Mg | 0 |
| | | | 1 | 1 | |
| 70 | WE | 1 | Total | Mg | 0 |
| | | | 1 | 1 | |
| 70 | WG | 1 | Total | Mg | 0 |
| | | | 1 | 1 | |
| 70 | WI | 1 | Total | Mg | 0 |
| | | | 1 | 1 | |
| 70 | WK | 1 | Total | Mg | 0 |
| | | | 1 | 1 | |
| 70 | WM | 1 | Total | Mg | 0 |
| | | | 1 | 1 | |

- Molecule 71 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|
| 71 | AA | 1 | Total | C | N | O | P | 0 |
| | | | 32 | 10 | 5 | 14 | 3 | |
| 71 | AC | 1 | Total | C | N | O | P | 0 |
| | | | 32 | 10 | 5 | 14 | 3 | |
| 71 | AE | 1 | Total | C | N | O | P | 0 |
| | | | 32 | 10 | 5 | 14 | 3 | |
| 71 | AG | 1 | Total | C | N | O | P | 0 |
| | | | 32 | 10 | 5 | 14 | 3 | |
| 71 | AI | 1 | Total | C | N | O | P | 0 |
| | | | 32 | 10 | 5 | 14 | 3 | |
| 71 | AK | 1 | Total | C | N | O | P | 0 |
| | | | 32 | 10 | 5 | 14 | 3 | |
| 71 | AM | 1 | Total | C | N | O | P | 0 |
| | | | 32 | 10 | 5 | 14 | 3 | |
| 71 | BA | 1 | Total | C | N | O | P | 0 |
| | | | 32 | 10 | 5 | 14 | 3 | |
| 71 | BC | 1 | Total | C | N | O | P | 0 |
| | | | 32 | 10 | 5 | 14 | 3 | |
| 71 | BE | 1 | Total | C | N | O | P | 0 |
| | | | 32 | 10 | 5 | 14 | 3 | |
| 71 | BG | 1 | Total | C | N | O | P | 0 |
| | | | 32 | 10 | 5 | 14 | 3 | |
| 71 | BI | 1 | Total | C | N | O | P | 0 |
| | | | 32 | 10 | 5 | 14 | 3 | |
| 71 | BK | 1 | Total | C | N | O | P | 0 |
| | | | 32 | 10 | 5 | 14 | 3 | |
| 71 | BM | 1 | Total | C | N | O | P | 0 |
| | | | 32 | 10 | 5 | 14 | 3 | |
| 71 | C | 1 | Total | C | N | O | P | 0 |
| | | | 32 | 10 | 5 | 14 | 3 | |
| 71 | CB | 1 | Total | C | N | O | P | 0 |
| | | | 32 | 10 | 5 | 14 | 3 | |
| 71 | CD | 1 | Total | C | N | O | P | 0 |
| | | | 32 | 10 | 5 | 14 | 3 | |
| 71 | CF | 1 | Total | C | N | O | P | 0 |
| | | | 32 | 10 | 5 | 14 | 3 | |
| 71 | CH | 1 | Total | C | N | O | P | 0 |
| | | | 32 | 10 | 5 | 14 | 3 | |
| 71 | CJ | 1 | Total | C | N | O | P | 0 |
| | | | 32 | 10 | 5 | 14 | 3 | |
| 71 | CL | 1 | Total | C | N | O | P | 0 |
| | | | 32 | 10 | 5 | 14 | 3 | |
| 71 | D | 1 | Total | C | N | O | P | 0 |
| | | | 32 | 10 | 5 | 14 | 3 | |

Continued on next page...

Continued from previous page...

| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------------|---------|--------|---------|--------|---------|
| 71 | DB | 1 | Total 32 | C 10 | N 5 | O 14 | P 3 | 0 |
| 71 | DD | 1 | Total 32 | C 10 | N 5 | O 14 | P 3 | 0 |
| 71 | DF | 1 | Total 32 | C 10 | N 5 | O 14 | P 3 | 0 |
| 71 | DH | 1 | Total 32 | C 10 | N 5 | O 14 | P 3 | 0 |
| 71 | DJ | 1 | Total 32 | C 10 | N 5 | O 14 | P 3 | 0 |
| 71 | DL | 1 | Total 32 | C 10 | N 5 | O 14 | P 3 | 0 |
| 71 | EA | 1 | Total 32 | C 10 | N 5 | O 14 | P 3 | 0 |
| 71 | EC | 1 | Total 32 | C 10 | N 5 | O 14 | P 3 | 0 |
| 71 | EE | 1 | Total 32 | C 10 | N 5 | O 14 | P 3 | 0 |
| 71 | EG | 1 | Total 32 | C 10 | N 5 | O 14 | P 3 | 0 |
| 71 | EI | 1 | Total 32 | C 10 | N 5 | O 14 | P 3 | 0 |
| 71 | EK | 1 | Total 32 | C 10 | N 5 | O 14 | P 3 | 0 |
| 71 | FA | 1 | Total 32 | C 10 | N 5 | O 14 | P 3 | 0 |
| 71 | FC | 1 | Total 32 | C 10 | N 5 | O 14 | P 3 | 0 |
| 71 | FE | 1 | Total 32 | C 10 | N 5 | O 14 | P 3 | 0 |
| 71 | FG | 1 | Total 32 | C 10 | N 5 | O 14 | P 3 | 0 |
| 71 | FI | 1 | Total 32 | C 10 | N 5 | O 14 | P 3 | 0 |
| 71 | FK | 1 | Total 32 | C 10 | N 5 | O 14 | P 3 | 0 |
| 71 | GA | 1 | Total 32 | C 10 | N 5 | O 14 | P 3 | 0 |
| 71 | GC | 1 | Total 32 | C 10 | N 5 | O 14 | P 3 | 0 |
| 71 | GE | 1 | Total 32 | C 10 | N 5 | O 14 | P 3 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------------|---------|--------|---------|--------|---------|
| 71 | GG | 1 | Total 32 | C 10 | N 5 | O 14 | P 3 | 0 |
| 71 | GI | 1 | Total 32 | C 10 | N 5 | O 14 | P 3 | 0 |
| 71 | GK | 1 | Total 32 | C 10 | N 5 | O 14 | P 3 | 0 |
| 71 | HA | 1 | Total 32 | C 10 | N 5 | O 14 | P 3 | 0 |
| 71 | HC | 1 | Total 32 | C 10 | N 5 | O 14 | P 3 | 0 |
| 71 | HE | 1 | Total 32 | C 10 | N 5 | O 14 | P 3 | 0 |
| 71 | HG | 1 | Total 32 | C 10 | N 5 | O 14 | P 3 | 0 |
| 71 | HI | 1 | Total 32 | C 10 | N 5 | O 14 | P 3 | 0 |
| 71 | HK | 1 | Total 32 | C 10 | N 5 | O 14 | P 3 | 0 |
| 71 | HM | 1 | Total 32 | C 10 | N 5 | O 14 | P 3 | 0 |
| 71 | IA | 1 | Total 32 | C 10 | N 5 | O 14 | P 3 | 0 |
| 71 | IC | 1 | Total 32 | C 10 | N 5 | O 14 | P 3 | 0 |
| 71 | IE | 1 | Total 32 | C 10 | N 5 | O 14 | P 3 | 0 |
| 71 | IG | 1 | Total 32 | C 10 | N 5 | O 14 | P 3 | 0 |
| 71 | II | 1 | Total 32 | C 10 | N 5 | O 14 | P 3 | 0 |
| 71 | IK | 1 | Total 32 | C 10 | N 5 | O 14 | P 3 | 0 |
| 71 | IM | 1 | Total 32 | C 10 | N 5 | O 14 | P 3 | 0 |
| 71 | J | 1 | Total 32 | C 10 | N 5 | O 14 | P 3 | 0 |
| 71 | JB | 1 | Total 32 | C 10 | N 5 | O 14 | P 3 | 0 |
| 71 | JD | 1 | Total 32 | C 10 | N 5 | O 14 | P 3 | 0 |
| 71 | JF | 1 | Total 32 | C 10 | N 5 | O 14 | P 3 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------------|---------|--------|---------|--------|---------|
| 71 | JH | 1 | Total 32 | C 10 | N 5 | O 14 | P 3 | 0 |
| 71 | JJ | 1 | Total 32 | C 10 | N 5 | O 14 | P 3 | 0 |
| 71 | JL | 1 | Total 32 | C 10 | N 5 | O 14 | P 3 | 0 |
| 71 | JN | 1 | Total 32 | C 10 | N 5 | O 14 | P 3 | 0 |
| 71 | K | 1 | Total 32 | C 10 | N 5 | O 14 | P 3 | 0 |
| 71 | KB | 1 | Total 32 | C 10 | N 5 | O 14 | P 3 | 0 |
| 71 | KD | 1 | Total 32 | C 10 | N 5 | O 14 | P 3 | 0 |
| 71 | KF | 1 | Total 32 | C 10 | N 5 | O 14 | P 3 | 0 |
| 71 | KH | 1 | Total 32 | C 10 | N 5 | O 14 | P 3 | 0 |
| 71 | KJ | 1 | Total 32 | C 10 | N 5 | O 14 | P 3 | 0 |
| 71 | KL | 1 | Total 32 | C 10 | N 5 | O 14 | P 3 | 0 |
| 71 | KN | 1 | Total 32 | C 10 | N 5 | O 14 | P 3 | 0 |
| 71 | L | 1 | Total 32 | C 10 | N 5 | O 14 | P 3 | 0 |
| 71 | LB | 1 | Total 32 | C 10 | N 5 | O 14 | P 3 | 0 |
| 71 | LD | 1 | Total 32 | C 10 | N 5 | O 14 | P 3 | 0 |
| 71 | LF | 1 | Total 32 | C 10 | N 5 | O 14 | P 3 | 0 |
| 71 | LH | 1 | Total 32 | C 10 | N 5 | O 14 | P 3 | 0 |
| 71 | LJ | 1 | Total 32 | C 10 | N 5 | O 14 | P 3 | 0 |
| 71 | LL | 1 | Total 32 | C 10 | N 5 | O 14 | P 3 | 0 |
| 71 | LN | 1 | Total 32 | C 10 | N 5 | O 14 | P 3 | 0 |
| 71 | MA | 1 | Total 32 | C 10 | N 5 | O 14 | P 3 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------------|---------|--------|---------|--------|---------|
| 71 | MC | 1 | Total 32 | C 10 | N 5 | O 14 | P 3 | 0 |
| 71 | ME | 1 | Total 32 | C 10 | N 5 | O 14 | P 3 | 0 |
| 71 | MG | 1 | Total 32 | C 10 | N 5 | O 14 | P 3 | 0 |
| 71 | MI | 1 | Total 32 | C 10 | N 5 | O 14 | P 3 | 0 |
| 71 | MK | 1 | Total 32 | C 10 | N 5 | O 14 | P 3 | 0 |
| 71 | MM | 1 | Total 32 | C 10 | N 5 | O 14 | P 3 | 0 |
| 71 | NA | 1 | Total 32 | C 10 | N 5 | O 14 | P 3 | 0 |
| 71 | NC | 1 | Total 32 | C 10 | N 5 | O 14 | P 3 | 0 |
| 71 | NE | 1 | Total 32 | C 10 | N 5 | O 14 | P 3 | 0 |
| 71 | NG | 1 | Total 32 | C 10 | N 5 | O 14 | P 3 | 0 |
| 71 | NI | 1 | Total 32 | C 10 | N 5 | O 14 | P 3 | 0 |
| 71 | NK | 1 | Total 32 | C 10 | N 5 | O 14 | P 3 | 0 |
| 71 | NM | 1 | Total 32 | C 10 | N 5 | O 14 | P 3 | 0 |
| 71 | OA | 1 | Total 32 | C 10 | N 5 | O 14 | P 3 | 0 |
| 71 | OC | 1 | Total 32 | C 10 | N 5 | O 14 | P 3 | 0 |
| 71 | OE | 1 | Total 32 | C 10 | N 5 | O 14 | P 3 | 0 |
| 71 | OG | 1 | Total 32 | C 10 | N 5 | O 14 | P 3 | 0 |
| 71 | OI | 1 | Total 32 | C 10 | N 5 | O 14 | P 3 | 0 |
| 71 | OK | 1 | Total 32 | C 10 | N 5 | O 14 | P 3 | 0 |
| 71 | OM | 1 | Total 32 | C 10 | N 5 | O 14 | P 3 | 0 |
| 71 | PA | 1 | Total 32 | C 10 | N 5 | O 14 | P 3 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|
| | | | Total | C | N | O | P | |
| 71 | PC | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| 71 | PE | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| 71 | PG | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| 71 | PI | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| 71 | PK | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| 71 | PM | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| 71 | Q | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| 71 | QB | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| 71 | QD | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| 71 | QF | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| 71 | QH | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| 71 | QJ | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| 71 | QL | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| 71 | R | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| 71 | RB | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| 71 | RD | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| 71 | RF | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| 71 | RH | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| 71 | RJ | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| 71 | RL | 1 | 32 | 10 | 5 | 14 | 3 | 0 |
| 71 | SA | 1 | 32 | 10 | 5 | 14 | 3 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------------|---------|--------|---------|--------|---------|
| 71 | SC | 1 | Total 32 | C 10 | N 5 | O 14 | P 3 | 0 |
| 71 | SE | 1 | Total 32 | C 10 | N 5 | O 14 | P 3 | 0 |
| 71 | SG | 1 | Total 32 | C 10 | N 5 | O 14 | P 3 | 0 |
| 71 | SI | 1 | Total 32 | C 10 | N 5 | O 14 | P 3 | 0 |
| 71 | SK | 1 | Total 32 | C 10 | N 5 | O 14 | P 3 | 0 |
| 71 | TA | 1 | Total 32 | C 10 | N 5 | O 14 | P 3 | 0 |
| 71 | TC | 1 | Total 32 | C 10 | N 5 | O 14 | P 3 | 0 |
| 71 | TE | 1 | Total 32 | C 10 | N 5 | O 14 | P 3 | 0 |
| 71 | TG | 1 | Total 32 | C 10 | N 5 | O 14 | P 3 | 0 |
| 71 | TI | 1 | Total 32 | C 10 | N 5 | O 14 | P 3 | 0 |
| 71 | TK | 1 | Total 32 | C 10 | N 5 | O 14 | P 3 | 0 |
| 71 | UA | 1 | Total 32 | C 10 | N 5 | O 14 | P 3 | 0 |
| 71 | UC | 1 | Total 32 | C 10 | N 5 | O 14 | P 3 | 0 |
| 71 | UE | 1 | Total 32 | C 10 | N 5 | O 14 | P 3 | 0 |
| 71 | UG | 1 | Total 32 | C 10 | N 5 | O 14 | P 3 | 0 |
| 71 | UI | 1 | Total 32 | C 10 | N 5 | O 14 | P 3 | 0 |
| 71 | UK | 1 | Total 32 | C 10 | N 5 | O 14 | P 3 | 0 |
| 71 | VA | 1 | Total 32 | C 10 | N 5 | O 14 | P 3 | 0 |
| 71 | VC | 1 | Total 32 | C 10 | N 5 | O 14 | P 3 | 0 |
| 71 | VE | 1 | Total 32 | C 10 | N 5 | O 14 | P 3 | 0 |
| 71 | VG | 1 | Total 32 | C 10 | N 5 | O 14 | P 3 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------|----|---|----|---|---------|
| 71 | VI | 1 | Total | C | N | O | P | 0 |
| | | | 32 | 10 | 5 | 14 | 3 | |
| 71 | VK | 1 | Total | C | N | O | P | 0 |
| | | | 32 | 10 | 5 | 14 | 3 | |
| 71 | VM | 1 | Total | C | N | O | P | 0 |
| | | | 32 | 10 | 5 | 14 | 3 | |
| 71 | WA | 1 | Total | C | N | O | P | 0 |
| | | | 32 | 10 | 5 | 14 | 3 | |
| 71 | WC | 1 | Total | C | N | O | P | 0 |
| | | | 32 | 10 | 5 | 14 | 3 | |
| 71 | WE | 1 | Total | C | N | O | P | 0 |
| | | | 32 | 10 | 5 | 14 | 3 | |
| 71 | WG | 1 | Total | C | N | O | P | 0 |
| | | | 32 | 10 | 5 | 14 | 3 | |
| 71 | WI | 1 | Total | C | N | O | P | 0 |
| | | | 32 | 10 | 5 | 14 | 3 | |
| 71 | WK | 1 | Total | C | N | O | P | 0 |
| | | | 32 | 10 | 5 | 14 | 3 | |
| 71 | WM | 1 | Total | C | N | O | P | 0 |
| | | | 32 | 10 | 5 | 14 | 3 | |

- Molecule 72 is ZINC ION (three-letter code: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms | | AltConf |
|-----|-------|----------|-------|----|---------|
| 72 | 0A | 1 | Total | Zn | 0 |
| | | | 1 | 1 | |
| 72 | 0 | 1 | Total | Zn | 0 |
| | | | 1 | 1 | |
| 72 | 0z | 1 | Total | Zn | 0 |
| | | | 1 | 1 | |
| 72 | 1V | 2 | Total | Zn | 0 |
| | | | 2 | 2 | |
| 72 | 1Y | 2 | Total | Zn | 0 |
| | | | 2 | 2 | |
| 72 | 1b | 2 | Total | Zn | 0 |
| | | | 2 | 2 | |
| 72 | 1c | 2 | Total | Zn | 0 |
| | | | 2 | 2 | |
| 72 | 1e | 2 | Total | Zn | 0 |
| | | | 2 | 2 | |
| 72 | 1h | 2 | Total | Zn | 0 |
| | | | 2 | 2 | |

Continued on next page...

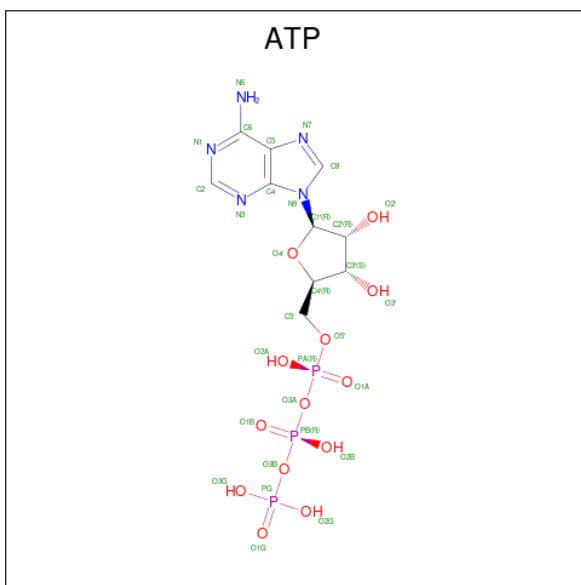
Continued from previous page...

| Mol | Chain | Residues | Atoms | | AltConf |
|-----|-------|----------|------------|---------|---------|
| 72 | 1q | 3 | Total 3 | Zn 3 | 0 |
| 72 | 1s | 1 | Total 1 | Zn 1 | 0 |
| 72 | 1t | 1 | Total 1 | Zn 1 | 0 |
| 72 | 1w | 2 | Total 2 | Zn 2 | 0 |
| 72 | 1x | 2 | Total 2 | Zn 2 | 0 |
| 72 | 3S | 1 | Total 1 | Zn 1 | 0 |
| 72 | 4W | 2 | Total 2 | Zn 2 | 0 |
| 72 | 5S | 1 | Total 1 | Zn 1 | 0 |
| 72 | 5T | 1 | Total 1 | Zn 1 | 0 |

- Molecule 73 is CALCIUM ION (three-letter code: CA) (formula: Ca).

| Mol | Chain | Residues | Atoms | | AltConf |
|-----|-------|----------|------------|---------|---------|
| 73 | 1S | 1 | Total 1 | Ca 1 | 0 |
| 73 | 2v | 1 | Total 1 | Ca 1 | 0 |
| 73 | 2w | 1 | Total 1 | Ca 1 | 0 |

- Molecule 74 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



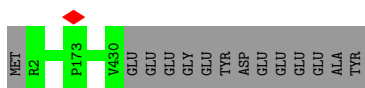
| Mol | Chain | Residues | Atoms | | | | | AltConf |
|-----|-------|----------|-------------|---------|--------|---------|--------|---------|
| 74 | 2v | 1 | Total 31 | C 10 | N 5 | O 13 | P 3 | 0 |
| 74 | 2w | 1 | Total 31 | C 10 | N 5 | O 13 | P 3 | 0 |

3 Residue-property plots

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 atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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.

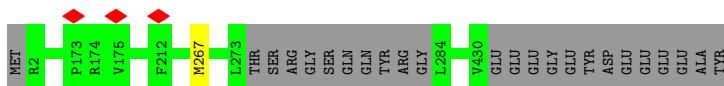
- Molecule 1: Tubulin beta chain

Chain A:  97% .



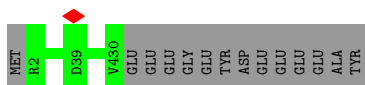
- Molecule 1: Tubulin beta chain

Chain AB:  94% 5% .



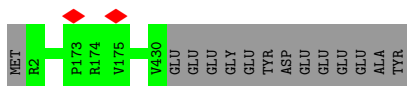
- Molecule 1: Tubulin beta chain

Chain AD:  97% .



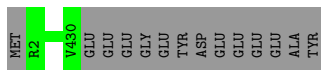
- Molecule 1: Tubulin beta chain

Chain AF:  97% .



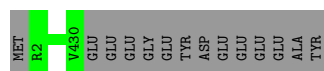
- Molecule 1: Tubulin beta chain

Chain AH:  97% .



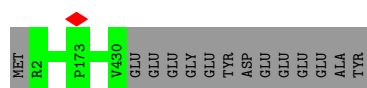
- Molecule 1: Tubulin beta chain

Chain AJ:  97% .



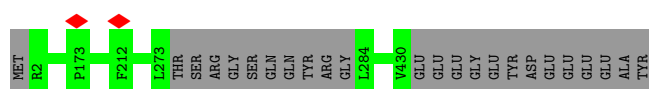
- Molecule 1: Tubulin beta chain

Chain AL:  97% .



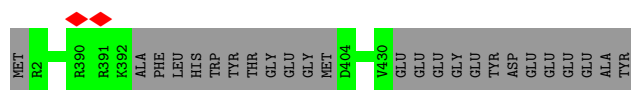
- Molecule 1: Tubulin beta chain

Chain AN:  95% 5%



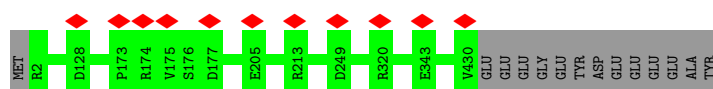
- Molecule 1: Tubulin beta chain

Chain B:  94% 6%



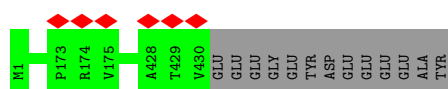
- Molecule 1: Tubulin beta chain

Chain BB:  97% .



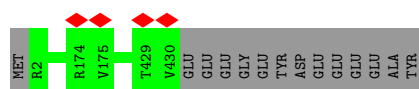
- Molecule 1: Tubulin beta chain

Chain BD:  97% .



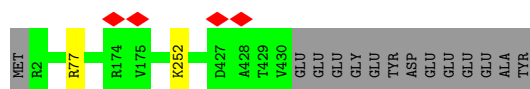
- Molecule 1: Tubulin beta chain

Chain BF:  97% .



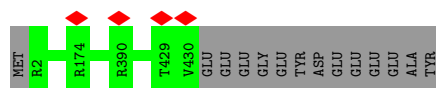
- Molecule 1: Tubulin beta chain

Chain BH:  96%



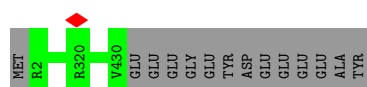
- Molecule 1: Tubulin beta chain

Chain BJ:  97%



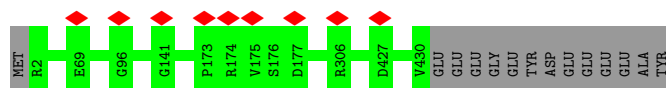
- Molecule 1: Tubulin beta chain

Chain BL:  97%



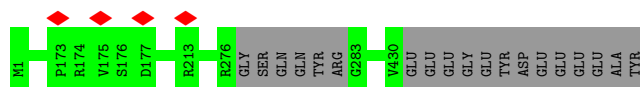
- Molecule 1: Tubulin beta chain

Chain BN:  97%



- Molecule 1: Tubulin beta chain

Chain CA:  96%




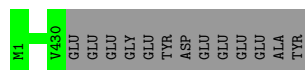
- Molecule 1: Tubulin beta chain

Chain CC:  97%



- Molecule 1: Tubulin beta chain

Chain CE:  97%



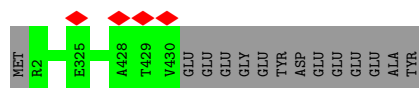
- Molecule 1: Tubulin beta chain

Chain CG:  97%



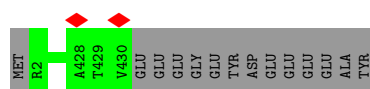
- Molecule 1: Tubulin beta chain

Chain CI:  97%



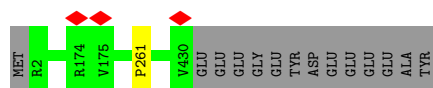
- Molecule 1: Tubulin beta chain

Chain CK:  97%



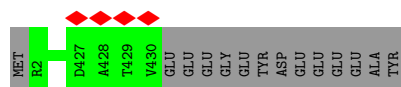
- Molecule 1: Tubulin beta chain

Chain CM:  97%



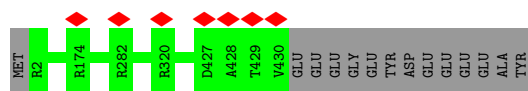
- Molecule 1: Tubulin beta chain

Chain DA:  97%



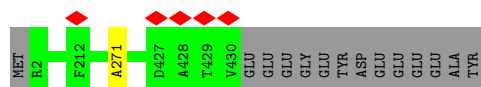
- Molecule 1: Tubulin beta chain

Chain DC:  97%



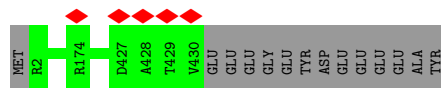
- Molecule 1: Tubulin beta chain

Chain DE:  97%



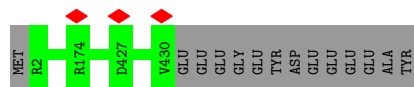
- Molecule 1: Tubulin beta chain

Chain DG:  97%



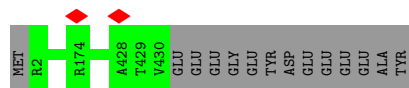
- Molecule 1: Tubulin beta chain

Chain DI:  97%



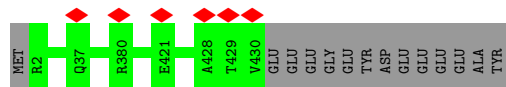
- Molecule 1: Tubulin beta chain

Chain DK:  97%



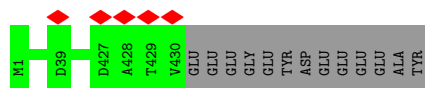
- Molecule 1: Tubulin beta chain

Chain DM:  97%



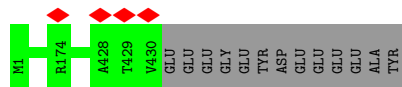
- Molecule 1: Tubulin beta chain

Chain E:  97%



- Molecule 1: Tubulin beta chain

Chain EB:  97%



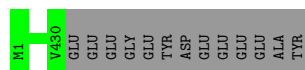
- Molecule 1: Tubulin beta chain

Chain ED:  97%



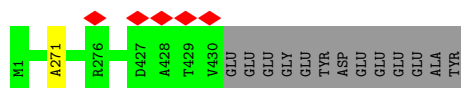
- Molecule 1: Tubulin beta chain

Chain EF: 97%



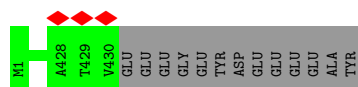
- Molecule 1: Tubulin beta chain

Chain EH: 97%



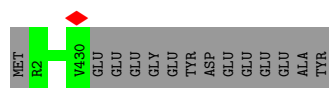
- Molecule 1: Tubulin beta chain

Chain EJ: 97%



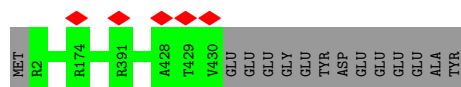
- Molecule 1: Tubulin beta chain

Chain EL: 97%



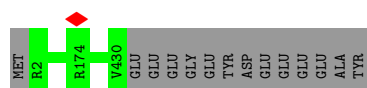
- Molecule 1: Tubulin beta chain

Chain F: 97%



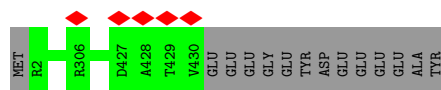
- Molecule 1: Tubulin beta chain

Chain FB: 97%



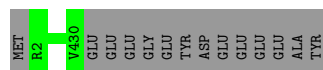
- Molecule 1: Tubulin beta chain

Chain FD: 97%



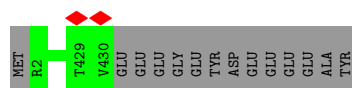
- Molecule 1: Tubulin beta chain

Chain FF: 97%



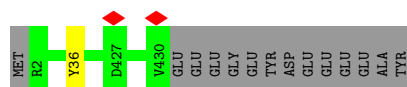
- Molecule 1: Tubulin beta chain

Chain FH: 97%



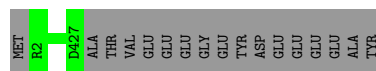
- Molecule 1: Tubulin beta chain

Chain FJ: 97%



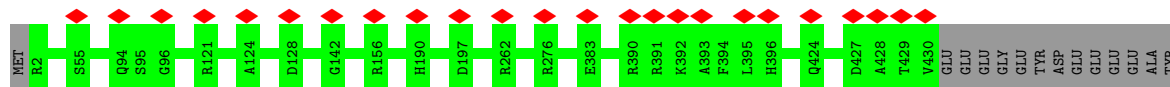
- Molecule 1: Tubulin beta chain

Chain FL: 96%



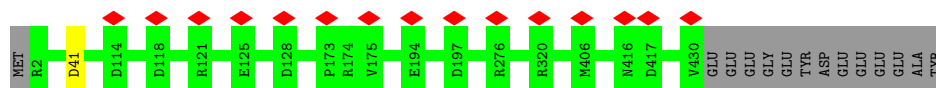
- Molecule 1: Tubulin beta chain

Chain G: 5% 97%



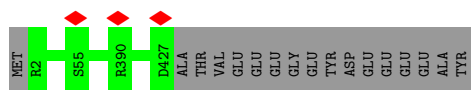
- Molecule 1: Tubulin beta chain

Chain GB: 97%

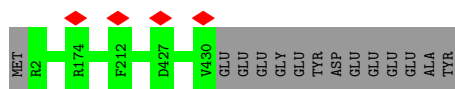


- Molecule 1: Tubulin beta chain

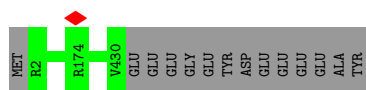
Chain GD: 96%



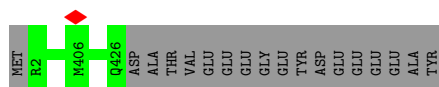
- Molecule 1: Tubulin beta chain



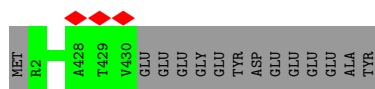
- Molecule 1: Tubulin beta chain



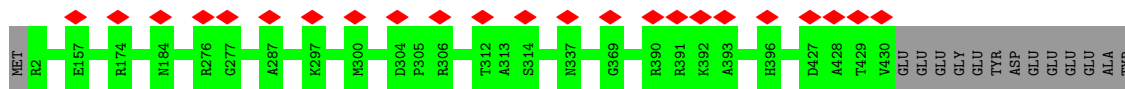
- Molecule 1: Tubulin beta chain



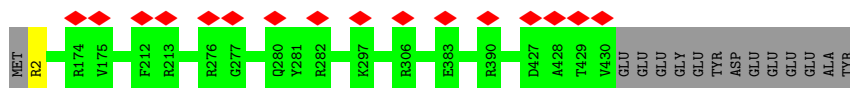
- Molecule 1: Tubulin beta chain



- Molecule 1: Tubulin beta chain

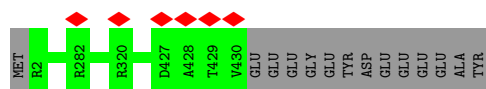


- Molecule 1: Tubulin beta chain



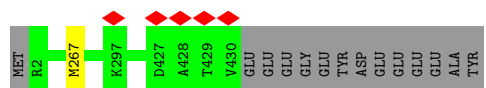
- Molecule 1: Tubulin beta chain

Chain HD:  97%



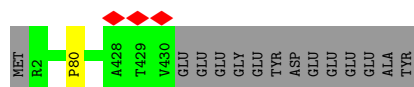
- Molecule 1: Tubulin beta chain

Chain HF:  97%



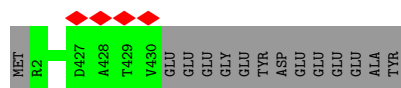
- Molecule 1: Tubulin beta chain

Chain HH:  97%



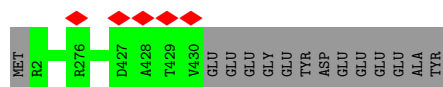
- Molecule 1: Tubulin beta chain

Chain HJ:  97%




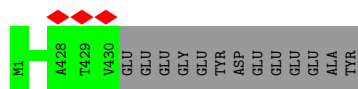
- Molecule 1: Tubulin beta chain

Chain HL:  97%



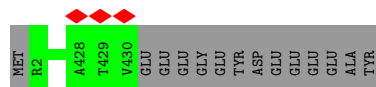
- Molecule 1: Tubulin beta chain

Chain I:  97%

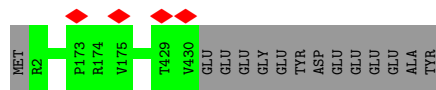


- Molecule 1: Tubulin beta chain

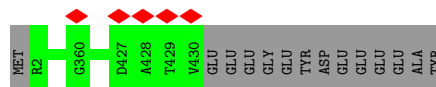
Chain IB:  97%



● Molecule 1: Tubulin beta chain

Chain ID:  97%

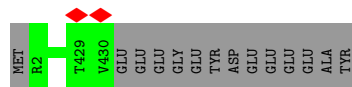
● Molecule 1: Tubulin beta chain

Chain IF:  97%

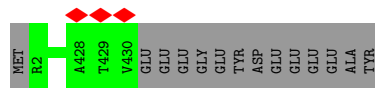
● Molecule 1: Tubulin beta chain

Chain IH:  97%

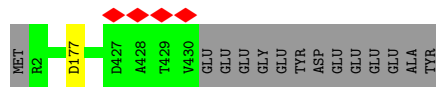
● Molecule 1: Tubulin beta chain

Chain IJ:  97%

● Molecule 1: Tubulin beta chain

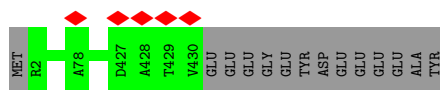
Chain IL:  97%

● Molecule 1: Tubulin beta chain

Chain JA:  97%

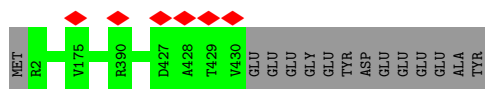
● Molecule 1: Tubulin beta chain

Chain JC:  97%



- Molecule 1: Tubulin beta chain

Chain JE:
97%



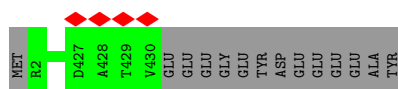
- Molecule 1: Tubulin beta chain

Chain JG:
97%



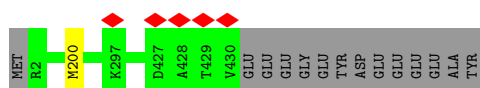
- Molecule 1: Tubulin beta chain

Chain JI:
97%



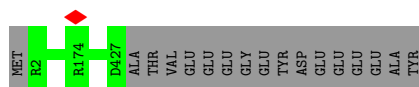
- Molecule 1: Tubulin beta chain

Chain JK:
97%



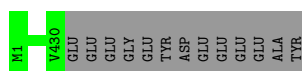
- Molecule 1: Tubulin beta chain

Chain JM:
96%



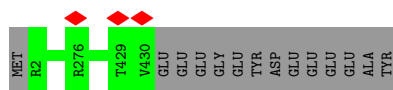
- Molecule 1: Tubulin beta chain

Chain KA:
97%



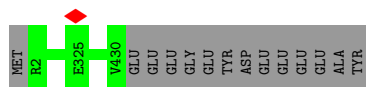
- Molecule 1: Tubulin beta chain

Chain KC:
97%



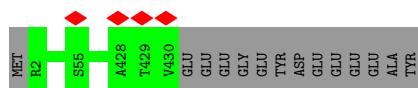
- Molecule 1: Tubulin beta chain

Chain KE: 97%



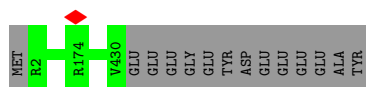
- Molecule 1: Tubulin beta chain

Chain KG: 97%



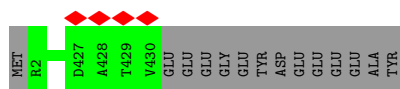
- Molecule 1: Tubulin beta chain

Chain KI: 97%



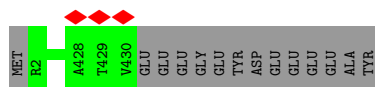
- Molecule 1: Tubulin beta chain

Chain KK: 97%



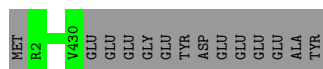
- Molecule 1: Tubulin beta chain

Chain KM: 97%



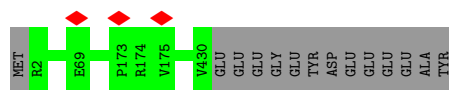
- Molecule 1: Tubulin beta chain

Chain LA: 97%



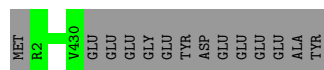
- Molecule 1: Tubulin beta chain

Chain LC: 97%



- Molecule 1: Tubulin beta chain

Chain LE: 97%



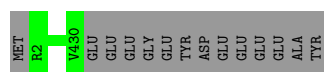
- Molecule 1: Tubulin beta chain

Chain LG: 97%



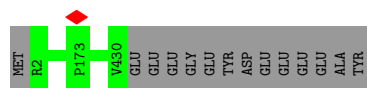
- Molecule 1: Tubulin beta chain

Chain LI: 97%



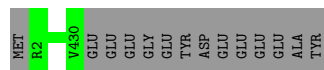
- Molecule 1: Tubulin beta chain

Chain LK: 97%



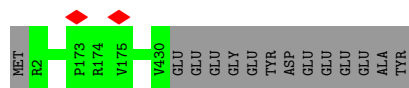
- Molecule 1: Tubulin beta chain

Chain LM: 97%



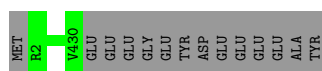
- Molecule 1: Tubulin beta chain

Chain LO: 97%



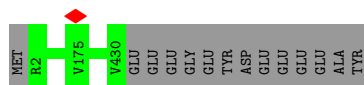
- Molecule 1: Tubulin beta chain

Chain M: 97%



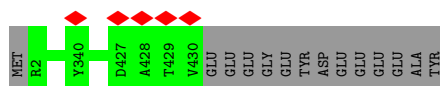
- Molecule 1: Tubulin beta chain

Chain MB:
97%



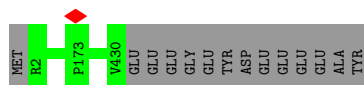
- Molecule 1: Tubulin beta chain

Chain MD:
97%



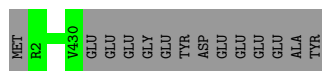
- Molecule 1: Tubulin beta chain

Chain MF:
97%



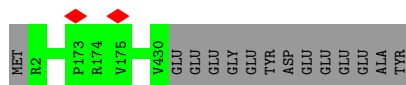
- Molecule 1: Tubulin beta chain

Chain MH:
97%



- Molecule 1: Tubulin beta chain

Chain MJ:
97%



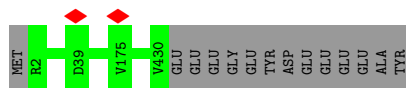
- Molecule 1: Tubulin beta chain

Chain ML:
97%

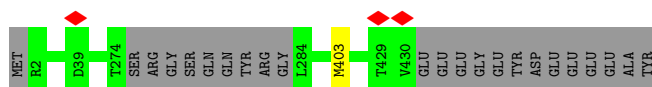


- Molecule 1: Tubulin beta chain

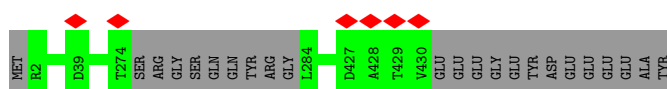
Chain MN:
97%



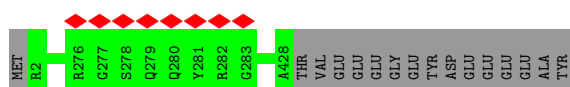
- Molecule 1: Tubulin beta chain



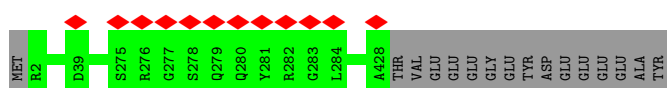
- Molecule 1: Tubulin beta chain



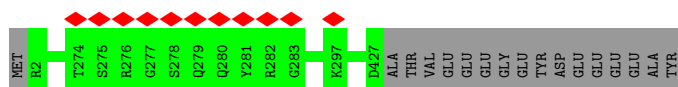
- Molecule 1: Tubulin beta chain



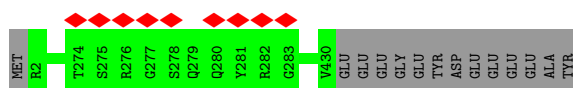
- Molecule 1: Tubulin beta chain



- Molecule 1: Tubulin beta chain

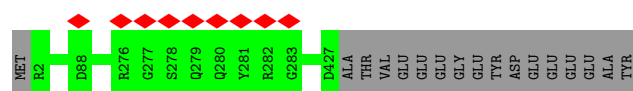


- Molecule 1: Tubulin beta chain



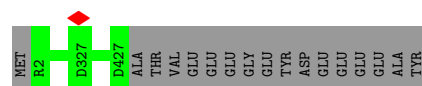
- Molecule 1: Tubulin beta chain

Chain NL:  96%



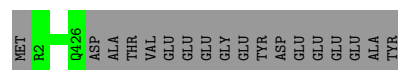
- Molecule 1: Tubulin beta chain

Chain O:  96%



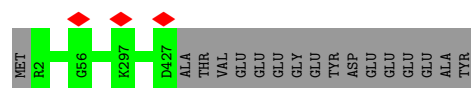
- Molecule 1: Tubulin beta chain

Chain OB:  96%



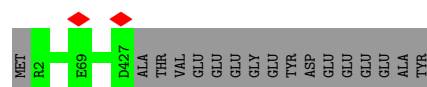
- Molecule 1: Tubulin beta chain

Chain OD:  96%



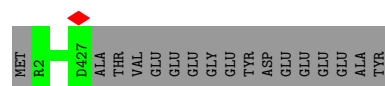
- Molecule 1: Tubulin beta chain

Chain OF:  96%



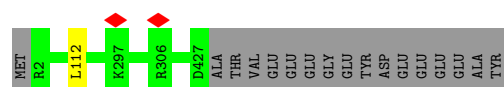
- Molecule 1: Tubulin beta chain

Chain OH:  96%



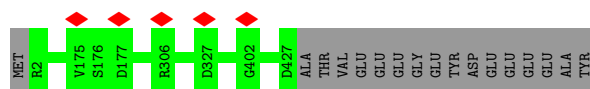
- Molecule 1: Tubulin beta chain

Chain OJ:  96%



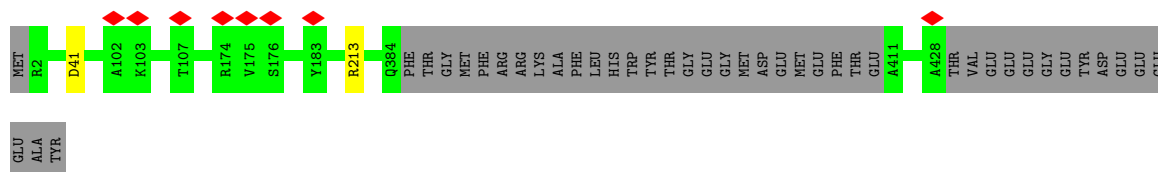
- Molecule 1: Tubulin beta chain

Chain OL:  96%



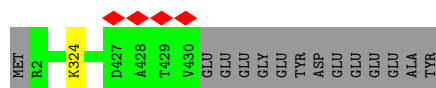
- Molecule 1: Tubulin beta chain

Chain P:  90%



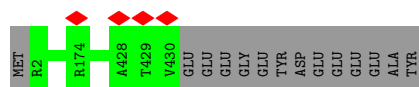
- Molecule 1: Tubulin beta chain

Chain PB:  97%



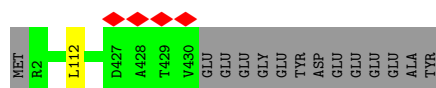
- Molecule 1: Tubulin beta chain

Chain PD:  97%



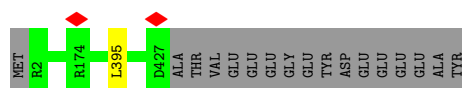
- Molecule 1: Tubulin beta chain

Chain PF:  97%



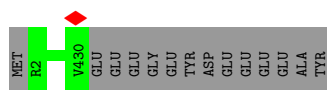
- Molecule 1: Tubulin beta chain

Chain PH:  96%

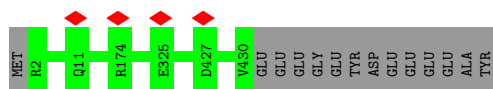


- Molecule 1: Tubulin beta chain

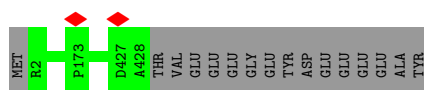
Chain PJ:  97%



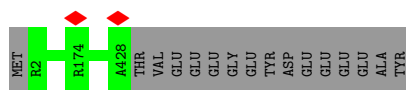
- Molecule 1: Tubulin beta chain



- Molecule 1: Tubulin beta chain



- Molecule 1: Tubulin beta chain



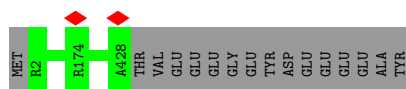
- Molecule 1: Tubulin beta chain



- Molecule 1: Tubulin beta chain

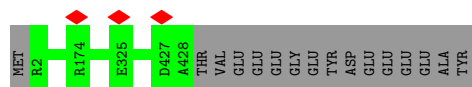


- Molecule 1: Tubulin beta chain



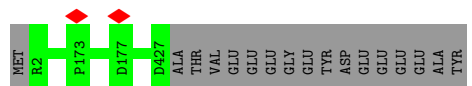
- Molecule 1: Tubulin beta chain

Chain QK:  96%



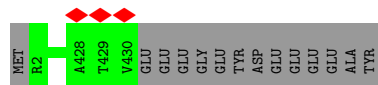
- Molecule 1: Tubulin beta chain

Chain RA:  96%



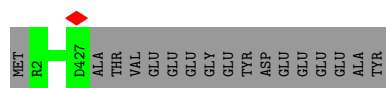
- Molecule 1: Tubulin beta chain

Chain RC:  97%



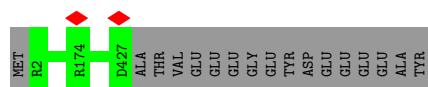
- Molecule 1: Tubulin beta chain

Chain RE:  96%



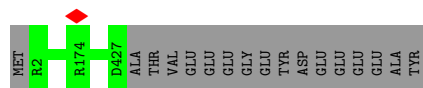
- Molecule 1: Tubulin beta chain

Chain RG:  96%



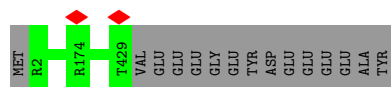
- Molecule 1: Tubulin beta chain

Chain RI:  96%



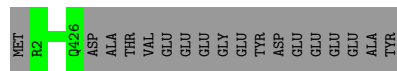
- Molecule 1: Tubulin beta chain

Chain RK:  97%



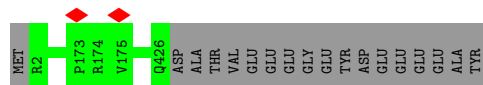
- Molecule 1: Tubulin beta chain

Chain S:  96%



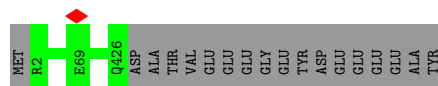
- Molecule 1: Tubulin beta chain

Chain SB:  96%



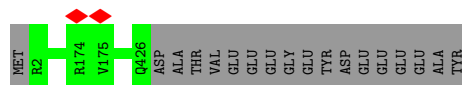
- Molecule 1: Tubulin beta chain

Chain SD:  96%



- Molecule 1: Tubulin beta chain

Chain SF:  96%



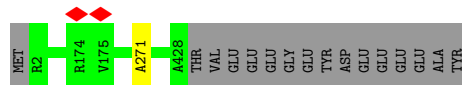
- Molecule 1: Tubulin beta chain

Chain SH:  96%



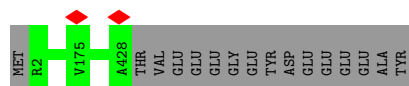
- Molecule 1: Tubulin beta chain

Chain SJ:  96%



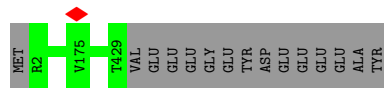
- Molecule 1: Tubulin beta chain

Chain T:  96%



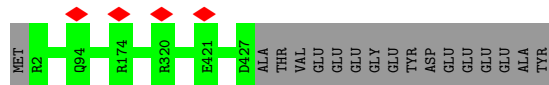
- Molecule 1: Tubulin beta chain

Chain TB:  97%



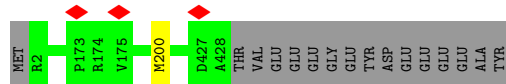
- Molecule 1: Tubulin beta chain

Chain TD:  96%



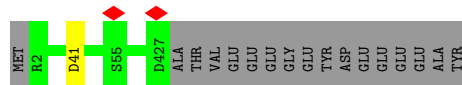
- Molecule 1: Tubulin beta chain

Chain TF:  96%



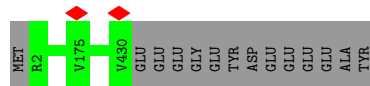
- Molecule 1: Tubulin beta chain

Chain TH:  96%



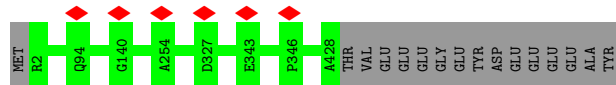
- Molecule 1: Tubulin beta chain

Chain TJ:  97%



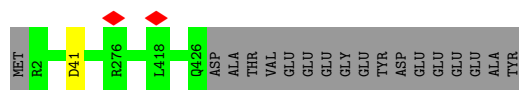
- Molecule 1: Tubulin beta chain

Chain TL:  96%

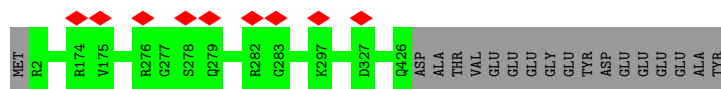


- Molecule 1: Tubulin beta chain

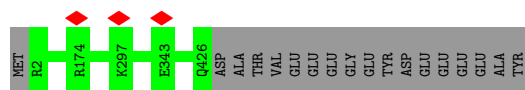
Chain U:  96%



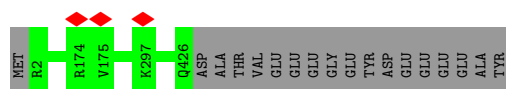
- Molecule 1: Tubulin beta chain



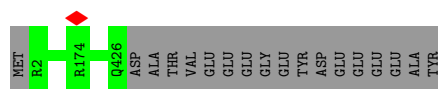
- Molecule 1: Tubulin beta chain



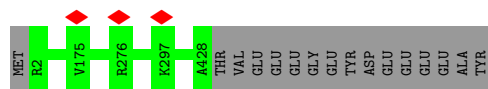
- Molecule 1: Tubulin beta chain



- Molecule 1: Tubulin beta chain




- Molecule 1: Tubulin beta chain

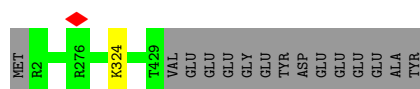


- Molecule 1: Tubulin beta chain



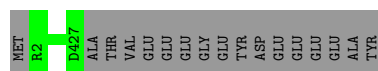
- Molecule 1: Tubulin beta chain

Chain V:  96%



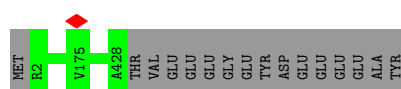
- Molecule 1: Tubulin beta chain

Chain VB:  96%



- Molecule 1: Tubulin beta chain

Chain VD:  96%



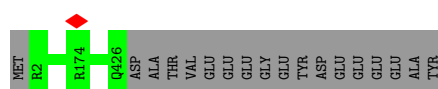
- Molecule 1: Tubulin beta chain

Chain VF:  97%



- Molecule 1: Tubulin beta chain

Chain VH:  96%



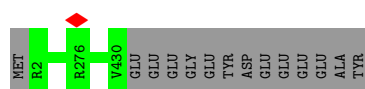
- Molecule 1: Tubulin beta chain

Chain VJ:  97%



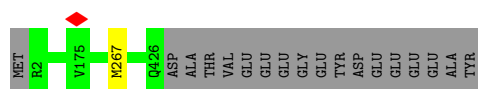
- Molecule 1: Tubulin beta chain

Chain VL:  97%



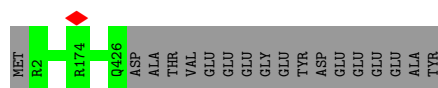
- Molecule 1: Tubulin beta chain

Chain W:  96%



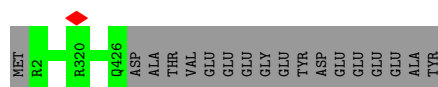
- Molecule 1: Tubulin beta chain

Chain WB:  96%



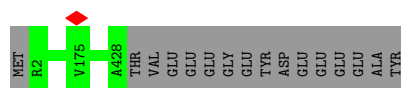
- Molecule 1: Tubulin beta chain

Chain WD:  96%



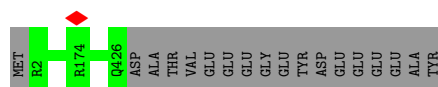
- Molecule 1: Tubulin beta chain

Chain WF:  96%



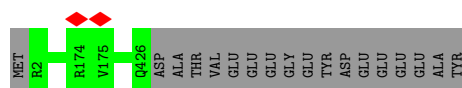
- Molecule 1: Tubulin beta chain

Chain WH:  96%



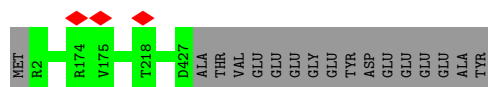
- Molecule 1: Tubulin beta chain

Chain WJ:  96%

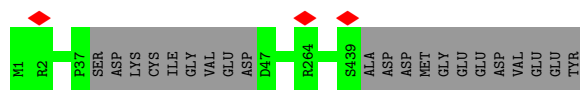


- Molecule 1: Tubulin beta chain

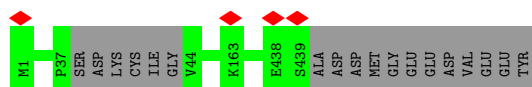
Chain WL:  96%



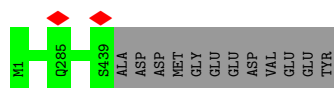
• Molecule 2: Tubulin alpha chain

Chain AA:  95% 5%

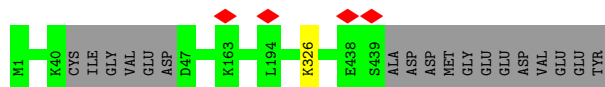
• Molecule 2: Tubulin alpha chain

Chain AC:  96% .

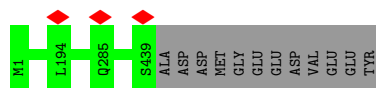
• Molecule 2: Tubulin alpha chain

Chain AE:  97% .

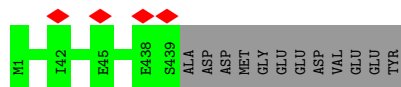
• Molecule 2: Tubulin alpha chain

Chain AG:  96% .

• Molecule 2: Tubulin alpha chain

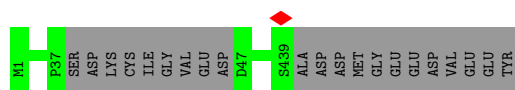
Chain AI:  97% .

• Molecule 2: Tubulin alpha chain

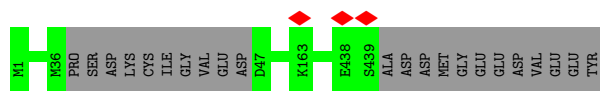
Chain AK:  97% .

• Molecule 2: Tubulin alpha chain

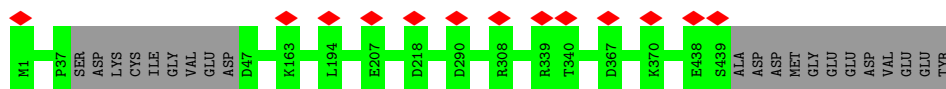
Chain AM:  95% 5%



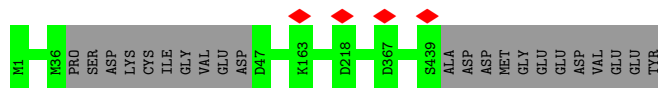
- Molecule 2: Tubulin alpha chain



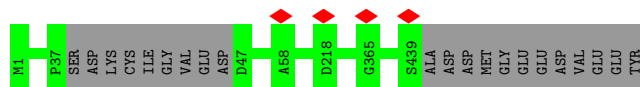
- Molecule 2: Tubulin alpha chain



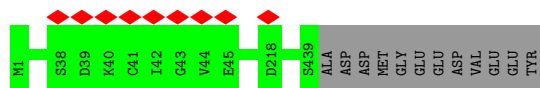
- Molecule 2: Tubulin alpha chain



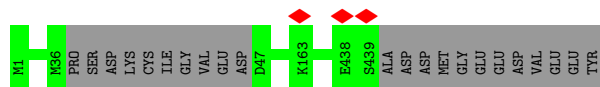
- Molecule 2: Tubulin alpha chain



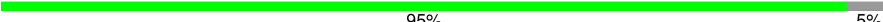
- Molecule 2: Tubulin alpha chain

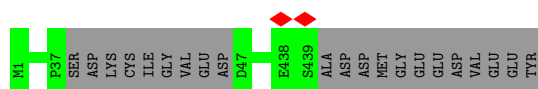


- Molecule 2: Tubulin alpha chain



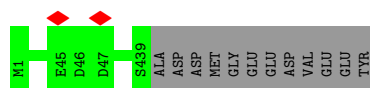
- Molecule 2: Tubulin alpha chain

Chain BM:  95% 5%



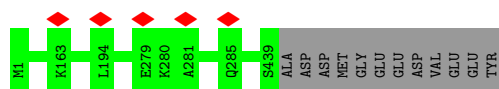
- Molecule 2: Tubulin alpha chain

Chain C:  97% .



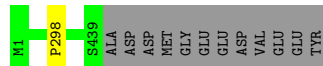
- Molecule 2: Tubulin alpha chain

Chain CB:  97% .



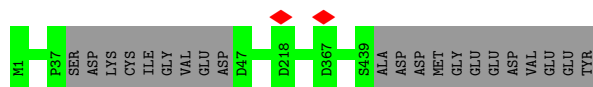
- Molecule 2: Tubulin alpha chain

Chain CD:  97% .



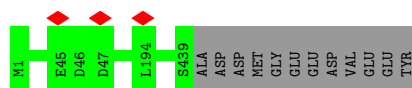
- Molecule 2: Tubulin alpha chain

Chain CF:  95% 5%



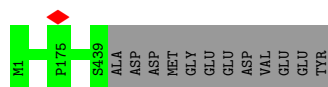
- Molecule 2: Tubulin alpha chain

Chain CH:  97% .

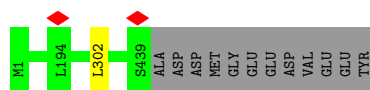


- Molecule 2: Tubulin alpha chain

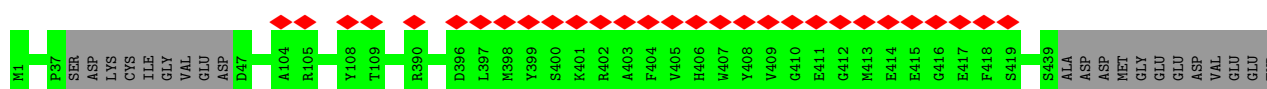
Chain CJ:  97% .



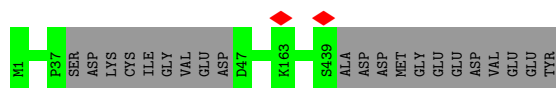
● Molecule 2: Tubulin alpha chain

Chain CL:  97%

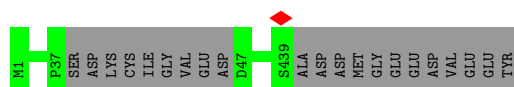
● Molecule 2: Tubulin alpha chain

Chain D:  95% 5% 6%

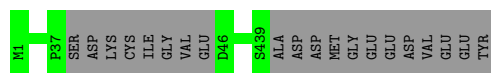
● Molecule 2: Tubulin alpha chain

Chain DB:  95% 5%

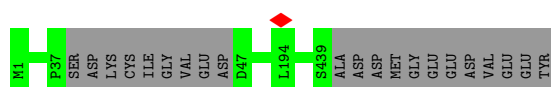
● Molecule 2: Tubulin alpha chain

Chain DD:  95% 5%

● Molecule 2: Tubulin alpha chain

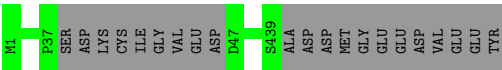
Chain DF:  96%

● Molecule 2: Tubulin alpha chain

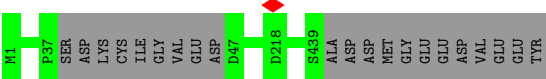
Chain DH:  95% 5%

● Molecule 2: Tubulin alpha chain

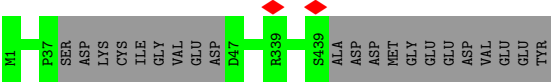
Chain DJ:  95% 5%



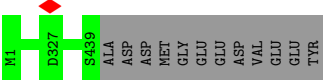
• Molecule 2: Tubulin alpha chain



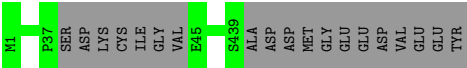
• Molecule 2: Tubulin alpha chain



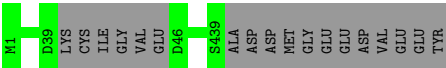
• Molecule 2: Tubulin alpha chain



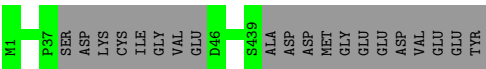
• Molecule 2: Tubulin alpha chain



• Molecule 2: Tubulin alpha chain

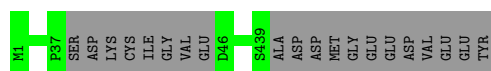


• Molecule 2: Tubulin alpha chain



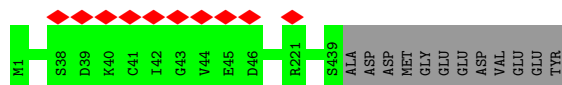
• Molecule 2: Tubulin alpha chain





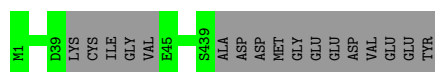
- Molecule 2: Tubulin alpha chain

Chain FA: 97%



- Molecule 2: Tubulin alpha chain

Chain FC: 96%



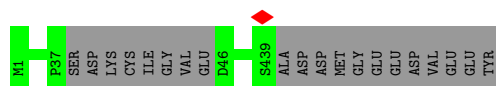
- Molecule 2: Tubulin alpha chain

Chain FE: 96%



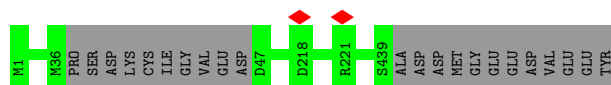
- Molecule 2: Tubulin alpha chain

Chain FG: 96%



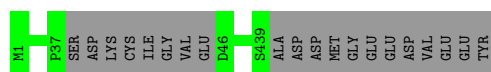
- Molecule 2: Tubulin alpha chain

Chain FI: 95%



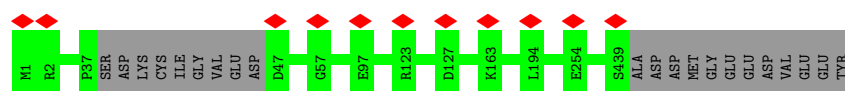
- Molecule 2: Tubulin alpha chain

Chain FK: 96%



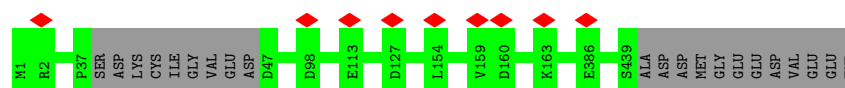
- Molecule 2: Tubulin alpha chain

Chain GA:  95% 5%



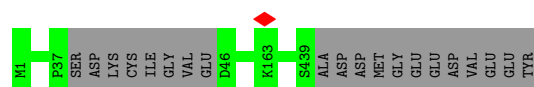
- Molecule 2: Tubulin alpha chain

Chain GC:  95% 5%



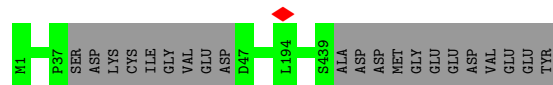
- Molecule 2: Tubulin alpha chain

Chain GE:  96%



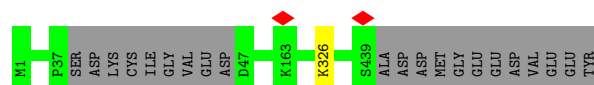
- Molecule 2: Tubulin alpha chain

Chain GG:  95% 5%



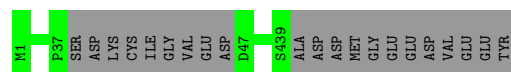
- Molecule 2: Tubulin alpha chain

Chain GI:  95% 5%



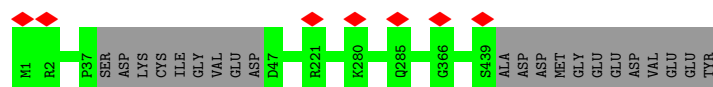
- Molecule 2: Tubulin alpha chain

Chain GK:  95% 5%

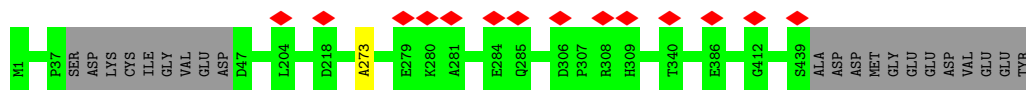


- Molecule 2: Tubulin alpha chain

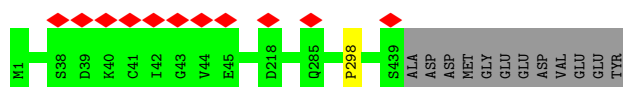
Chain HA:  95% 5%



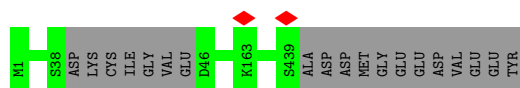
• Molecule 2: Tubulin alpha chain

Chain HC:  95% 5%

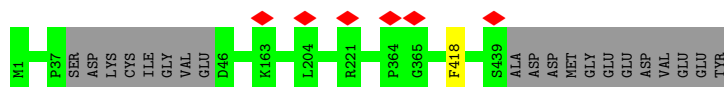
• Molecule 2: Tubulin alpha chain

Chain HE:  97% .

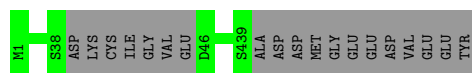
• Molecule 2: Tubulin alpha chain

Chain HG:  96% .

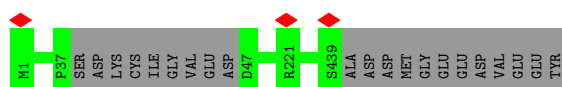
• Molecule 2: Tubulin alpha chain

Chain HI:  95% .

• Molecule 2: Tubulin alpha chain

Chain HK:  96% .

• Molecule 2: Tubulin alpha chain

Chain HM:  95% 5%

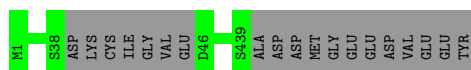
• Molecule 2: Tubulin alpha chain

Chain IA:  95% 5%



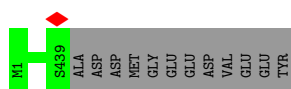
- Molecule 2: Tubulin alpha chain

Chain IC: 96%



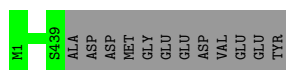
- Molecule 2: Tubulin alpha chain

Chain IE: 97%



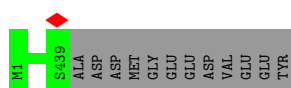
- Molecule 2: Tubulin alpha chain

Chain IG: 97%



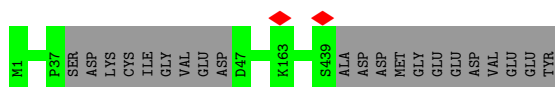
- Molecule 2: Tubulin alpha chain

Chain II: 97%



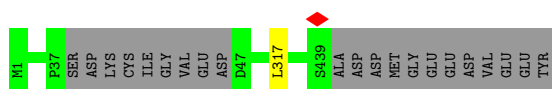
- Molecule 2: Tubulin alpha chain

Chain IK: 95%



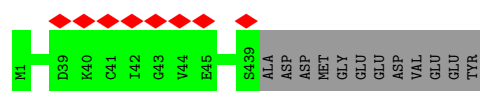
- Molecule 2: Tubulin alpha chain

Chain IM: 95%



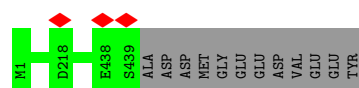
- Molecule 2: Tubulin alpha chain

Chain J:  97%



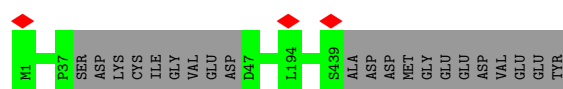
- Molecule 2: Tubulin alpha chain

Chain JB:  97%



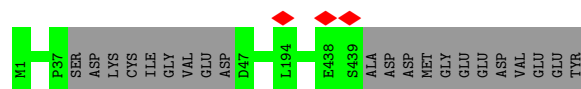
- Molecule 2: Tubulin alpha chain

Chain JD:  95% 5%



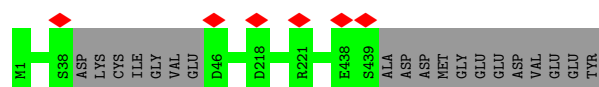
- Molecule 2: Tubulin alpha chain

Chain JF:  95% 5%



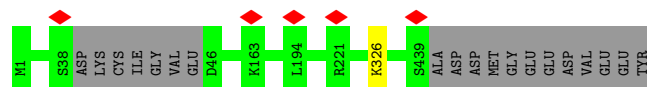
- Molecule 2: Tubulin alpha chain

Chain JH:  96%



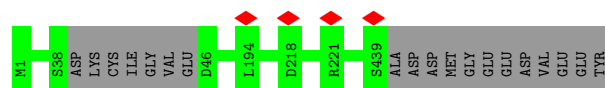
- Molecule 2: Tubulin alpha chain

Chain JJ:  96%

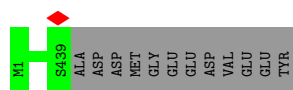


- Molecule 2: Tubulin alpha chain

Chain JL:  96%



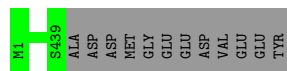
● Molecule 2: Tubulin alpha chain

Chain JN:  97%

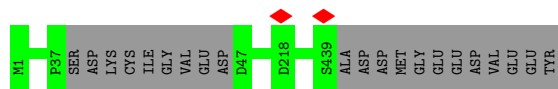
● Molecule 2: Tubulin alpha chain

Chain K:  96%

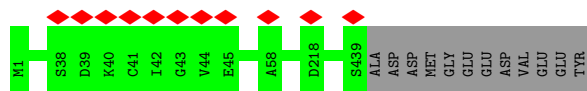
● Molecule 2: Tubulin alpha chain

Chain KB:  97%

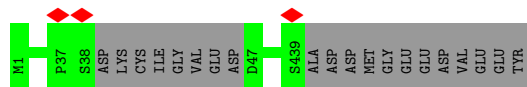
● Molecule 2: Tubulin alpha chain

Chain KD:  95%

● Molecule 2: Tubulin alpha chain

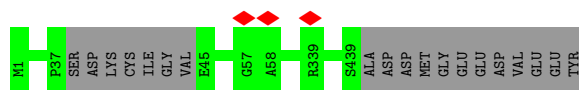
Chain KF:  97%

● Molecule 2: Tubulin alpha chain

Chain KH:  96%

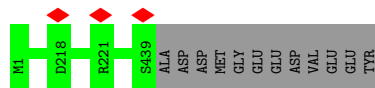
● Molecule 2: Tubulin alpha chain

Chain KJ:  96%



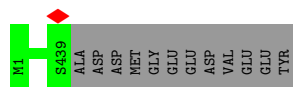
- Molecule 2: Tubulin alpha chain

Chain KL: 97%



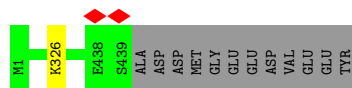
- Molecule 2: Tubulin alpha chain

Chain KN: 97%



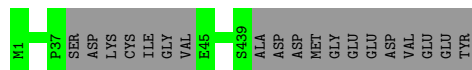
- Molecule 2: Tubulin alpha chain

Chain L: 97%



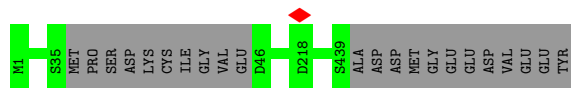
- Molecule 2: Tubulin alpha chain

Chain LB: 96%



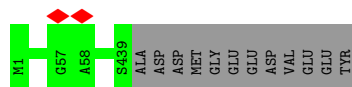
- Molecule 2: Tubulin alpha chain

Chain LD: 95% 5%



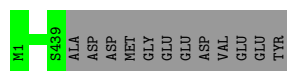
- Molecule 2: Tubulin alpha chain

Chain LF: 97%



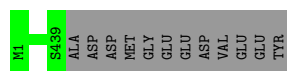
- Molecule 2: Tubulin alpha chain

Chain LH:  97%



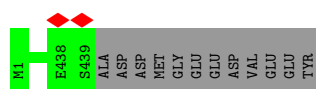
- Molecule 2: Tubulin alpha chain

Chain LJ:  97%



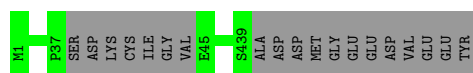
- Molecule 2: Tubulin alpha chain

Chain LL:  97%



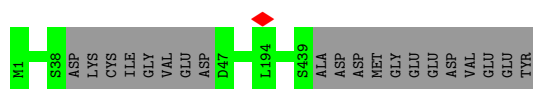
- Molecule 2: Tubulin alpha chain

Chain LN:  96%



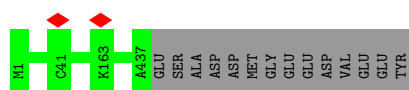
- Molecule 2: Tubulin alpha chain

Chain MA:  96%



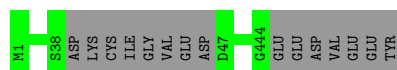
- Molecule 2: Tubulin alpha chain

Chain MC:  97%



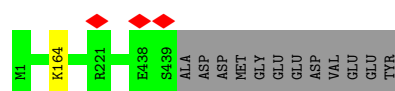
- Molecule 2: Tubulin alpha chain

Chain ME:  97%



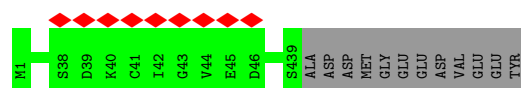
- Molecule 2: Tubulin alpha chain

Chain MG:  97%



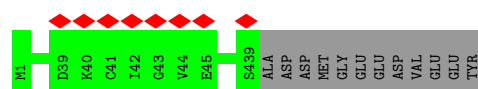
- Molecule 2: Tubulin alpha chain

Chain MI:  97%



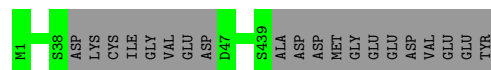
- Molecule 2: Tubulin alpha chain

Chain MK:  97%



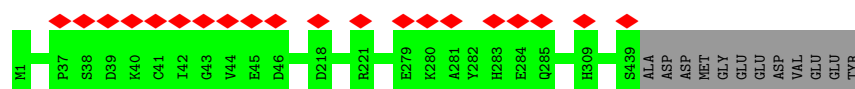
- Molecule 2: Tubulin alpha chain

Chain MM:  96%



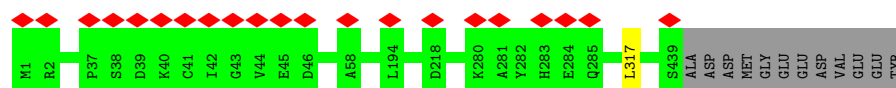
- Molecule 2: Tubulin alpha chain

Chain NA:  97%



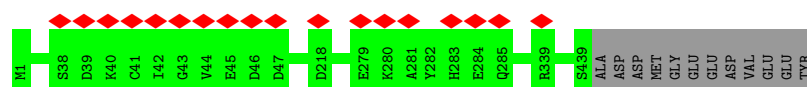
- Molecule 2: Tubulin alpha chain

Chain NC:  5% 97%

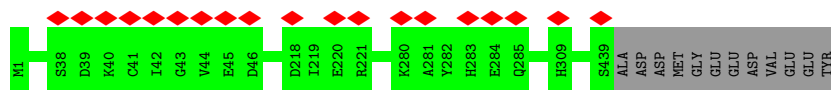


- Molecule 2: Tubulin alpha chain

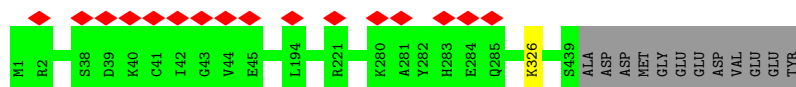
Chain NE:  97%



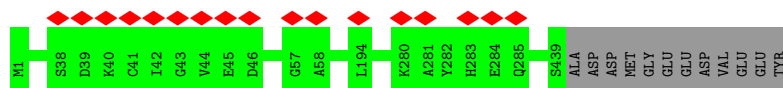
● Molecule 2: Tubulin alpha chain

Chain NG:  97%

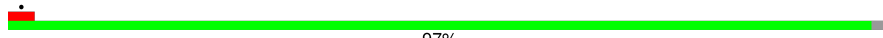
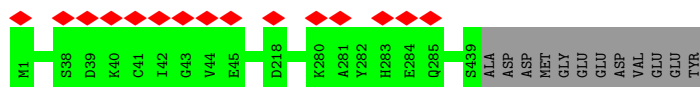
● Molecule 2: Tubulin alpha chain

Chain NI:  97%

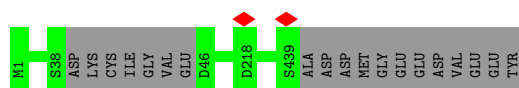
● Molecule 2: Tubulin alpha chain

Chain NK:  97%

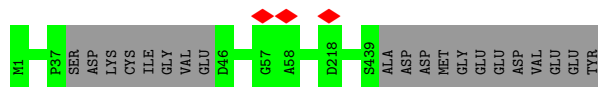
● Molecule 2: Tubulin alpha chain

Chain NM:  97%

● Molecule 2: Tubulin alpha chain

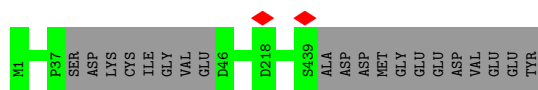
Chain OA:  96%

● Molecule 2: Tubulin alpha chain

Chain OC:  96%

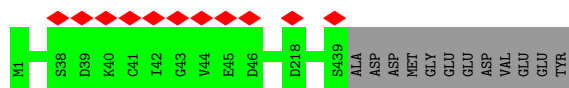
● Molecule 2: Tubulin alpha chain

Chain OE:  96%



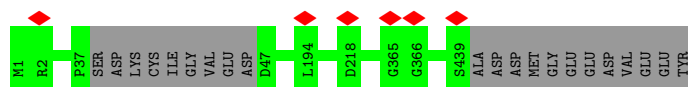
- Molecule 2: Tubulin alpha chain

Chain OG: 97%



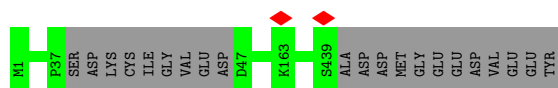
- Molecule 2: Tubulin alpha chain

Chain OI: 95%



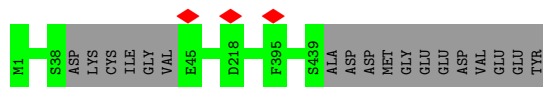
- Molecule 2: Tubulin alpha chain

Chain OK: 95%



- Molecule 2: Tubulin alpha chain

Chain OM: 96%



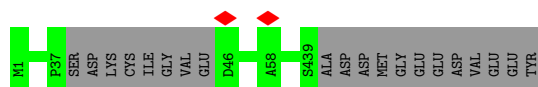
- Molecule 2: Tubulin alpha chain

Chain PA: 95%



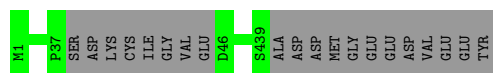
- Molecule 2: Tubulin alpha chain

Chain PC: 96%



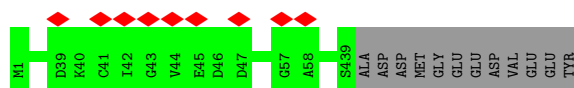
- Molecule 2: Tubulin alpha chain

Chain PE:  96%



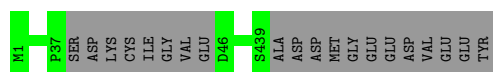
- Molecule 2: Tubulin alpha chain

Chain PG:  97%



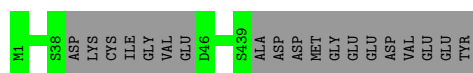
- Molecule 2: Tubulin alpha chain

Chain PI:  96%



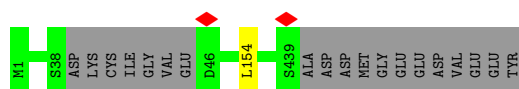
- Molecule 2: Tubulin alpha chain

Chain PK:  96%



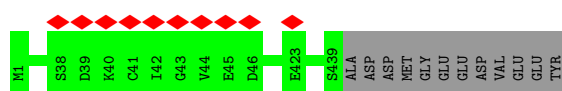
- Molecule 2: Tubulin alpha chain

Chain PM:  96%



- Molecule 2: Tubulin alpha chain

Chain Q:  97%



- Molecule 2: Tubulin alpha chain

Chain QB:  95%



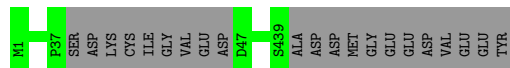
- Molecule 2: Tubulin alpha chain

Chain QD:  95% 5%



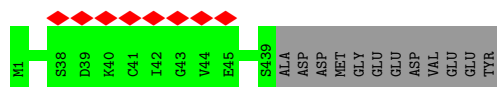
- Molecule 2: Tubulin alpha chain

Chain QF:  95% 5%



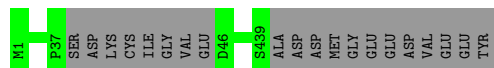
- Molecule 2: Tubulin alpha chain

Chain QH:  97% .



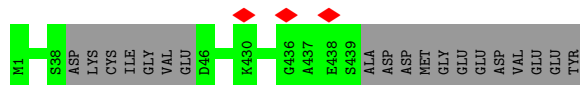
- Molecule 2: Tubulin alpha chain

Chain QJ:  96% .



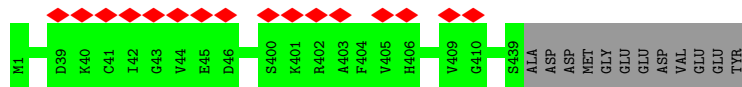
- Molecule 2: Tubulin alpha chain

Chain QL:  96% .



- Molecule 2: Tubulin alpha chain

Chain R:  97% .

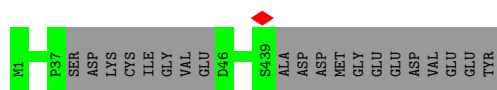


- Molecule 2: Tubulin alpha chain

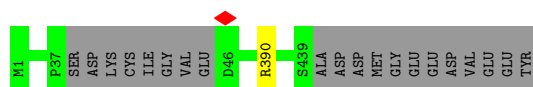
Chain RB:  95% .



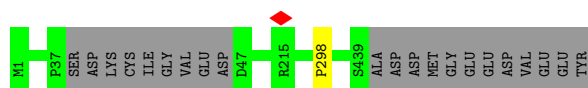
• Molecule 2: Tubulin alpha chain

Chain RD:  96%

• Molecule 2: Tubulin alpha chain

Chain RF:  95%

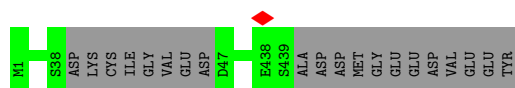
• Molecule 2: Tubulin alpha chain

Chain RH:  95% 5%

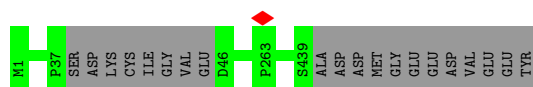
• Molecule 2: Tubulin alpha chain

Chain RJ:  95% 5%

• Molecule 2: Tubulin alpha chain

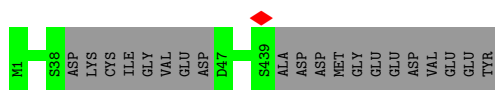
Chain RL:  96%

• Molecule 2: Tubulin alpha chain

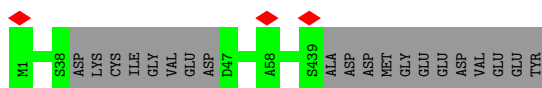
Chain SA:  96%

• Molecule 2: Tubulin alpha chain

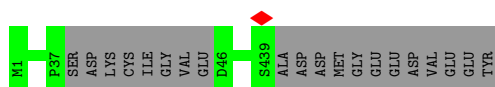
Chain SC:  96%



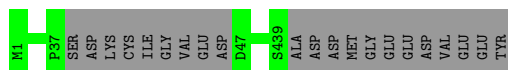
- Molecule 2: Tubulin alpha chain



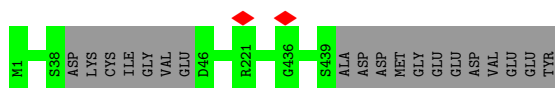
- Molecule 2: Tubulin alpha chain



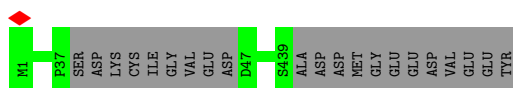
- Molecule 2: Tubulin alpha chain



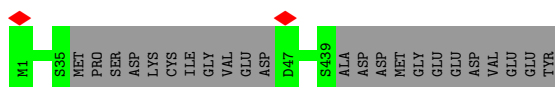
- Molecule 2: Tubulin alpha chain



- Molecule 2: Tubulin alpha chain

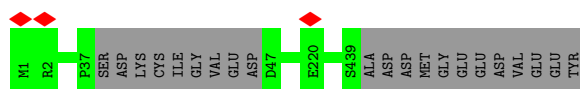


- Molecule 2: Tubulin alpha chain



- Molecule 2: Tubulin alpha chain

Chain TE:  95% 5%



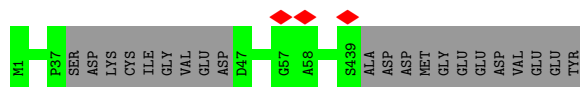
- Molecule 2: Tubulin alpha chain

Chain TG:  96% 4%



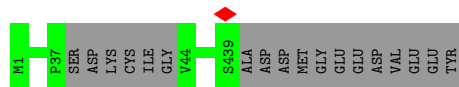
- Molecule 2: Tubulin alpha chain

Chain TI:  95% 5%



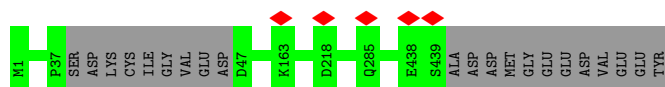
- Molecule 2: Tubulin alpha chain

Chain TK:  96% 4%



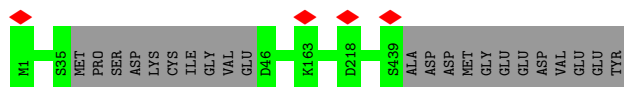
- Molecule 2: Tubulin alpha chain

Chain UA:  95% 5%



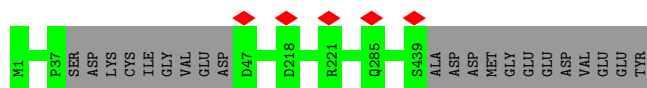
- Molecule 2: Tubulin alpha chain

Chain UC:  95% 5%

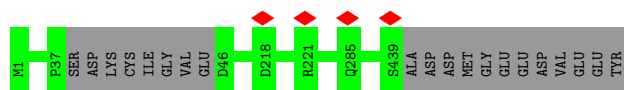


- Molecule 2: Tubulin alpha chain

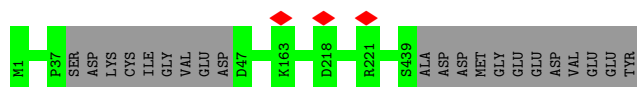
Chain UE:  95% 5%



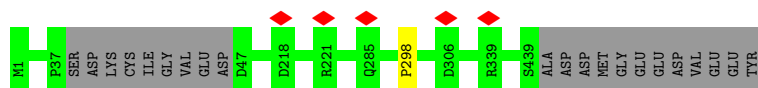
• Molecule 2: Tubulin alpha chain

Chain UG:  96%

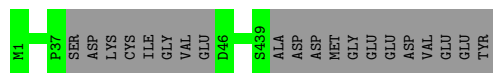
• Molecule 2: Tubulin alpha chain

Chain UI:  95% 5%

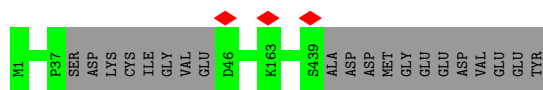
• Molecule 2: Tubulin alpha chain

Chain UK:  95% 5%

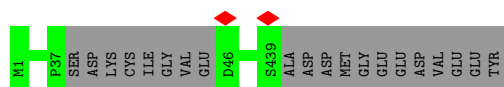
• Molecule 2: Tubulin alpha chain

Chain VA:  96%

• Molecule 2: Tubulin alpha chain

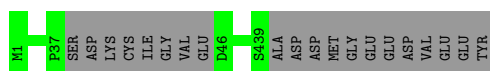
Chain VC:  96%

• Molecule 2: Tubulin alpha chain

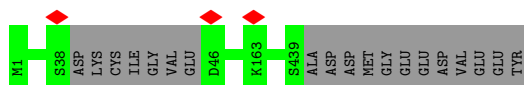
Chain VE:  96%

• Molecule 2: Tubulin alpha chain

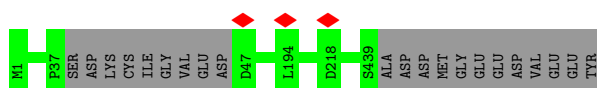
Chain VG:  96%



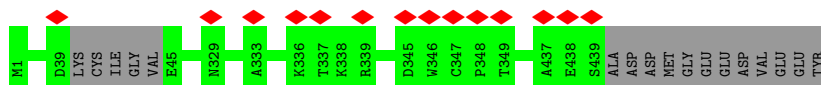
- Molecule 2: Tubulin alpha chain



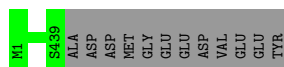
- Molecule 2: Tubulin alpha chain



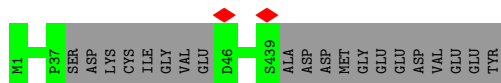
- Molecule 2: Tubulin alpha chain



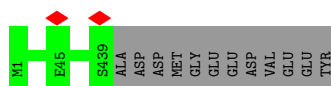
- Molecule 2: Tubulin alpha chain



- Molecule 2: Tubulin alpha chain

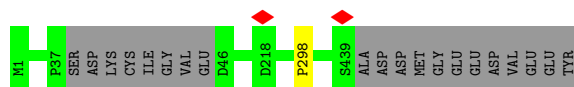


- Molecule 2: Tubulin alpha chain



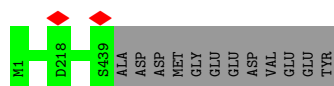
- Molecule 2: Tubulin alpha chain

Chain WG:  95%



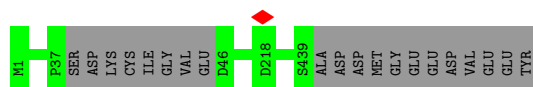
- Molecule 2: Tubulin alpha chain

Chain WI:  97%



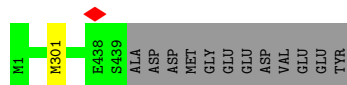
- Molecule 2: Tubulin alpha chain

Chain WK:  96%





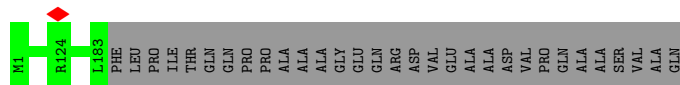
- Molecule 2: Tubulin alpha chain

Chain WM:  97%





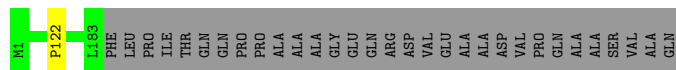
- Molecule 3: CFAP20

Chain X:  86%  14%





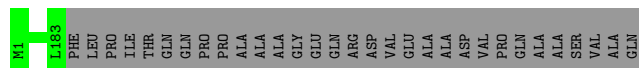
- Molecule 3: CFAP20

Chain XA:  85%  14%




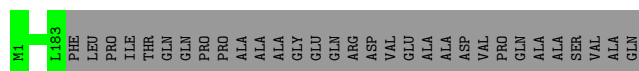
- Molecule 3: CFAP20

Chain XB:  86%  14%




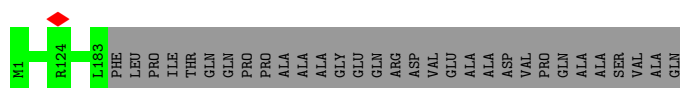
- Molecule 3: CFAP20

Chain XC:  86% 14%




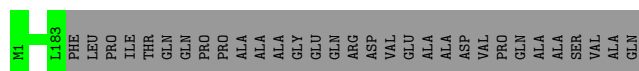
• Molecule 3: CFAP20

Chain XD:  86% 14%




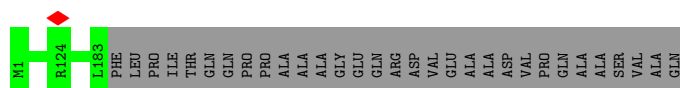
• Molecule 3: CFAP20

Chain XE:  86% 14%




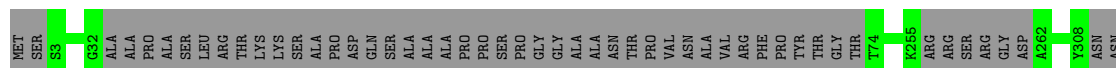
• Molecule 3: CFAP20

Chain XF:  86% 14%




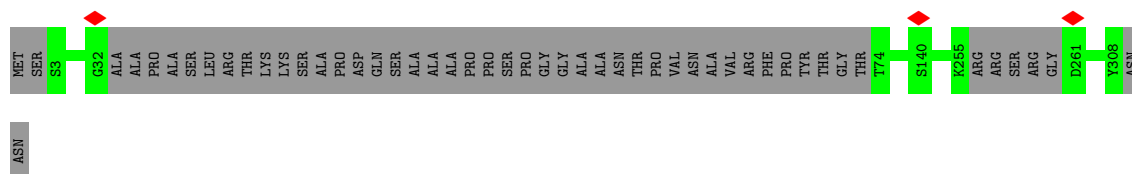
• Molecule 4: PACRGA

Chain XM:  84% 16%




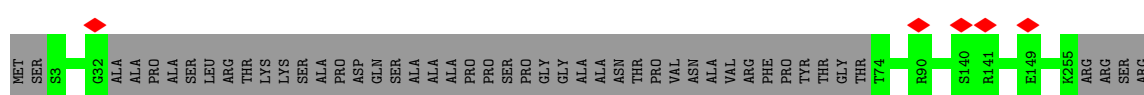
• Molecule 4: PACRGA

Chain XO:  84% 16%

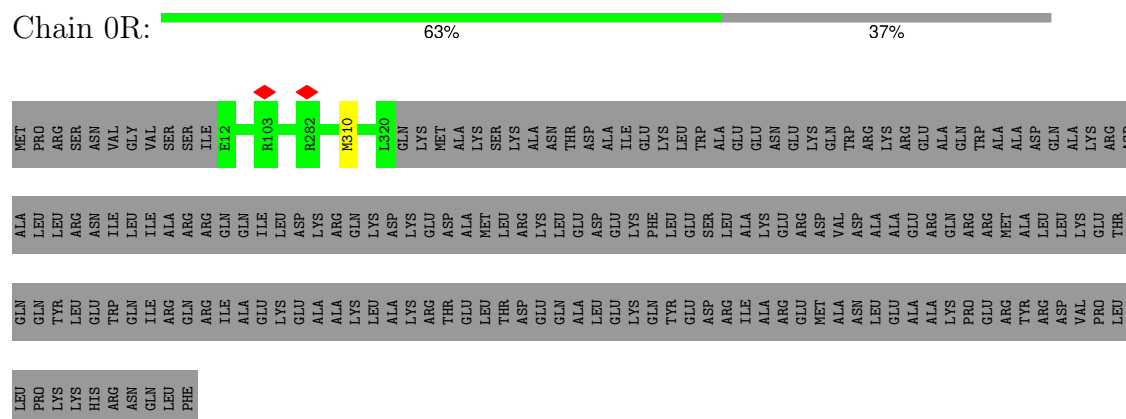


• Molecule 4: PACRGA

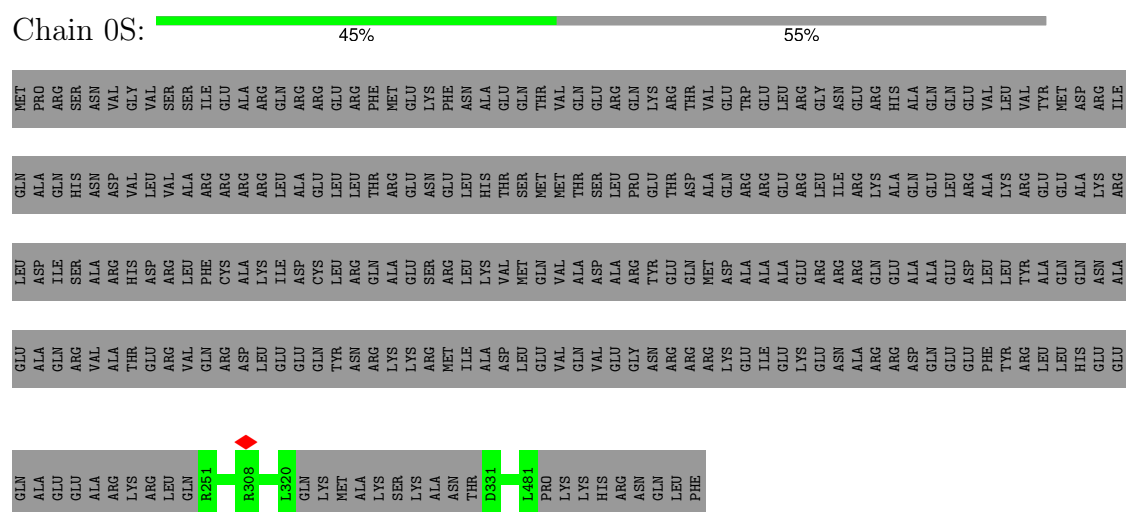
Chain XQ:  84% 16%



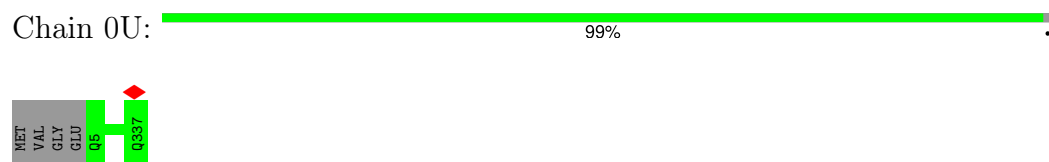
- Molecule 10: CFAP53



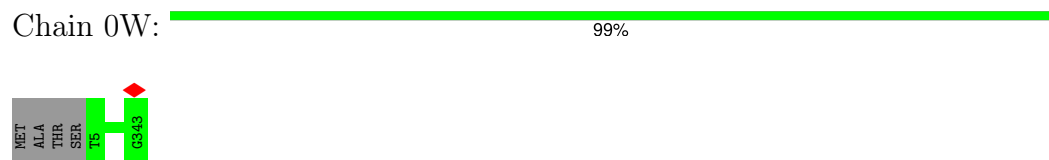
- Molecule 10: CFAP53



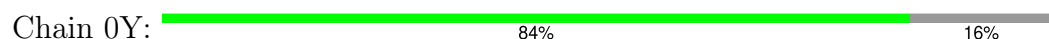
- Molecule 11: CFAP67A

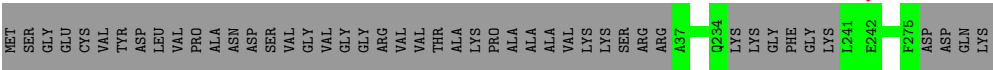


- Molecule 12: CFAP67B

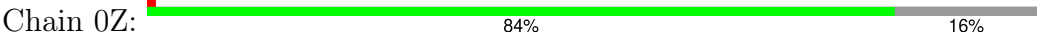


- Molecule 13: CFAP106A





• Molecule 13: CFAP106A



• Molecule 13: CFAP106A



• Molecule 14: CFAP106B



• Molecule 14: CFAP106B



S370

• Molecule 15: CFAP107

Chain 0f: 58% 42%

| | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| MET | ALA | THR | ASN | LEU | ALA | THR | GLY | GLU | GLN | SER | VAL | LYS | SER | ALA | TYR | HIS | CYS | ALA | THR | LEU | LEU | ASP | ASN | TRP | ALA | GLU | ASP | ARG | HIS | GLN | PHE | GLY | GLN | PRO | VAL | THR | ASN | PRO | THR | THR | SER | HIS | ALA | ASP | THR | ARG | GLY | PHE | ASP | P46 | M135 | GLY | PHE | SER | THR | THR | SER | GLY | SER | GLY | SER | HIS | ALA | GLY | THR |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|

| | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|
| SER | THR | GLY | LEU | ALA | ASP | GLN | SER | VAL | ALA | LYS | ALA | VAL | GLN | TYR | HIS | ARG | GLY | ALA | ALA | TYR | LEU | GLN | ASP | ASN | MET | ALA | SER | THR | MET | ARG | SER | THR | GLN | HIS | ALA | VAL | THR | ASN | GLY | THR | GLN | SER | ALA | THR | ASP | THR | ASP | PRO | GLY | SER | GLU | THR | THR | GLU | THR | LYS | THR | THR | GLY | SER | GLY | TYR | ALA | GLY | THR | A206 |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|

D275
ASP
TYR

• Molecule 15: CFAP107

Chain 0g: 11% 89%

| | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| MET | ALA | THR | LEU | ALA | THR | GLY | GLU | GLN | SER | VAL | LYS | SER | ALA | TYR | HIS | CYS | ALA | THR | LEU | LEU | ASP | ASN | TRP | ALA | GLU | ASP | ARG | HIS | GLN | PHE | GLY | GLN | PRO | VAL | THR | ASN | PRO | THR | THR | SER | HIS | ALA | ASP | THR | ARG | GLY | PHE | ASP | P46 | A76 | PRO | ARG | MET | THR | LEU | LEU | PHE | HIS | GLY | ASP | ILE | GLY |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|

| | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| ASN | ILE | GLU | THR | TYR | GLY | TYR | ALA | THR | SER | VAL | LEU | ALA | HIS | THR | ASP | ARG | LYS | LYS | GLN | VAL | TYR | THR | ASN | ASP | GLU | VAL | LEU | ASP | MET | THR | GLY | GLN | HIS | THR | ASN | ARG | THR | GLN | LYS | THR | ALA | THR | ALA | LEU | GLN | ARG | ASP | THR | GLY | THR | GLY | PHE | SER | THR | THR | GLY | GLY | GLY | HIS | ALA | GLY | THR |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|

| | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| SER | THR | ASN | GLY | LEU | PRO | GLY | ARG | ASP | VAL | GLU | SER | ALA | ALA | VAL | GLN | ARG | GLU | ALA | TYR | LEU | GLN | SER | MET | ALA | SER | THR | THR | THR | ARG | THR | GLN | HIS | TRP | ASN | GLY | THR | ASN | GLN | LYS | THR | SER | THR | ALA | THR | ARG | ASP | PRO | GLY | GLY | SER | THR | THR | GLY | THR | LYS | THR | GLY | GLY | GLY | TYR | ALA | PRO |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|

| | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| PRO | ARG | LEU | LEU | PRO | MET | GLY | ARG | VAL | GLU | GLU | ARG | LEU | THR | THR | LYS | ASN | VAL | SER | ILE | THR | ASP | ALA | SER | GLY | THR | TYR | THR | PHE | ASP | ASN | GLU | LEU | ALA | THR | PRO | LEU | THR | SER | THR | GLN | CYS | VAL | GLY | LYS | MET | THR | LYS | THR | TRP | CYS | ASP | ASN | PRO | MET | HIS | LYS | THR | ASN |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|

| | | | | | | | | | |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| LEU | ARG | ILE | HIS | TYR | MET | GLU | ASP | ASP | TYR |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|

• Molecule 16: CFAP115

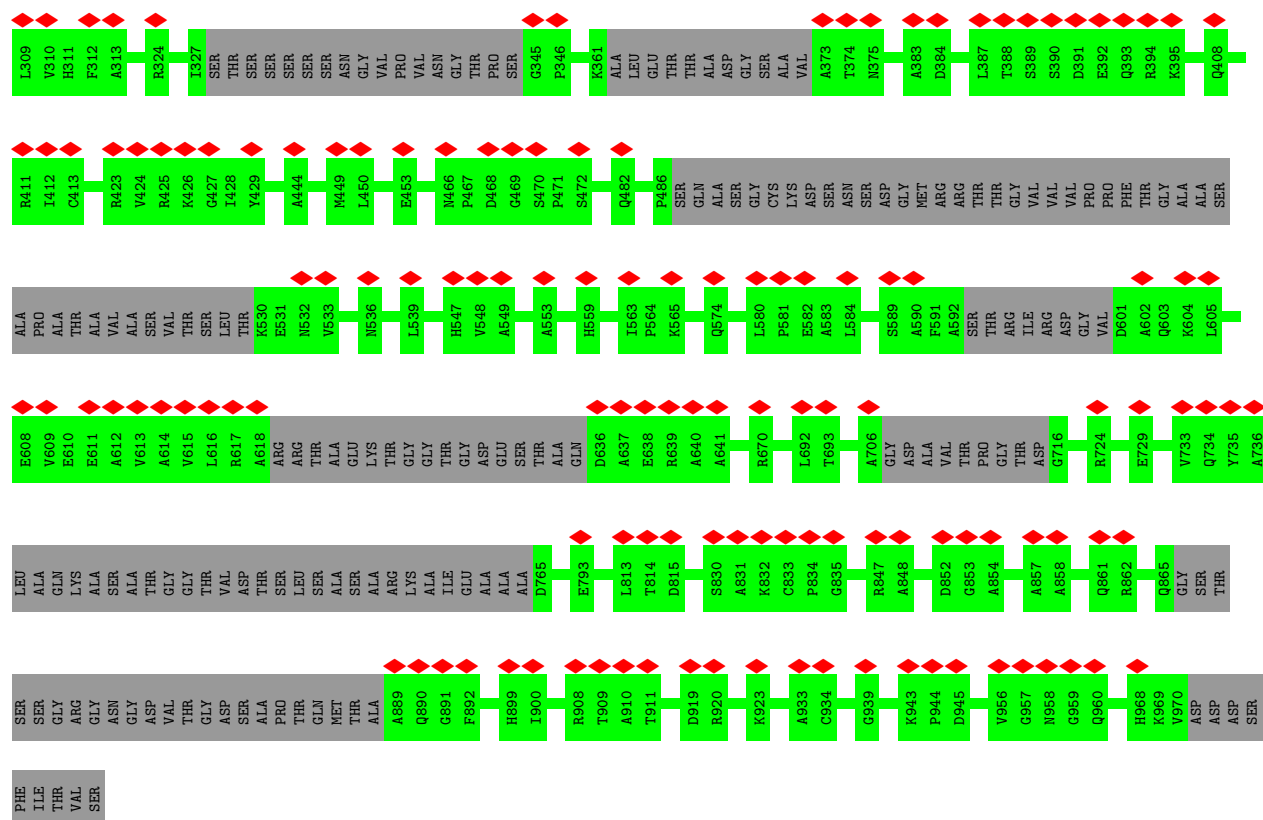
Chain 0l: 19% 65% 35%

| | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
|-----|-----|-----|-----|-----|-----|----|----|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| MET | SER | SER | SER | VAL | PRO | S7 | F8 | D9 | R13 | R16 | A17 | Q18 | V19 | G20 | K21 | R22 | R23 | I24 | F25 | L26 | A31 | D32 | D34 | F33 | R35 | L36 | R37 | C38 | G39 | R40 | T51 | N52 | N53 | D54 | V55 | H56 | M62 | R63 | R67 | R68 | F69 | A70 | F71 | A72 | VAL | ALA | ALA | GLY | THR | SER | ALA | ALA |
|-----|-----|-----|-----|-----|-----|----|----|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|

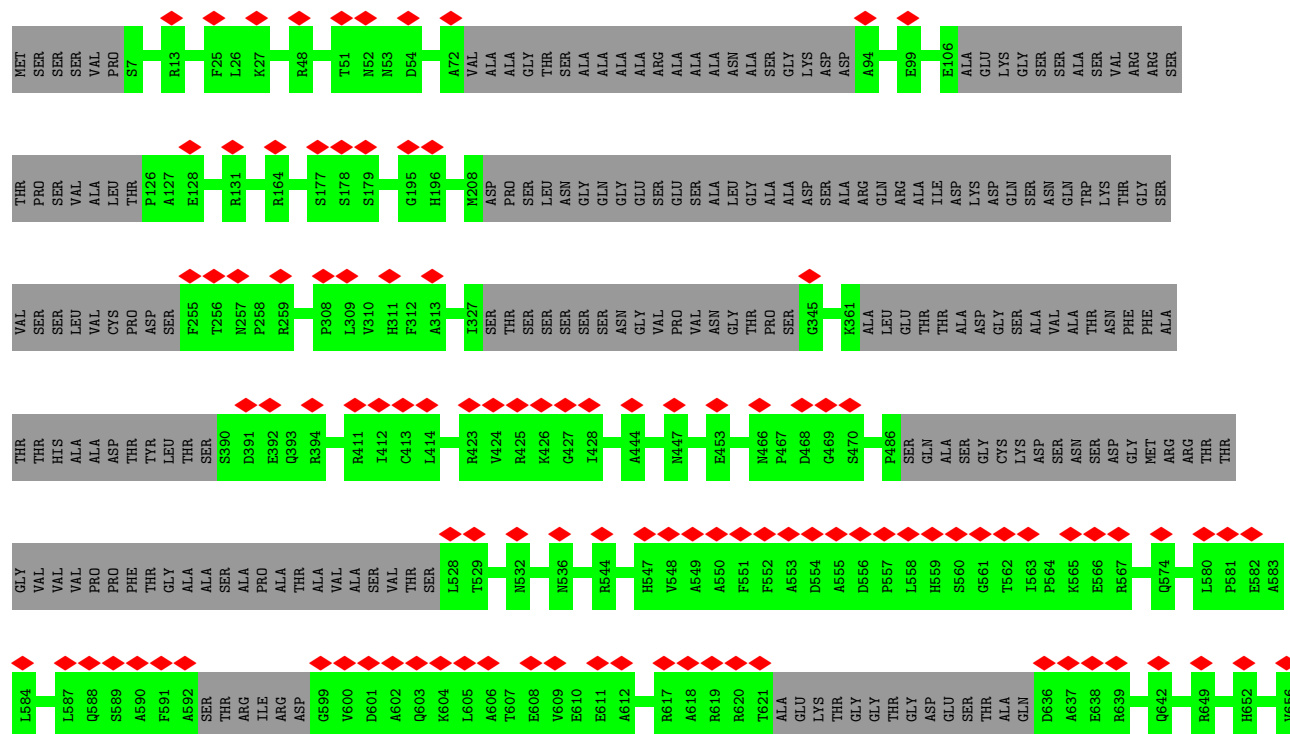
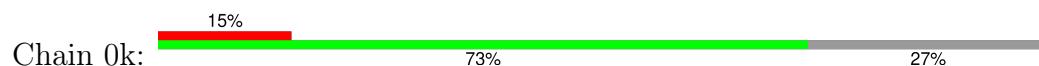
| | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| ALA | ARG | ALA | ALA | ALA | ASN | ALA | SER | GLY | LYS | ASP | A94 | E95 | E99 | D100 | F101 | L102 | A103 | A104 | L105 | E106 | ALA | GLU | LYS | GLY | SER | ALA | ALA | SER | VAL | ARG | THR | SER | PRO | SER | VAL | ALA | LEU | THR | PRO | ALA | GLU | GLY | ALA | ARG | ALA | LEU | LYS | PRO | PHE | GLN | THR | MET | LEU | ARG | GLN | ALA | ILE |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|

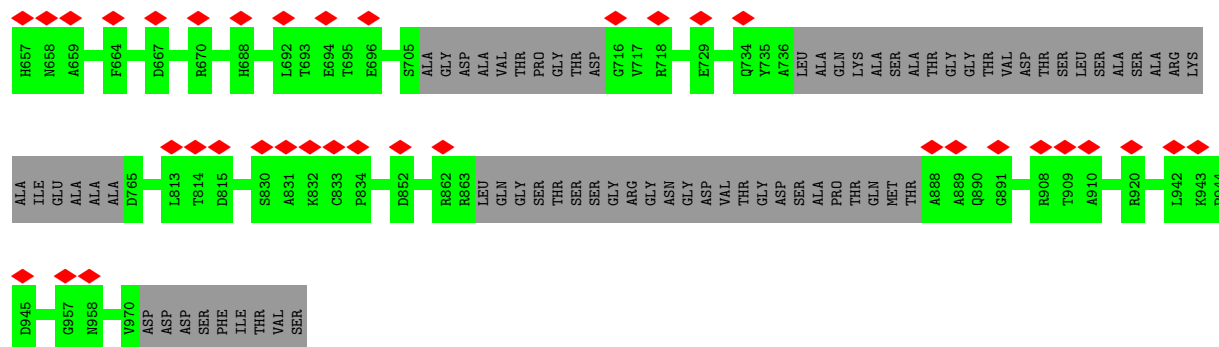
| | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|
| GLN | ALA | HIS | GLY | THR | SER | SER | LEU | THR | ALA | PRO | ASN | GLY | ARG | ASP | LEU | ASP | PRO | LEU | ARG | THR | GLY | VAL | THR | ASP | ALA | ALA | VAL | ALA | GLN | PHE | ARG | GLY | ILE | CYS | ARG | LEU | PRO | PHE | ASP | GLN | SER | THR | ASN | GLN | TRP | LYS | THR | GLY | VAL | SER | LEU | LEU | ALA | VAL | CYS | PRO | ASP | S254 | F255 | T256 | R259 | R279 | F287 |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|

| | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|
| TRP | CYS | ARG | ALA | MET | ASP | PRO | SER | LEU | ASN | GLY | GLY | GLU | SER | GLU | ALA | ALA | ASP | SER | ALA | ARG | GLN | PHE | ARG | ALA | ILE | LYS | ASP | GLN | ASN | GLN | TRP | LYS | THR | GLY | VAL | SER | SER | LEU | VAL | CYS | PRO | ASP | S254 | F255 | T256 | R259 | R279 | F287 |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|

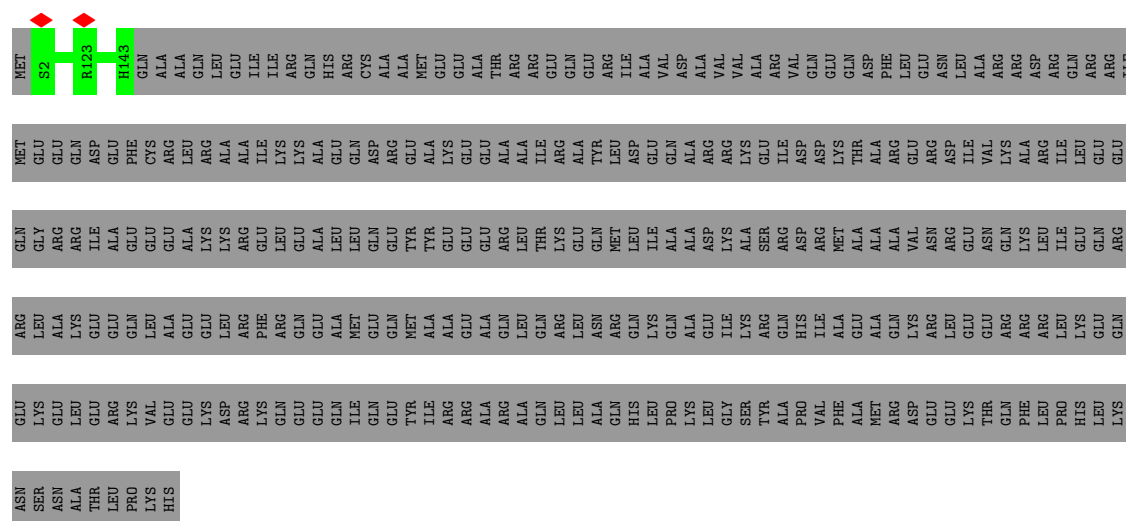


• Molecule 16: CFAP115

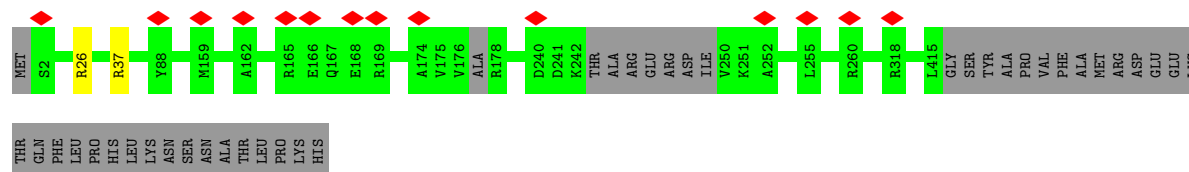
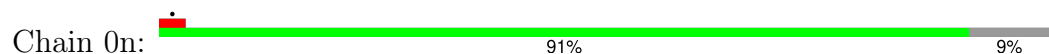




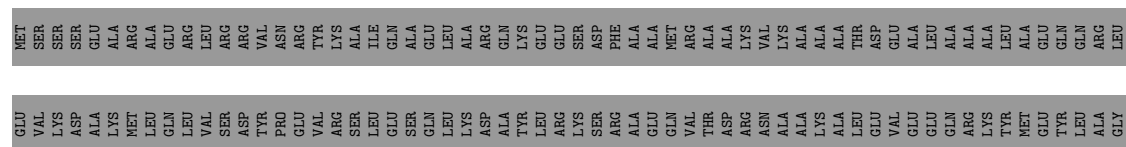
- Molecule 17: CFAP127



- Molecule 17: CFAP127



- Molecule 17: CFAP127



[illegible]

- Molecule 22: DMIP5

[illegible]

- Molecule 22: DMIP5

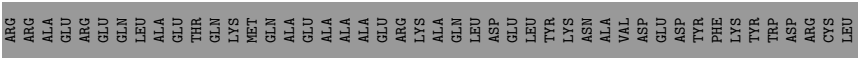
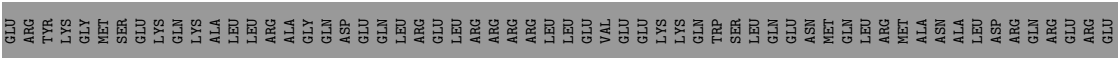
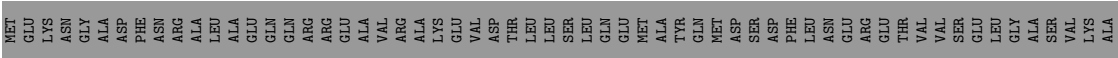
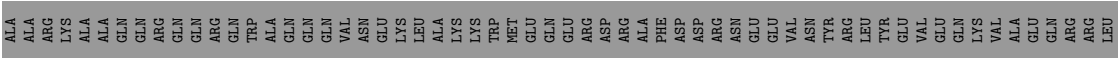
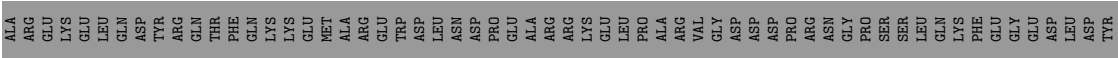


| Amino Acid | Information Content (bits) |
|------------|----------------------------|
| MET | 0.38 |
| SER | 0.35 |
| THR | 0.05 |
| LEU | 0.05 |
| ALA | 0.05 |
| SER | 0.05 |
| THR | 0.05 |
| LEU | 0.05 |
| PRO | 0.05 |
| PRO | 0.05 |
| VAL | 0.05 |
| LYS | 0.05 |
| GLY | 0.05 |
| THR | 0.05 |
| SER | 0.05 |
| SER | 0.05 |
| LYS | 0.05 |
| LYS | 0.05 |
| SER | 0.05 |
| GLN | 0.05 |
| LYS | 0.05 |
| LYS | 0.05 |
| GLY | 0.05 |
| ARG | 0.05 |
| ARG | 0.05 |
| PRO | 0.05 |
| ALA | 0.05 |
| ASP | 0.05 |
| SER | 0.05 |
| LYS | 0.05 |
| GLY | 0.05 |
| ASN | 0.05 |
| GLY | 0.05 |
| THR | 0.05 |
| ALA | 0.05 |
| PRO | 0.05 |
| ALA | 0.05 |
| ALA | 0.05 |
| ASN | 0.05 |
| PRO | 0.05 |
| HIS | 0.05 |
| CYS | 0.05 |
| Y42 | 0.05 |
| R46 | 0.05 |
| R50 | 0.05 |
| VAL | 0.05 |
| ALA | 0.05 |
| ALA | 0.05 |
| HIS | 0.05 |
| PRO | 0.05 |
| GLY | 0.05 |
| SER | 0.05 |
| TRP | 0.05 |
| ARG | 0.05 |
| LEU | 0.05 |
| LYS | 0.05 |
| GLU | 0.05 |
| GLY | 0.05 |
| GLN | 0.05 |

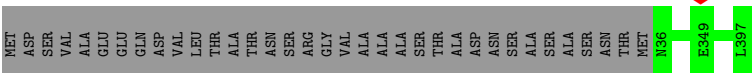
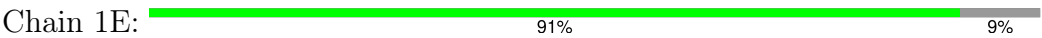
| | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| ARG | GLN | THR | PHE | GLY | LYS | GLU | MET | ALA | ARG | GLU | TRP | ASP | LEU | ASN | ASP | PRO | GLU | ALA | ARG | ARG | LYS | GLU | LEU | PRO | ALA | ARG | VAL | GLY | ASP | ASP | ASP | PRO | PRO | ARG | GLY | GLY | PRO | SER | SER | LEU | GLN | LYS | PHE | GLU | GLY | GLU | GLU | ASP | LEU | ASP | TYR | ALA | ALA | ALA | ARG | LYS | ALA | ALA | GLN | GLN | ARG |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|



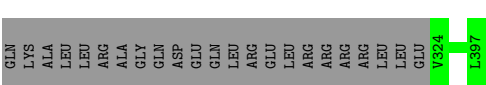
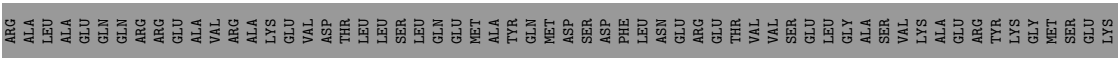
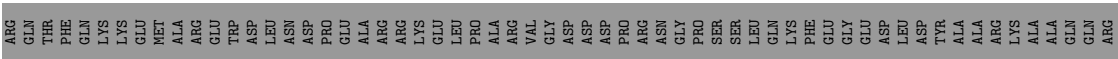
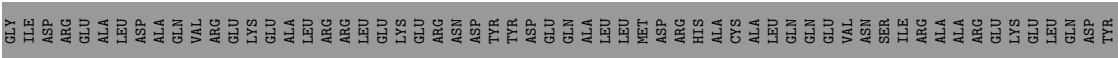
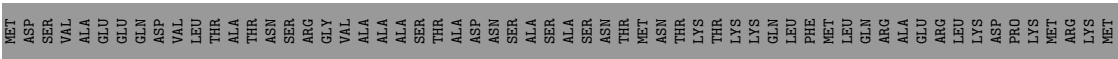
● Molecule 23: RIB43



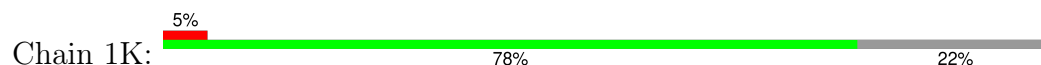
● Molecule 23: RIB43



● Molecule 23: RIB43



● Molecule 24: RIB72A



74%

- Molecule 28: DMIP1

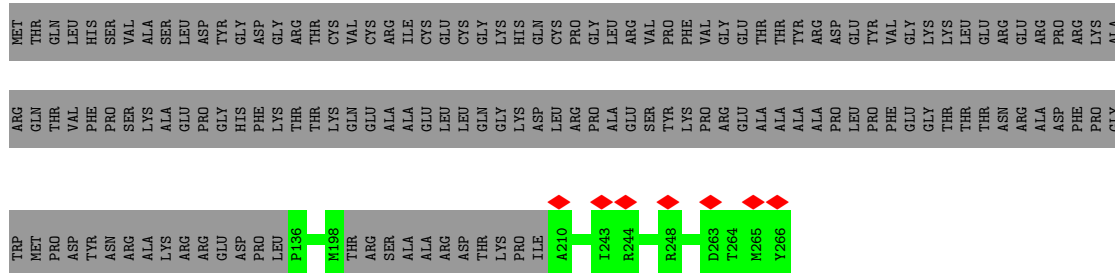
55%

- Molecule 28: DMIP1

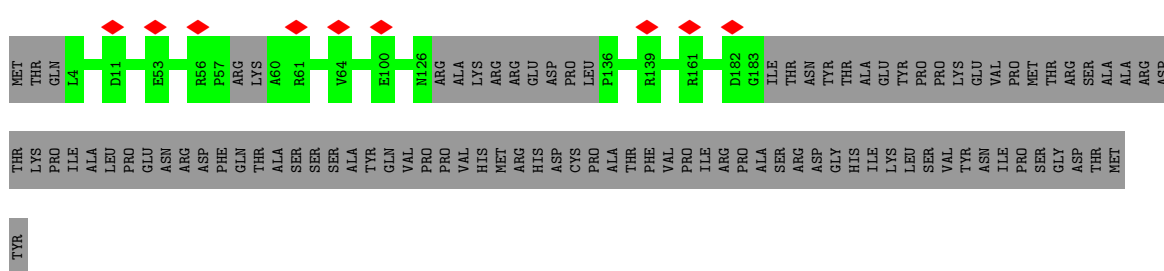
82%

MET
 THR
 GLN
 L4
 L4
 G13
 K51
 LEU
 GLU
 ARG
 GLU
 ARG
 ARG
 PRO
 ARG
 ARG
 LYS
 ALA
 ARG
 GLN
 THR
 VAL
 PHE
 PRO
 SER
 LYS
 ALA
 ALA
 GLU
 GLU
 PRO
 GLY
 HIS
 PHE
 LYS
 THR
 THR
 LYS
 GLN
 GLU
 ALA
 ALA
 ALA
 GLU
 LEU
 LEU
 GLN
 GLY
 LYS
 ASP
 LEU
 ARG
 ARG
 PRO
 PRO
 GLU
 GLU
 SER
 THR
 LYS
 PRO
 ARG
 ARG
 GLU
 ALA
 ALA

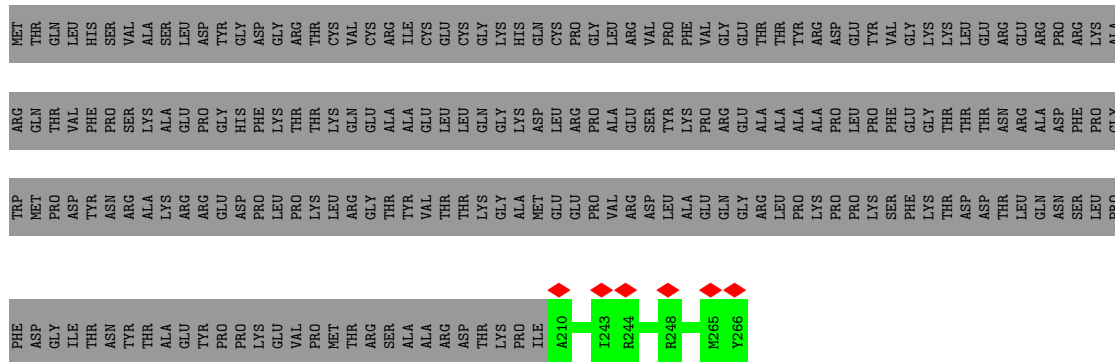
- Molecule 28: DMIP1



- Molecule 28: DMIP1

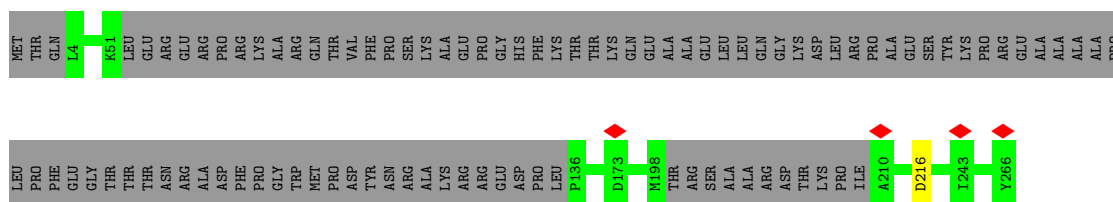


- Molecule 28: DMIP1



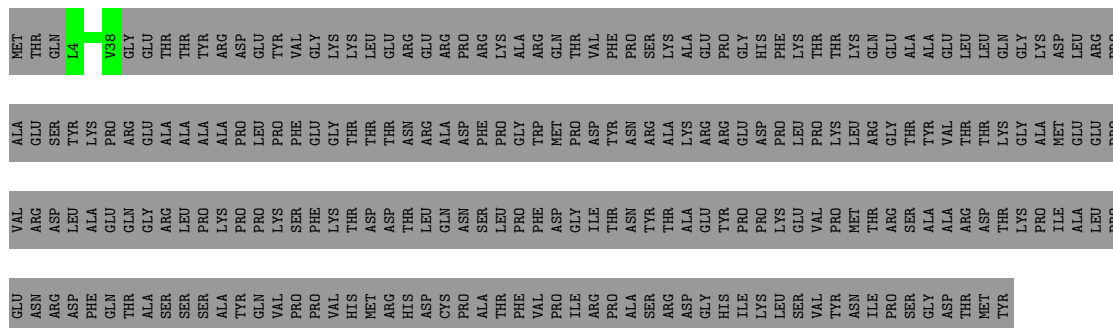
- Molecule 28: DMIP1





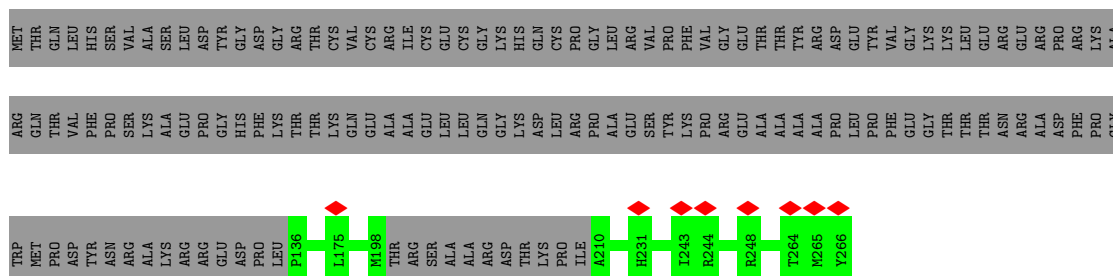
- Molecule 28: DMIP1

Chain 1c: 13% 87%



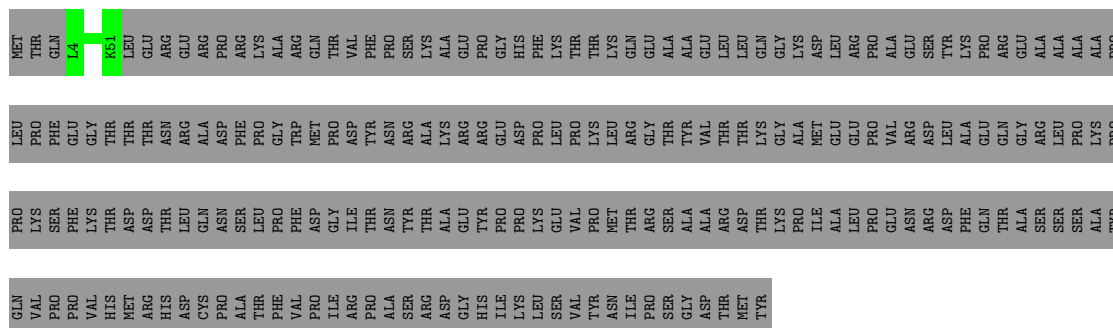
- Molecule 28: DMIP1

Chain 1d: 45% 55%



- Molecule 28: DMIP1

Chain 1e: 18% 82%



- Molecule 28: DMIP1

Chain 1g: 6% 45% 55%

- Molecule 28: DMIP1



- Molecule 28: DMIP1



- Molecule 28: DMIP1




- Molecule 29: DMIP2



Chain 1t: 

Chain 2B: 87% 13%

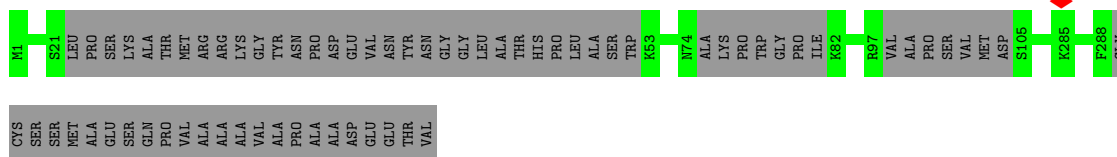
Chain 2C: 

Chain 2F:  91% 9%

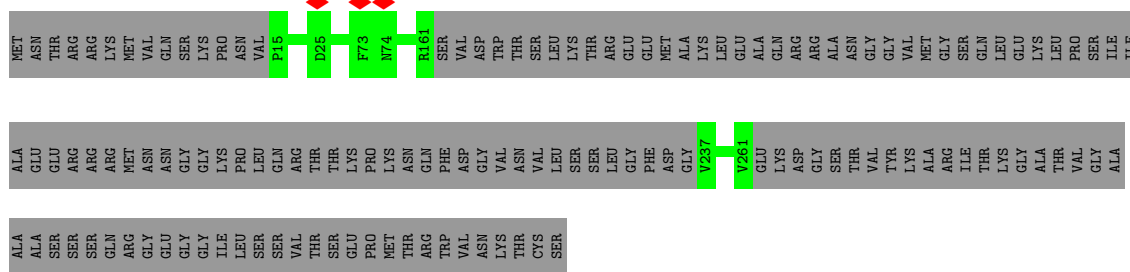
Chain 2G:  91% 9%

Chain 2H:  92% 8%

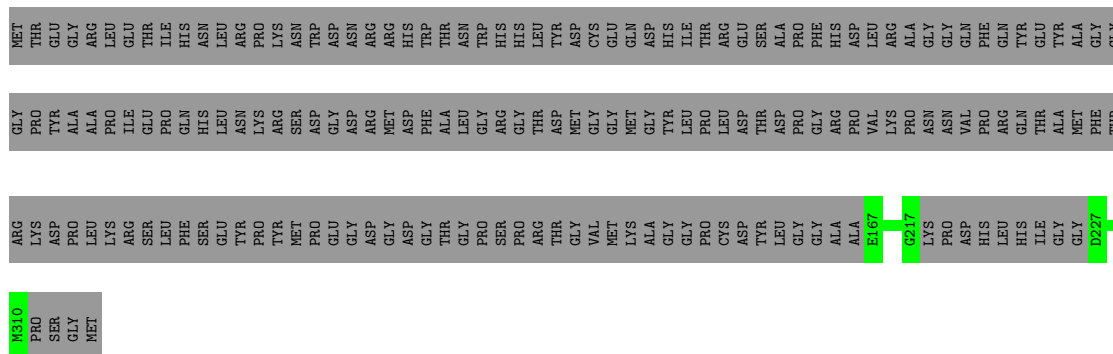
- Molecule 33: DMIP7



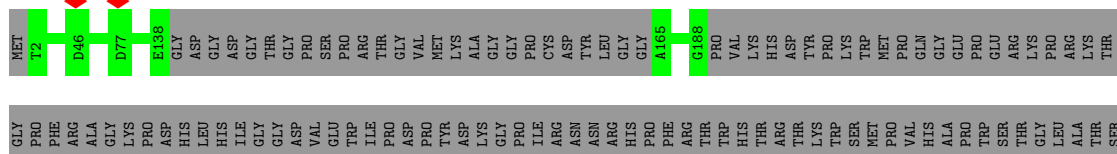
- Molecule 34: DMIP8



- Molecule 35: DMIP9

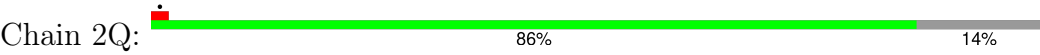


- Molecule 35: DMIP9



GLU
ALA
ARG
LYS
GLY
ALA
GLY
LEU
ASP
LEU
THR
THR
GLU
ASN
ASN
LEU
PRO
SER
SER
LEU
LYS
THR
TYR
TYR
LYS
LYS
ALA
ASN
LEU
THR
GLN
THR
ILE
ILE
GLY
ALA
GLU
ALA
ALA
LEU
SER
SER
SER
MET
PRO
SER
GLY
MET

● Molecule 36: DMIP10



MI
DE4
RI44
ARG
GLN
VAL
ALA
GLY
ALA
SER
PRO
ASP
ASP
SER
GLY
HIS
GLN
SER
PHE
GLY
SER
SER
GLY
GLY
ALA
ALA
HIS
ASN
ASP
LEU
F169
E227
G228
D242
P269
L272
G315
LEU
CYS
GLY
LYS
TYR
PHE
SER
LYS
LEU
VAL
ALA
PRO
LYS
LEU
SER
SER
ALA
THR

GLY
ILE
ASN
MET

● Molecule 37: DMIP11



MET
ASN
HIS
LEU
SER
THR
ARG
ARG
PRO
ALA
GLY
ALA
T112
T248
MET
ARG
LEU
ALA
SER
PRO
SER
SER
SER
ALA
ALA
VAL
PRO
GLN
ALA
TRP
MET
ILE
ILE
GLU
THR
ALA
THR
PRO
SER
SER
SER
ALA
PHE
GLU
GLY
LYS
LYS
THR
THR
ALA
THR
TPP
GLU
VAL
ALA
PRO
CYS
GLU
PRO
GLU
ILE

LEU
GLN
LEU
GLN
HIS
HIS
ALA
ASP
ASP
GLY
SER
VAL
MET
ALA
VAL
SER
PRO
ARG
VAL
ALA
ASP
MET
THR
THR
SER
THR
SER
PHE
GLY
GLN
PRO
LEU
LYS
SER
SER
LEU
ALA
PHE
LYS
LYS
THR
THR
ALA
ALA
TPP
GLU
LYS
ALA
ARG
HIS
ASP
LYS
HIS
ILE

SER
TYR
GLN
LEU

● Molecule 38: DMIP12



MET
SER
ASP
VAL
LEU
CYS
LYS
THR
VAL
ALA
ASN
THR
ARG
ALA
SER
LEU
ALA
SER
GLY
GLY
ALA
ALA
T783
Y190
R162
E279
HIS
GLY
GLY
GLY
VAL
HIS
ARG
LYS
ILE
ALA
ILE
GLU
THR
THR
ASP
THR
THR
ALA
VAL
THR
VAL
ARG
HIS
SER
HIS
PRO
ALA
ARG
CYS
PHE
LYS
THR
VAL
GLY
ALA

ASP
GLY
ALA
THR
GLU
CYS
HIS
LEU
ALA
ALA
ASP
ASP
GLY
THR
ALA
LEU
SER
SER
GLY
GLY
GLN
THR
T783
Y190
R162
E279
HIS
GLY
GLY
GLY
VAL
HIS
ARG
LYS
ILE
ALA
ILE
GLU
THR
THR
ASP
THR
THR
ALA
VAL
THR
VAL
ARG
HIS
SER
HIS
PRO
ALA
ARG
CYS
PHE
LYS
THR
VAL
GLY
ALA

H341
ILE
ARG
GLU
ASP
ALA
GLN
HIS
ARG
TYR
PHE

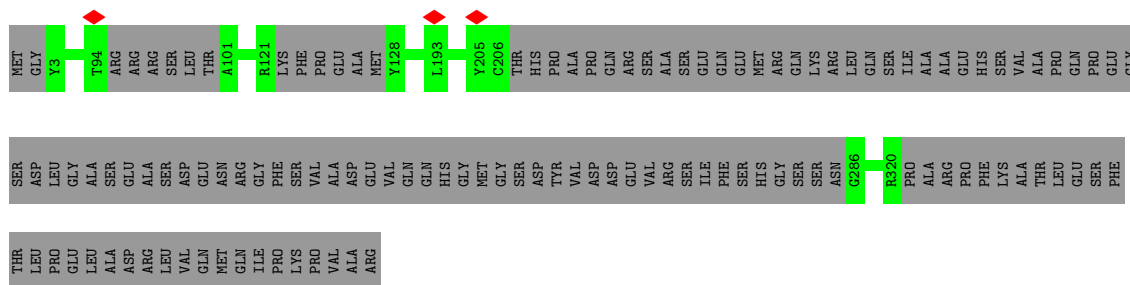
● Molecule 38: DMIP12



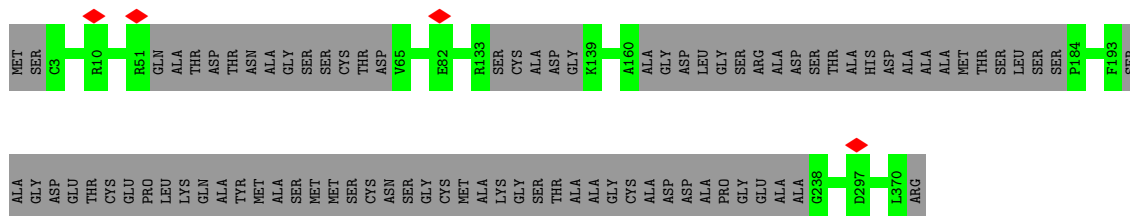
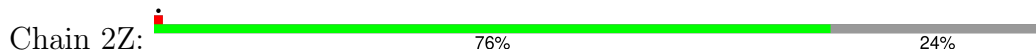
MET
SER
ASN
VAL
THR
CYS
LYS
THR
ALA
ALA
ASN
THR
ARG
ALA
SER
LEU
ALA
SER
SER
GLY
GLY
GLN
LEU
PRO
THR
TYR
LYS
LYS
ARG
GLU
GLU
VAL
PRO
THR
THR
ALA
SER
SER
TYR
ASP
ILE
SER
CYS
PRO
HIS
GLY
LEU
SER
ASN
ASP
ILE
ARG
CYS
GLY
THR
PHE
ALA
LYS
SER
THR
MET
THR
MET
SER
GLU
HIS
LYS
VAL
THR
ILE
GLY
VAL
GLY
ASP
MET
ILE

ASP
GLY
ALA
THR
GLU
CYS
HIS
LEU
ALA
ALA
ASP
ASP
GLY
THR
ALA
LEU
SER
SER
GLY
GLY
GLN
LEU
PRO
THR
TYR
LYS
TYR
VAL
PRO
ILE
ALA
LYS
HIS
ASN
VAL
PRO
CYS
ILE
SER
ASN
ASP
ILE
ARG
CYS
GLY
THR
PHE
ALA
LYS
SER
THR
MET
THR
MET
SER
GLU
HIS
LYS
VAL
THR
ILE
GLY
VAL
GLY
ASP
MET
ILE

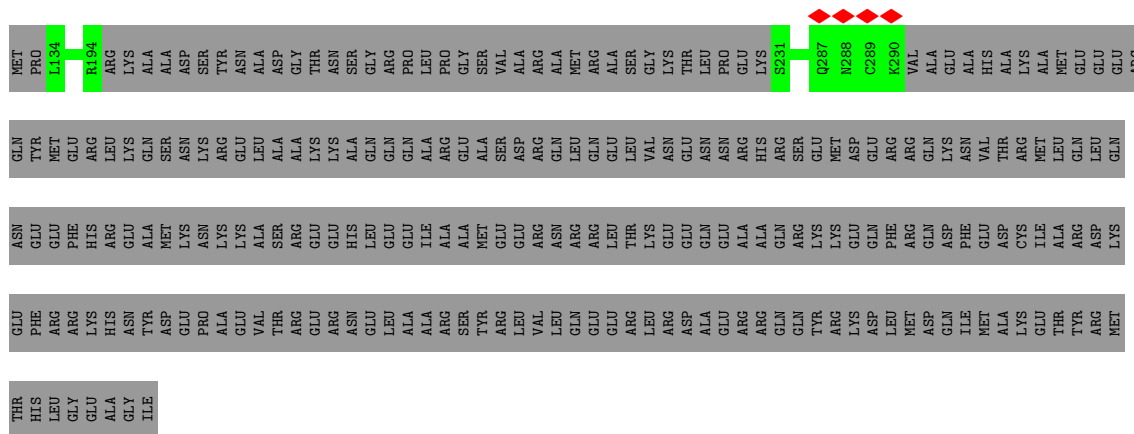
- Molecule 39: DMIP13



- Molecule 40: DMIP14

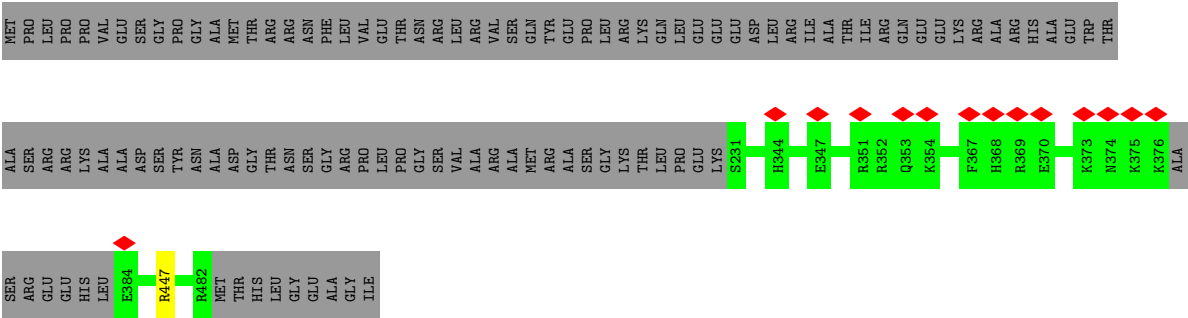


- Molecule 41: DMIP15

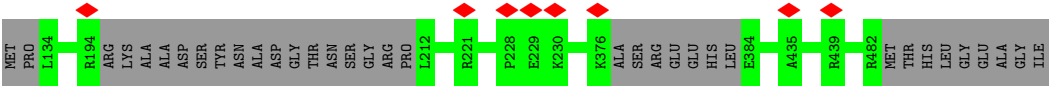
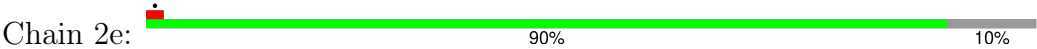


- Molecule 41: DMIP15

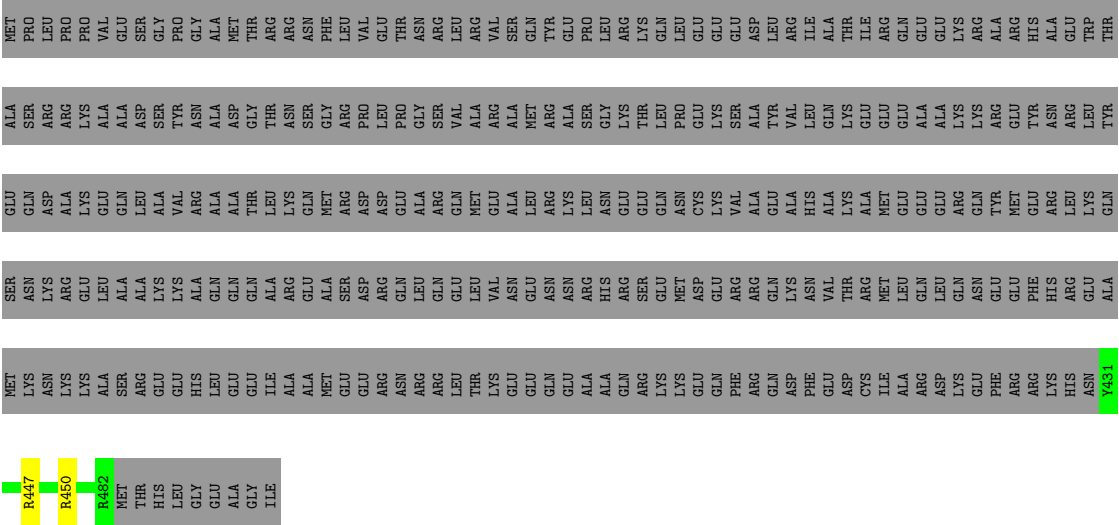




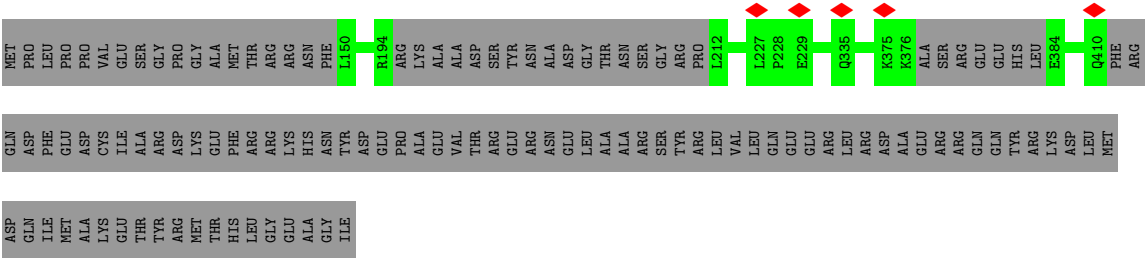
• Molecule 41: DMIP15



• Molecule 41: DMIP15



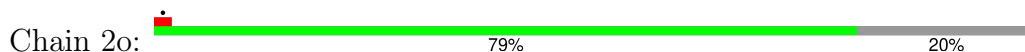
• Molecule 41: DMIP15



• Molecule 41: DMIP15

[illegible]

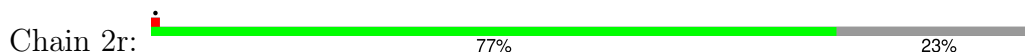
- Molecule 41: DMIP15

[illegible]

- Molecule 41: DMIP15

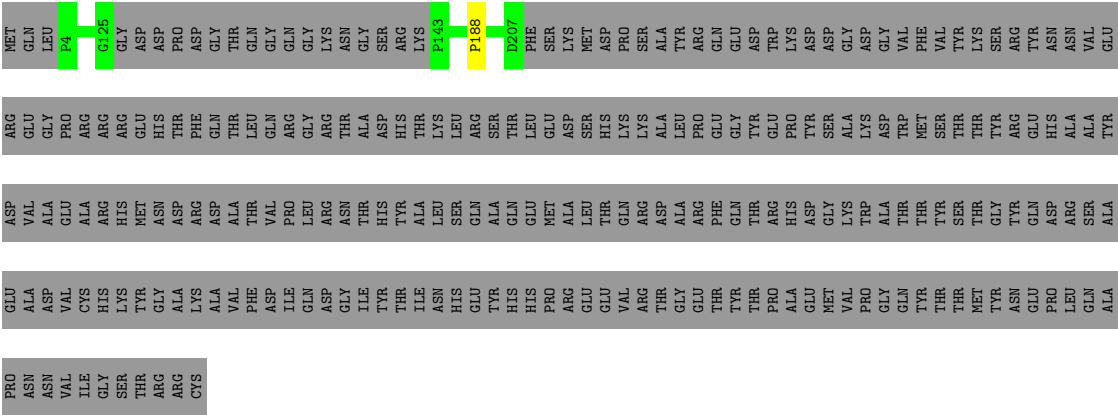
[illegible]

- Molecule 42: DMIP16

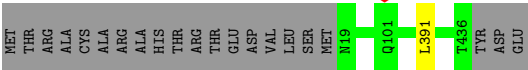


MET PRO ILE ARG ARG
 A6 L7
 R52 ALA VAL ALA ALA SER ASP LYS SER THR
 SER SER ALA ALA LEU PRO SER SER LEU LEU PRO GLY PHE
 PRO PRO PRO PRO GLN THR ARG ARG VAL ALA ALA VAL GLY HIS
 ARG ALA ASP PHE SER ASN SER SER PHE VAL VAL VAL PRO GLN ILE
 S100 R403
 F171 SER THR LEU PRO LEU SER SER CYS VAL A180
 R204 ALA VAL D207 G237 P272 S272
 GLN LEU LEU PRO PRO ALA LEU LEU ALA SER PRO PRO SER
 GLN GLY GLY ALA SER PRO LEU LEU ALA ALA ALA MET ALA THR
 SER SER THR ASN SER SER A303 Y407 R403
 LEU LEU ALA

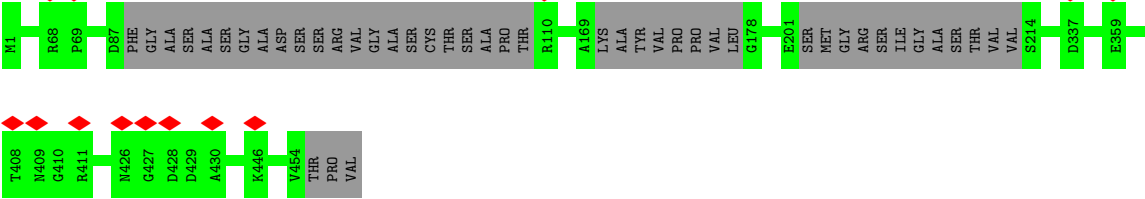
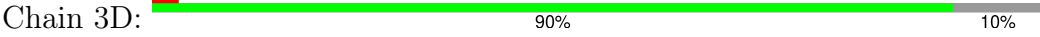




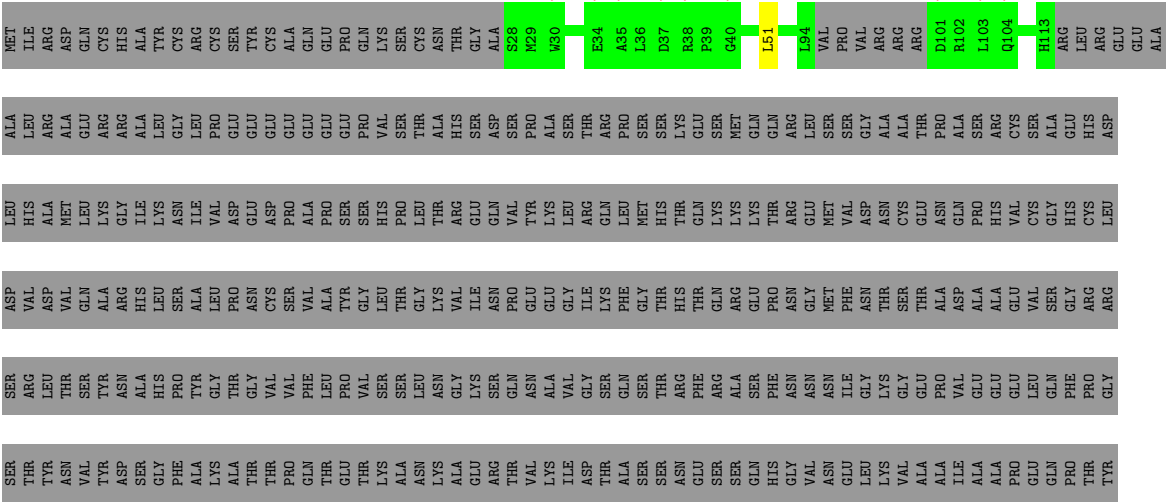
• Molecule 46: DMIP20



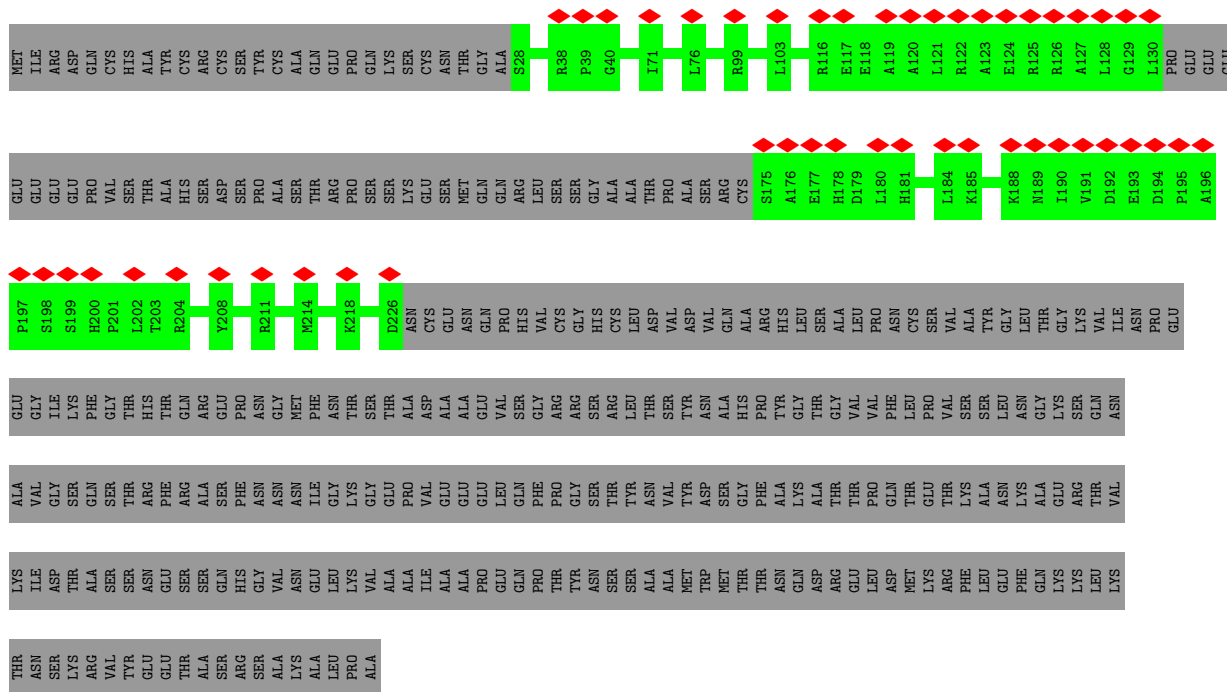
• Molecule 47: DMIP21



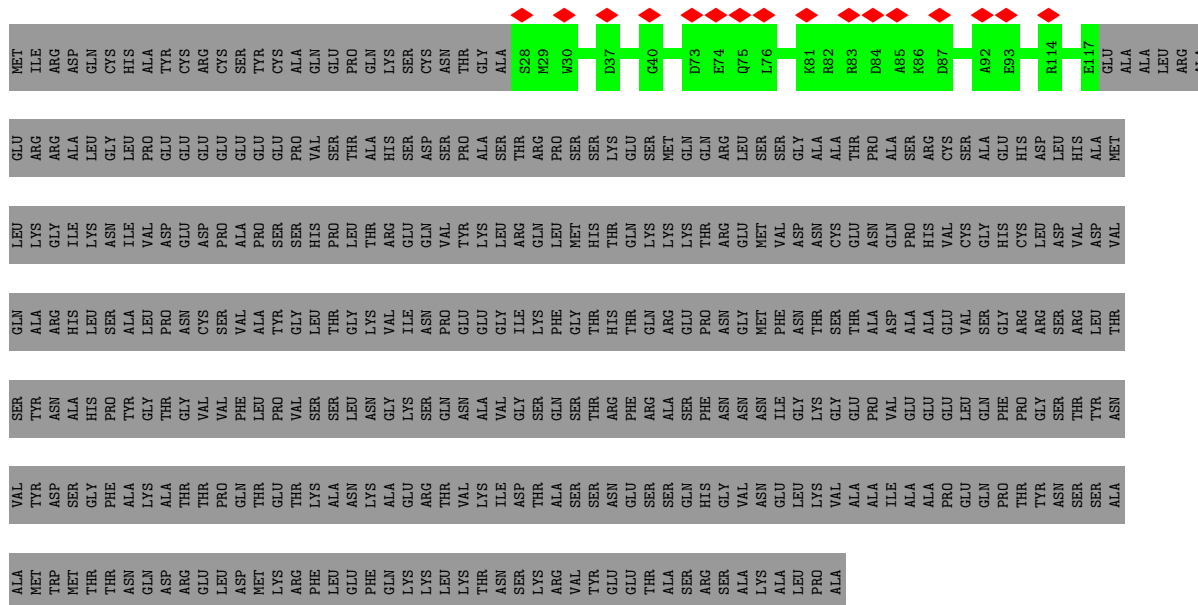
• Molecule 48: DMIP22



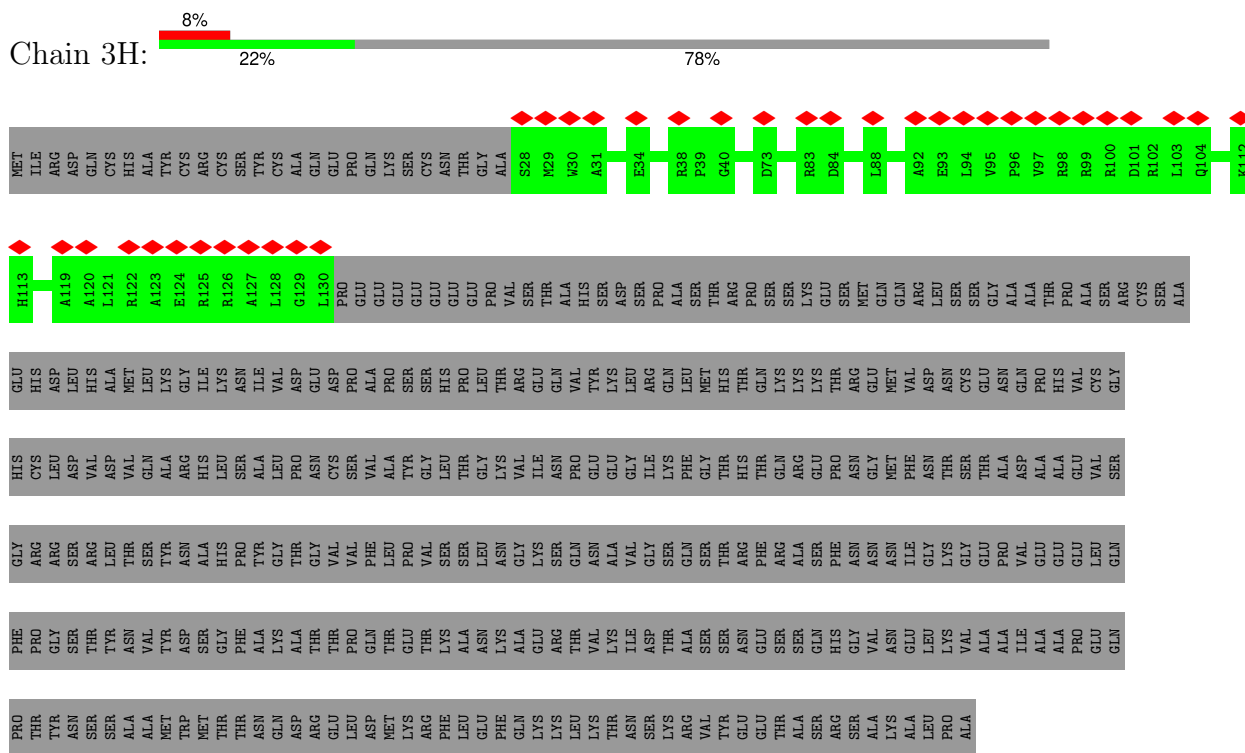
- Molecule 48: DMIP22



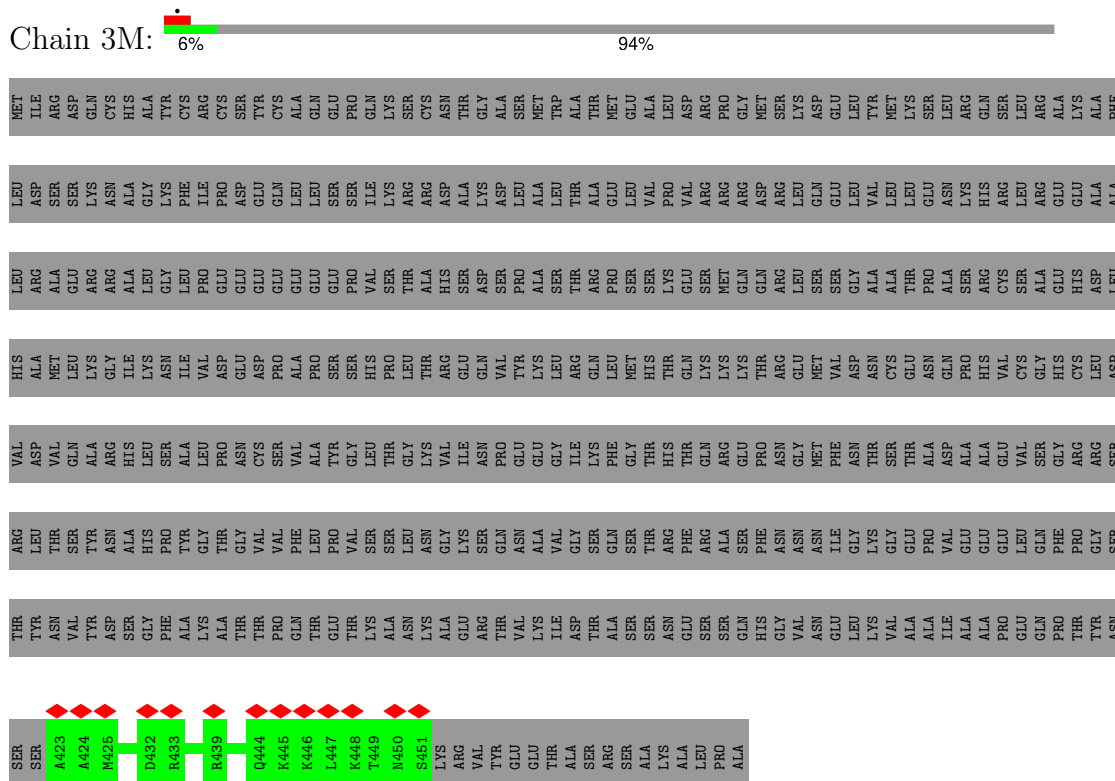
- Molecule 48: DMIP22



- Molecule 48: DMIP22



- Molecule 48: DMIP22



- Molecule 48: DMIP22

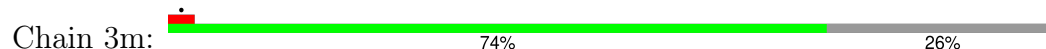


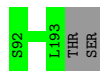


| Satisfaction Level | Percentage |
|--------------------|------------|
| Very satisfied | 20% |
| Satisfied | 80% |

• 96%

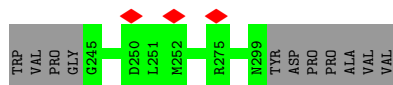
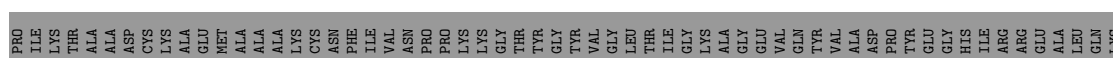
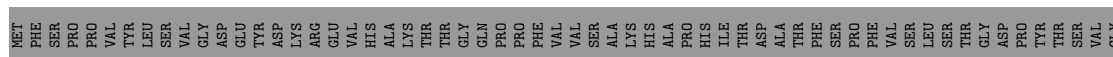
| Response | Percentage |
|--------------|------------|
| Democracy | 74% |
| Dictatorship | 26% |





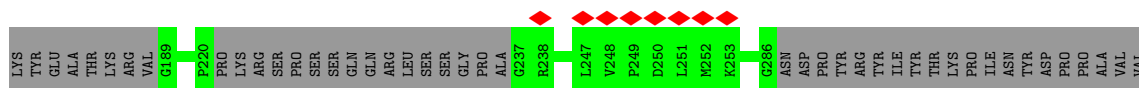
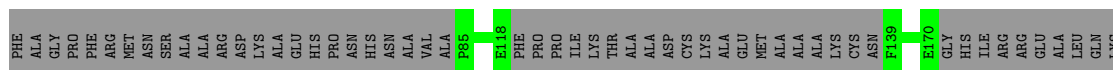
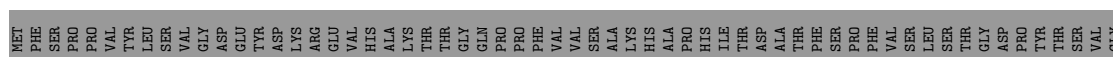
- Molecule 59: CFAP96

Chain 3o:



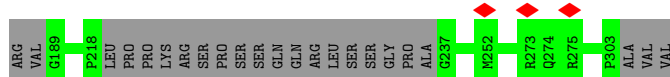
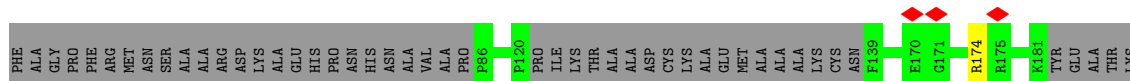
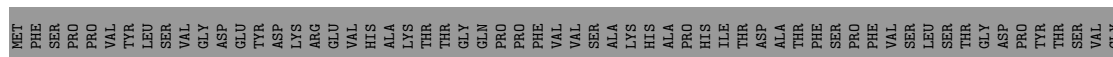
- Molecule 59: CFAP96

Chain 3p:

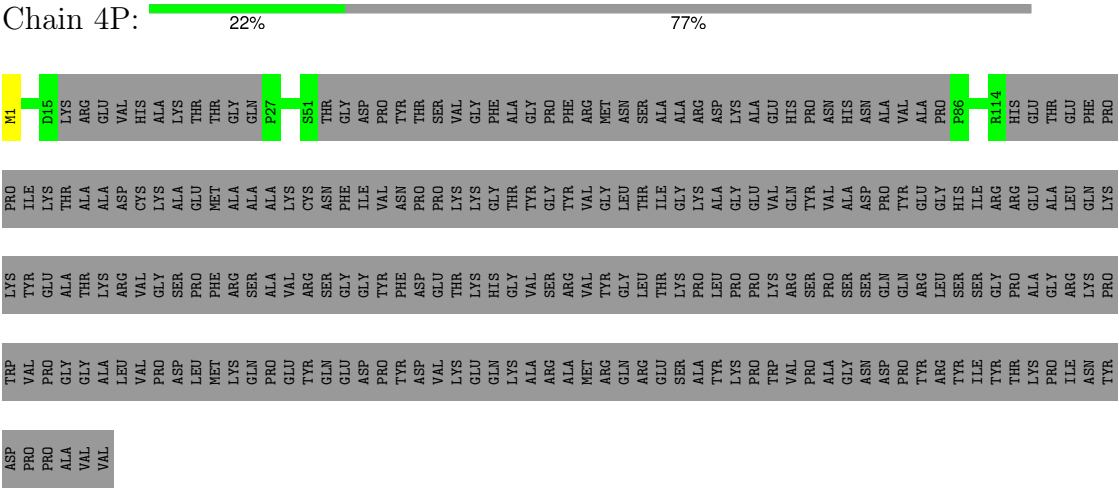


- Molecule 59: CFAP96

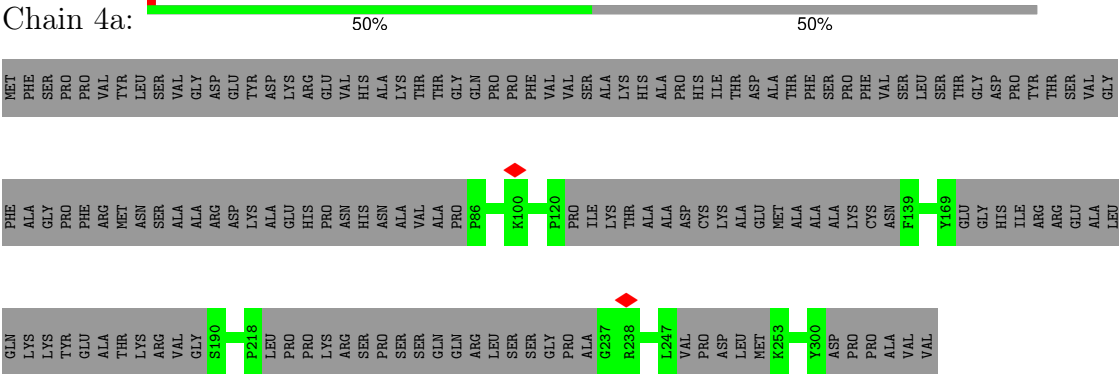
Chain 40:



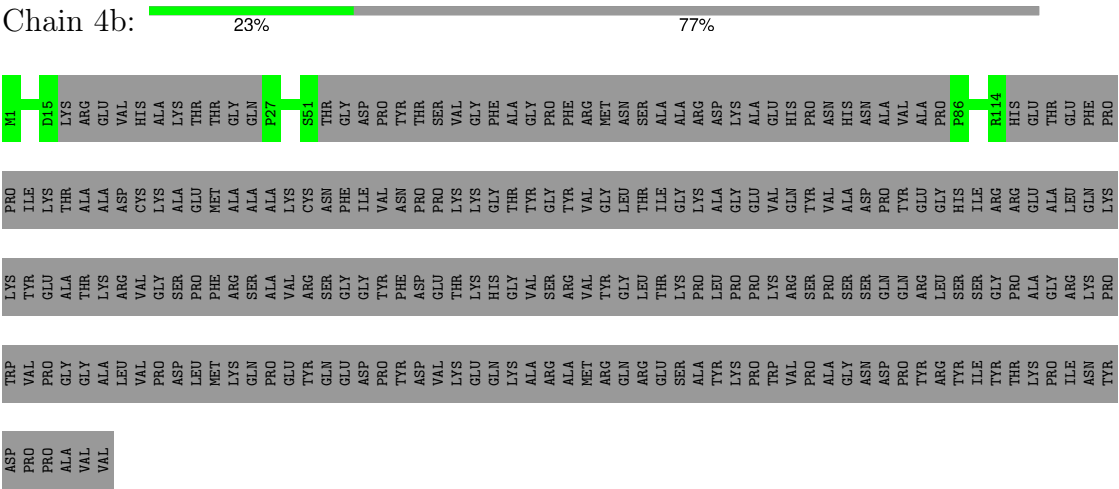
● Molecule 59: CFAP96



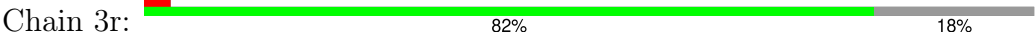
● Molecule 59: CFAP96

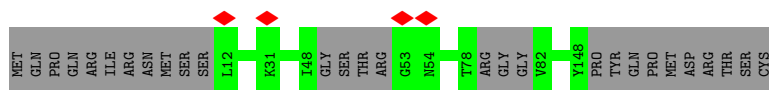


● Molecule 59: CFAP96

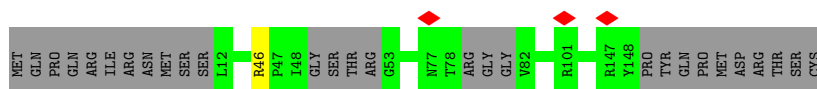
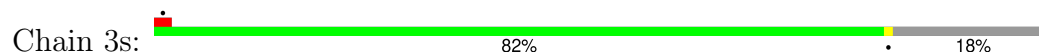


● Molecule 60: CFAP97

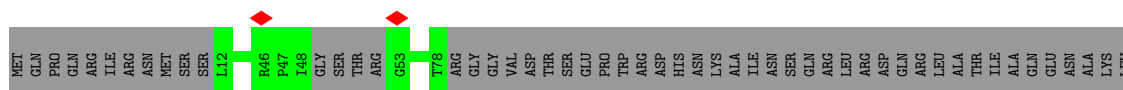




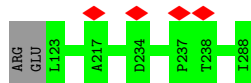
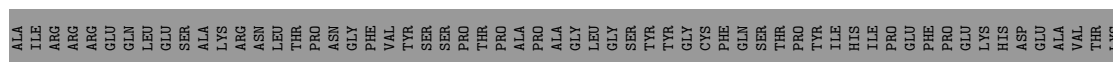
● Molecule 60: CFAP97



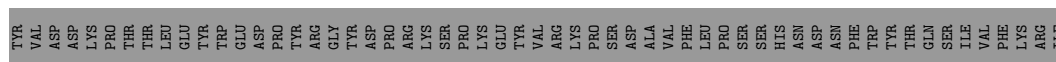
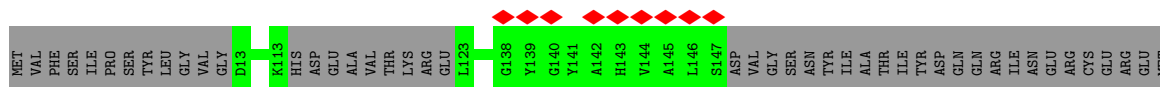
● Molecule 60: CFAP97



● Molecule 61: DMAP1

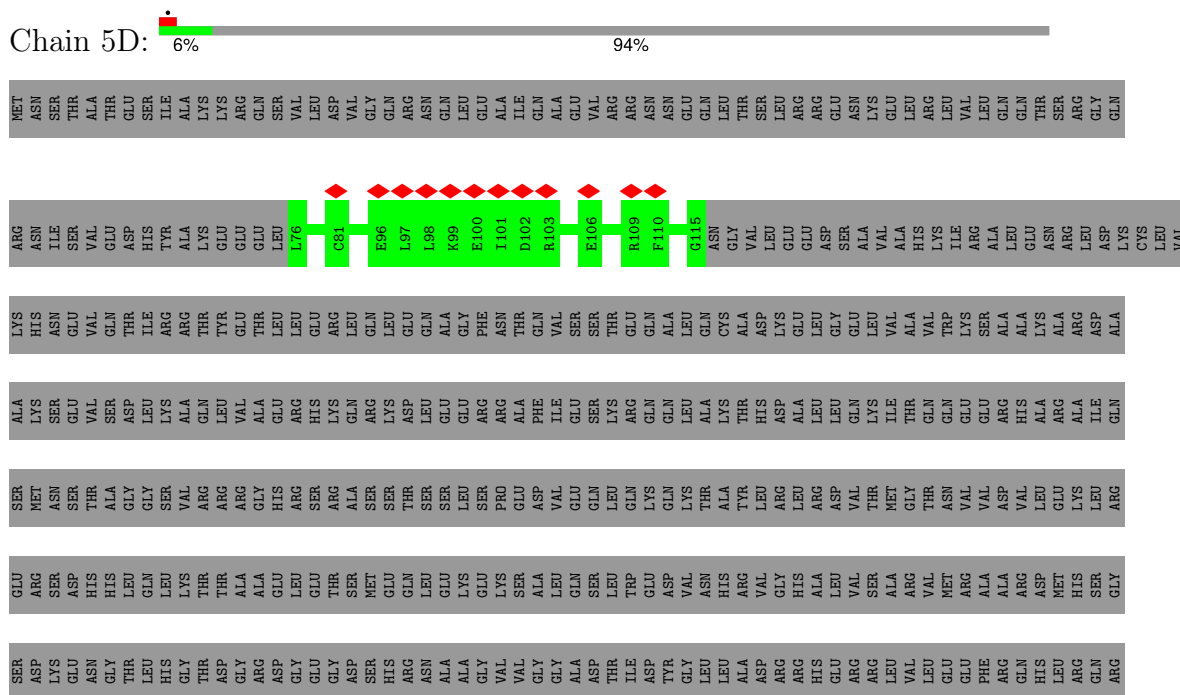
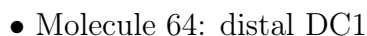


● Molecule 61: DMAP1



● Molecule 62: DMAP2





- Molecule 65: distal DC2

[illegible]

- Molecule 65: distal DC2

[illegible]

[illegible]

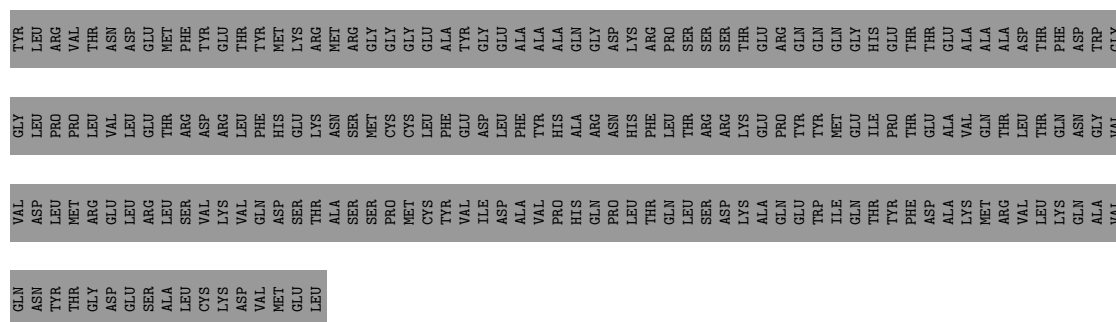
- Molecule 65: distal DC2

[illegible]

- Molecule 66: distal DC4

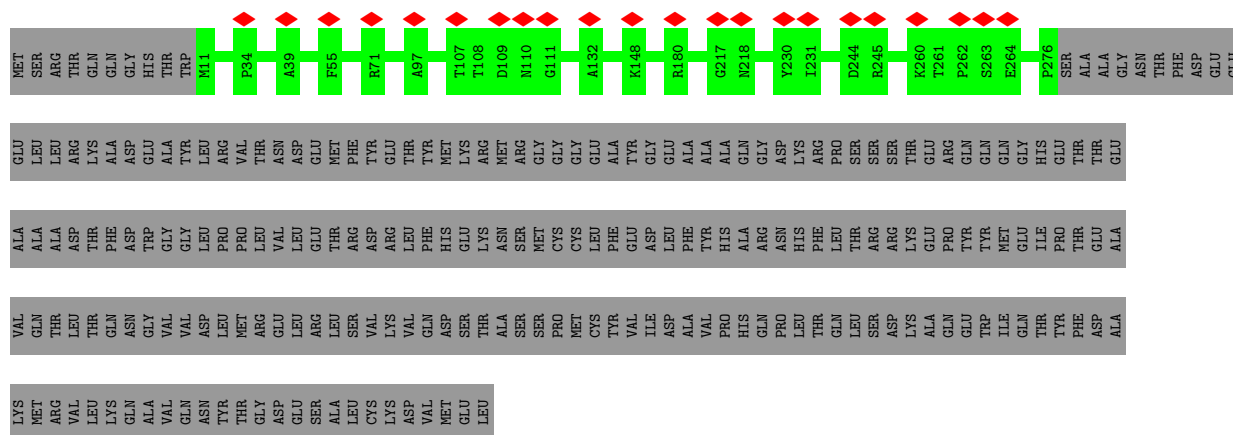


| | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|------|------|------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| MET | SER | ARG | THR | GLN | GLN | GLY | HIS | THR | TRP | M11 | R32 | A39 | F55 | G74 | K75 | D76 | N89 | L90 | Y91 | D92 | D109 | N110 | E114 | R245 | K260 | T261 | P262 | S263 | E264 | P276 | SER | ALA | ALA | GLY | ASN | THR | PHE | ASP | GLU | GLU | GLU | LEU | LEU | ARG | LYS | ALA | ASP | GLU |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|------|------|------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|



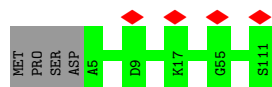
- Molecule 66: distal DC4

Chain 5L: 



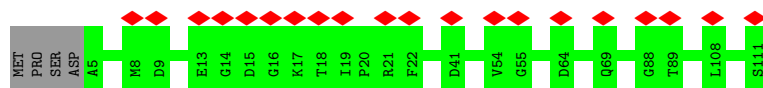
- Molecule 67: DC5

Chain 50:  96%



- Molecule 67: DC5

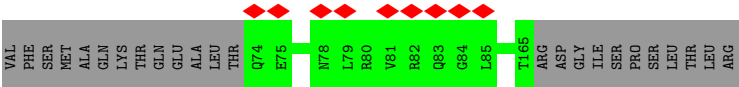
Chain 5P:  18% 96%



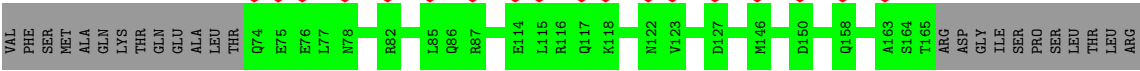
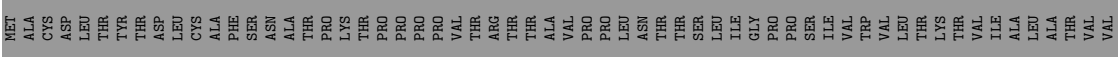
- Molecule 68: DC6

Chain 5S: 





● Molecule 68: DC6



4 Experimental information

| Property | Value | Source |
|--------------------------------------|-----------------------------------------|-----------|
| EM reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, Not provided | |
| Number of particles used | 533420 | Depositor |
| Resolution determination method | FSC 0.143 CUT-OFF | Depositor |
| CTF correction method | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope | TFS KRIOS | Depositor |
| Voltage (kV) | 300 | Depositor |
| Electron dose ($e^-/\text{\AA}^2$) | 62.6 | Depositor |
| Minimum defocus (nm) | 500 | Depositor |
| Maximum defocus (nm) | 2000 | Depositor |
| Magnification | Not provided | |
| Image detector | GATAN K3 (6k x 4k) | Depositor |
| Maximum map value | 1.841 | Depositor |
| Minimum map value | -0.012 | Depositor |
| Average map value | 0.010 | Depositor |
| Map value standard deviation | 0.058 | Depositor |
| Recommended contour level | 0.0435 | Depositor |
| Map size (\AA) | 680.96, 680.96, 680.96 | wwPDB |
| Map dimensions | 512, 512, 512 | wwPDB |
| Map angles ($^\circ$) | 90.0, 90.0, 90.0 | wwPDB |
| Pixel spacing (\AA) | 1.33, 1.33, 1.33 | Depositor |

