# Full wwPDB EM Validation Report

Mar 22, 2025 – 06:59 am GMT

| | | |
|---|---|---|
| PDB ID | : | 9F5X |
| EMDB ID | : | EMD-50202 |
| Title | : | Structure of the Chlamydomonas reinhardtii respiratory supercomplex I1 III2 IV2 |
| Authors | : | Waltz, F.; Righetto, R.; Kotecha, A.; Engel, B.D. |
| Deposited on | : | 2024-04-30 |
| Resolution | : | 2.82 Å(reported) |

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.

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

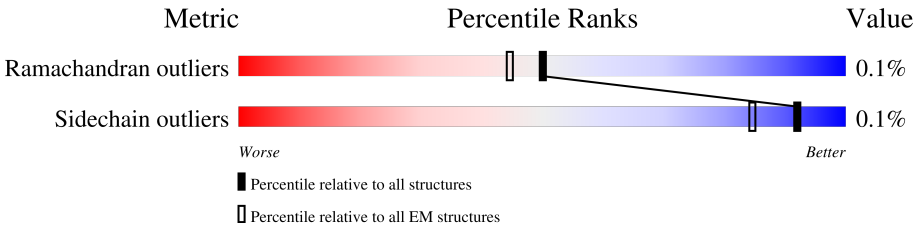
| | | |
|---|---|---|
| EMDB validation analysis | : | 0.0.1.dev117 |
| Mogul | : | 1.8.4, CSD as541be (2020) |
| MolProbity | : | 4.02b-467 |
| buster-report | : | 1.1.7 (2018) |
| Percentile statistics | : | 20231227.v01 (using entries in the PDB archive December 27th 2023) |
| MapQ | : | FAILED |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | 2.41.5 |

# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.82 Å.

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




| Metric | Whole archive (#Entries) | EM structures (#Entries) |
|---|---|---|
| Ramachandran outliers | 207382 | 16835 |
| Sidechain outliers | 206894 | 16415 |

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 <=5%

| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | 1A | 381 | 98% |
| 1 | 1B | 381 | 98% |
| 2 | 1C | 262 | 79% 21% |
| 2 | 1D | 262 | 79% 21% |
| 3 | 1E | 314 | 77% 23% |
| 3 | 1F | 314 | 77% 23% |
| 4 | 1G | 60 | 98% |
| 4 | 1H | 60 | 98% |
| 5 | 1I | 69 | 99% |
| 5 | 1J | 69 | 99% |