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GTP, CA, ATP, GDP, MG, ZN

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 | 0.27 | 0/3432 | 0.54 | 0/4637 |
| 1 | AB | 0.27 | 0/3351 | 0.52 | 0/4528 |
| 1 | AD | 0.27 | 0/3432 | 0.53 | 0/4637 |
| 1 | AF | 0.27 | 0/3432 | 0.52 | 0/4637 |
| 1 | AH | 0.29 | 0/3432 | 0.54 | 0/4637 |
| 1 | AJ | 0.27 | 0/3432 | 0.52 | 0/4637 |
| 1 | AL | 0.27 | 0/3432 | 0.53 | 0/4637 |
| 1 | AN | 0.27 | 0/3351 | 0.52 | 0/4528 |
| 1 | B | 0.27 | 0/3334 | 0.53 | 0/4502 |
| 1 | BB | 0.27 | 0/3432 | 0.52 | 0/4637 |
| 1 | BD | 0.28 | 0/3440 | 0.53 | 0/4647 |
| 1 | BF | 0.27 | 0/3432 | 0.52 | 0/4637 |
| 1 | BH | 0.32 | 0/3432 | 0.56 | 1/4637 (0.0%) |
| 1 | BJ | 0.27 | 0/3432 | 0.53 | 0/4637 |
| 1 | BL | 0.27 | 0/3432 | 0.53 | 0/4637 |
| 1 | BN | 0.27 | 0/3432 | 0.54 | 0/4637 |
| 1 | CA | 0.29 | 0/3387 | 0.53 | 0/4575 |
| 1 | CC | 0.27 | 0/3440 | 0.53 | 0/4647 |
| 1 | CE | 0.27 | 0/3440 | 0.54 | 0/4647 |
| 1 | CG | 0.26 | 0/3440 | 0.51 | 0/4647 |
| 1 | CI | 0.27 | 0/3432 | 0.52 | 0/4637 |
| 1 | CK | 0.26 | 0/3432 | 0.52 | 0/4637 |
| 1 | CM | 0.28 | 0/3432 | 0.59 | 1/4637 (0.0%) |
| 1 | DA | 0.27 | 0/3432 | 0.51 | 0/4637 |
| 1 | DC | 0.27 | 0/3432 | 0.52 | 0/4637 |
| 1 | DE | 0.27 | 0/3432 | 0.54 | 0/4637 |
| 1 | DG | 0.27 | 0/3432 | 0.53 | 0/4637 |
| 1 | DI | 0.26 | 0/3432 | 0.52 | 0/4637 |
| 1 | DK | 0.26 | 0/3432 | 0.52 | 0/4637 |
| 1 | DM | 0.28 | 0/3432 | 0.54 | 0/4637 |
| 1 | E | 0.28 | 0/3440 | 0.53 | 0/4647 |
| 1 | EB | 0.27 | 0/3440 | 0.53 | 0/4647 |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|---------|-------------|---------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 1 | ED | 0.27 | 0/3440 | 0.53 | 0/4647 |
| 1 | EF | 0.27 | 0/3440 | 0.53 | 0/4647 |
| 1 | EH | 0.27 | 0/3440 | 0.52 | 0/4647 |
| 1 | EJ | 0.27 | 0/3440 | 0.53 | 0/4647 |
| 1 | EL | 0.30 | 0/3432 | 0.57 | 0/4637 |
| 1 | F | 0.28 | 0/3432 | 0.55 | 0/4637 |
| 1 | FB | 0.28 | 0/3432 | 0.53 | 0/4637 |
| 1 | FD | 0.28 | 0/3432 | 0.53 | 0/4637 |
| 1 | FF | 0.27 | 0/3432 | 0.53 | 0/4637 |
| 1 | FH | 0.27 | 0/3432 | 0.53 | 0/4637 |
| 1 | FJ | 0.27 | 0/3430 | 0.54 | 2/4633 (0.0%) |
| 1 | FL | 0.27 | 0/3413 | 0.55 | 0/4610 |
| 1 | G | 0.26 | 0/3432 | 0.53 | 0/4637 |
| 1 | GB | 0.26 | 0/3432 | 0.54 | 1/4637 (0.0%) |
| 1 | GD | 0.29 | 0/3413 | 0.53 | 0/4610 |
| 1 | GF | 0.28 | 0/3432 | 0.55 | 0/4637 |
| 1 | GH | 0.28 | 0/3432 | 0.54 | 0/4637 |
| 1 | GJ | 0.27 | 0/3405 | 0.54 | 0/4599 |
| 1 | GL | 0.27 | 0/3432 | 0.54 | 0/4637 |
| 1 | H | 0.28 | 0/3432 | 0.54 | 0/4637 |
| 1 | HB | 0.28 | 0/3432 | 0.55 | 0/4637 |
| 1 | HD | 0.27 | 0/3432 | 0.55 | 0/4637 |
| 1 | HF | 0.27 | 0/3432 | 0.52 | 0/4637 |
| 1 | HH | 0.27 | 0/3432 | 0.53 | 1/4637 (0.0%) |
| 1 | HJ | 0.26 | 0/3432 | 0.52 | 0/4637 |
| 1 | HL | 0.27 | 0/3432 | 0.54 | 0/4637 |
| 1 | I | 0.28 | 0/3440 | 0.54 | 0/4647 |
| 1 | IB | 0.27 | 0/3432 | 0.53 | 0/4637 |
| 1 | ID | 0.26 | 0/3432 | 0.52 | 0/4637 |
| 1 | IF | 0.27 | 0/3432 | 0.53 | 0/4637 |
| 1 | IH | 0.27 | 0/3432 | 0.51 | 0/4637 |
| 1 | IJ | 0.27 | 0/3432 | 0.52 | 0/4637 |
| 1 | IL | 0.28 | 0/3432 | 0.57 | 0/4637 |
| 1 | JA | 0.27 | 0/3432 | 0.54 | 1/4637 (0.0%) |
| 1 | JC | 0.26 | 0/3432 | 0.54 | 0/4637 |
| 1 | JE | 0.27 | 0/3432 | 0.54 | 0/4637 |
| 1 | JG | 0.27 | 0/3432 | 0.53 | 0/4637 |
| 1 | JI | 0.27 | 0/3432 | 0.52 | 0/4637 |
| 1 | JK | 0.28 | 0/3432 | 0.57 | 0/4637 |
| 1 | JM | 0.27 | 0/3413 | 0.53 | 0/4610 |
| 1 | KA | 0.27 | 0/3440 | 0.51 | 0/4647 |
| 1 | KC | 0.26 | 0/3432 | 0.52 | 0/4637 |
| 1 | KE | 0.27 | 0/3432 | 0.53 | 0/4637 |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|---------|-------------|---------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 1 | KG | 0.27 | 0/3432 | 0.51 | 0/4637 |
| 1 | KI | 0.26 | 0/3432 | 0.51 | 0/4637 |
| 1 | KK | 0.27 | 0/3432 | 0.53 | 0/4637 |
| 1 | KM | 0.27 | 0/3432 | 0.52 | 0/4637 |
| 1 | LA | 0.27 | 0/3432 | 0.54 | 0/4637 |
| 1 | LC | 0.27 | 0/3432 | 0.51 | 0/4637 |
| 1 | LE | 0.27 | 0/3432 | 0.54 | 0/4637 |
| 1 | LG | 0.28 | 0/3432 | 0.53 | 1/4637 (0.0%) |
| 1 | LI | 0.27 | 0/3432 | 0.52 | 0/4637 |
| 1 | LK | 0.27 | 0/3432 | 0.52 | 0/4637 |
| 1 | LM | 0.28 | 0/3432 | 0.54 | 0/4637 |
| 1 | LO | 0.27 | 0/3432 | 0.53 | 0/4637 |
| 1 | M | 0.26 | 0/3432 | 0.51 | 0/4637 |
| 1 | MB | 0.27 | 0/3432 | 0.52 | 0/4637 |
| 1 | MD | 0.27 | 0/3432 | 0.51 | 0/4637 |
| 1 | MF | 0.28 | 0/3432 | 0.54 | 0/4637 |
| 1 | MH | 0.27 | 0/3432 | 0.53 | 0/4637 |
| 1 | MJ | 0.28 | 0/3432 | 0.55 | 0/4637 |
| 1 | ML | 0.26 | 0/3432 | 0.52 | 0/4637 |
| 1 | MN | 0.28 | 0/3432 | 0.53 | 0/4637 |
| 1 | N | 0.28 | 0/3358 | 0.56 | 1/4538 (0.0%) |
| 1 | NB | 0.26 | 0/3358 | 0.53 | 0/4538 |
| 1 | ND | 0.27 | 0/3418 | 0.54 | 0/4617 |
| 1 | NF | 0.26 | 0/3418 | 0.52 | 0/4617 |
| 1 | NH | 0.28 | 0/3413 | 0.54 | 0/4610 |
| 1 | NJ | 0.27 | 0/3432 | 0.52 | 0/4637 |
| 1 | NL | 0.28 | 0/3413 | 0.56 | 0/4610 |
| 1 | O | 0.27 | 0/3413 | 0.56 | 0/4610 |
| 1 | OB | 0.27 | 0/3405 | 0.52 | 0/4599 |
| 1 | OD | 0.26 | 0/3413 | 0.51 | 0/4610 |
| 1 | OF | 0.27 | 0/3413 | 0.53 | 0/4610 |
| 1 | OH | 0.27 | 0/3413 | 0.53 | 0/4610 |
| 1 | OJ | 0.28 | 0/3413 | 0.55 | 1/4610 (0.0%) |
| 1 | OL | 0.29 | 0/3413 | 0.57 | 0/4610 |
| 1 | P | 0.28 | 0/3184 | 0.55 | 2/4303 (0.0%) |
| 1 | PB | 0.27 | 0/3432 | 0.53 | 1/4637 (0.0%) |
| 1 | PD | 0.28 | 0/3432 | 0.54 | 0/4637 |
| 1 | PF | 0.27 | 0/3432 | 0.53 | 1/4637 (0.0%) |
| 1 | PH | 0.28 | 0/3412 | 0.54 | 1/4608 (0.0%) |
| 1 | PJ | 0.27 | 0/3432 | 0.52 | 0/4637 |
| 1 | PL | 0.28 | 0/3432 | 0.55 | 0/4637 |
| 1 | QA | 0.27 | 0/3418 | 0.55 | 0/4617 |
| 1 | QC | 0.27 | 0/3418 | 0.51 | 0/4617 |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|---------|-------------|---------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 1 | QE | 0.28 | 0/3413 | 0.52 | 0/4610 |
| 1 | QG | 0.27 | 0/3418 | 0.52 | 0/4617 |
| 1 | QI | 0.27 | 0/3418 | 0.52 | 0/4617 |
| 1 | QK | 0.28 | 0/3418 | 0.53 | 0/4617 |
| 1 | RA | 0.27 | 0/3413 | 0.53 | 0/4610 |
| 1 | RC | 0.28 | 0/3432 | 0.53 | 0/4637 |
| 1 | RE | 0.27 | 0/3413 | 0.50 | 0/4610 |
| 1 | RG | 0.27 | 0/3413 | 0.52 | 0/4610 |
| 1 | RI | 0.27 | 0/3411 | 0.52 | 0/4606 |
| 1 | RK | 0.27 | 0/3425 | 0.53 | 0/4627 |
| 1 | S | 0.27 | 0/3405 | 0.52 | 0/4599 |
| 1 | SB | 0.28 | 0/3405 | 0.52 | 0/4599 |
| 1 | SD | 0.28 | 0/3405 | 0.53 | 0/4599 |
| 1 | SF | 0.27 | 0/3405 | 0.53 | 0/4599 |
| 1 | SH | 0.27 | 0/3425 | 0.55 | 0/4627 |
| 1 | SJ | 0.27 | 0/3418 | 0.54 | 0/4617 |
| 1 | T | 0.28 | 0/3418 | 0.54 | 0/4617 |
| 1 | TB | 0.28 | 0/3425 | 0.54 | 0/4627 |
| 1 | TD | 0.28 | 0/3413 | 0.55 | 0/4610 |
| 1 | TF | 0.27 | 0/3418 | 0.54 | 0/4617 |
| 1 | TH | 0.26 | 0/3413 | 0.54 | 1/4610 (0.0%) |
| 1 | TJ | 0.27 | 0/3432 | 0.54 | 0/4637 |
| 1 | TL | 0.28 | 0/3418 | 0.55 | 0/4617 |
| 1 | U | 0.27 | 0/3405 | 0.52 | 1/4599 (0.0%) |
| 1 | UB | 0.26 | 0/3405 | 0.51 | 0/4599 |
| 1 | UD | 0.27 | 0/3405 | 0.52 | 0/4599 |
| 1 | UF | 0.27 | 0/3405 | 0.53 | 0/4599 |
| 1 | UH | 0.27 | 0/3405 | 0.52 | 0/4599 |
| 1 | UJ | 0.27 | 0/3418 | 0.52 | 0/4617 |
| 1 | UL | 0.27 | 0/3413 | 0.55 | 0/4610 |
| 1 | V | 0.28 | 0/3425 | 0.55 | 1/4627 (0.0%) |
| 1 | VB | 0.27 | 0/3413 | 0.51 | 0/4610 |
| 1 | VD | 0.27 | 0/3418 | 0.54 | 0/4617 |
| 1 | VF | 0.27 | 0/3425 | 0.52 | 0/4627 |
| 1 | VH | 0.27 | 0/3405 | 0.52 | 0/4599 |
| 1 | VJ | 0.27 | 0/3432 | 0.53 | 0/4637 |
| 1 | VL | 0.26 | 0/3432 | 0.52 | 0/4637 |
| 1 | W | 0.27 | 0/3405 | 0.52 | 0/4599 |
| 1 | WB | 0.26 | 0/3405 | 0.52 | 0/4599 |
| 1 | WD | 0.27 | 0/3405 | 0.52 | 0/4599 |
| 1 | WF | 0.27 | 0/3418 | 0.52 | 0/4617 |
| 1 | WH | 0.26 | 0/3405 | 0.52 | 0/4599 |
| 1 | WJ | 0.27 | 0/3405 | 0.52 | 0/4599 |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|---------|-------------|---------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 1 | WL | 0.27 | 0/3413 | 0.52 | 0/4610 |
| 2 | AA | 0.27 | 0/3400 | 0.52 | 0/4614 |
| 2 | AC | 0.27 | 0/3424 | 0.52 | 0/4647 |
| 2 | AE | 0.27 | 0/3466 | 0.51 | 0/4704 |
| 2 | AG | 0.27 | 0/3423 | 0.53 | 2/4644 (0.0%) |
| 2 | AI | 0.27 | 0/3466 | 0.53 | 0/4704 |
| 2 | AK | 0.27 | 0/3466 | 0.52 | 0/4704 |
| 2 | AM | 0.28 | 0/3400 | 0.52 | 0/4614 |
| 2 | BA | 0.27 | 0/3392 | 0.52 | 0/4602 |
| 2 | BC | 0.28 | 0/3400 | 0.54 | 0/4614 |
| 2 | BE | 0.27 | 0/3392 | 0.52 | 0/4602 |
| 2 | BG | 0.27 | 0/3400 | 0.54 | 0/4614 |
| 2 | BI | 0.29 | 0/3466 | 0.54 | 0/4704 |
| 2 | BK | 0.27 | 0/3392 | 0.52 | 0/4602 |
| 2 | BM | 0.28 | 0/3400 | 0.53 | 0/4614 |
| 2 | C | 0.28 | 0/3466 | 0.51 | 0/4704 |
| 2 | CB | 0.28 | 0/3466 | 0.53 | 0/4704 |
| 2 | CD | 0.28 | 0/3466 | 0.54 | 1/4704 (0.0%) |
| 2 | CF | 0.26 | 0/3400 | 0.49 | 0/4614 |
| 2 | CH | 0.27 | 0/3466 | 0.53 | 0/4704 |
| 2 | CJ | 0.26 | 0/3466 | 0.51 | 0/4704 |
| 2 | CL | 0.28 | 0/3466 | 0.53 | 1/4704 (0.0%) |
| 2 | D | 0.27 | 0/3400 | 0.52 | 0/4614 |
| 2 | DB | 0.27 | 0/3400 | 0.51 | 0/4614 |
| 2 | DD | 0.28 | 0/3400 | 0.52 | 0/4614 |
| 2 | DF | 0.26 | 0/3408 | 0.51 | 0/4625 |
| 2 | DH | 0.27 | 0/3398 | 0.51 | 0/4610 |
| 2 | DJ | 0.27 | 0/3400 | 0.50 | 0/4614 |
| 2 | DL | 0.28 | 0/3400 | 0.54 | 0/4614 |
| 2 | EA | 0.27 | 0/3400 | 0.52 | 0/4614 |
| 2 | EC | 0.27 | 0/3466 | 0.51 | 0/4704 |
| 2 | EE | 0.26 | 0/3417 | 0.50 | 0/4637 |
| 2 | EG | 0.28 | 0/3422 | 0.53 | 0/4644 |
| 2 | EI | 0.26 | 0/3408 | 0.52 | 0/4625 |
| 2 | EK | 0.28 | 0/3408 | 0.52 | 0/4625 |
| 2 | FA | 0.27 | 0/3466 | 0.53 | 0/4704 |
| 2 | FC | 0.28 | 0/3431 | 0.53 | 0/4656 |
| 2 | FE | 0.28 | 0/3414 | 0.53 | 0/4633 |
| 2 | FG | 0.29 | 0/3408 | 0.53 | 0/4625 |
| 2 | FI | 0.26 | 0/3392 | 0.50 | 0/4602 |
| 2 | FK | 0.29 | 0/3408 | 0.54 | 0/4625 |
| 2 | GA | 0.28 | 0/3400 | 0.54 | 0/4614 |
| 2 | GC | 0.27 | 0/3400 | 0.53 | 0/4614 |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|---------|-------------|---------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 2 | GE | 0.28 | 0/3408 | 0.53 | 0/4625 |
| 2 | GG | 0.27 | 0/3400 | 0.52 | 0/4614 |
| 2 | GI | 0.28 | 0/3400 | 0.53 | 1/4614 (0.0%) |
| 2 | GK | 0.27 | 0/3400 | 0.53 | 0/4614 |
| 2 | HA | 0.27 | 0/3400 | 0.54 | 0/4614 |
| 2 | HC | 0.26 | 0/3400 | 0.52 | 1/4614 (0.0%) |
| 2 | HE | 0.27 | 0/3466 | 0.53 | 1/4704 (0.0%) |
| 2 | HG | 0.28 | 0/3414 | 0.53 | 0/4633 |
| 2 | HI | 0.28 | 0/3406 | 0.53 | 1/4621 (0.0%) |
| 2 | HK | 0.28 | 0/3414 | 0.54 | 0/4633 |
| 2 | HM | 0.28 | 0/3400 | 0.55 | 0/4614 |
| 2 | IA | 0.28 | 0/3400 | 0.54 | 0/4614 |
| 2 | IC | 0.27 | 0/3414 | 0.53 | 0/4633 |
| 2 | IE | 0.27 | 0/3466 | 0.52 | 0/4704 |
| 2 | IG | 0.26 | 0/3466 | 0.52 | 0/4704 |
| 2 | II | 0.27 | 0/3466 | 0.52 | 0/4704 |
| 2 | IK | 0.29 | 0/3400 | 0.54 | 0/4614 |
| 2 | IM | 0.28 | 0/3400 | 0.54 | 1/4614 (0.0%) |
| 2 | J | 0.29 | 0/3466 | 0.56 | 0/4704 |
| 2 | JB | 0.27 | 0/3466 | 0.52 | 0/4704 |
| 2 | JD | 0.28 | 0/3400 | 0.52 | 0/4614 |
| 2 | JF | 0.28 | 0/3400 | 0.53 | 0/4614 |
| 2 | JH | 0.28 | 0/3413 | 0.52 | 0/4631 |
| 2 | JJ | 0.28 | 0/3414 | 0.52 | 1/4633 (0.0%) |
| 2 | JL | 0.29 | 0/3414 | 0.55 | 0/4633 |
| 2 | JN | 0.28 | 0/3466 | 0.56 | 0/4704 |
| 2 | K | 0.28 | 0/3429 | 0.55 | 1/4652 (0.0%) |
| 2 | KB | 0.27 | 0/3466 | 0.54 | 0/4704 |
| 2 | KD | 0.27 | 0/3400 | 0.52 | 0/4614 |
| 2 | KF | 0.27 | 0/3466 | 0.53 | 0/4704 |
| 2 | KH | 0.28 | 0/3406 | 0.54 | 0/4622 |
| 2 | KJ | 0.26 | 0/3417 | 0.51 | 0/4637 |
| 2 | KL | 0.28 | 0/3466 | 0.53 | 0/4704 |
| 2 | KN | 0.27 | 0/3466 | 0.52 | 0/4704 |
| 2 | L | 0.27 | 0/3466 | 0.52 | 1/4704 (0.0%) |
| 2 | LB | 0.28 | 0/3417 | 0.51 | 0/4637 |
| 2 | LD | 0.28 | 0/3392 | 0.51 | 0/4603 |
| 2 | LF | 0.27 | 0/3466 | 0.52 | 0/4704 |
| 2 | LH | 0.29 | 0/3466 | 0.53 | 0/4704 |
| 2 | LJ | 0.27 | 0/3466 | 0.53 | 0/4704 |
| 2 | LL | 0.28 | 0/3466 | 0.53 | 0/4704 |
| 2 | LN | 0.27 | 0/3417 | 0.52 | 0/4637 |
| 2 | MA | 0.28 | 0/3406 | 0.52 | 0/4622 |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|---------|-------------|---------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 2 | MC | 0.28 | 0/3451 | 0.53 | 0/4684 |
| 2 | ME | 0.28 | 0/3439 | 0.53 | 0/4666 |
| 2 | MG | 0.27 | 0/3466 | 0.52 | 0/4704 |
| 2 | MI | 0.27 | 0/3466 | 0.52 | 0/4704 |
| 2 | MK | 0.28 | 0/3466 | 0.54 | 0/4704 |
| 2 | MM | 0.28 | 0/3406 | 0.53 | 0/4622 |
| 2 | NA | 0.27 | 0/3466 | 0.53 | 0/4704 |
| 2 | NC | 0.27 | 0/3466 | 0.54 | 1/4704 (0.0%) |
| 2 | NE | 0.27 | 0/3466 | 0.53 | 0/4704 |
| 2 | NG | 0.27 | 0/3466 | 0.53 | 0/4704 |
| 2 | NI | 0.28 | 0/3466 | 0.53 | 1/4704 (0.0%) |
| 2 | NK | 0.28 | 0/3466 | 0.54 | 0/4704 |
| 2 | NM | 0.28 | 0/3466 | 0.55 | 0/4704 |
| 2 | OA | 0.28 | 0/3414 | 0.53 | 0/4633 |
| 2 | OC | 0.27 | 0/3408 | 0.53 | 0/4625 |
| 2 | OE | 0.27 | 0/3408 | 0.52 | 0/4625 |
| 2 | OG | 0.28 | 0/3466 | 0.52 | 0/4704 |
| 2 | OI | 0.27 | 0/3400 | 0.53 | 0/4614 |
| 2 | OK | 0.28 | 0/3400 | 0.55 | 0/4614 |
| 2 | OM | 0.29 | 0/3423 | 0.53 | 0/4645 |
| 2 | PA | 0.27 | 0/3400 | 0.53 | 0/4614 |
| 2 | PC | 0.27 | 0/3408 | 0.51 | 0/4625 |
| 2 | PE | 0.29 | 0/3408 | 0.52 | 0/4625 |
| 2 | PG | 0.28 | 0/3466 | 0.52 | 0/4704 |
| 2 | PI | 0.28 | 0/3408 | 0.53 | 0/4625 |
| 2 | PK | 0.29 | 0/3414 | 0.53 | 0/4633 |
| 2 | PM | 0.30 | 0/3414 | 0.56 | 1/4633 (0.0%) |
| 2 | Q | 0.28 | 0/3466 | 0.53 | 0/4704 |
| 2 | QB | 0.28 | 0/3394 | 0.53 | 0/4606 |
| 2 | QD | 0.29 | 0/3400 | 0.54 | 0/4614 |
| 2 | QF | 0.28 | 0/3400 | 0.52 | 0/4614 |
| 2 | QH | 0.29 | 0/3466 | 0.53 | 0/4704 |
| 2 | QJ | 0.28 | 0/3408 | 0.52 | 0/4625 |
| 2 | QL | 0.29 | 0/3414 | 0.56 | 0/4633 |
| 2 | R | 0.27 | 0/3466 | 0.53 | 0/4704 |
| 2 | RB | 0.29 | 0/3408 | 0.55 | 2/4625 (0.0%) |
| 2 | RD | 0.29 | 0/3408 | 0.53 | 0/4625 |
| 2 | RF | 0.28 | 0/3408 | 0.52 | 0/4625 |
| 2 | RH | 0.29 | 0/3400 | 0.55 | 1/4614 (0.0%) |
| 2 | RJ | 0.29 | 0/3400 | 0.56 | 1/4614 (0.0%) |
| 2 | RL | 0.28 | 0/3406 | 0.55 | 0/4622 |
| 2 | SA | 0.28 | 0/3408 | 0.53 | 0/4625 |
| 2 | SC | 0.28 | 0/3406 | 0.53 | 0/4622 |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|---------|-------------|---------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 2 | SE | 0.27 | 0/3406 | 0.51 | 0/4622 |
| 2 | SG | 0.27 | 0/3408 | 0.50 | 0/4625 |
| 2 | SI | 0.28 | 0/3400 | 0.52 | 0/4614 |
| 2 | SK | 0.29 | 0/3414 | 0.54 | 0/4633 |
| 2 | TA | 0.28 | 0/3400 | 0.52 | 0/4614 |
| 2 | TC | 0.28 | 0/3384 | 0.54 | 0/4592 |
| 2 | TE | 0.27 | 0/3400 | 0.51 | 0/4614 |
| 2 | TG | 0.27 | 0/3408 | 0.51 | 0/4625 |
| 2 | TI | 0.27 | 0/3400 | 0.51 | 0/4614 |
| 2 | TK | 0.28 | 0/3424 | 0.53 | 0/4647 |
| 2 | UA | 0.28 | 0/3400 | 0.53 | 0/4614 |
| 2 | UC | 0.27 | 0/3392 | 0.51 | 0/4603 |
| 2 | UE | 0.28 | 0/3400 | 0.53 | 0/4614 |
| 2 | UG | 0.28 | 0/3408 | 0.52 | 0/4625 |
| 2 | UI | 0.27 | 0/3400 | 0.52 | 0/4614 |
| 2 | UK | 0.28 | 0/3400 | 0.52 | 1/4614 (0.0%) |
| 2 | VA | 0.28 | 0/3408 | 0.53 | 0/4625 |
| 2 | VC | 0.28 | 0/3408 | 0.54 | 0/4625 |
| 2 | VE | 0.27 | 0/3408 | 0.51 | 0/4625 |
| 2 | VG | 0.27 | 0/3408 | 0.52 | 0/4625 |
| 2 | VI | 0.27 | 0/3412 | 0.51 | 0/4629 |
| 2 | VK | 0.28 | 0/3400 | 0.51 | 0/4614 |
| 2 | VM | 0.28 | 0/3431 | 0.55 | 0/4656 |
| 2 | WA | 0.27 | 0/3466 | 0.51 | 0/4704 |
| 2 | WC | 0.27 | 0/3408 | 0.52 | 0/4625 |
| 2 | WE | 0.26 | 0/3466 | 0.52 | 0/4704 |
| 2 | WG | 0.28 | 0/3408 | 0.52 | 1/4625 (0.0%) |
| 2 | WI | 0.28 | 0/3466 | 0.54 | 0/4704 |
| 2 | WK | 0.27 | 0/3408 | 0.51 | 0/4625 |
| 2 | WM | 0.28 | 0/3466 | 0.52 | 0/4704 |
| 3 | X | 0.27 | 0/1544 | 0.54 | 0/2083 |
| 3 | XA | 0.27 | 0/1544 | 0.55 | 1/2083 (0.0%) |
| 3 | XB | 0.27 | 0/1544 | 0.54 | 0/2083 |
| 3 | XC | 0.27 | 0/1544 | 0.55 | 0/2083 |
| 3 | XD | 0.26 | 0/1544 | 0.54 | 0/2083 |
| 3 | XE | 0.27 | 0/1544 | 0.56 | 0/2083 |
| 3 | XF | 0.26 | 0/1544 | 0.54 | 0/2083 |
| 4 | XM | 0.28 | 0/2094 | 0.51 | 0/2833 |
| 4 | XO | 0.27 | 0/2102 | 0.50 | 0/2844 |
| 4 | XQ | 0.26 | 0/2102 | 0.52 | 0/2844 |
| 4 | XR | 0.29 | 0/2105 | 0.52 | 0/2847 |
| 5 | XN | 0.27 | 0/2172 | 0.51 | 0/2940 |
| 5 | XP | 0.27 | 0/2172 | 0.51 | 0/2940 |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|---------|-------------|---------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 6 | 0 | 0.27 | 0/2040 | 0.54 | 0/2754 |
| 6 | 0A | 0.29 | 0/2040 | 0.55 | 0/2754 |
| 7 | 0C | 0.27 | 0/955 | 0.52 | 0/1293 |
| 7 | 0D | 0.26 | 0/2785 | 0.57 | 2/3777 (0.1%) |
| 8 | 0F | 0.25 | 0/1449 | 0.57 | 0/1930 |
| 8 | 0G | 0.28 | 0/2966 | 0.60 | 0/3932 |
| 8 | 0H | 0.28 | 0/230 | 0.62 | 0/307 |
| 8 | 0I | 0.27 | 0/2384 | 0.62 | 0/3167 |
| 8 | 0J | 0.27 | 0/1910 | 0.64 | 0/2530 |
| 9 | 0L | 0.26 | 0/4845 | 0.55 | 1/6569 (0.0%) |
| 9 | 0M | 0.26 | 0/4845 | 0.55 | 0/6569 |
| 9 | 0N | 0.27 | 0/4845 | 0.56 | 0/6569 |
| 9 | 0O | 0.29 | 0/2401 | 0.59 | 0/3253 |
| 10 | 0R | 0.29 | 0/2646 | 0.62 | 1/3521 (0.0%) |
| 10 | 0S | 0.30 | 0/1888 | 0.62 | 0/2513 |
| 11 | 0U | 0.27 | 0/2621 | 0.51 | 0/3555 |
| 12 | 0W | 0.26 | 0/2645 | 0.52 | 0/3600 |
| 13 | 0Y | 0.26 | 0/1875 | 0.50 | 0/2538 |
| 13 | 0Z | 0.27 | 0/1888 | 0.50 | 0/2554 |
| 13 | 0a | 0.25 | 0/430 | 0.53 | 0/584 |
| 14 | 0c | 0.27 | 0/1965 | 0.50 | 0/2631 |
| 14 | 0d | 0.29 | 0/2190 | 0.56 | 0/2934 |
| 15 | 0f | 0.26 | 0/1283 | 0.52 | 0/1737 |
| 15 | 0g | 0.28 | 0/223 | 0.45 | 0/303 |
| 16 | 0k | 0.26 | 0/5705 | 0.55 | 0/7710 |
| 16 | 0l | 0.25 | 0/5141 | 0.53 | 0/6953 |
| 17 | 0m | 0.27 | 0/1164 | 0.61 | 0/1550 |
| 17 | 0n | 0.29 | 0/3406 | 0.62 | 0/4525 |
| 17 | 0o | 0.24 | 0/173 | 0.56 | 0/232 |
| 18 | 0p | 0.27 | 0/915 | 0.62 | 0/1222 |
| 19 | 0r | 0.27 | 0/2076 | 0.59 | 1/2806 (0.0%) |
| 20 | 0t | 0.27 | 0/2117 | 0.53 | 0/2877 |
| 20 | 0u | 0.27 | 0/1819 | 0.53 | 0/2476 |
| 21 | 0v | 0.24 | 0/588 | 0.57 | 0/788 |
| 21 | 0w | 0.28 | 0/3753 | 0.58 | 0/5006 |
| 21 | 0x | 0.26 | 0/917 | 0.54 | 0/1228 |
| 22 | 0z | 0.30 | 0/1177 | 0.56 | 0/1585 |
| 22 | 1w | 0.26 | 0/1509 | 0.56 | 0/2035 |
| 22 | 1x | 0.27 | 0/1714 | 0.57 | 1/2310 (0.0%) |
| 22 | 1y | 0.28 | 0/733 | 0.57 | 0/989 |
| 23 | 1A | 0.27 | 0/2310 | 0.59 | 0/3075 |
| 23 | 1B | 0.29 | 0/1682 | 0.61 | 0/2236 |
| 23 | 1D | 0.26 | 0/467 | 0.67 | 0/616 |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|---------|-------------|---------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 23 | 1E | 0.28 | 0/3083 | 0.57 | 0/4112 |
| 23 | 1F | 0.27 | 0/642 | 0.60 | 0/856 |
| 24 | 1H | 0.27 | 0/4800 | 0.52 | 1/6491 (0.0%) |
| 24 | 1I | 0.26 | 0/5391 | 0.53 | 0/7280 |
| 24 | 1J | 0.26 | 0/5470 | 0.53 | 0/7387 |
| 24 | 1K | 0.27 | 0/4799 | 0.53 | 0/6489 |
| 25 | 1O | 0.26 | 0/5862 | 0.51 | 0/7901 |
| 26 | 1Q | 0.26 | 0/5371 | 0.54 | 0/7261 |
| 27 | 1S | 0.26 | 0/5967 | 0.53 | 0/8066 |
| 27 | 1T | 0.27 | 0/1822 | 0.60 | 1/2458 (0.0%) |
| 28 | 1U | 0.27 | 0/969 | 0.50 | 0/1318 |
| 28 | 1V | 0.27 | 0/378 | 0.55 | 0/508 |
| 28 | 1X | 0.26 | 0/969 | 0.51 | 0/1318 |
| 28 | 1Y | 0.26 | 0/1357 | 0.54 | 0/1833 |
| 28 | 1a | 0.26 | 0/460 | 0.48 | 0/627 |
| 28 | 1b | 0.39 | 0/1347 | 0.59 | 1/1826 (0.1%) |
| 28 | 1c | 0.27 | 0/268 | 0.57 | 0/361 |
| 28 | 1d | 0.27 | 0/969 | 0.48 | 0/1318 |
| 28 | 1e | 0.26 | 0/378 | 0.51 | 0/508 |
| 28 | 1g | 0.27 | 0/969 | 0.51 | 0/1318 |
| 28 | 1h | 0.30 | 0/1248 | 0.55 | 0/1685 |
| 28 | 4V | 0.27 | 0/500 | 0.50 | 0/679 |
| 28 | 4W | 0.33 | 0/1512 | 0.70 | 5/2048 (0.2%) |
| 29 | 1j | 0.26 | 0/936 | 0.50 | 0/1267 |
| 29 | 1k | 0.29 | 0/826 | 0.50 | 0/1128 |
| 29 | 1l | 0.26 | 0/936 | 0.53 | 0/1267 |
| 29 | 1m | 0.27 | 0/433 | 0.50 | 0/591 |
| 30 | 1o | 0.25 | 0/1059 | 0.51 | 0/1435 |
| 31 | 1q | 0.26 | 0/1708 | 0.54 | 0/2297 |
| 31 | 1r | 0.27 | 0/875 | 0.53 | 0/1164 |
| 31 | 1s | 0.27 | 0/1471 | 0.50 | 0/1978 |
| 31 | 1t | 0.26 | 0/620 | 0.59 | 0/817 |
| 32 | 2B | 0.27 | 0/2020 | 0.52 | 0/2728 |
| 32 | 2C | 0.28 | 0/1852 | 0.56 | 0/2496 |
| 33 | 2F | 0.30 | 0/2316 | 0.56 | 0/3146 |
| 33 | 2G | 0.29 | 0/2308 | 0.54 | 0/3135 |
| 33 | 2H | 0.29 | 0/2346 | 0.55 | 0/3188 |
| 33 | 2I | 0.30 | 0/1986 | 0.55 | 0/2689 |
| 34 | 2L | 0.26 | 0/1473 | 0.54 | 0/2003 |
| 35 | 2N | 0.26 | 0/1143 | 0.55 | 0/1555 |
| 35 | 2O | 0.27 | 0/1369 | 0.56 | 0/1856 |
| 36 | 2Q | 0.27 | 0/2383 | 0.50 | 0/3232 |
| 37 | 2S | 0.26 | 0/1845 | 0.52 | 0/2506 |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|---------|-------------|---------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 38 | 2U | 0.26 | 0/1840 | 0.55 | 0/2491 |
| 38 | 2V | 0.26 | 0/888 | 0.58 | 0/1202 |
| 39 | 2X | 0.27 | 0/1809 | 0.54 | 0/2439 |
| 40 | 2Z | 0.26 | 0/2305 | 0.55 | 0/3116 |
| 41 | 2b | 0.30 | 0/1016 | 0.57 | 0/1358 |
| 41 | 2c | 0.29 | 0/2107 | 0.55 | 0/2794 |
| 41 | 2e | 0.31 | 0/2760 | 0.63 | 0/3672 |
| 41 | 2f | 0.33 | 0/458 | 0.62 | 0/611 |
| 41 | 2h | 0.28 | 0/1990 | 0.57 | 0/2642 |
| 41 | 2i | 0.27 | 0/1311 | 0.57 | 0/1737 |
| 41 | 2k | 0.32 | 0/1383 | 0.59 | 0/1846 |
| 41 | 2l | 0.26 | 0/2245 | 0.57 | 0/2979 |
| 41 | 2n | 0.26 | 0/365 | 0.67 | 0/489 |
| 41 | 2o | 0.29 | 0/2472 | 0.62 | 0/3283 |
| 41 | 2p | 0.32 | 0/428 | 0.69 | 0/569 |
| 42 | 2r | 0.27 | 0/2528 | 0.52 | 0/3431 |
| 43 | 2t | 0.26 | 0/1750 | 0.55 | 0/2372 |
| 44 | 2v | 0.29 | 0/2308 | 0.53 | 0/3111 |
| 44 | 2w | 0.28 | 0/3370 | 0.54 | 0/4575 |
| 45 | 2y | 0.25 | 0/2372 | 0.53 | 0/3216 |
| 45 | 2z | 0.40 | 0/1465 | 0.64 | 2/1989 (0.1%) |
| 46 | 3B | 0.25 | 0/3375 | 0.52 | 1/4571 (0.0%) |
| 47 | 3D | 0.28 | 0/3268 | 0.53 | 0/4423 |
| 48 | 3F | 0.26 | 0/1269 | 0.60 | 0/1696 |
| 48 | 3G | 0.24 | 0/741 | 0.59 | 0/989 |
| 48 | 3H | 0.27 | 0/840 | 0.59 | 0/1121 |
| 48 | 3I | 0.26 | 0/646 | 0.62 | 1/861 (0.1%) |
| 48 | 3L | 0.25 | 0/250 | 0.48 | 0/331 |
| 48 | 3M | 0.24 | 0/250 | 0.43 | 0/331 |
| 49 | 3P | 0.26 | 0/2031 | 0.56 | 0/2750 |
| 49 | 3Q | 0.27 | 0/3890 | 0.54 | 0/5277 |
| 50 | 3S | 0.25 | 0/183 | 0.44 | 0/242 |
| 51 | X1 | 0.26 | 0/310 | 0.53 | 0/422 |
| 52 | 3U | 0.25 | 0/1100 | 0.51 | 0/1501 |
| 53 | 3W | 0.25 | 0/1282 | 0.52 | 0/1717 |
| 53 | 3X | 0.25 | 0/393 | 0.60 | 0/530 |
| 54 | 3Z | 0.27 | 0/1431 | 0.54 | 0/1933 |
| 54 | 3a | 0.26 | 0/734 | 0.50 | 0/998 |
| 54 | 4Y | 0.23 | 0/125 | 0.42 | 0/170 |
| 55 | 3b | 0.27 | 0/1139 | 0.53 | 0/1526 |
| 56 | 3d | 0.26 | 0/1259 | 0.57 | 0/1692 |
| 57 | 3f | 0.25 | 0/1426 | 0.55 | 0/1897 |
| 57 | 3g | 0.25 | 0/1426 | 0.55 | 0/1897 |

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|-----------|-------------|-------------------|
| | | RMSZ | # Z >5 | RMSZ | # Z >5 |
| 57 | 3h | 0.24 | 0/1426 | 0.53 | 0/1897 |
| 57 | 3i | 0.32 | 0/1426 | 0.72 | 1/1897 (0.1%) |
| 58 | 3m | 0.27 | 0/1229 | 0.56 | 0/1638 |
| 59 | 3o | 0.27 | 0/473 | 0.61 | 0/642 |
| 59 | 3p | 0.28 | 0/1195 | 0.53 | 0/1614 |
| 59 | 4O | 0.31 | 0/1444 | 0.51 | 0/1951 |
| 59 | 4P | 0.28 | 0/548 | 0.47 | 0/742 |
| 59 | 4a | 0.27 | 0/1273 | 0.49 | 0/1719 |
| 59 | 4b | 0.28 | 0/548 | 0.45 | 0/742 |
| 60 | 3r | 0.28 | 0/1115 | 0.59 | 0/1497 |
| 60 | 3s | 0.28 | 0/1115 | 0.60 | 0/1497 |
| 60 | 3t | 0.31 | 0/541 | 0.59 | 0/726 |
| 61 | 3w | 0.31 | 0/1410 | 0.51 | 0/1916 |
| 61 | 3x | 0.33 | 0/1018 | 0.56 | 0/1381 |
| 62 | 4A | 0.25 | 0/236 | 0.48 | 0/322 |
| 62 | 4B | 0.32 | 0/1637 | 0.50 | 0/2225 |
| 63 | 4I | 0.26 | 0/639 | 0.57 | 0/863 |
| 64 | 5B | 0.23 | 0/1356 | 0.49 | 0/1811 |
| 64 | 5C | 0.27 | 0/1356 | 0.62 | 1/1811 (0.1%) |
| 64 | 5D | 0.37 | 0/321 | 0.67 | 0/425 |
| 65 | 5G | 0.24 | 0/1552 | 0.52 | 0/2068 |
| 65 | 5H | 0.27 | 0/1552 | 0.61 | 0/2068 |
| 65 | 5I | 0.26 | 0/405 | 0.55 | 0/537 |
| 66 | 5K | 0.25 | 0/2204 | 0.49 | 0/2980 |
| 66 | 5L | 0.26 | 0/2204 | 0.53 | 0/2980 |
| 67 | 5O | 0.27 | 0/826 | 0.51 | 0/1117 |
| 67 | 5P | 0.28 | 0/826 | 0.53 | 0/1117 |
| 68 | 5S | 0.29 | 0/762 | 0.56 | 0/1022 |
| 68 | 5T | 0.27 | 0/762 | 0.56 | 0/1022 |
| All | All | 0.27 | 0/1389933 | 0.53 | 60/1880072 (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 | AB | 0 | 1 |
| 1 | BH | 0 | 1 |
| 1 | DE | 0 | 1 |
| 1 | EH | 0 | 1 |
| 1 | HB | 0 | 1 |

Continued on next page...

Continued from previous page...

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 1 | HF | 0 | 1 |
| 1 | JK | 0 | 1 |
| 1 | SH | 0 | 1 |
| 1 | SJ | 0 | 1 |
| 1 | TF | 0 | 1 |
| 1 | W | 0 | 1 |
| 2 | FE | 0 | 1 |
| 2 | MG | 0 | 1 |
| 2 | QD | 0 | 1 |
| 2 | RF | 0 | 1 |
| 2 | WM | 0 | 1 |
| 6 | 0A | 0 | 1 |
| 8 | 0I | 0 | 1 |
| 9 | 0O | 0 | 1 |
| 17 | 0n | 0 | 2 |
| 27 | 1S | 0 | 1 |
| 28 | 4W | 0 | 1 |
| 33 | 2H | 0 | 1 |
| 41 | 2c | 0 | 1 |
| 41 | 2f | 0 | 2 |
| 41 | 2i | 0 | 1 |
| 41 | 2k | 0 | 1 |
| 41 | 2l | 0 | 1 |
| 41 | 2o | 0 | 1 |
| 44 | 2v | 0 | 1 |
| 44 | 2w | 0 | 1 |
| 59 | 4O | 0 | 1 |
| 59 | 4P | 0 | 1 |
| 60 | 3s | 0 | 1 |
| All | All | 0 | 36 |

There are no bond length outliers.

All (60) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|--------|-------------|----------|
| 45 | 2z | 188 | PRO | CA-N-CD | -11.42 | 95.51 | 111.50 |
| 2 | RH | 298 | PRO | CA-N-CD | -10.86 | 96.30 | 111.50 |
| 28 | 4W | 20 | CYS | CA-CB-SG | -10.76 | 94.63 | 114.00 |
| 28 | 4W | 20 | CYS | CB-CA-C | -10.20 | 90.00 | 110.40 |
| 1 | HH | 80 | PRO | CA-N-CD | -8.61 | 99.45 | 111.50 |
| 2 | HE | 298 | PRO | CA-N-CD | -8.39 | 99.75 | 111.50 |
| 1 | V | 324 | LYS | CD-CE-NZ | -8.26 | 92.70 | 111.70 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 2 | RB | 298 | PRO | CA-N-CD | -8.09 | 100.17 | 111.50 |
| 1 | PH | 395 | LEU | CB-CG-CD2 | -7.65 | 98.00 | 111.00 |
| 2 | RJ | 175 | PRO | CA-N-CD | -7.56 | 100.92 | 111.50 |
| 28 | 4W | 30 | CYS | CB-CA-C | 7.43 | 125.26 | 110.40 |
| 45 | 2z | 188 | PRO | N-CD-CG | -7.02 | 92.67 | 103.20 |
| 1 | CM | 261 | PRO | CA-N-CD | -6.99 | 101.71 | 111.50 |
| 2 | WG | 298 | PRO | CA-N-CD | -6.96 | 101.75 | 111.50 |
| 2 | L | 326 | LYS | CD-CE-NZ | -6.84 | 95.97 | 111.70 |
| 1 | FJ | 36 | TYR | CG-CD2-CE2 | 6.73 | 126.68 | 121.30 |
| 57 | 3i | 99 | MET | CA-CB-CG | 6.36 | 124.11 | 113.30 |
| 48 | 3I | 51 | LEU | CA-CB-CG | 6.25 | 129.66 | 115.30 |
| 7 | 0D | 117 | LEU | CA-CB-CG | 6.20 | 129.57 | 115.30 |
| 2 | PM | 154 | LEU | CA-CB-CG | 6.05 | 129.22 | 115.30 |
| 46 | 3B | 391 | LEU | CA-CB-CG | 6.03 | 129.16 | 115.30 |
| 1 | P | 213 | ARG | CG-CD-NE | 5.91 | 124.20 | 111.80 |
| 2 | AG | 326 | LYS | CB-CG-CD | -5.89 | 96.29 | 111.60 |
| 2 | CL | 302 | LEU | CB-CG-CD1 | -5.80 | 101.14 | 111.00 |
| 2 | K | 326 | LYS | CD-CE-NZ | -5.80 | 98.36 | 111.70 |
| 2 | GI | 326 | LYS | CD-CE-NZ | -5.79 | 98.38 | 111.70 |
| 10 | 0R | 310 | MET | CA-CB-CG | 5.77 | 123.11 | 113.30 |
| 1 | OJ | 112 | LEU | CA-CB-CG | 5.75 | 128.52 | 115.30 |
| 1 | FJ | 36 | TYR | CZ-CE2-CD2 | 5.68 | 124.91 | 119.80 |
| 2 | NC | 317 | LEU | CA-CB-CG | 5.66 | 128.31 | 115.30 |
| 24 | 1H | 648 | MET | CA-CB-CG | 5.65 | 122.91 | 113.30 |
| 64 | 5C | 178 | LEU | CA-CB-CG | 5.64 | 128.28 | 115.30 |
| 2 | IM | 317 | LEU | CA-CB-CG | 5.62 | 128.24 | 115.30 |
| 2 | HC | 273 | ALA | C-N-CD | -5.56 | 108.36 | 120.60 |
| 1 | PF | 112 | LEU | CA-CB-CG | 5.55 | 128.07 | 115.30 |
| 3 | XA | 122 | PRO | CA-N-CD | -5.47 | 103.84 | 111.50 |
| 1 | GB | 41 | ASP | CB-CG-OD1 | 5.45 | 123.20 | 118.30 |
| 2 | NI | 326 | LYS | CG-CD-CE | -5.44 | 95.57 | 111.90 |
| 1 | N | 403 | MET | CA-CB-CG | 5.43 | 122.53 | 113.30 |
| 2 | AG | 326 | LYS | CD-CE-NZ | -5.34 | 99.42 | 111.70 |
| 1 | PB | 324 | LYS | CD-CE-NZ | -5.33 | 99.44 | 111.70 |
| 1 | JA | 177 | ASP | CB-CG-OD1 | 5.32 | 123.09 | 118.30 |
| 1 | U | 41 | ASP | CB-CG-OD1 | 5.31 | 123.08 | 118.30 |
| 27 | 1T | 722 | LEU | CA-CB-CG | 5.30 | 127.50 | 115.30 |
| 1 | BH | 252 | LYS | CD-CE-NZ | -5.29 | 99.52 | 111.70 |
| 19 | 0r | 194 | MET | CA-CB-CG | 5.29 | 122.28 | 113.30 |
| 1 | TH | 41 | ASP | CB-CG-OD1 | 5.27 | 123.05 | 118.30 |
| 1 | P | 41 | ASP | CB-CG-OD1 | 5.26 | 123.03 | 118.30 |
| 22 | 1x | 146 | ASP | CB-CG-OD2 | 5.25 | 123.02 | 118.30 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 1 | LG | 336 | LYS | CD-CE-NZ | 5.24 | 123.75 | 111.70 |
| 2 | CD | 298 | PRO | CA-N-CD | -5.18 | 104.25 | 111.50 |
| 2 | JJ | 326 | LYS | CB-CG-CD | -5.16 | 98.20 | 111.60 |
| 7 | 0D | 74 | PRO | CA-N-CD | -5.12 | 104.33 | 111.50 |
| 28 | 4W | 30 | CYS | N-CA-CB | -5.11 | 101.40 | 110.60 |
| 2 | HI | 418 | PHE | CD1-CE1-CZ | 5.08 | 126.20 | 120.10 |
| 9 | 0L | 106 | LEU | CA-CB-CG | 5.07 | 126.96 | 115.30 |
| 28 | 1b | 216 | ASP | CB-CG-OD1 | 5.05 | 122.84 | 118.30 |
| 28 | 4W | 20 | CYS | N-CA-CB | -5.04 | 101.52 | 110.60 |
| 2 | UK | 298 | PRO | CA-N-CD | -5.03 | 104.46 | 111.50 |
| 2 | RB | 298 | PRO | N-CD-CG | -5.00 | 95.69 | 103.20 |

There are no chirality outliers.

All (36) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|-----------|
| 6 | 0A | 160 | ALA | Peptide |
| 8 | 0I | 99 | ARG | Peptide |
| 9 | 0O | 74 | ARG | Peptide |
| 17 | 0n | 26 | ARG | Sidechain |
| 17 | 0n | 37 | ARG | Sidechain |
| 27 | 1S | 281 | LYS | Peptide |
| 33 | 2H | 218 | ARG | Sidechain |
| 41 | 2c | 447 | ARG | Sidechain |
| 41 | 2f | 447 | ARG | Sidechain |
| 41 | 2f | 450 | ARG | Sidechain |
| 41 | 2i | 447 | ARG | Sidechain |
| 41 | 2k | 315 | ARG | Sidechain |
| 41 | 2l | 447 | ARG | Sidechain |
| 41 | 2o | 447 | ARG | Sidechain |
| 44 | 2v | 240 | SER | Peptide |
| 44 | 2w | 218 | ARG | Sidechain |
| 60 | 3s | 46 | ARG | Sidechain |
| 59 | 4O | 174 | ARG | Sidechain |
| 59 | 4P | 1 | MET | Peptide |
| 28 | 4W | 21 | ARG | Sidechain |
| 1 | AB | 267 | MET | Peptide |
| 1 | BH | 77 | ARG | Sidechain |
| 1 | DE | 271 | ALA | Peptide |
| 1 | EH | 271 | ALA | Peptide |
| 2 | FE | 338 | LYS | Peptide |
| 1 | HB | 2 | ARG | Sidechain |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|-----------|
| 1 | HF | 267 | MET | Peptide |
| 1 | JK | 200 | MET | Peptide |
| 2 | MG | 164 | LYS | Peptide |
| 2 | QD | 326 | LYS | Peptide |
| 2 | RF | 390 | ARG | Sidechain |
| 1 | SH | 200 | MET | Peptide |
| 1 | SJ | 271 | ALA | Peptide |
| 1 | TF | 200 | MET | Peptide |
| 1 | W | 267 | MET | Peptide |
| 2 | WM | 301 | MET | Peptide |

5.2 Too-close contacts [i](#)

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

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains [i](#)

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

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 511 ligands modelled in this entry, 190 are monoatomic - leaving 321 for Mogul analysis.

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 |
| 69 | GDP | CE | 500 | - | 25,30,30 | 0.96 | 1 (4%) | 30,47,47 | 1.07 | 1 (3%) |
| 69 | GDP | HF | 500 | - | 25,30,30 | 0.95 | 1 (4%) | 30,47,47 | 1.03 | 1 (3%) |
| 71 | GTP | MK | 501 | 70 | 29,34,34 | 1.25 | 2 (6%) | 35,54,54 | 1.28 | 4 (11%) |
| 71 | GTP | HK | 501 | 70 | 29,34,34 | 1.21 | 2 (6%) | 35,54,54 | 1.27 | 4 (11%) |
| 69 | GDP | GB | 500 | - | 25,30,30 | 0.98 | 1 (4%) | 30,47,47 | 1.07 | 2 (6%) |
| 69 | GDP | UJ | 500 | - | 25,30,30 | 0.95 | 1 (4%) | 30,47,47 | 1.06 | 2 (6%) |
| 69 | GDP | TD | 500 | - | 25,30,30 | 0.95 | 1 (4%) | 30,47,47 | 1.10 | 2 (6%) |
| 71 | GTP | NC | 501 | 70 | 29,34,34 | 1.25 | 2 (6%) | 35,54,54 | 1.25 | 4 (11%) |
| 71 | GTP | IA | 501 | 70 | 29,34,34 | 1.21 | 2 (6%) | 35,54,54 | 1.27 | 4 (11%) |
| 69 | GDP | EH | 500 | - | 25,30,30 | 0.93 | 1 (4%) | 30,47,47 | 1.06 | 1 (3%) |
| 71 | GTP | TG | 501 | 70 | 29,34,34 | 1.24 | 2 (6%) | 35,54,54 | 1.26 | 4 (11%) |
| 69 | GDP | VF | 500 | - | 25,30,30 | 0.96 | 1 (4%) | 30,47,47 | 1.09 | 2 (6%) |
| 71 | GTP | LB | 501 | 70 | 29,34,34 | 1.26 | 3 (10%) | 35,54,54 | 1.25 | 4 (11%) |
| 69 | GDP | MB | 500 | - | 25,30,30 | 0.96 | 1 (4%) | 30,47,47 | 1.05 | 2 (6%) |
| 71 | GTP | HG | 501 | 70 | 29,34,34 | 1.21 | 2 (6%) | 35,54,54 | 1.33 | 5 (14%) |
| 71 | GTP | EK | 501 | 70 | 29,34,34 | 1.27 | 3 (10%) | 35,54,54 | 1.32 | 5 (14%) |
| 71 | GTP | UI | 501 | 70 | 29,34,34 | 1.25 | 2 (6%) | 35,54,54 | 1.30 | 4 (11%) |
| 69 | GDP | V | 500 | - | 25,30,30 | 0.95 | 1 (4%) | 30,47,47 | 1.06 | 2 (6%) |
| 71 | GTP | JL | 501 | 70 | 29,34,34 | 1.21 | 2 (6%) | 35,54,54 | 1.34 | 4 (11%) |
| 71 | GTP | QH | 501 | 70 | 29,34,34 | 1.25 | 2 (6%) | 35,54,54 | 1.38 | 6 (17%) |
| 71 | GTP | WI | 501 | 70 | 29,34,34 | 1.26 | 2 (6%) | 35,54,54 | 1.26 | 4 (11%) |
| 69 | GDP | QE | 500 | - | 25,30,30 | 0.94 | 1 (4%) | 30,47,47 | 1.09 | 2 (6%) |
| 71 | GTP | GI | 501 | 70 | 29,34,34 | 1.20 | 2 (6%) | 35,54,54 | 1.27 | 4 (11%) |
| 71 | GTP | SA | 501 | 70 | 29,34,34 | 1.23 | 2 (6%) | 35,54,54 | 1.25 | 4 (11%) |
| 71 | GTP | PC | 501 | 70 | 29,34,34 | 1.26 | 2 (6%) | 35,54,54 | 1.27 | 4 (11%) |
| 69 | GDP | LI | 500 | - | 25,30,30 | 0.96 | 1 (4%) | 30,47,47 | 1.05 | 2 (6%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 71 | GTP | MI | 501 | 70 | 29,34,34 | 1.26 | 2 (6%) | 35,54,54 | 1.24 | 4 (11%) |
| 71 | GTP | RJ | 501 | - | 29,34,34 | 1.26 | 2 (6%) | 35,54,54 | 1.30 | 4 (11%) |
| 69 | GDP | JC | 500 | - | 25,30,30 | 0.95 | 1 (4%) | 30,47,47 | 1.06 | 2 (6%) |
| 69 | GDP | ID | 500 | - | 25,30,30 | 0.96 | 1 (4%) | 30,47,47 | 1.06 | 2 (6%) |
| 69 | GDP | KG | 500 | - | 25,30,30 | 0.97 | 1 (4%) | 30,47,47 | 1.08 | 1 (3%) |
| 71 | GTP | FK | 501 | - | 29,34,34 | 1.24 | 2 (6%) | 35,54,54 | 1.33 | 4 (11%) |
| 69 | GDP | RC | 500 | - | 25,30,30 | 0.95 | 1 (4%) | 30,47,47 | 1.07 | 2 (6%) |
| 69 | GDP | JA | 500 | - | 25,30,30 | 0.97 | 1 (4%) | 30,47,47 | 1.07 | 2 (6%) |
| 69 | GDP | DE | 500 | - | 25,30,30 | 0.96 | 1 (4%) | 30,47,47 | 1.08 | 2 (6%) |
| 71 | GTP | RH | 501 | 70 | 29,34,34 | 1.23 | 2 (6%) | 35,54,54 | 1.31 | 4 (11%) |
| 71 | GTP | CF | 501 | 70 | 29,34,34 | 1.28 | 3 (10%) | 35,54,54 | 1.26 | 3 (8%) |
| 69 | GDP | LK | 500 | - | 25,30,30 | 0.97 | 1 (4%) | 30,47,47 | 1.08 | 2 (6%) |
| 71 | GTP | WK | 501 | 70 | 29,34,34 | 1.25 | 2 (6%) | 35,54,54 | 1.25 | 4 (11%) |
| 69 | GDP | NF | 500 | - | 25,30,30 | 0.96 | 1 (4%) | 30,47,47 | 1.06 | 1 (3%) |
| 71 | GTP | DD | 501 | 70 | 29,34,34 | 1.28 | 3 (10%) | 35,54,54 | 1.24 | 4 (11%) |
| 69 | GDP | CC | 500 | - | 25,30,30 | 0.97 | 1 (4%) | 30,47,47 | 1.06 | 2 (6%) |
| 71 | GTP | OK | 501 | - | 29,34,34 | 1.21 | 2 (6%) | 35,54,54 | 1.32 | 4 (11%) |
| 69 | GDP | BF | 500 | - | 25,30,30 | 0.95 | 1 (4%) | 30,47,47 | 1.09 | 2 (6%) |
| 69 | GDP | HH | 500 | - | 25,30,30 | 0.94 | 1 (4%) | 30,47,47 | 1.08 | 2 (6%) |
| 71 | GTP | ME | 501 | 70 | 29,34,34 | 1.28 | 4 (13%) | 35,54,54 | 1.32 | 4 (11%) |
| 71 | GTP | RB | 501 | 70 | 29,34,34 | 1.28 | 3 (10%) | 35,54,54 | 1.27 | 4 (11%) |
| 69 | GDP | H | 500 | - | 25,30,30 | 0.98 | 1 (4%) | 30,47,47 | 1.05 | 2 (6%) |
| 69 | GDP | VJ | 500 | - | 25,30,30 | 0.95 | 1 (4%) | 30,47,47 | 1.08 | 3 (10%) |
| 71 | GTP | RL | 501 | 70 | 29,34,34 | 1.24 | 2 (6%) | 35,54,54 | 1.32 | 4 (11%) |
| 71 | GTP | PE | 501 | 70 | 29,34,34 | 1.25 | 2 (6%) | 35,54,54 | 1.31 | 4 (11%) |
| 71 | GTP | LH | 501 | 70 | 29,34,34 | 1.24 | 2 (6%) | 35,54,54 | 1.36 | 5 (14%) |
| 69 | GDP | PF | 500 | - | 25,30,30 | 0.94 | 1 (4%) | 30,47,47 | 1.04 | 2 (6%) |
| 69 | GDP | G | 500 | - | 25,30,30 | 0.98 | 1 (4%) | 30,47,47 | 1.03 | 2 (6%) |
| 71 | GTP | WC | 501 | 70 | 29,34,34 | 1.25 | 2 (6%) | 35,54,54 | 1.25 | 4 (11%) |
| 69 | GDP | PL | 500 | - | 25,30,30 | 0.96 | 1 (4%) | 30,47,47 | 1.07 | 1 (3%) |
| 69 | GDP | JE | 500 | - | 25,30,30 | 0.95 | 1 (4%) | 30,47,47 | 1.07 | 2 (6%) |
| 69 | GDP | DG | 500 | - | 25,30,30 | 0.96 | 1 (4%) | 30,47,47 | 1.09 | 2 (6%) |
| 71 | GTP | J | 501 | 70 | 29,34,34 | 1.24 | 2 (6%) | 35,54,54 | 1.23 | 4 (11%) |
| 71 | GTP | R | 501 | 70 | 29,34,34 | 1.24 | 2 (6%) | 35,54,54 | 1.28 | 4 (11%) |
| 69 | GDP | IB | 500 | - | 25,30,30 | 0.96 | 1 (4%) | 30,47,47 | 1.06 | 1 (3%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 71 | GTP | LF | 501 | 70 | 29,34,34 | 1.21 | 2 (6%) | 35,54,54 | 1.35 | 5 (14%) |
| 71 | GTP | KJ | 501 | 70 | 29,34,34 | 1.24 | 2 (6%) | 35,54,54 | 1.29 | 4 (11%) |
| 69 | GDP | JI | 500 | - | 25,30,30 | 0.97 | 1 (4%) | 30,47,47 | 1.07 | 2 (6%) |
| 69 | GDP | RK | 500 | - | 25,30,30 | 0.96 | 1 (4%) | 30,47,47 | 1.07 | 2 (6%) |
| 71 | GTP | SC | 501 | 70 | 29,34,34 | 1.20 | 2 (6%) | 35,54,54 | 1.27 | 4 (11%) |
| 69 | GDP | WJ | 500 | - | 25,30,30 | 0.95 | 1 (4%) | 30,47,47 | 1.05 | 2 (6%) |
| 69 | GDP | LO | 500 | - | 25,30,30 | 0.95 | 1 (4%) | 30,47,47 | 1.08 | 2 (6%) |
| 71 | GTP | KD | 501 | 70 | 29,34,34 | 1.26 | 2 (6%) | 35,54,54 | 1.26 | 4 (11%) |
| 71 | GTP | NI | 501 | 70 | 29,34,34 | 1.22 | 2 (6%) | 35,54,54 | 1.27 | 4 (11%) |
| 69 | GDP | MJ | 500 | - | 25,30,30 | 0.98 | 1 (4%) | 30,47,47 | 1.17 | 3 (10%) |
| 69 | GDP | KM | 500 | - | 25,30,30 | 0.95 | 1 (4%) | 30,47,47 | 1.06 | 2 (6%) |
| 71 | GTP | D | 501 | - | 29,34,34 | 1.29 | 4 (13%) | 35,54,54 | 1.30 | 5 (14%) |
| 71 | GTP | VC | 501 | 70 | 29,34,34 | 1.28 | 3 (10%) | 35,54,54 | 1.24 | 4 (11%) |
| 69 | GDP | NH | 500 | - | 25,30,30 | 0.97 | 1 (4%) | 30,47,47 | 1.08 | 2 (6%) |
| 69 | GDP | RE | 500 | - | 25,30,30 | 0.97 | 1 (4%) | 30,47,47 | 1.18 | 4 (13%) |
| 71 | GTP | QJ | 501 | 70 | 29,34,34 | 1.24 | 3 (10%) | 35,54,54 | 1.30 | 4 (11%) |
| 71 | GTP | CB | 501 | 70 | 29,34,34 | 1.27 | 2 (6%) | 35,54,54 | 1.27 | 4 (11%) |
| 71 | GTP | AM | 501 | 70 | 29,34,34 | 1.24 | 2 (6%) | 35,54,54 | 1.26 | 3 (8%) |
| 71 | GTP | NE | 501 | 70 | 29,34,34 | 1.28 | 3 (10%) | 35,54,54 | 1.24 | 4 (11%) |
| 69 | GDP | PH | 500 | - | 25,30,30 | 0.94 | 1 (4%) | 30,47,47 | 1.06 | 2 (6%) |
| 69 | GDP | FF | 500 | - | 25,30,30 | 0.95 | 1 (4%) | 30,47,47 | 1.06 | 1 (3%) |
| 71 | GTP | HC | 501 | 70 | 29,34,34 | 1.26 | 3 (10%) | 35,54,54 | 1.28 | 4 (11%) |
| 69 | GDP | UH | 500 | - | 25,30,30 | 0.97 | 1 (4%) | 30,47,47 | 1.07 | 2 (6%) |
| 71 | GTP | K | 501 | 70 | 29,34,34 | 1.26 | 3 (10%) | 35,54,54 | 1.30 | 4 (11%) |
| 71 | GTP | CL | 501 | 70 | 29,34,34 | 1.30 | 4 (13%) | 35,54,54 | 1.25 | 4 (11%) |
| 71 | GTP | MC | 501 | 70 | 29,34,34 | 1.22 | 2 (6%) | 35,54,54 | 1.28 | 4 (11%) |
| 71 | GTP | AI | 501 | 70 | 29,34,34 | 1.21 | 2 (6%) | 35,54,54 | 1.28 | 4 (11%) |
| 69 | GDP | F | 500 | - | 25,30,30 | 0.95 | 1 (4%) | 30,47,47 | 1.08 | 2 (6%) |
| 71 | GTP | BC | 501 | 70 | 29,34,34 | 1.27 | 3 (10%) | 35,54,54 | 1.25 | 4 (11%) |
| 69 | GDP | MH | 500 | - | 25,30,30 | 0.96 | 1 (4%) | 30,47,47 | 1.08 | 2 (6%) |
| 69 | GDP | TF | 500 | - | 25,30,30 | 0.94 | 1 (4%) | 30,47,47 | 1.07 | 2 (6%) |
| 71 | GTP | FC | 501 | 70 | 29,34,34 | 1.24 | 2 (6%) | 35,54,54 | 1.25 | 4 (11%) |
| 71 | GTP | VA | 501 | 70 | 29,34,34 | 1.24 | 2 (6%) | 35,54,54 | 1.24 | 4 (11%) |
| 69 | GDP | QA | 500 | - | 25,30,30 | 0.97 | 1 (4%) | 30,47,47 | 1.07 | 2 (6%) |
| 71 | GTP | FI | 501 | 70 | 29,34,34 | 1.22 | 2 (6%) | 35,54,54 | 1.30 | 5 (14%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 69 | GDP | DC | 500 | - | 25,30,30 | 0.96 | 1 (4%) | 30,47,47 | 1.06 | 2 (6%) |
| 69 | GDP | MF | 500 | - | 25,30,30 | 0.95 | 1 (4%) | 30,47,47 | 1.07 | 2 (6%) |
| 71 | GTP | MG | 501 | 70 | 29,34,34 | 1.19 | 2 (6%) | 35,54,54 | 1.29 | 4 (11%) |
| 69 | GDP | AL | 500 | - | 25,30,30 | 0.95 | 1 (4%) | 30,47,47 | 1.06 | 2 (6%) |
| 71 | GTP | LD | 501 | 70 | 29,34,34 | 1.25 | 2 (6%) | 35,54,54 | 1.26 | 4 (11%) |
| 71 | GTP | UG | 501 | 70 | 29,34,34 | 1.20 | 2 (6%) | 35,54,54 | 1.28 | 4 (11%) |
| 69 | GDP | DM | 500 | - | 25,30,30 | 0.98 | 1 (4%) | 30,47,47 | 1.08 | 2 (6%) |
| 69 | GDP | S | 500 | - | 25,30,30 | 0.93 | 1 (4%) | 30,47,47 | 1.08 | 2 (6%) |
| 69 | GDP | TB | 500 | - | 25,30,30 | 0.95 | 1 (4%) | 30,47,47 | 1.09 | 2 (6%) |
| 71 | GTP | KF | 501 | 70 | 29,34,34 | 1.27 | 3 (10%) | 35,54,54 | 1.24 | 4 (11%) |
| 71 | GTP | JN | 501 | 70 | 29,34,34 | 1.23 | 2 (6%) | 35,54,54 | 1.25 | 4 (11%) |
| 69 | GDP | W | 500 | - | 25,30,30 | 0.95 | 1 (4%) | 30,47,47 | 1.07 | 2 (6%) |
| 69 | GDP | BH | 500 | - | 25,30,30 | 0.96 | 1 (4%) | 30,47,47 | 1.10 | 2 (6%) |
| 69 | GDP | IL | 500 | - | 25,30,30 | 0.96 | 1 (4%) | 30,47,47 | 1.09 | 2 (6%) |
| 71 | GTP | JJ | 501 | 70 | 29,34,34 | 1.26 | 2 (6%) | 35,54,54 | 1.25 | 3 (8%) |
| 69 | GDP | GF | 500 | - | 25,30,30 | 0.95 | 1 (4%) | 30,47,47 | 1.08 | 2 (6%) |
| 71 | GTP | KH | 501 | 70 | 29,34,34 | 1.23 | 2 (6%) | 35,54,54 | 1.35 | 4 (11%) |
| 69 | GDP | BD | 500 | - | 25,30,30 | 0.97 | 1 (4%) | 30,47,47 | 1.06 | 2 (6%) |
| 69 | GDP | KA | 500 | - | 25,30,30 | 0.95 | 1 (4%) | 30,47,47 | 1.07 | 1 (3%) |
| 71 | GTP | RD | 501 | 70 | 29,34,34 | 1.27 | 3 (10%) | 35,54,54 | 1.26 | 4 (11%) |
| 69 | GDP | ED | 500 | - | 25,30,30 | 0.96 | 1 (4%) | 30,47,47 | 1.06 | 2 (6%) |
| 69 | GDP | NB | 500 | - | 25,30,30 | 0.96 | 1 (4%) | 30,47,47 | 1.09 | 1 (3%) |
| 69 | GDP | KI | 500 | - | 25,30,30 | 0.95 | 1 (4%) | 30,47,47 | 1.08 | 2 (6%) |
| 71 | GTP | DL | 501 | - | 29,34,34 | 1.26 | 2 (6%) | 35,54,54 | 1.28 | 5 (14%) |
| 69 | GDP | AF | 500 | - | 25,30,30 | 0.95 | 1 (4%) | 30,47,47 | 1.08 | 2 (6%) |
| 69 | GDP | CI | 500 | - | 25,30,30 | 0.96 | 1 (4%) | 30,47,47 | 1.06 | 2 (6%) |
| 71 | GTP | PM | 501 | 70 | 29,34,34 | 1.26 | 2 (6%) | 35,54,54 | 1.25 | 4 (11%) |
| 69 | GDP | N | 500 | - | 25,30,30 | 0.98 | 1 (4%) | 30,47,47 | 1.06 | 2 (6%) |
| 69 | GDP | LE | 500 | - | 25,30,30 | 0.95 | 1 (4%) | 30,47,47 | 1.07 | 1 (3%) |
| 69 | GDP | QI | 500 | - | 25,30,30 | 0.94 | 1 (4%) | 30,47,47 | 1.08 | 2 (6%) |
| 71 | GTP | LN | 501 | 70 | 29,34,34 | 1.26 | 2 (6%) | 35,54,54 | 1.25 | 4 (11%) |
| 71 | GTP | DB | 501 | 70 | 29,34,34 | 1.28 | 3 (10%) | 35,54,54 | 1.25 | 4 (11%) |
| 71 | GTP | JH | 501 | 70 | 29,34,34 | 1.22 | 2 (6%) | 35,54,54 | 1.26 | 4 (11%) |
| 71 | GTP | II | 501 | 70 | 29,34,34 | 1.20 | 2 (6%) | 35,54,54 | 1.30 | 4 (11%) |
| 71 | GTP | KL | 501 | 70 | 29,34,34 | 1.25 | 3 (10%) | 35,54,54 | 1.28 | 4 (11%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 69 | GDP | CA | 500 | - | 25,30,30 | 0.97 | 1 (4%) | 30,47,47 | 1.08 | 3 (10%) |
| 71 | GTP | UE | 501 | 70 | 29,34,34 | 1.21 | 2 (6%) | 35,54,54 | 1.24 | 4 (11%) |
| 71 | GTP | HA | 501 | 70 | 29,34,34 | 1.22 | 2 (6%) | 35,54,54 | 1.23 | 4 (11%) |
| 69 | GDP | ND | 500 | - | 25,30,30 | 0.99 | 1 (4%) | 30,47,47 | 1.11 | 3 (10%) |
| 69 | GDP | SB | 500 | - | 25,30,30 | 0.95 | 1 (4%) | 30,47,47 | 1.07 | 2 (6%) |
| 69 | GDP | FH | 500 | - | 25,30,30 | 0.95 | 1 (4%) | 30,47,47 | 1.08 | 2 (6%) |
| 71 | GTP | TC | 501 | 70 | 29,34,34 | 1.21 | 2 (6%) | 35,54,54 | 1.32 | 4 (11%) |
| 69 | GDP | GH | 500 | - | 25,30,30 | 0.95 | 1 (4%) | 30,47,47 | 1.09 | 2 (6%) |
| 69 | GDP | RA | 500 | - | 25,30,30 | 0.94 | 1 (4%) | 30,47,47 | 1.07 | 2 (6%) |
| 71 | GTP | GA | 501 | 70 | 29,34,34 | 1.25 | 2 (6%) | 35,54,54 | 1.35 | 5 (14%) |
| 71 | GTP | KN | 501 | 70 | 29,34,34 | 1.21 | 2 (6%) | 35,54,54 | 1.29 | 4 (11%) |
| 71 | GTP | BG | 501 | 70 | 29,34,34 | 1.20 | 2 (6%) | 35,54,54 | 1.27 | 4 (11%) |
| 69 | GDP | VB | 500 | - | 25,30,30 | 0.94 | 1 (4%) | 30,47,47 | 1.09 | 2 (6%) |
| 71 | GTP | JF | 501 | 70 | 29,34,34 | 1.20 | 2 (6%) | 35,54,54 | 1.35 | 5 (14%) |
| 71 | GTP | GE | 501 | 70 | 29,34,34 | 1.23 | 2 (6%) | 35,54,54 | 1.33 | 4 (11%) |
| 71 | GTP | PG | 501 | - | 29,34,34 | 1.21 | 2 (6%) | 35,54,54 | 1.30 | 4 (11%) |
| 69 | GDP | SD | 500 | - | 25,30,30 | 0.94 | 1 (4%) | 30,47,47 | 1.07 | 2 (6%) |
| 71 | GTP | VG | 501 | 70 | 29,34,34 | 1.29 | 4 (13%) | 35,54,54 | 1.26 | 4 (11%) |
| 69 | GDP | AH | 500 | - | 25,30,30 | 0.95 | 1 (4%) | 30,47,47 | 1.03 | 1 (3%) |
| 71 | GTP | DJ | 501 | 70 | 29,34,34 | 1.27 | 3 (10%) | 35,54,54 | 1.29 | 4 (11%) |
| 69 | GDP | TL | 500 | - | 25,30,30 | 0.98 | 1 (4%) | 30,47,47 | 1.05 | 2 (6%) |
| 71 | GTP | AA | 501 | 70 | 29,34,34 | 1.26 | 2 (6%) | 35,54,54 | 1.23 | 4 (11%) |
| 71 | GTP | QB | 501 | 70 | 29,34,34 | 1.26 | 2 (6%) | 35,54,54 | 1.29 | 4 (11%) |
| 71 | GTP | UA | 501 | 70 | 29,34,34 | 1.25 | 2 (6%) | 35,54,54 | 1.22 | 4 (11%) |
| 71 | GTP | BA | 501 | 70 | 29,34,34 | 1.27 | 2 (6%) | 35,54,54 | 1.24 | 4 (11%) |
| 69 | GDP | FJ | 500 | - | 25,30,30 | 0.95 | 1 (4%) | 30,47,47 | 1.06 | 2 (6%) |
| 69 | GDP | WL | 500 | - | 25,30,30 | 0.95 | 1 (4%) | 30,47,47 | 1.07 | 2 (6%) |
| 69 | GDP | KK | 500 | - | 25,30,30 | 0.96 | 1 (4%) | 30,47,47 | 1.06 | 2 (6%) |
| 71 | GTP | OI | 501 | 70 | 29,34,34 | 1.22 | 2 (6%) | 35,54,54 | 1.29 | 4 (11%) |
| 69 | GDP | IJ | 500 | - | 25,30,30 | 0.95 | 1 (4%) | 30,47,47 | 1.08 | 2 (6%) |
| 71 | GTP | NA | 501 | - | 29,34,34 | 1.24 | 2 (6%) | 35,54,54 | 1.26 | 4 (11%) |
| 71 | GTP | TK | 501 | 70 | 29,34,34 | 1.22 | 2 (6%) | 35,54,54 | 1.24 | 4 (11%) |
| 71 | GTP | BM | 501 | 70 | 29,34,34 | 1.29 | 4 (13%) | 35,54,54 | 1.23 | 4 (11%) |
| 71 | GTP | LJ | 501 | 70 | 29,34,34 | 1.21 | 2 (6%) | 35,54,54 | 1.31 | 4 (11%) |
| 69 | GDP | AB | 500 | - | 25,30,30 | 0.94 | 1 (4%) | 30,47,47 | 1.07 | 1 (3%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 69 | GDP | HD | 500 | - | 25,30,30 | 0.96 | 1 (4%) | 30,47,47 | 1.08 | 2 (6%) |
| 71 | GTP | AK | 501 | 70 | 29,34,34 | 1.26 | 2 (6%) | 35,54,54 | 1.25 | 4 (11%) |
| 69 | GDP | PD | 500 | - | 25,30,30 | 0.94 | 1 (4%) | 30,47,47 | 1.06 | 2 (6%) |
| 69 | GDP | EB | 500 | - | 25,30,30 | 0.95 | 1 (4%) | 30,47,47 | 1.05 | 1 (3%) |
| 71 | GTP | OC | 501 | 70 | 29,34,34 | 1.25 | 2 (6%) | 35,54,54 | 1.28 | 4 (11%) |
| 71 | GTP | PA | 501 | 70 | 29,34,34 | 1.28 | 2 (6%) | 35,54,54 | 1.27 | 4 (11%) |
| 69 | GDP | I | 500 | - | 25,30,30 | 0.94 | 1 (4%) | 30,47,47 | 1.09 | 2 (6%) |
| 69 | GDP | OB | 500 | - | 25,30,30 | 0.95 | 1 (4%) | 30,47,47 | 1.11 | 2 (6%) |
| 71 | GTP | IE | 501 | 70 | 29,34,34 | 1.26 | 2 (6%) | 35,54,54 | 1.41 | 5 (14%) |
| 69 | GDP | AJ | 500 | - | 25,30,30 | 0.96 | 1 (4%) | 30,47,47 | 1.07 | 3 (10%) |
| 69 | GDP | LM | 500 | - | 25,30,30 | 0.95 | 1 (4%) | 30,47,47 | 1.06 | 2 (6%) |
| 71 | GTP | CJ | 501 | 70 | 29,34,34 | 1.26 | 2 (6%) | 35,54,54 | 1.25 | 4 (11%) |
| 71 | GTP | NK | 501 | - | 29,34,34 | 1.20 | 2 (6%) | 35,54,54 | 1.37 | 5 (14%) |
| 69 | GDP | PB | 500 | - | 25,30,30 | 0.95 | 1 (4%) | 30,47,47 | 1.07 | 1 (3%) |
| 71 | GTP | QD | 501 | 70 | 29,34,34 | 1.27 | 3 (10%) | 35,54,54 | 1.31 | 5 (14%) |
| 69 | GDP | LC | 500 | - | 25,30,30 | 0.95 | 1 (4%) | 30,47,47 | 1.08 | 2 (6%) |
| 69 | GDP | OH | 500 | - | 25,30,30 | 0.95 | 1 (4%) | 30,47,47 | 1.06 | 1 (3%) |
| 69 | GDP | MN | 500 | - | 25,30,30 | 0.96 | 1 (4%) | 30,47,47 | 1.07 | 3 (10%) |
| 69 | GDP | KE | 500 | - | 25,30,30 | 0.98 | 1 (4%) | 30,47,47 | 1.07 | 2 (6%) |
| 69 | GDP | VH | 500 | - | 25,30,30 | 0.95 | 1 (4%) | 30,47,47 | 1.07 | 2 (6%) |
| 71 | GTP | HM | 501 | 70 | 29,34,34 | 1.21 | 2 (6%) | 35,54,54 | 1.22 | 4 (11%) |
| 71 | GTP | WA | 501 | 70 | 29,34,34 | 1.26 | 2 (6%) | 35,54,54 | 1.24 | 4 (11%) |
| 71 | GTP | AE | 501 | 70 | 29,34,34 | 1.23 | 2 (6%) | 35,54,54 | 1.28 | 4 (11%) |
| 69 | GDP | JM | 500 | - | 25,30,30 | 0.95 | 1 (4%) | 30,47,47 | 1.05 | 2 (6%) |
| 71 | GTP | EC | 501 | 70 | 29,34,34 | 1.22 | 2 (6%) | 35,54,54 | 1.26 | 4 (11%) |
| 69 | GDP | QC | 500 | - | 25,30,30 | 0.94 | 1 (4%) | 30,47,47 | 1.09 | 2 (6%) |
| 69 | GDP | BJ | 500 | - | 25,30,30 | 0.93 | 1 (4%) | 30,47,47 | 1.08 | 1 (3%) |
| 71 | GTP | RF | 501 | 70 | 29,34,34 | 1.21 | 2 (6%) | 35,54,54 | 1.33 | 4 (11%) |
| 69 | GDP | IH | 500 | - | 25,30,30 | 0.95 | 1 (4%) | 30,47,47 | 1.06 | 2 (6%) |
| 69 | GDP | FB | 500 | - | 25,30,30 | 0.98 | 1 (4%) | 30,47,47 | 1.15 | 3 (10%) |
| 69 | GDP | PJ | 500 | - | 25,30,30 | 0.93 | 1 (4%) | 30,47,47 | 1.04 | 2 (6%) |
| 71 | GTP | CD | 501 | 70 | 29,34,34 | 1.30 | 4 (13%) | 35,54,54 | 1.30 | 5 (14%) |
| 69 | GDP | CK | 500 | - | 25,30,30 | 0.97 | 1 (4%) | 30,47,47 | 1.10 | 2 (6%) |
| 71 | GTP | LL | 501 | 70 | 29,34,34 | 1.25 | 2 (6%) | 35,54,54 | 1.23 | 4 (11%) |
| 69 | GDP | OL | 500 | - | 25,30,30 | 0.96 | 1 (4%) | 30,47,47 | 1.06 | 2 (6%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 74 | ATP | 2w | 501 | - | 28,33,33 | 0.67 | 0 | 34,52,52 | 0.59 | 1 (2%) |
| 69 | GDP | VL | 500 | - | 25,30,30 | 0.96 | 1 (4%) | 30,47,47 | 1.06 | 2 (6%) |
| 71 | GTP | AG | 501 | 70 | 29,34,34 | 1.20 | 2 (6%) | 35,54,54 | 1.23 | 4 (11%) |
| 71 | GTP | SK | 501 | 70 | 29,34,34 | 1.26 | 2 (6%) | 35,54,54 | 1.27 | 4 (11%) |
| 69 | GDP | CG | 500 | - | 25,30,30 | 0.95 | 1 (4%) | 30,47,47 | 1.08 | 2 (6%) |
| 71 | GTP | OA | 501 | 70 | 29,34,34 | 1.24 | 2 (6%) | 35,54,54 | 1.25 | 4 (11%) |
| 71 | GTP | SI | 501 | 70 | 29,34,34 | 1.20 | 2 (6%) | 35,54,54 | 1.30 | 4 (11%) |
| 71 | GTP | NM | 501 | 70 | 29,34,34 | 1.25 | 2 (6%) | 35,54,54 | 1.25 | 4 (11%) |
| 69 | GDP | M | 500 | - | 25,30,30 | 0.97 | 1 (4%) | 30,47,47 | 1.07 | 2 (6%) |
| 71 | GTP | WG | 501 | 70 | 29,34,34 | 1.18 | 2 (6%) | 35,54,54 | 1.29 | 4 (11%) |
| 69 | GDP | OF | 500 | - | 25,30,30 | 0.95 | 1 (4%) | 30,47,47 | 1.09 | 2 (6%) |
| 69 | GDP | RI | 500 | - | 25,30,30 | 0.95 | 1 (4%) | 30,47,47 | 1.06 | 1 (3%) |
| 69 | GDP | EF | 500 | - | 25,30,30 | 0.95 | 1 (4%) | 30,47,47 | 1.09 | 2 (6%) |
| 69 | GDP | WB | 500 | - | 25,30,30 | 0.94 | 1 (4%) | 30,47,47 | 1.07 | 2 (6%) |
| 69 | GDP | TH | 500 | - | 25,30,30 | 0.95 | 1 (4%) | 30,47,47 | 1.05 | 2 (6%) |
| 71 | GTP | JB | 501 | 70 | 29,34,34 | 1.22 | 2 (6%) | 35,54,54 | 1.26 | 4 (11%) |
| 69 | GDP | AN | 500 | - | 25,30,30 | 0.94 | 1 (4%) | 30,47,47 | 1.07 | 2 (6%) |
| 71 | GTP | BE | 501 | 70 | 29,34,34 | 1.20 | 2 (6%) | 35,54,54 | 1.25 | 4 (11%) |
| 71 | GTP | CH | 501 | 70 | 29,34,34 | 1.26 | 2 (6%) | 35,54,54 | 1.33 | 5 (14%) |
| 69 | GDP | MD | 500 | - | 25,30,30 | 0.95 | 1 (4%) | 30,47,47 | 1.09 | 2 (6%) |
| 69 | GDP | A | 500 | - | 25,30,30 | 0.98 | 1 (4%) | 30,47,47 | 1.07 | 2 (6%) |
| 69 | GDP | GD | 500 | - | 25,30,30 | 0.98 | 1 (4%) | 30,47,47 | 1.11 | 2 (6%) |
| 71 | GTP | OG | 501 | 70 | 29,34,34 | 1.21 | 2 (6%) | 35,54,54 | 1.37 | 5 (14%) |
| 71 | GTP | VK | 501 | 70 | 29,34,34 | 1.25 | 2 (6%) | 35,54,54 | 1.27 | 4 (11%) |
| 69 | GDP | WH | 500 | - | 25,30,30 | 0.96 | 1 (4%) | 30,47,47 | 1.08 | 2 (6%) |
| 69 | GDP | QK | 500 | - | 25,30,30 | 0.99 | 1 (4%) | 30,47,47 | 1.01 | 1 (3%) |
| 71 | GTP | Q | 501 | 70 | 29,34,34 | 1.24 | 2 (6%) | 35,54,54 | 1.26 | 4 (11%) |
| 69 | GDP | RG | 500 | - | 25,30,30 | 0.95 | 1 (4%) | 30,47,47 | 1.06 | 2 (6%) |
| 71 | GTP | OE | 501 | 70 | 29,34,34 | 1.25 | 3 (10%) | 35,54,54 | 1.32 | 5 (14%) |
| 69 | GDP | CM | 500 | - | 25,30,30 | 0.97 | 1 (4%) | 30,47,47 | 1.22 | 3 (10%) |
| 69 | GDP | GL | 500 | - | 25,30,30 | 0.93 | 1 (4%) | 30,47,47 | 1.08 | 2 (6%) |
| 69 | GDP | UL | 500 | - | 25,30,30 | 0.96 | 1 (4%) | 30,47,47 | 1.07 | 2 (6%) |
| 71 | GTP | GC | 501 | 70 | 29,34,34 | 1.21 | 2 (6%) | 35,54,54 | 1.38 | 5 (14%) |
| 71 | GTP | FA | 501 | 70 | 29,34,34 | 1.24 | 2 (6%) | 35,54,54 | 1.25 | 4 (11%) |
| 69 | GDP | SJ | 500 | - | 25,30,30 | 0.95 | 1 (4%) | 30,47,47 | 1.06 | 2 (6%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 71 | GTP | IG | 501 | 70 | 29,34,34 | 1.21 | 2 (6%) | 35,54,54 | 1.25 | 4 (11%) |
| 69 | GDP | DI | 500 | - | 25,30,30 | 0.95 | 1 (4%) | 30,47,47 | 1.08 | 2 (6%) |
| 71 | GTP | WM | 501 | 70 | 29,34,34 | 1.27 | 2 (6%) | 35,54,54 | 1.25 | 4 (11%) |
| 69 | GDP | E | 500 | - | 25,30,30 | 0.99 | 1 (4%) | 30,47,47 | 1.03 | 2 (6%) |
| 69 | GDP | U | 500 | - | 25,30,30 | 0.95 | 1 (4%) | 30,47,47 | 1.09 | 2 (6%) |
| 69 | GDP | VD | 500 | - | 25,30,30 | 0.95 | 1 (4%) | 30,47,47 | 1.07 | 2 (6%) |
| 71 | GTP | BK | 501 | 70 | 29,34,34 | 1.24 | 2 (6%) | 35,54,54 | 1.27 | 4 (11%) |
| 71 | GTP | SE | 501 | 70 | 29,34,34 | 1.21 | 1 (3%) | 35,54,54 | 1.32 | 5 (14%) |
| 71 | GTP | HE | 501 | 70 | 29,34,34 | 1.22 | 2 (6%) | 35,54,54 | 1.24 | 4 (11%) |
| 71 | GTP | L | 501 | 70 | 29,34,34 | 1.24 | 2 (6%) | 35,54,54 | 1.26 | 4 (11%) |
| 69 | GDP | OJ | 500 | - | 25,30,30 | 0.95 | 1 (4%) | 30,47,47 | 1.07 | 2 (6%) |
| 71 | GTP | EG | 501 | 70 | 29,34,34 | 1.25 | 2 (6%) | 35,54,54 | 1.32 | 5 (14%) |
| 71 | GTP | JD | 501 | 70 | 29,34,34 | 1.24 | 2 (6%) | 35,54,54 | 1.25 | 3 (8%) |
| 71 | GTP | VE | 501 | 70 | 29,34,34 | 1.22 | 2 (6%) | 35,54,54 | 1.34 | 5 (14%) |
| 71 | GTP | DH | 501 | 70 | 29,34,34 | 1.17 | 2 (6%) | 35,54,54 | 1.32 | 4 (11%) |
| 71 | GTP | DF | 501 | 70 | 29,34,34 | 1.25 | 3 (10%) | 35,54,54 | 1.32 | 5 (14%) |
| 74 | ATP | 2v | 501 | - | 28,33,33 | 0.64 | 0 | 34,52,52 | 0.60 | 1 (2%) |
| 69 | GDP | WD | 500 | - | 25,30,30 | 0.95 | 1 (4%) | 30,47,47 | 1.07 | 2 (6%) |
| 71 | GTP | VM | 501 | 70 | 29,34,34 | 1.26 | 2 (6%) | 35,54,54 | 1.23 | 4 (11%) |
| 69 | GDP | HB | 500 | - | 25,30,30 | 0.96 | 1 (4%) | 30,47,47 | 1.07 | 2 (6%) |
| 69 | GDP | OD | 500 | - | 25,30,30 | 0.96 | 1 (4%) | 30,47,47 | 1.08 | 2 (6%) |
| 71 | GTP | QL | 501 | - | 29,34,34 | 1.25 | 2 (6%) | 35,54,54 | 1.26 | 4 (11%) |
| 71 | GTP | UC | 501 | 70 | 29,34,34 | 1.24 | 2 (6%) | 35,54,54 | 1.27 | 4 (11%) |
| 69 | GDP | NJ | 500 | - | 25,30,30 | 0.96 | 1 (4%) | 30,47,47 | 1.08 | 2 (6%) |
| 71 | GTP | QF | 501 | 70 | 29,34,34 | 1.19 | 2 (6%) | 35,54,54 | 1.31 | 4 (11%) |
| 71 | GTP | PI | 501 | 70 | 29,34,34 | 1.22 | 2 (6%) | 35,54,54 | 1.27 | 4 (11%) |
| 71 | GTP | IK | 501 | 70 | 29,34,34 | 1.49 | 6 (20%) | 35,54,54 | 1.36 | 5 (14%) |
| 69 | GDP | IF | 500 | - | 25,30,30 | 0.95 | 1 (4%) | 30,47,47 | 1.07 | 2 (6%) |
| 71 | GTP | GK | 501 | 70 | 29,34,34 | 1.26 | 3 (10%) | 35,54,54 | 1.27 | 4 (11%) |
| 71 | GTP | EA | 501 | 70 | 29,34,34 | 1.26 | 2 (6%) | 35,54,54 | 1.34 | 5 (14%) |
| 71 | GTP | OM | 501 | 70 | 29,34,34 | 1.23 | 2 (6%) | 35,54,54 | 1.26 | 4 (11%) |
| 69 | GDP | JG | 500 | - | 25,30,30 | 0.96 | 1 (4%) | 30,47,47 | 1.05 | 2 (6%) |
| 71 | GTP | KB | 501 | 70 | 29,34,34 | 1.23 | 2 (6%) | 35,54,54 | 1.23 | 4 (11%) |
| 71 | GTP | MA | 501 | 70 | 29,34,34 | 1.26 | 2 (6%) | 35,54,54 | 1.25 | 4 (11%) |
| 69 | GDP | FD | 500 | - | 25,30,30 | 0.95 | 1 (4%) | 30,47,47 | 1.06 | 2 (6%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 71 | GTP | FE | 501 | 70 | 29,34,34 | 1.24 | 2 (6%) | 35,54,54 | 1.22 | 4 (11%) |
| 69 | GDP | HJ | 500 | - | 25,30,30 | 0.95 | 1 (4%) | 30,47,47 | 1.06 | 2 (6%) |
| 69 | GDP | DK | 500 | - | 25,30,30 | 0.95 | 1 (4%) | 30,47,47 | 1.06 | 2 (6%) |
| 69 | GDP | LA | 500 | - | 25,30,30 | 0.96 | 1 (4%) | 30,47,47 | 1.06 | 2 (6%) |
| 69 | GDP | FL | 500 | - | 25,30,30 | 0.95 | 1 (4%) | 30,47,47 | 1.09 | 2 (6%) |
| 69 | GDP | HL | 500 | - | 25,30,30 | 0.96 | 1 (4%) | 30,47,47 | 1.03 | 1 (3%) |
| 71 | GTP | MM | 501 | 70 | 29,34,34 | 1.26 | 2 (6%) | 35,54,54 | 1.28 | 4 (11%) |
| 71 | GTP | WE | 501 | 70 | 29,34,34 | 1.25 | 2 (6%) | 35,54,54 | 1.31 | 5 (14%) |
| 71 | GTP | TE | 501 | 70 | 29,34,34 | 1.20 | 2 (6%) | 35,54,54 | 1.25 | 4 (11%) |
| 69 | GDP | NL | 500 | - | 25,30,30 | 0.95 | 1 (4%) | 30,47,47 | 1.05 | 1 (3%) |
| 71 | GTP | HI | 501 | 70 | 29,34,34 | 1.19 | 2 (6%) | 35,54,54 | 1.26 | 4 (11%) |
| 71 | GTP | BI | 501 | 70 | 29,34,34 | 1.29 | 4 (13%) | 35,54,54 | 1.31 | 4 (11%) |
| 69 | GDP | EL | 500 | - | 25,30,30 | 0.98 | 1 (4%) | 30,47,47 | 1.07 | 2 (6%) |
| 71 | GTP | C | 501 | 70 | 29,34,34 | 1.26 | 2 (6%) | 35,54,54 | 1.27 | 4 (11%) |
| 69 | GDP | UF | 500 | - | 25,30,30 | 0.95 | 1 (4%) | 30,47,47 | 1.08 | 2 (6%) |
| 71 | GTP | GG | 501 | 70 | 29,34,34 | 1.21 | 2 (6%) | 35,54,54 | 1.34 | 5 (14%) |
| 69 | GDP | UD | 500 | - | 25,30,30 | 0.96 | 1 (4%) | 30,47,47 | 1.07 | 1 (3%) |
| 69 | GDP | DA | 500 | - | 25,30,30 | 0.95 | 1 (4%) | 30,47,47 | 1.10 | 2 (6%) |
| 71 | GTP | TI | 501 | 70 | 29,34,34 | 1.27 | 2 (6%) | 35,54,54 | 1.26 | 4 (11%) |
| 69 | GDP | SF | 500 | - | 25,30,30 | 0.94 | 1 (4%) | 30,47,47 | 1.05 | 1 (3%) |
| 69 | GDP | P | 500 | - | 25,30,30 | 0.97 | 1 (4%) | 30,47,47 | 1.16 | 3 (10%) |
| 71 | GTP | NG | 501 | - | 29,34,34 | 1.31 | 4 (13%) | 35,54,54 | 1.30 | 4 (11%) |
| 71 | GTP | FG | 501 | 70 | 29,34,34 | 1.24 | 2 (6%) | 35,54,54 | 1.30 | 4 (11%) |
| 69 | GDP | ML | 500 | - | 25,30,30 | 0.97 | 1 (4%) | 30,47,47 | 1.07 | 2 (6%) |
| 69 | GDP | QG | 500 | - | 25,30,30 | 0.94 | 1 (4%) | 30,47,47 | 1.10 | 2 (6%) |
| 69 | GDP | O | 500 | - | 25,30,30 | 0.97 | 1 (4%) | 30,47,47 | 1.04 | 1 (3%) |
| 71 | GTP | EE | 501 | 70 | 29,34,34 | 1.30 | 4 (13%) | 35,54,54 | 1.28 | 5 (14%) |
| 69 | GDP | EJ | 500 | - | 25,30,30 | 0.96 | 1 (4%) | 30,47,47 | 1.07 | 2 (6%) |
| 69 | GDP | JK | 500 | - | 25,30,30 | 0.95 | 1 (4%) | 30,47,47 | 1.03 | 2 (6%) |
| 71 | GTP | VI | 501 | 70 | 29,34,34 | 1.24 | 2 (6%) | 35,54,54 | 1.31 | 4 (11%) |
| 71 | GTP | SG | 501 | 70 | 29,34,34 | 1.23 | 2 (6%) | 35,54,54 | 1.30 | 5 (14%) |
| 69 | GDP | KC | 500 | - | 25,30,30 | 0.95 | 1 (4%) | 30,47,47 | 1.07 | 2 (6%) |
| 69 | GDP | BB | 500 | - | 25,30,30 | 0.97 | 1 (4%) | 30,47,47 | 1.09 | 2 (6%) |
| 71 | GTP | UK | 501 | 70 | 29,34,34 | 1.25 | 2 (6%) | 35,54,54 | 1.26 | 4 (11%) |
| 71 | GTP | PK | 501 | 70 | 29,34,34 | 1.23 | 2 (6%) | 35,54,54 | 1.30 | 4 (11%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 69 | GDP | BL | 500 | - | 25,30,30 | 0.95 | 1 (4%) | 30,47,47 | 1.08 | 2 (6%) |
| 69 | GDP | LG | 500 | - | 25,30,30 | 0.96 | 1 (4%) | 30,47,47 | 1.09 | 2 (6%) |
| 71 | GTP | TA | 501 | 70 | 29,34,34 | 1.27 | 3 (10%) | 35,54,54 | 1.31 | 5 (14%) |
| 69 | GDP | T | 500 | - | 25,30,30 | 0.92 | 1 (4%) | 30,47,47 | 1.05 | 2 (6%) |
| 69 | GDP | BN | 500 | - | 25,30,30 | 0.99 | 1 (4%) | 30,47,47 | 1.14 | 3 (10%) |
| 69 | GDP | GJ | 500 | - | 25,30,30 | 0.94 | 1 (4%) | 30,47,47 | 1.09 | 2 (6%) |
| 69 | GDP | UB | 500 | - | 25,30,30 | 0.97 | 1 (4%) | 30,47,47 | 1.10 | 2 (6%) |
| 69 | GDP | AD | 500 | - | 25,30,30 | 0.95 | 1 (4%) | 30,47,47 | 1.08 | 2 (6%) |
| 71 | GTP | EI | 501 | 70 | 29,34,34 | 1.22 | 2 (6%) | 35,54,54 | 1.26 | 4 (11%) |
| 69 | GDP | TJ | 500 | - | 25,30,30 | 0.95 | 1 (4%) | 30,47,47 | 1.08 | 2 (6%) |
| 69 | GDP | WF | 500 | - | 25,30,30 | 0.94 | 1 (4%) | 30,47,47 | 1.07 | 2 (6%) |
| 69 | GDP | SH | 500 | - | 25,30,30 | 0.96 | 1 (4%) | 30,47,47 | 1.08 | 2 (6%) |
| 71 | GTP | AC | 501 | 70 | 29,34,34 | 1.22 | 2 (6%) | 35,54,54 | 1.23 | 4 (11%) |
| 71 | GTP | IC | 501 | 70 | 29,34,34 | 1.28 | 3 (10%) | 35,54,54 | 1.31 | 4 (11%) |
| 71 | GTP | IM | 501 | 70 | 29,34,34 | 1.24 | 2 (6%) | 35,54,54 | 1.25 | 4 (11%) |

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 |
|-----|------|-------|-----|------|---------|------------|---------|
| 69 | GDP | CE | 500 | - | - | 1/12/32/32 | 0/3/3/3 |
| 69 | GDP | HF | 500 | - | - | 2/12/32/32 | 0/3/3/3 |
| 71 | GTP | MK | 501 | 70 | - | 5/18/38/38 | 0/3/3/3 |
| 71 | GTP | HK | 501 | 70 | - | 4/18/38/38 | 0/3/3/3 |
| 69 | GDP | GB | 500 | - | - | 1/12/32/32 | 0/3/3/3 |
| 69 | GDP | UJ | 500 | - | - | 1/12/32/32 | 0/3/3/3 |
| 69 | GDP | TD | 500 | - | - | 1/12/32/32 | 0/3/3/3 |
| 71 | GTP | NC | 501 | 70 | - | 3/18/38/38 | 0/3/3/3 |
| 71 | GTP | IA | 501 | 70 | - | 6/18/38/38 | 0/3/3/3 |
| 69 | GDP | EH | 500 | - | - | 1/12/32/32 | 0/3/3/3 |
| 71 | GTP | TG | 501 | 70 | - | 1/18/38/38 | 0/3/3/3 |
| 69 | GDP | VF | 500 | - | - | 1/12/32/32 | 0/3/3/3 |
| 71 | GTP | LB | 501 | 70 | - | 3/18/38/38 | 0/3/3/3 |
| 69 | GDP | MB | 500 | - | - | 2/12/32/32 | 0/3/3/3 |
| 71 | GTP | HG | 501 | 70 | - | 3/18/38/38 | 0/3/3/3 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|-------------|---------|
| 71 | GTP | EK | 501 | 70 | - | 3/18/38/38 | 0/3/3/3 |
| 71 | GTP | UI | 501 | 70 | - | 3/18/38/38 | 0/3/3/3 |
| 69 | GDP | V | 500 | - | - | 1/12/32/32 | 0/3/3/3 |
| 71 | GTP | JL | 501 | 70 | - | 3/18/38/38 | 0/3/3/3 |
| 71 | GTP | QH | 501 | 70 | - | 10/18/38/38 | 0/3/3/3 |
| 71 | GTP | WI | 501 | 70 | - | 3/18/38/38 | 0/3/3/3 |
| 69 | GDP | QE | 500 | - | - | 2/12/32/32 | 0/3/3/3 |
| 71 | GTP | GI | 501 | 70 | - | 0/18/38/38 | 0/3/3/3 |
| 71 | GTP | SA | 501 | 70 | - | 3/18/38/38 | 0/3/3/3 |
| 71 | GTP | PC | 501 | 70 | - | 3/18/38/38 | 0/3/3/3 |
| 69 | GDP | LI | 500 | - | - | 3/12/32/32 | 0/3/3/3 |
| 71 | GTP | MI | 501 | 70 | - | 5/18/38/38 | 0/3/3/3 |
| 71 | GTP | RJ | 501 | - | - | 1/18/38/38 | 0/3/3/3 |
| 69 | GDP | JC | 500 | - | - | 2/12/32/32 | 0/3/3/3 |
| 69 | GDP | ID | 500 | - | - | 1/12/32/32 | 0/3/3/3 |
| 69 | GDP | KG | 500 | - | - | 2/12/32/32 | 0/3/3/3 |
| 71 | GTP | FK | 501 | - | - | 3/18/38/38 | 0/3/3/3 |
| 69 | GDP | RC | 500 | - | - | 1/12/32/32 | 0/3/3/3 |
| 69 | GDP | JA | 500 | - | - | 1/12/32/32 | 0/3/3/3 |
| 69 | GDP | DE | 500 | - | - | 1/12/32/32 | 0/3/3/3 |
| 71 | GTP | RH | 501 | 70 | - | 2/18/38/38 | 0/3/3/3 |
| 71 | GTP | CF | 501 | 70 | - | 7/18/38/38 | 0/3/3/3 |
| 69 | GDP | LK | 500 | - | - | 1/12/32/32 | 0/3/3/3 |
| 71 | GTP | WK | 501 | 70 | - | 5/18/38/38 | 0/3/3/3 |
| 69 | GDP | NF | 500 | - | - | 3/12/32/32 | 0/3/3/3 |
| 71 | GTP | DD | 501 | 70 | - | 3/18/38/38 | 0/3/3/3 |
| 69 | GDP | CC | 500 | - | - | 2/12/32/32 | 0/3/3/3 |
| 71 | GTP | OK | 501 | - | - | 6/18/38/38 | 0/3/3/3 |
| 69 | GDP | BF | 500 | - | - | 1/12/32/32 | 0/3/3/3 |
| 69 | GDP | HH | 500 | - | - | 1/12/32/32 | 0/3/3/3 |
| 71 | GTP | ME | 501 | 70 | - | 5/18/38/38 | 0/3/3/3 |
| 71 | GTP | RB | 501 | 70 | - | 3/18/38/38 | 0/3/3/3 |
| 69 | GDP | H | 500 | - | - | 1/12/32/32 | 0/3/3/3 |
| 69 | GDP | VJ | 500 | - | - | 2/12/32/32 | 0/3/3/3 |
| 71 | GTP | RL | 501 | 70 | - | 9/18/38/38 | 0/3/3/3 |
| 71 | GTP | PE | 501 | 70 | - | 0/18/38/38 | 0/3/3/3 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|-------------|---------|
| 71 | GTP | LH | 501 | 70 | - | 3/18/38/38 | 0/3/3/3 |
| 69 | GDP | PF | 500 | - | - | 3/12/32/32 | 0/3/3/3 |
| 69 | GDP | G | 500 | - | - | 0/12/32/32 | 0/3/3/3 |
| 71 | GTP | WC | 501 | 70 | - | 2/18/38/38 | 0/3/3/3 |
| 69 | GDP | PL | 500 | - | - | 1/12/32/32 | 0/3/3/3 |
| 69 | GDP | JE | 500 | - | - | 1/12/32/32 | 0/3/3/3 |
| 69 | GDP | DG | 500 | - | - | 2/12/32/32 | 0/3/3/3 |
| 71 | GTP | J | 501 | 70 | - | 8/18/38/38 | 0/3/3/3 |
| 71 | GTP | R | 501 | 70 | - | 6/18/38/38 | 0/3/3/3 |
| 69 | GDP | IB | 500 | - | - | 3/12/32/32 | 0/3/3/3 |
| 71 | GTP | LF | 501 | 70 | - | 2/18/38/38 | 0/3/3/3 |
| 71 | GTP | KJ | 501 | 70 | - | 3/18/38/38 | 0/3/3/3 |
| 69 | GDP | JI | 500 | - | - | 1/12/32/32 | 0/3/3/3 |
| 69 | GDP | RK | 500 | - | - | 2/12/32/32 | 0/3/3/3 |
| 71 | GTP | SC | 501 | 70 | - | 6/18/38/38 | 0/3/3/3 |
| 69 | GDP | WJ | 500 | - | - | 1/12/32/32 | 0/3/3/3 |
| 69 | GDP | LO | 500 | - | - | 3/12/32/32 | 0/3/3/3 |
| 71 | GTP | KD | 501 | 70 | - | 3/18/38/38 | 0/3/3/3 |
| 71 | GTP | NI | 501 | 70 | - | 1/18/38/38 | 0/3/3/3 |
| 69 | GDP | MJ | 500 | - | - | 3/12/32/32 | 0/3/3/3 |
| 69 | GDP | KM | 500 | - | - | 2/12/32/32 | 0/3/3/3 |
| 71 | GTP | D | 501 | - | - | 12/18/38/38 | 0/3/3/3 |
| 71 | GTP | VC | 501 | 70 | - | 6/18/38/38 | 0/3/3/3 |
| 69 | GDP | NH | 500 | - | - | 2/12/32/32 | 0/3/3/3 |
| 69 | GDP | RE | 500 | - | - | 0/12/32/32 | 0/3/3/3 |
| 71 | GTP | QJ | 501 | 70 | - | 4/18/38/38 | 0/3/3/3 |
| 71 | GTP | CB | 501 | 70 | - | 3/18/38/38 | 0/3/3/3 |
| 71 | GTP | AM | 501 | 70 | - | 5/18/38/38 | 0/3/3/3 |
| 71 | GTP | NE | 501 | 70 | - | 4/18/38/38 | 0/3/3/3 |
| 69 | GDP | PH | 500 | - | - | 1/12/32/32 | 0/3/3/3 |
| 69 | GDP | FF | 500 | - | - | 2/12/32/32 | 0/3/3/3 |
| 71 | GTP | HC | 501 | 70 | - | 7/18/38/38 | 0/3/3/3 |
| 69 | GDP | UH | 500 | - | - | 1/12/32/32 | 0/3/3/3 |
| 71 | GTP | K | 501 | 70 | - | 2/18/38/38 | 0/3/3/3 |
| 71 | GTP | CL | 501 | 70 | - | 8/18/38/38 | 0/3/3/3 |
| 71 | GTP | MC | 501 | 70 | - | 4/18/38/38 | 0/3/3/3 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|------------|---------|
| 71 | GTP | AI | 501 | 70 | - | 0/18/38/38 | 0/3/3/3 |
| 69 | GDP | F | 500 | - | - | 3/12/32/32 | 0/3/3/3 |
| 71 | GTP | BC | 501 | 70 | - | 0/18/38/38 | 0/3/3/3 |
| 69 | GDP | MH | 500 | - | - | 1/12/32/32 | 0/3/3/3 |
| 69 | GDP | TF | 500 | - | - | 1/12/32/32 | 0/3/3/3 |
| 71 | GTP | FC | 501 | 70 | - | 4/18/38/38 | 0/3/3/3 |
| 71 | GTP | VA | 501 | 70 | - | 4/18/38/38 | 0/3/3/3 |
| 69 | GDP | QA | 500 | - | - | 1/12/32/32 | 0/3/3/3 |
| 71 | GTP | FI | 501 | 70 | - | 3/18/38/38 | 0/3/3/3 |
| 69 | GDP | DC | 500 | - | - | 1/12/32/32 | 0/3/3/3 |
| 69 | GDP | MF | 500 | - | - | 3/12/32/32 | 0/3/3/3 |
| 71 | GTP | MG | 501 | 70 | - | 5/18/38/38 | 0/3/3/3 |
| 69 | GDP | AL | 500 | - | - | 2/12/32/32 | 0/3/3/3 |
| 71 | GTP | LD | 501 | 70 | - | 6/18/38/38 | 0/3/3/3 |
| 71 | GTP | UG | 501 | 70 | - | 5/18/38/38 | 0/3/3/3 |
| 69 | GDP | DM | 500 | - | - | 1/12/32/32 | 0/3/3/3 |
| 69 | GDP | S | 500 | - | - | 2/12/32/32 | 0/3/3/3 |
| 69 | GDP | TB | 500 | - | - | 3/12/32/32 | 0/3/3/3 |
| 71 | GTP | KF | 501 | 70 | - | 6/18/38/38 | 0/3/3/3 |
| 71 | GTP | JN | 501 | 70 | - | 3/18/38/38 | 0/3/3/3 |
| 69 | GDP | W | 500 | - | - | 1/12/32/32 | 0/3/3/3 |
| 69 | GDP | BH | 500 | - | - | 2/12/32/32 | 0/3/3/3 |
| 69 | GDP | IL | 500 | - | - | 0/12/32/32 | 0/3/3/3 |
| 71 | GTP | JJ | 501 | 70 | - | 3/18/38/38 | 0/3/3/3 |
| 69 | GDP | GF | 500 | - | - | 4/12/32/32 | 0/3/3/3 |
| 71 | GTP | KH | 501 | 70 | - | 5/18/38/38 | 0/3/3/3 |
| 69 | GDP | BD | 500 | - | - | 1/12/32/32 | 0/3/3/3 |
| 69 | GDP | KA | 500 | - | - | 3/12/32/32 | 0/3/3/3 |
| 71 | GTP | RD | 501 | 70 | - | 7/18/38/38 | 0/3/3/3 |
| 69 | GDP | ED | 500 | - | - | 4/12/32/32 | 0/3/3/3 |
| 69 | GDP | NB | 500 | - | - | 3/12/32/32 | 0/3/3/3 |
| 69 | GDP | KI | 500 | - | - | 3/12/32/32 | 0/3/3/3 |
| 71 | GTP | DL | 501 | - | - | 8/18/38/38 | 0/3/3/3 |
| 69 | GDP | AF | 500 | - | - | 1/12/32/32 | 0/3/3/3 |
| 69 | GDP | CI | 500 | - | - | 1/12/32/32 | 0/3/3/3 |
| 71 | GTP | PM | 501 | 70 | - | 3/18/38/38 | 0/3/3/3 |
| 69 | GDP | N | 500 | - | - | 1/12/32/32 | 0/3/3/3 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|------------|---------|
| 69 | GDP | LE | 500 | - | - | 2/12/32/32 | 0/3/3/3 |
| 69 | GDP | QI | 500 | - | - | 2/12/32/32 | 0/3/3/3 |
| 71 | GTP | LN | 501 | 70 | - | 3/18/38/38 | 0/3/3/3 |
| 71 | GTP | DB | 501 | 70 | - | 3/18/38/38 | 0/3/3/3 |
| 71 | GTP | JH | 501 | 70 | - | 5/18/38/38 | 0/3/3/3 |
| 71 | GTP | II | 501 | 70 | - | 3/18/38/38 | 0/3/3/3 |
| 71 | GTP | KL | 501 | 70 | - | 2/18/38/38 | 0/3/3/3 |
| 69 | GDP | CA | 500 | - | - | 3/12/32/32 | 0/3/3/3 |
| 71 | GTP | UE | 501 | 70 | - | 9/18/38/38 | 0/3/3/3 |
| 71 | GTP | HA | 501 | 70 | - | 3/18/38/38 | 0/3/3/3 |
| 69 | GDP | ND | 500 | - | - | 0/12/32/32 | 0/3/3/3 |
| 69 | GDP | SB | 500 | - | - | 3/12/32/32 | 0/3/3/3 |
| 69 | GDP | FH | 500 | - | - | 1/12/32/32 | 0/3/3/3 |
| 71 | GTP | TC | 501 | 70 | - | 5/18/38/38 | 0/3/3/3 |
| 69 | GDP | GH | 500 | - | - | 3/12/32/32 | 0/3/3/3 |
| 69 | GDP | RA | 500 | - | - | 1/12/32/32 | 0/3/3/3 |
| 71 | GTP | GA | 501 | 70 | - | 8/18/38/38 | 0/3/3/3 |
| 71 | GTP | KN | 501 | 70 | - | 3/18/38/38 | 0/3/3/3 |
| 71 | GTP | BG | 501 | 70 | - | 0/18/38/38 | 0/3/3/3 |
| 69 | GDP | VB | 500 | - | - | 1/12/32/32 | 0/3/3/3 |
| 71 | GTP | JF | 501 | 70 | - | 3/18/38/38 | 0/3/3/3 |
| 71 | GTP | GE | 501 | 70 | - | 4/18/38/38 | 0/3/3/3 |
| 71 | GTP | PG | 501 | - | - | 5/18/38/38 | 0/3/3/3 |
| 69 | GDP | SD | 500 | - | - | 3/12/32/32 | 0/3/3/3 |
| 71 | GTP | VG | 501 | 70 | - | 4/18/38/38 | 0/3/3/3 |
| 69 | GDP | AH | 500 | - | - | 2/12/32/32 | 0/3/3/3 |
| 71 | GTP | DJ | 501 | 70 | - | 4/18/38/38 | 0/3/3/3 |
| 69 | GDP | TL | 500 | - | - | 0/12/32/32 | 0/3/3/3 |
| 71 | GTP | AA | 501 | 70 | - | 4/18/38/38 | 0/3/3/3 |
| 71 | GTP | QB | 501 | 70 | - | 2/18/38/38 | 0/3/3/3 |
| 71 | GTP | UA | 501 | 70 | - | 5/18/38/38 | 0/3/3/3 |
| 71 | GTP | BA | 501 | 70 | - | 3/18/38/38 | 0/3/3/3 |
| 69 | GDP | FJ | 500 | - | - | 2/12/32/32 | 0/3/3/3 |
| 69 | GDP | WL | 500 | - | - | 1/12/32/32 | 0/3/3/3 |
| 69 | GDP | KK | 500 | - | - | 1/12/32/32 | 0/3/3/3 |
| 71 | GTP | OI | 501 | 70 | - | 6/18/38/38 | 0/3/3/3 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|------------|---------|
| 69 | GDP | IJ | 500 | - | - | 2/12/32/32 | 0/3/3/3 |
| 71 | GTP | NA | 501 | - | - | 7/18/38/38 | 0/3/3/3 |
| 71 | GTP | TK | 501 | 70 | - | 5/18/38/38 | 0/3/3/3 |
| 71 | GTP | BM | 501 | 70 | - | 6/18/38/38 | 0/3/3/3 |
| 71 | GTP | LJ | 501 | 70 | - | 4/18/38/38 | 0/3/3/3 |
| 69 | GDP | AB | 500 | - | - | 1/12/32/32 | 0/3/3/3 |
| 69 | GDP | HD | 500 | - | - | 3/12/32/32 | 0/3/3/3 |
| 71 | GTP | AK | 501 | 70 | - | 3/18/38/38 | 0/3/3/3 |
| 69 | GDP | PD | 500 | - | - | 4/12/32/32 | 0/3/3/3 |
| 69 | GDP | EB | 500 | - | - | 4/12/32/32 | 0/3/3/3 |
| 71 | GTP | OC | 501 | 70 | - | 1/18/38/38 | 0/3/3/3 |
| 71 | GTP | PA | 501 | 70 | - | 0/18/38/38 | 0/3/3/3 |
| 69 | GDP | I | 500 | - | - | 0/12/32/32 | 0/3/3/3 |
| 69 | GDP | OB | 500 | - | - | 5/12/32/32 | 0/3/3/3 |
| 71 | GTP | IE | 501 | 70 | - | 2/18/38/38 | 0/3/3/3 |
| 69 | GDP | AJ | 500 | - | - | 1/12/32/32 | 0/3/3/3 |
| 69 | GDP | LM | 500 | - | - | 1/12/32/32 | 0/3/3/3 |
| 71 | GTP | CJ | 501 | 70 | - | 3/18/38/38 | 0/3/3/3 |
| 71 | GTP | NK | 501 | - | - | 3/18/38/38 | 0/3/3/3 |
| 69 | GDP | PB | 500 | - | - | 1/12/32/32 | 0/3/3/3 |
| 71 | GTP | QD | 501 | 70 | - | 5/18/38/38 | 0/3/3/3 |
| 69 | GDP | LC | 500 | - | - | 2/12/32/32 | 0/3/3/3 |
| 69 | GDP | OH | 500 | - | - | 3/12/32/32 | 0/3/3/3 |
| 69 | GDP | MN | 500 | - | - | 2/12/32/32 | 0/3/3/3 |
| 69 | GDP | KE | 500 | - | - | 1/12/32/32 | 0/3/3/3 |
| 69 | GDP | VH | 500 | - | - | 1/12/32/32 | 0/3/3/3 |
| 71 | GTP | HM | 501 | 70 | - | 3/18/38/38 | 0/3/3/3 |
| 71 | GTP | WA | 501 | 70 | - | 2/18/38/38 | 0/3/3/3 |
| 71 | GTP | AE | 501 | 70 | - | 4/18/38/38 | 0/3/3/3 |
| 69 | GDP | JM | 500 | - | - | 0/12/32/32 | 0/3/3/3 |
| 71 | GTP | EC | 501 | 70 | - | 4/18/38/38 | 0/3/3/3 |
| 69 | GDP | QC | 500 | - | - | 2/12/32/32 | 0/3/3/3 |
| 69 | GDP | BJ | 500 | - | - | 2/12/32/32 | 0/3/3/3 |
| 71 | GTP | RF | 501 | 70 | - | 1/18/38/38 | 0/3/3/3 |
| 69 | GDP | IH | 500 | - | - | 2/12/32/32 | 0/3/3/3 |
| 69 | GDP | FB | 500 | - | - | 0/12/32/32 | 0/3/3/3 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|------------|---------|
| 69 | GDP | PJ | 500 | - | - | 3/12/32/32 | 0/3/3/3 |
| 71 | GTP | CD | 501 | 70 | - | 3/18/38/38 | 0/3/3/3 |
| 69 | GDP | CK | 500 | - | - | 3/12/32/32 | 0/3/3/3 |
| 71 | GTP | LL | 501 | 70 | - | 4/18/38/38 | 0/3/3/3 |
| 69 | GDP | OL | 500 | - | - | 2/12/32/32 | 0/3/3/3 |
| 74 | ATP | 2w | 501 | - | - | 5/18/38/38 | 0/3/3/3 |
| 69 | GDP | VL | 500 | - | - | 1/12/32/32 | 0/3/3/3 |
| 71 | GTP | AG | 501 | 70 | - | 7/18/38/38 | 0/3/3/3 |
| 71 | GTP | SK | 501 | 70 | - | 0/18/38/38 | 0/3/3/3 |
| 69 | GDP | CG | 500 | - | - | 2/12/32/32 | 0/3/3/3 |
| 71 | GTP | OA | 501 | 70 | - | 4/18/38/38 | 0/3/3/3 |
| 71 | GTP | SI | 501 | 70 | - | 3/18/38/38 | 0/3/3/3 |
| 71 | GTP | NM | 501 | 70 | - | 4/18/38/38 | 0/3/3/3 |
| 69 | GDP | M | 500 | - | - | 3/12/32/32 | 0/3/3/3 |
| 71 | GTP | WG | 501 | 70 | - | 1/18/38/38 | 0/3/3/3 |
| 69 | GDP | OF | 500 | - | - | 1/12/32/32 | 0/3/3/3 |
| 69 | GDP | RI | 500 | - | - | 0/12/32/32 | 0/3/3/3 |
| 69 | GDP | EF | 500 | - | - | 3/12/32/32 | 0/3/3/3 |
| 69 | GDP | WB | 500 | - | - | 1/12/32/32 | 0/3/3/3 |
| 69 | GDP | TH | 500 | - | - | 1/12/32/32 | 0/3/3/3 |
| 71 | GTP | JB | 501 | 70 | - | 2/18/38/38 | 0/3/3/3 |
| 69 | GDP | AN | 500 | - | - | 1/12/32/32 | 0/3/3/3 |
| 71 | GTP | BE | 501 | 70 | - | 9/18/38/38 | 0/3/3/3 |
| 71 | GTP | CH | 501 | 70 | - | 5/18/38/38 | 0/3/3/3 |
| 69 | GDP | MD | 500 | - | - | 1/12/32/32 | 0/3/3/3 |
| 69 | GDP | A | 500 | - | - | 2/12/32/32 | 0/3/3/3 |
| 69 | GDP | GD | 500 | - | - | 1/12/32/32 | 0/3/3/3 |
| 71 | GTP | OG | 501 | 70 | - | 3/18/38/38 | 0/3/3/3 |
| 71 | GTP | VK | 501 | 70 | - | 5/18/38/38 | 0/3/3/3 |
| 69 | GDP | WH | 500 | - | - | 2/12/32/32 | 0/3/3/3 |
| 69 | GDP | QK | 500 | - | - | 5/12/32/32 | 0/3/3/3 |
| 71 | GTP | Q | 501 | 70 | - | 3/18/38/38 | 0/3/3/3 |
| 69 | GDP | RG | 500 | - | - | 1/12/32/32 | 0/3/3/3 |
| 71 | GTP | OE | 501 | 70 | - | 4/18/38/38 | 0/3/3/3 |
| 69 | GDP | CM | 500 | - | - | 3/12/32/32 | 0/3/3/3 |
| 69 | GDP | GL | 500 | - | - | 3/12/32/32 | 0/3/3/3 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|------------|---------|
| 69 | GDP | UL | 500 | - | - | 1/12/32/32 | 0/3/3/3 |
| 71 | GTP | GC | 501 | 70 | - | 3/18/38/38 | 0/3/3/3 |
| 71 | GTP | FA | 501 | 70 | - | 3/18/38/38 | 0/3/3/3 |
| 69 | GDP | SJ | 500 | - | - | 2/12/32/32 | 0/3/3/3 |
| 71 | GTP | IG | 501 | 70 | - | 7/18/38/38 | 0/3/3/3 |
| 69 | GDP | DI | 500 | - | - | 2/12/32/32 | 0/3/3/3 |
| 71 | GTP | WM | 501 | 70 | - | 3/18/38/38 | 0/3/3/3 |
| 69 | GDP | E | 500 | - | - | 4/12/32/32 | 0/3/3/3 |
| 69 | GDP | U | 500 | - | - | 2/12/32/32 | 0/3/3/3 |
| 69 | GDP | VD | 500 | - | - | 1/12/32/32 | 0/3/3/3 |
| 71 | GTP | BK | 501 | 70 | - | 5/18/38/38 | 0/3/3/3 |
| 71 | GTP | SE | 501 | 70 | - | 5/18/38/38 | 0/3/3/3 |
| 71 | GTP | HE | 501 | 70 | - | 4/18/38/38 | 0/3/3/3 |
| 71 | GTP | L | 501 | 70 | - | 4/18/38/38 | 0/3/3/3 |
| 69 | GDP | OJ | 500 | - | - | 3/12/32/32 | 0/3/3/3 |
| 71 | GTP | EG | 501 | 70 | - | 6/18/38/38 | 0/3/3/3 |
| 71 | GTP | JD | 501 | 70 | - | 5/18/38/38 | 0/3/3/3 |
| 71 | GTP | VE | 501 | 70 | - | 1/18/38/38 | 0/3/3/3 |
| 71 | GTP | DH | 501 | 70 | - | 2/18/38/38 | 0/3/3/3 |
| 71 | GTP | DF | 501 | 70 | - | 6/18/38/38 | 0/3/3/3 |
| 74 | ATP | 2v | 501 | - | - | 2/18/38/38 | 0/3/3/3 |
| 69 | GDP | WD | 500 | - | - | 2/12/32/32 | 0/3/3/3 |
| 71 | GTP | VM | 501 | 70 | - | 5/18/38/38 | 0/3/3/3 |
| 69 | GDP | HB | 500 | - | - | 3/12/32/32 | 0/3/3/3 |
| 69 | GDP | OD | 500 | - | - | 2/12/32/32 | 0/3/3/3 |
| 71 | GTP | QL | 501 | - | - | 3/18/38/38 | 0/3/3/3 |
| 71 | GTP | UC | 501 | 70 | - | 3/18/38/38 | 0/3/3/3 |
| 69 | GDP | NJ | 500 | - | - | 1/12/32/32 | 0/3/3/3 |
| 71 | GTP | QF | 501 | 70 | - | 2/18/38/38 | 0/3/3/3 |
| 71 | GTP | PI | 501 | 70 | - | 4/18/38/38 | 0/3/3/3 |
| 71 | GTP | IK | 501 | 70 | - | 3/18/38/38 | 0/3/3/3 |
| 69 | GDP | IF | 500 | - | - | 3/12/32/32 | 0/3/3/3 |
| 71 | GTP | GK | 501 | 70 | - | 3/18/38/38 | 0/3/3/3 |
| 71 | GTP | EA | 501 | 70 | - | 8/18/38/38 | 0/3/3/3 |
| 71 | GTP | OM | 501 | 70 | - | 5/18/38/38 | 0/3/3/3 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|------------|---------|
| 69 | GDP | JG | 500 | - | - | 2/12/32/32 | 0/3/3/3 |
| 71 | GTP | KB | 501 | 70 | - | 4/18/38/38 | 0/3/3/3 |
| 71 | GTP | MA | 501 | 70 | - | 0/18/38/38 | 0/3/3/3 |
| 69 | GDP | FD | 500 | - | - | 2/12/32/32 | 0/3/3/3 |
| 71 | GTP | FE | 501 | 70 | - | 5/18/38/38 | 0/3/3/3 |
| 69 | GDP | HJ | 500 | - | - | 2/12/32/32 | 0/3/3/3 |
| 69 | GDP | DK | 500 | - | - | 1/12/32/32 | 0/3/3/3 |
| 69 | GDP | LA | 500 | - | - | 2/12/32/32 | 0/3/3/3 |
| 69 | GDP | FL | 500 | - | - | 3/12/32/32 | 0/3/3/3 |
| 69 | GDP | HL | 500 | - | - | 1/12/32/32 | 0/3/3/3 |
| 71 | GTP | MM | 501 | 70 | - | 2/18/38/38 | 0/3/3/3 |
| 71 | GTP | WE | 501 | 70 | - | 8/18/38/38 | 0/3/3/3 |
| 71 | GTP | TE | 501 | 70 | - | 6/18/38/38 | 0/3/3/3 |
| 69 | GDP | NL | 500 | - | - | 1/12/32/32 | 0/3/3/3 |
| 71 | GTP | HI | 501 | 70 | - | 2/18/38/38 | 0/3/3/3 |
| 71 | GTP | BI | 501 | 70 | - | 6/18/38/38 | 0/3/3/3 |
| 69 | GDP | EL | 500 | - | - | 3/12/32/32 | 0/3/3/3 |
| 71 | GTP | C | 501 | 70 | - | 6/18/38/38 | 0/3/3/3 |
| 69 | GDP | UF | 500 | - | - | 1/12/32/32 | 0/3/3/3 |
| 71 | GTP | GG | 501 | 70 | - | 4/18/38/38 | 0/3/3/3 |
| 69 | GDP | UD | 500 | - | - | 3/12/32/32 | 0/3/3/3 |
| 69 | GDP | DA | 500 | - | - | 4/12/32/32 | 0/3/3/3 |
| 71 | GTP | TI | 501 | 70 | - | 4/18/38/38 | 0/3/3/3 |
| 69 | GDP | SF | 500 | - | - | 1/12/32/32 | 0/3/3/3 |
| 69 | GDP | P | 500 | - | - | 2/12/32/32 | 0/3/3/3 |
| 71 | GTP | NG | 501 | - | - | 6/18/38/38 | 0/3/3/3 |
| 71 | GTP | FG | 501 | 70 | - | 7/18/38/38 | 0/3/3/3 |
| 69 | GDP | ML | 500 | - | - | 1/12/32/32 | 0/3/3/3 |
| 69 | GDP | QG | 500 | - | - | 1/12/32/32 | 0/3/3/3 |
| 69 | GDP | O | 500 | - | - | 2/12/32/32 | 0/3/3/3 |
| 71 | GTP | EE | 501 | 70 | - | 5/18/38/38 | 0/3/3/3 |
| 69 | GDP | EJ | 500 | - | - | 1/12/32/32 | 0/3/3/3 |
| 69 | GDP | JK | 500 | - | - | 3/12/32/32 | 0/3/3/3 |
| 71 | GTP | VI | 501 | 70 | - | 4/18/38/38 | 0/3/3/3 |
| 71 | GTP | SG | 501 | 70 | - | 8/18/38/38 | 0/3/3/3 |
| 69 | GDP | KC | 500 | - | - | 1/12/32/32 | 0/3/3/3 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|------------|---------|
| 69 | GDP | BB | 500 | - | - | 2/12/32/32 | 0/3/3/3 |
| 71 | GTP | UK | 501 | 70 | - | 5/18/38/38 | 0/3/3/3 |
| 71 | GTP | PK | 501 | 70 | - | 3/18/38/38 | 0/3/3/3 |
| 69 | GDP | BL | 500 | - | - | 3/12/32/32 | 0/3/3/3 |
| 69 | GDP | LG | 500 | - | - | 2/12/32/32 | 0/3/3/3 |
| 71 | GTP | TA | 501 | 70 | - | 7/18/38/38 | 0/3/3/3 |
| 69 | GDP | T | 500 | - | - | 1/12/32/32 | 0/3/3/3 |
| 69 | GDP | BN | 500 | - | - | 2/12/32/32 | 0/3/3/3 |
| 69 | GDP | GJ | 500 | - | - | 2/12/32/32 | 0/3/3/3 |
| 69 | GDP | UB | 500 | - | - | 3/12/32/32 | 0/3/3/3 |
| 69 | GDP | AD | 500 | - | - | 2/12/32/32 | 0/3/3/3 |
| 71 | GTP | EI | 501 | 70 | - | 2/18/38/38 | 0/3/3/3 |
| 69 | GDP | TJ | 500 | - | - | 2/12/32/32 | 0/3/3/3 |
| 69 | GDP | WF | 500 | - | - | 1/12/32/32 | 0/3/3/3 |
| 69 | GDP | SH | 500 | - | - | 2/12/32/32 | 0/3/3/3 |
| 71 | GTP | AC | 501 | 70 | - | 4/18/38/38 | 0/3/3/3 |
| 71 | GTP | IC | 501 | 70 | - | 4/18/38/38 | 0/3/3/3 |
| 71 | GTP | IM | 501 | 70 | - | 4/18/38/38 | 0/3/3/3 |

All (520) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 71 | RD | 501 | GTP | C5-C6 | -4.37 | 1.38 | 1.47 |
| 71 | PA | 501 | GTP | C5-C6 | -4.36 | 1.38 | 1.47 |
| 71 | RH | 501 | GTP | C5-C6 | -4.35 | 1.38 | 1.47 |
| 71 | PI | 501 | GTP | C5-C6 | -4.33 | 1.38 | 1.47 |
| 71 | IE | 501 | GTP | C5-C6 | -4.31 | 1.38 | 1.47 |
| 71 | PK | 501 | GTP | C5-C6 | -4.31 | 1.38 | 1.47 |
| 71 | HI | 501 | GTP | C5-C6 | -4.31 | 1.38 | 1.47 |
| 71 | SC | 501 | GTP | C5-C6 | -4.30 | 1.38 | 1.47 |
| 71 | FE | 501 | GTP | C5-C6 | -4.30 | 1.38 | 1.47 |
| 71 | IC | 501 | GTP | C5-C6 | -4.30 | 1.38 | 1.47 |
| 71 | EC | 501 | GTP | C5-C6 | -4.30 | 1.38 | 1.47 |
| 71 | TG | 501 | GTP | C5-C6 | -4.30 | 1.39 | 1.47 |
| 71 | HA | 501 | GTP | C5-C6 | -4.29 | 1.39 | 1.47 |
| 71 | QD | 501 | GTP | C5-C6 | -4.29 | 1.39 | 1.47 |
| 71 | LH | 501 | GTP | C5-C6 | -4.29 | 1.39 | 1.47 |
| 71 | QH | 501 | GTP | C5-C6 | -4.29 | 1.39 | 1.47 |
| 71 | KH | 501 | GTP | C5-C6 | -4.29 | 1.39 | 1.47 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 71 | FK | 501 | GTP | C5-C6 | -4.29 | 1.39 | 1.47 |
| 71 | DD | 501 | GTP | C5-C6 | -4.29 | 1.39 | 1.47 |
| 71 | GA | 501 | GTP | C5-C6 | -4.29 | 1.39 | 1.47 |
| 71 | MK | 501 | GTP | C5-C6 | -4.29 | 1.39 | 1.47 |
| 71 | FC | 501 | GTP | C5-C6 | -4.28 | 1.39 | 1.47 |
| 71 | VE | 501 | GTP | C5-C6 | -4.28 | 1.39 | 1.47 |
| 71 | BI | 501 | GTP | C5-C6 | -4.28 | 1.39 | 1.47 |
| 71 | JH | 501 | GTP | C5-C6 | -4.28 | 1.39 | 1.47 |
| 71 | JN | 501 | GTP | C5-C6 | -4.28 | 1.39 | 1.47 |
| 71 | UK | 501 | GTP | C5-C6 | -4.28 | 1.39 | 1.47 |
| 71 | WM | 501 | GTP | C5-C6 | -4.28 | 1.39 | 1.47 |
| 71 | UA | 501 | GTP | C5-C6 | -4.27 | 1.39 | 1.47 |
| 71 | C | 501 | GTP | C5-C6 | -4.27 | 1.39 | 1.47 |
| 71 | OG | 501 | GTP | C5-C6 | -4.27 | 1.39 | 1.47 |
| 71 | CH | 501 | GTP | C5-C6 | -4.27 | 1.39 | 1.47 |
| 71 | SA | 501 | GTP | C5-C6 | -4.27 | 1.39 | 1.47 |
| 71 | VG | 501 | GTP | C5-C6 | -4.27 | 1.39 | 1.47 |
| 71 | TC | 501 | GTP | C5-C6 | -4.26 | 1.39 | 1.47 |
| 71 | HE | 501 | GTP | C5-C6 | -4.26 | 1.39 | 1.47 |
| 71 | HG | 501 | GTP | C5-C6 | -4.26 | 1.39 | 1.47 |
| 71 | JF | 501 | GTP | C5-C6 | -4.26 | 1.39 | 1.47 |
| 71 | FG | 501 | GTP | C5-C6 | -4.26 | 1.39 | 1.47 |
| 71 | HM | 501 | GTP | C5-C6 | -4.26 | 1.39 | 1.47 |
| 71 | NI | 501 | GTP | C5-C6 | -4.26 | 1.39 | 1.47 |
| 71 | GE | 501 | GTP | C5-C6 | -4.26 | 1.39 | 1.47 |
| 71 | RB | 501 | GTP | C5-C6 | -4.25 | 1.39 | 1.47 |
| 71 | NK | 501 | GTP | C5-C6 | -4.25 | 1.39 | 1.47 |
| 71 | PE | 501 | GTP | C5-C6 | -4.25 | 1.39 | 1.47 |
| 71 | LL | 501 | GTP | C5-C6 | -4.25 | 1.39 | 1.47 |
| 71 | OI | 501 | GTP | C5-C6 | -4.25 | 1.39 | 1.47 |
| 71 | J | 501 | GTP | C5-C6 | -4.25 | 1.39 | 1.47 |
| 71 | GI | 501 | GTP | C5-C6 | -4.25 | 1.39 | 1.47 |
| 71 | GG | 501 | GTP | C5-C6 | -4.25 | 1.39 | 1.47 |
| 71 | FA | 501 | GTP | C5-C6 | -4.25 | 1.39 | 1.47 |
| 71 | QJ | 501 | GTP | C5-C6 | -4.25 | 1.39 | 1.47 |
| 71 | SE | 501 | GTP | C5-C6 | -4.25 | 1.39 | 1.47 |
| 71 | SI | 501 | GTP | C5-C6 | -4.24 | 1.39 | 1.47 |
| 71 | R | 501 | GTP | C5-C6 | -4.24 | 1.39 | 1.47 |
| 71 | HK | 501 | GTP | C5-C6 | -4.24 | 1.39 | 1.47 |
| 71 | OA | 501 | GTP | C5-C6 | -4.24 | 1.39 | 1.47 |
| 71 | PG | 501 | GTP | C5-C6 | -4.24 | 1.39 | 1.47 |
| 71 | SK | 501 | GTP | C5-C6 | -4.24 | 1.39 | 1.47 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 71 | SG | 501 | GTP | C5-C6 | -4.24 | 1.39 | 1.47 |
| 71 | NG | 501 | GTP | C5-C6 | -4.24 | 1.39 | 1.47 |
| 71 | KJ | 501 | GTP | C5-C6 | -4.24 | 1.39 | 1.47 |
| 71 | FI | 501 | GTP | C5-C6 | -4.24 | 1.39 | 1.47 |
| 71 | VM | 501 | GTP | C5-C6 | -4.24 | 1.39 | 1.47 |
| 71 | AC | 501 | GTP | C5-C6 | -4.24 | 1.39 | 1.47 |
| 71 | LF | 501 | GTP | C5-C6 | -4.24 | 1.39 | 1.47 |
| 71 | TE | 501 | GTP | C5-C6 | -4.24 | 1.39 | 1.47 |
| 71 | KL | 501 | GTP | C5-C6 | -4.23 | 1.39 | 1.47 |
| 71 | CL | 501 | GTP | C5-C6 | -4.23 | 1.39 | 1.47 |
| 71 | UE | 501 | GTP | C5-C6 | -4.23 | 1.39 | 1.47 |
| 71 | LJ | 501 | GTP | C5-C6 | -4.23 | 1.39 | 1.47 |
| 71 | RF | 501 | GTP | C5-C6 | -4.23 | 1.39 | 1.47 |
| 71 | GC | 501 | GTP | C5-C6 | -4.23 | 1.39 | 1.47 |
| 71 | AI | 501 | GTP | C5-C6 | -4.23 | 1.39 | 1.47 |
| 71 | OE | 501 | GTP | C5-C6 | -4.23 | 1.39 | 1.47 |
| 71 | UG | 501 | GTP | C5-C6 | -4.23 | 1.39 | 1.47 |
| 71 | GK | 501 | GTP | C5-C6 | -4.23 | 1.39 | 1.47 |
| 71 | QL | 501 | GTP | C5-C6 | -4.23 | 1.39 | 1.47 |
| 71 | RL | 501 | GTP | C5-C6 | -4.23 | 1.39 | 1.47 |
| 71 | JJ | 501 | GTP | C5-C6 | -4.23 | 1.39 | 1.47 |
| 71 | VC | 501 | GTP | C5-C6 | -4.23 | 1.39 | 1.47 |
| 71 | DB | 501 | GTP | C5-C6 | -4.22 | 1.39 | 1.47 |
| 71 | K | 501 | GTP | C5-C6 | -4.22 | 1.39 | 1.47 |
| 71 | VI | 501 | GTP | C5-C6 | -4.22 | 1.39 | 1.47 |
| 71 | AG | 501 | GTP | C5-C6 | -4.22 | 1.39 | 1.47 |
| 71 | BG | 501 | GTP | C5-C6 | -4.22 | 1.39 | 1.47 |
| 71 | EE | 501 | GTP | C5-C6 | -4.22 | 1.39 | 1.47 |
| 71 | EG | 501 | GTP | C5-C6 | -4.22 | 1.39 | 1.47 |
| 71 | VK | 501 | GTP | C5-C6 | -4.22 | 1.39 | 1.47 |
| 71 | TA | 501 | GTP | C5-C6 | -4.22 | 1.39 | 1.47 |
| 71 | OK | 501 | GTP | C5-C6 | -4.22 | 1.39 | 1.47 |
| 71 | BM | 501 | GTP | C5-C6 | -4.21 | 1.39 | 1.47 |
| 71 | IA | 501 | GTP | C5-C6 | -4.21 | 1.39 | 1.47 |
| 71 | HC | 501 | GTP | C5-C6 | -4.21 | 1.39 | 1.47 |
| 71 | MG | 501 | GTP | C5-C6 | -4.21 | 1.39 | 1.47 |
| 71 | EI | 501 | GTP | C5-C6 | -4.21 | 1.39 | 1.47 |
| 71 | L | 501 | GTP | C5-C6 | -4.21 | 1.39 | 1.47 |
| 71 | AE | 501 | GTP | C5-C6 | -4.21 | 1.39 | 1.47 |
| 71 | MM | 501 | GTP | C5-C6 | -4.21 | 1.39 | 1.47 |
| 71 | CF | 501 | GTP | C5-C6 | -4.21 | 1.39 | 1.47 |
| 71 | IG | 501 | GTP | C5-C6 | -4.21 | 1.39 | 1.47 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 71 | LB | 501 | GTP | C5-C6 | -4.20 | 1.39 | 1.47 |
| 71 | MI | 501 | GTP | C5-C6 | -4.20 | 1.39 | 1.47 |
| 71 | WA | 501 | GTP | C5-C6 | -4.20 | 1.39 | 1.47 |
| 71 | WE | 501 | GTP | C5-C6 | -4.20 | 1.39 | 1.47 |
| 71 | BA | 501 | GTP | C5-C6 | -4.20 | 1.39 | 1.47 |
| 71 | NM | 501 | GTP | C5-C6 | -4.20 | 1.39 | 1.47 |
| 71 | KB | 501 | GTP | C5-C6 | -4.20 | 1.39 | 1.47 |
| 71 | KF | 501 | GTP | C5-C6 | -4.20 | 1.39 | 1.47 |
| 71 | WK | 501 | GTP | C5-C6 | -4.20 | 1.39 | 1.47 |
| 71 | NC | 501 | GTP | C5-C6 | -4.20 | 1.39 | 1.47 |
| 71 | NE | 501 | GTP | C5-C6 | -4.20 | 1.39 | 1.47 |
| 71 | KN | 501 | GTP | C5-C6 | -4.20 | 1.39 | 1.47 |
| 71 | DH | 501 | GTP | C5-C6 | -4.19 | 1.39 | 1.47 |
| 71 | BE | 501 | GTP | C5-C6 | -4.19 | 1.39 | 1.47 |
| 71 | TI | 501 | GTP | C5-C6 | -4.19 | 1.39 | 1.47 |
| 71 | PM | 501 | GTP | C5-C6 | -4.19 | 1.39 | 1.47 |
| 71 | CD | 501 | GTP | C5-C6 | -4.19 | 1.39 | 1.47 |
| 71 | WC | 501 | GTP | C5-C6 | -4.19 | 1.39 | 1.47 |
| 71 | AK | 501 | GTP | C5-C6 | -4.19 | 1.39 | 1.47 |
| 71 | LD | 501 | GTP | C5-C6 | -4.19 | 1.39 | 1.47 |
| 71 | WG | 501 | GTP | C5-C6 | -4.19 | 1.39 | 1.47 |
| 71 | Q | 501 | GTP | C5-C6 | -4.19 | 1.39 | 1.47 |
| 71 | IM | 501 | GTP | C5-C6 | -4.19 | 1.39 | 1.47 |
| 71 | DF | 501 | GTP | C5-C6 | -4.19 | 1.39 | 1.47 |
| 71 | WI | 501 | GTP | C5-C6 | -4.19 | 1.39 | 1.47 |
| 71 | VA | 501 | GTP | C5-C6 | -4.18 | 1.39 | 1.47 |
| 71 | MA | 501 | GTP | C5-C6 | -4.18 | 1.39 | 1.47 |
| 71 | MC | 501 | GTP | C5-C6 | -4.18 | 1.39 | 1.47 |
| 71 | NA | 501 | GTP | C5-C6 | -4.18 | 1.39 | 1.47 |
| 71 | LN | 501 | GTP | C5-C6 | -4.18 | 1.39 | 1.47 |
| 71 | ME | 501 | GTP | C5-C6 | -4.18 | 1.39 | 1.47 |
| 71 | AA | 501 | GTP | C5-C6 | -4.18 | 1.39 | 1.47 |
| 71 | QF | 501 | GTP | C5-C6 | -4.18 | 1.39 | 1.47 |
| 71 | II | 501 | GTP | C5-C6 | -4.18 | 1.39 | 1.47 |
| 71 | PC | 501 | GTP | C5-C6 | -4.17 | 1.39 | 1.47 |
| 71 | UI | 501 | GTP | C5-C6 | -4.17 | 1.39 | 1.47 |
| 71 | DJ | 501 | GTP | C5-C6 | -4.16 | 1.39 | 1.47 |
| 71 | UC | 501 | GTP | C5-C6 | -4.16 | 1.39 | 1.47 |
| 71 | TK | 501 | GTP | C5-C6 | -4.16 | 1.39 | 1.47 |
| 71 | OM | 501 | GTP | C5-C6 | -4.16 | 1.39 | 1.47 |
| 71 | AM | 501 | GTP | C5-C6 | -4.16 | 1.39 | 1.47 |
| 71 | DL | 501 | GTP | C5-C6 | -4.16 | 1.39 | 1.47 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 71 | EA | 501 | GTP | C5-C6 | -4.16 | 1.39 | 1.47 |
| 71 | CB | 501 | GTP | C5-C6 | -4.16 | 1.39 | 1.47 |
| 71 | KD | 501 | GTP | C5-C6 | -4.16 | 1.39 | 1.47 |
| 71 | CJ | 501 | GTP | C5-C6 | -4.15 | 1.39 | 1.47 |
| 71 | JB | 501 | GTP | C5-C6 | -4.15 | 1.39 | 1.47 |
| 71 | OC | 501 | GTP | C5-C6 | -4.15 | 1.39 | 1.47 |
| 71 | D | 501 | GTP | C5-C6 | -4.15 | 1.39 | 1.47 |
| 71 | JL | 501 | GTP | C5-C6 | -4.15 | 1.39 | 1.47 |
| 71 | RJ | 501 | GTP | C5-C6 | -4.14 | 1.39 | 1.47 |
| 71 | EK | 501 | GTP | C5-C6 | -4.14 | 1.39 | 1.47 |
| 71 | JD | 501 | GTP | C5-C6 | -4.13 | 1.39 | 1.47 |
| 71 | BK | 501 | GTP | C5-C6 | -4.13 | 1.39 | 1.47 |
| 71 | BC | 501 | GTP | C5-C6 | -4.13 | 1.39 | 1.47 |
| 71 | QB | 501 | GTP | C5-C6 | -4.12 | 1.39 | 1.47 |
| 71 | IK | 501 | GTP | C5-C6 | -4.00 | 1.39 | 1.47 |
| 71 | IK | 501 | GTP | PB-O3A | 3.42 | 1.63 | 1.59 |
| 71 | IK | 501 | GTP | PA-O3A | 3.04 | 1.62 | 1.59 |
| 69 | A | 500 | GDP | C6-N1 | -2.46 | 1.34 | 1.37 |
| 69 | PL | 500 | GDP | C6-N1 | -2.46 | 1.34 | 1.37 |
| 69 | UD | 500 | GDP | C6-N1 | -2.45 | 1.34 | 1.37 |
| 69 | CM | 500 | GDP | C6-N1 | -2.45 | 1.34 | 1.37 |
| 69 | ED | 500 | GDP | C6-N1 | -2.44 | 1.34 | 1.37 |
| 71 | IK | 501 | GTP | PB-O3B | 2.44 | 1.62 | 1.59 |
| 69 | QI | 500 | GDP | C6-N1 | -2.43 | 1.34 | 1.37 |
| 69 | TH | 500 | GDP | C6-N1 | -2.42 | 1.34 | 1.37 |
| 69 | DE | 500 | GDP | C6-N1 | -2.42 | 1.34 | 1.37 |
| 69 | H | 500 | GDP | C6-N1 | -2.41 | 1.34 | 1.37 |
| 69 | BN | 500 | GDP | C6-N1 | -2.41 | 1.34 | 1.37 |
| 69 | VL | 500 | GDP | C6-N1 | -2.41 | 1.34 | 1.37 |
| 69 | N | 500 | GDP | C6-N1 | -2.41 | 1.34 | 1.37 |
| 69 | JI | 500 | GDP | C6-N1 | -2.41 | 1.34 | 1.37 |
| 69 | FL | 500 | GDP | C6-N1 | -2.41 | 1.34 | 1.37 |
| 69 | QG | 500 | GDP | C6-N1 | -2.41 | 1.34 | 1.37 |
| 69 | RE | 500 | GDP | C6-N1 | -2.41 | 1.34 | 1.37 |
| 69 | TL | 500 | GDP | C6-N1 | -2.40 | 1.34 | 1.37 |
| 69 | NB | 500 | GDP | C6-N1 | -2.40 | 1.34 | 1.37 |
| 69 | KG | 500 | GDP | C6-N1 | -2.40 | 1.34 | 1.37 |
| 69 | UB | 500 | GDP | C6-N1 | -2.40 | 1.34 | 1.37 |
| 69 | JK | 500 | GDP | C6-N1 | -2.40 | 1.34 | 1.37 |
| 69 | EL | 500 | GDP | C6-N1 | -2.40 | 1.34 | 1.37 |
| 69 | HF | 500 | GDP | C6-N1 | -2.40 | 1.34 | 1.37 |
| 69 | WD | 500 | GDP | C6-N1 | -2.40 | 1.34 | 1.37 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 69 | HL | 500 | GDP | C6-N1 | -2.39 | 1.34 | 1.37 |
| 71 | CD | 501 | GTP | PB-O3B | 2.39 | 1.62 | 1.59 |
| 69 | IH | 500 | GDP | C6-N1 | -2.39 | 1.34 | 1.37 |
| 69 | RC | 500 | GDP | C6-N1 | -2.39 | 1.34 | 1.37 |
| 69 | U | 500 | GDP | C6-N1 | -2.39 | 1.34 | 1.37 |
| 69 | WH | 500 | GDP | C6-N1 | -2.39 | 1.34 | 1.37 |
| 69 | PH | 500 | GDP | C6-N1 | -2.39 | 1.34 | 1.37 |
| 69 | UL | 500 | GDP | C6-N1 | -2.39 | 1.34 | 1.37 |
| 69 | CC | 500 | GDP | C6-N1 | -2.39 | 1.34 | 1.37 |
| 69 | JC | 500 | GDP | C6-N1 | -2.39 | 1.34 | 1.37 |
| 69 | KK | 500 | GDP | C6-N1 | -2.39 | 1.34 | 1.37 |
| 69 | IJ | 500 | GDP | C6-N1 | -2.39 | 1.34 | 1.37 |
| 69 | CA | 500 | GDP | C6-N1 | -2.38 | 1.34 | 1.37 |
| 69 | CE | 500 | GDP | C6-N1 | -2.38 | 1.34 | 1.37 |
| 69 | FD | 500 | GDP | C6-N1 | -2.38 | 1.34 | 1.37 |
| 69 | EB | 500 | GDP | C6-N1 | -2.38 | 1.34 | 1.37 |
| 69 | F | 500 | GDP | C6-N1 | -2.38 | 1.34 | 1.37 |
| 69 | OL | 500 | GDP | C6-N1 | -2.38 | 1.34 | 1.37 |
| 69 | TD | 500 | GDP | C6-N1 | -2.38 | 1.34 | 1.37 |
| 69 | O | 500 | GDP | C6-N1 | -2.38 | 1.34 | 1.37 |
| 69 | IB | 500 | GDP | C6-N1 | -2.38 | 1.34 | 1.37 |
| 69 | RK | 500 | GDP | C6-N1 | -2.38 | 1.34 | 1.37 |
| 69 | DA | 500 | GDP | C6-N1 | -2.38 | 1.34 | 1.37 |
| 69 | PF | 500 | GDP | C6-N1 | -2.38 | 1.34 | 1.37 |
| 69 | JG | 500 | GDP | C6-N1 | -2.38 | 1.34 | 1.37 |
| 69 | GF | 500 | GDP | C6-N1 | -2.38 | 1.34 | 1.37 |
| 69 | BH | 500 | GDP | C6-N1 | -2.37 | 1.34 | 1.37 |
| 69 | DK | 500 | GDP | C6-N1 | -2.37 | 1.34 | 1.37 |
| 69 | HH | 500 | GDP | C6-N1 | -2.37 | 1.34 | 1.37 |
| 69 | NJ | 500 | GDP | C6-N1 | -2.37 | 1.34 | 1.37 |
| 69 | QC | 500 | GDP | C6-N1 | -2.37 | 1.34 | 1.37 |
| 69 | JM | 500 | GDP | C6-N1 | -2.37 | 1.34 | 1.37 |
| 69 | VB | 500 | GDP | C6-N1 | -2.37 | 1.34 | 1.37 |
| 69 | BD | 500 | GDP | C6-N1 | -2.37 | 1.34 | 1.37 |
| 69 | DC | 500 | GDP | C6-N1 | -2.37 | 1.34 | 1.37 |
| 69 | FH | 500 | GDP | C6-N1 | -2.37 | 1.34 | 1.37 |
| 69 | HD | 500 | GDP | C6-N1 | -2.37 | 1.34 | 1.37 |
| 69 | OJ | 500 | GDP | C6-N1 | -2.37 | 1.34 | 1.37 |
| 69 | NF | 500 | GDP | C6-N1 | -2.37 | 1.34 | 1.37 |
| 69 | UH | 500 | GDP | C6-N1 | -2.37 | 1.34 | 1.37 |
| 71 | NG | 501 | GTP | PA-O3A | 2.37 | 1.62 | 1.59 |
| 69 | LI | 500 | GDP | C6-N1 | -2.37 | 1.34 | 1.37 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 69 | ID | 500 | GDP | C6-N1 | -2.37 | 1.34 | 1.37 |
| 71 | CF | 501 | GTP | PB-O3B | 2.36 | 1.62 | 1.59 |
| 69 | SJ | 500 | GDP | C6-N1 | -2.36 | 1.34 | 1.37 |
| 69 | KE | 500 | GDP | C6-N1 | -2.36 | 1.34 | 1.37 |
| 69 | WJ | 500 | GDP | C6-N1 | -2.36 | 1.34 | 1.37 |
| 69 | GD | 500 | GDP | C6-N1 | -2.36 | 1.34 | 1.37 |
| 69 | LA | 500 | GDP | C6-N1 | -2.36 | 1.34 | 1.37 |
| 69 | SD | 500 | GDP | C6-N1 | -2.36 | 1.34 | 1.37 |
| 69 | VF | 500 | GDP | C6-N1 | -2.36 | 1.34 | 1.37 |
| 69 | AJ | 500 | GDP | C6-N1 | -2.36 | 1.34 | 1.37 |
| 69 | FF | 500 | GDP | C6-N1 | -2.36 | 1.34 | 1.37 |
| 69 | LK | 500 | GDP | C6-N1 | -2.36 | 1.34 | 1.37 |
| 69 | BF | 500 | GDP | C6-N1 | -2.35 | 1.34 | 1.37 |
| 69 | VJ | 500 | GDP | C6-N1 | -2.35 | 1.34 | 1.37 |
| 69 | TB | 500 | GDP | C6-N1 | -2.35 | 1.34 | 1.37 |
| 69 | QA | 500 | GDP | C6-N1 | -2.35 | 1.34 | 1.37 |
| 69 | V | 500 | GDP | C6-N1 | -2.35 | 1.34 | 1.37 |
| 69 | JA | 500 | GDP | C6-N1 | -2.35 | 1.34 | 1.37 |
| 69 | AH | 500 | GDP | C6-N1 | -2.35 | 1.34 | 1.37 |
| 69 | E | 500 | GDP | C6-N1 | -2.35 | 1.34 | 1.37 |
| 69 | OB | 500 | GDP | C6-N1 | -2.35 | 1.34 | 1.37 |
| 69 | VD | 500 | GDP | C6-N1 | -2.35 | 1.34 | 1.37 |
| 69 | ML | 500 | GDP | C6-N1 | -2.35 | 1.34 | 1.37 |
| 69 | S | 500 | GDP | C6-N1 | -2.35 | 1.34 | 1.37 |
| 69 | MH | 500 | GDP | C6-N1 | -2.35 | 1.34 | 1.37 |
| 69 | PJ | 500 | GDP | C6-N1 | -2.35 | 1.34 | 1.37 |
| 69 | RG | 500 | GDP | C6-N1 | -2.35 | 1.34 | 1.37 |
| 69 | GJ | 500 | GDP | C6-N1 | -2.35 | 1.34 | 1.37 |
| 69 | KM | 500 | GDP | C6-N1 | -2.35 | 1.34 | 1.37 |
| 69 | PD | 500 | GDP | C6-N1 | -2.35 | 1.34 | 1.37 |
| 69 | NH | 500 | GDP | C6-N1 | -2.35 | 1.34 | 1.37 |
| 69 | SF | 500 | GDP | C6-N1 | -2.34 | 1.34 | 1.37 |
| 69 | WL | 500 | GDP | C6-N1 | -2.34 | 1.34 | 1.37 |
| 69 | MB | 500 | GDP | C6-N1 | -2.34 | 1.34 | 1.37 |
| 69 | BB | 500 | GDP | C6-N1 | -2.34 | 1.34 | 1.37 |
| 69 | I | 500 | GDP | C6-N1 | -2.34 | 1.34 | 1.37 |
| 69 | WB | 500 | GDP | C6-N1 | -2.34 | 1.34 | 1.37 |
| 69 | AL | 500 | GDP | C6-N1 | -2.34 | 1.34 | 1.37 |
| 69 | FB | 500 | GDP | C6-N1 | -2.34 | 1.34 | 1.37 |
| 69 | G | 500 | GDP | C6-N1 | -2.34 | 1.34 | 1.37 |
| 69 | LG | 500 | GDP | C6-N1 | -2.34 | 1.34 | 1.37 |
| 69 | OD | 500 | GDP | C6-N1 | -2.34 | 1.34 | 1.37 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 69 | RI | 500 | GDP | C6-N1 | -2.34 | 1.34 | 1.37 |
| 69 | SH | 500 | GDP | C6-N1 | -2.34 | 1.34 | 1.37 |
| 69 | LM | 500 | GDP | C6-N1 | -2.34 | 1.34 | 1.37 |
| 69 | MD | 500 | GDP | C6-N1 | -2.34 | 1.34 | 1.37 |
| 69 | DI | 500 | GDP | C6-N1 | -2.33 | 1.34 | 1.37 |
| 69 | EH | 500 | GDP | C6-N1 | -2.33 | 1.34 | 1.37 |
| 69 | PB | 500 | GDP | C6-N1 | -2.33 | 1.34 | 1.37 |
| 69 | SB | 500 | GDP | C6-N1 | -2.33 | 1.34 | 1.37 |
| 69 | KI | 500 | GDP | C6-N1 | -2.33 | 1.34 | 1.37 |
| 69 | QE | 500 | GDP | C6-N1 | -2.33 | 1.34 | 1.37 |
| 69 | DM | 500 | GDP | C6-N1 | -2.33 | 1.34 | 1.37 |
| 71 | EE | 501 | GTP | PB-O3B | 2.33 | 1.62 | 1.59 |
| 69 | IL | 500 | GDP | C6-N1 | -2.33 | 1.34 | 1.37 |
| 69 | GH | 500 | GDP | C6-N1 | -2.33 | 1.34 | 1.37 |
| 69 | NL | 500 | GDP | C6-N1 | -2.33 | 1.34 | 1.37 |
| 69 | CG | 500 | GDP | C6-N1 | -2.32 | 1.34 | 1.37 |
| 69 | FJ | 500 | GDP | C6-N1 | -2.32 | 1.34 | 1.37 |
| 69 | UJ | 500 | GDP | C6-N1 | -2.32 | 1.34 | 1.37 |
| 69 | JE | 500 | GDP | C6-N1 | -2.32 | 1.34 | 1.37 |
| 69 | UF | 500 | GDP | C6-N1 | -2.32 | 1.34 | 1.37 |
| 69 | EJ | 500 | GDP | C6-N1 | -2.32 | 1.34 | 1.37 |
| 69 | P | 500 | GDP | C6-N1 | -2.32 | 1.34 | 1.37 |
| 69 | WF | 500 | GDP | C6-N1 | -2.32 | 1.34 | 1.37 |
| 69 | DG | 500 | GDP | C6-N1 | -2.32 | 1.34 | 1.37 |
| 69 | HJ | 500 | GDP | C6-N1 | -2.31 | 1.34 | 1.37 |
| 69 | BL | 500 | GDP | C6-N1 | -2.31 | 1.34 | 1.37 |
| 69 | LO | 500 | GDP | C6-N1 | -2.31 | 1.34 | 1.37 |
| 69 | AD | 500 | GDP | C6-N1 | -2.31 | 1.34 | 1.37 |
| 69 | EF | 500 | GDP | C6-N1 | -2.31 | 1.34 | 1.37 |
| 69 | GL | 500 | GDP | C6-N1 | -2.31 | 1.34 | 1.37 |
| 69 | GB | 500 | GDP | C6-N1 | -2.31 | 1.34 | 1.37 |
| 69 | MF | 500 | GDP | C6-N1 | -2.31 | 1.34 | 1.37 |
| 69 | CK | 500 | GDP | C6-N1 | -2.31 | 1.34 | 1.37 |
| 71 | TA | 501 | GTP | PB-O3B | 2.31 | 1.62 | 1.59 |
| 69 | AN | 500 | GDP | C6-N1 | -2.31 | 1.34 | 1.37 |
| 69 | HB | 500 | GDP | C6-N1 | -2.31 | 1.34 | 1.37 |
| 69 | LE | 500 | GDP | C6-N1 | -2.31 | 1.34 | 1.37 |
| 69 | TF | 500 | GDP | C6-N1 | -2.31 | 1.34 | 1.37 |
| 69 | OH | 500 | GDP | C6-N1 | -2.30 | 1.34 | 1.37 |
| 69 | M | 500 | GDP | C6-N1 | -2.30 | 1.34 | 1.37 |
| 69 | MN | 500 | GDP | C6-N1 | -2.30 | 1.34 | 1.37 |
| 69 | KC | 500 | GDP | C6-N1 | -2.30 | 1.34 | 1.37 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 69 | CI | 500 | GDP | C6-N1 | -2.29 | 1.34 | 1.37 |
| 71 | D | 501 | GTP | PA-O3A | 2.29 | 1.62 | 1.59 |
| 69 | OF | 500 | GDP | C6-N1 | -2.29 | 1.34 | 1.37 |
| 69 | AB | 500 | GDP | C6-N1 | -2.29 | 1.34 | 1.37 |
| 69 | IF | 500 | GDP | C6-N1 | -2.29 | 1.34 | 1.37 |
| 69 | ND | 500 | GDP | C6-N1 | -2.29 | 1.34 | 1.37 |
| 69 | RA | 500 | GDP | C6-N1 | -2.28 | 1.34 | 1.37 |
| 69 | KA | 500 | GDP | C6-N1 | -2.28 | 1.34 | 1.37 |
| 69 | LC | 500 | GDP | C6-N1 | -2.28 | 1.34 | 1.37 |
| 69 | W | 500 | GDP | C6-N1 | -2.27 | 1.34 | 1.37 |
| 69 | VH | 500 | GDP | C6-N1 | -2.27 | 1.34 | 1.37 |
| 69 | MJ | 500 | GDP | C6-N1 | -2.27 | 1.34 | 1.37 |
| 69 | TJ | 500 | GDP | C6-N1 | -2.26 | 1.34 | 1.37 |
| 69 | QK | 500 | GDP | C6-N1 | -2.26 | 1.34 | 1.37 |
| 69 | AF | 500 | GDP | C6-N1 | -2.26 | 1.34 | 1.37 |
| 69 | BJ | 500 | GDP | C6-N1 | -2.26 | 1.34 | 1.37 |
| 71 | QD | 501 | GTP | PB-O3B | 2.25 | 1.61 | 1.59 |
| 71 | VC | 501 | GTP | PB-O3B | 2.25 | 1.61 | 1.59 |
| 69 | T | 500 | GDP | C6-N1 | -2.24 | 1.34 | 1.37 |
| 71 | DF | 501 | GTP | PB-O3B | 2.24 | 1.61 | 1.59 |
| 71 | VG | 501 | GTP | PB-O3B | 2.24 | 1.61 | 1.59 |
| 71 | EK | 501 | GTP | PB-O3B | 2.23 | 1.61 | 1.59 |
| 71 | IC | 501 | GTP | C2-N3 | 2.23 | 1.38 | 1.33 |
| 71 | HK | 501 | GTP | C2-N3 | 2.21 | 1.38 | 1.33 |
| 71 | HC | 501 | GTP | C2-N3 | 2.20 | 1.38 | 1.33 |
| 71 | BG | 501 | GTP | C2-N3 | 2.20 | 1.38 | 1.33 |
| 71 | KL | 501 | GTP | C2-N3 | 2.19 | 1.38 | 1.33 |
| 71 | VE | 501 | GTP | C2-N3 | 2.18 | 1.38 | 1.33 |
| 71 | KH | 501 | GTP | C2-N3 | 2.18 | 1.38 | 1.33 |
| 71 | FE | 501 | GTP | C2-N3 | 2.18 | 1.38 | 1.33 |
| 71 | IK | 501 | GTP | C2-N3 | 2.18 | 1.38 | 1.33 |
| 71 | BC | 501 | GTP | C2-N3 | 2.18 | 1.38 | 1.33 |
| 71 | OK | 501 | GTP | C2-N3 | 2.18 | 1.38 | 1.33 |
| 71 | OE | 501 | GTP | PB-O3B | 2.17 | 1.61 | 1.59 |
| 71 | QF | 501 | GTP | C2-N3 | 2.17 | 1.38 | 1.33 |
| 71 | QH | 501 | GTP | C2-N3 | 2.17 | 1.38 | 1.33 |
| 71 | NM | 501 | GTP | C2-N3 | 2.17 | 1.38 | 1.33 |
| 71 | SG | 501 | GTP | C2-N3 | 2.16 | 1.38 | 1.33 |
| 71 | LH | 501 | GTP | C2-N3 | 2.16 | 1.38 | 1.33 |
| 71 | IK | 501 | GTP | O4'-C4' | -2.16 | 1.40 | 1.45 |
| 71 | NE | 501 | GTP | C2-N3 | 2.16 | 1.38 | 1.33 |
| 71 | KL | 501 | GTP | PB-O3A | 2.15 | 1.61 | 1.59 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 71 | IG | 501 | GTP | C2-N3 | 2.15 | 1.38 | 1.33 |
| 71 | TI | 501 | GTP | C2-N3 | 2.15 | 1.38 | 1.33 |
| 71 | II | 501 | GTP | C2-N3 | 2.15 | 1.38 | 1.33 |
| 71 | DH | 501 | GTP | C2-N3 | 2.15 | 1.38 | 1.33 |
| 71 | RD | 501 | GTP | PB-O3B | 2.15 | 1.61 | 1.59 |
| 71 | NG | 501 | GTP | C2-N3 | 2.15 | 1.38 | 1.33 |
| 71 | CH | 501 | GTP | C2-N3 | 2.15 | 1.38 | 1.33 |
| 71 | EC | 501 | GTP | C2-N3 | 2.15 | 1.38 | 1.33 |
| 71 | AC | 501 | GTP | C2-N3 | 2.14 | 1.38 | 1.33 |
| 71 | IM | 501 | GTP | C2-N3 | 2.14 | 1.38 | 1.33 |
| 71 | UI | 501 | GTP | C2-N3 | 2.14 | 1.38 | 1.33 |
| 71 | BM | 501 | GTP | PB-O3B | 2.14 | 1.61 | 1.59 |
| 71 | AK | 501 | GTP | C2-N3 | 2.14 | 1.38 | 1.33 |
| 71 | IA | 501 | GTP | C2-N3 | 2.14 | 1.38 | 1.33 |
| 71 | HE | 501 | GTP | C2-N3 | 2.14 | 1.38 | 1.33 |
| 71 | WG | 501 | GTP | C2-N3 | 2.14 | 1.38 | 1.33 |
| 71 | VG | 501 | GTP | C2-N3 | 2.14 | 1.38 | 1.33 |
| 71 | HM | 501 | GTP | C2-N3 | 2.14 | 1.38 | 1.33 |
| 71 | UC | 501 | GTP | C2-N3 | 2.14 | 1.38 | 1.33 |
| 71 | RD | 501 | GTP | C2-N3 | 2.13 | 1.38 | 1.33 |
| 71 | VC | 501 | GTP | C2-N3 | 2.13 | 1.38 | 1.33 |
| 71 | WE | 501 | GTP | C2-N3 | 2.13 | 1.38 | 1.33 |
| 71 | AM | 501 | GTP | C2-N3 | 2.13 | 1.38 | 1.33 |
| 71 | VM | 501 | GTP | C2-N3 | 2.13 | 1.38 | 1.33 |
| 71 | BI | 501 | GTP | C2-N3 | 2.13 | 1.38 | 1.33 |
| 71 | NI | 501 | GTP | C2-N3 | 2.13 | 1.38 | 1.33 |
| 71 | Q | 501 | GTP | C2-N3 | 2.13 | 1.38 | 1.33 |
| 71 | IC | 501 | GTP | PB-O3B | 2.13 | 1.61 | 1.59 |
| 71 | NG | 501 | GTP | PB-O3A | 2.13 | 1.61 | 1.59 |
| 71 | J | 501 | GTP | C2-N3 | 2.13 | 1.38 | 1.33 |
| 71 | CF | 501 | GTP | C2-N3 | 2.13 | 1.38 | 1.33 |
| 71 | K | 501 | GTP | PB-O3A | 2.13 | 1.61 | 1.59 |
| 71 | FK | 501 | GTP | C2-N3 | 2.13 | 1.38 | 1.33 |
| 71 | IE | 501 | GTP | C2-N3 | 2.13 | 1.38 | 1.33 |
| 71 | KB | 501 | GTP | C2-N3 | 2.13 | 1.38 | 1.33 |
| 71 | KN | 501 | GTP | C2-N3 | 2.12 | 1.38 | 1.33 |
| 71 | AI | 501 | GTP | C2-N3 | 2.12 | 1.38 | 1.33 |
| 71 | NC | 501 | GTP | C2-N3 | 2.12 | 1.38 | 1.33 |
| 71 | JB | 501 | GTP | C2-N3 | 2.12 | 1.38 | 1.33 |
| 71 | AA | 501 | GTP | C2-N3 | 2.12 | 1.38 | 1.33 |
| 71 | JH | 501 | GTP | C2-N3 | 2.12 | 1.38 | 1.33 |
| 71 | DF | 501 | GTP | C2-N3 | 2.12 | 1.38 | 1.33 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 71 | LJ | 501 | GTP | C2-N3 | 2.12 | 1.38 | 1.33 |
| 71 | BA | 501 | GTP | C2-N3 | 2.12 | 1.38 | 1.33 |
| 71 | BE | 501 | GTP | C2-N3 | 2.12 | 1.38 | 1.33 |
| 71 | JF | 501 | GTP | C2-N3 | 2.12 | 1.38 | 1.33 |
| 71 | R | 501 | GTP | C2-N3 | 2.12 | 1.38 | 1.33 |
| 71 | EE | 501 | GTP | C2-N3 | 2.12 | 1.38 | 1.33 |
| 71 | VI | 501 | GTP | C2-N3 | 2.12 | 1.38 | 1.33 |
| 71 | QJ | 501 | GTP | PB-O3B | 2.12 | 1.61 | 1.59 |
| 71 | MK | 501 | GTP | C2-N3 | 2.12 | 1.38 | 1.33 |
| 71 | PA | 501 | GTP | C2-N3 | 2.11 | 1.38 | 1.33 |
| 71 | KD | 501 | GTP | C2-N3 | 2.11 | 1.38 | 1.33 |
| 71 | GI | 501 | GTP | C2-N3 | 2.11 | 1.38 | 1.33 |
| 71 | OI | 501 | GTP | C2-N3 | 2.11 | 1.38 | 1.33 |
| 71 | KF | 501 | GTP | C2-N3 | 2.11 | 1.38 | 1.33 |
| 71 | SC | 501 | GTP | C2-N3 | 2.11 | 1.38 | 1.33 |
| 71 | EA | 501 | GTP | C2-N3 | 2.11 | 1.38 | 1.33 |
| 71 | JN | 501 | GTP | C2-N3 | 2.11 | 1.38 | 1.33 |
| 71 | L | 501 | GTP | C2-N3 | 2.11 | 1.38 | 1.33 |
| 71 | GA | 501 | GTP | C2-N3 | 2.11 | 1.38 | 1.33 |
| 71 | CD | 501 | GTP | C2-N3 | 2.11 | 1.38 | 1.33 |
| 71 | OM | 501 | GTP | C2-N3 | 2.11 | 1.38 | 1.33 |
| 71 | EI | 501 | GTP | C2-N3 | 2.11 | 1.38 | 1.33 |
| 71 | VA | 501 | GTP | C2-N3 | 2.11 | 1.38 | 1.33 |
| 71 | UG | 501 | GTP | C2-N3 | 2.11 | 1.38 | 1.33 |
| 71 | C | 501 | GTP | C2-N3 | 2.10 | 1.38 | 1.33 |
| 71 | UK | 501 | GTP | C2-N3 | 2.10 | 1.38 | 1.33 |
| 71 | D | 501 | GTP | C2-N3 | 2.10 | 1.38 | 1.33 |
| 71 | EG | 501 | GTP | C2-N3 | 2.10 | 1.38 | 1.33 |
| 71 | K | 501 | GTP | C2-N3 | 2.10 | 1.38 | 1.33 |
| 71 | FI | 501 | GTP | C2-N3 | 2.10 | 1.38 | 1.33 |
| 71 | AG | 501 | GTP | C2-N3 | 2.10 | 1.38 | 1.33 |
| 71 | FC | 501 | GTP | C2-N3 | 2.10 | 1.38 | 1.33 |
| 71 | HA | 501 | GTP | C2-N3 | 2.10 | 1.38 | 1.33 |
| 71 | OA | 501 | GTP | C2-N3 | 2.10 | 1.38 | 1.33 |
| 71 | TE | 501 | GTP | C2-N3 | 2.10 | 1.38 | 1.33 |
| 71 | JJ | 501 | GTP | C2-N3 | 2.10 | 1.38 | 1.33 |
| 71 | MG | 501 | GTP | C2-N3 | 2.10 | 1.38 | 1.33 |
| 71 | BK | 501 | GTP | C2-N3 | 2.10 | 1.38 | 1.33 |
| 71 | SK | 501 | GTP | C2-N3 | 2.10 | 1.38 | 1.33 |
| 71 | BC | 501 | GTP | PA-O3A | 2.10 | 1.61 | 1.59 |
| 71 | DL | 501 | GTP | C2-N3 | 2.10 | 1.38 | 1.33 |
| 71 | UE | 501 | GTP | C2-N3 | 2.10 | 1.38 | 1.33 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 71 | DJ | 501 | GTP | C2-N3 | 2.10 | 1.38 | 1.33 |
| 71 | WM | 501 | GTP | C2-N3 | 2.09 | 1.38 | 1.33 |
| 71 | WC | 501 | GTP | C2-N3 | 2.09 | 1.38 | 1.33 |
| 71 | UA | 501 | GTP | C2-N3 | 2.09 | 1.38 | 1.33 |
| 71 | QL | 501 | GTP | C2-N3 | 2.09 | 1.38 | 1.33 |
| 71 | DB | 501 | GTP | C2-N3 | 2.09 | 1.38 | 1.33 |
| 71 | WA | 501 | GTP | C2-N3 | 2.09 | 1.38 | 1.33 |
| 71 | OE | 501 | GTP | C2-N3 | 2.09 | 1.38 | 1.33 |
| 71 | JL | 501 | GTP | C2-N3 | 2.09 | 1.38 | 1.33 |
| 71 | AE | 501 | GTP | C2-N3 | 2.09 | 1.38 | 1.33 |
| 71 | FG | 501 | GTP | C2-N3 | 2.09 | 1.38 | 1.33 |
| 71 | PM | 501 | GTP | C2-N3 | 2.09 | 1.38 | 1.33 |
| 71 | TG | 501 | GTP | C2-N3 | 2.09 | 1.38 | 1.33 |
| 71 | RH | 501 | GTP | C2-N3 | 2.08 | 1.38 | 1.33 |
| 71 | CL | 501 | GTP | PA-O3A | 2.08 | 1.61 | 1.59 |
| 71 | MC | 501 | GTP | C2-N3 | 2.08 | 1.38 | 1.33 |
| 71 | RF | 501 | GTP | C2-N3 | 2.08 | 1.38 | 1.33 |
| 71 | LL | 501 | GTP | C2-N3 | 2.08 | 1.38 | 1.33 |
| 71 | PC | 501 | GTP | C2-N3 | 2.08 | 1.38 | 1.33 |
| 71 | HG | 501 | GTP | C2-N3 | 2.08 | 1.38 | 1.33 |
| 71 | HI | 501 | GTP | C2-N3 | 2.08 | 1.38 | 1.33 |
| 71 | PE | 501 | GTP | C2-N3 | 2.08 | 1.38 | 1.33 |
| 71 | KF | 501 | GTP | PB-O3B | 2.08 | 1.61 | 1.59 |
| 71 | NE | 501 | GTP | PB-O3B | 2.08 | 1.61 | 1.59 |
| 71 | NA | 501 | GTP | C2-N3 | 2.07 | 1.38 | 1.33 |
| 71 | GE | 501 | GTP | C2-N3 | 2.07 | 1.38 | 1.33 |
| 71 | RL | 501 | GTP | C2-N3 | 2.07 | 1.38 | 1.33 |
| 71 | VK | 501 | GTP | C2-N3 | 2.07 | 1.38 | 1.33 |
| 71 | CJ | 501 | GTP | C2-N3 | 2.07 | 1.38 | 1.33 |
| 71 | MA | 501 | GTP | C2-N3 | 2.07 | 1.38 | 1.33 |
| 71 | KJ | 501 | GTP | C2-N3 | 2.07 | 1.38 | 1.33 |
| 71 | GK | 501 | GTP | C2-N3 | 2.07 | 1.38 | 1.33 |
| 71 | OG | 501 | GTP | C2-N3 | 2.07 | 1.38 | 1.33 |
| 71 | QJ | 501 | GTP | C2-N3 | 2.07 | 1.38 | 1.33 |
| 71 | SA | 501 | GTP | C2-N3 | 2.07 | 1.38 | 1.33 |
| 71 | MM | 501 | GTP | C2-N3 | 2.07 | 1.38 | 1.33 |
| 71 | HC | 501 | GTP | PB-O3B | 2.07 | 1.61 | 1.59 |
| 71 | LB | 501 | GTP | PA-O3A | 2.07 | 1.61 | 1.59 |
| 71 | TA | 501 | GTP | C2-N3 | 2.06 | 1.38 | 1.33 |
| 71 | FA | 501 | GTP | C2-N3 | 2.06 | 1.38 | 1.33 |
| 71 | EK | 501 | GTP | C2-N3 | 2.06 | 1.38 | 1.33 |
| 71 | CL | 501 | GTP | PB-O3A | 2.06 | 1.61 | 1.59 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 71 | CL | 501 | GTP | C2-N3 | 2.06 | 1.38 | 1.33 |
| 71 | NK | 501 | GTP | C2-N3 | 2.05 | 1.38 | 1.33 |
| 71 | WI | 501 | GTP | C2-N3 | 2.05 | 1.38 | 1.33 |
| 71 | LD | 501 | GTP | C2-N3 | 2.05 | 1.38 | 1.33 |
| 71 | WK | 501 | GTP | C2-N3 | 2.05 | 1.38 | 1.33 |
| 71 | BM | 501 | GTP | C2-N3 | 2.05 | 1.38 | 1.33 |
| 71 | DB | 501 | GTP | PA-O3A | 2.05 | 1.61 | 1.59 |
| 71 | LB | 501 | GTP | C2-N3 | 2.05 | 1.38 | 1.33 |
| 71 | PI | 501 | GTP | C2-N3 | 2.05 | 1.38 | 1.33 |
| 71 | LN | 501 | GTP | C2-N3 | 2.05 | 1.38 | 1.33 |
| 71 | DD | 501 | GTP | PA-O3A | 2.05 | 1.61 | 1.59 |
| 71 | DJ | 501 | GTP | PA-O3A | 2.04 | 1.61 | 1.59 |
| 71 | JD | 501 | GTP | C2-N3 | 2.04 | 1.38 | 1.33 |
| 71 | TK | 501 | GTP | C2-N3 | 2.04 | 1.38 | 1.33 |
| 71 | BI | 501 | GTP | PB-O3B | 2.04 | 1.61 | 1.59 |
| 71 | VG | 501 | GTP | PB-O3A | 2.04 | 1.61 | 1.59 |
| 71 | RB | 501 | GTP | C2-N3 | 2.04 | 1.38 | 1.33 |
| 71 | DD | 501 | GTP | C2-N3 | 2.04 | 1.38 | 1.33 |
| 71 | RJ | 501 | GTP | C2-N3 | 2.03 | 1.38 | 1.33 |
| 71 | QB | 501 | GTP | PA-O3A | 2.03 | 1.61 | 1.59 |
| 71 | MI | 501 | GTP | C2-N3 | 2.03 | 1.38 | 1.33 |
| 71 | EE | 501 | GTP | PA-O3A | 2.03 | 1.61 | 1.59 |
| 71 | BI | 501 | GTP | PB-O3A | 2.03 | 1.61 | 1.59 |
| 71 | CD | 501 | GTP | PB-O3A | 2.03 | 1.61 | 1.59 |
| 71 | ME | 501 | GTP | C2-N3 | 2.03 | 1.38 | 1.33 |
| 71 | PK | 501 | GTP | C2-N3 | 2.03 | 1.38 | 1.33 |
| 71 | CB | 501 | GTP | C2-N3 | 2.03 | 1.38 | 1.33 |
| 71 | GG | 501 | GTP | C2-N3 | 2.03 | 1.38 | 1.33 |
| 71 | TC | 501 | GTP | C2-N3 | 2.02 | 1.38 | 1.33 |
| 71 | GK | 501 | GTP | PA-O3A | 2.02 | 1.61 | 1.59 |
| 71 | BM | 501 | GTP | PB-O3A | 2.02 | 1.61 | 1.59 |
| 71 | LF | 501 | GTP | C2-N3 | 2.02 | 1.38 | 1.33 |
| 71 | ME | 501 | GTP | PB-O3A | 2.02 | 1.61 | 1.59 |
| 71 | GC | 501 | GTP | C2-N3 | 2.02 | 1.38 | 1.33 |
| 71 | ME | 501 | GTP | PA-O3A | 2.01 | 1.61 | 1.59 |
| 71 | OC | 501 | GTP | C2-N3 | 2.01 | 1.38 | 1.33 |
| 71 | RB | 501 | GTP | PA-O3A | 2.01 | 1.61 | 1.59 |
| 71 | SI | 501 | GTP | C2-N3 | 2.01 | 1.38 | 1.33 |
| 71 | QD | 501 | GTP | C2-N3 | 2.01 | 1.38 | 1.33 |
| 71 | PG | 501 | GTP | C2-N3 | 2.00 | 1.38 | 1.33 |
| 71 | D | 501 | GTP | PB-O3A | 2.00 | 1.61 | 1.59 |

All (970) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|------|-------------|----------|
| 71 | IK | 501 | GTP | C8-N7-C5 | 3.82 | 109.05 | 102.55 |
| 71 | OC | 501 | GTP | C8-N7-C5 | 3.73 | 108.90 | 102.55 |
| 71 | PE | 501 | GTP | C8-N7-C5 | 3.72 | 108.88 | 102.55 |
| 71 | DJ | 501 | GTP | C8-N7-C5 | 3.71 | 108.86 | 102.55 |
| 71 | EE | 501 | GTP | C8-N7-C5 | 3.70 | 108.85 | 102.55 |
| 71 | KN | 501 | GTP | C8-N7-C5 | 3.70 | 108.85 | 102.55 |
| 71 | EA | 501 | GTP | C8-N7-C5 | 3.70 | 108.84 | 102.55 |
| 71 | AM | 501 | GTP | C8-N7-C5 | 3.69 | 108.83 | 102.55 |
| 71 | SA | 501 | GTP | C8-N7-C5 | 3.69 | 108.83 | 102.55 |
| 71 | UC | 501 | GTP | C8-N7-C5 | 3.69 | 108.83 | 102.55 |
| 71 | JD | 501 | GTP | C8-N7-C5 | 3.68 | 108.81 | 102.55 |
| 71 | NM | 501 | GTP | C8-N7-C5 | 3.68 | 108.81 | 102.55 |
| 71 | AE | 501 | GTP | C8-N7-C5 | 3.67 | 108.81 | 102.55 |
| 71 | CF | 501 | GTP | C8-N7-C5 | 3.67 | 108.80 | 102.55 |
| 71 | UI | 501 | GTP | C8-N7-C5 | 3.67 | 108.80 | 102.55 |
| 71 | PM | 501 | GTP | C8-N7-C5 | 3.67 | 108.79 | 102.55 |
| 71 | OM | 501 | GTP | C8-N7-C5 | 3.67 | 108.79 | 102.55 |
| 71 | OK | 501 | GTP | C8-N7-C5 | 3.67 | 108.79 | 102.55 |
| 71 | HC | 501 | GTP | C8-N7-C5 | 3.67 | 108.79 | 102.55 |
| 71 | IM | 501 | GTP | C8-N7-C5 | 3.66 | 108.79 | 102.55 |
| 71 | EK | 501 | GTP | C8-N7-C5 | 3.66 | 108.78 | 102.55 |
| 71 | L | 501 | GTP | C8-N7-C5 | 3.66 | 108.78 | 102.55 |
| 71 | UA | 501 | GTP | C8-N7-C5 | 3.66 | 108.78 | 102.55 |
| 71 | LD | 501 | GTP | C8-N7-C5 | 3.66 | 108.78 | 102.55 |
| 71 | CB | 501 | GTP | C8-N7-C5 | 3.66 | 108.78 | 102.55 |
| 71 | RJ | 501 | GTP | C8-N7-C5 | 3.66 | 108.78 | 102.55 |
| 71 | CL | 501 | GTP | C8-N7-C5 | 3.66 | 108.78 | 102.55 |
| 71 | WG | 501 | GTP | C8-N7-C5 | 3.66 | 108.78 | 102.55 |
| 71 | BK | 501 | GTP | C8-N7-C5 | 3.66 | 108.77 | 102.55 |
| 71 | WI | 501 | GTP | C8-N7-C5 | 3.66 | 108.77 | 102.55 |
| 71 | DF | 501 | GTP | C8-N7-C5 | 3.66 | 108.77 | 102.55 |
| 71 | MI | 501 | GTP | C8-N7-C5 | 3.65 | 108.77 | 102.55 |
| 71 | BA | 501 | GTP | C8-N7-C5 | 3.65 | 108.77 | 102.55 |
| 71 | OI | 501 | GTP | C8-N7-C5 | 3.65 | 108.77 | 102.55 |
| 71 | SI | 501 | GTP | C8-N7-C5 | 3.65 | 108.77 | 102.55 |
| 71 | IA | 501 | GTP | C8-N7-C5 | 3.65 | 108.77 | 102.55 |
| 71 | JJ | 501 | GTP | C8-N7-C5 | 3.65 | 108.77 | 102.55 |
| 71 | KD | 501 | GTP | C8-N7-C5 | 3.65 | 108.76 | 102.55 |
| 71 | TI | 501 | GTP | C8-N7-C5 | 3.65 | 108.76 | 102.55 |
| 71 | AA | 501 | GTP | C8-N7-C5 | 3.65 | 108.76 | 102.55 |
| 71 | CJ | 501 | GTP | C8-N7-C5 | 3.65 | 108.76 | 102.55 |
| 71 | ME | 501 | GTP | C8-N7-C5 | 3.65 | 108.76 | 102.55 |
| 71 | NC | 501 | GTP | C8-N7-C5 | 3.65 | 108.76 | 102.55 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|------|-------------|----------|
| 71 | SE | 501 | GTP | C8-N7-C5 | 3.65 | 108.76 | 102.55 |
| 71 | QJ | 501 | GTP | C8-N7-C5 | 3.65 | 108.76 | 102.55 |
| 71 | AK | 501 | GTP | C8-N7-C5 | 3.65 | 108.76 | 102.55 |
| 71 | KL | 501 | GTP | C8-N7-C5 | 3.65 | 108.76 | 102.55 |
| 71 | HM | 501 | GTP | C8-N7-C5 | 3.64 | 108.75 | 102.55 |
| 71 | JB | 501 | GTP | C8-N7-C5 | 3.64 | 108.75 | 102.55 |
| 71 | QL | 501 | GTP | C8-N7-C5 | 3.64 | 108.75 | 102.55 |
| 71 | D | 501 | GTP | C8-N7-C5 | 3.64 | 108.75 | 102.55 |
| 71 | NG | 501 | GTP | C8-N7-C5 | 3.64 | 108.75 | 102.55 |
| 71 | KJ | 501 | GTP | C8-N7-C5 | 3.64 | 108.75 | 102.55 |
| 71 | SK | 501 | GTP | C8-N7-C5 | 3.64 | 108.75 | 102.55 |
| 71 | NA | 501 | GTP | C8-N7-C5 | 3.64 | 108.75 | 102.55 |
| 71 | DH | 501 | GTP | C8-N7-C5 | 3.64 | 108.75 | 102.55 |
| 71 | FE | 501 | GTP | C8-N7-C5 | 3.64 | 108.75 | 102.55 |
| 71 | NK | 501 | GTP | C8-N7-C5 | 3.64 | 108.75 | 102.55 |
| 71 | LN | 501 | GTP | C8-N7-C5 | 3.64 | 108.75 | 102.55 |
| 71 | QB | 501 | GTP | C8-N7-C5 | 3.64 | 108.74 | 102.55 |
| 71 | BC | 501 | GTP | C8-N7-C5 | 3.64 | 108.74 | 102.55 |
| 71 | RF | 501 | GTP | C8-N7-C5 | 3.64 | 108.74 | 102.55 |
| 71 | CD | 501 | GTP | C8-N7-C5 | 3.64 | 108.74 | 102.55 |
| 71 | PI | 501 | GTP | C8-N7-C5 | 3.64 | 108.74 | 102.55 |
| 71 | WK | 501 | GTP | C8-N7-C5 | 3.64 | 108.74 | 102.55 |
| 71 | PC | 501 | GTP | C8-N7-C5 | 3.64 | 108.74 | 102.55 |
| 71 | AC | 501 | GTP | C8-N7-C5 | 3.63 | 108.74 | 102.55 |
| 71 | TC | 501 | GTP | C8-N7-C5 | 3.63 | 108.74 | 102.55 |
| 71 | EI | 501 | GTP | C8-N7-C5 | 3.63 | 108.74 | 102.55 |
| 71 | WC | 501 | GTP | C8-N7-C5 | 3.63 | 108.74 | 102.55 |
| 71 | LL | 501 | GTP | C8-N7-C5 | 3.63 | 108.73 | 102.55 |
| 71 | QH | 501 | GTP | C8-N7-C5 | 3.63 | 108.73 | 102.55 |
| 71 | TA | 501 | GTP | C8-N7-C5 | 3.63 | 108.73 | 102.55 |
| 71 | EG | 501 | GTP | C8-N7-C5 | 3.63 | 108.73 | 102.55 |
| 71 | KF | 501 | GTP | C8-N7-C5 | 3.63 | 108.73 | 102.55 |
| 71 | MA | 501 | GTP | C8-N7-C5 | 3.63 | 108.73 | 102.55 |
| 71 | DL | 501 | GTP | C8-N7-C5 | 3.63 | 108.73 | 102.55 |
| 71 | QF | 501 | GTP | C8-N7-C5 | 3.63 | 108.73 | 102.55 |
| 71 | RL | 501 | GTP | C8-N7-C5 | 3.63 | 108.73 | 102.55 |
| 71 | VA | 501 | GTP | C8-N7-C5 | 3.63 | 108.73 | 102.55 |
| 71 | VG | 501 | GTP | C8-N7-C5 | 3.63 | 108.73 | 102.55 |
| 71 | MG | 501 | GTP | C8-N7-C5 | 3.63 | 108.73 | 102.55 |
| 71 | OE | 501 | GTP | C8-N7-C5 | 3.63 | 108.73 | 102.55 |
| 71 | FA | 501 | GTP | C8-N7-C5 | 3.63 | 108.72 | 102.55 |
| 71 | GK | 501 | GTP | C8-N7-C5 | 3.63 | 108.72 | 102.55 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|------|-------------|----------|
| 71 | MM | 501 | GTP | C8-N7-C5 | 3.63 | 108.72 | 102.55 |
| 71 | AG | 501 | GTP | C8-N7-C5 | 3.63 | 108.72 | 102.55 |
| 71 | UG | 501 | GTP | C8-N7-C5 | 3.63 | 108.72 | 102.55 |
| 71 | SC | 501 | GTP | C8-N7-C5 | 3.62 | 108.72 | 102.55 |
| 71 | VC | 501 | GTP | C8-N7-C5 | 3.62 | 108.72 | 102.55 |
| 71 | DB | 501 | GTP | C8-N7-C5 | 3.62 | 108.72 | 102.55 |
| 71 | FC | 501 | GTP | C8-N7-C5 | 3.62 | 108.72 | 102.55 |
| 71 | HK | 501 | GTP | C8-N7-C5 | 3.62 | 108.72 | 102.55 |
| 71 | DD | 501 | GTP | C8-N7-C5 | 3.62 | 108.72 | 102.55 |
| 71 | NE | 501 | GTP | C8-N7-C5 | 3.62 | 108.72 | 102.55 |
| 71 | WA | 501 | GTP | C8-N7-C5 | 3.62 | 108.72 | 102.55 |
| 71 | BM | 501 | GTP | C8-N7-C5 | 3.62 | 108.71 | 102.55 |
| 71 | JF | 501 | GTP | C8-N7-C5 | 3.62 | 108.71 | 102.55 |
| 71 | JN | 501 | GTP | C8-N7-C5 | 3.62 | 108.71 | 102.55 |
| 71 | GI | 501 | GTP | C8-N7-C5 | 3.62 | 108.71 | 102.55 |
| 71 | JL | 501 | GTP | C8-N7-C5 | 3.62 | 108.70 | 102.55 |
| 71 | PG | 501 | GTP | C8-N7-C5 | 3.62 | 108.70 | 102.55 |
| 71 | VK | 501 | GTP | C8-N7-C5 | 3.62 | 108.70 | 102.55 |
| 71 | FK | 501 | GTP | C8-N7-C5 | 3.61 | 108.70 | 102.55 |
| 71 | RH | 501 | GTP | C8-N7-C5 | 3.61 | 108.70 | 102.55 |
| 71 | II | 501 | GTP | C8-N7-C5 | 3.61 | 108.70 | 102.55 |
| 71 | KB | 501 | GTP | C8-N7-C5 | 3.61 | 108.70 | 102.55 |
| 71 | IC | 501 | GTP | C8-N7-C5 | 3.61 | 108.69 | 102.55 |
| 71 | K | 501 | GTP | C8-N7-C5 | 3.61 | 108.69 | 102.55 |
| 71 | MC | 501 | GTP | C8-N7-C5 | 3.61 | 108.69 | 102.55 |
| 71 | OA | 501 | GTP | C8-N7-C5 | 3.61 | 108.69 | 102.55 |
| 71 | BG | 501 | GTP | C8-N7-C5 | 3.61 | 108.69 | 102.55 |
| 71 | FG | 501 | GTP | C8-N7-C5 | 3.61 | 108.69 | 102.55 |
| 71 | OG | 501 | GTP | C8-N7-C5 | 3.61 | 108.69 | 102.55 |
| 71 | VM | 501 | GTP | C8-N7-C5 | 3.61 | 108.69 | 102.55 |
| 71 | QD | 501 | GTP | C8-N7-C5 | 3.61 | 108.69 | 102.55 |
| 71 | WM | 501 | GTP | C8-N7-C5 | 3.61 | 108.69 | 102.55 |
| 71 | FI | 501 | GTP | C8-N7-C5 | 3.60 | 108.69 | 102.55 |
| 71 | PK | 501 | GTP | C8-N7-C5 | 3.60 | 108.69 | 102.55 |
| 71 | LJ | 501 | GTP | C8-N7-C5 | 3.60 | 108.68 | 102.55 |
| 71 | C | 501 | GTP | C8-N7-C5 | 3.60 | 108.67 | 102.55 |
| 71 | AI | 501 | GTP | C8-N7-C5 | 3.59 | 108.67 | 102.55 |
| 71 | HA | 501 | GTP | C8-N7-C5 | 3.59 | 108.67 | 102.55 |
| 71 | CH | 501 | GTP | C8-N7-C5 | 3.59 | 108.67 | 102.55 |
| 71 | GG | 501 | GTP | C8-N7-C5 | 3.59 | 108.67 | 102.55 |
| 71 | WE | 501 | GTP | C8-N7-C5 | 3.59 | 108.67 | 102.55 |
| 71 | SG | 501 | GTP | C8-N7-C5 | 3.59 | 108.66 | 102.55 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 71 | TG | 501 | GTP | C8-N7-C5 | 3.59 | 108.66 | 102.55 |
| 71 | VE | 501 | GTP | C8-N7-C5 | 3.59 | 108.66 | 102.55 |
| 71 | IG | 501 | GTP | C8-N7-C5 | 3.59 | 108.66 | 102.55 |
| 71 | GE | 501 | GTP | C8-N7-C5 | 3.59 | 108.66 | 102.55 |
| 71 | J | 501 | GTP | C8-N7-C5 | 3.59 | 108.66 | 102.55 |
| 71 | EC | 501 | GTP | C8-N7-C5 | 3.59 | 108.66 | 102.55 |
| 71 | UK | 501 | GTP | C8-N7-C5 | 3.59 | 108.66 | 102.55 |
| 71 | JH | 501 | GTP | C8-N7-C5 | 3.59 | 108.66 | 102.55 |
| 71 | RB | 501 | GTP | C8-N7-C5 | 3.59 | 108.66 | 102.55 |
| 71 | BE | 501 | GTP | C8-N7-C5 | 3.59 | 108.65 | 102.55 |
| 71 | Q | 501 | GTP | C8-N7-C5 | 3.59 | 108.65 | 102.55 |
| 71 | LB | 501 | GTP | C8-N7-C5 | 3.58 | 108.65 | 102.55 |
| 71 | R | 501 | GTP | C8-N7-C5 | 3.58 | 108.65 | 102.55 |
| 71 | LF | 501 | GTP | C8-N7-C5 | 3.58 | 108.65 | 102.55 |
| 71 | VI | 501 | GTP | C8-N7-C5 | 3.58 | 108.65 | 102.55 |
| 71 | TE | 501 | GTP | C8-N7-C5 | 3.58 | 108.65 | 102.55 |
| 71 | TK | 501 | GTP | C8-N7-C5 | 3.58 | 108.65 | 102.55 |
| 71 | NI | 501 | GTP | C8-N7-C5 | 3.58 | 108.64 | 102.55 |
| 71 | HG | 501 | GTP | C8-N7-C5 | 3.58 | 108.64 | 102.55 |
| 71 | PA | 501 | GTP | C8-N7-C5 | 3.57 | 108.63 | 102.55 |
| 71 | GA | 501 | GTP | C8-N7-C5 | 3.57 | 108.63 | 102.55 |
| 71 | MK | 501 | GTP | C8-N7-C5 | 3.57 | 108.63 | 102.55 |
| 71 | KH | 501 | GTP | C8-N7-C5 | 3.57 | 108.62 | 102.55 |
| 71 | GC | 501 | GTP | C8-N7-C5 | 3.57 | 108.62 | 102.55 |
| 71 | UE | 501 | GTP | C8-N7-C5 | 3.57 | 108.62 | 102.55 |
| 71 | LH | 501 | GTP | C8-N7-C5 | 3.56 | 108.62 | 102.55 |
| 71 | HE | 501 | GTP | C8-N7-C5 | 3.56 | 108.62 | 102.55 |
| 71 | BI | 501 | GTP | C8-N7-C5 | 3.56 | 108.61 | 102.55 |
| 71 | IE | 501 | GTP | C8-N7-C5 | 3.52 | 108.55 | 102.55 |
| 71 | HI | 501 | GTP | C8-N7-C5 | 3.52 | 108.54 | 102.55 |
| 71 | RD | 501 | GTP | C8-N7-C5 | 3.51 | 108.53 | 102.55 |
| 69 | CM | 500 | GDP | O4'-C1'-N9 | 3.29 | 113.11 | 108.75 |
| 69 | CK | 500 | GDP | C8-N7-C5 | 3.06 | 107.76 | 102.55 |
| 71 | IA | 501 | GTP | C5-C6-N1 | 3.06 | 119.90 | 114.07 |
| 71 | IA | 501 | GTP | C2-N1-C6 | -3.05 | 119.53 | 125.11 |
| 71 | LH | 501 | GTP | C5-C6-N1 | 3.03 | 119.86 | 114.07 |
| 71 | PA | 501 | GTP | C5-C6-N1 | 3.03 | 119.86 | 114.07 |
| 71 | HK | 501 | GTP | C2-N1-C6 | -3.03 | 119.56 | 125.11 |
| 71 | IE | 501 | GTP | C5-C6-N1 | 3.03 | 119.85 | 114.07 |
| 71 | VM | 501 | GTP | C5-C6-N1 | 3.03 | 119.85 | 114.07 |
| 71 | HK | 501 | GTP | C5-C6-N1 | 3.02 | 119.83 | 114.07 |
| 71 | EA | 501 | GTP | C2-N1-C6 | -3.02 | 119.59 | 125.11 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 71 | IC | 501 | GTP | C2-N1-C6 | -3.02 | 119.59 | 125.11 |
| 71 | JB | 501 | GTP | C5-C6-N1 | 3.01 | 119.80 | 114.07 |
| 71 | KL | 501 | GTP | C5-C6-N1 | 3.00 | 119.80 | 114.07 |
| 71 | OK | 501 | GTP | C5-C6-N1 | 3.00 | 119.80 | 114.07 |
| 71 | KD | 501 | GTP | C5-C6-N1 | 3.00 | 119.79 | 114.07 |
| 71 | JJ | 501 | GTP | C5-C6-N1 | 3.00 | 119.79 | 114.07 |
| 71 | JH | 501 | GTP | C5-C6-N1 | 3.00 | 119.79 | 114.07 |
| 71 | EA | 501 | GTP | C5-C6-N1 | 3.00 | 119.79 | 114.07 |
| 71 | WG | 501 | GTP | C5-C6-N1 | 2.99 | 119.78 | 114.07 |
| 71 | QB | 501 | GTP | C2-N1-C6 | -2.99 | 119.63 | 125.11 |
| 71 | AM | 501 | GTP | C5-C6-N1 | 2.99 | 119.78 | 114.07 |
| 71 | QH | 501 | GTP | C5-C6-N1 | 2.99 | 119.78 | 114.07 |
| 71 | LF | 501 | GTP | C2-N1-C6 | -2.99 | 119.63 | 125.11 |
| 71 | WM | 501 | GTP | C2-N1-C6 | -2.99 | 119.63 | 125.11 |
| 71 | BA | 501 | GTP | C5-C6-N1 | 2.99 | 119.77 | 114.07 |
| 71 | C | 501 | GTP | C5-C6-N1 | 2.99 | 119.77 | 114.07 |
| 71 | PA | 501 | GTP | C2-N1-C6 | -2.99 | 119.64 | 125.11 |
| 71 | CF | 501 | GTP | C5-C6-N1 | 2.99 | 119.77 | 114.07 |
| 71 | PK | 501 | GTP | C2-N1-C6 | -2.98 | 119.65 | 125.11 |
| 71 | WE | 501 | GTP | C5-C6-N1 | 2.98 | 119.76 | 114.07 |
| 71 | KH | 501 | GTP | C2-N1-C6 | -2.98 | 119.65 | 125.11 |
| 71 | KH | 501 | GTP | C5-C6-N1 | 2.98 | 119.76 | 114.07 |
| 71 | RJ | 501 | GTP | C5-C6-N1 | 2.98 | 119.76 | 114.07 |
| 71 | VK | 501 | GTP | C5-C6-N1 | 2.98 | 119.76 | 114.07 |
| 71 | AK | 501 | GTP | C5-C6-N1 | 2.98 | 119.75 | 114.07 |
| 71 | PE | 501 | GTP | C5-C6-N1 | 2.98 | 119.75 | 114.07 |
| 71 | IC | 501 | GTP | C5-C6-N1 | 2.98 | 119.75 | 114.07 |
| 71 | TE | 501 | GTP | C2-N1-C6 | -2.98 | 119.66 | 125.11 |
| 71 | SI | 501 | GTP | C5-C6-N1 | 2.98 | 119.75 | 114.07 |
| 71 | QJ | 501 | GTP | C5-C6-N1 | 2.98 | 119.75 | 114.07 |
| 71 | DJ | 501 | GTP | C5-C6-N1 | 2.97 | 119.75 | 114.07 |
| 71 | II | 501 | GTP | C5-C6-N1 | 2.97 | 119.75 | 114.07 |
| 71 | QL | 501 | GTP | C5-C6-N1 | 2.97 | 119.75 | 114.07 |
| 71 | TE | 501 | GTP | C5-C6-N1 | 2.97 | 119.74 | 114.07 |
| 71 | LH | 501 | GTP | C2-N1-C6 | -2.97 | 119.67 | 125.11 |
| 71 | LB | 501 | GTP | C2-N1-C6 | -2.97 | 119.67 | 125.11 |
| 71 | QF | 501 | GTP | C5-C6-N1 | 2.97 | 119.74 | 114.07 |
| 71 | KB | 501 | GTP | C5-C6-N1 | 2.97 | 119.74 | 114.07 |
| 71 | OA | 501 | GTP | C5-C6-N1 | 2.97 | 119.73 | 114.07 |
| 71 | RJ | 501 | GTP | C2-N1-C6 | -2.97 | 119.68 | 125.11 |
| 71 | KF | 501 | GTP | C5-C6-N1 | 2.97 | 119.73 | 114.07 |
| 71 | UI | 501 | GTP | C5-C6-N1 | 2.97 | 119.73 | 114.07 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 71 | FE | 501 | GTP | C5-C6-N1 | 2.97 | 119.73 | 114.07 |
| 71 | DB | 501 | GTP | C5-C6-N1 | 2.97 | 119.73 | 114.07 |
| 71 | LF | 501 | GTP | C5-C6-N1 | 2.97 | 119.73 | 114.07 |
| 71 | LJ | 501 | GTP | C5-C6-N1 | 2.97 | 119.73 | 114.07 |
| 71 | KN | 501 | GTP | C5-C6-N1 | 2.97 | 119.73 | 114.07 |
| 71 | QL | 501 | GTP | C2-N1-C6 | -2.97 | 119.68 | 125.11 |
| 71 | DJ | 501 | GTP | C2-N1-C6 | -2.96 | 119.68 | 125.11 |
| 69 | EL | 500 | GDP | C8-N7-C5 | 2.96 | 107.59 | 102.55 |
| 71 | OM | 501 | GTP | C5-C6-N1 | 2.96 | 119.72 | 114.07 |
| 71 | BK | 501 | GTP | C5-C6-N1 | 2.96 | 119.72 | 114.07 |
| 71 | CH | 501 | GTP | C5-C6-N1 | 2.96 | 119.72 | 114.07 |
| 71 | IM | 501 | GTP | C5-C6-N1 | 2.96 | 119.72 | 114.07 |
| 71 | UC | 501 | GTP | C5-C6-N1 | 2.96 | 119.72 | 114.07 |
| 71 | NM | 501 | GTP | C2-N1-C6 | -2.96 | 119.69 | 125.11 |
| 71 | VE | 501 | GTP | C5-C6-N1 | 2.96 | 119.72 | 114.07 |
| 71 | II | 501 | GTP | C2-N1-C6 | -2.96 | 119.69 | 125.11 |
| 71 | KB | 501 | GTP | C2-N1-C6 | -2.96 | 119.69 | 125.11 |
| 71 | VI | 501 | GTP | C5-C6-N1 | 2.96 | 119.72 | 114.07 |
| 71 | MA | 501 | GTP | C5-C6-N1 | 2.96 | 119.72 | 114.07 |
| 71 | JH | 501 | GTP | C2-N1-C6 | -2.96 | 119.69 | 125.11 |
| 71 | WM | 501 | GTP | C5-C6-N1 | 2.96 | 119.72 | 114.07 |
| 71 | CB | 501 | GTP | C5-C6-N1 | 2.96 | 119.72 | 114.07 |
| 71 | CL | 501 | GTP | C2-N1-C6 | -2.96 | 119.69 | 125.11 |
| 71 | PC | 501 | GTP | C5-C6-N1 | 2.96 | 119.71 | 114.07 |
| 71 | UE | 501 | GTP | C5-C6-N1 | 2.96 | 119.71 | 114.07 |
| 71 | VG | 501 | GTP | C5-C6-N1 | 2.96 | 119.71 | 114.07 |
| 71 | OC | 501 | GTP | C2-N1-C6 | -2.96 | 119.70 | 125.11 |
| 71 | FK | 501 | GTP | C5-C6-N1 | 2.96 | 119.71 | 114.07 |
| 71 | JL | 501 | GTP | C5-C6-N1 | 2.95 | 119.71 | 114.07 |
| 71 | CH | 501 | GTP | C2-N1-C6 | -2.95 | 119.70 | 125.11 |
| 71 | SE | 501 | GTP | C2-N1-C6 | -2.95 | 119.70 | 125.11 |
| 71 | MM | 501 | GTP | C2-N1-C6 | -2.95 | 119.70 | 125.11 |
| 71 | QD | 501 | GTP | C2-N1-C6 | -2.95 | 119.70 | 125.11 |
| 71 | FC | 501 | GTP | C2-N1-C6 | -2.95 | 119.71 | 125.11 |
| 71 | EI | 501 | GTP | C2-N1-C6 | -2.95 | 119.71 | 125.11 |
| 71 | QH | 501 | GTP | C2-N1-C6 | -2.95 | 119.71 | 125.11 |
| 71 | MA | 501 | GTP | C2-N1-C6 | -2.95 | 119.71 | 125.11 |
| 71 | MK | 501 | GTP | C5-C6-N1 | 2.95 | 119.70 | 114.07 |
| 71 | CD | 501 | GTP | C5-C6-N1 | 2.95 | 119.70 | 114.07 |
| 71 | VC | 501 | GTP | C5-C6-N1 | 2.95 | 119.70 | 114.07 |
| 69 | E | 500 | GDP | C8-N7-C5 | 2.95 | 107.57 | 102.55 |
| 71 | OC | 501 | GTP | C5-C6-N1 | 2.95 | 119.70 | 114.07 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 71 | R | 501 | GTP | C5-C6-N1 | 2.95 | 119.70 | 114.07 |
| 71 | CJ | 501 | GTP | C2-N1-C6 | -2.95 | 119.71 | 125.11 |
| 71 | EE | 501 | GTP | C5-C6-N1 | 2.95 | 119.69 | 114.07 |
| 71 | EG | 501 | GTP | C5-C6-N1 | 2.95 | 119.69 | 114.07 |
| 71 | EG | 501 | GTP | C2-N1-C6 | -2.95 | 119.71 | 125.11 |
| 71 | OK | 501 | GTP | C2-N1-C6 | -2.95 | 119.72 | 125.11 |
| 71 | GE | 501 | GTP | C5-C6-N1 | 2.95 | 119.69 | 114.07 |
| 71 | WK | 501 | GTP | C5-C6-N1 | 2.95 | 119.69 | 114.07 |
| 71 | SK | 501 | GTP | C5-C6-N1 | 2.95 | 119.69 | 114.07 |
| 71 | VI | 501 | GTP | C2-N1-C6 | -2.94 | 119.72 | 125.11 |
| 71 | WC | 501 | GTP | C5-C6-N1 | 2.94 | 119.69 | 114.07 |
| 71 | IM | 501 | GTP | C2-N1-C6 | -2.94 | 119.72 | 125.11 |
| 71 | VA | 501 | GTP | C2-N1-C6 | -2.94 | 119.72 | 125.11 |
| 71 | RB | 501 | GTP | C5-C6-N1 | 2.94 | 119.68 | 114.07 |
| 71 | AC | 501 | GTP | C5-C6-N1 | 2.94 | 119.68 | 114.07 |
| 71 | DF | 501 | GTP | C5-C6-N1 | 2.94 | 119.68 | 114.07 |
| 71 | CB | 501 | GTP | C2-N1-C6 | -2.94 | 119.72 | 125.11 |
| 71 | NG | 501 | GTP | C2-N1-C6 | -2.94 | 119.72 | 125.11 |
| 71 | QF | 501 | GTP | C2-N1-C6 | -2.94 | 119.72 | 125.11 |
| 71 | EC | 501 | GTP | C5-C6-N1 | 2.94 | 119.68 | 114.07 |
| 71 | UG | 501 | GTP | C5-C6-N1 | 2.94 | 119.68 | 114.07 |
| 71 | D | 501 | GTP | C2-N1-C6 | -2.94 | 119.73 | 125.11 |
| 71 | KD | 501 | GTP | C2-N1-C6 | -2.94 | 119.73 | 125.11 |
| 71 | GI | 501 | GTP | C5-C6-N1 | 2.94 | 119.68 | 114.07 |
| 71 | QB | 501 | GTP | C5-C6-N1 | 2.94 | 119.68 | 114.07 |
| 71 | NC | 501 | GTP | C2-N1-C6 | -2.94 | 119.73 | 125.11 |
| 71 | RF | 501 | GTP | C5-C6-N1 | 2.94 | 119.68 | 114.07 |
| 71 | IE | 501 | GTP | C2-N1-C6 | -2.94 | 119.73 | 125.11 |
| 71 | PC | 501 | GTP | C2-N1-C6 | -2.94 | 119.73 | 125.11 |
| 71 | PI | 501 | GTP | C2-N1-C6 | -2.94 | 119.73 | 125.11 |
| 71 | PI | 501 | GTP | C5-C6-N1 | 2.94 | 119.68 | 114.07 |
| 71 | DH | 501 | GTP | C2-N1-C6 | -2.94 | 119.73 | 125.11 |
| 71 | NI | 501 | GTP | C2-N1-C6 | -2.94 | 119.73 | 125.11 |
| 71 | JD | 501 | GTP | C2-N1-C6 | -2.94 | 119.73 | 125.11 |
| 71 | UA | 501 | GTP | C2-N1-C6 | -2.94 | 119.73 | 125.11 |
| 71 | OE | 501 | GTP | C2-N1-C6 | -2.94 | 119.73 | 125.11 |
| 71 | SG | 501 | GTP | C2-N1-C6 | -2.94 | 119.73 | 125.11 |
| 71 | NA | 501 | GTP | C5-C6-N1 | 2.94 | 119.67 | 114.07 |
| 71 | NM | 501 | GTP | C5-C6-N1 | 2.94 | 119.67 | 114.07 |
| 71 | PK | 501 | GTP | C5-C6-N1 | 2.94 | 119.67 | 114.07 |
| 71 | TC | 501 | GTP | C5-C6-N1 | 2.94 | 119.67 | 114.07 |
| 71 | NA | 501 | GTP | C2-N1-C6 | -2.94 | 119.73 | 125.11 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 71 | FC | 501 | GTP | C5-C6-N1 | 2.94 | 119.67 | 114.07 |
| 71 | KF | 501 | GTP | C2-N1-C6 | -2.94 | 119.73 | 125.11 |
| 71 | BG | 501 | GTP | C5-C6-N1 | 2.94 | 119.67 | 114.07 |
| 71 | DH | 501 | GTP | C5-C6-N1 | 2.94 | 119.67 | 114.07 |
| 71 | IG | 501 | GTP | C2-N1-C6 | -2.94 | 119.74 | 125.11 |
| 71 | UI | 501 | GTP | C2-N1-C6 | -2.94 | 119.74 | 125.11 |
| 71 | VC | 501 | GTP | C2-N1-C6 | -2.94 | 119.74 | 125.11 |
| 71 | QD | 501 | GTP | C5-C6-N1 | 2.94 | 119.67 | 114.07 |
| 69 | DM | 500 | GDP | C8-N7-C5 | 2.93 | 107.55 | 102.55 |
| 71 | JD | 501 | GTP | C5-C6-N1 | 2.93 | 119.67 | 114.07 |
| 71 | SI | 501 | GTP | C2-N1-C6 | -2.93 | 119.74 | 125.11 |
| 71 | FG | 501 | GTP | C5-C6-N1 | 2.93 | 119.67 | 114.07 |
| 71 | Q | 501 | GTP | C5-C6-N1 | 2.93 | 119.67 | 114.07 |
| 71 | EE | 501 | GTP | C2-N1-C6 | -2.93 | 119.74 | 125.11 |
| 71 | HC | 501 | GTP | C5-C6-N1 | 2.93 | 119.67 | 114.07 |
| 71 | WI | 501 | GTP | C5-C6-N1 | 2.93 | 119.67 | 114.07 |
| 71 | NC | 501 | GTP | C5-C6-N1 | 2.93 | 119.67 | 114.07 |
| 71 | EK | 501 | GTP | C5-C6-N1 | 2.93 | 119.67 | 114.07 |
| 71 | JN | 501 | GTP | C5-C6-N1 | 2.93 | 119.67 | 114.07 |
| 71 | AK | 501 | GTP | C2-N1-C6 | -2.93 | 119.74 | 125.11 |
| 71 | CL | 501 | GTP | C5-C6-N1 | 2.93 | 119.66 | 114.07 |
| 71 | DD | 501 | GTP | C2-N1-C6 | -2.93 | 119.74 | 125.11 |
| 71 | JJ | 501 | GTP | C2-N1-C6 | -2.93 | 119.74 | 125.11 |
| 71 | PE | 501 | GTP | C2-N1-C6 | -2.93 | 119.74 | 125.11 |
| 71 | AA | 501 | GTP | C5-C6-N1 | 2.93 | 119.66 | 114.07 |
| 71 | L | 501 | GTP | C5-C6-N1 | 2.93 | 119.66 | 114.07 |
| 71 | QJ | 501 | GTP | C2-N1-C6 | -2.93 | 119.75 | 125.11 |
| 71 | TI | 501 | GTP | C2-N1-C6 | -2.93 | 119.75 | 125.11 |
| 71 | EI | 501 | GTP | C5-C6-N1 | 2.93 | 119.66 | 114.07 |
| 71 | SE | 501 | GTP | C5-C6-N1 | 2.93 | 119.66 | 114.07 |
| 69 | PL | 500 | GDP | C8-N7-C5 | 2.93 | 107.54 | 102.55 |
| 71 | BG | 501 | GTP | C2-N1-C6 | -2.93 | 119.75 | 125.11 |
| 71 | AI | 501 | GTP | C5-C6-N1 | 2.93 | 119.66 | 114.07 |
| 71 | LN | 501 | GTP | C2-N1-C6 | -2.93 | 119.75 | 125.11 |
| 71 | OE | 501 | GTP | C5-C6-N1 | 2.93 | 119.66 | 114.07 |
| 71 | TI | 501 | GTP | C5-C6-N1 | 2.93 | 119.66 | 114.07 |
| 71 | AI | 501 | GTP | C2-N1-C6 | -2.93 | 119.75 | 125.11 |
| 71 | JF | 501 | GTP | C2-N1-C6 | -2.93 | 119.75 | 125.11 |
| 71 | OI | 501 | GTP | C5-C6-N1 | 2.93 | 119.66 | 114.07 |
| 69 | H | 500 | GDP | C8-N7-C5 | 2.93 | 107.53 | 102.55 |
| 71 | BC | 501 | GTP | C5-C6-N1 | 2.93 | 119.66 | 114.07 |
| 71 | JF | 501 | GTP | C5-C6-N1 | 2.93 | 119.66 | 114.07 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 71 | SG | 501 | GTP | C5-C6-N1 | 2.93 | 119.66 | 114.07 |
| 71 | K | 501 | GTP | C2-N1-C6 | -2.93 | 119.75 | 125.11 |
| 71 | L | 501 | GTP | C2-N1-C6 | -2.93 | 119.75 | 125.11 |
| 71 | BE | 501 | GTP | C5-C6-N1 | 2.93 | 119.65 | 114.07 |
| 71 | DF | 501 | GTP | C2-N1-C6 | -2.93 | 119.75 | 125.11 |
| 71 | J | 501 | GTP | C2-N1-C6 | -2.93 | 119.75 | 125.11 |
| 71 | KL | 501 | GTP | C2-N1-C6 | -2.93 | 119.75 | 125.11 |
| 71 | VG | 501 | GTP | C2-N1-C6 | -2.93 | 119.75 | 125.11 |
| 69 | DE | 500 | GDP | C8-N7-C5 | 2.93 | 107.53 | 102.55 |
| 71 | UA | 501 | GTP | C5-C6-N1 | 2.93 | 119.65 | 114.07 |
| 71 | AE | 501 | GTP | C2-N1-C6 | -2.93 | 119.75 | 125.11 |
| 71 | BK | 501 | GTP | C2-N1-C6 | -2.93 | 119.75 | 125.11 |
| 71 | GG | 501 | GTP | C5-C6-N1 | 2.93 | 119.65 | 114.07 |
| 71 | TG | 501 | GTP | C5-C6-N1 | 2.92 | 119.65 | 114.07 |
| 71 | CJ | 501 | GTP | C5-C6-N1 | 2.92 | 119.65 | 114.07 |
| 71 | J | 501 | GTP | C5-C6-N1 | 2.92 | 119.65 | 114.07 |
| 71 | NI | 501 | GTP | C5-C6-N1 | 2.92 | 119.65 | 114.07 |
| 71 | SC | 501 | GTP | C5-C6-N1 | 2.92 | 119.65 | 114.07 |
| 71 | OG | 501 | GTP | C2-N1-C6 | -2.92 | 119.76 | 125.11 |
| 69 | CC | 500 | GDP | C8-N7-C5 | 2.92 | 107.53 | 102.55 |
| 69 | TL | 500 | GDP | C8-N7-C5 | 2.92 | 107.53 | 102.55 |
| 71 | DB | 501 | GTP | C2-N1-C6 | -2.92 | 119.76 | 125.11 |
| 69 | U | 500 | GDP | C8-N7-C5 | 2.92 | 107.53 | 102.55 |
| 71 | NE | 501 | GTP | C5-C6-N1 | 2.92 | 119.65 | 114.07 |
| 71 | BE | 501 | GTP | C2-N1-C6 | -2.92 | 119.76 | 125.11 |
| 71 | TG | 501 | GTP | C2-N1-C6 | -2.92 | 119.76 | 125.11 |
| 71 | VM | 501 | GTP | C2-N1-C6 | -2.92 | 119.76 | 125.11 |
| 71 | DL | 501 | GTP | C5-C6-N1 | 2.92 | 119.64 | 114.07 |
| 71 | NK | 501 | GTP | C5-C6-N1 | 2.92 | 119.64 | 114.07 |
| 71 | NG | 501 | GTP | C5-C6-N1 | 2.92 | 119.64 | 114.07 |
| 71 | GK | 501 | GTP | C2-N1-C6 | -2.92 | 119.76 | 125.11 |
| 69 | TD | 500 | GDP | C8-N7-C5 | 2.92 | 107.52 | 102.55 |
| 71 | K | 501 | GTP | C5-C6-N1 | 2.92 | 119.64 | 114.07 |
| 71 | AM | 501 | GTP | C2-N1-C6 | -2.92 | 119.77 | 125.11 |
| 71 | DL | 501 | GTP | C2-N1-C6 | -2.92 | 119.77 | 125.11 |
| 71 | VA | 501 | GTP | C5-C6-N1 | 2.92 | 119.64 | 114.07 |
| 69 | DA | 500 | GDP | C8-N7-C5 | 2.92 | 107.52 | 102.55 |
| 69 | QK | 500 | GDP | C8-N7-C5 | 2.92 | 107.52 | 102.55 |
| 71 | JN | 501 | GTP | C2-N1-C6 | -2.92 | 119.77 | 125.11 |
| 71 | TK | 501 | GTP | C2-N1-C6 | -2.92 | 119.77 | 125.11 |
| 71 | UC | 501 | GTP | C2-N1-C6 | -2.92 | 119.77 | 125.11 |
| 71 | OI | 501 | GTP | C2-N1-C6 | -2.92 | 119.77 | 125.11 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 71 | OG | 501 | GTP | C5-C6-N1 | 2.92 | 119.64 | 114.07 |
| 71 | TA | 501 | GTP | C5-C6-N1 | 2.92 | 119.64 | 114.07 |
| 69 | WH | 500 | GDP | C8-N7-C5 | 2.92 | 107.52 | 102.55 |
| 71 | MM | 501 | GTP | C5-C6-N1 | 2.92 | 119.64 | 114.07 |
| 71 | PM | 501 | GTP | C5-C6-N1 | 2.92 | 119.64 | 114.07 |
| 71 | SA | 501 | GTP | C5-C6-N1 | 2.92 | 119.64 | 114.07 |
| 71 | WA | 501 | GTP | C5-C6-N1 | 2.92 | 119.64 | 114.07 |
| 69 | P | 500 | GDP | C8-N7-C5 | 2.92 | 107.52 | 102.55 |
| 71 | MK | 501 | GTP | C2-N1-C6 | -2.92 | 119.77 | 125.11 |
| 71 | NE | 501 | GTP | C2-N1-C6 | -2.92 | 119.77 | 125.11 |
| 71 | LD | 501 | GTP | C5-C6-N1 | 2.92 | 119.64 | 114.07 |
| 71 | GC | 501 | GTP | C2-N1-C6 | -2.92 | 119.77 | 125.11 |
| 71 | RB | 501 | GTP | C2-N1-C6 | -2.92 | 119.77 | 125.11 |
| 71 | LN | 501 | GTP | C5-C6-N1 | 2.92 | 119.64 | 114.07 |
| 71 | RD | 501 | GTP | C5-C6-N1 | 2.92 | 119.64 | 114.07 |
| 71 | FG | 501 | GTP | C2-N1-C6 | -2.92 | 119.77 | 125.11 |
| 71 | WC | 501 | GTP | C2-N1-C6 | -2.92 | 119.77 | 125.11 |
| 71 | LL | 501 | GTP | C5-C6-N1 | 2.91 | 119.63 | 114.07 |
| 71 | RF | 501 | GTP | C2-N1-C6 | -2.91 | 119.78 | 125.11 |
| 71 | WA | 501 | GTP | C2-N1-C6 | -2.91 | 119.78 | 125.11 |
| 69 | S | 500 | GDP | C8-N7-C5 | 2.91 | 107.51 | 102.55 |
| 71 | ME | 501 | GTP | C5-C6-N1 | 2.91 | 119.63 | 114.07 |
| 71 | R | 501 | GTP | C2-N1-C6 | -2.91 | 119.78 | 125.11 |
| 69 | CG | 500 | GDP | C8-N7-C5 | 2.91 | 107.51 | 102.55 |
| 69 | UL | 500 | GDP | C8-N7-C5 | 2.91 | 107.51 | 102.55 |
| 71 | KJ | 501 | GTP | C5-C6-N1 | 2.91 | 119.63 | 114.07 |
| 71 | GK | 501 | GTP | C5-C6-N1 | 2.91 | 119.63 | 114.07 |
| 71 | EK | 501 | GTP | C2-N1-C6 | -2.91 | 119.78 | 125.11 |
| 71 | WG | 501 | GTP | C2-N1-C6 | -2.91 | 119.78 | 125.11 |
| 69 | SF | 500 | GDP | C8-N7-C5 | 2.91 | 107.51 | 102.55 |
| 71 | RH | 501 | GTP | C5-C6-N1 | 2.91 | 119.62 | 114.07 |
| 71 | OM | 501 | GTP | C2-N1-C6 | -2.91 | 119.78 | 125.11 |
| 71 | SK | 501 | GTP | C2-N1-C6 | -2.91 | 119.78 | 125.11 |
| 69 | FL | 500 | GDP | C8-N7-C5 | 2.91 | 107.50 | 102.55 |
| 71 | FK | 501 | GTP | C2-N1-C6 | -2.91 | 119.78 | 125.11 |
| 71 | PG | 501 | GTP | C5-C6-N1 | 2.91 | 119.62 | 114.07 |
| 71 | CF | 501 | GTP | C2-N1-C6 | -2.91 | 119.78 | 125.11 |
| 71 | Q | 501 | GTP | C2-N1-C6 | -2.91 | 119.78 | 125.11 |
| 71 | AE | 501 | GTP | C5-C6-N1 | 2.91 | 119.62 | 114.07 |
| 71 | IG | 501 | GTP | C5-C6-N1 | 2.91 | 119.62 | 114.07 |
| 71 | WI | 501 | GTP | C2-N1-C6 | -2.91 | 119.78 | 125.11 |
| 71 | LD | 501 | GTP | C2-N1-C6 | -2.91 | 119.79 | 125.11 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 71 | HE | 501 | GTP | C5-C6-N1 | 2.91 | 119.62 | 114.07 |
| 71 | MI | 501 | GTP | C2-N1-C6 | -2.91 | 119.79 | 125.11 |
| 71 | KN | 501 | GTP | C2-N1-C6 | -2.91 | 119.79 | 125.11 |
| 71 | PG | 501 | GTP | C2-N1-C6 | -2.91 | 119.79 | 125.11 |
| 71 | WE | 501 | GTP | C2-N1-C6 | -2.91 | 119.79 | 125.11 |
| 71 | NK | 501 | GTP | C2-N1-C6 | -2.91 | 119.79 | 125.11 |
| 71 | FA | 501 | GTP | C5-C6-N1 | 2.91 | 119.61 | 114.07 |
| 71 | MG | 501 | GTP | C5-C6-N1 | 2.91 | 119.61 | 114.07 |
| 69 | NJ | 500 | GDP | C8-N7-C5 | 2.90 | 107.50 | 102.55 |
| 71 | C | 501 | GTP | C2-N1-C6 | -2.90 | 119.79 | 125.11 |
| 71 | AG | 501 | GTP | C5-C6-N1 | 2.90 | 119.61 | 114.07 |
| 69 | DI | 500 | GDP | C8-N7-C5 | 2.90 | 107.49 | 102.55 |
| 69 | UF | 500 | GDP | C8-N7-C5 | 2.90 | 107.49 | 102.55 |
| 71 | BM | 501 | GTP | C2-N1-C6 | -2.90 | 119.80 | 125.11 |
| 71 | MI | 501 | GTP | C5-C6-N1 | 2.90 | 119.61 | 114.07 |
| 71 | JL | 501 | GTP | C2-N1-C6 | -2.90 | 119.80 | 125.11 |
| 69 | KM | 500 | GDP | C8-N7-C5 | 2.90 | 107.49 | 102.55 |
| 69 | KA | 500 | GDP | C8-N7-C5 | 2.90 | 107.49 | 102.55 |
| 71 | UG | 501 | GTP | C2-N1-C6 | -2.90 | 119.80 | 125.11 |
| 71 | DD | 501 | GTP | C5-C6-N1 | 2.90 | 119.60 | 114.07 |
| 71 | HM | 501 | GTP | C5-C6-N1 | 2.90 | 119.60 | 114.07 |
| 69 | T | 500 | GDP | C8-N7-C5 | 2.90 | 107.49 | 102.55 |
| 71 | BA | 501 | GTP | C2-N1-C6 | -2.90 | 119.80 | 125.11 |
| 69 | GL | 500 | GDP | C8-N7-C5 | 2.90 | 107.48 | 102.55 |
| 71 | HC | 501 | GTP | C2-N1-C6 | -2.90 | 119.80 | 125.11 |
| 71 | OA | 501 | GTP | C2-N1-C6 | -2.90 | 119.81 | 125.11 |
| 69 | LG | 500 | GDP | C8-N7-C5 | 2.90 | 107.48 | 102.55 |
| 71 | AA | 501 | GTP | C2-N1-C6 | -2.90 | 119.81 | 125.11 |
| 71 | GE | 501 | GTP | C2-N1-C6 | -2.90 | 119.81 | 125.11 |
| 69 | VB | 500 | GDP | C8-N7-C5 | 2.90 | 107.48 | 102.55 |
| 71 | AG | 501 | GTP | C2-N1-C6 | -2.90 | 119.81 | 125.11 |
| 69 | UJ | 500 | GDP | C8-N7-C5 | 2.90 | 107.48 | 102.55 |
| 69 | V | 500 | GDP | C8-N7-C5 | 2.90 | 107.48 | 102.55 |
| 71 | D | 501 | GTP | C5-C6-N1 | 2.90 | 119.60 | 114.07 |
| 71 | VK | 501 | GTP | C2-N1-C6 | -2.90 | 119.81 | 125.11 |
| 71 | LB | 501 | GTP | C5-C6-N1 | 2.90 | 119.60 | 114.07 |
| 69 | BB | 500 | GDP | C8-N7-C5 | 2.90 | 107.48 | 102.55 |
| 71 | LL | 501 | GTP | C2-N1-C6 | -2.89 | 119.81 | 125.11 |
| 71 | HG | 501 | GTP | C2-N1-C6 | -2.89 | 119.81 | 125.11 |
| 69 | EJ | 500 | GDP | C8-N7-C5 | 2.89 | 107.47 | 102.55 |
| 69 | GH | 500 | GDP | C8-N7-C5 | 2.89 | 107.47 | 102.55 |
| 71 | GI | 501 | GTP | C2-N1-C6 | -2.89 | 119.81 | 125.11 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 71 | HE | 501 | GTP | C2-N1-C6 | -2.89 | 119.81 | 125.11 |
| 69 | JM | 500 | GDP | C8-N7-C5 | 2.89 | 107.47 | 102.55 |
| 71 | BC | 501 | GTP | C2-N1-C6 | -2.89 | 119.82 | 125.11 |
| 71 | BM | 501 | GTP | C5-C6-N1 | 2.89 | 119.59 | 114.07 |
| 71 | FI | 501 | GTP | C2-N1-C6 | -2.89 | 119.82 | 125.11 |
| 71 | WK | 501 | GTP | C2-N1-C6 | -2.89 | 119.82 | 125.11 |
| 69 | TF | 500 | GDP | C8-N7-C5 | 2.89 | 107.47 | 102.55 |
| 71 | GA | 501 | GTP | C2-N1-C6 | -2.89 | 119.82 | 125.11 |
| 71 | JB | 501 | GTP | C2-N1-C6 | -2.89 | 119.82 | 125.11 |
| 71 | GA | 501 | GTP | C5-C6-N1 | 2.89 | 119.58 | 114.07 |
| 69 | KI | 500 | GDP | C8-N7-C5 | 2.89 | 107.47 | 102.55 |
| 71 | RH | 501 | GTP | C2-N1-C6 | -2.89 | 119.82 | 125.11 |
| 71 | AC | 501 | GTP | C2-N1-C6 | -2.89 | 119.82 | 125.11 |
| 69 | AB | 500 | GDP | C8-N7-C5 | 2.89 | 107.47 | 102.55 |
| 69 | EF | 500 | GDP | C8-N7-C5 | 2.89 | 107.47 | 102.55 |
| 69 | IF | 500 | GDP | C8-N7-C5 | 2.89 | 107.47 | 102.55 |
| 69 | PD | 500 | GDP | C8-N7-C5 | 2.89 | 107.46 | 102.55 |
| 71 | PM | 501 | GTP | C2-N1-C6 | -2.89 | 119.83 | 125.11 |
| 69 | SB | 500 | GDP | C8-N7-C5 | 2.89 | 107.46 | 102.55 |
| 69 | HB | 500 | GDP | C8-N7-C5 | 2.89 | 107.46 | 102.55 |
| 71 | MG | 501 | GTP | C2-N1-C6 | -2.88 | 119.83 | 125.11 |
| 69 | BJ | 500 | GDP | C8-N7-C5 | 2.88 | 107.46 | 102.55 |
| 71 | UE | 501 | GTP | C2-N1-C6 | -2.88 | 119.83 | 125.11 |
| 71 | MC | 501 | GTP | C2-N1-C6 | -2.88 | 119.83 | 125.11 |
| 71 | SC | 501 | GTP | C2-N1-C6 | -2.88 | 119.83 | 125.11 |
| 71 | FI | 501 | GTP | C5-C6-N1 | 2.88 | 119.57 | 114.07 |
| 71 | GG | 501 | GTP | C2-N1-C6 | -2.88 | 119.83 | 125.11 |
| 69 | OL | 500 | GDP | C8-N7-C5 | 2.88 | 107.46 | 102.55 |
| 69 | ML | 500 | GDP | C8-N7-C5 | 2.88 | 107.46 | 102.55 |
| 71 | UK | 501 | GTP | C5-C6-N1 | 2.88 | 119.57 | 114.07 |
| 71 | FE | 501 | GTP | C2-N1-C6 | -2.88 | 119.84 | 125.11 |
| 69 | N | 500 | GDP | C8-N7-C5 | 2.88 | 107.45 | 102.55 |
| 69 | VH | 500 | GDP | C8-N7-C5 | 2.88 | 107.45 | 102.55 |
| 69 | VL | 500 | GDP | C8-N7-C5 | 2.88 | 107.45 | 102.55 |
| 71 | VE | 501 | GTP | C2-N1-C6 | -2.88 | 119.84 | 125.11 |
| 69 | VJ | 500 | GDP | C8-N7-C5 | 2.88 | 107.45 | 102.55 |
| 71 | CD | 501 | GTP | C2-N1-C6 | -2.88 | 119.84 | 125.11 |
| 69 | F | 500 | GDP | C8-N7-C5 | 2.88 | 107.45 | 102.55 |
| 71 | RD | 501 | GTP | C2-N1-C6 | -2.88 | 119.84 | 125.11 |
| 71 | UK | 501 | GTP | C2-N1-C6 | -2.88 | 119.84 | 125.11 |
| 71 | BI | 501 | GTP | C5-C6-N1 | 2.88 | 119.56 | 114.07 |
| 69 | JG | 500 | GDP | C8-N7-C5 | 2.88 | 107.45 | 102.55 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 71 | FA | 501 | GTP | C2-N1-C6 | -2.88 | 119.84 | 125.11 |
| 69 | WF | 500 | GDP | C8-N7-C5 | 2.88 | 107.45 | 102.55 |
| 71 | ME | 501 | GTP | C2-N1-C6 | -2.88 | 119.84 | 125.11 |
| 71 | SA | 501 | GTP | C2-N1-C6 | -2.88 | 119.84 | 125.11 |
| 69 | O | 500 | GDP | C8-N7-C5 | 2.88 | 107.44 | 102.55 |
| 69 | TH | 500 | GDP | C8-N7-C5 | 2.88 | 107.44 | 102.55 |
| 71 | EC | 501 | GTP | C2-N1-C6 | -2.88 | 119.85 | 125.11 |
| 71 | KJ | 501 | GTP | C2-N1-C6 | -2.88 | 119.85 | 125.11 |
| 69 | HD | 500 | GDP | C8-N7-C5 | 2.88 | 107.44 | 102.55 |
| 69 | LC | 500 | GDP | C8-N7-C5 | 2.87 | 107.44 | 102.55 |
| 69 | BF | 500 | GDP | C8-N7-C5 | 2.87 | 107.44 | 102.55 |
| 69 | CI | 500 | GDP | C8-N7-C5 | 2.87 | 107.44 | 102.55 |
| 69 | KK | 500 | GDP | C8-N7-C5 | 2.87 | 107.44 | 102.55 |
| 69 | NL | 500 | GDP | C8-N7-C5 | 2.87 | 107.44 | 102.55 |
| 69 | PH | 500 | GDP | C8-N7-C5 | 2.87 | 107.44 | 102.55 |
| 69 | WB | 500 | GDP | C8-N7-C5 | 2.87 | 107.44 | 102.55 |
| 69 | ED | 500 | GDP | C8-N7-C5 | 2.87 | 107.44 | 102.55 |
| 69 | DC | 500 | GDP | C8-N7-C5 | 2.87 | 107.44 | 102.55 |
| 69 | HJ | 500 | GDP | C8-N7-C5 | 2.87 | 107.44 | 102.55 |
| 71 | HG | 501 | GTP | C5-C6-N1 | 2.87 | 119.55 | 114.07 |
| 69 | BN | 500 | GDP | C8-N7-C5 | 2.87 | 107.44 | 102.55 |
| 71 | MC | 501 | GTP | C5-C6-N1 | 2.87 | 119.55 | 114.07 |
| 69 | NH | 500 | GDP | C8-N7-C5 | 2.87 | 107.43 | 102.55 |
| 69 | MB | 500 | GDP | C8-N7-C5 | 2.87 | 107.43 | 102.55 |
| 69 | RA | 500 | GDP | C8-N7-C5 | 2.87 | 107.43 | 102.55 |
| 69 | RK | 500 | GDP | C8-N7-C5 | 2.87 | 107.43 | 102.55 |
| 69 | MN | 500 | GDP | C8-N7-C5 | 2.87 | 107.43 | 102.55 |
| 71 | RL | 501 | GTP | C5-C6-N1 | 2.87 | 119.54 | 114.07 |
| 69 | QI | 500 | GDP | C8-N7-C5 | 2.87 | 107.43 | 102.55 |
| 69 | A | 500 | GDP | C8-N7-C5 | 2.87 | 107.43 | 102.55 |
| 69 | G | 500 | GDP | C8-N7-C5 | 2.87 | 107.43 | 102.55 |
| 69 | QE | 500 | GDP | C8-N7-C5 | 2.87 | 107.43 | 102.55 |
| 69 | ND | 500 | GDP | C8-N7-C5 | 2.87 | 107.43 | 102.55 |
| 69 | PB | 500 | GDP | C8-N7-C5 | 2.87 | 107.43 | 102.55 |
| 69 | LI | 500 | GDP | C8-N7-C5 | 2.86 | 107.43 | 102.55 |
| 69 | BD | 500 | GDP | C8-N7-C5 | 2.86 | 107.42 | 102.55 |
| 69 | W | 500 | GDP | C8-N7-C5 | 2.86 | 107.42 | 102.55 |
| 69 | PJ | 500 | GDP | C8-N7-C5 | 2.86 | 107.42 | 102.55 |
| 69 | JI | 500 | GDP | C8-N7-C5 | 2.86 | 107.42 | 102.55 |
| 69 | OF | 500 | GDP | C8-N7-C5 | 2.86 | 107.42 | 102.55 |
| 71 | TA | 501 | GTP | C2-N1-C6 | -2.86 | 119.87 | 125.11 |
| 69 | ID | 500 | GDP | C8-N7-C5 | 2.86 | 107.42 | 102.55 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 69 | SH | 500 | GDP | C8-N7-C5 | 2.86 | 107.42 | 102.55 |
| 69 | M | 500 | GDP | C8-N7-C5 | 2.86 | 107.42 | 102.55 |
| 69 | AL | 500 | GDP | C8-N7-C5 | 2.86 | 107.42 | 102.55 |
| 69 | AD | 500 | GDP | C8-N7-C5 | 2.86 | 107.42 | 102.55 |
| 69 | PF | 500 | GDP | C8-N7-C5 | 2.86 | 107.42 | 102.55 |
| 69 | KC | 500 | GDP | C8-N7-C5 | 2.86 | 107.42 | 102.55 |
| 69 | JC | 500 | GDP | C8-N7-C5 | 2.86 | 107.42 | 102.55 |
| 69 | UH | 500 | GDP | C8-N7-C5 | 2.86 | 107.42 | 102.55 |
| 69 | AN | 500 | GDP | C8-N7-C5 | 2.86 | 107.42 | 102.55 |
| 69 | DK | 500 | GDP | C8-N7-C5 | 2.86 | 107.42 | 102.55 |
| 69 | SD | 500 | GDP | C8-N7-C5 | 2.86 | 107.42 | 102.55 |
| 69 | AF | 500 | GDP | C8-N7-C5 | 2.86 | 107.42 | 102.55 |
| 69 | GB | 500 | GDP | C8-N7-C5 | 2.86 | 107.41 | 102.55 |
| 69 | GF | 500 | GDP | C8-N7-C5 | 2.86 | 107.41 | 102.55 |
| 69 | MH | 500 | GDP | C8-N7-C5 | 2.86 | 107.41 | 102.55 |
| 69 | OJ | 500 | GDP | C8-N7-C5 | 2.86 | 107.41 | 102.55 |
| 69 | DG | 500 | GDP | C8-N7-C5 | 2.86 | 107.41 | 102.55 |
| 69 | OD | 500 | GDP | C8-N7-C5 | 2.86 | 107.41 | 102.55 |
| 69 | JE | 500 | GDP | C8-N7-C5 | 2.85 | 107.41 | 102.55 |
| 71 | TK | 501 | GTP | C5-C6-N1 | 2.85 | 119.51 | 114.07 |
| 69 | TJ | 500 | GDP | C8-N7-C5 | 2.85 | 107.40 | 102.55 |
| 69 | FJ | 500 | GDP | C8-N7-C5 | 2.85 | 107.40 | 102.55 |
| 69 | IL | 500 | GDP | C8-N7-C5 | 2.85 | 107.40 | 102.55 |
| 69 | VF | 500 | GDP | C8-N7-C5 | 2.85 | 107.40 | 102.55 |
| 69 | IH | 500 | GDP | C8-N7-C5 | 2.85 | 107.40 | 102.55 |
| 69 | LK | 500 | GDP | C8-N7-C5 | 2.85 | 107.40 | 102.55 |
| 69 | BL | 500 | GDP | C8-N7-C5 | 2.85 | 107.40 | 102.55 |
| 69 | LA | 500 | GDP | C8-N7-C5 | 2.85 | 107.40 | 102.55 |
| 69 | QC | 500 | GDP | C8-N7-C5 | 2.85 | 107.40 | 102.55 |
| 71 | TC | 501 | GTP | C2-N1-C6 | -2.85 | 119.90 | 125.11 |
| 69 | FD | 500 | GDP | C8-N7-C5 | 2.85 | 107.39 | 102.55 |
| 69 | WD | 500 | GDP | C8-N7-C5 | 2.84 | 107.39 | 102.55 |
| 71 | HM | 501 | GTP | C2-N1-C6 | -2.84 | 119.90 | 125.11 |
| 71 | LJ | 501 | GTP | C2-N1-C6 | -2.84 | 119.91 | 125.11 |
| 71 | GC | 501 | GTP | C5-C6-N1 | 2.84 | 119.49 | 114.07 |
| 71 | HI | 501 | GTP | C5-C6-N1 | 2.84 | 119.49 | 114.07 |
| 69 | UB | 500 | GDP | C8-N7-C5 | 2.84 | 107.39 | 102.55 |
| 69 | VD | 500 | GDP | C8-N7-C5 | 2.84 | 107.39 | 102.55 |
| 69 | MF | 500 | GDP | C8-N7-C5 | 2.84 | 107.39 | 102.55 |
| 69 | SJ | 500 | GDP | C8-N7-C5 | 2.84 | 107.39 | 102.55 |
| 71 | BI | 501 | GTP | C2-N1-C6 | -2.84 | 119.91 | 125.11 |
| 69 | EH | 500 | GDP | C8-N7-C5 | 2.84 | 107.39 | 102.55 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 69 | JK | 500 | GDP | C8-N7-C5 | 2.84 | 107.39 | 102.55 |
| 69 | KE | 500 | GDP | C8-N7-C5 | 2.84 | 107.39 | 102.55 |
| 69 | BH | 500 | GDP | C8-N7-C5 | 2.84 | 107.38 | 102.55 |
| 69 | CE | 500 | GDP | C8-N7-C5 | 2.84 | 107.38 | 102.55 |
| 69 | RG | 500 | GDP | C8-N7-C5 | 2.84 | 107.38 | 102.55 |
| 69 | RE | 500 | GDP | C8-N7-C5 | 2.84 | 107.38 | 102.55 |
| 69 | JA | 500 | GDP | C8-N7-C5 | 2.84 | 107.38 | 102.55 |
| 69 | NF | 500 | GDP | C8-N7-C5 | 2.84 | 107.38 | 102.55 |
| 69 | MD | 500 | GDP | C8-N7-C5 | 2.84 | 107.38 | 102.55 |
| 69 | QG | 500 | GDP | C8-N7-C5 | 2.84 | 107.38 | 102.55 |
| 69 | FH | 500 | GDP | C8-N7-C5 | 2.83 | 107.38 | 102.55 |
| 69 | QA | 500 | GDP | C8-N7-C5 | 2.83 | 107.37 | 102.55 |
| 69 | WL | 500 | GDP | C8-N7-C5 | 2.83 | 107.37 | 102.55 |
| 69 | LM | 500 | GDP | C8-N7-C5 | 2.83 | 107.37 | 102.55 |
| 71 | HA | 501 | GTP | C5-C6-N1 | 2.83 | 119.47 | 114.07 |
| 69 | GJ | 500 | GDP | C8-N7-C5 | 2.83 | 107.37 | 102.55 |
| 69 | IJ | 500 | GDP | C8-N7-C5 | 2.83 | 107.37 | 102.55 |
| 69 | EB | 500 | GDP | C8-N7-C5 | 2.83 | 107.36 | 102.55 |
| 69 | WJ | 500 | GDP | C8-N7-C5 | 2.83 | 107.36 | 102.55 |
| 69 | HF | 500 | GDP | C8-N7-C5 | 2.82 | 107.36 | 102.55 |
| 69 | FF | 500 | GDP | C8-N7-C5 | 2.82 | 107.36 | 102.55 |
| 69 | OH | 500 | GDP | C8-N7-C5 | 2.82 | 107.36 | 102.55 |
| 69 | RC | 500 | GDP | C8-N7-C5 | 2.82 | 107.35 | 102.55 |
| 71 | RL | 501 | GTP | C2-N1-C6 | -2.82 | 119.94 | 125.11 |
| 69 | CA | 500 | GDP | C8-N7-C5 | 2.82 | 107.35 | 102.55 |
| 69 | HH | 500 | GDP | C8-N7-C5 | 2.82 | 107.34 | 102.55 |
| 69 | IB | 500 | GDP | C8-N7-C5 | 2.82 | 107.34 | 102.55 |
| 69 | TB | 500 | GDP | C8-N7-C5 | 2.82 | 107.34 | 102.55 |
| 69 | KG | 500 | GDP | C8-N7-C5 | 2.81 | 107.34 | 102.55 |
| 71 | HI | 501 | GTP | C2-N1-C6 | -2.81 | 119.96 | 125.11 |
| 69 | FB | 500 | GDP | C8-N7-C5 | 2.81 | 107.33 | 102.55 |
| 69 | NB | 500 | GDP | C8-N7-C5 | 2.81 | 107.33 | 102.55 |
| 69 | GD | 500 | GDP | C8-N7-C5 | 2.81 | 107.33 | 102.55 |
| 69 | UD | 500 | GDP | C8-N7-C5 | 2.80 | 107.32 | 102.55 |
| 69 | AJ | 500 | GDP | C8-N7-C5 | 2.80 | 107.32 | 102.55 |
| 69 | I | 500 | GDP | C8-N7-C5 | 2.80 | 107.32 | 102.55 |
| 69 | LO | 500 | GDP | C8-N7-C5 | 2.80 | 107.32 | 102.55 |
| 69 | HL | 500 | GDP | C8-N7-C5 | 2.80 | 107.31 | 102.55 |
| 69 | LE | 500 | GDP | C8-N7-C5 | 2.80 | 107.31 | 102.55 |
| 71 | GC | 501 | GTP | C4'-O4'-C1' | 2.79 | 112.48 | 109.92 |
| 69 | CM | 500 | GDP | C8-N7-C5 | 2.79 | 107.30 | 102.55 |
| 69 | RI | 500 | GDP | C8-N7-C5 | 2.79 | 107.30 | 102.55 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 69 | AH | 500 | GDP | C8-N7-C5 | 2.78 | 107.27 | 102.55 |
| 71 | IE | 501 | GTP | C4'-O4'-C1' | 2.75 | 112.44 | 109.92 |
| 69 | RE | 500 | GDP | C4'-O4'-C1' | 2.73 | 112.43 | 109.92 |
| 71 | HA | 501 | GTP | C2-N1-C6 | -2.73 | 120.11 | 125.11 |
| 69 | MJ | 500 | GDP | C8-N7-C5 | 2.68 | 107.12 | 102.55 |
| 71 | VE | 501 | GTP | C4'-O4'-C1' | 2.68 | 112.38 | 109.92 |
| 69 | OB | 500 | GDP | C8-N7-C5 | 2.68 | 107.11 | 102.55 |
| 71 | IK | 501 | GTP | O2A-PA-O5' | 2.63 | 119.48 | 107.57 |
| 71 | IK | 501 | GTP | C2-N1-C6 | -2.58 | 120.38 | 125.11 |
| 71 | CD | 501 | GTP | O3G-PG-O3B | 2.58 | 113.30 | 104.64 |
| 71 | GA | 501 | GTP | C4'-O4'-C1' | 2.58 | 112.29 | 109.92 |
| 71 | OG | 501 | GTP | C4'-O4'-C1' | 2.58 | 112.29 | 109.92 |
| 71 | IK | 501 | GTP | C5-C6-N1 | 2.56 | 118.96 | 114.07 |
| 71 | JF | 501 | GTP | C4'-O4'-C1' | 2.56 | 112.27 | 109.92 |
| 71 | LH | 501 | GTP | C4'-O4'-C1' | 2.52 | 112.23 | 109.92 |
| 71 | WE | 501 | GTP | O3G-PG-O3B | 2.44 | 112.83 | 104.64 |
| 71 | NK | 501 | GTP | C4'-O4'-C1' | 2.42 | 112.14 | 109.92 |
| 71 | PA | 501 | GTP | O6-C6-C5 | -2.39 | 119.58 | 124.32 |
| 71 | CH | 501 | GTP | O3G-PG-O3B | 2.39 | 112.64 | 104.64 |
| 71 | QH | 501 | GTP | O3G-PG-O3B | 2.37 | 112.57 | 104.64 |
| 71 | EK | 501 | GTP | O3G-PG-O3B | 2.35 | 112.51 | 104.64 |
| 69 | MJ | 500 | GDP | C2'-C3'-C4' | 2.34 | 107.14 | 102.61 |
| 71 | HG | 501 | GTP | C4'-O4'-C1' | 2.32 | 112.05 | 109.92 |
| 74 | 2v | 501 | ATP | C5-C6-N6 | 2.32 | 123.85 | 120.31 |
| 71 | EA | 501 | GTP | O3G-PG-O3B | 2.31 | 112.37 | 104.64 |
| 71 | IC | 501 | GTP | O6-C6-C5 | -2.30 | 119.75 | 124.32 |
| 71 | IK | 501 | GTP | O2A-PA-O1A | -2.30 | 101.74 | 112.44 |
| 74 | 2w | 501 | ATP | C5-C6-N6 | 2.29 | 123.80 | 120.31 |
| 71 | QH | 501 | GTP | O2B-PB-O3A | 2.29 | 113.45 | 107.27 |
| 71 | LF | 501 | GTP | C4'-O4'-C1' | 2.27 | 112.00 | 109.92 |
| 71 | KH | 501 | GTP | O6-C6-C5 | -2.27 | 119.82 | 124.32 |
| 71 | D | 501 | GTP | O3G-PG-O3B | 2.26 | 112.21 | 104.64 |
| 71 | RB | 501 | GTP | O6-C6-C5 | -2.25 | 119.87 | 124.32 |
| 71 | IE | 501 | GTP | O6-C6-C5 | -2.24 | 119.87 | 124.32 |
| 71 | FK | 501 | GTP | O6-C6-C5 | -2.24 | 119.88 | 124.32 |
| 71 | GG | 501 | GTP | C4'-O4'-C1' | 2.23 | 111.97 | 109.92 |
| 69 | FB | 500 | GDP | C2'-C3'-C4' | 2.22 | 106.90 | 102.61 |
| 71 | MK | 501 | GTP | O6-C6-C5 | -2.22 | 119.92 | 124.32 |
| 71 | RL | 501 | GTP | O3G-PG-O3B | 2.21 | 112.05 | 104.64 |
| 71 | SG | 501 | GTP | O3G-PG-O3B | 2.21 | 112.04 | 104.64 |
| 71 | HK | 501 | GTP | O6-C6-C5 | -2.20 | 119.95 | 124.32 |
| 71 | QD | 501 | GTP | O3G-PG-O3B | 2.20 | 112.02 | 104.64 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 71 | IA | 501 | GTP | O6-C6-C5 | -2.19 | 119.98 | 124.32 |
| 71 | JH | 501 | GTP | O6-C6-C5 | -2.18 | 120.00 | 124.32 |
| 71 | QH | 501 | GTP | O6-C6-C5 | -2.18 | 120.01 | 124.32 |
| 71 | LH | 501 | GTP | O6-C6-C5 | -2.17 | 120.01 | 124.32 |
| 69 | CA | 500 | GDP | O4'-C1'-N9 | 2.17 | 111.63 | 108.75 |
| 71 | WE | 501 | GTP | O6-C6-C5 | -2.17 | 120.02 | 124.32 |
| 71 | RD | 501 | GTP | O6-C6-C5 | -2.17 | 120.02 | 124.32 |
| 71 | EE | 501 | GTP | O3G-PG-O3B | 2.17 | 111.90 | 104.64 |
| 71 | TG | 501 | GTP | O6-C6-C5 | -2.16 | 120.03 | 124.32 |
| 71 | RF | 501 | GTP | O6-C6-C5 | -2.16 | 120.04 | 124.32 |
| 71 | IM | 501 | GTP | O6-C6-C5 | -2.16 | 120.04 | 124.32 |
| 71 | WM | 501 | GTP | O6-C6-C5 | -2.16 | 120.04 | 124.32 |
| 71 | FE | 501 | GTP | O6-C6-C5 | -2.15 | 120.05 | 124.32 |
| 69 | CC | 500 | GDP | C5-C6-N1 | 2.15 | 118.17 | 114.07 |
| 69 | CM | 500 | GDP | C5-C6-N1 | 2.15 | 118.17 | 114.07 |
| 69 | EL | 500 | GDP | C5-C6-N1 | 2.15 | 118.17 | 114.07 |
| 69 | MJ | 500 | GDP | C5-C6-N1 | 2.15 | 118.16 | 114.07 |
| 71 | OE | 501 | GTP | O6-C6-C5 | -2.15 | 120.07 | 124.32 |
| 71 | SG | 501 | GTP | O6-C6-C5 | -2.14 | 120.07 | 124.32 |
| 69 | BD | 500 | GDP | C5-C6-N1 | 2.14 | 118.16 | 114.07 |
| 71 | LB | 501 | GTP | O6-C6-C5 | -2.14 | 120.08 | 124.32 |
| 71 | GG | 501 | GTP | O6-C6-C5 | -2.14 | 120.08 | 124.32 |
| 71 | K | 501 | GTP | O6-C6-C5 | -2.14 | 120.08 | 124.32 |
| 71 | SC | 501 | GTP | O6-C6-C5 | -2.14 | 120.08 | 124.32 |
| 69 | UJ | 500 | GDP | C5-C6-N1 | 2.14 | 118.15 | 114.07 |
| 71 | R | 501 | GTP | O6-C6-C5 | -2.14 | 120.08 | 124.32 |
| 69 | DE | 500 | GDP | C5-C6-N1 | 2.14 | 118.15 | 114.07 |
| 69 | P | 500 | GDP | O6-C6-C5 | -2.14 | 120.09 | 124.32 |
| 71 | C | 501 | GTP | O6-C6-C5 | -2.14 | 120.09 | 124.32 |
| 71 | VE | 501 | GTP | O6-C6-C5 | -2.14 | 120.09 | 124.32 |
| 71 | EC | 501 | GTP | O6-C6-C5 | -2.13 | 120.09 | 124.32 |
| 71 | FC | 501 | GTP | O6-C6-C5 | -2.13 | 120.09 | 124.32 |
| 69 | QG | 500 | GDP | C5-C6-N1 | 2.13 | 118.14 | 114.07 |
| 69 | BH | 500 | GDP | C5-C6-N1 | 2.13 | 118.14 | 114.07 |
| 71 | DF | 501 | GTP | O6-C6-C5 | -2.13 | 120.09 | 124.32 |
| 71 | PK | 501 | GTP | O6-C6-C5 | -2.13 | 120.10 | 124.32 |
| 71 | GI | 501 | GTP | O6-C6-C5 | -2.13 | 120.10 | 124.32 |
| 71 | JF | 501 | GTP | O6-C6-C5 | -2.13 | 120.10 | 124.32 |
| 69 | OB | 500 | GDP | C4'-O4'-C1' | 2.13 | 111.87 | 109.92 |
| 71 | GE | 501 | GTP | O6-C6-C5 | -2.13 | 120.10 | 124.32 |
| 71 | KB | 501 | GTP | O6-C6-C5 | -2.13 | 120.10 | 124.32 |
| 71 | II | 501 | GTP | O6-C6-C5 | -2.13 | 120.11 | 124.32 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 71 | WA | 501 | GTP | O6-C6-C5 | -2.13 | 120.11 | 124.32 |
| 71 | EA | 501 | GTP | O6-C6-C5 | -2.12 | 120.11 | 124.32 |
| 71 | TE | 501 | GTP | O6-C6-C5 | -2.12 | 120.11 | 124.32 |
| 71 | SE | 501 | GTP | O2A-PA-O3A | 2.12 | 113.01 | 107.27 |
| 71 | FG | 501 | GTP | O6-C6-C5 | -2.12 | 120.11 | 124.32 |
| 71 | NG | 501 | GTP | O6-C6-C5 | -2.12 | 120.11 | 124.32 |
| 69 | KK | 500 | GDP | C5-C6-N1 | 2.12 | 118.12 | 114.07 |
| 69 | VJ | 500 | GDP | C5-C6-N1 | 2.12 | 118.12 | 114.07 |
| 71 | GA | 501 | GTP | O6-C6-C5 | -2.12 | 120.11 | 124.32 |
| 71 | HE | 501 | GTP | O6-C6-C5 | -2.12 | 120.11 | 124.32 |
| 71 | TA | 501 | GTP | O3G-PG-O3B | 2.12 | 111.75 | 104.64 |
| 71 | EG | 501 | GTP | O6-C6-C5 | -2.12 | 120.12 | 124.32 |
| 71 | GC | 501 | GTP | O6-C6-C5 | -2.12 | 120.12 | 124.32 |
| 71 | TC | 501 | GTP | O6-C6-C5 | -2.12 | 120.12 | 124.32 |
| 71 | HG | 501 | GTP | O6-C6-C5 | -2.12 | 120.12 | 124.32 |
| 71 | VC | 501 | GTP | O6-C6-C5 | -2.12 | 120.12 | 124.32 |
| 69 | FL | 500 | GDP | C5-C6-N1 | 2.12 | 118.11 | 114.07 |
| 71 | UI | 501 | GTP | O6-C6-C5 | -2.12 | 120.12 | 124.32 |
| 71 | AE | 501 | GTP | O6-C6-C5 | -2.12 | 120.13 | 124.32 |
| 71 | NE | 501 | GTP | O6-C6-C5 | -2.11 | 120.13 | 124.32 |
| 71 | AC | 501 | GTP | O6-C6-C5 | -2.11 | 120.13 | 124.32 |
| 71 | J | 501 | GTP | O6-C6-C5 | -2.11 | 120.13 | 124.32 |
| 71 | RH | 501 | GTP | O6-C6-C5 | -2.11 | 120.13 | 124.32 |
| 71 | AI | 501 | GTP | O6-C6-C5 | -2.11 | 120.13 | 124.32 |
| 71 | PI | 501 | GTP | O6-C6-C5 | -2.11 | 120.13 | 124.32 |
| 69 | JG | 500 | GDP | C5-C6-N1 | 2.11 | 118.10 | 114.07 |
| 69 | SJ | 500 | GDP | C5-C6-N1 | 2.11 | 118.10 | 114.07 |
| 71 | KJ | 501 | GTP | O6-C6-C5 | -2.11 | 120.14 | 124.32 |
| 71 | Q | 501 | GTP | O6-C6-C5 | -2.11 | 120.14 | 124.32 |
| 69 | FJ | 500 | GDP | C5-C6-N1 | 2.11 | 118.09 | 114.07 |
| 69 | TF | 500 | GDP | C5-C6-N1 | 2.11 | 118.09 | 114.07 |
| 71 | IG | 501 | GTP | O6-C6-C5 | -2.11 | 120.14 | 124.32 |
| 71 | NK | 501 | GTP | O6-C6-C5 | -2.11 | 120.14 | 124.32 |
| 71 | UG | 501 | GTP | O6-C6-C5 | -2.11 | 120.14 | 124.32 |
| 71 | DL | 501 | GTP | O3G-PG-O3B | 2.11 | 111.70 | 104.64 |
| 71 | DJ | 501 | GTP | O6-C6-C5 | -2.11 | 120.15 | 124.32 |
| 69 | HD | 500 | GDP | C5-C6-N1 | 2.10 | 118.08 | 114.07 |
| 69 | LG | 500 | GDP | C5-C6-N1 | 2.10 | 118.08 | 114.07 |
| 69 | U | 500 | GDP | C5-C6-N1 | 2.10 | 118.08 | 114.07 |
| 71 | FI | 501 | GTP | O6-C6-C5 | -2.10 | 120.15 | 124.32 |
| 71 | LN | 501 | GTP | O6-C6-C5 | -2.10 | 120.15 | 124.32 |
| 71 | WC | 501 | GTP | O6-C6-C5 | -2.10 | 120.15 | 124.32 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 71 | CL | 501 | GTP | O6-C6-C5 | -2.10 | 120.15 | 124.32 |
| 71 | LL | 501 | GTP | O6-C6-C5 | -2.10 | 120.15 | 124.32 |
| 71 | QB | 501 | GTP | O6-C6-C5 | -2.10 | 120.15 | 124.32 |
| 71 | BI | 501 | GTP | O6-C6-C5 | -2.10 | 120.15 | 124.32 |
| 71 | GK | 501 | GTP | O6-C6-C5 | -2.10 | 120.15 | 124.32 |
| 69 | BN | 500 | GDP | C2'-C3'-C4' | 2.10 | 106.67 | 102.61 |
| 71 | OG | 501 | GTP | O6-C6-C5 | -2.10 | 120.15 | 124.32 |
| 71 | TA | 501 | GTP | O6-C6-C5 | -2.10 | 120.15 | 124.32 |
| 71 | EI | 501 | GTP | O6-C6-C5 | -2.10 | 120.15 | 124.32 |
| 69 | HJ | 500 | GDP | C5-C6-N1 | 2.10 | 118.08 | 114.07 |
| 71 | BC | 501 | GTP | O6-C6-C5 | -2.10 | 120.16 | 124.32 |
| 71 | KF | 501 | GTP | O6-C6-C5 | -2.10 | 120.16 | 124.32 |
| 69 | DK | 500 | GDP | C5-C6-N1 | 2.10 | 118.08 | 114.07 |
| 69 | LA | 500 | GDP | C5-C6-N1 | 2.10 | 118.08 | 114.07 |
| 69 | GD | 500 | GDP | C5-C6-N1 | 2.10 | 118.08 | 114.07 |
| 71 | BA | 501 | GTP | O6-C6-C5 | -2.10 | 120.16 | 124.32 |
| 71 | MC | 501 | GTP | O6-C6-C5 | -2.10 | 120.16 | 124.32 |
| 71 | MM | 501 | GTP | O6-C6-C5 | -2.10 | 120.16 | 124.32 |
| 71 | NI | 501 | GTP | O6-C6-C5 | -2.10 | 120.16 | 124.32 |
| 69 | VB | 500 | GDP | C5-C6-N1 | 2.10 | 118.07 | 114.07 |
| 71 | BE | 501 | GTP | O6-C6-C5 | -2.10 | 120.16 | 124.32 |
| 71 | MA | 501 | GTP | O6-C6-C5 | -2.10 | 120.17 | 124.32 |
| 71 | QD | 501 | GTP | O6-C6-C5 | -2.10 | 120.17 | 124.32 |
| 69 | HH | 500 | GDP | C5-C6-N1 | 2.10 | 118.07 | 114.07 |
| 71 | HM | 501 | GTP | O6-C6-C5 | -2.10 | 120.17 | 124.32 |
| 69 | GH | 500 | GDP | C5-C6-N1 | 2.09 | 118.07 | 114.07 |
| 71 | HI | 501 | GTP | O6-C6-C5 | -2.09 | 120.17 | 124.32 |
| 71 | PG | 501 | GTP | O6-C6-C5 | -2.09 | 120.17 | 124.32 |
| 71 | AG | 501 | GTP | O6-C6-C5 | -2.09 | 120.17 | 124.32 |
| 71 | CJ | 501 | GTP | O6-C6-C5 | -2.09 | 120.17 | 124.32 |
| 71 | MG | 501 | GTP | O6-C6-C5 | -2.09 | 120.17 | 124.32 |
| 71 | QL | 501 | GTP | O6-C6-C5 | -2.09 | 120.17 | 124.32 |
| 71 | SA | 501 | GTP | O6-C6-C5 | -2.09 | 120.17 | 124.32 |
| 71 | OC | 501 | GTP | O6-C6-C5 | -2.09 | 120.17 | 124.32 |
| 71 | OK | 501 | GTP | O6-C6-C5 | -2.09 | 120.17 | 124.32 |
| 69 | WH | 500 | GDP | C5-C6-N1 | 2.09 | 118.06 | 114.07 |
| 71 | DD | 501 | GTP | O6-C6-C5 | -2.09 | 120.18 | 124.32 |
| 71 | LF | 501 | GTP | O6-C6-C5 | -2.09 | 120.18 | 124.32 |
| 71 | ME | 501 | GTP | O6-C6-C5 | -2.09 | 120.18 | 124.32 |
| 69 | DA | 500 | GDP | C5-C6-N1 | 2.09 | 118.06 | 114.07 |
| 71 | AA | 501 | GTP | O6-C6-C5 | -2.09 | 120.18 | 124.32 |
| 71 | MI | 501 | GTP | O6-C6-C5 | -2.09 | 120.18 | 124.32 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 71 | NA | 501 | GTP | O6-C6-C5 | -2.09 | 120.18 | 124.32 |
| 69 | I | 500 | GDP | C5-C6-N1 | 2.09 | 118.05 | 114.07 |
| 71 | FA | 501 | GTP | O6-C6-C5 | -2.09 | 120.18 | 124.32 |
| 69 | LK | 500 | GDP | C5-C6-N1 | 2.08 | 118.05 | 114.07 |
| 71 | SK | 501 | GTP | O6-C6-C5 | -2.08 | 120.19 | 124.32 |
| 69 | AD | 500 | GDP | C5-C6-N1 | 2.08 | 118.05 | 114.07 |
| 69 | FD | 500 | GDP | C5-C6-N1 | 2.08 | 118.05 | 114.07 |
| 69 | ED | 500 | GDP | C5-C6-N1 | 2.08 | 118.04 | 114.07 |
| 71 | UC | 501 | GTP | O6-C6-C5 | -2.08 | 120.19 | 124.32 |
| 71 | BG | 501 | GTP | O6-C6-C5 | -2.08 | 120.19 | 124.32 |
| 71 | LD | 501 | GTP | O6-C6-C5 | -2.08 | 120.19 | 124.32 |
| 71 | TI | 501 | GTP | O6-C6-C5 | -2.08 | 120.19 | 124.32 |
| 69 | WD | 500 | GDP | C5-C6-N1 | 2.08 | 118.04 | 114.07 |
| 69 | E | 500 | GDP | C5-C6-N1 | 2.08 | 118.04 | 114.07 |
| 69 | MD | 500 | GDP | C5-C6-N1 | 2.08 | 118.04 | 114.07 |
| 71 | UE | 501 | GTP | O6-C6-C5 | -2.08 | 120.20 | 124.32 |
| 71 | DH | 501 | GTP | O6-C6-C5 | -2.08 | 120.20 | 124.32 |
| 71 | EE | 501 | GTP | O6-C6-C5 | -2.08 | 120.20 | 124.32 |
| 71 | VI | 501 | GTP | O6-C6-C5 | -2.08 | 120.20 | 124.32 |
| 69 | GL | 500 | GDP | C5-C6-N1 | 2.08 | 118.04 | 114.07 |
| 69 | OF | 500 | GDP | C5-C6-N1 | 2.08 | 118.04 | 114.07 |
| 69 | CA | 500 | GDP | C5-C6-N1 | 2.08 | 118.03 | 114.07 |
| 69 | BN | 500 | GDP | C5-C6-N1 | 2.08 | 118.03 | 114.07 |
| 69 | PJ | 500 | GDP | C5-C6-N1 | 2.08 | 118.03 | 114.07 |
| 71 | VA | 501 | GTP | O6-C6-C5 | -2.08 | 120.20 | 124.32 |
| 71 | JL | 501 | GTP | O4'-C1'-N9 | 2.08 | 111.50 | 108.75 |
| 71 | NC | 501 | GTP | O6-C6-C5 | -2.08 | 120.20 | 124.32 |
| 71 | SE | 501 | GTP | O6-C6-C5 | -2.08 | 120.20 | 124.32 |
| 69 | NJ | 500 | GDP | C5-C6-N1 | 2.08 | 118.03 | 114.07 |
| 71 | L | 501 | GTP | O6-C6-C5 | -2.08 | 120.21 | 124.32 |
| 69 | A | 500 | GDP | C5-C6-N1 | 2.07 | 118.03 | 114.07 |
| 69 | CG | 500 | GDP | C5-C6-N1 | 2.07 | 118.03 | 114.07 |
| 69 | LO | 500 | GDP | C5-C6-N1 | 2.07 | 118.03 | 114.07 |
| 69 | NH | 500 | GDP | C5-C6-N1 | 2.07 | 118.03 | 114.07 |
| 69 | TL | 500 | GDP | C5-C6-N1 | 2.07 | 118.03 | 114.07 |
| 69 | VF | 500 | GDP | C5-C6-N1 | 2.07 | 118.03 | 114.07 |
| 69 | TD | 500 | GDP | C5-C6-N1 | 2.07 | 118.03 | 114.07 |
| 71 | JN | 501 | GTP | O6-C6-C5 | -2.07 | 120.21 | 124.32 |
| 69 | VL | 500 | GDP | C5-C6-N1 | 2.07 | 118.02 | 114.07 |
| 71 | PM | 501 | GTP | O6-C6-C5 | -2.07 | 120.22 | 124.32 |
| 69 | JA | 500 | GDP | C5-C6-N1 | 2.07 | 118.02 | 114.07 |
| 71 | QF | 501 | GTP | O6-C6-C5 | -2.07 | 120.22 | 124.32 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|------------|-------|-------------|----------|
| 69 | EF | 500 | GDP | C5-C6-N1 | 2.07 | 118.02 | 114.07 |
| 69 | IH | 500 | GDP | C5-C6-N1 | 2.07 | 118.02 | 114.07 |
| 69 | LM | 500 | GDP | C5-C6-N1 | 2.07 | 118.02 | 114.07 |
| 69 | W | 500 | GDP | C5-C6-N1 | 2.07 | 118.02 | 114.07 |
| 71 | PC | 501 | GTP | O6-C6-C5 | -2.07 | 120.22 | 124.32 |
| 71 | BK | 501 | GTP | O6-C6-C5 | -2.07 | 120.22 | 124.32 |
| 71 | CD | 501 | GTP | O6-C6-C5 | -2.07 | 120.22 | 124.32 |
| 71 | OI | 501 | GTP | O6-C6-C5 | -2.07 | 120.22 | 124.32 |
| 69 | UH | 500 | GDP | C5-C6-N1 | 2.07 | 118.01 | 114.07 |
| 71 | WK | 501 | GTP | O6-C6-C5 | -2.07 | 120.22 | 124.32 |
| 69 | OD | 500 | GDP | C5-C6-N1 | 2.07 | 118.01 | 114.07 |
| 71 | D | 501 | GTP | O6-C6-C5 | -2.06 | 120.23 | 124.32 |
| 71 | VG | 501 | GTP | O6-C6-C5 | -2.06 | 120.23 | 124.32 |
| 69 | GJ | 500 | GDP | C5-C6-N1 | 2.06 | 118.01 | 114.07 |
| 69 | TH | 500 | GDP | C5-C6-N1 | 2.06 | 118.01 | 114.07 |
| 71 | DB | 501 | GTP | O6-C6-C5 | -2.06 | 120.23 | 124.32 |
| 69 | SH | 500 | GDP | C5-C6-N1 | 2.06 | 118.01 | 114.07 |
| 69 | MH | 500 | GDP | C5-C6-N1 | 2.06 | 118.01 | 114.07 |
| 71 | BM | 501 | GTP | O6-C6-C5 | -2.06 | 120.23 | 124.32 |
| 69 | IL | 500 | GDP | C5-C6-N1 | 2.06 | 118.00 | 114.07 |
| 69 | CK | 500 | GDP | C5-C6-N1 | 2.06 | 118.00 | 114.07 |
| 69 | UL | 500 | GDP | C5-C6-N1 | 2.06 | 118.00 | 114.07 |
| 69 | WL | 500 | GDP | C5-C6-N1 | 2.06 | 118.00 | 114.07 |
| 69 | EJ | 500 | GDP | C5-C6-N1 | 2.06 | 118.00 | 114.07 |
| 69 | S | 500 | GDP | C5-C6-N1 | 2.06 | 118.00 | 114.07 |
| 71 | DF | 501 | GTP | O3G-PG-O3B | 2.06 | 111.55 | 104.64 |
| 69 | BB | 500 | GDP | C5-C6-N1 | 2.06 | 118.00 | 114.07 |
| 69 | DI | 500 | GDP | C5-C6-N1 | 2.06 | 118.00 | 114.07 |
| 69 | OJ | 500 | GDP | C5-C6-N1 | 2.06 | 118.00 | 114.07 |
| 71 | HC | 501 | GTP | O6-C6-C5 | -2.06 | 120.24 | 124.32 |
| 69 | AF | 500 | GDP | C5-C6-N1 | 2.06 | 118.00 | 114.07 |
| 71 | DL | 501 | GTP | O6-C6-C5 | -2.06 | 120.24 | 124.32 |
| 69 | WJ | 500 | GDP | C5-C6-N1 | 2.06 | 118.00 | 114.07 |
| 71 | HA | 501 | GTP | O6-C6-C5 | -2.06 | 120.24 | 124.32 |
| 69 | G | 500 | GDP | C5-C6-N1 | 2.06 | 118.00 | 114.07 |
| 69 | ID | 500 | GDP | C5-C6-N1 | 2.06 | 118.00 | 114.07 |
| 71 | CB | 501 | GTP | O6-C6-C5 | -2.06 | 120.24 | 124.32 |
| 69 | JK | 500 | GDP | C5-C6-N1 | 2.06 | 117.99 | 114.07 |
| 69 | FH | 500 | GDP | C5-C6-N1 | 2.06 | 117.99 | 114.07 |
| 69 | QC | 500 | GDP | C5-C6-N1 | 2.06 | 117.99 | 114.07 |
| 71 | KN | 501 | GTP | O6-C6-C5 | -2.06 | 120.25 | 124.32 |
| 71 | QJ | 501 | GTP | O3G-PG-O3B | 2.05 | 111.53 | 104.64 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 69 | CI | 500 | GDP | C5-C6-N1 | 2.05 | 117.99 | 114.07 |
| 69 | DC | 500 | GDP | C5-C6-N1 | 2.05 | 117.99 | 114.07 |
| 69 | WF | 500 | GDP | C5-C6-N1 | 2.05 | 117.99 | 114.07 |
| 71 | CH | 501 | GTP | O6-C6-C5 | -2.05 | 120.25 | 124.32 |
| 69 | AN | 500 | GDP | C5-C6-N1 | 2.05 | 117.99 | 114.07 |
| 69 | JE | 500 | GDP | C5-C6-N1 | 2.05 | 117.98 | 114.07 |
| 69 | RK | 500 | GDP | C5-C6-N1 | 2.05 | 117.98 | 114.07 |
| 71 | TK | 501 | GTP | O6-C6-C5 | -2.05 | 120.25 | 124.32 |
| 71 | OE | 501 | GTP | O3G-PG-O3B | 2.05 | 111.51 | 104.64 |
| 69 | DM | 500 | GDP | C5-C6-N1 | 2.05 | 117.98 | 114.07 |
| 69 | VH | 500 | GDP | C5-C6-N1 | 2.05 | 117.98 | 114.07 |
| 71 | OA | 501 | GTP | O6-C6-C5 | -2.05 | 120.25 | 124.32 |
| 69 | WB | 500 | GDP | C5-C6-N1 | 2.05 | 117.98 | 114.07 |
| 71 | KD | 501 | GTP | O6-C6-C5 | -2.05 | 120.26 | 124.32 |
| 71 | SI | 501 | GTP | O6-C6-C5 | -2.05 | 120.26 | 124.32 |
| 69 | F | 500 | GDP | C5-C6-N1 | 2.05 | 117.98 | 114.07 |
| 69 | UF | 500 | GDP | C5-C6-N1 | 2.05 | 117.98 | 114.07 |
| 69 | FB | 500 | GDP | C4'-O4'-C1' | 2.05 | 111.80 | 109.92 |
| 69 | RA | 500 | GDP | C2'-C3'-C4' | 2.05 | 106.57 | 102.61 |
| 69 | OL | 500 | GDP | C5-C6-N1 | 2.05 | 117.98 | 114.07 |
| 69 | PH | 500 | GDP | C5-C6-N1 | 2.05 | 117.98 | 114.07 |
| 69 | QI | 500 | GDP | C5-C6-N1 | 2.05 | 117.98 | 114.07 |
| 71 | KL | 501 | GTP | O6-C6-C5 | -2.05 | 120.26 | 124.32 |
| 69 | LC | 500 | GDP | C5-C6-N1 | 2.05 | 117.98 | 114.07 |
| 69 | SD | 500 | GDP | C5-C6-N1 | 2.05 | 117.98 | 114.07 |
| 71 | VK | 501 | GTP | O6-C6-C5 | -2.05 | 120.26 | 124.32 |
| 69 | JC | 500 | GDP | C5-C6-N1 | 2.05 | 117.97 | 114.07 |
| 69 | PD | 500 | GDP | C5-C6-N1 | 2.05 | 117.97 | 114.07 |
| 69 | KE | 500 | GDP | C5-C6-N1 | 2.05 | 117.97 | 114.07 |
| 71 | NM | 501 | GTP | O6-C6-C5 | -2.05 | 120.27 | 124.32 |
| 71 | WG | 501 | GTP | O6-C6-C5 | -2.05 | 120.27 | 124.32 |
| 69 | TJ | 500 | GDP | C5-C6-N1 | 2.05 | 117.97 | 114.07 |
| 69 | GB | 500 | GDP | C5-C6-N1 | 2.04 | 117.97 | 114.07 |
| 71 | PE | 501 | GTP | O6-C6-C5 | -2.04 | 120.27 | 124.32 |
| 69 | RE | 500 | GDP | C5-C6-N1 | 2.04 | 117.97 | 114.07 |
| 69 | M | 500 | GDP | C5-C6-N1 | 2.04 | 117.97 | 114.07 |
| 71 | OM | 501 | GTP | O6-C6-C5 | -2.04 | 120.27 | 124.32 |
| 69 | QE | 500 | GDP | C5-C6-N1 | 2.04 | 117.96 | 114.07 |
| 71 | AK | 501 | GTP | O6-C6-C5 | -2.04 | 120.27 | 124.32 |
| 71 | UK | 501 | GTP | O6-C6-C5 | -2.04 | 120.27 | 124.32 |
| 69 | VJ | 500 | GDP | C2'-C3'-C4' | 2.04 | 106.55 | 102.61 |
| 69 | JM | 500 | GDP | C5-C6-N1 | 2.04 | 117.96 | 114.07 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|-------|-------------|----------|
| 69 | MN | 500 | GDP | C5-C6-N1 | 2.04 | 117.96 | 114.07 |
| 69 | RC | 500 | GDP | C5-C6-N1 | 2.04 | 117.96 | 114.07 |
| 69 | UB | 500 | GDP | C5-C6-N1 | 2.04 | 117.96 | 114.07 |
| 69 | ML | 500 | GDP | C5-C6-N1 | 2.04 | 117.96 | 114.07 |
| 69 | N | 500 | GDP | C5-C6-N1 | 2.04 | 117.96 | 114.07 |
| 69 | IF | 500 | GDP | C5-C6-N1 | 2.04 | 117.96 | 114.07 |
| 69 | DG | 500 | GDP | C5-C6-N1 | 2.04 | 117.95 | 114.07 |
| 71 | EK | 501 | GTP | O6-C6-C5 | -2.04 | 120.28 | 124.32 |
| 69 | KM | 500 | GDP | C5-C6-N1 | 2.04 | 117.95 | 114.07 |
| 71 | UA | 501 | GTP | O6-C6-C5 | -2.04 | 120.28 | 124.32 |
| 69 | T | 500 | GDP | C5-C6-N1 | 2.04 | 117.95 | 114.07 |
| 69 | RE | 500 | GDP | C2'-C3'-C4' | 2.04 | 106.54 | 102.61 |
| 69 | MN | 500 | GDP | C2'-C3'-C4' | 2.03 | 106.53 | 102.61 |
| 71 | WI | 501 | GTP | O6-C6-C5 | -2.03 | 120.29 | 124.32 |
| 69 | TB | 500 | GDP | C5-C6-N1 | 2.03 | 117.94 | 114.07 |
| 69 | AJ | 500 | GDP | C2'-C3'-C4' | 2.03 | 106.53 | 102.61 |
| 69 | H | 500 | GDP | C5-C6-N1 | 2.03 | 117.94 | 114.07 |
| 69 | MF | 500 | GDP | C2'-C3'-C4' | 2.03 | 106.53 | 102.61 |
| 69 | MB | 500 | GDP | C5-C6-N1 | 2.03 | 117.94 | 114.07 |
| 69 | V | 500 | GDP | C5-C6-N1 | 2.03 | 117.94 | 114.07 |
| 71 | JB | 501 | GTP | O6-C6-C5 | -2.03 | 120.30 | 124.32 |
| 69 | BL | 500 | GDP | C5-C6-N1 | 2.03 | 117.94 | 114.07 |
| 69 | ND | 500 | GDP | C5-C6-N1 | 2.03 | 117.94 | 114.07 |
| 69 | KI | 500 | GDP | C5-C6-N1 | 2.03 | 117.94 | 114.07 |
| 69 | SB | 500 | GDP | C5-C6-N1 | 2.03 | 117.94 | 114.07 |
| 71 | VM | 501 | GTP | O6-C6-C5 | -2.03 | 120.31 | 124.32 |
| 71 | LJ | 501 | GTP | O6-C6-C5 | -2.02 | 120.31 | 124.32 |
| 69 | AJ | 500 | GDP | C5-C6-N1 | 2.02 | 117.93 | 114.07 |
| 69 | HB | 500 | GDP | C5-C6-N1 | 2.02 | 117.93 | 114.07 |
| 71 | RJ | 501 | GTP | O6-C6-C5 | -2.02 | 120.31 | 124.32 |
| 69 | IJ | 500 | GDP | C5-C6-N1 | 2.02 | 117.92 | 114.07 |
| 69 | RG | 500 | GDP | C5-C6-N1 | 2.02 | 117.92 | 114.07 |
| 69 | ND | 500 | GDP | O2A-PA-O3A | 2.02 | 112.73 | 107.27 |
| 69 | VD | 500 | GDP | C5-C6-N1 | 2.02 | 117.92 | 114.07 |
| 69 | AL | 500 | GDP | C2'-C3'-C4' | 2.02 | 106.50 | 102.61 |
| 69 | P | 500 | GDP | C5-C6-N1 | 2.02 | 117.92 | 114.07 |
| 71 | FI | 501 | GTP | C4'-O4'-C1' | 2.01 | 111.77 | 109.92 |
| 69 | KC | 500 | GDP | C5-C6-N1 | 2.01 | 117.91 | 114.07 |
| 71 | EG | 501 | GTP | O2A-PA-O3A | 2.01 | 112.71 | 107.27 |
| 69 | QA | 500 | GDP | C5-C6-N1 | 2.01 | 117.91 | 114.07 |
| 69 | BF | 500 | GDP | C5-C6-N1 | 2.01 | 117.90 | 114.07 |
| 69 | JI | 500 | GDP | C5-C6-N1 | 2.01 | 117.90 | 114.07 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|------|-------------|----------|
| 69 | LI | 500 | GDP | C5-C6-N1 | 2.01 | 117.89 | 114.07 |
| 69 | PF | 500 | GDP | C5-C6-N1 | 2.01 | 117.89 | 114.07 |
| 69 | GF | 500 | GDP | C5-C6-N1 | 2.00 | 117.89 | 114.07 |

There are no chirality outliers.

All (941) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 69 | AB | 500 | GDP | C5'-O5'-PA-O1A |
| 69 | AD | 500 | GDP | C5'-O5'-PA-O1A |
| 69 | AF | 500 | GDP | C5'-O5'-PA-O1A |
| 69 | AH | 500 | GDP | C5'-O5'-PA-O1A |
| 69 | AJ | 500 | GDP | C5'-O5'-PA-O1A |
| 69 | AN | 500 | GDP | C5'-O5'-PA-O1A |
| 69 | BB | 500 | GDP | C5'-O5'-PA-O3A |
| 69 | BD | 500 | GDP | C5'-O5'-PA-O1A |
| 69 | BF | 500 | GDP | C5'-O5'-PA-O1A |
| 69 | BH | 500 | GDP | C5'-O5'-PA-O3A |
| 69 | BJ | 500 | GDP | C5'-O5'-PA-O3A |
| 69 | BJ | 500 | GDP | C5'-O5'-PA-O1A |
| 69 | BL | 500 | GDP | C5'-O5'-PA-O1A |
| 69 | BN | 500 | GDP | C5'-O5'-PA-O3A |
| 69 | CA | 500 | GDP | C5'-O5'-PA-O3A |
| 69 | CA | 500 | GDP | C5'-O5'-PA-O1A |
| 69 | CA | 500 | GDP | C5'-O5'-PA-O2A |
| 69 | CE | 500 | GDP | C5'-O5'-PA-O1A |
| 69 | CG | 500 | GDP | C5'-O5'-PA-O3A |
| 69 | CG | 500 | GDP | C5'-O5'-PA-O1A |
| 69 | CK | 500 | GDP | C5'-O5'-PA-O1A |
| 69 | CK | 500 | GDP | O4'-C4'-C5'-O5' |
| 69 | CM | 500 | GDP | C5'-O5'-PA-O3A |
| 69 | CM | 500 | GDP | C5'-O5'-PA-O1A |
| 69 | CM | 500 | GDP | C5'-O5'-PA-O2A |
| 69 | DA | 500 | GDP | C5'-O5'-PA-O3A |
| 69 | DA | 500 | GDP | C5'-O5'-PA-O1A |
| 69 | DC | 500 | GDP | C5'-O5'-PA-O1A |
| 69 | DE | 500 | GDP | C5'-O5'-PA-O1A |
| 69 | DG | 500 | GDP | C5'-O5'-PA-O3A |
| 69 | DI | 500 | GDP | C5'-O5'-PA-O1A |
| 69 | DK | 500 | GDP | C5'-O5'-PA-O1A |
| 69 | E | 500 | GDP | C5'-O5'-PA-O3A |
| 69 | E | 500 | GDP | C5'-O5'-PA-O2A |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 69 | EB | 500 | GDP | C5'-O5'-PA-O3A |
| 69 | EB | 500 | GDP | C5'-O5'-PA-O1A |
| 69 | ED | 500 | GDP | C5'-O5'-PA-O3A |
| 69 | ED | 500 | GDP | C5'-O5'-PA-O1A |
| 69 | EF | 500 | GDP | C5'-O5'-PA-O3A |
| 69 | EF | 500 | GDP | C5'-O5'-PA-O2A |
| 69 | EJ | 500 | GDP | C5'-O5'-PA-O1A |
| 69 | EL | 500 | GDP | C5'-O5'-PA-O3A |
| 69 | EL | 500 | GDP | C5'-O5'-PA-O2A |
| 69 | FH | 500 | GDP | C5'-O5'-PA-O1A |
| 69 | GD | 500 | GDP | C5'-O5'-PA-O1A |
| 69 | GF | 500 | GDP | C5'-O5'-PA-O1A |
| 69 | GH | 500 | GDP | C5'-O5'-PA-O3A |
| 69 | GH | 500 | GDP | C5'-O5'-PA-O2A |
| 69 | GJ | 500 | GDP | C5'-O5'-PA-O3A |
| 69 | H | 500 | GDP | C5'-O5'-PA-O1A |
| 69 | HD | 500 | GDP | C5'-O5'-PA-O1A |
| 69 | HH | 500 | GDP | C5'-O5'-PA-O1A |
| 69 | HJ | 500 | GDP | C5'-O5'-PA-O3A |
| 69 | HJ | 500 | GDP | C5'-O5'-PA-O1A |
| 69 | IB | 500 | GDP | C5'-O5'-PA-O1A |
| 69 | IF | 500 | GDP | C5'-O5'-PA-O1A |
| 69 | IJ | 500 | GDP | C5'-O5'-PA-O3A |
| 69 | IJ | 500 | GDP | C5'-O5'-PA-O1A |
| 69 | JI | 500 | GDP | C5'-O5'-PA-O1A |
| 69 | JK | 500 | GDP | C5'-O5'-PA-O3A |
| 69 | JK | 500 | GDP | C5'-O5'-PA-O1A |
| 69 | JK | 500 | GDP | C5'-O5'-PA-O2A |
| 69 | KC | 500 | GDP | C5'-O5'-PA-O1A |
| 69 | KG | 500 | GDP | C5'-O5'-PA-O3A |
| 69 | KG | 500 | GDP | C5'-O5'-PA-O1A |
| 69 | LC | 500 | GDP | C5'-O5'-PA-O3A |
| 69 | LC | 500 | GDP | C5'-O5'-PA-O1A |
| 69 | LE | 500 | GDP | C5'-O5'-PA-O1A |
| 69 | LG | 500 | GDP | C5'-O5'-PA-O1A |
| 69 | LO | 500 | GDP | C5'-O5'-PA-O3A |
| 69 | LO | 500 | GDP | C5'-O5'-PA-O1A |
| 69 | M | 500 | GDP | C5'-O5'-PA-O1A |
| 69 | MD | 500 | GDP | C5'-O5'-PA-O1A |
| 69 | MH | 500 | GDP | C5'-O5'-PA-O1A |
| 69 | MJ | 500 | GDP | O4'-C4'-C5'-O5' |
| 69 | N | 500 | GDP | C5'-O5'-PA-O1A |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 69 | NB | 500 | GDP | C5'-O5'-PA-O1A |
| 69 | NF | 500 | GDP | C5'-O5'-PA-O1A |
| 69 | NH | 500 | GDP | C5'-O5'-PA-O1A |
| 69 | OB | 500 | GDP | C5'-O5'-PA-O3A |
| 69 | OB | 500 | GDP | C5'-O5'-PA-O1A |
| 69 | OB | 500 | GDP | C5'-O5'-PA-O2A |
| 69 | OF | 500 | GDP | C5'-O5'-PA-O1A |
| 69 | OH | 500 | GDP | C5'-O5'-PA-O1A |
| 69 | PB | 500 | GDP | C5'-O5'-PA-O1A |
| 69 | PD | 500 | GDP | C5'-O5'-PA-O1A |
| 69 | PH | 500 | GDP | C5'-O5'-PA-O1A |
| 69 | PL | 500 | GDP | C5'-O5'-PA-O1A |
| 69 | QA | 500 | GDP | C5'-O5'-PA-O1A |
| 69 | QC | 500 | GDP | C5'-O5'-PA-O3A |
| 69 | QE | 500 | GDP | C5'-O5'-PA-O1A |
| 69 | QG | 500 | GDP | C5'-O5'-PA-O1A |
| 69 | QI | 500 | GDP | C5'-O5'-PA-O3A |
| 69 | QK | 500 | GDP | C5'-O5'-PA-O3A |
| 69 | QK | 500 | GDP | C5'-O5'-PA-O2A |
| 69 | QK | 500 | GDP | C3'-C4'-C5'-O5' |
| 69 | RA | 500 | GDP | C5'-O5'-PA-O1A |
| 69 | RC | 500 | GDP | C5'-O5'-PA-O1A |
| 69 | RG | 500 | GDP | C5'-O5'-PA-O1A |
| 69 | S | 500 | GDP | C5'-O5'-PA-O3A |
| 69 | S | 500 | GDP | C5'-O5'-PA-O1A |
| 69 | SB | 500 | GDP | C5'-O5'-PA-O1A |
| 69 | SD | 500 | GDP | C5'-O5'-PA-O1A |
| 69 | SF | 500 | GDP | C5'-O5'-PA-O1A |
| 69 | TB | 500 | GDP | C5'-O5'-PA-O3A |
| 69 | TB | 500 | GDP | C5'-O5'-PA-O1A |
| 69 | TB | 500 | GDP | C5'-O5'-PA-O2A |
| 69 | TF | 500 | GDP | C5'-O5'-PA-O1A |
| 69 | TH | 500 | GDP | C5'-O5'-PA-O1A |
| 69 | TJ | 500 | GDP | C5'-O5'-PA-O3A |
| 69 | TJ | 500 | GDP | C5'-O5'-PA-O1A |
| 69 | U | 500 | GDP | C5'-O5'-PA-O3A |
| 69 | U | 500 | GDP | C5'-O5'-PA-O1A |
| 69 | UB | 500 | GDP | C5'-O5'-PA-O3A |
| 69 | UB | 500 | GDP | C5'-O5'-PA-O2A |
| 69 | UD | 500 | GDP | C5'-O5'-PA-O3A |
| 69 | UD | 500 | GDP | C5'-O5'-PA-O1A |
| 69 | UD | 500 | GDP | C5'-O5'-PA-O2A |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|----------------|
| 69 | UF | 500 | GDP | C5'-O5'-PA-O1A |
| 69 | UH | 500 | GDP | C5'-O5'-PA-O1A |
| 69 | VB | 500 | GDP | C5'-O5'-PA-O1A |
| 69 | VD | 500 | GDP | C5'-O5'-PA-O1A |
| 69 | VF | 500 | GDP | C5'-O5'-PA-O1A |
| 69 | VJ | 500 | GDP | C5'-O5'-PA-O3A |
| 69 | VJ | 500 | GDP | C5'-O5'-PA-O1A |
| 69 | VL | 500 | GDP | C5'-O5'-PA-O1A |
| 69 | WD | 500 | GDP | C5'-O5'-PA-O3A |
| 69 | WD | 500 | GDP | C5'-O5'-PA-O1A |
| 69 | WH | 500 | GDP | C5'-O5'-PA-O1A |
| 69 | WJ | 500 | GDP | C5'-O5'-PA-O1A |
| 69 | WL | 500 | GDP | C5'-O5'-PA-O1A |
| 71 | AA | 501 | GTP | C5'-O5'-PA-O1A |
| 71 | AC | 501 | GTP | C5'-O5'-PA-O3A |
| 71 | AC | 501 | GTP | C5'-O5'-PA-O1A |
| 71 | AC | 501 | GTP | C5'-O5'-PA-O2A |
| 71 | AE | 501 | GTP | C5'-O5'-PA-O3A |
| 71 | AE | 501 | GTP | C5'-O5'-PA-O1A |
| 71 | AE | 501 | GTP | C5'-O5'-PA-O2A |
| 71 | AG | 501 | GTP | C5'-O5'-PA-O3A |
| 71 | AG | 501 | GTP | C5'-O5'-PA-O1A |
| 71 | AG | 501 | GTP | C5'-O5'-PA-O2A |
| 71 | AK | 501 | GTP | C5'-O5'-PA-O2A |
| 71 | AM | 501 | GTP | C5'-O5'-PA-O1A |
| 71 | BA | 501 | GTP | C5'-O5'-PA-O3A |
| 71 | BE | 501 | GTP | C5'-O5'-PA-O3A |
| 71 | BE | 501 | GTP | C5'-O5'-PA-O1A |
| 71 | BE | 501 | GTP | C5'-O5'-PA-O2A |
| 71 | BI | 501 | GTP | C5'-O5'-PA-O3A |
| 71 | BI | 501 | GTP | C5'-O5'-PA-O1A |
| 71 | BI | 501 | GTP | C5'-O5'-PA-O2A |
| 71 | BK | 501 | GTP | C5'-O5'-PA-O3A |
| 71 | BK | 501 | GTP | C5'-O5'-PA-O1A |
| 71 | BM | 501 | GTP | C5'-O5'-PA-O3A |
| 71 | BM | 501 | GTP | C5'-O5'-PA-O2A |
| 71 | C | 501 | GTP | PB-O3A-PA-O5' |
| 71 | C | 501 | GTP | C5'-O5'-PA-O3A |
| 71 | CB | 501 | GTP | C5'-O5'-PA-O3A |
| 71 | CB | 501 | GTP | C5'-O5'-PA-O1A |
| 71 | CB | 501 | GTP | C5'-O5'-PA-O2A |
| 71 | CD | 501 | GTP | C5'-O5'-PA-O3A |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 71 | CD | 501 | GTP | C5'-O5'-PA-O2A |
| 71 | CF | 501 | GTP | C5'-O5'-PA-O3A |
| 71 | CF | 501 | GTP | C5'-O5'-PA-O1A |
| 71 | CH | 501 | GTP | PB-O3B-PG-O3G |
| 71 | CH | 501 | GTP | O4'-C4'-C5'-O5' |
| 71 | CH | 501 | GTP | C3'-C4'-C5'-O5' |
| 71 | CJ | 501 | GTP | C5'-O5'-PA-O3A |
| 71 | CJ | 501 | GTP | C5'-O5'-PA-O2A |
| 71 | CL | 501 | GTP | PB-O3B-PG-O3G |
| 71 | CL | 501 | GTP | C5'-O5'-PA-O3A |
| 71 | CL | 501 | GTP | C5'-O5'-PA-O1A |
| 71 | D | 501 | GTP | PB-O3B-PG-O2G |
| 71 | D | 501 | GTP | PB-O3B-PG-O3G |
| 71 | D | 501 | GTP | C5'-O5'-PA-O3A |
| 71 | D | 501 | GTP | C5'-O5'-PA-O1A |
| 71 | D | 501 | GTP | C5'-O5'-PA-O2A |
| 71 | DB | 501 | GTP | C5'-O5'-PA-O3A |
| 71 | DB | 501 | GTP | C5'-O5'-PA-O1A |
| 71 | DB | 501 | GTP | C5'-O5'-PA-O2A |
| 71 | DD | 501 | GTP | C5'-O5'-PA-O3A |
| 71 | DD | 501 | GTP | C5'-O5'-PA-O1A |
| 71 | DD | 501 | GTP | C5'-O5'-PA-O2A |
| 71 | DF | 501 | GTP | C5'-O5'-PA-O3A |
| 71 | DF | 501 | GTP | C5'-O5'-PA-O1A |
| 71 | DJ | 501 | GTP | C5'-O5'-PA-O3A |
| 71 | DJ | 501 | GTP | C5'-O5'-PA-O1A |
| 71 | DJ | 501 | GTP | C5'-O5'-PA-O2A |
| 71 | DL | 501 | GTP | PB-O3B-PG-O3G |
| 71 | DL | 501 | GTP | C5'-O5'-PA-O3A |
| 71 | EA | 501 | GTP | PB-O3B-PG-O3G |
| 71 | EA | 501 | GTP | C5'-O5'-PA-O1A |
| 71 | EC | 501 | GTP | C5'-O5'-PA-O3A |
| 71 | EC | 501 | GTP | C5'-O5'-PA-O1A |
| 71 | EC | 501 | GTP | C5'-O5'-PA-O2A |
| 71 | EE | 501 | GTP | C5'-O5'-PA-O3A |
| 71 | EE | 501 | GTP | C5'-O5'-PA-O2A |
| 71 | EG | 501 | GTP | C5'-O5'-PA-O3A |
| 71 | EG | 501 | GTP | C5'-O5'-PA-O2A |
| 71 | EI | 501 | GTP | O4'-C4'-C5'-O5' |
| 71 | EK | 501 | GTP | C5'-O5'-PA-O3A |
| 71 | EK | 501 | GTP | C5'-O5'-PA-O2A |
| 71 | FA | 501 | GTP | C5'-O5'-PA-O3A |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 71 | FC | 501 | GTP | C5'-O5'-PA-O3A |
| 71 | FC | 501 | GTP | C5'-O5'-PA-O1A |
| 71 | FC | 501 | GTP | C5'-O5'-PA-O2A |
| 71 | FE | 501 | GTP | PB-O3B-PG-O2G |
| 71 | FE | 501 | GTP | C5'-O5'-PA-O3A |
| 71 | FE | 501 | GTP | C5'-O5'-PA-O1A |
| 71 | FE | 501 | GTP | C5'-O5'-PA-O2A |
| 71 | FG | 501 | GTP | C5'-O5'-PA-O3A |
| 71 | FG | 501 | GTP | C5'-O5'-PA-O1A |
| 71 | FG | 501 | GTP | C5'-O5'-PA-O2A |
| 71 | FI | 501 | GTP | O4'-C4'-C5'-O5' |
| 71 | FI | 501 | GTP | C3'-C4'-C5'-O5' |
| 71 | FK | 501 | GTP | C5'-O5'-PA-O3A |
| 71 | FK | 501 | GTP | C5'-O5'-PA-O2A |
| 71 | GA | 501 | GTP | PB-O3B-PG-O2G |
| 71 | GA | 501 | GTP | PB-O3B-PG-O3G |
| 71 | GA | 501 | GTP | C5'-O5'-PA-O3A |
| 71 | GA | 501 | GTP | C5'-O5'-PA-O1A |
| 71 | GA | 501 | GTP | C5'-O5'-PA-O2A |
| 71 | GC | 501 | GTP | C5'-O5'-PA-O3A |
| 71 | GC | 501 | GTP | C5'-O5'-PA-O2A |
| 71 | GC | 501 | GTP | C4'-C5'-O5'-PA |
| 71 | GE | 501 | GTP | C5'-O5'-PA-O3A |
| 71 | GE | 501 | GTP | C5'-O5'-PA-O2A |
| 71 | GG | 501 | GTP | C5'-O5'-PA-O3A |
| 71 | GG | 501 | GTP | C5'-O5'-PA-O1A |
| 71 | GG | 501 | GTP | C5'-O5'-PA-O2A |
| 71 | GK | 501 | GTP | C5'-O5'-PA-O3A |
| 71 | GK | 501 | GTP | C5'-O5'-PA-O1A |
| 71 | GK | 501 | GTP | C5'-O5'-PA-O2A |
| 71 | HA | 501 | GTP | C5'-O5'-PA-O3A |
| 71 | HA | 501 | GTP | C5'-O5'-PA-O2A |
| 71 | HC | 501 | GTP | C5'-O5'-PA-O3A |
| 71 | HC | 501 | GTP | C5'-O5'-PA-O1A |
| 71 | HC | 501 | GTP | C5'-O5'-PA-O2A |
| 71 | HE | 501 | GTP | C5'-O5'-PA-O3A |
| 71 | HE | 501 | GTP | C5'-O5'-PA-O1A |
| 71 | HE | 501 | GTP | C5'-O5'-PA-O2A |
| 71 | HG | 501 | GTP | C5'-O5'-PA-O3A |
| 71 | HG | 501 | GTP | C5'-O5'-PA-O2A |
| 71 | HK | 501 | GTP | C5'-O5'-PA-O3A |
| 71 | HK | 501 | GTP | C5'-O5'-PA-O1A |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 71 | HK | 501 | GTP | C5'-O5'-PA-O2A |
| 71 | HM | 501 | GTP | C5'-O5'-PA-O3A |
| 71 | HM | 501 | GTP | C5'-O5'-PA-O2A |
| 71 | IA | 501 | GTP | PB-O3A-PA-O5' |
| 71 | IA | 501 | GTP | C5'-O5'-PA-O3A |
| 71 | IA | 501 | GTP | C5'-O5'-PA-O1A |
| 71 | IC | 501 | GTP | C5'-O5'-PA-O3A |
| 71 | IC | 501 | GTP | C5'-O5'-PA-O1A |
| 71 | IC | 501 | GTP | C5'-O5'-PA-O2A |
| 71 | IG | 501 | GTP | C5'-O5'-PA-O3A |
| 71 | IG | 501 | GTP | C5'-O5'-PA-O1A |
| 71 | IG | 501 | GTP | C5'-O5'-PA-O2A |
| 71 | IG | 501 | GTP | O4'-C4'-C5'-O5' |
| 71 | IM | 501 | GTP | PB-O3A-PA-O5' |
| 71 | IM | 501 | GTP | C5'-O5'-PA-O3A |
| 71 | J | 501 | GTP | C5'-O5'-PA-O3A |
| 71 | J | 501 | GTP | C5'-O5'-PA-O1A |
| 71 | JB | 501 | GTP | C5'-O5'-PA-O3A |
| 71 | JD | 501 | GTP | C5'-O5'-PA-O3A |
| 71 | JD | 501 | GTP | C5'-O5'-PA-O2A |
| 71 | JF | 501 | GTP | C5'-O5'-PA-O3A |
| 71 | JF | 501 | GTP | C5'-O5'-PA-O2A |
| 71 | JF | 501 | GTP | C4'-C5'-O5'-PA |
| 71 | JH | 501 | GTP | C5'-O5'-PA-O2A |
| 71 | JH | 501 | GTP | O4'-C4'-C5'-O5' |
| 71 | JH | 501 | GTP | C3'-C4'-C5'-O5' |
| 71 | JJ | 501 | GTP | C5'-O5'-PA-O3A |
| 71 | JJ | 501 | GTP | C5'-O5'-PA-O1A |
| 71 | JJ | 501 | GTP | C5'-O5'-PA-O2A |
| 71 | JN | 501 | GTP | C5'-O5'-PA-O3A |
| 71 | JN | 501 | GTP | C5'-O5'-PA-O2A |
| 71 | K | 501 | GTP | O4'-C4'-C5'-O5' |
| 71 | KB | 501 | GTP | C5'-O5'-PA-O3A |
| 71 | KB | 501 | GTP | C5'-O5'-PA-O2A |
| 71 | KD | 501 | GTP | C5'-O5'-PA-O3A |
| 71 | KD | 501 | GTP | C5'-O5'-PA-O2A |
| 71 | KF | 501 | GTP | C5'-O5'-PA-O3A |
| 71 | KF | 501 | GTP | C5'-O5'-PA-O1A |
| 71 | KF | 501 | GTP | C5'-O5'-PA-O2A |
| 71 | KH | 501 | GTP | PB-O3B-PG-O3G |
| 71 | KH | 501 | GTP | O4'-C4'-C5'-O5' |
| 71 | KH | 501 | GTP | C3'-C4'-C5'-O5' |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 71 | KJ | 501 | GTP | C5'-O5'-PA-O3A |
| 71 | KJ | 501 | GTP | C5'-O5'-PA-O1A |
| 71 | KL | 501 | GTP | O4'-C4'-C5'-O5' |
| 71 | KN | 501 | GTP | O4'-C4'-C5'-O5' |
| 71 | L | 501 | GTP | C5'-O5'-PA-O1A |
| 71 | LB | 501 | GTP | C5'-O5'-PA-O3A |
| 71 | LB | 501 | GTP | C5'-O5'-PA-O2A |
| 71 | LD | 501 | GTP | C5'-O5'-PA-O3A |
| 71 | LF | 501 | GTP | C5'-O5'-PA-O3A |
| 71 | LJ | 501 | GTP | C5'-O5'-PA-O3A |
| 71 | LJ | 501 | GTP | C5'-O5'-PA-O1A |
| 71 | LJ | 501 | GTP | C5'-O5'-PA-O2A |
| 71 | LN | 501 | GTP | C5'-O5'-PA-O3A |
| 71 | LN | 501 | GTP | C5'-O5'-PA-O1A |
| 71 | LN | 501 | GTP | C5'-O5'-PA-O2A |
| 71 | MC | 501 | GTP | C5'-O5'-PA-O3A |
| 71 | MC | 501 | GTP | C5'-O5'-PA-O1A |
| 71 | ME | 501 | GTP | C5'-O5'-PA-O3A |
| 71 | ME | 501 | GTP | C5'-O5'-PA-O2A |
| 71 | MG | 501 | GTP | C5'-O5'-PA-O3A |
| 71 | MG | 501 | GTP | O4'-C4'-C5'-O5' |
| 71 | MG | 501 | GTP | C3'-C4'-C5'-O5' |
| 71 | MI | 501 | GTP | PB-O3B-PG-O3G |
| 71 | MI | 501 | GTP | C5'-O5'-PA-O3A |
| 71 | MI | 501 | GTP | C5'-O5'-PA-O1A |
| 71 | MI | 501 | GTP | C5'-O5'-PA-O2A |
| 71 | MK | 501 | GTP | PB-O3A-PA-O5' |
| 71 | MK | 501 | GTP | C5'-O5'-PA-O3A |
| 71 | NA | 501 | GTP | PB-O3B-PG-O3G |
| 71 | NA | 501 | GTP | PB-O3A-PA-O5' |
| 71 | NA | 501 | GTP | C5'-O5'-PA-O3A |
| 71 | NA | 501 | GTP | C5'-O5'-PA-O2A |
| 71 | NC | 501 | GTP | C5'-O5'-PA-O3A |
| 71 | NC | 501 | GTP | C5'-O5'-PA-O2A |
| 71 | NE | 501 | GTP | PB-O3B-PG-O2G |
| 71 | NE | 501 | GTP | C5'-O5'-PA-O3A |
| 71 | NE | 501 | GTP | C5'-O5'-PA-O1A |
| 71 | NE | 501 | GTP | C5'-O5'-PA-O2A |
| 71 | NG | 501 | GTP | C5'-O5'-PA-O3A |
| 71 | NG | 501 | GTP | C5'-O5'-PA-O1A |
| 71 | NK | 501 | GTP | C5'-O5'-PA-O3A |
| 71 | NK | 501 | GTP | C4'-C5'-O5'-PA |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 71 | NM | 501 | GTP | C5'-O5'-PA-O3A |
| 71 | OA | 501 | GTP | PB-O3A-PA-O5' |
| 71 | OA | 501 | GTP | C5'-O5'-PA-O3A |
| 71 | OA | 501 | GTP | C5'-O5'-PA-O1A |
| 71 | OE | 501 | GTP | C5'-O5'-PA-O3A |
| 71 | OE | 501 | GTP | C5'-O5'-PA-O1A |
| 71 | OE | 501 | GTP | C5'-O5'-PA-O2A |
| 71 | OG | 501 | GTP | C5'-O5'-PA-O3A |
| 71 | OG | 501 | GTP | C5'-O5'-PA-O2A |
| 71 | OG | 501 | GTP | C4'-C5'-O5'-PA |
| 71 | OI | 501 | GTP | C5'-O5'-PA-O3A |
| 71 | OI | 501 | GTP | C5'-O5'-PA-O2A |
| 71 | OI | 501 | GTP | O4'-C4'-C5'-O5' |
| 71 | OI | 501 | GTP | C3'-C4'-C5'-O5' |
| 71 | OK | 501 | GTP | C5'-O5'-PA-O3A |
| 71 | OK | 501 | GTP | C5'-O5'-PA-O1A |
| 71 | OK | 501 | GTP | C5'-O5'-PA-O2A |
| 71 | OM | 501 | GTP | PB-O3A-PA-O5' |
| 71 | OM | 501 | GTP | C5'-O5'-PA-O3A |
| 71 | OM | 501 | GTP | C5'-O5'-PA-O1A |
| 71 | PC | 501 | GTP | C5'-O5'-PA-O3A |
| 71 | PC | 501 | GTP | C5'-O5'-PA-O1A |
| 71 | PC | 501 | GTP | C5'-O5'-PA-O2A |
| 71 | PG | 501 | GTP | C5'-O5'-PA-O1A |
| 71 | PI | 501 | GTP | C5'-O5'-PA-O3A |
| 71 | PI | 501 | GTP | C5'-O5'-PA-O2A |
| 71 | PI | 501 | GTP | O4'-C4'-C5'-O5' |
| 71 | PK | 501 | GTP | C5'-O5'-PA-O1A |
| 71 | PM | 501 | GTP | C5'-O5'-PA-O3A |
| 71 | PM | 501 | GTP | C5'-O5'-PA-O1A |
| 71 | PM | 501 | GTP | C5'-O5'-PA-O2A |
| 71 | Q | 501 | GTP | C5'-O5'-PA-O3A |
| 71 | Q | 501 | GTP | C5'-O5'-PA-O2A |
| 71 | QD | 501 | GTP | C5'-O5'-PA-O3A |
| 71 | QD | 501 | GTP | C5'-O5'-PA-O1A |
| 71 | QD | 501 | GTP | C5'-O5'-PA-O2A |
| 71 | QH | 501 | GTP | PB-O3B-PG-O2G |
| 71 | QH | 501 | GTP | PB-O3B-PG-O3G |
| 71 | QH | 501 | GTP | C5'-O5'-PA-O3A |
| 71 | QH | 501 | GTP | C5'-O5'-PA-O1A |
| 71 | QH | 501 | GTP | C5'-O5'-PA-O2A |
| 71 | QH | 501 | GTP | C4'-C5'-O5'-PA |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 71 | QH | 501 | GTP | O4'-C4'-C5'-O5' |
| 71 | QJ | 501 | GTP | C5'-O5'-PA-O3A |
| 71 | QJ | 501 | GTP | C5'-O5'-PA-O1A |
| 71 | QJ | 501 | GTP | C5'-O5'-PA-O2A |
| 71 | QL | 501 | GTP | C5'-O5'-PA-O3A |
| 71 | QL | 501 | GTP | C5'-O5'-PA-O1A |
| 71 | QL | 501 | GTP | C5'-O5'-PA-O2A |
| 71 | R | 501 | GTP | C5'-O5'-PA-O3A |
| 71 | R | 501 | GTP | C5'-O5'-PA-O1A |
| 71 | R | 501 | GTP | C5'-O5'-PA-O2A |
| 71 | RB | 501 | GTP | C5'-O5'-PA-O3A |
| 71 | RB | 501 | GTP | C5'-O5'-PA-O1A |
| 71 | RB | 501 | GTP | C5'-O5'-PA-O2A |
| 71 | RD | 501 | GTP | PB-O3A-PA-O5' |
| 71 | RD | 501 | GTP | C5'-O5'-PA-O3A |
| 71 | RD | 501 | GTP | C5'-O5'-PA-O1A |
| 71 | RH | 501 | GTP | O4'-C4'-C5'-O5' |
| 71 | RL | 501 | GTP | PB-O3A-PA-O5' |
| 71 | RL | 501 | GTP | C5'-O5'-PA-O3A |
| 71 | SA | 501 | GTP | C5'-O5'-PA-O3A |
| 71 | SA | 501 | GTP | C5'-O5'-PA-O2A |
| 71 | SC | 501 | GTP | C5'-O5'-PA-O3A |
| 71 | SC | 501 | GTP | C5'-O5'-PA-O1A |
| 71 | SE | 501 | GTP | C5'-O5'-PA-O3A |
| 71 | SE | 501 | GTP | C5'-O5'-PA-O1A |
| 71 | SE | 501 | GTP | C5'-O5'-PA-O2A |
| 71 | SG | 501 | GTP | PB-O3B-PG-O3G |
| 71 | SG | 501 | GTP | C5'-O5'-PA-O2A |
| 71 | SG | 501 | GTP | O4'-C4'-C5'-O5' |
| 71 | SI | 501 | GTP | C5'-O5'-PA-O3A |
| 71 | SI | 501 | GTP | C5'-O5'-PA-O2A |
| 71 | TA | 501 | GTP | C5'-O5'-PA-O3A |
| 71 | TA | 501 | GTP | C5'-O5'-PA-O1A |
| 71 | TA | 501 | GTP | C5'-O5'-PA-O2A |
| 71 | TC | 501 | GTP | C5'-O5'-PA-O1A |
| 71 | TE | 501 | GTP | C5'-O5'-PA-O3A |
| 71 | TE | 501 | GTP | C5'-O5'-PA-O1A |
| 71 | TE | 501 | GTP | C5'-O5'-PA-O2A |
| 71 | TI | 501 | GTP | C5'-O5'-PA-O3A |
| 71 | TI | 501 | GTP | C5'-O5'-PA-O1A |
| 71 | TI | 501 | GTP | C5'-O5'-PA-O2A |
| 71 | UA | 501 | GTP | PB-O3B-PG-O3G |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 71 | UA | 501 | GTP | C5'-O5'-PA-O3A |
| 71 | UA | 501 | GTP | C5'-O5'-PA-O2A |
| 71 | UC | 501 | GTP | C5'-O5'-PA-O3A |
| 71 | UC | 501 | GTP | C5'-O5'-PA-O1A |
| 71 | UC | 501 | GTP | C5'-O5'-PA-O2A |
| 71 | UE | 501 | GTP | C5'-O5'-PA-O3A |
| 71 | UE | 501 | GTP | C5'-O5'-PA-O1A |
| 71 | UE | 501 | GTP | C5'-O5'-PA-O2A |
| 71 | UG | 501 | GTP | C5'-O5'-PA-O3A |
| 71 | UG | 501 | GTP | C5'-O5'-PA-O2A |
| 71 | UG | 501 | GTP | O4'-C4'-C5'-O5' |
| 71 | UI | 501 | GTP | C5'-O5'-PA-O3A |
| 71 | UI | 501 | GTP | C5'-O5'-PA-O1A |
| 71 | UI | 501 | GTP | C5'-O5'-PA-O2A |
| 71 | UK | 501 | GTP | C5'-O5'-PA-O1A |
| 71 | VA | 501 | GTP | C5'-O5'-PA-O3A |
| 71 | VA | 501 | GTP | C5'-O5'-PA-O1A |
| 71 | VC | 501 | GTP | C5'-O5'-PA-O3A |
| 71 | VC | 501 | GTP | C5'-O5'-PA-O1A |
| 71 | VC | 501 | GTP | C5'-O5'-PA-O2A |
| 71 | VG | 501 | GTP | O4'-C4'-C5'-O5' |
| 71 | VI | 501 | GTP | C5'-O5'-PA-O3A |
| 71 | VI | 501 | GTP | C5'-O5'-PA-O1A |
| 71 | VI | 501 | GTP | C5'-O5'-PA-O2A |
| 71 | VM | 501 | GTP | C5'-O5'-PA-O3A |
| 71 | VM | 501 | GTP | C5'-O5'-PA-O2A |
| 71 | WE | 501 | GTP | PB-O3B-PG-O3G |
| 71 | WI | 501 | GTP | C5'-O5'-PA-O3A |
| 71 | WI | 501 | GTP | C5'-O5'-PA-O1A |
| 71 | WI | 501 | GTP | C5'-O5'-PA-O2A |
| 71 | WK | 501 | GTP | C5'-O5'-PA-O3A |
| 71 | WK | 501 | GTP | C5'-O5'-PA-O1A |
| 71 | WM | 501 | GTP | C5'-O5'-PA-O3A |
| 71 | WM | 501 | GTP | C5'-O5'-PA-O2A |
| 74 | 2v | 501 | ATP | O4'-C4'-C5'-O5' |
| 69 | CK | 500 | GDP | C3'-C4'-C5'-O5' |
| 69 | EB | 500 | GDP | C3'-C4'-C5'-O5' |
| 69 | MJ | 500 | GDP | C3'-C4'-C5'-O5' |
| 69 | O | 500 | GDP | C3'-C4'-C5'-O5' |
| 69 | PF | 500 | GDP | O4'-C4'-C5'-O5' |
| 69 | PF | 500 | GDP | C3'-C4'-C5'-O5' |
| 71 | AG | 501 | GTP | O4'-C4'-C5'-O5' |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 71 | AG | 501 | GTP | C3'-C4'-C5'-O5' |
| 71 | BE | 501 | GTP | O4'-C4'-C5'-O5' |
| 71 | BE | 501 | GTP | C3'-C4'-C5'-O5' |
| 71 | DF | 501 | GTP | O4'-C4'-C5'-O5' |
| 71 | DF | 501 | GTP | C3'-C4'-C5'-O5' |
| 71 | EA | 501 | GTP | C3'-C4'-C5'-O5' |
| 71 | EI | 501 | GTP | C3'-C4'-C5'-O5' |
| 71 | IG | 501 | GTP | C3'-C4'-C5'-O5' |
| 71 | K | 501 | GTP | C3'-C4'-C5'-O5' |
| 71 | KL | 501 | GTP | C3'-C4'-C5'-O5' |
| 71 | L | 501 | GTP | O4'-C4'-C5'-O5' |
| 71 | L | 501 | GTP | C3'-C4'-C5'-O5' |
| 71 | LL | 501 | GTP | O4'-C4'-C5'-O5' |
| 71 | LL | 501 | GTP | C3'-C4'-C5'-O5' |
| 71 | QH | 501 | GTP | C3'-C4'-C5'-O5' |
| 71 | RH | 501 | GTP | C3'-C4'-C5'-O5' |
| 71 | SC | 501 | GTP | O4'-C4'-C5'-O5' |
| 71 | SC | 501 | GTP | C3'-C4'-C5'-O5' |
| 71 | TE | 501 | GTP | O4'-C4'-C5'-O5' |
| 71 | TE | 501 | GTP | C3'-C4'-C5'-O5' |
| 71 | UE | 501 | GTP | O4'-C4'-C5'-O5' |
| 71 | UE | 501 | GTP | C3'-C4'-C5'-O5' |
| 71 | UG | 501 | GTP | C3'-C4'-C5'-O5' |
| 71 | VA | 501 | GTP | O4'-C4'-C5'-O5' |
| 71 | VA | 501 | GTP | C3'-C4'-C5'-O5' |
| 71 | SI | 501 | GTP | C4'-C5'-O5'-PA |
| 69 | DA | 500 | GDP | O4'-C4'-C5'-O5' |
| 69 | DA | 500 | GDP | C3'-C4'-C5'-O5' |
| 69 | EB | 500 | GDP | O4'-C4'-C5'-O5' |
| 69 | O | 500 | GDP | O4'-C4'-C5'-O5' |
| 69 | PJ | 500 | GDP | O4'-C4'-C5'-O5' |
| 69 | PJ | 500 | GDP | C3'-C4'-C5'-O5' |
| 69 | QK | 500 | GDP | O4'-C4'-C5'-O5' |
| 71 | BK | 501 | GTP | O4'-C4'-C5'-O5' |
| 71 | BK | 501 | GTP | C3'-C4'-C5'-O5' |
| 71 | EA | 501 | GTP | O4'-C4'-C5'-O5' |
| 71 | IE | 501 | GTP | O4'-C4'-C5'-O5' |
| 71 | JL | 501 | GTP | O4'-C4'-C5'-O5' |
| 71 | JL | 501 | GTP | C3'-C4'-C5'-O5' |
| 71 | LH | 501 | GTP | O4'-C4'-C5'-O5' |
| 71 | TK | 501 | GTP | O4'-C4'-C5'-O5' |
| 71 | TK | 501 | GTP | C3'-C4'-C5'-O5' |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 74 | 2v | 501 | ATP | C3'-C4'-C5'-O5' |
| 74 | 2w | 501 | ATP | O4'-C4'-C5'-O5' |
| 74 | 2w | 501 | ATP | C3'-C4'-C5'-O5' |
| 71 | FK | 501 | GTP | C4'-C5'-O5'-PA |
| 71 | HG | 501 | GTP | C4'-C5'-O5'-PA |
| 71 | PI | 501 | GTP | C3'-C4'-C5'-O5' |
| 71 | SG | 501 | GTP | C3'-C4'-C5'-O5' |
| 71 | VG | 501 | GTP | C3'-C4'-C5'-O5' |
| 71 | VK | 501 | GTP | C3'-C4'-C5'-O5' |
| 71 | GA | 501 | GTP | C4'-C5'-O5'-PA |
| 71 | RF | 501 | GTP | C4'-C5'-O5'-PA |
| 69 | ED | 500 | GDP | C3'-C4'-C5'-O5' |
| 69 | GF | 500 | GDP | C3'-C4'-C5'-O5' |
| 69 | LI | 500 | GDP | C3'-C4'-C5'-O5' |
| 69 | M | 500 | GDP | C3'-C4'-C5'-O5' |
| 69 | OB | 500 | GDP | O4'-C4'-C5'-O5' |
| 69 | OH | 500 | GDP | C3'-C4'-C5'-O5' |
| 71 | AM | 501 | GTP | C3'-C4'-C5'-O5' |
| 71 | DL | 501 | GTP | C3'-C4'-C5'-O5' |
| 71 | IE | 501 | GTP | C3'-C4'-C5'-O5' |
| 71 | KN | 501 | GTP | C3'-C4'-C5'-O5' |
| 71 | LH | 501 | GTP | C3'-C4'-C5'-O5' |
| 71 | QB | 501 | GTP | C3'-C4'-C5'-O5' |
| 71 | RD | 501 | GTP | C3'-C4'-C5'-O5' |
| 71 | UK | 501 | GTP | C3'-C4'-C5'-O5' |
| 71 | WE | 501 | GTP | C3'-C4'-C5'-O5' |
| 71 | BI | 501 | GTP | C4'-C5'-O5'-PA |
| 71 | GG | 501 | GTP | C4'-C5'-O5'-PA |
| 69 | ED | 500 | GDP | O4'-C4'-C5'-O5' |
| 69 | IB | 500 | GDP | C3'-C4'-C5'-O5' |
| 69 | IF | 500 | GDP | C3'-C4'-C5'-O5' |
| 69 | PD | 500 | GDP | C3'-C4'-C5'-O5' |
| 69 | SD | 500 | GDP | C3'-C4'-C5'-O5' |
| 71 | DL | 501 | GTP | O4'-C4'-C5'-O5' |
| 71 | HI | 501 | GTP | O4'-C4'-C5'-O5' |
| 71 | HI | 501 | GTP | C3'-C4'-C5'-O5' |
| 71 | IA | 501 | GTP | C3'-C4'-C5'-O5' |
| 71 | VK | 501 | GTP | O4'-C4'-C5'-O5' |
| 69 | F | 500 | GDP | C3'-C4'-C5'-O5' |
| 69 | OJ | 500 | GDP | C3'-C4'-C5'-O5' |
| 71 | AM | 501 | GTP | O4'-C4'-C5'-O5' |
| 71 | CF | 501 | GTP | C3'-C4'-C5'-O5' |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 71 | DH | 501 | GTP | O4'-C4'-C5'-O5' |
| 71 | EE | 501 | GTP | C3'-C4'-C5'-O5' |
| 71 | WE | 501 | GTP | O4'-C4'-C5'-O5' |
| 71 | RL | 501 | GTP | PB-O3B-PG-O1G |
| 69 | NB | 500 | GDP | C3'-C4'-C5'-O5' |
| 69 | OL | 500 | GDP | C3'-C4'-C5'-O5' |
| 71 | DH | 501 | GTP | C3'-C4'-C5'-O5' |
| 71 | PG | 501 | GTP | C3'-C4'-C5'-O5' |
| 71 | D | 501 | GTP | PG-O3B-PB-O1B |
| 71 | FG | 501 | GTP | PB-O3A-PA-O1A |
| 71 | ME | 501 | GTP | PA-O3A-PB-O1B |
| 71 | NG | 501 | GTP | PB-O3A-PA-O1A |
| 71 | VG | 501 | GTP | PB-O3A-PA-O1A |
| 71 | EG | 501 | GTP | C4'-C5'-O5'-PA |
| 71 | GE | 501 | GTP | C4'-C5'-O5'-PA |
| 71 | LF | 501 | GTP | C4'-C5'-O5'-PA |
| 71 | LJ | 501 | GTP | C4'-C5'-O5'-PA |
| 71 | OI | 501 | GTP | C4'-C5'-O5'-PA |
| 71 | OK | 501 | GTP | C4'-C5'-O5'-PA |
| 69 | GF | 500 | GDP | O4'-C4'-C5'-O5' |
| 69 | M | 500 | GDP | O4'-C4'-C5'-O5' |
| 71 | UK | 501 | GTP | O4'-C4'-C5'-O5' |
| 71 | FG | 501 | GTP | C4'-C5'-O5'-PA |
| 71 | FI | 501 | GTP | C4'-C5'-O5'-PA |
| 71 | IC | 501 | GTP | C4'-C5'-O5'-PA |
| 71 | ME | 501 | GTP | C4'-C5'-O5'-PA |
| 71 | QF | 501 | GTP | C4'-C5'-O5'-PA |
| 69 | LI | 500 | GDP | O4'-C4'-C5'-O5' |
| 69 | OH | 500 | GDP | O4'-C4'-C5'-O5' |
| 71 | IA | 501 | GTP | O4'-C4'-C5'-O5' |
| 71 | RD | 501 | GTP | O4'-C4'-C5'-O5' |
| 71 | AM | 501 | GTP | PB-O3A-PA-O5' |
| 71 | CF | 501 | GTP | PB-O3A-PA-O5' |
| 71 | CL | 501 | GTP | PB-O3A-PA-O5' |
| 71 | D | 501 | GTP | PB-O3A-PA-O5' |
| 71 | DL | 501 | GTP | PB-O3A-PA-O5' |
| 71 | KB | 501 | GTP | PB-O3A-PA-O5' |
| 71 | LD | 501 | GTP | PB-O3A-PA-O5' |
| 71 | NM | 501 | GTP | PB-O3A-PA-O5' |
| 71 | QH | 501 | GTP | PB-O3A-PA-O5' |
| 71 | R | 501 | GTP | PB-O3A-PA-O5' |
| 71 | UA | 501 | GTP | PB-O3A-PA-O5' |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 71 | UE | 501 | GTP | PB-O3A-PA-O5' |
| 71 | UK | 501 | GTP | PB-O3A-PA-O5' |
| 71 | VK | 501 | GTP | PB-O3A-PA-O5' |
| 71 | WE | 501 | GTP | PB-O3A-PA-O5' |
| 71 | WK | 501 | GTP | PB-O3A-PA-O5' |
| 71 | TC | 501 | GTP | C3'-C4'-C5'-O5' |
| 71 | VM | 501 | GTP | C3'-C4'-C5'-O5' |
| 71 | KF | 501 | GTP | PB-O3B-PG-O1G |
| 71 | TA | 501 | GTP | PB-O3B-PG-O1G |
| 71 | VC | 501 | GTP | PB-O3B-PG-O1G |
| 71 | WE | 501 | GTP | PB-O3B-PG-O1G |
| 71 | BE | 501 | GTP | PB-O3B-PG-O2G |
| 71 | BE | 501 | GTP | PB-O3B-PG-O3G |
| 71 | C | 501 | GTP | PB-O3B-PG-O3G |
| 71 | CF | 501 | GTP | PB-O3B-PG-O2G |
| 71 | CL | 501 | GTP | PB-O3B-PG-O2G |
| 71 | NA | 501 | GTP | PB-O3B-PG-O2G |
| 71 | RD | 501 | GTP | PB-O3B-PG-O2G |
| 71 | RL | 501 | GTP | PB-O3B-PG-O3G |
| 71 | SG | 501 | GTP | PB-O3B-PG-O2G |
| 69 | HD | 500 | GDP | C3'-C4'-C5'-O5' |
| 69 | IB | 500 | GDP | O4'-C4'-C5'-O5' |
| 69 | JG | 500 | GDP | C3'-C4'-C5'-O5' |
| 69 | KI | 500 | GDP | C3'-C4'-C5'-O5' |
| 69 | MF | 500 | GDP | C3'-C4'-C5'-O5' |
| 69 | NF | 500 | GDP | C3'-C4'-C5'-O5' |
| 71 | AA | 501 | GTP | C3'-C4'-C5'-O5' |
| 71 | II | 501 | GTP | C3'-C4'-C5'-O5' |
| 71 | JD | 501 | GTP | C3'-C4'-C5'-O5' |
| 71 | DF | 501 | GTP | C4'-C5'-O5'-PA |
| 71 | DL | 501 | GTP | C4'-C5'-O5'-PA |
| 71 | NA | 501 | GTP | C4'-C5'-O5'-PA |
| 71 | BE | 501 | GTP | PA-O3A-PB-O1B |
| 71 | QH | 501 | GTP | PA-O3A-PB-O2B |
| 71 | UE | 501 | GTP | PA-O3A-PB-O1B |
| 74 | 2w | 501 | ATP | PA-O3A-PB-O1B |
| 69 | GL | 500 | GDP | C3'-C4'-C5'-O5' |
| 71 | D | 501 | GTP | C3'-C4'-C5'-O5' |
| 71 | EE | 501 | GTP | O4'-C4'-C5'-O5' |
| 71 | LD | 501 | GTP | C3'-C4'-C5'-O5' |
| 71 | MK | 501 | GTP | C4'-C5'-O5'-PA |
| 69 | F | 500 | GDP | O4'-C4'-C5'-O5' |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 69 | FL | 500 | GDP | C3'-C4'-C5'-O5' |
| 69 | IF | 500 | GDP | O4'-C4'-C5'-O5' |
| 69 | OJ | 500 | GDP | O4'-C4'-C5'-O5' |
| 69 | PD | 500 | GDP | O4'-C4'-C5'-O5' |
| 69 | SB | 500 | GDP | C3'-C4'-C5'-O5' |
| 69 | SD | 500 | GDP | O4'-C4'-C5'-O5' |
| 71 | CF | 501 | GTP | O4'-C4'-C5'-O5' |
| 71 | II | 501 | GTP | O4'-C4'-C5'-O5' |
| 71 | RL | 501 | GTP | C3'-C4'-C5'-O5' |
| 69 | A | 500 | GDP | C5'-O5'-PA-O1A |
| 69 | AL | 500 | GDP | C5'-O5'-PA-O1A |
| 69 | BB | 500 | GDP | C5'-O5'-PA-O1A |
| 69 | BH | 500 | GDP | C5'-O5'-PA-O1A |
| 69 | BN | 500 | GDP | C5'-O5'-PA-O1A |
| 69 | CC | 500 | GDP | C5'-O5'-PA-O1A |
| 69 | CI | 500 | GDP | C5'-O5'-PA-O1A |
| 69 | DG | 500 | GDP | C5'-O5'-PA-O1A |
| 69 | DI | 500 | GDP | C5'-O5'-PA-O3A |
| 69 | EF | 500 | GDP | C5'-O5'-PA-O1A |
| 69 | EH | 500 | GDP | C5'-O5'-PA-O1A |
| 69 | F | 500 | GDP | C5'-O5'-PA-O1A |
| 69 | FD | 500 | GDP | C5'-O5'-PA-O1A |
| 69 | FF | 500 | GDP | C5'-O5'-PA-O1A |
| 69 | FJ | 500 | GDP | C5'-O5'-PA-O1A |
| 69 | FL | 500 | GDP | C5'-O5'-PA-O1A |
| 69 | GB | 500 | GDP | C5'-O5'-PA-O1A |
| 69 | GF | 500 | GDP | C5'-O5'-PA-O3A |
| 69 | GH | 500 | GDP | C5'-O5'-PA-O1A |
| 69 | GJ | 500 | GDP | C5'-O5'-PA-O1A |
| 69 | GL | 500 | GDP | C5'-O5'-PA-O1A |
| 69 | HB | 500 | GDP | C5'-O5'-PA-O1A |
| 69 | HL | 500 | GDP | C5'-O5'-PA-O1A |
| 69 | ID | 500 | GDP | C5'-O5'-PA-O1A |
| 69 | IH | 500 | GDP | C5'-O5'-PA-O1A |
| 69 | JA | 500 | GDP | C5'-O5'-PA-O1A |
| 69 | JC | 500 | GDP | C5'-O5'-PA-O1A |
| 69 | JE | 500 | GDP | C5'-O5'-PA-O1A |
| 69 | KA | 500 | GDP | C5'-O5'-PA-O1A |
| 69 | KE | 500 | GDP | C5'-O5'-PA-O1A |
| 69 | KI | 500 | GDP | C5'-O5'-PA-O1A |
| 69 | KK | 500 | GDP | C5'-O5'-PA-O1A |
| 69 | KM | 500 | GDP | C5'-O5'-PA-O1A |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|----------------|
| 69 | LA | 500 | GDP | C5'-O5'-PA-O1A |
| 69 | LE | 500 | GDP | C5'-O5'-PA-O3A |
| 69 | LI | 500 | GDP | C5'-O5'-PA-O1A |
| 69 | LK | 500 | GDP | C5'-O5'-PA-O1A |
| 69 | MB | 500 | GDP | C5'-O5'-PA-O1A |
| 69 | MF | 500 | GDP | C5'-O5'-PA-O1A |
| 69 | MJ | 500 | GDP | C5'-O5'-PA-O1A |
| 69 | ML | 500 | GDP | C5'-O5'-PA-O1A |
| 69 | MN | 500 | GDP | C5'-O5'-PA-O1A |
| 69 | NJ | 500 | GDP | C5'-O5'-PA-O1A |
| 69 | NL | 500 | GDP | C5'-O5'-PA-O1A |
| 69 | OD | 500 | GDP | C5'-O5'-PA-O1A |
| 69 | OJ | 500 | GDP | C5'-O5'-PA-O1A |
| 69 | P | 500 | GDP | C5'-O5'-PA-O1A |
| 69 | PD | 500 | GDP | C5'-O5'-PA-O3A |
| 69 | PF | 500 | GDP | C5'-O5'-PA-O1A |
| 69 | PJ | 500 | GDP | C5'-O5'-PA-O1A |
| 69 | QC | 500 | GDP | C5'-O5'-PA-O1A |
| 69 | QI | 500 | GDP | C5'-O5'-PA-O1A |
| 69 | RK | 500 | GDP | C5'-O5'-PA-O1A |
| 69 | SH | 500 | GDP | C5'-O5'-PA-O1A |
| 69 | SJ | 500 | GDP | C5'-O5'-PA-O1A |
| 69 | T | 500 | GDP | C5'-O5'-PA-O1A |
| 69 | TD | 500 | GDP | C5'-O5'-PA-O1A |
| 69 | UB | 500 | GDP | C5'-O5'-PA-O1A |
| 69 | UJ | 500 | GDP | C5'-O5'-PA-O1A |
| 69 | UL | 500 | GDP | C5'-O5'-PA-O1A |
| 69 | V | 500 | GDP | C5'-O5'-PA-O1A |
| 69 | VH | 500 | GDP | C5'-O5'-PA-O1A |
| 69 | W | 500 | GDP | C5'-O5'-PA-O1A |
| 69 | WB | 500 | GDP | C5'-O5'-PA-O1A |
| 69 | WF | 500 | GDP | C5'-O5'-PA-O1A |
| 69 | WH | 500 | GDP | C5'-O5'-PA-O3A |
| 71 | AA | 501 | GTP | C5'-O5'-PA-O3A |
| 71 | AK | 501 | GTP | C5'-O5'-PA-O3A |
| 71 | AK | 501 | GTP | C5'-O5'-PA-O1A |
| 71 | BA | 501 | GTP | C5'-O5'-PA-O1A |
| 71 | BM | 501 | GTP | C5'-O5'-PA-O1A |
| 71 | C | 501 | GTP | C5'-O5'-PA-O1A |
| 71 | CD | 501 | GTP | C5'-O5'-PA-O1A |
| 71 | CJ | 501 | GTP | C5'-O5'-PA-O1A |
| 71 | DF | 501 | GTP | C5'-O5'-PA-O2A |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|----------------|
| 71 | DL | 501 | GTP | C5'-O5'-PA-O1A |
| 71 | EE | 501 | GTP | C5'-O5'-PA-O1A |
| 71 | EK | 501 | GTP | C5'-O5'-PA-O1A |
| 71 | FA | 501 | GTP | C5'-O5'-PA-O2A |
| 71 | IM | 501 | GTP | C5'-O5'-PA-O1A |
| 71 | JD | 501 | GTP | C5'-O5'-PA-O1A |
| 71 | JH | 501 | GTP | C5'-O5'-PA-O3A |
| 71 | JH | 501 | GTP | C5'-O5'-PA-O1A |
| 71 | KD | 501 | GTP | C5'-O5'-PA-O1A |
| 71 | LB | 501 | GTP | C5'-O5'-PA-O1A |
| 71 | LD | 501 | GTP | C5'-O5'-PA-O1A |
| 71 | LL | 501 | GTP | C5'-O5'-PA-O1A |
| 71 | ME | 501 | GTP | C5'-O5'-PA-O1A |
| 71 | MG | 501 | GTP | C5'-O5'-PA-O2A |
| 71 | MK | 501 | GTP | C5'-O5'-PA-O1A |
| 71 | MM | 501 | GTP | C5'-O5'-PA-O3A |
| 71 | MM | 501 | GTP | C5'-O5'-PA-O1A |
| 71 | NA | 501 | GTP | C5'-O5'-PA-O1A |
| 71 | NC | 501 | GTP | C5'-O5'-PA-O1A |
| 71 | NG | 501 | GTP | C5'-O5'-PA-O2A |
| 71 | NM | 501 | GTP | C5'-O5'-PA-O1A |
| 71 | OI | 501 | GTP | C5'-O5'-PA-O1A |
| 71 | PG | 501 | GTP | C5'-O5'-PA-O3A |
| 71 | Q | 501 | GTP | C5'-O5'-PA-O1A |
| 71 | QF | 501 | GTP | C5'-O5'-PA-O3A |
| 71 | RL | 501 | GTP | C5'-O5'-PA-O1A |
| 71 | SC | 501 | GTP | C5'-O5'-PA-O2A |
| 71 | SG | 501 | GTP | C5'-O5'-PA-O3A |
| 71 | SG | 501 | GTP | C5'-O5'-PA-O1A |
| 71 | TC | 501 | GTP | C5'-O5'-PA-O3A |
| 71 | TK | 501 | GTP | C5'-O5'-PA-O1A |
| 71 | UG | 501 | GTP | C5'-O5'-PA-O1A |
| 71 | VK | 501 | GTP | C5'-O5'-PA-O1A |
| 71 | VM | 501 | GTP | C5'-O5'-PA-O1A |
| 71 | WA | 501 | GTP | C5'-O5'-PA-O3A |
| 71 | WA | 501 | GTP | C5'-O5'-PA-O1A |
| 71 | WC | 501 | GTP | C5'-O5'-PA-O3A |
| 71 | WC | 501 | GTP | C5'-O5'-PA-O1A |
| 71 | WE | 501 | GTP | C5'-O5'-PA-O1A |
| 71 | WM | 501 | GTP | C5'-O5'-PA-O1A |
| 74 | 2w | 501 | ATP | C5'-O5'-PA-O1A |
| 71 | AG | 501 | GTP | C4'-C5'-O5'-PA |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 71 | BE | 501 | GTP | C4'-C5'-O5'-PA |
| 71 | D | 501 | GTP | C4'-C5'-O5'-PA |
| 71 | HA | 501 | GTP | C4'-C5'-O5'-PA |
| 71 | HC | 501 | GTP | C4'-C5'-O5'-PA |
| 71 | IG | 501 | GTP | C4'-C5'-O5'-PA |
| 71 | J | 501 | GTP | C4'-C5'-O5'-PA |
| 71 | JL | 501 | GTP | C4'-C5'-O5'-PA |
| 71 | KJ | 501 | GTP | C4'-C5'-O5'-PA |
| 71 | KN | 501 | GTP | C4'-C5'-O5'-PA |
| 71 | NG | 501 | GTP | C4'-C5'-O5'-PA |
| 71 | OA | 501 | GTP | C4'-C5'-O5'-PA |
| 71 | OM | 501 | GTP | C4'-C5'-O5'-PA |
| 71 | RD | 501 | GTP | C4'-C5'-O5'-PA |
| 71 | RL | 501 | GTP | C4'-C5'-O5'-PA |
| 71 | SC | 501 | GTP | C4'-C5'-O5'-PA |
| 71 | SE | 501 | GTP | C4'-C5'-O5'-PA |
| 71 | TA | 501 | GTP | C4'-C5'-O5'-PA |
| 71 | TC | 501 | GTP | C4'-C5'-O5'-PA |
| 71 | TE | 501 | GTP | C4'-C5'-O5'-PA |
| 71 | UE | 501 | GTP | C4'-C5'-O5'-PA |
| 71 | VE | 501 | GTP | C4'-C5'-O5'-PA |
| 69 | HB | 500 | GDP | C3'-C4'-C5'-O5' |
| 69 | KA | 500 | GDP | C3'-C4'-C5'-O5' |
| 69 | NB | 500 | GDP | O4'-C4'-C5'-O5' |
| 69 | SH | 500 | GDP | C3'-C4'-C5'-O5' |
| 71 | CL | 501 | GTP | C3'-C4'-C5'-O5' |
| 71 | RJ | 501 | GTP | C3'-C4'-C5'-O5' |
| 69 | QK | 500 | GDP | PB-O3A-PA-O2A |
| 71 | CH | 501 | GTP | PB-O3A-PA-O1A |
| 71 | EG | 501 | GTP | PB-O3A-PA-O1A |
| 71 | IK | 501 | GTP | PG-O3B-PB-O1B |
| 71 | J | 501 | GTP | PG-O3B-PB-O2B |
| 71 | RL | 501 | GTP | PG-O3B-PB-O1B |
| 71 | SE | 501 | GTP | PB-O3A-PA-O2A |
| 69 | CC | 500 | GDP | C3'-C4'-C5'-O5' |
| 69 | HF | 500 | GDP | C3'-C4'-C5'-O5' |
| 69 | SJ | 500 | GDP | C3'-C4'-C5'-O5' |
| 71 | FA | 501 | GTP | C4'-C5'-O5'-PA |
| 71 | LD | 501 | GTP | C4'-C5'-O5'-PA |
| 71 | PG | 501 | GTP | C4'-C5'-O5'-PA |
| 71 | J | 501 | GTP | PA-O3A-PB-O3B |
| 69 | BL | 500 | GDP | C3'-C4'-C5'-O5' |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 71 | QB | 501 | GTP | O4'-C4'-C5'-O5' |
| 71 | AC | 501 | GTP | C4'-C5'-O5'-PA |
| 71 | AM | 501 | GTP | C4'-C5'-O5'-PA |
| 71 | BK | 501 | GTP | C4'-C5'-O5'-PA |
| 71 | CF | 501 | GTP | C4'-C5'-O5'-PA |
| 71 | EA | 501 | GTP | C4'-C5'-O5'-PA |
| 71 | FC | 501 | GTP | C4'-C5'-O5'-PA |
| 71 | JB | 501 | GTP | C4'-C5'-O5'-PA |
| 71 | JN | 501 | GTP | C4'-C5'-O5'-PA |
| 71 | MC | 501 | GTP | C4'-C5'-O5'-PA |
| 71 | TK | 501 | GTP | C4'-C5'-O5'-PA |
| 71 | UK | 501 | GTP | C4'-C5'-O5'-PA |
| 71 | BM | 501 | GTP | PB-O3B-PG-O1G |
| 71 | HC | 501 | GTP | PB-O3B-PG-O1G |
| 69 | IH | 500 | GDP | C3'-C4'-C5'-O5' |
| 69 | OL | 500 | GDP | O4'-C4'-C5'-O5' |
| 71 | IK | 501 | GTP | PA-O3A-PB-O3B |
| 71 | AE | 501 | GTP | C4'-C5'-O5'-PA |
| 71 | FE | 501 | GTP | C4'-C5'-O5'-PA |
| 71 | KB | 501 | GTP | C4'-C5'-O5'-PA |
| 71 | NM | 501 | GTP | C4'-C5'-O5'-PA |
| 71 | QD | 501 | GTP | C4'-C5'-O5'-PA |
| 71 | WK | 501 | GTP | C4'-C5'-O5'-PA |
| 69 | AH | 500 | GDP | C3'-C4'-C5'-O5' |
| 69 | FD | 500 | GDP | C3'-C4'-C5'-O5' |
| 69 | KM | 500 | GDP | C3'-C4'-C5'-O5' |
| 71 | AA | 501 | GTP | O4'-C4'-C5'-O5' |
| 71 | OK | 501 | GTP | C3'-C4'-C5'-O5' |
| 71 | PG | 501 | GTP | O4'-C4'-C5'-O5' |
| 71 | PK | 501 | GTP | C3'-C4'-C5'-O5' |
| 71 | TC | 501 | GTP | O4'-C4'-C5'-O5' |
| 71 | TI | 501 | GTP | C3'-C4'-C5'-O5' |
| 71 | VM | 501 | GTP | O4'-C4'-C5'-O5' |
| 71 | BI | 501 | GTP | PB-O3A-PA-O1A |
| 71 | EA | 501 | GTP | PG-O3B-PB-O1B |
| 71 | IK | 501 | GTP | PA-O3A-PB-O1B |
| 71 | OK | 501 | GTP | PA-O3A-PB-O1B |
| 71 | OM | 501 | GTP | PG-O3B-PB-O1B |
| 71 | R | 501 | GTP | PG-O3B-PB-O1B |
| 71 | WE | 501 | GTP | PG-O3B-PB-O1B |
| 71 | TK | 501 | GTP | PB-O3A-PA-O5' |
| 71 | CL | 501 | GTP | C4'-C5'-O5'-PA |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 71 | HE | 501 | GTP | C4'-C5'-O5'-PA |
| 71 | HM | 501 | GTP | C4'-C5'-O5'-PA |
| 71 | IA | 501 | GTP | C4'-C5'-O5'-PA |
| 71 | IM | 501 | GTP | C4'-C5'-O5'-PA |
| 71 | L | 501 | GTP | C4'-C5'-O5'-PA |
| 71 | OE | 501 | GTP | C4'-C5'-O5'-PA |
| 71 | R | 501 | GTP | C4'-C5'-O5'-PA |
| 71 | SA | 501 | GTP | C4'-C5'-O5'-PA |
| 71 | VI | 501 | GTP | C4'-C5'-O5'-PA |
| 71 | VK | 501 | GTP | C4'-C5'-O5'-PA |
| 69 | AD | 500 | GDP | C3'-C4'-C5'-O5' |
| 69 | E | 500 | GDP | C3'-C4'-C5'-O5' |
| 69 | HD | 500 | GDP | O4'-C4'-C5'-O5' |
| 69 | JG | 500 | GDP | O4'-C4'-C5'-O5' |
| 69 | LA | 500 | GDP | C3'-C4'-C5'-O5' |
| 69 | LO | 500 | GDP | C3'-C4'-C5'-O5' |
| 69 | MF | 500 | GDP | O4'-C4'-C5'-O5' |
| 71 | BA | 501 | GTP | C3'-C4'-C5'-O5' |
| 71 | C | 501 | GTP | C4'-C5'-O5'-PA |
| 71 | HK | 501 | GTP | C4'-C5'-O5'-PA |
| 71 | LL | 501 | GTP | C4'-C5'-O5'-PA |
| 71 | PK | 501 | GTP | C4'-C5'-O5'-PA |
| 71 | UA | 501 | GTP | C4'-C5'-O5'-PA |
| 71 | WE | 501 | GTP | C4'-C5'-O5'-PA |
| 69 | EL | 500 | GDP | C3'-C4'-C5'-O5' |
| 69 | JC | 500 | GDP | C3'-C4'-C5'-O5' |
| 69 | KI | 500 | GDP | O4'-C4'-C5'-O5' |
| 69 | MN | 500 | GDP | C3'-C4'-C5'-O5' |
| 69 | NF | 500 | GDP | O4'-C4'-C5'-O5' |
| 71 | JD | 501 | GTP | O4'-C4'-C5'-O5' |
| 71 | EA | 501 | GTP | PB-O3B-PG-O1G |
| 71 | SG | 501 | GTP | PB-O3B-PG-O1G |
| 69 | E | 500 | GDP | PA-O3A-PB-O2B |
| 71 | BM | 501 | GTP | PB-O3B-PG-O2G |
| 71 | BM | 501 | GTP | PB-O3B-PG-O3G |
| 71 | C | 501 | GTP | PB-O3B-PG-O2G |
| 71 | CH | 501 | GTP | PB-O3B-PG-O2G |
| 71 | DJ | 501 | GTP | PB-O3B-PG-O2G |
| 71 | DL | 501 | GTP | PB-O3B-PG-O2G |
| 71 | EA | 501 | GTP | PB-O3B-PG-O2G |
| 71 | HC | 501 | GTP | PB-O3B-PG-O2G |
| 71 | HC | 501 | GTP | PB-O3B-PG-O3G |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 71 | KF | 501 | GTP | PB-O3B-PG-O2G |
| 71 | KF | 501 | GTP | PB-O3B-PG-O3G |
| 71 | KH | 501 | GTP | PB-O3B-PG-O2G |
| 71 | QD | 501 | GTP | PB-O3B-PG-O2G |
| 71 | TA | 501 | GTP | PB-O3B-PG-O2G |
| 71 | TA | 501 | GTP | PB-O3B-PG-O3G |
| 71 | VC | 501 | GTP | PB-O3B-PG-O2G |
| 71 | VC | 501 | GTP | PB-O3B-PG-O3G |
| 71 | EC | 501 | GTP | C4'-C5'-O5'-PA |
| 71 | KH | 501 | GTP | C4'-C5'-O5'-PA |
| 71 | MI | 501 | GTP | C4'-C5'-O5'-PA |
| 71 | QJ | 501 | GTP | C4'-C5'-O5'-PA |
| 69 | MB | 500 | GDP | C3'-C4'-C5'-O5' |
| 69 | QE | 500 | GDP | C3'-C4'-C5'-O5' |
| 69 | RK | 500 | GDP | C3'-C4'-C5'-O5' |
| 71 | LD | 501 | GTP | O4'-C4'-C5'-O5' |
| 69 | A | 500 | GDP | C3'-C4'-C5'-O5' |
| 69 | AL | 500 | GDP | C3'-C4'-C5'-O5' |
| 69 | FF | 500 | GDP | C3'-C4'-C5'-O5' |
| 69 | GL | 500 | GDP | O4'-C4'-C5'-O5' |
| 69 | OD | 500 | GDP | C3'-C4'-C5'-O5' |
| 71 | FG | 501 | GTP | C3'-C4'-C5'-O5' |
| 71 | MK | 501 | GTP | C3'-C4'-C5'-O5' |
| 71 | NK | 501 | GTP | C3'-C4'-C5'-O5' |
| 71 | OC | 501 | GTP | C3'-C4'-C5'-O5' |
| 71 | WK | 501 | GTP | C3'-C4'-C5'-O5' |
| 71 | AG | 501 | GTP | PA-O3A-PB-O2B |
| 71 | EG | 501 | GTP | PB-O3A-PA-O2A |
| 71 | FG | 501 | GTP | PB-O3A-PA-O2A |
| 71 | GA | 501 | GTP | PA-O3A-PB-O1B |
| 71 | IG | 501 | GTP | PA-O3A-PB-O2B |
| 71 | II | 501 | GTP | PB-O3A-PA-O2A |
| 71 | J | 501 | GTP | PA-O3A-PB-O1B |
| 71 | NG | 501 | GTP | PB-O3A-PA-O2A |
| 71 | NI | 501 | GTP | PB-O3A-PA-O2A |
| 71 | TG | 501 | GTP | PB-O3A-PA-O2A |
| 71 | VG | 501 | GTP | PB-O3A-PA-O2A |
| 71 | WG | 501 | GTP | PG-O3B-PB-O2B |
| 71 | J | 501 | GTP | C3'-C4'-C5'-O5' |
| 71 | D | 501 | GTP | PB-O3B-PG-O1G |
| 69 | FL | 500 | GDP | O4'-C4'-C5'-O5' |
| 69 | HB | 500 | GDP | O4'-C4'-C5'-O5' |

Continued on next page...

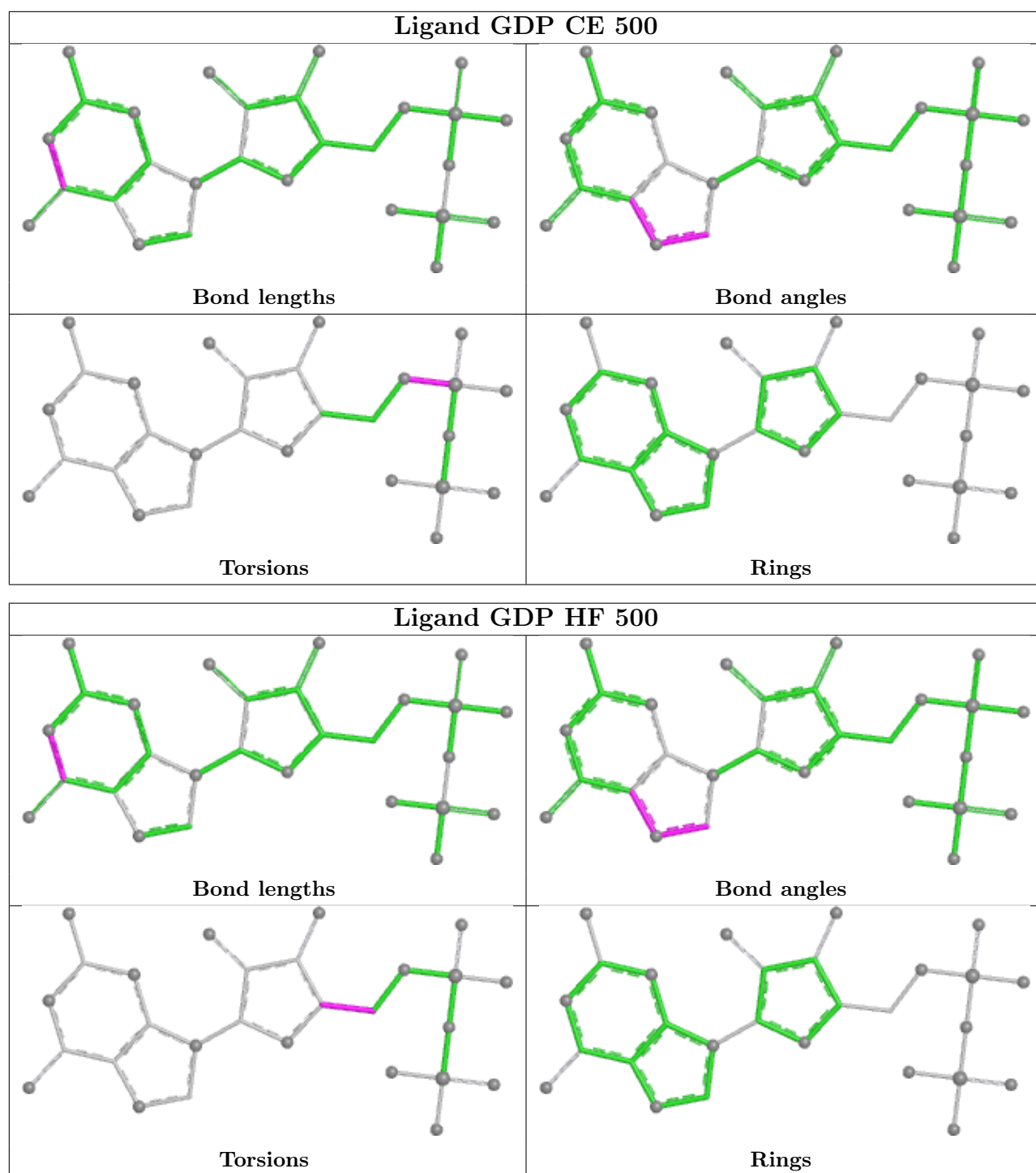
Continued from previous page...

| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-----------------|
| 69 | HF | 500 | GDP | O4'-C4'-C5'-O5' |
| 69 | LM | 500 | GDP | C3'-C4'-C5'-O5' |
| 69 | SB | 500 | GDP | O4'-C4'-C5'-O5' |
| 71 | CL | 501 | GTP | O4'-C4'-C5'-O5' |
| 71 | D | 501 | GTP | O4'-C4'-C5'-O5' |
| 71 | MC | 501 | GTP | C3'-C4'-C5'-O5' |
| 71 | RL | 501 | GTP | O4'-C4'-C5'-O5' |
| 69 | OB | 500 | GDP | C3'-C4'-C5'-O5' |
| 71 | BI | 501 | GTP | PB-O3A-PA-O2A |
| 71 | D | 501 | GTP | PG-O3B-PB-O2B |
| 71 | EG | 501 | GTP | PA-O3A-PB-O2B |
| 71 | GA | 501 | GTP | PA-O3A-PB-O2B |
| 71 | GE | 501 | GTP | PB-O3A-PA-O1A |
| 71 | J | 501 | GTP | PG-O3B-PB-O1B |
| 71 | LH | 501 | GTP | PB-O3A-PA-O2A |
| 71 | MG | 501 | GTP | PG-O3B-PB-O2B |
| 71 | UE | 501 | GTP | PA-O3A-PB-O2B |
| 74 | 2w | 501 | ATP | PA-O3A-PB-O2B |
| 69 | BL | 500 | GDP | O4'-C4'-C5'-O5' |
| 69 | DM | 500 | GDP | C3'-C4'-C5'-O5' |
| 69 | FJ | 500 | GDP | C3'-C4'-C5'-O5' |
| 69 | KA | 500 | GDP | O4'-C4'-C5'-O5' |
| 69 | LG | 500 | GDP | C3'-C4'-C5'-O5' |
| 69 | NH | 500 | GDP | C3'-C4'-C5'-O5' |
| 69 | P | 500 | GDP | C3'-C4'-C5'-O5' |

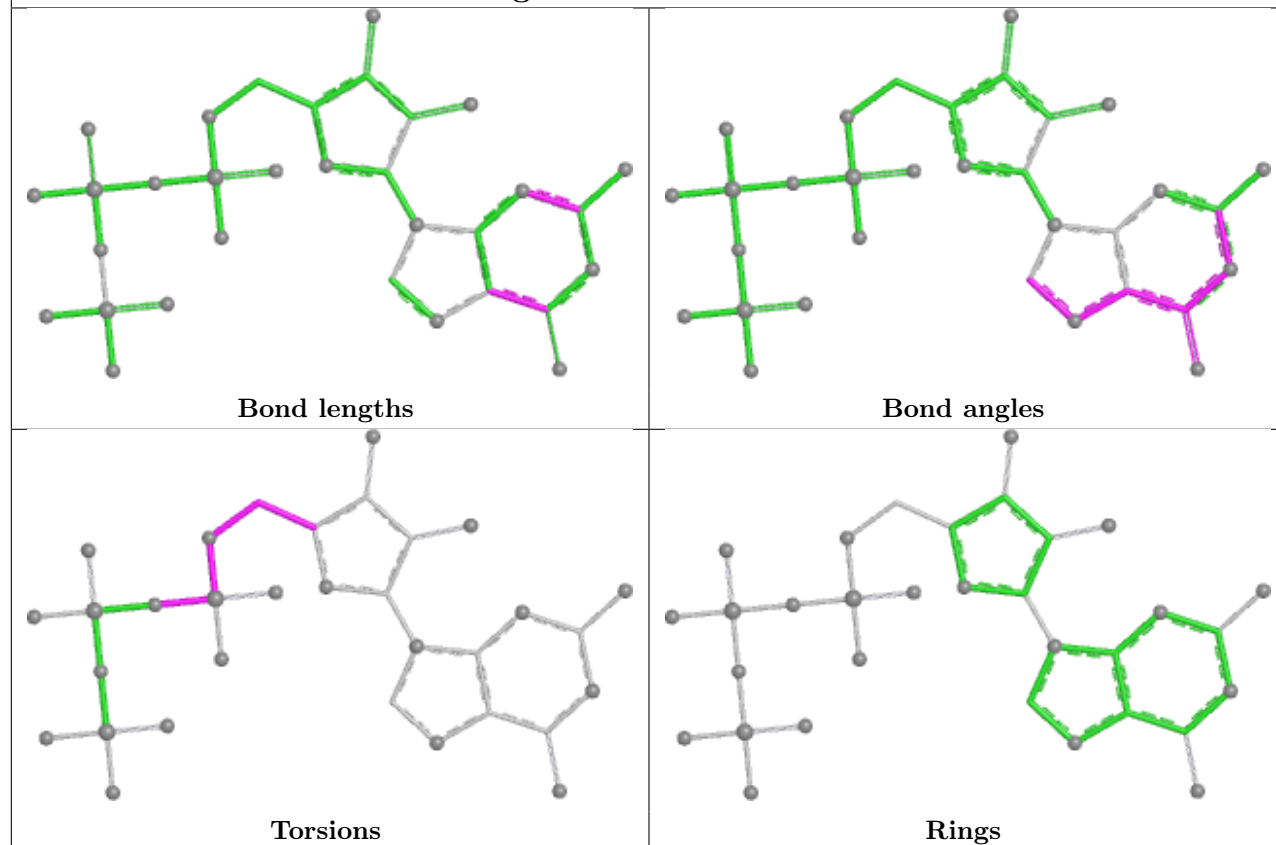
There are no ring outliers.

No monomer is involved in short contacts.

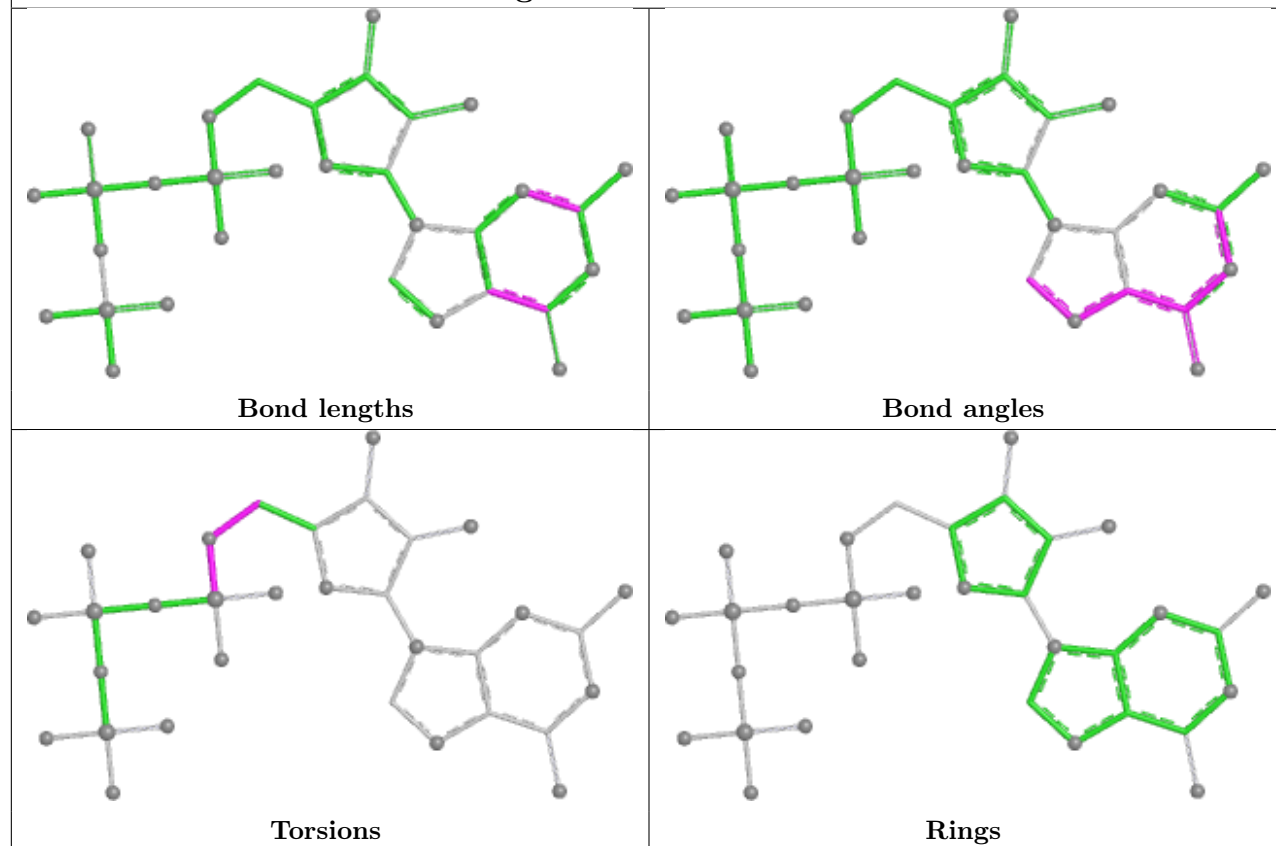
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

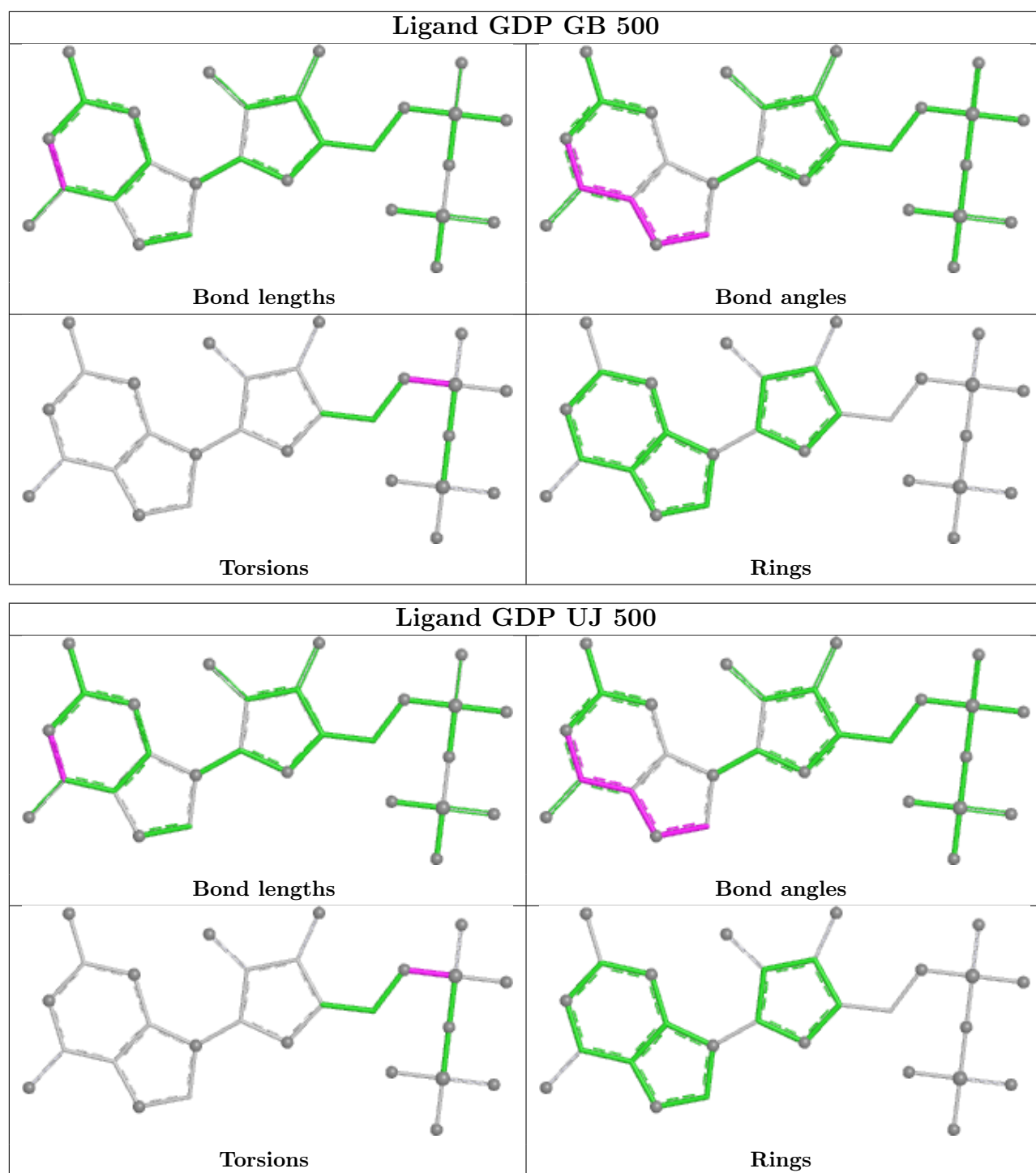


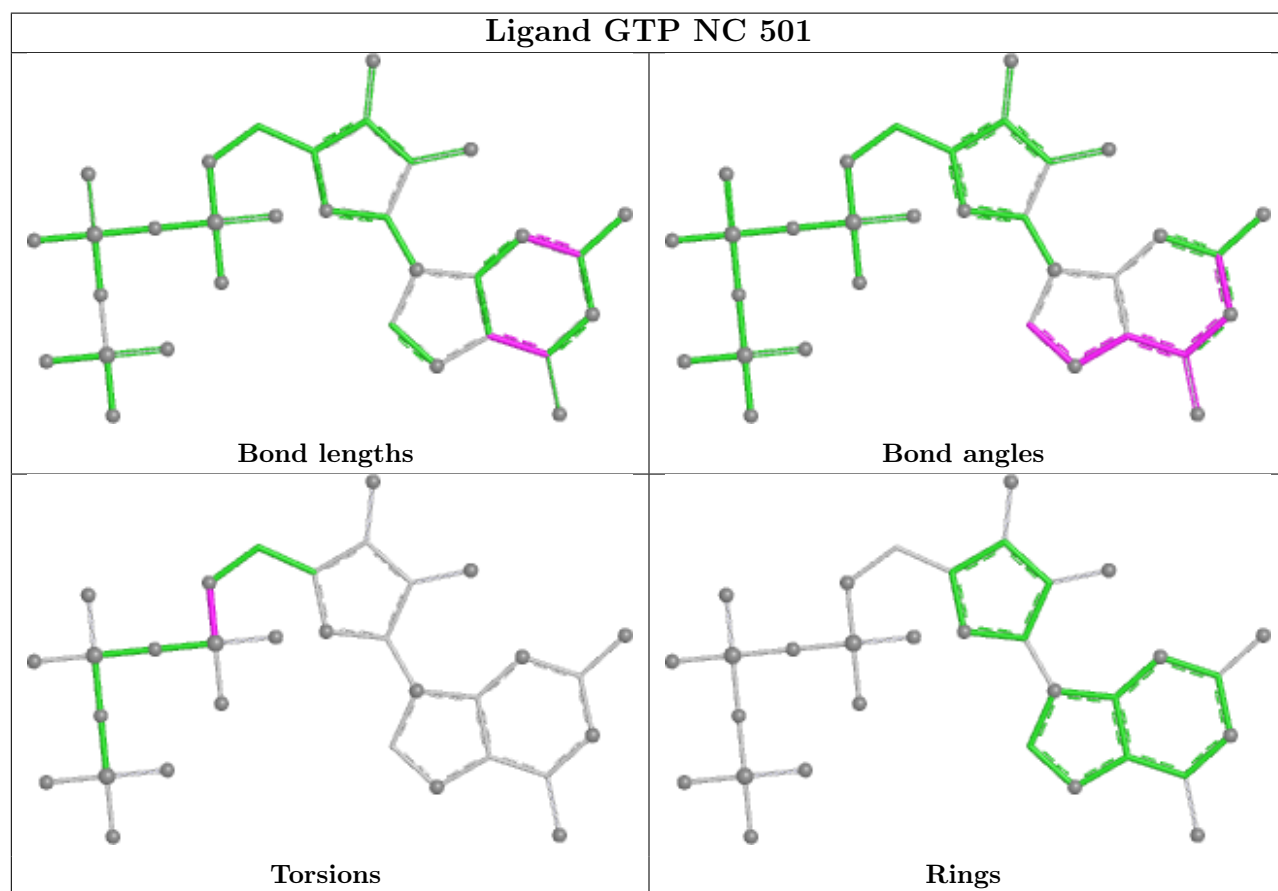
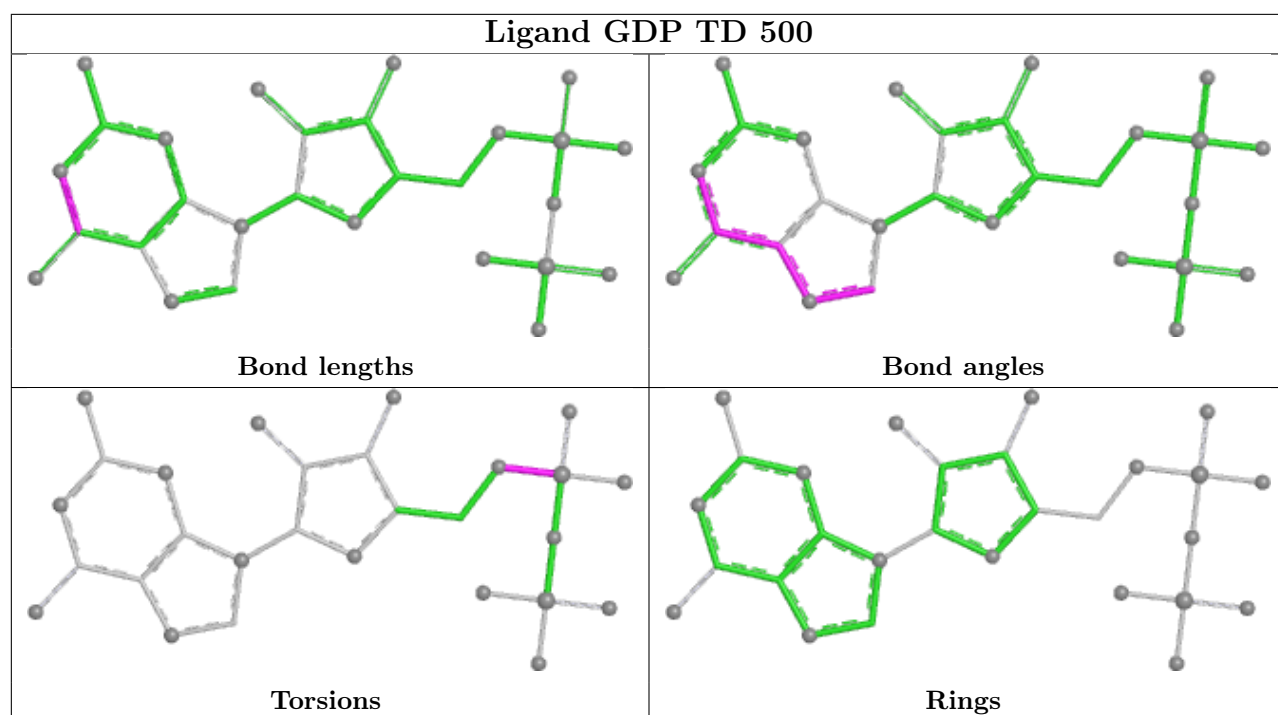
Ligand GTP MK 501

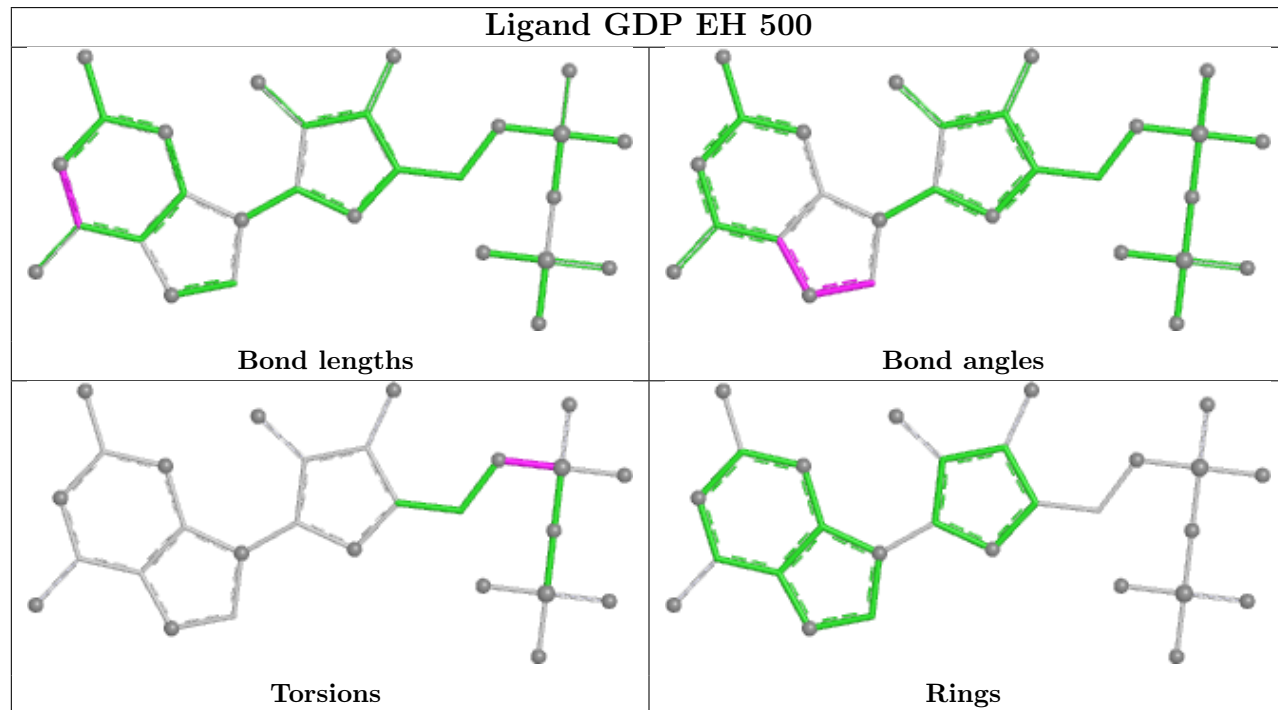
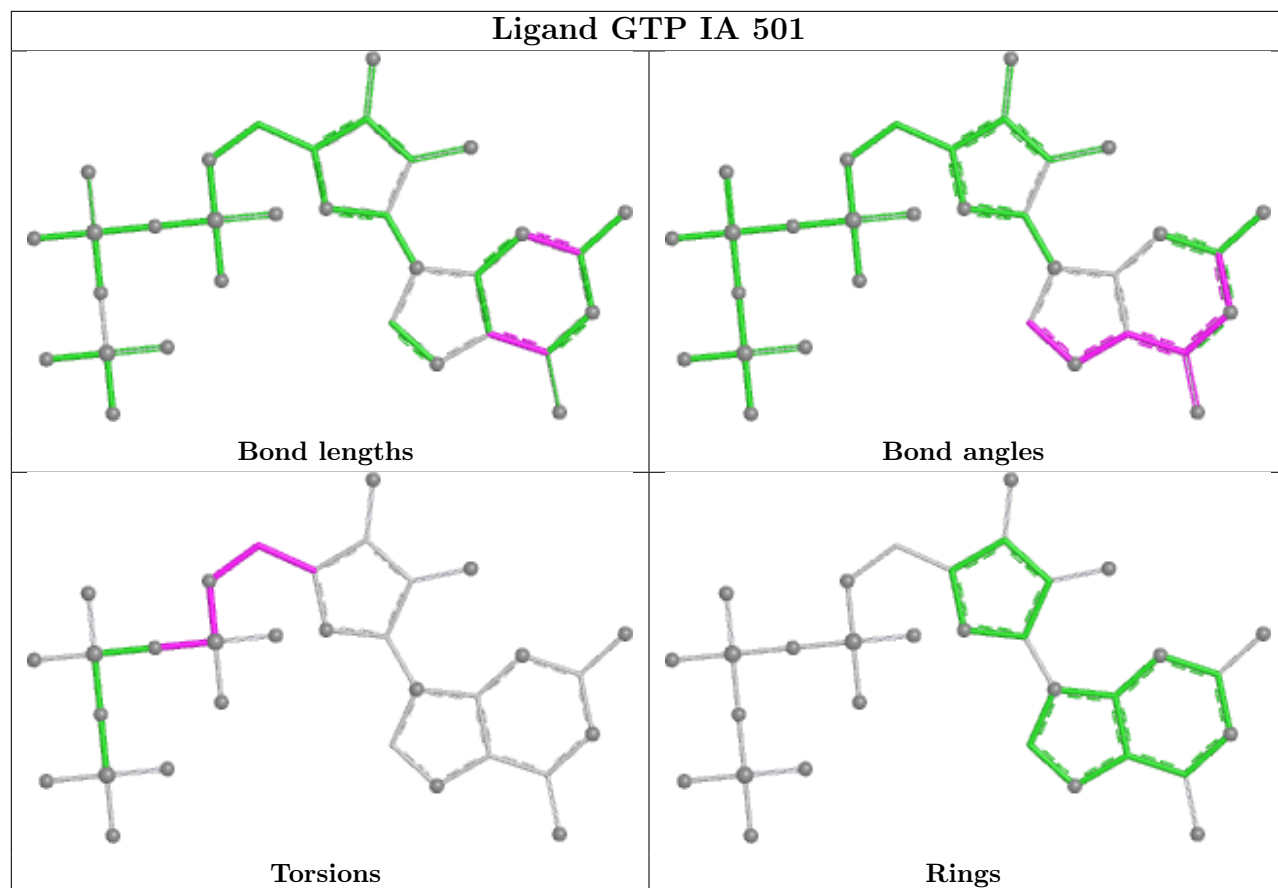


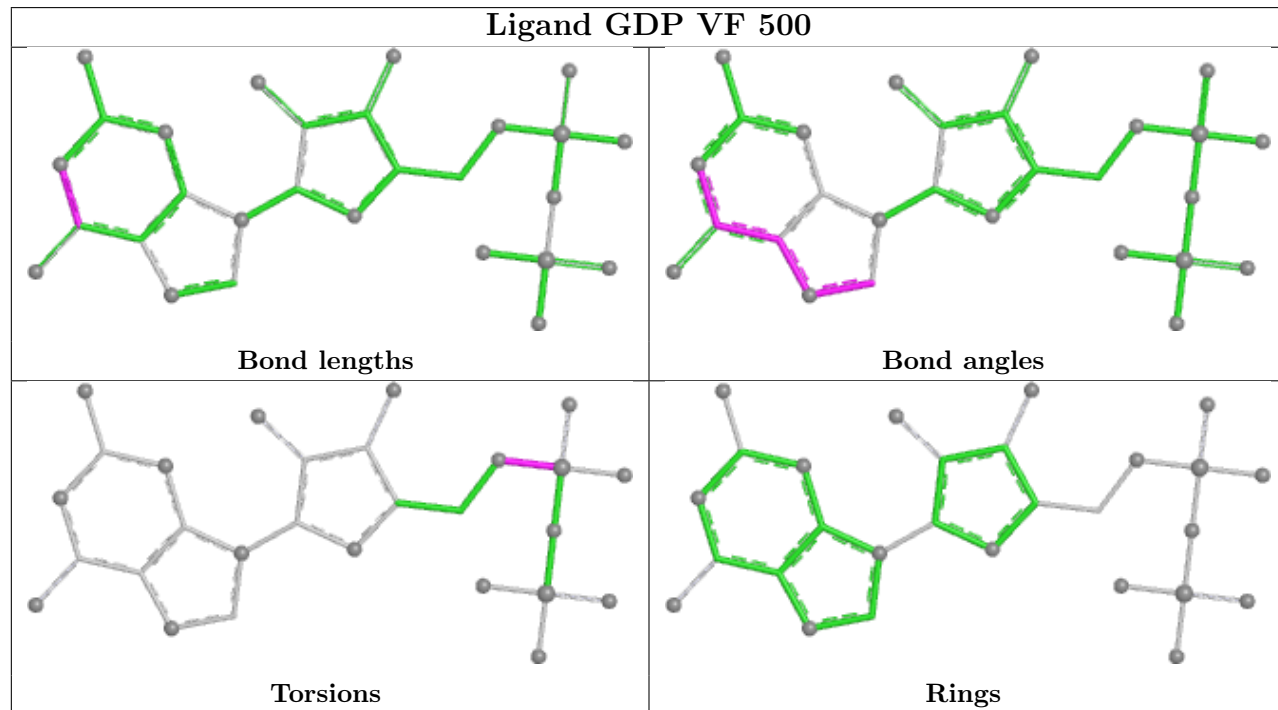
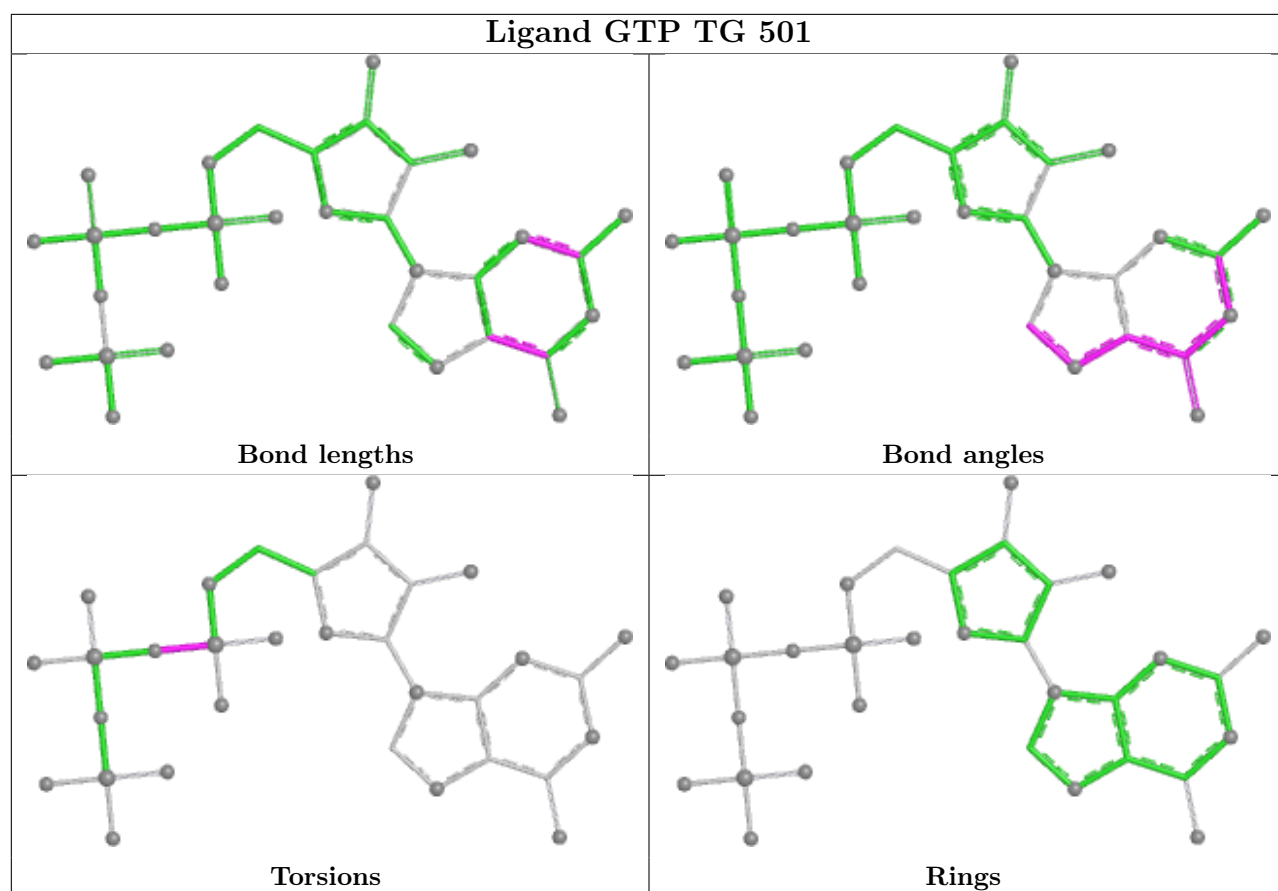
Ligand GTP HK 501

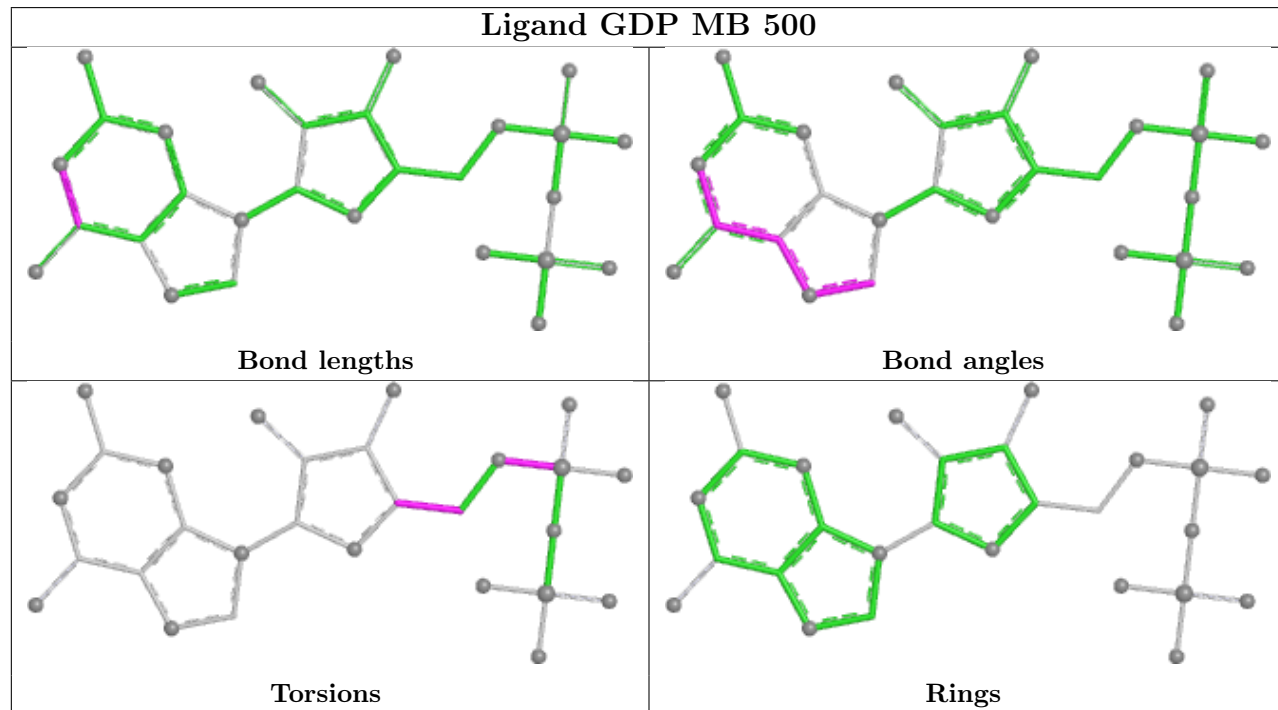
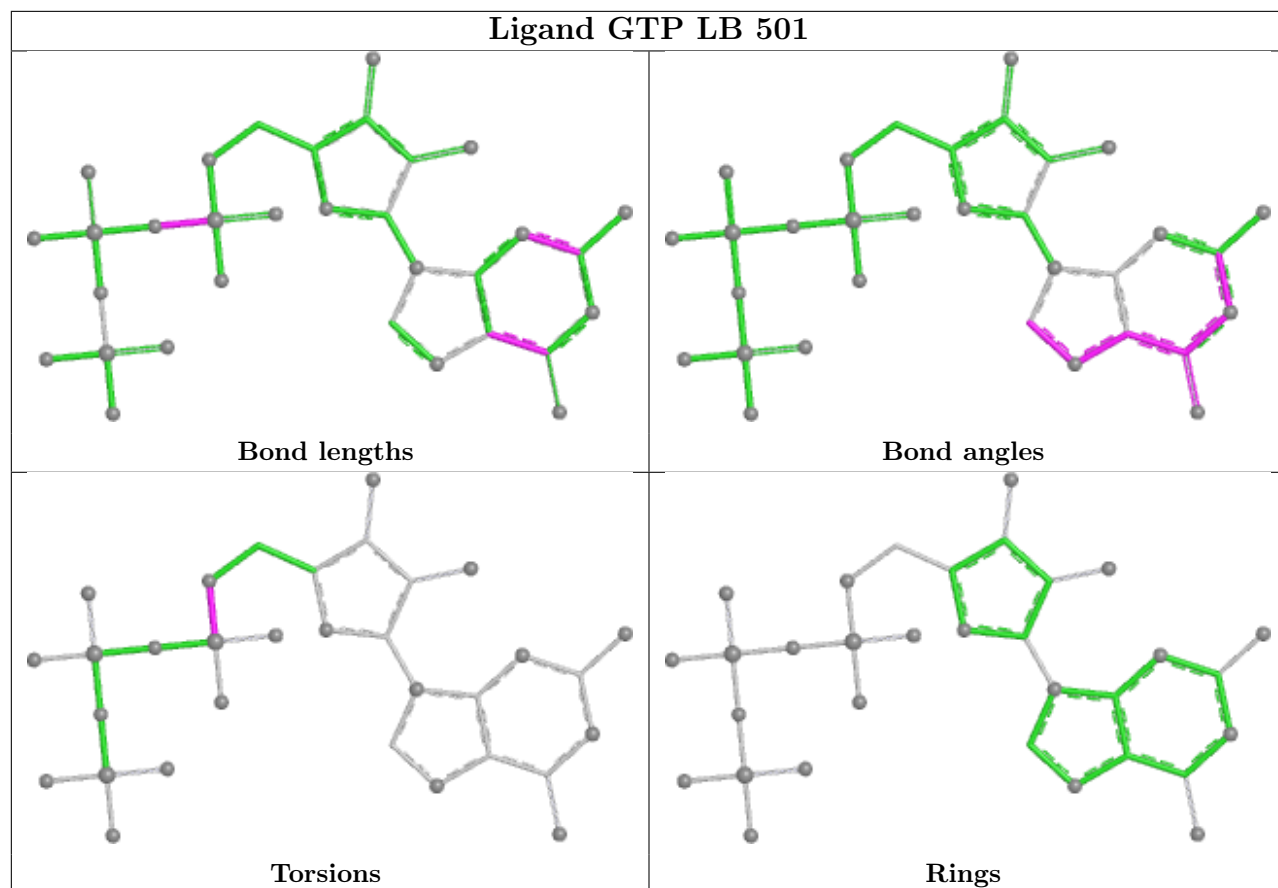




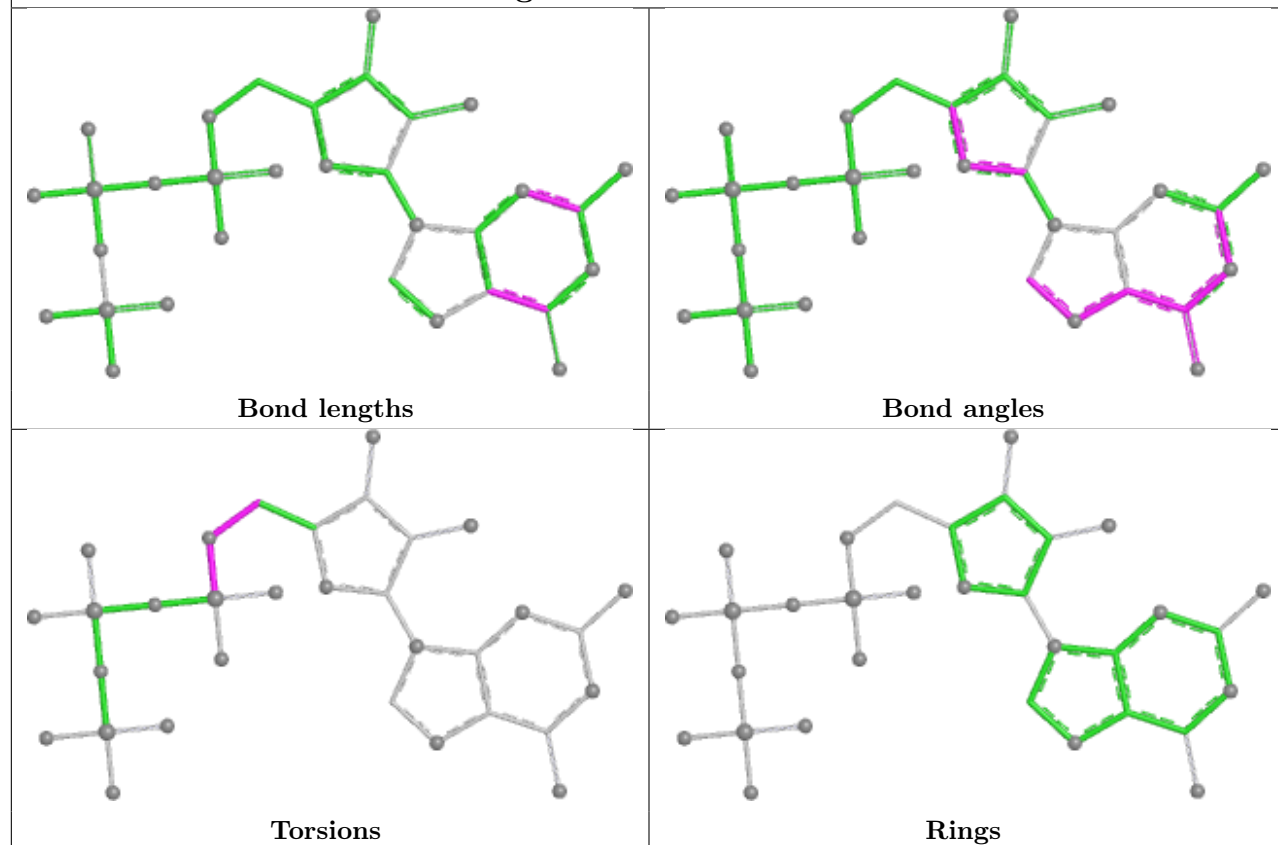




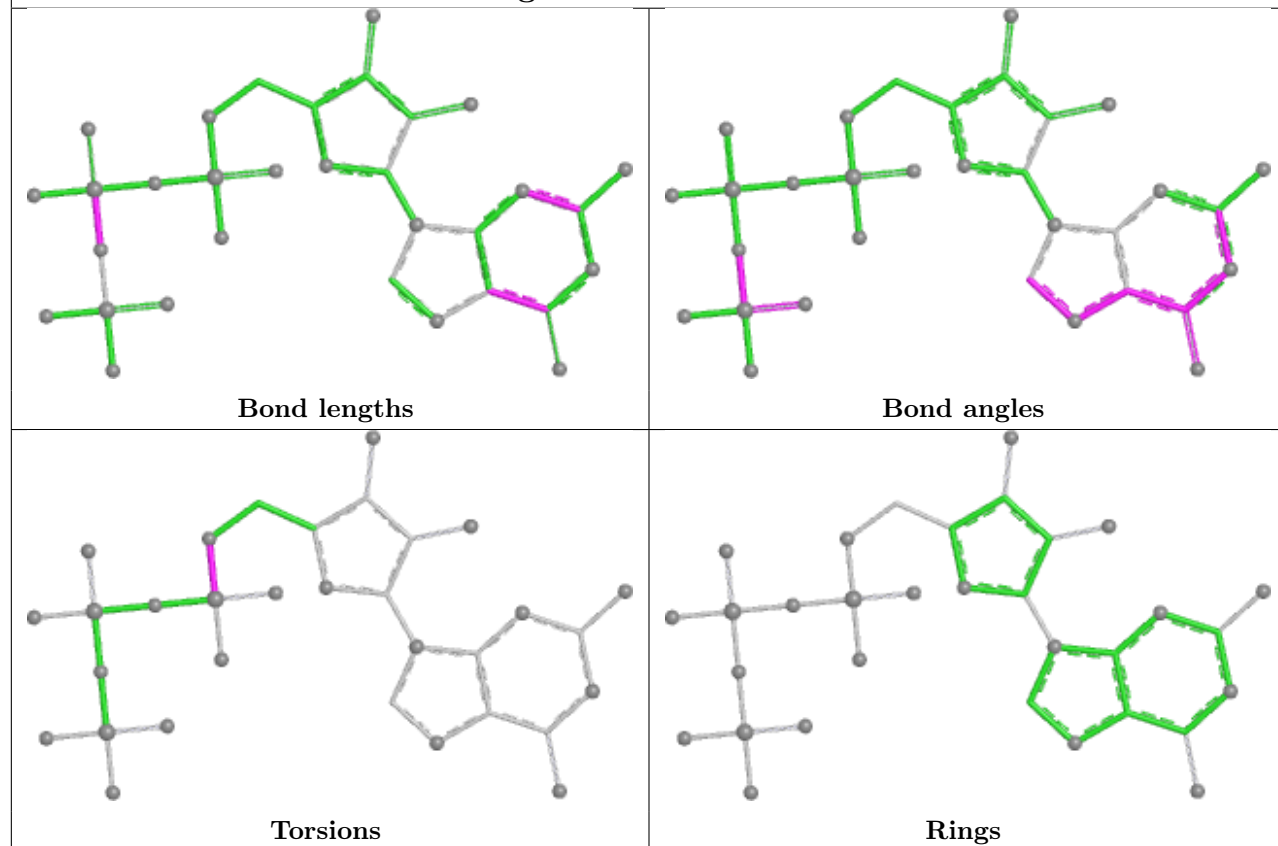


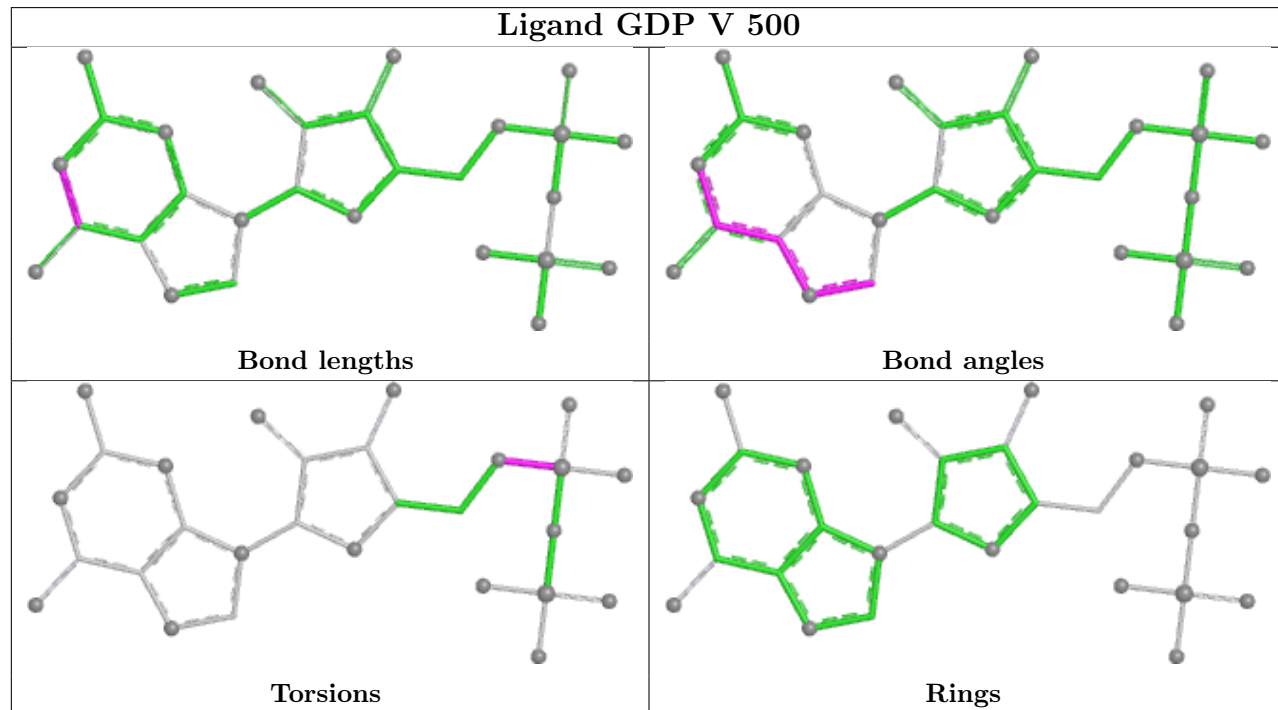
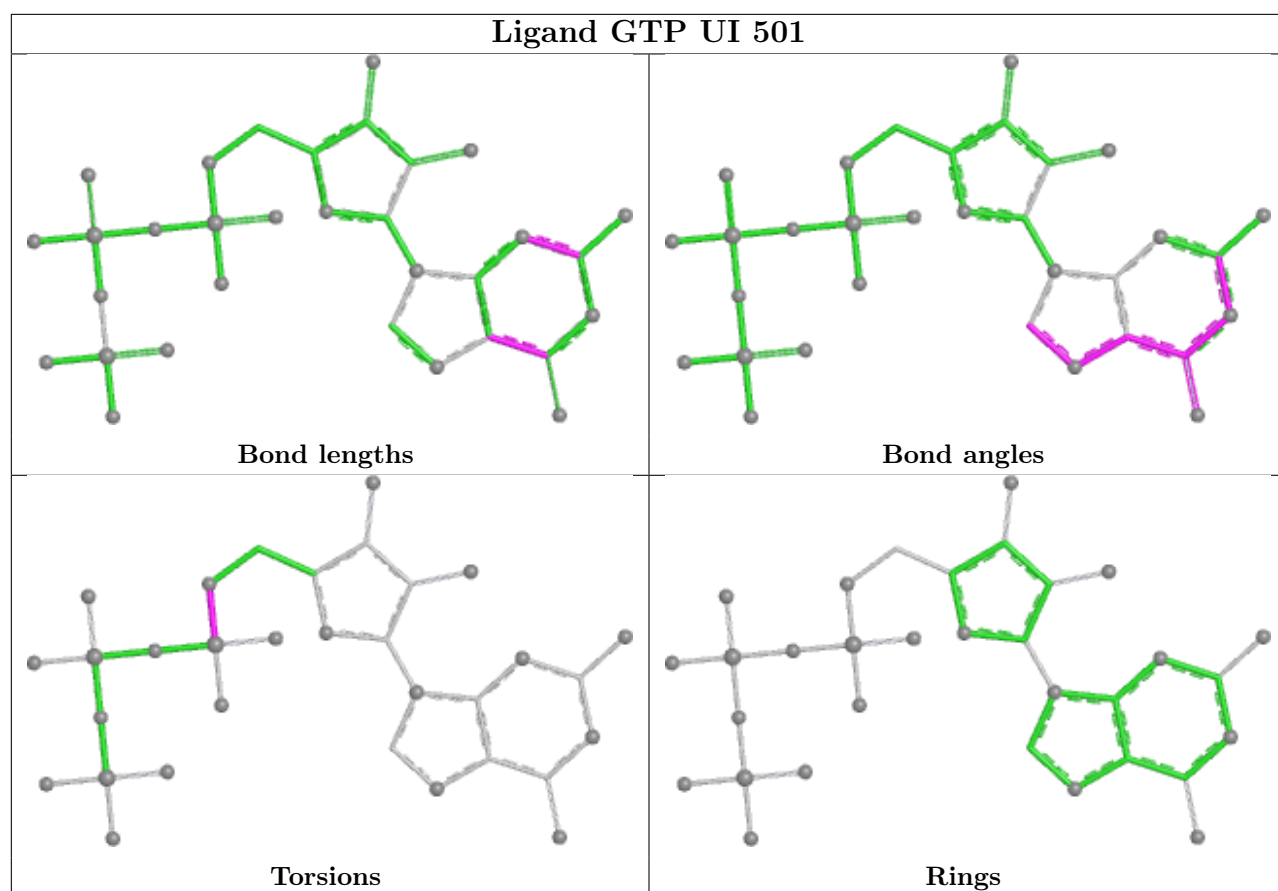