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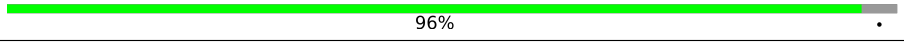
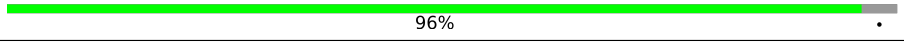
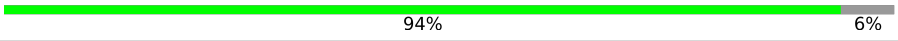
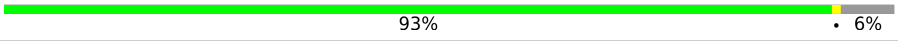
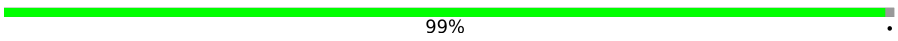
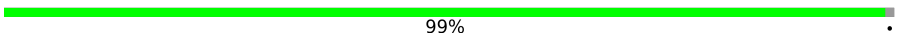
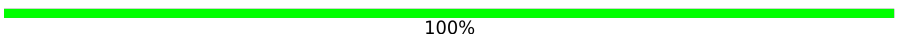
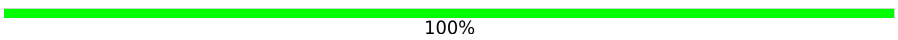
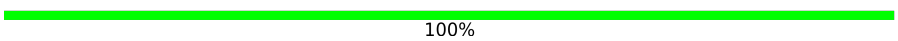
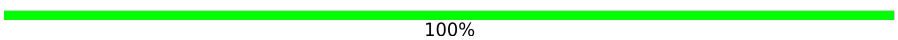
| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 6 | 1K | 73 |   |
| 6 | 1L | 73 |   |
| 7 | 1M | 495 |   |
| 7 | 1N | 495 |   |
| 8 | 1O | 59 |   |
| 8 | 1P | 59 |   |
| 9 | 1Q | 485 |   |
| 9 | 1S | 485 |   |
| 10 | 1R | 123 |   |
| 10 | 1T | 123 |   |
| 11 | 2A | 504 |   |
| 11 | 3A | 504 |   |
| 12 | 2B | 284 |   |
| 12 | 3B | 284 |   |
| 13 | 2C | 153 |   |
| 13 | 3C | 153 |   |
| 14 | 2D | 382 |   |
| 14 | 3D | 382 |   |
| 15 | 2E | 175 |   |
| 15 | 3E | 175 |   |
| 16 | 2F | 96 |   |
| 16 | 3F | 96 |   |
| 17 | 2G | 125 |   |
| 17 | 3G | 125 |   |
| 18 | 2H | 148 |   |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 18 | 3H | 148 | 77% 23% |
| 19 | 2I | 101 | 71% 29% |
| 19 | 3I | 101 | 71% 29% |
| 20 | 2J | 105 | 99% |
| 20 | 3J | 105 | 99% |
| 21 | 2K | 58 | 81% 19% |
| 21 | 3K | 58 | 81% 19% |
| 22 | 2L | 87 | 87% 13% |
| 22 | 3L | 87 | 90% 10% |
| 23 | A | 282 | 85% 15% |
| 24 | B | 484 | 90% 10% |
| 25 | C | 733 | 94% 6% |
| 26 | D | 282 | 77% 23% |
| 27 | E | 467 | 82% 18% |
| 28 | F | 164 | 96% |
| 29 | G | 231 | 86% 14% |
| 30 | H | 118 | 75% 24% |
| 31 | I | 165 | 82% 18% |
| 32 | J | 128 | 66% 34% |
| 32 | r | 128 | 69% 31% |
| 33 | K | 138 | 86% 14% |
| 34 | L | 187 | 88% 12% |
| 35 | M | 154 | 79% 21% |
| 36 | N | 156 | 96% |
| 37 | O | 101 | 98% |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 38 | P | 397 | 91% 9% |
| 39 | Q | 292 | 98% |
| 40 | R | 387 | 100% |
| 41 | S | 279 | 48% 52% |
| 42 | T | 443 | 100% |
| 43 | U | 227 | 46% 54% |
| 44 | V | 546 | 100% |
| 45 | W | 162 | 97% |
| 46 | X | 149 | 84% 16% |
| 47 | Y | 64 | 84% 16% |
| 48 | Z | 124 | 86% 14% |
| 49 | a | 129 | 63% 36% |
| 50 | b | 172 | 84% 16% |
| 51 | c | 67 | 88% 12% |
| 52 | d | 86 | 99% |
| 53 | e | 219 | 99% |
| 54 | f | 65 | 98% |
| 55 | g | 55 | 91% 9% |
| 56 | h | 142 | 76% 24% |
| 57 | i | 81 | 94% 6% |
| 58 | j | 86 | 99% |
| 59 | k | 117 | 100% |
| 60 | l | 121 | 95% |
| 61 | m | 142 | 97% |
| 62 | n | 106 | 98% |

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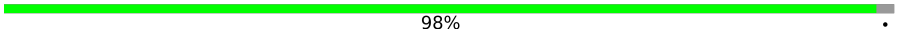
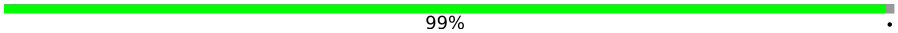
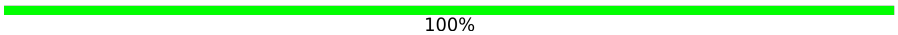
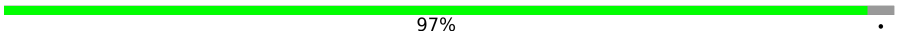
| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 63 | o | 155 |   |
| 64 | p | 130 |   |
| 65 | q | 197 |   |
| 66 | s | 312 |   |
| 67 | t | 279 |   |
| 68 | u | 229 |   |
| 69 | v | 45 |   |
| 70 | w | 109 |   |
| 71 | x | 157 |   |
| 72 | y | 118 |   |