Ligand GTP HG 501

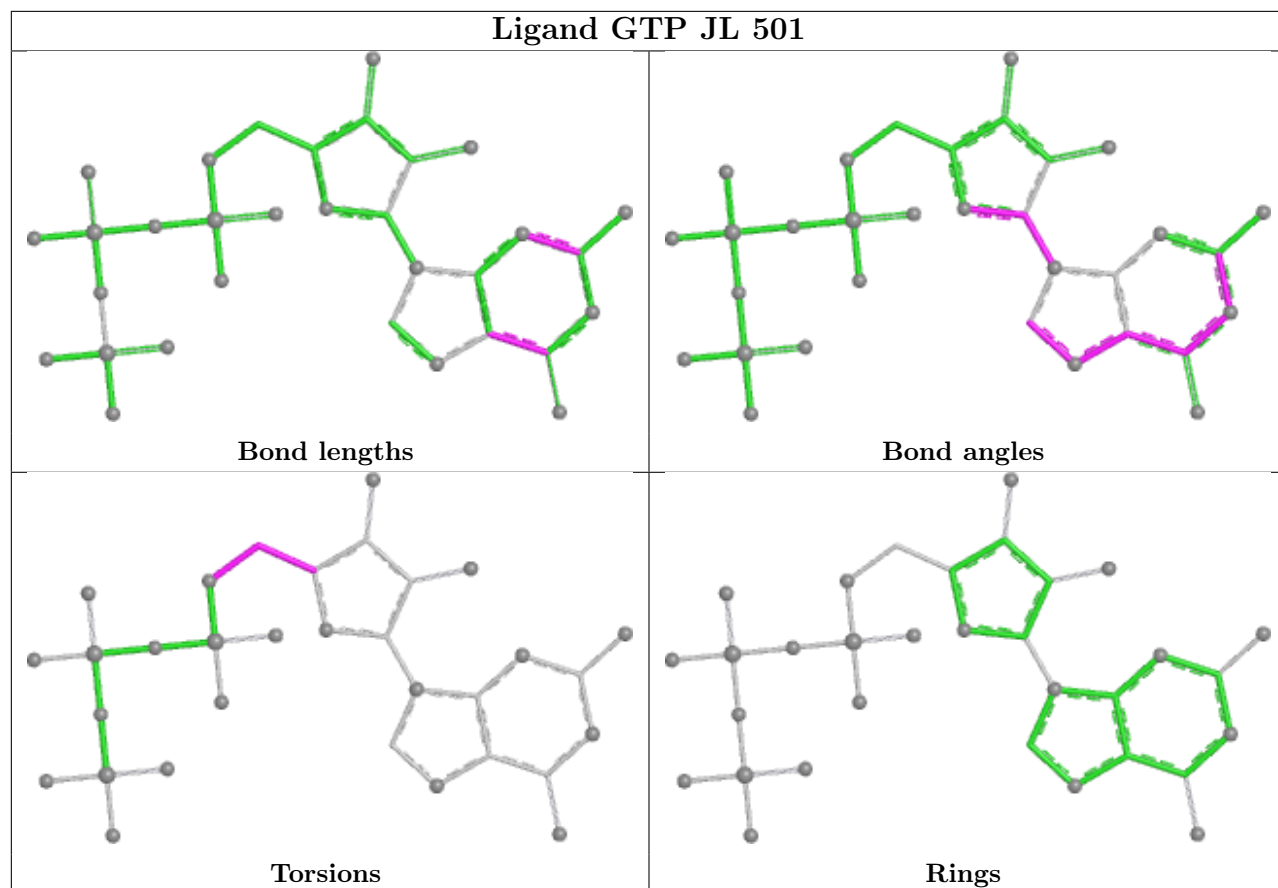


Ligand GTP EK 501

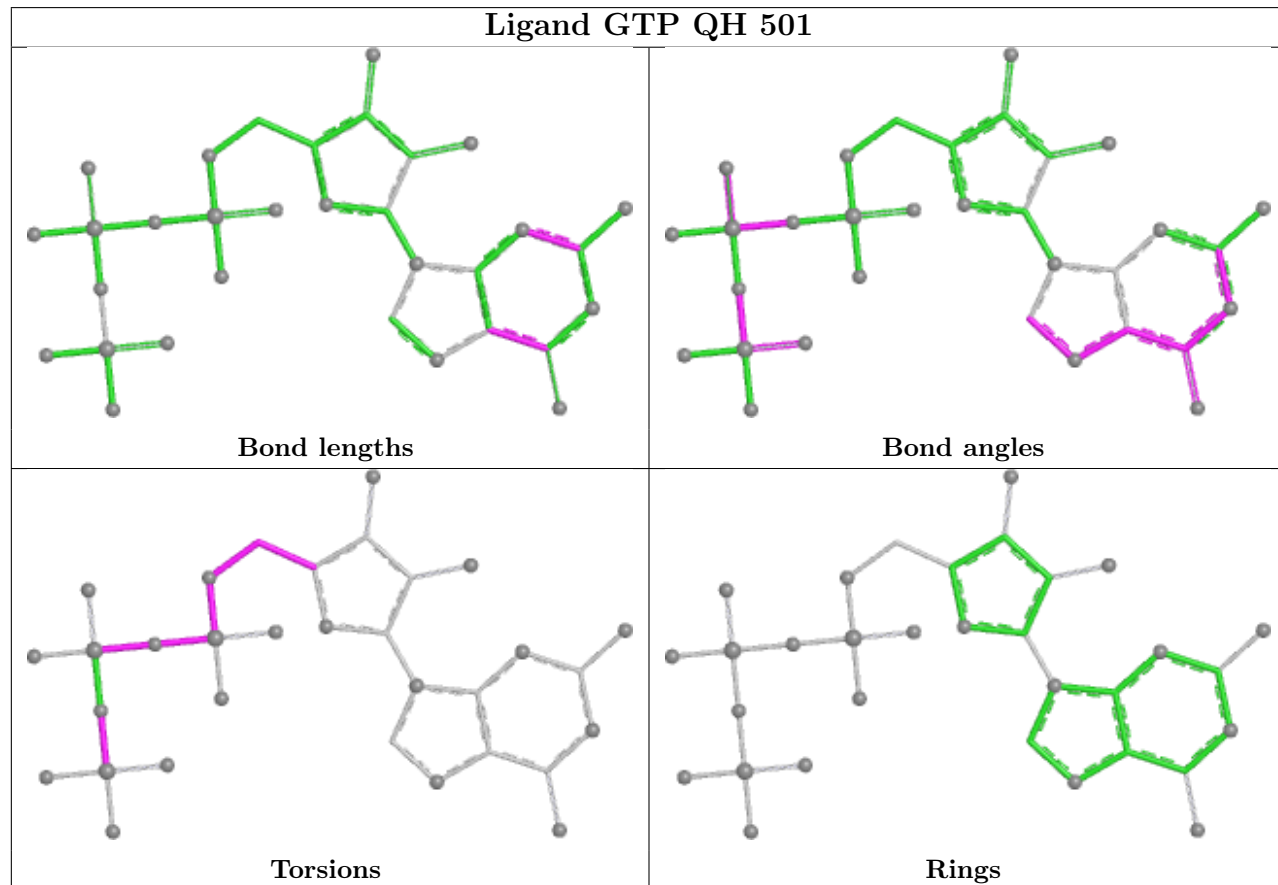


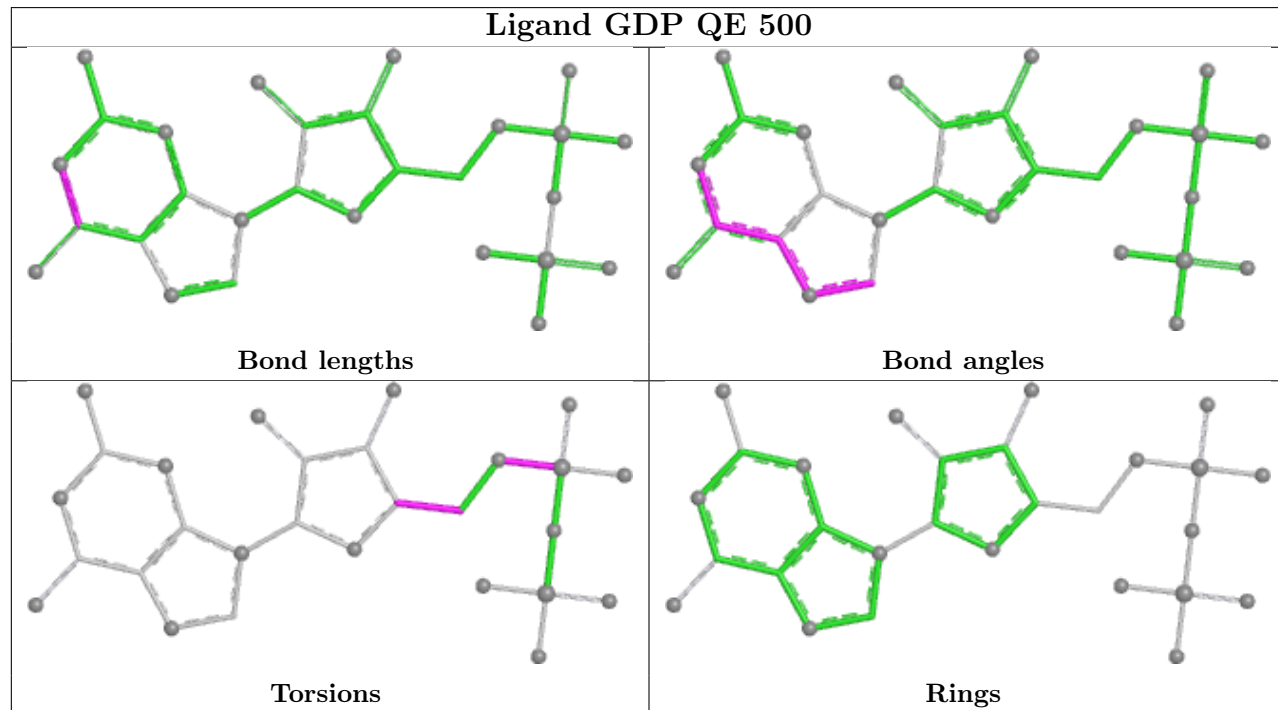
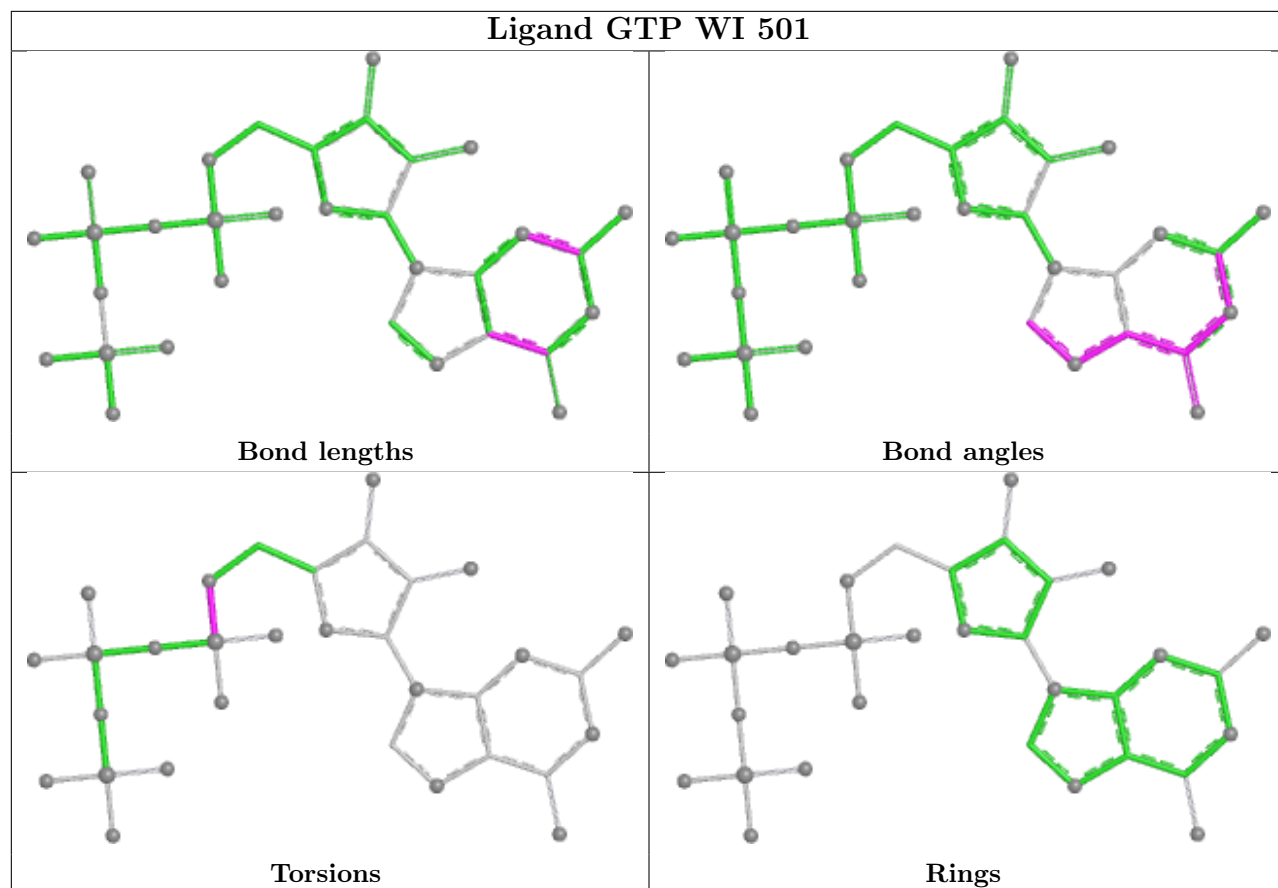


Ligand GTP JL 501

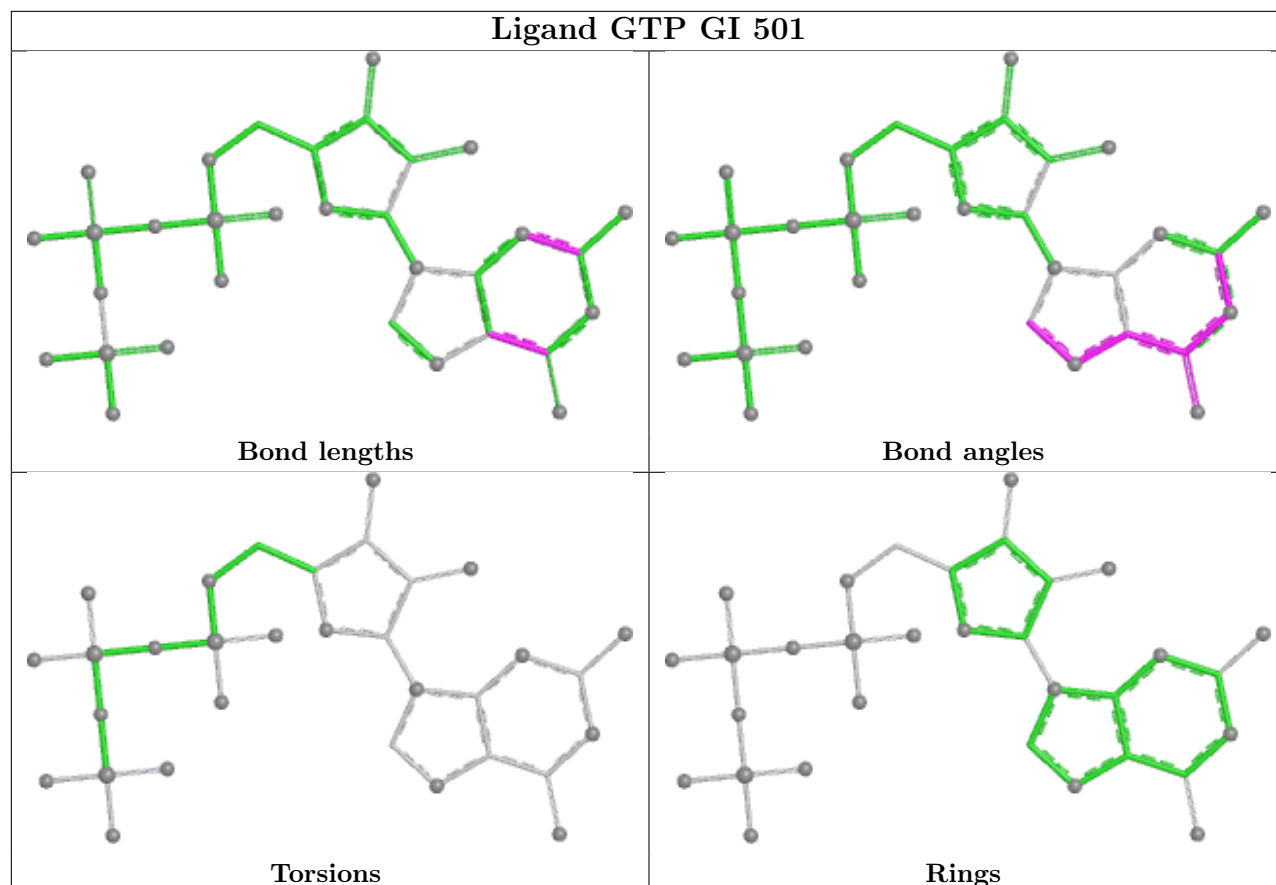


Ligand GTP QH 501

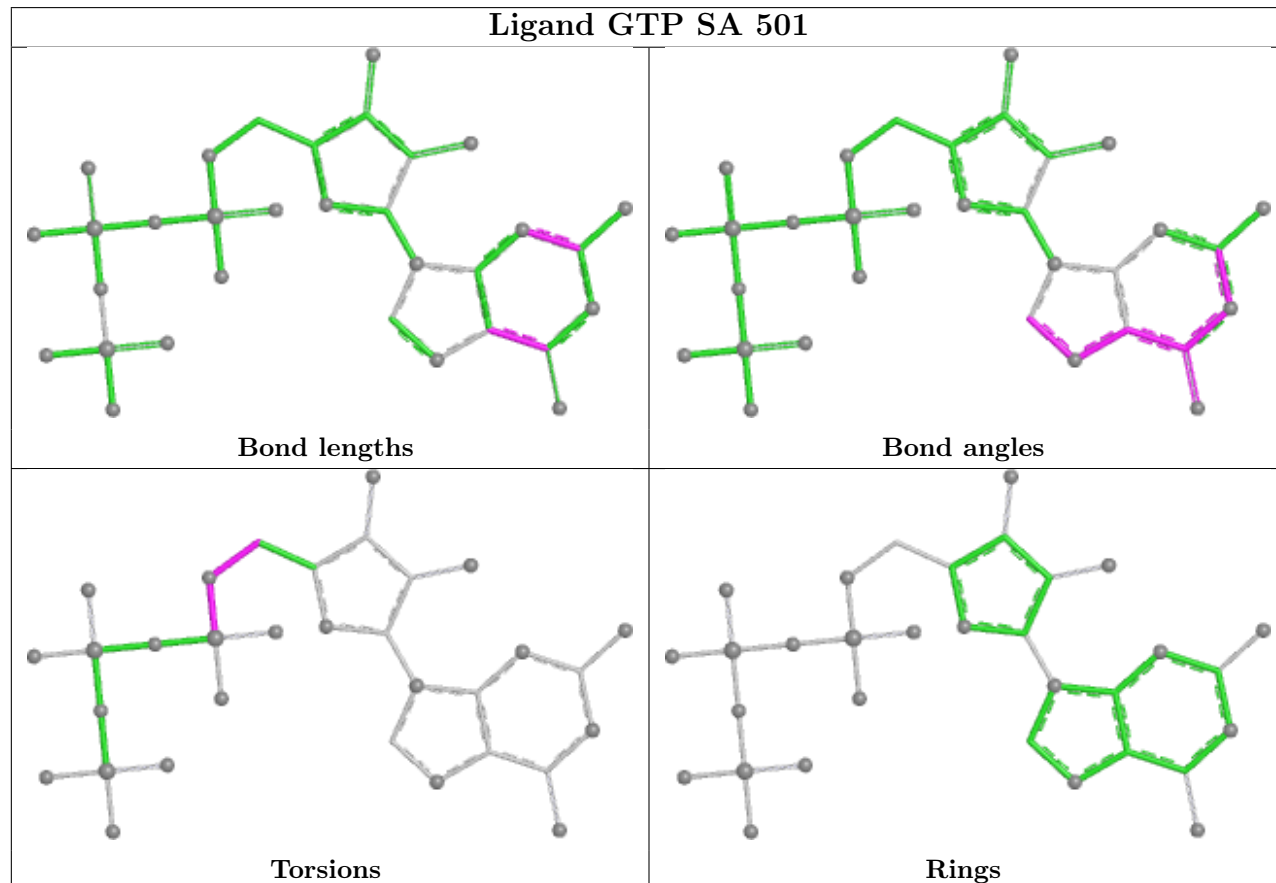


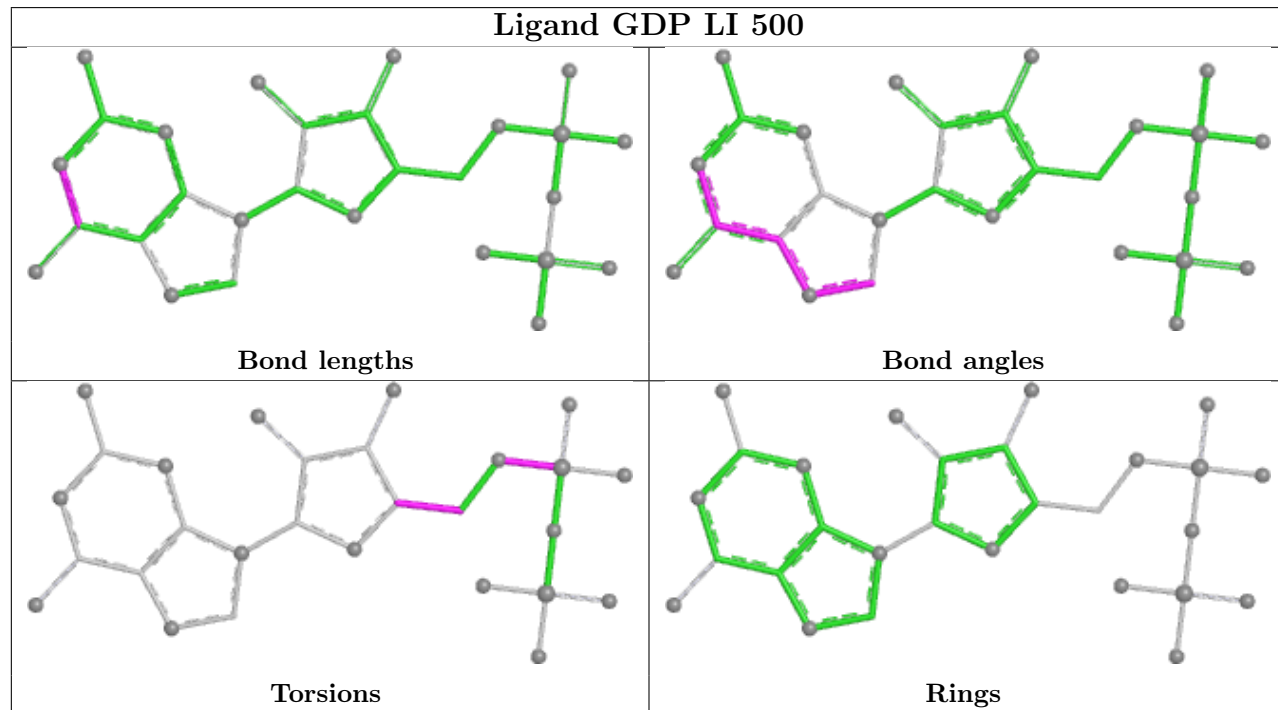
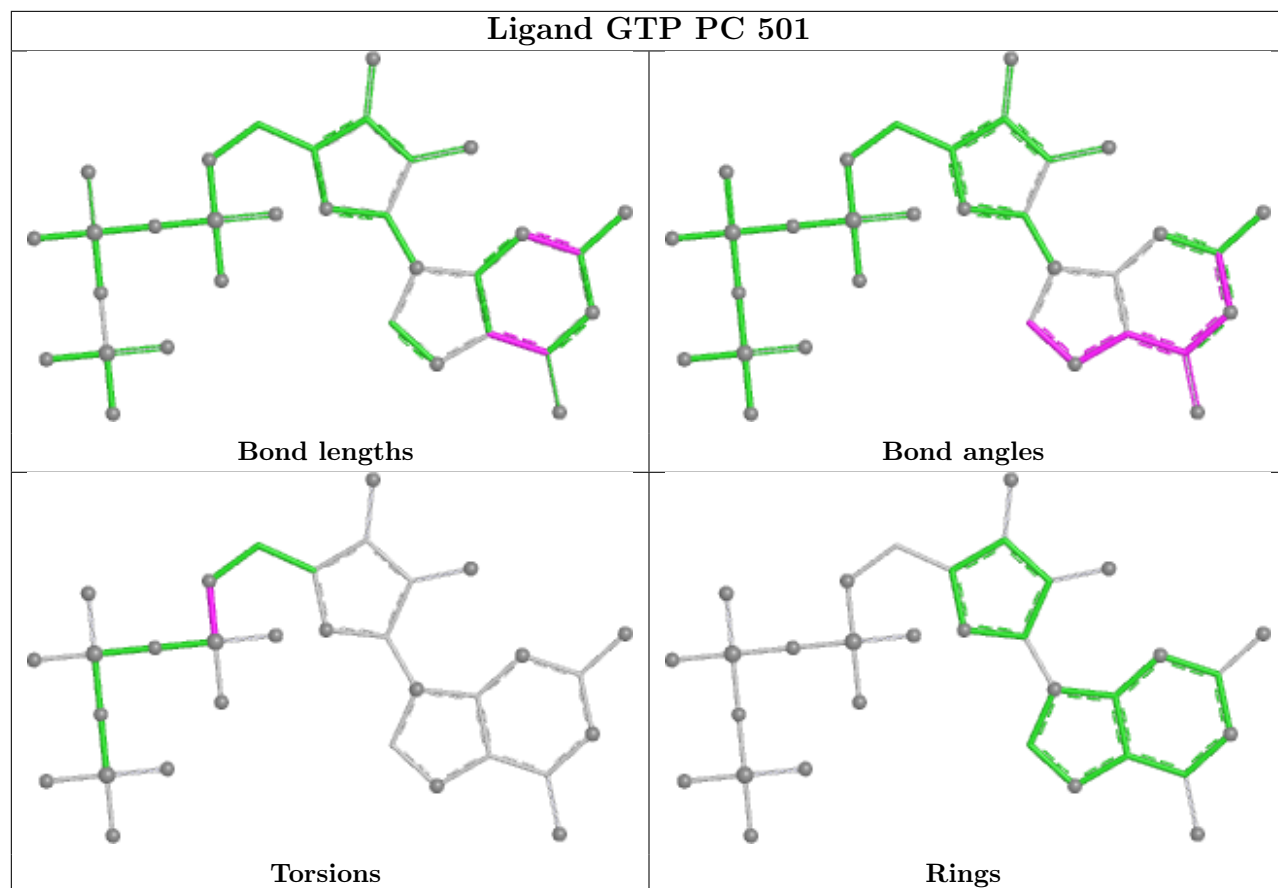


Ligand GTP GI 501

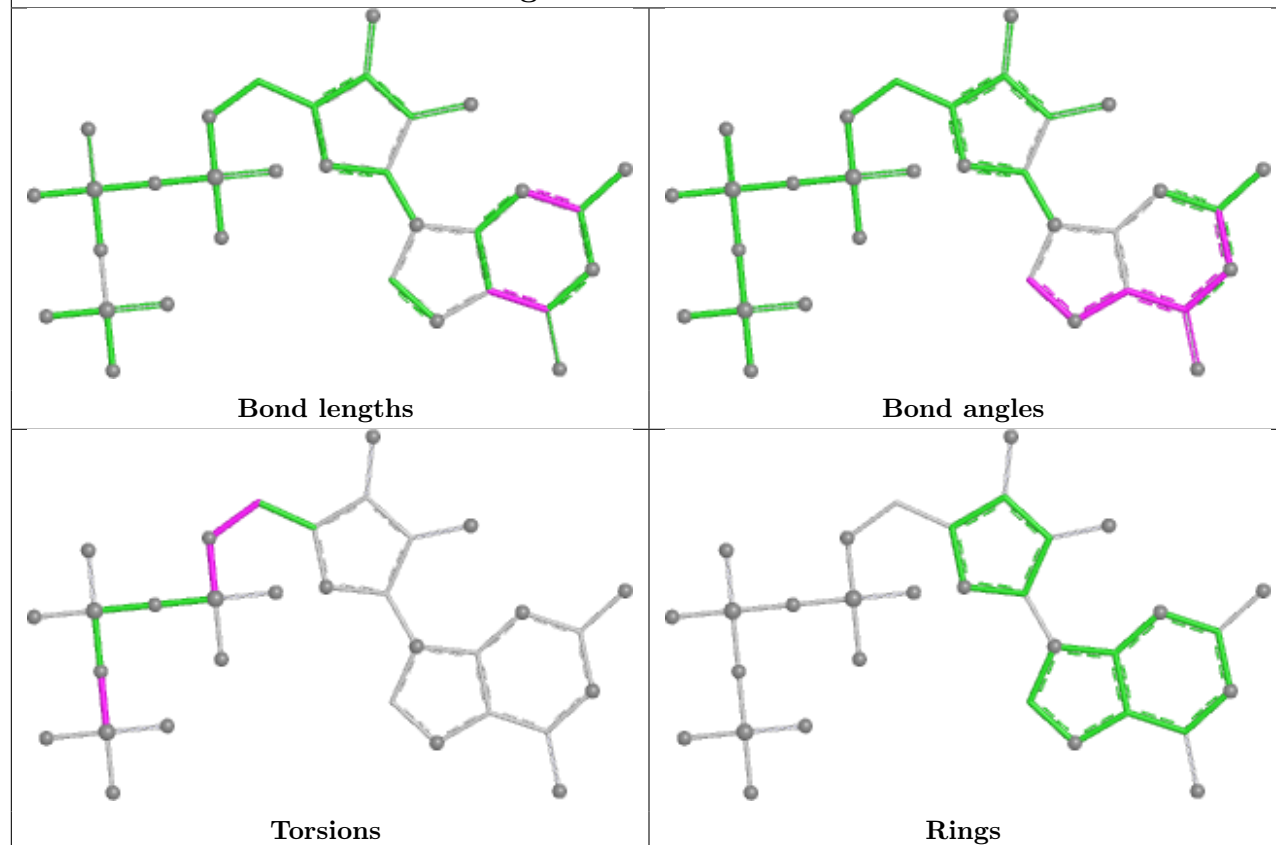


Ligand GTP SA 501

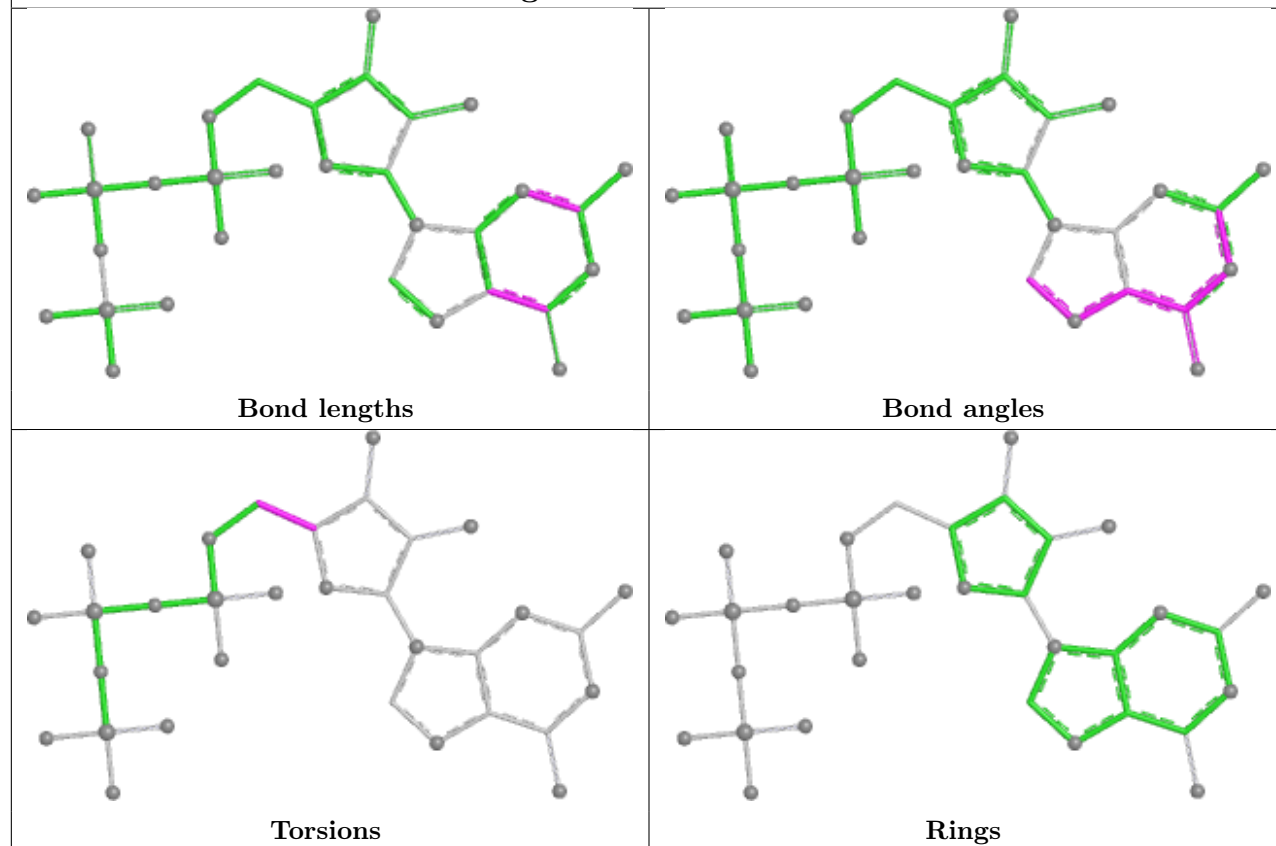


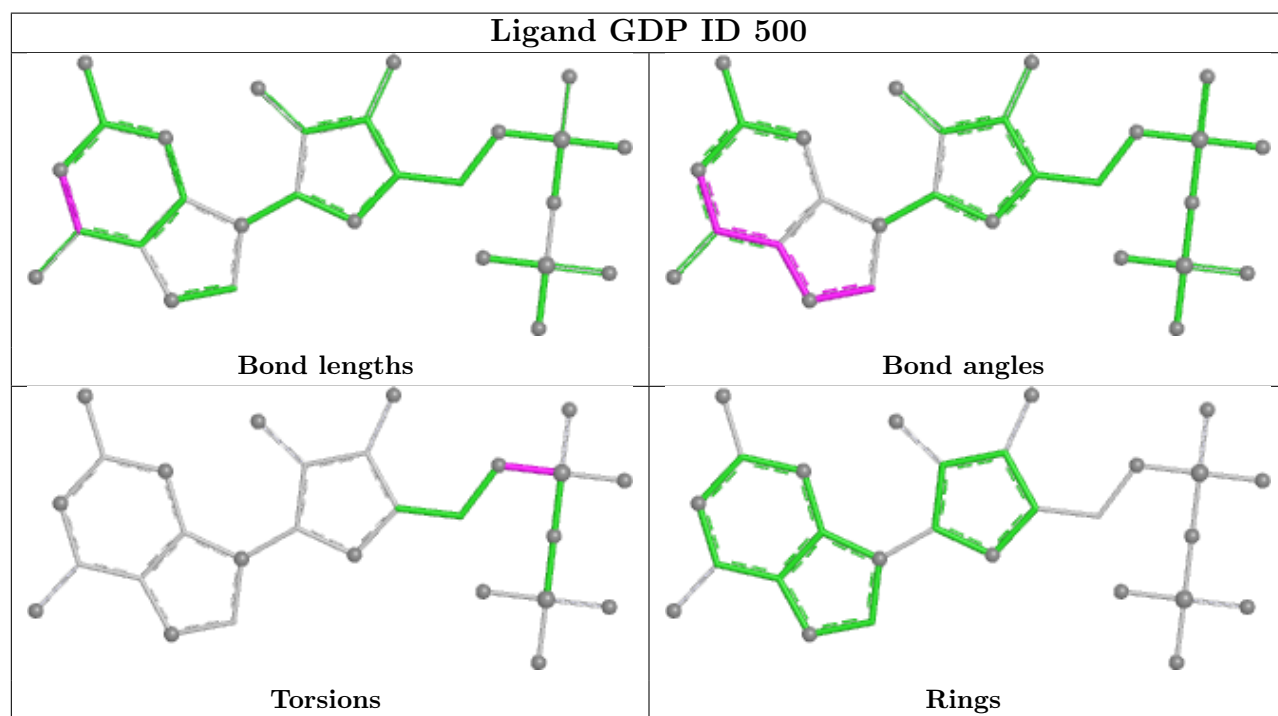
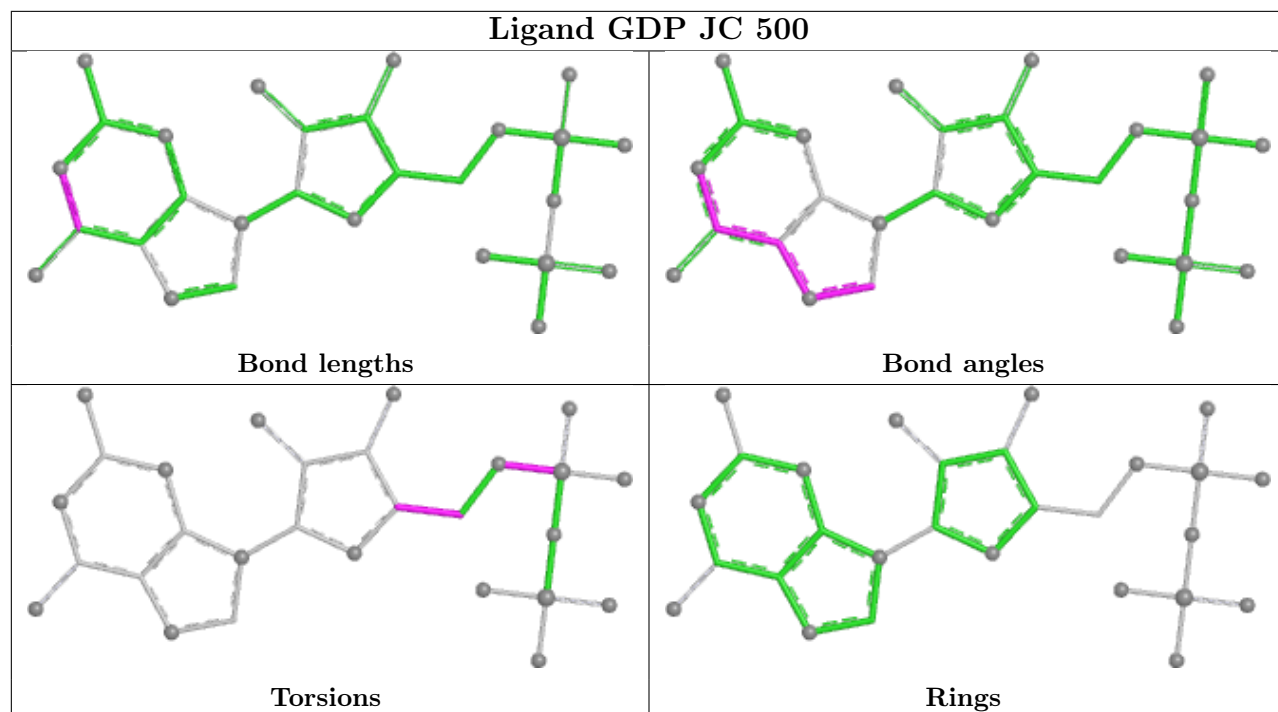


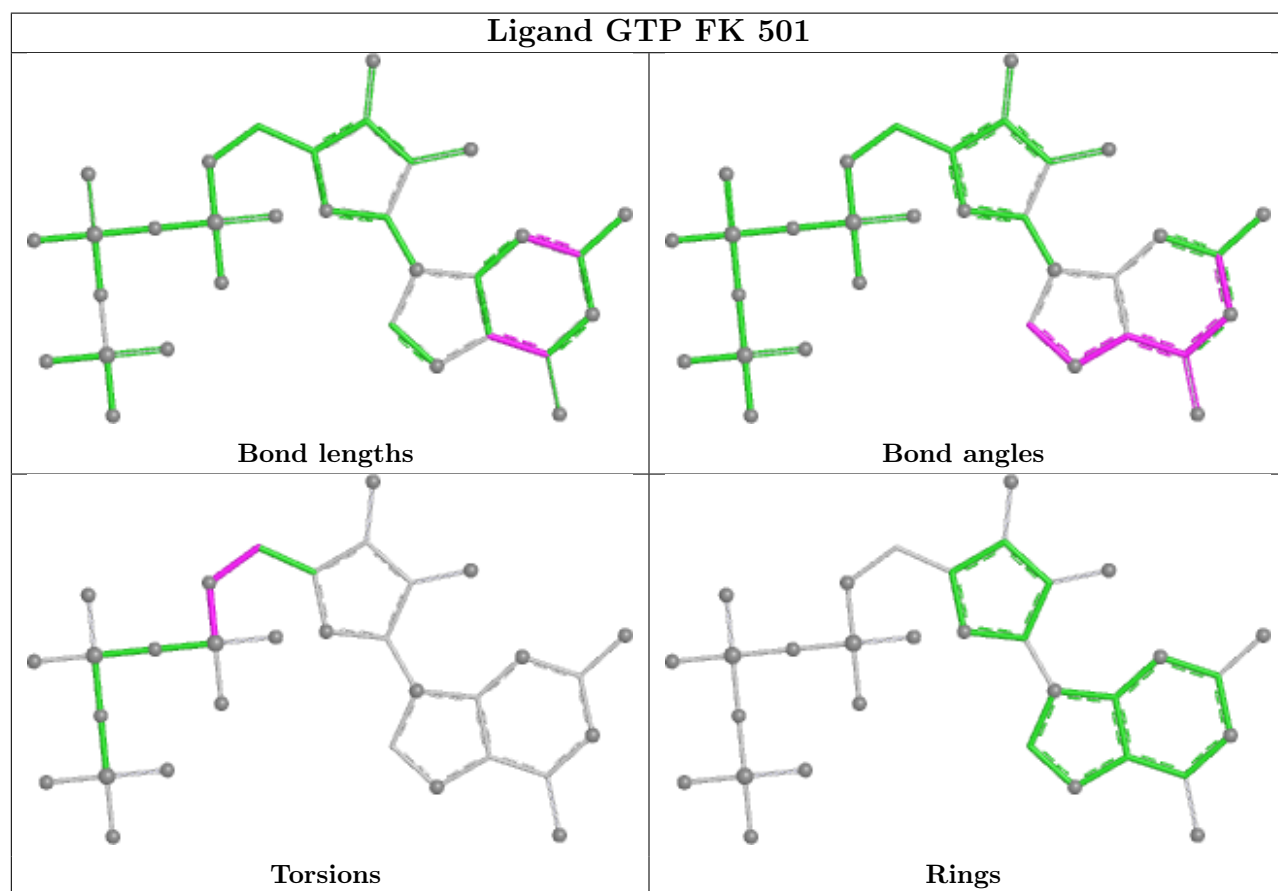
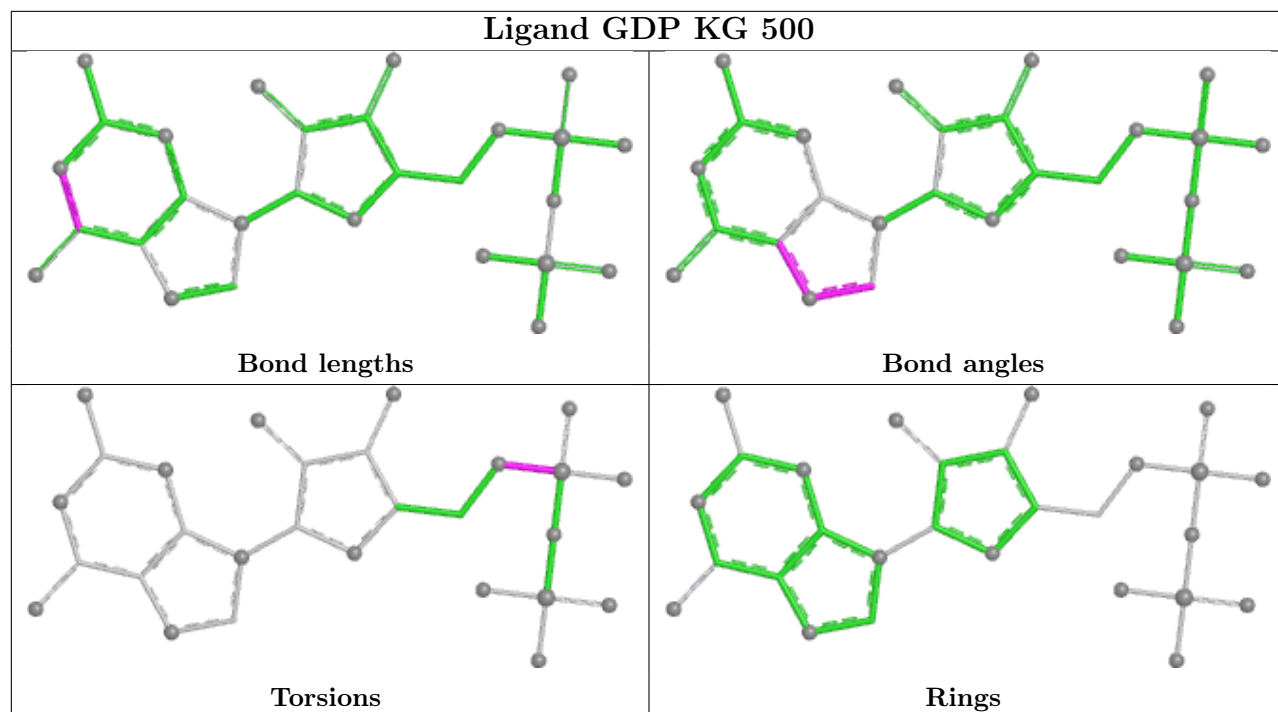
Ligand GTP MI 501

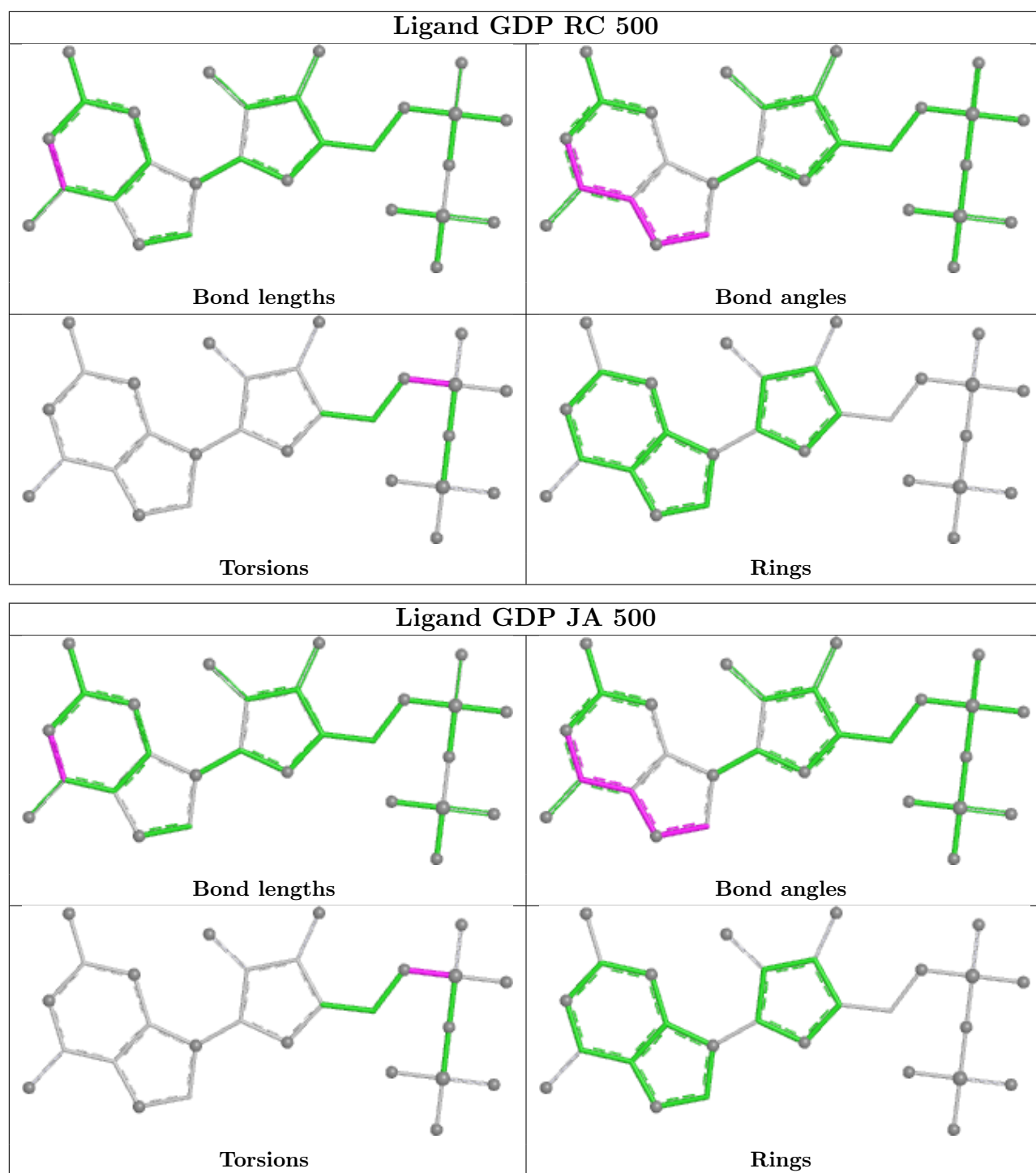


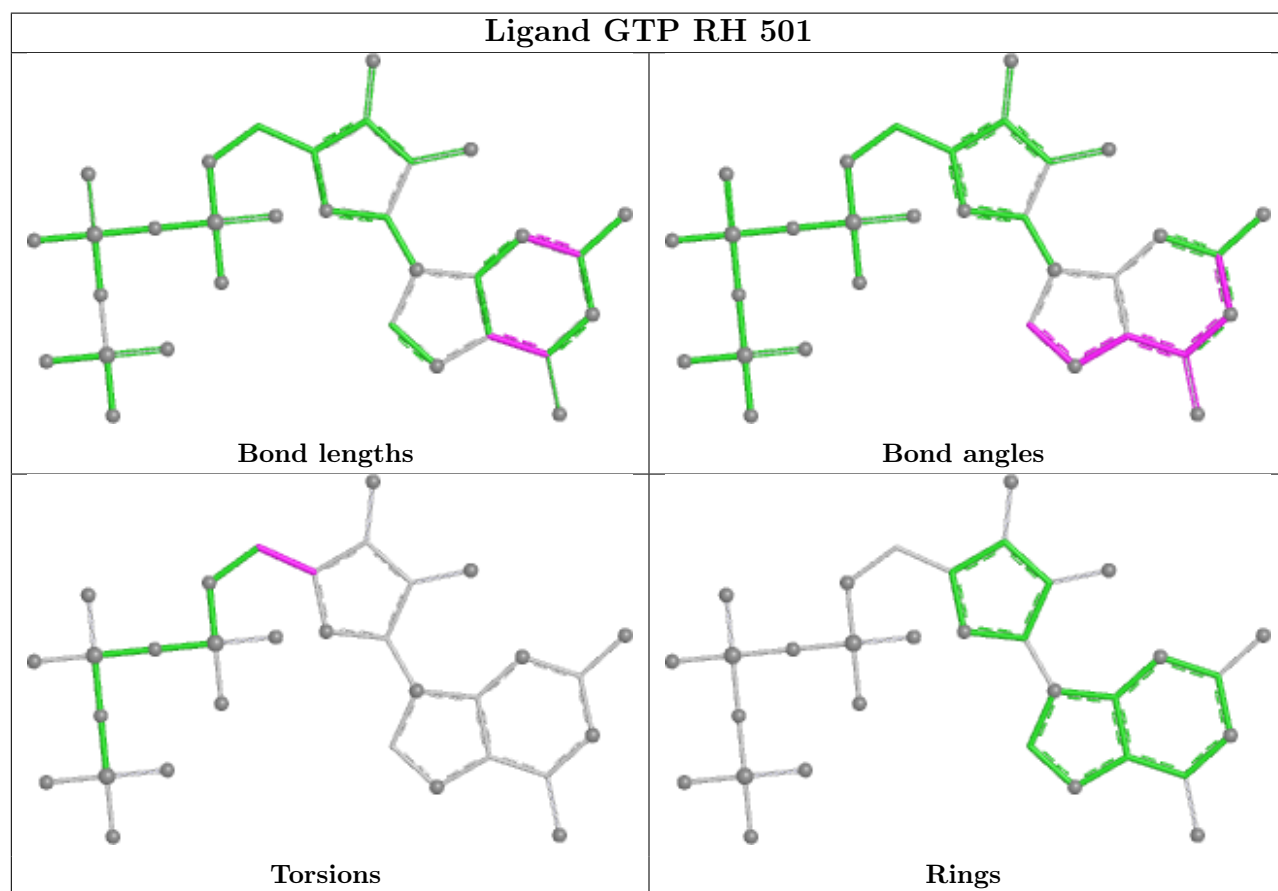
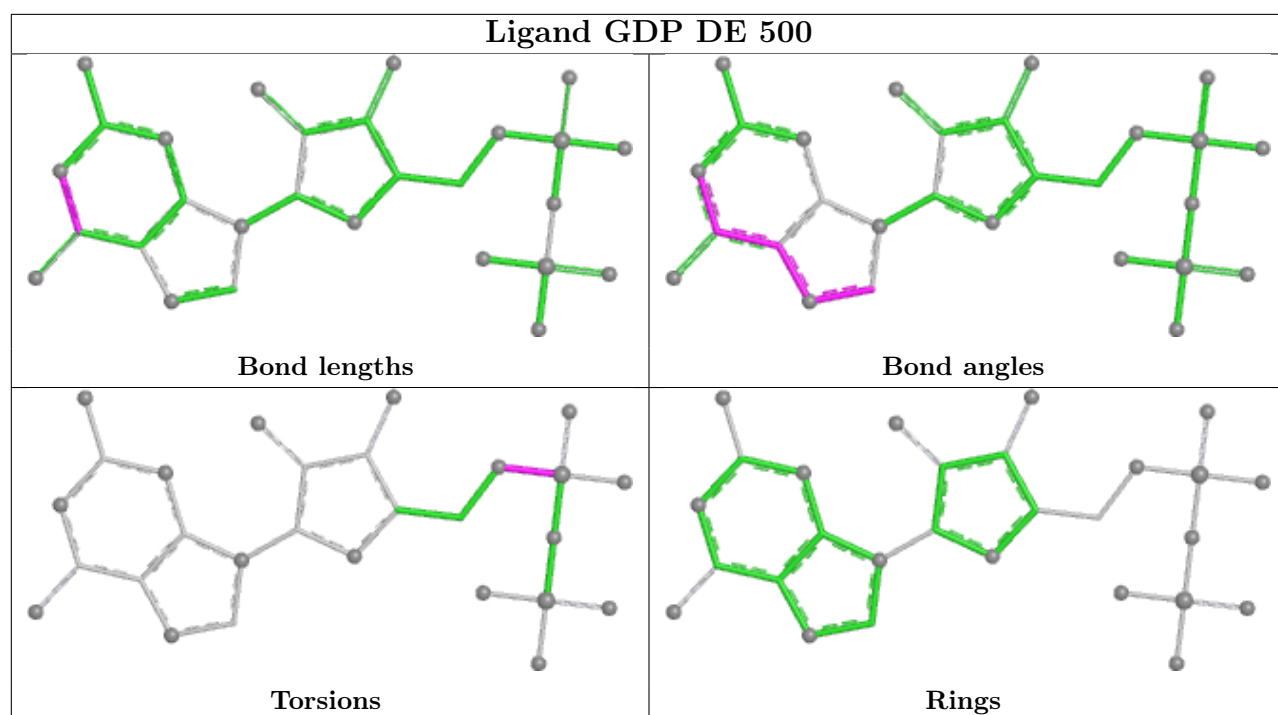
Ligand GTP RJ 501

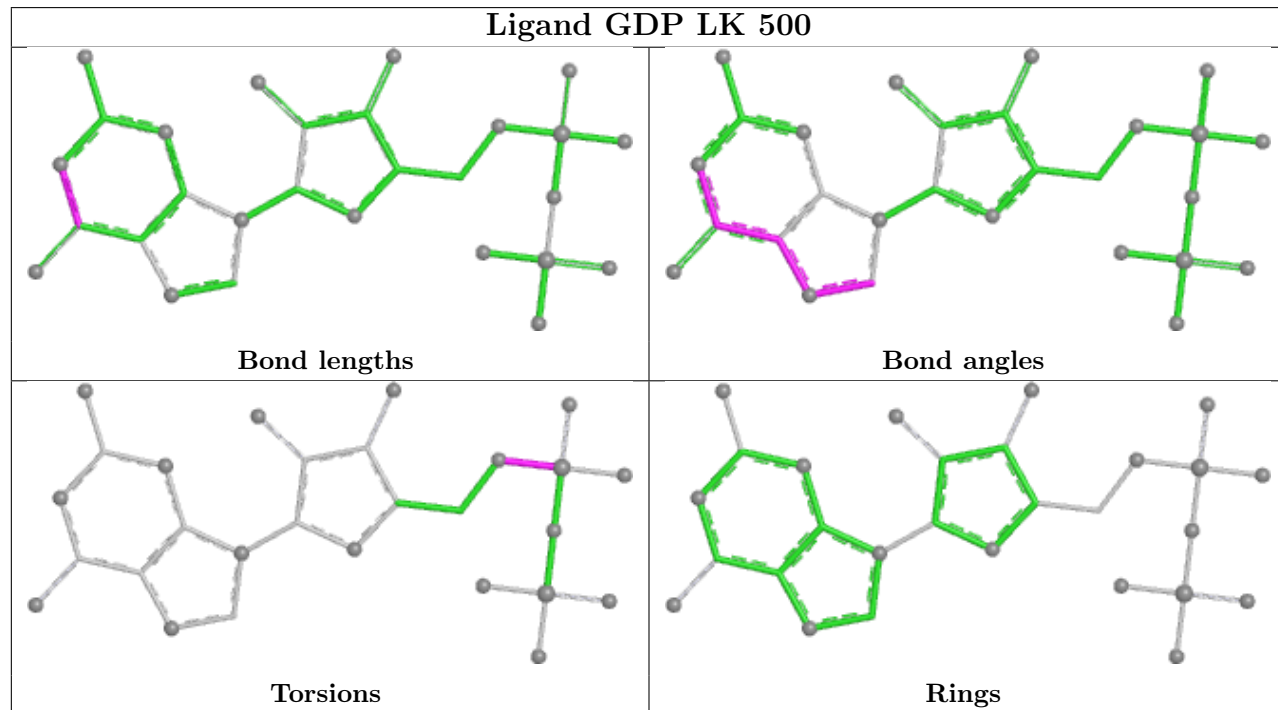
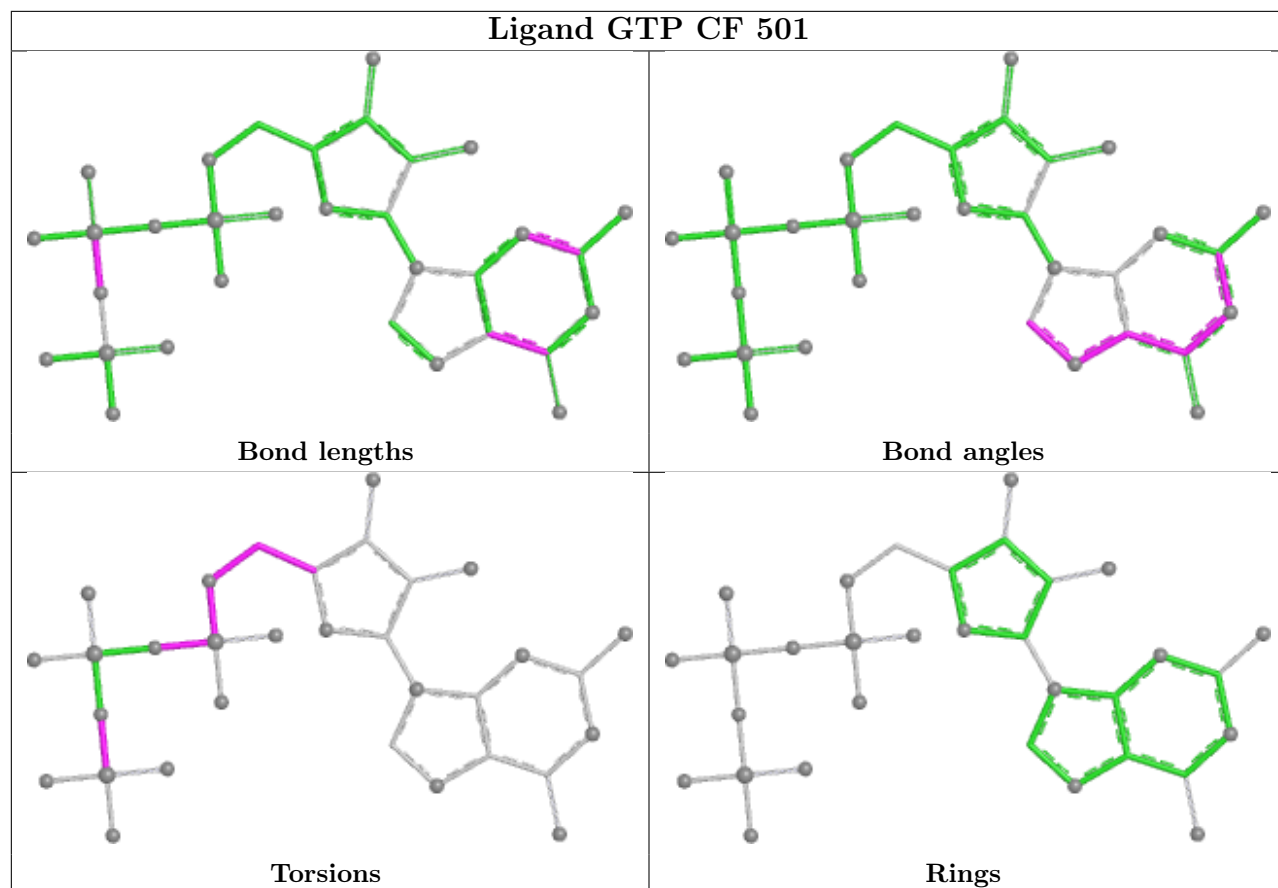


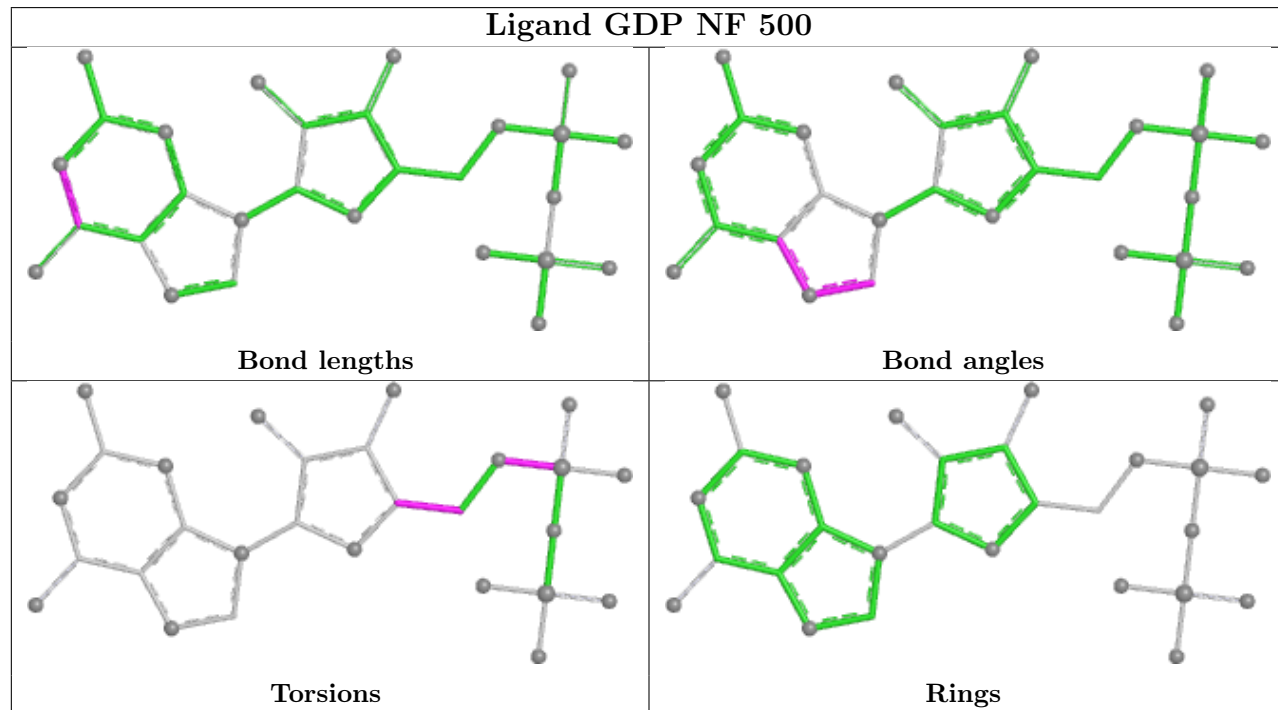
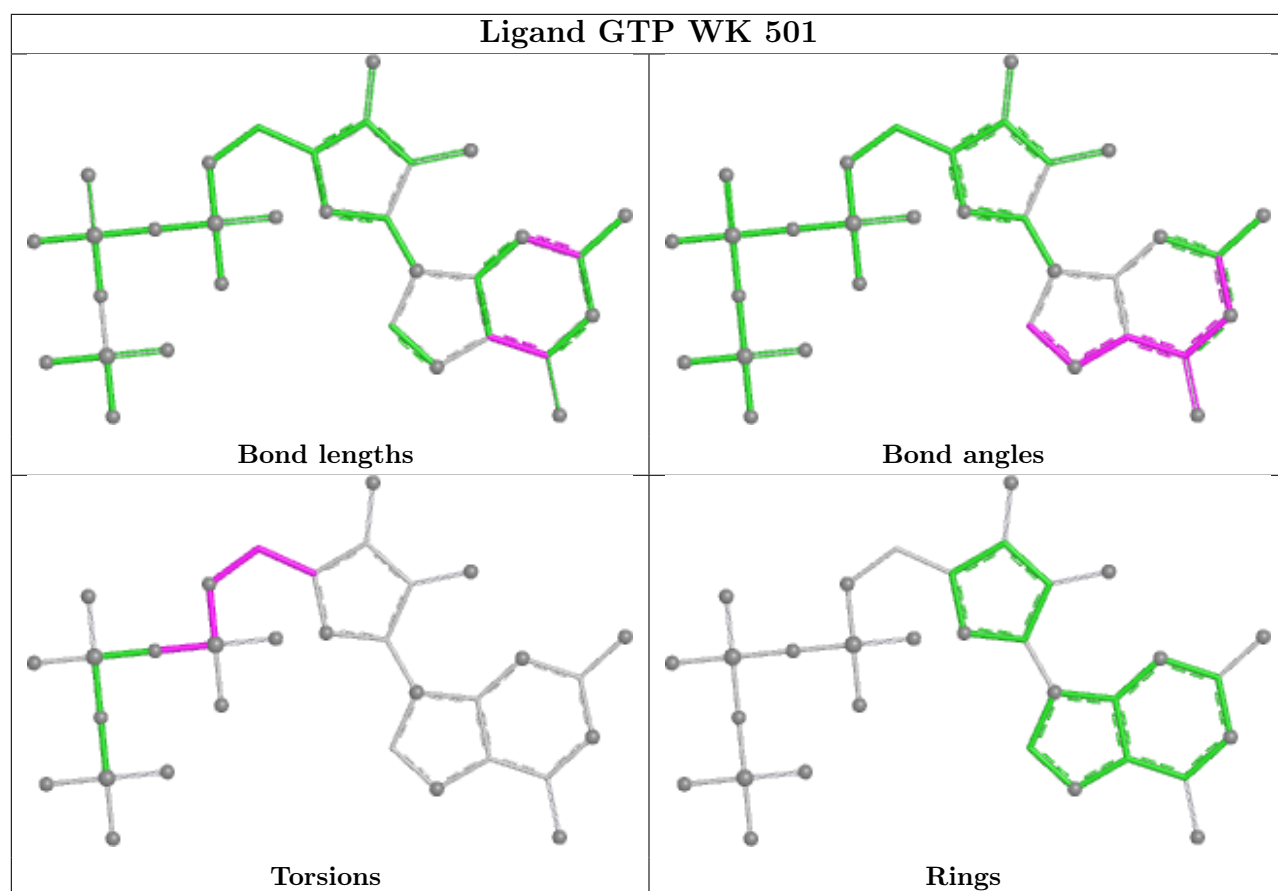


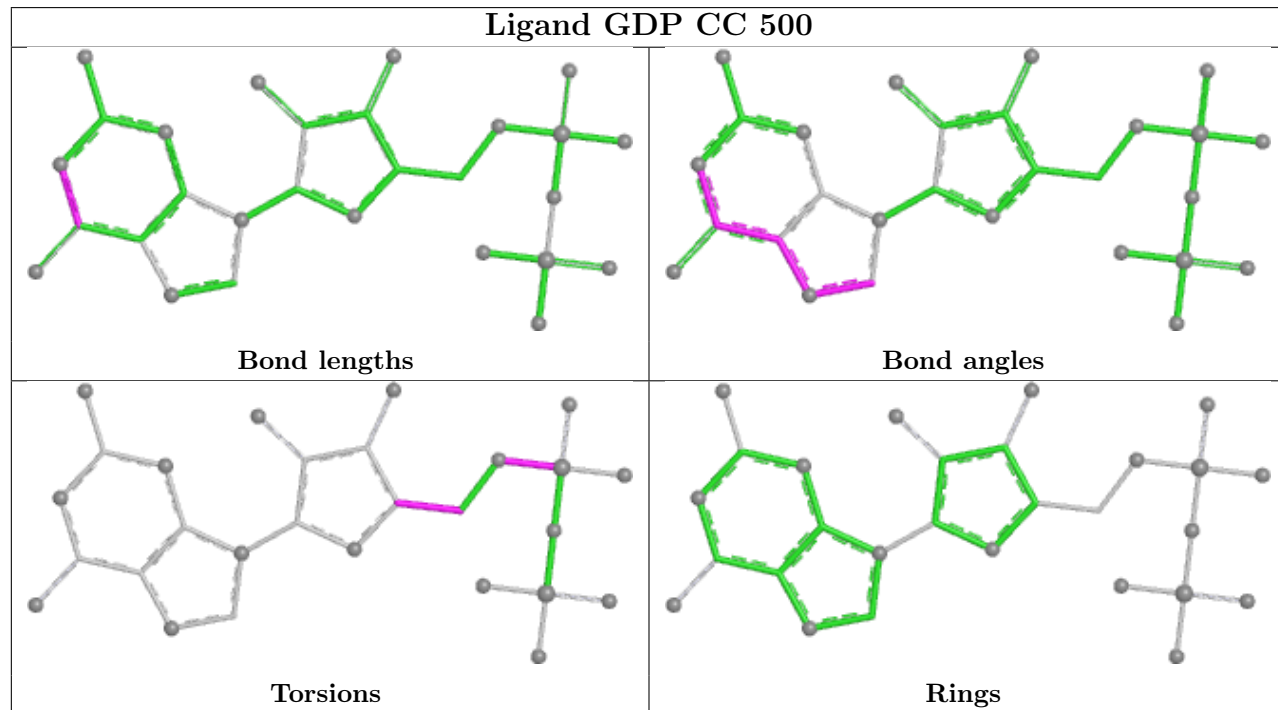
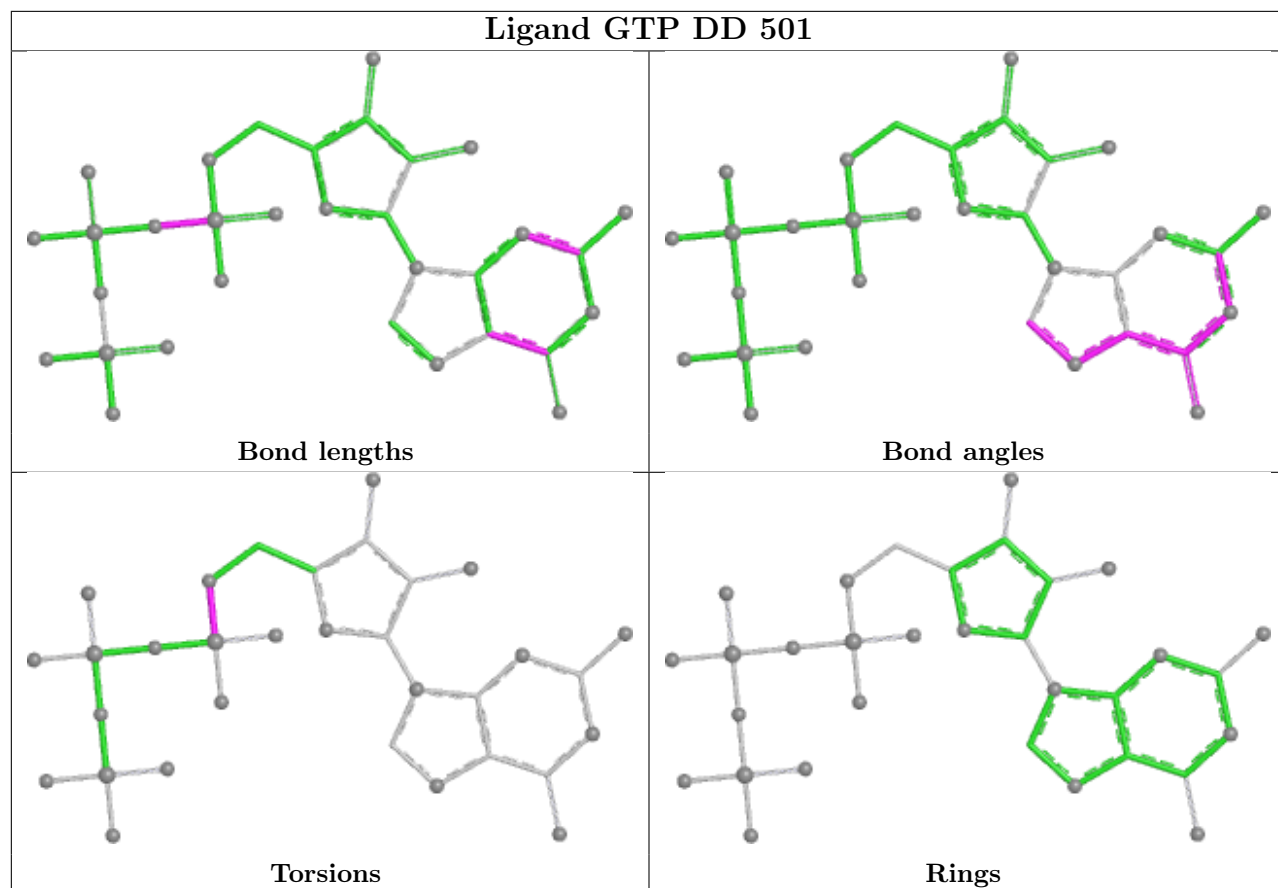


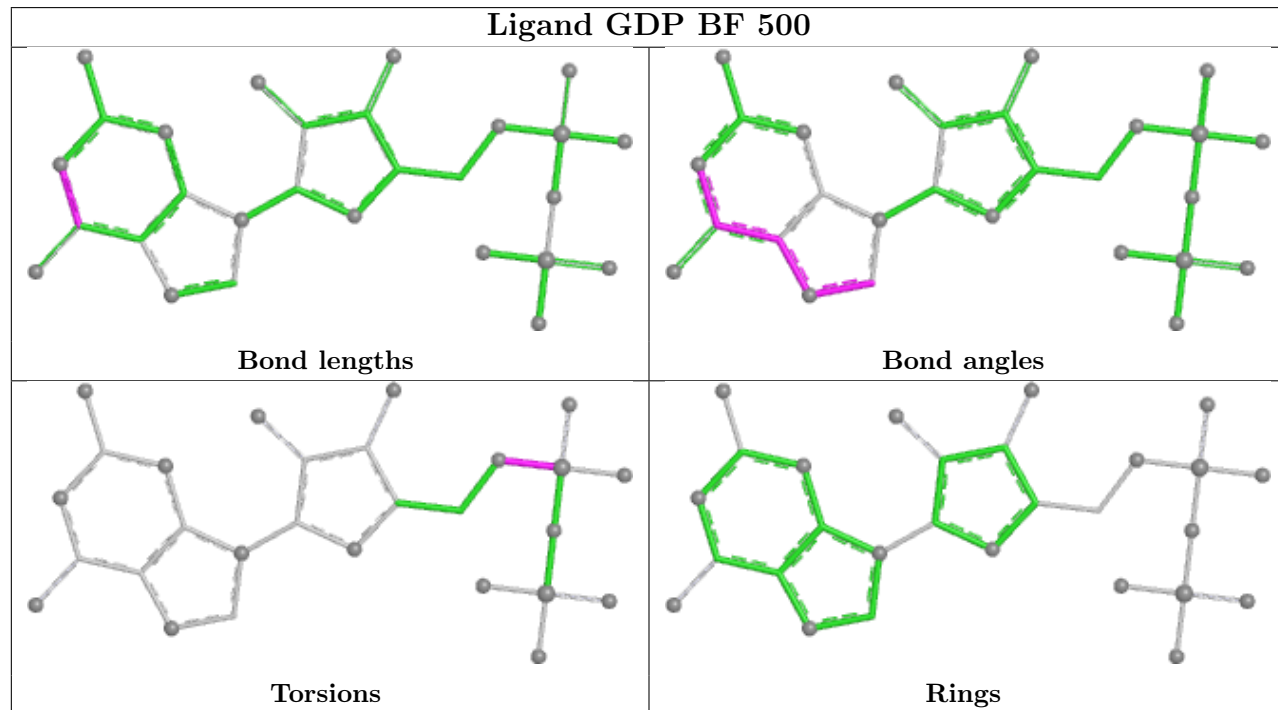
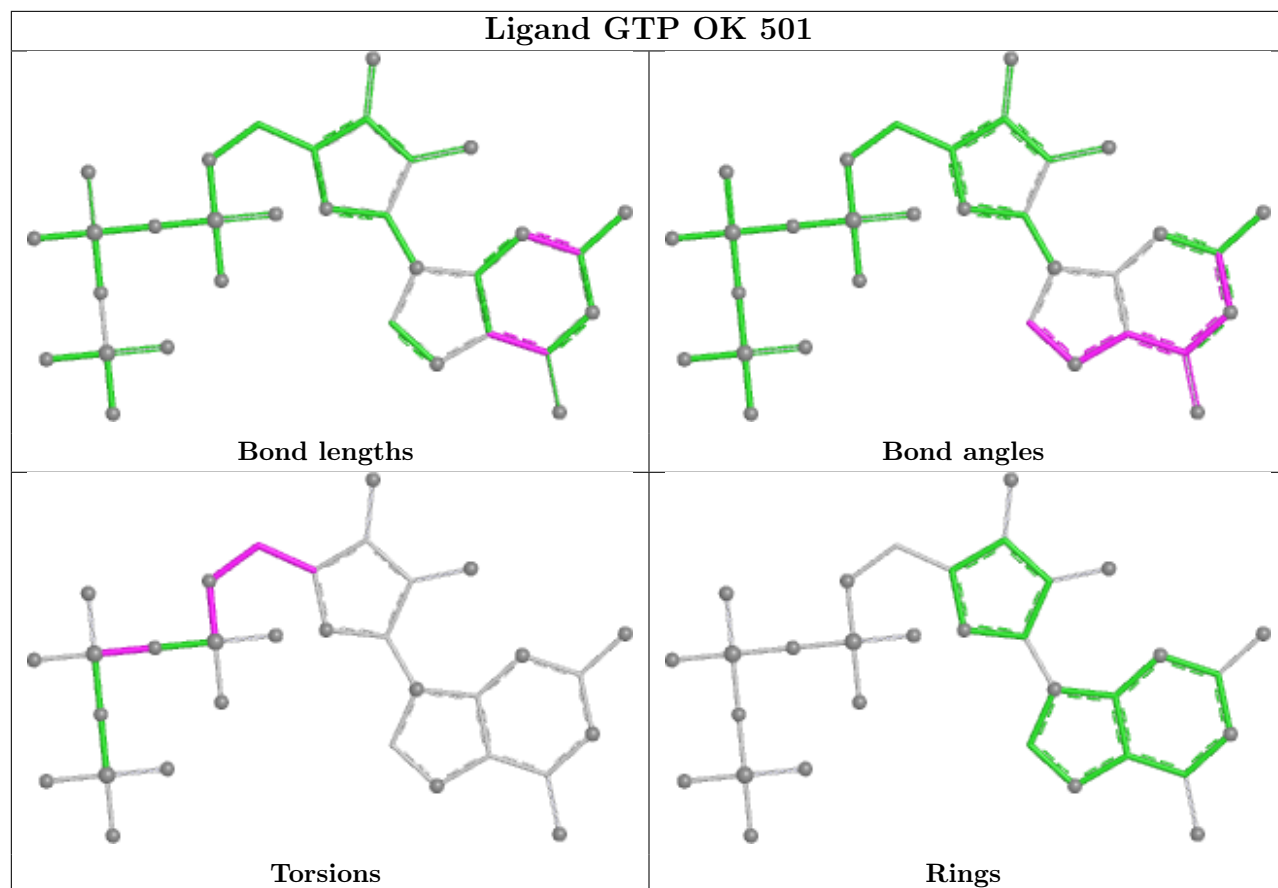


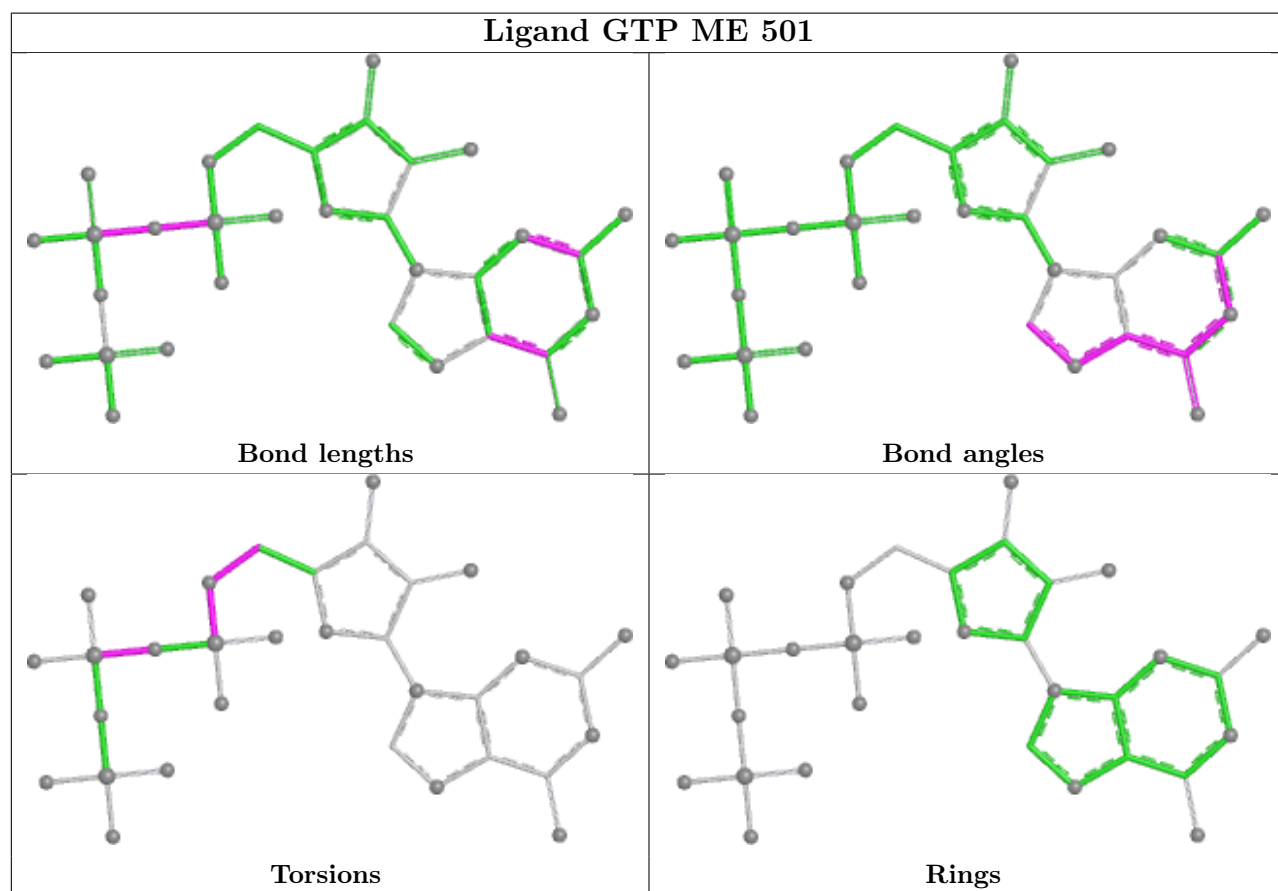
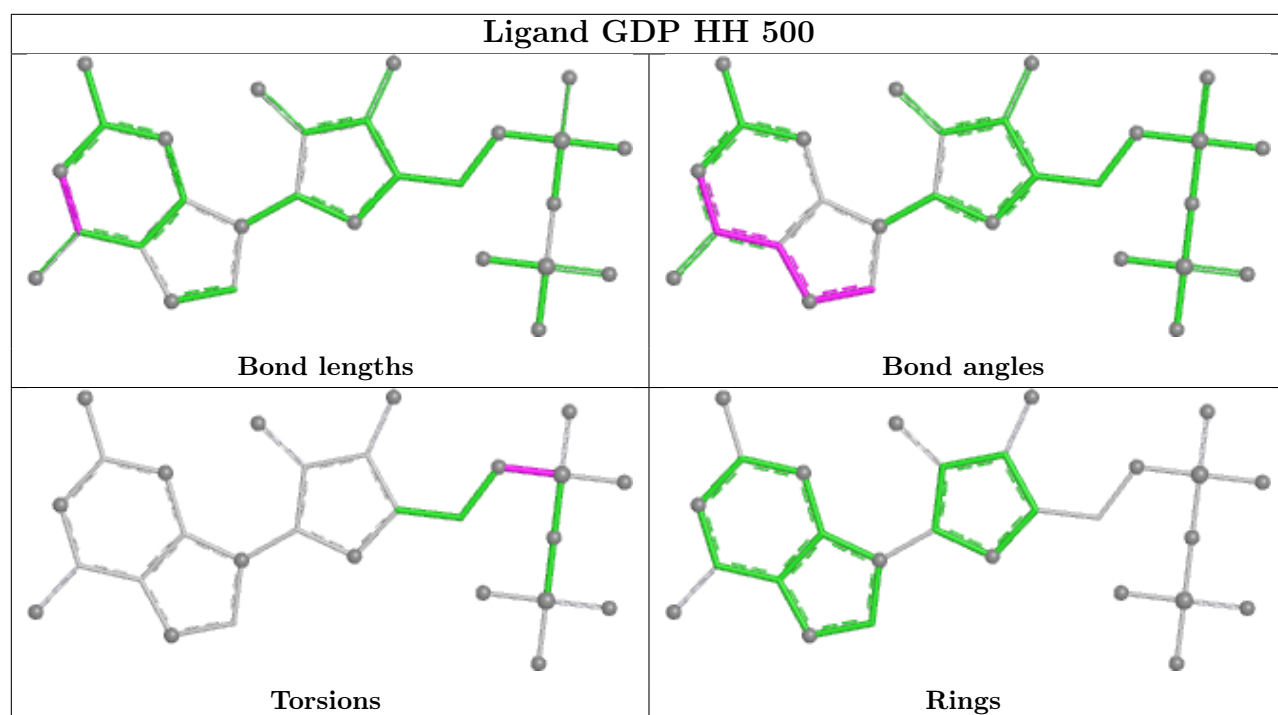


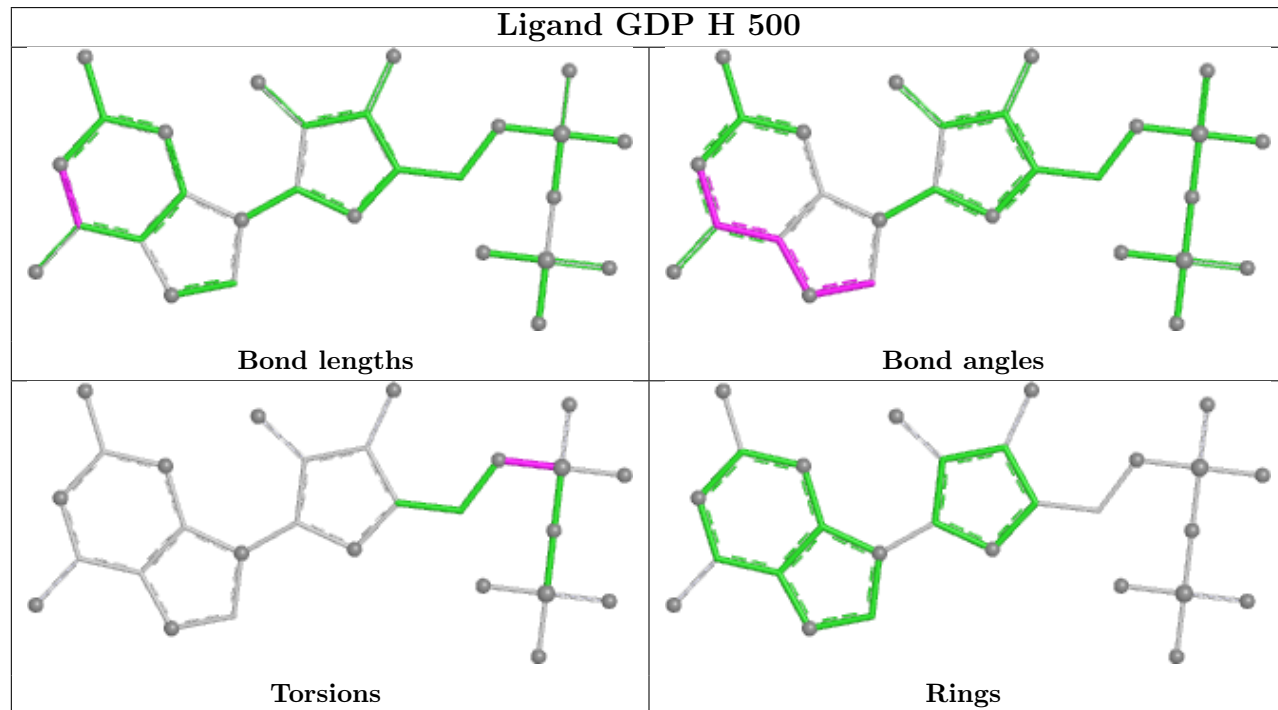
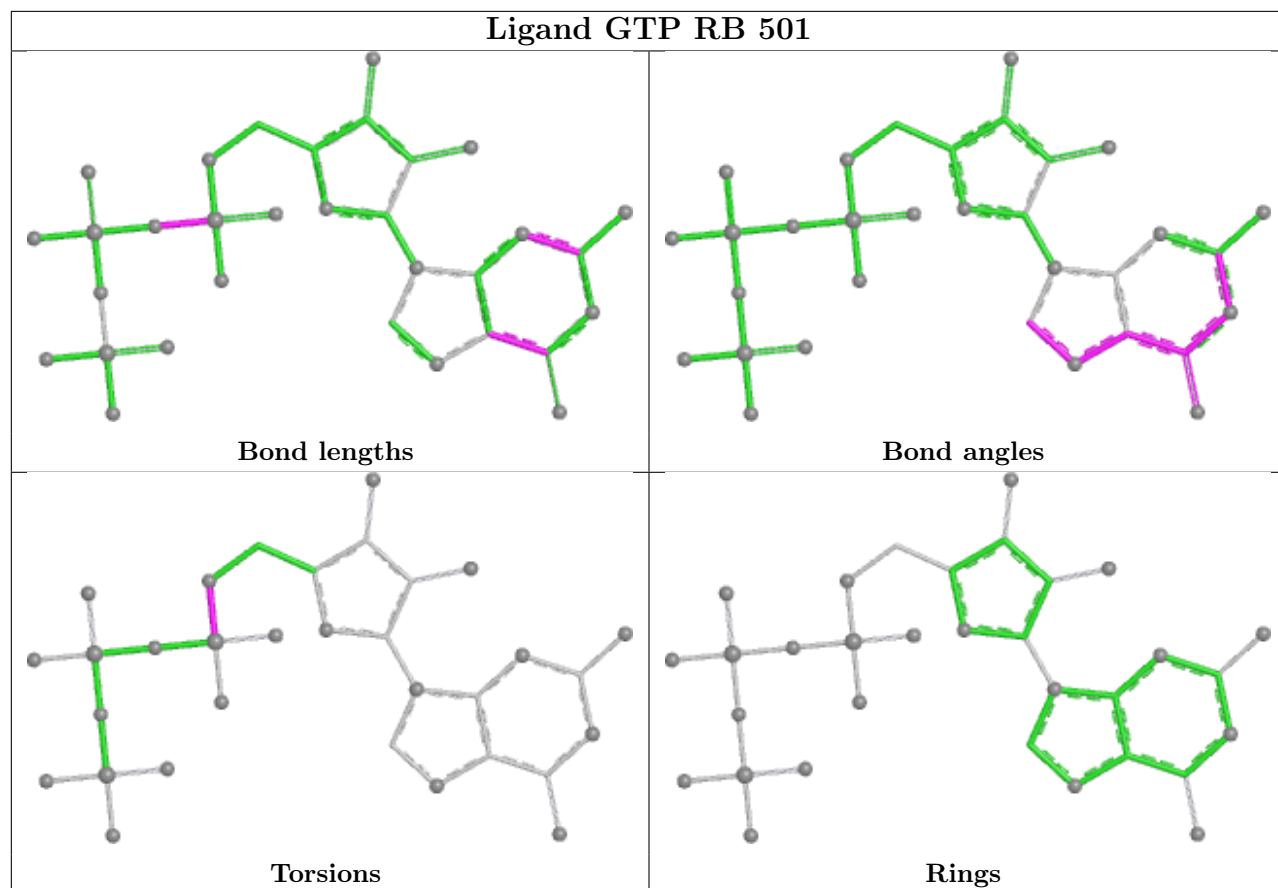


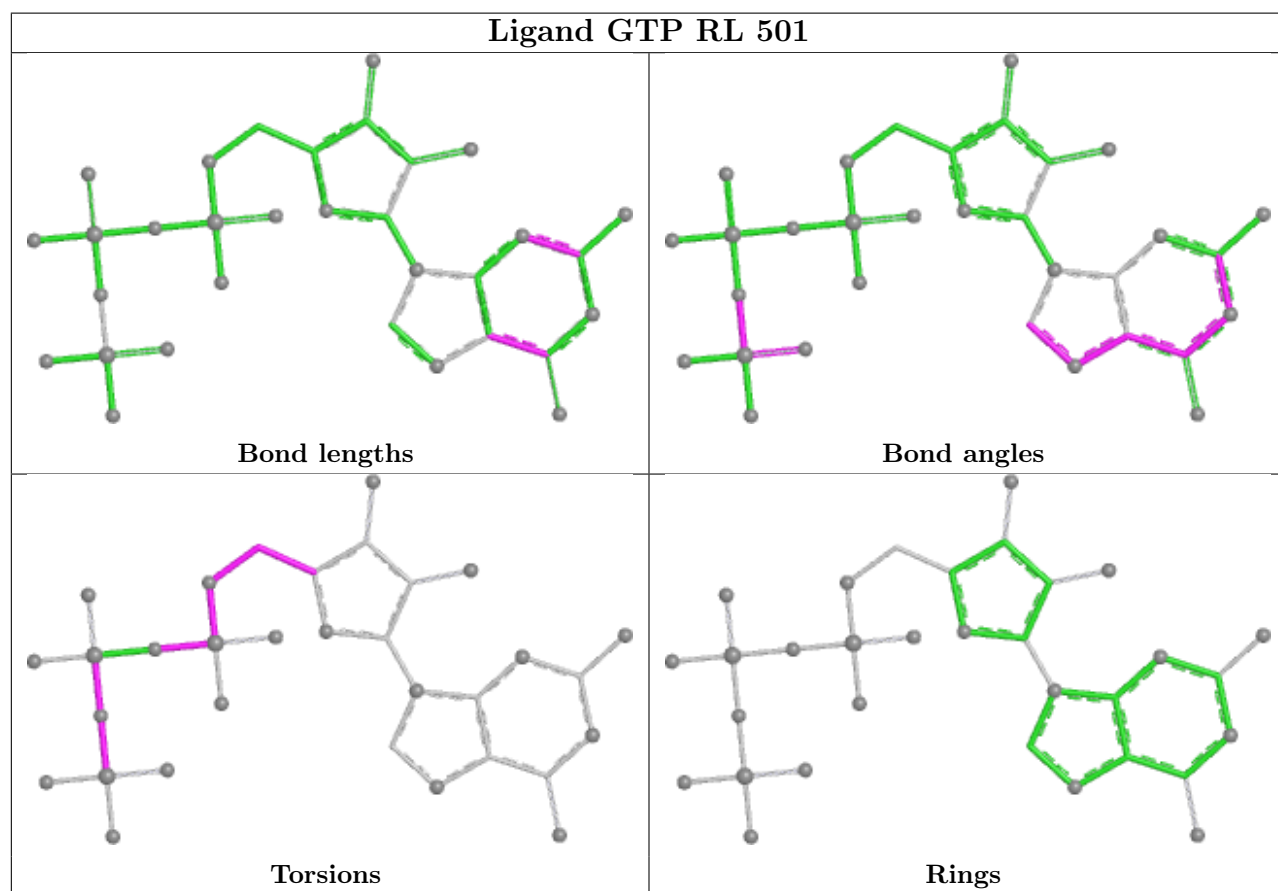
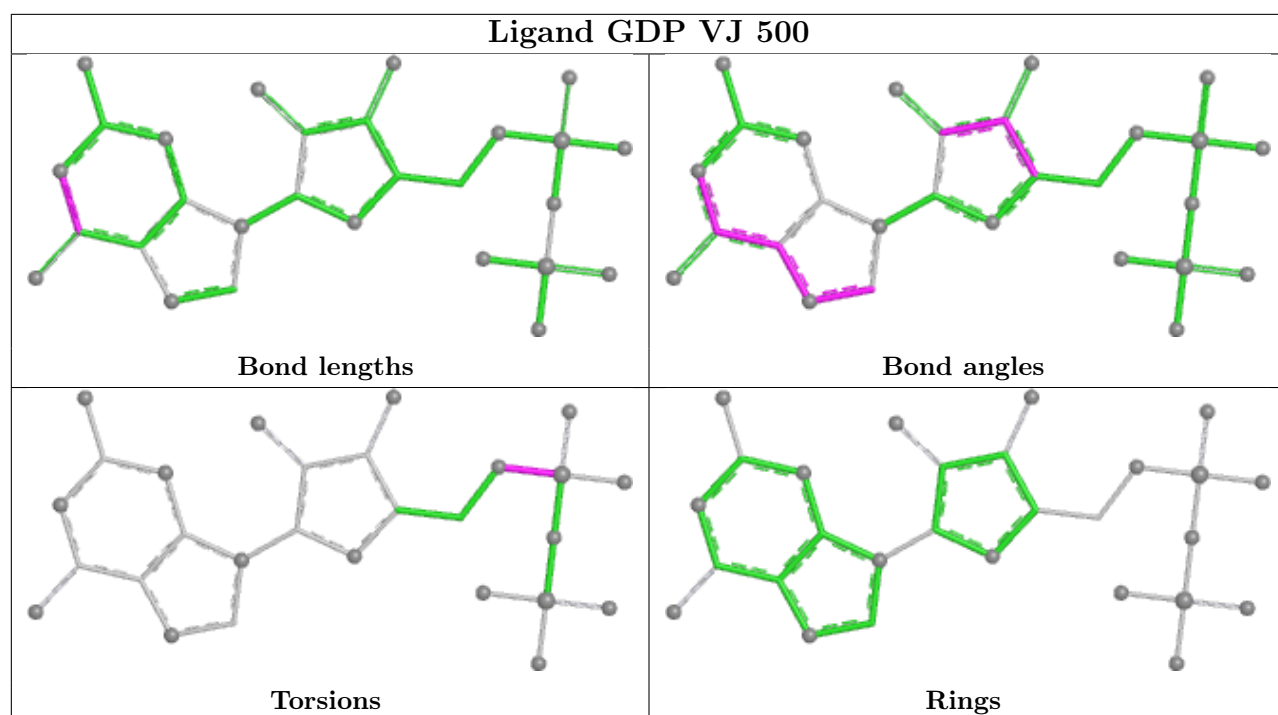




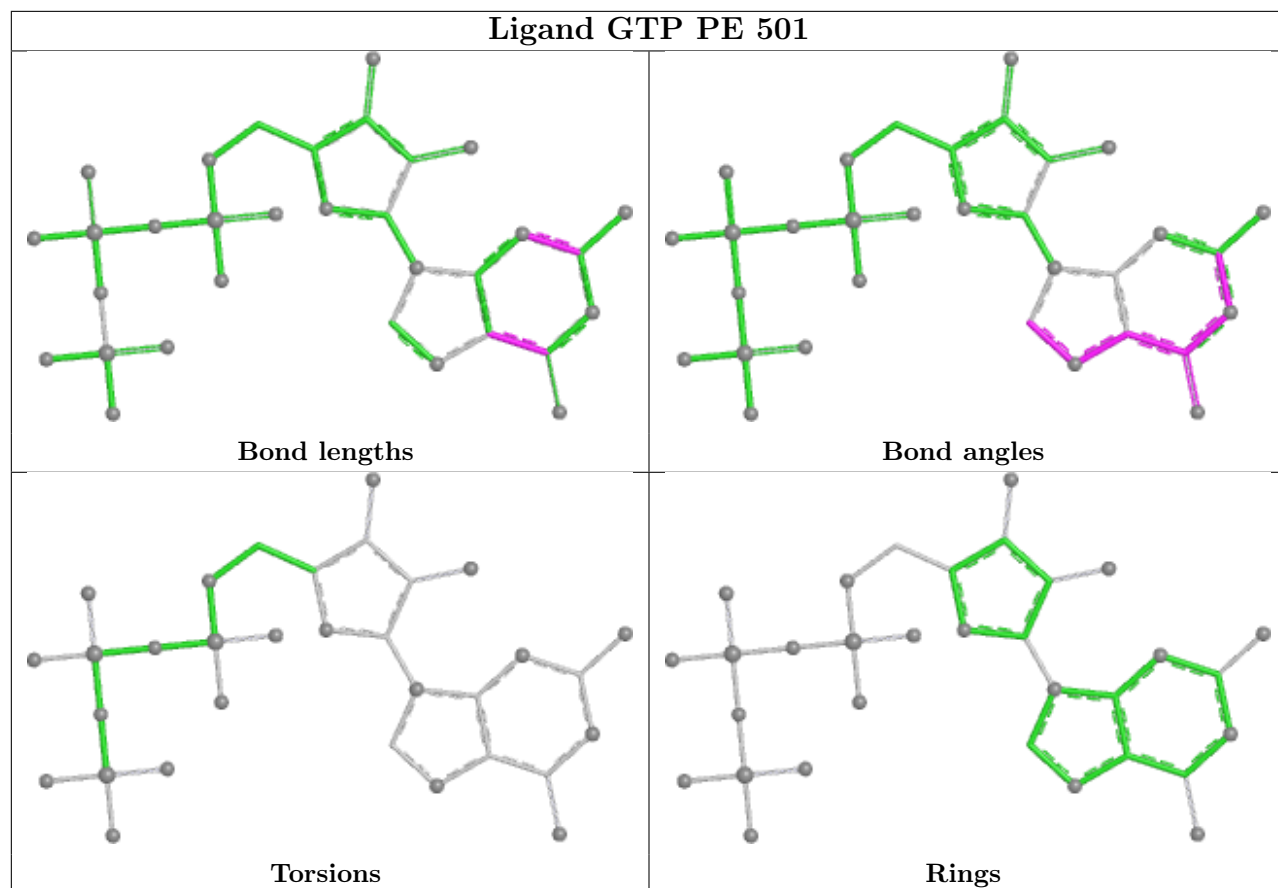




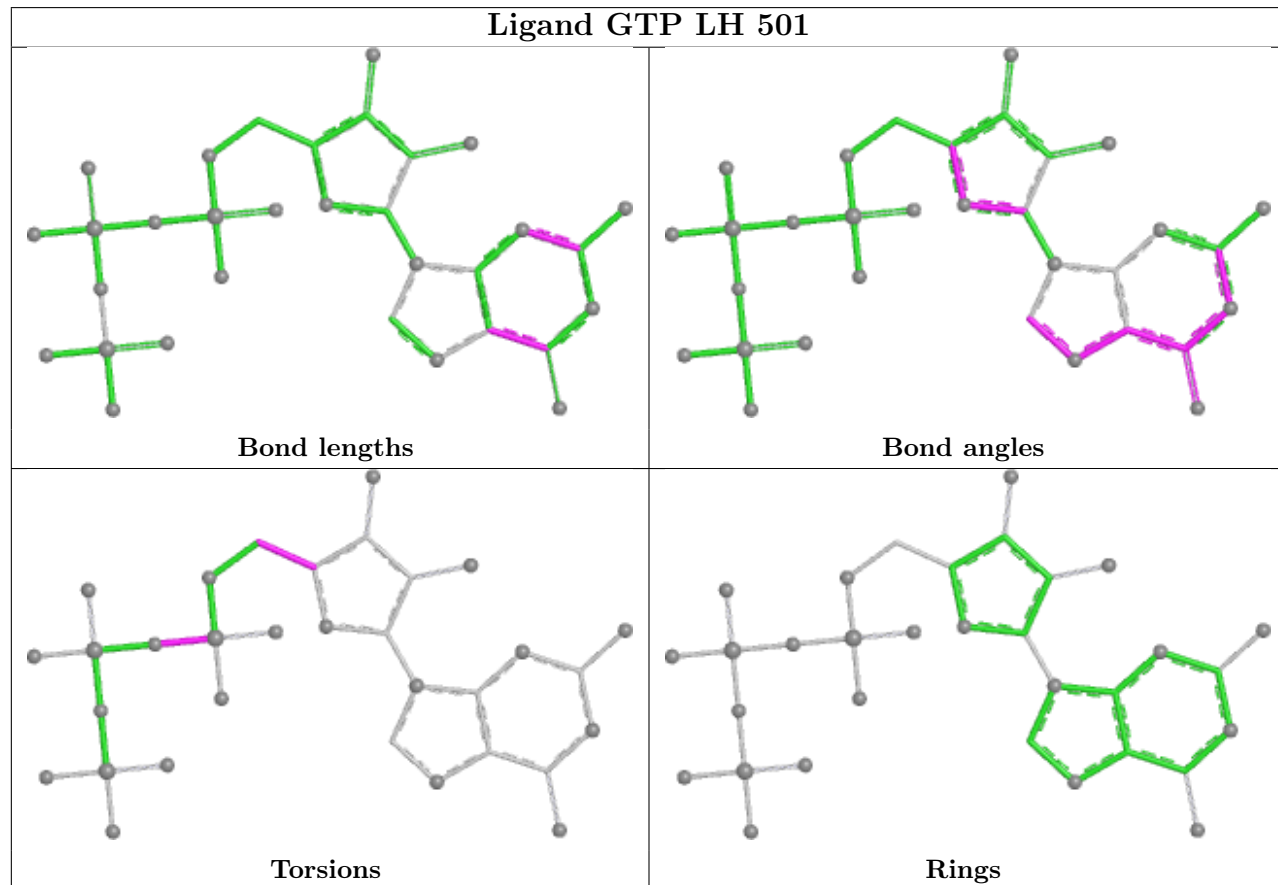


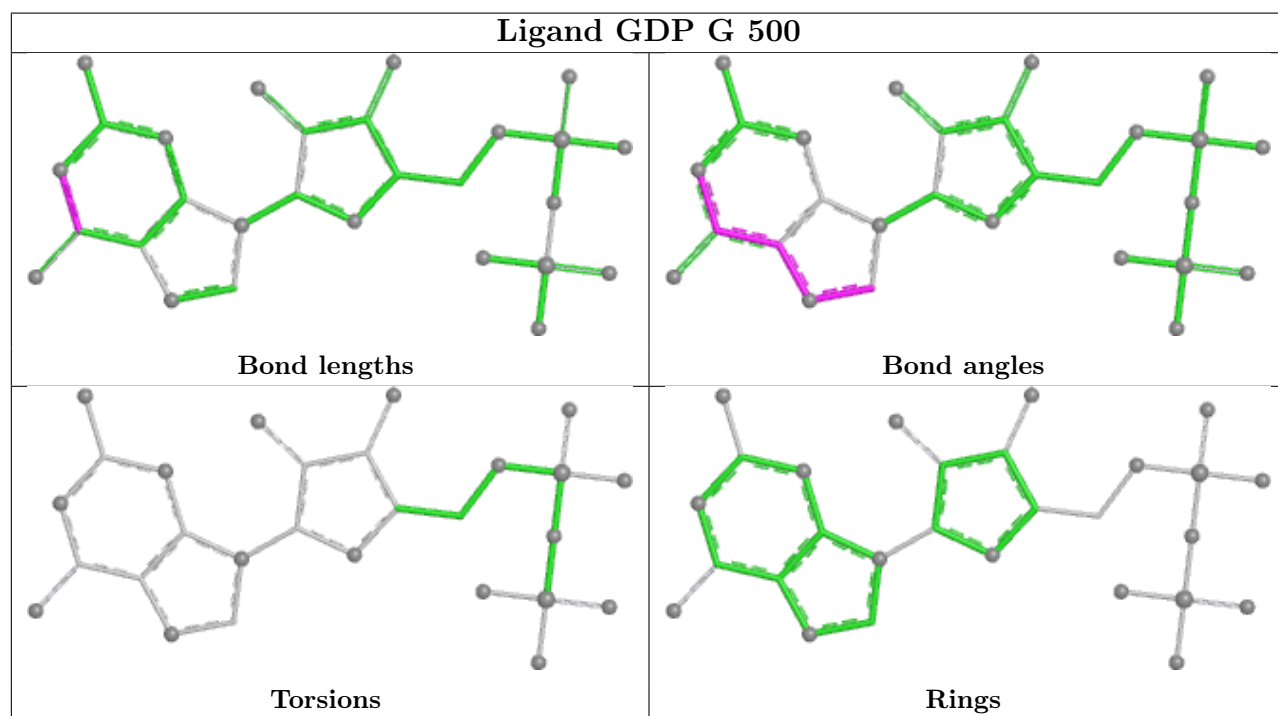
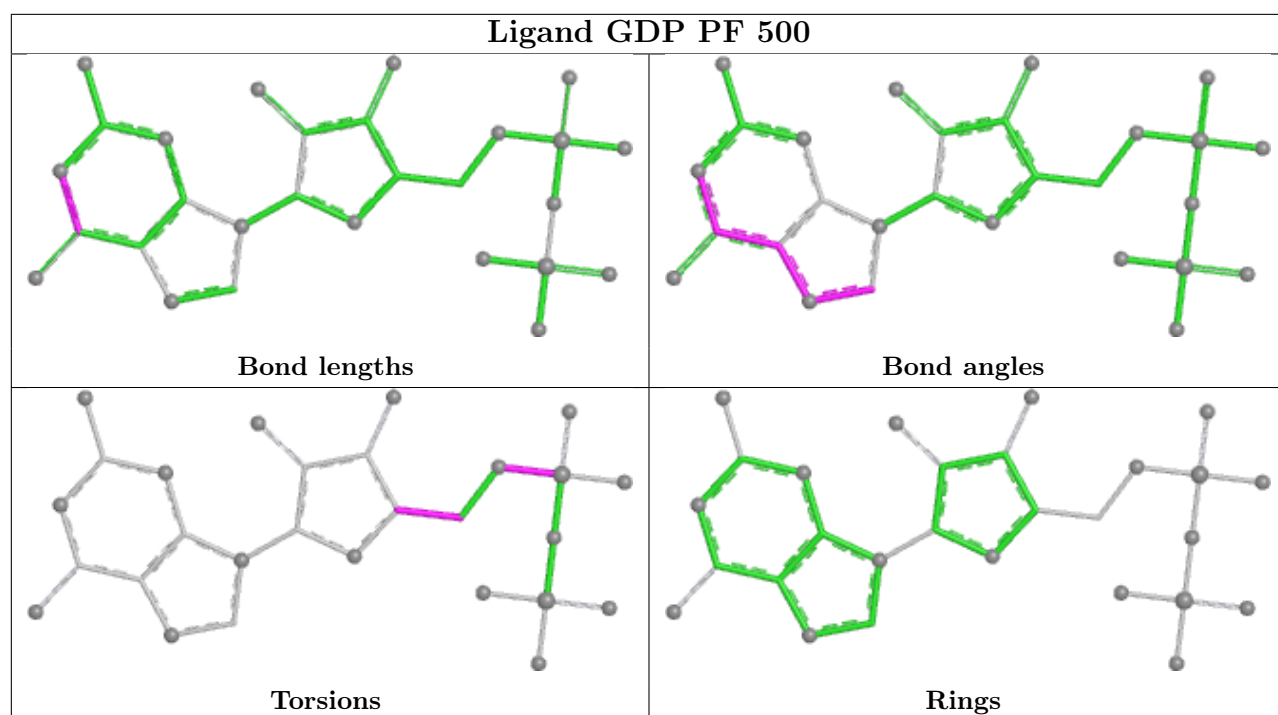


Ligand GTP PE 501

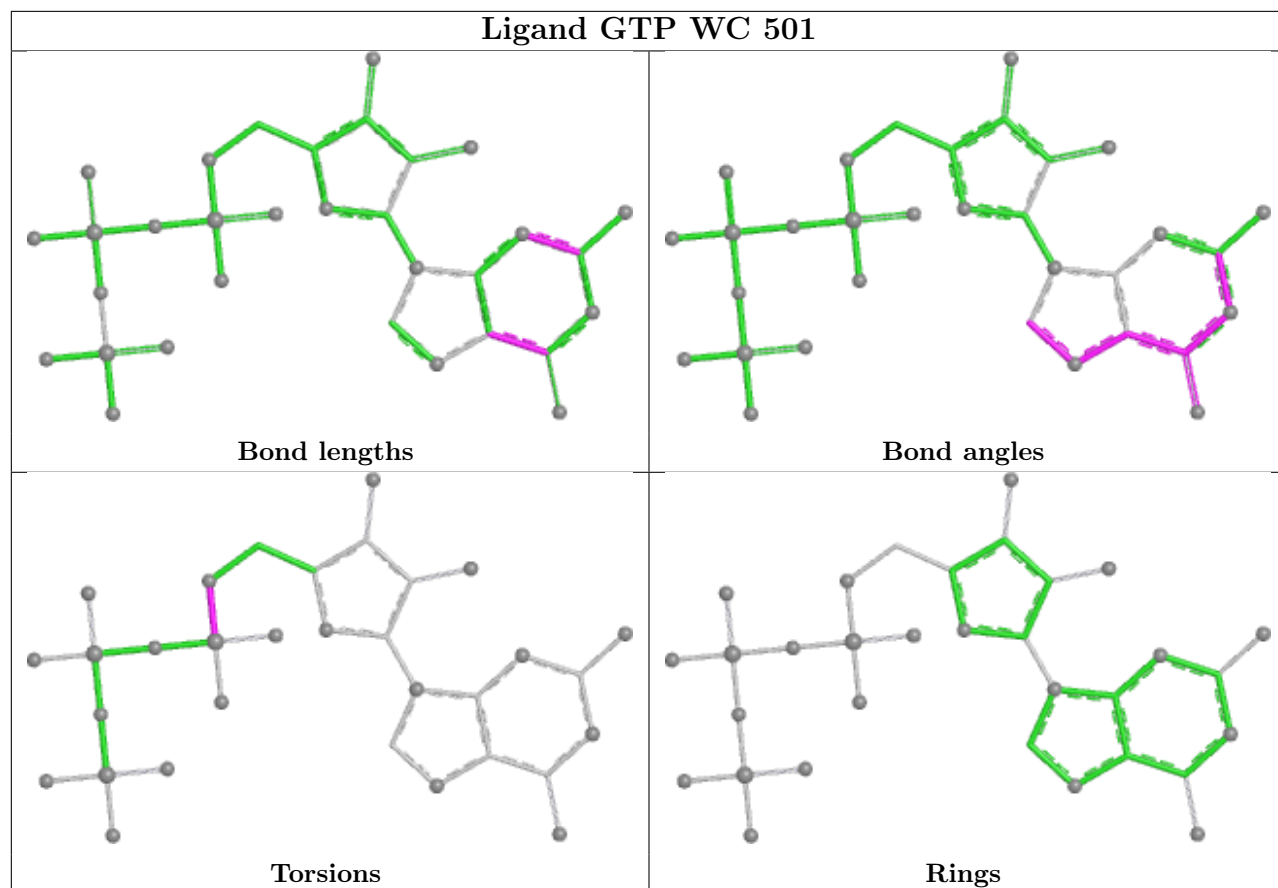


Ligand GTP LH 501

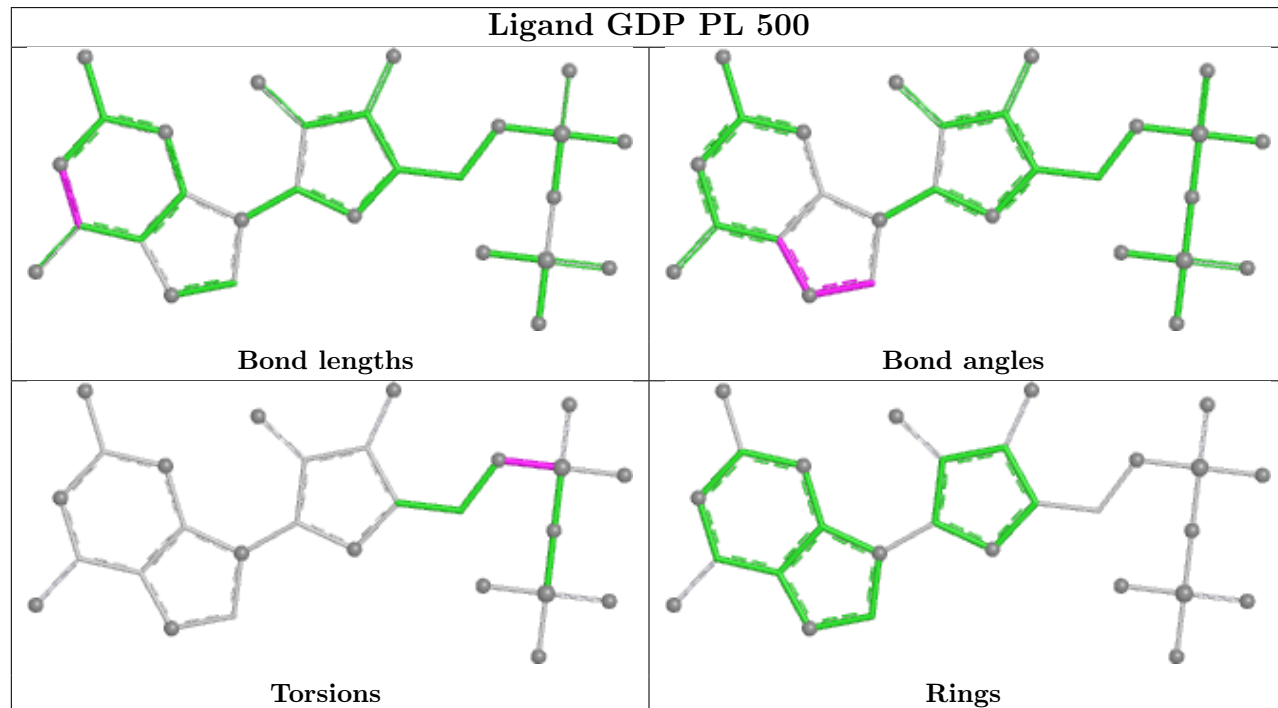


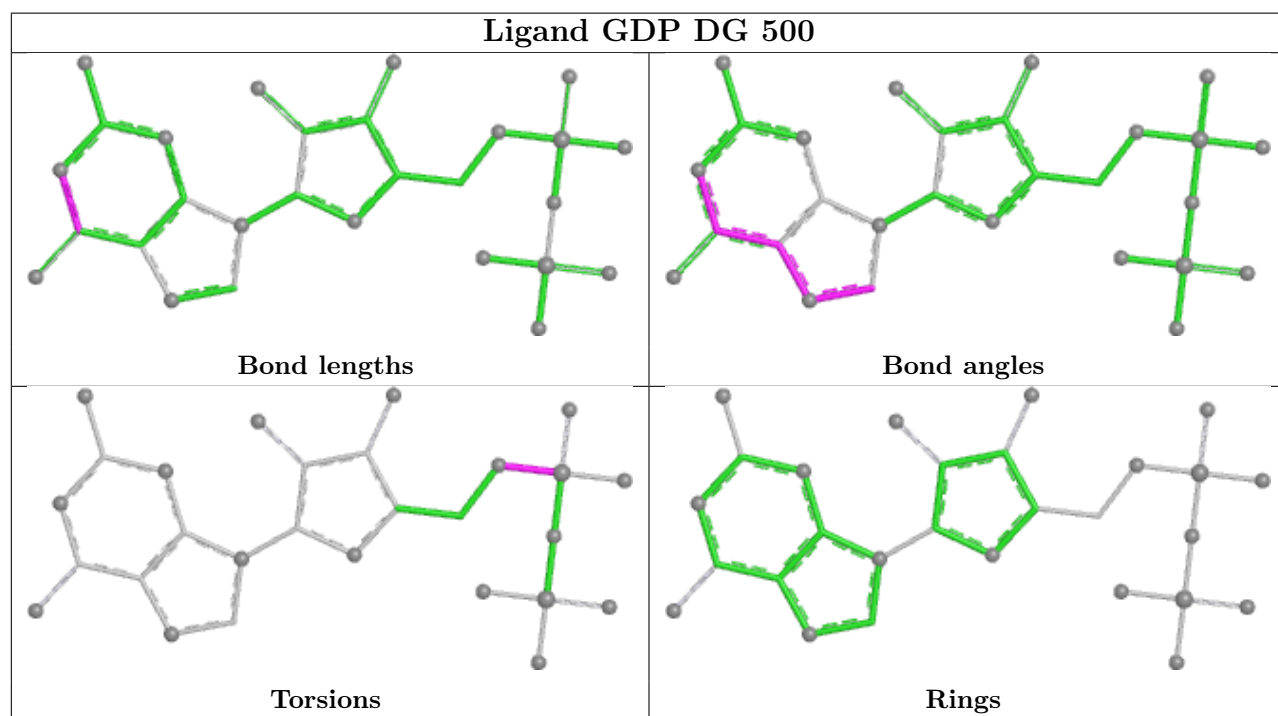
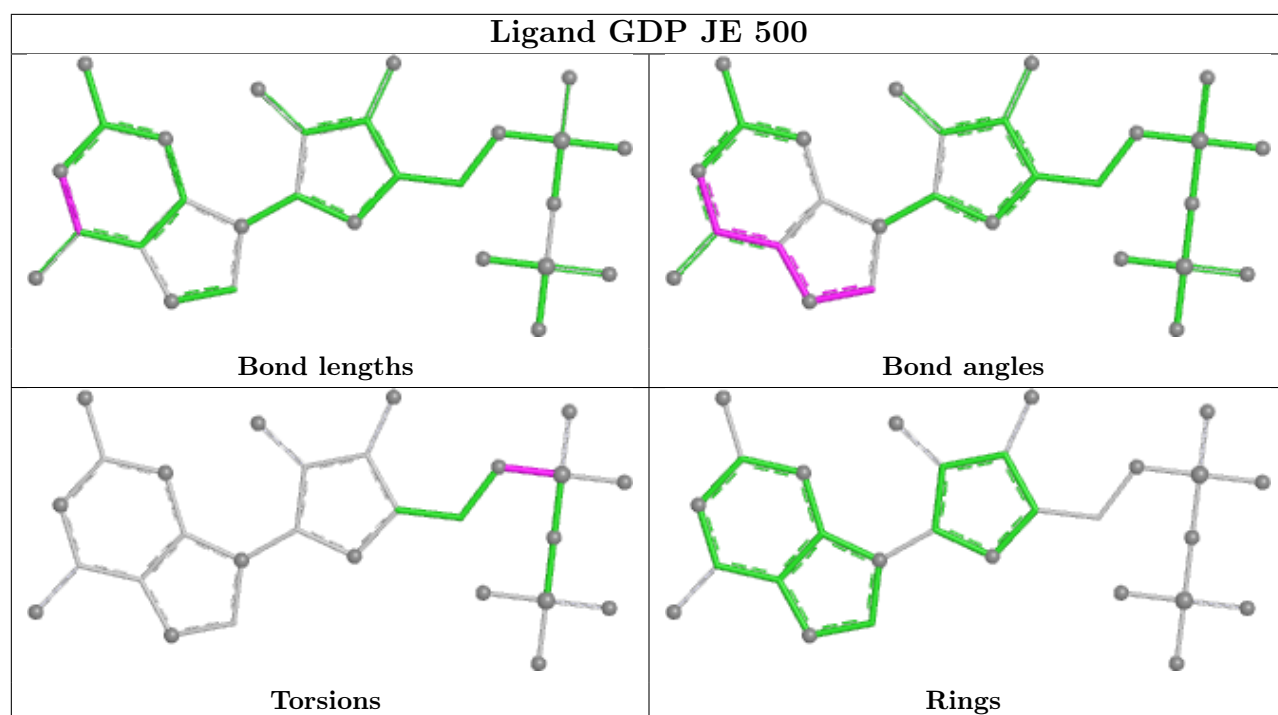


Ligand GTP WC 501

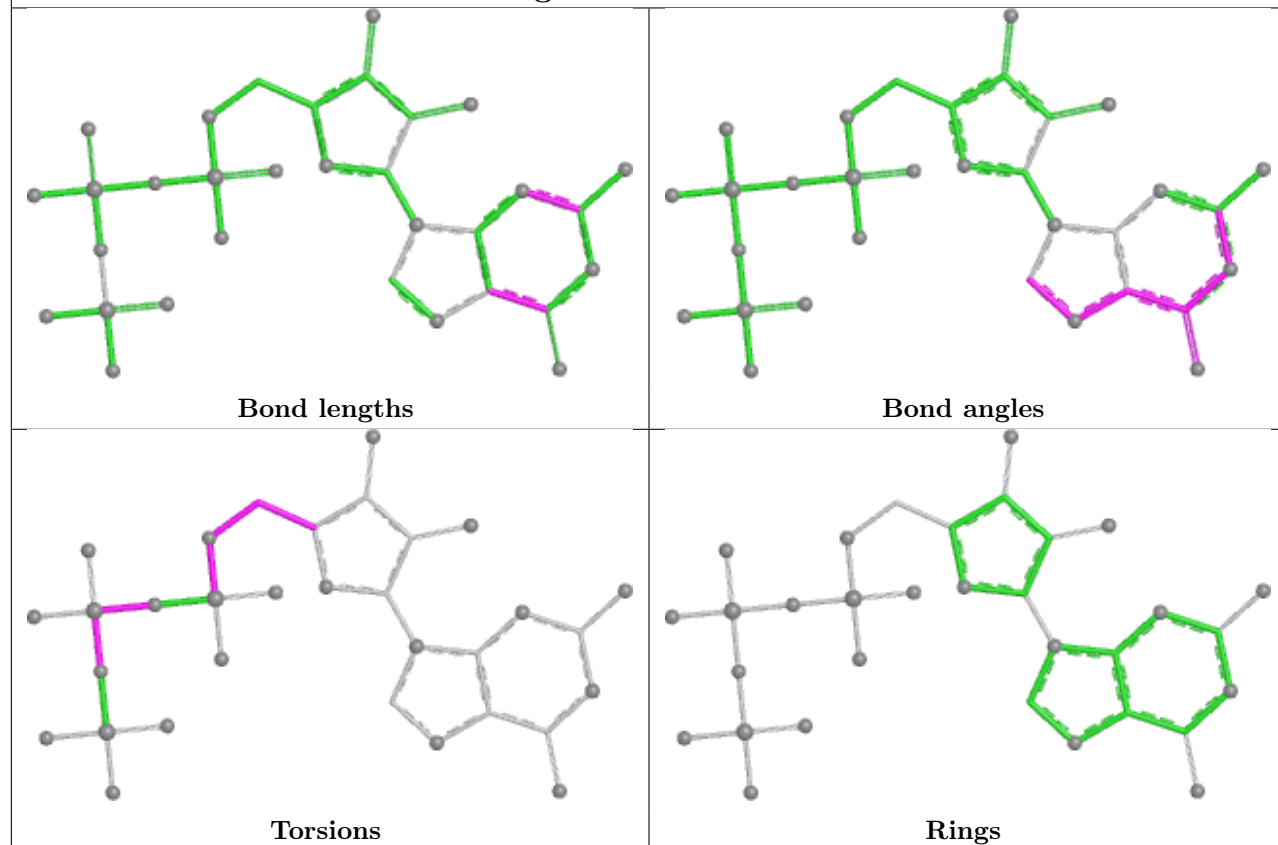


Ligand GDP PL 500

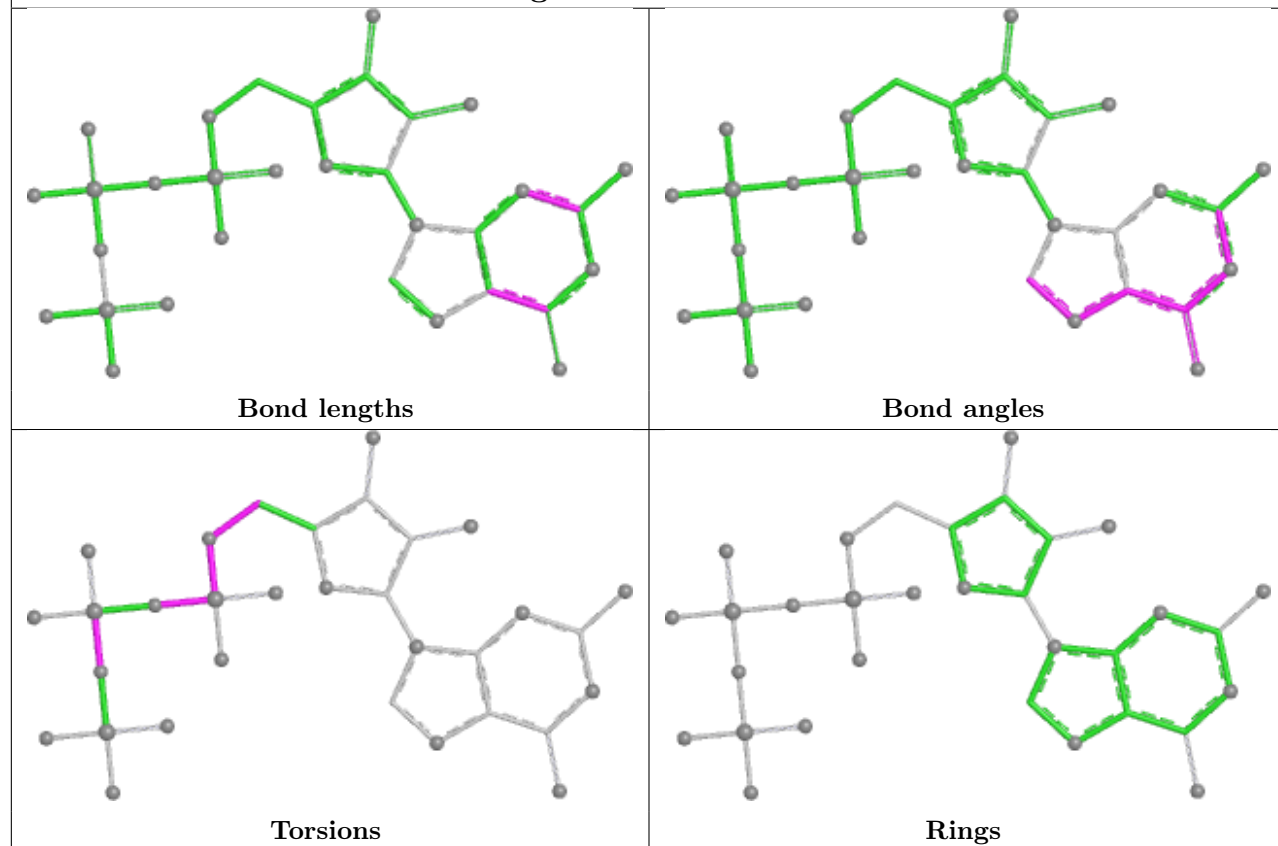


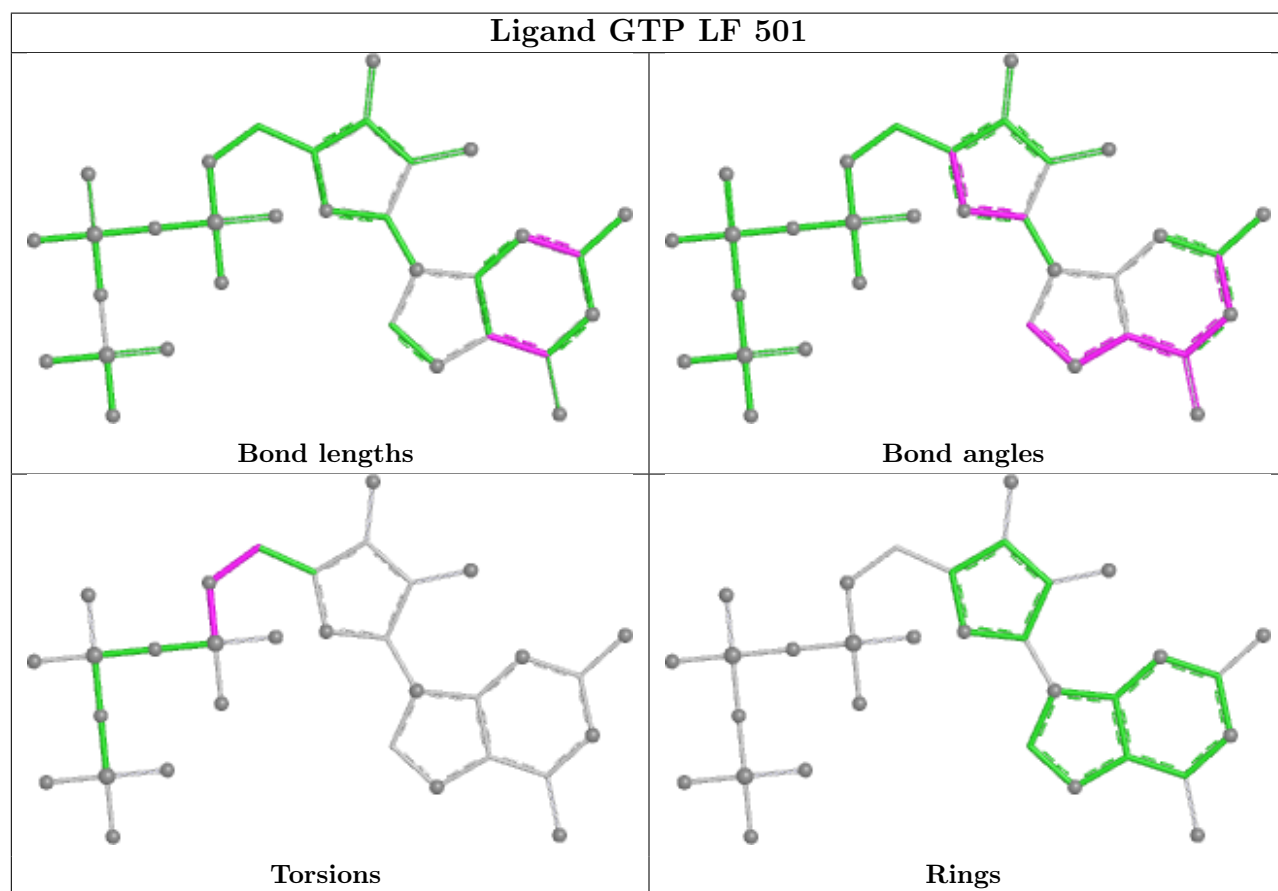
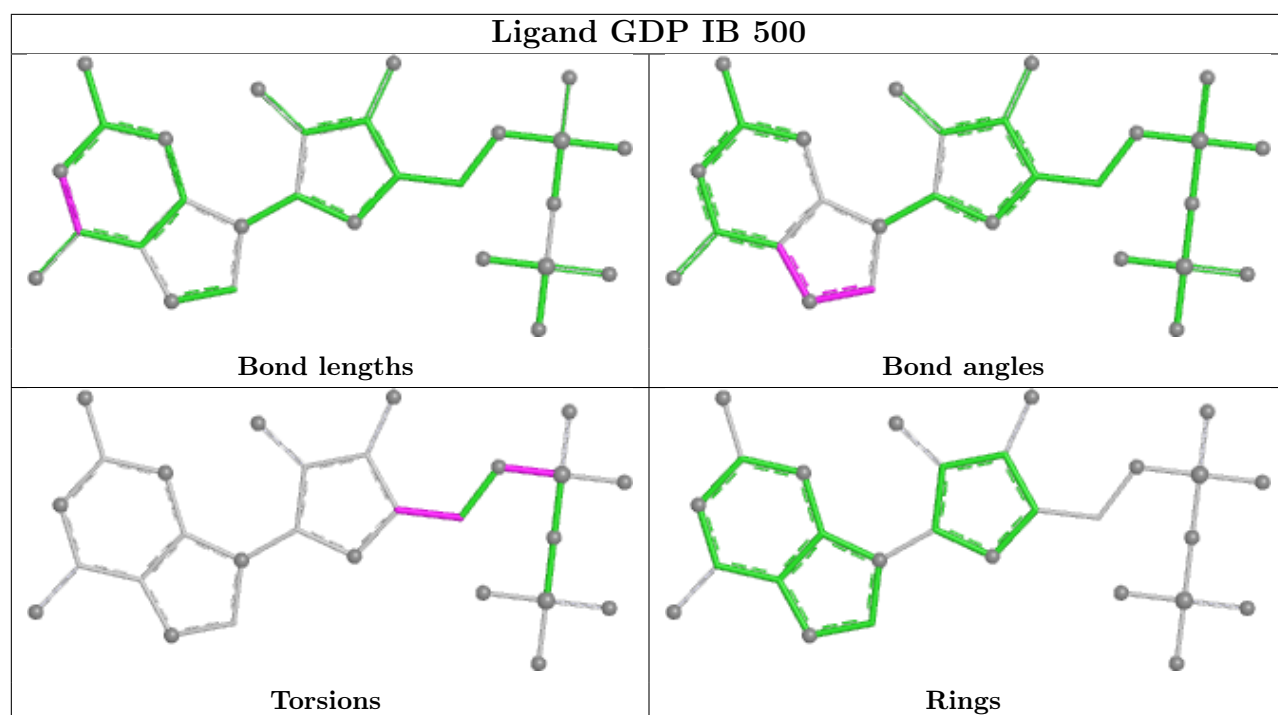


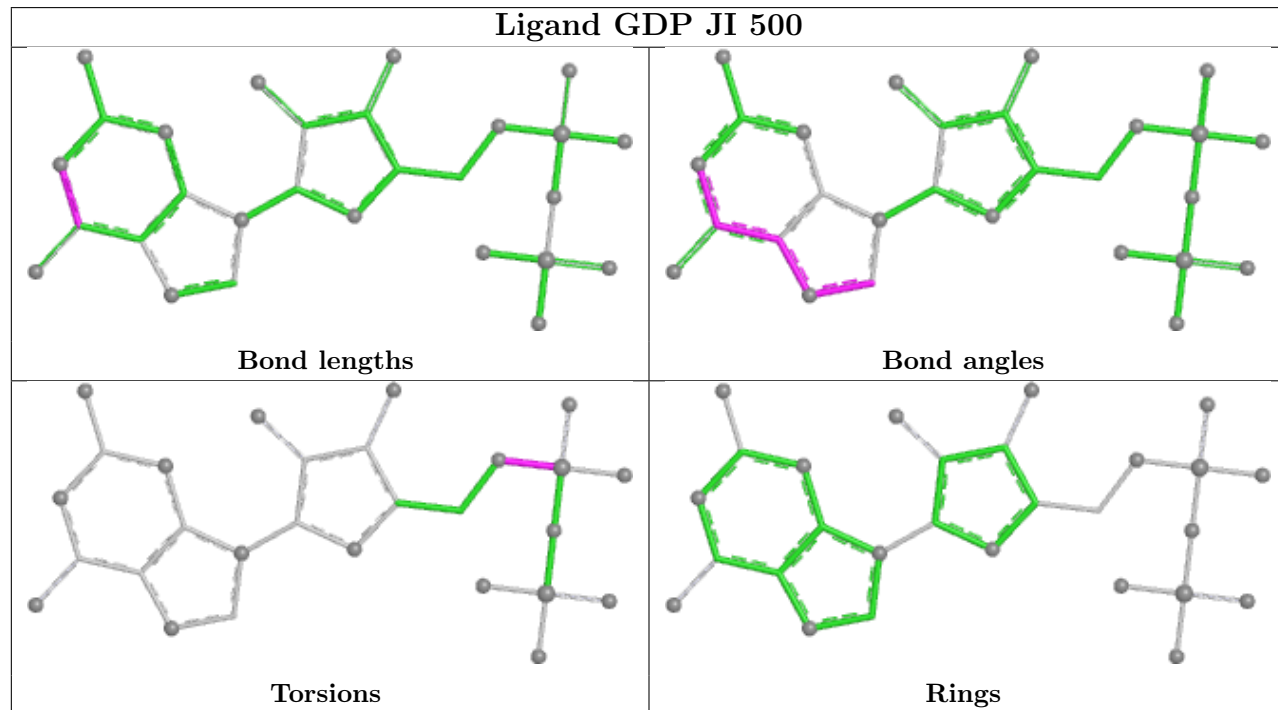
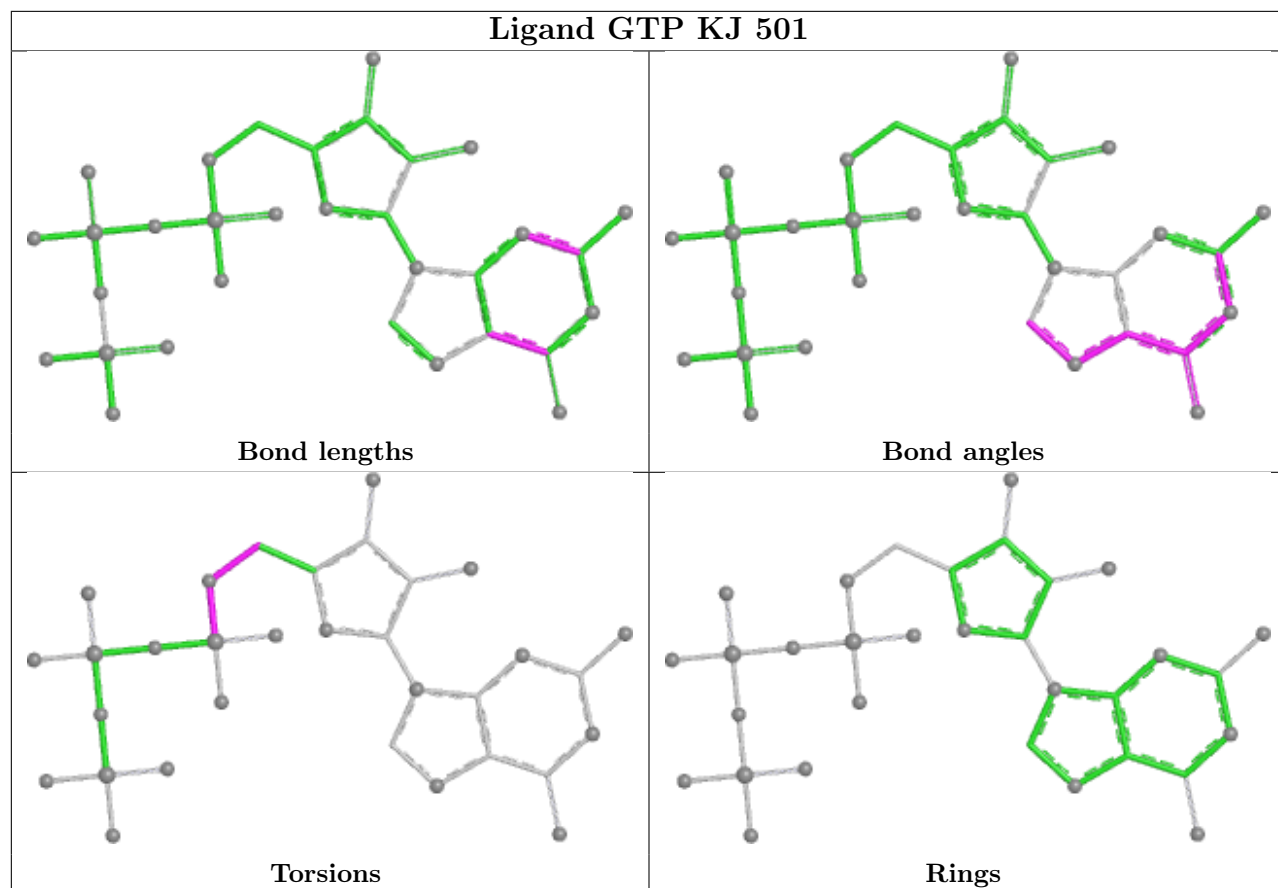
Ligand GTP J 501

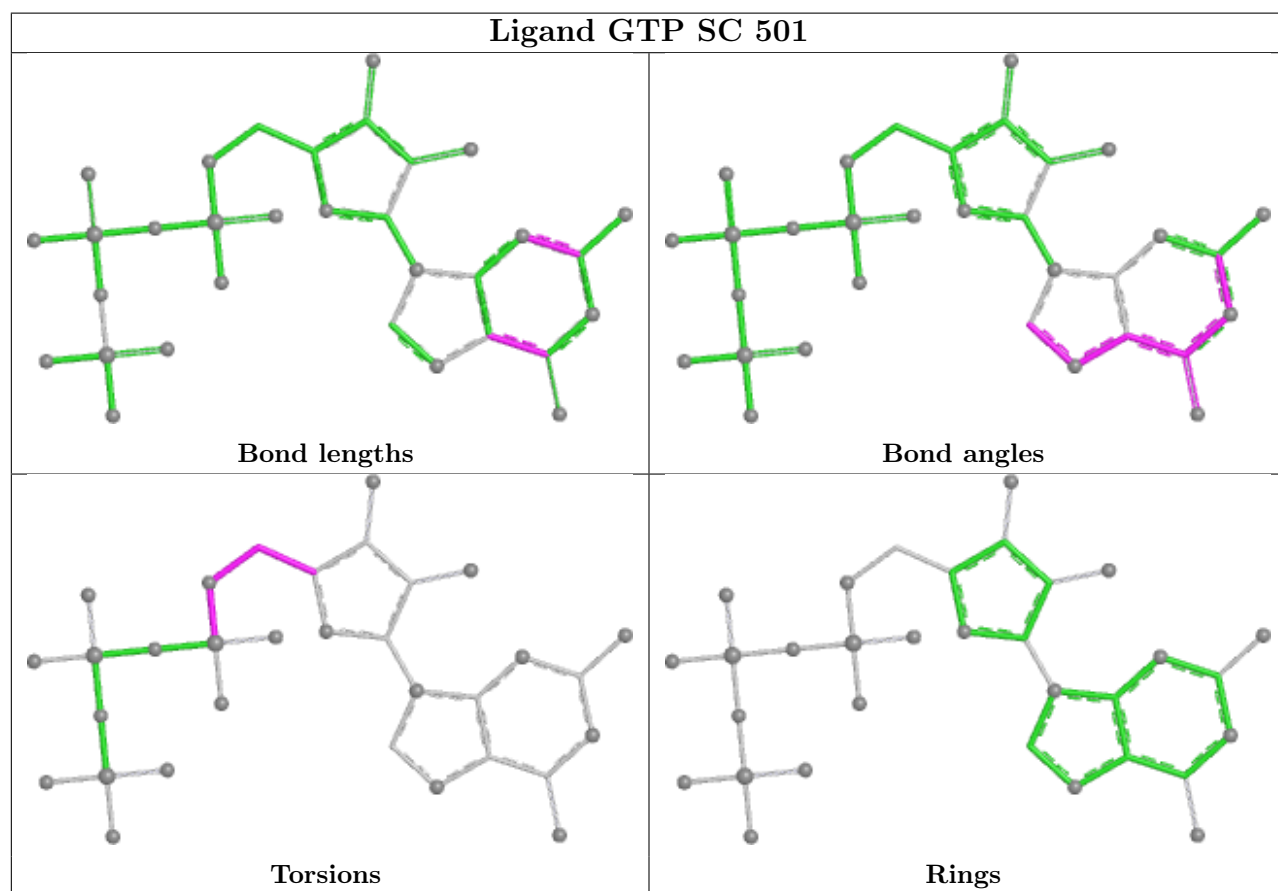
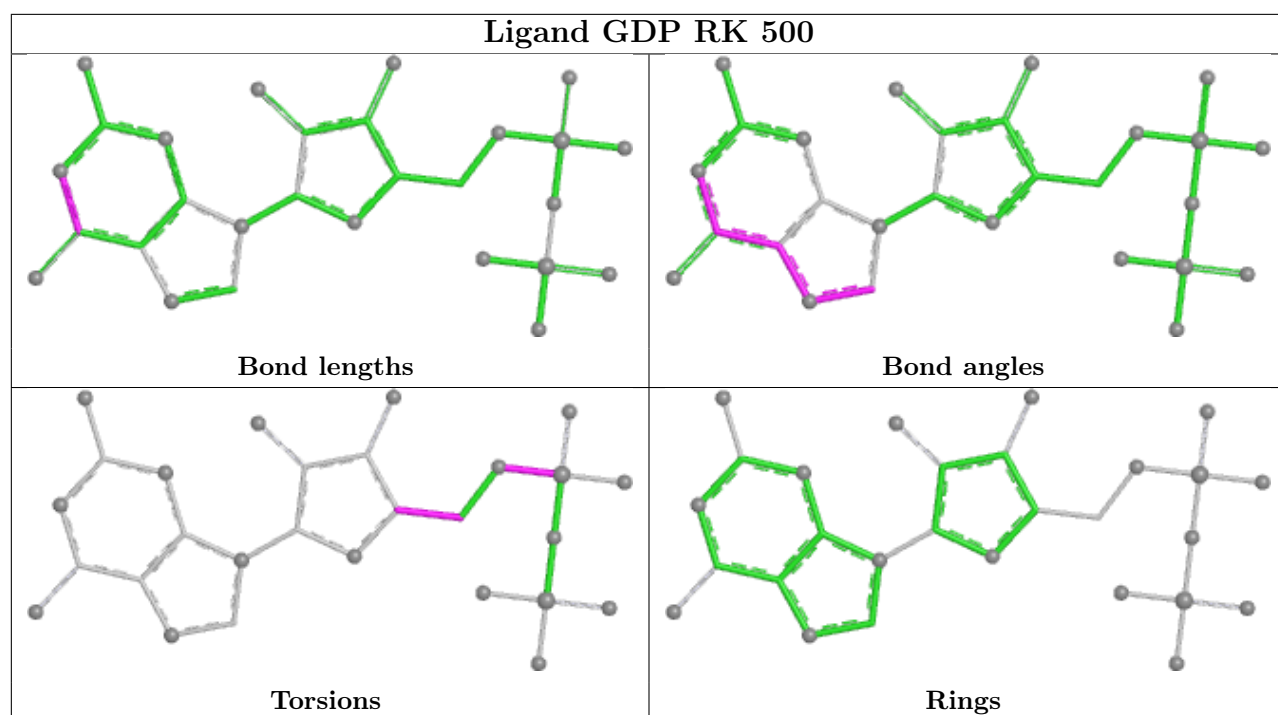


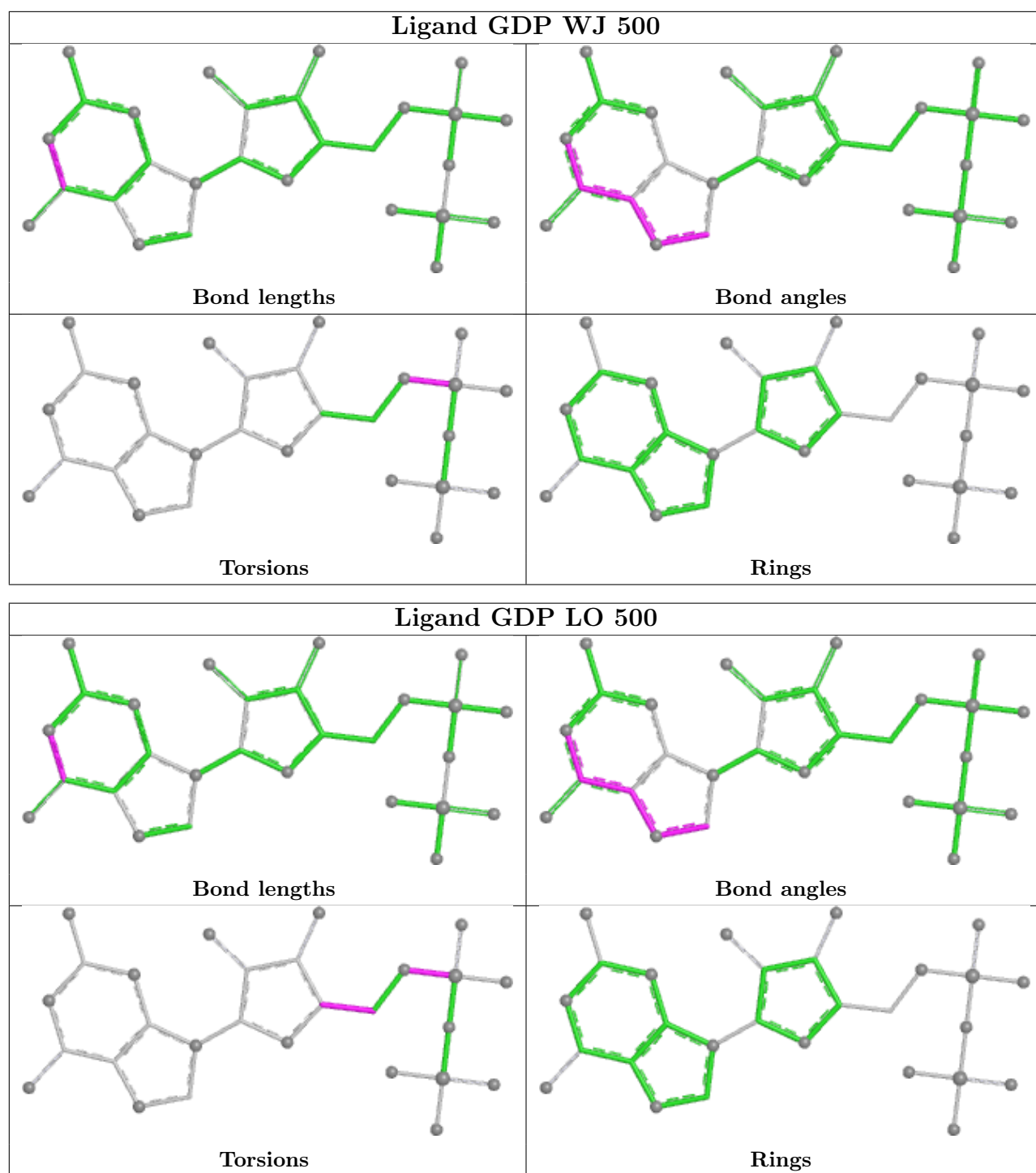
Ligand GTP R 501



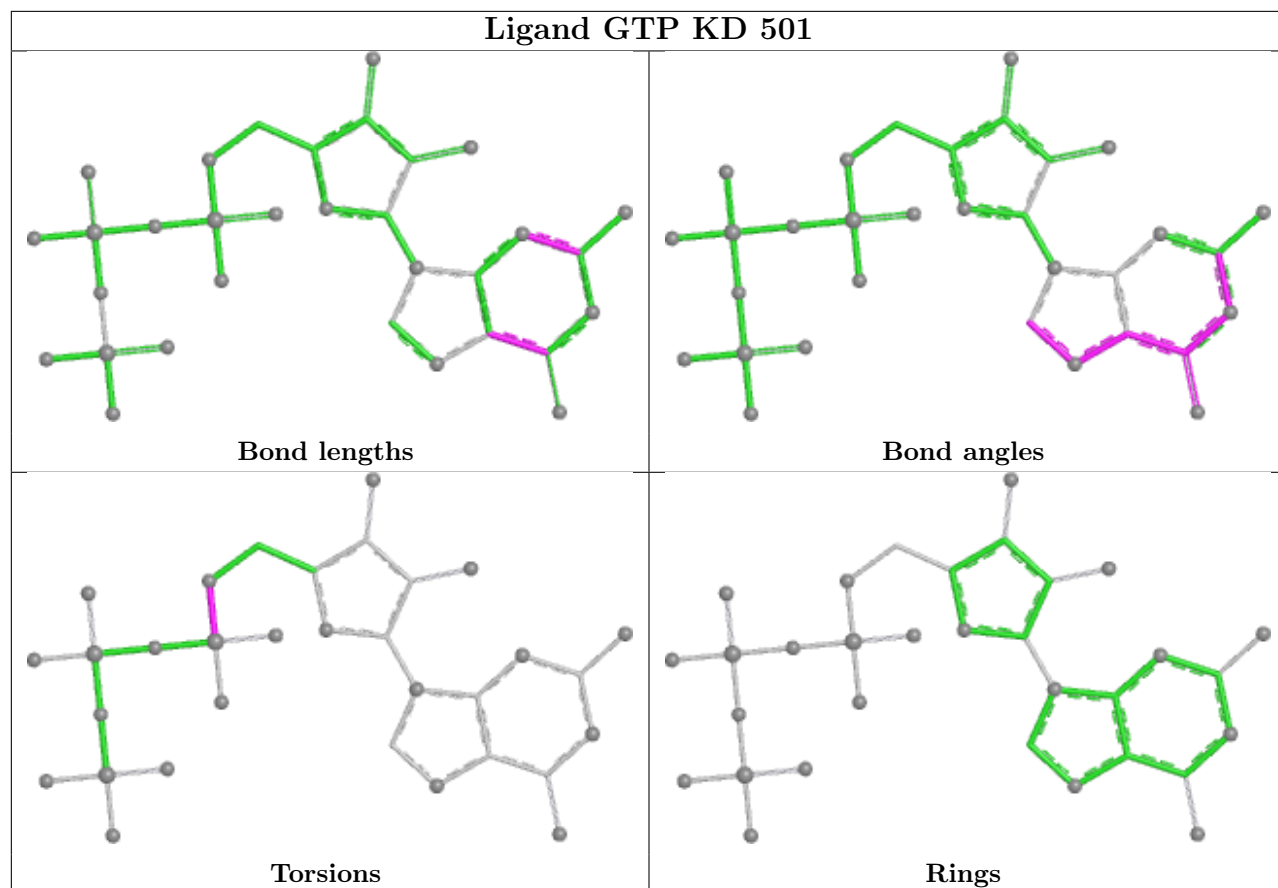




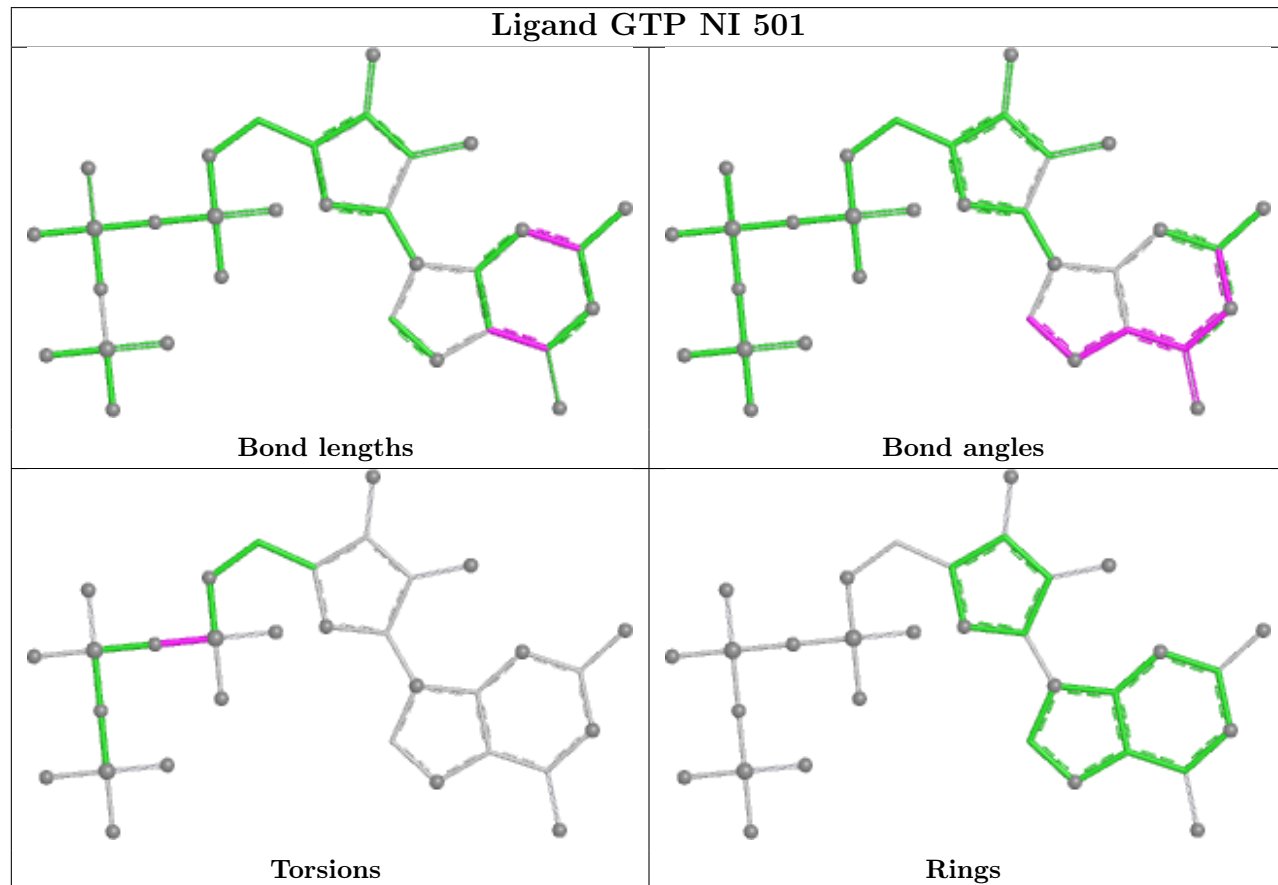


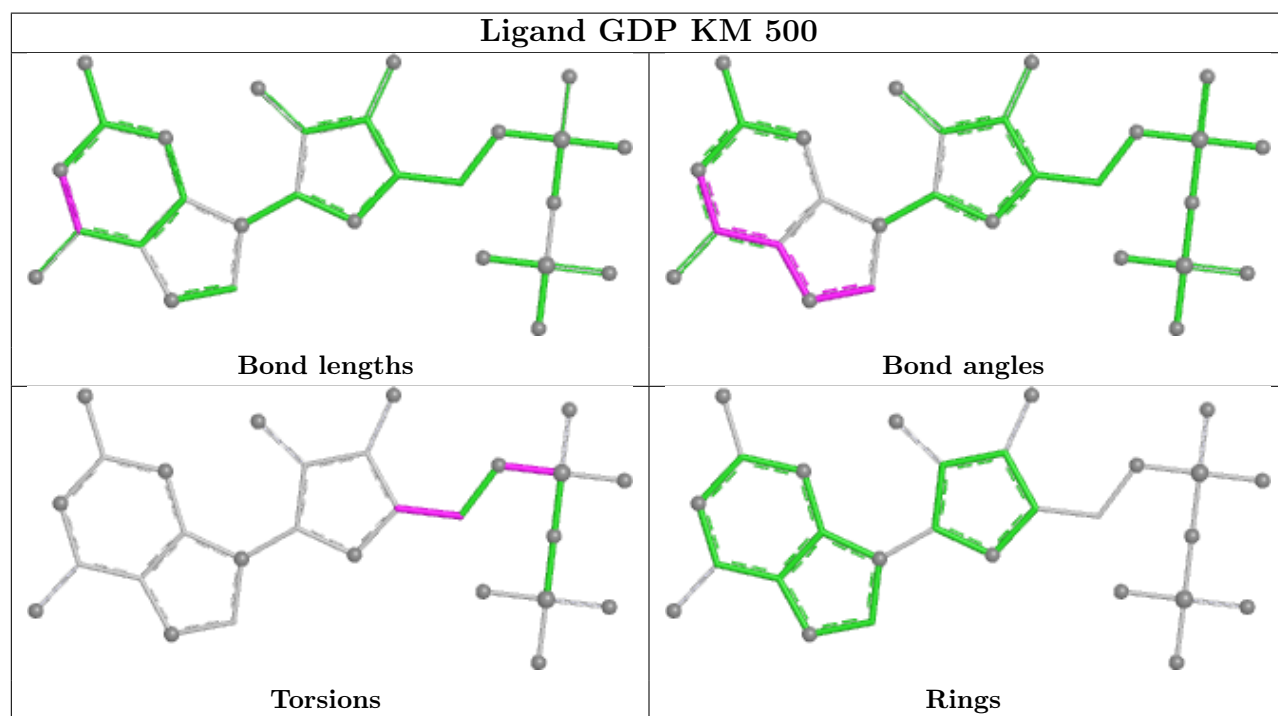
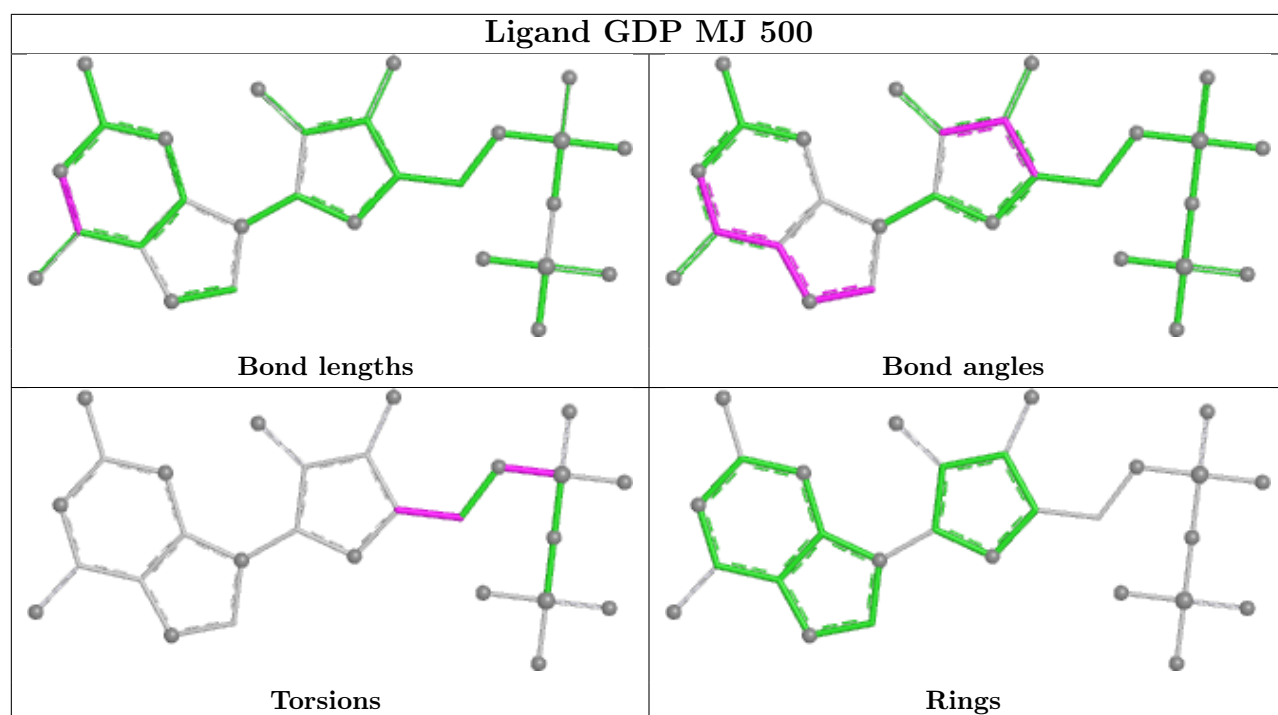


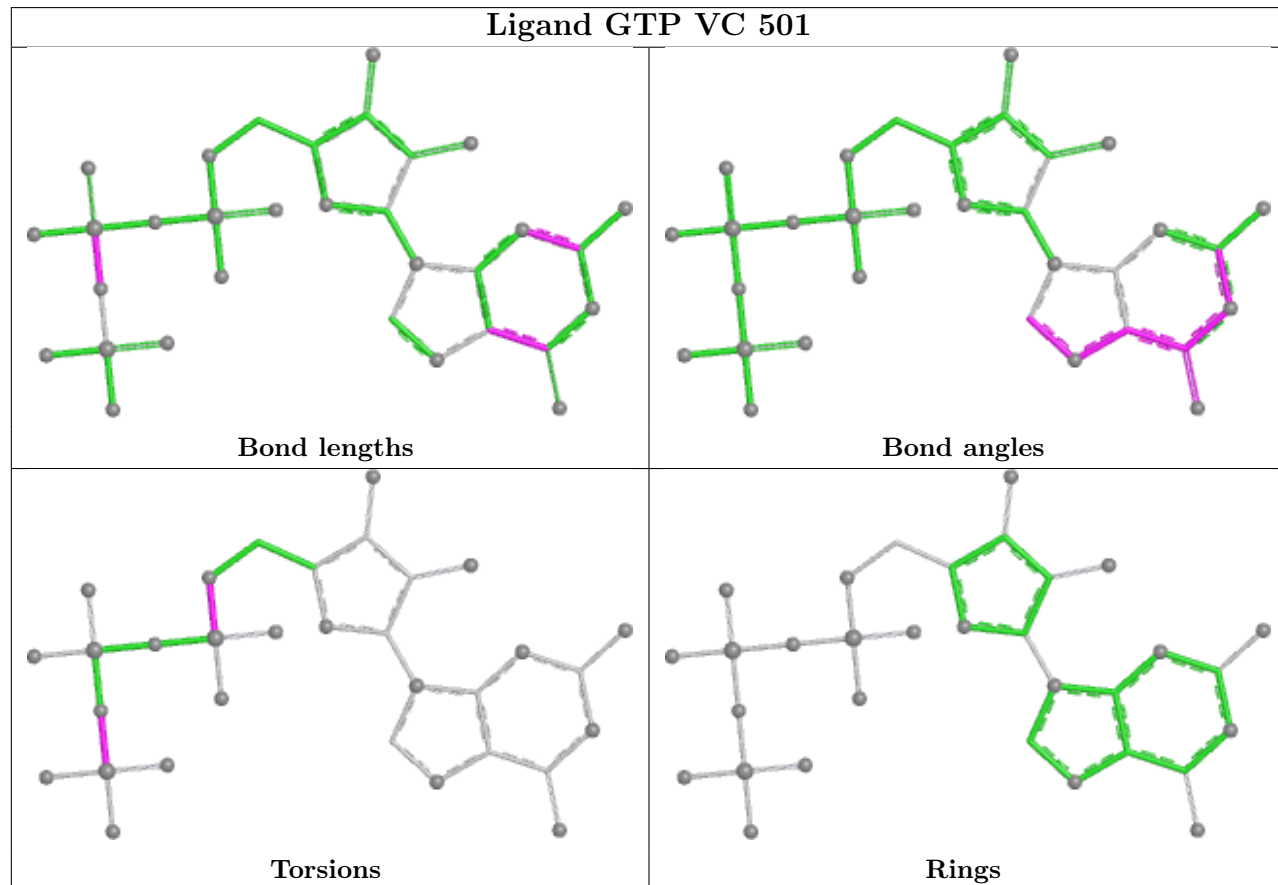
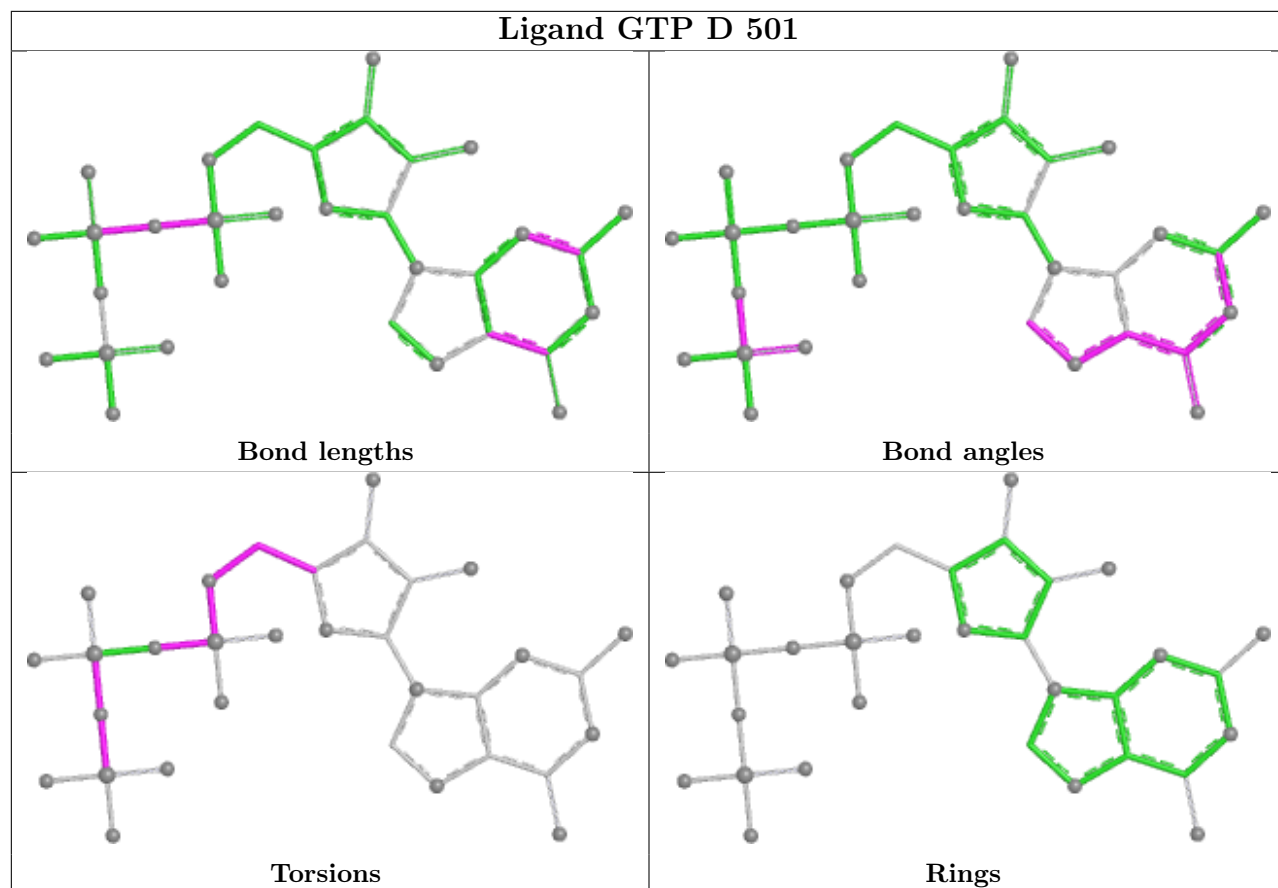
Ligand GTP KD 501

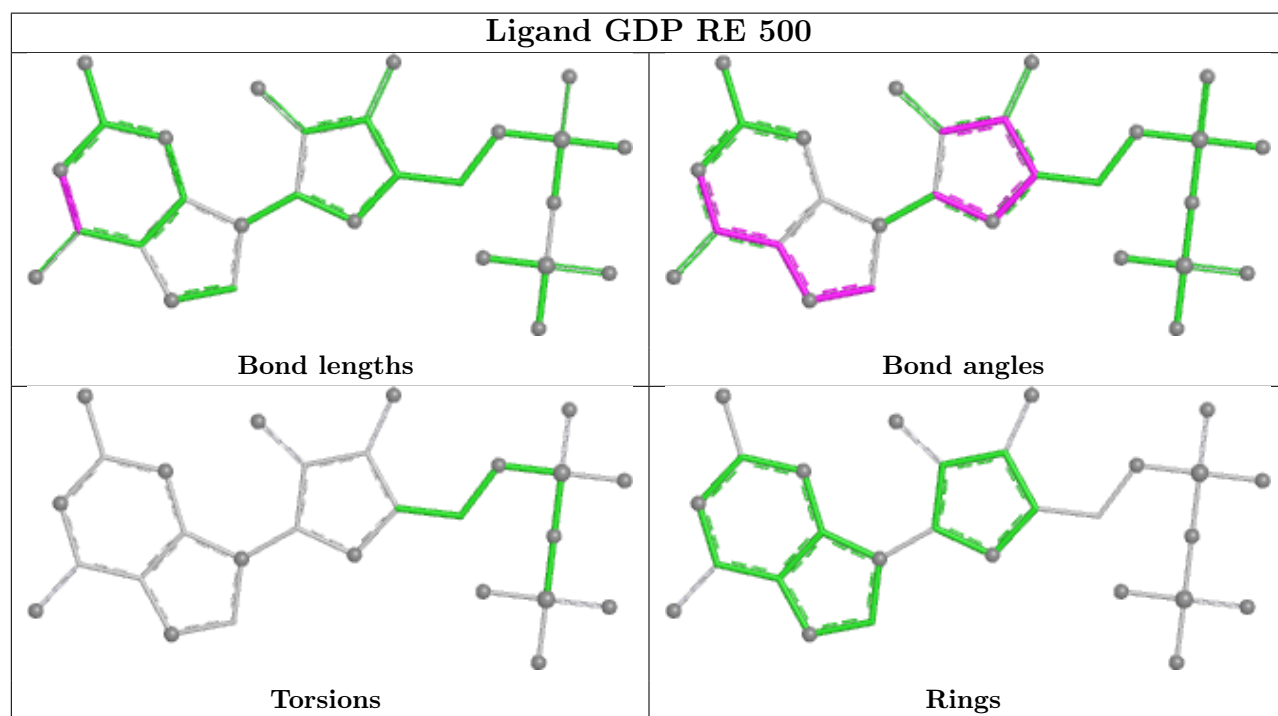
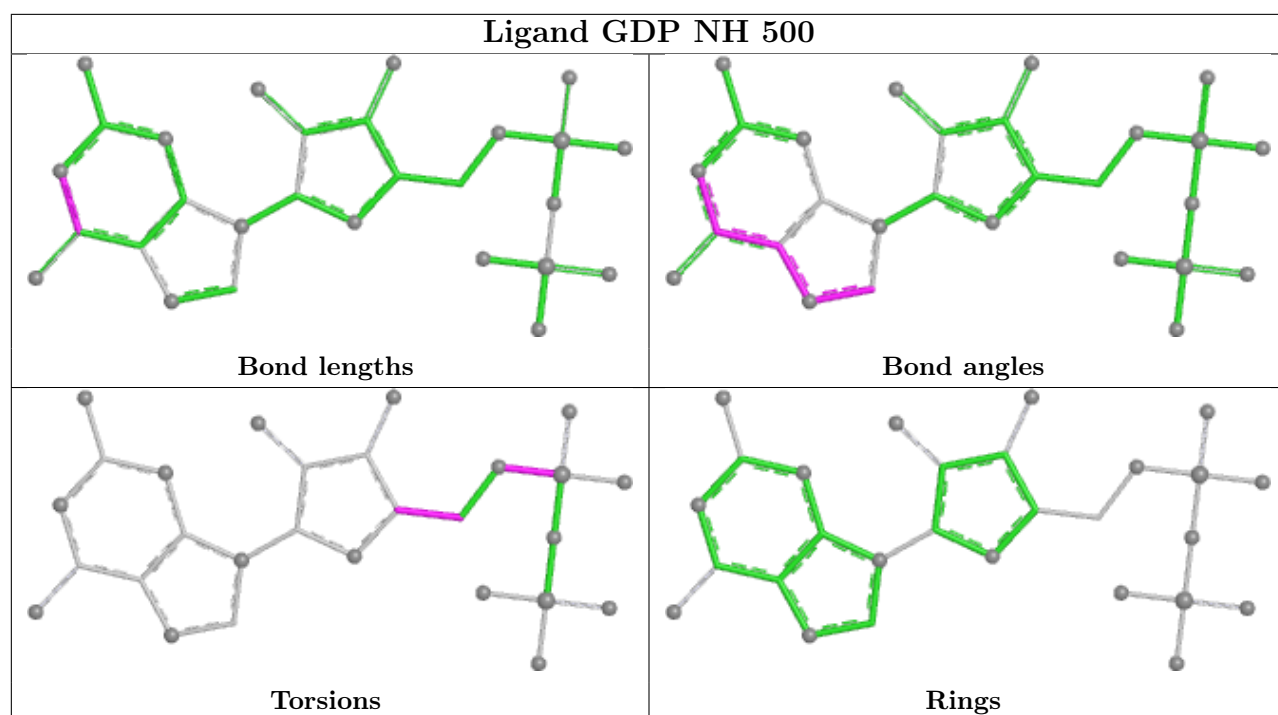


Ligand GTP NI 501

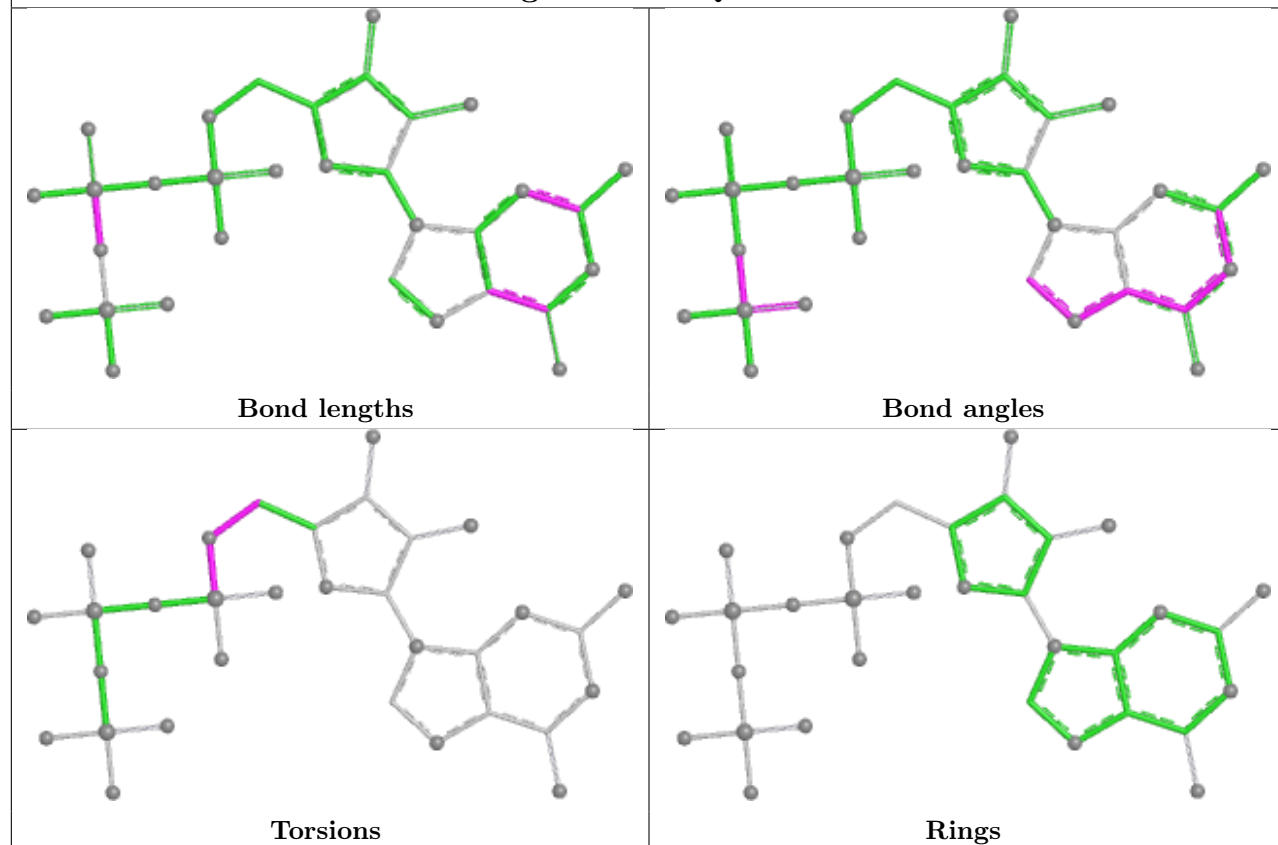




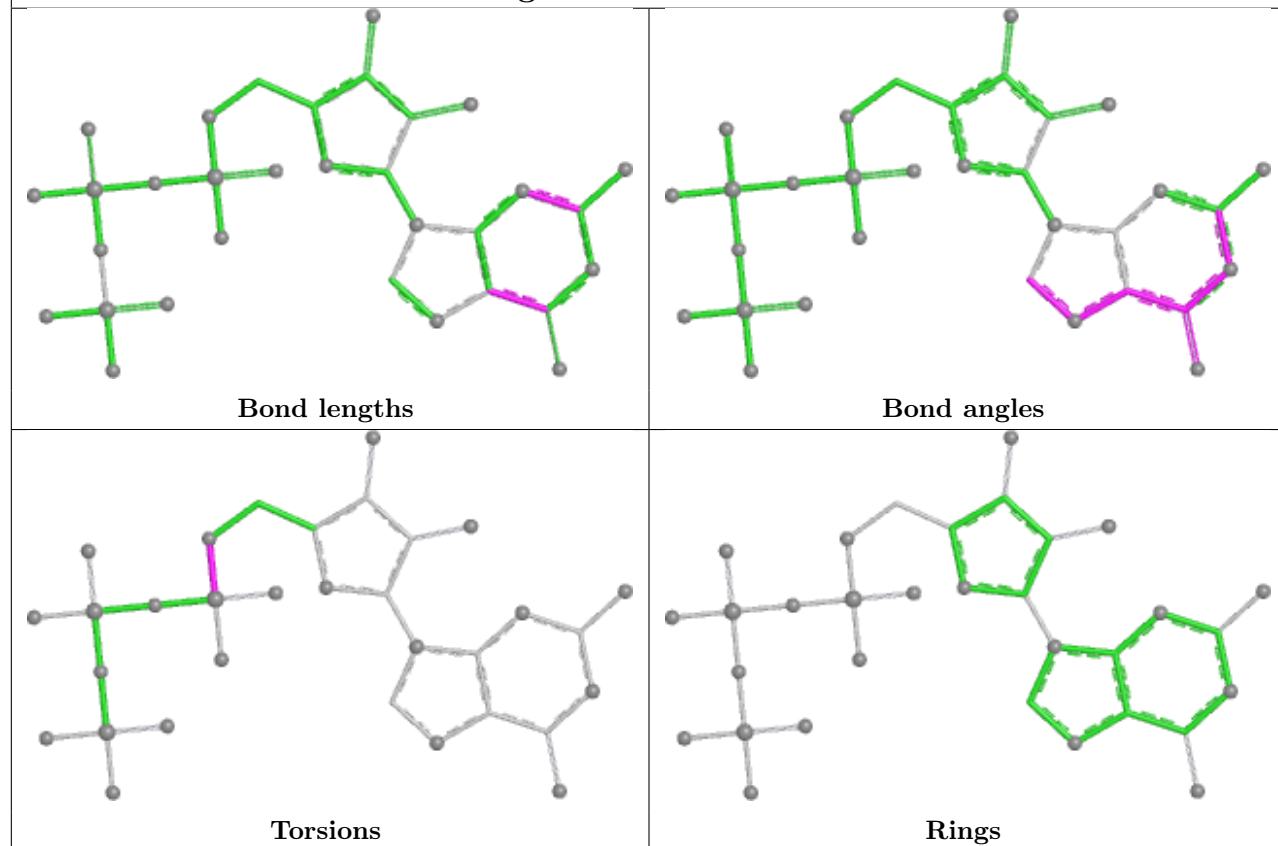




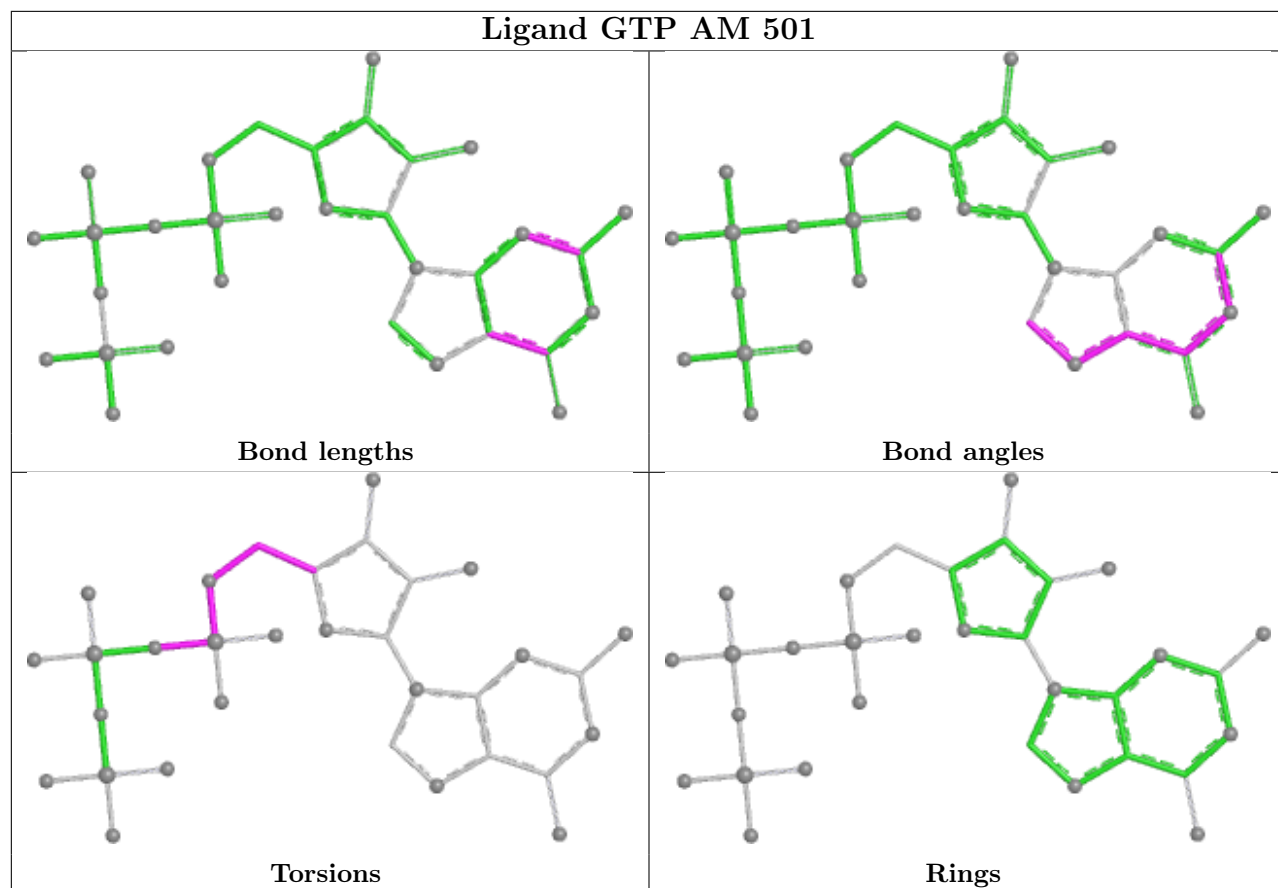
Ligand GTP QJ 501



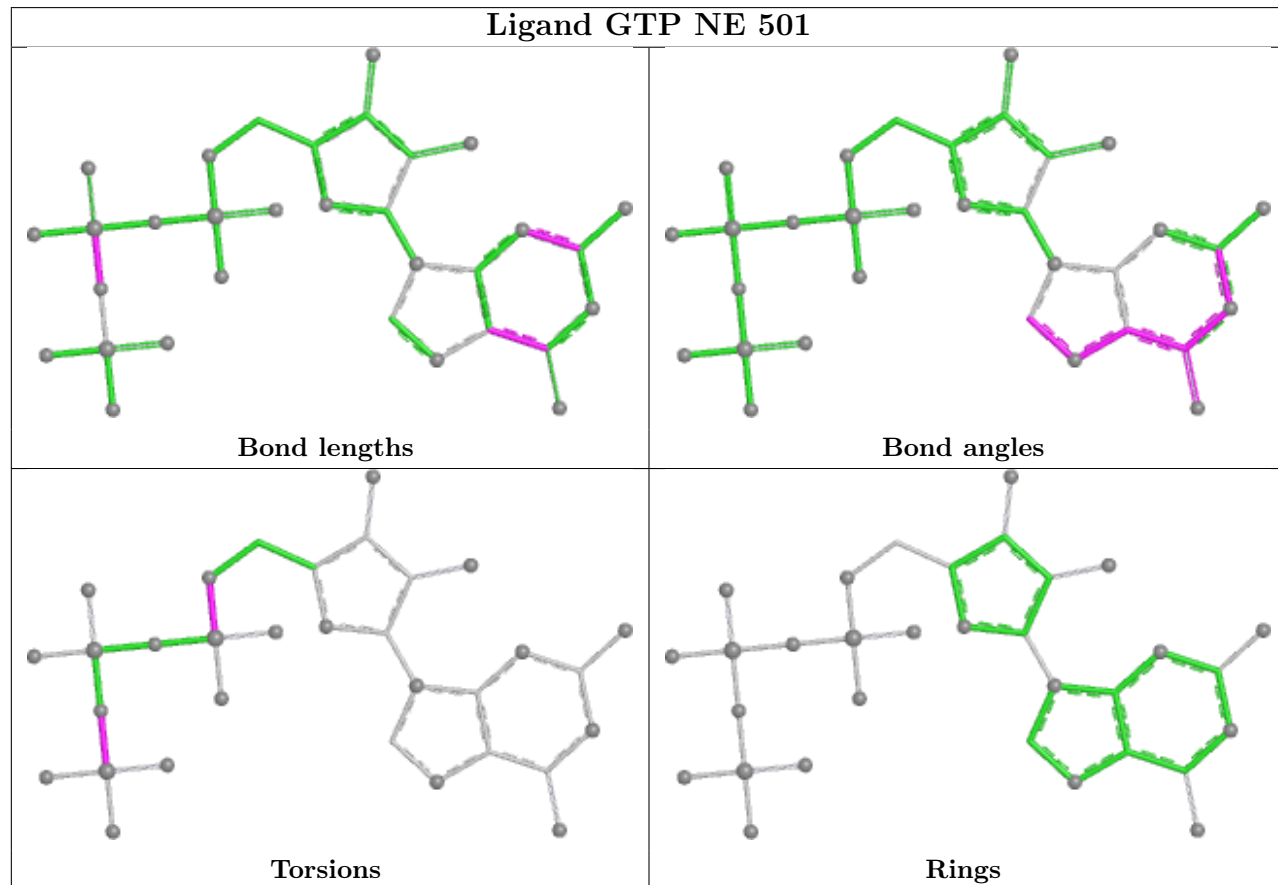
Ligand GTP CB 501

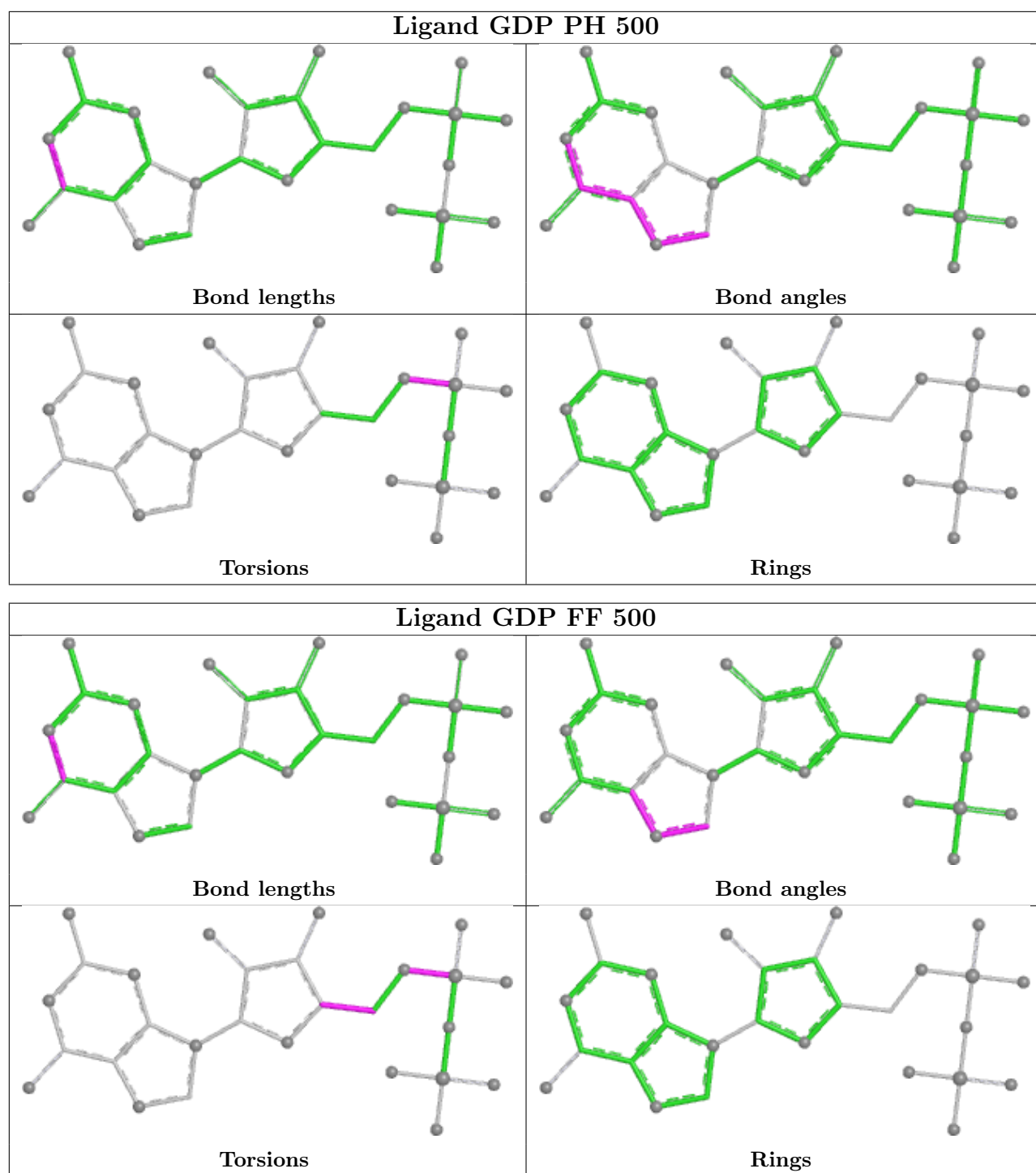


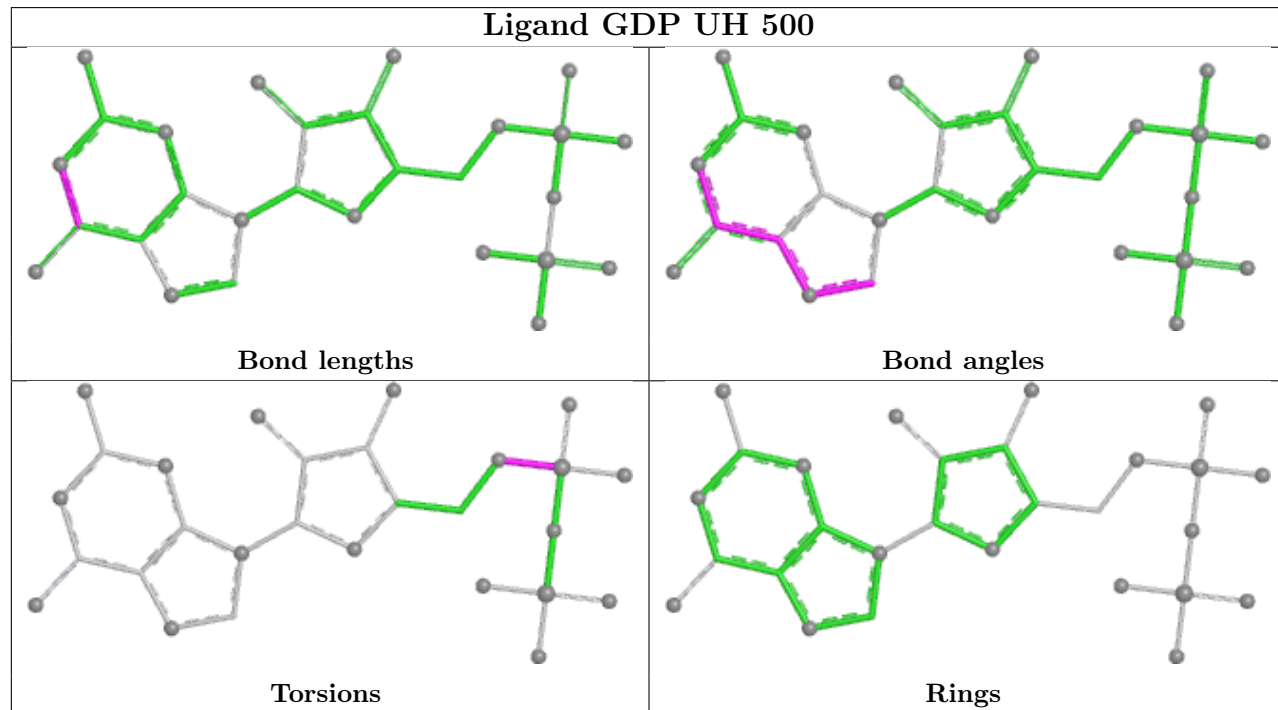
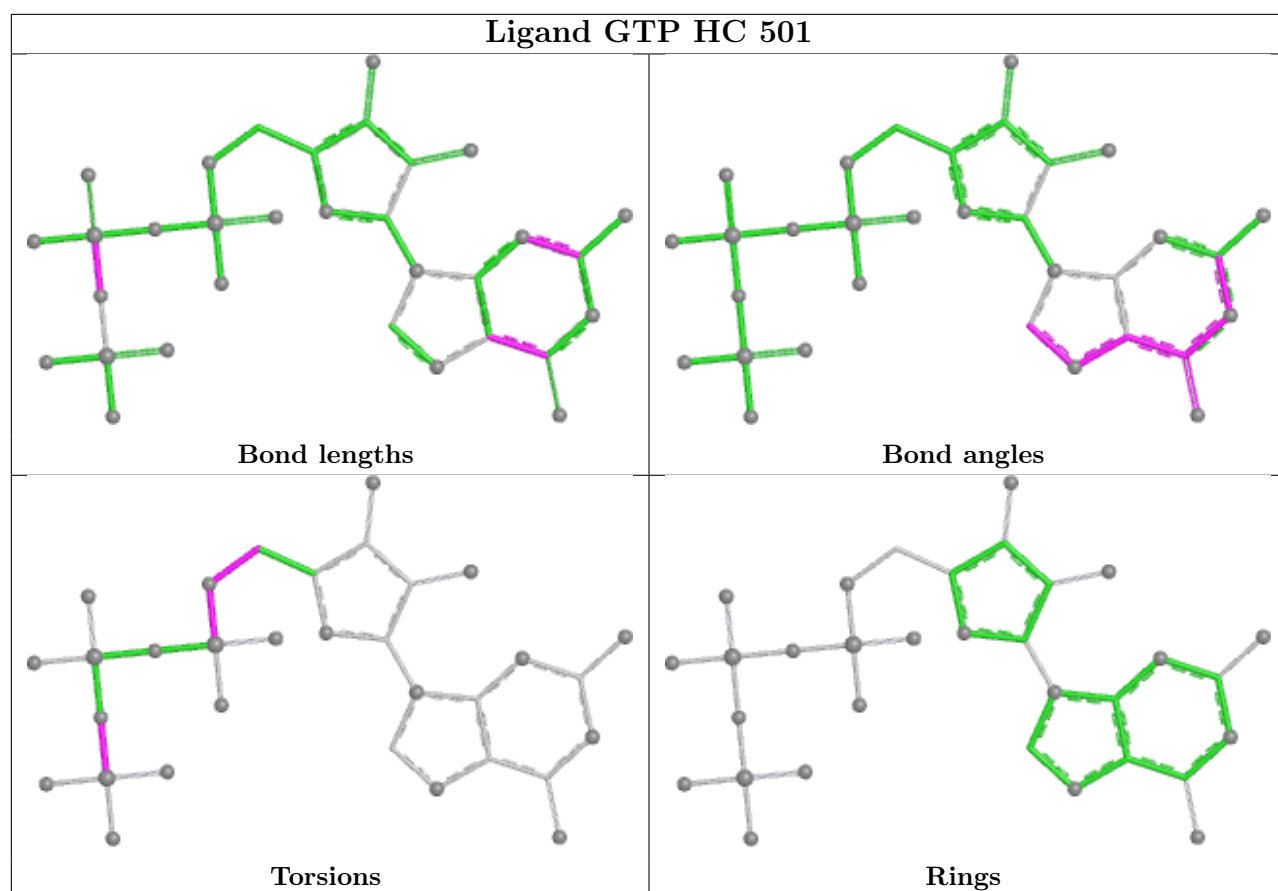
Ligand GTP AM 501