# 2 Entry composition

There are 92 unique types of molecules in this entry. The entry contains 137999 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 Cytochrome b.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 1 | 1A | 376 | Total | C | N | O | S | 0 | 0 |
| | | | 2958 | 1984 | 466 | 491 | 17 | | |
| 1 | 1B | 376 | Total | C | N | O | S | 0 | 0 |
| | | | 2958 | 1984 | 466 | 491 | 17 | | |

- Molecule 2 is a protein called Cytochrome b-c1 complex subunit Rieske, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 2 | 1C | 207 | Total | C | N | O | S | 0 | 0 |
| | | | 1602 | 1017 | 279 | 299 | 7 | | |
| 2 | 1D | 207 | Total | C | N | O | S | 0 | 0 |
| | | | 1602 | 1017 | 279 | 299 | 7 | | |

- Molecule 3 is a protein called Cytochrome c1.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 3 | 1E | 243 | Total | C | N | O | S | 0 | 0 |
| | | | 1898 | 1204 | 326 | 356 | 12 | | |
| 3 | 1F | 243 | Total | C | N | O | S | 0 | 0 |
| | | | 1898 | 1204 | 326 | 356 | 12 | | |

- Molecule 4 is a protein called Complex III subunit 9.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 4 | 1G | 59 | Total | C | N | O | S | 0 | 0 |
| | | | 486 | 316 | 79 | 88 | 3 | | |
| 4 | 1H | 59 | Total | C | N | O | S | 0 | 0 |
| | | | 486 | 316 | 79 | 88 | 3 | | |

- Molecule 5 is a protein called Cytochrome b-c1 complex subunit 6.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 5 | 1I | 68 | Total | C | N | O | S | 0 | 0 |
| | | | 550 | 347 | 92 | 105 | 6 | | |
| 5 | 1J | 68 | Total | C | N | O | S | 0 | 0 |
| | | | 550 | 347 | 92 | 105 | 6 | | |

- Molecule 6 is a protein called Mitochondrial ubiquinol-cytochrome c oxidoreductase subunit 8.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 6 | 1K | 70 | Total | C | N | O | S | 0 | 0 |
| | | | 594 | 386 | 104 | 103 | 1 | | |
| 6 | 1L | 70 | Total | C | N | O | S | 0 | 0 |
| | | | 594 | 386 | 104 | 103 | 1 | | |

- Molecule 7 is a protein called MPP-Beta.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 7 | 1M | 464 | Total | C | N | O | S | 0 | 0 |
| | | | 3646 | 2290 | 641 | 696 | 19 | | |
| 7 | 1N | 464 | Total | C | N | O | S | 0 | 0 |
| | | | 3646 | 2290 | 641 | 696 | 19 | | |

- Molecule 8 is a protein called Mitochondrial ubiquinol-cytochrome c oxidoreductase subunit 10.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 8 | 1O | 48 | Total | C | N | O | S | 0 | 0 |
| | | | 371 | 249 | 61 | 60 | 1 | | |
| 8 | 1P | 48 | Total | C | N | O | S | 0 | 0 |
| | | | 371 | 249 | 61 | 60 | 1 | | |

- Molecule 9 is a protein called Alpha-MPP.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 9 | 1Q | 441 | Total | C | N | O | S | 0 | 0 |
| | | | 3204 | 2018 | 562 | 619 | 5 | | |
| 9 | 1S | 441 | Total | C | N | O | S | 0 | 0 |
| | | | 3204 | 2018 | 562 | 619 | 5 | | |