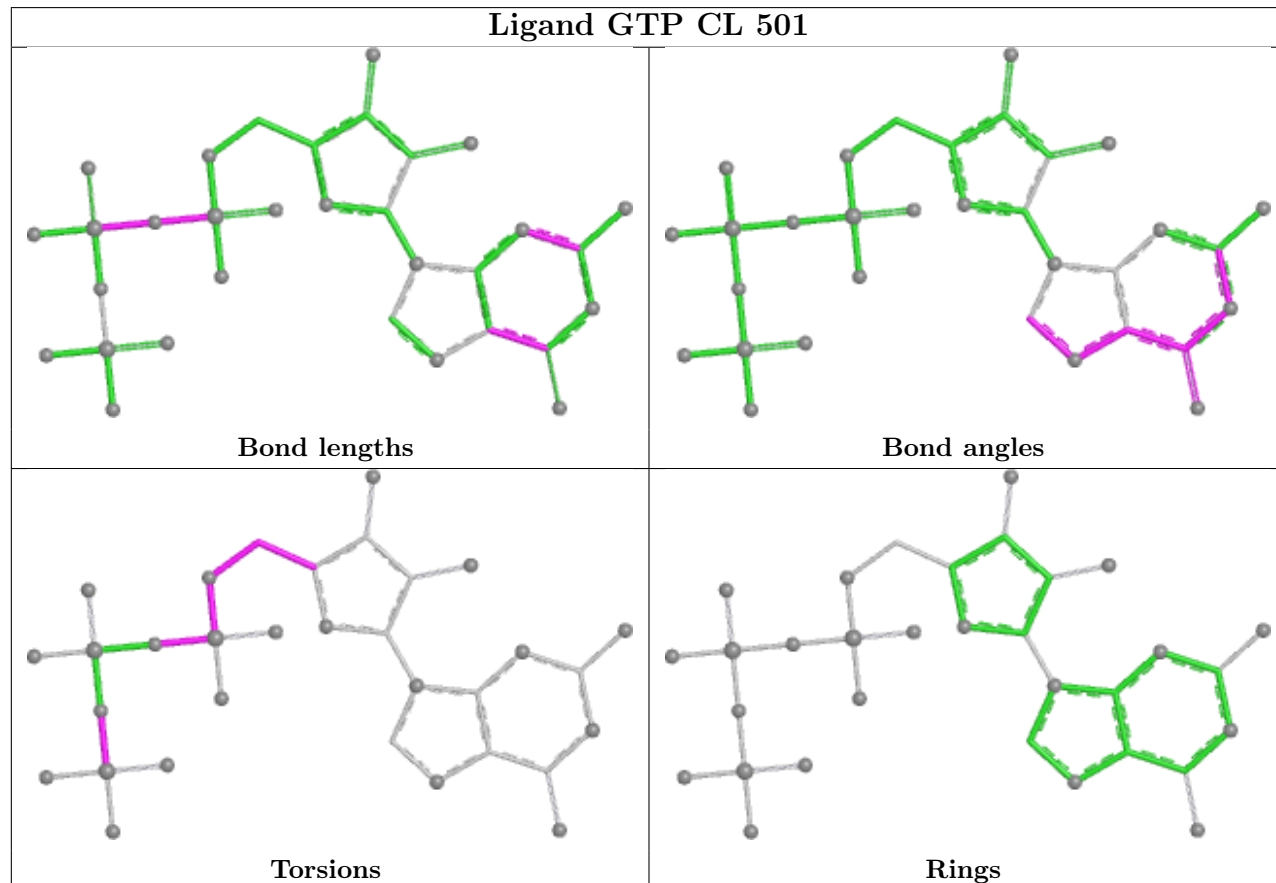
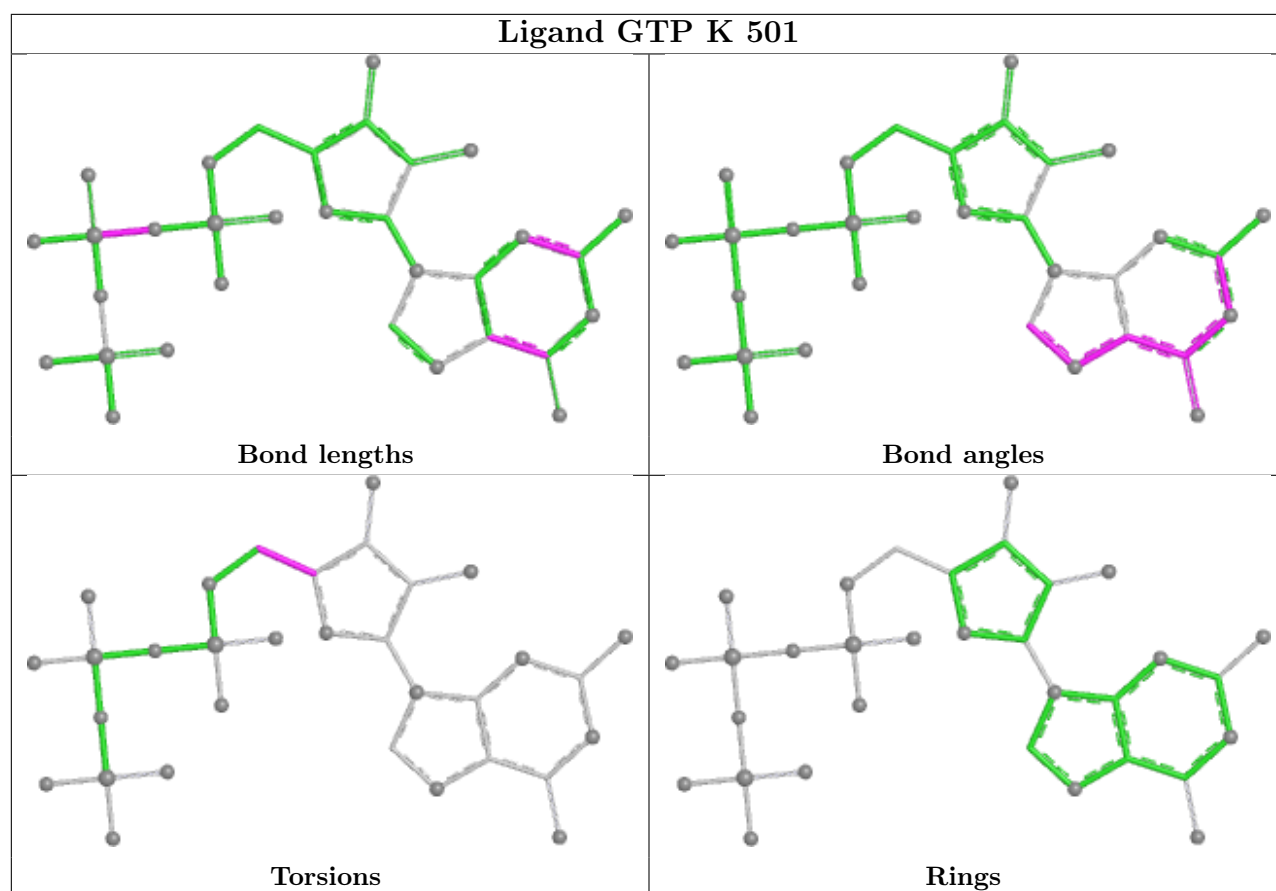


Ligand GTP NE 501

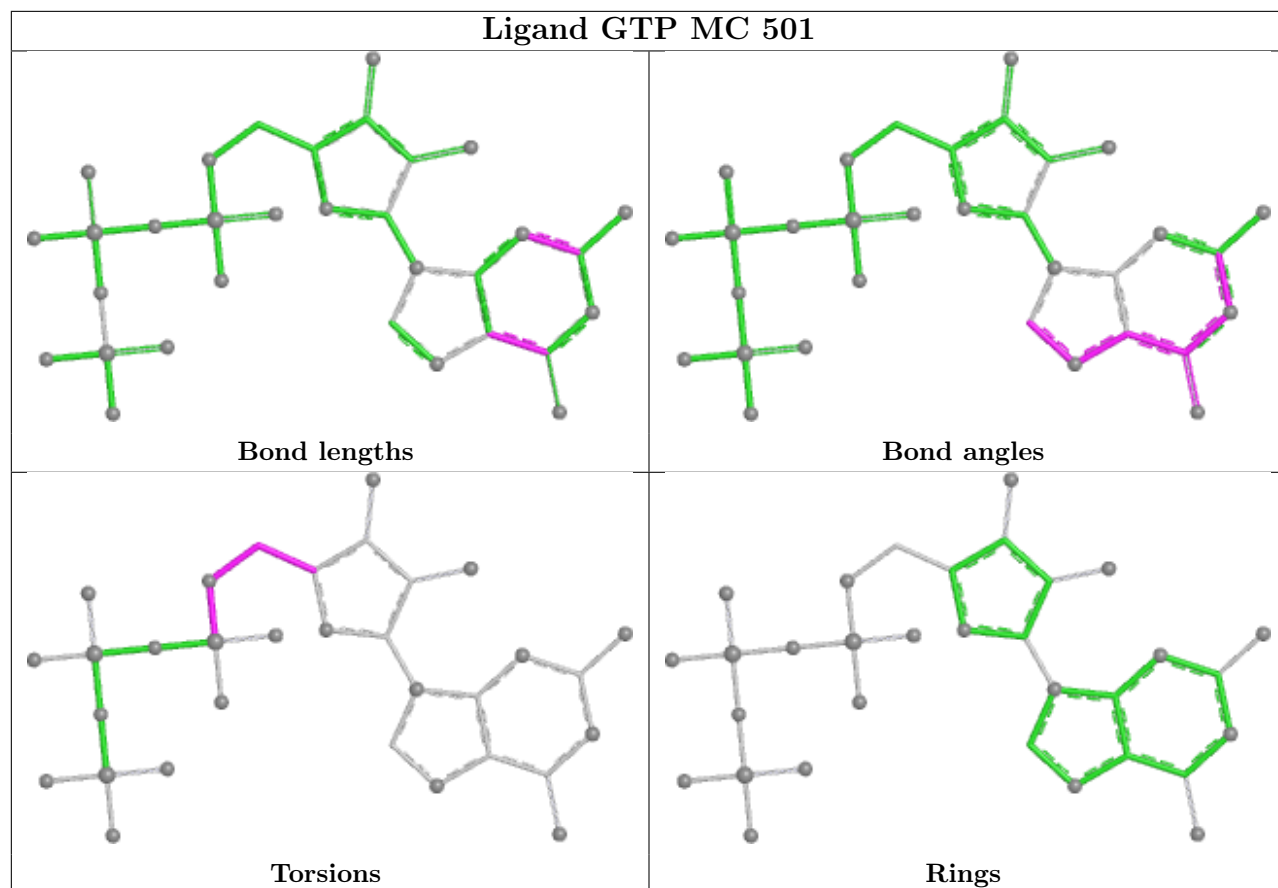




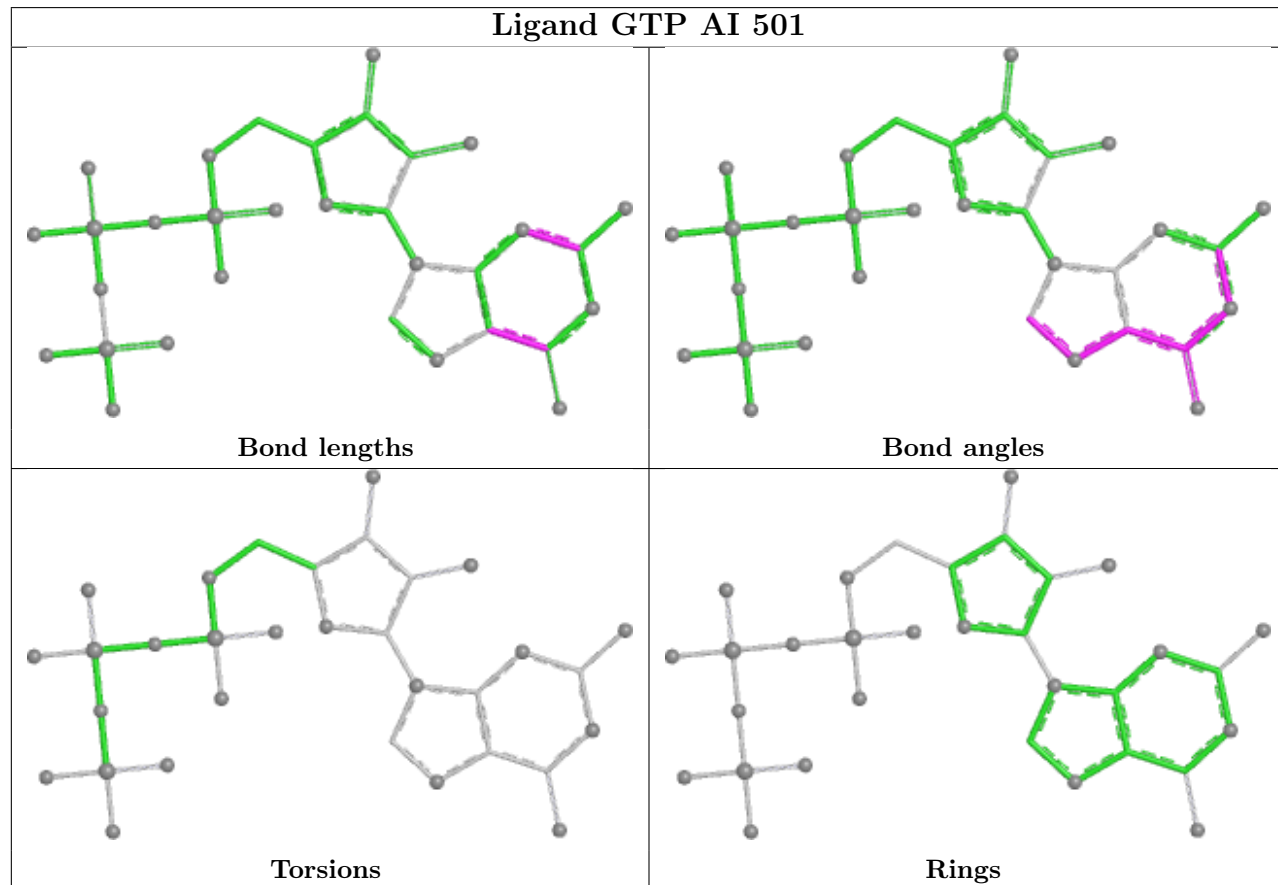


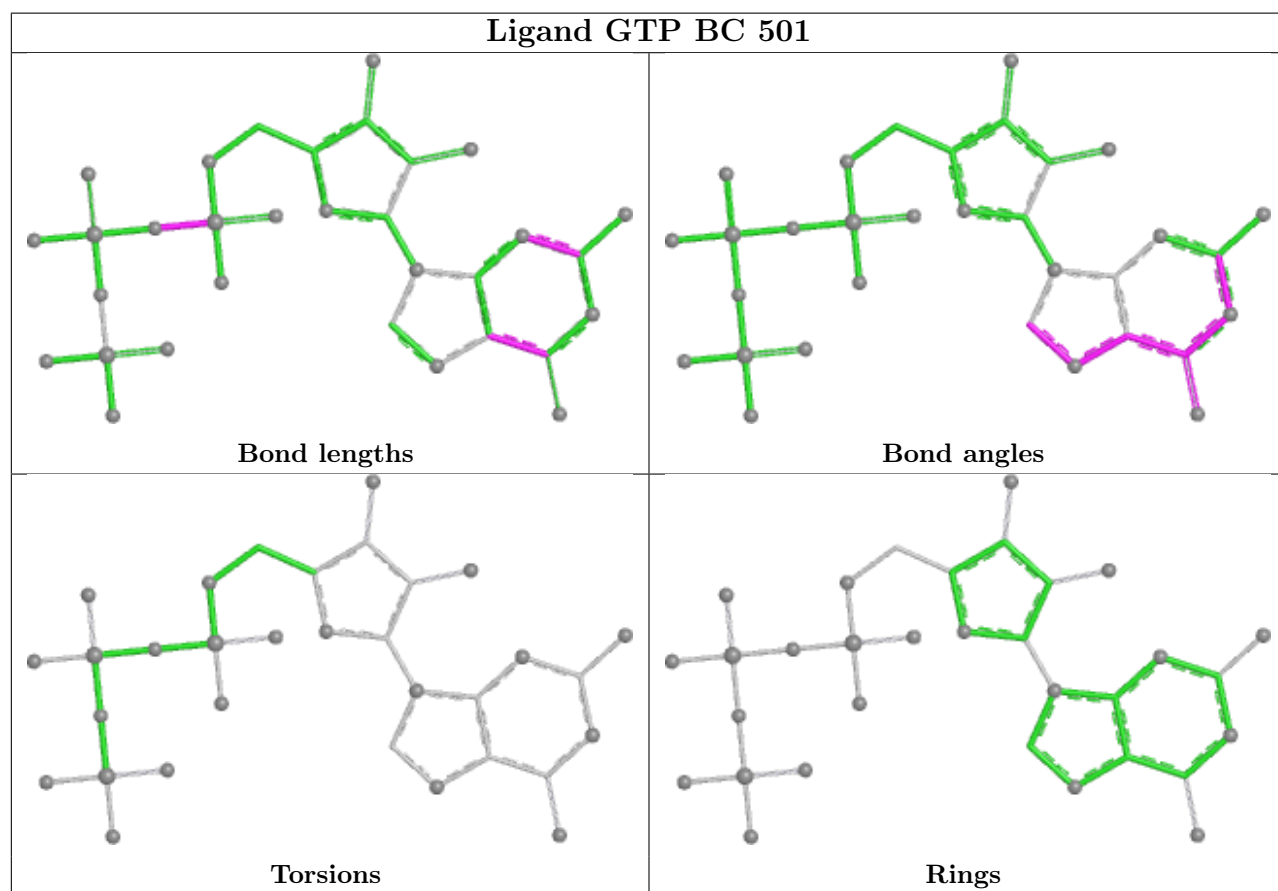
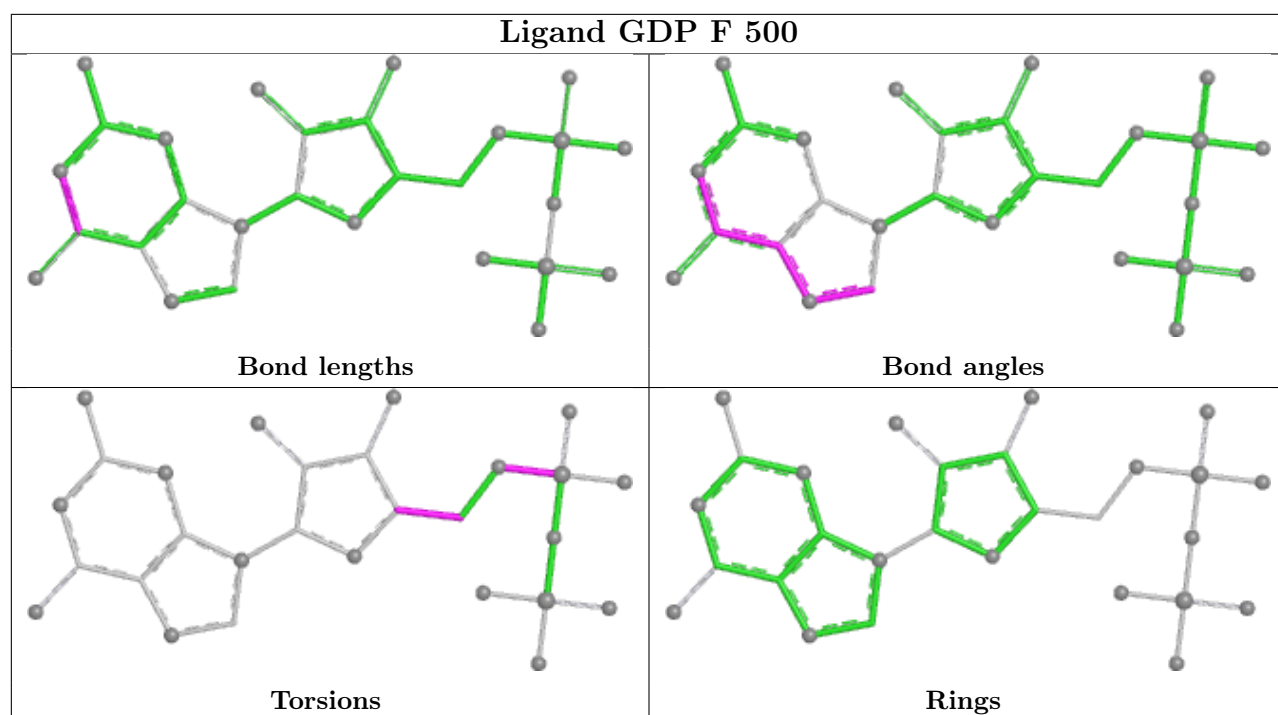


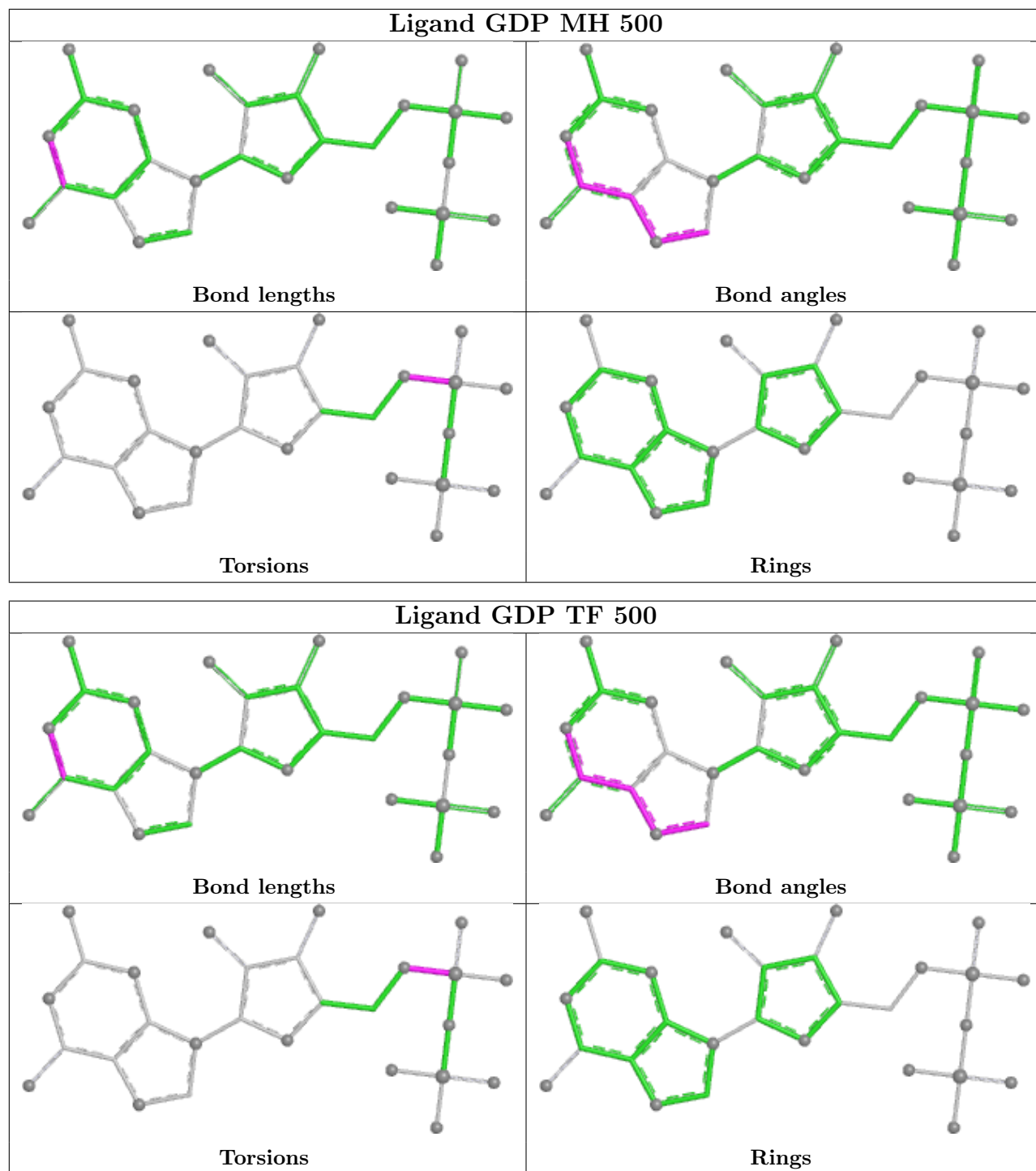
Ligand GTP MC 501



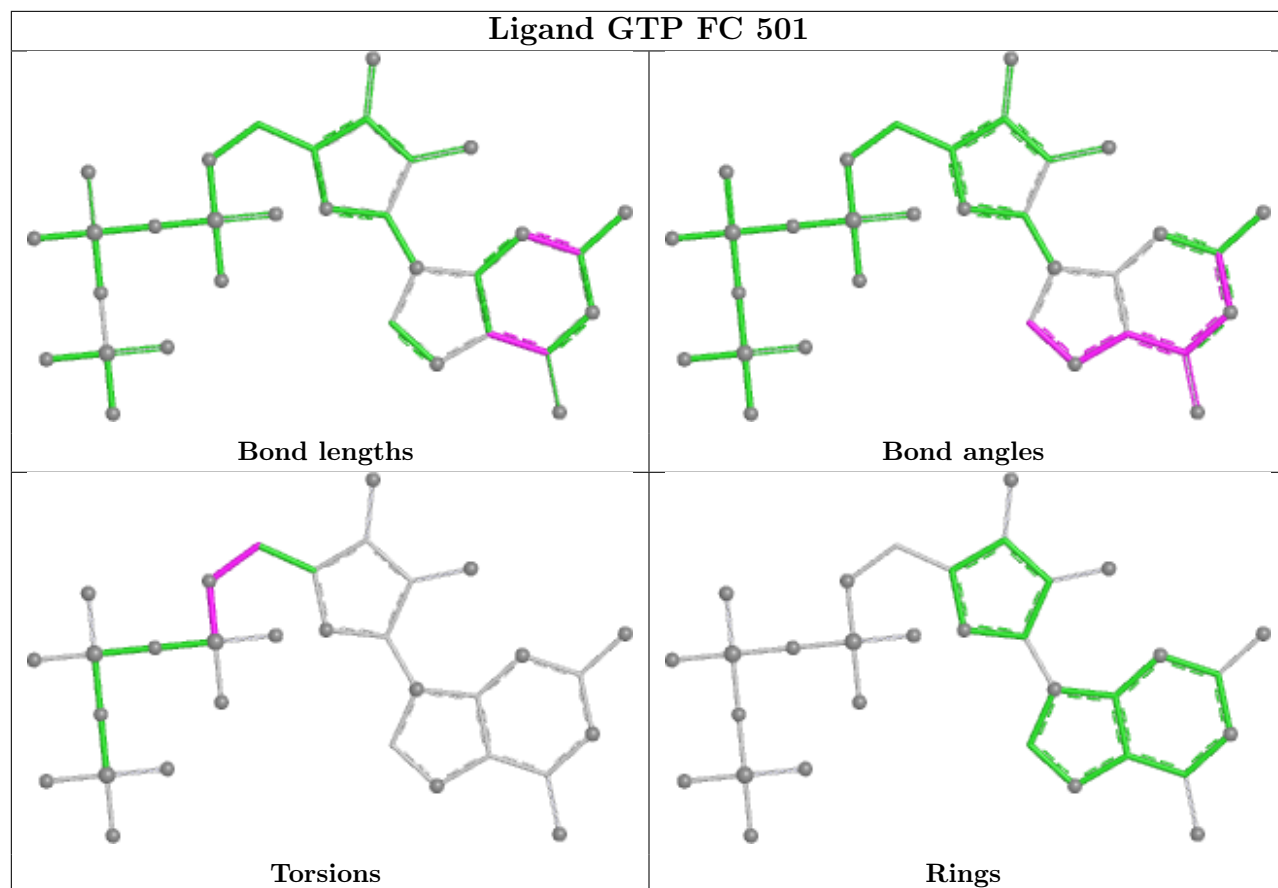
Ligand GTP AI 501



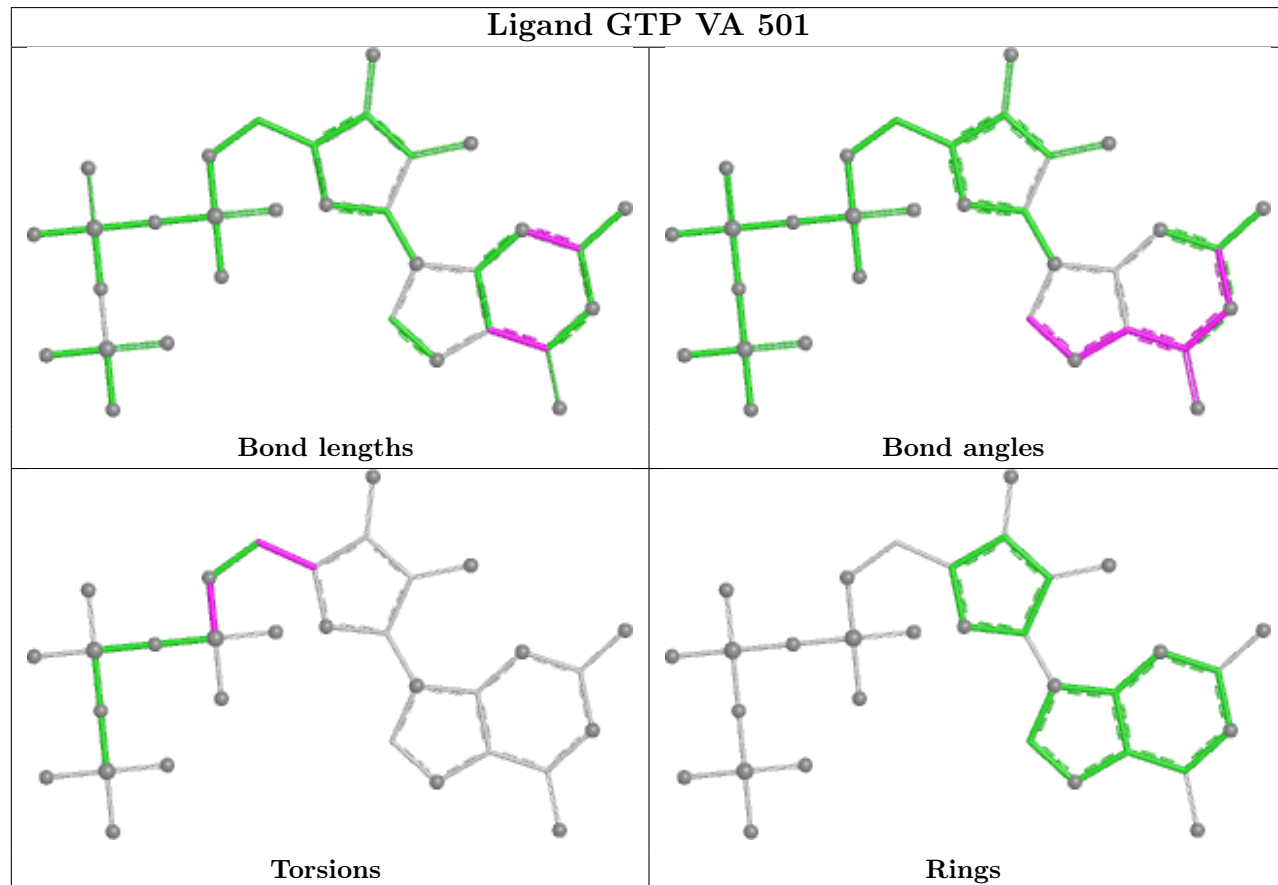


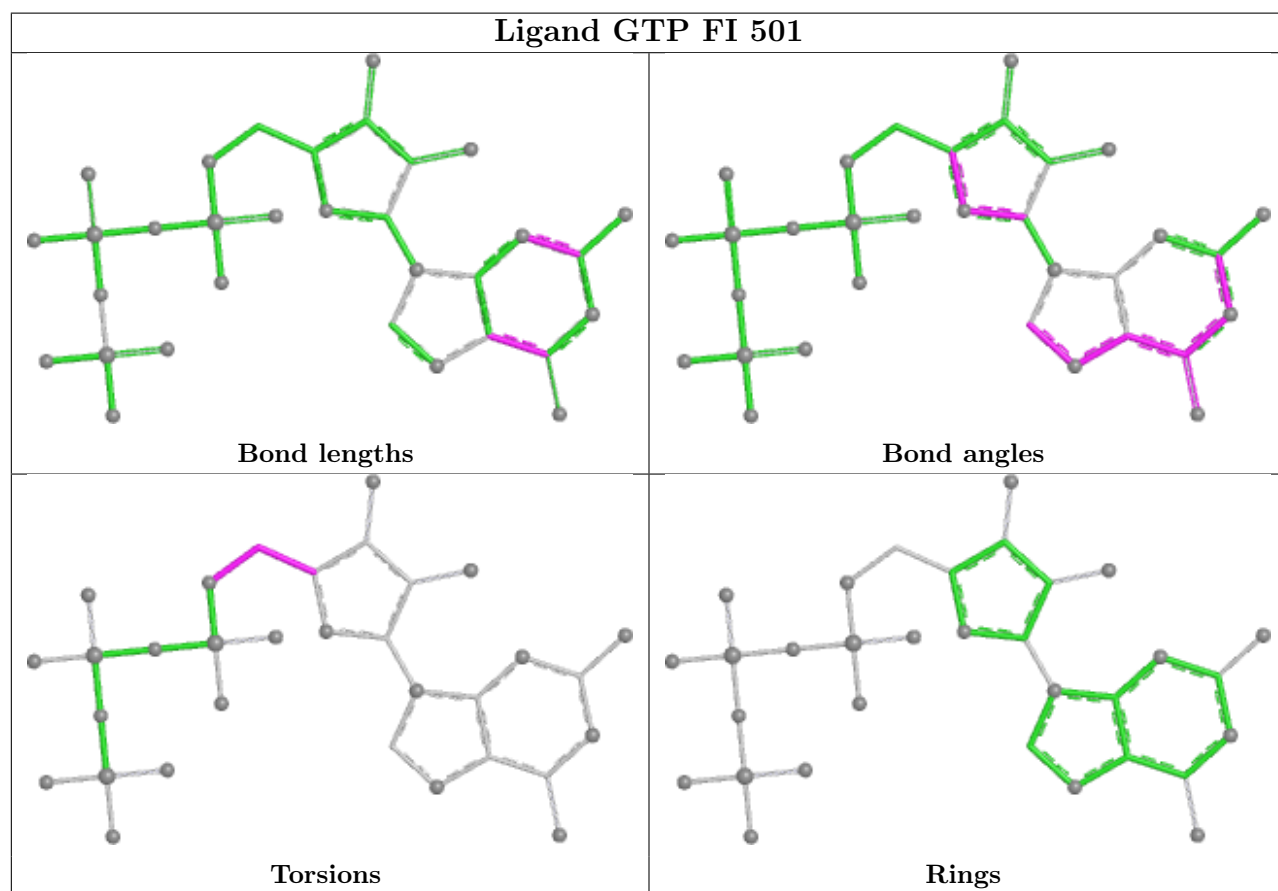
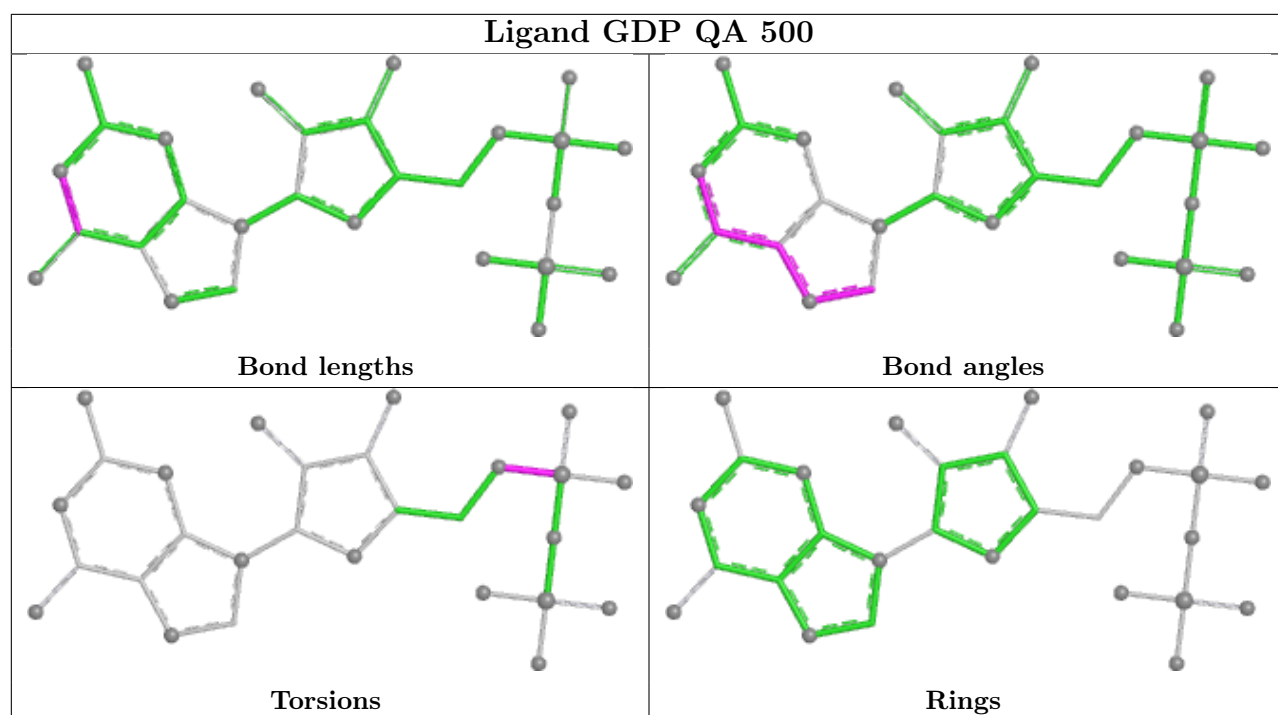


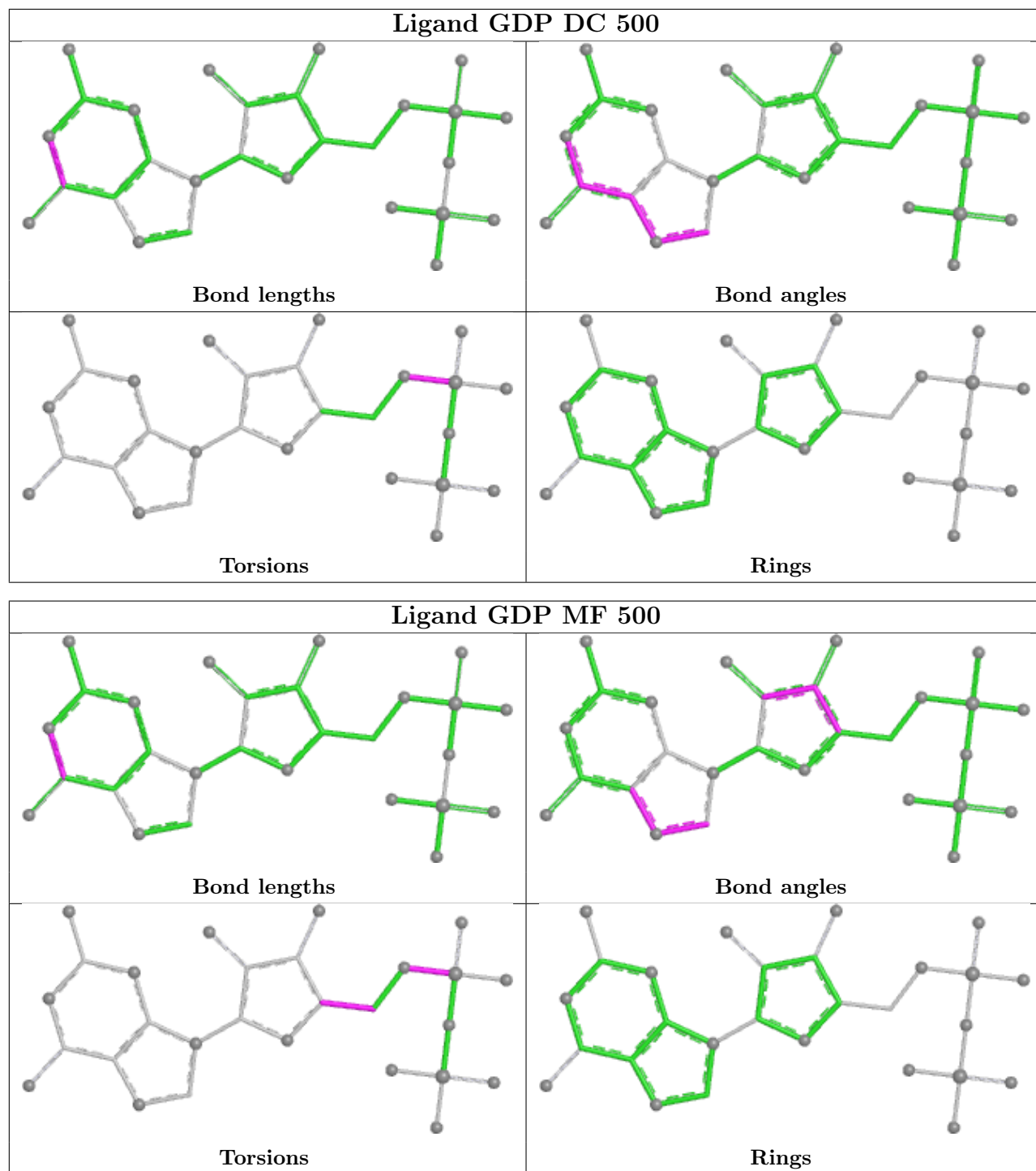
Ligand GTP FC 501



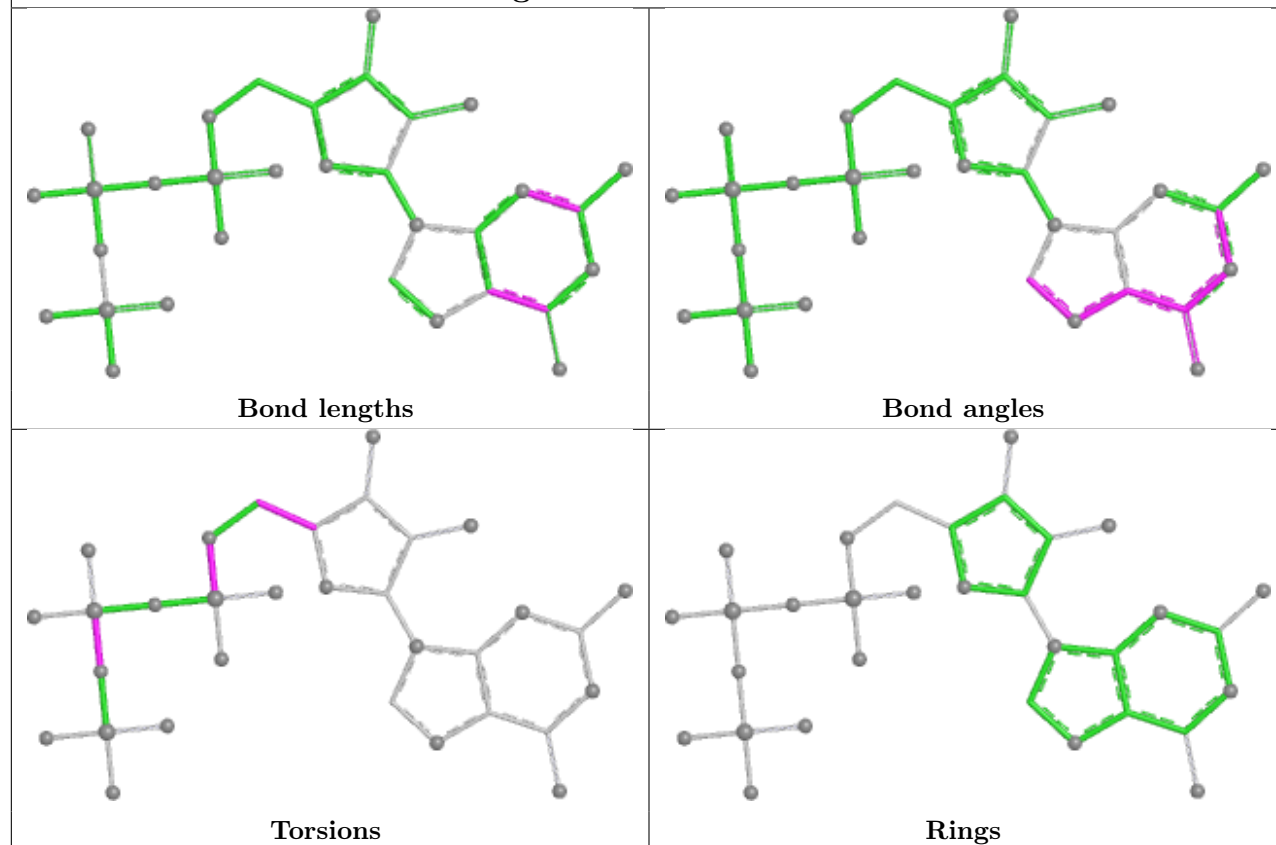
Ligand GTP VA 501



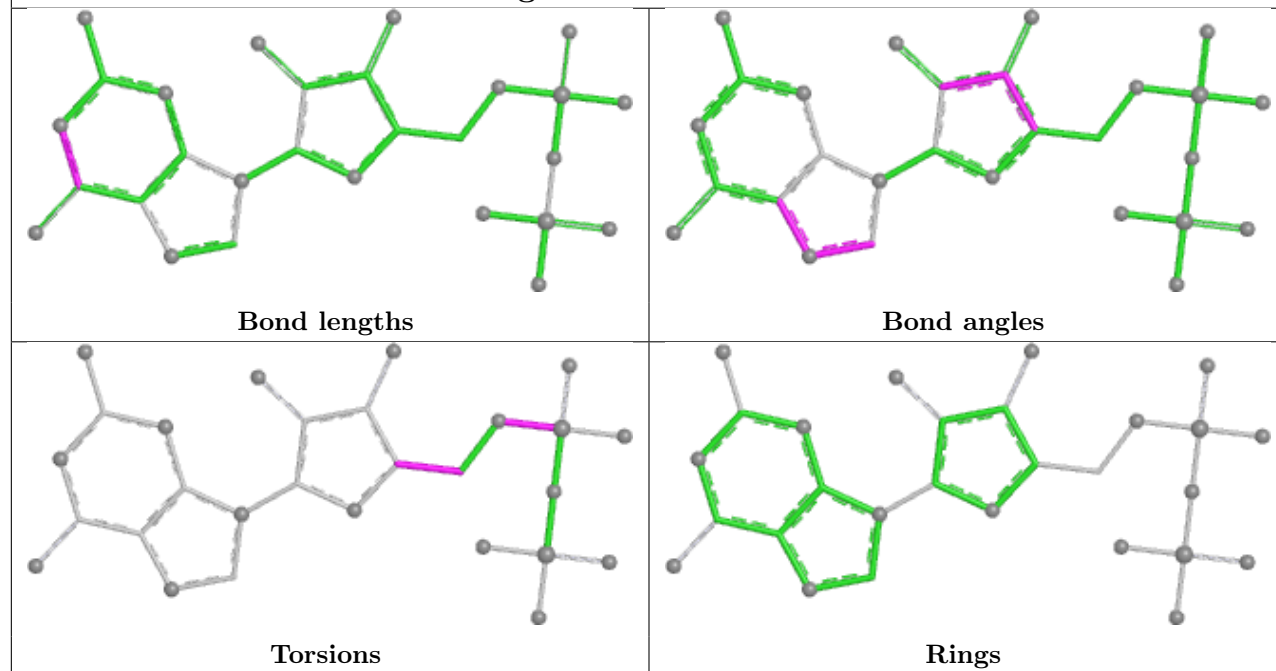




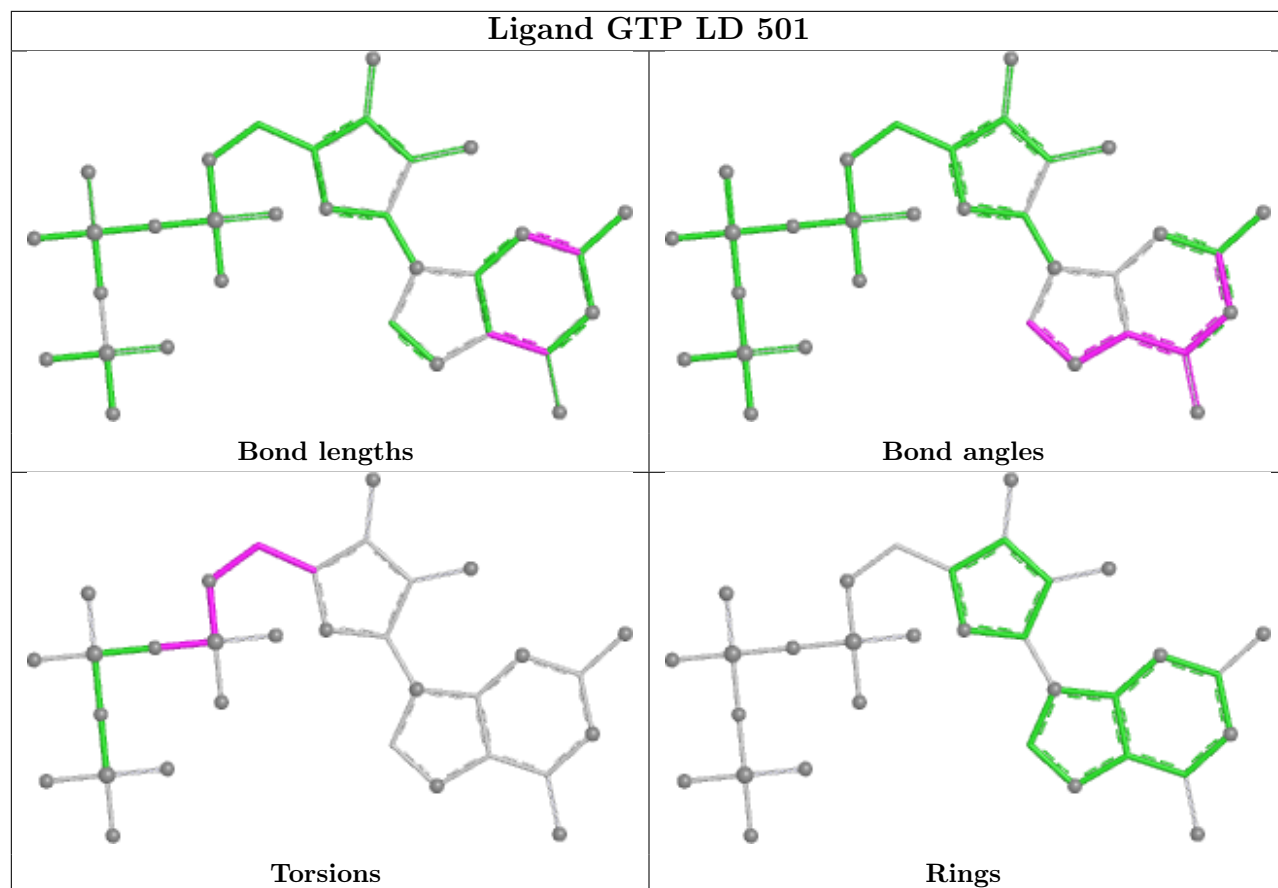
Ligand GTP MG 501



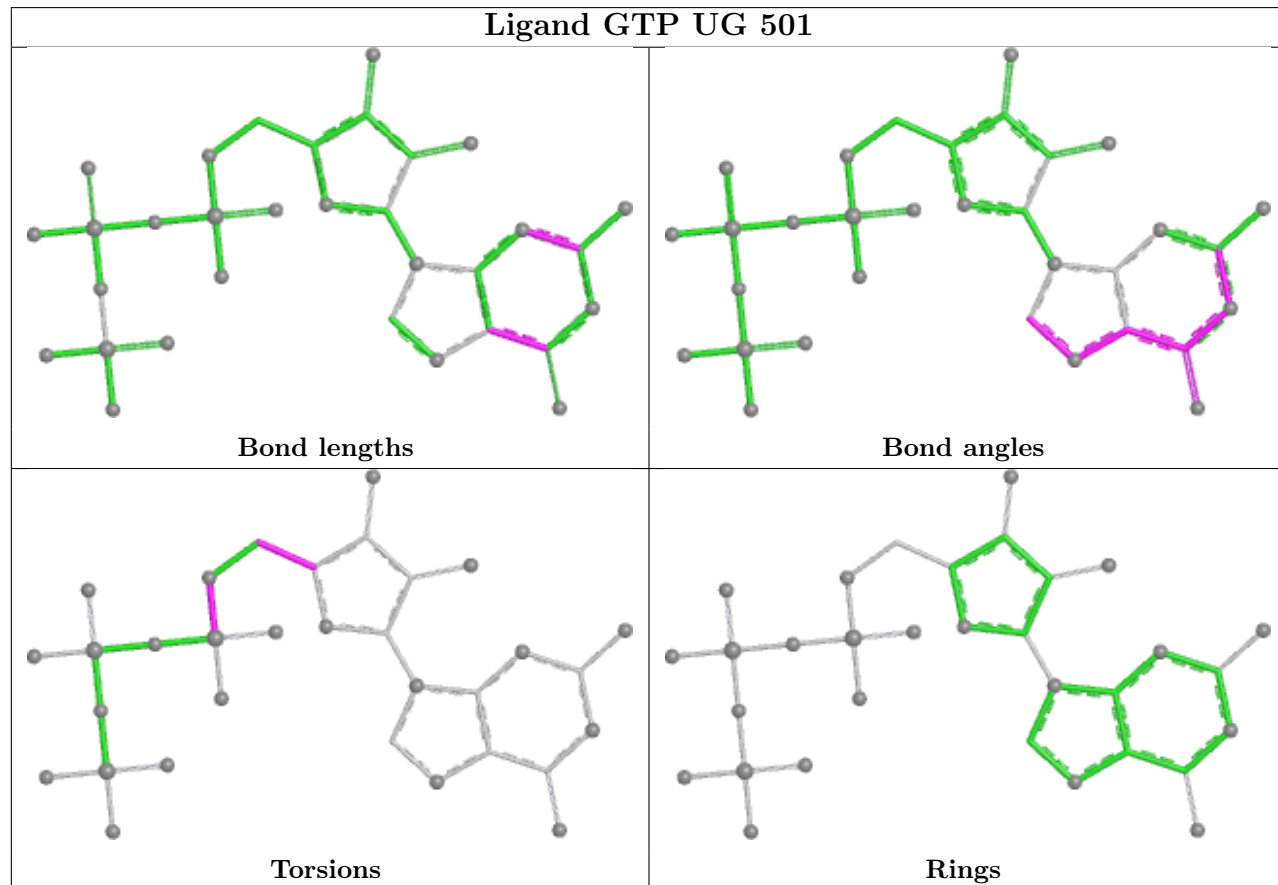
Ligand GDP AL 500

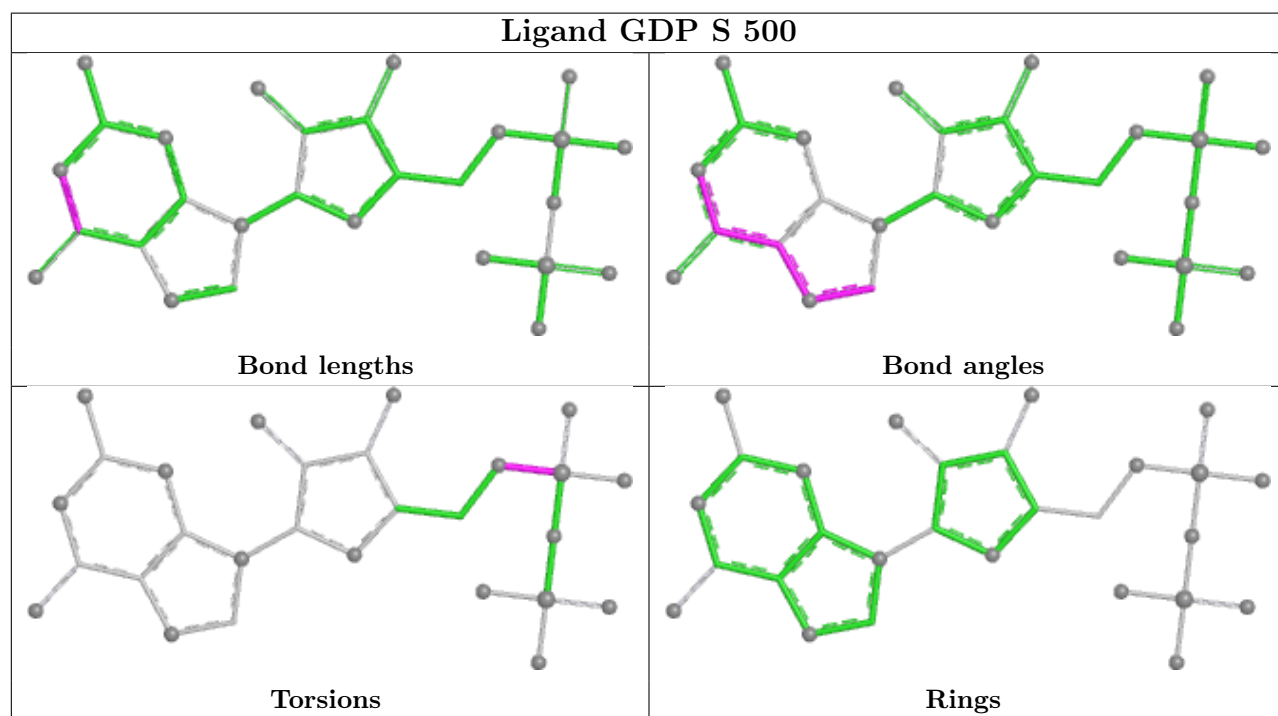
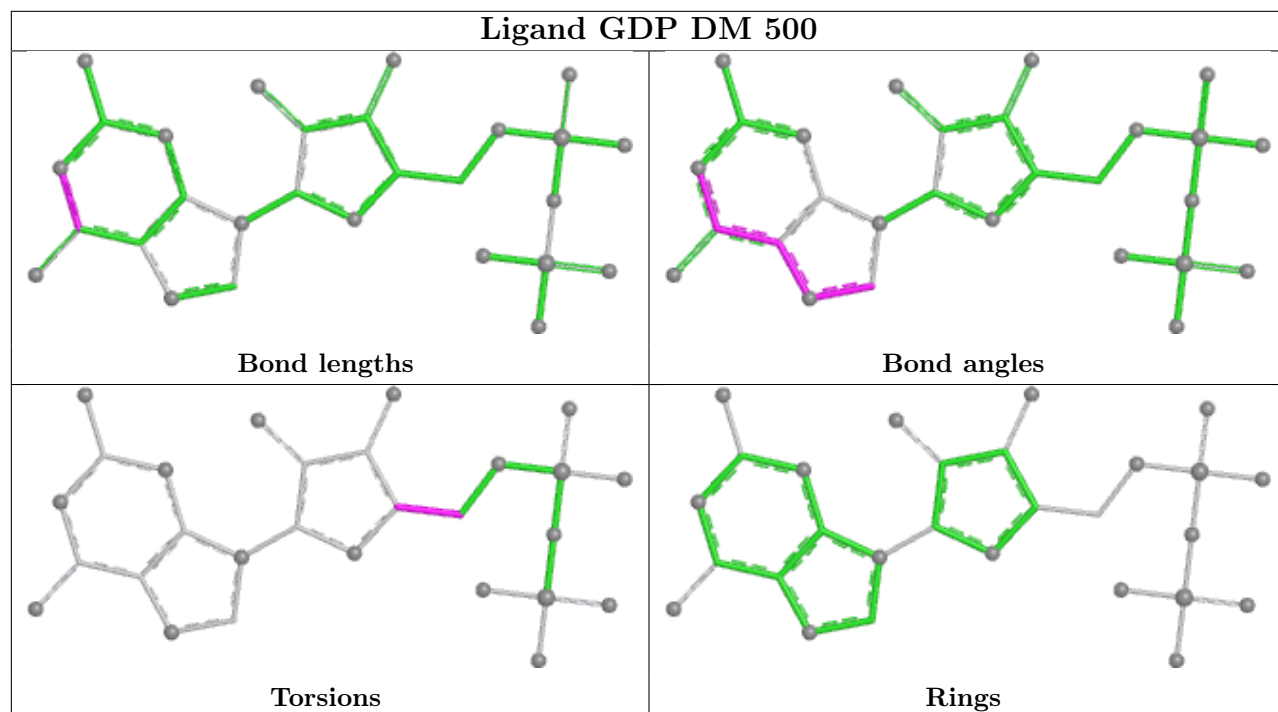


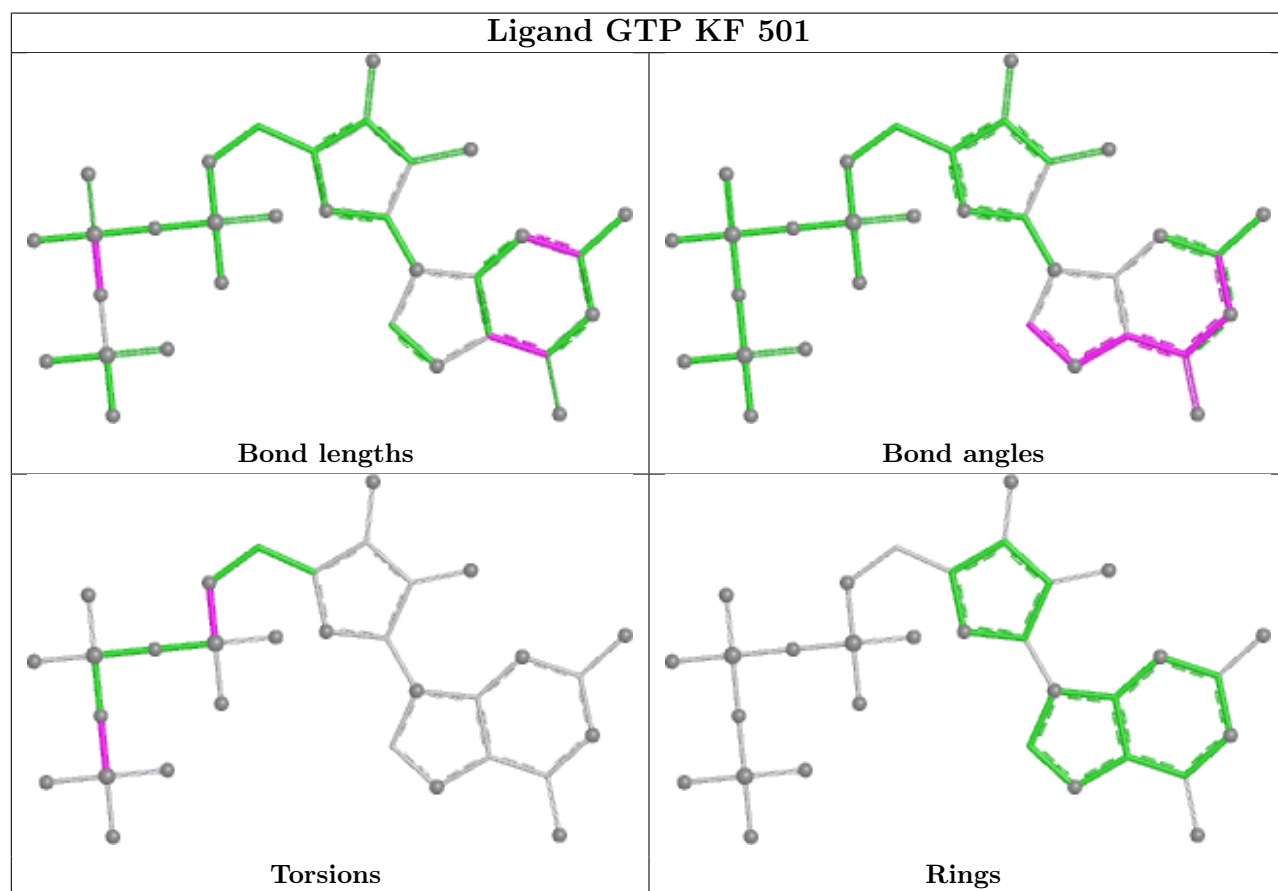
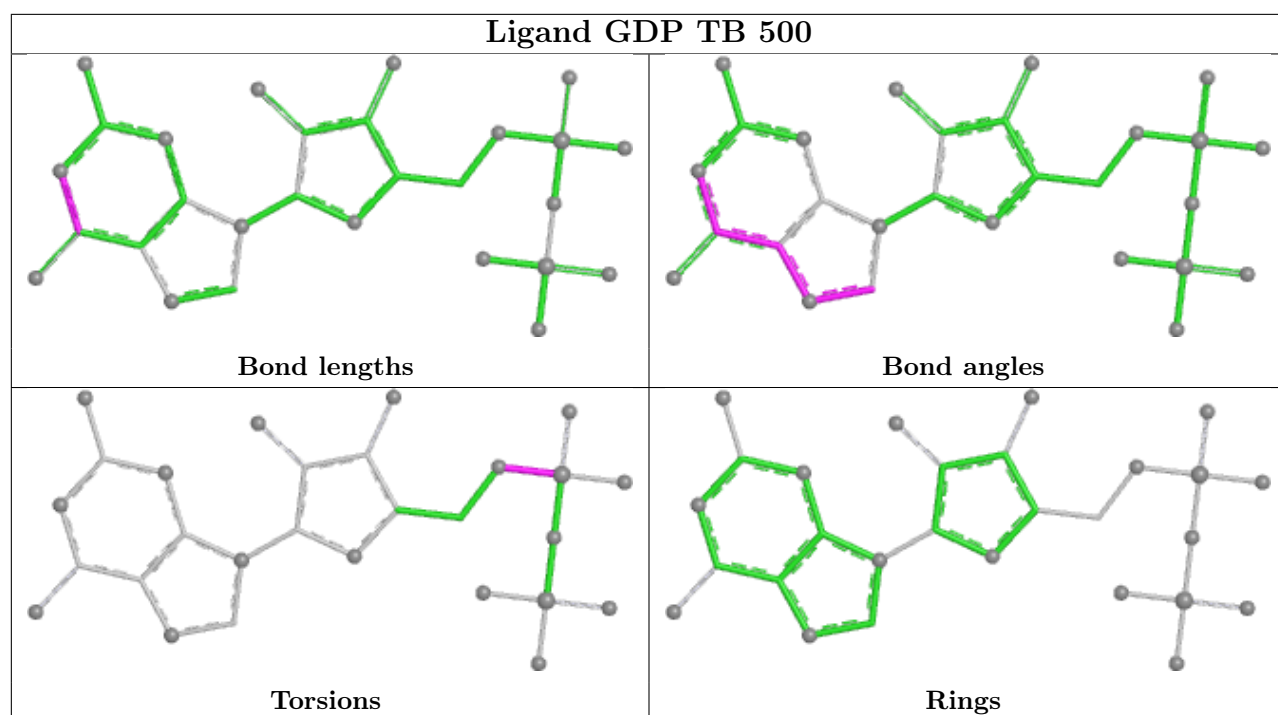
Ligand GTP LD 501

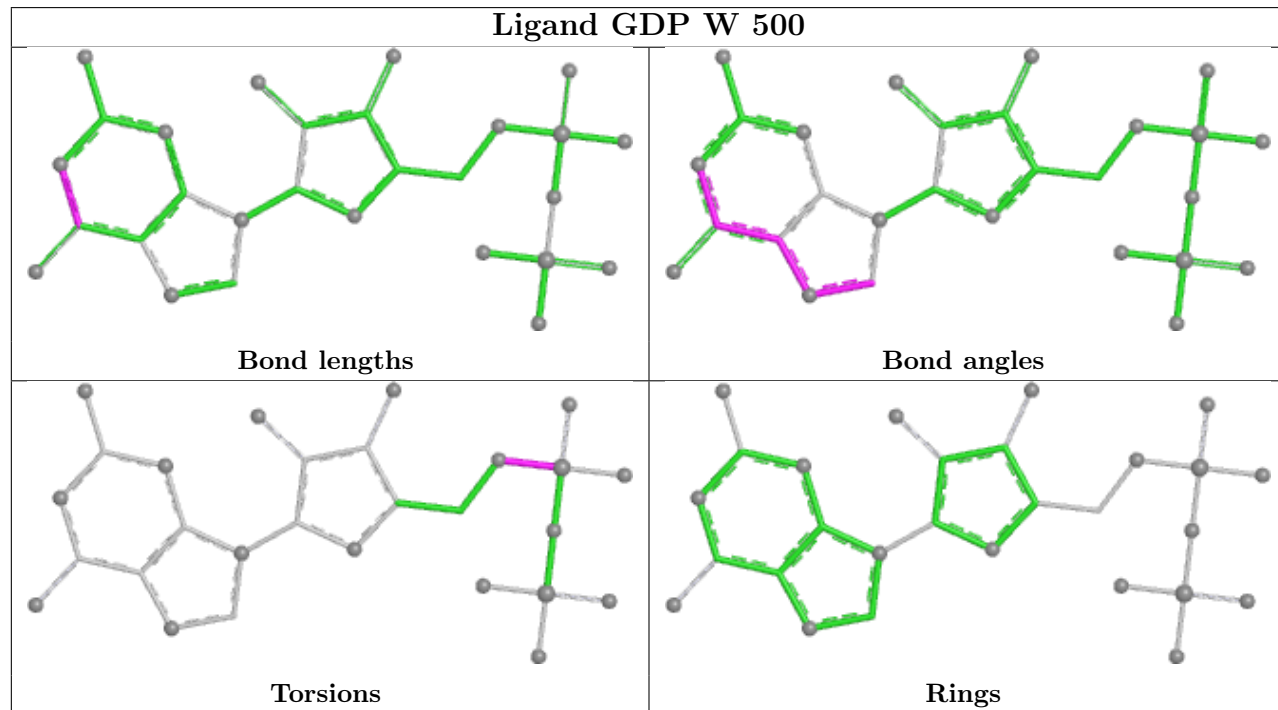
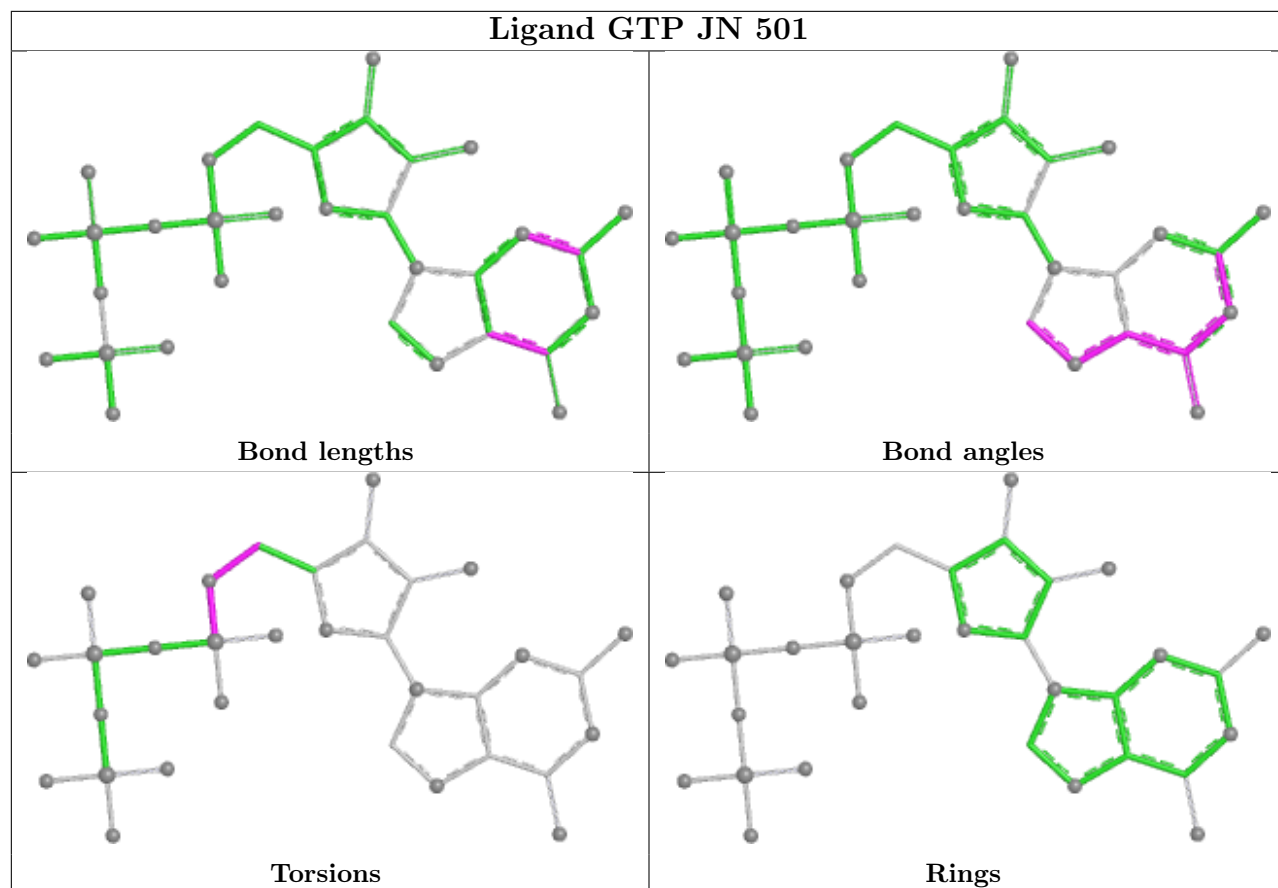


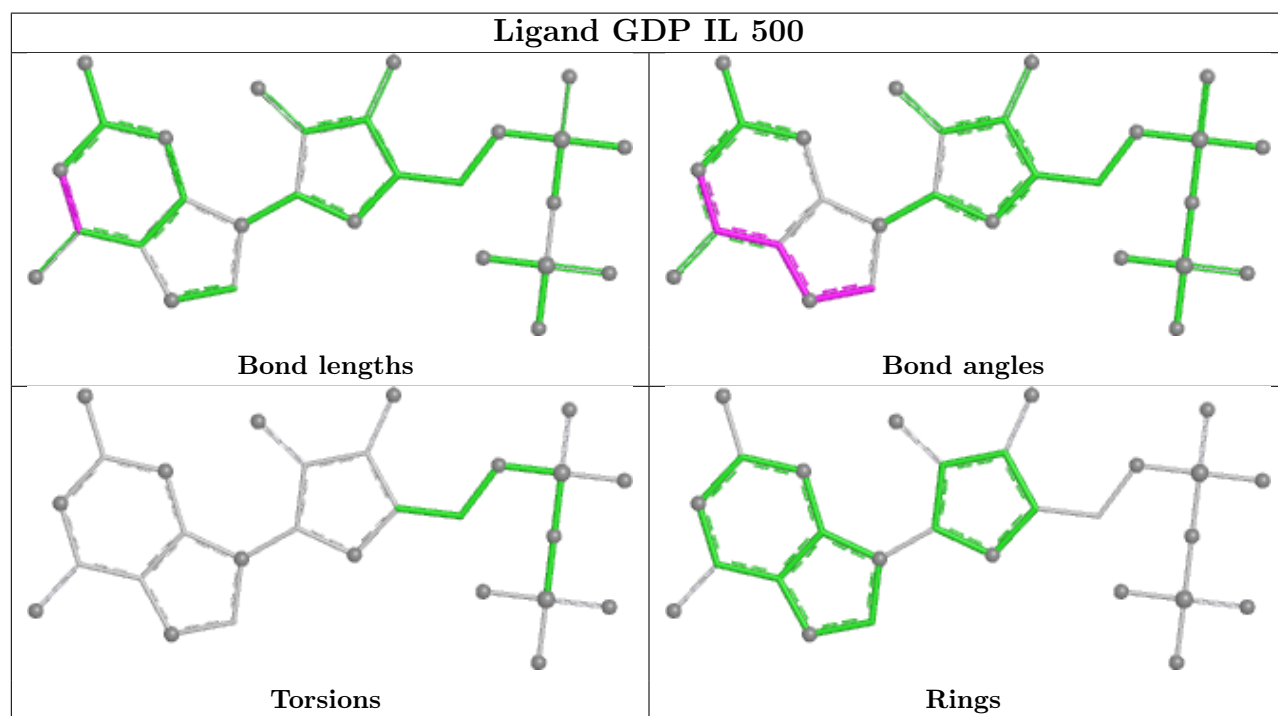
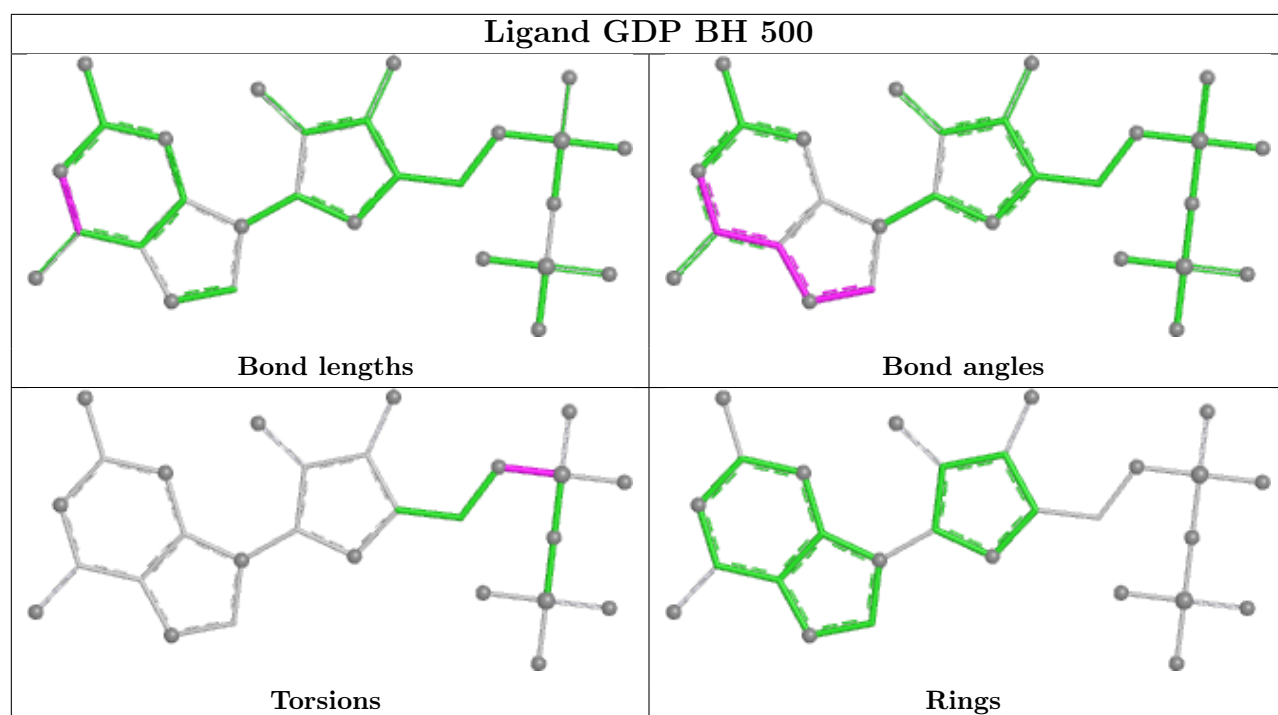
Ligand GTP UG 501

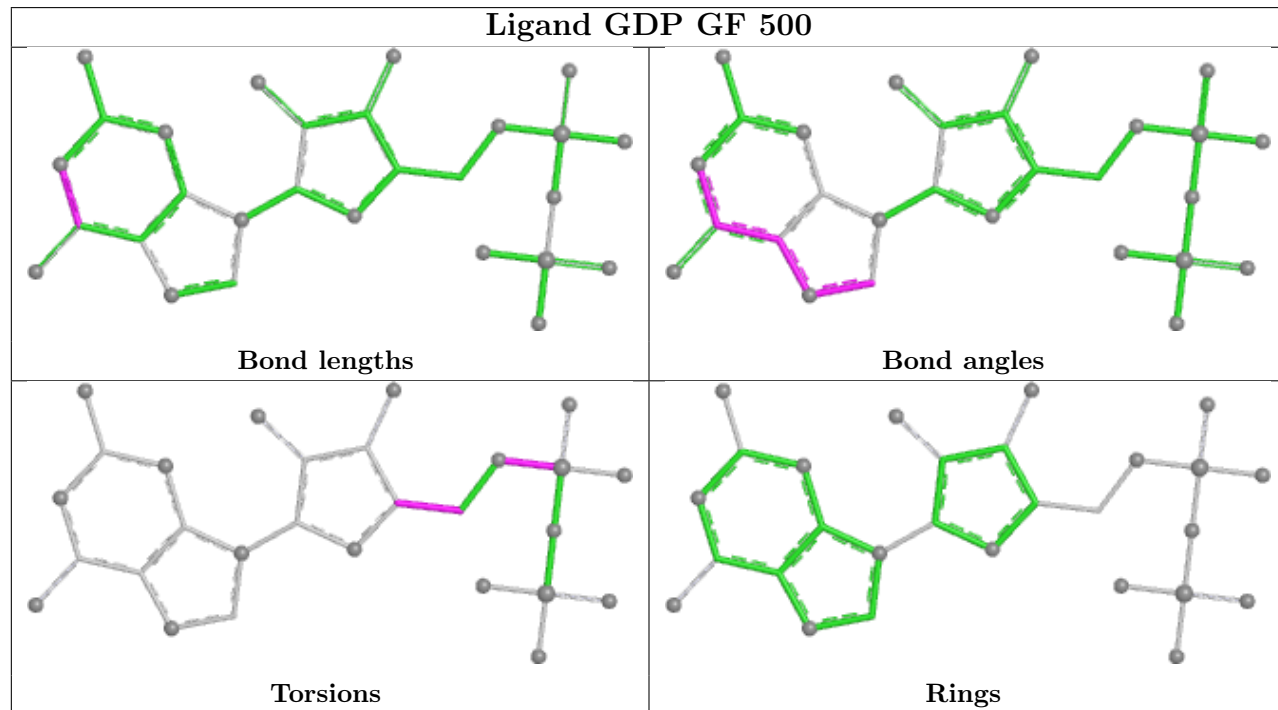
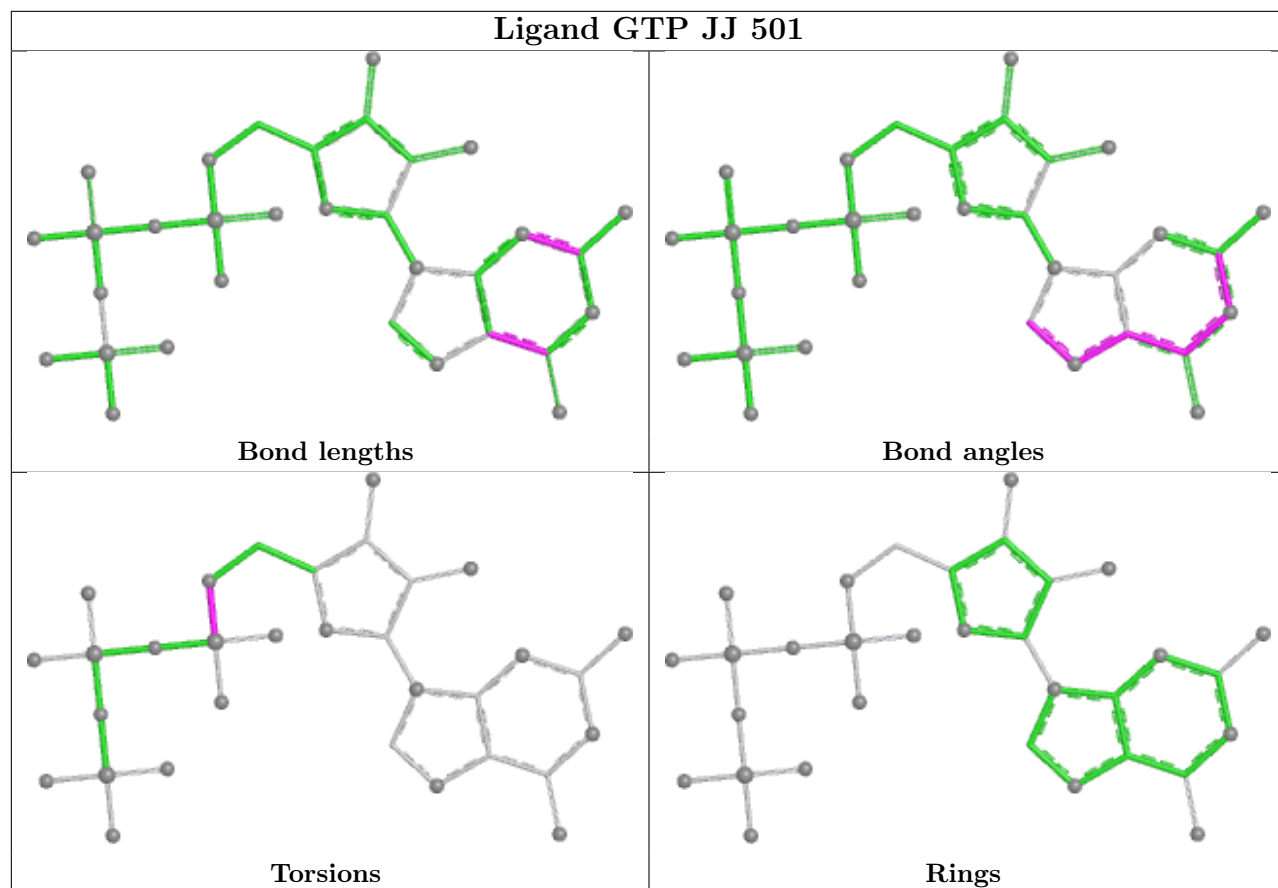


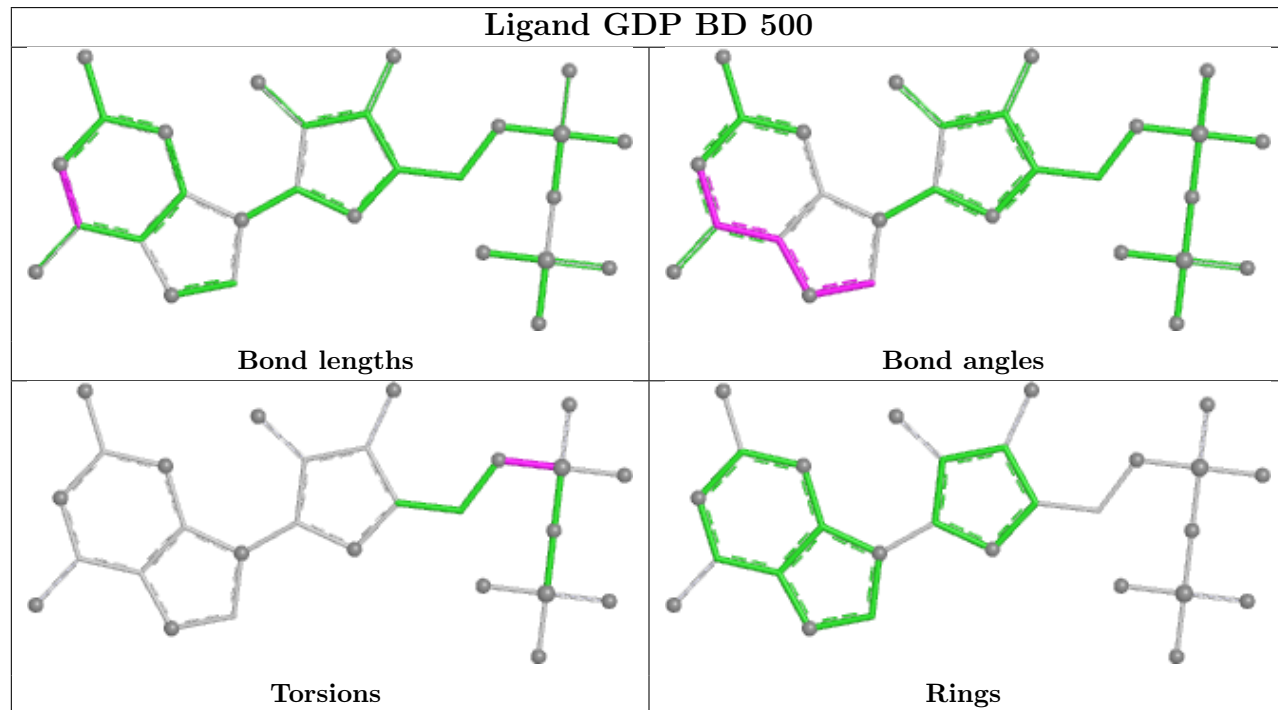
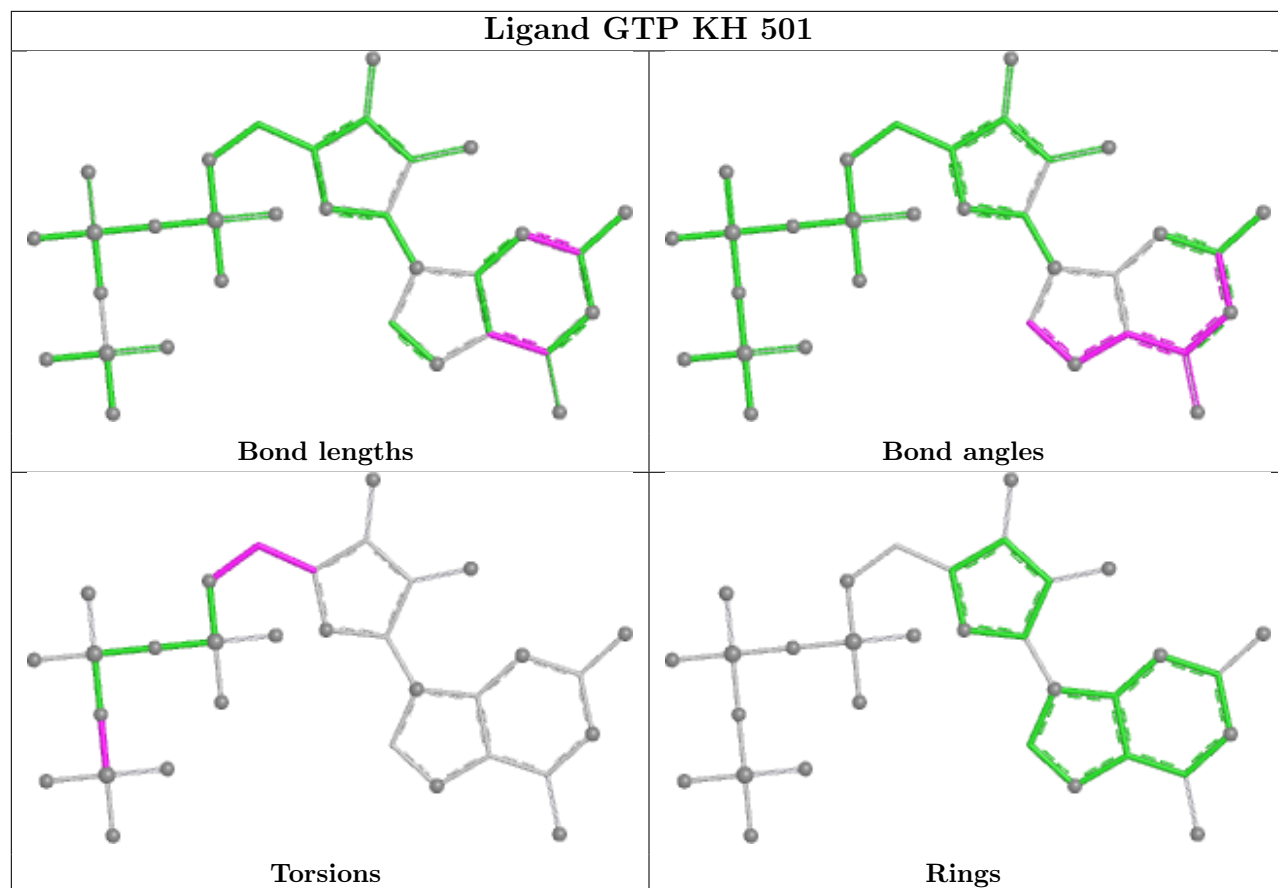




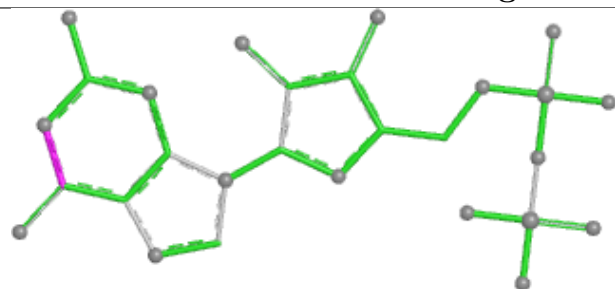




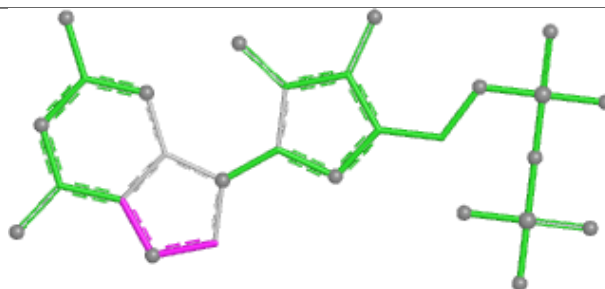




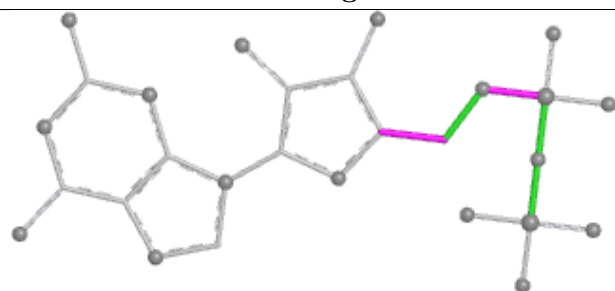
Ligand GDP KA 500



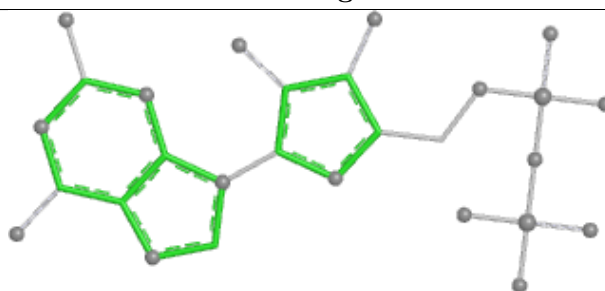
Bond lengths



Bond angles

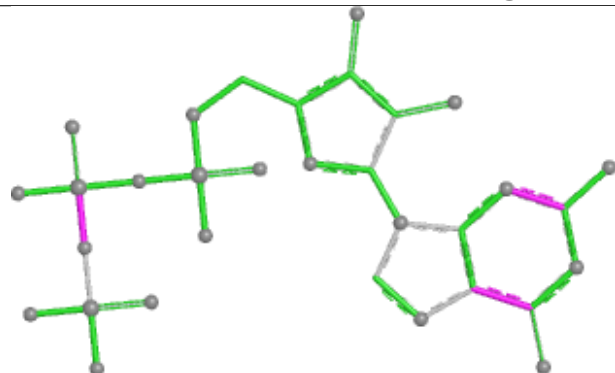


Torsions

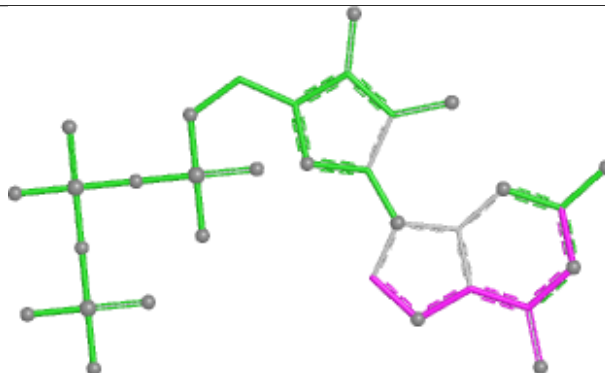


Rings

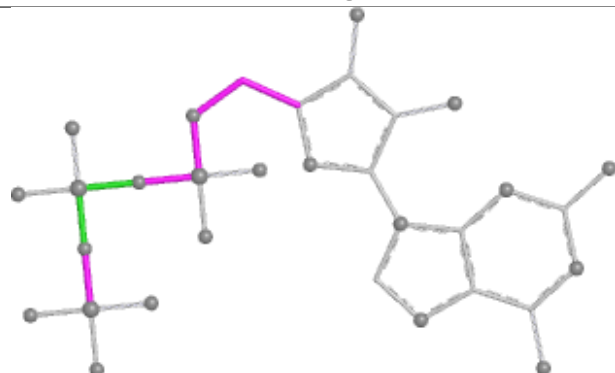
Ligand GTP RD 501



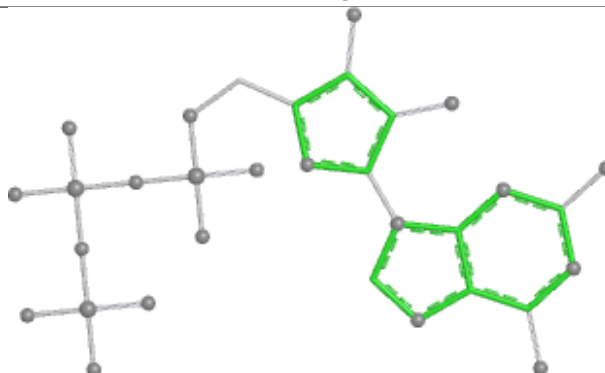
Bond lengths



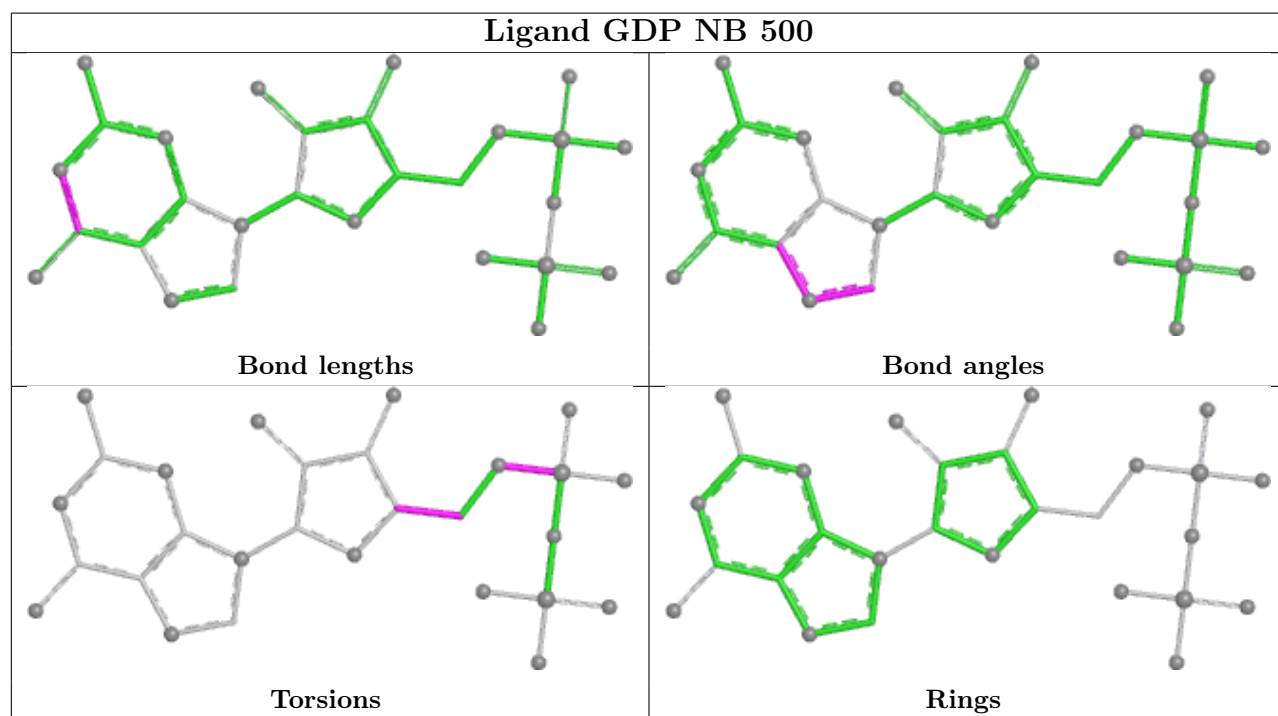
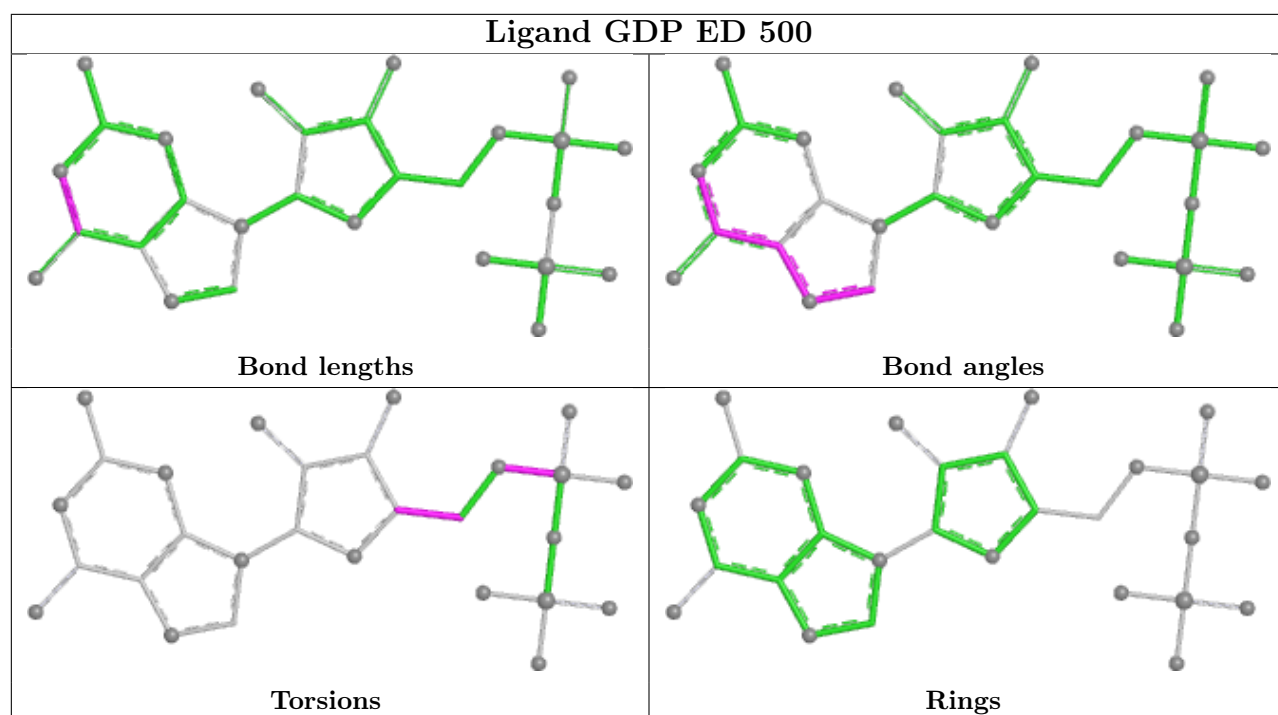
Bond angles

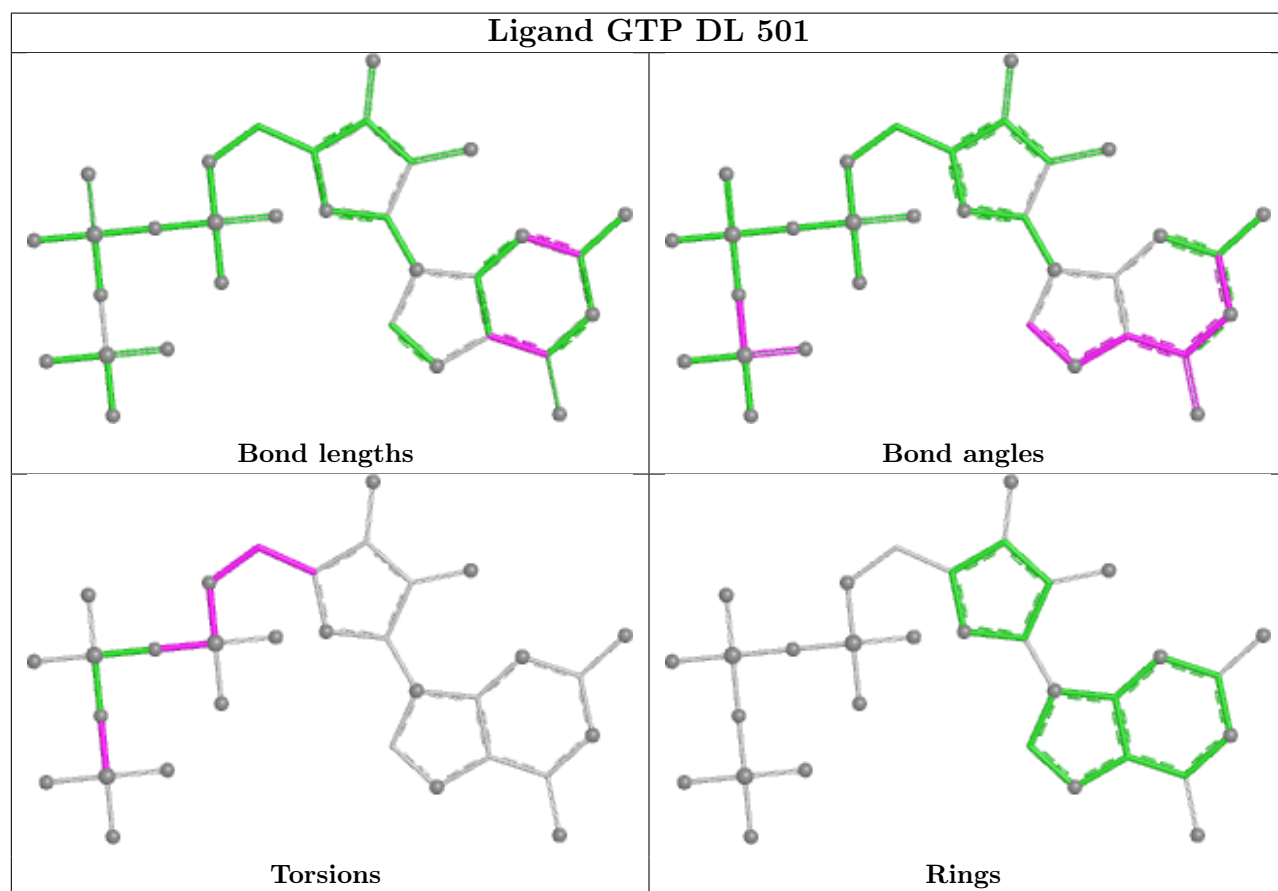
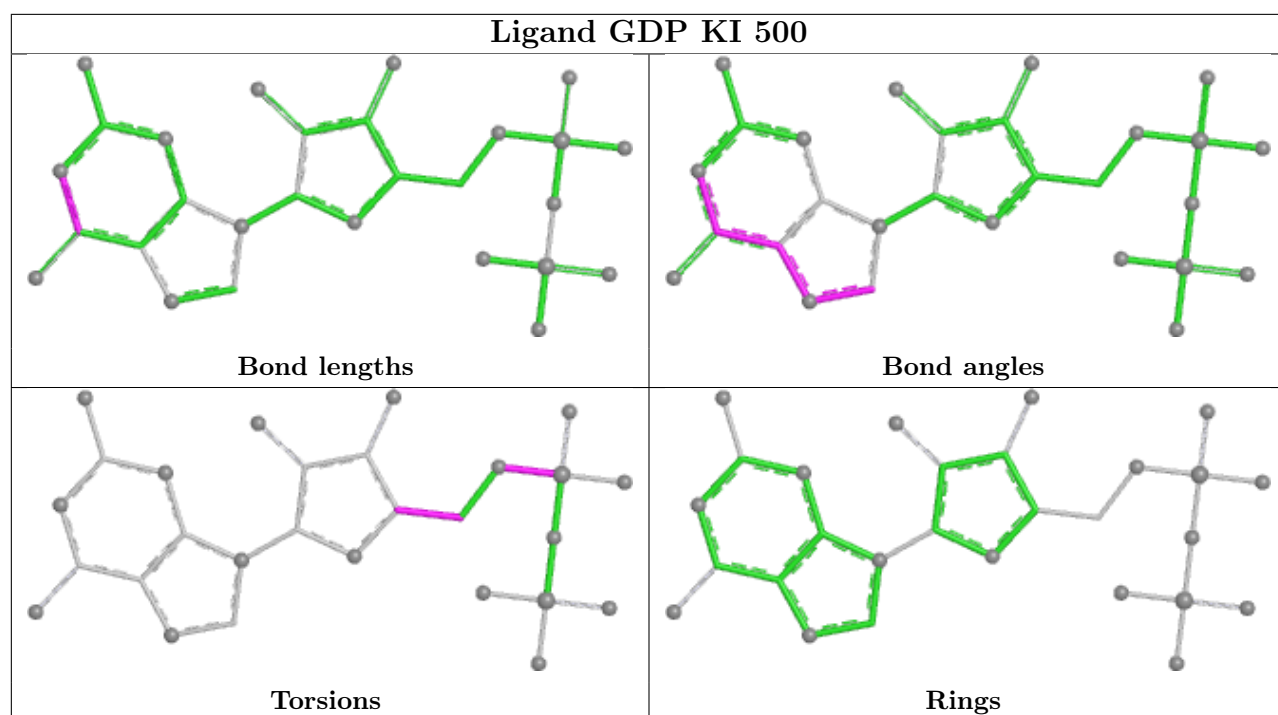


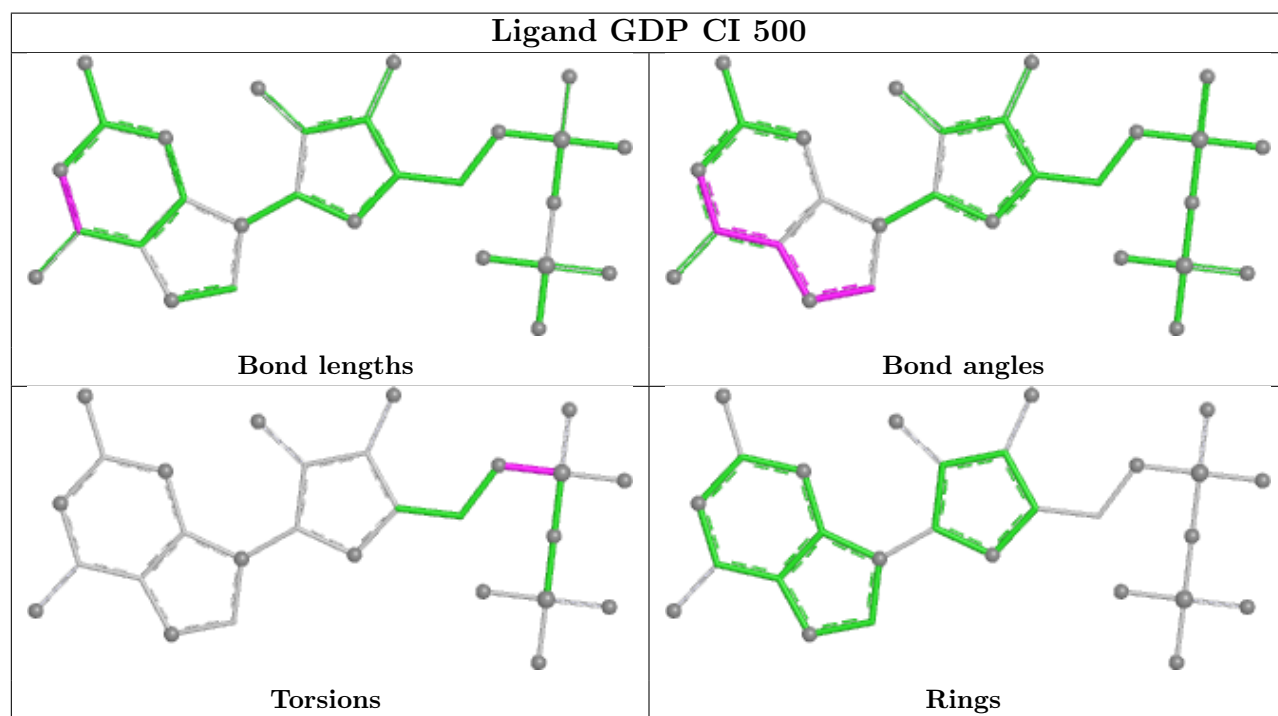
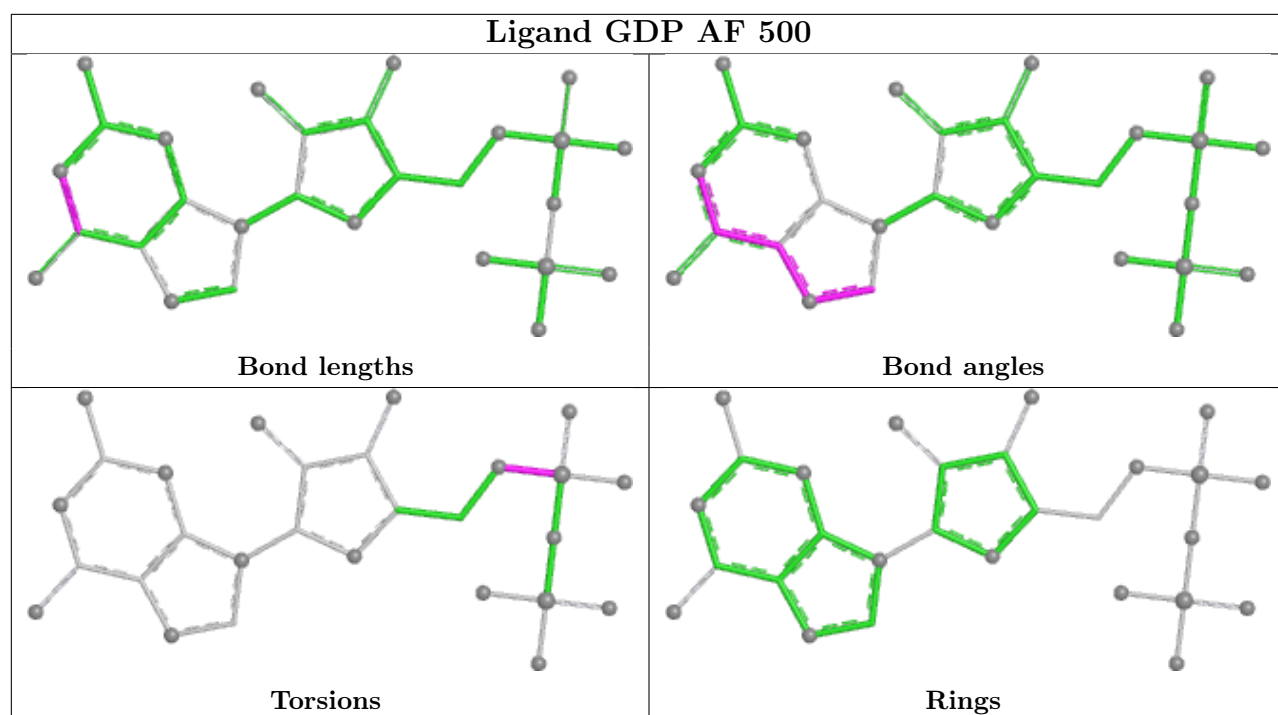
Torsions



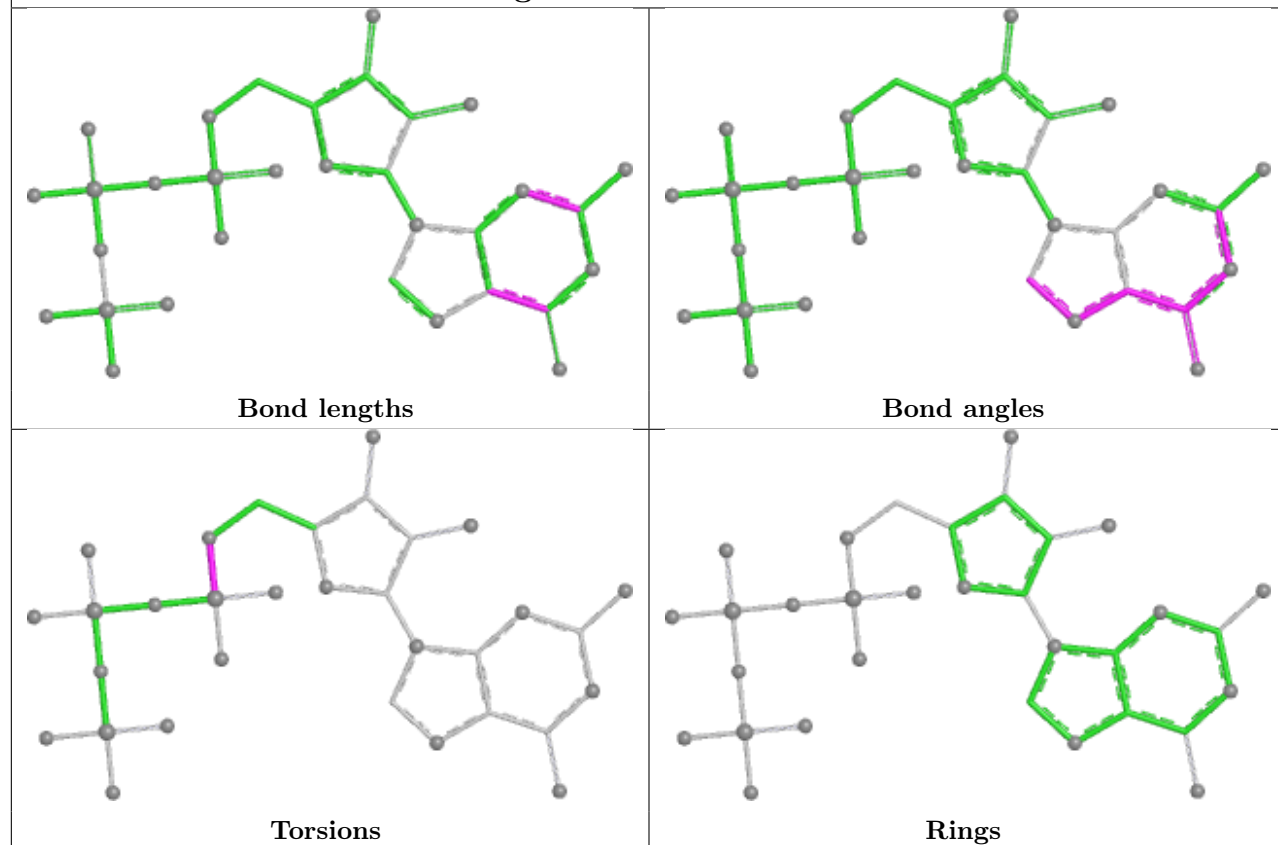
Rings



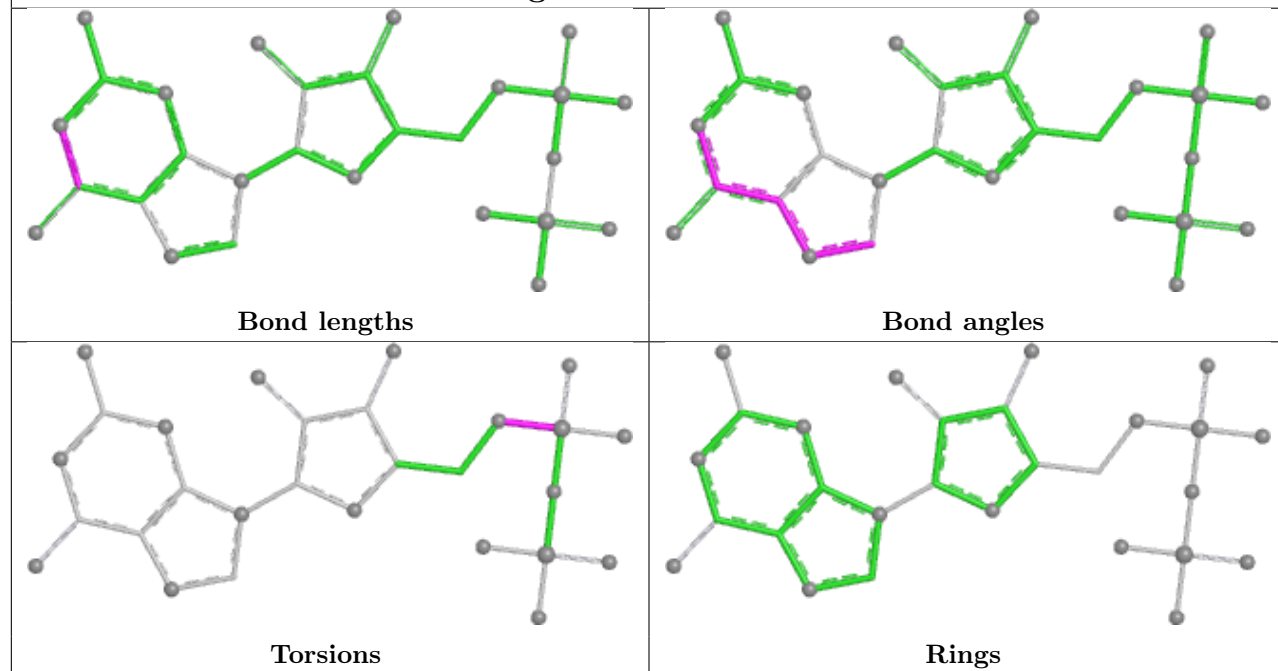


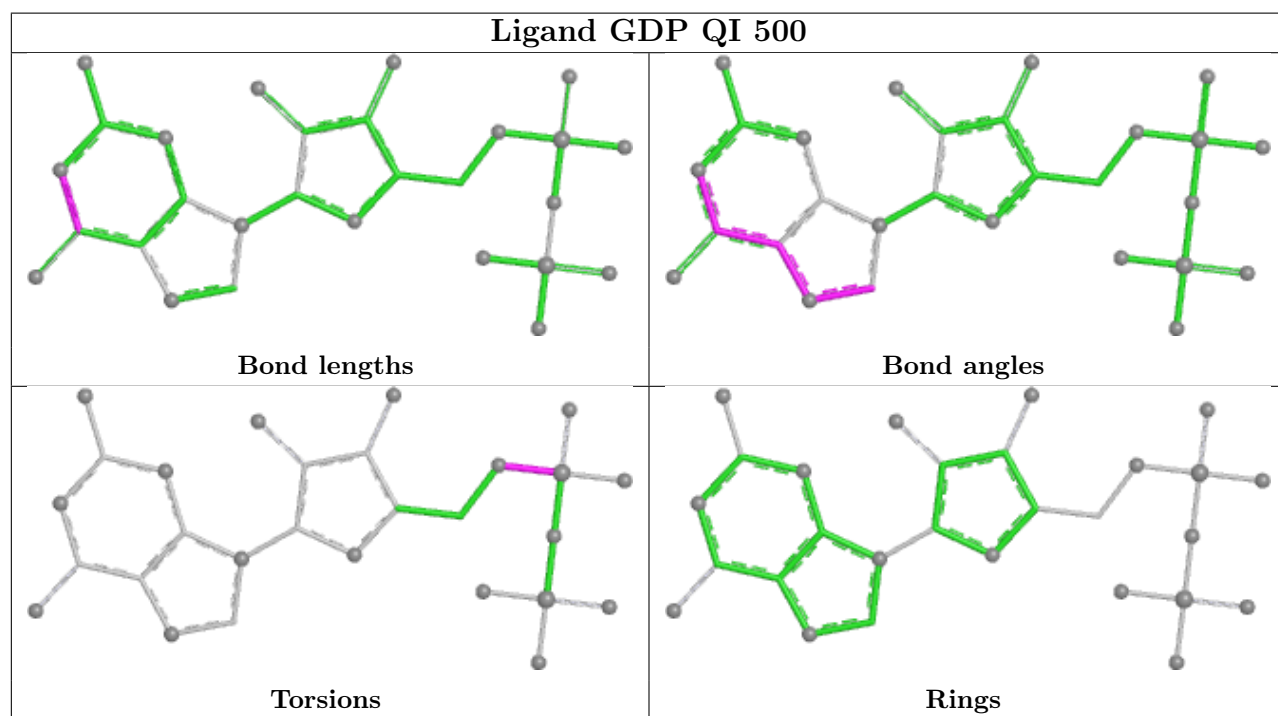
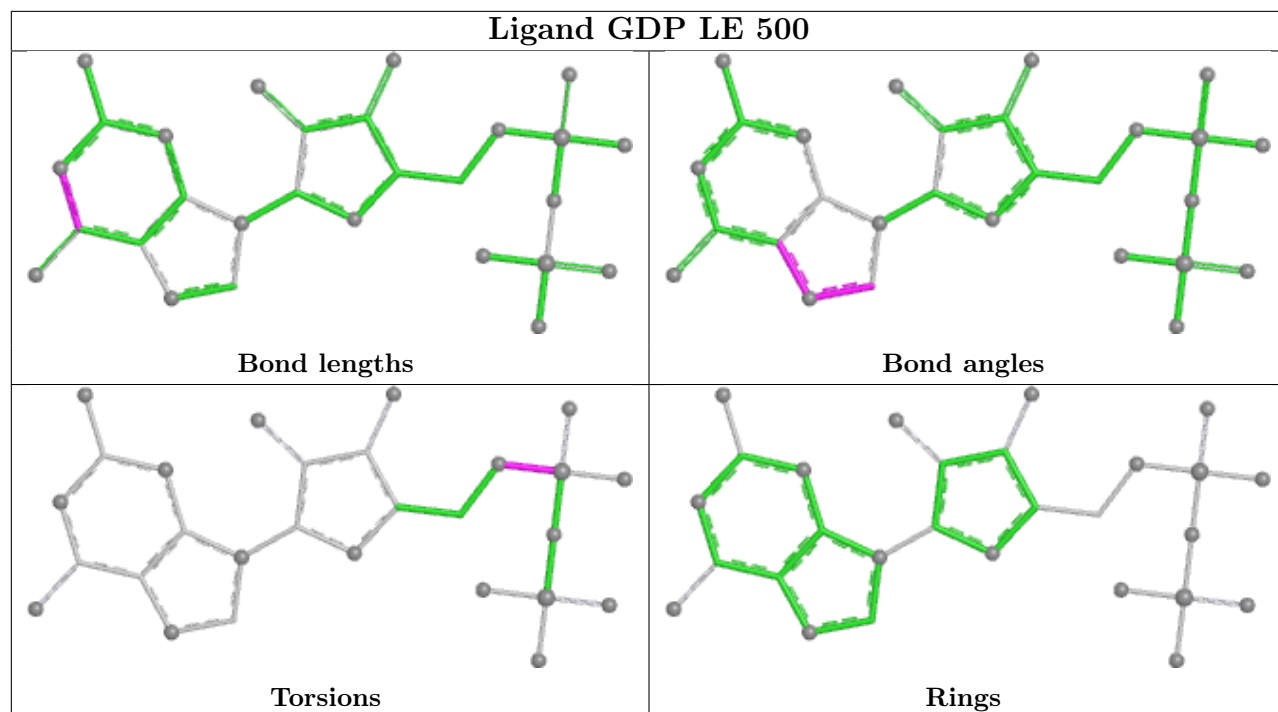


Ligand GTP PM 501

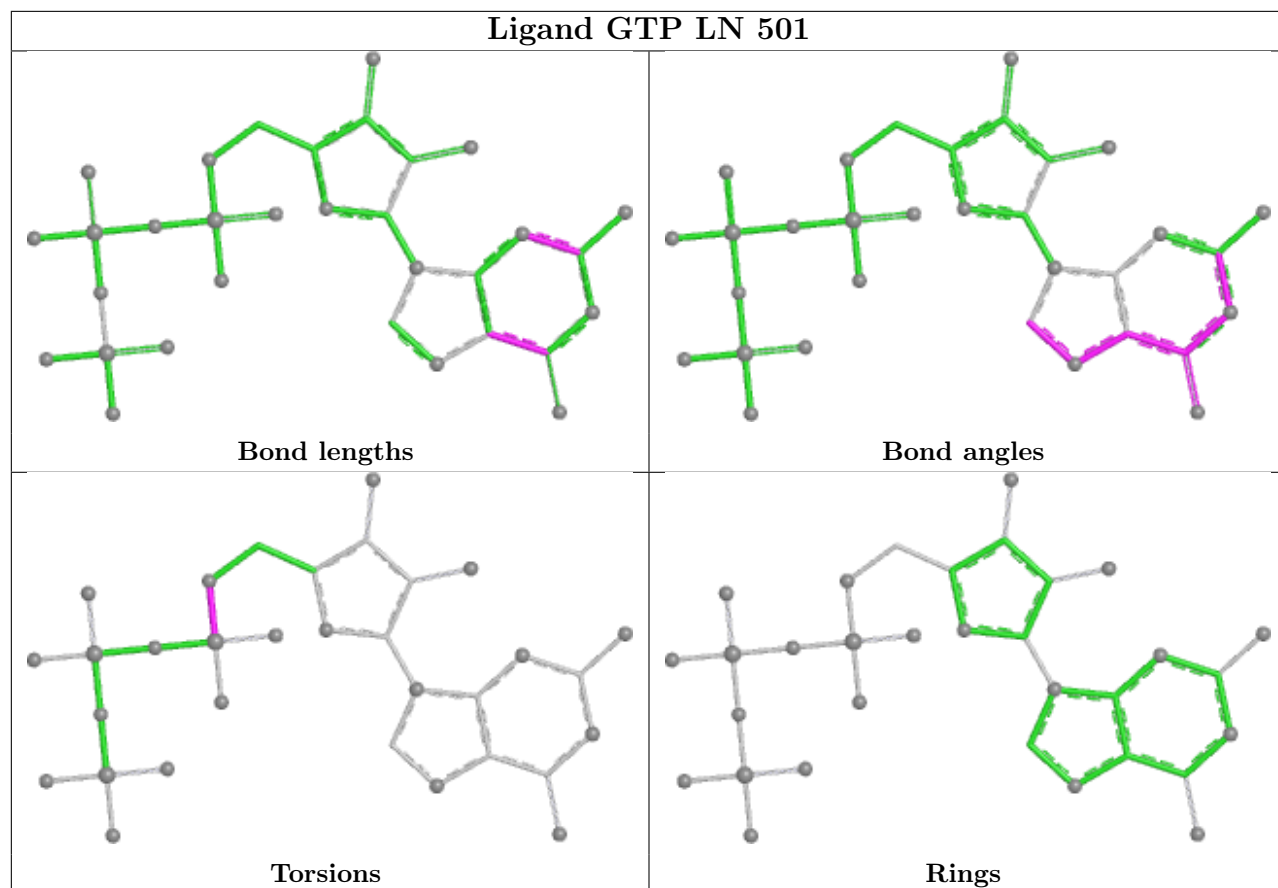


Ligand GDP N 500

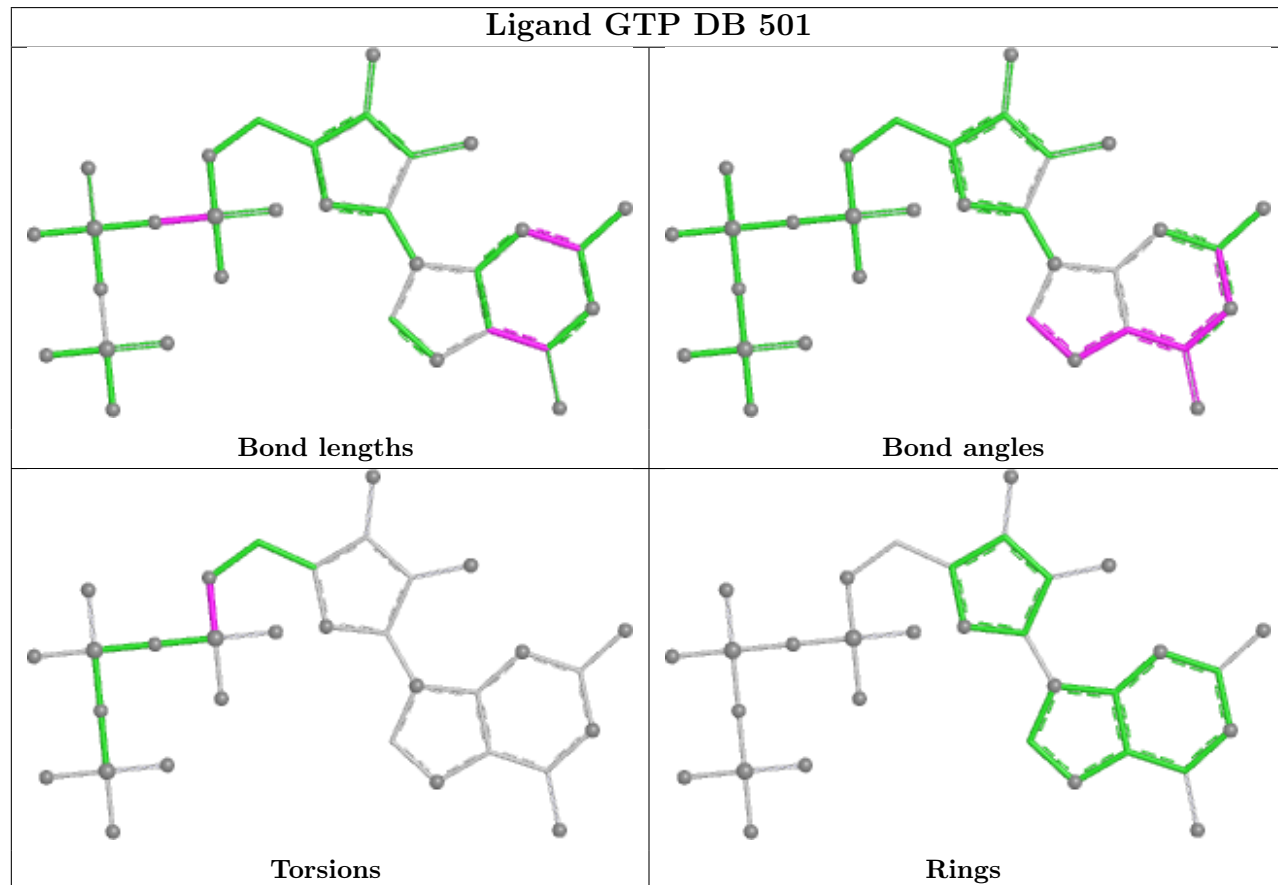




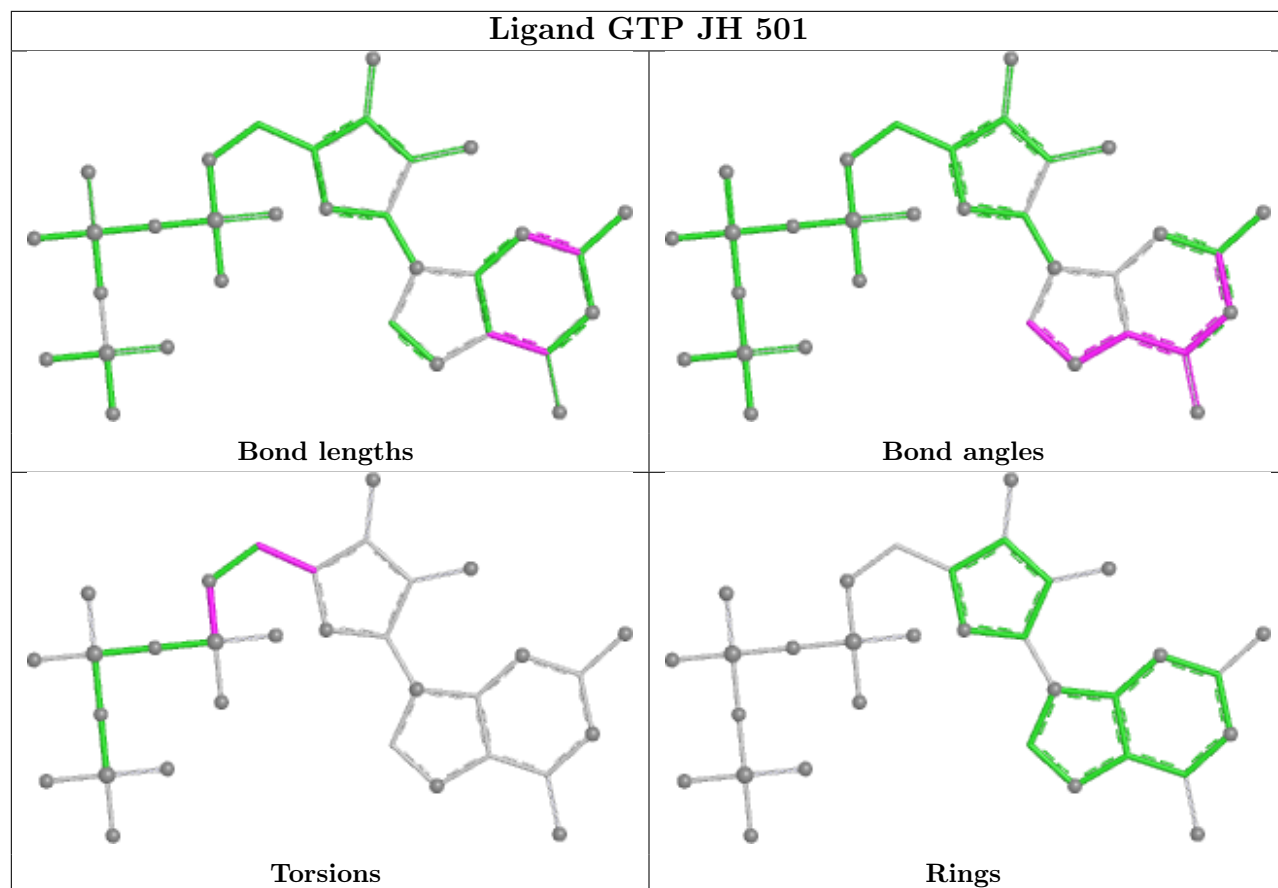
Ligand GTP LN 501



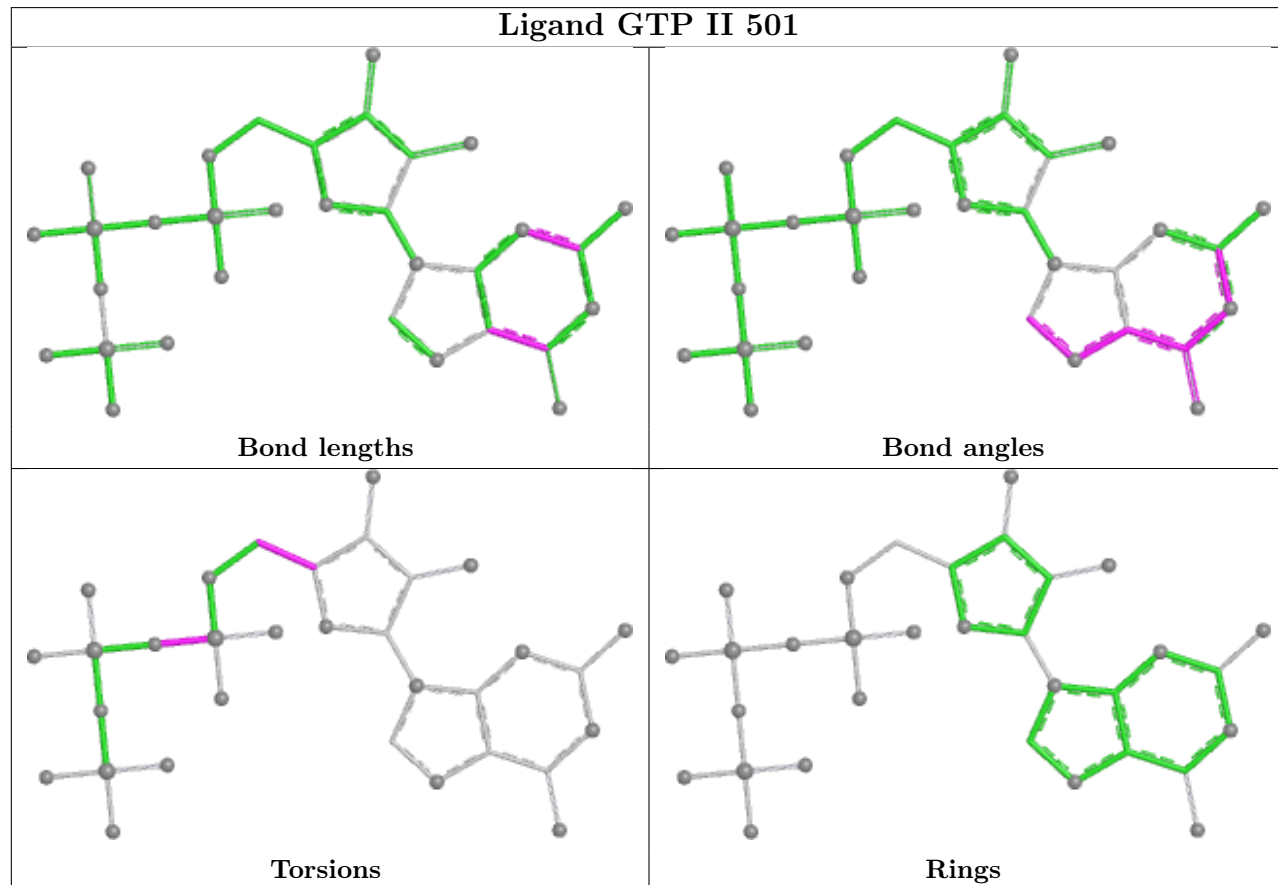
Ligand GTP DB 501



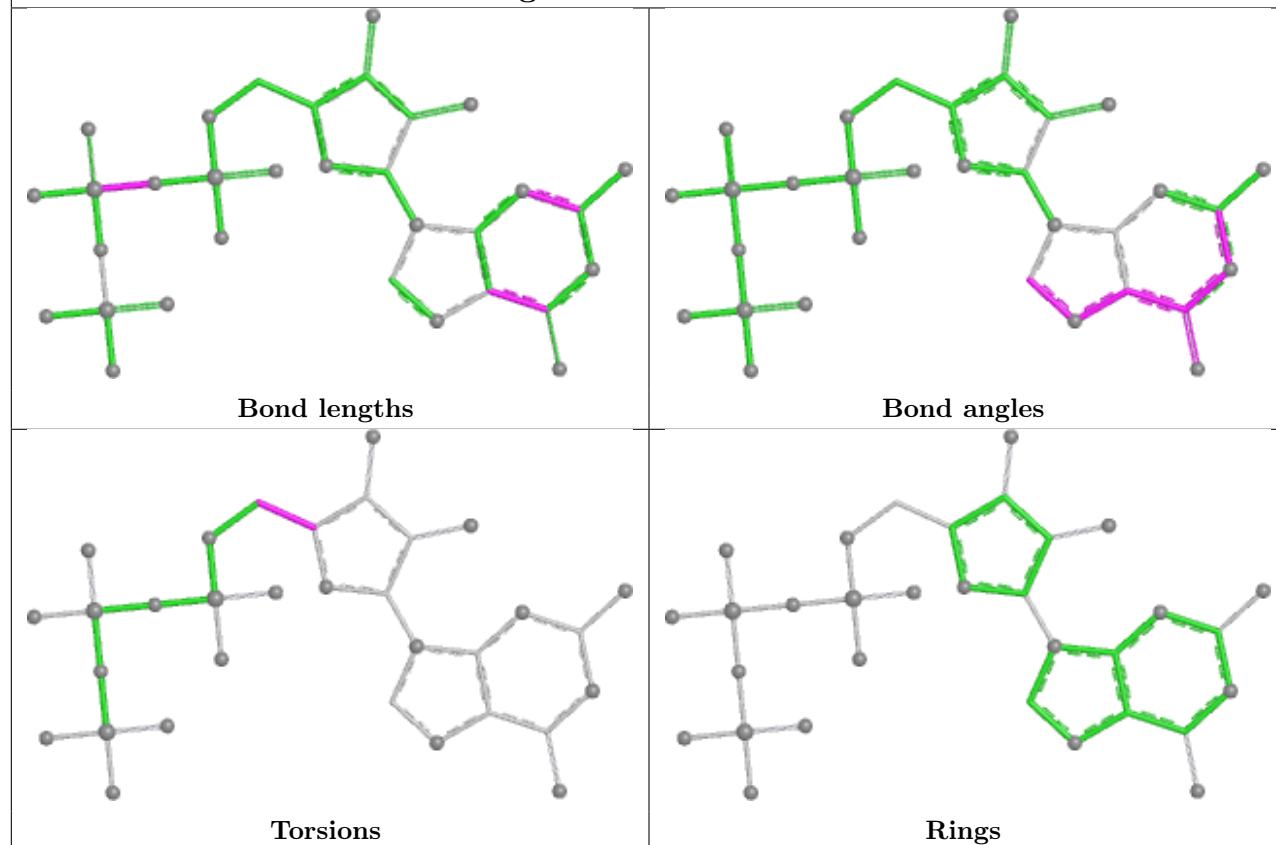
Ligand GTP JH 501



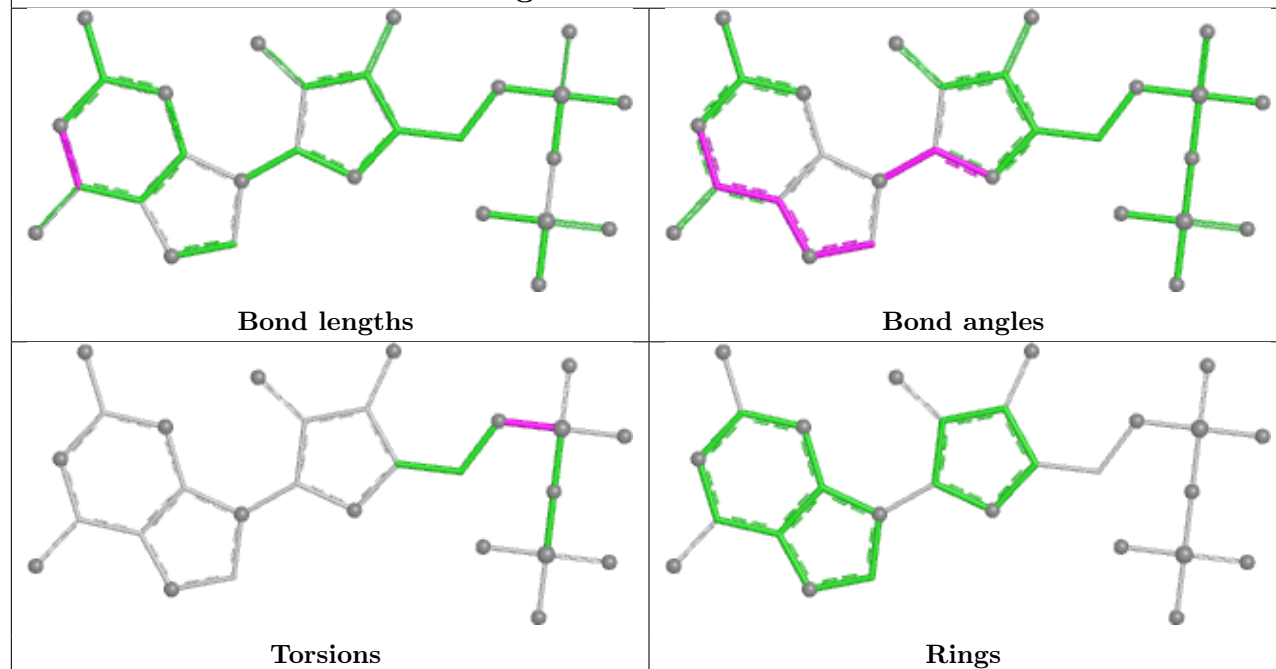
Ligand GTP II 501



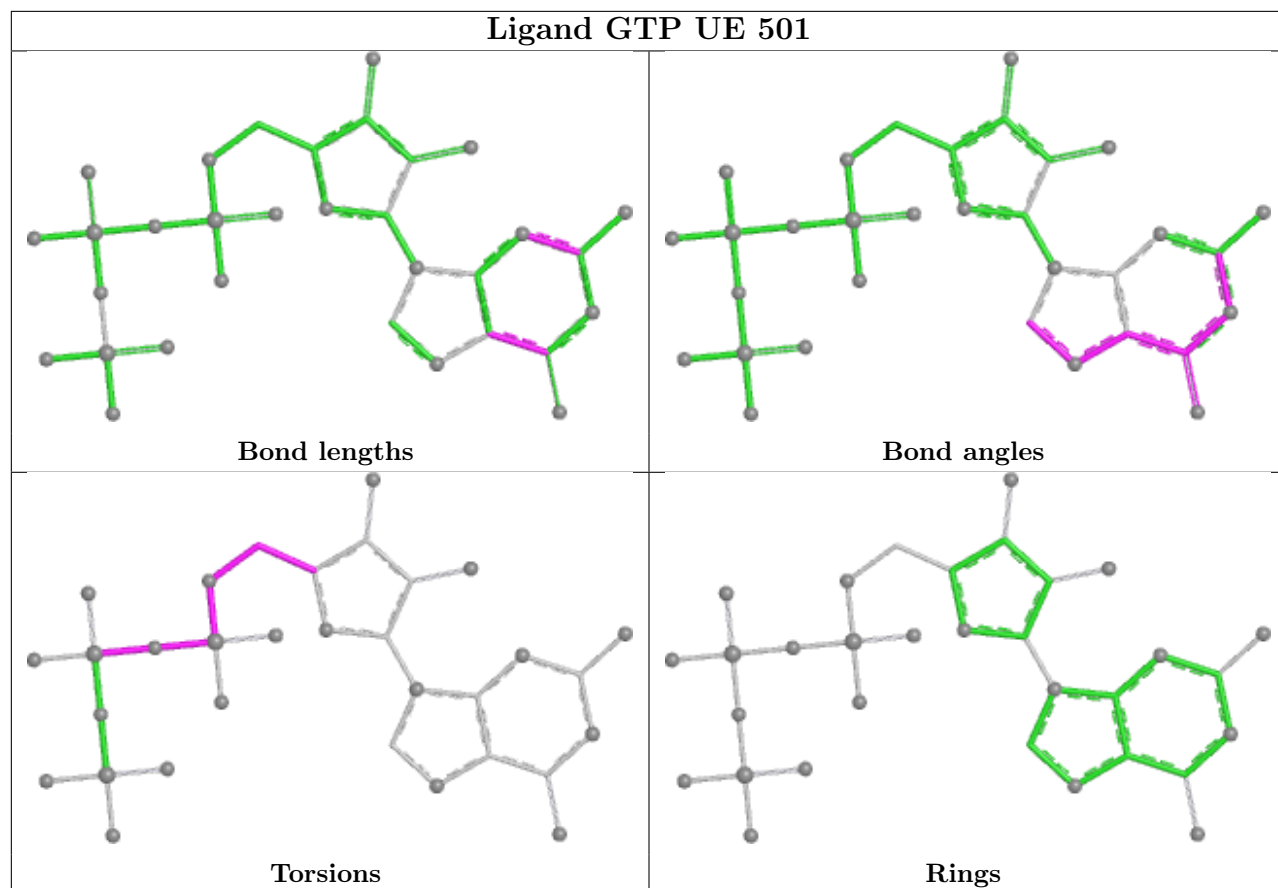
Ligand GTP KL 501



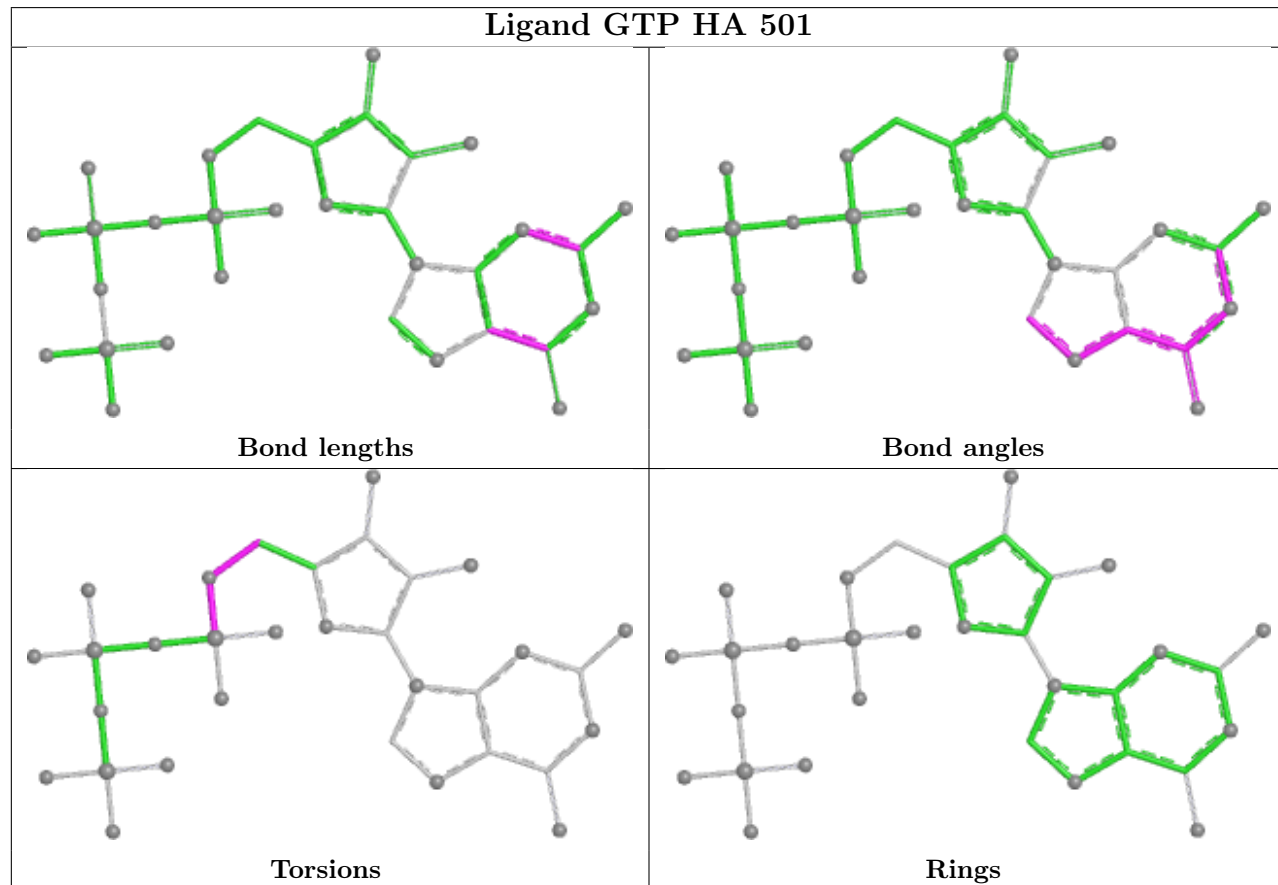
Ligand GDP CA 500

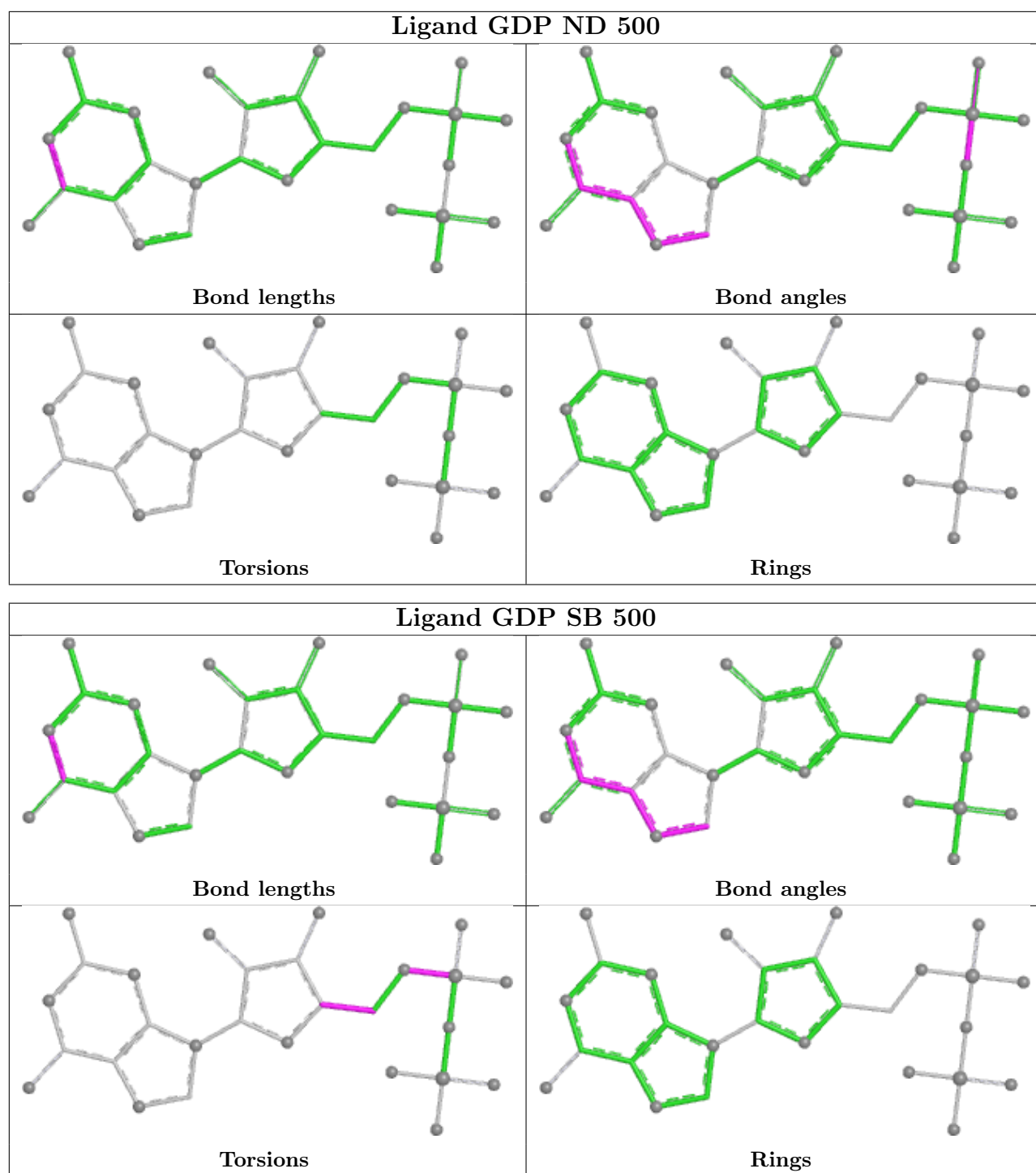


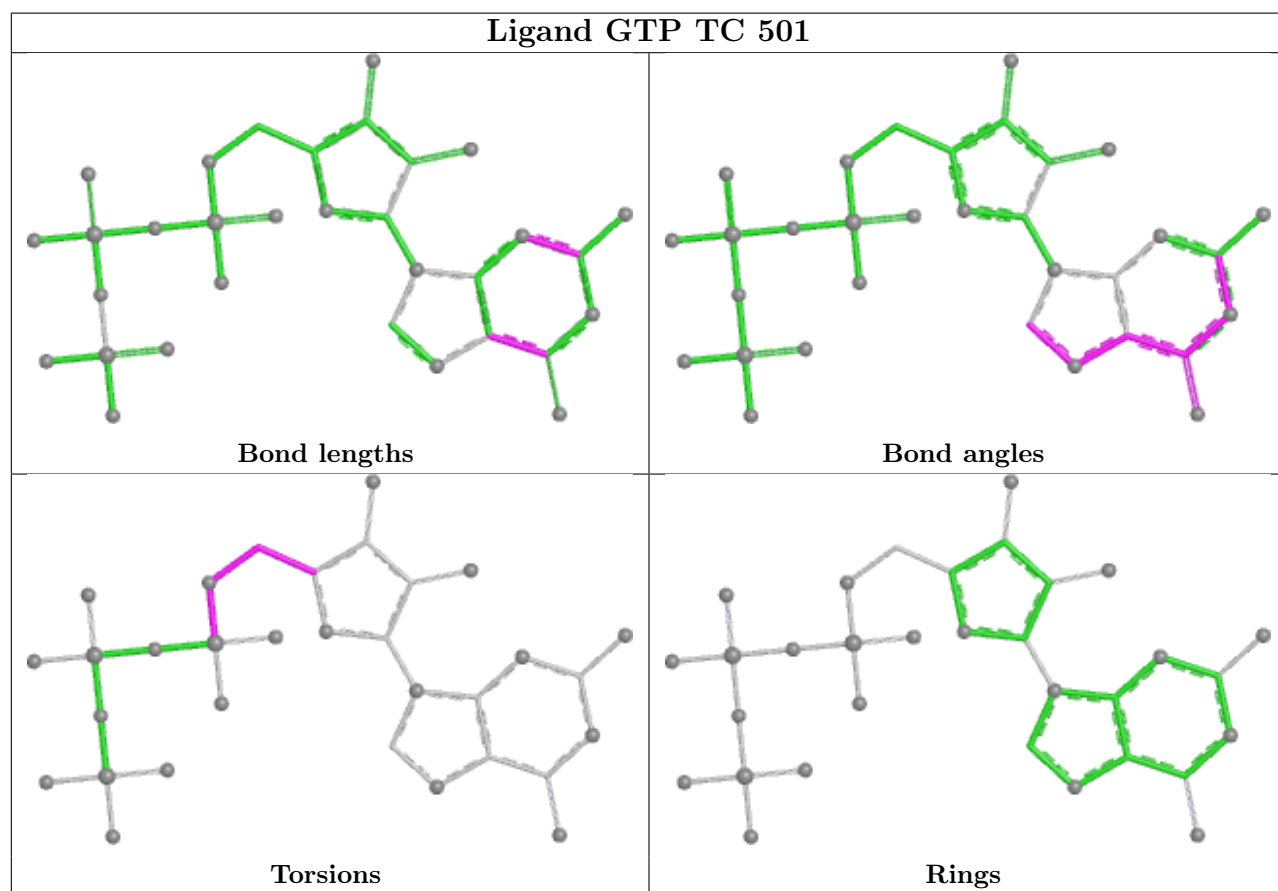
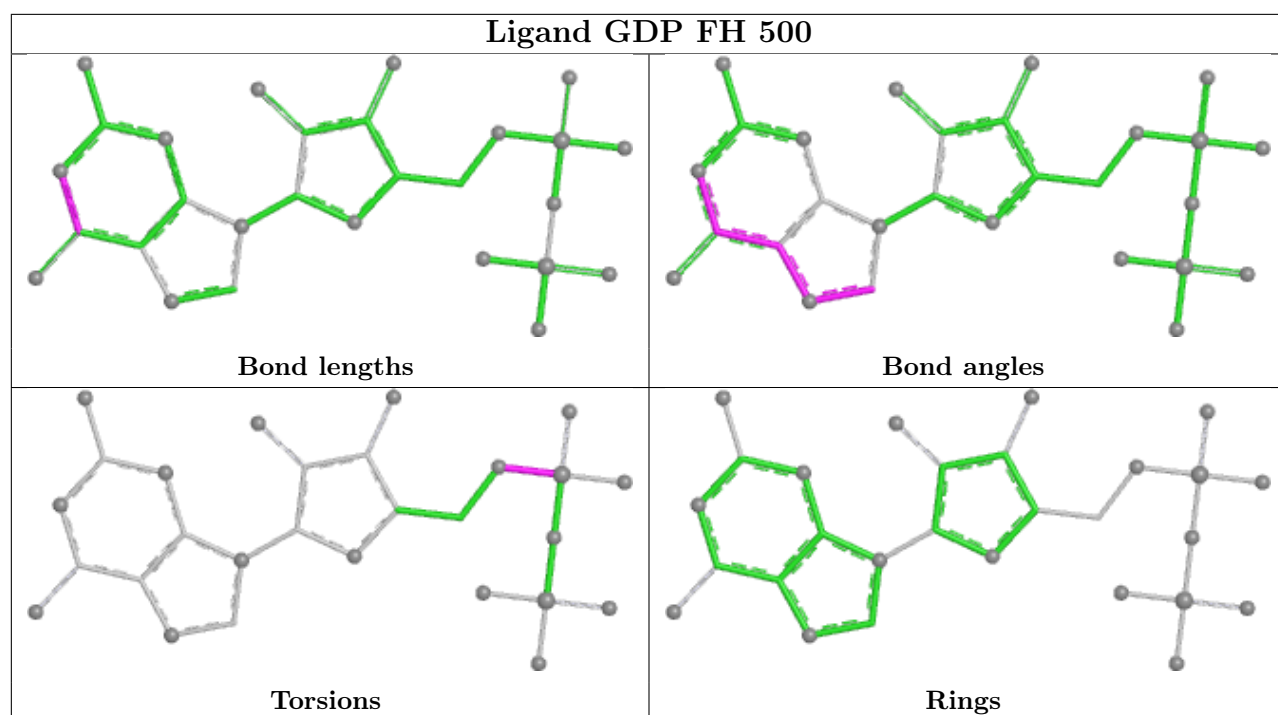
Ligand GTP UE 501

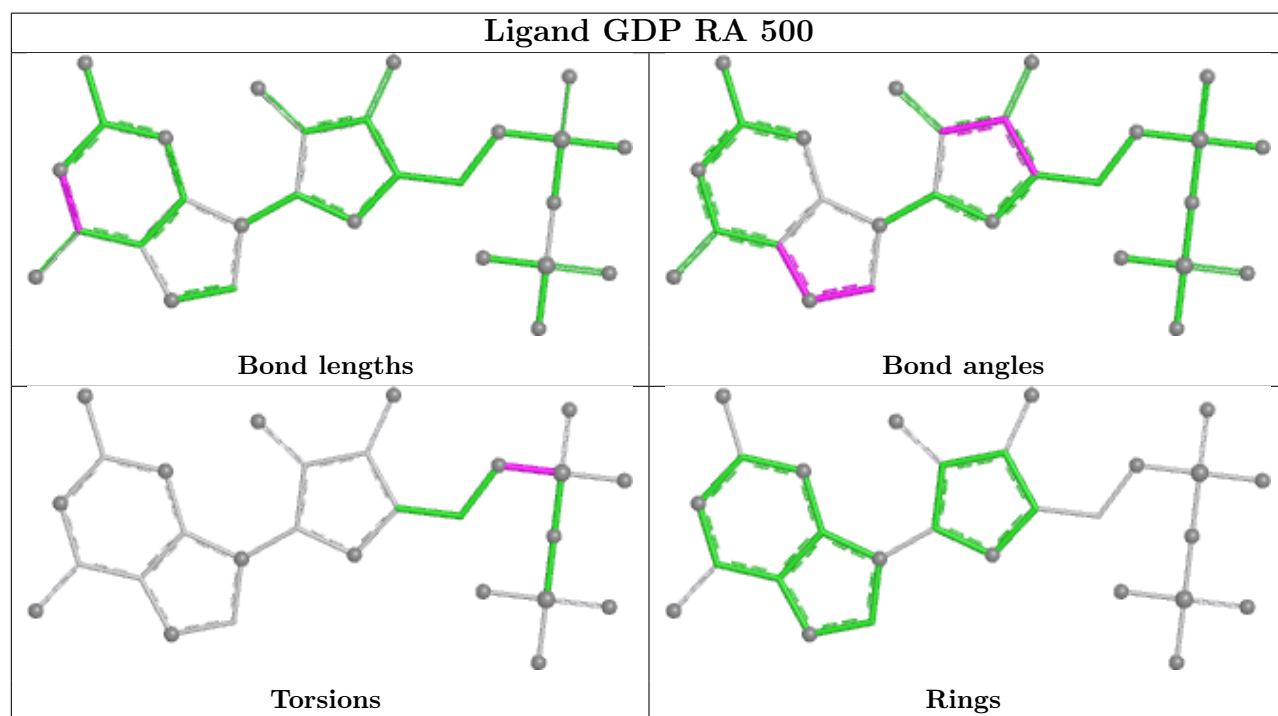
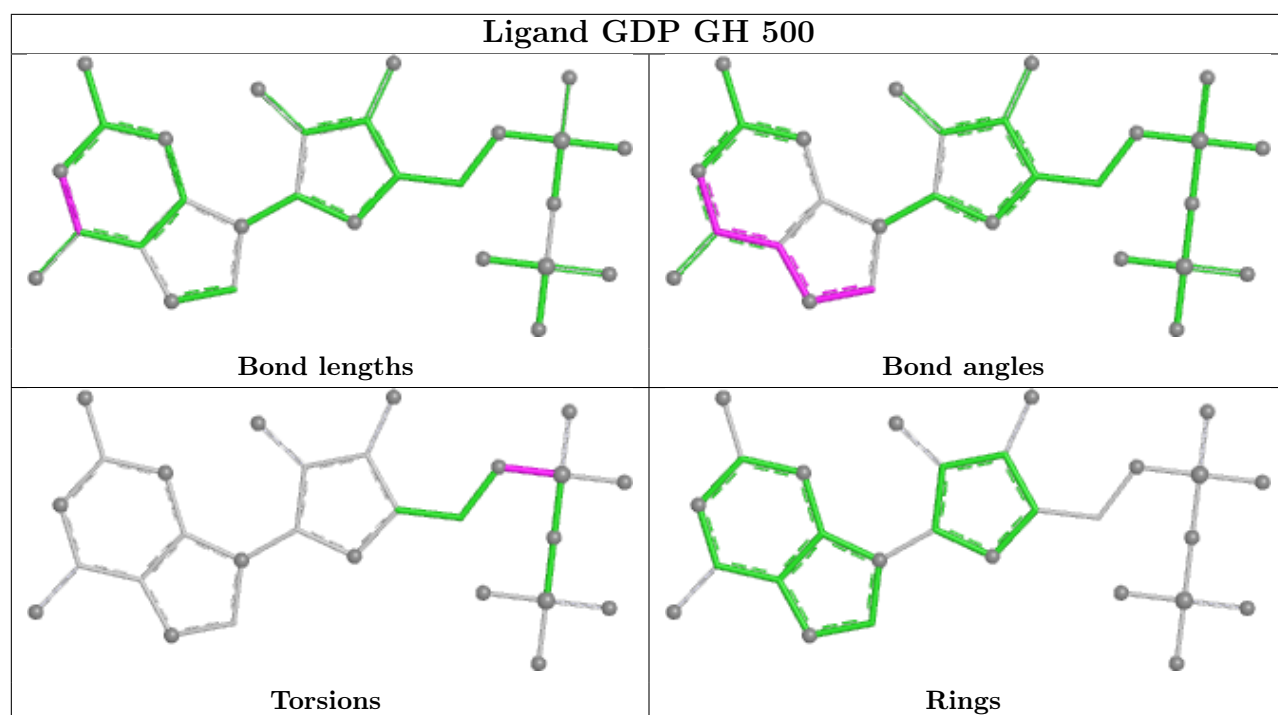


Ligand GTP HA 501

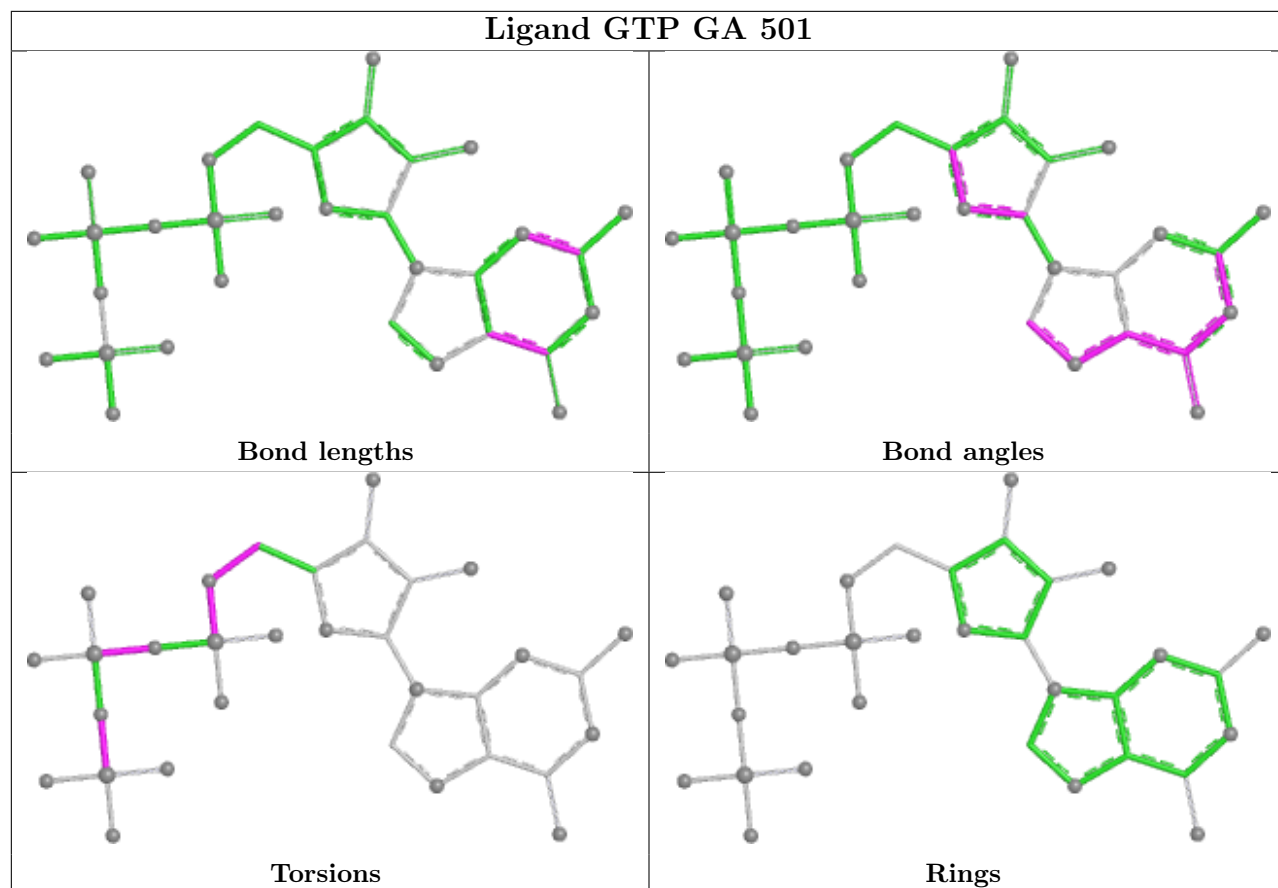




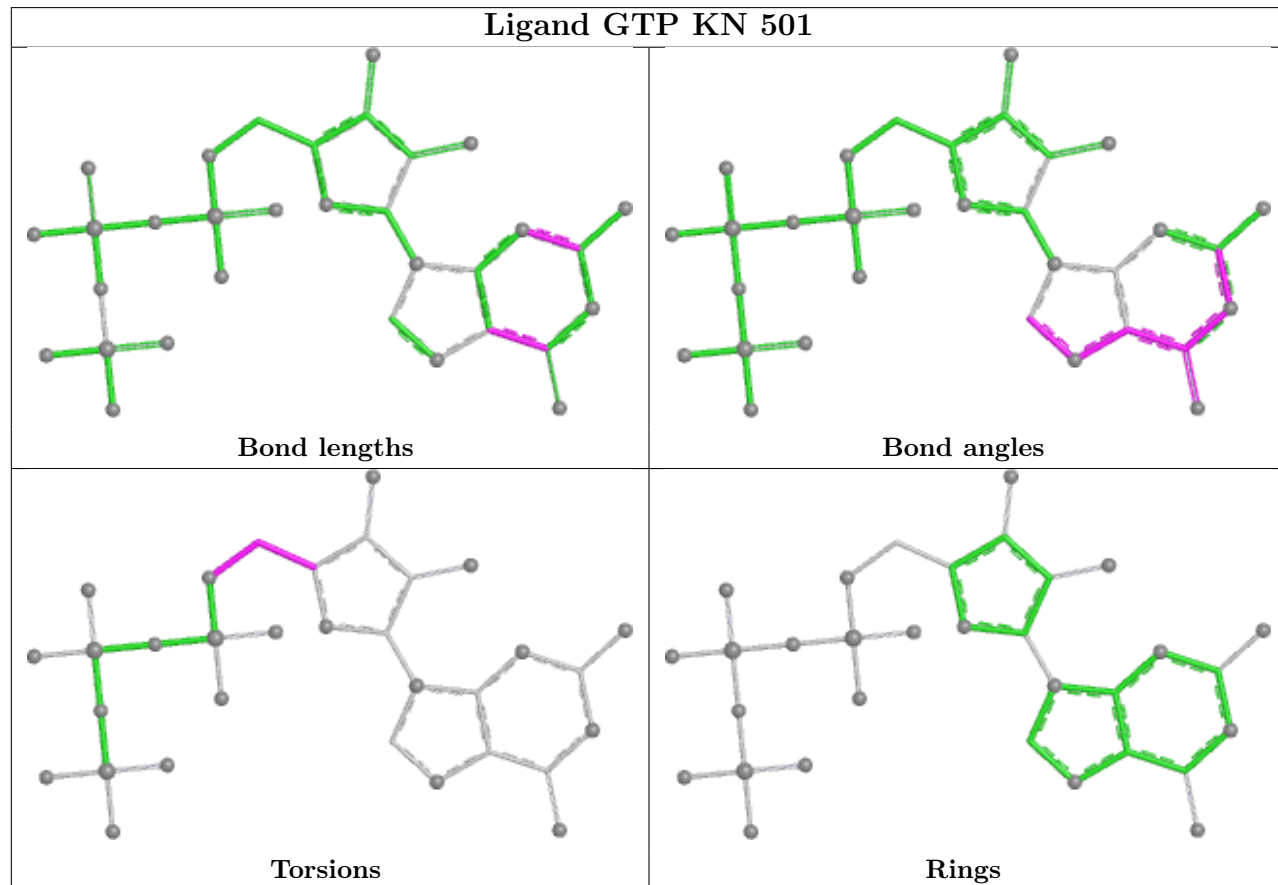


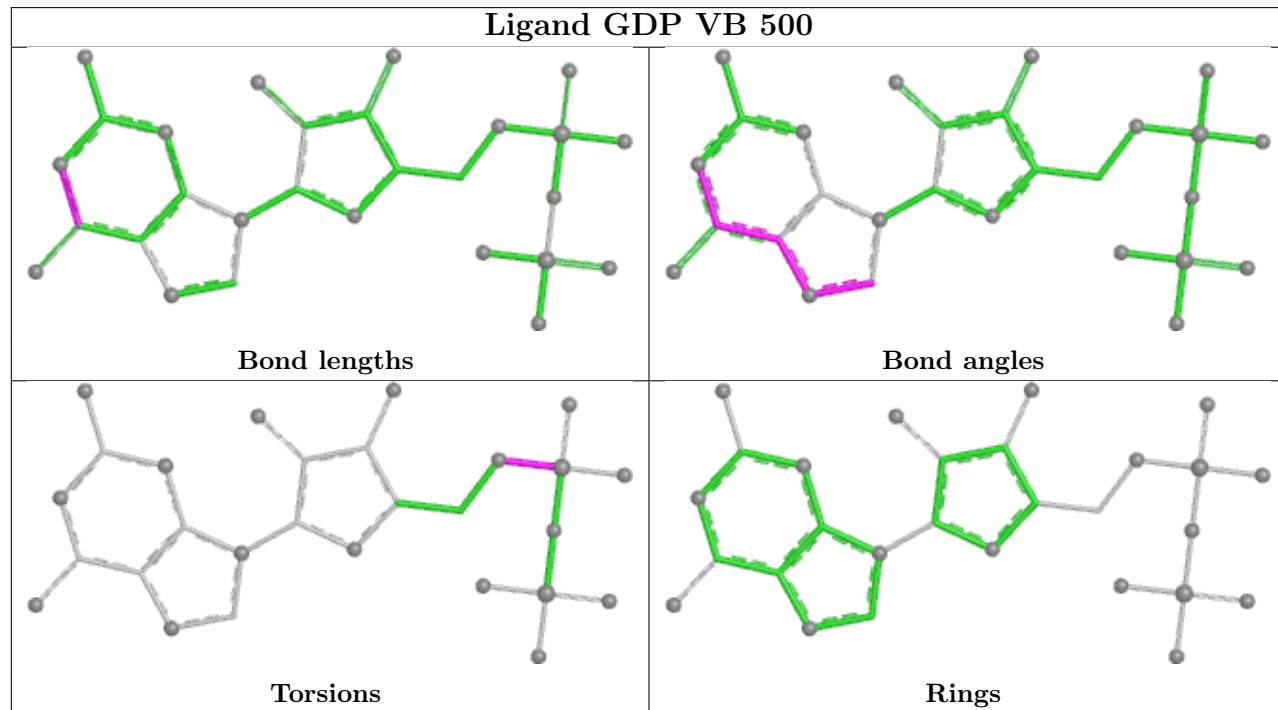
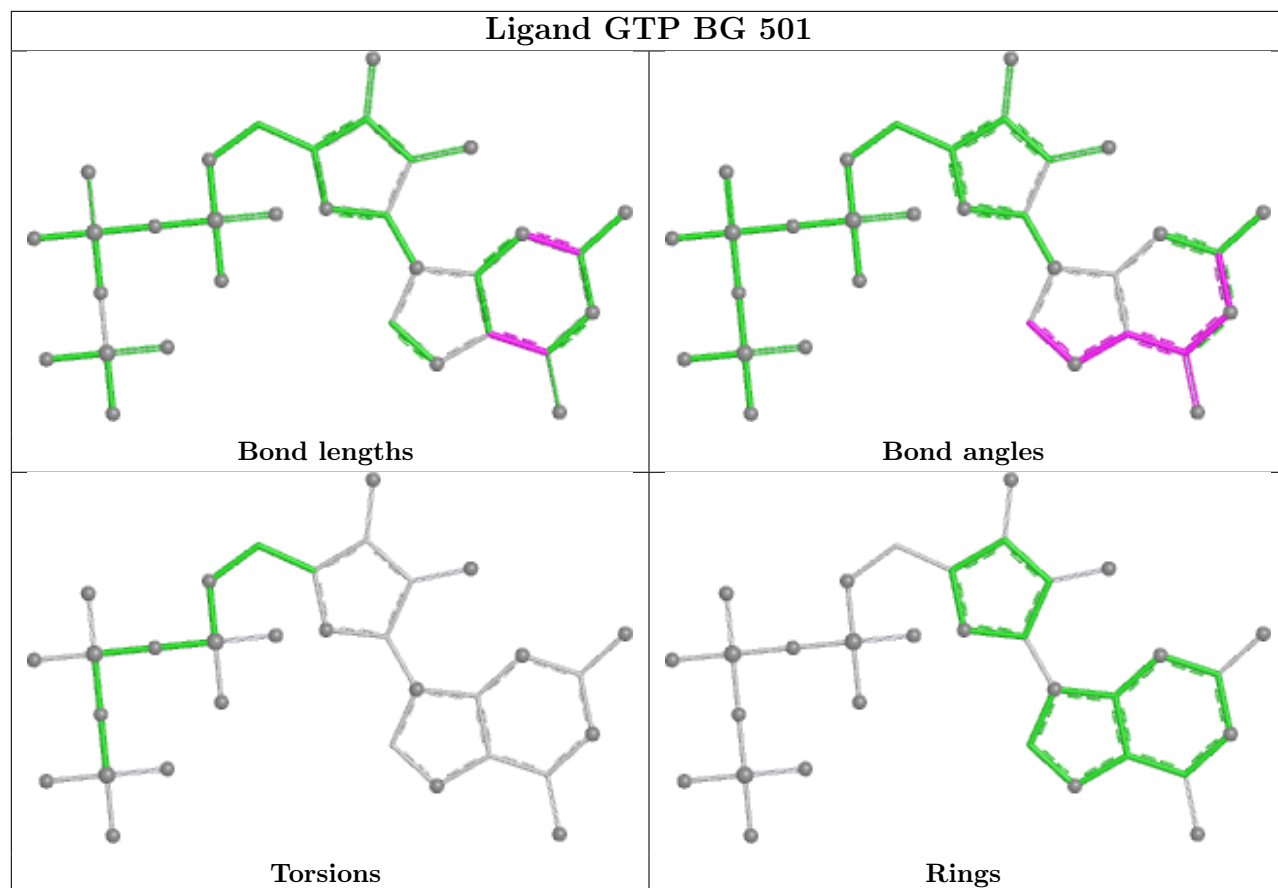


Ligand GTP GA 501

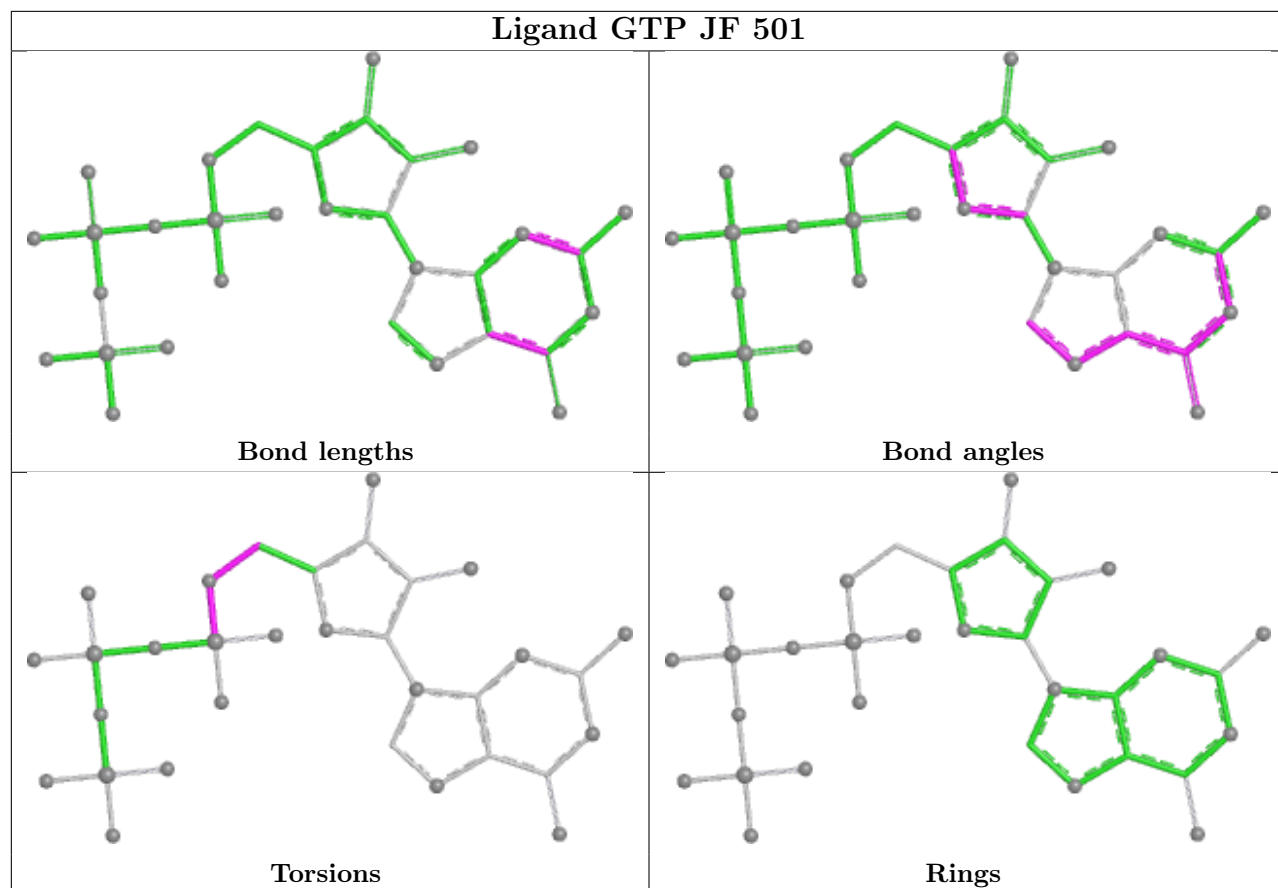


Ligand GTP KN 501

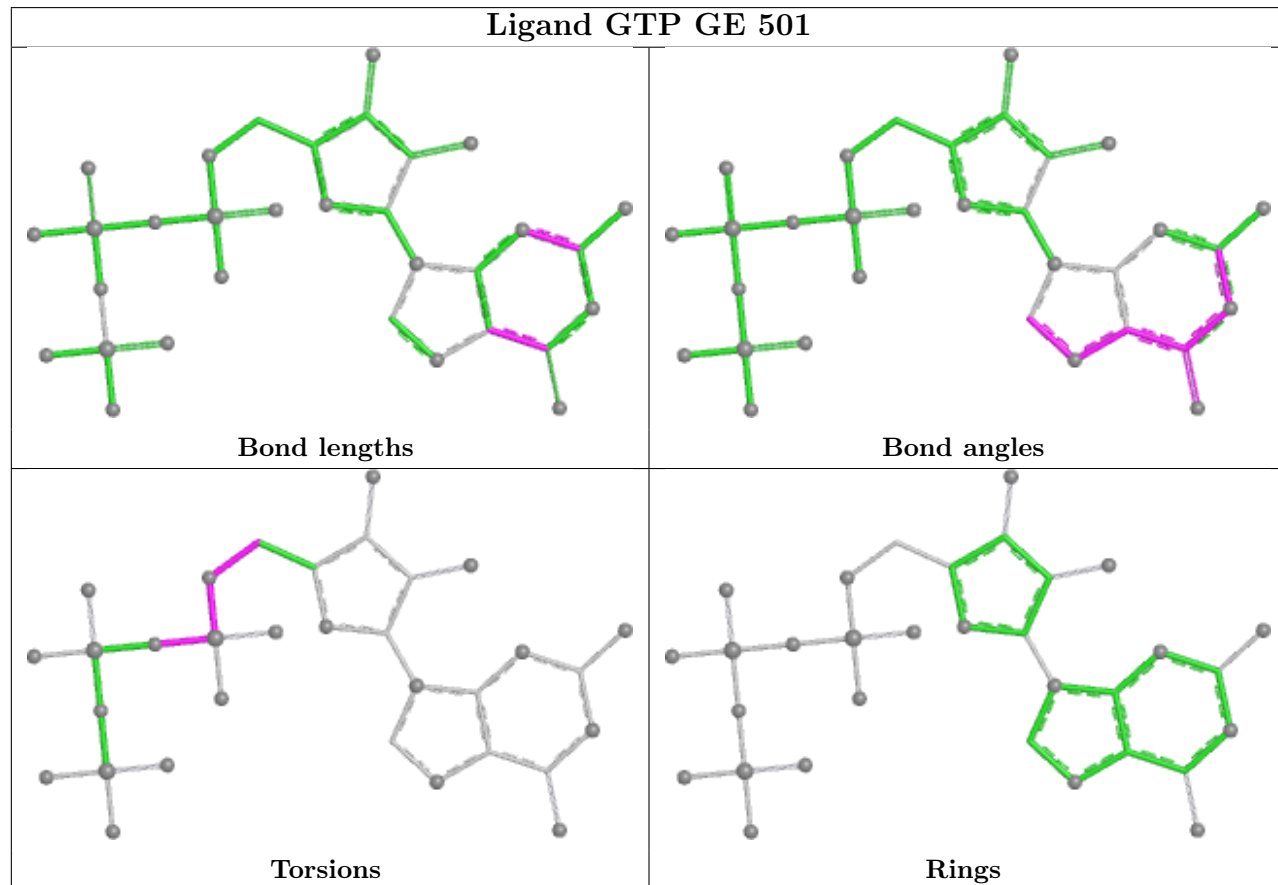




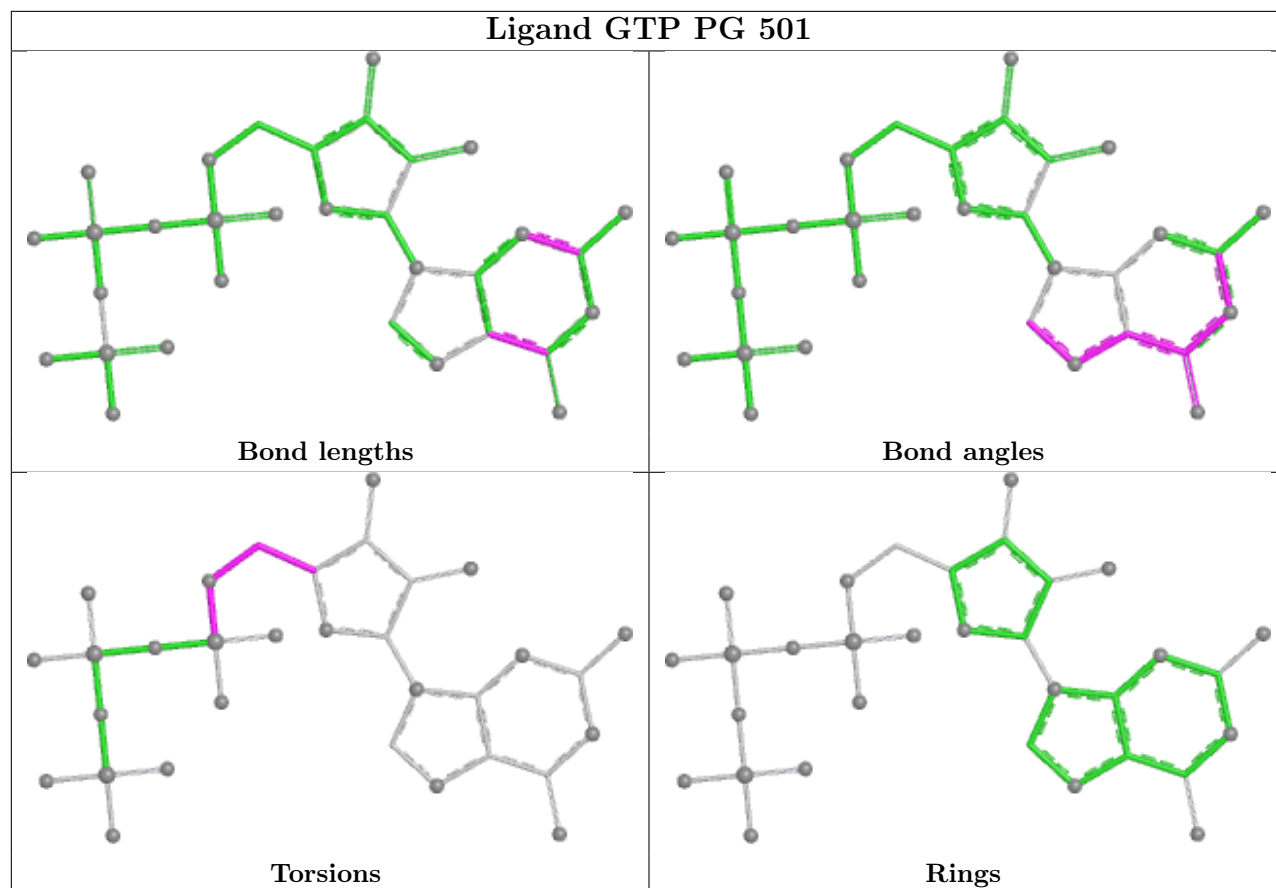
Ligand GTP JF 501



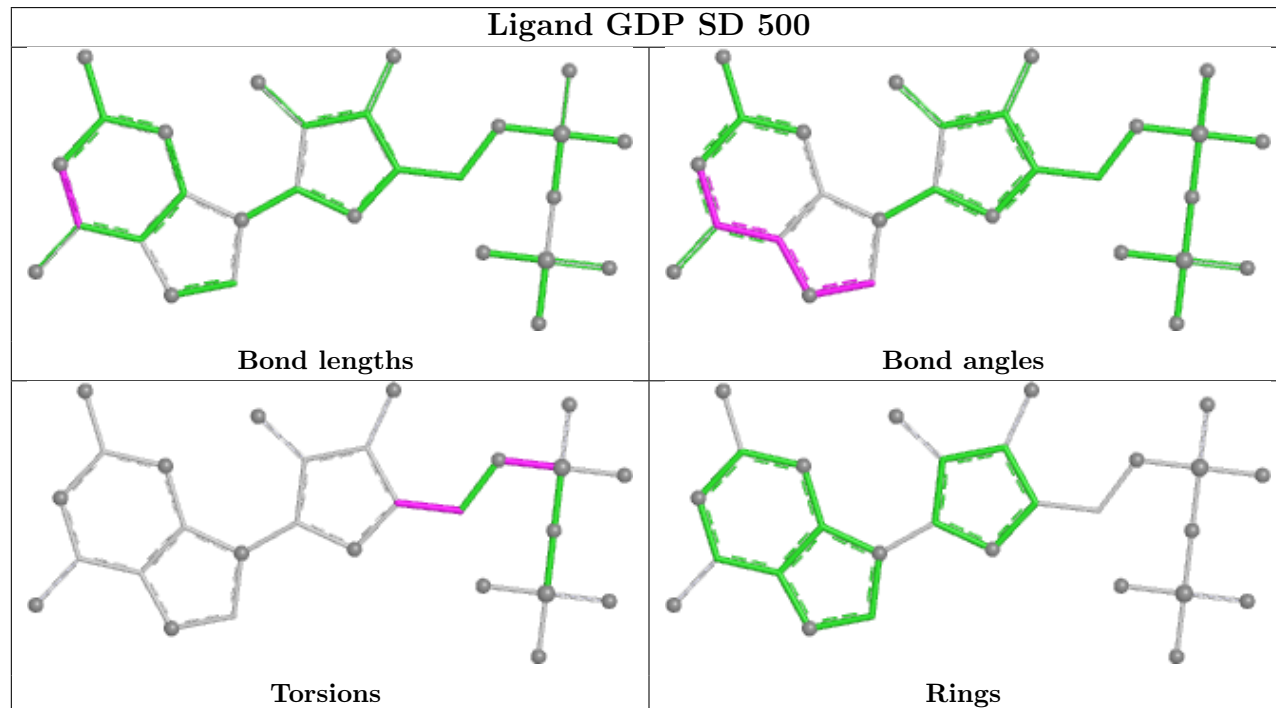
Ligand GTP GE 501



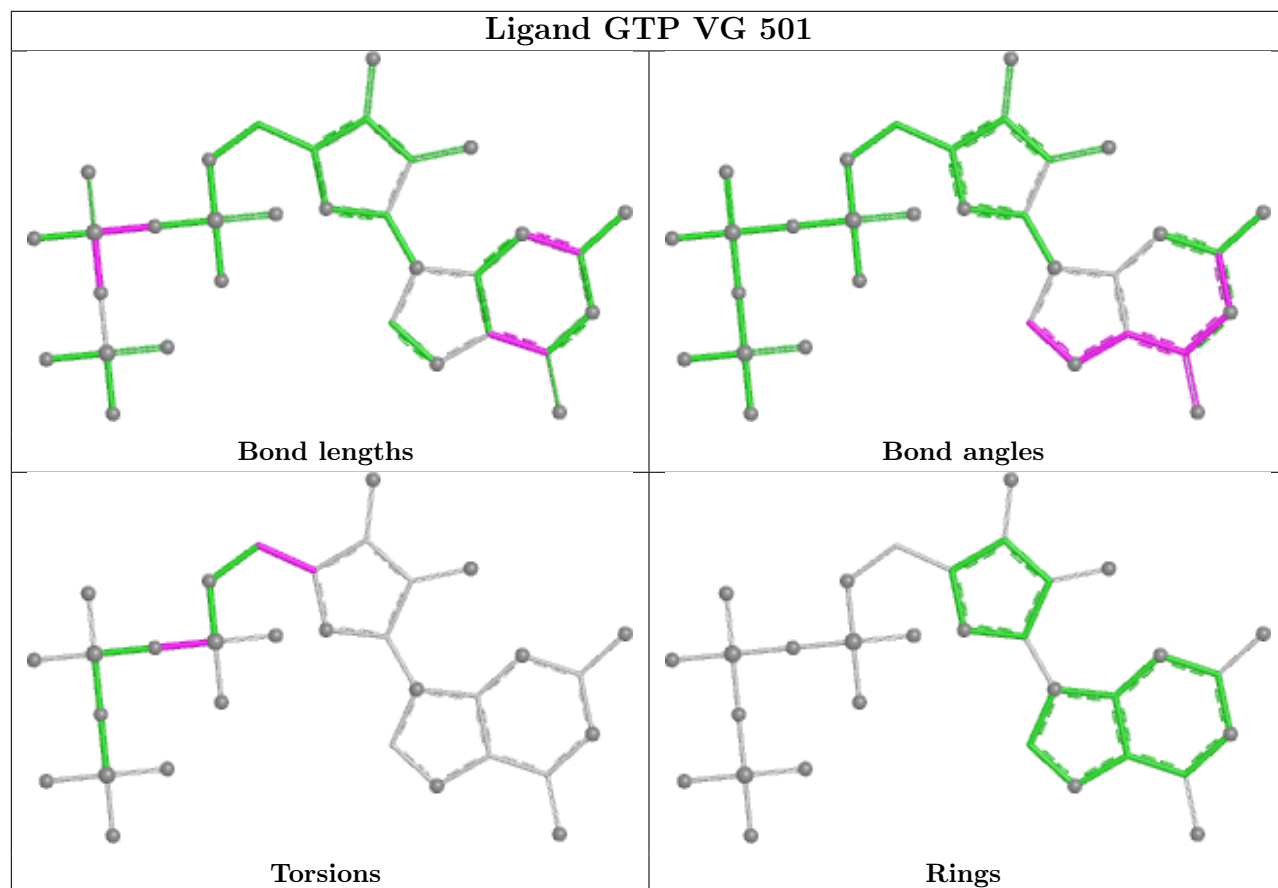
Ligand GTP PG 501



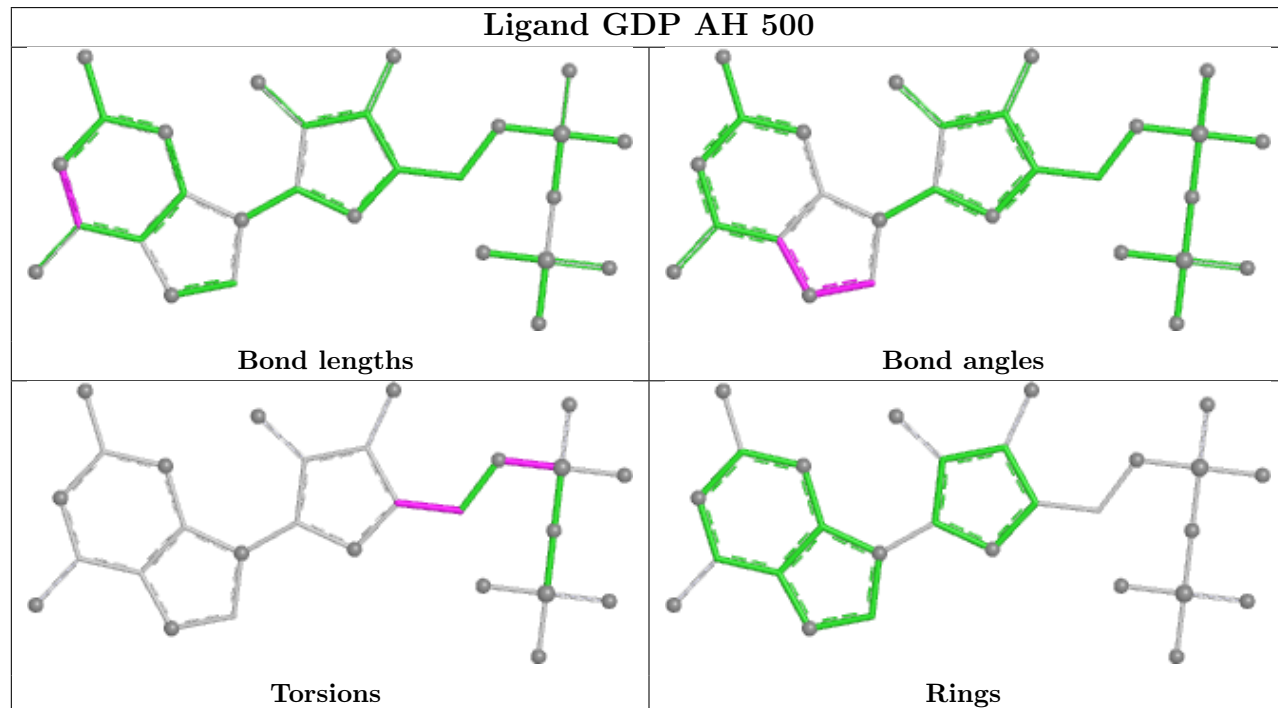
Ligand GDP SD 500

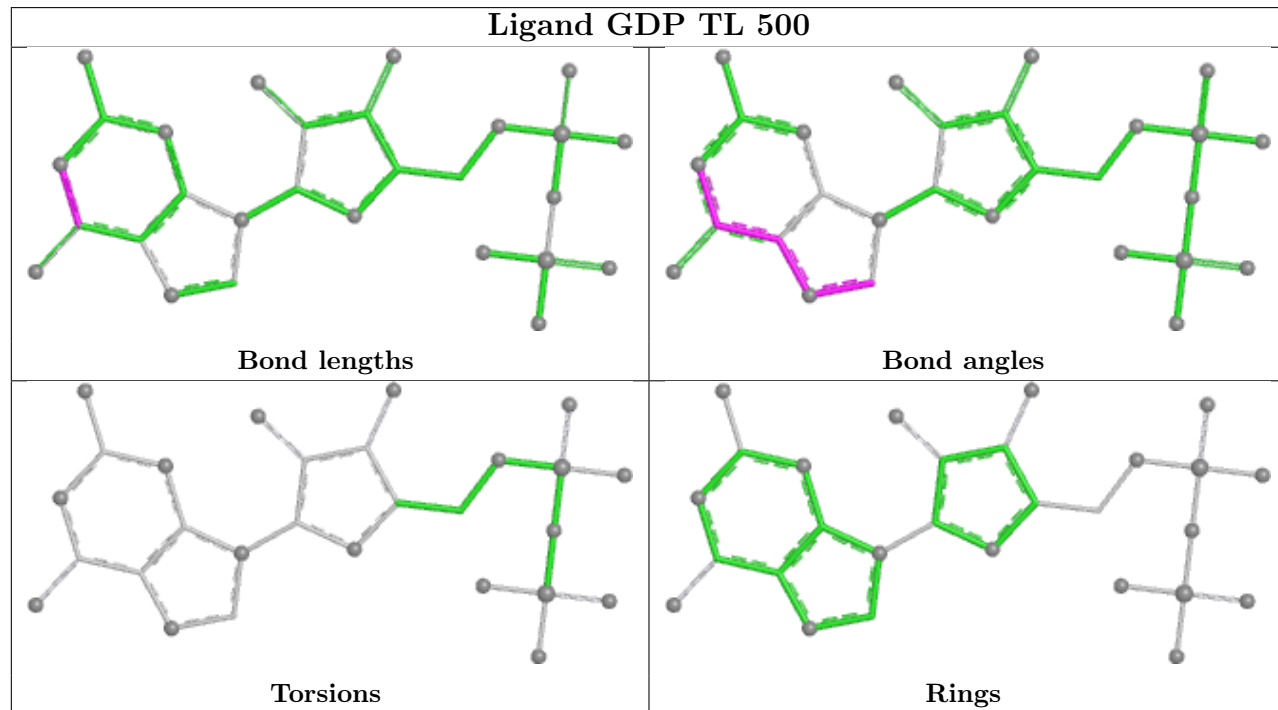
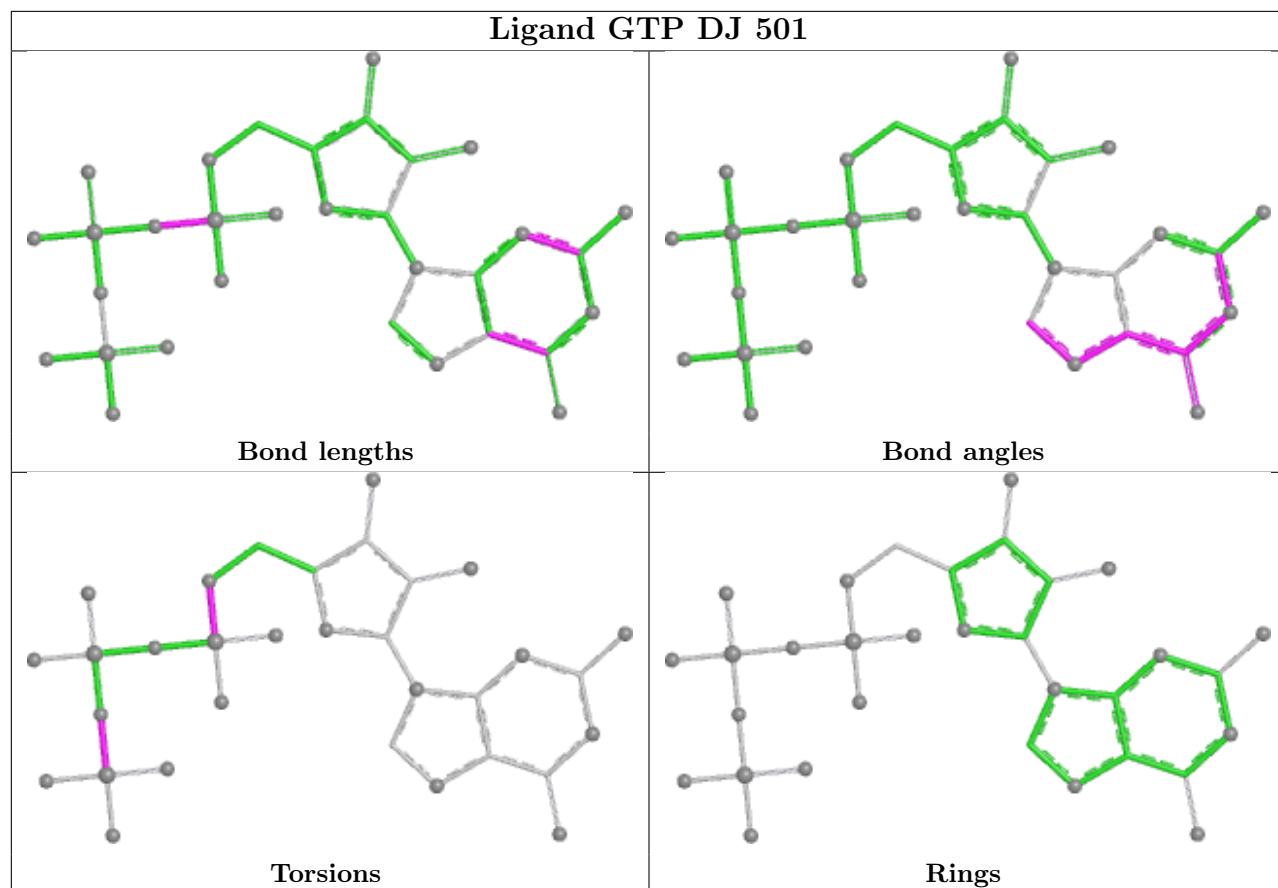


Ligand GTP VG 501

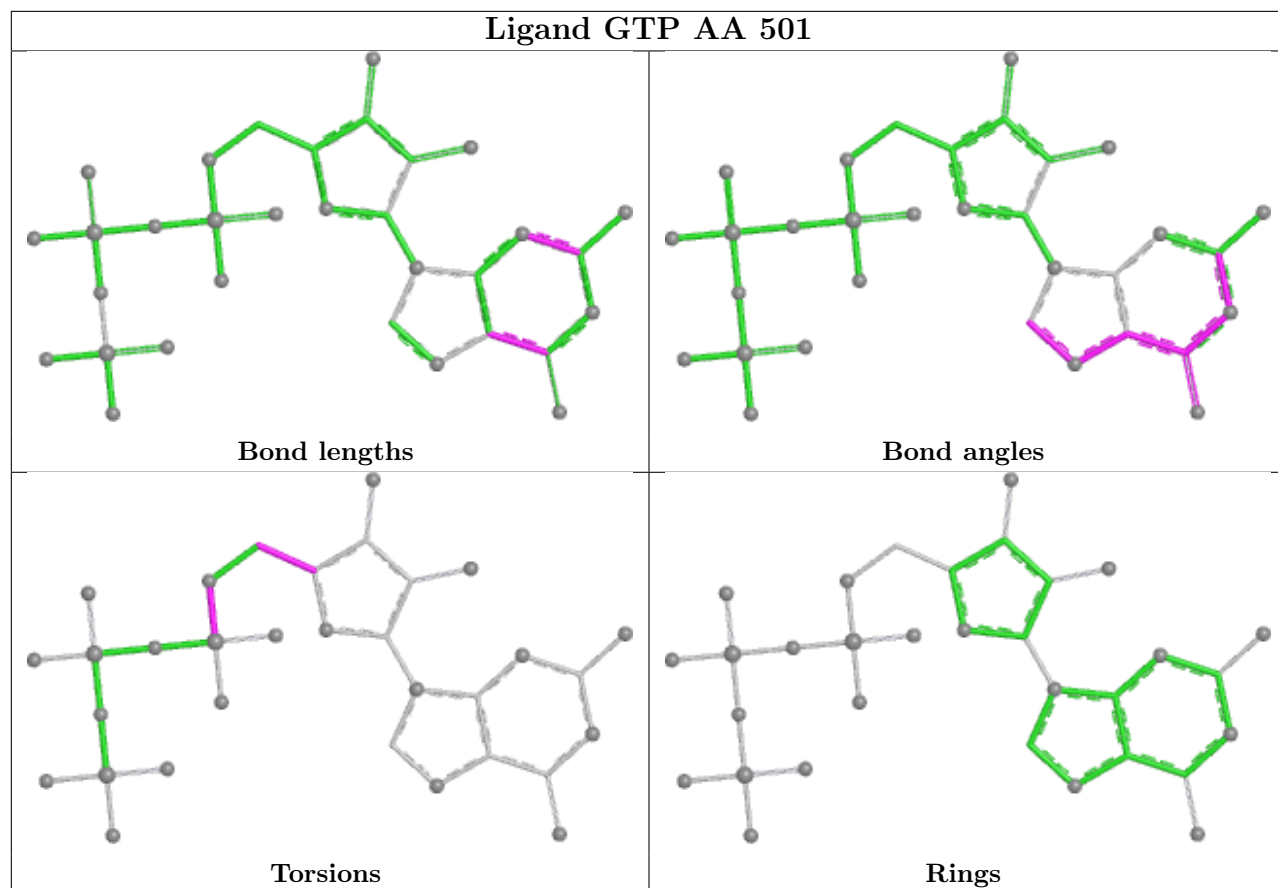


Ligand GDP AH 500

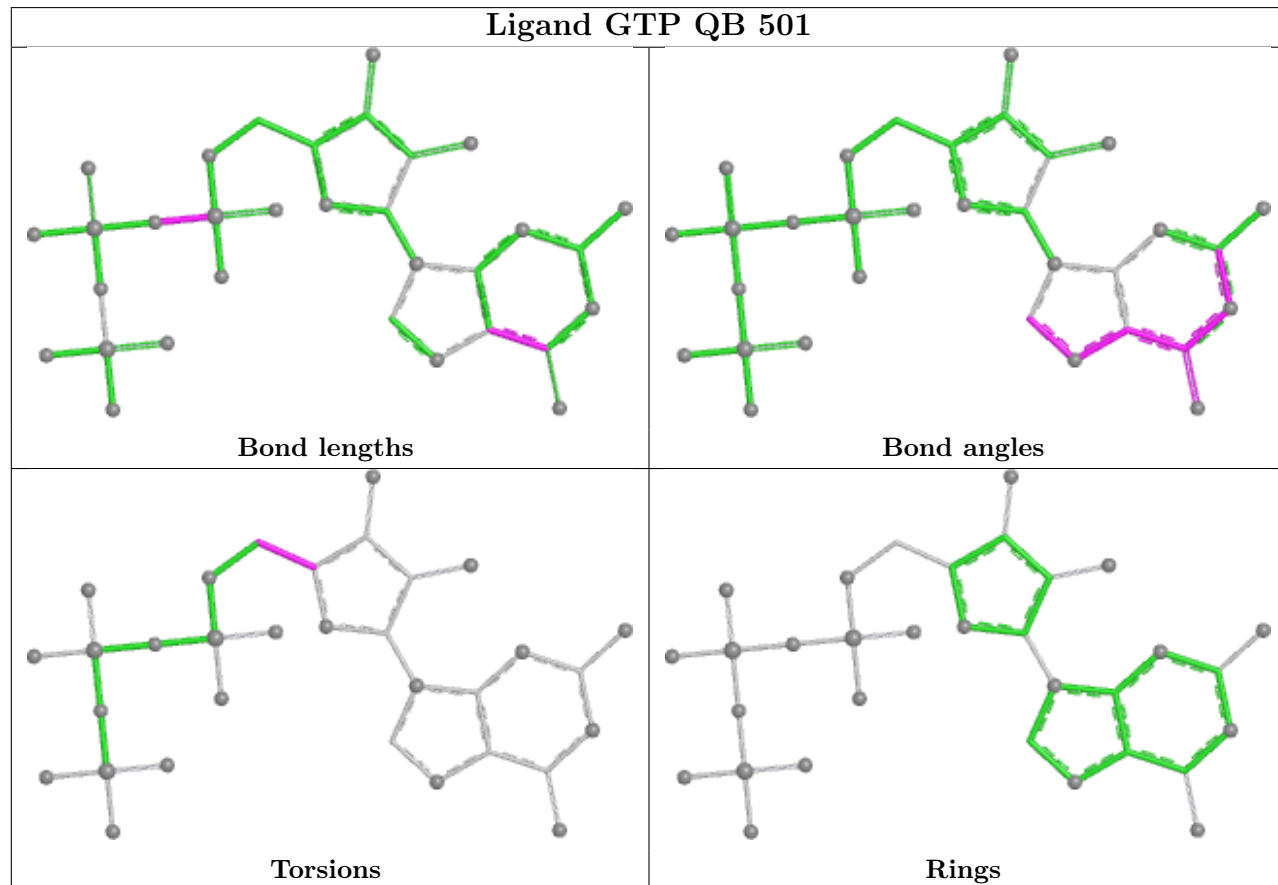




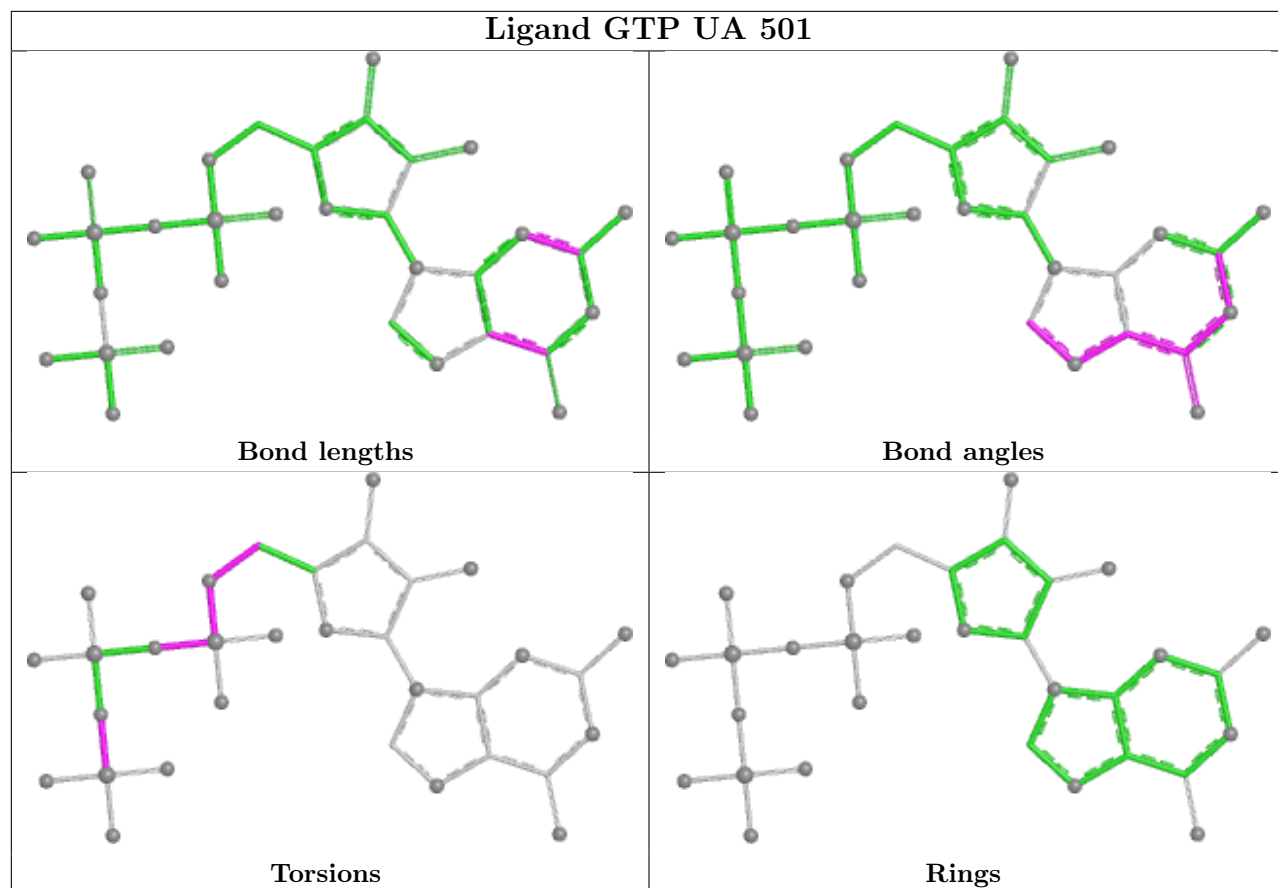
Ligand GTP AA 501



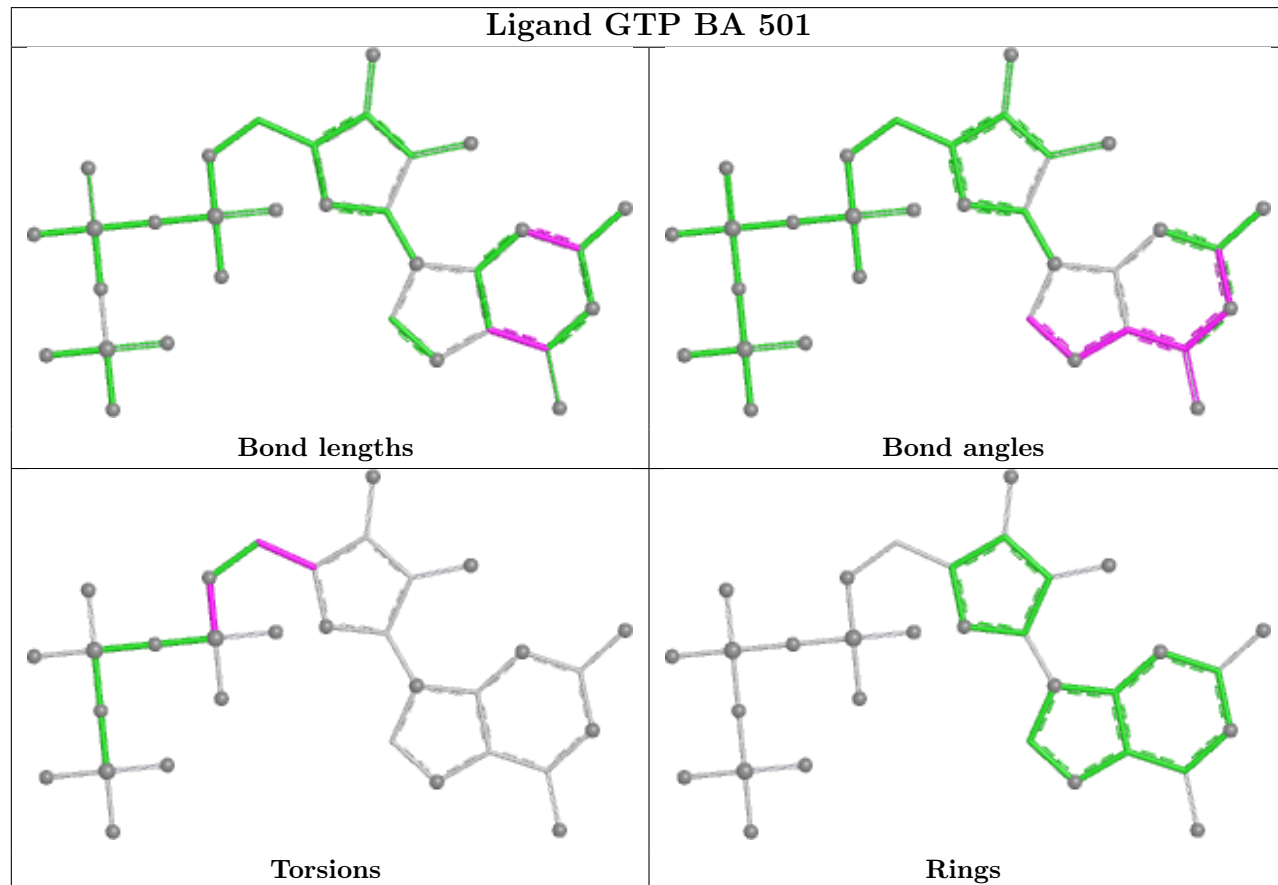
Ligand GTP QB 501

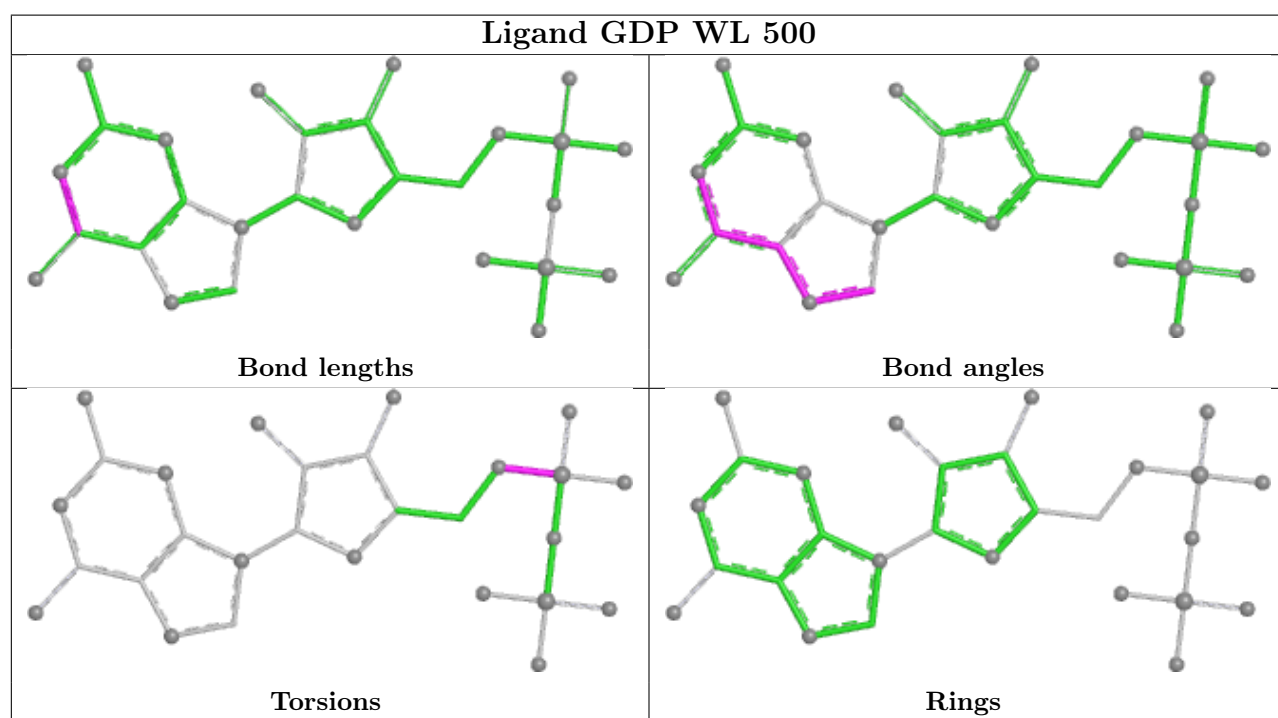
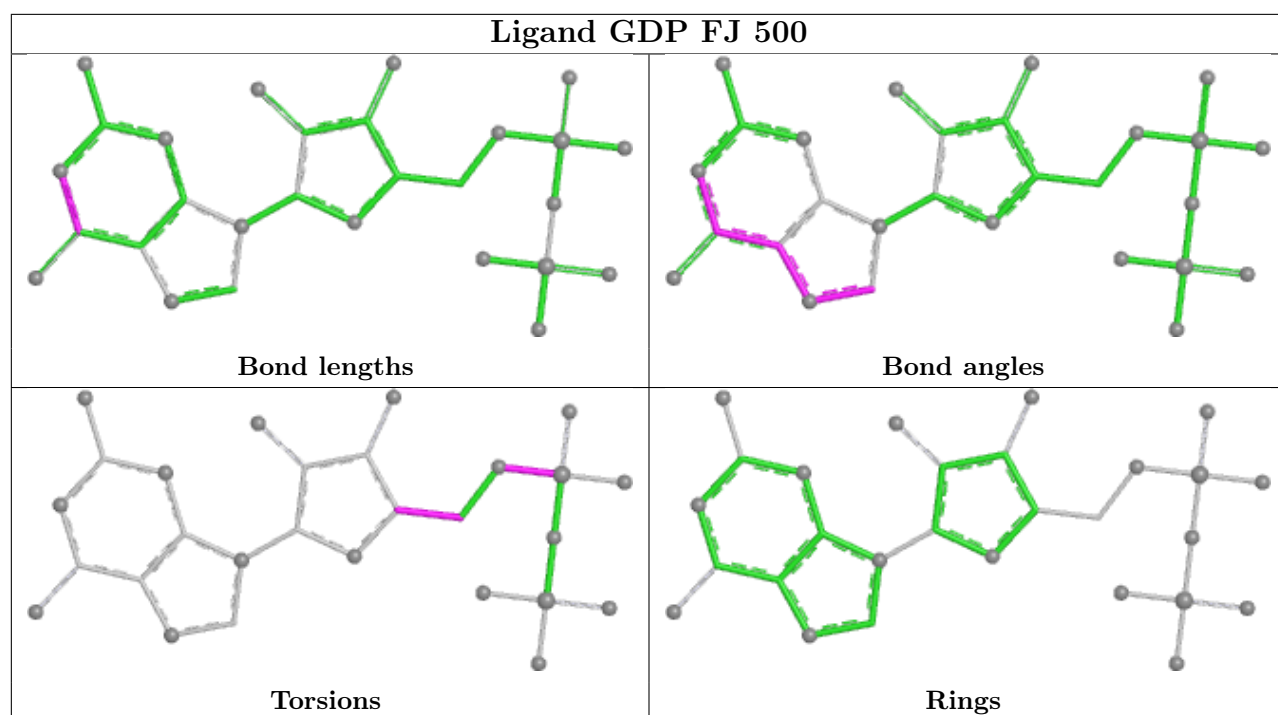


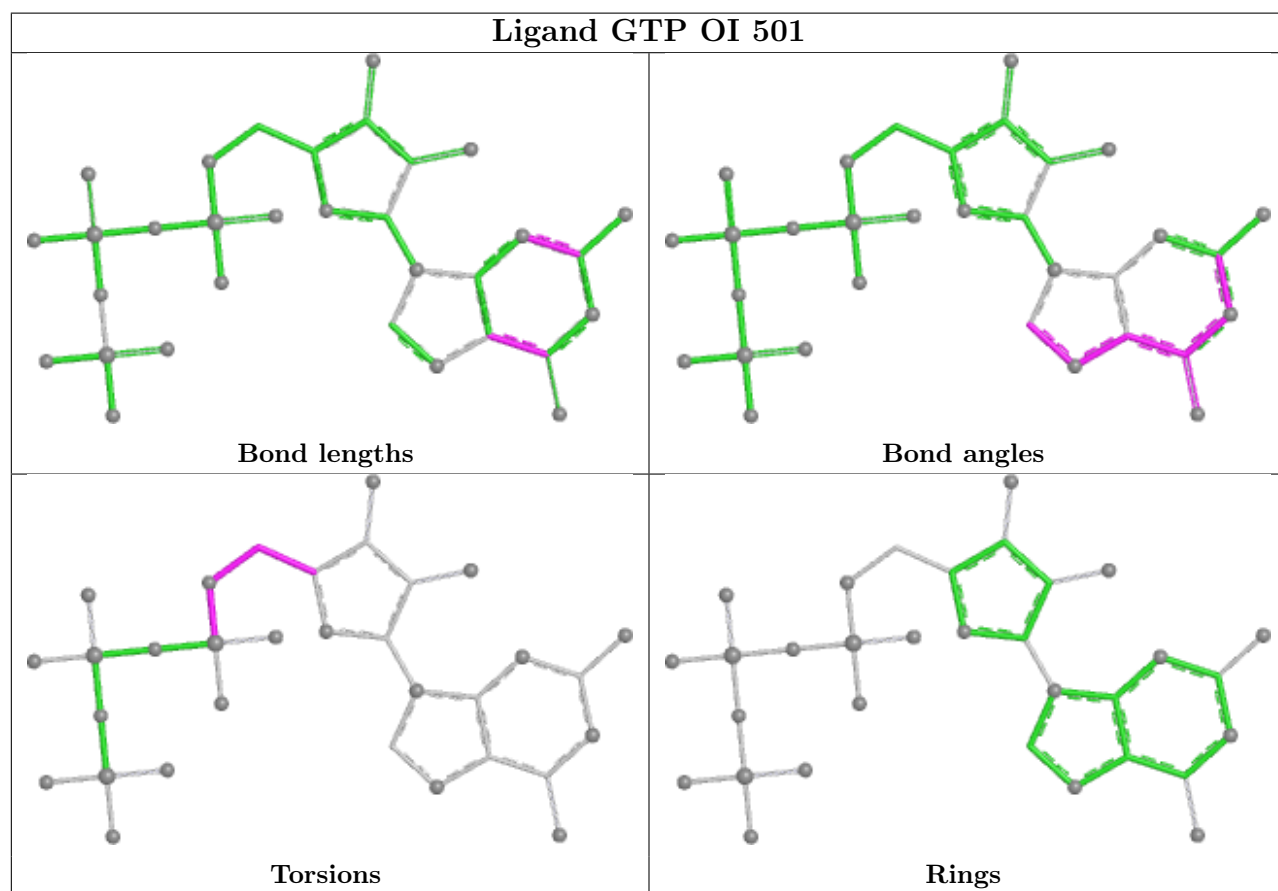
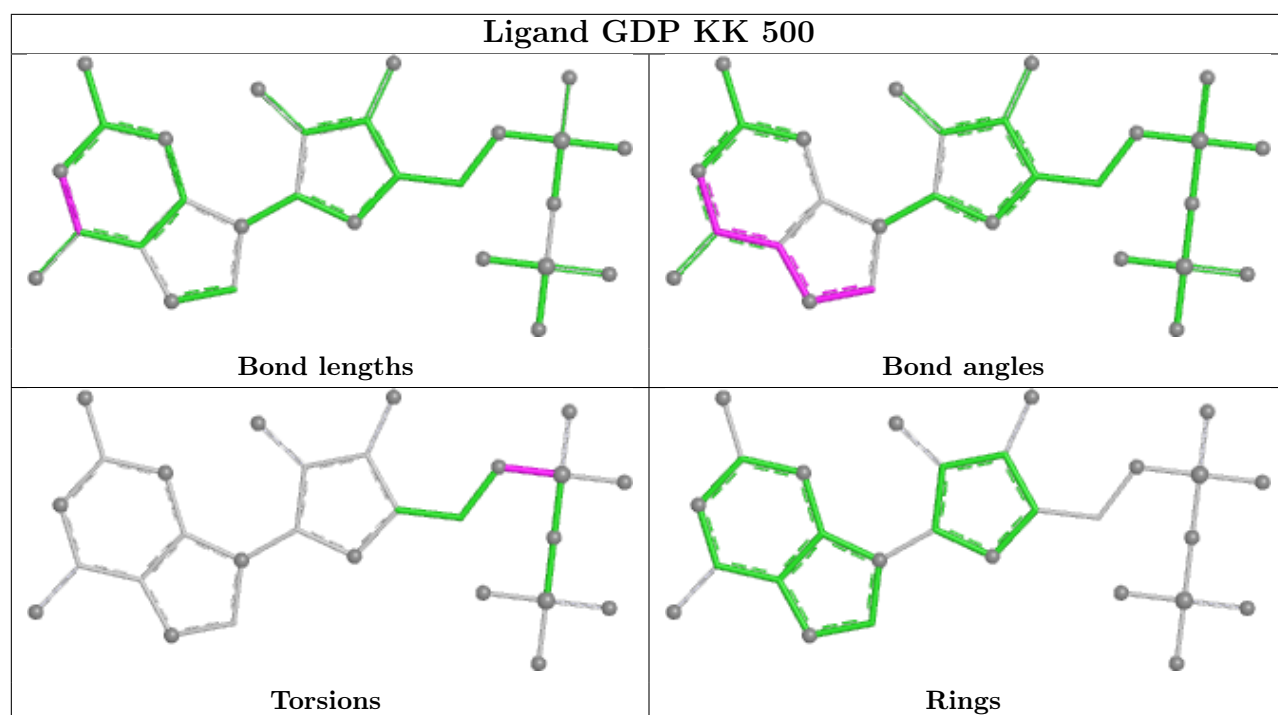
Ligand GTP UA 501

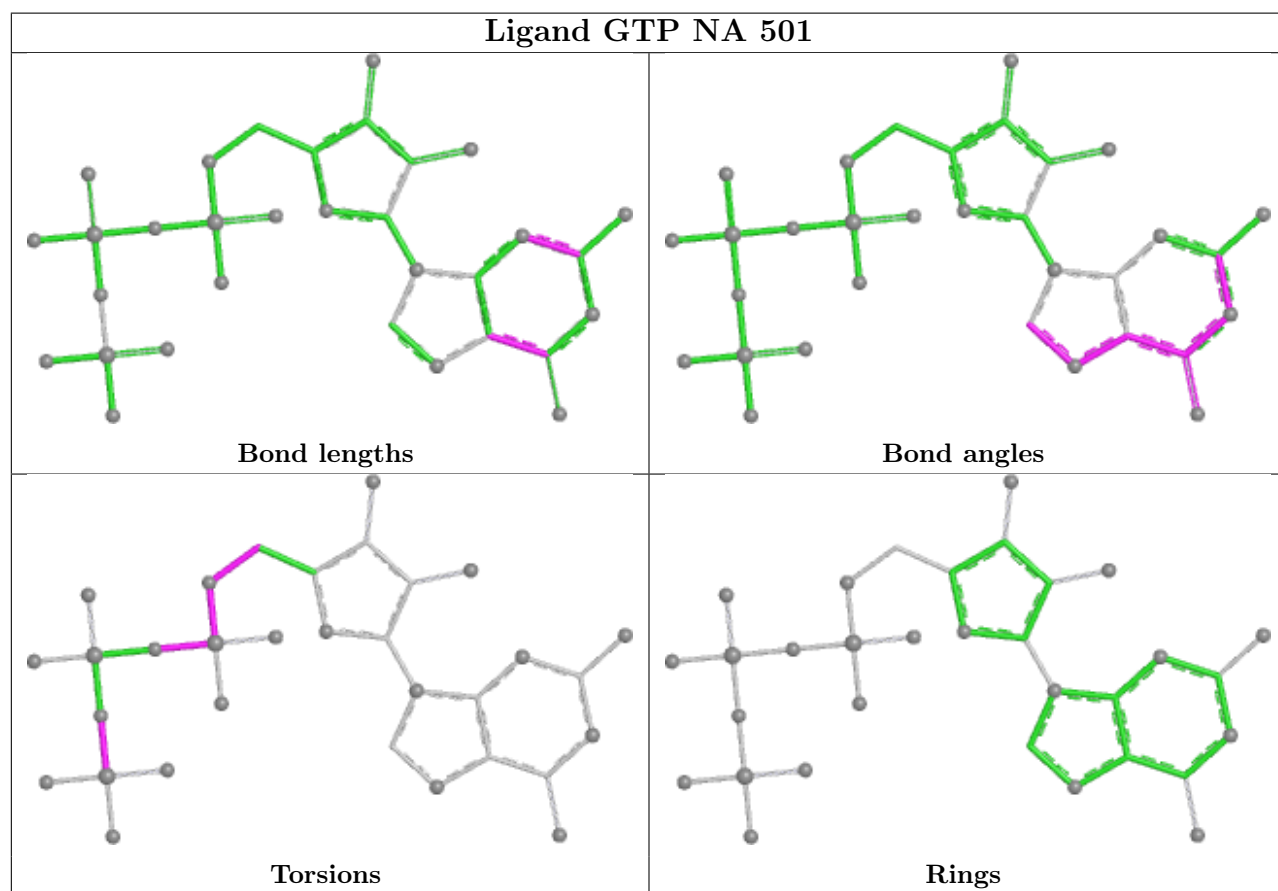
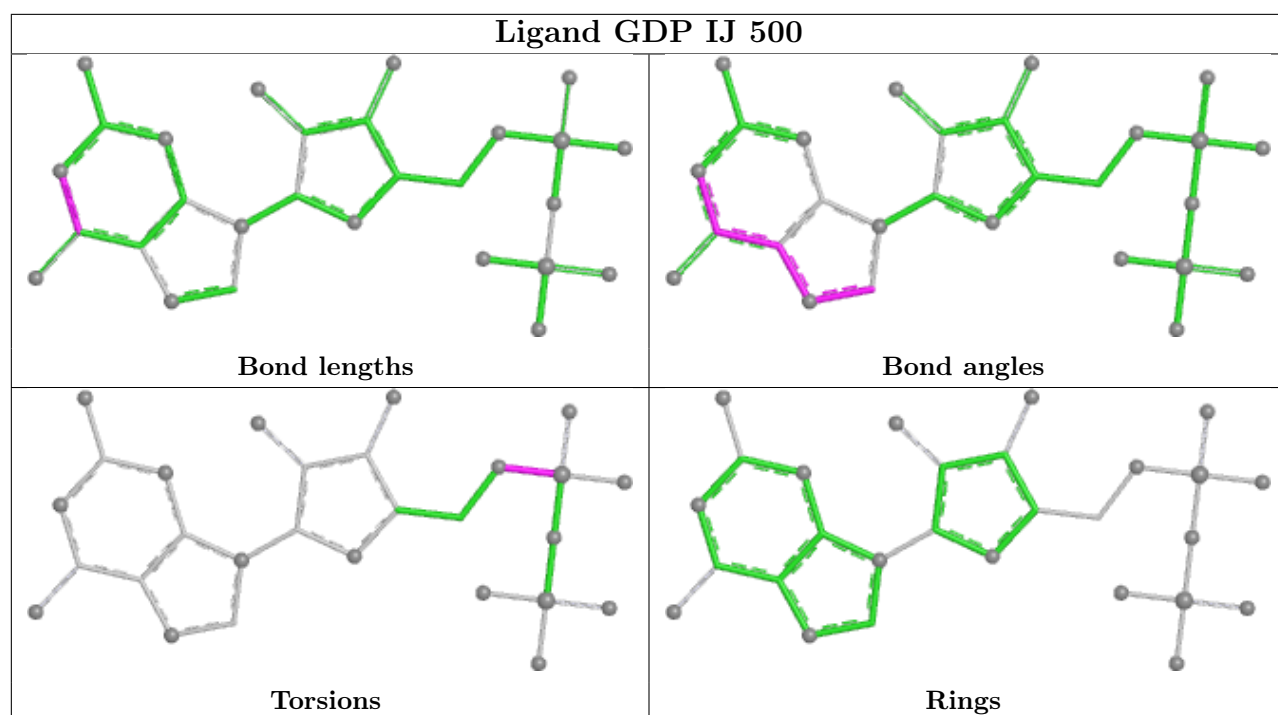


Ligand GTP BA 501

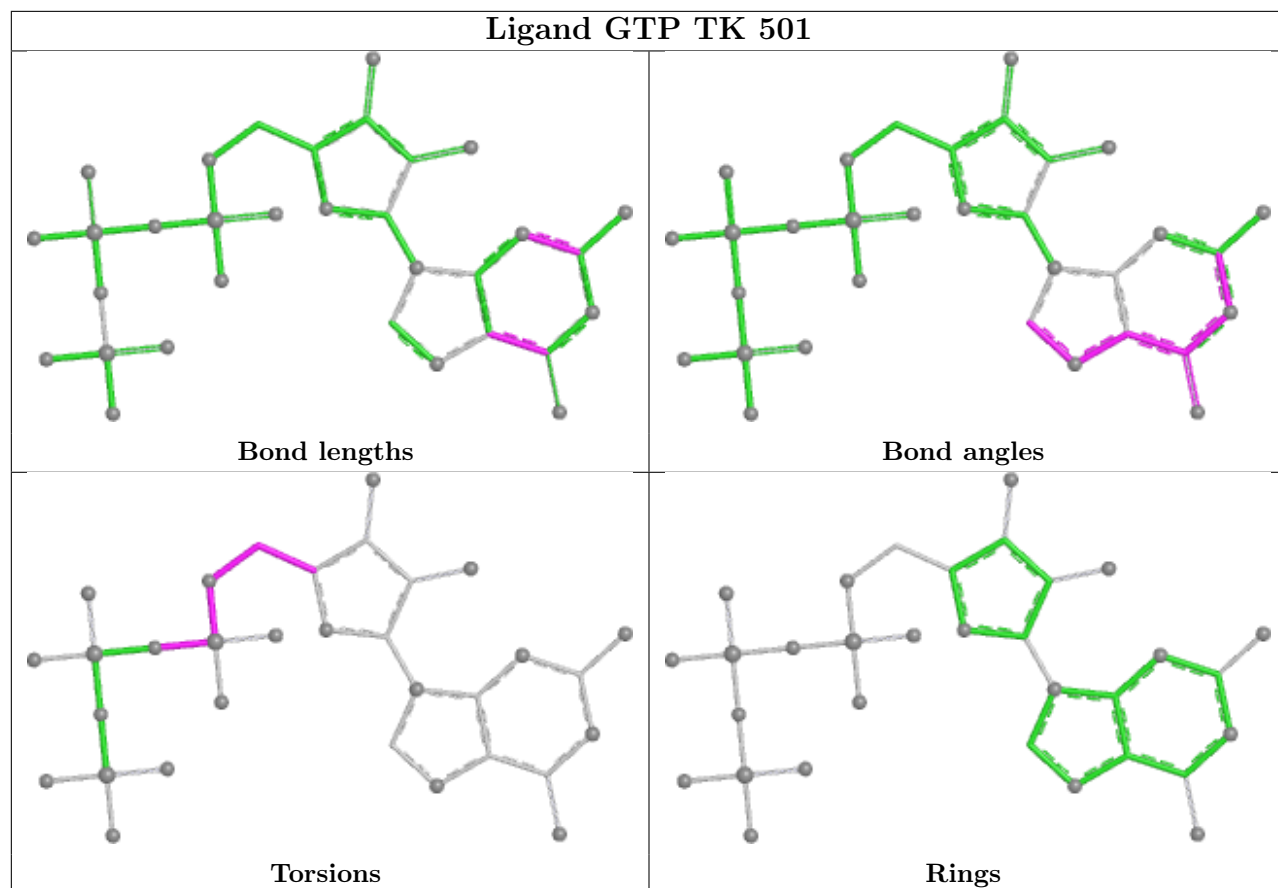




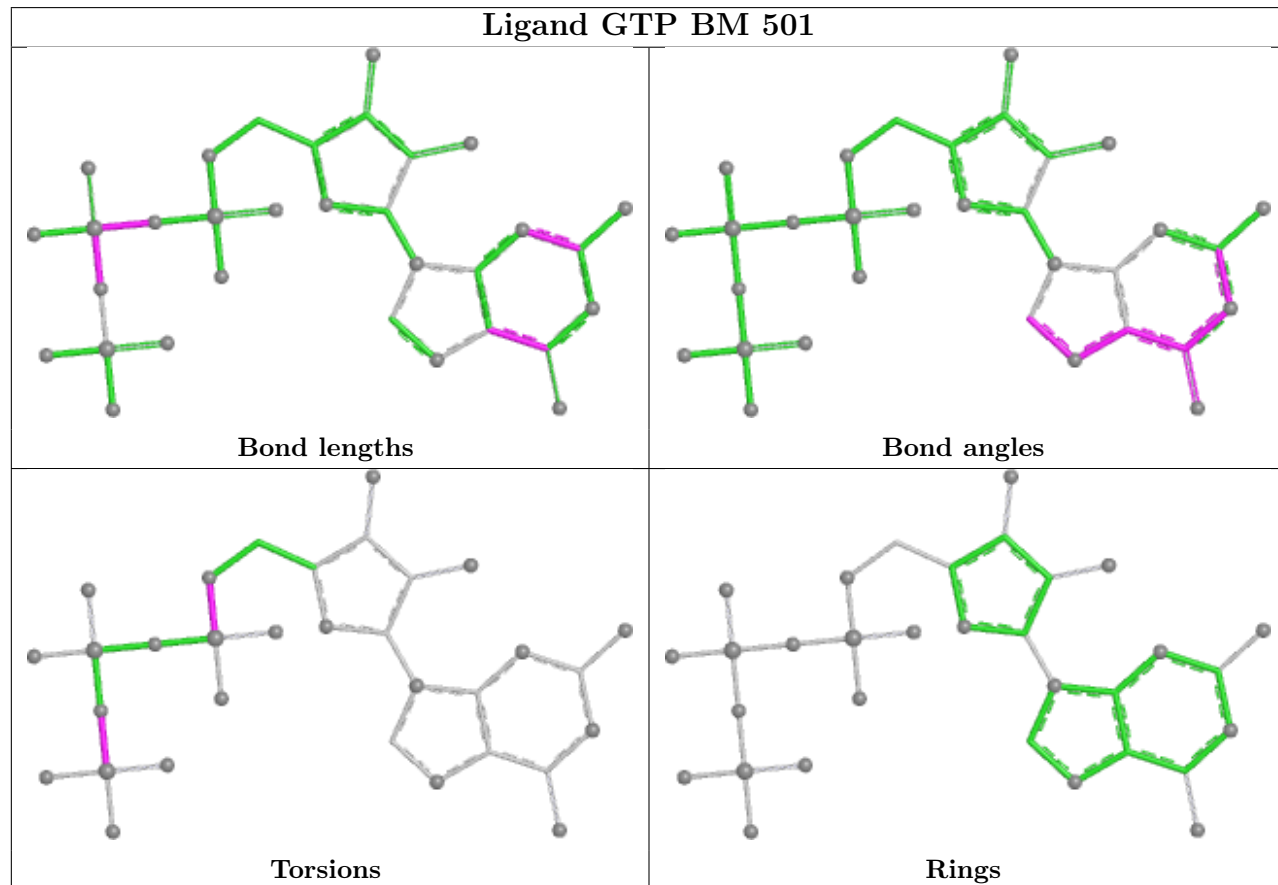


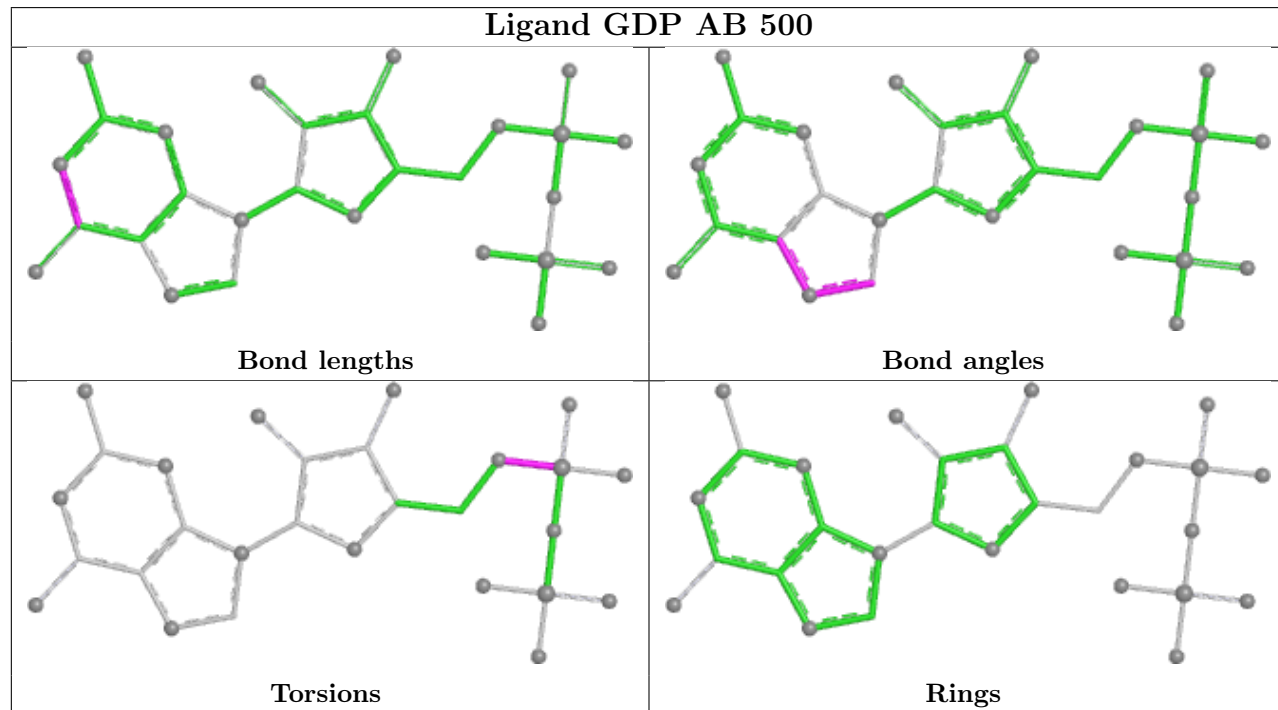
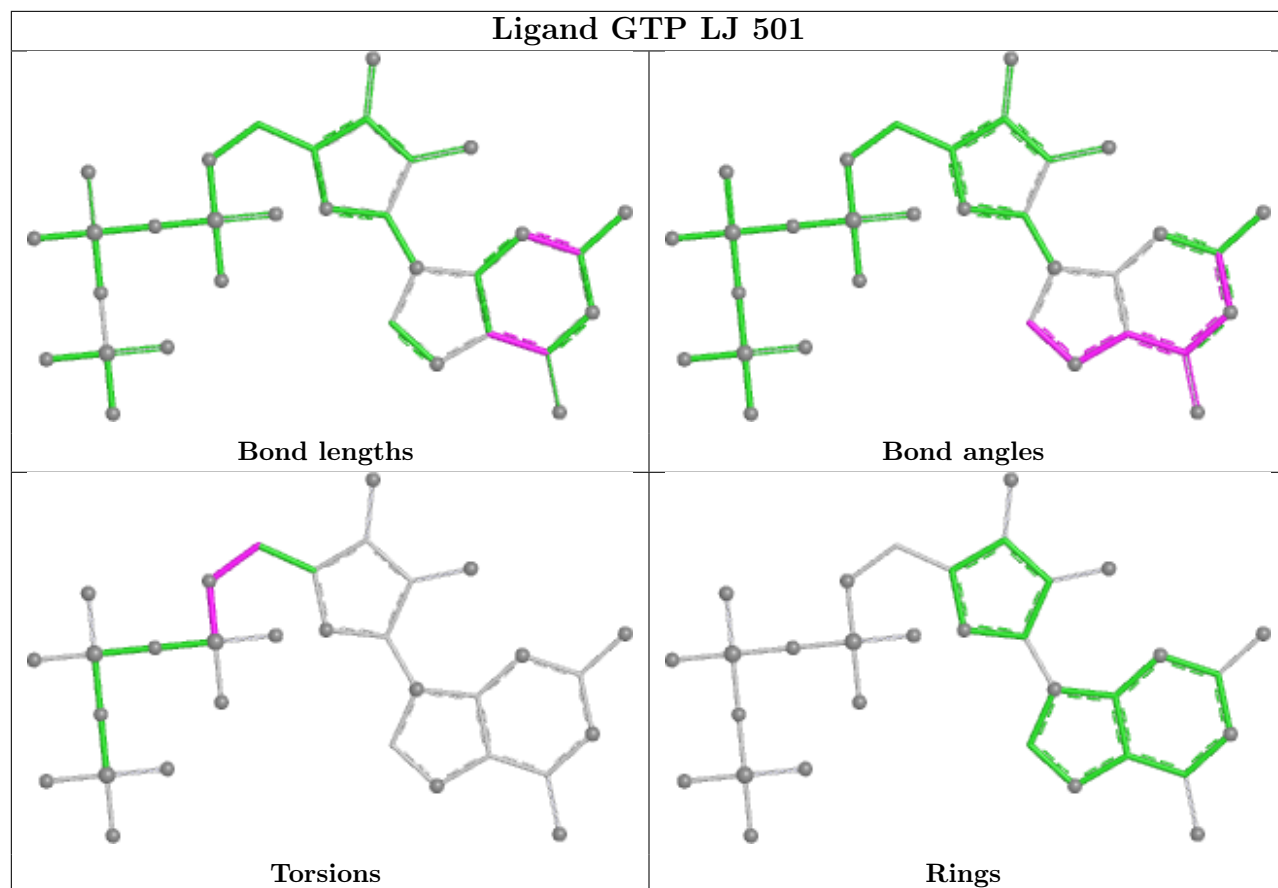


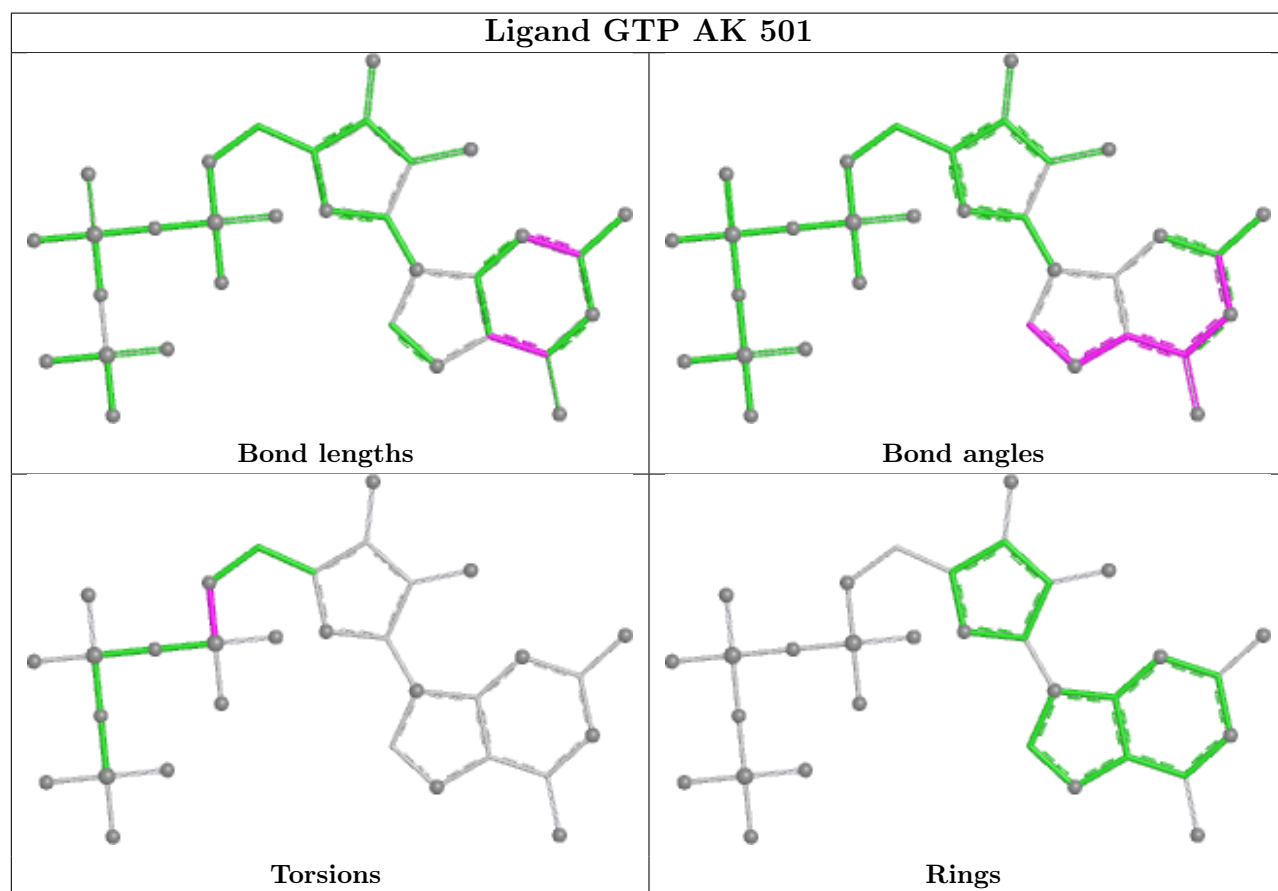
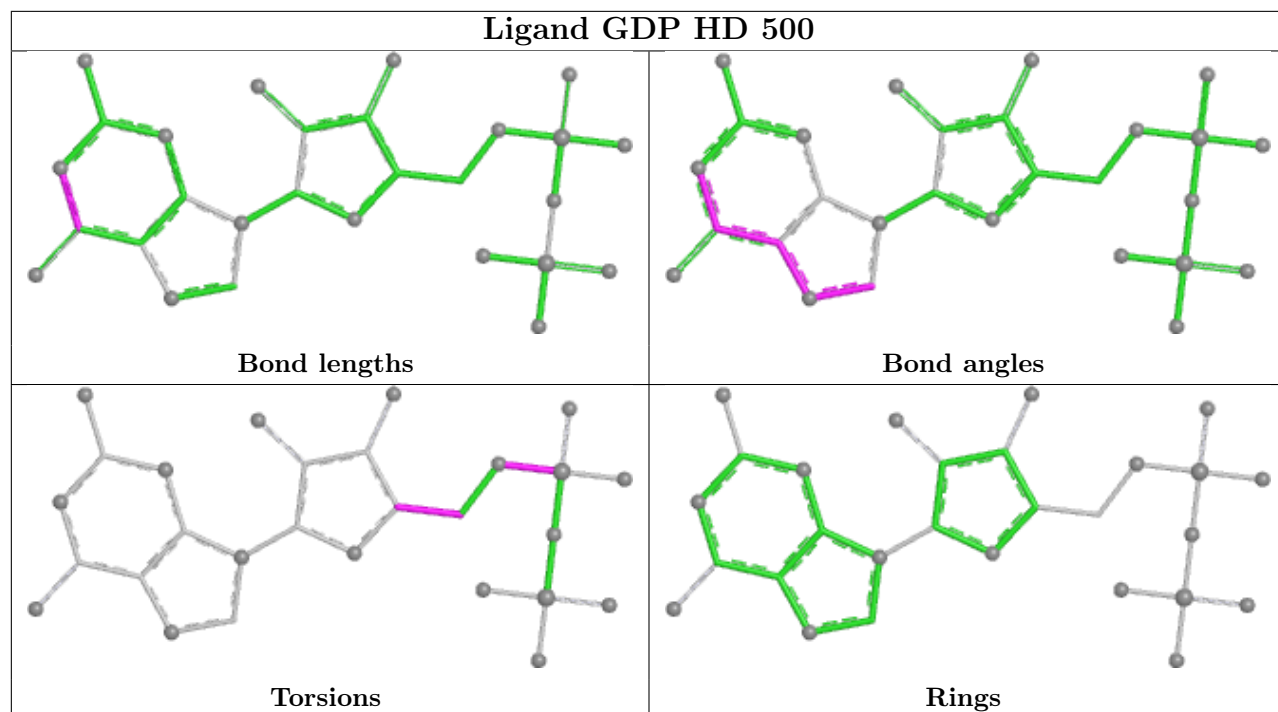
Ligand GTP TK 501

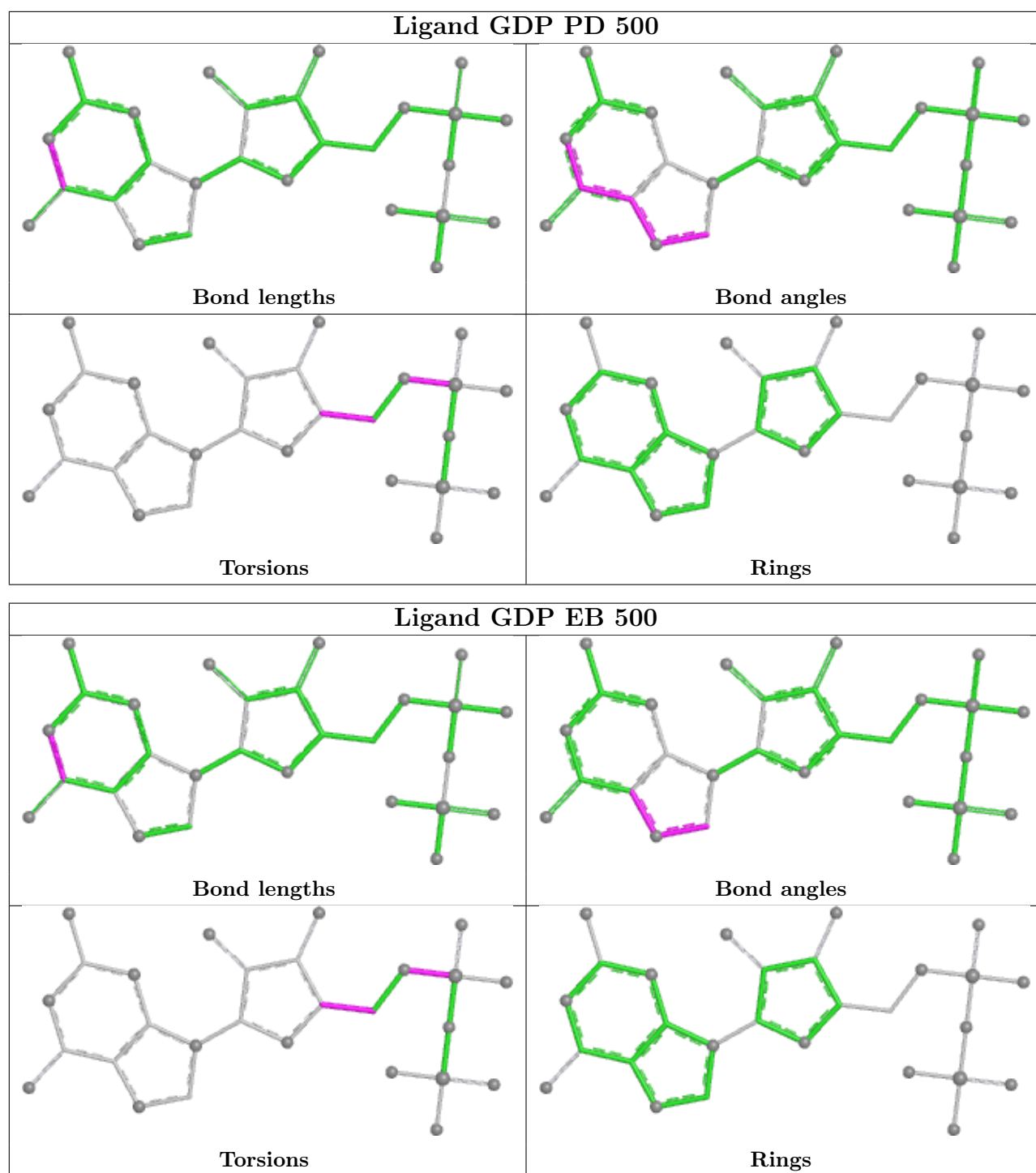


Ligand GTP BM 501

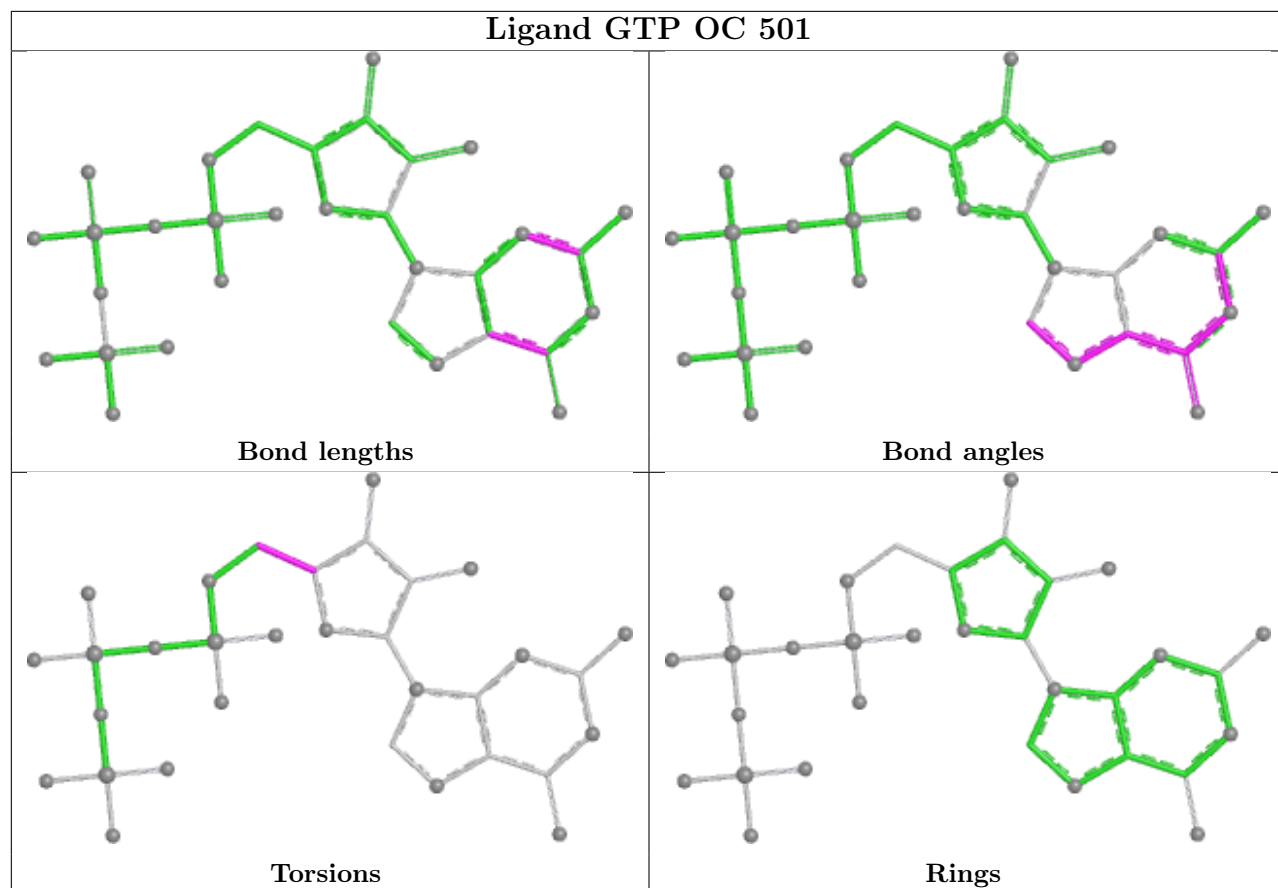




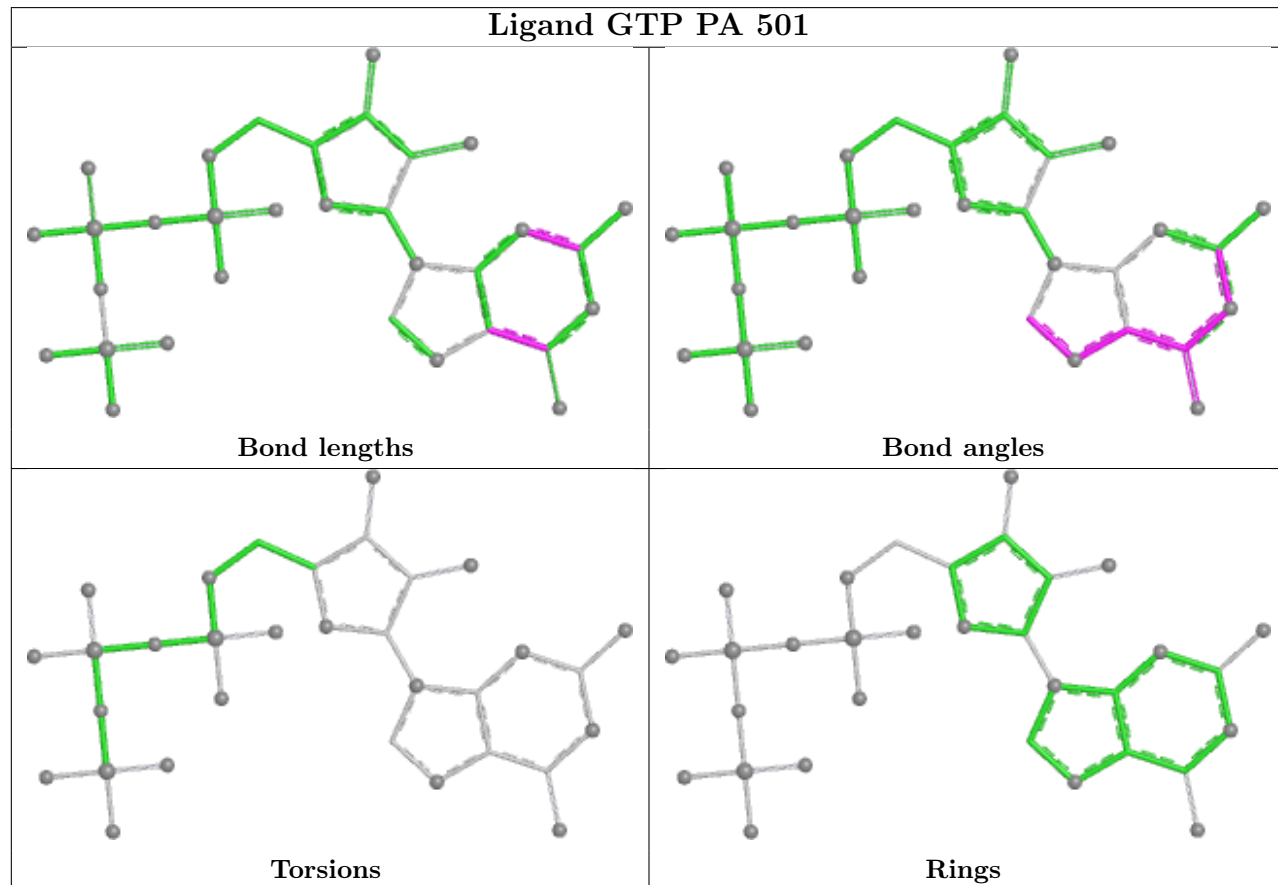


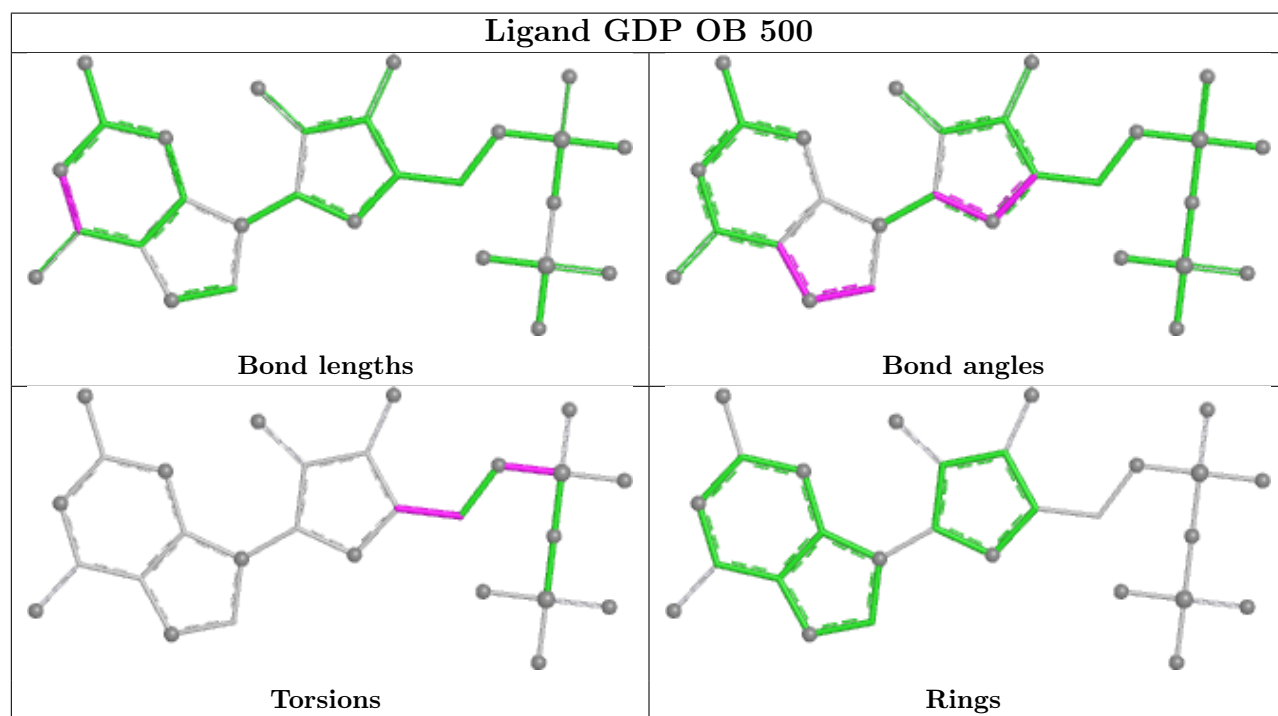
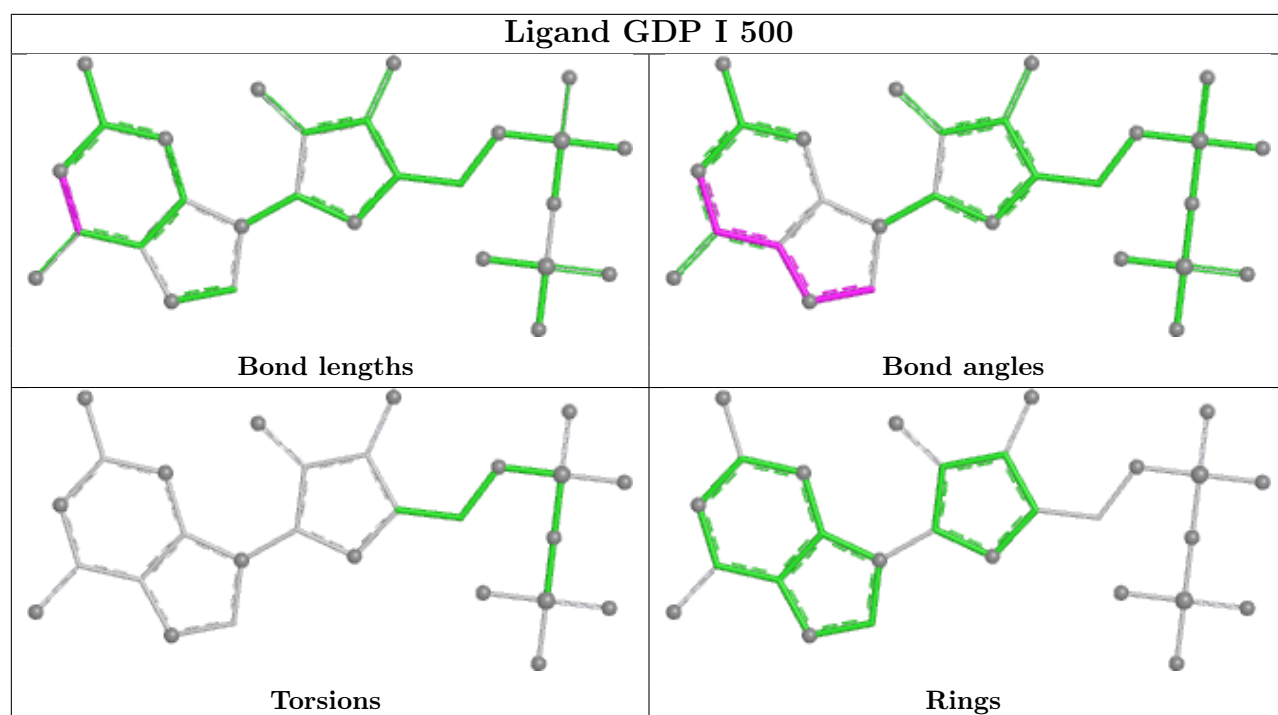


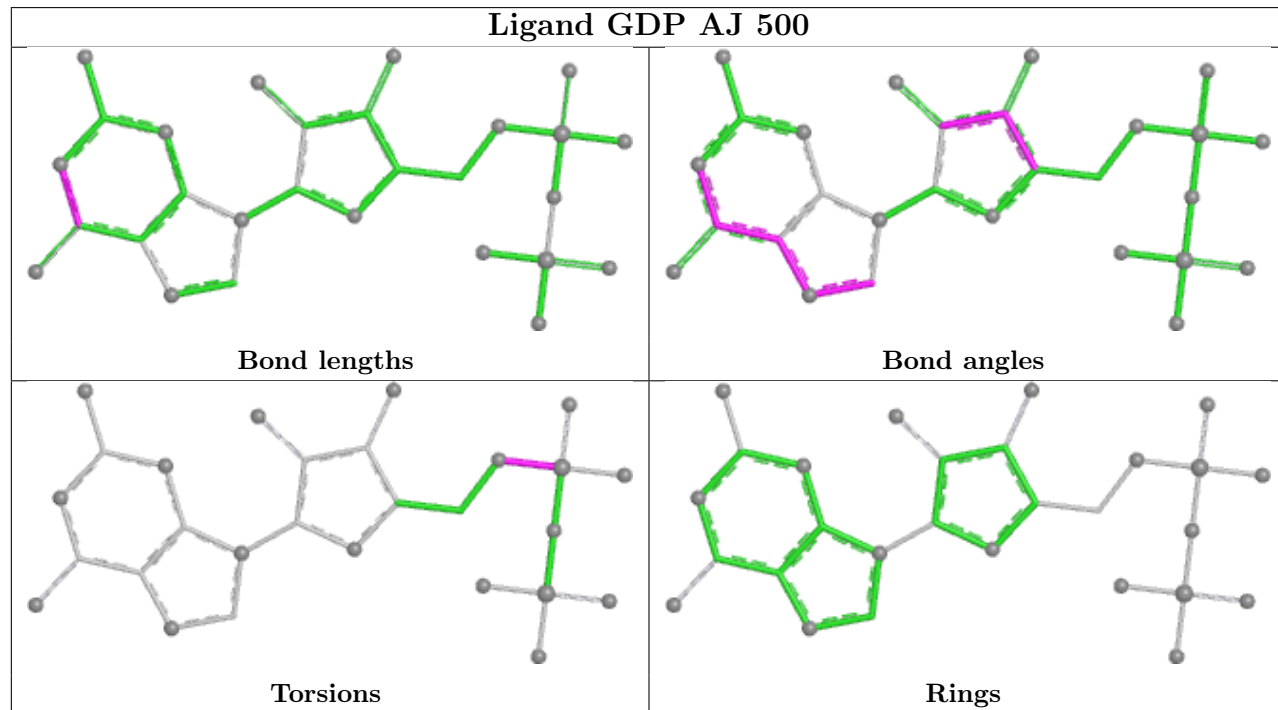
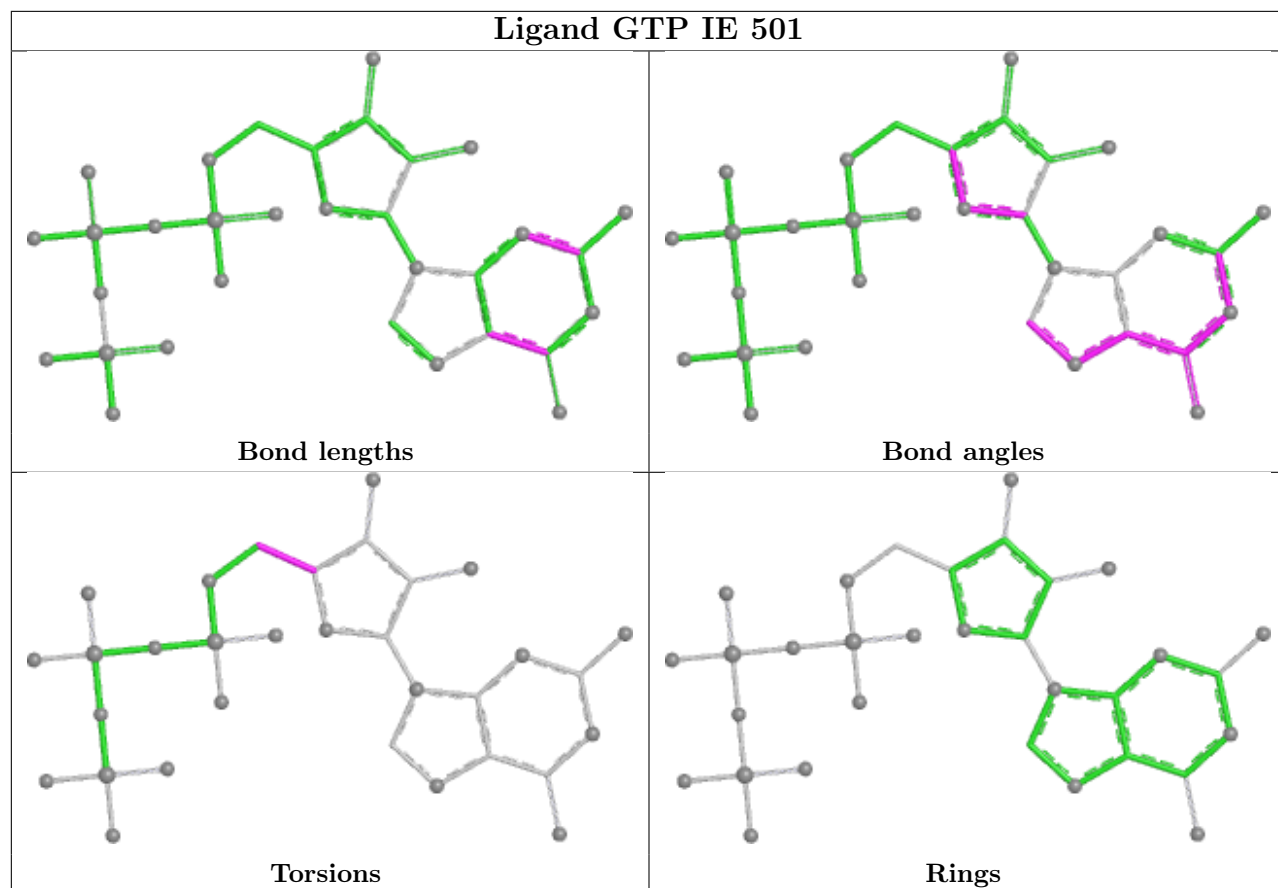
Ligand GTP OC 501

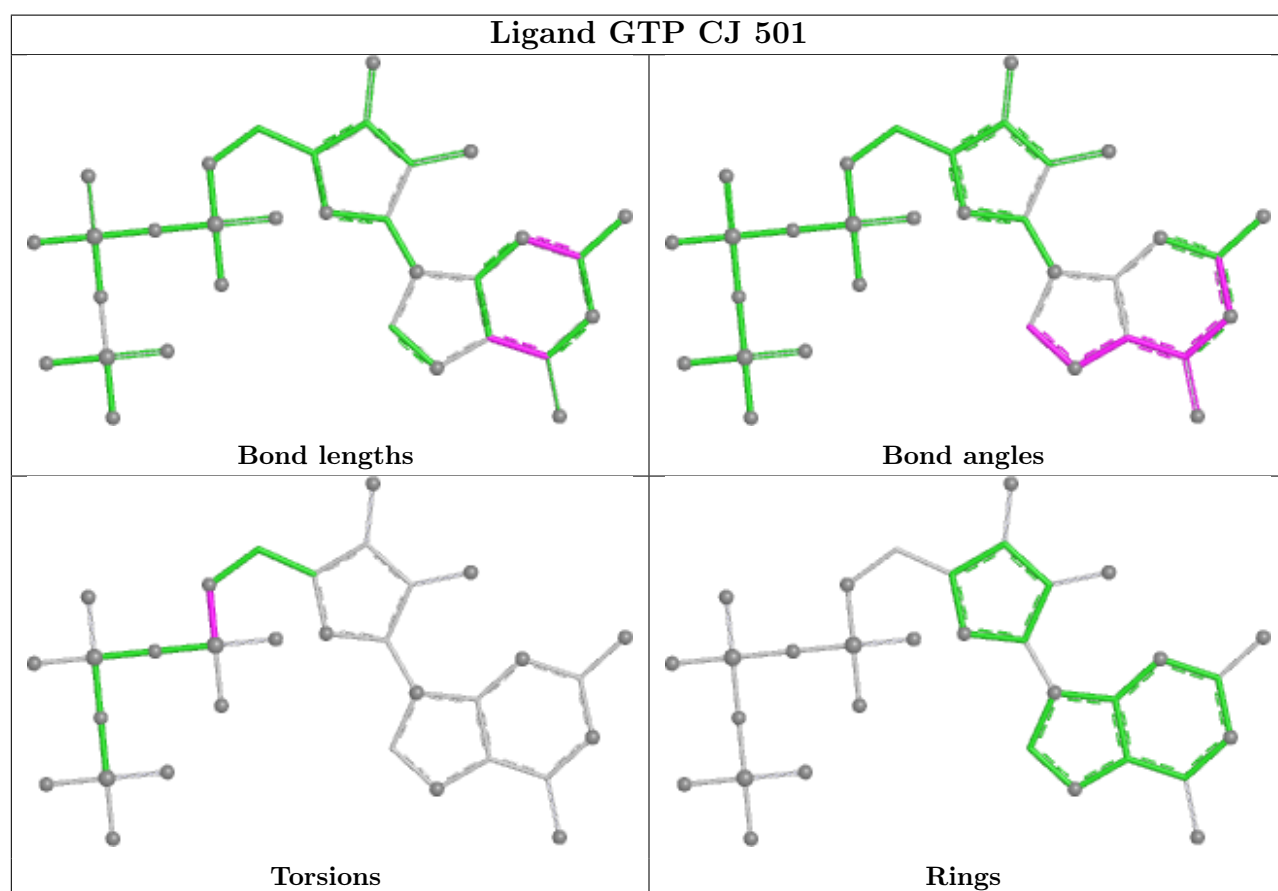
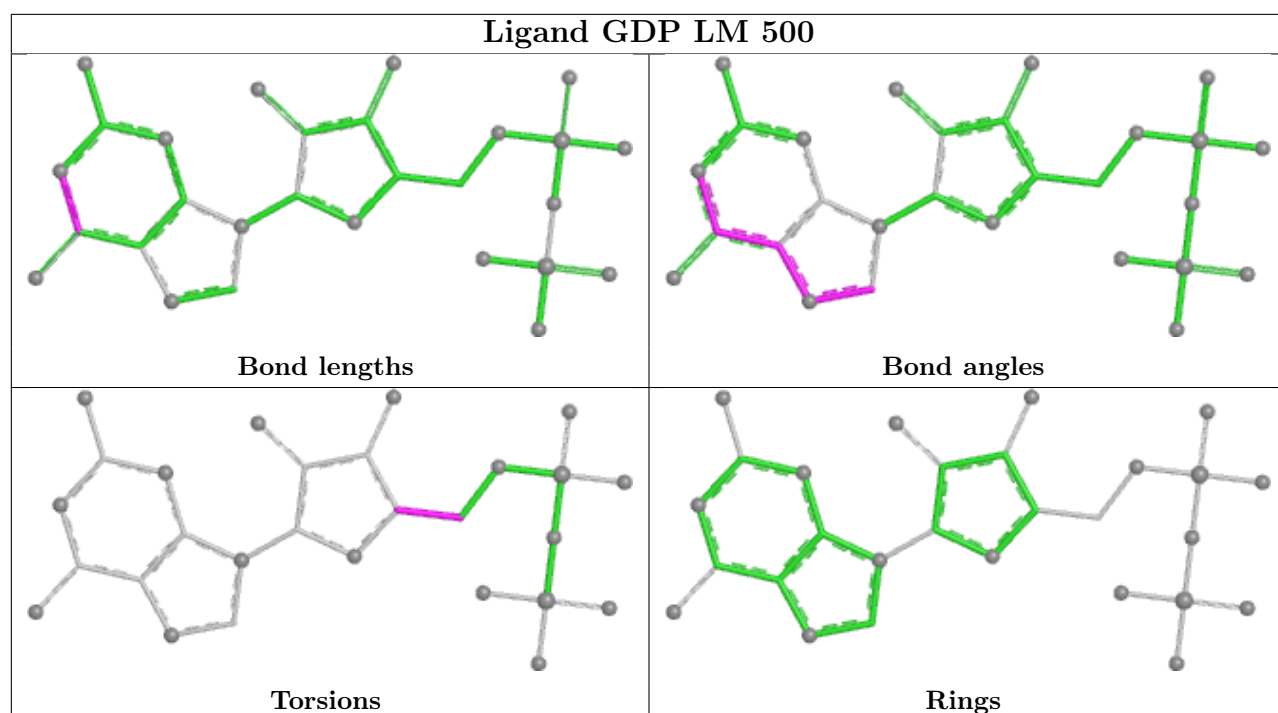


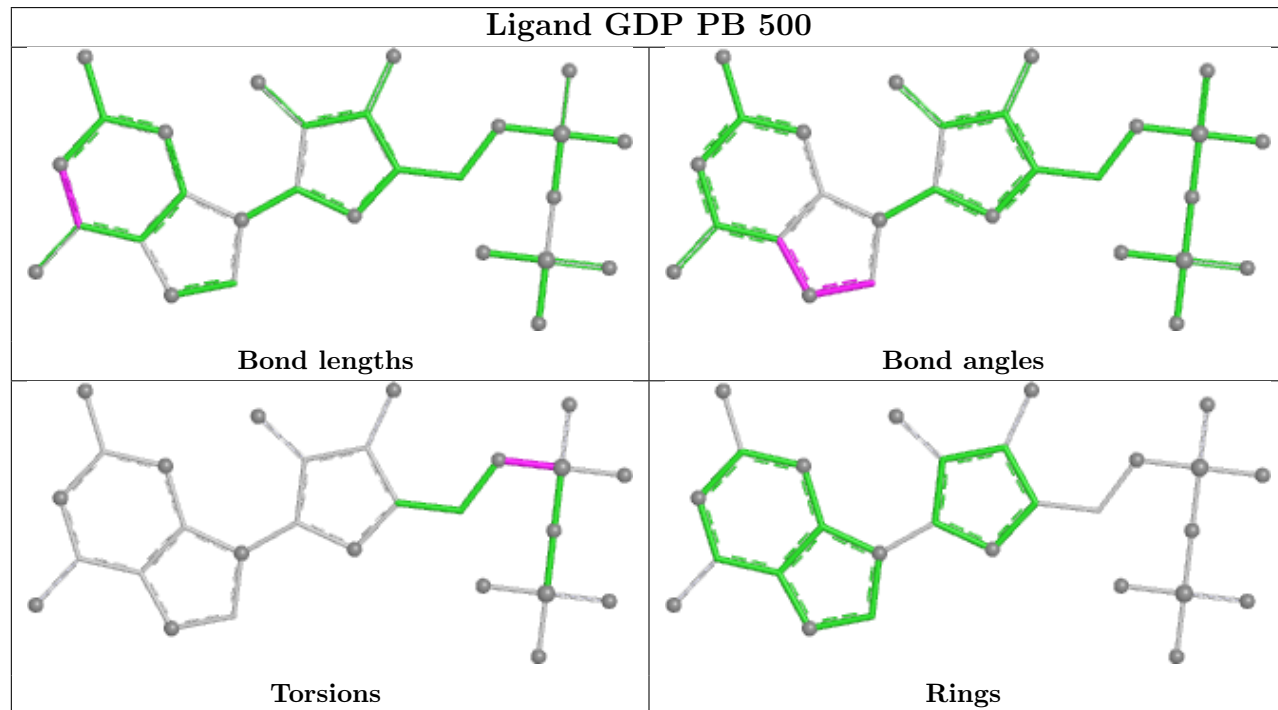
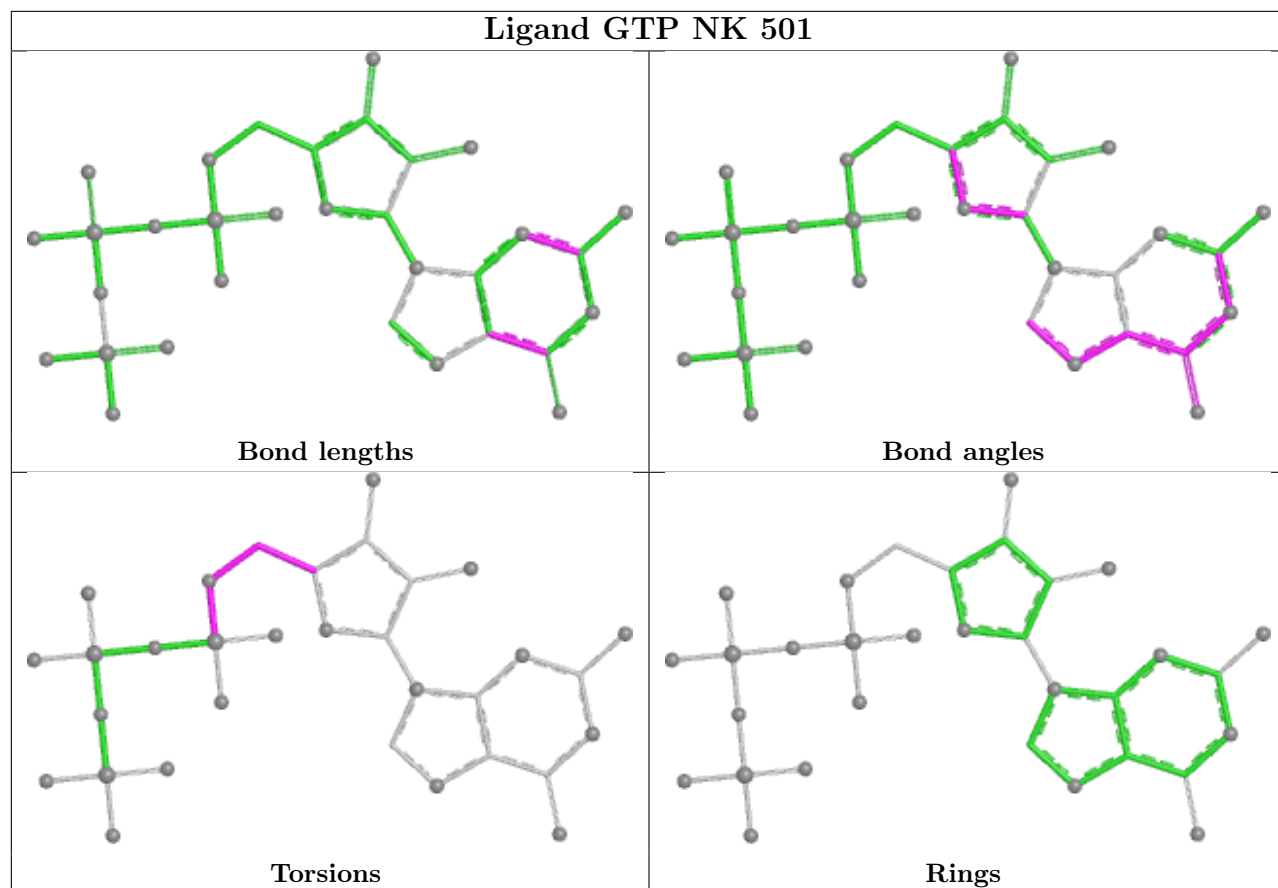
Ligand GTP PA 501

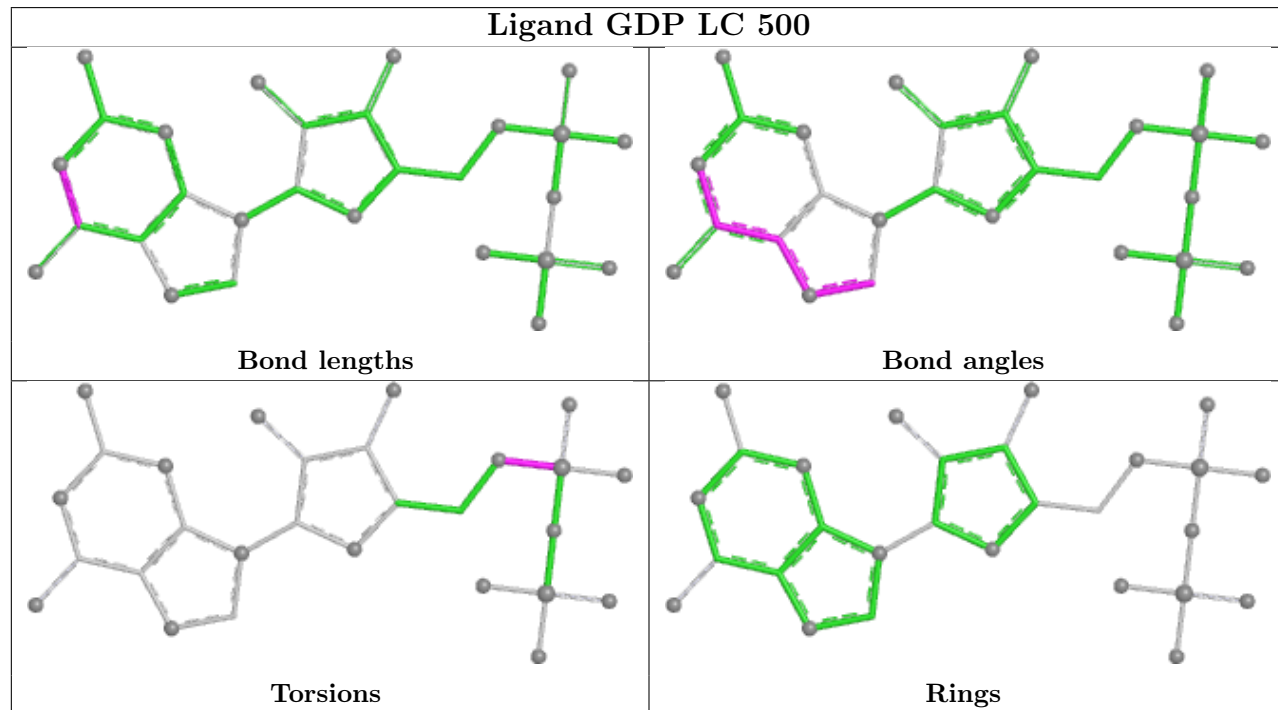
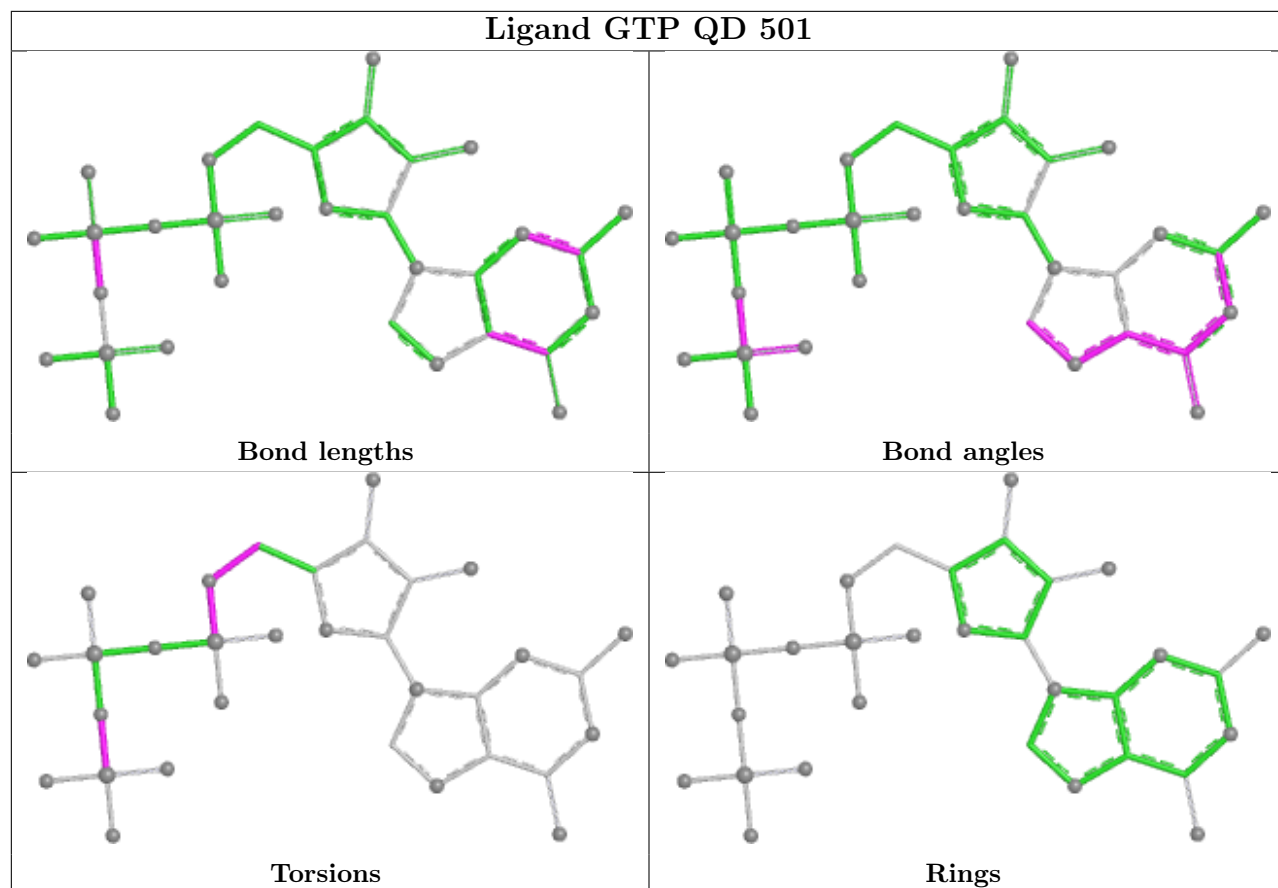


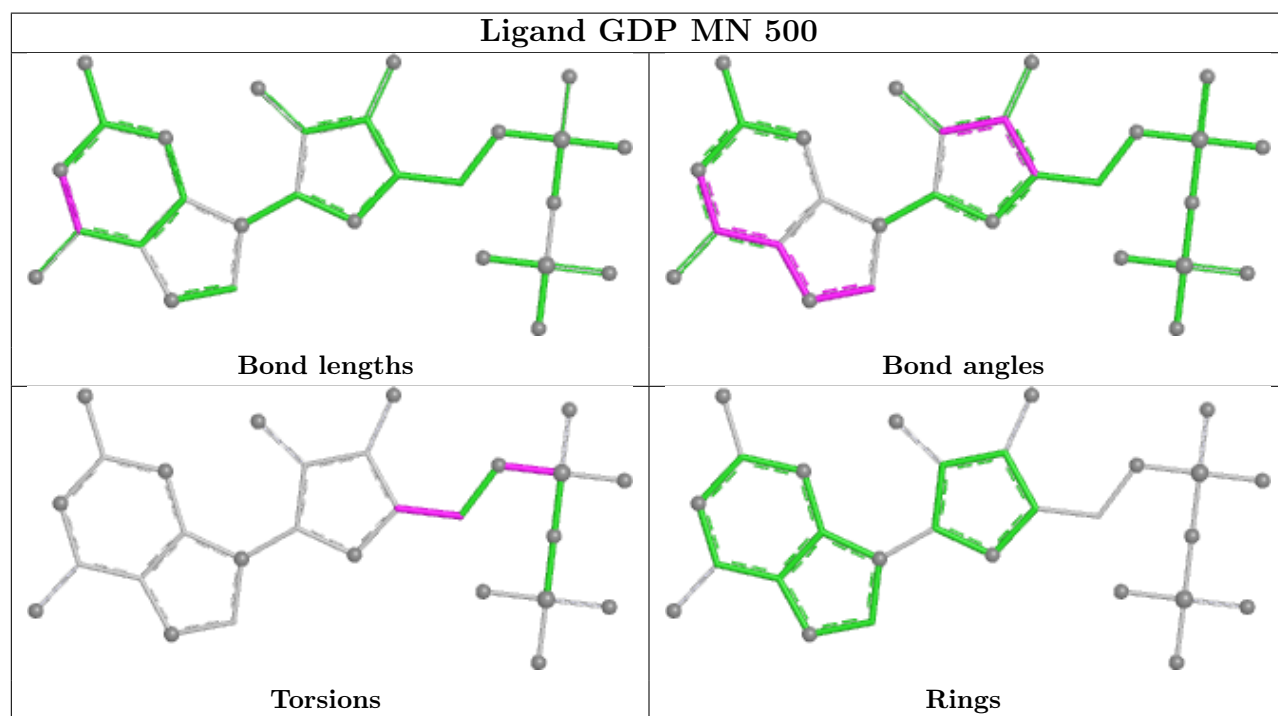
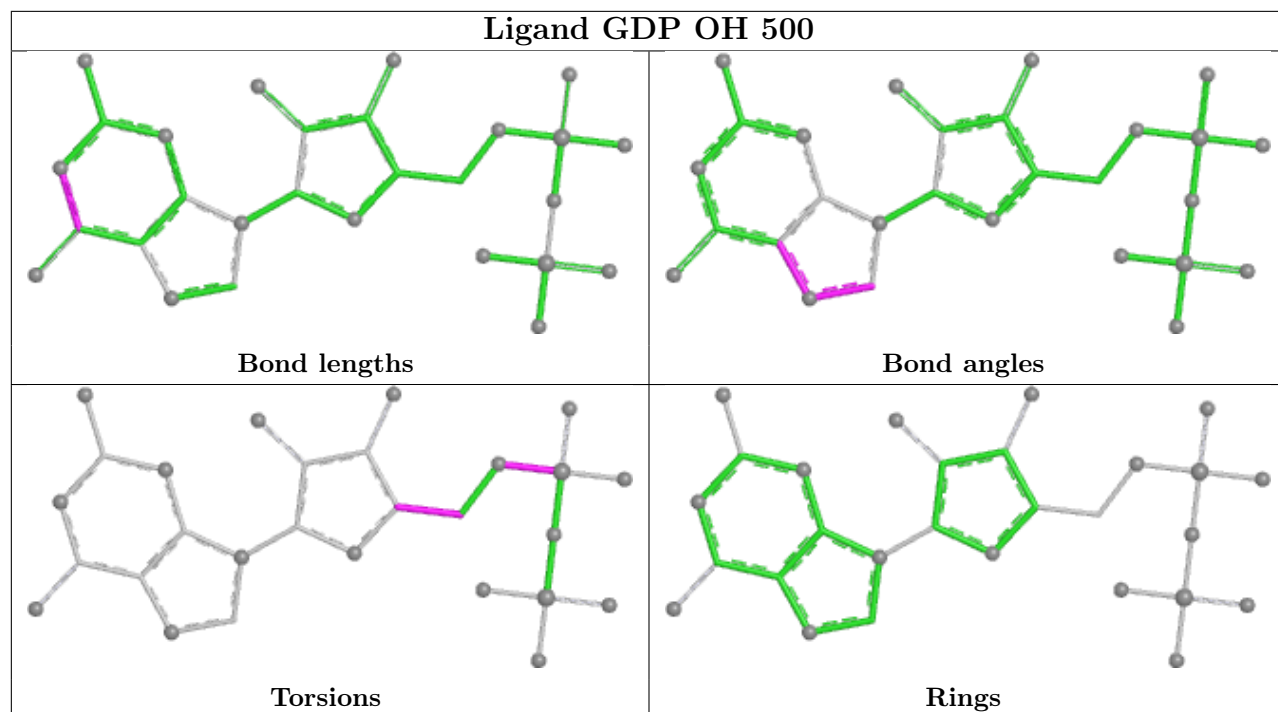


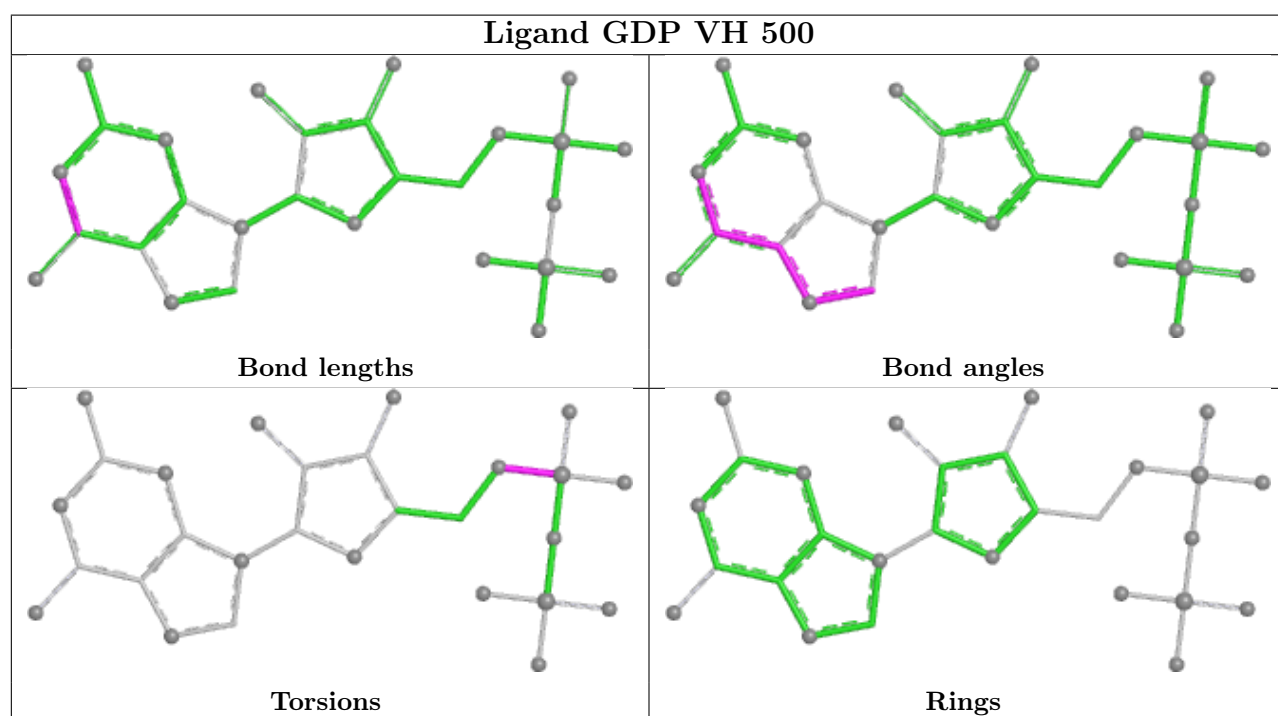
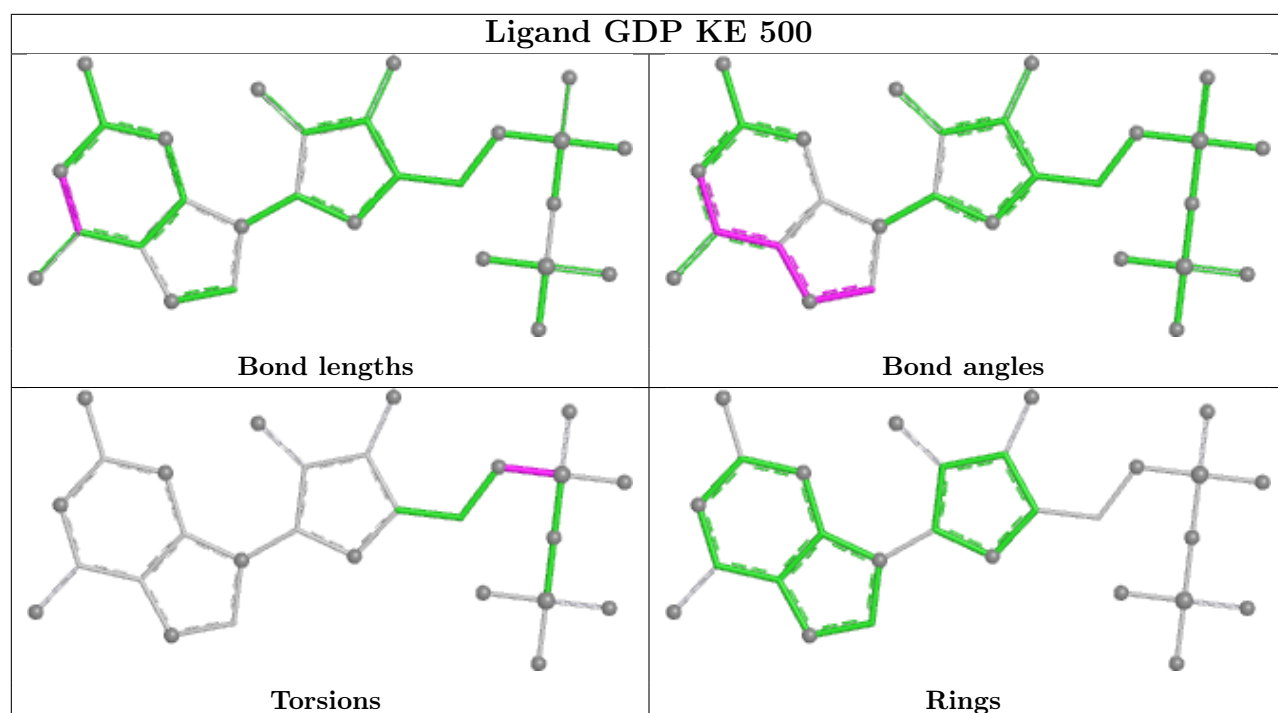




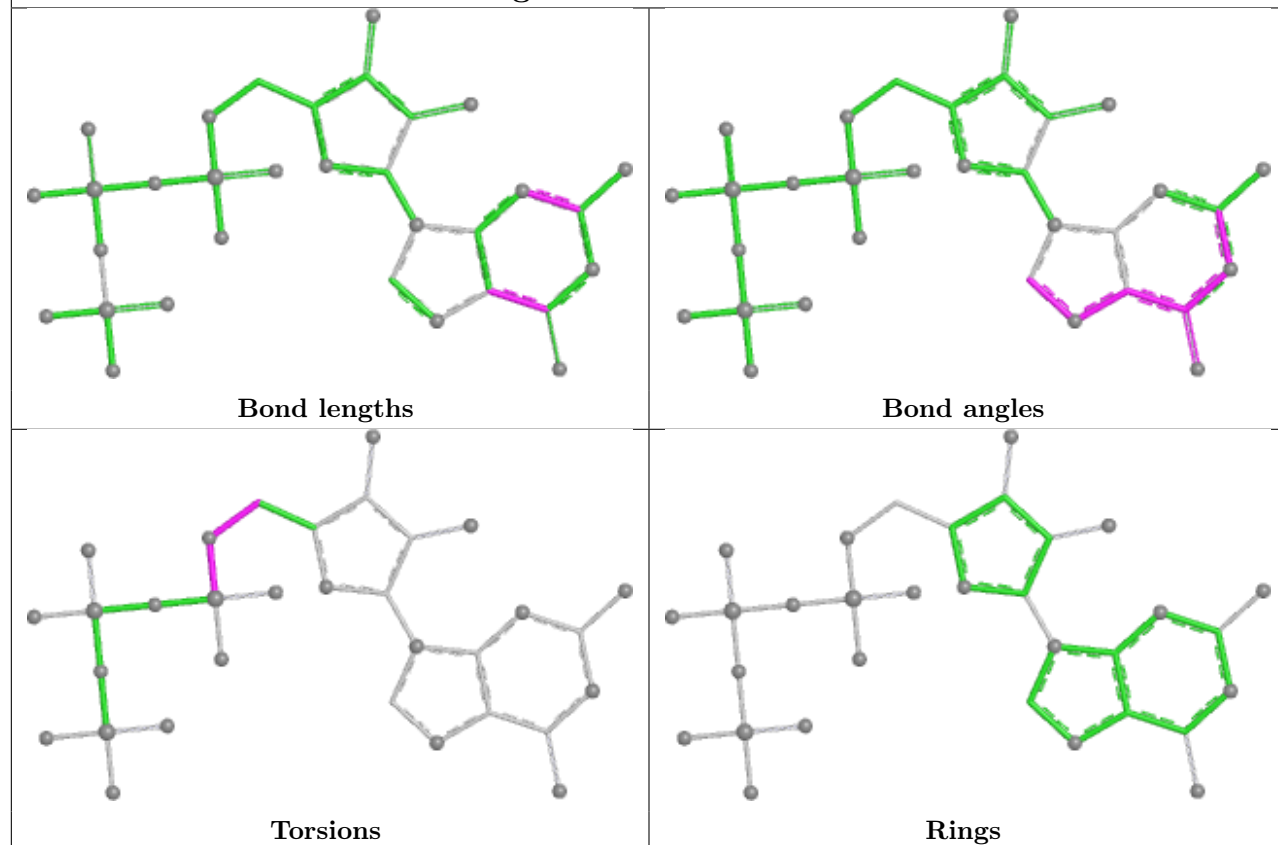




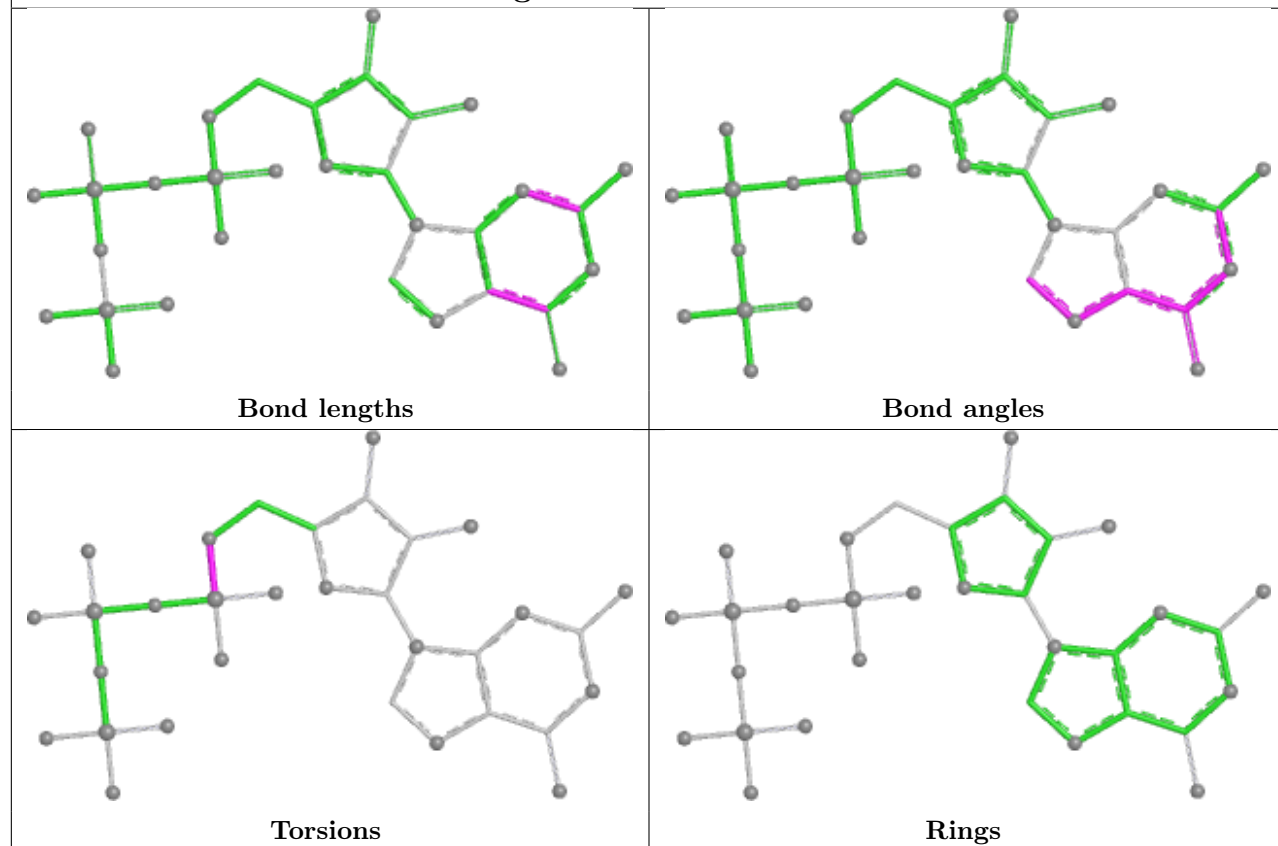


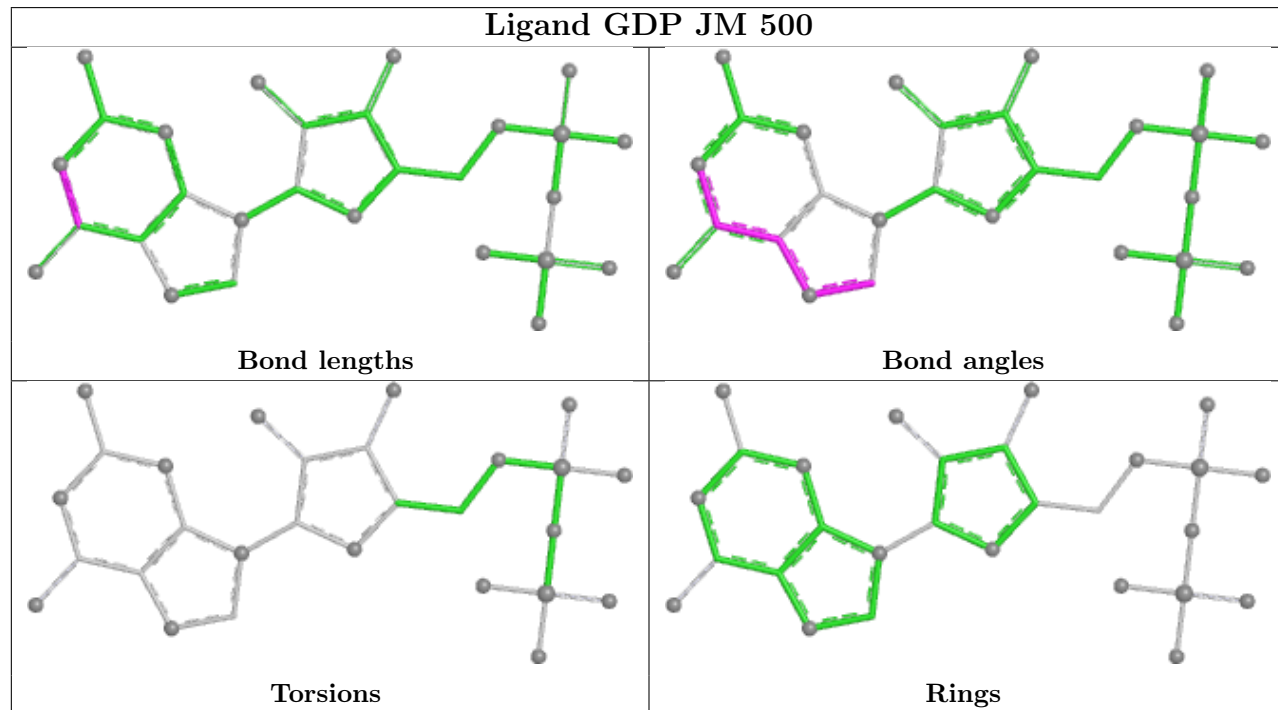
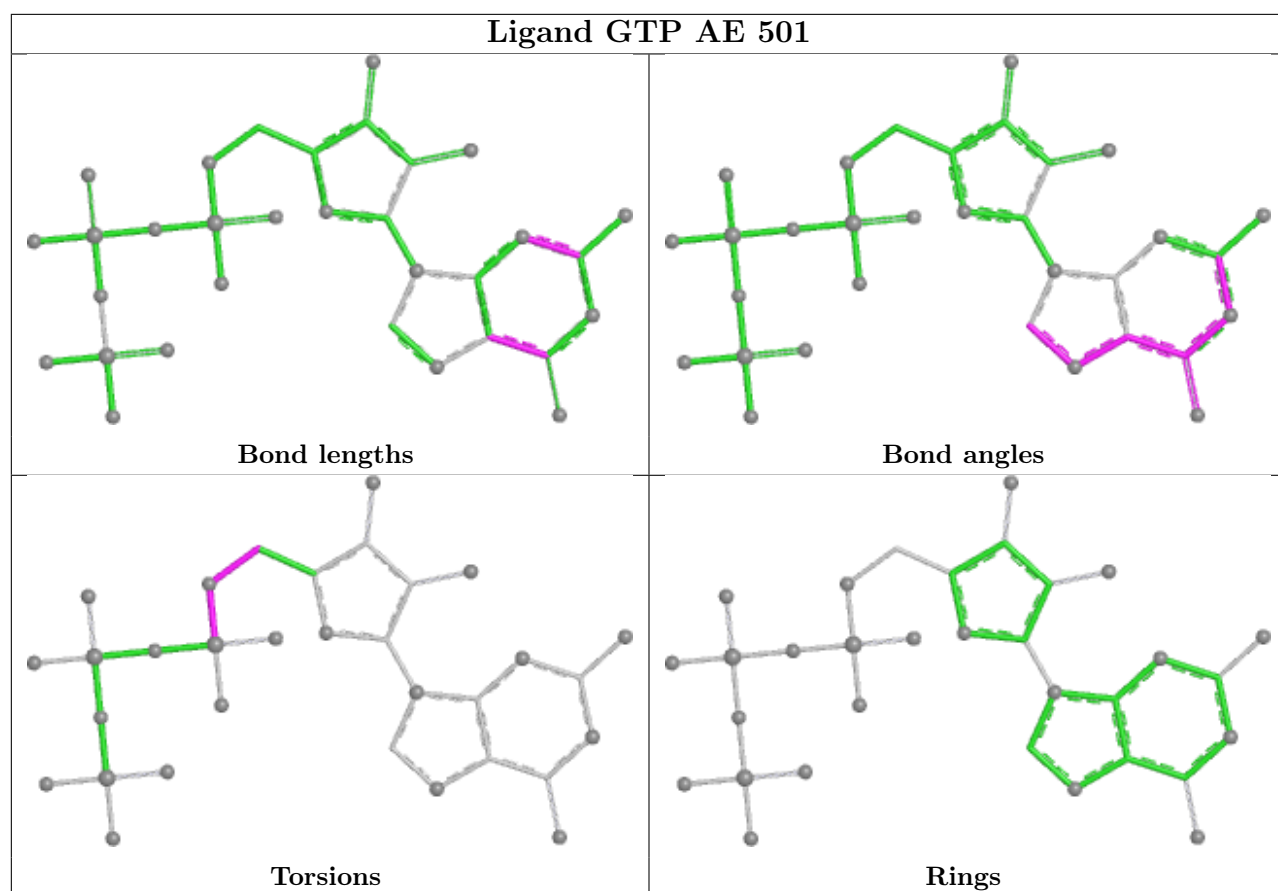


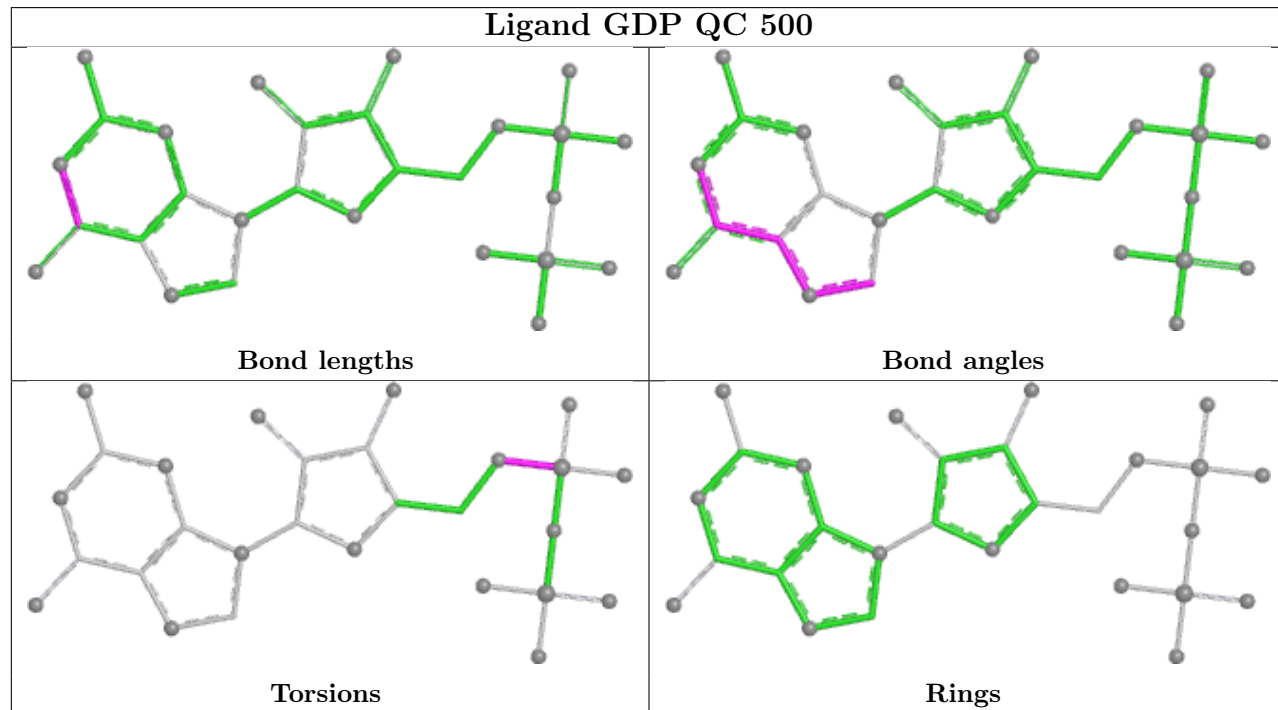
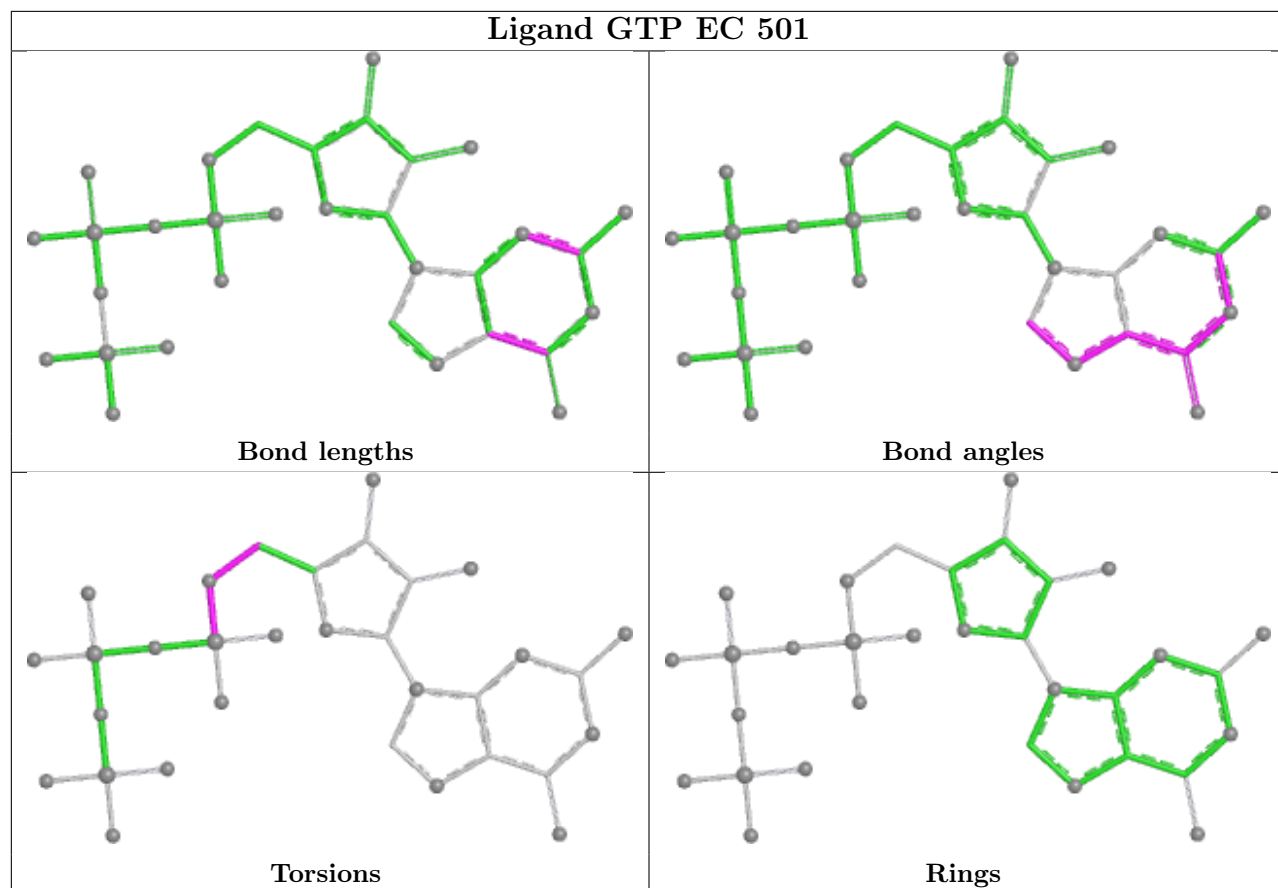
Ligand GTP HM 501

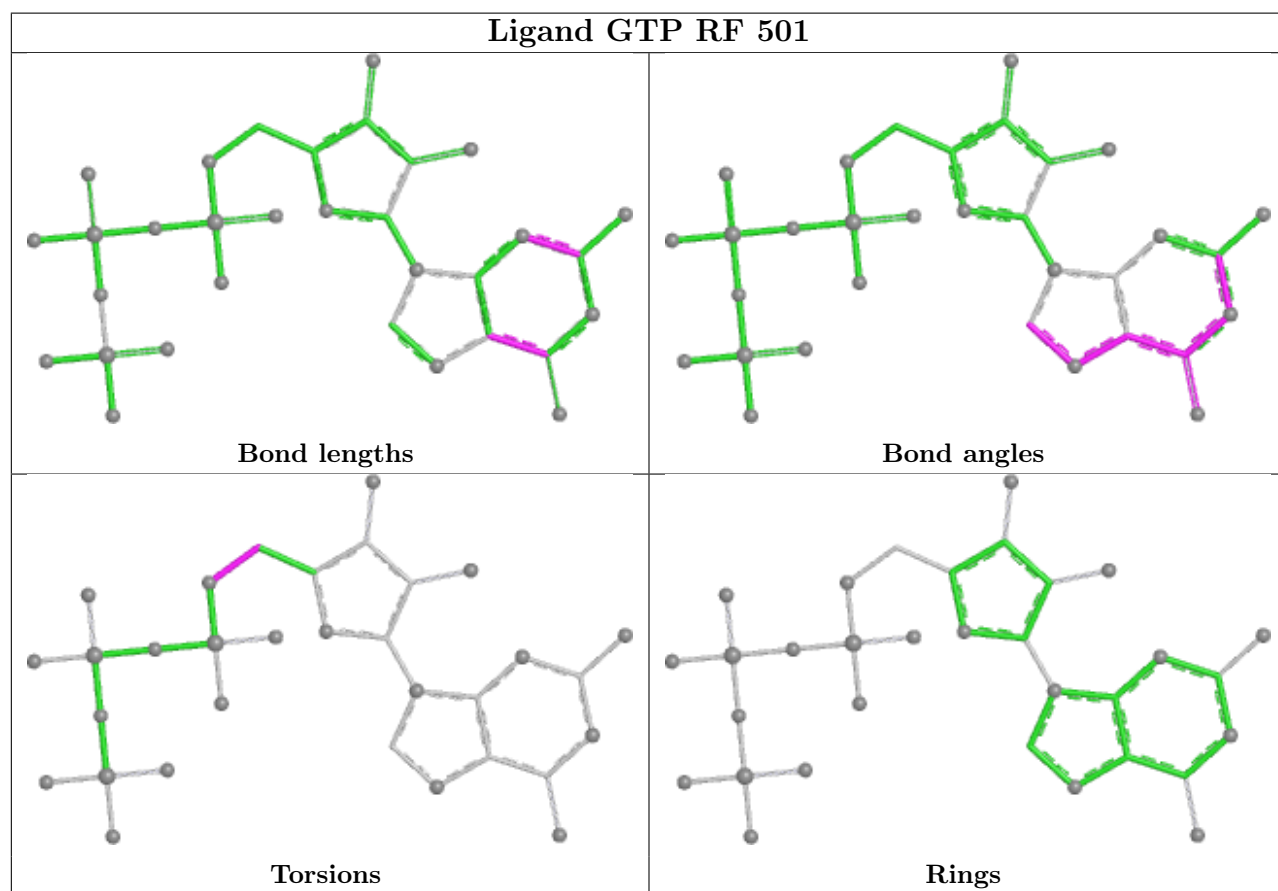
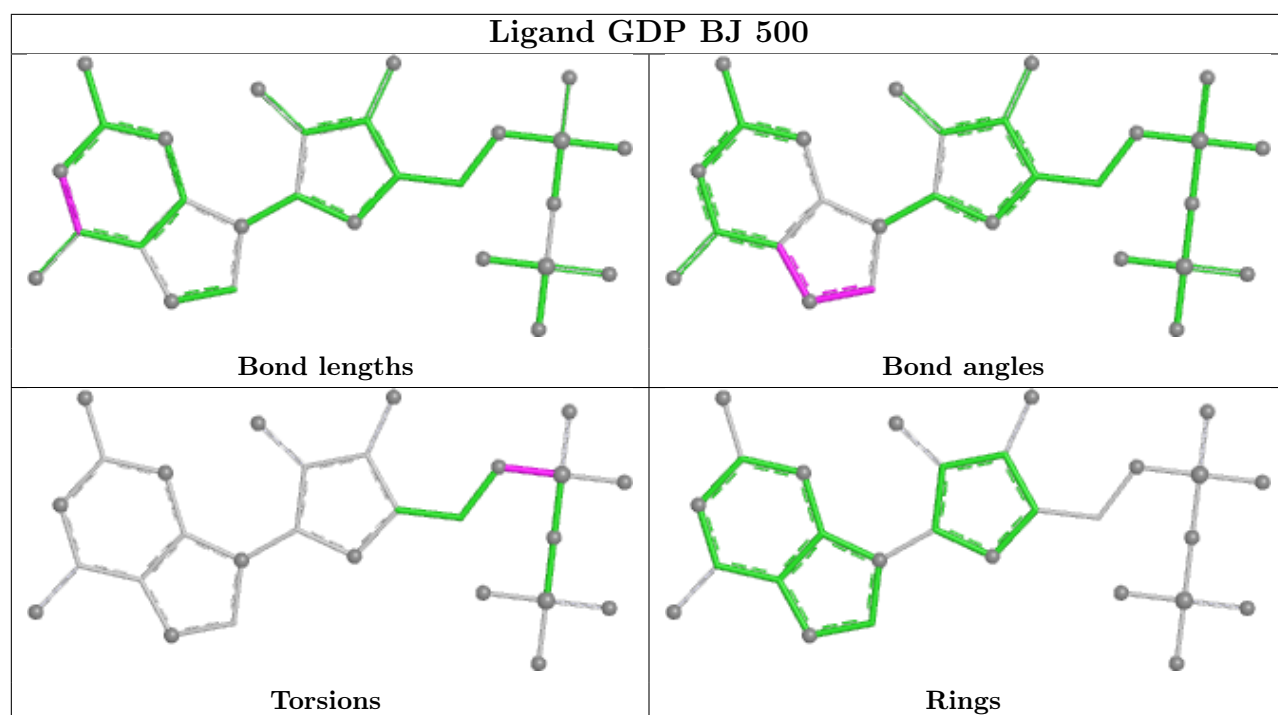


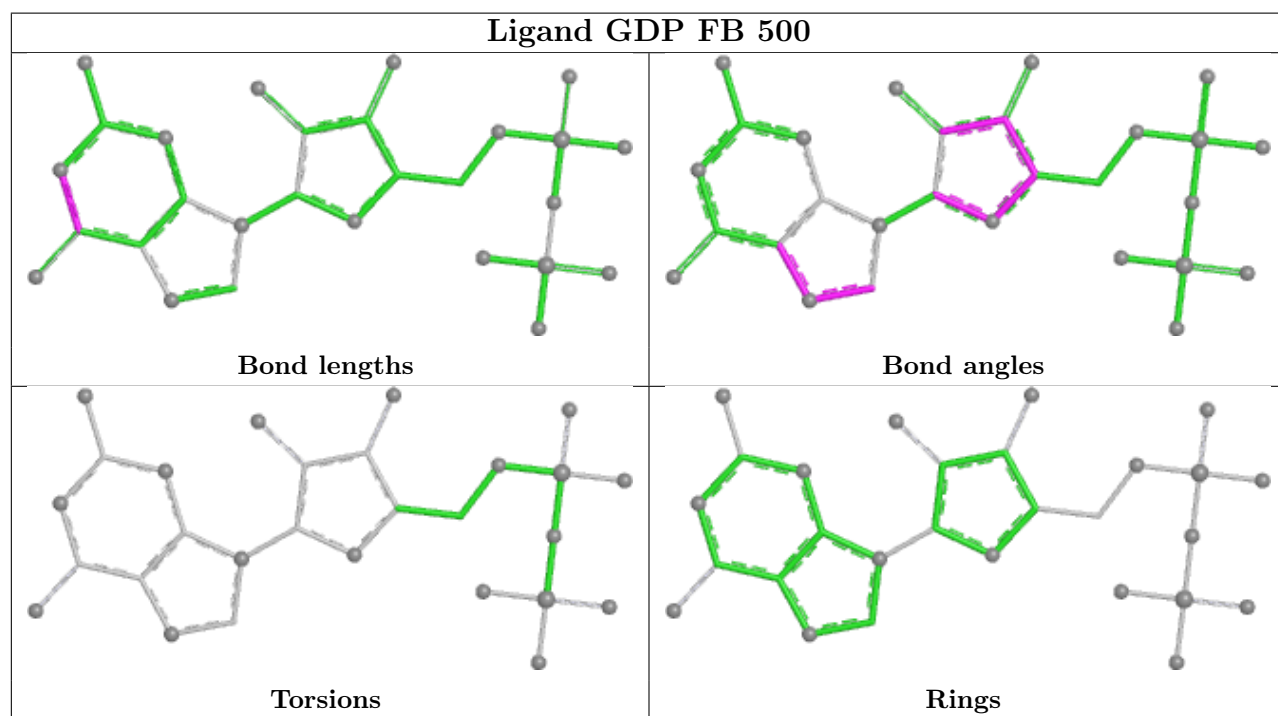
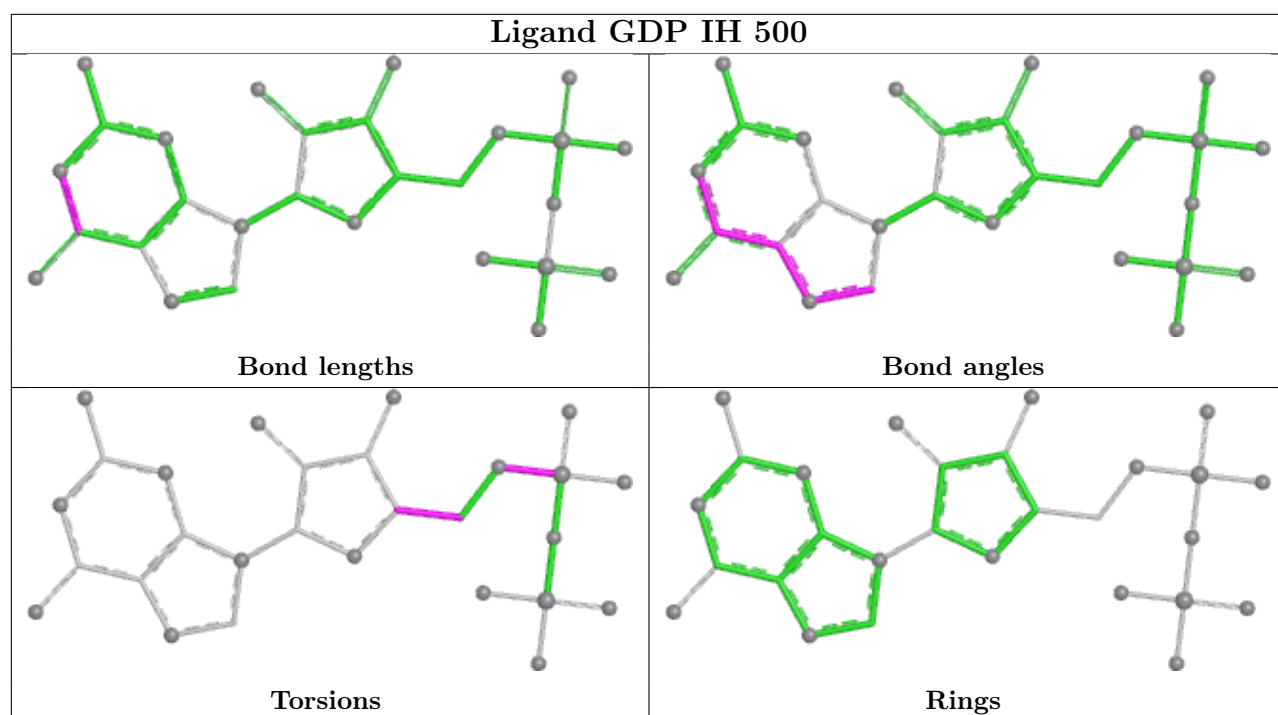
Ligand GTP WA 501

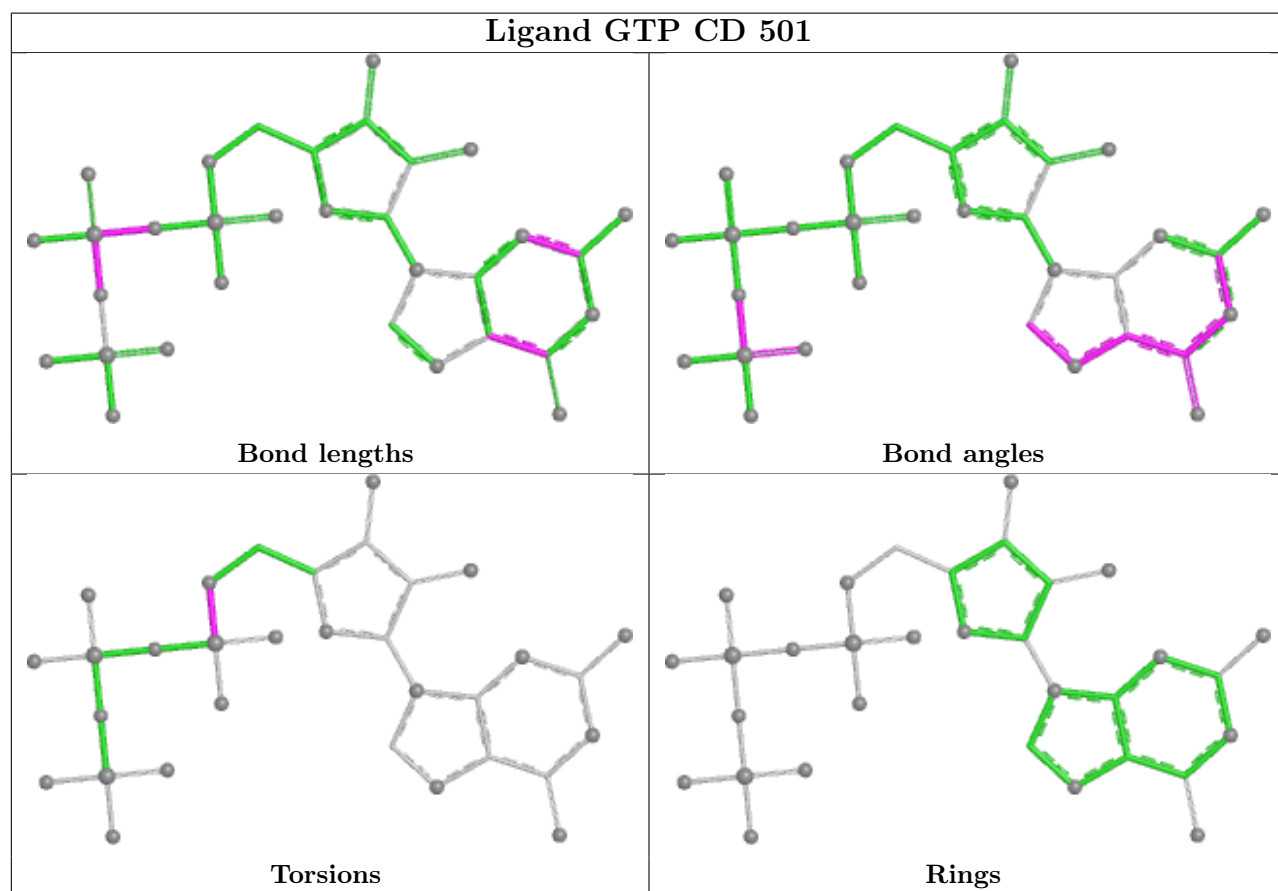
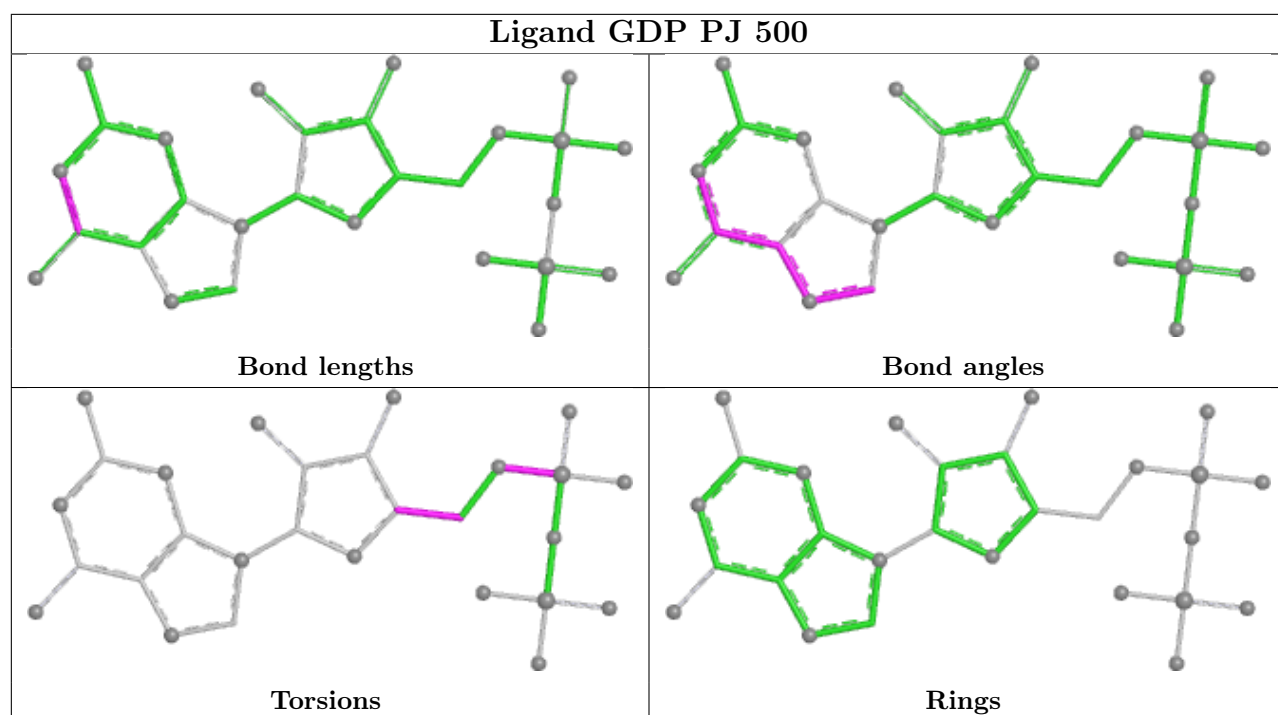


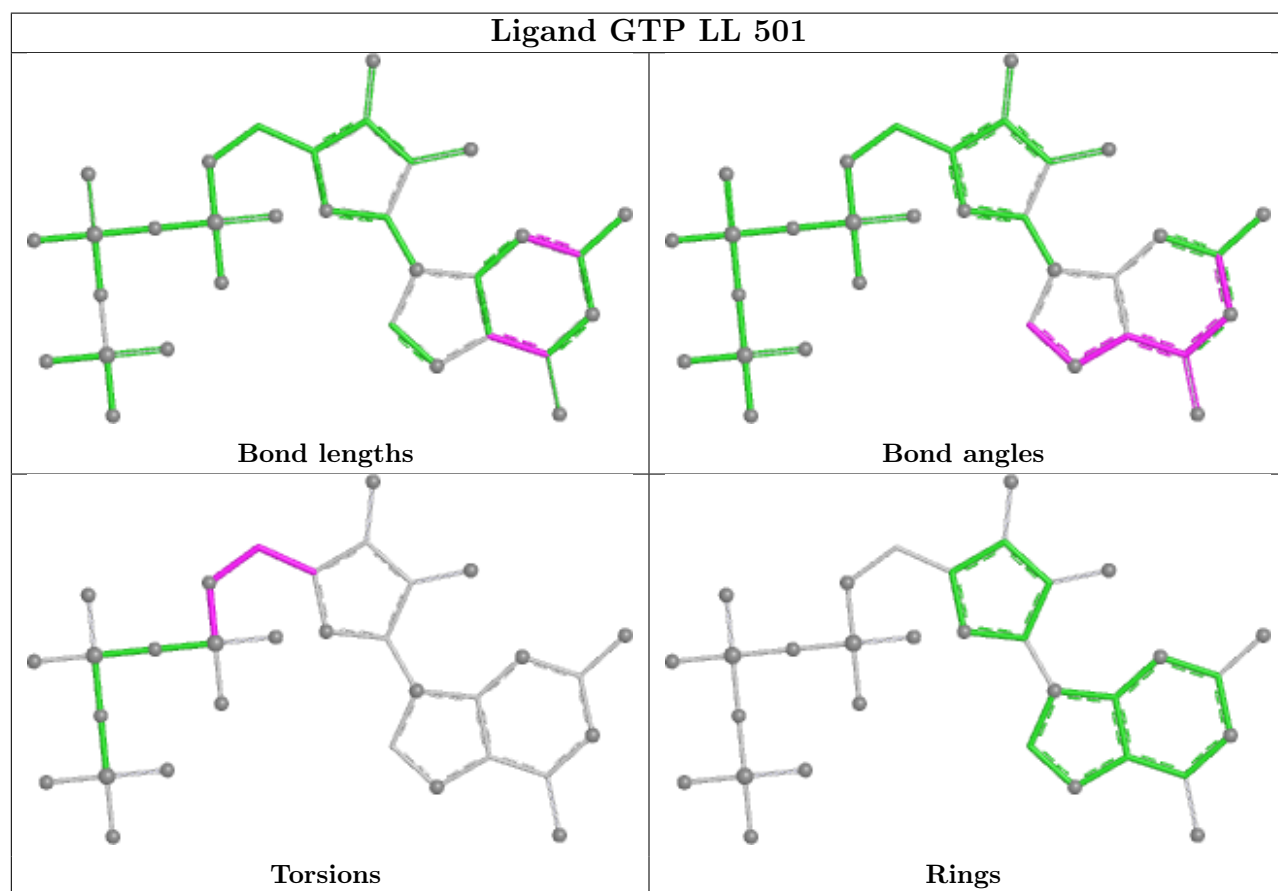
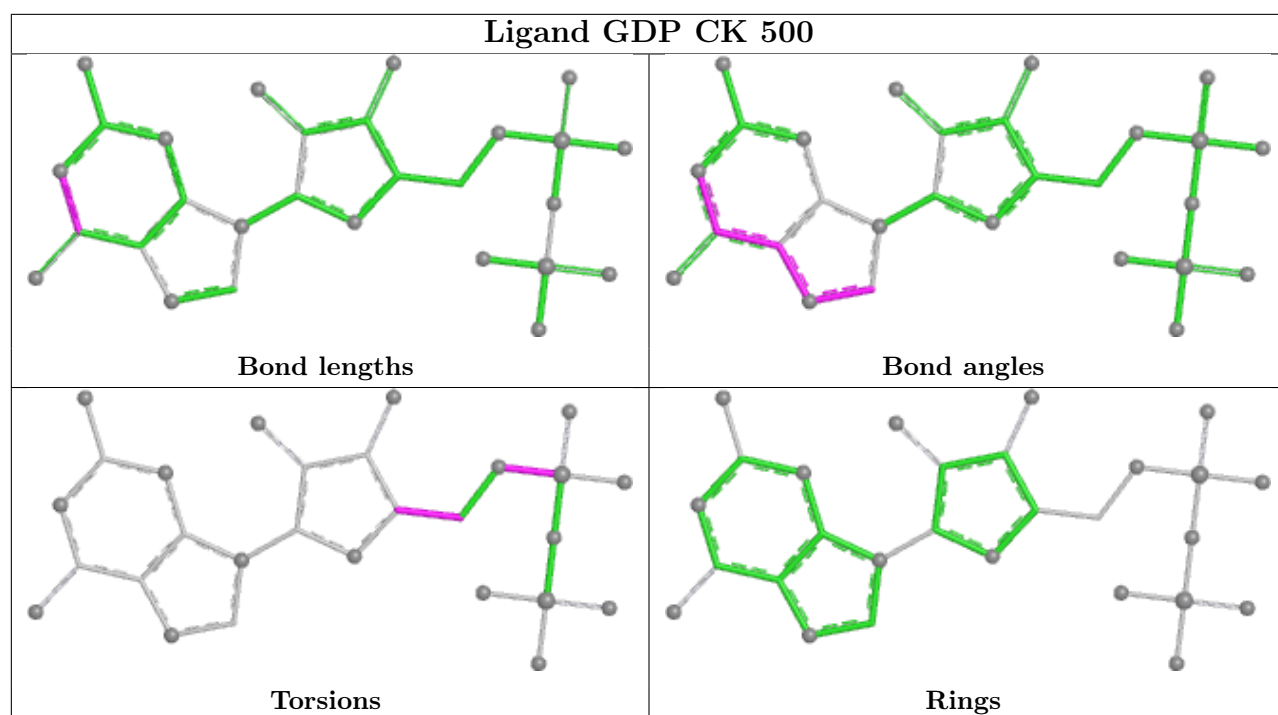


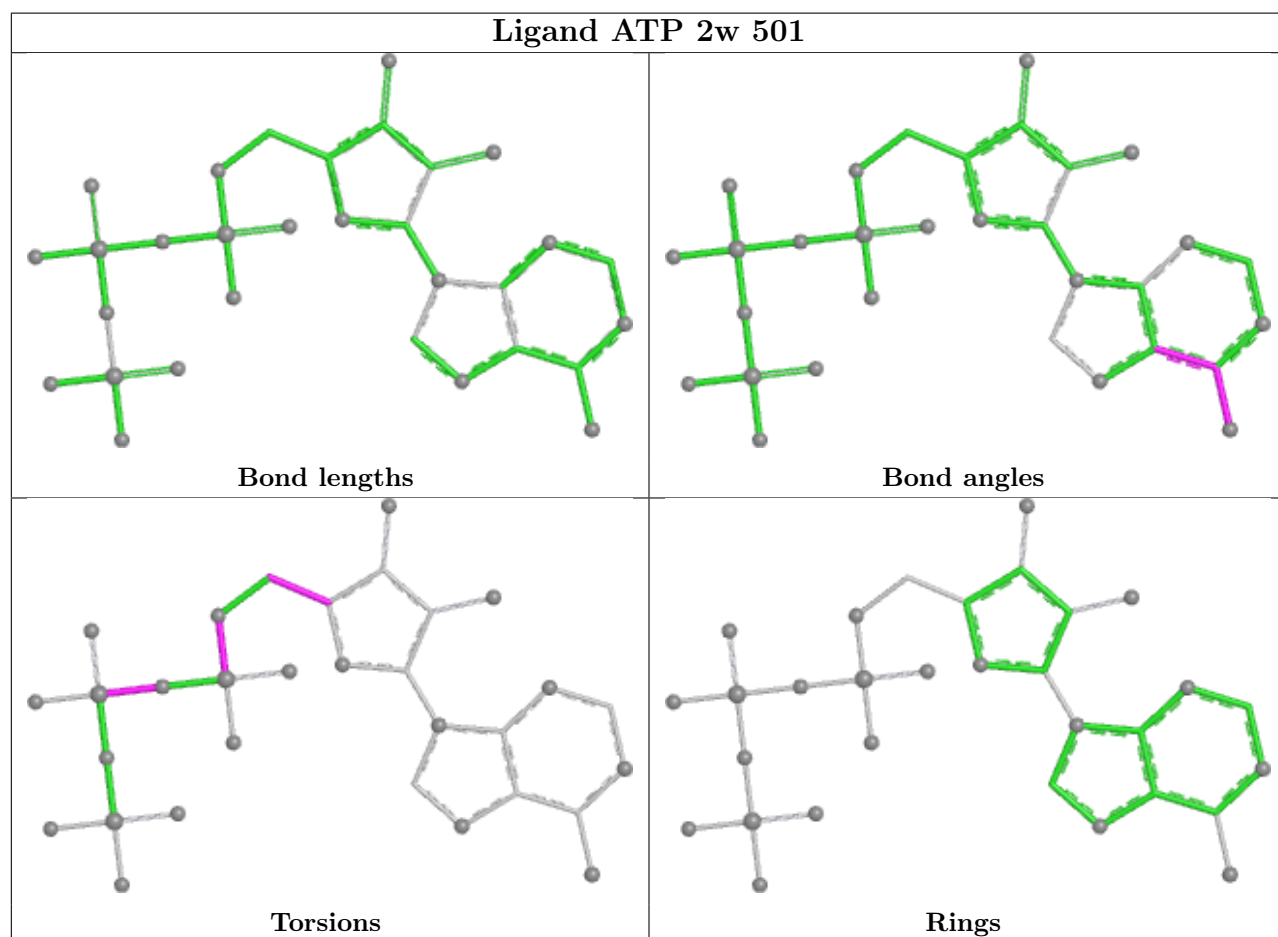
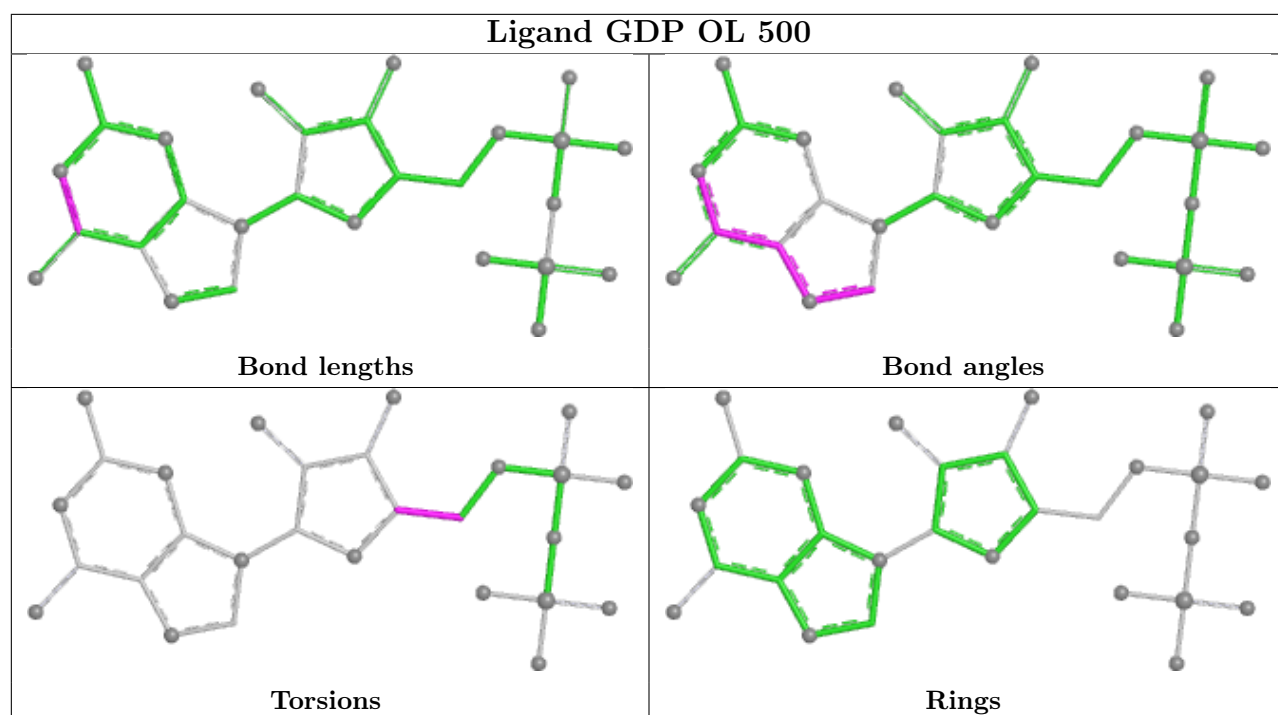


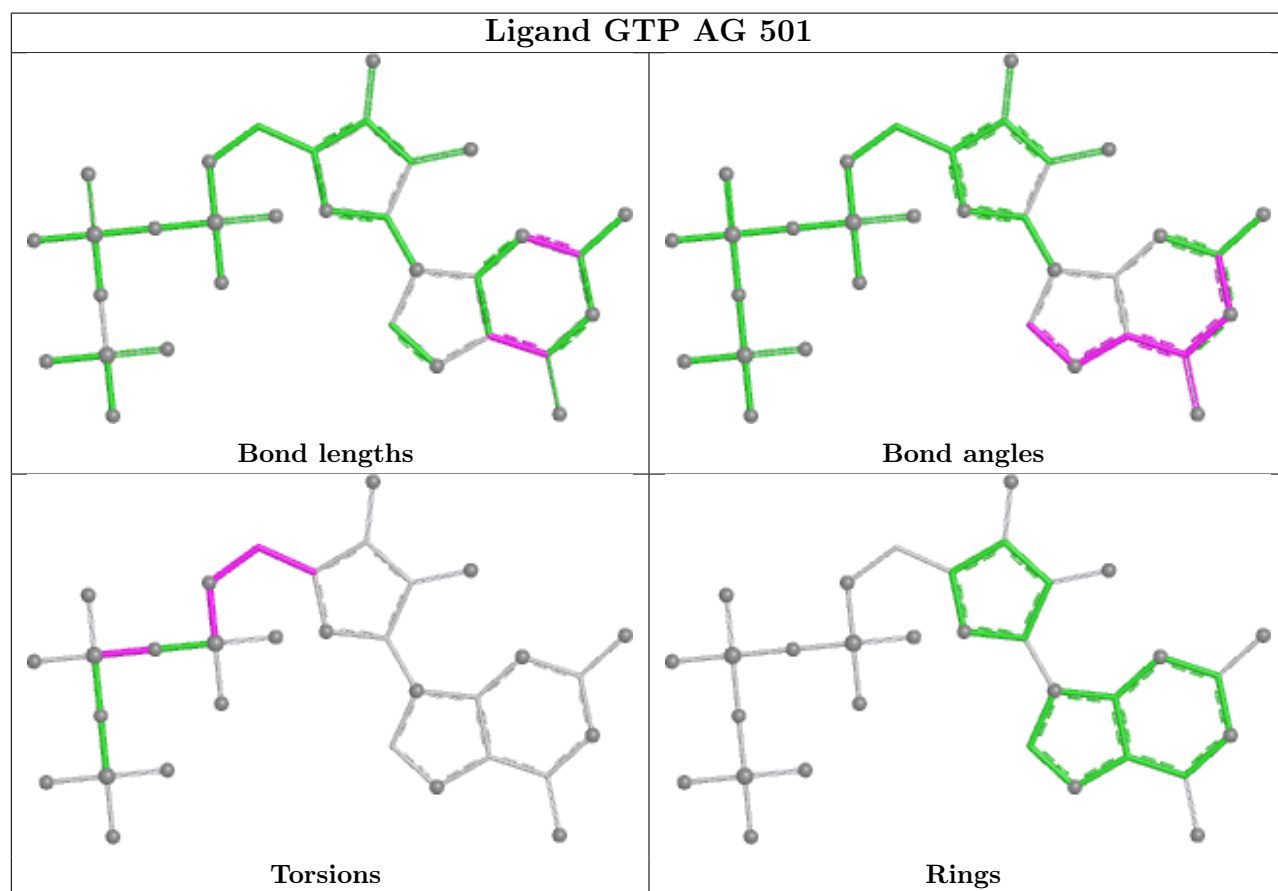
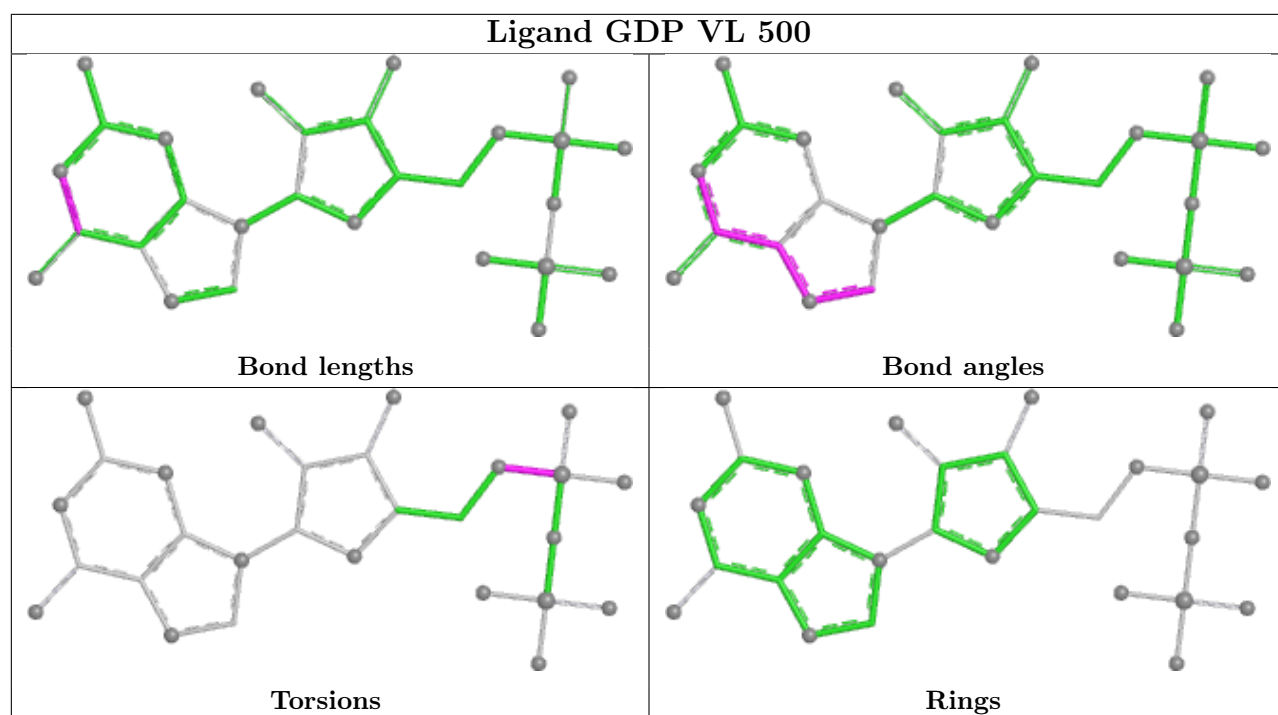


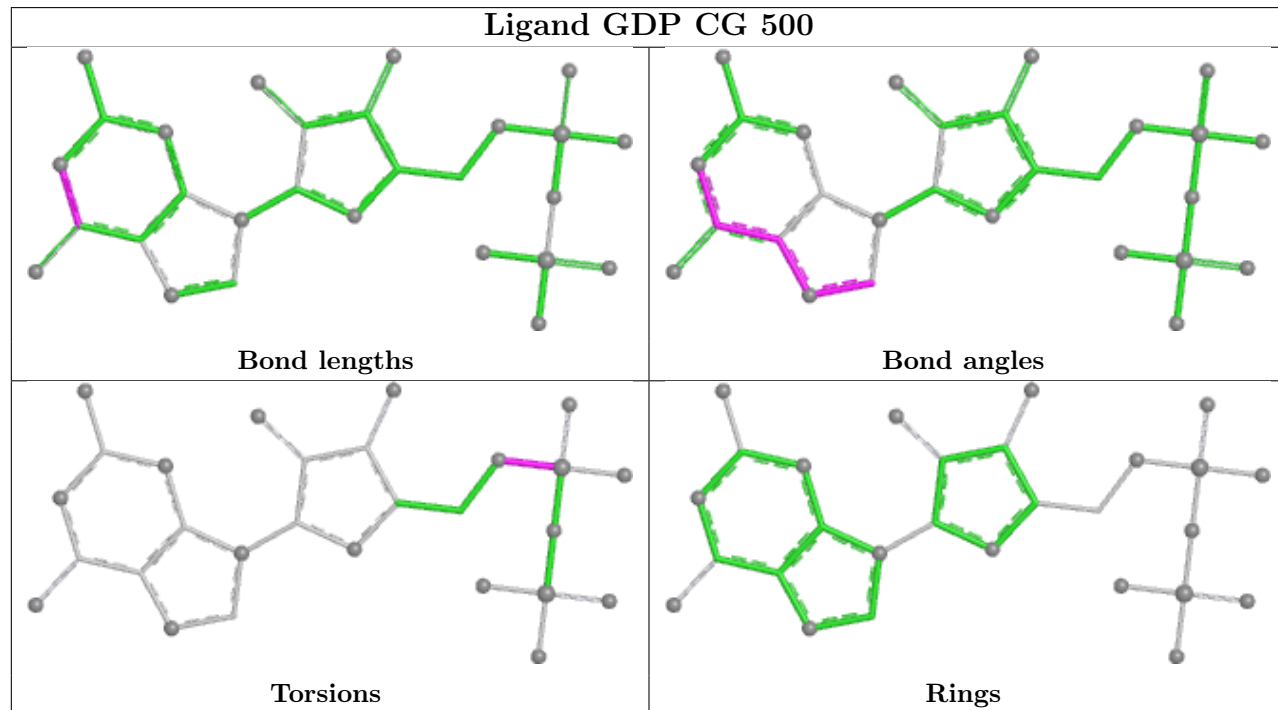
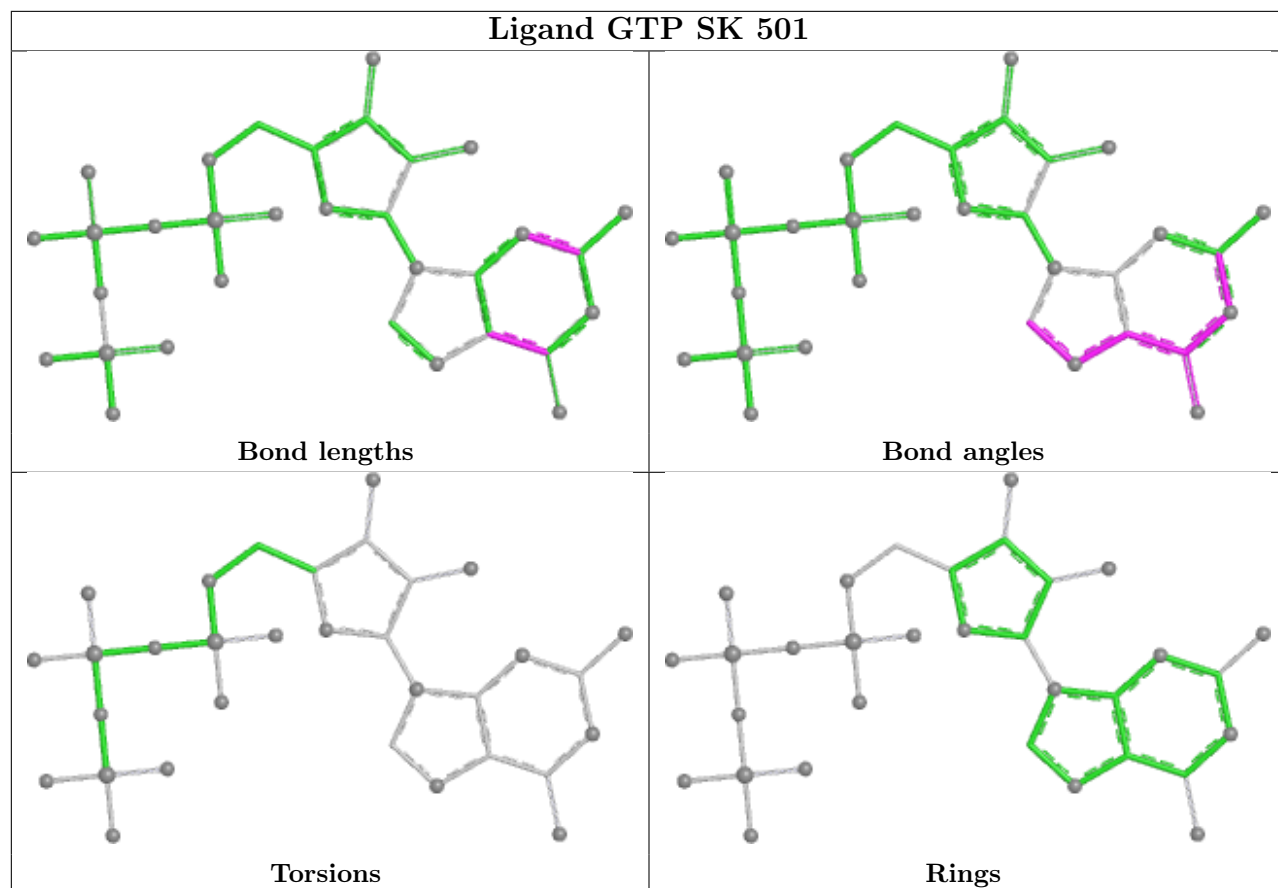




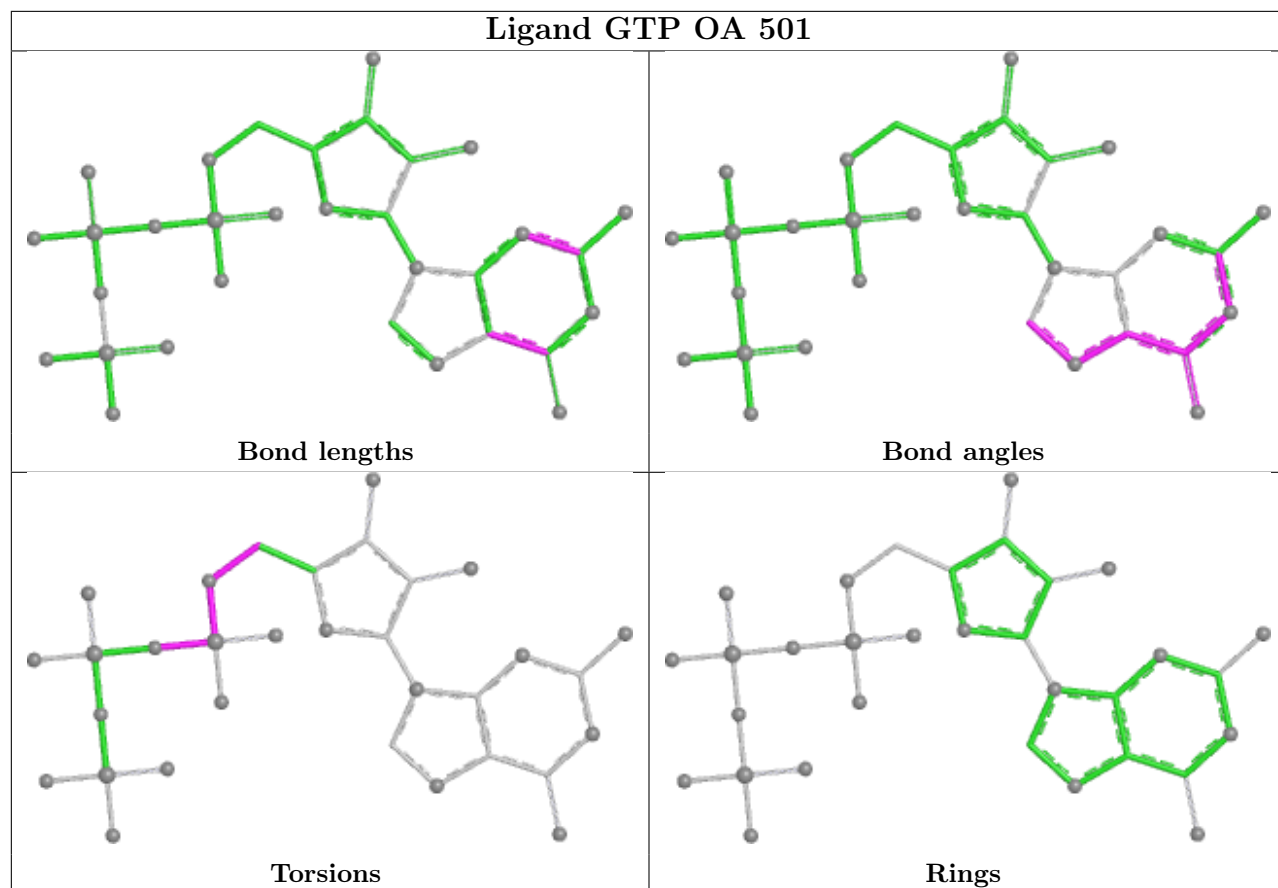




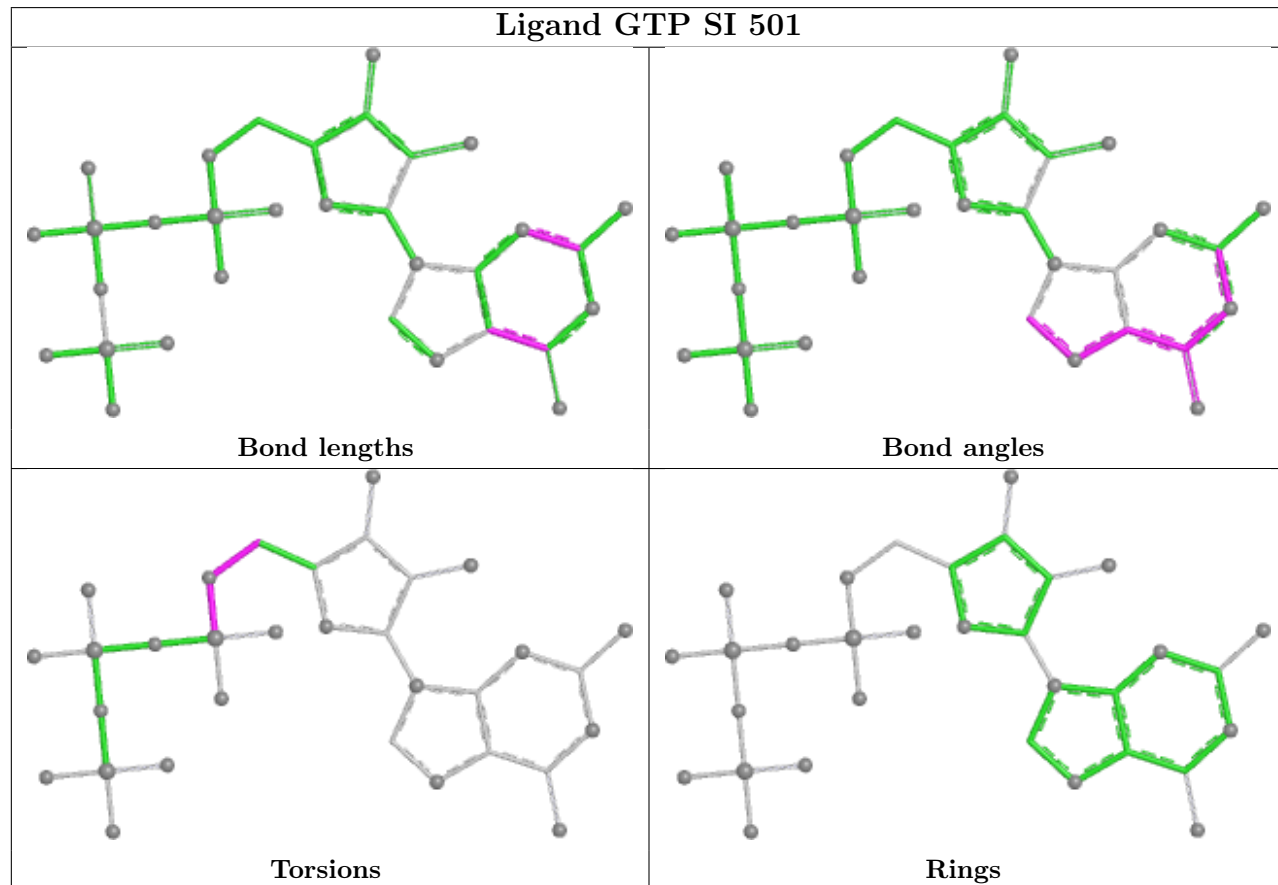




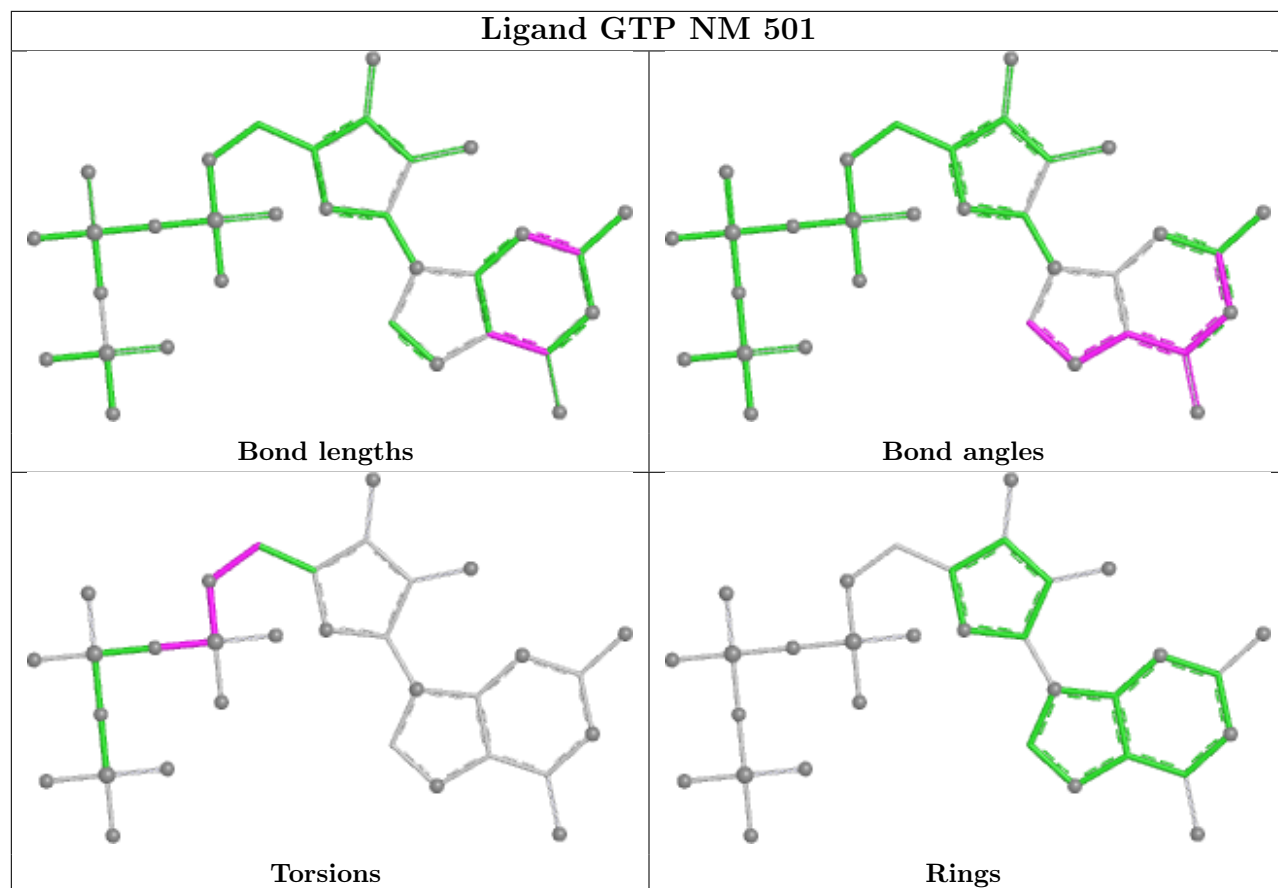
Ligand GTP OA 501



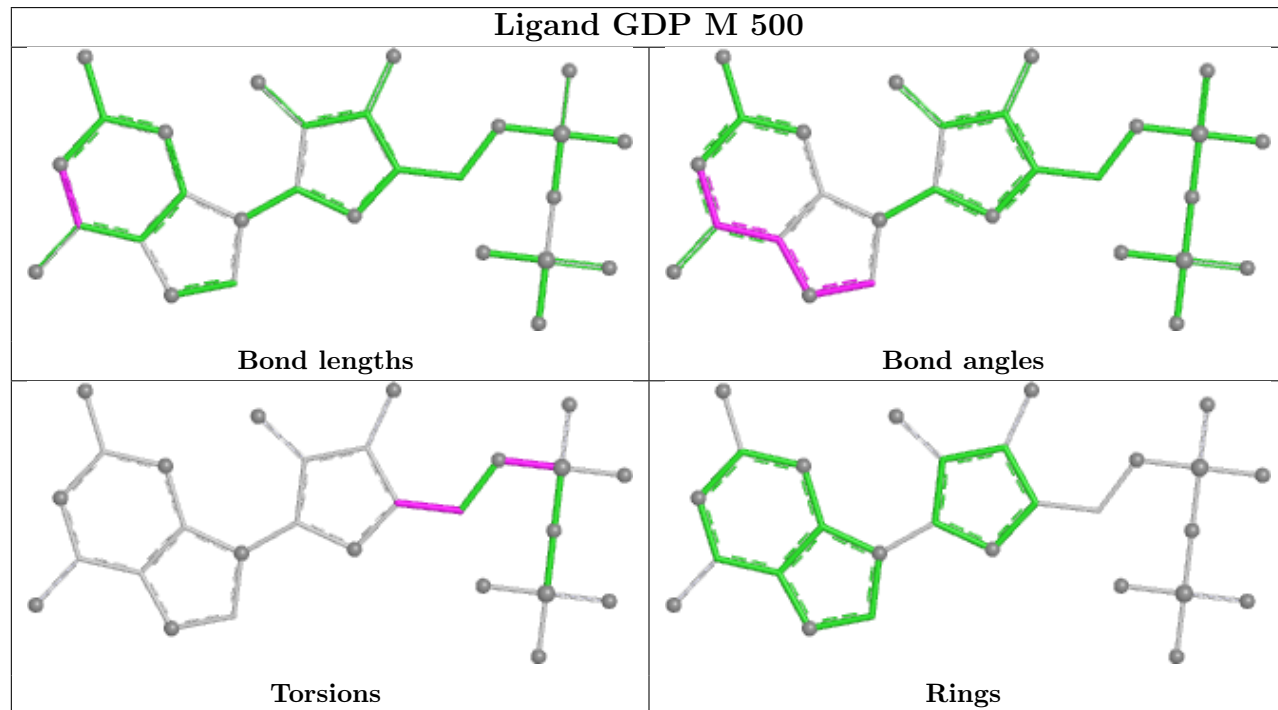
Ligand GTP SI 501

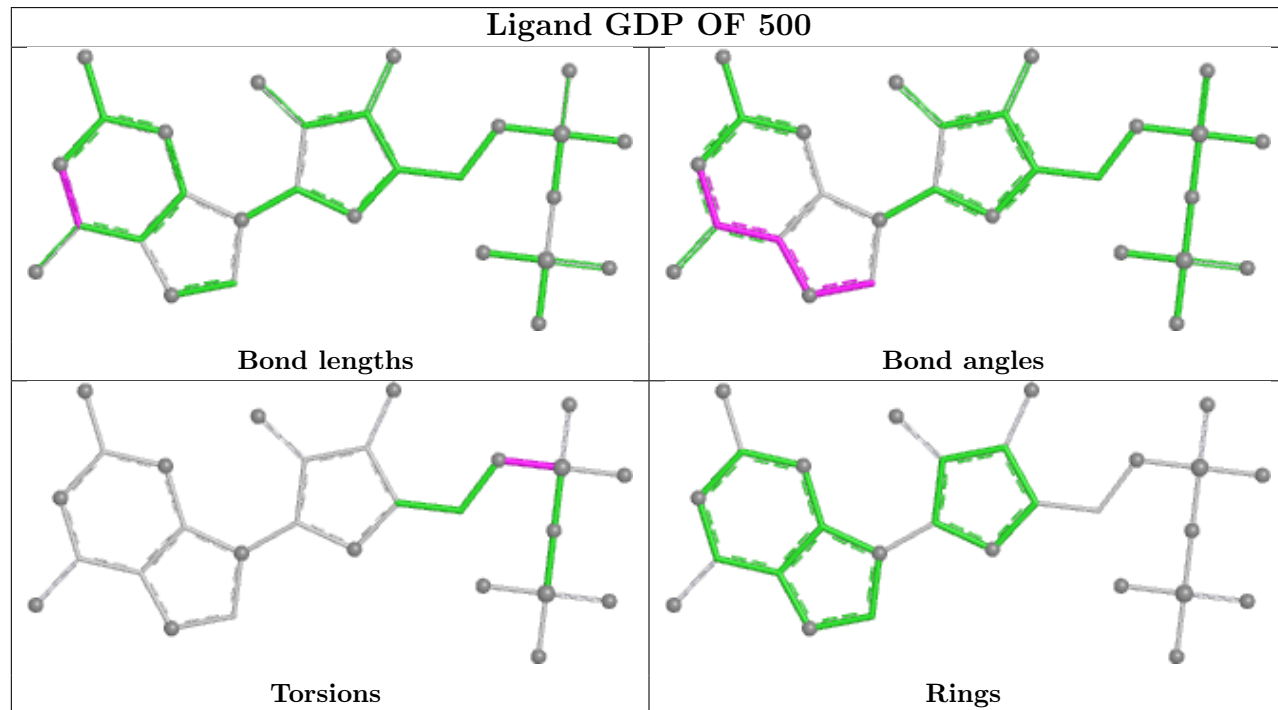
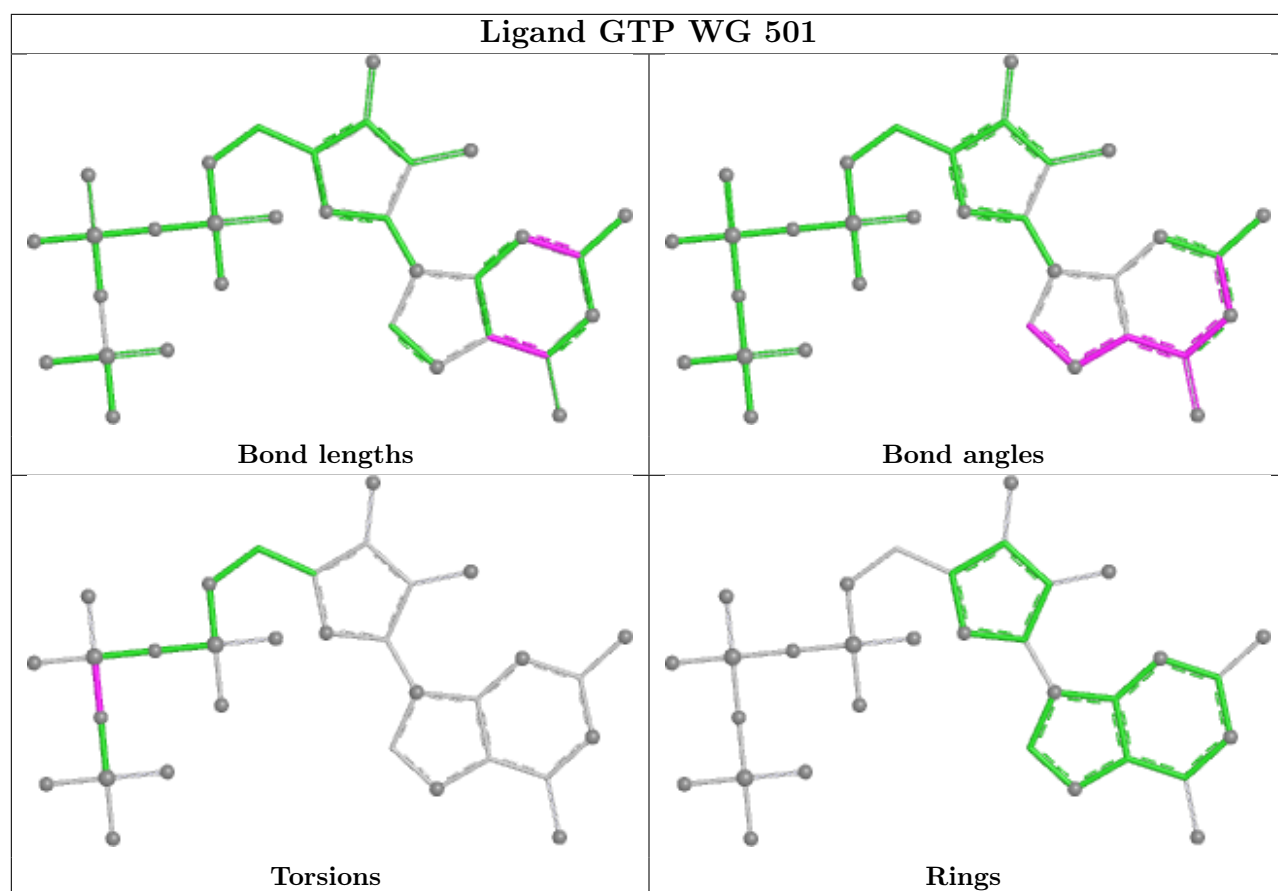


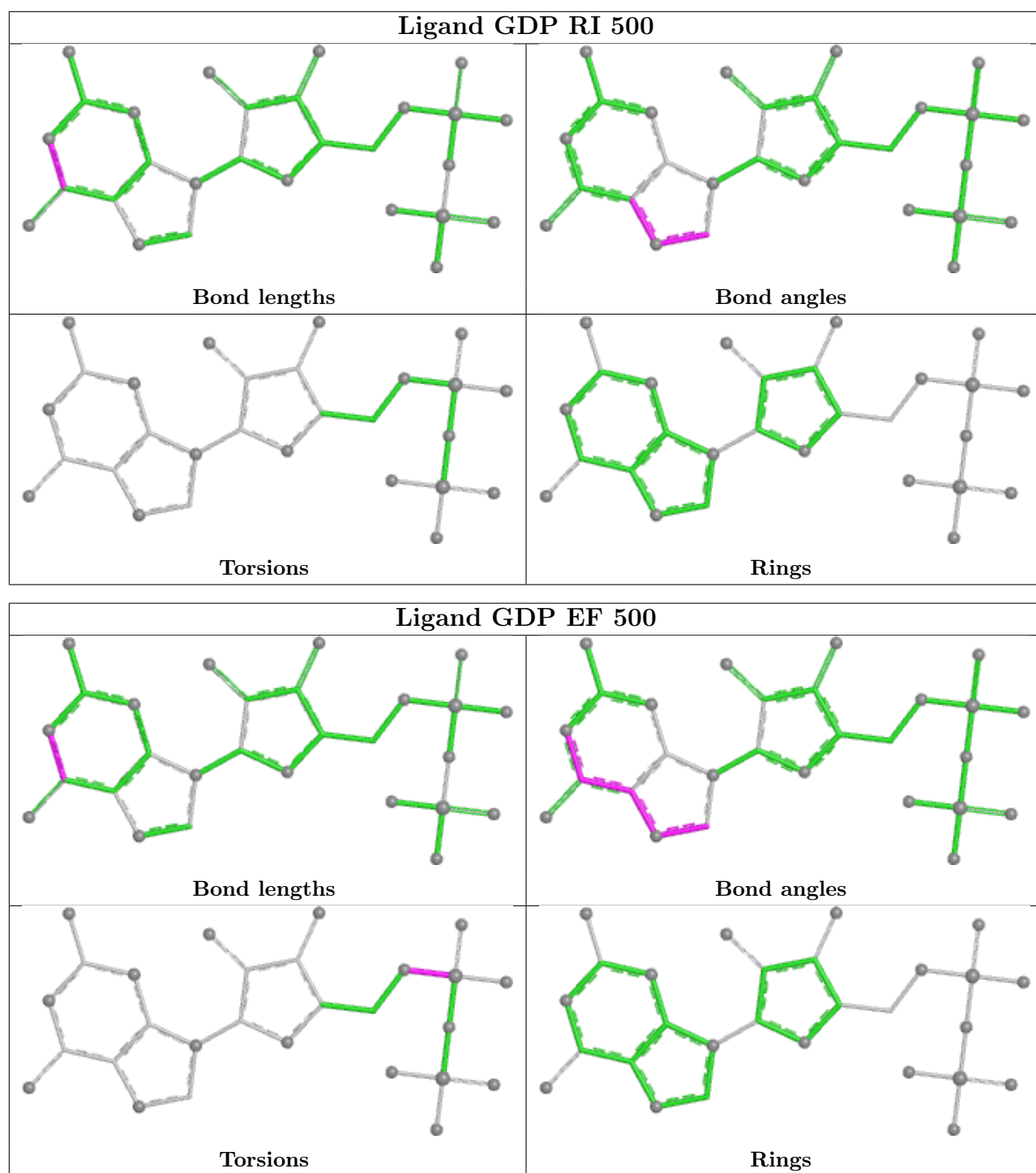
Ligand GTP NM 501

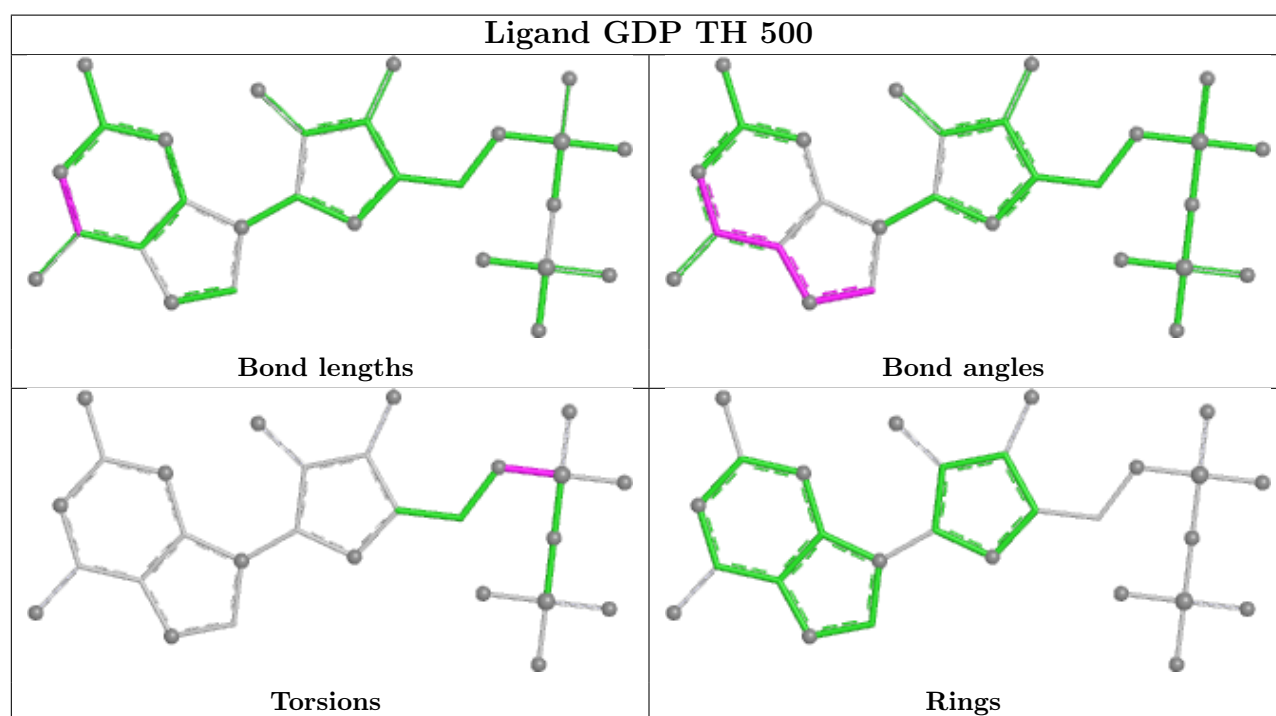
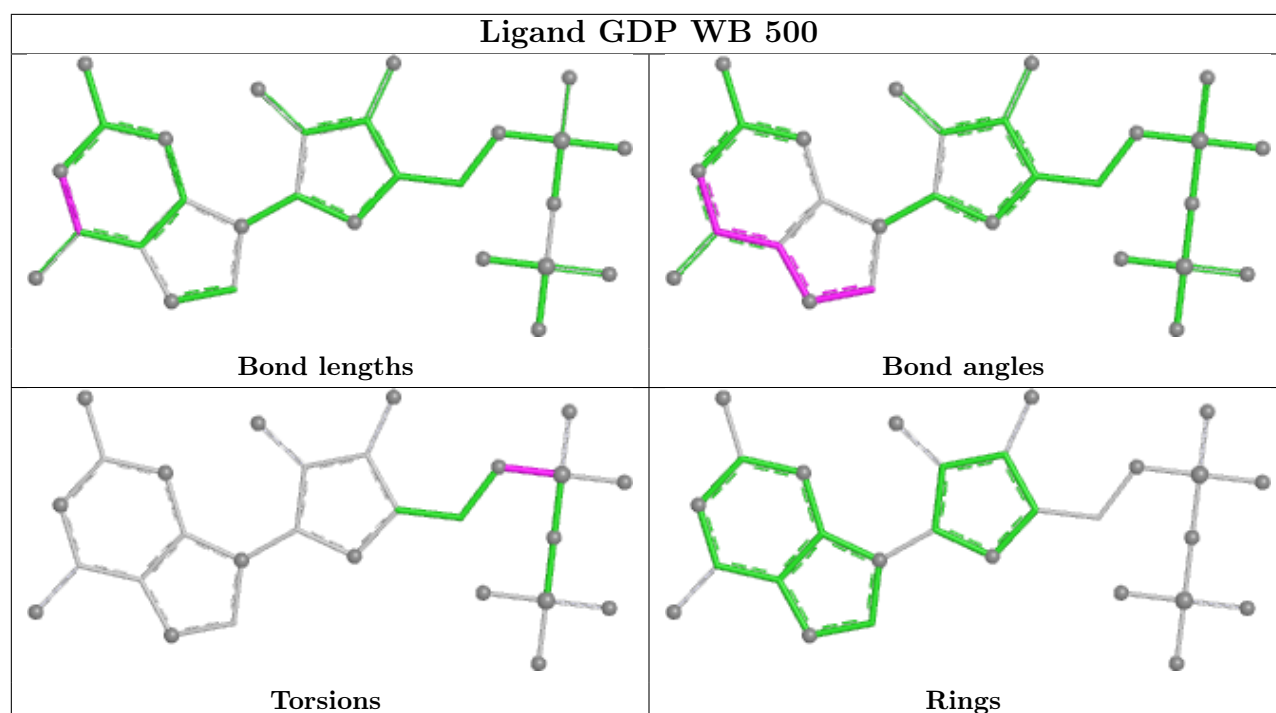


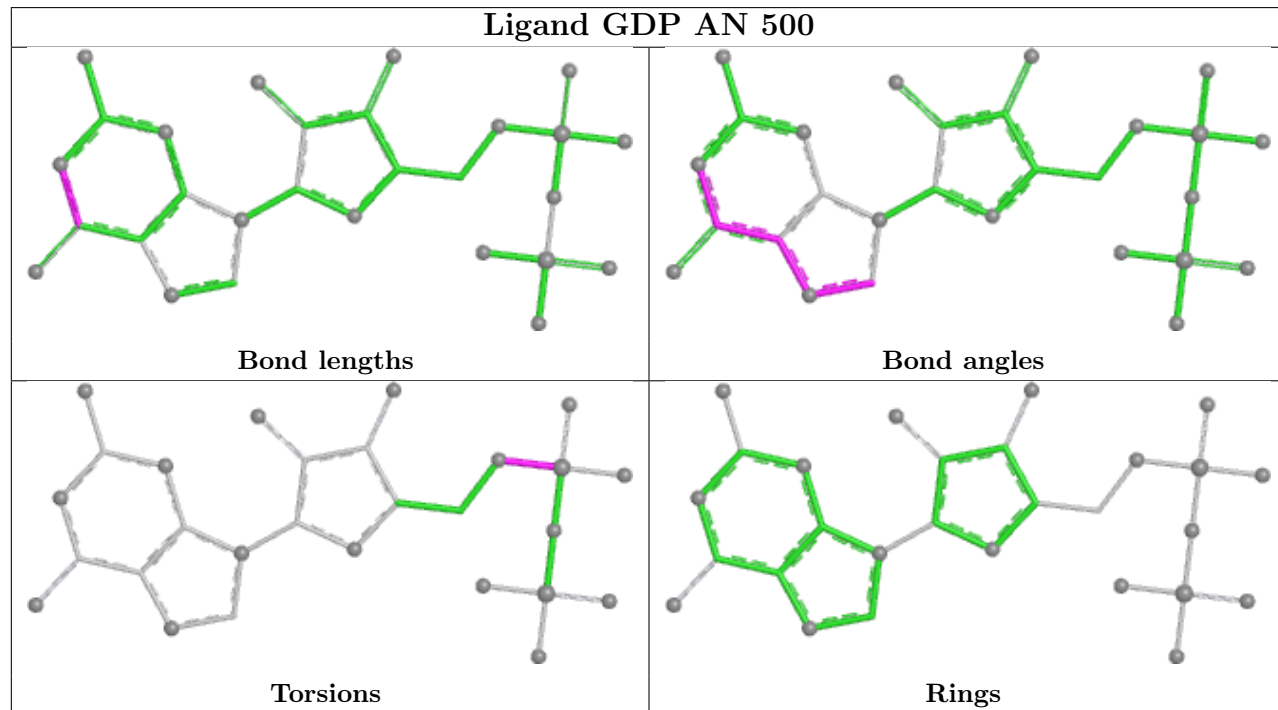
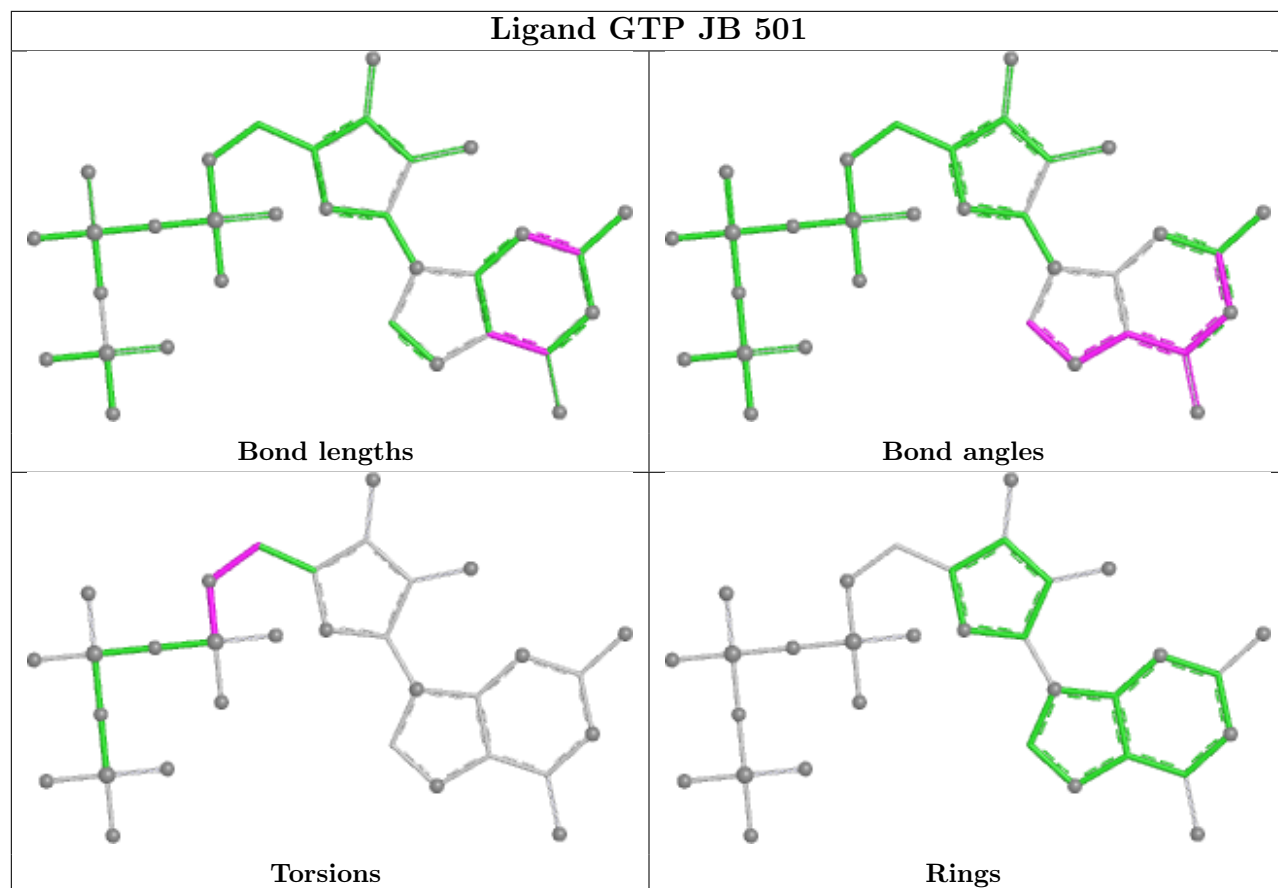
Ligand GDP M 500



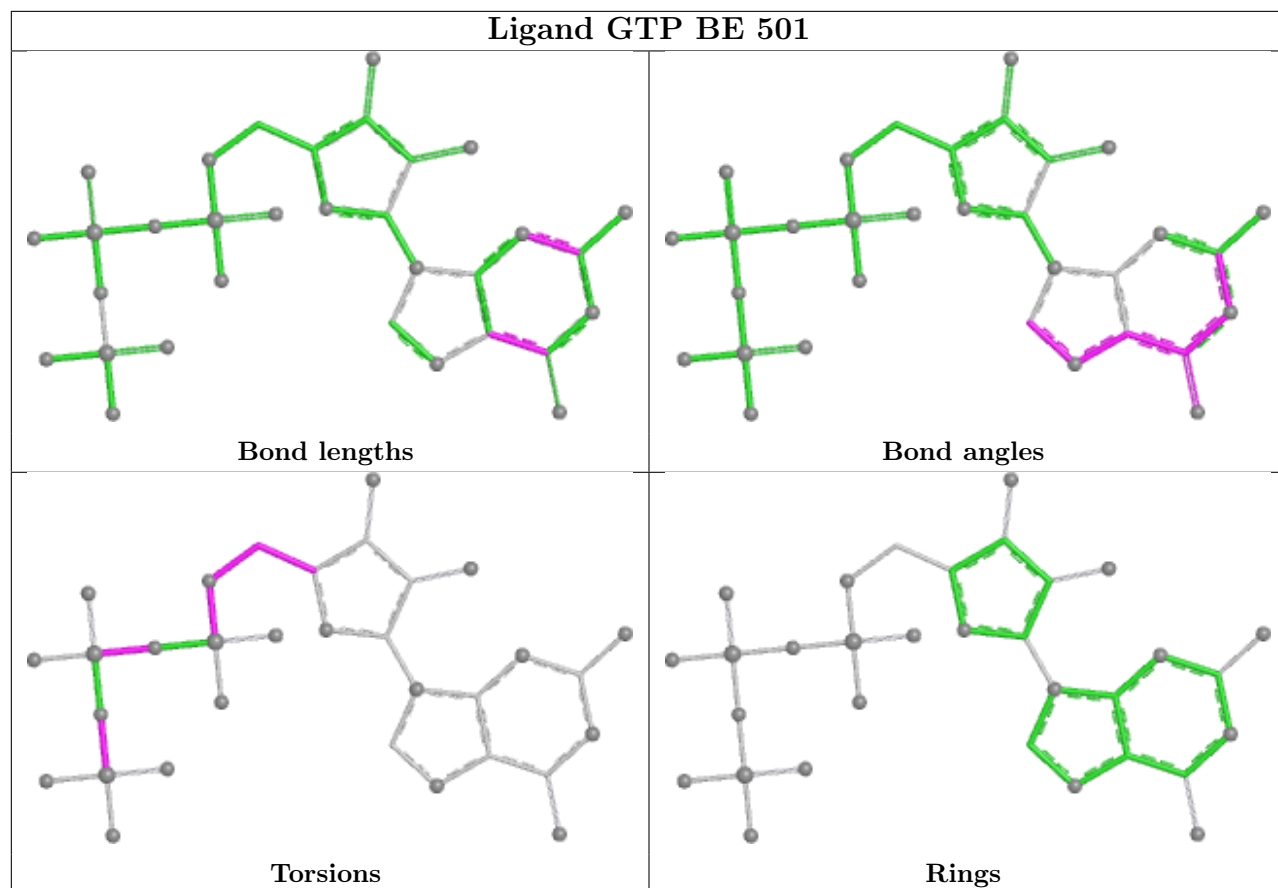




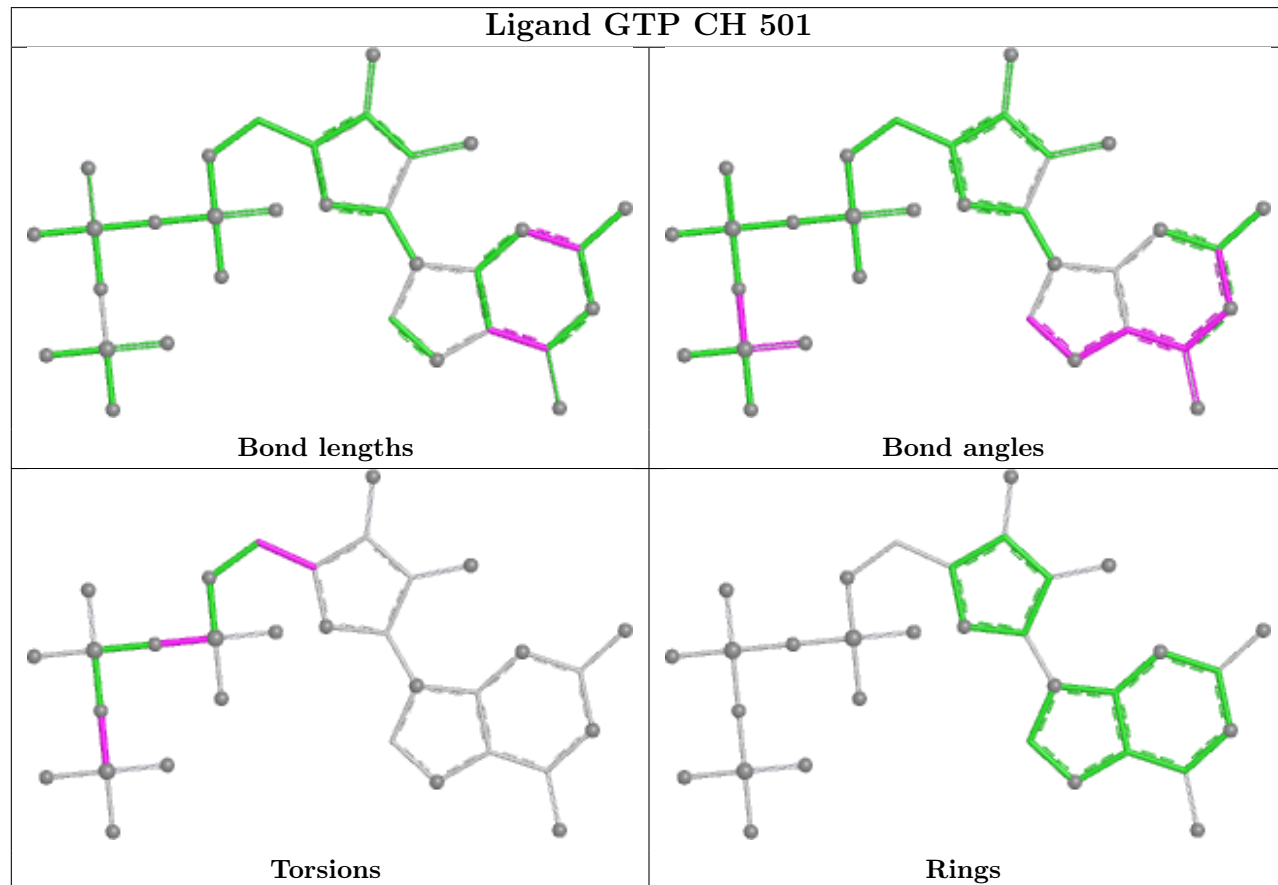


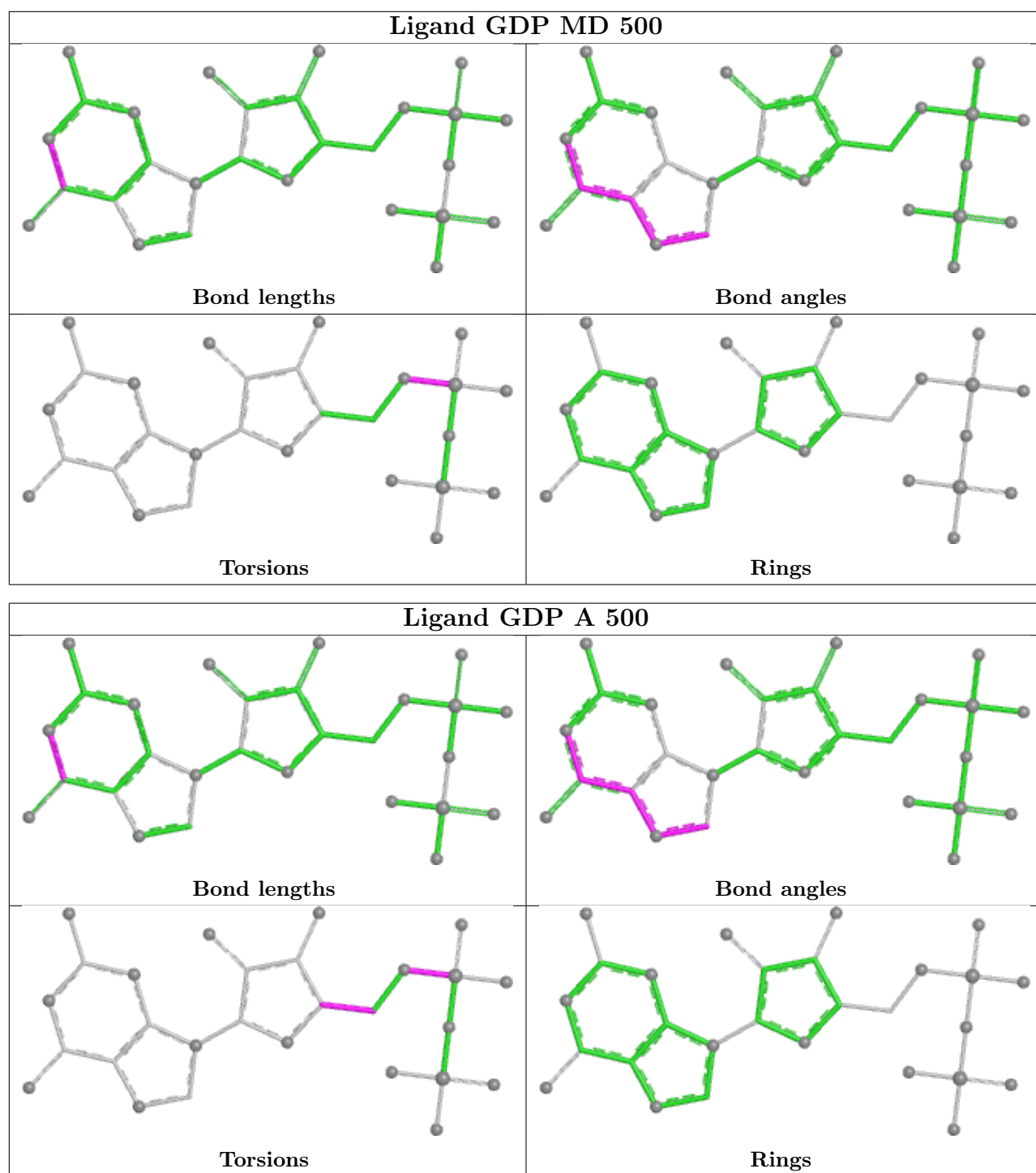


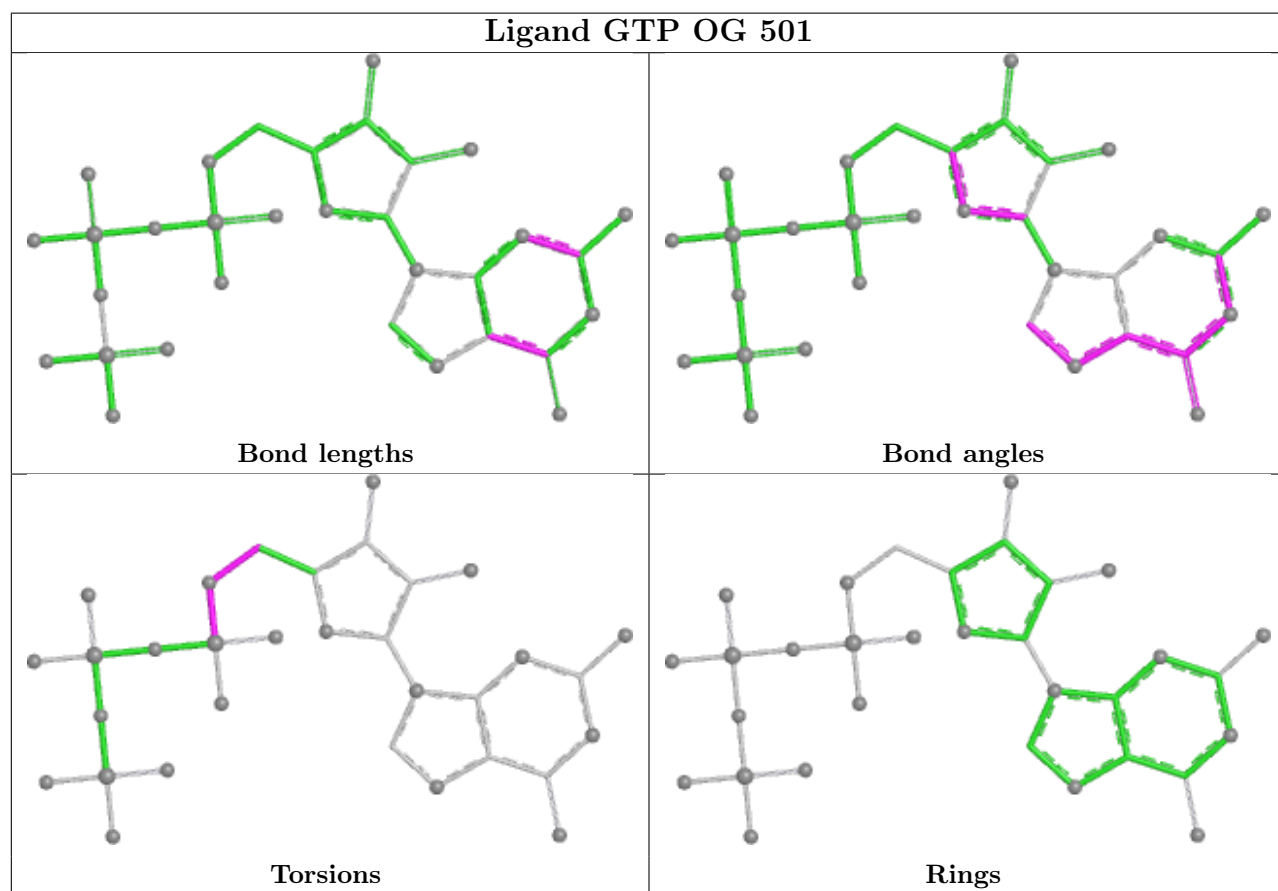
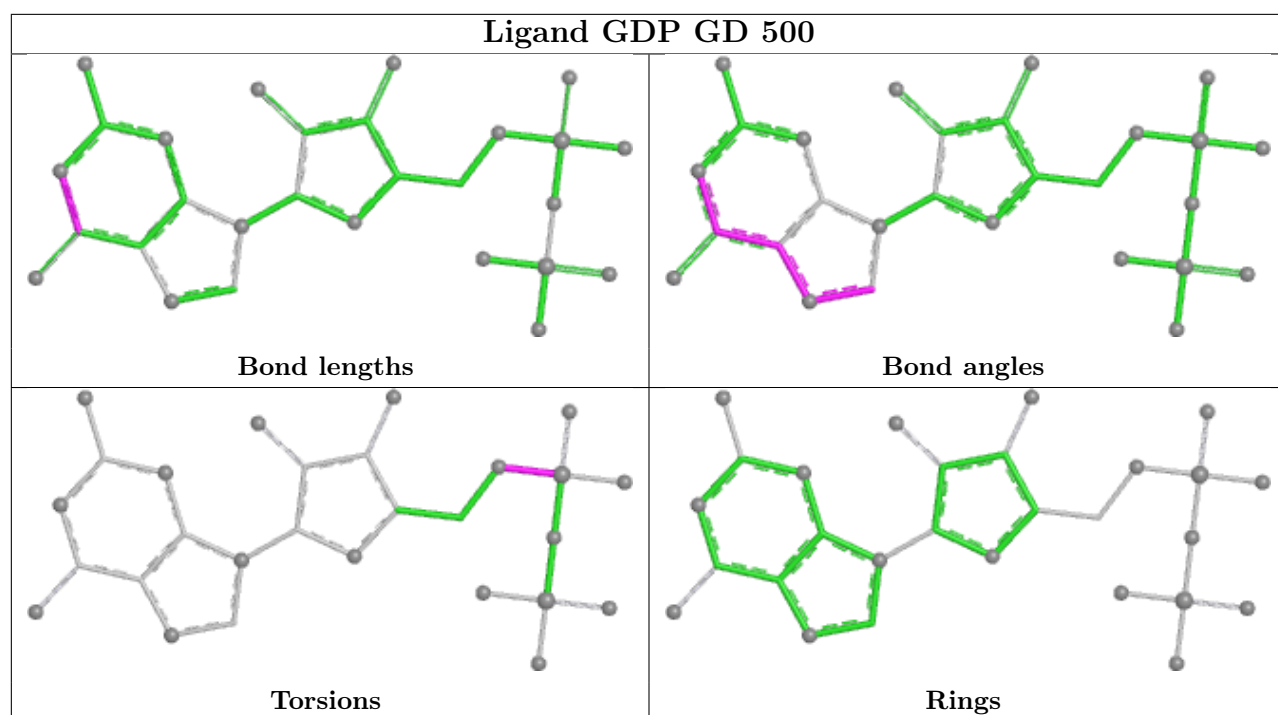
Ligand GTP BE 501

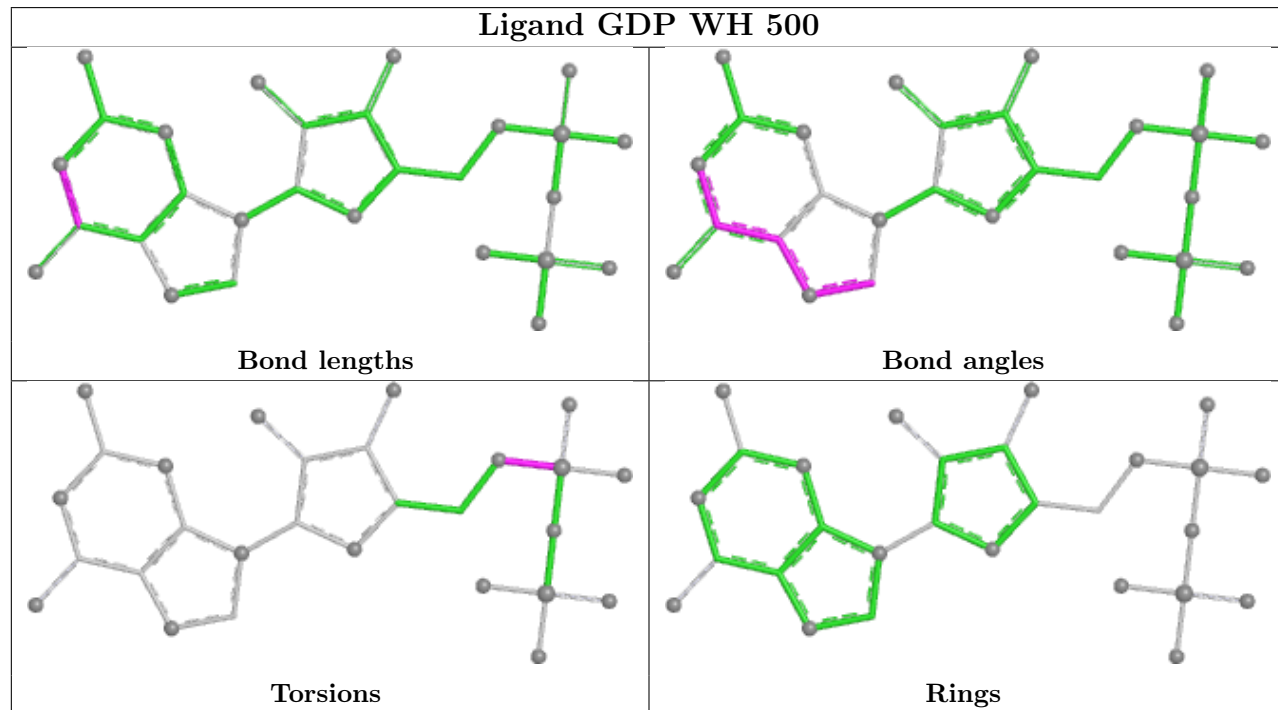
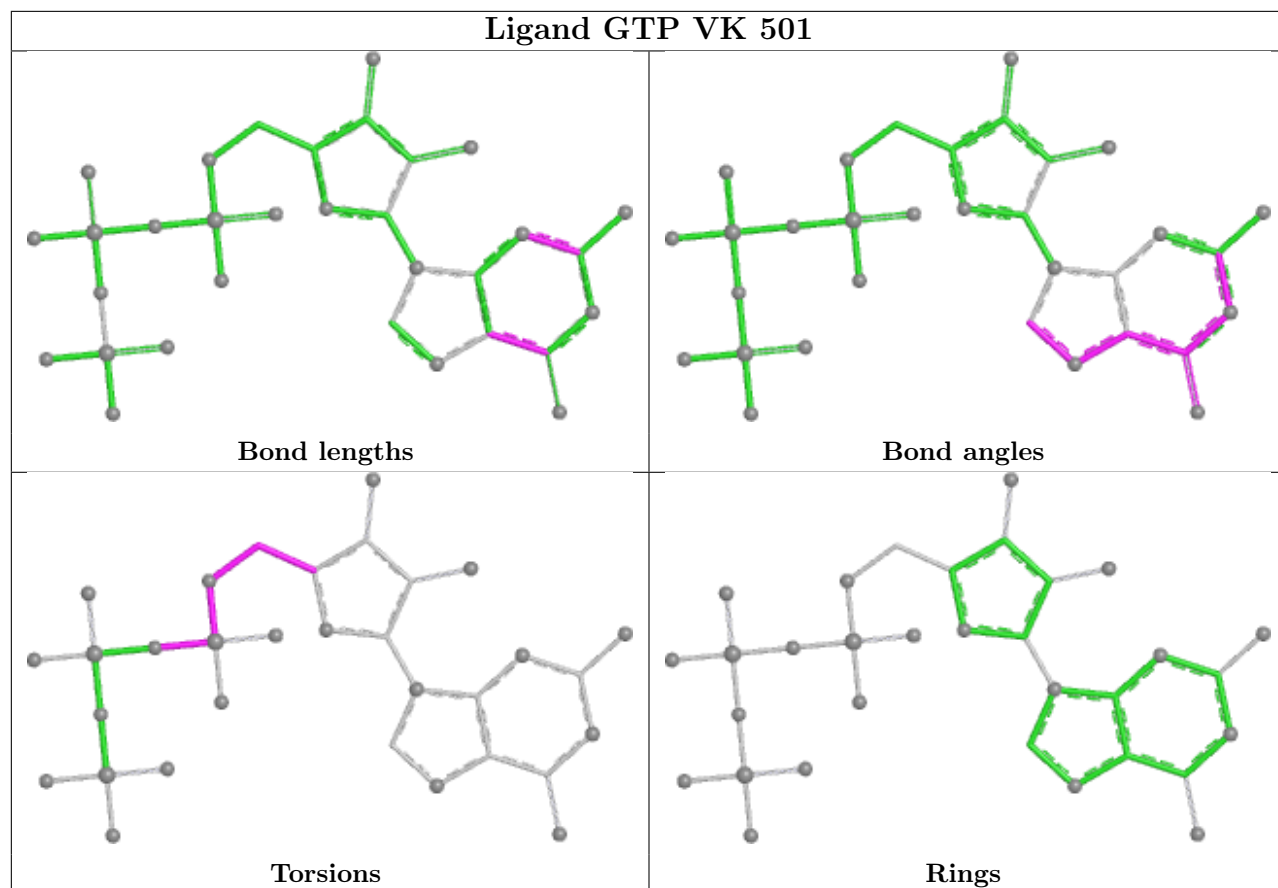


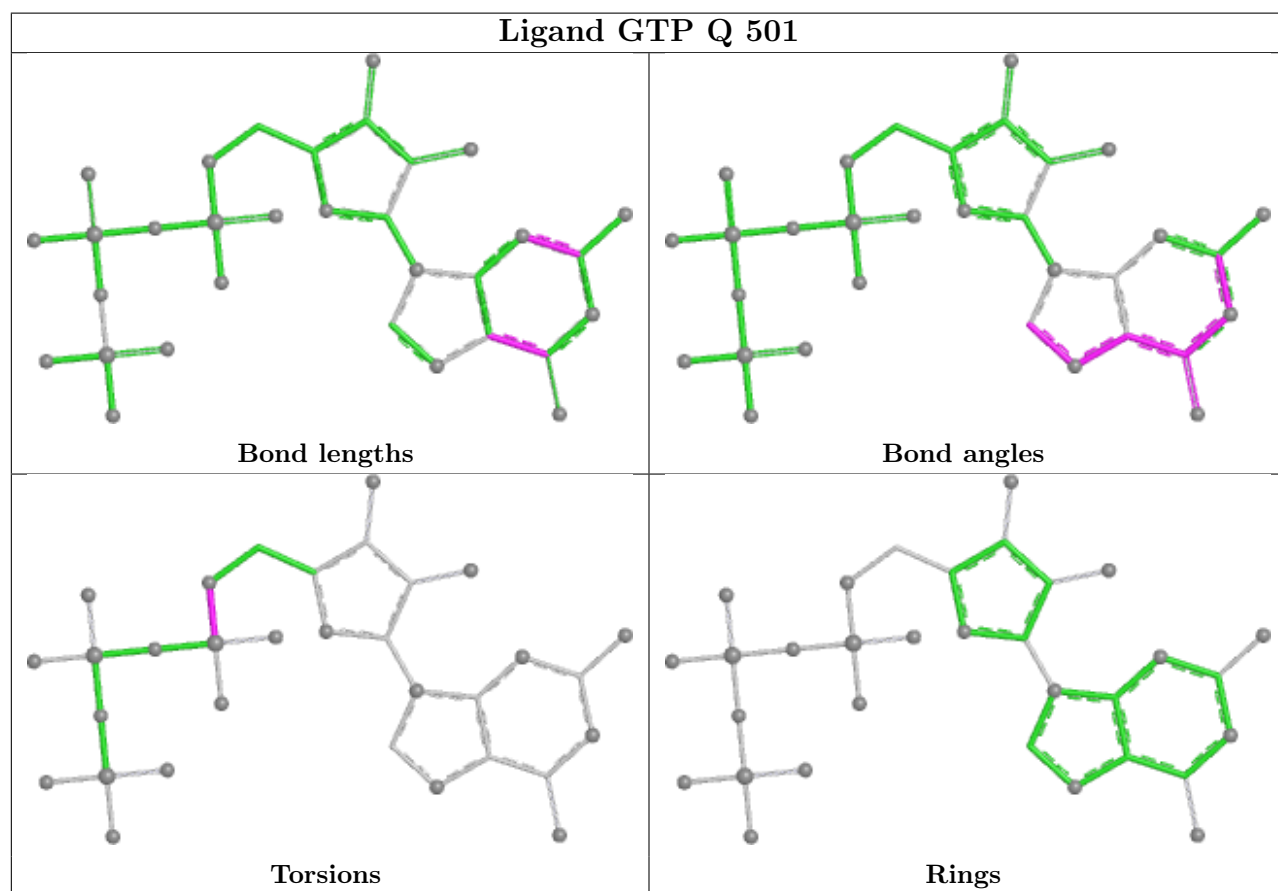
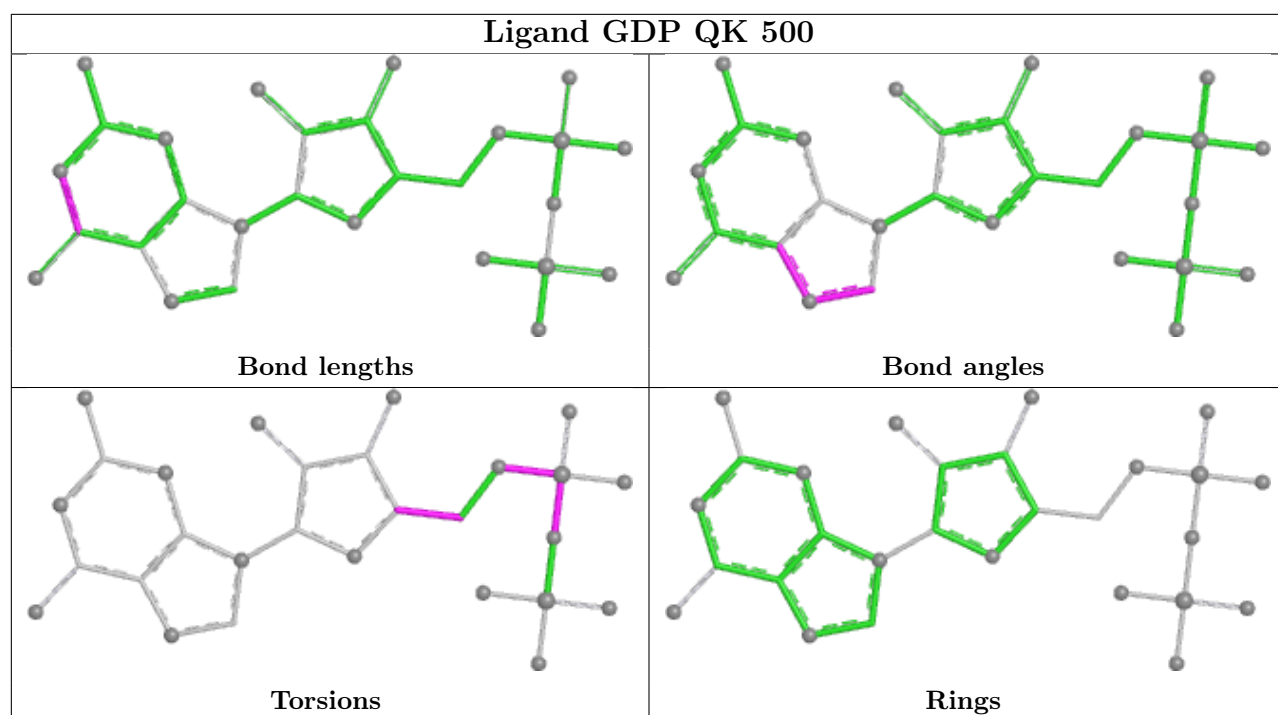
Ligand GTP CH 501

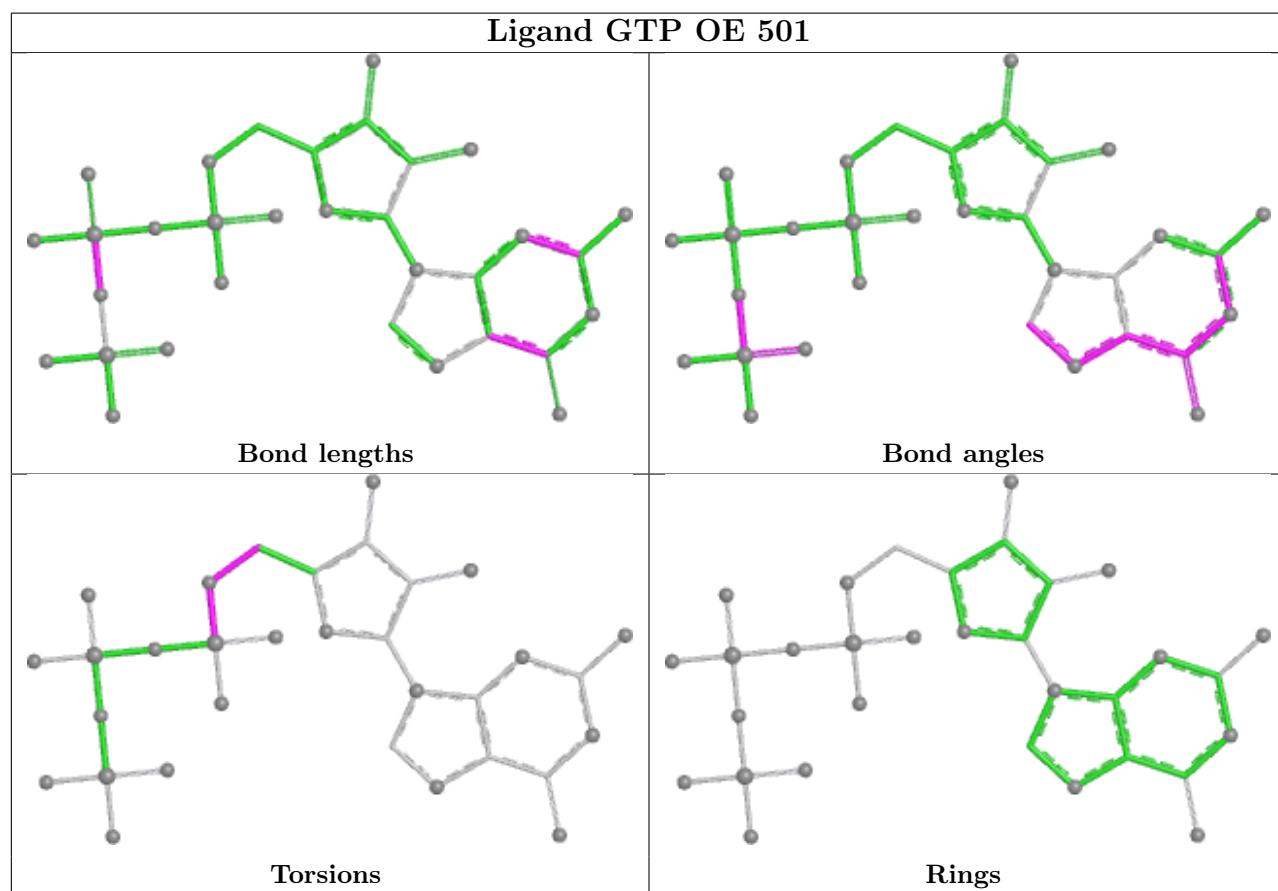
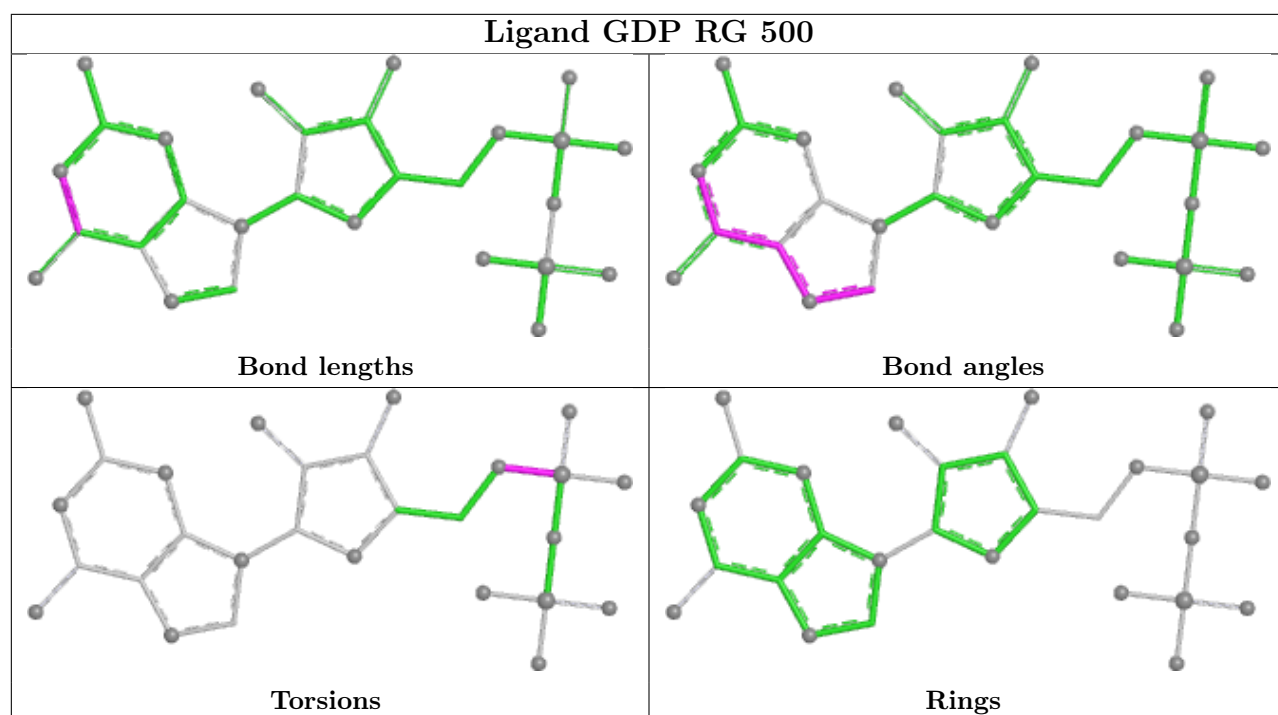


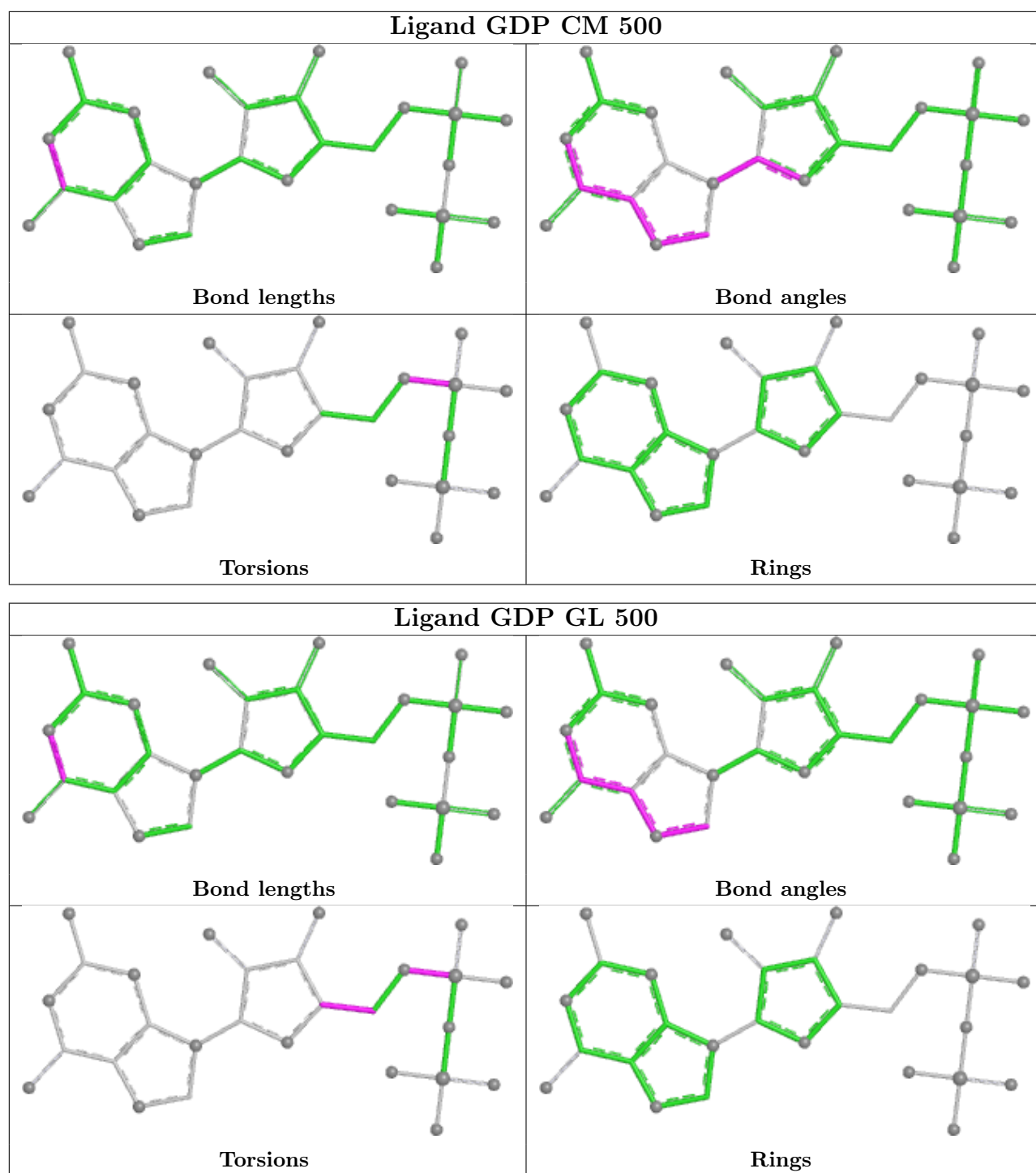


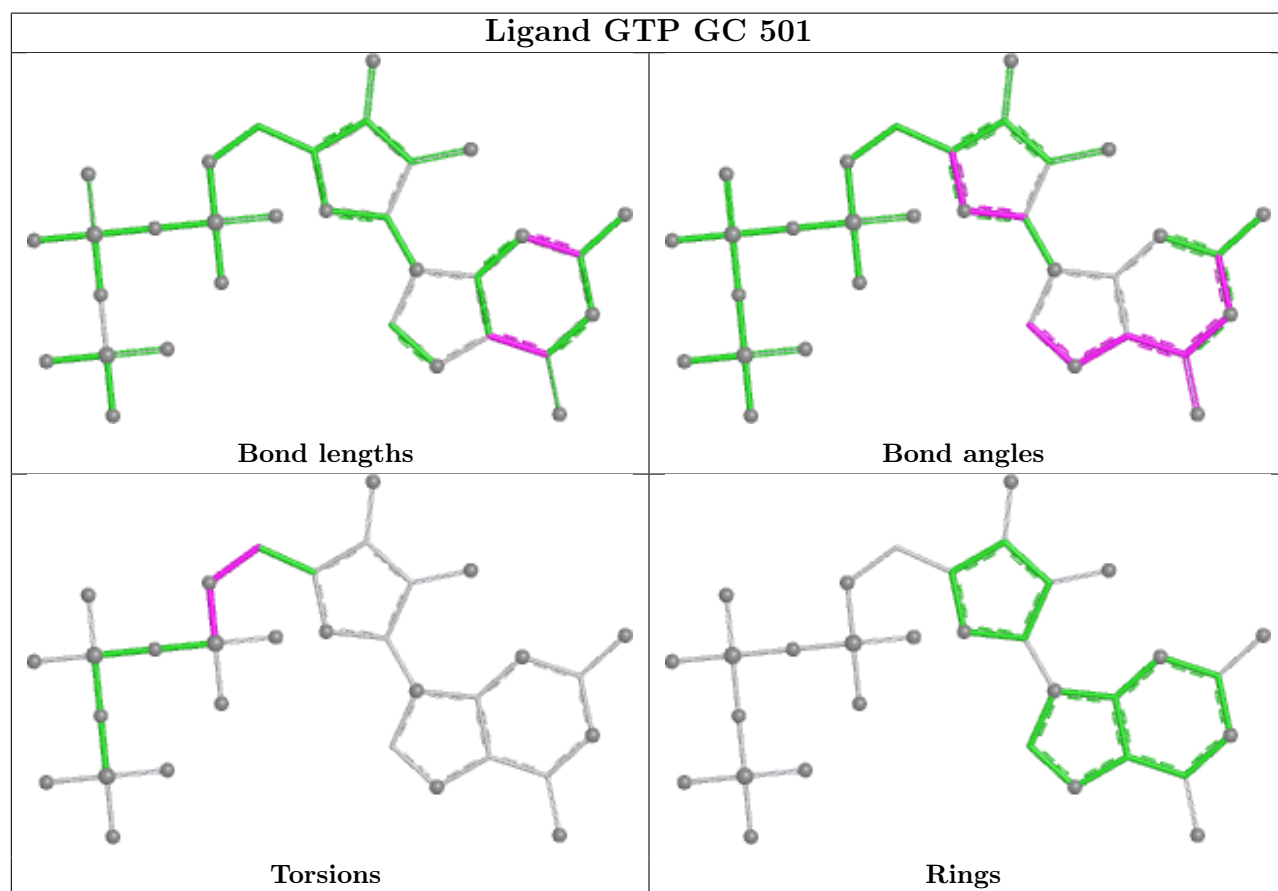
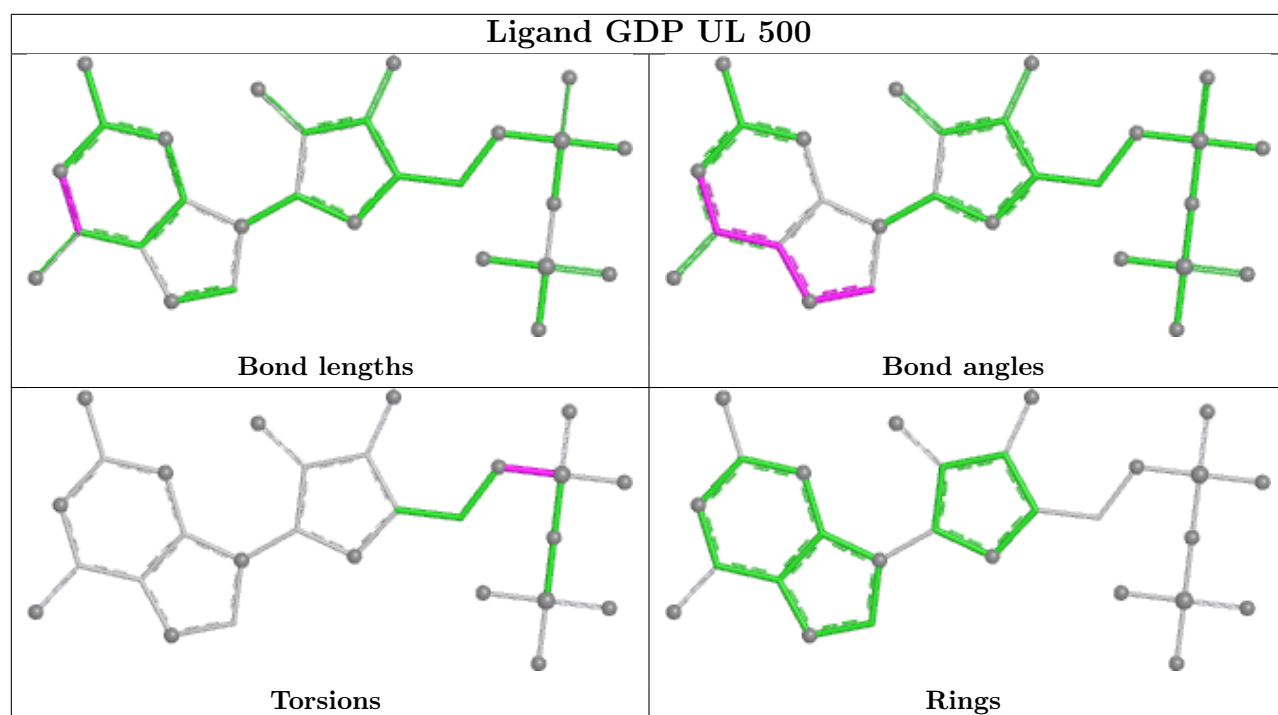


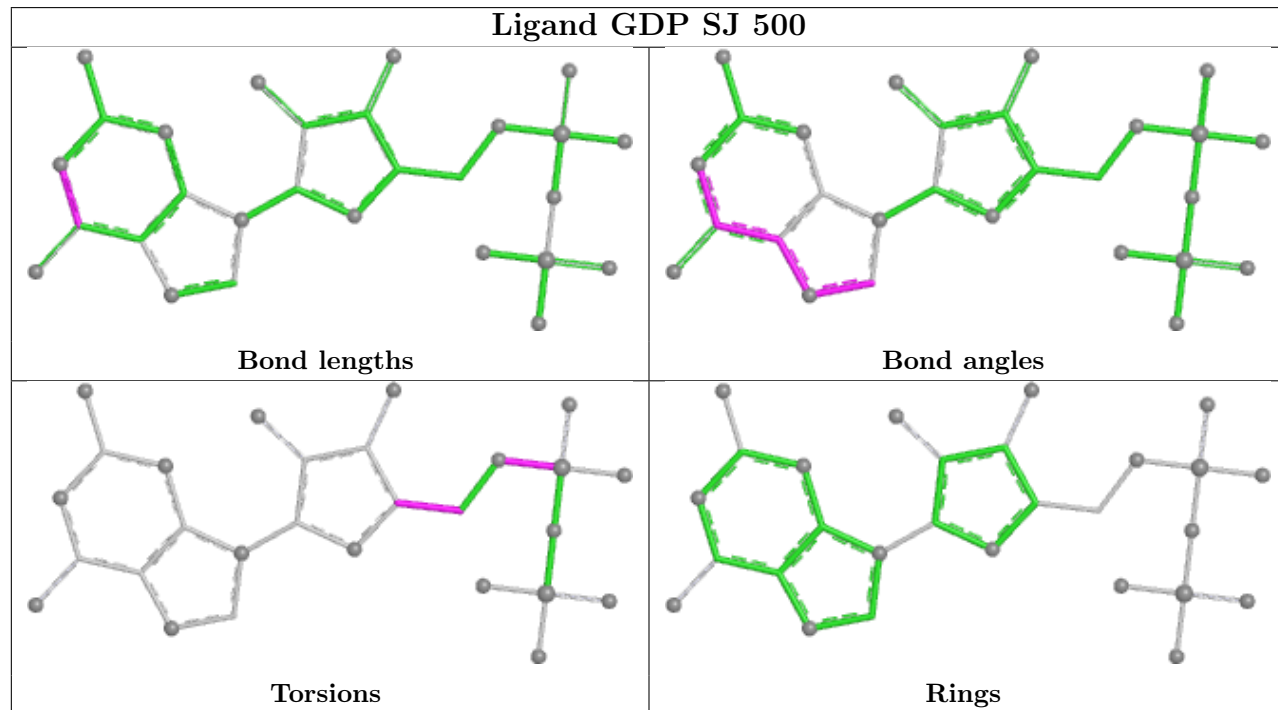
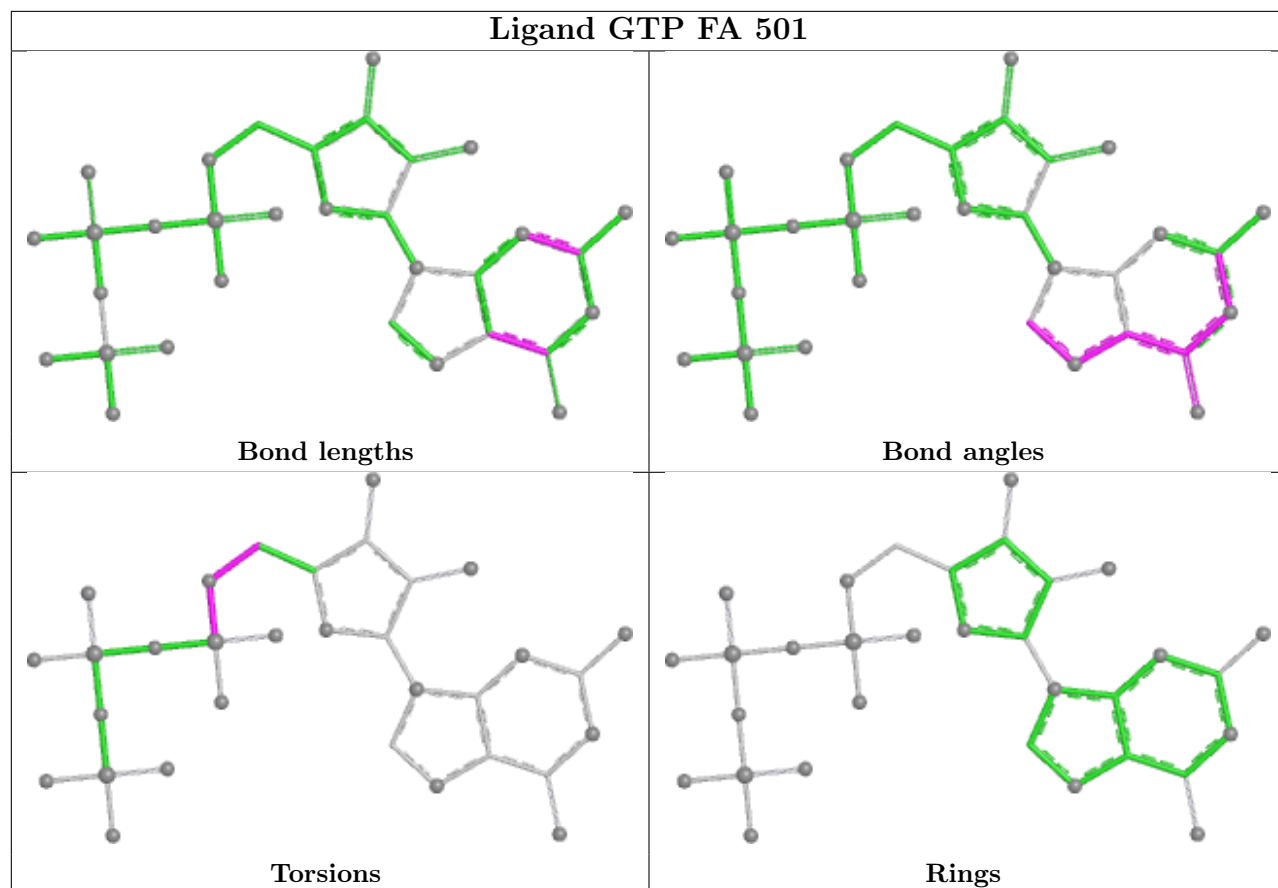


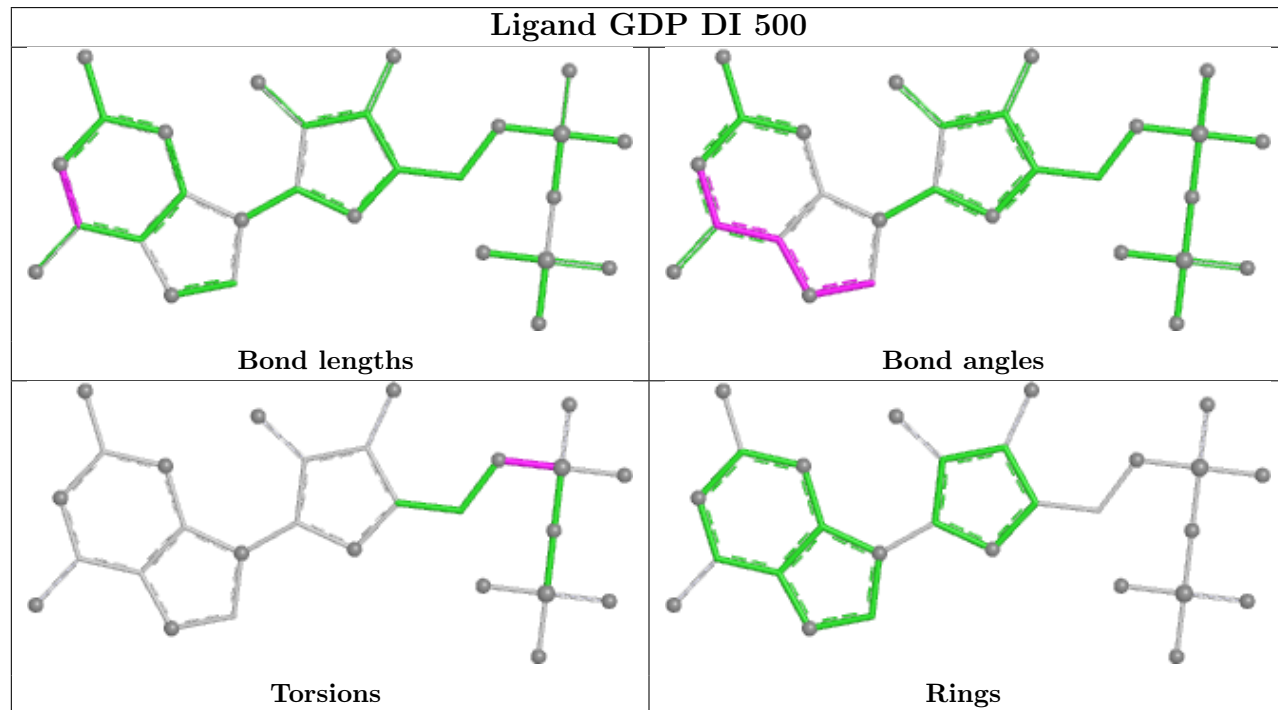
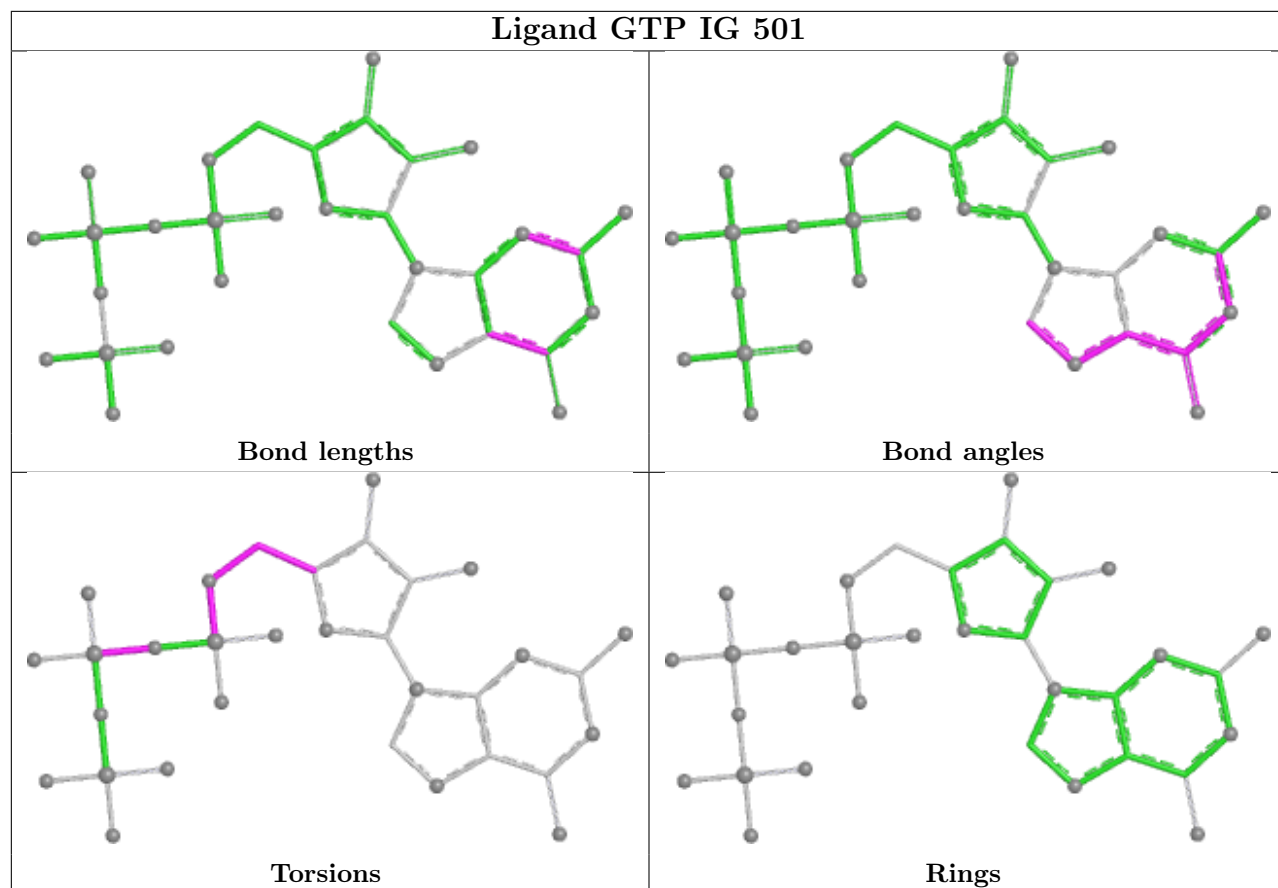


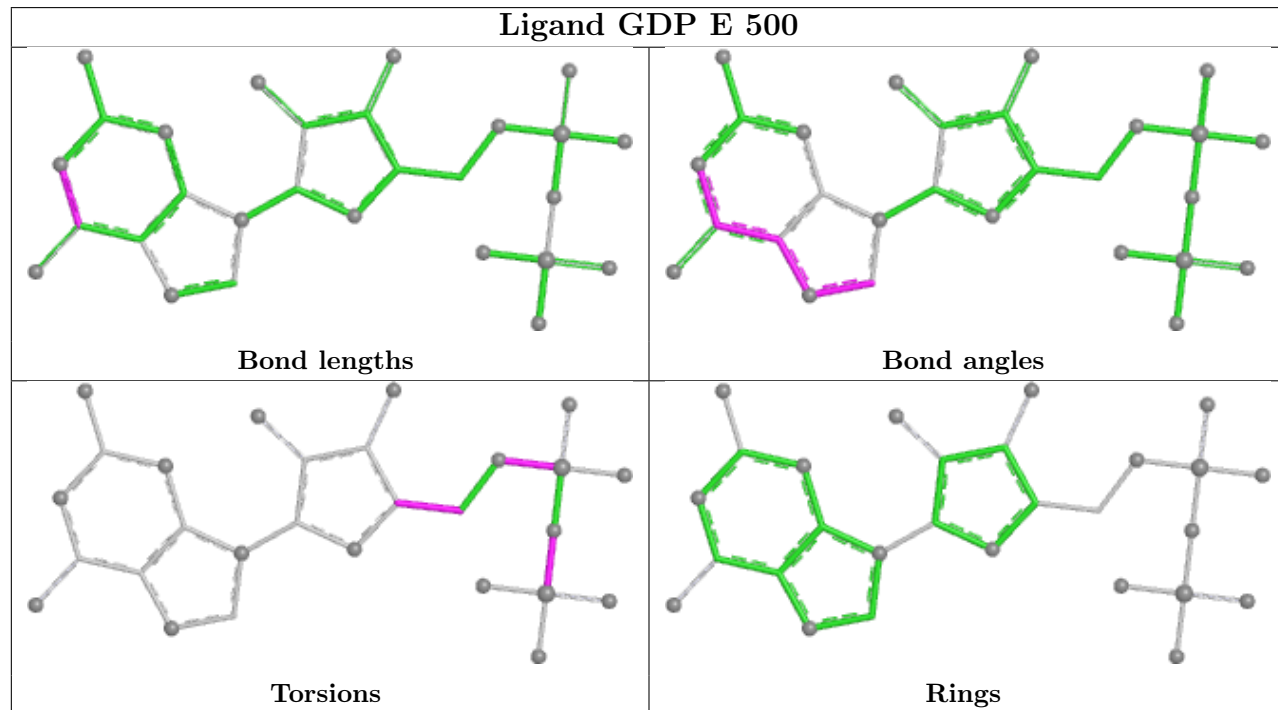
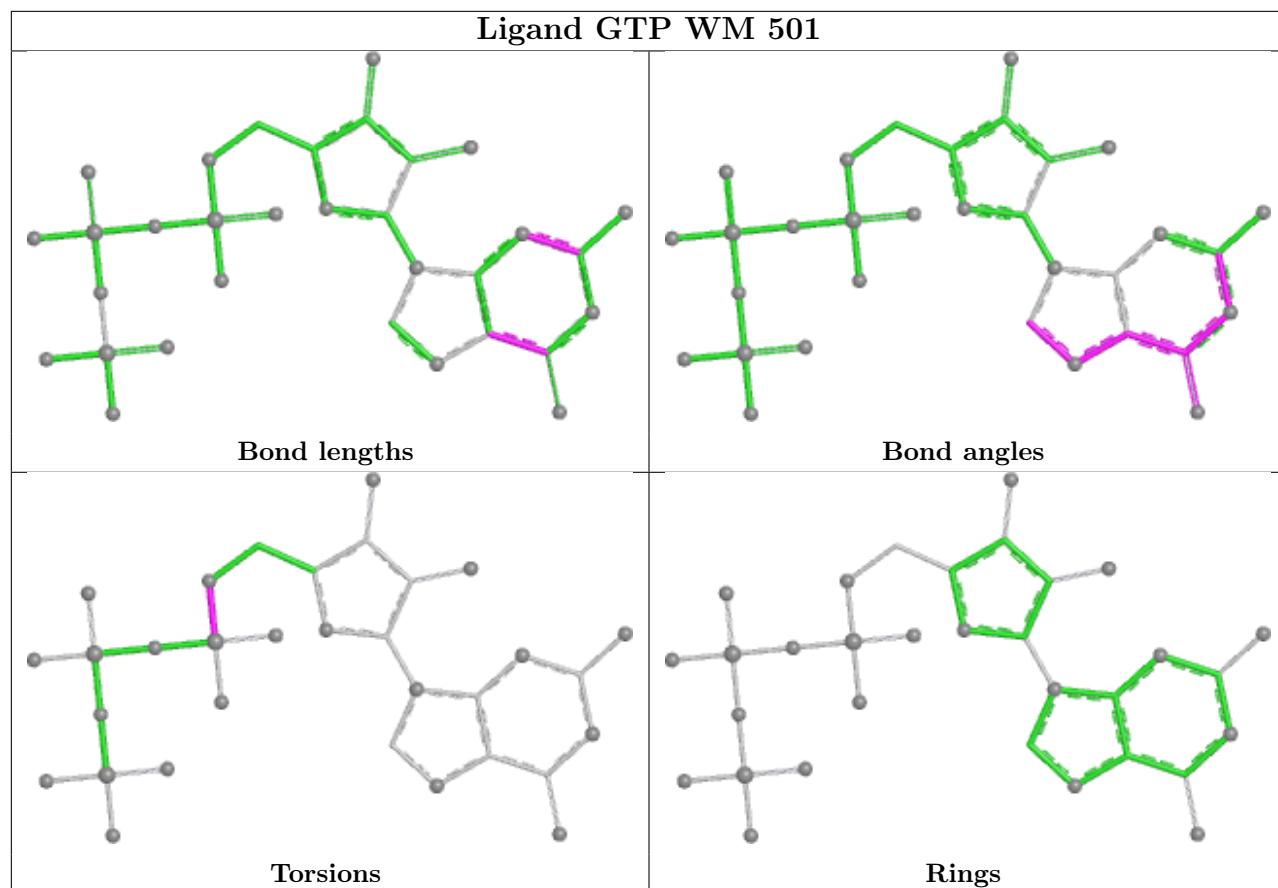


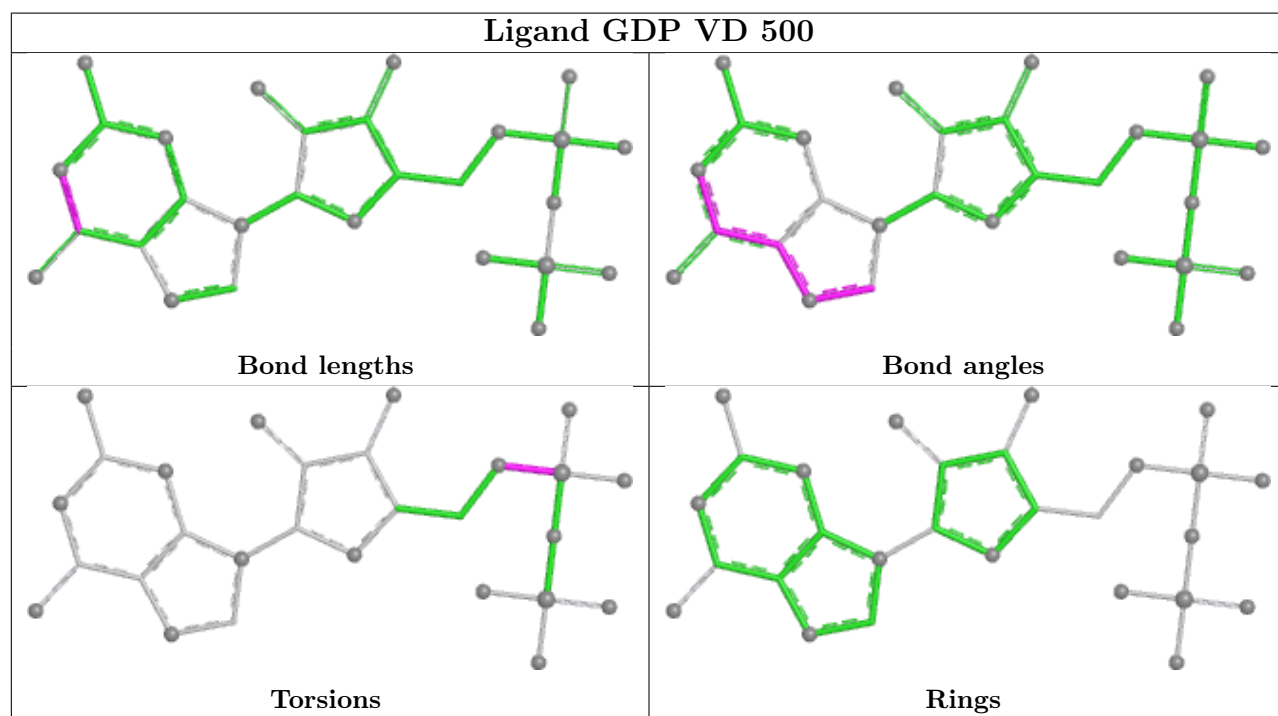
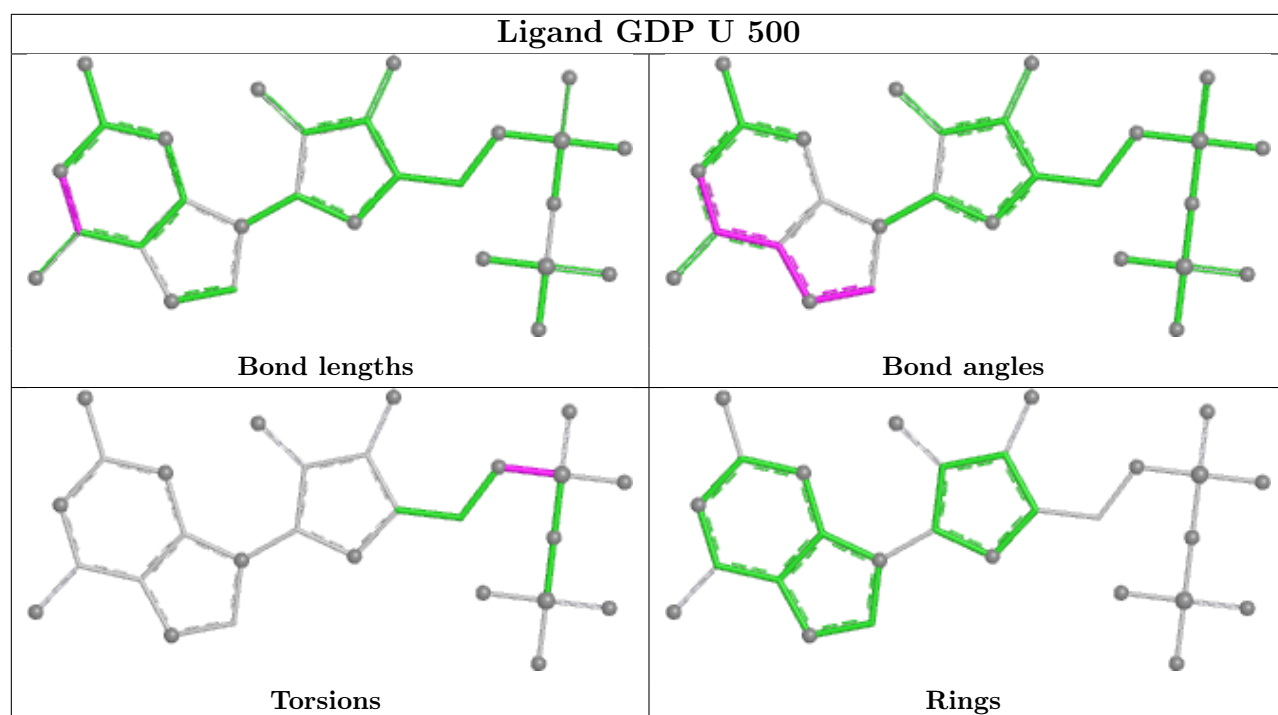




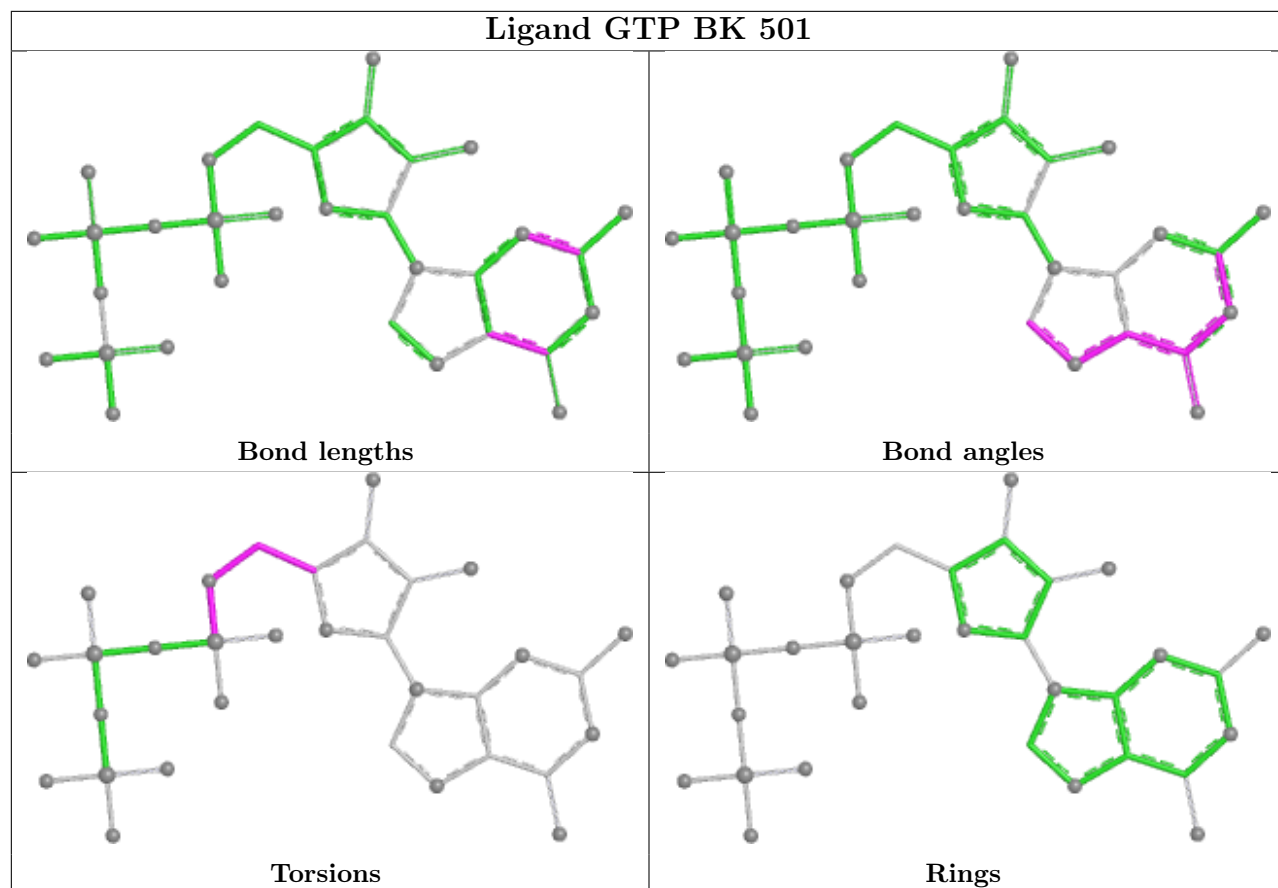




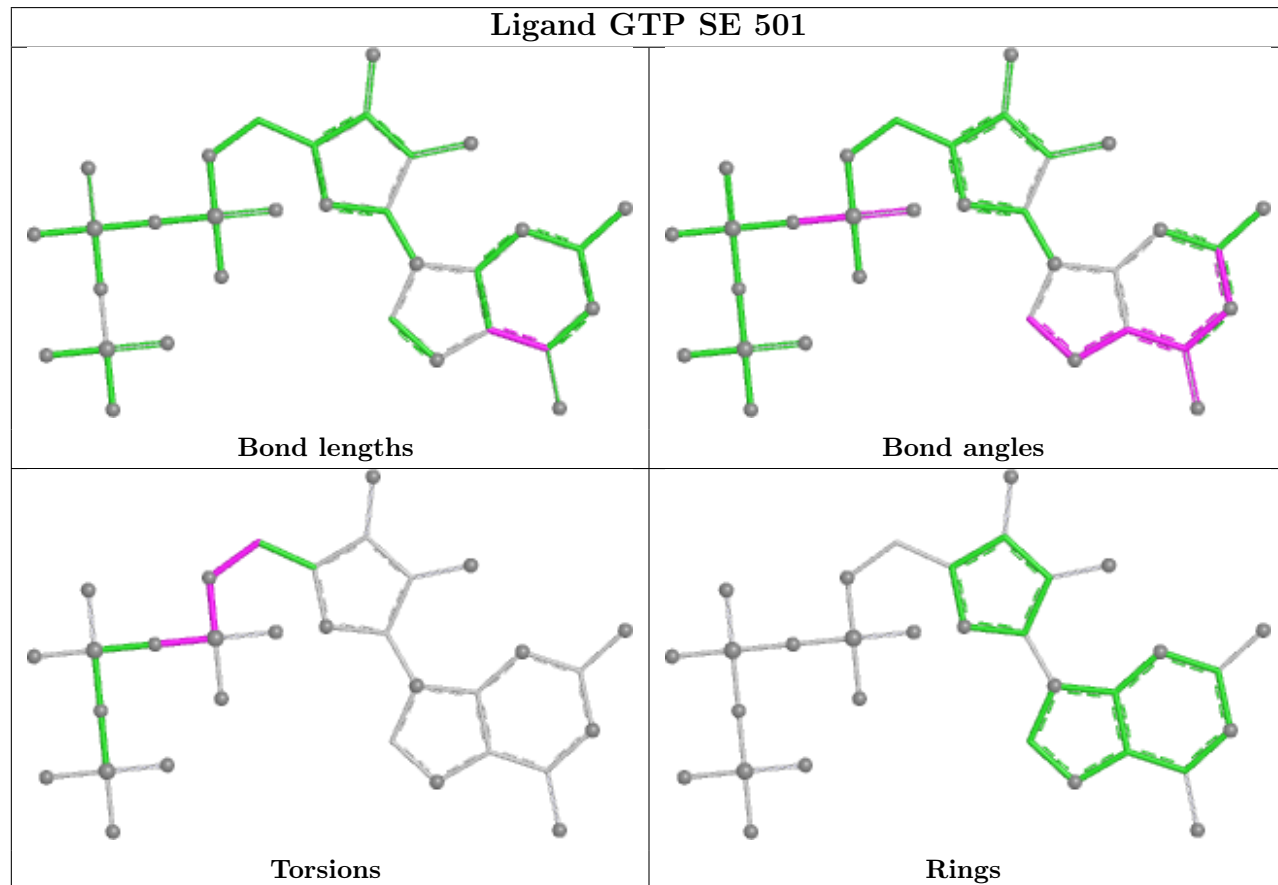




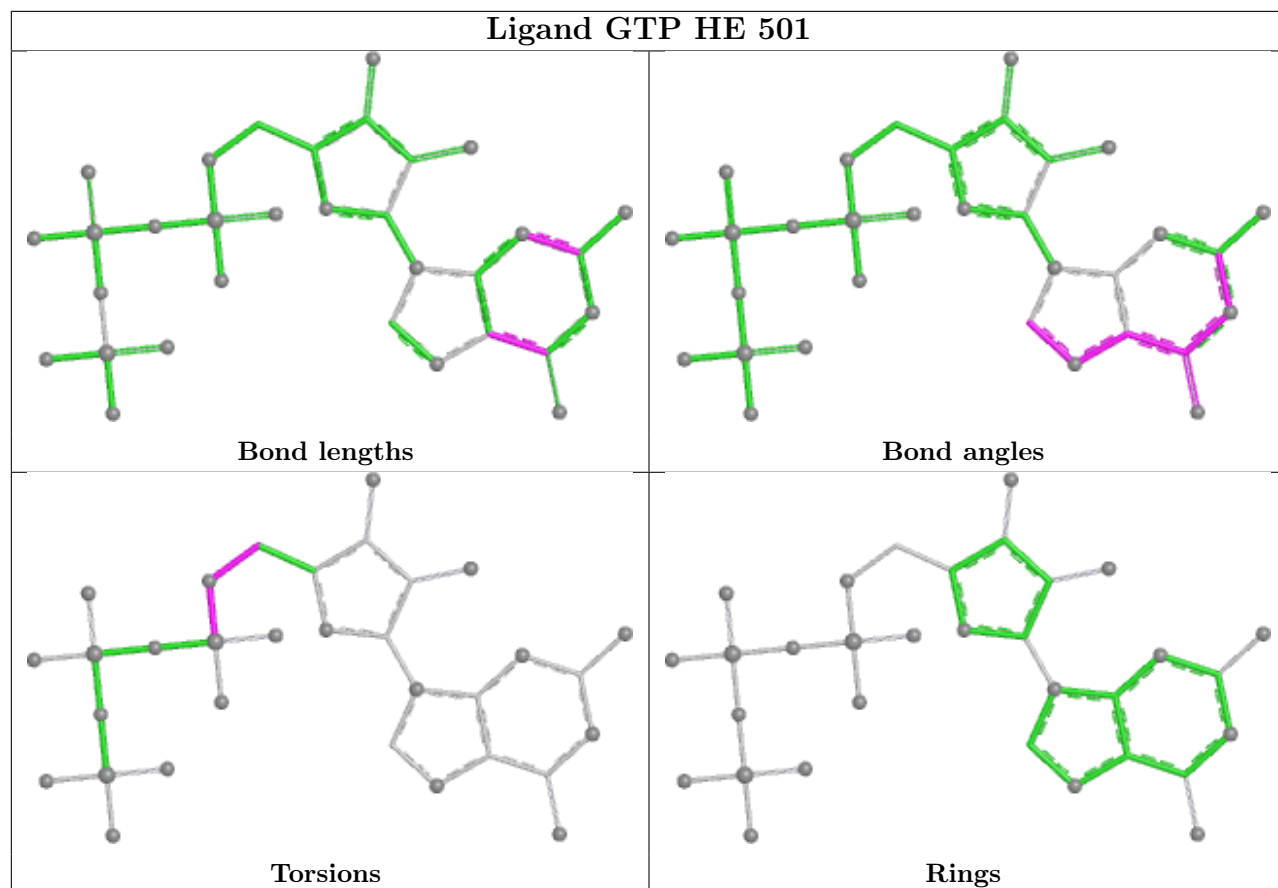
Ligand GTP BK 501



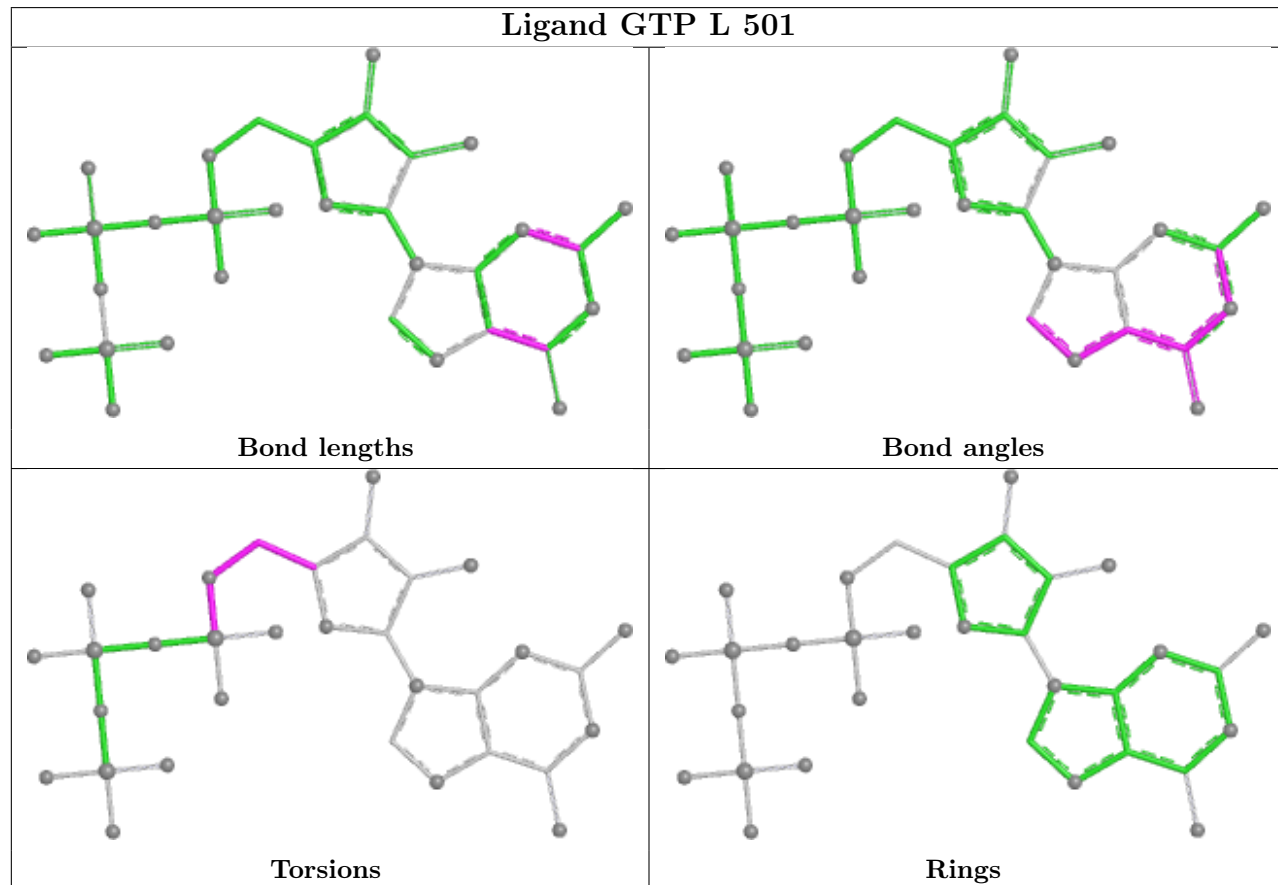
Ligand GTP SE 501

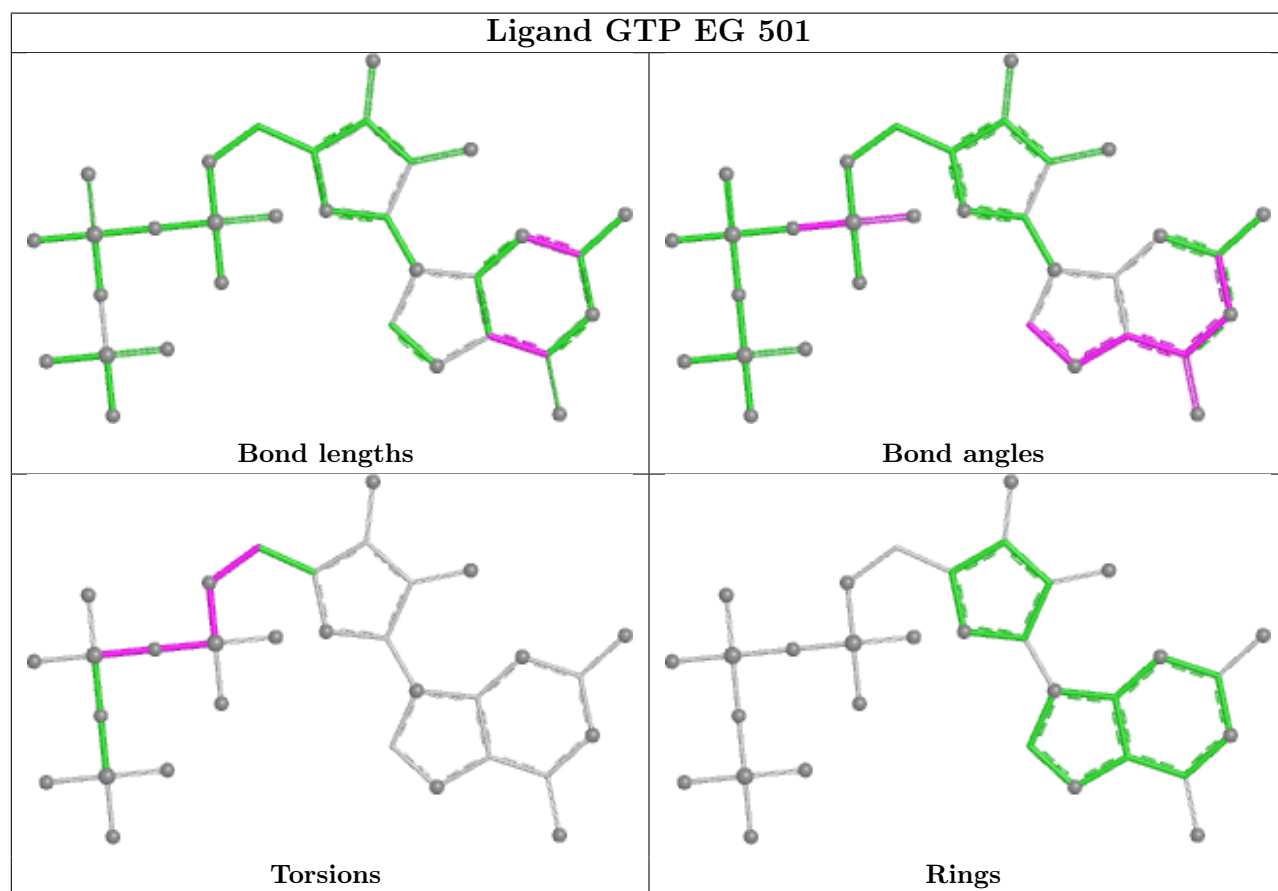
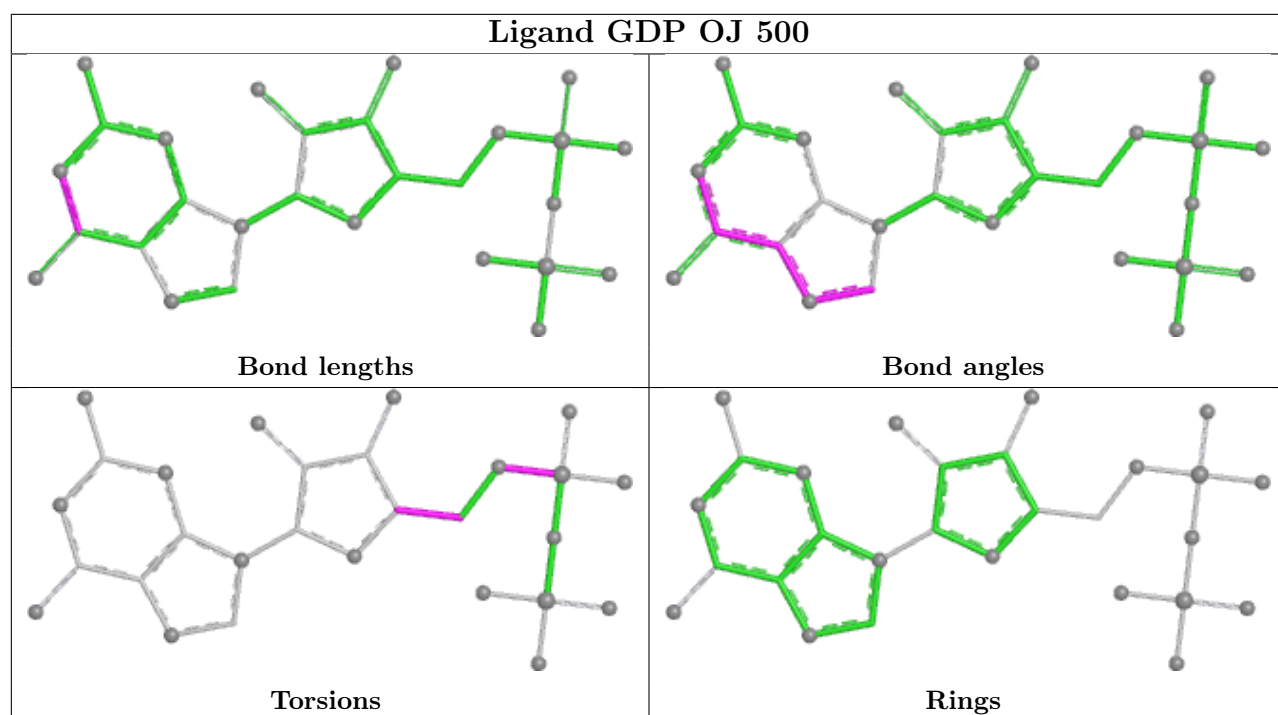


Ligand GTP HE 501

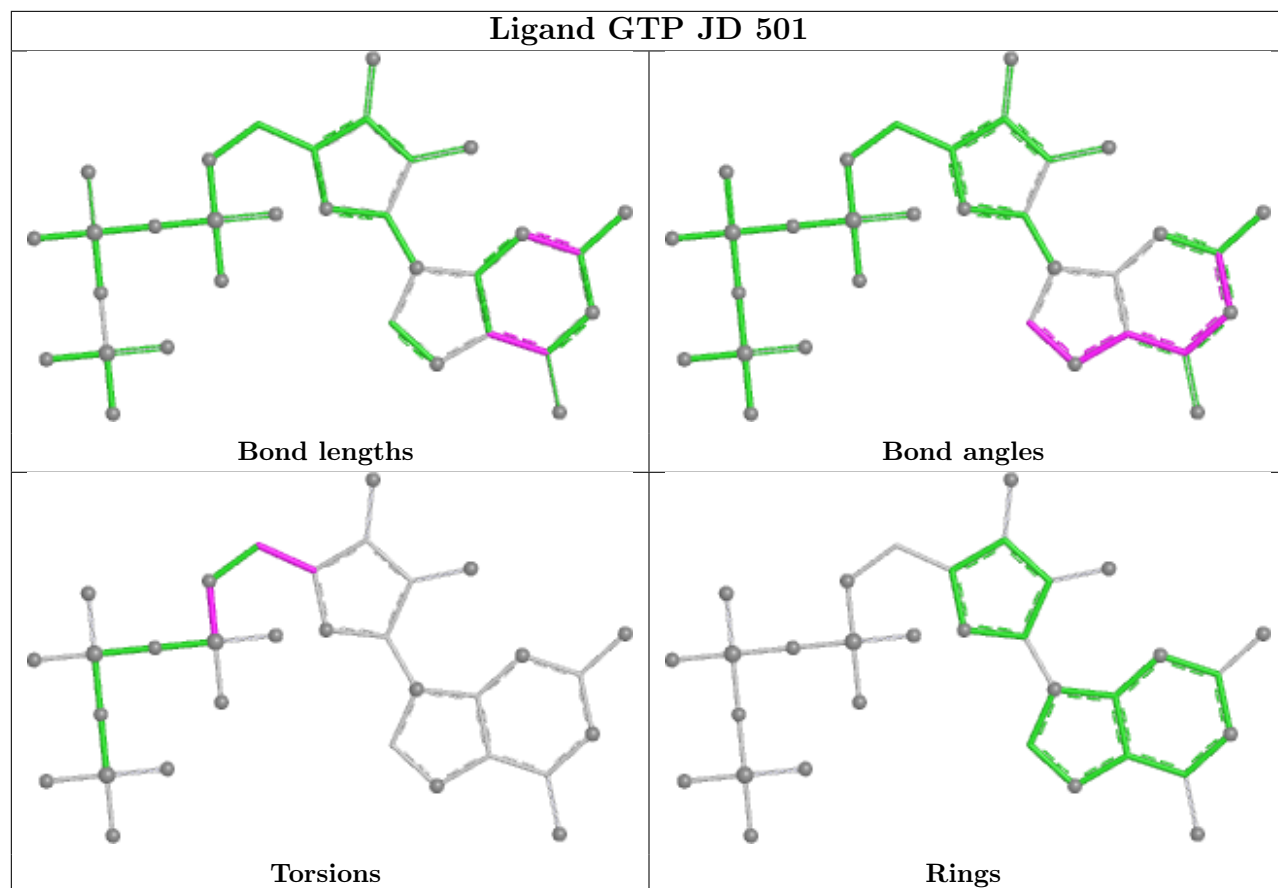


Ligand GTP L 501

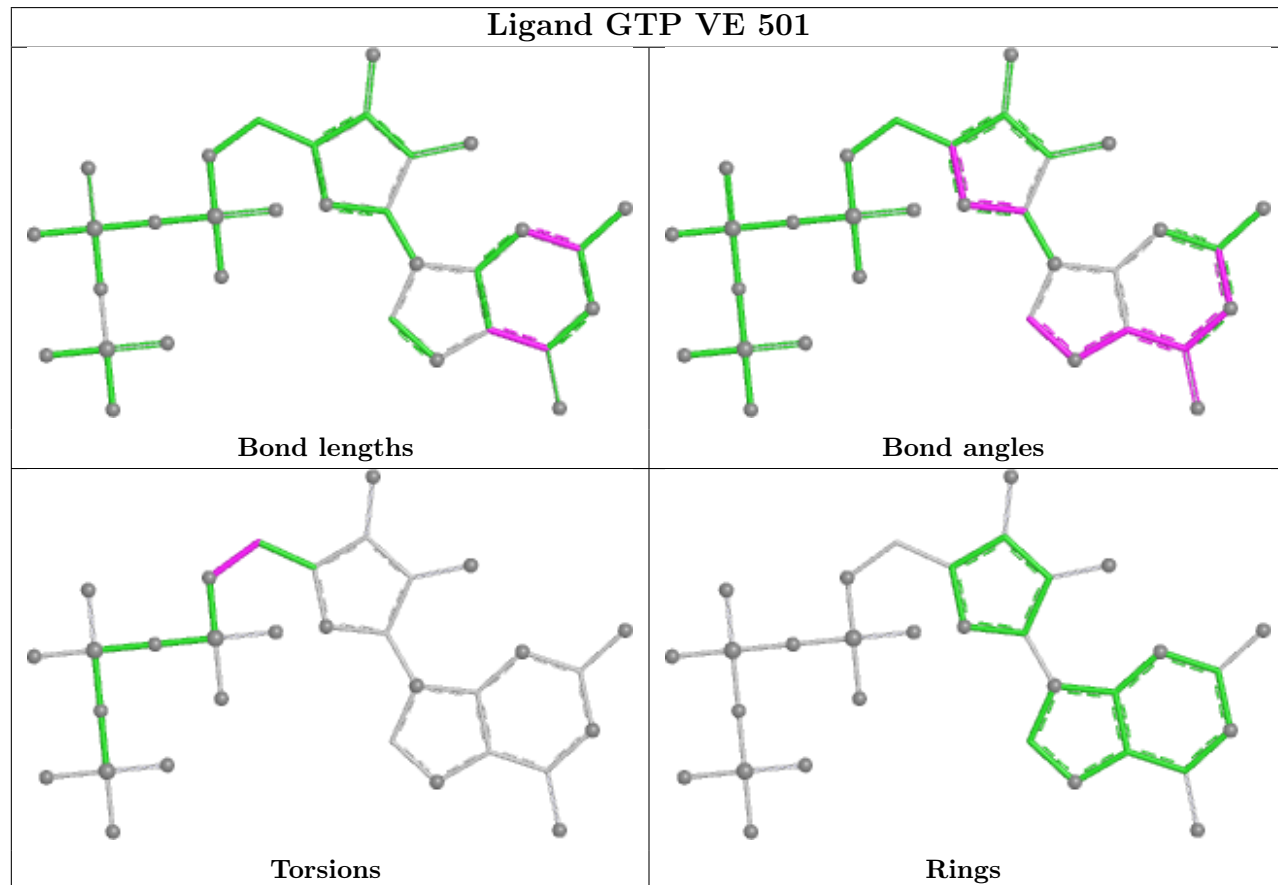




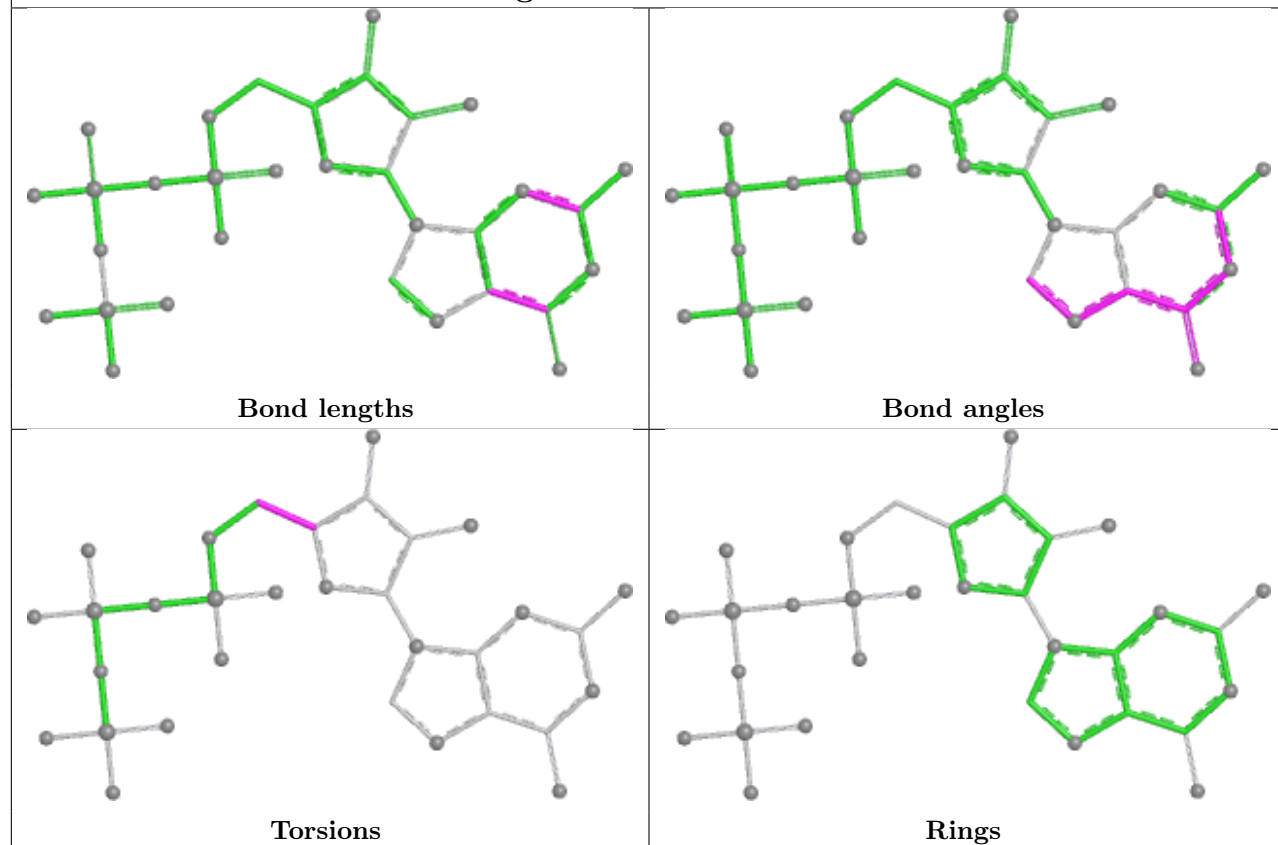
Ligand GTP JD 501



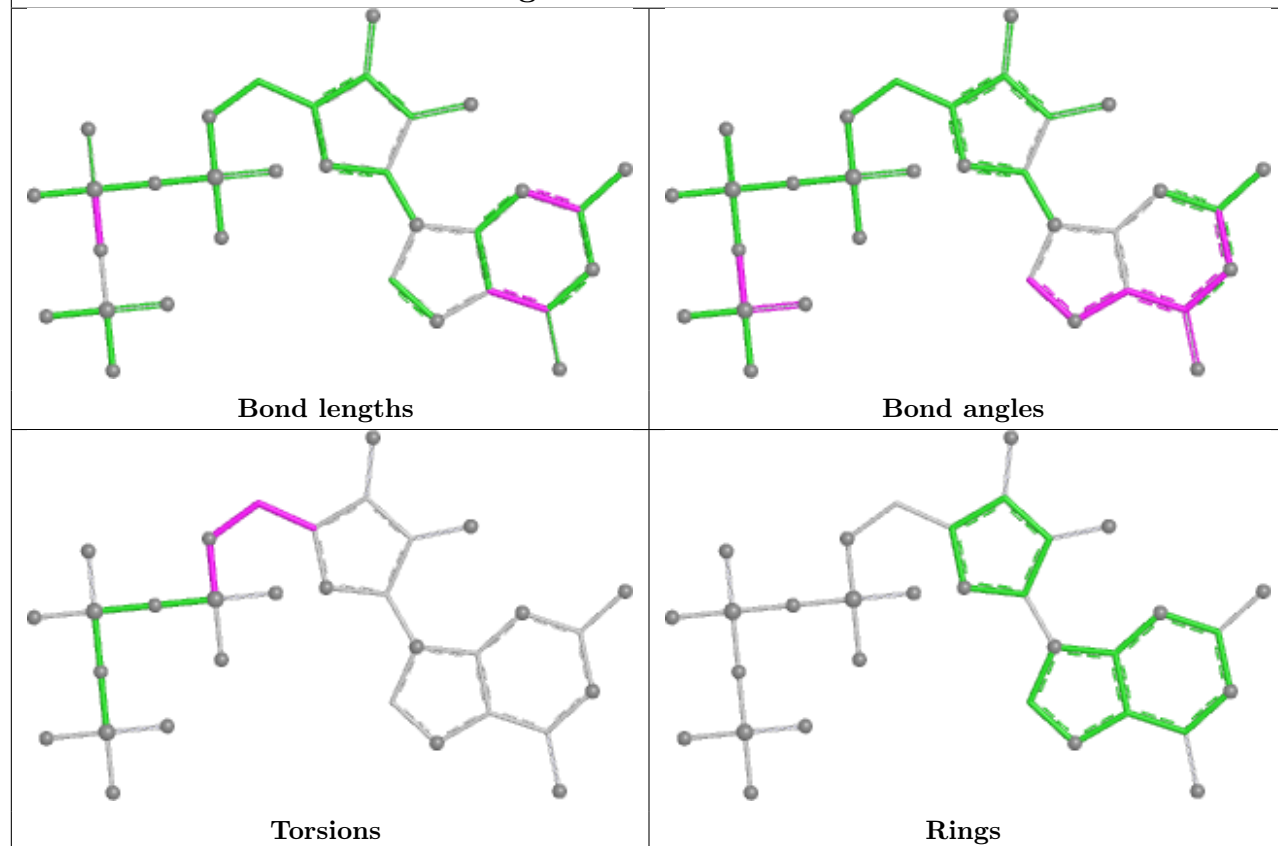
Ligand GTP VE 501

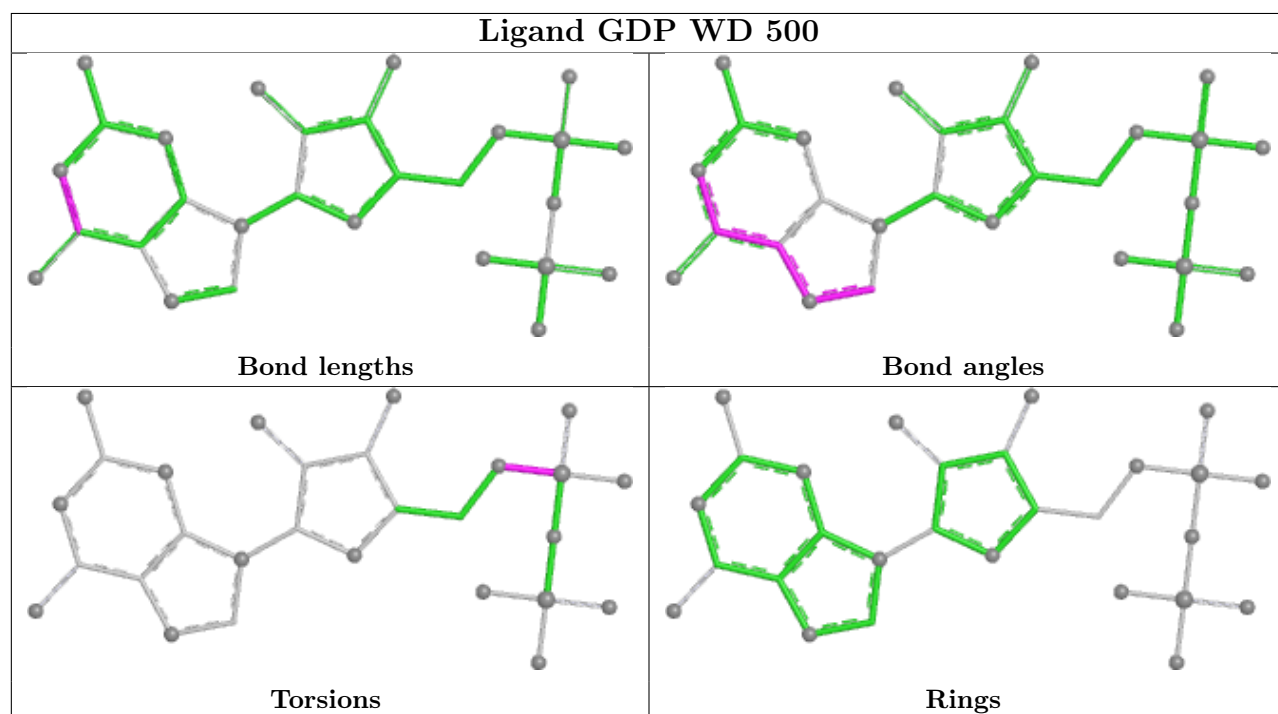
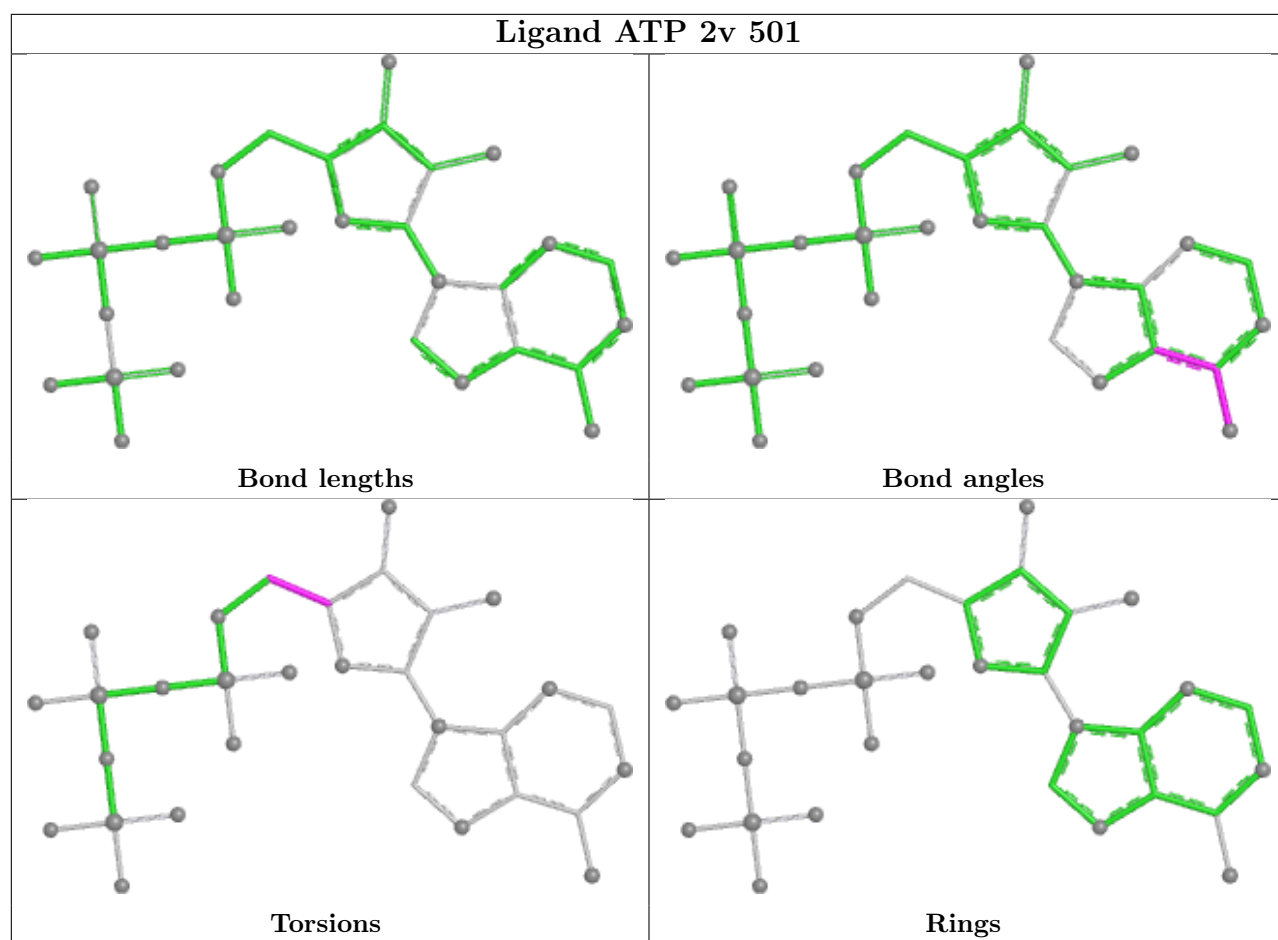


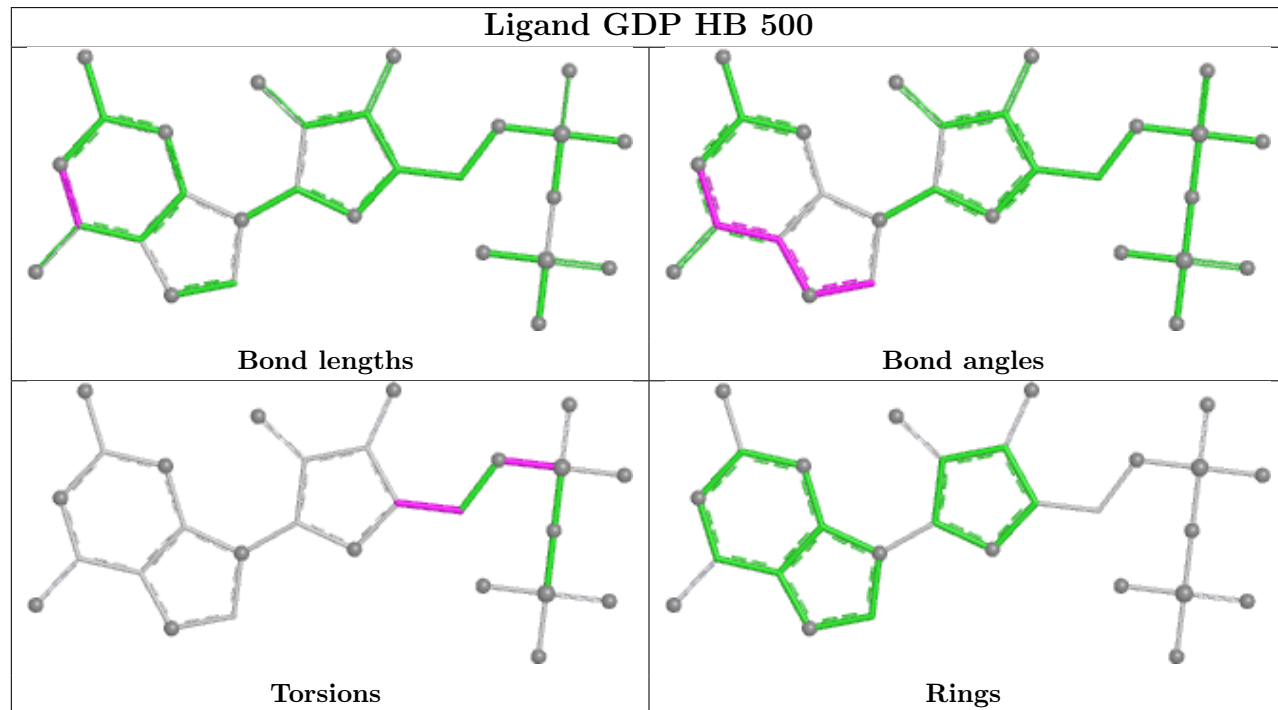
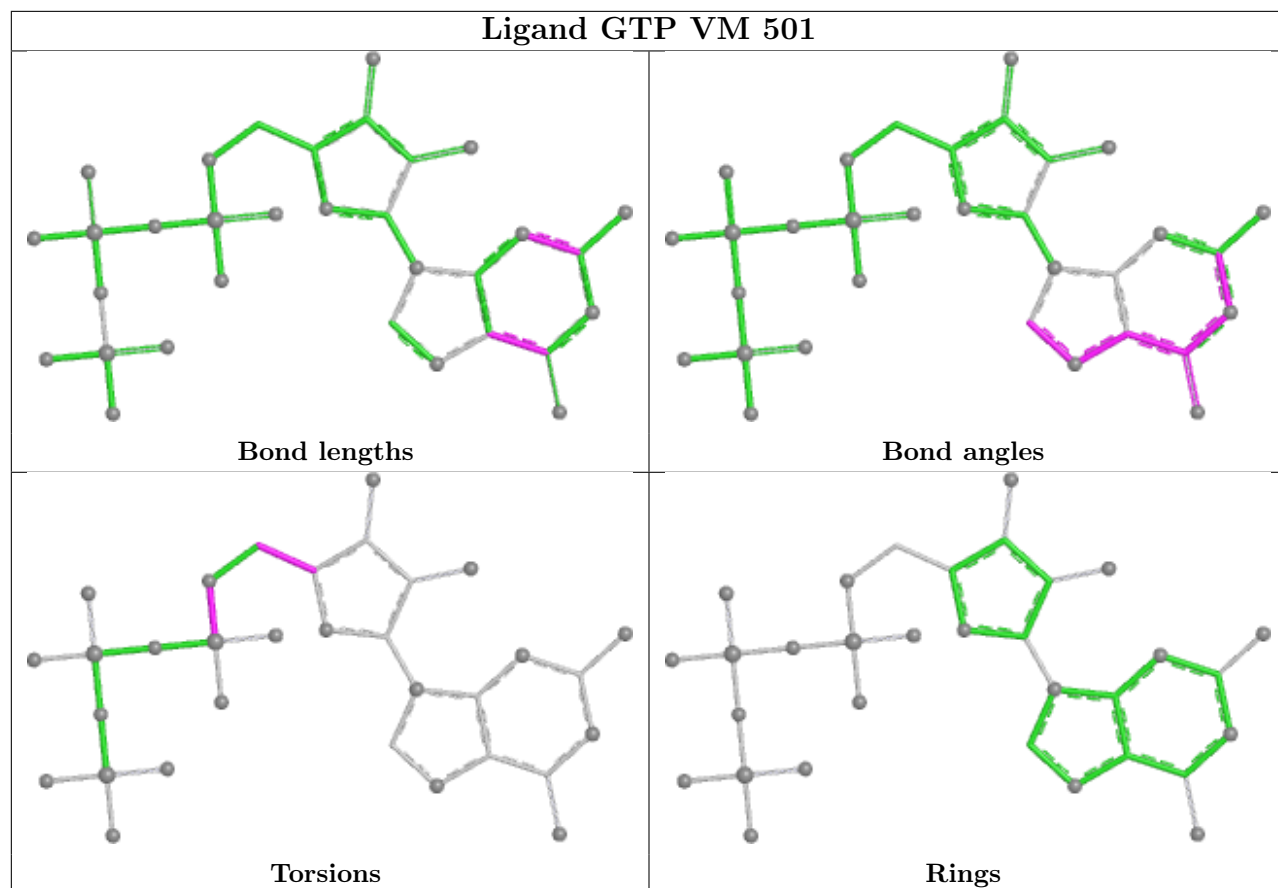
Ligand GTP DH 501

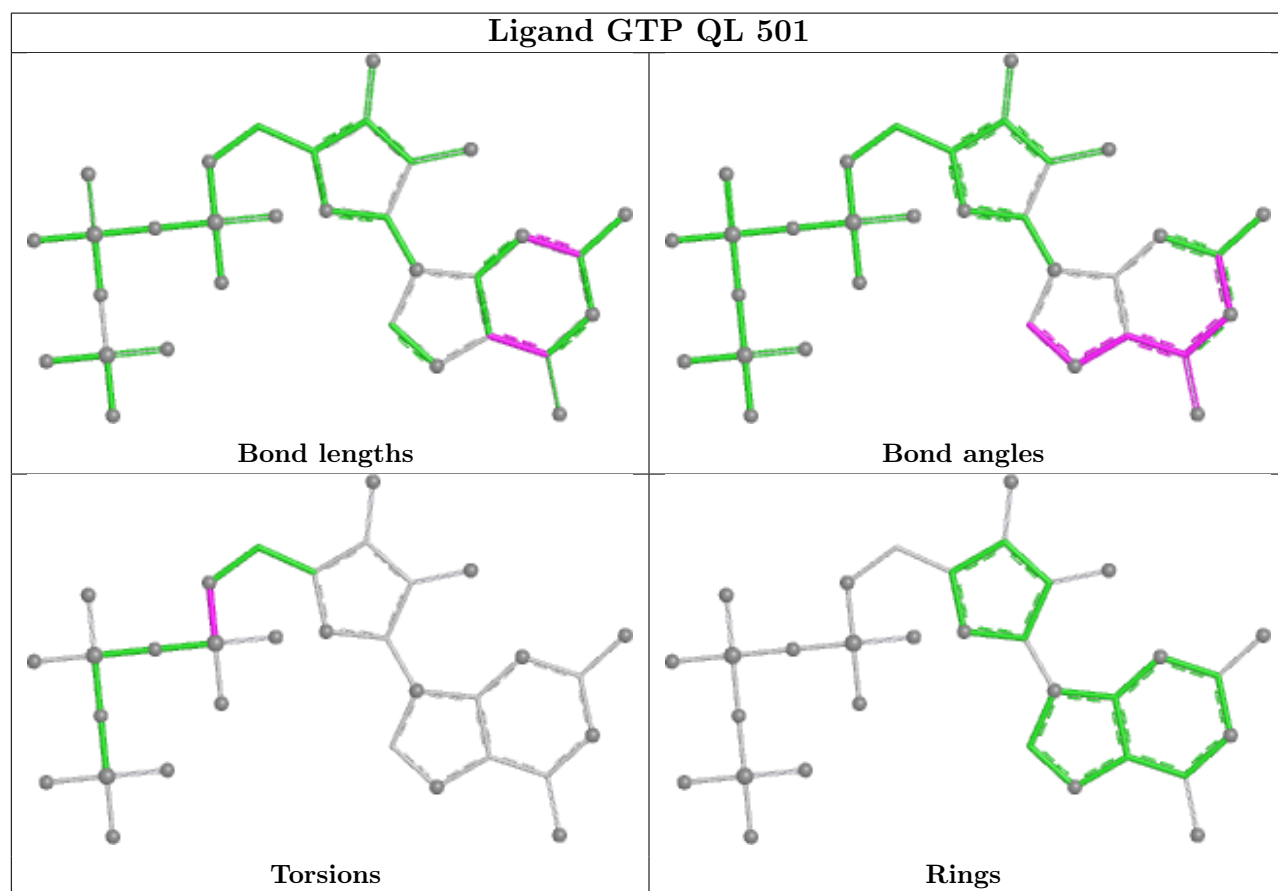
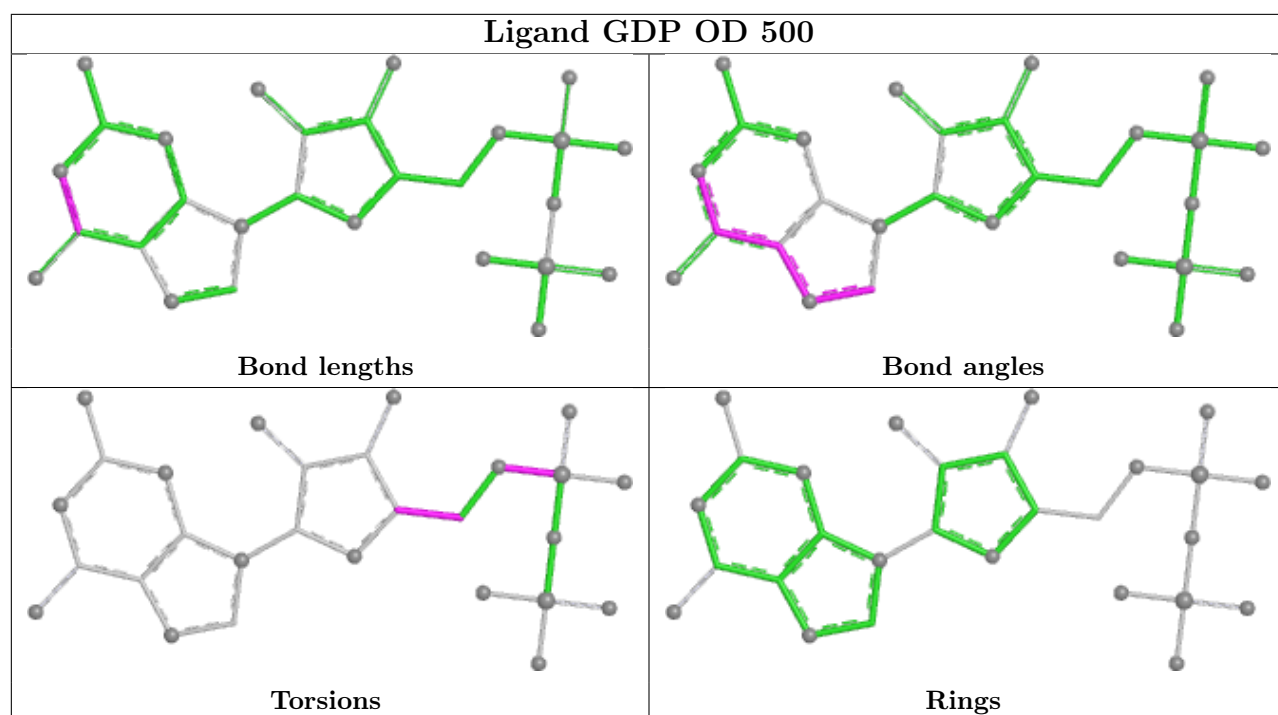


Ligand GTP DF 501

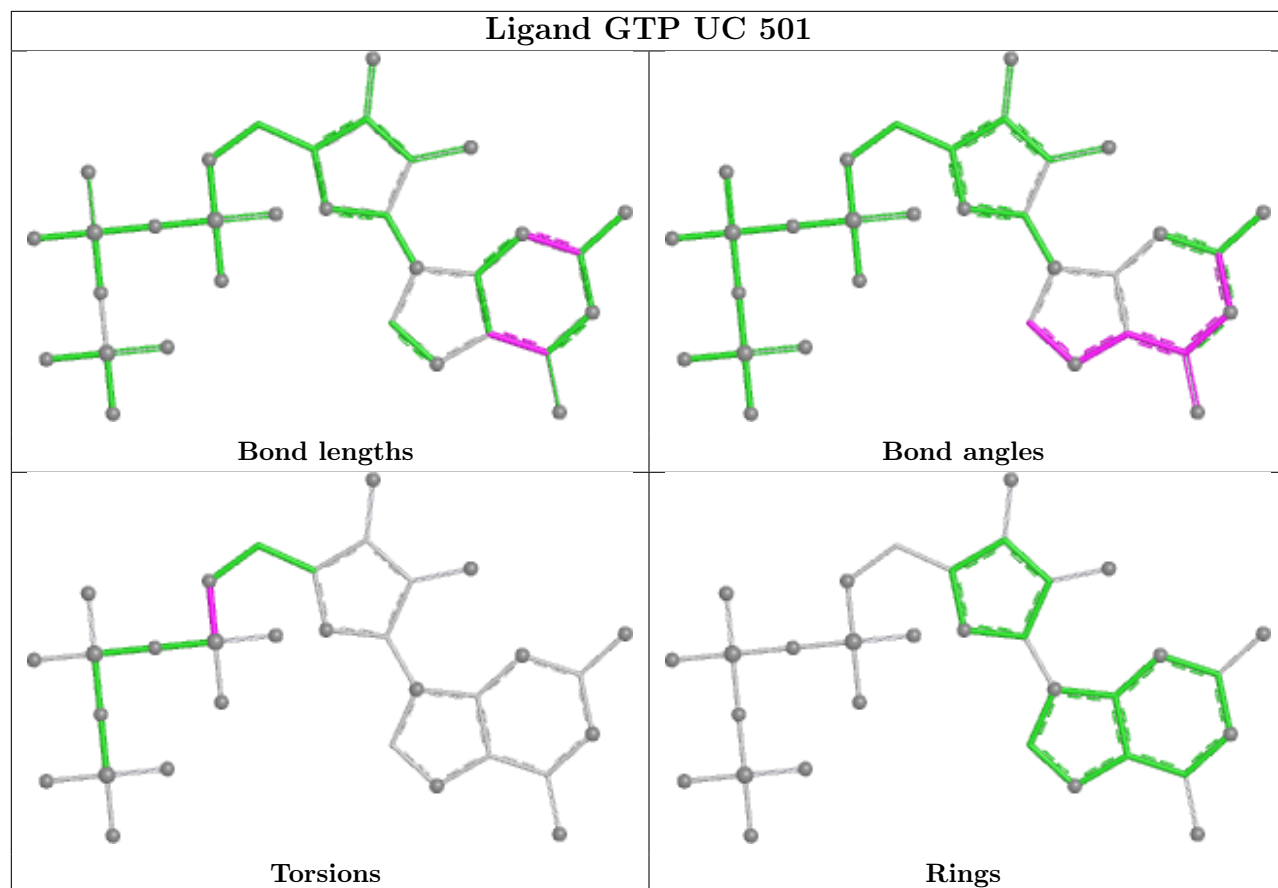




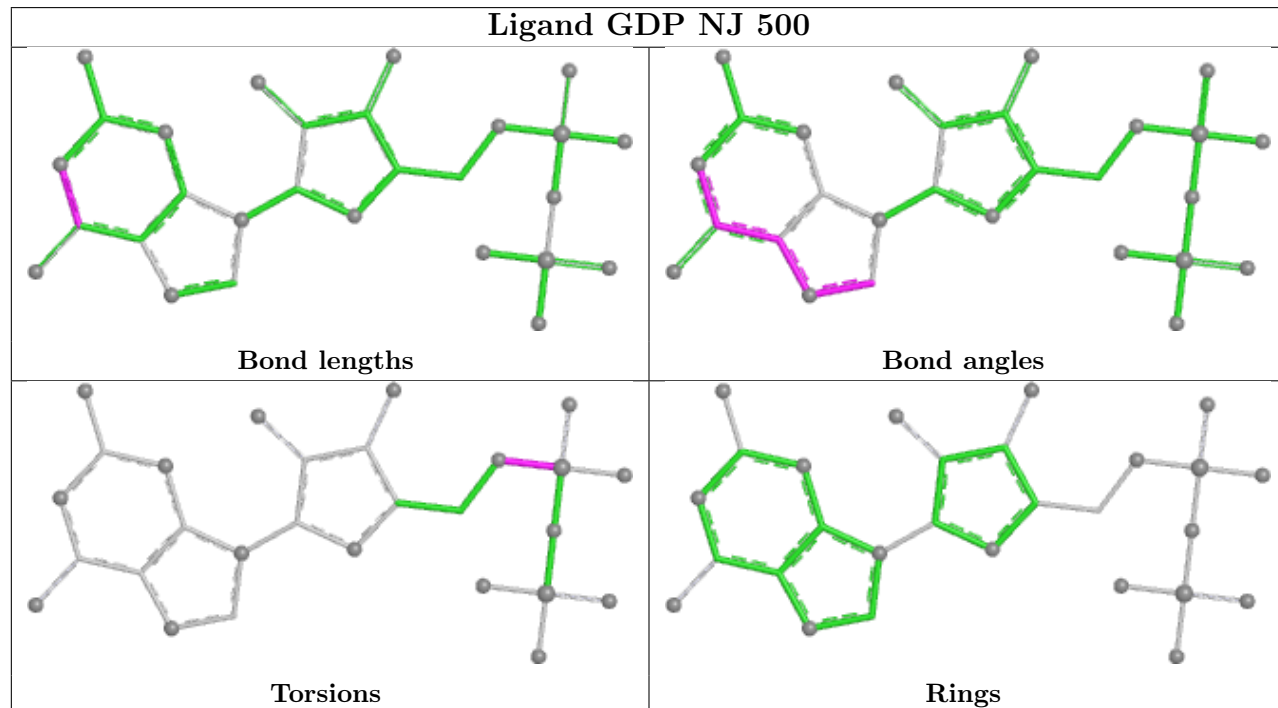




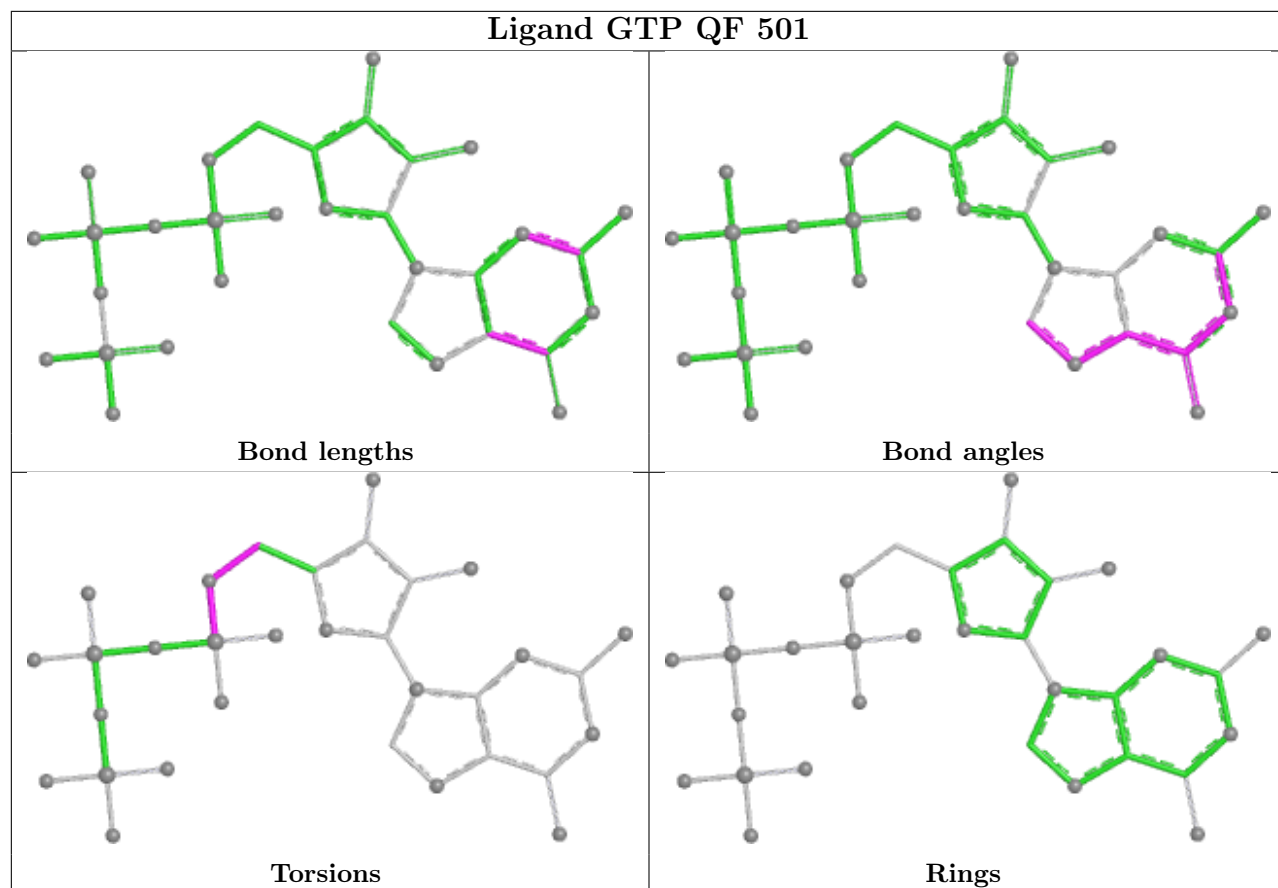
Ligand GTP UC 501



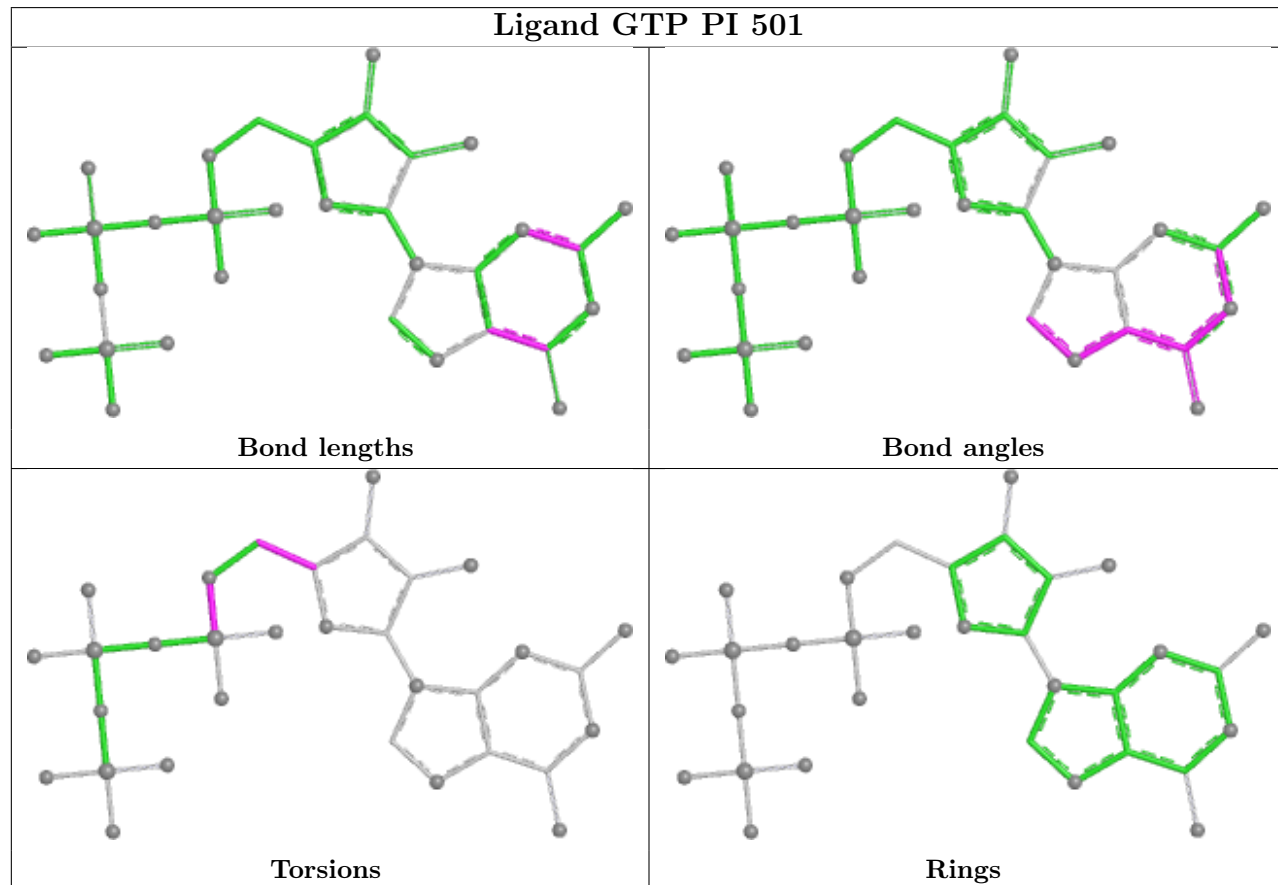
Ligand GDP NJ 500

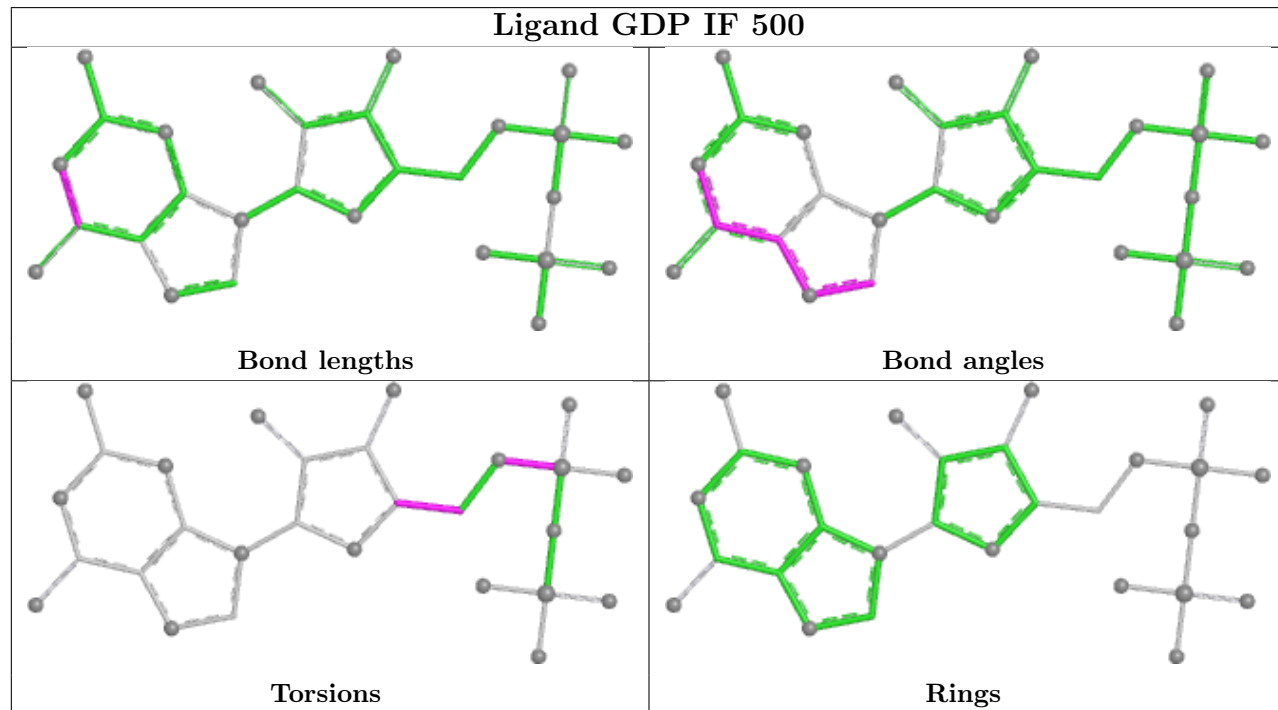
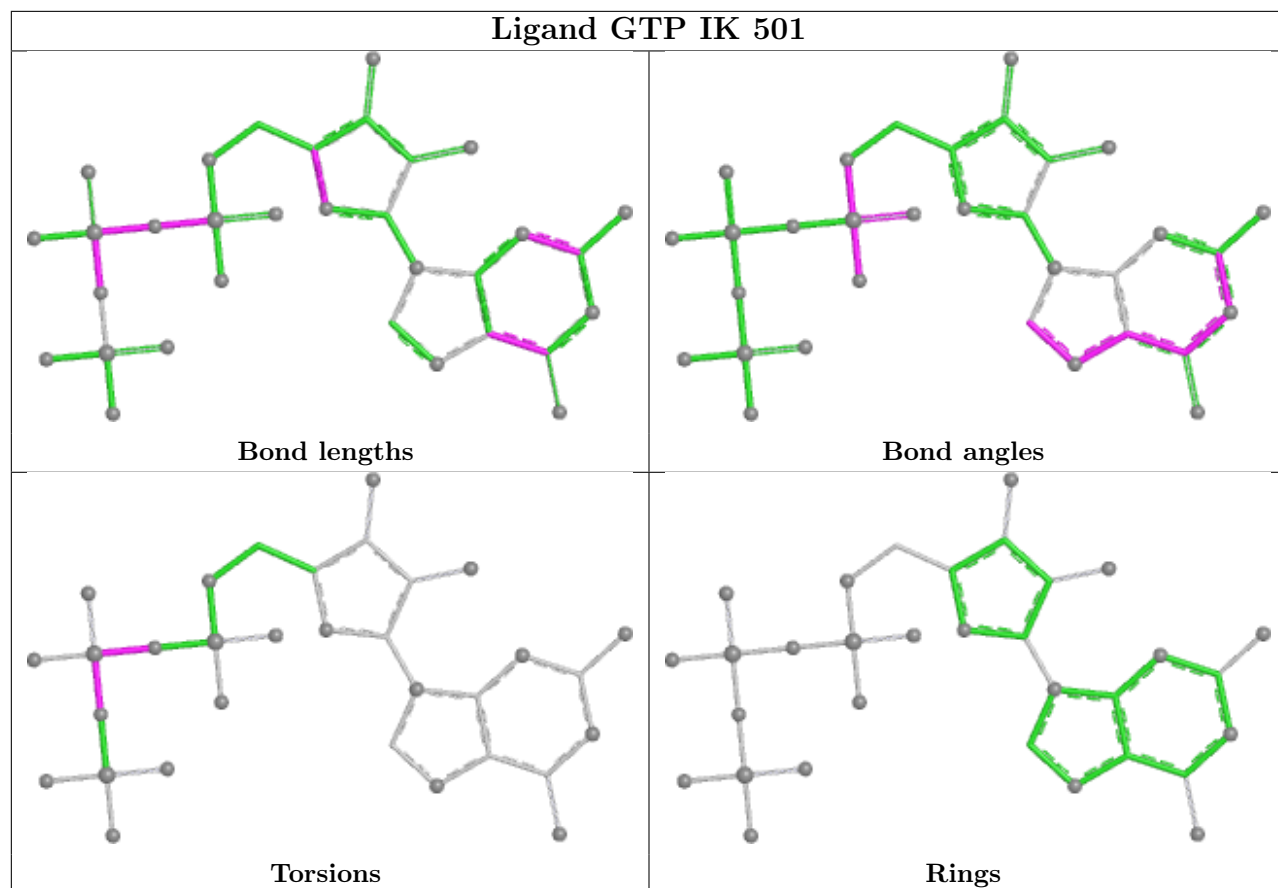


Ligand GTP QF 501

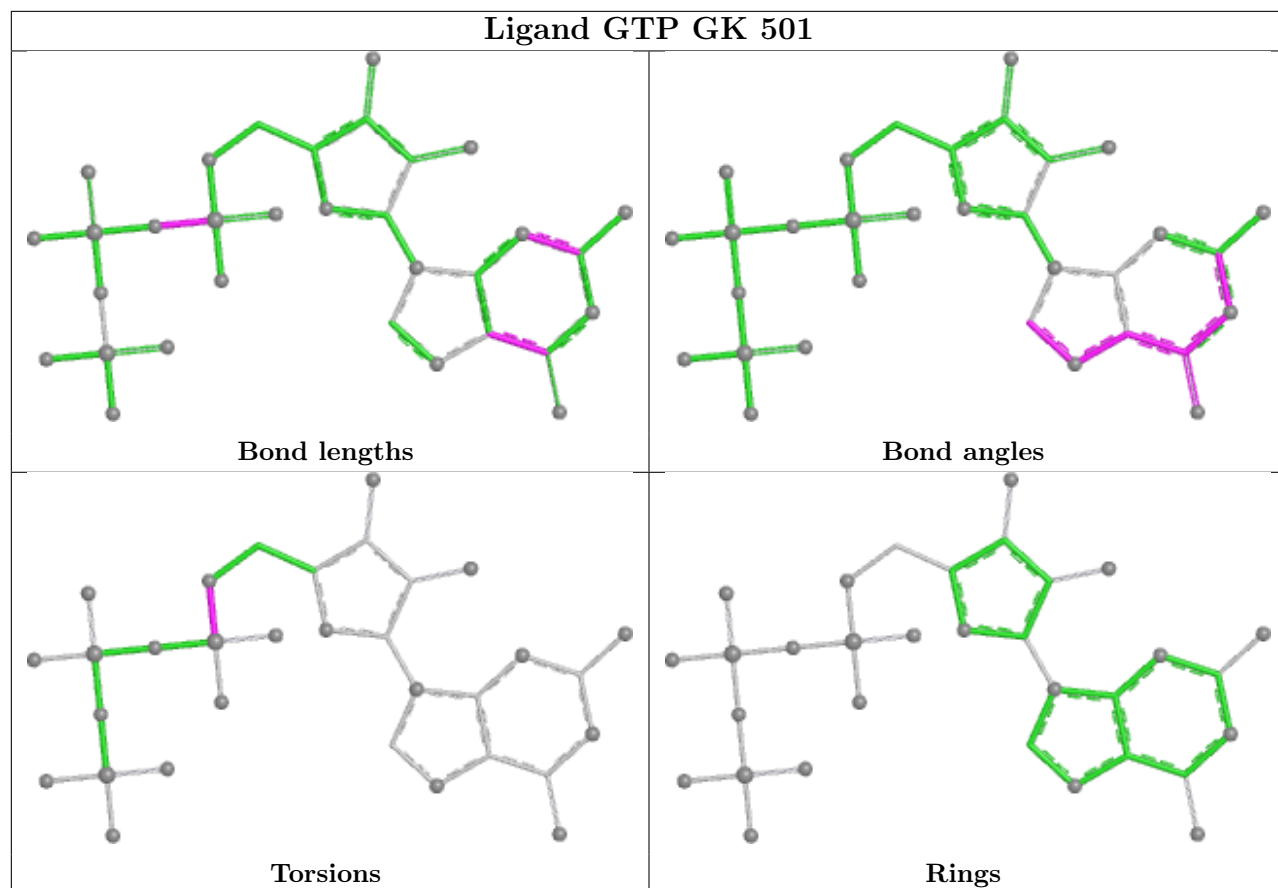


Ligand GTP PI 501

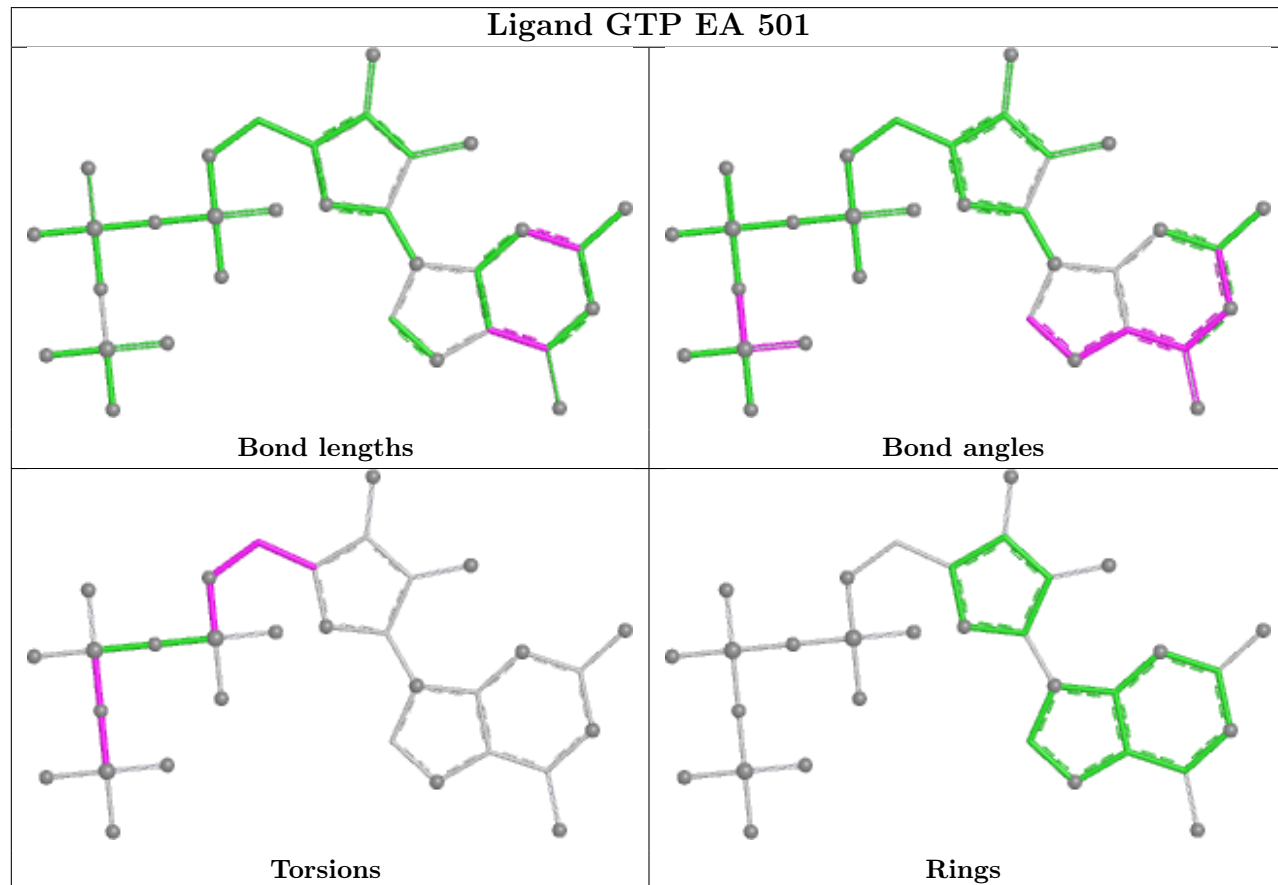


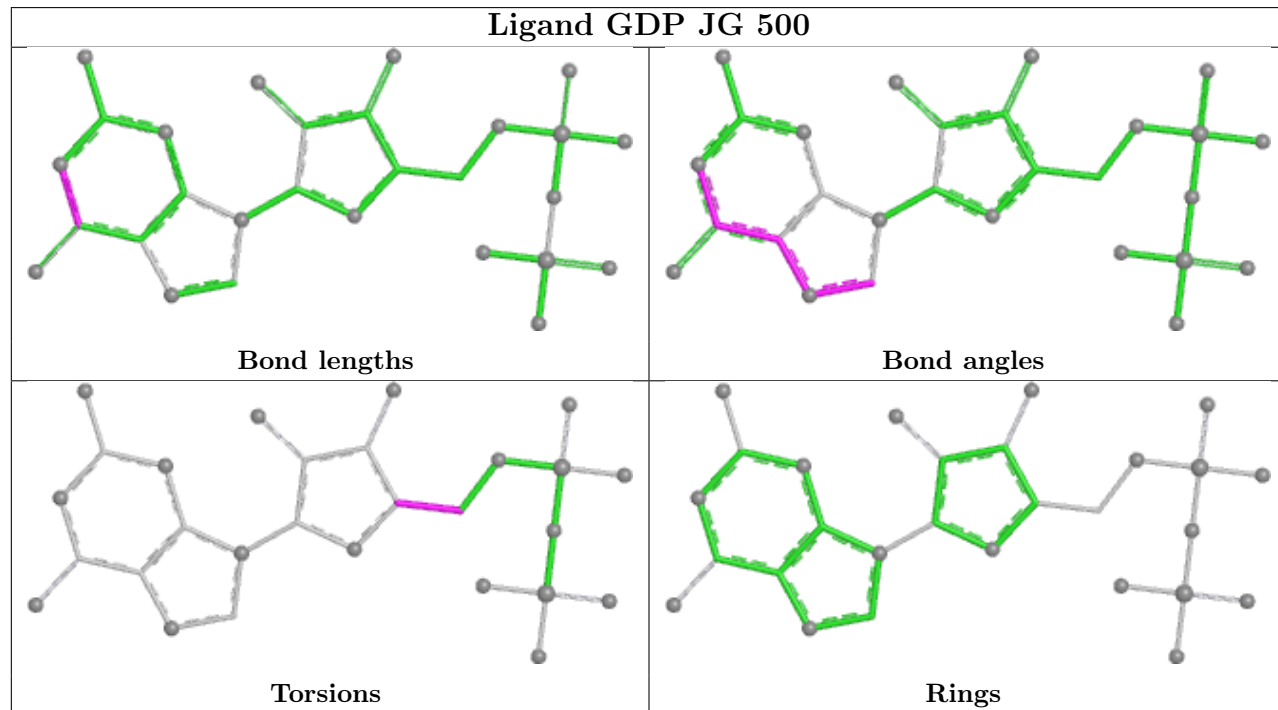
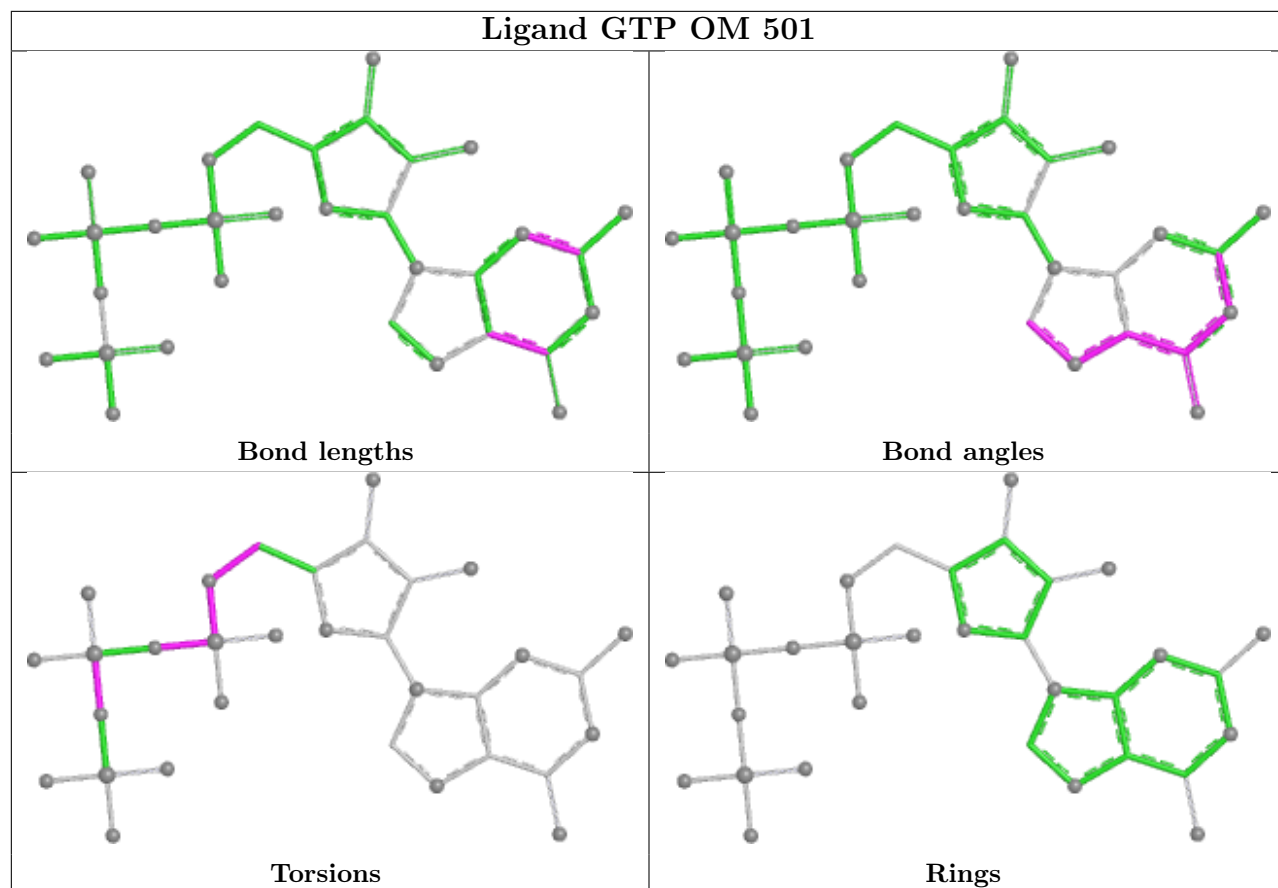


Ligand GTP GK 501

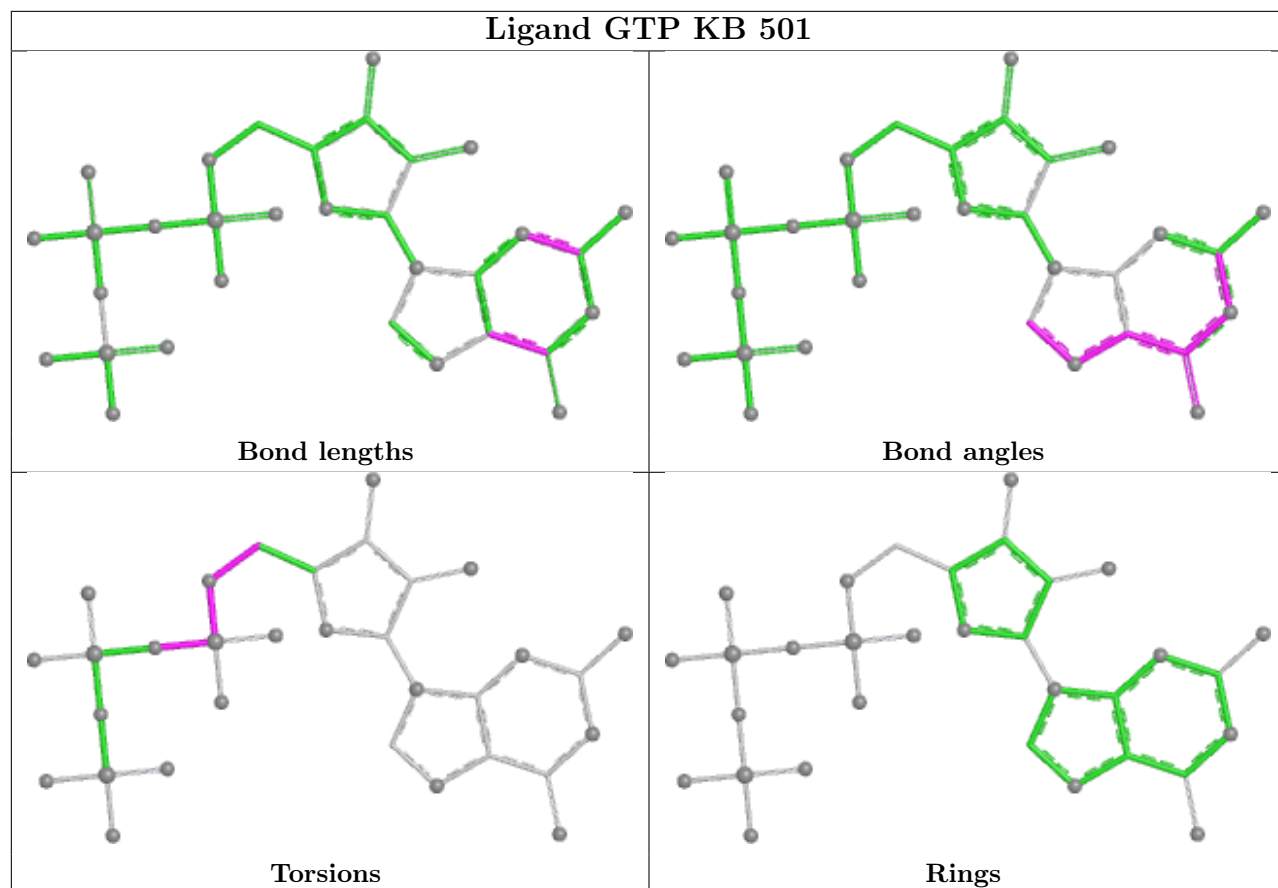


Ligand GTP EA 501

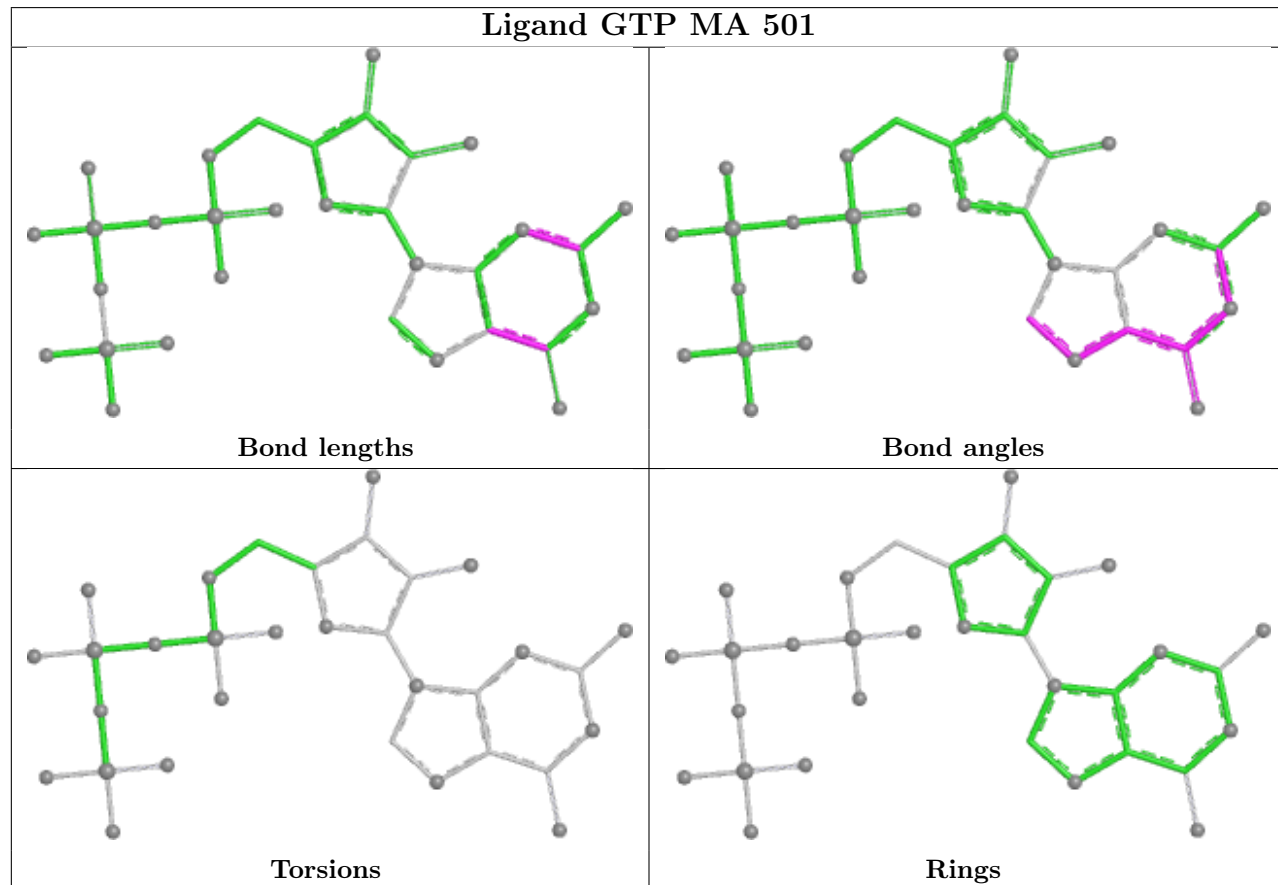


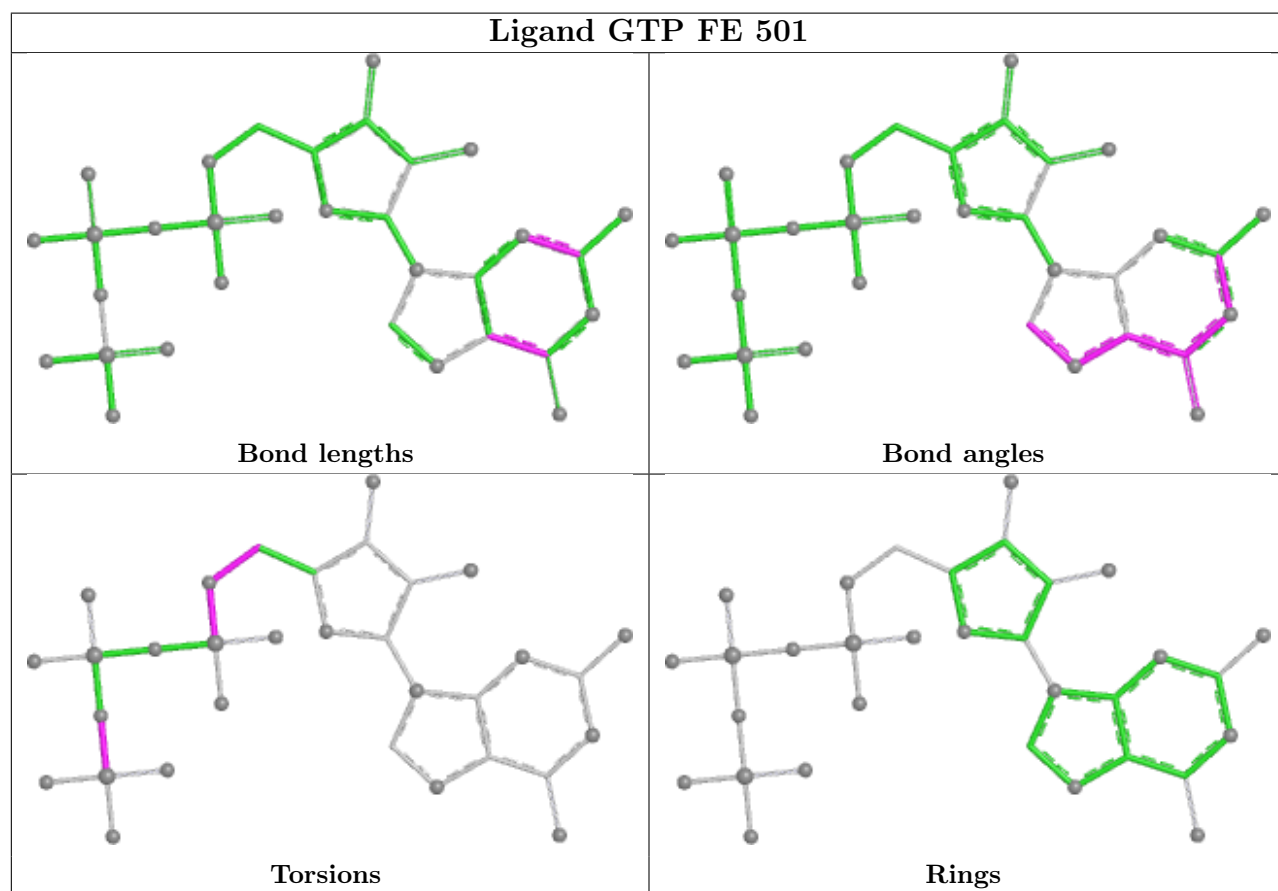
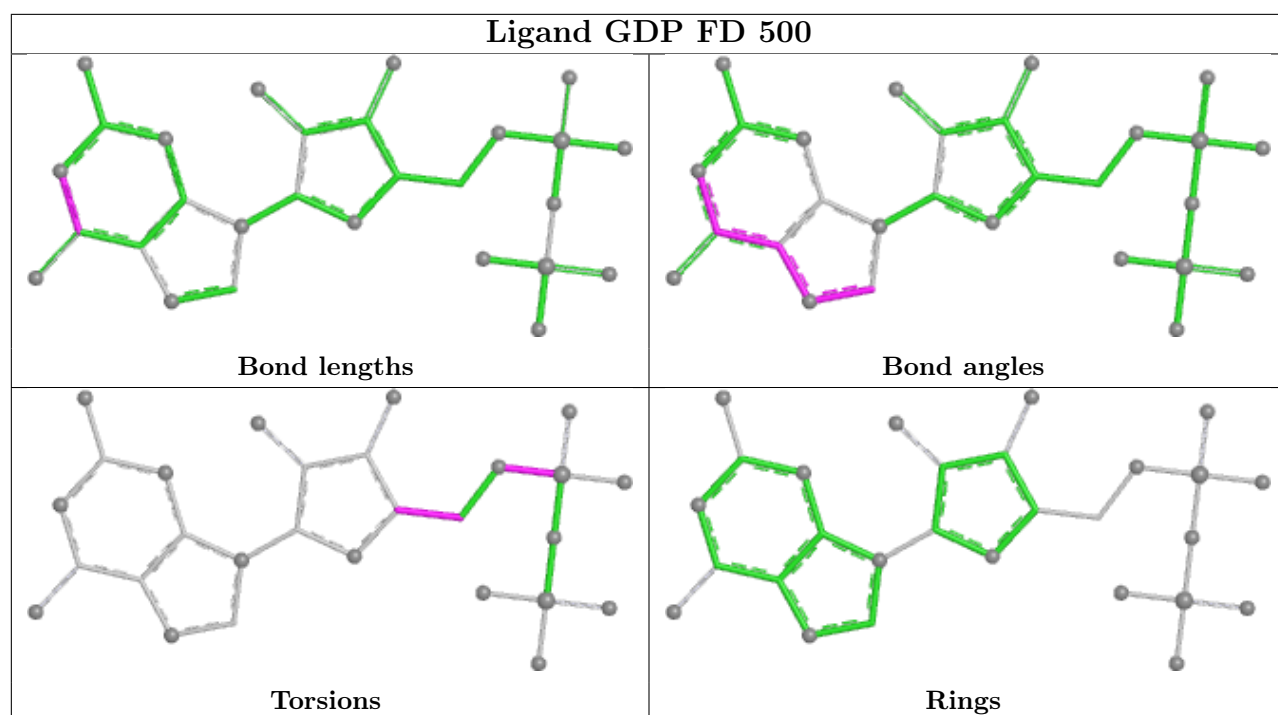


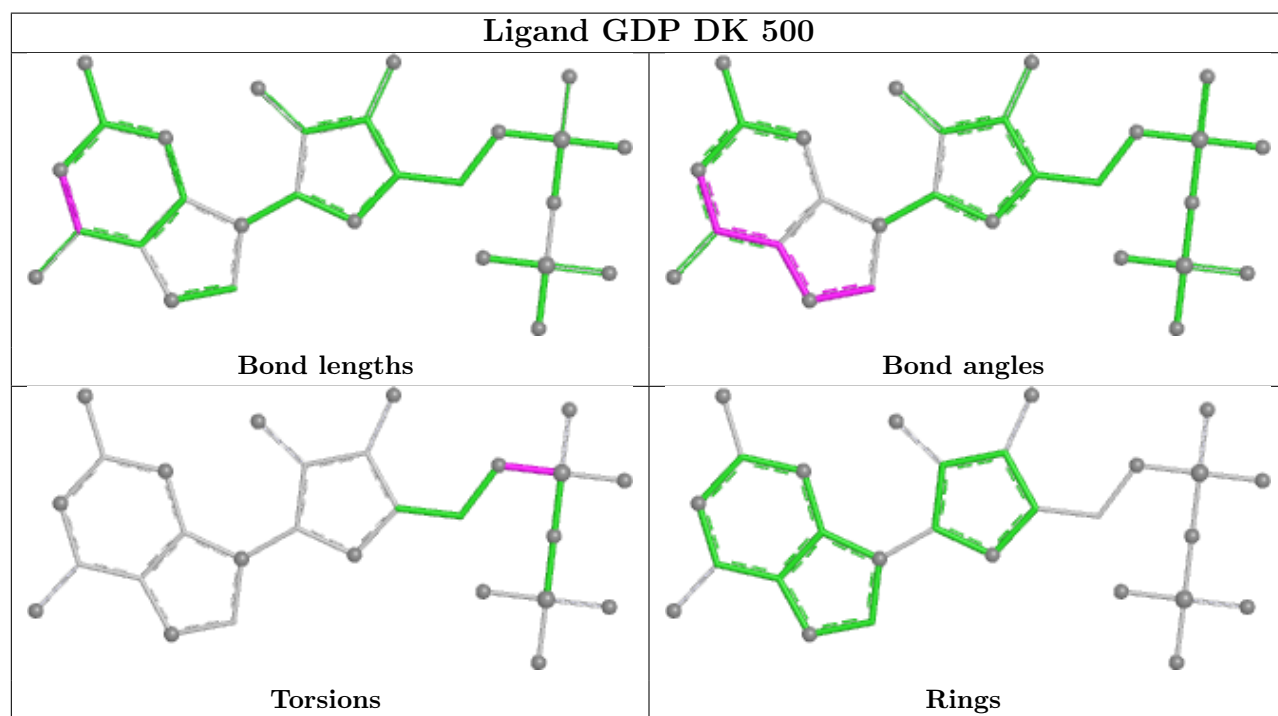
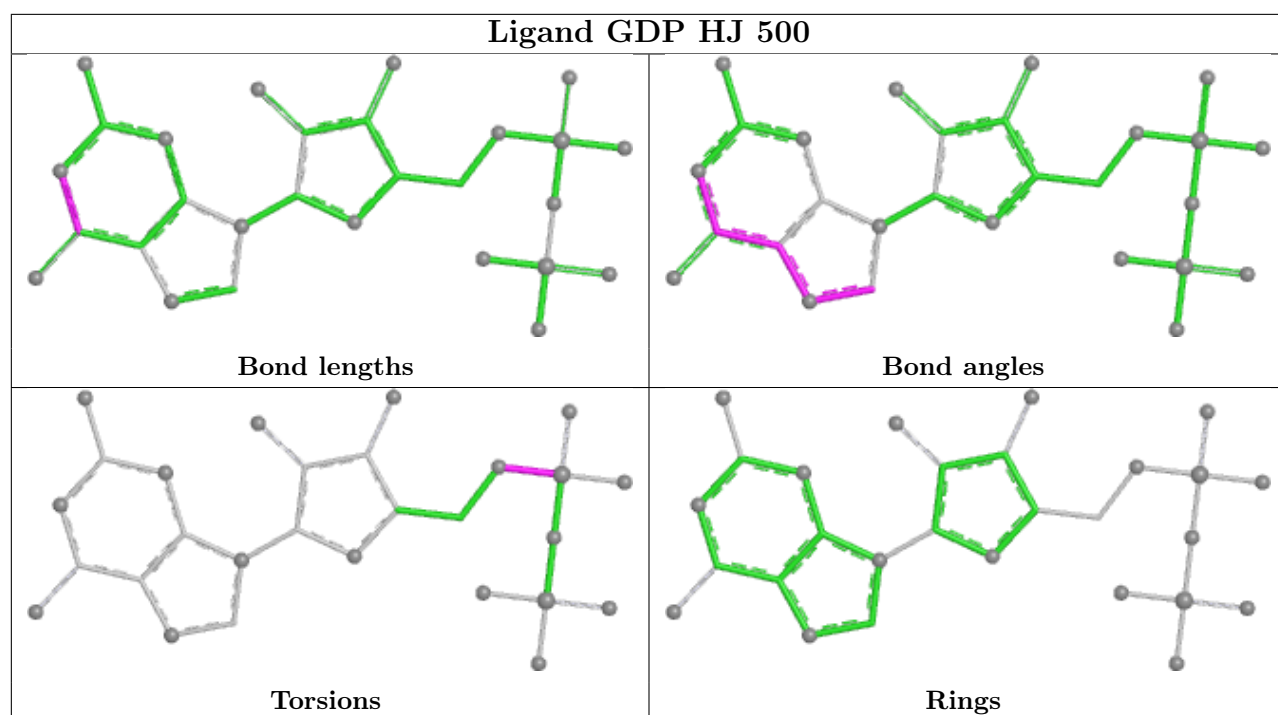
Ligand GTP KB 501

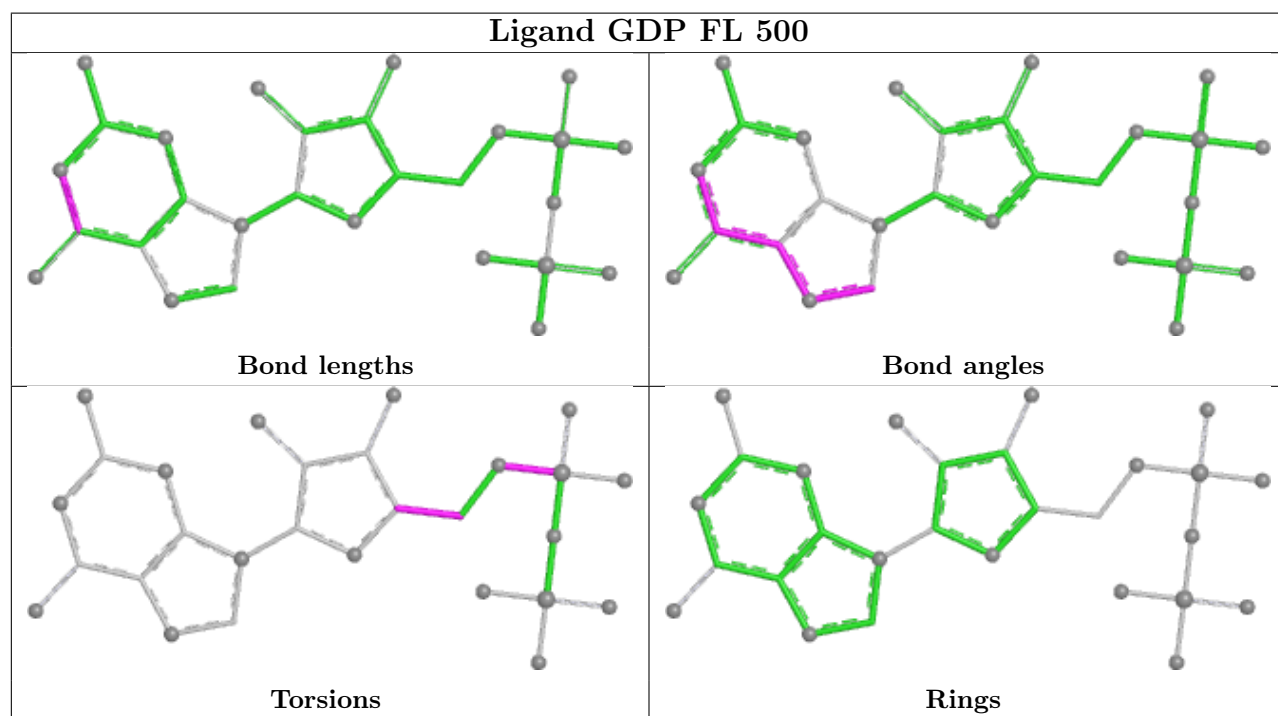
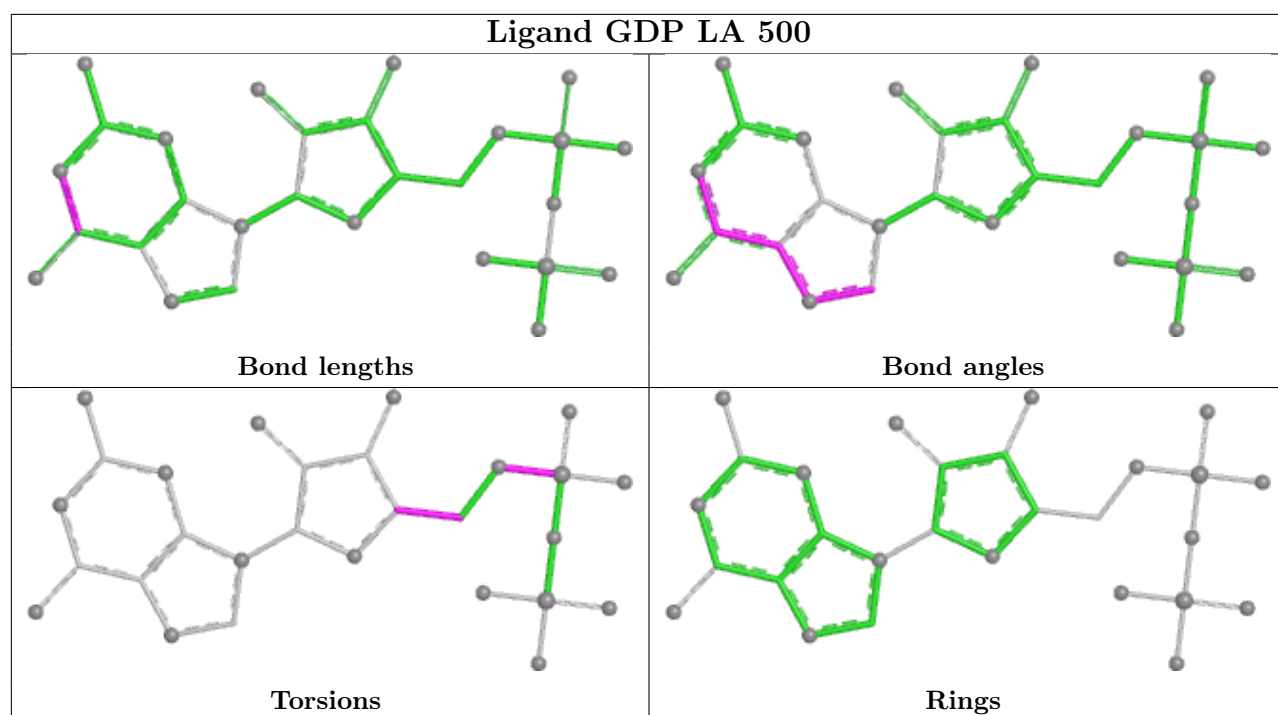


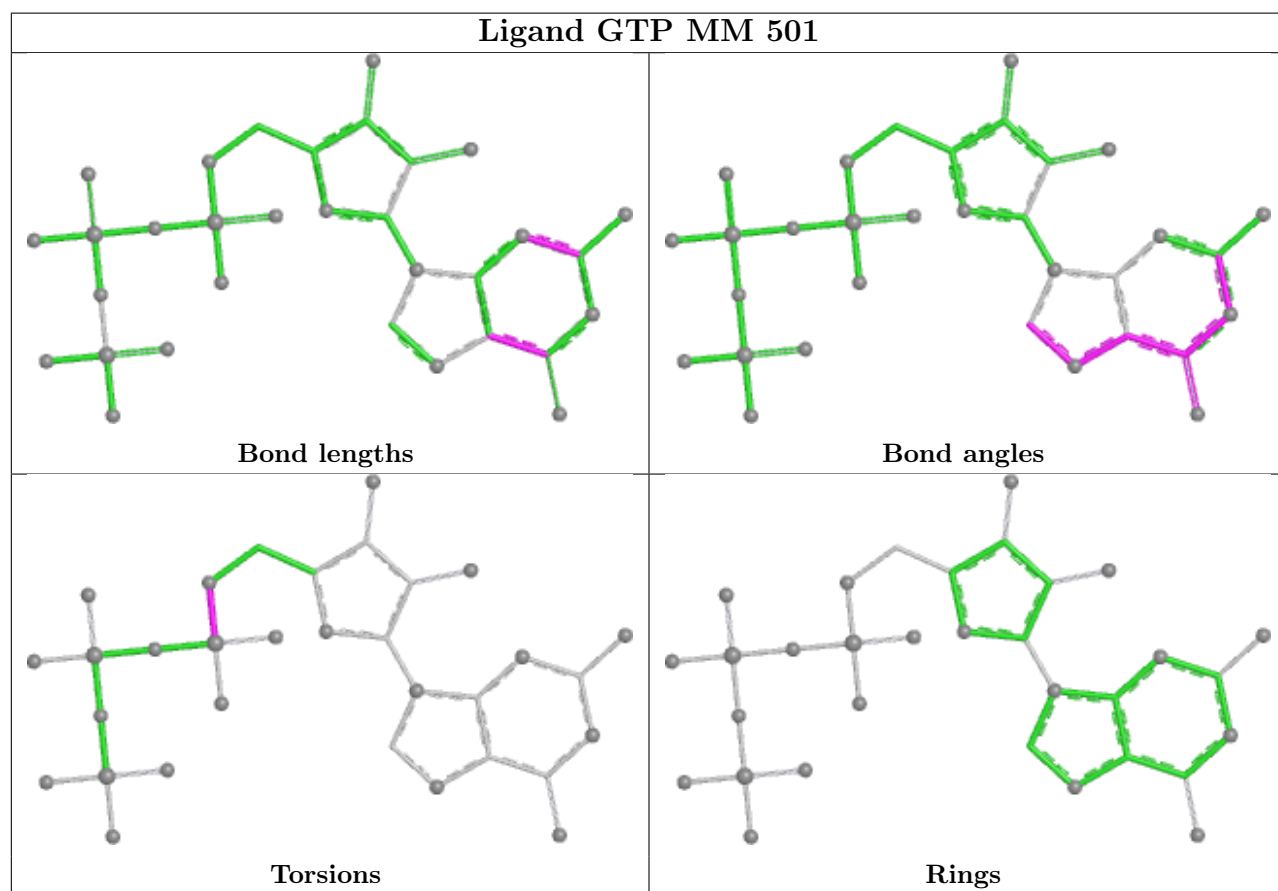
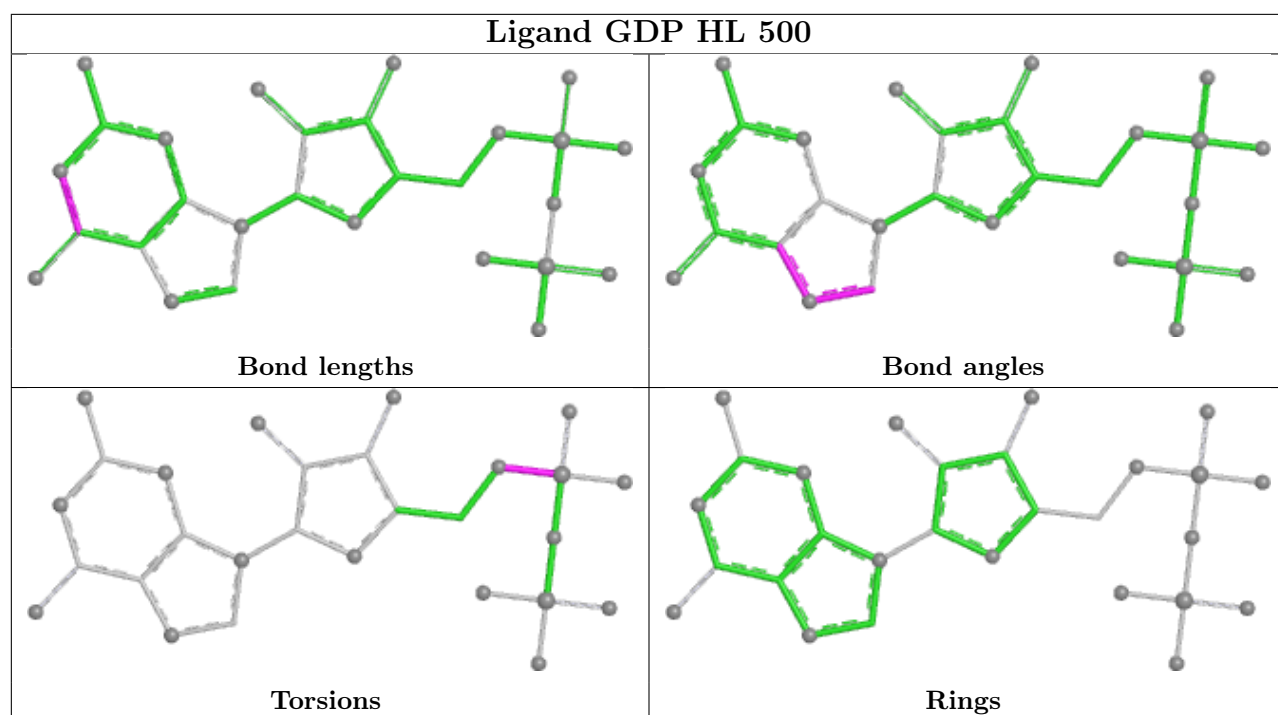
Ligand GTP MA 501



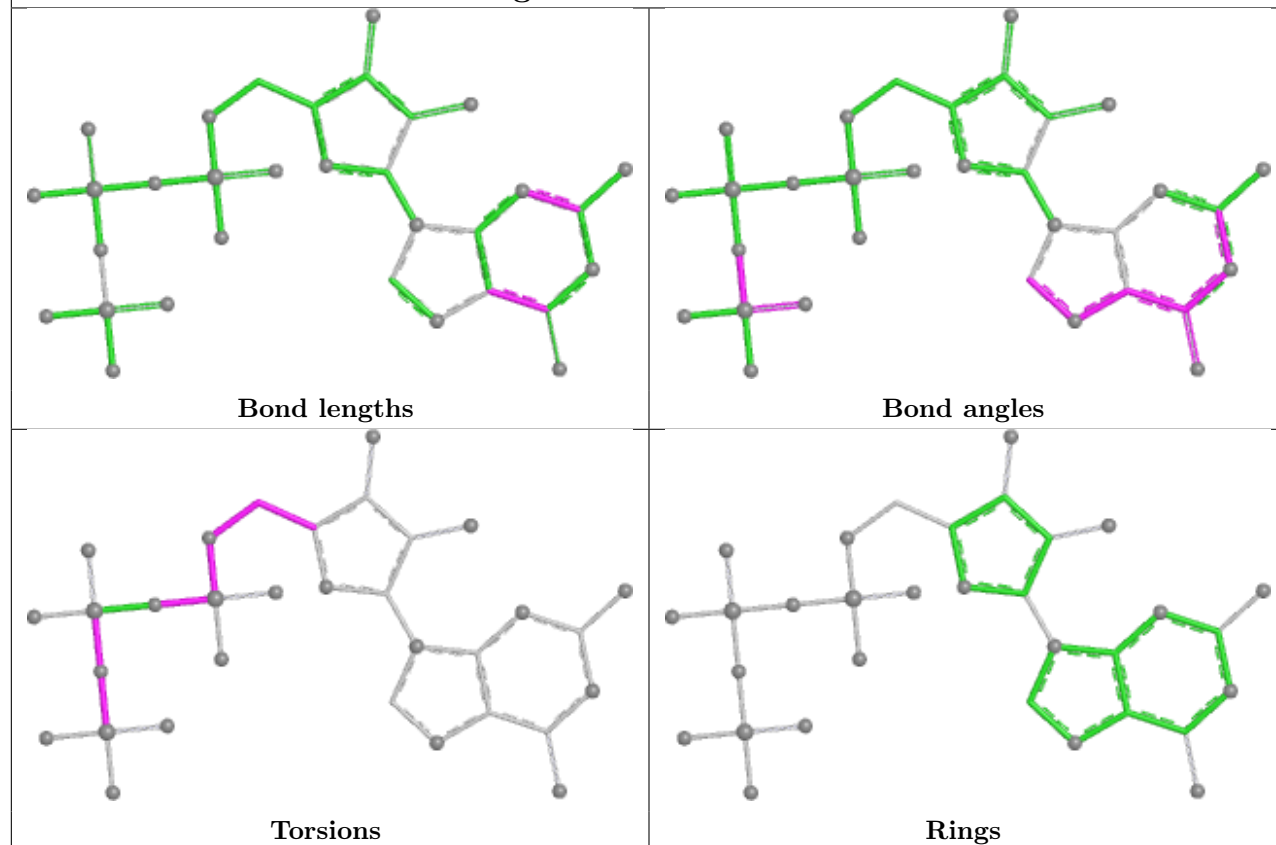




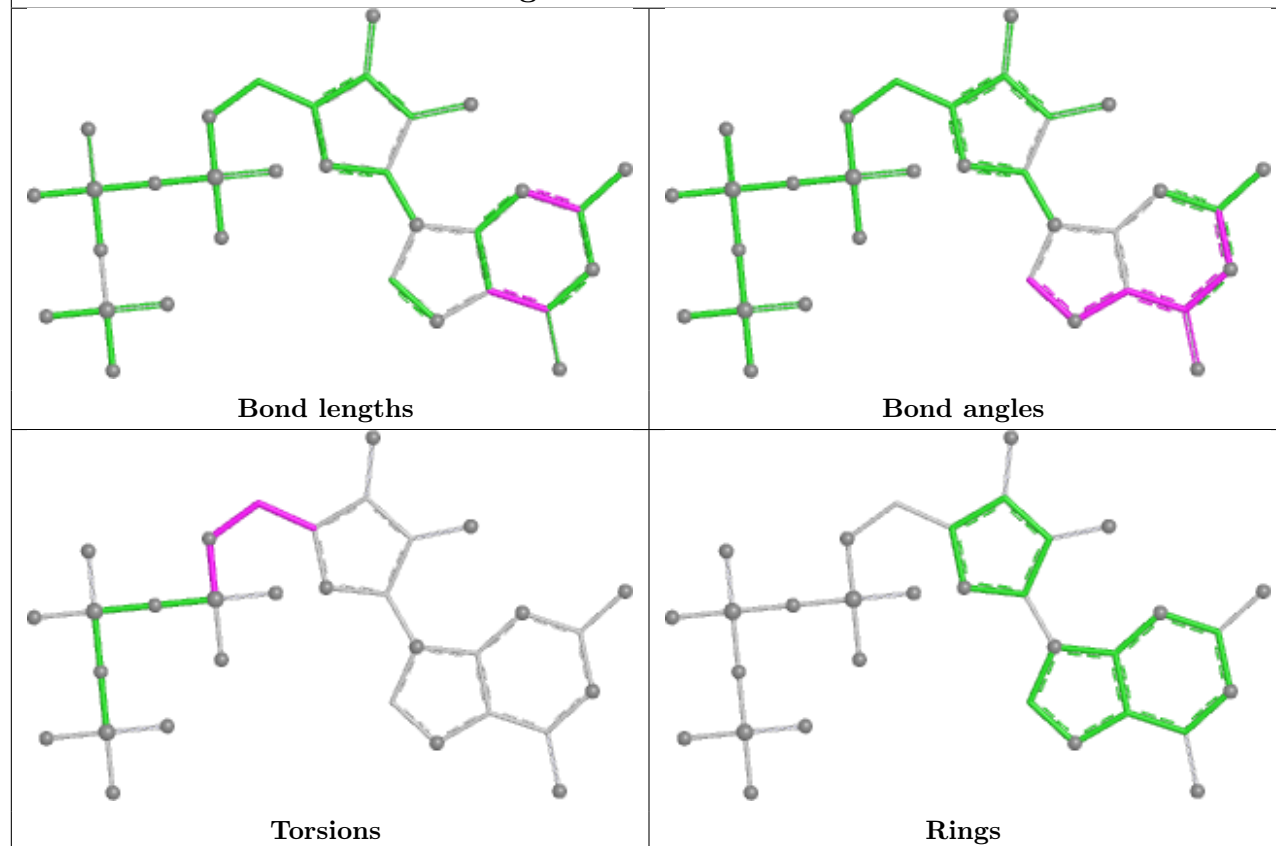


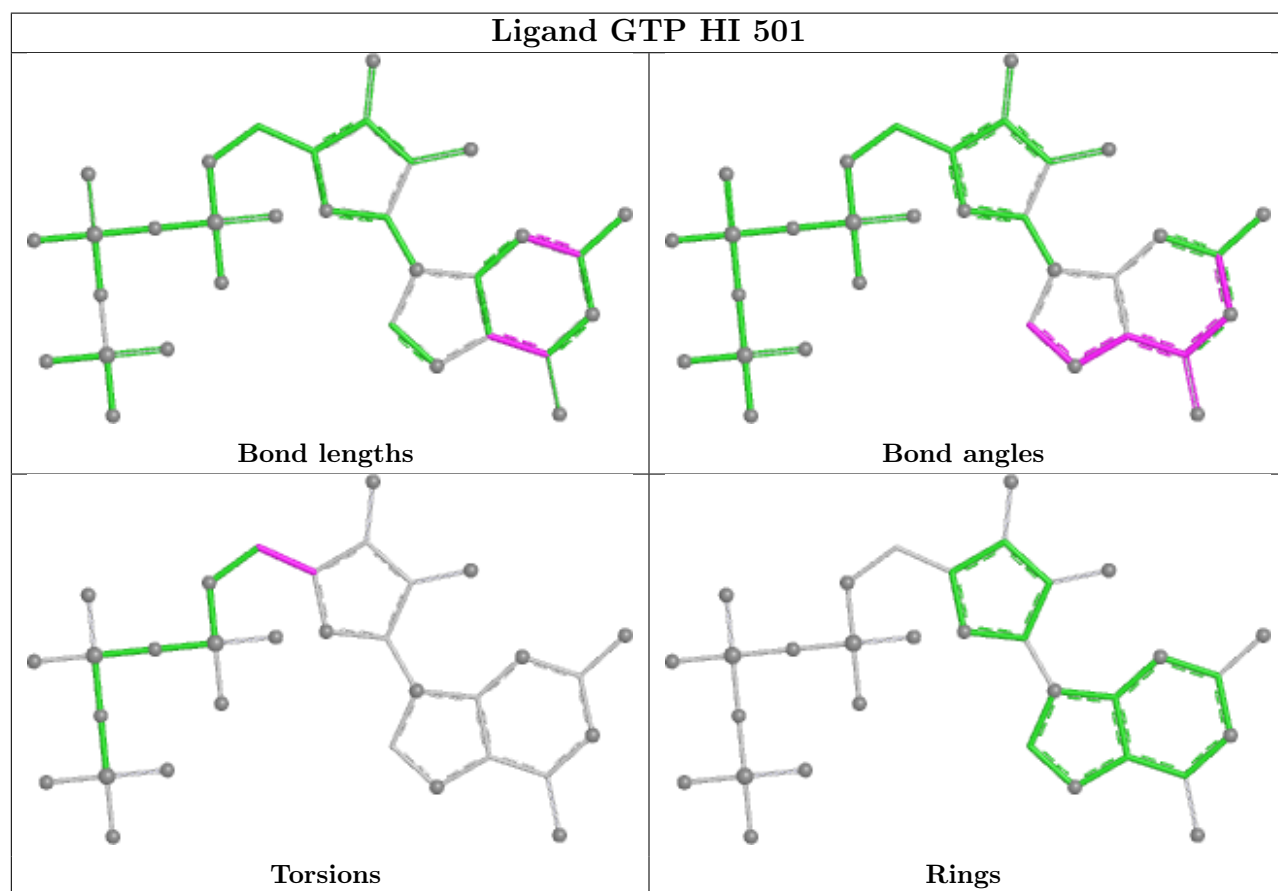
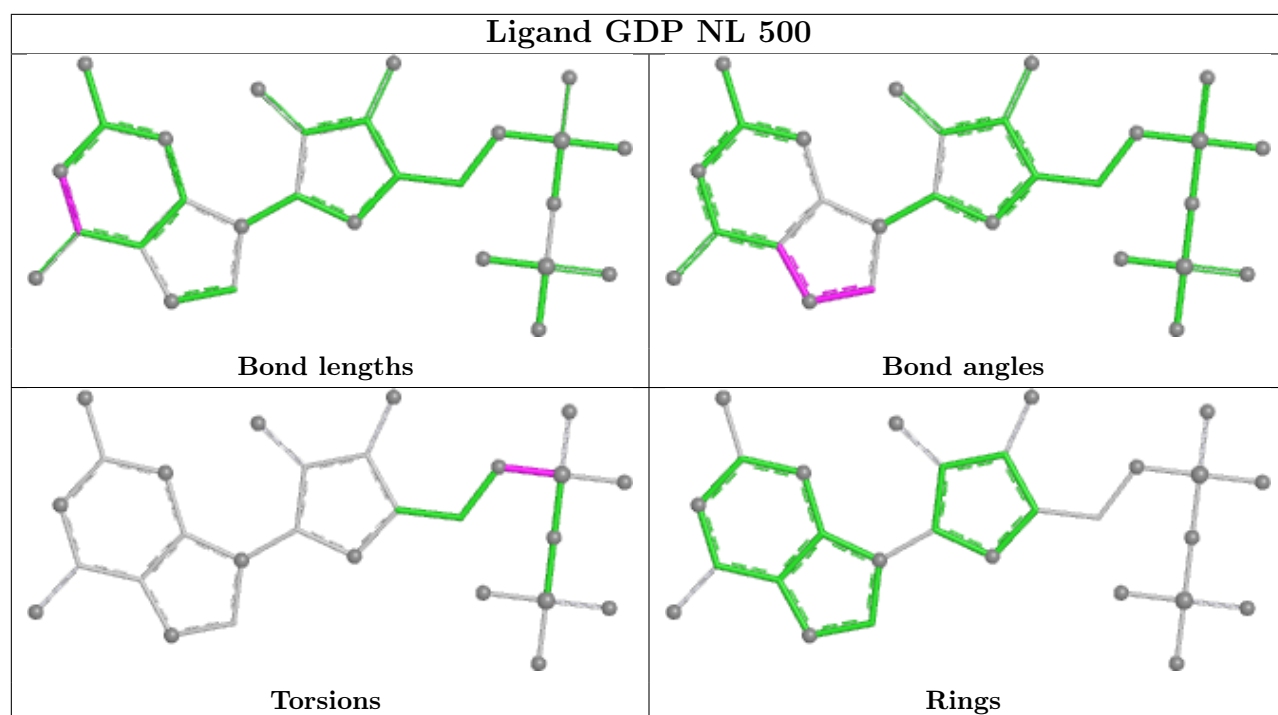


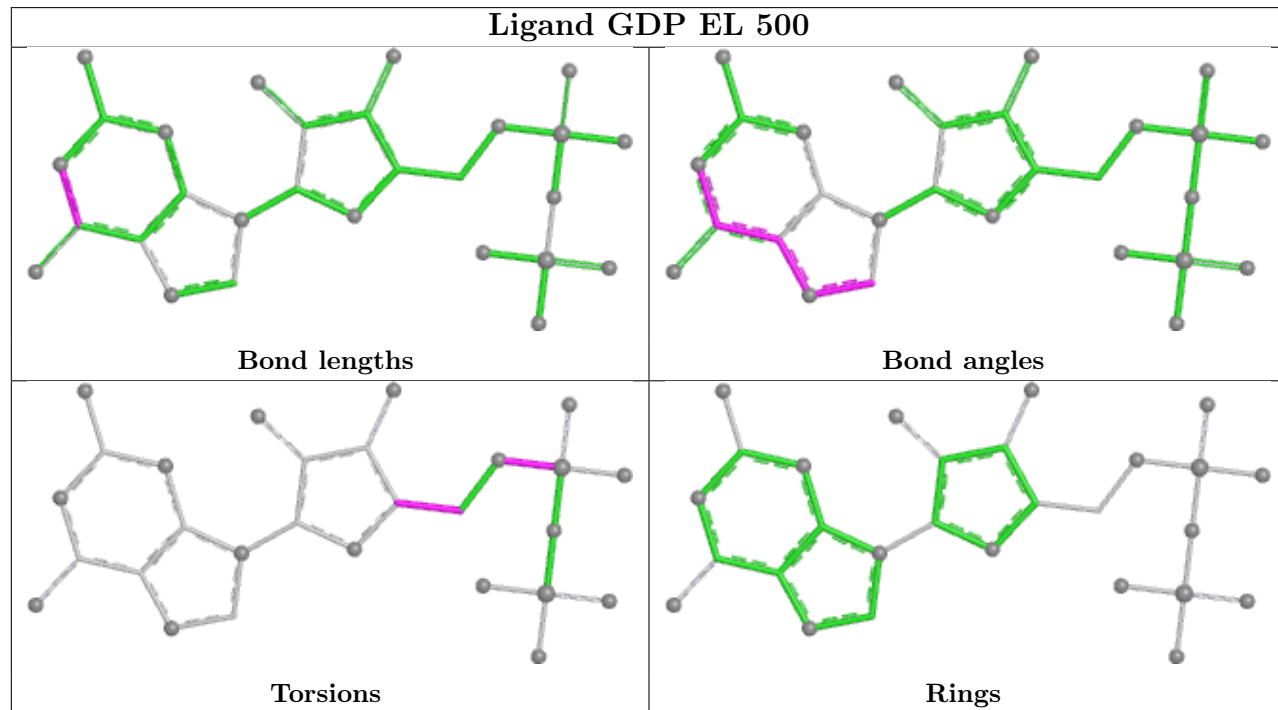
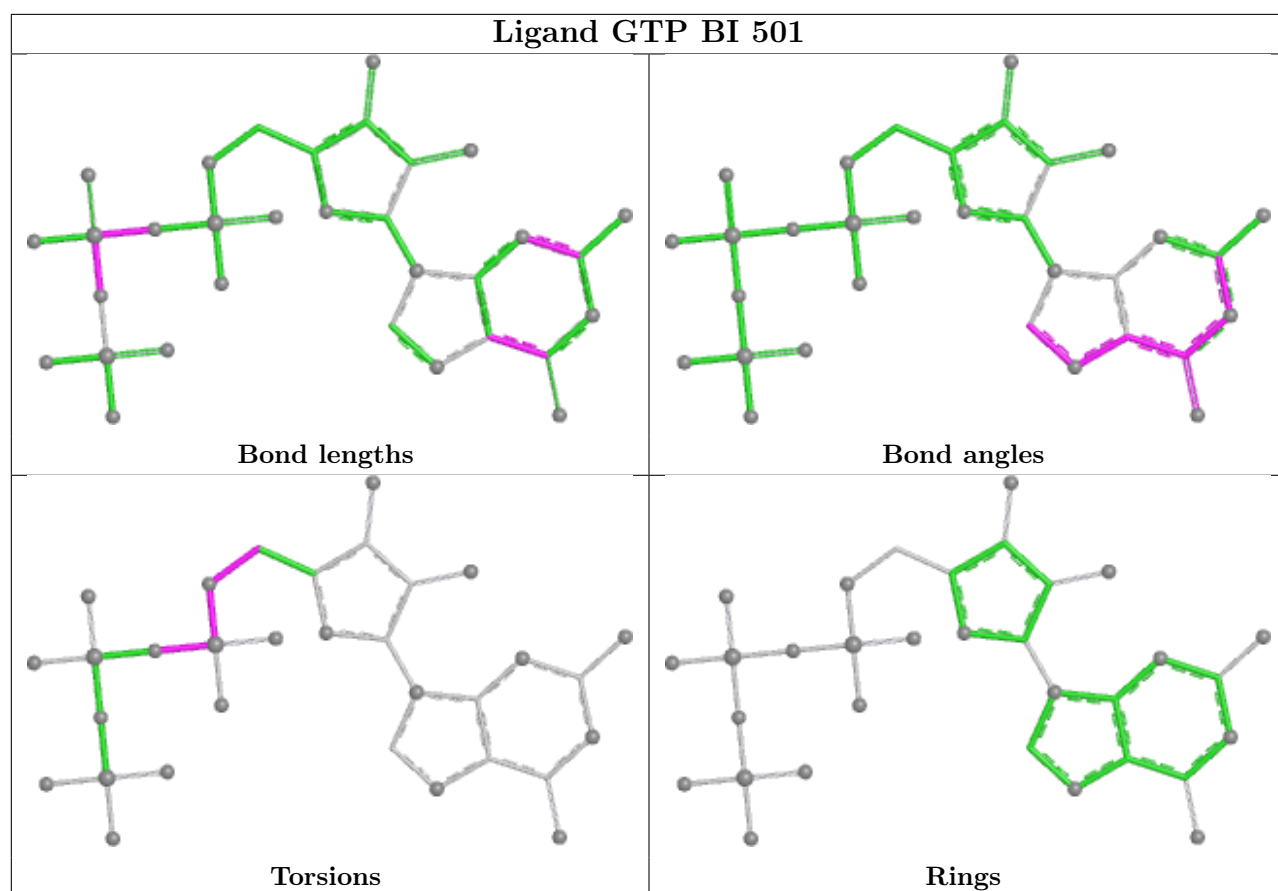
Ligand GTP WE 501

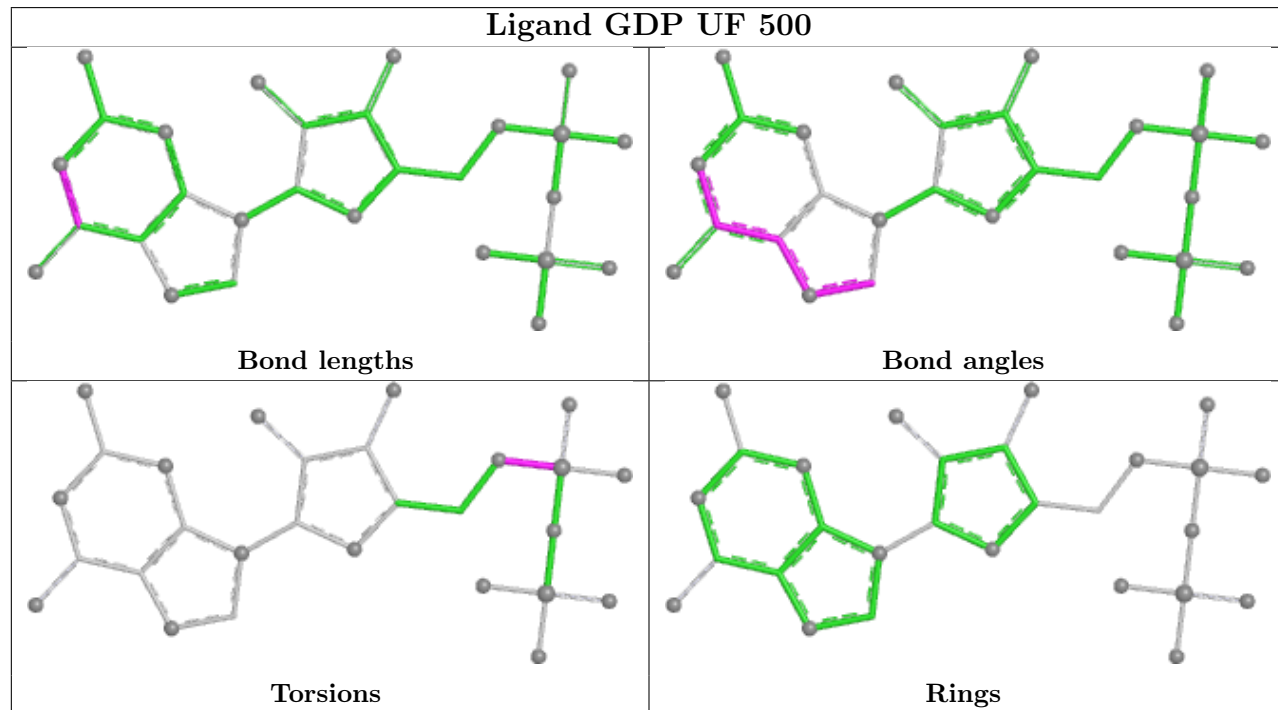
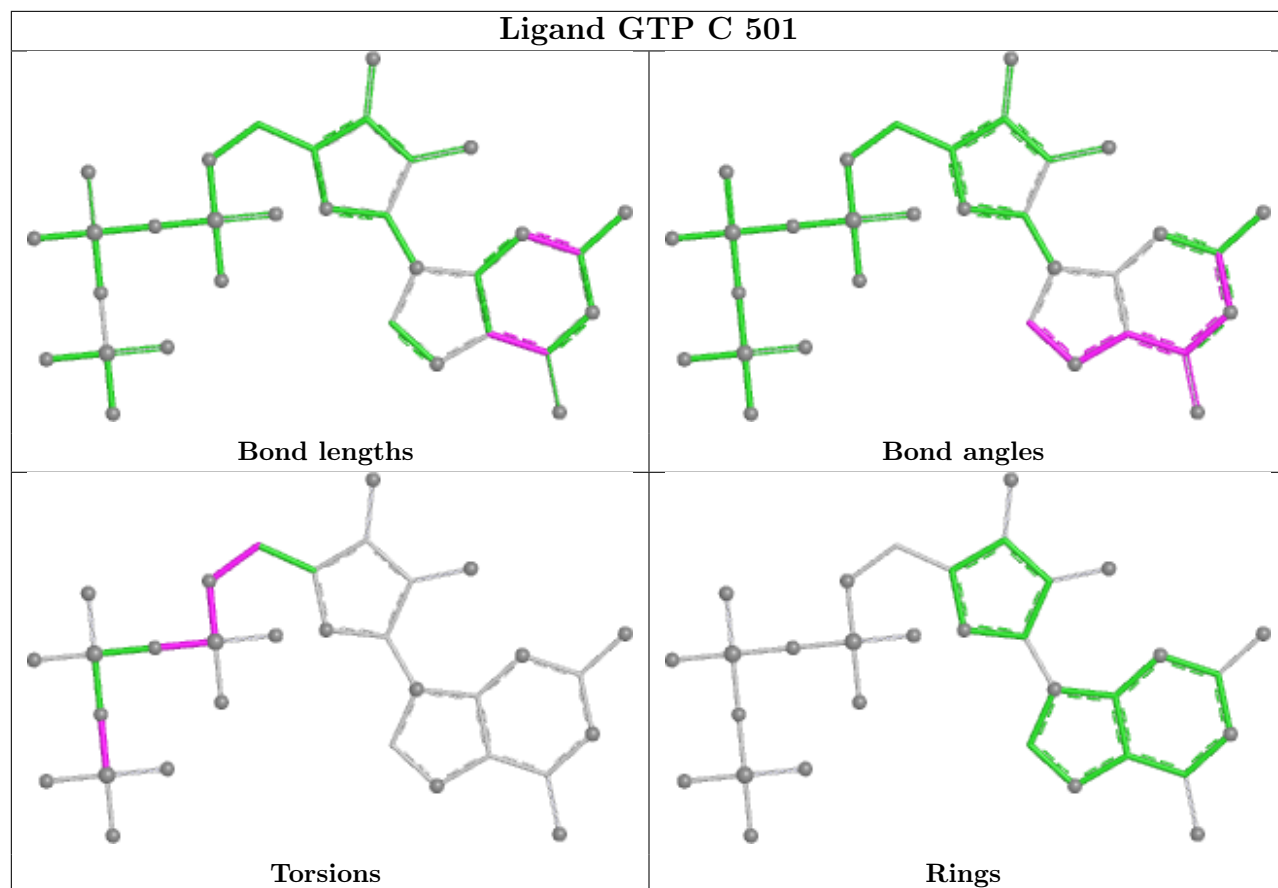


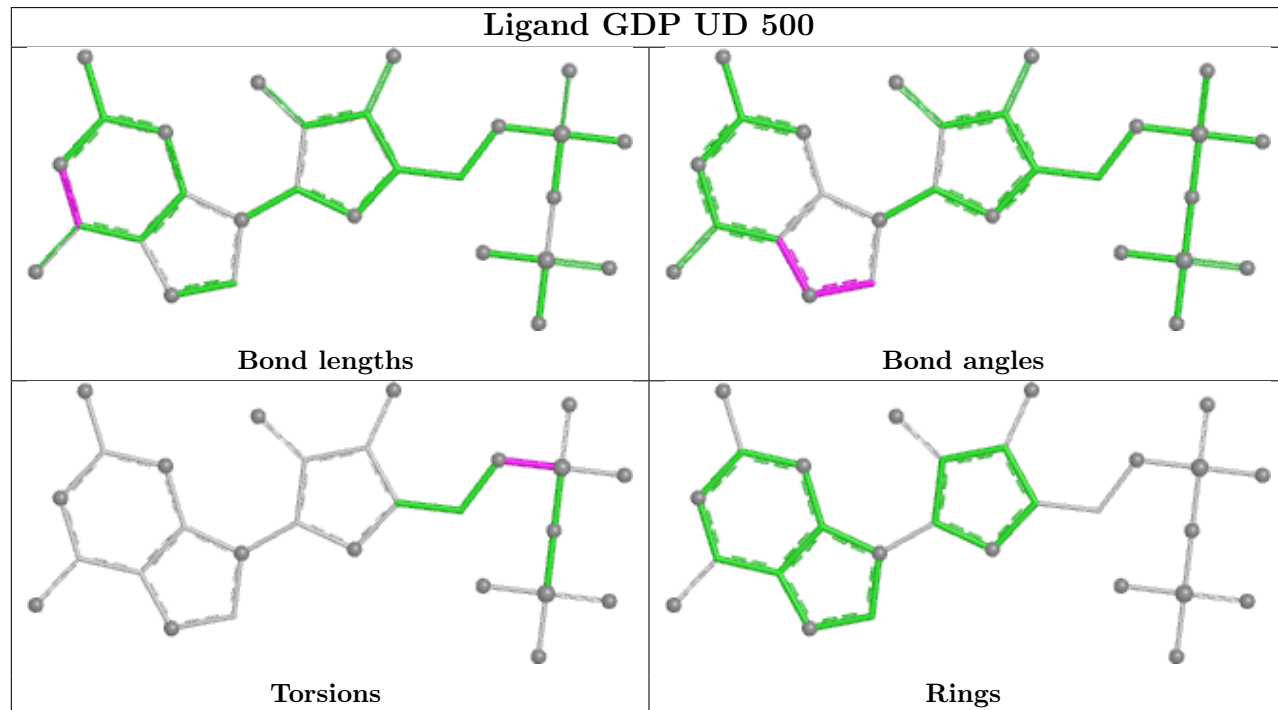
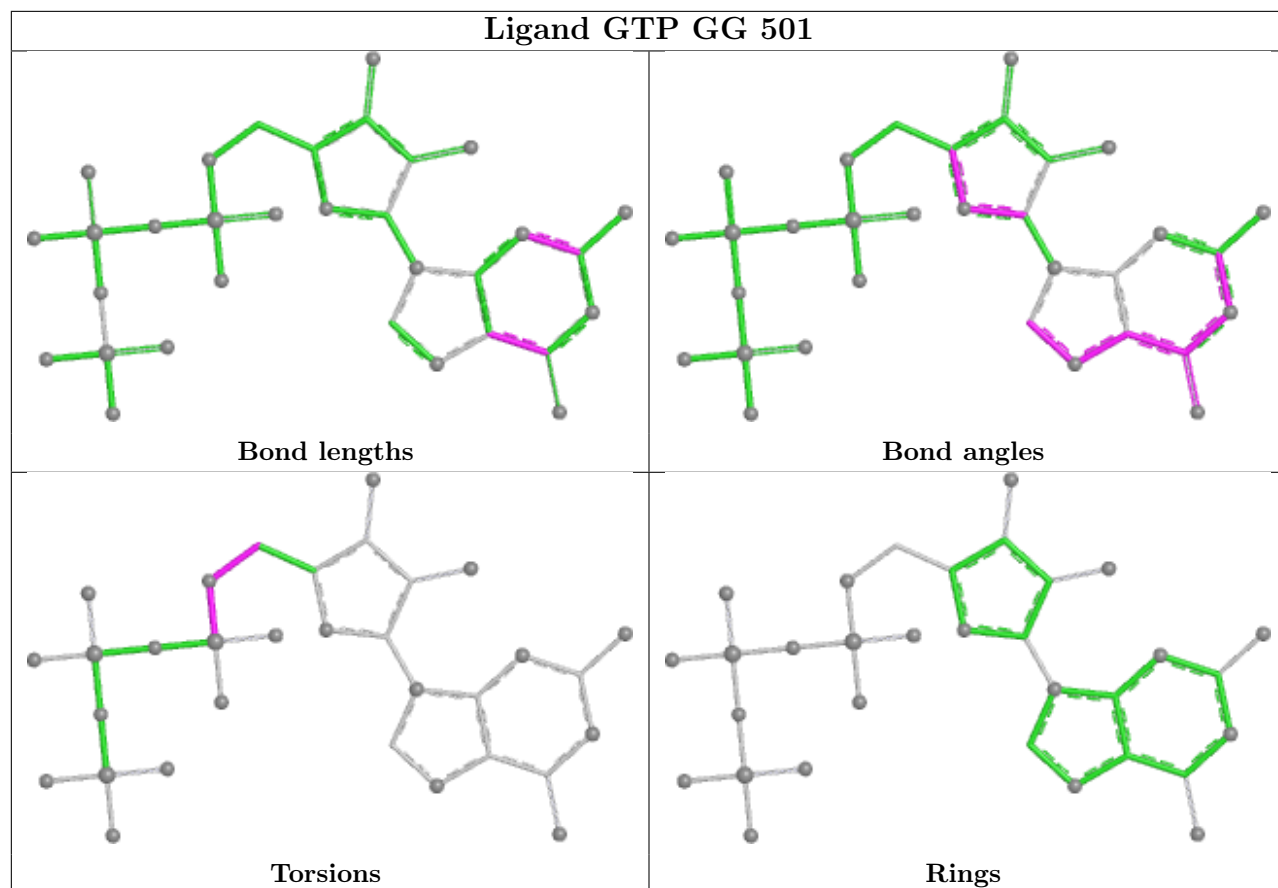
Ligand GTP TE 501

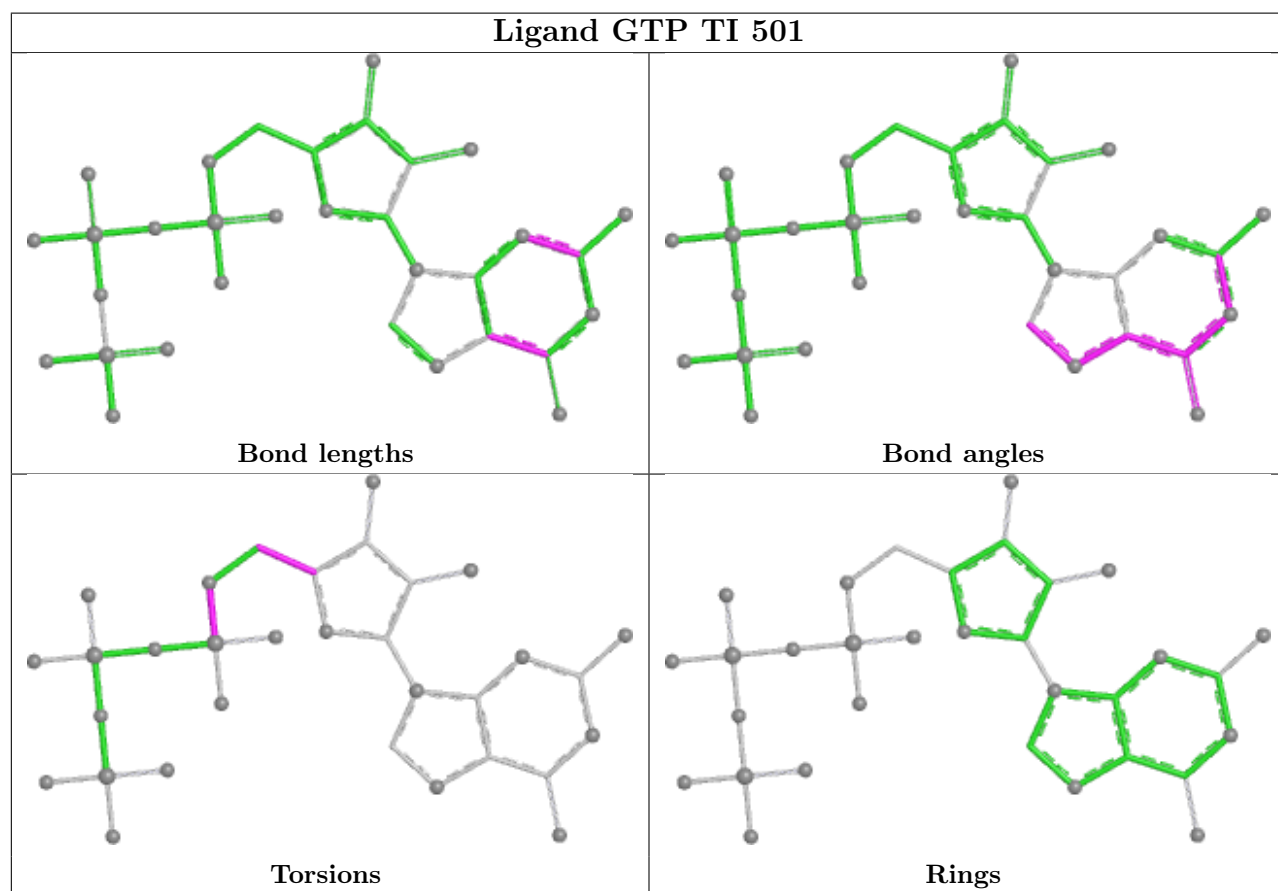
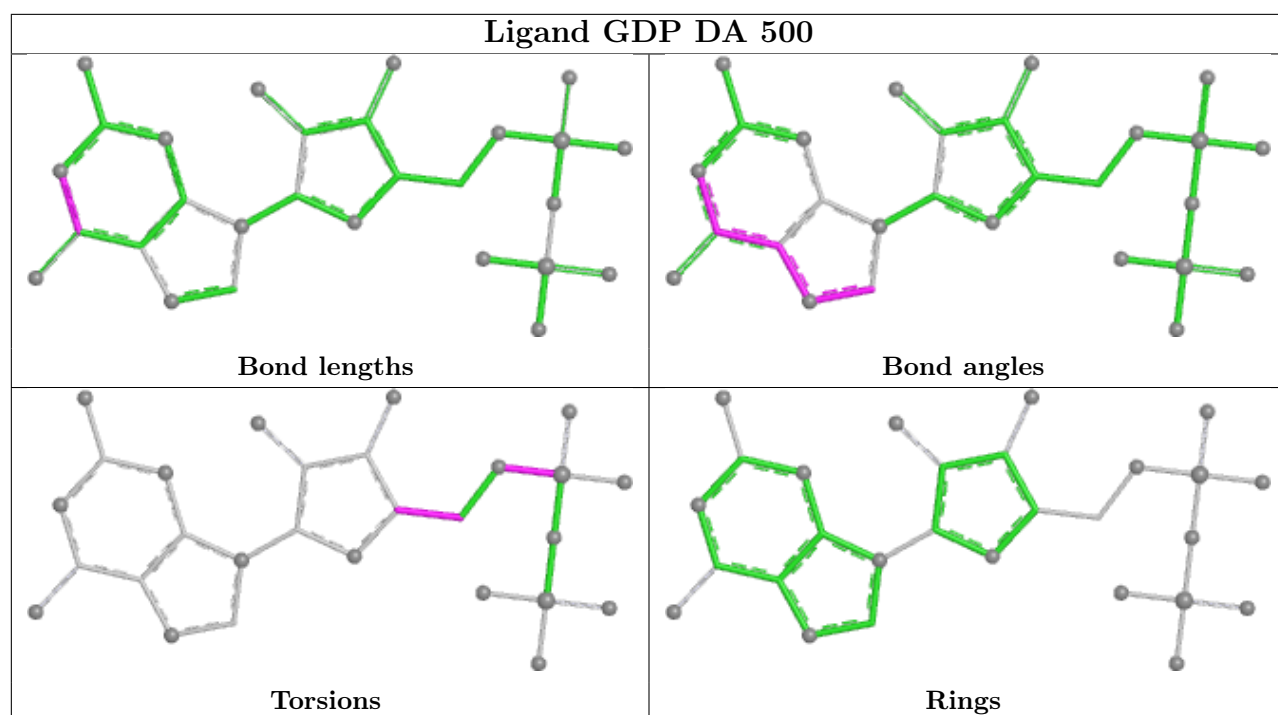


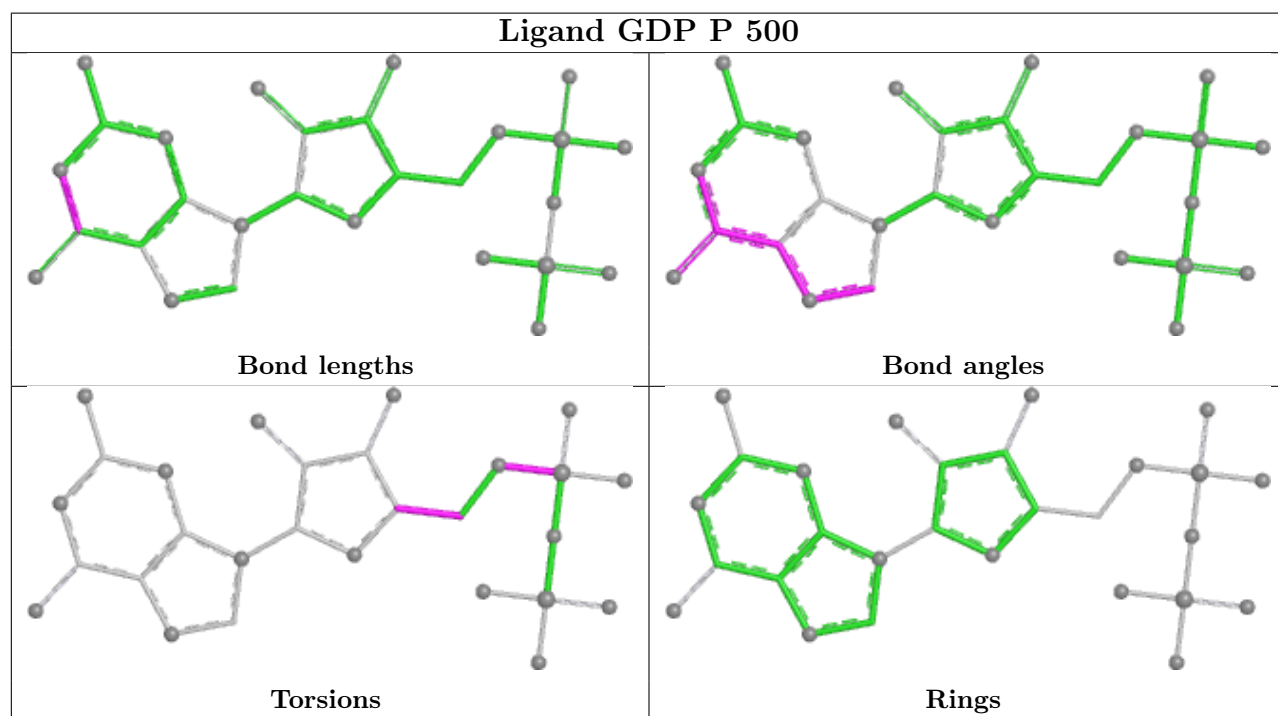
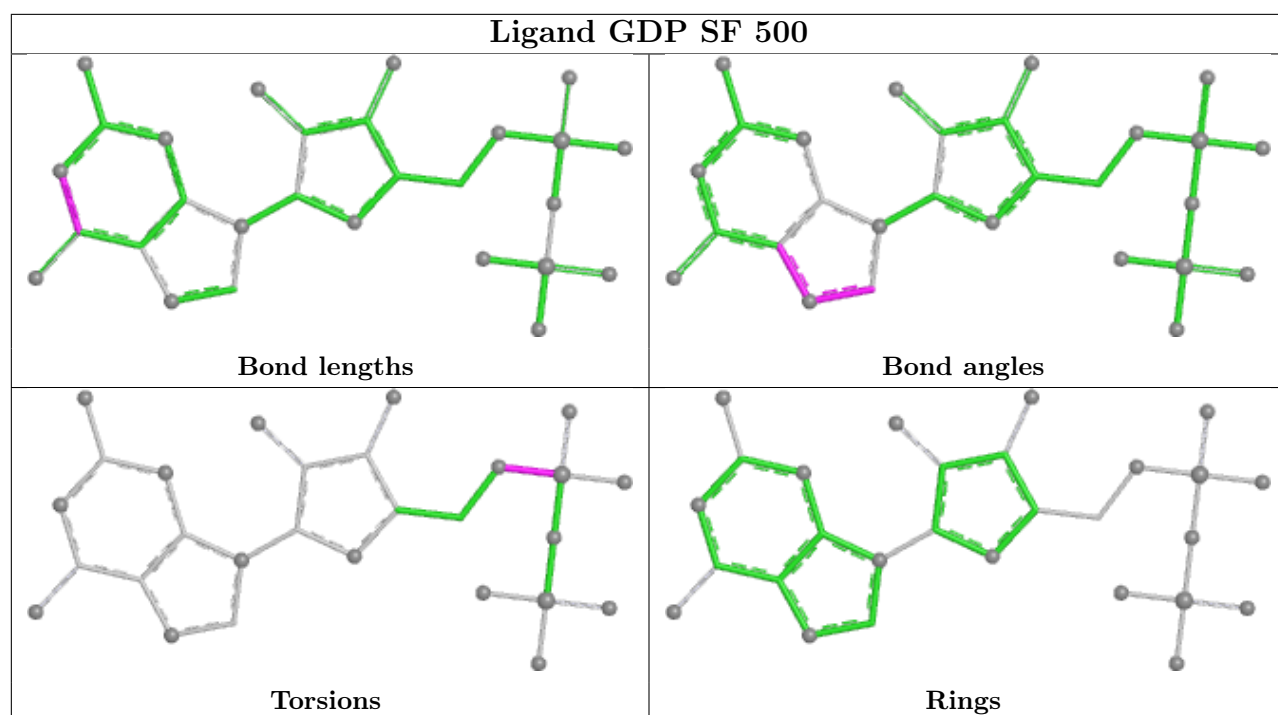




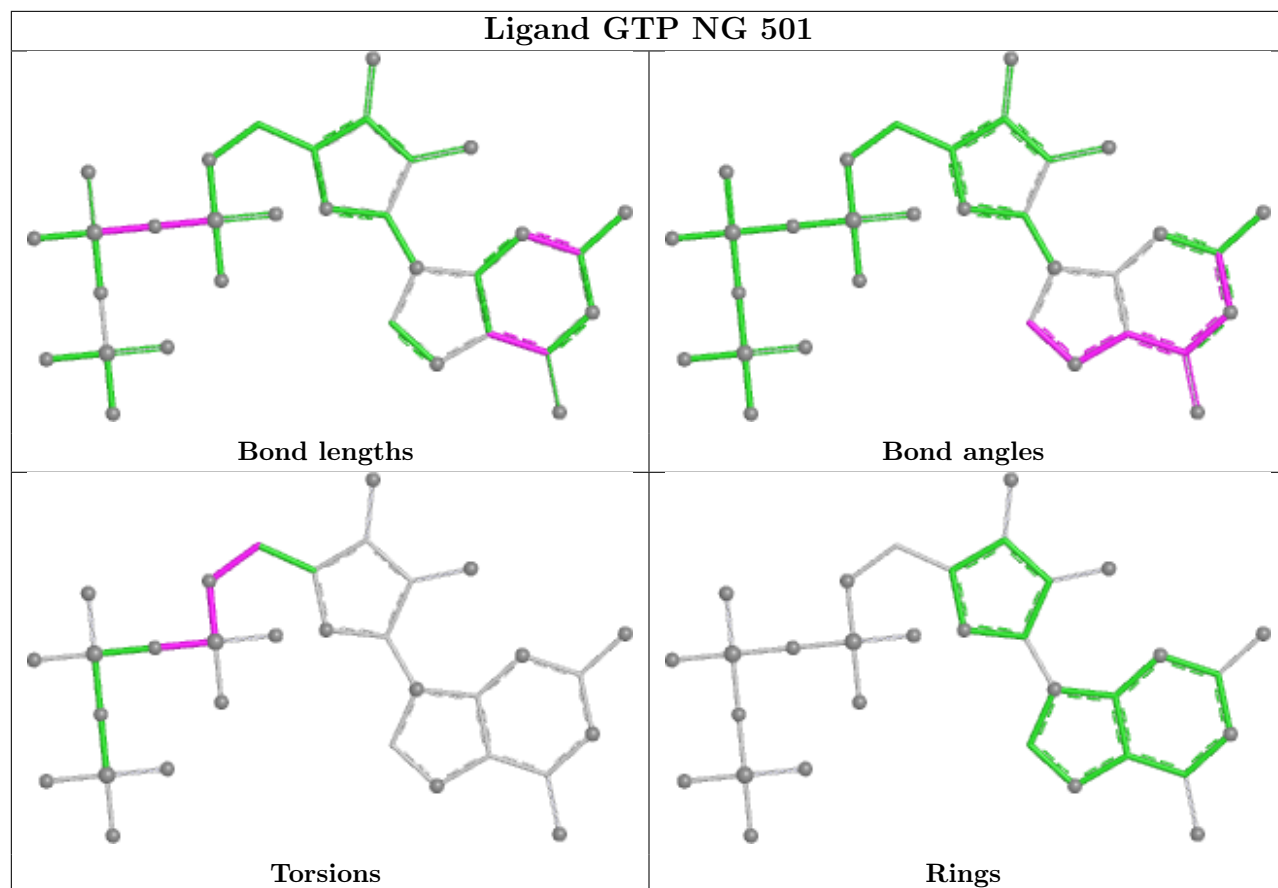




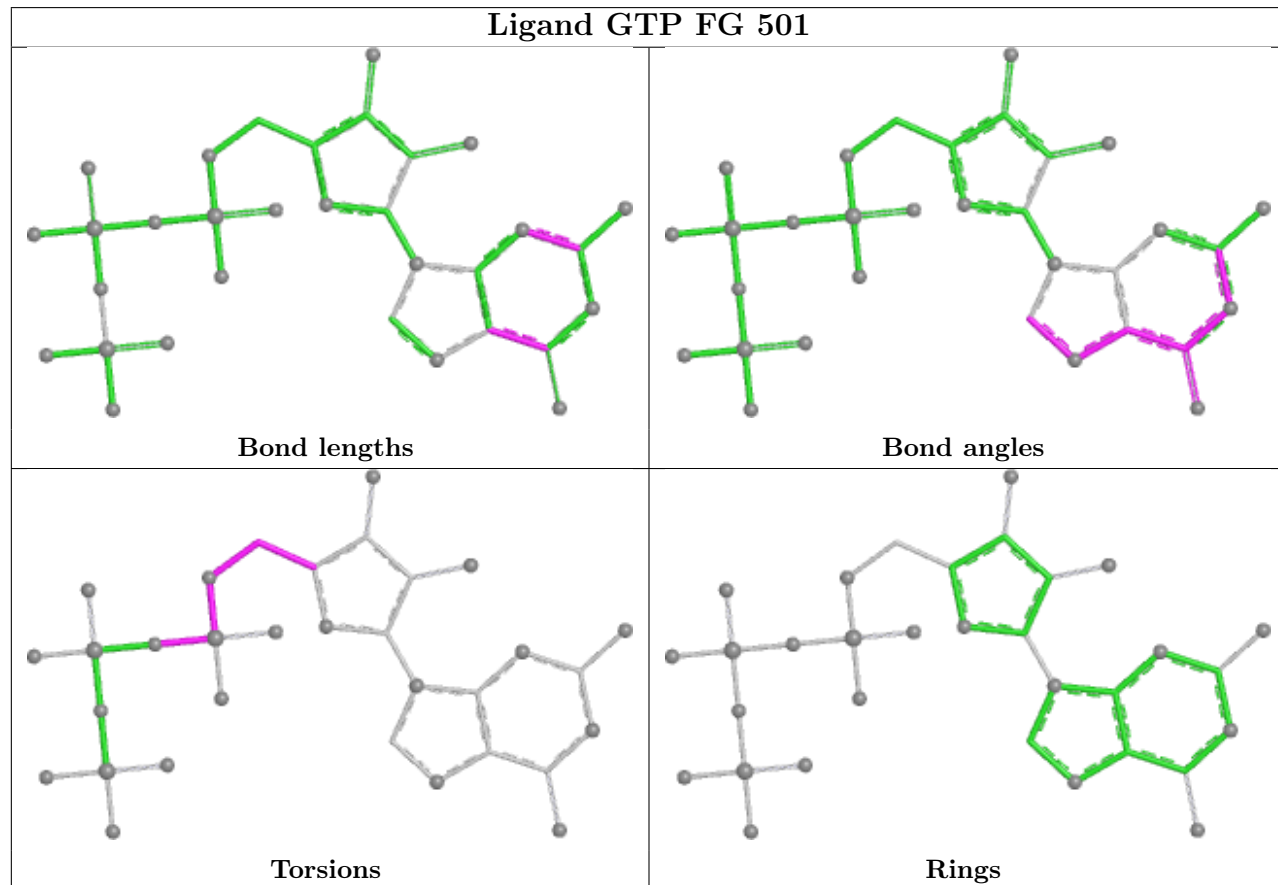


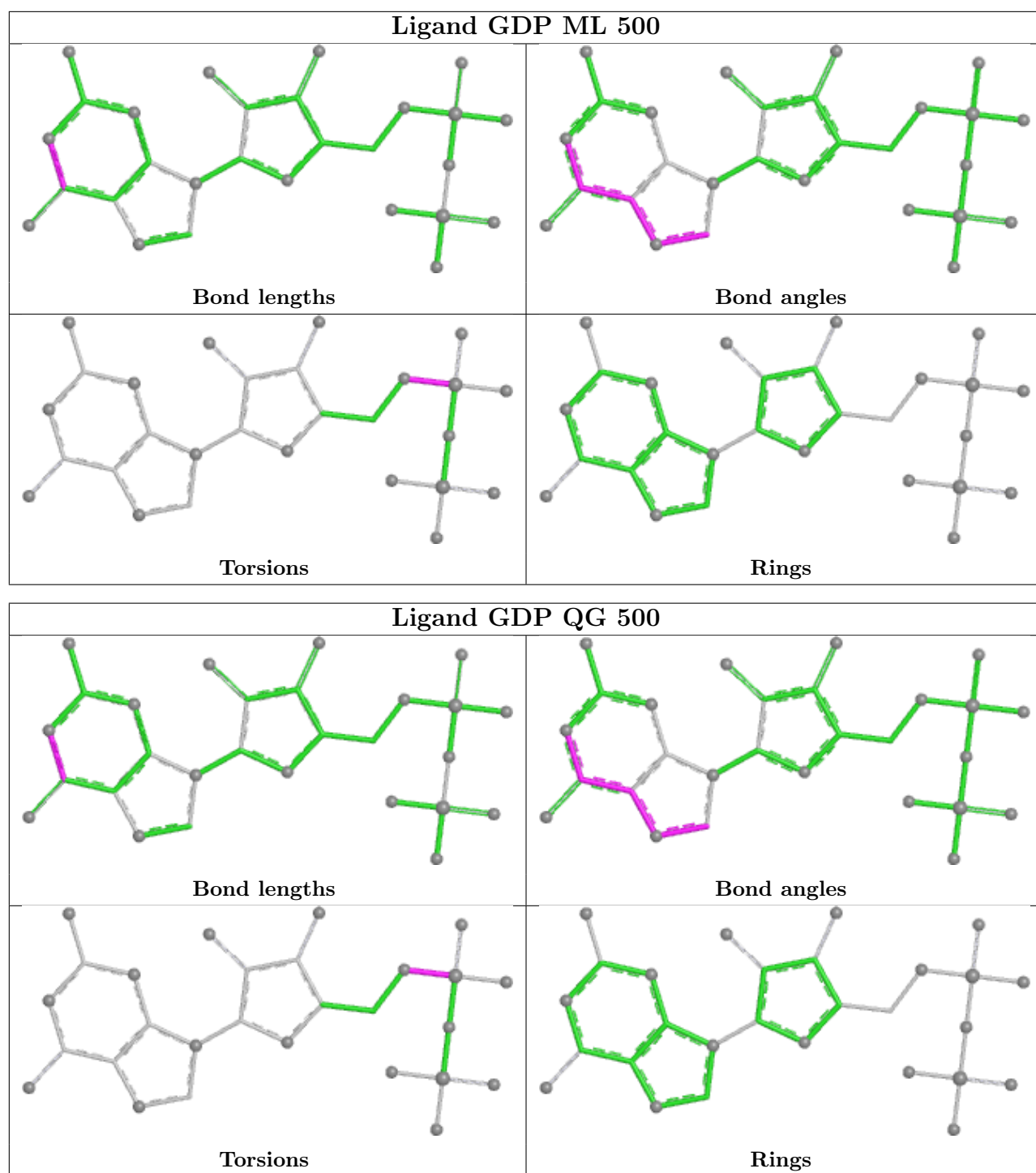


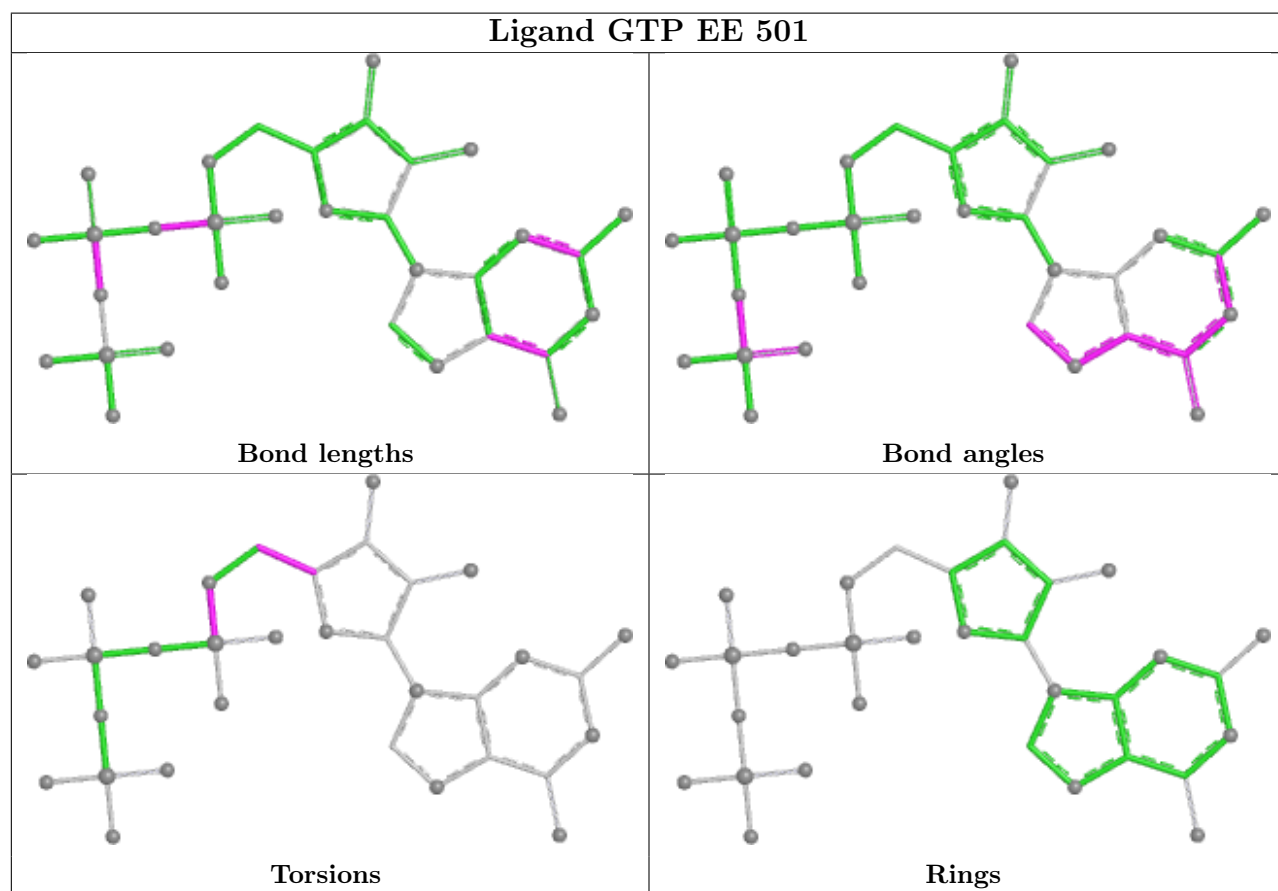
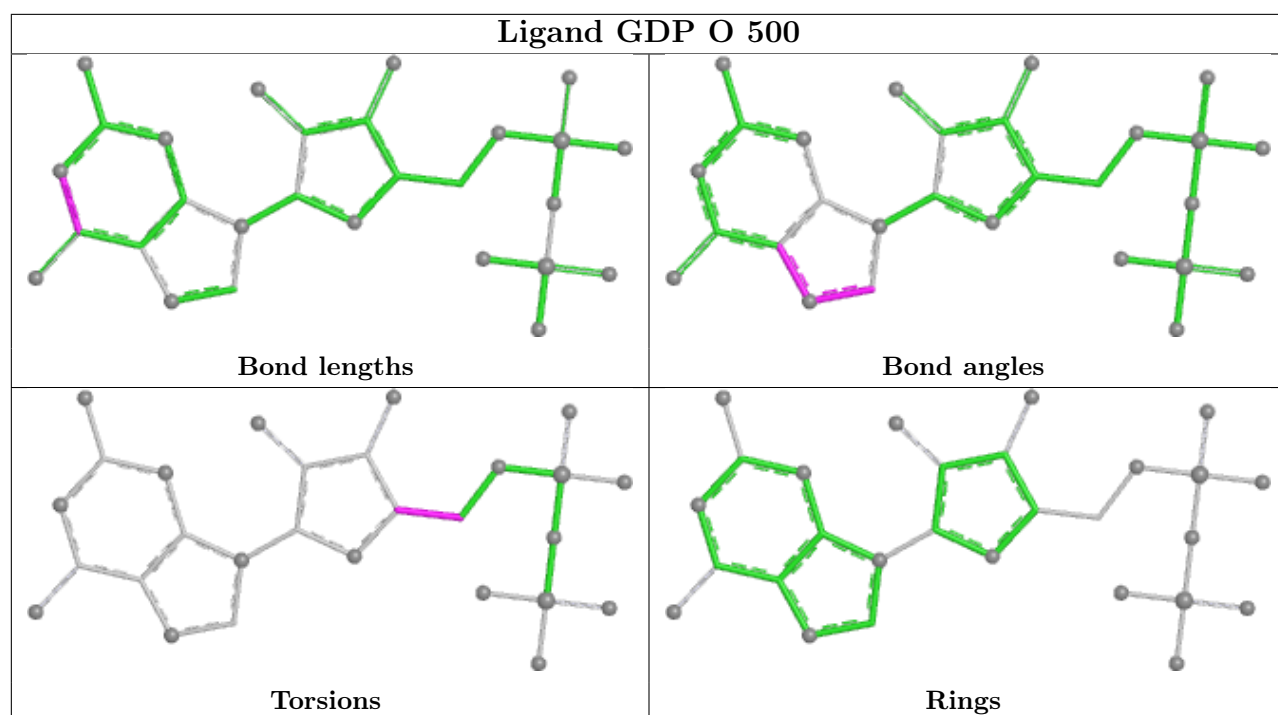
Ligand GTP NG 501

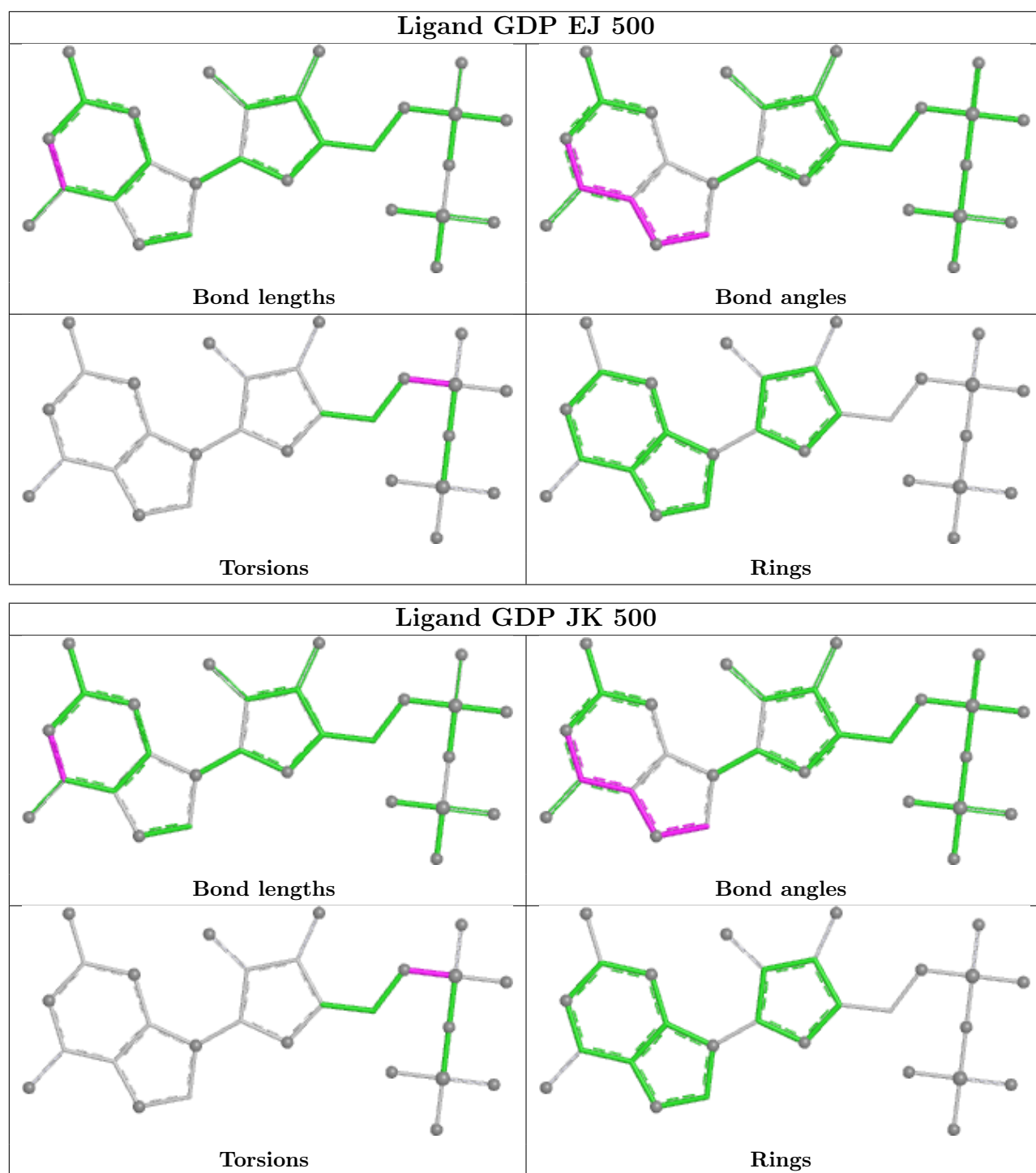


Ligand GTP FG 501

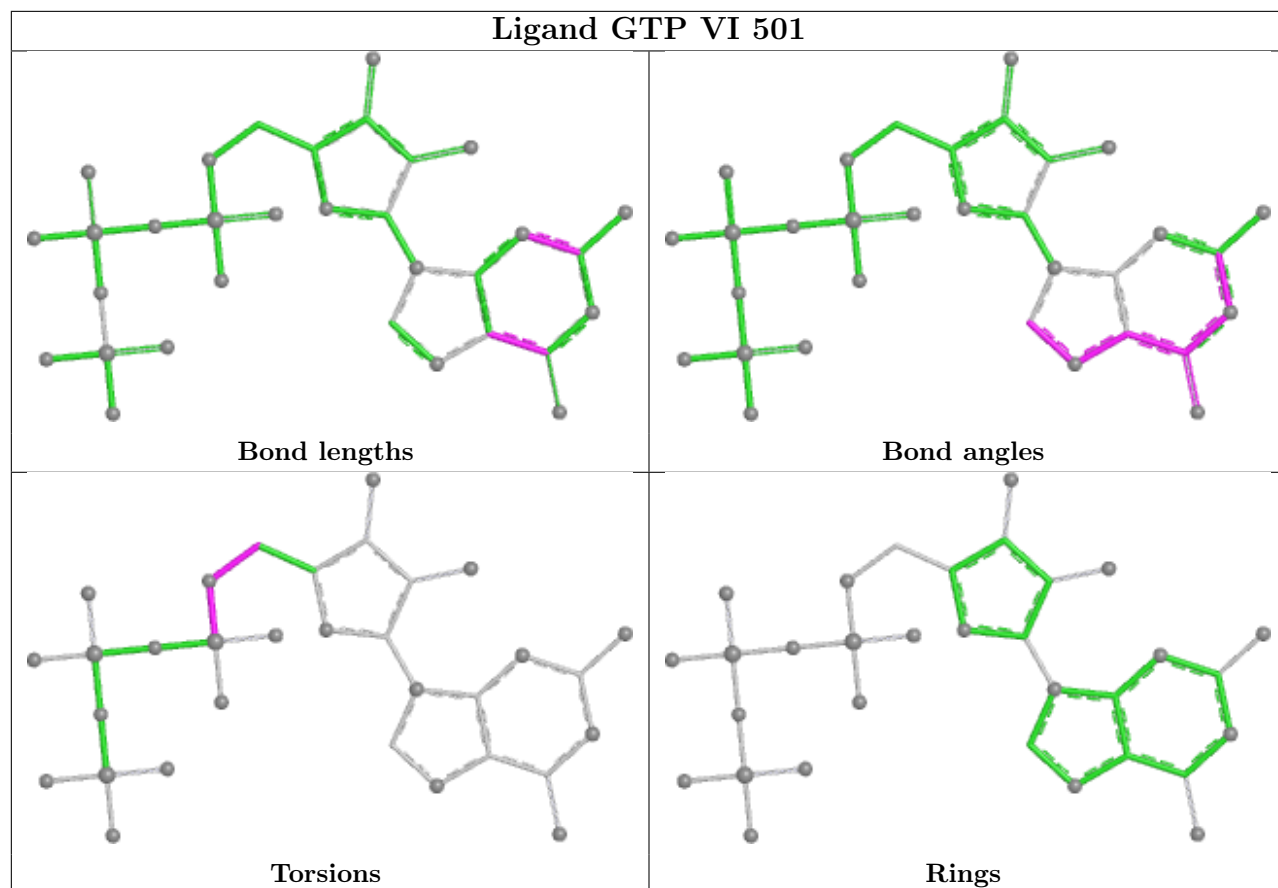




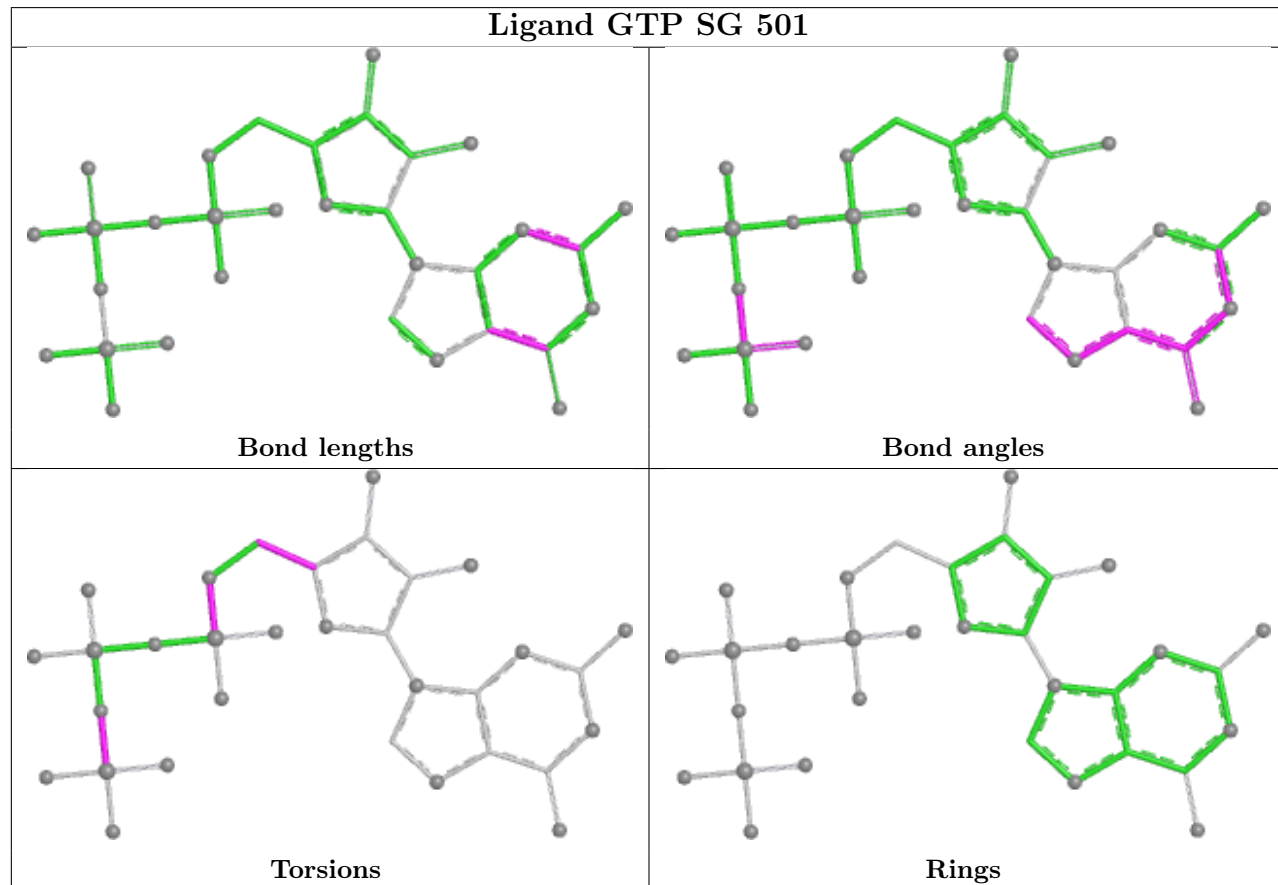


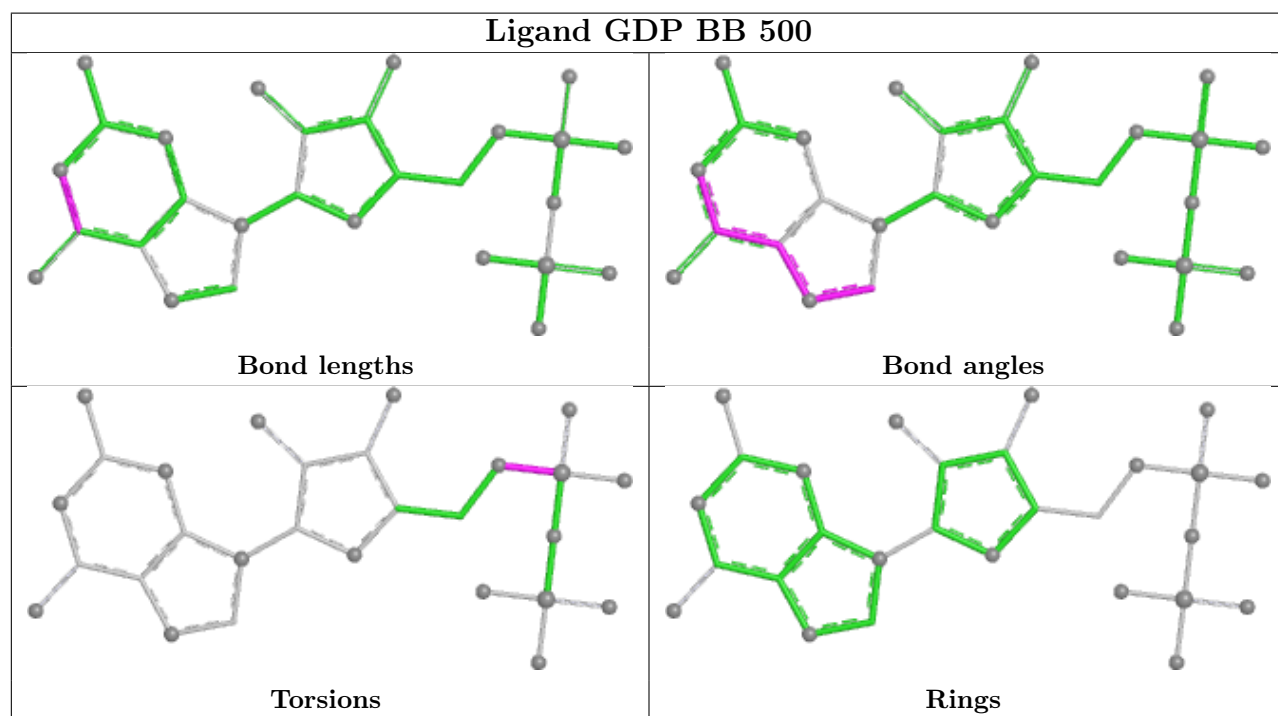
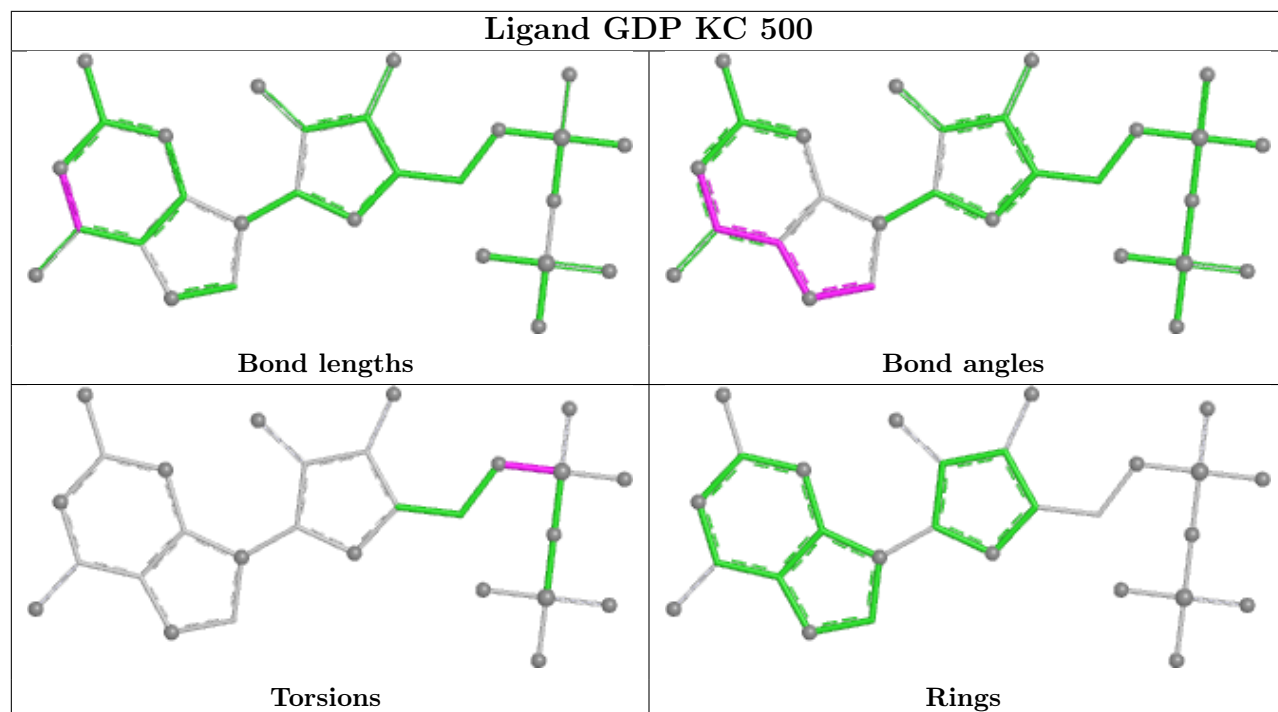


Ligand GTP VI 501

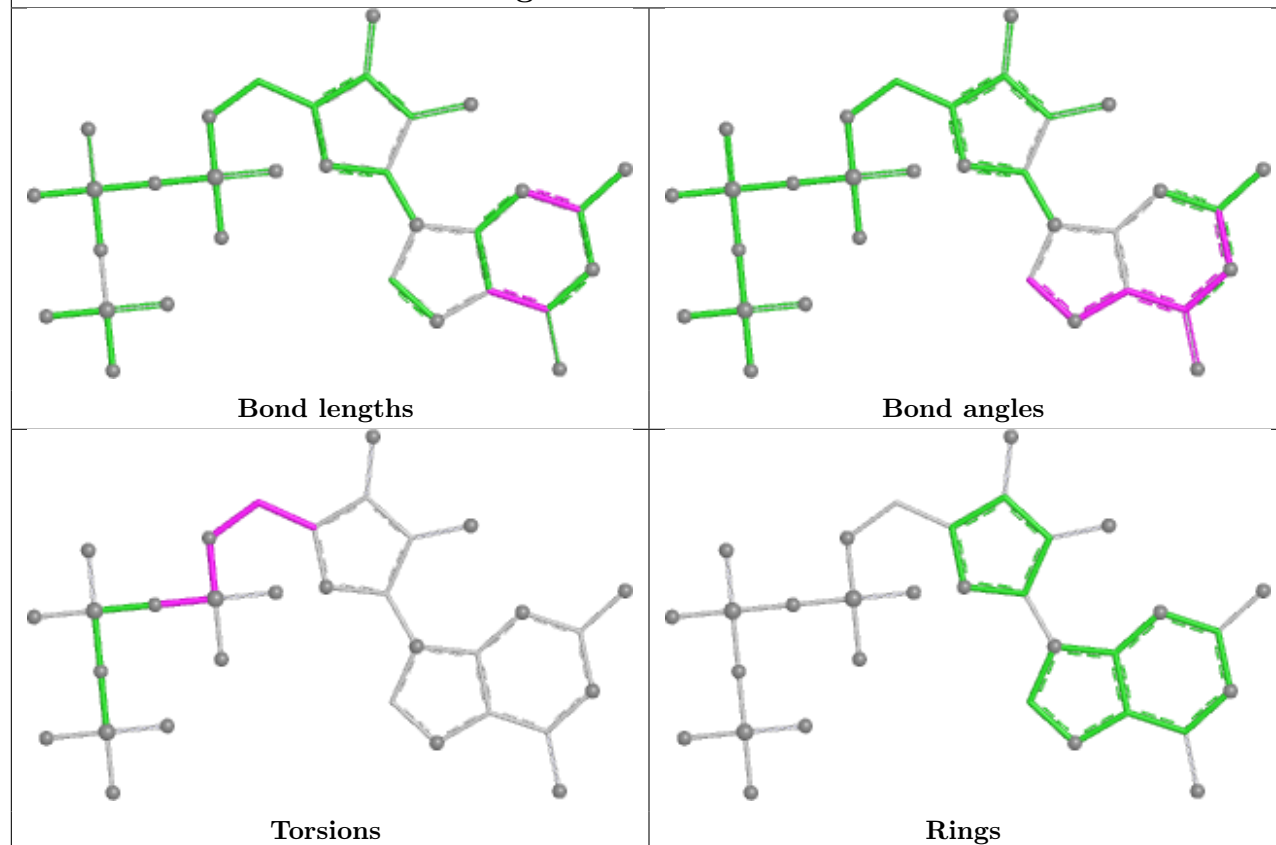


Ligand GTP SG 501

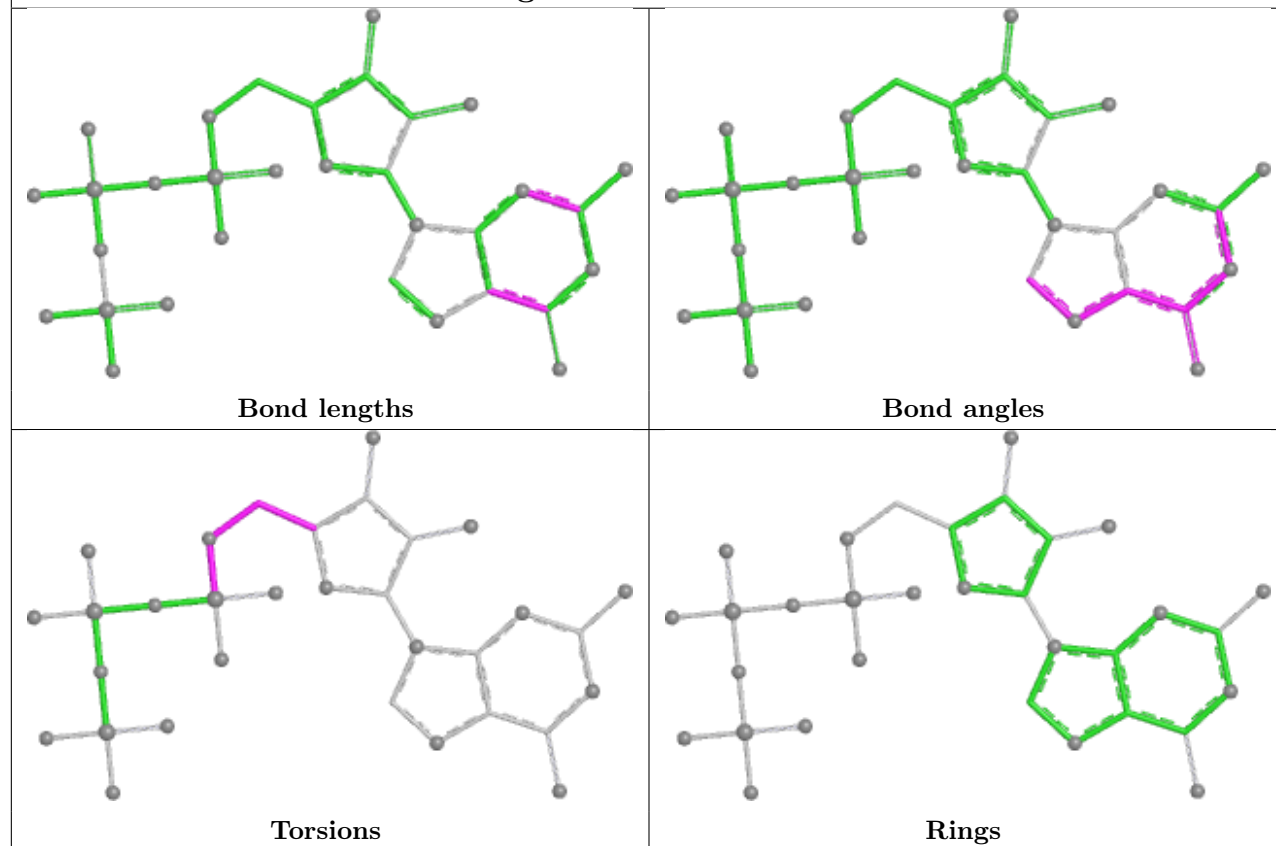


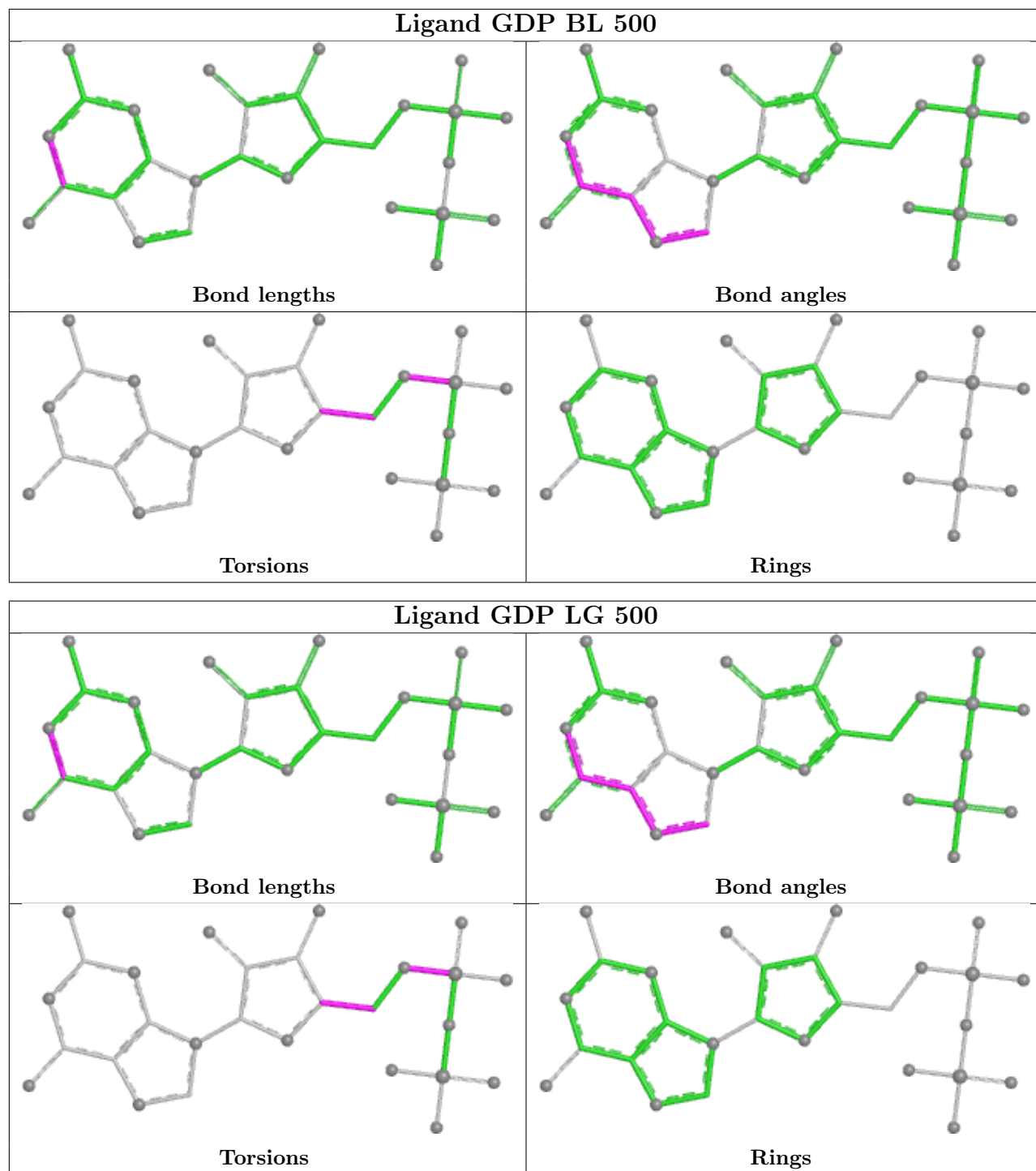


Ligand GTP UK 501

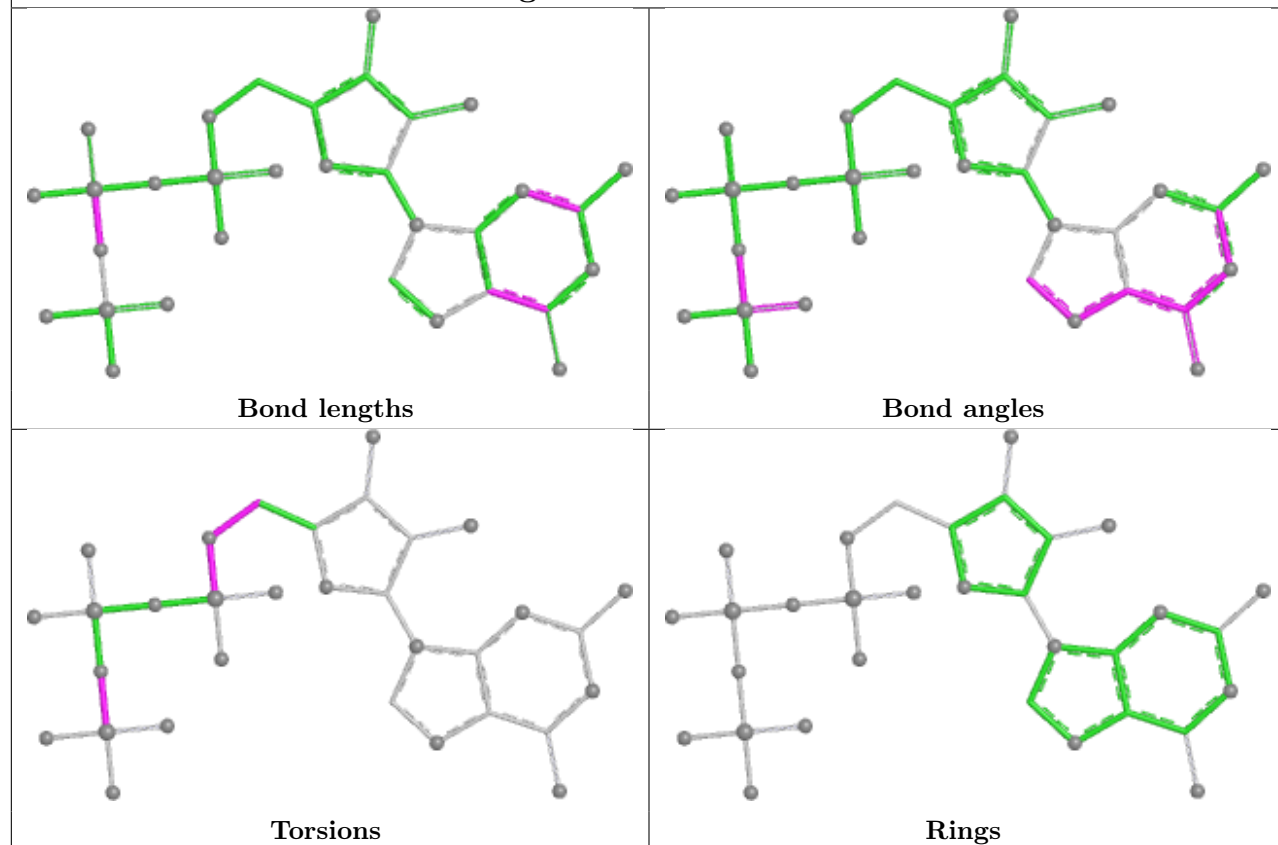


Ligand GTP PK 501

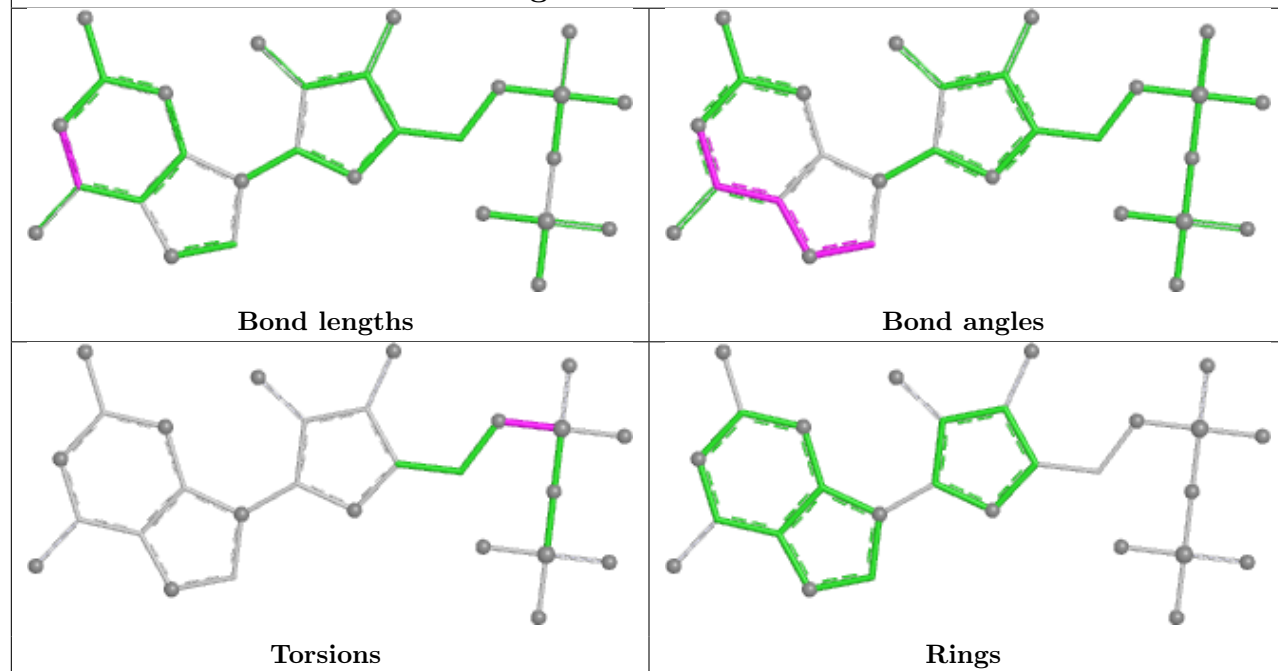


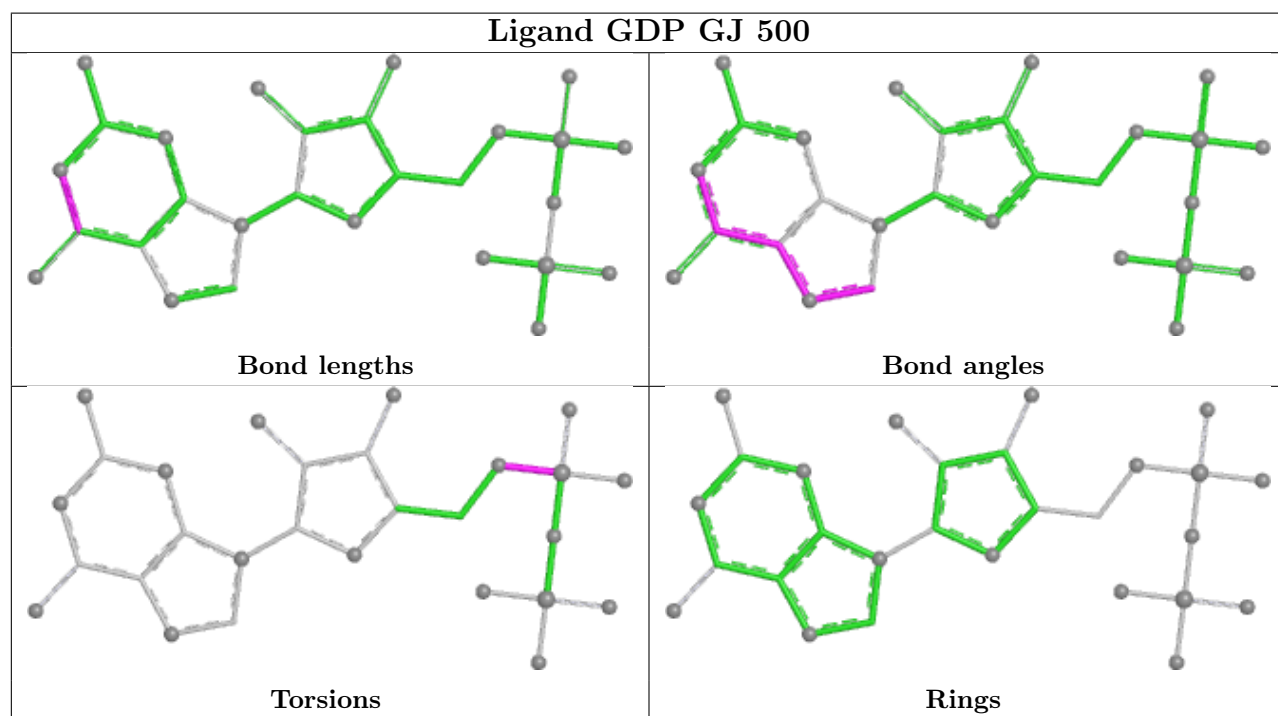
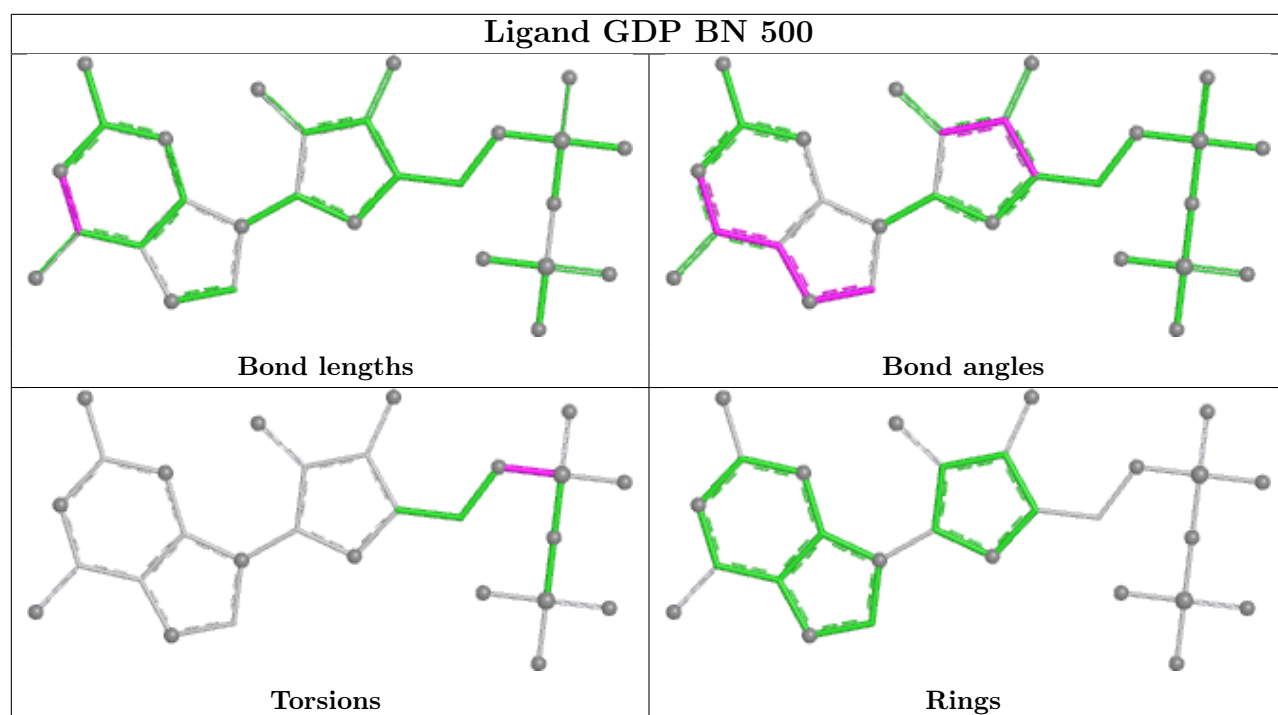


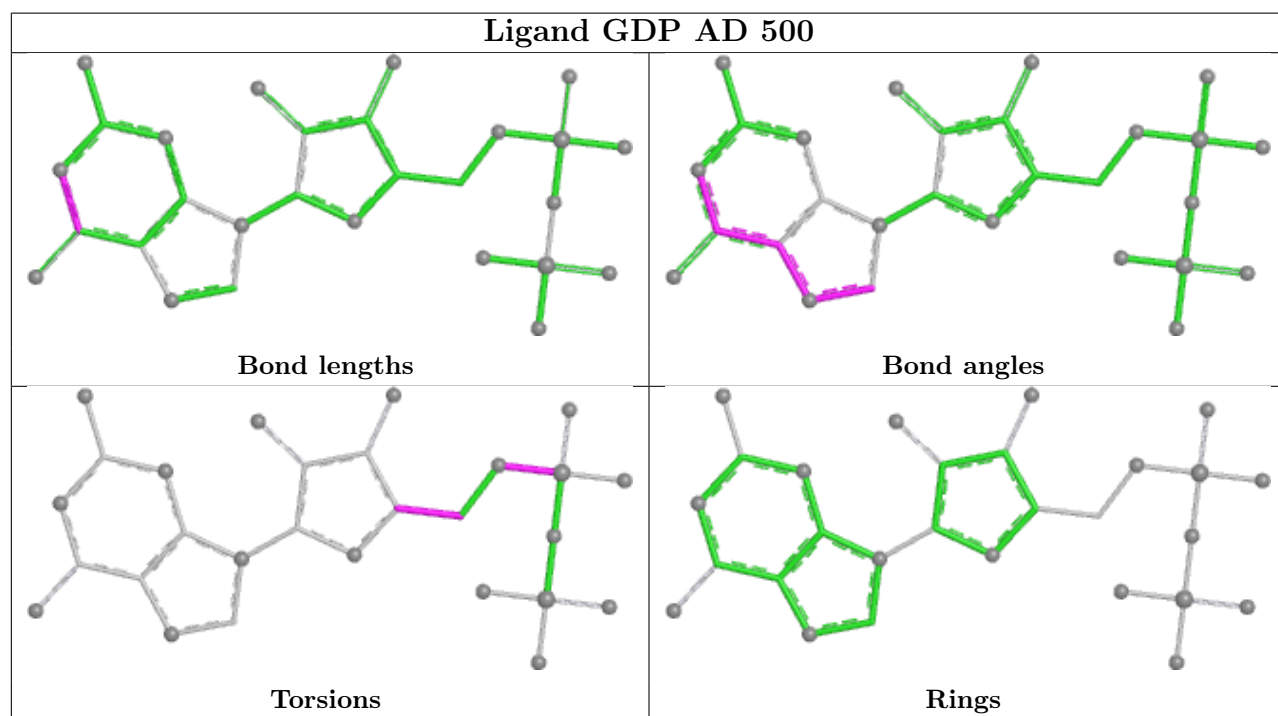
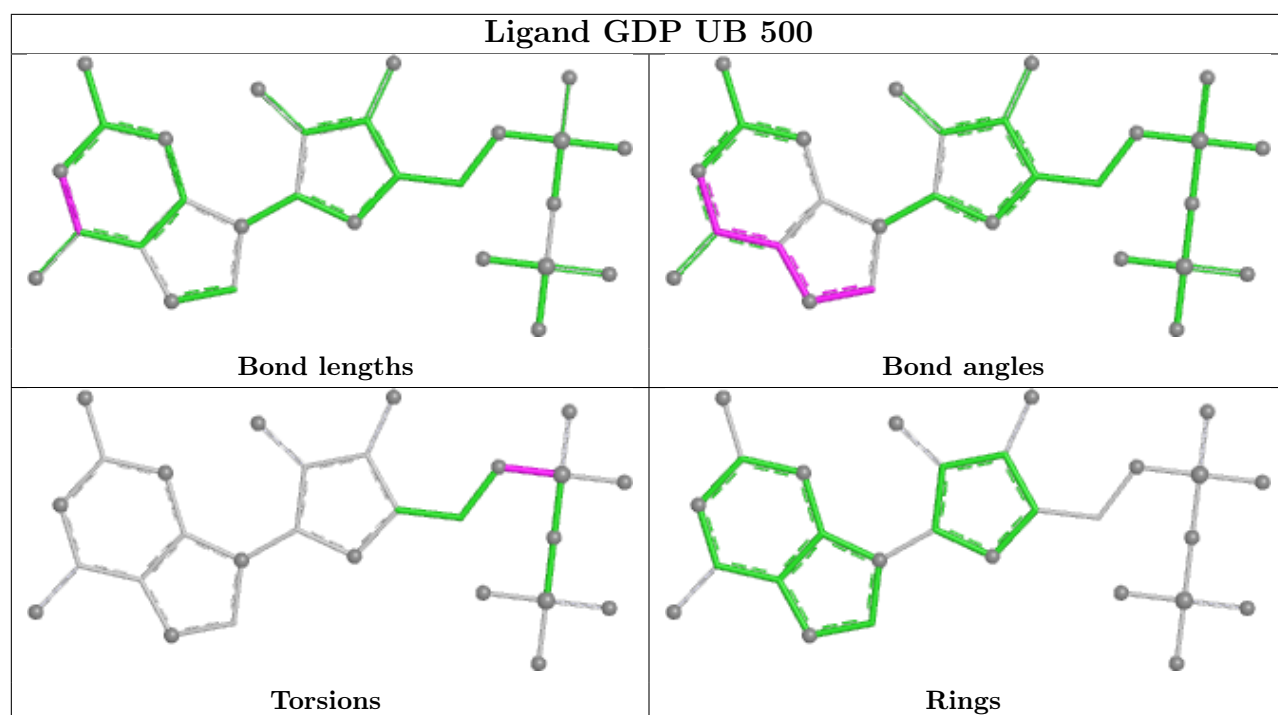
Ligand GTP TA 501

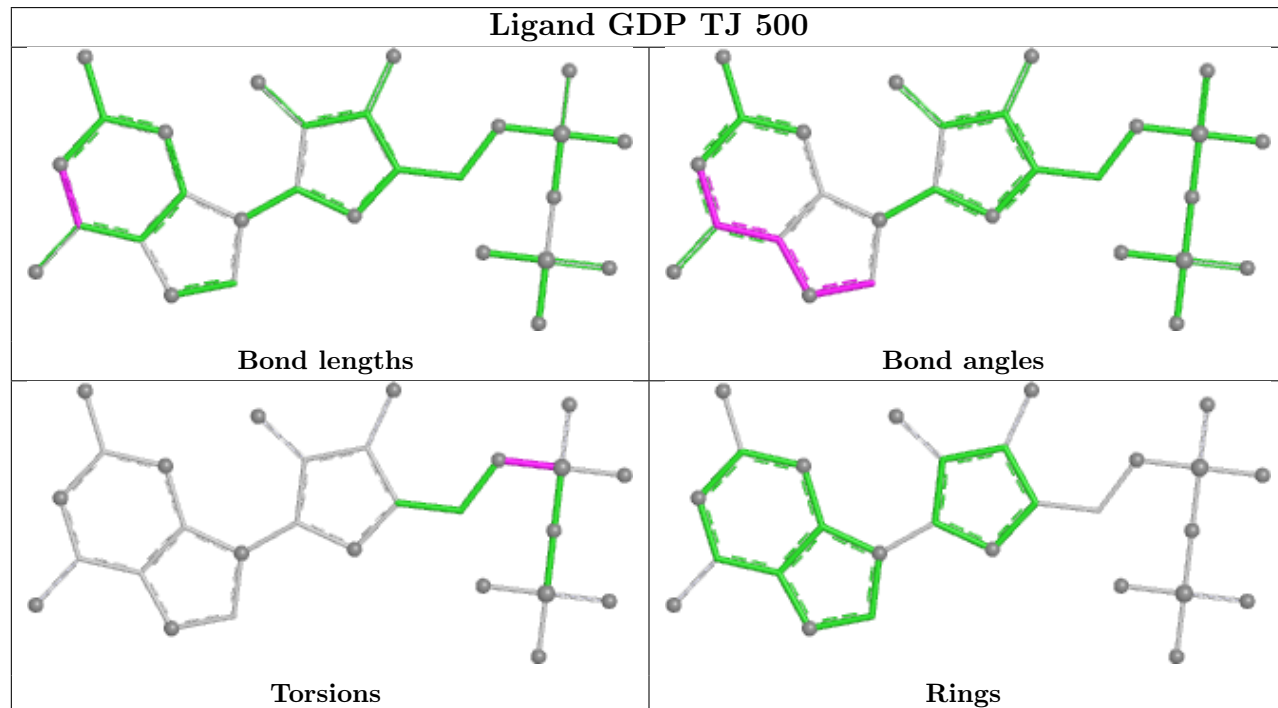
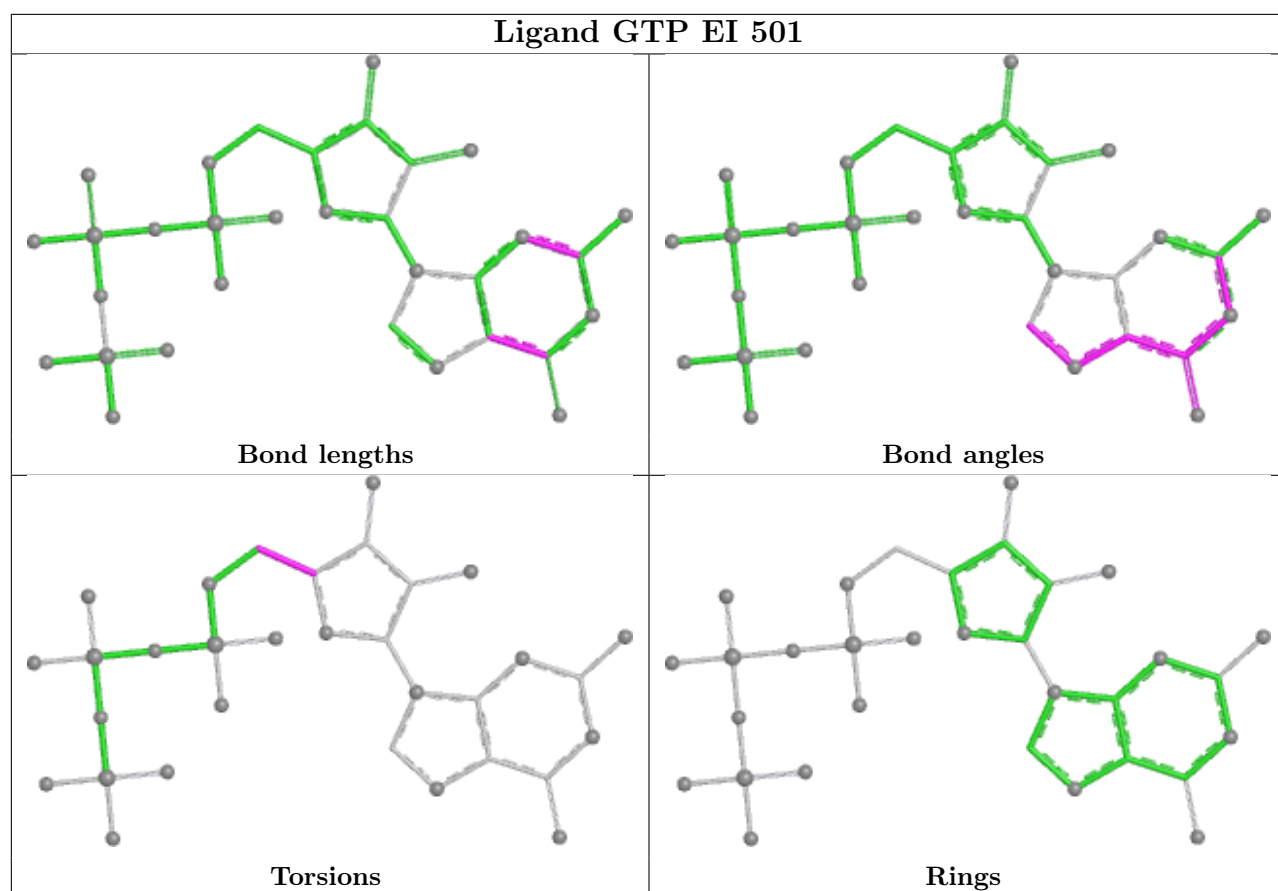


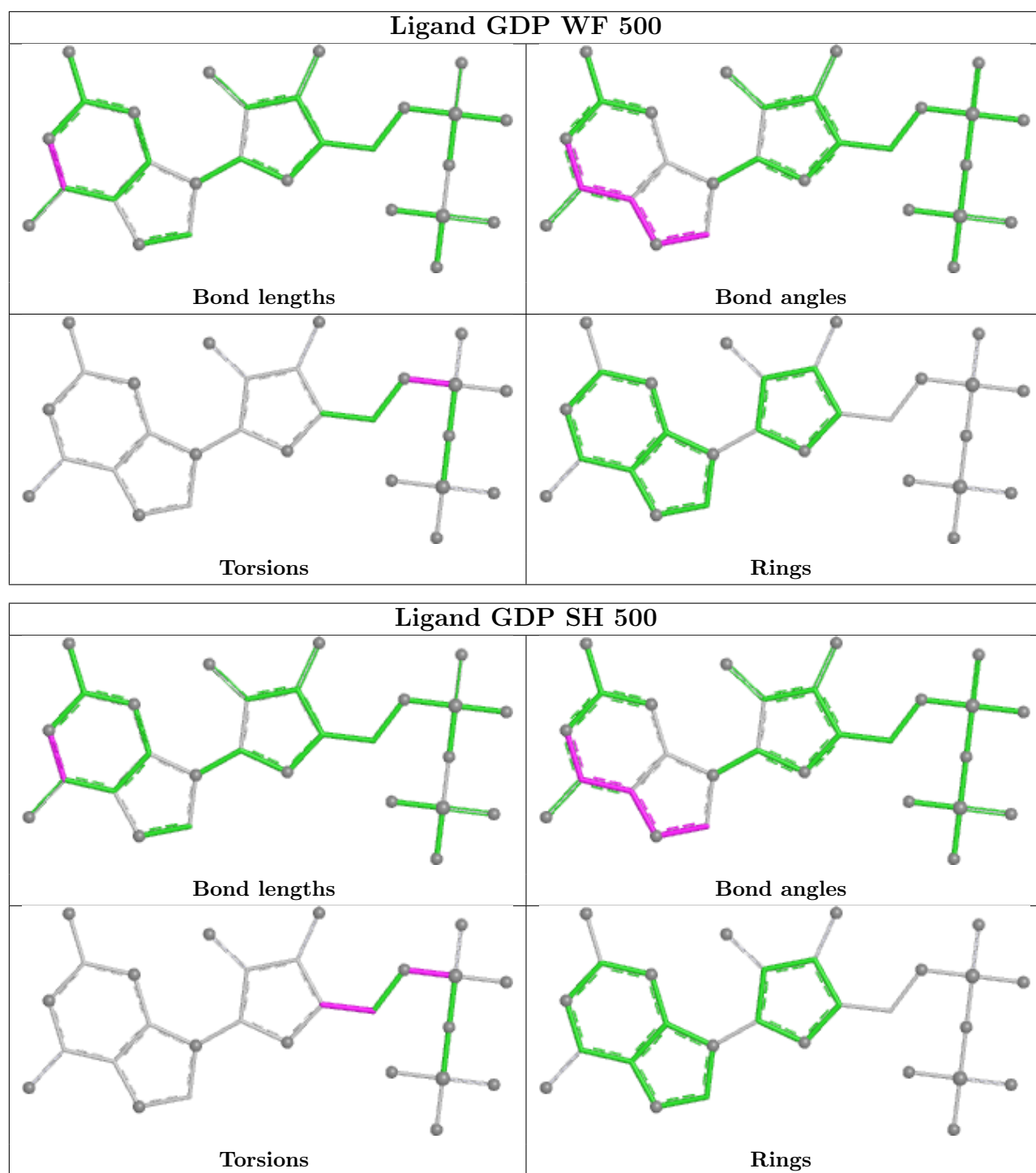
Ligand GDP T 500



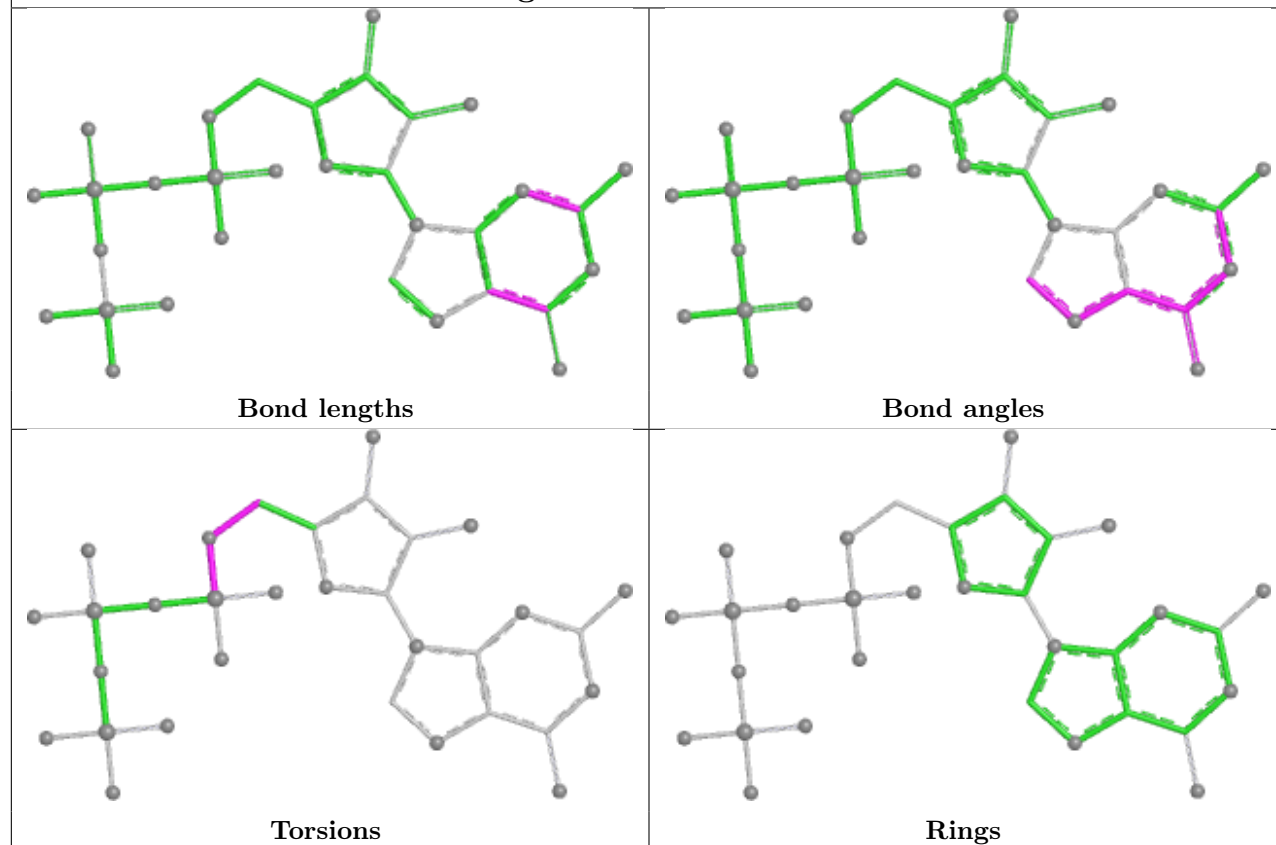




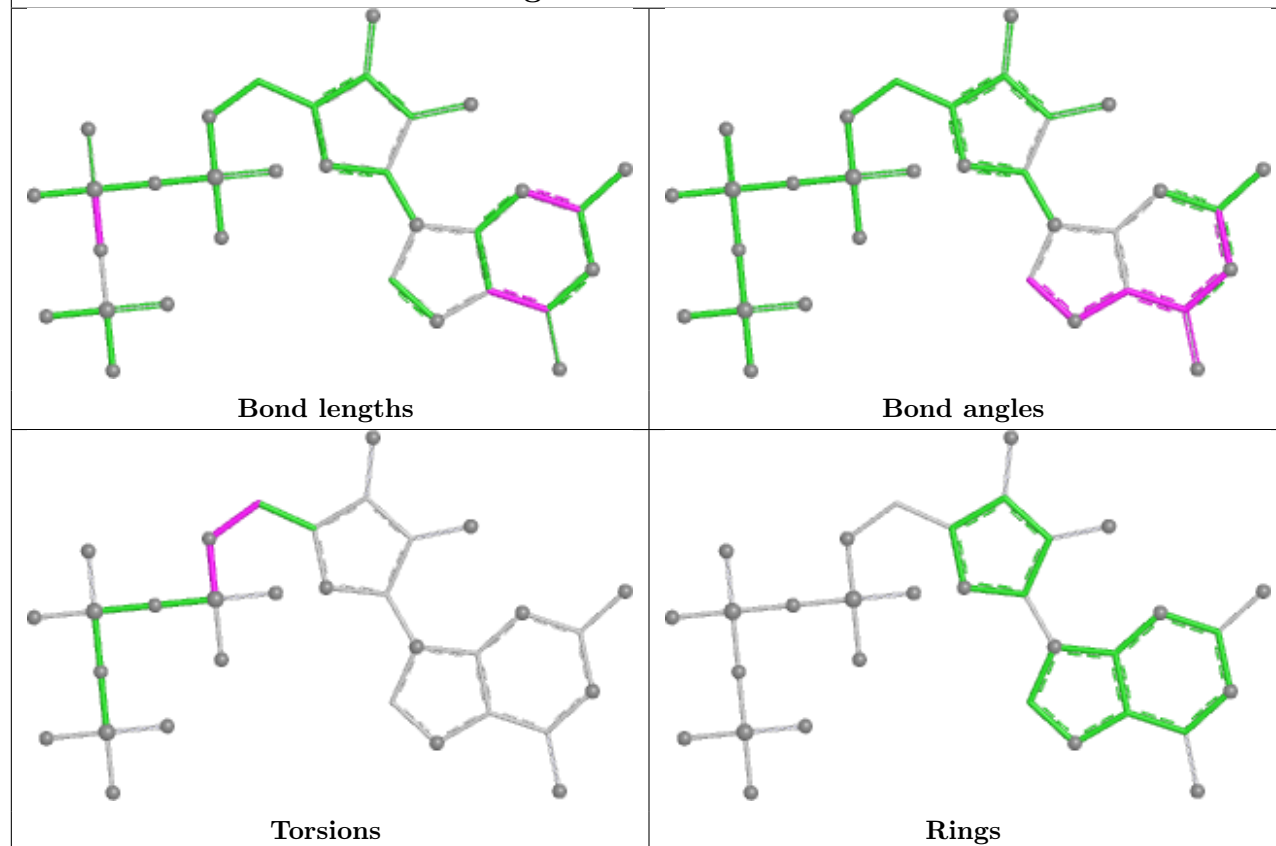


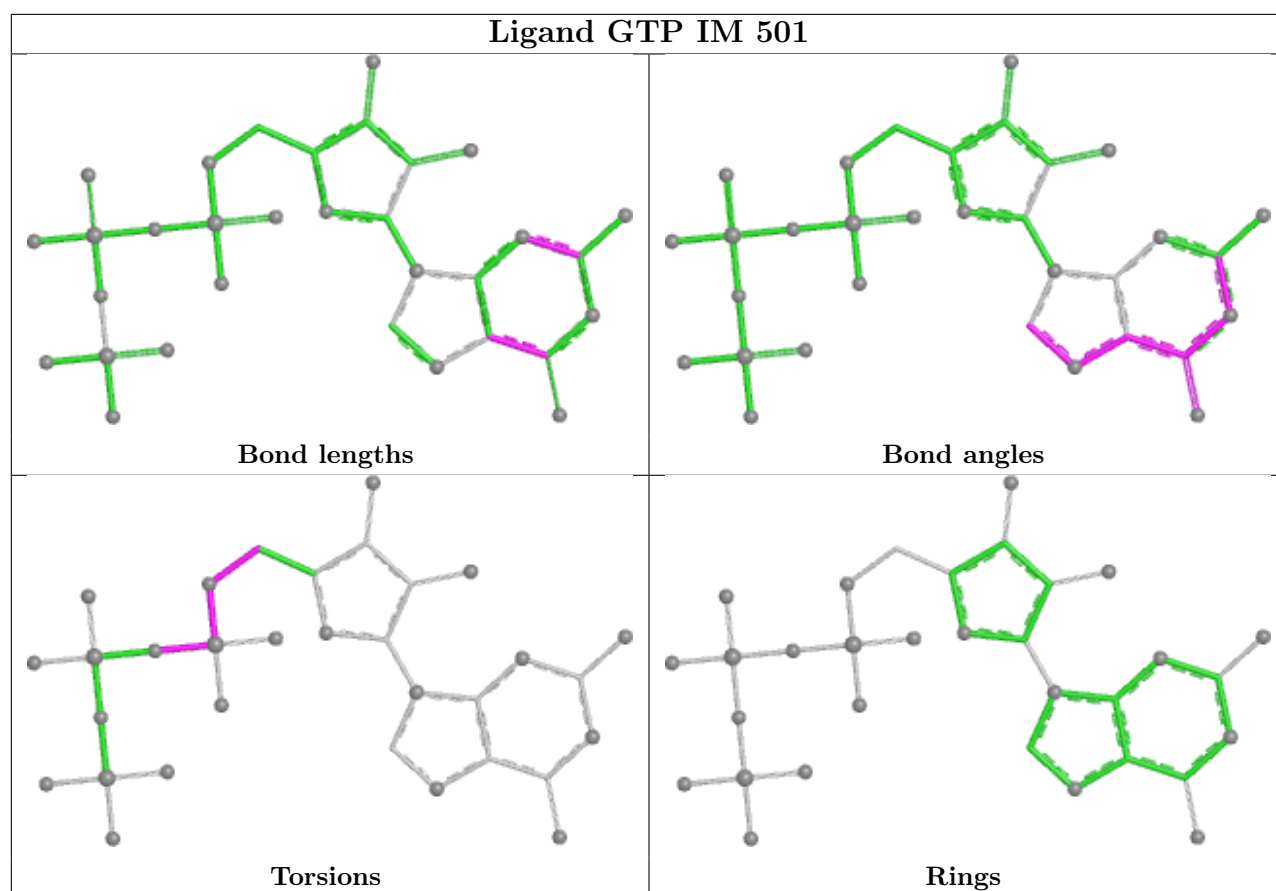


Ligand GTP AC 501



Ligand GTP IC 501





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.

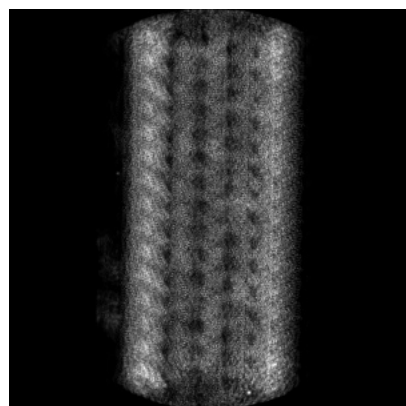
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-47661. These allow visual inspection of the internal detail of the map and identification of artifacts.

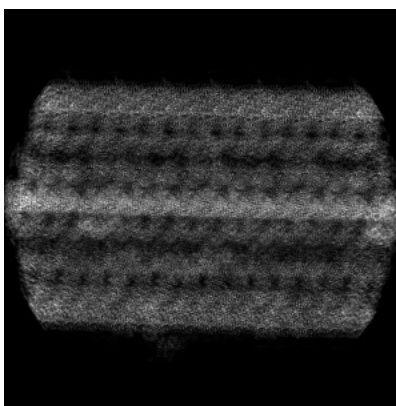
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

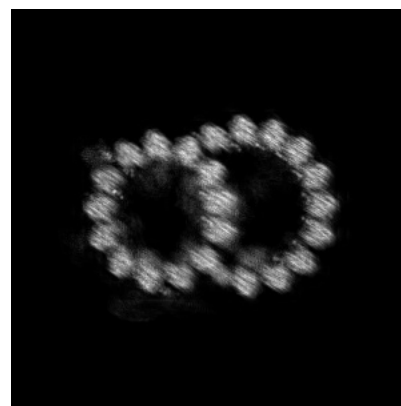
6.1.1 Primary map



X

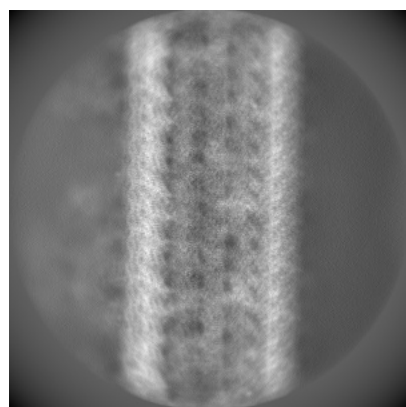


Y

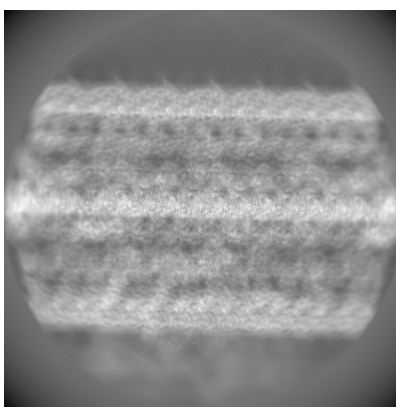


Z

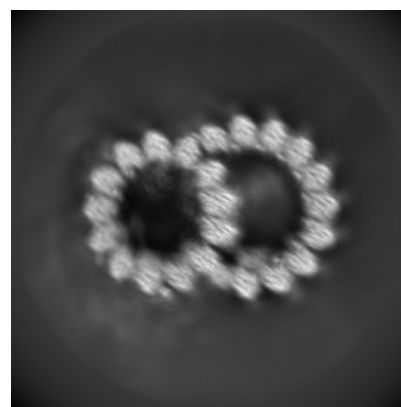
6.1.2 Raw map



X



Y

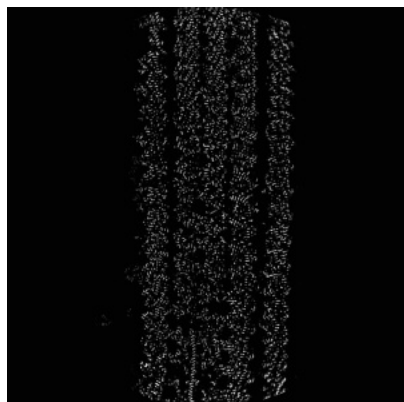


Z

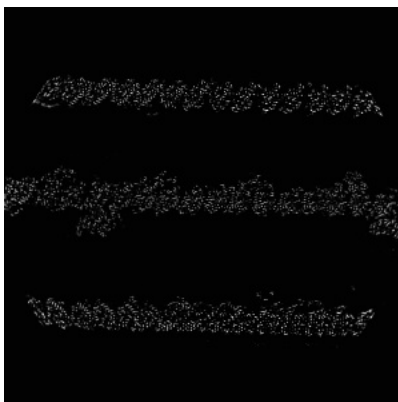
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

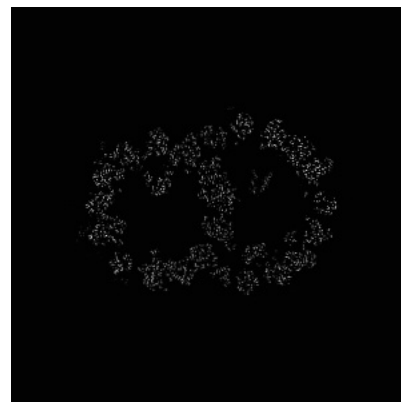
6.2.1 Primary map



X Index: 256

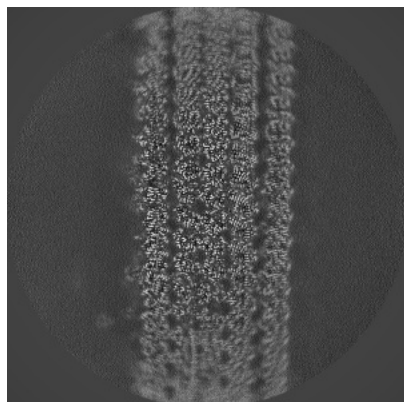


Y Index: 256

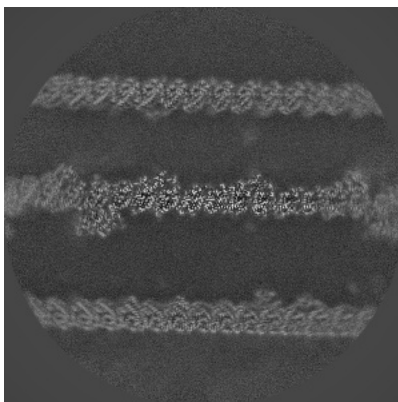


Z Index: 256

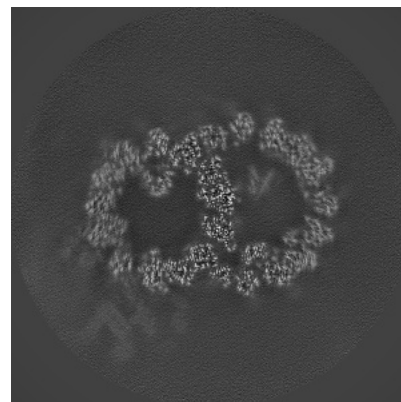
6.2.2 Raw map



X Index: 256



Y Index: 256

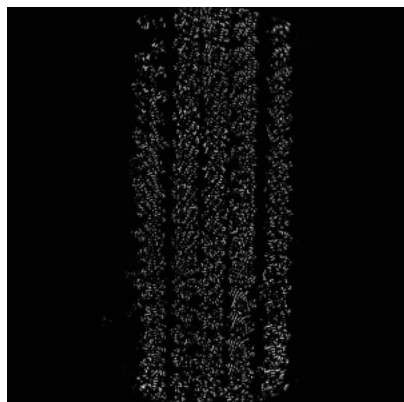


Z Index: 256

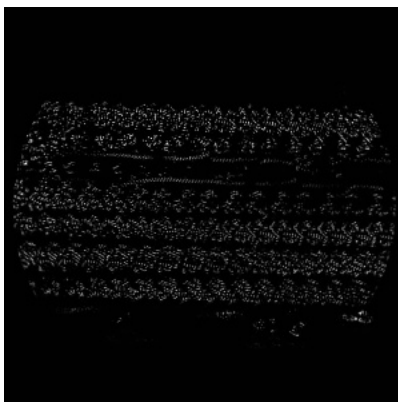
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 260

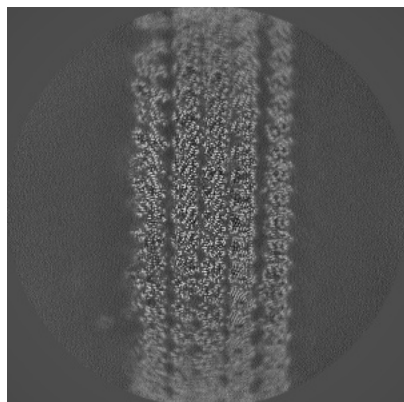


Y Index: 335

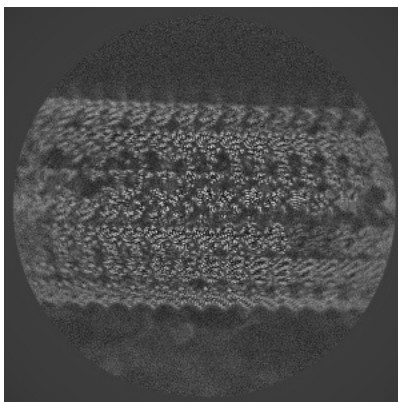


Z Index: 57

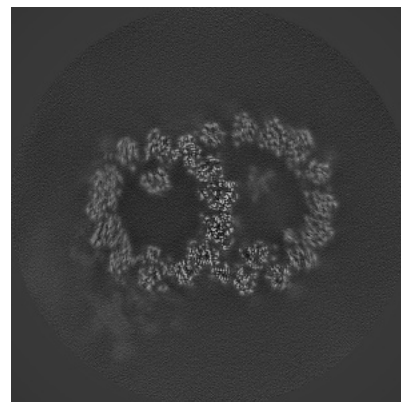
6.3.2 Raw map



X Index: 260



Y Index: 176

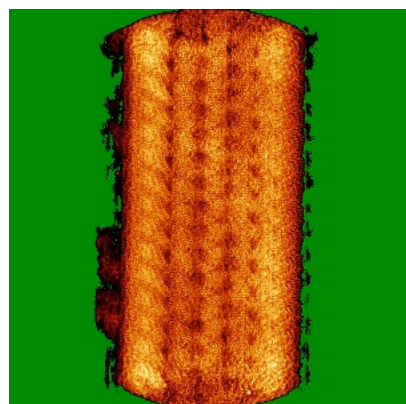


Z Index: 250

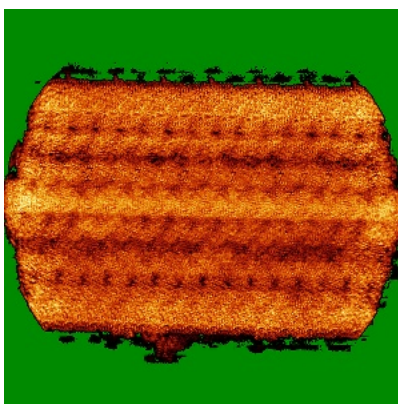
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

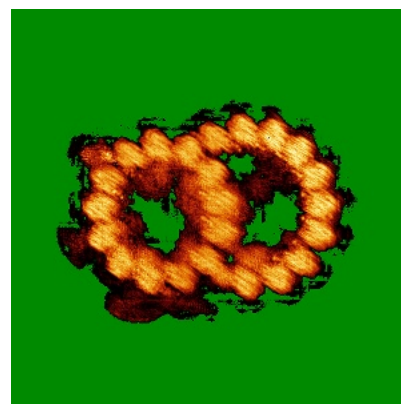
6.4.1 Primary map



X

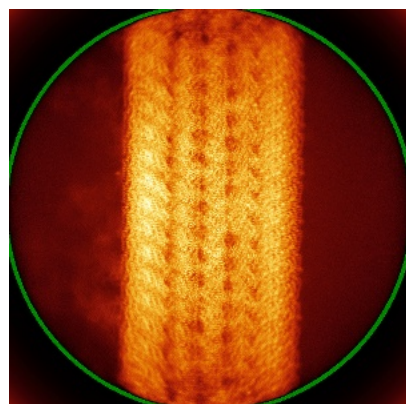


Y

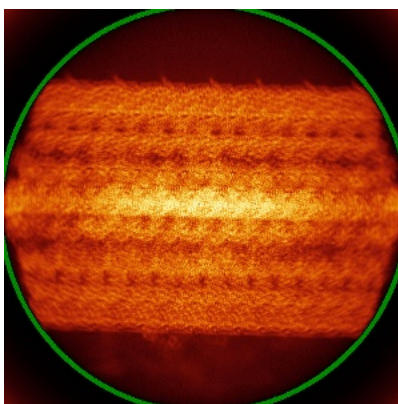


Z

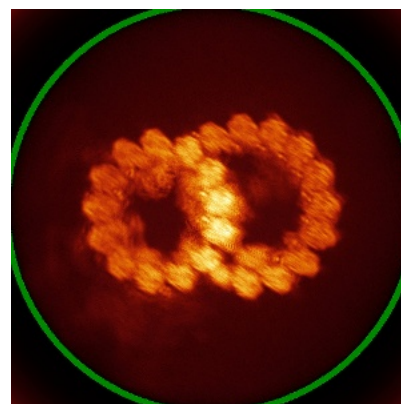
6.4.2 Raw map



X



Y

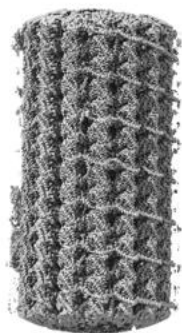


Z

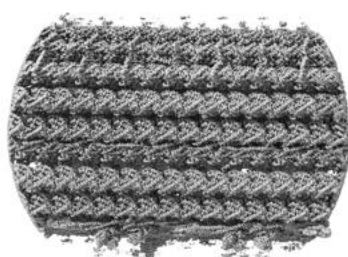
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

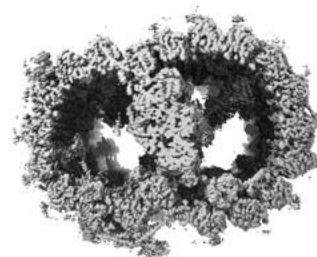
6.5.1 Primary map



X



Y



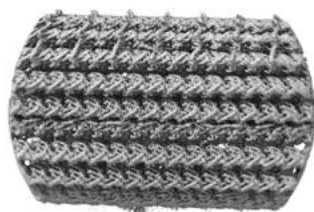
Z

The images above show the 3D surface view of the map at the recommended contour level 0.0435. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

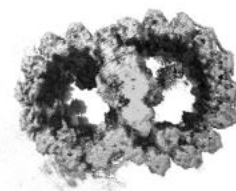
6.5.2 Raw map



X



Y



Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

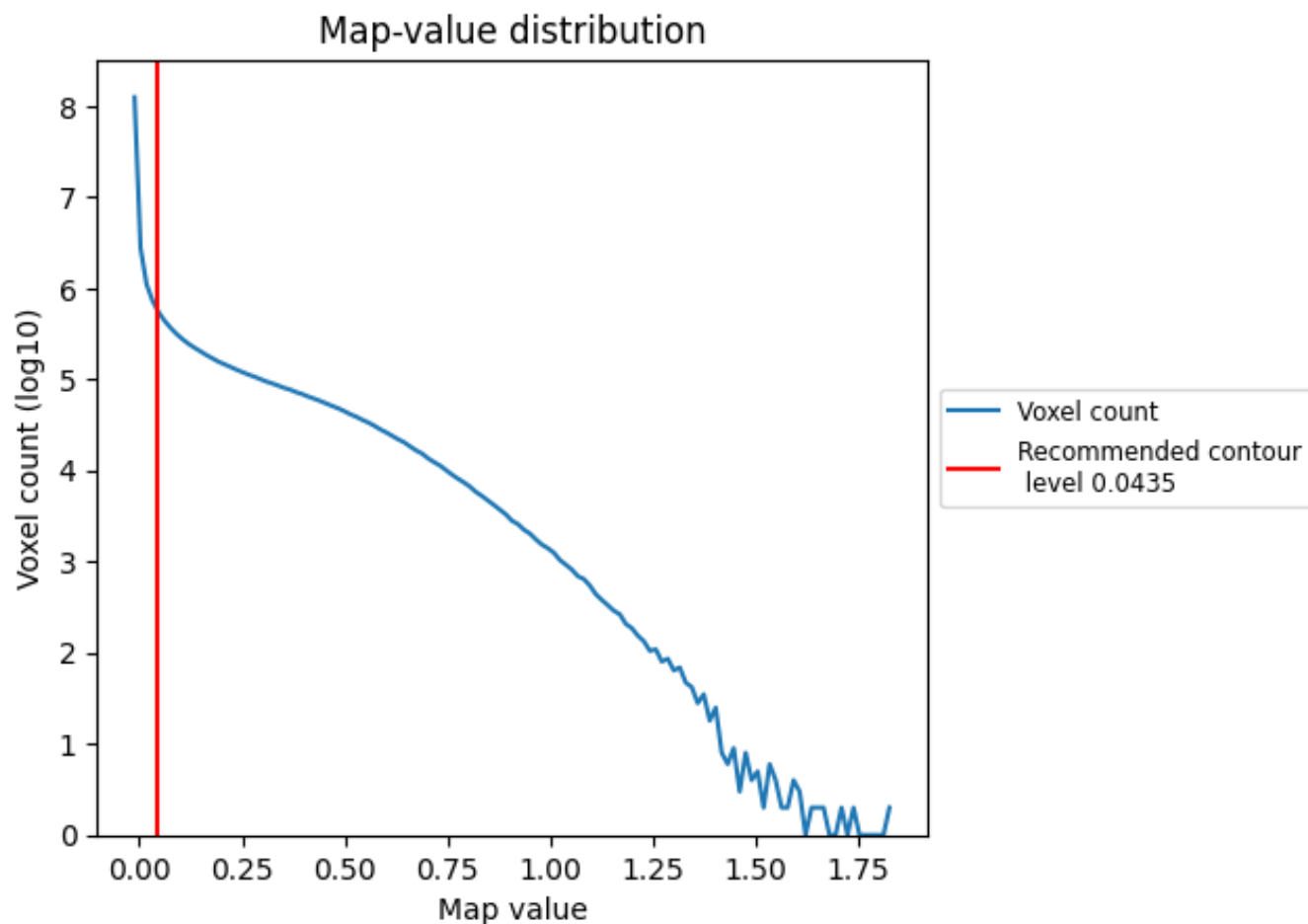
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

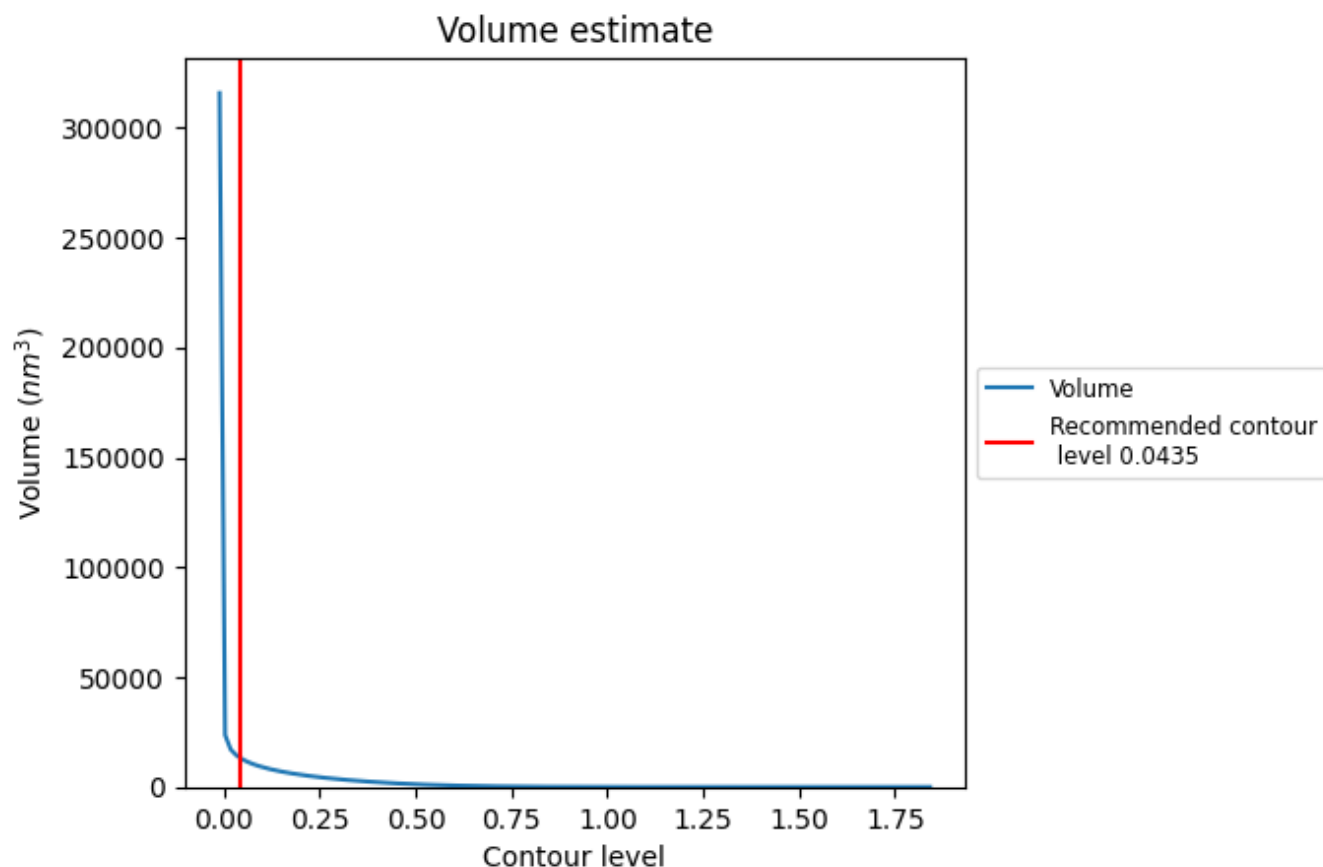
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

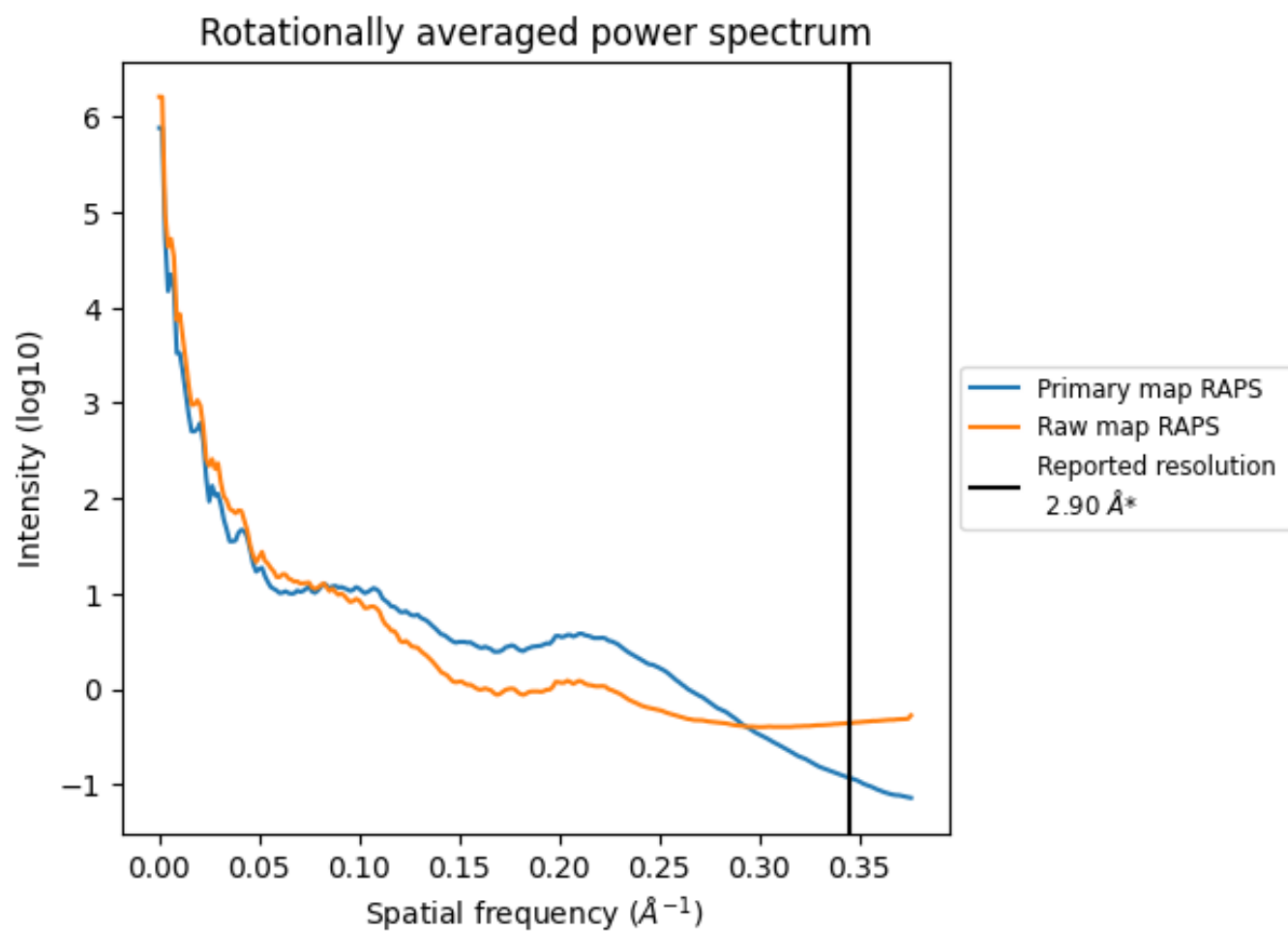
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 13083 nm^3 ; this corresponds to an approximate mass of 11818 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

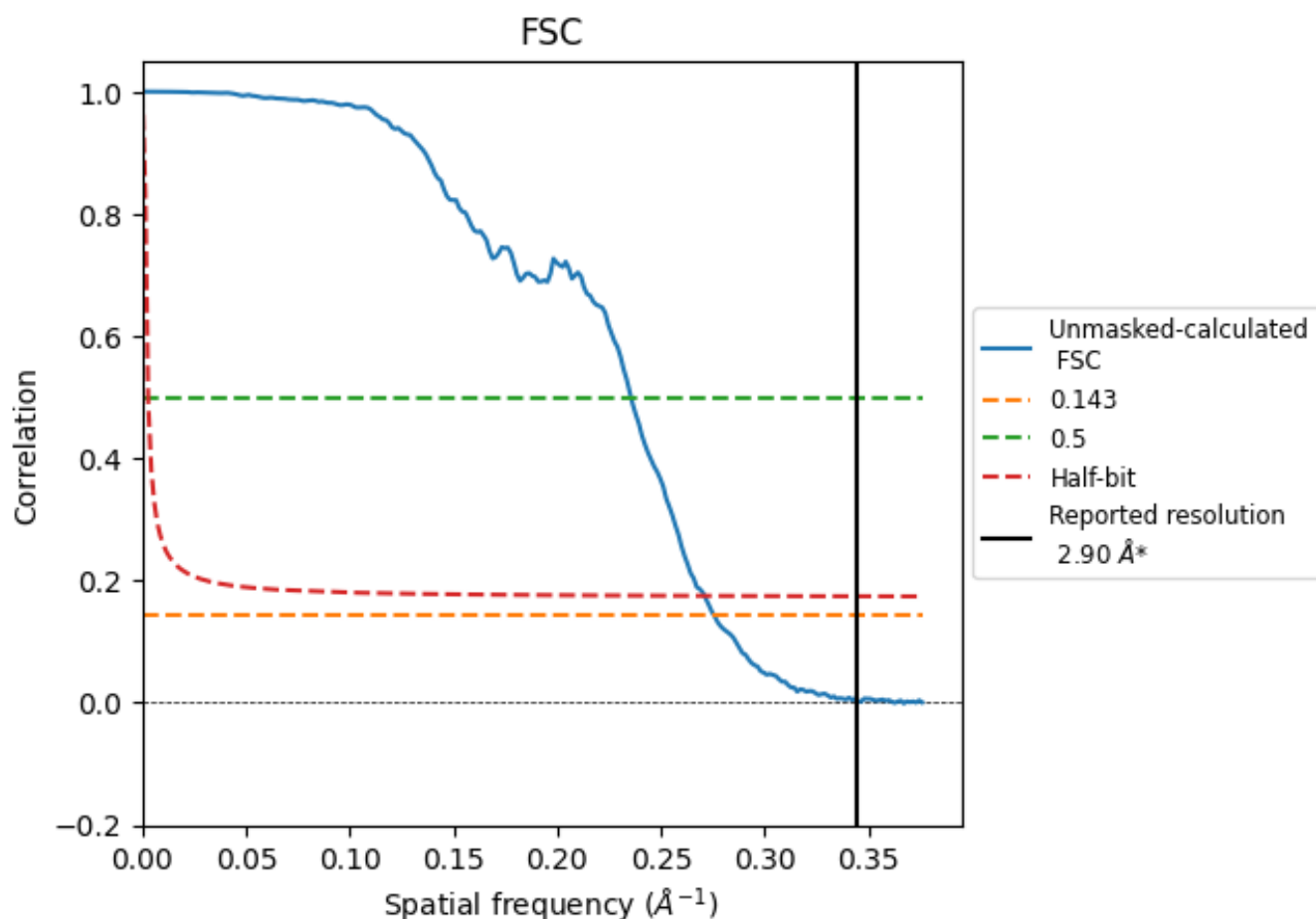


*Reported resolution corresponds to spatial frequency of 0.345 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.345 \AA^{-1}

8.2 Resolution estimates [i](#)

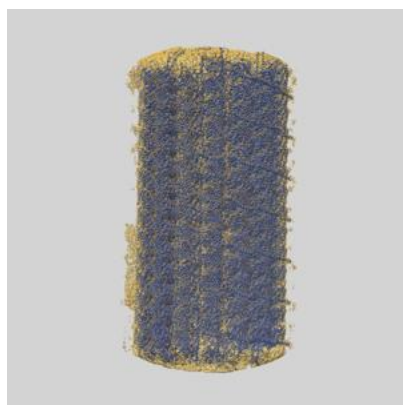
| Resolution estimate (Å) | Estimation criterion (FSC cut-off) | | |
|---------------------------|------------------------------------|------|----------|
| | 0.143 | 0.5 | Half-bit |
| Reported by author | 2.90 | - | - |
| Author-provided FSC curve | - | - | - |
| Unmasked-calculated* | 3.63 | 4.25 | 3.69 |

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.63 differs from the reported value 2.9 by more than 10 %

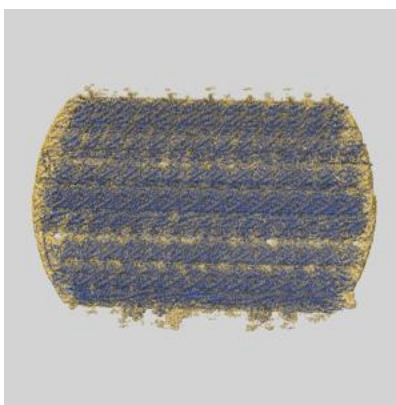
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-47661 and PDB model 9E78. Per-residue inclusion information can be found in section [3](#) on page [78](#).

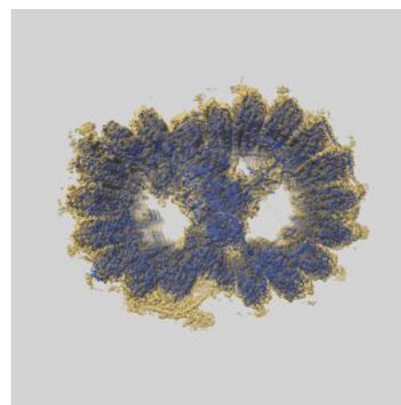
9.1 Map-model overlay [i](#)



X



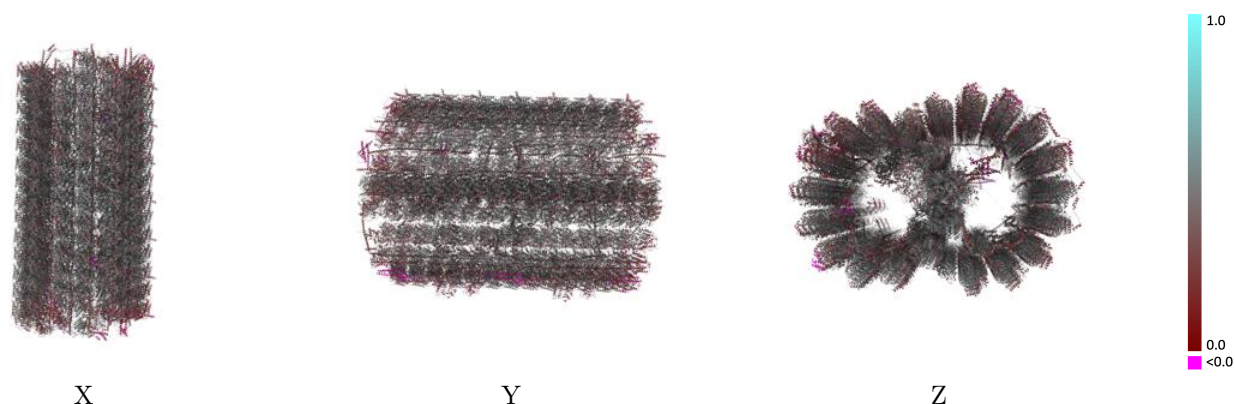
Y



Z

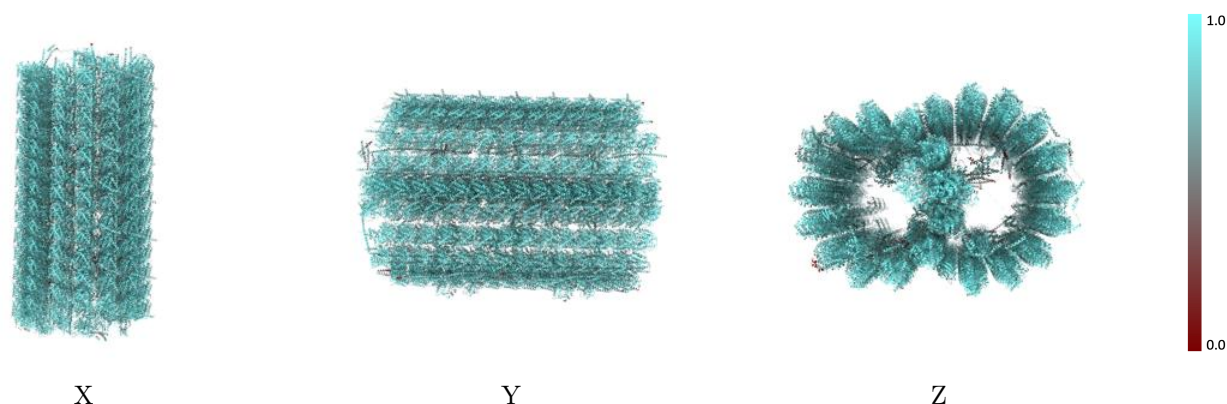
The images above show the 3D surface view of the map at the recommended contour level 0.0435 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



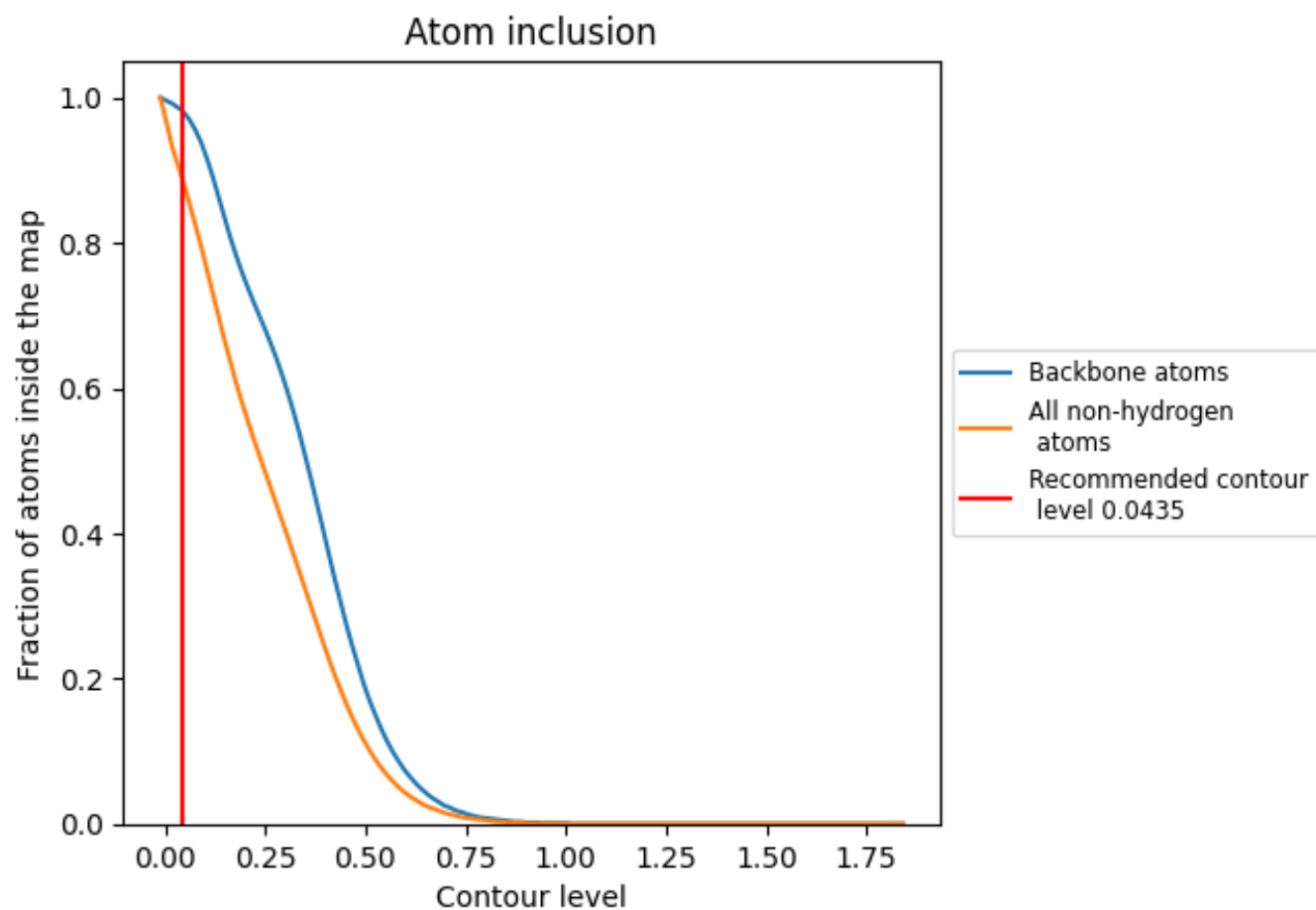
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0435).







































































9.4 Atom inclusion ⓘ



At the recommended contour level, 98% of all backbone atoms, 89% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ





















































































The table lists the average atom inclusion at the recommended contour level (0.0435) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion | Q-score |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| All |  0.8880 |  0.4210 |
| 0 |  0.9160 |  0.4480 |
| 0A |  0.8850 |  0.4350 |
| 0C |  0.8910 |  0.3690 |
| 0D |  0.8720 |  0.3660 |
| 0F |  0.7950 |  0.3640 |
| 0G |  0.7170 |  0.3190 |
| 0H |  0.7580 |  0.2040 |
| 0I |  0.7390 |  0.3240 |
| 0J |  0.6720 |  0.2350 |
| 0L |  0.8890 |  0.4600 |
| 0M |  0.8840 |  0.4480 |
| 0N |  0.8950 |  0.4530 |
| 0O |  0.8840 |  0.3550 |
| 0R |  0.8060 |  0.3460 |
| 0S |  0.7640 |  0.2880 |
| 0U |  0.9020 |  0.4490 |
| 0W |  0.8800 |  0.4120 |
| 0Y |  0.8680 |  0.4330 |
| 0Z |  0.8530 |  0.4300 |
| 0a |  0.9300 |  0.4500 |
| 0c |  0.8520 |  0.3860 |
| 0d |  0.8200 |  0.3890 |
| 0f |  0.9100 |  0.4450 |
| 0g |  0.9630 |  0.4340 |
| 0k |  0.6530 |  0.3150 |
| 0l |  0.6000 |  0.2870 |
| 0m |  0.7810 |  0.3010 |
| 0n |  0.7260 |  0.2490 |
| 0o |  0.8230 |  0.2330 |
| 0p |  0.7980 |  0.3660 |
| 0r |  0.8720 |  0.4170 |
| 0t |  0.9170 |  0.4450 |
| 0u |  0.9330 |  0.3880 |
| 0v |  0.8010 |  0.2720 |























































































Continued on next page...

Continued from previous page...

| Chain | Atom inclusion | Q-score |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| 0w |  0.8000 |  0.3660 |
| 0x |  0.8590 |  0.3840 |
| 0z |  0.6470 |  0.2820 |
| 1A |  0.9000 |  0.4510 |
| 1B |  0.8750 |  0.4150 |
| 1D |  0.9080 |  0.4130 |
| 1E |  0.8990 |  0.4500 |
| 1F |  0.9150 |  0.4370 |
| 1H |  0.8070 |  0.3570 |
| 1I |  0.8390 |  0.3890 |
| 1J |  0.8380 |  0.3950 |
| 1K |  0.8160 |  0.3610 |
| 1O |  0.8620 |  0.4220 |
| 1Q |  0.8580 |  0.4180 |
| 1S |  0.8690 |  0.4380 |
| 1T |  0.8940 |  0.3180 |
| 1U |  0.7920 |  0.3710 |
| 1V |  0.8590 |  0.3940 |
| 1X |  0.8000 |  0.3550 |
| 1Y |  0.8010 |  0.3670 |
| 1a |  0.7680 |  0.3020 |
| 1b |  0.8410 |  0.3670 |
| 1c |  0.8800 |  0.3020 |
| 1d |  0.7740 |  0.3520 |
| 1e |  0.8810 |  0.4110 |
| 1g |  0.7090 |  0.3340 |
| 1h |  0.7740 |  0.3420 |
| 1j |  0.9090 |  0.4510 |
| 1k |  0.8890 |  0.4250 |
| 1l |  0.9060 |  0.4540 |
| 1m |  0.9510 |  0.4220 |
| 1o |  0.8860 |  0.4380 |
| 1q |  0.7780 |  0.3830 |
| 1r |  0.6860 |  0.2710 |
| 1s |  0.6750 |  0.2930 |
| 1t |  0.5320 |  0.0680 |
| 1w |  0.7560 |  0.3270 |
| 1x |  0.7860 |  0.3480 |
| 1y |  0.7280 |  0.2370 |
| 2B |  0.8930 |  0.4620 |
| 2C |  0.8960 |  0.4540 |
| 2F |  0.9060 |  0.4620 |





















































































Continued on next page...

Continued from previous page...

| Chain | Atom inclusion | Q-score |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| 2G |  0.8950 |  0.4600 |
| 2H |  0.8950 |  0.4490 |
| 2I |  0.9160 |  0.4440 |
| 2L |  0.8160 |  0.3620 |
| 2N |  0.8980 |  0.4500 |
| 2O |  0.8930 |  0.4300 |
| 2Q |  0.8320 |  0.3880 |
| 2S |  0.8920 |  0.4610 |
| 2U |  0.8670 |  0.3950 |
| 2V |  0.8510 |  0.3620 |
| 2X |  0.8130 |  0.3930 |
| 2Z |  0.8650 |  0.4380 |
| 2b |  0.8390 |  0.3770 |
| 2c |  0.7420 |  0.3070 |
| 2e |  0.7770 |  0.3410 |
| 2f |  0.8440 |  0.3040 |
| 2h |  0.7640 |  0.3220 |
| 2i |  0.7280 |  0.2720 |
| 2k |  0.7740 |  0.3290 |
| 2l |  0.7340 |  0.2760 |
| 2n |  0.7450 |  0.2540 |
| 2o |  0.7050 |  0.2880 |
| 2p |  0.7240 |  0.1920 |
| 2r |  0.8400 |  0.3680 |
| 2t |  0.8660 |  0.3870 |
| 2v |  0.9380 |  0.4070 |
| 2w |  0.9270 |  0.4560 |
| 2y |  0.8830 |  0.4480 |
| 2z |  0.8970 |  0.4320 |
| 3B |  0.8900 |  0.4300 |
| 3D |  0.8480 |  0.4040 |
| 3F |  0.5500 |  0.1620 |
| 3G |  0.6840 |  0.2400 |
| 3H |  0.5300 |  0.1880 |
| 3I |  0.6770 |  0.2210 |
| 3L |  0.8060 |  0.4230 |
| 3M |  0.3800 |  0.2070 |
| 3P |  0.9170 |  0.4040 |
| 3Q |  0.9120 |  0.4390 |
| 3S |  0.8660 |  0.4270 |
| 3U |  0.8770 |  0.4240 |
| 3W |  0.7950 |  0.3860 |





















































































Continued on next page...

Continued from previous page...

| Chain | Atom inclusion | Q-score |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| 3X |  0.7930 |  0.3590 |
| 3Z |  0.7920 |  0.4000 |
| 3a |  0.8620 |  0.4370 |
| 3b |  0.8100 |  0.3510 |
| 3d |  0.7290 |  0.3150 |
| 3f |  0.7670 |  0.2750 |
| 3g |  0.7660 |  0.3530 |
| 3h |  0.7410 |  0.3130 |
| 3i |  0.7600 |  0.2080 |
| 3m |  0.7850 |  0.3700 |
| 3o |  0.8040 |  0.3350 |
| 3p |  0.8160 |  0.3940 |
| 3r |  0.7720 |  0.3230 |
| 3s |  0.7770 |  0.3470 |
| 3t |  0.7420 |  0.2640 |
| 3w |  0.8640 |  0.4210 |
| 3x |  0.8260 |  0.3810 |
| 4A |  0.8190 |  0.3750 |
| 4B |  0.8280 |  0.4110 |
| 4I |  0.5320 |  0.2360 |
| 4O |  0.8310 |  0.3900 |
| 4P |  0.8790 |  0.4120 |
| 4V |  0.8320 |  0.3940 |
| 4W |  0.8170 |  0.3940 |
| 4Y |  0.7560 |  0.3100 |
| 4a |  0.8030 |  0.3660 |
| 4b |  0.8520 |  0.4110 |
| 5B |  0.7560 |  0.2440 |
| 5C |  0.6470 |  0.1700 |
| 5D |  0.5490 |  0.0640 |
| 5G |  0.7830 |  0.2690 |
| 5H |  0.6710 |  0.1750 |
| 5I |  0.5360 |  0.0410 |
| 5K |  0.7980 |  0.3300 |
| 5L |  0.7240 |  0.2430 |
| 5O |  0.8050 |  0.3160 |
| 5P |  0.6270 |  0.1820 |
| 5S |  0.7540 |  0.3230 |
| 5T |  0.6320 |  0.2100 |
| A |  0.9280 |  0.4400 |
| AA |  0.9150 |  0.4540 |
| AB |  0.9190 |  0.4630 |





















































































Continued on next page...

Continued from previous page...

| Chain | Atom inclusion | Q-score |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| AC |  0.9080 |  0.4530 |
| AD |  0.9210 |  0.4610 |
| AE |  0.9100 |  0.4490 |
| AF |  0.9190 |  0.4580 |
| AG |  0.9000 |  0.4470 |
| AH |  0.9220 |  0.4510 |
| AI |  0.9140 |  0.4460 |
| AJ |  0.9210 |  0.4560 |
| AK |  0.9030 |  0.4480 |
| AL |  0.9250 |  0.4610 |
| AM |  0.9280 |  0.4610 |
| AN |  0.9270 |  0.4280 |
| B |  0.9080 |  0.4110 |
| BA |  0.9010 |  0.4380 |
| BB |  0.8440 |  0.4250 |
| BC |  0.8100 |  0.4050 |
| BD |  0.9030 |  0.4400 |
| BE |  0.9120 |  0.4380 |
| BF |  0.9110 |  0.4510 |
| BG |  0.9100 |  0.4370 |
| BH |  0.9120 |  0.4410 |
| BI |  0.8940 |  0.4200 |
| BJ |  0.9060 |  0.4360 |
| BK |  0.9100 |  0.4500 |
| BL |  0.9230 |  0.4550 |
| BM |  0.9160 |  0.4370 |
| BN |  0.8530 |  0.3720 |
| C |  0.9040 |  0.4260 |
| CA |  0.9150 |  0.4690 |
| CB |  0.9050 |  0.4580 |
| CC |  0.9090 |  0.4500 |
| CD |  0.9150 |  0.4340 |
| CE |  0.9150 |  0.4520 |
| CF |  0.9120 |  0.4510 |
| CG |  0.9090 |  0.4450 |
| CH |  0.9110 |  0.4270 |
| CI |  0.9150 |  0.4410 |
| CJ |  0.9160 |  0.4540 |
| CK |  0.9040 |  0.4350 |
| CL |  0.9130 |  0.4330 |
| CM |  0.9100 |  0.3410 |
| D |  0.8050 |  0.3160 |





















































































Continued on next page...

Continued from previous page...

| Chain | Atom inclusion | Q-score |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| DA |  0.8960 |  0.4500 |
| DB |  0.8980 |  0.4630 |
| DC |  0.9000 |  0.4510 |
| DD |  0.9050 |  0.4450 |
| DE |  0.9100 |  0.4490 |
| DF |  0.9130 |  0.4570 |
| DG |  0.9070 |  0.4440 |
| DH |  0.9160 |  0.4430 |
| DI |  0.9190 |  0.4440 |
| DJ |  0.9180 |  0.4530 |
| DK |  0.9180 |  0.4490 |
| DL |  0.9160 |  0.4300 |
| DM |  0.8830 |  0.3200 |
| E |  0.8940 |  0.4210 |
| EA |  0.8950 |  0.4500 |
| EB |  0.8930 |  0.4610 |
| EC |  0.9010 |  0.4570 |
| ED |  0.9050 |  0.4560 |
| EE |  0.9030 |  0.4540 |
| EF |  0.9120 |  0.4600 |
| EG |  0.9140 |  0.4400 |
| EH |  0.9110 |  0.4340 |
| EI |  0.9070 |  0.4420 |
| EJ |  0.9070 |  0.4460 |
| EK |  0.9140 |  0.4360 |
| EL |  0.9040 |  0.3670 |
| F |  0.9040 |  0.4010 |
| FA |  0.8880 |  0.4290 |
| FB |  0.9090 |  0.4650 |
| FC |  0.9170 |  0.4680 |
| FD |  0.9010 |  0.4590 |
| FE |  0.9060 |  0.4660 |
| FF |  0.9220 |  0.4660 |
| FG |  0.9240 |  0.4580 |
| FH |  0.9230 |  0.4530 |
| FI |  0.9210 |  0.4520 |
| FJ |  0.9200 |  0.4490 |
| FK |  0.9210 |  0.4380 |
| FL |  0.9290 |  0.4100 |
| G |  0.7650 |  0.2810 |
| GA |  0.8330 |  0.3440 |
| GB |  0.8000 |  0.3760 |





















































































Continued on next page...

Continued from previous page...

| Chain | Atom inclusion | Q-score |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| GC |  0.8420 |  0.3790 |
| GD |  0.8750 |  0.4130 |
| GE |  0.8940 |  0.4380 |
| GF |  0.8930 |  0.4410 |
| GG |  0.9000 |  0.4450 |
| GH |  0.9080 |  0.4350 |
| GI |  0.9060 |  0.4310 |
| GJ |  0.9070 |  0.4310 |
| GK |  0.9110 |  0.4320 |
| GL |  0.9020 |  0.3870 |
| H |  0.8110 |  0.2930 |
| HA |  0.8780 |  0.3640 |
| HB |  0.8430 |  0.3840 |
| HC |  0.8480 |  0.3890 |
| HD |  0.8810 |  0.4070 |
| HE |  0.8770 |  0.4100 |
| HF |  0.8910 |  0.4200 |
| HG |  0.8930 |  0.4230 |
| HH |  0.8970 |  0.4210 |
| HI |  0.8870 |  0.4120 |
| HJ |  0.8960 |  0.4160 |
| HK |  0.9110 |  0.4270 |
| HL |  0.8920 |  0.3840 |
| HM |  0.9110 |  0.3570 |
| I |  0.9050 |  0.3480 |
| IA |  0.9070 |  0.4040 |
| IB |  0.9200 |  0.4310 |
| IC |  0.9180 |  0.4330 |
| ID |  0.9100 |  0.4310 |
| IE |  0.9050 |  0.4260 |
| IF |  0.9050 |  0.4300 |
| IG |  0.9150 |  0.4450 |
| IH |  0.9120 |  0.4390 |
| II |  0.9070 |  0.4390 |
| IJ |  0.9100 |  0.4370 |
| IK |  0.9080 |  0.4180 |
| IL |  0.9030 |  0.3860 |
| IM |  0.9150 |  0.3820 |
| J |  0.9080 |  0.3680 |
| JA |  0.9170 |  0.4230 |
| JB |  0.9130 |  0.4330 |
| JC |  0.9130 |  0.4310 |





















































































Continued on next page...

Continued from previous page...

| Chain | Atom inclusion | Q-score |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| JD |  0.9120 |  0.4360 |
| JE |  0.9120 |  0.4370 |
| JF |  0.9030 |  0.4410 |
| JG |  0.9050 |  0.4440 |
| JH |  0.8960 |  0.4340 |
| JI |  0.9050 |  0.4500 |
| JJ |  0.9020 |  0.4380 |
| JK |  0.9040 |  0.4190 |
| JL |  0.9090 |  0.4190 |
| JM |  0.9190 |  0.4020 |
| JN |  0.9210 |  0.3650 |
| K |  0.9360 |  0.4230 |
| KA |  0.9290 |  0.4480 |
| KB |  0.9280 |  0.4540 |
| KC |  0.9150 |  0.4550 |
| KD |  0.9230 |  0.4600 |
| KE |  0.9250 |  0.4590 |
| KF |  0.8960 |  0.4460 |
| KG |  0.9090 |  0.4570 |
| KH |  0.9000 |  0.4530 |
| KI |  0.9110 |  0.4650 |
| KJ |  0.9200 |  0.4600 |
| KK |  0.9110 |  0.4430 |
| KL |  0.9180 |  0.4360 |
| KM |  0.9210 |  0.4350 |
| KN |  0.9350 |  0.4250 |
| L |  0.9450 |  0.4420 |
| LA |  0.9500 |  0.4670 |
| LB |  0.9390 |  0.4660 |
| LC |  0.9340 |  0.4750 |
| LD |  0.9300 |  0.4680 |
| LE |  0.9330 |  0.4730 |
| LF |  0.9200 |  0.4730 |
| LG |  0.9140 |  0.4730 |
| LH |  0.9290 |  0.4770 |
| LI |  0.9350 |  0.4810 |
| LJ |  0.9240 |  0.4630 |
| LK |  0.9280 |  0.4720 |
| LL |  0.9320 |  0.4560 |
| LM |  0.9440 |  0.4620 |
| LN |  0.9420 |  0.4580 |
| LO |  0.9440 |  0.4340 |





















































































Continued on next page...

Continued from previous page...

| Chain | Atom inclusion | Q-score |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| M |  0.9390 |  0.4720 |
| MA |  0.9330 |  0.4770 |
| MB |  0.9300 |  0.4780 |
| MC |  0.9160 |  0.4650 |
| MD |  0.9170 |  0.4610 |
| ME |  0.9240 |  0.4710 |
| MF |  0.9220 |  0.4710 |
| MG |  0.9050 |  0.4550 |
| MH |  0.9140 |  0.4560 |
| MI |  0.9060 |  0.4510 |
| MJ |  0.9270 |  0.4590 |
| MK |  0.9050 |  0.4380 |
| ML |  0.9150 |  0.4600 |
| MM |  0.9390 |  0.4680 |
| MN |  0.9400 |  0.4590 |
| N |  0.8900 |  0.3720 |
| NA |  0.8560 |  0.3730 |
| NB |  0.8830 |  0.4050 |
| NC |  0.8640 |  0.3980 |
| ND |  0.8830 |  0.4140 |
| NE |  0.8620 |  0.4020 |
| NF |  0.8600 |  0.4090 |
| NG |  0.8400 |  0.3940 |
| NH |  0.8730 |  0.4170 |
| NI |  0.8680 |  0.4170 |
| NJ |  0.8820 |  0.4230 |
| NK |  0.8640 |  0.3950 |
| NL |  0.8730 |  0.3780 |
| NM |  0.8660 |  0.3410 |
| O |  0.8820 |  0.3260 |
| OA |  0.9030 |  0.3900 |
| OB |  0.9070 |  0.4190 |
| OC |  0.9010 |  0.4210 |
| OD |  0.9040 |  0.4250 |
| OE |  0.9110 |  0.4310 |
| OF |  0.9010 |  0.4330 |
| OG |  0.8860 |  0.4200 |
| OH |  0.9090 |  0.4380 |
| OI |  0.8940 |  0.4370 |
| OJ |  0.8990 |  0.4300 |
| OK |  0.8870 |  0.4120 |
| OL |  0.8740 |  0.3610 |





















































































Continued on next page...

Continued from previous page...

| Chain | Atom inclusion | Q-score |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| OM |  0.8740 |  0.3230 |
| P |  0.8820 |  0.3310 |
| PA |  0.9080 |  0.3870 |
| PB |  0.9120 |  0.4380 |
| PC |  0.9140 |  0.4440 |
| PD |  0.9130 |  0.4390 |
| PE |  0.9140 |  0.4380 |
| PF |  0.9100 |  0.4500 |
| PG |  0.8980 |  0.4460 |
| PH |  0.9110 |  0.4580 |
| PI |  0.9080 |  0.4590 |
| PJ |  0.9080 |  0.4590 |
| PK |  0.9050 |  0.4500 |
| PL |  0.8880 |  0.3930 |
| PM |  0.8900 |  0.3560 |
| Q |  0.8860 |  0.3640 |
| QA |  0.9160 |  0.4420 |
| QB |  0.9190 |  0.4540 |
| QC |  0.9150 |  0.4550 |
| QD |  0.9140 |  0.4460 |
| QE |  0.9130 |  0.4560 |
| QF |  0.9100 |  0.4560 |
| QG |  0.9150 |  0.4720 |
| QH |  0.8940 |  0.4530 |
| QI |  0.9130 |  0.4630 |
| QJ |  0.9240 |  0.4610 |
| QK |  0.8930 |  0.4020 |
| QL |  0.9100 |  0.3670 |
| R |  0.8710 |  0.3580 |
| RA |  0.9130 |  0.4400 |
| RB |  0.9140 |  0.4440 |
| RC |  0.9080 |  0.4450 |
| RD |  0.9100 |  0.4380 |
| RE |  0.9100 |  0.4500 |
| RF |  0.9080 |  0.4610 |
| RG |  0.9060 |  0.4690 |
| RH |  0.9060 |  0.4550 |
| RI |  0.9190 |  0.4530 |
| RJ |  0.9040 |  0.4310 |
| RK |  0.9040 |  0.4220 |
| RL |  0.9100 |  0.3860 |
| S |  0.9250 |  0.4520 |











































































Continued on next page...

Continued from previous page...

| Chain | Atom inclusion | Q-score |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| SA |  0.9210 |  0.4590 |
| SB |  0.9130 |  0.4540 |
| SC |  0.9160 |  0.4470 |
| SD |  0.9160 |  0.4610 |
| SE |  0.9140 |  0.4740 |
| SF |  0.9180 |  0.4760 |
| SG |  0.9240 |  0.4750 |
| SH |  0.9170 |  0.4470 |
| SI |  0.9210 |  0.4500 |
| SJ |  0.9110 |  0.4520 |
| SK |  0.9170 |  0.4210 |
| T |  0.9130 |  0.4200 |
| TA |  0.9000 |  0.4420 |
| TB |  0.9000 |  0.4420 |
| TC |  0.8910 |  0.4120 |
| TD |  0.8990 |  0.4220 |
| TE |  0.9120 |  0.4630 |
| TF |  0.9180 |  0.4650 |
| TG |  0.9140 |  0.4600 |
| TH |  0.9150 |  0.4440 |
| TI |  0.9130 |  0.4440 |
| TJ |  0.9130 |  0.4440 |
| TK |  0.9140 |  0.4340 |
| TL |  0.8410 |  0.2440 |
| U |  0.8820 |  0.3880 |
| UA |  0.8790 |  0.4190 |
| UB |  0.8760 |  0.4210 |
| UC |  0.8900 |  0.4210 |
| UD |  0.9020 |  0.4400 |
| UE |  0.8950 |  0.4400 |
| UF |  0.9010 |  0.4490 |
| UG |  0.9040 |  0.4410 |
| UH |  0.9030 |  0.4290 |
| UI |  0.9030 |  0.4310 |
| UJ |  0.8970 |  0.4320 |
| UK |  0.8920 |  0.4190 |
| UL |  0.8710 |  0.3490 |
| V |  0.9120 |  0.4190 |
| VA |  0.9070 |  0.4440 |
| VB |  0.9120 |  0.4620 |
| VC |  0.9150 |  0.4570 |
| VD |  0.9170 |  0.4550 |

Continued on next page...

Continued from previous page...

| Chain | Atom inclusion | Q-score |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| VE |  0.9070 |  0.4540 |
| VF |  0.9150 |  0.4660 |
| VG |  0.9070 |  0.4570 |
| VH |  0.9100 |  0.4530 |
| VI |  0.9140 |  0.4580 |
| VJ |  0.9180 |  0.4690 |
| VK |  0.9160 |  0.4680 |
| VL |  0.9160 |  0.4510 |
| VM |  0.8750 |  0.3870 |
| W |  0.9130 |  0.4280 |
| WA |  0.9160 |  0.4520 |
| WB |  0.9150 |  0.4580 |
| WC |  0.9160 |  0.4520 |
| WD |  0.9050 |  0.4400 |
| WE |  0.9100 |  0.4450 |
| WF |  0.9100 |  0.4480 |
| WG |  0.9080 |  0.4500 |
| WH |  0.9040 |  0.4460 |
| WI |  0.9120 |  0.4450 |
| WJ |  0.9160 |  0.4680 |
| WK |  0.9140 |  0.4680 |
| WL |  0.9030 |  0.4480 |
| WM |  0.9080 |  0.4230 |
| X |  0.9080 |  0.4630 |
| X1 |  0.8840 |  0.4300 |
| XA |  0.8990 |  0.4670 |
| XB |  0.9250 |  0.4630 |
| XC |  0.9050 |  0.4600 |
| XD |  0.9140 |  0.4670 |
| XE |  0.9150 |  0.4710 |
| XF |  0.9140 |  0.4650 |
| XM |  0.8950 |  0.4500 |
| XN |  0.8770 |  0.4240 |
| XO |  0.8980 |  0.4450 |
| XP |  0.8640 |  0.4220 |
| XQ |  0.9010 |  0.4530 |
| XR |  0.9110 |  0.4260 |