- Molecule 10 is a protein called Cytochrome b-c1 complex subunit 7.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 10 | 1R | 122 | Total | C | N | O | S | 0 | 0 |
| | | | 980 | 617 | 178 | 183 | 2 | | |
| 10 | 1T | 122 | Total | C | N | O | S | 0 | 0 |
| | | | 980 | 617 | 178 | 183 | 2 | | |

- Molecule 11 is a protein called Cytochrome c oxidase subunit 1.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 11 | 2A | 504 | Total | C | N | O | S | 0 | 0 |
| | | | 3888 | 2600 | 618 | 643 | 27 | | |
| 11 | 3A | 504 | Total | C | N | O | S | 0 | 0 |
| | | | 3888 | 2600 | 618 | 643 | 27 | | |

- Molecule 12 is a protein called Cytochrome c oxidase polypeptide II.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 12 | 2B | 141 | Total | C | N | O | S | 0 | 0 |
| | | | 1169 | 774 | 188 | 201 | 6 | | |
| 12 | 3B | 141 | Total | C | N | O | S | 0 | 0 |
| | | | 1169 | 774 | 188 | 201 | 6 | | |

- Molecule 13 is a protein called cytochrome-c oxidase.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 13 | 2C | 153 | Total | C | N | O | S | 0 | 0 |
| | | | 1212 | 776 | 206 | 223 | 7 | | |
| 13 | 3C | 153 | Total | C | N | O | S | 0 | 0 |
| | | | 1212 | 776 | 206 | 223 | 7 | | |

- Molecule 14 is a protein called Cytochrome c oxidase subunit 3.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 14 | 2D | 266 | Total | C | N | O | S | 0 | 0 |
| | | | 2079 | 1373 | 334 | 351 | 21 | | |
| 14 | 3D | 266 | Total | C | N | O | S | 0 | 0 |
| | | | 2079 | 1373 | 334 | 351 | 21 | | |

- Molecule 15 is a protein called Cox5b.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 15 | 2E | 90 | Total | C | N | O | S | 0 | 0 |
| | | | 737 | 478 | 114 | 144 | 1 | | |

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| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 15 | 3E | 90 | Total | C | N | O | S | 0 | 0 |
| | | | 737 | 478 | 114 | 144 | 1 | | |

- Molecule 16 is a protein called Cox5c.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 16 | 2F | 86 | Total | C | N | O | S | 0 | 0 |
| | | | 706 | 456 | 122 | 126 | 2 | | |
| 16 | 3F | 86 | Total | C | N | O | S | 0 | 0 |
| | | | 706 | 456 | 122 | 126 | 2 | | |

- Molecule 17 is a protein called Cox6a.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 17 | 2G | 91 | Total | C | N | O | S | 0 | 0 |
| | | | 733 | 484 | 120 | 124 | 5 | | |
| 17 | 3G | 91 | Total | C | N | O | S | 0 | 0 |
| | | | 733 | 484 | 120 | 124 | 5 | | |

- Molecule 18 is a protein called Cox6b.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 18 | 2H | 114 | Total | C | N | O | S | 0 | 0 |
| | | | 954 | 606 | 159 | 185 | 4 | | |
| 18 | 3H | 114 | Total | C | N | O | S | 0 | 0 |
| | | | 954 | 606 | 159 | 185 | 4 | | |

- Molecule 19 is a protein called Cox7c.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| 19 | 2I | 72 | Total | C | N | O | 0 | 0 |
| | | | 594 | 393 | 98 | 103 | | |
| 19 | 3I | 72 | Total | C | N | O | 0 | 0 |
| | | | 594 | 393 | 98 | 103 | | |

- Molecule 20 is a protein called Cytochrome c oxidase subunit.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 20 | 2J | 104 | Total | C | N | O | S | 0 | 0 |
| | | | 816 | 522 | 144 | 147 | 3 | | |
| 20 | 3J | 104 | Total | C | N | O | S | 0 | 0 |
| | | | 816 | 522 | 144 | 147 | 3 | | |

- Molecule 21 is a protein called Cox7a.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| 21 | 2K | 47 | Total | C | N | O | 0 | 0 |
| | | | 382 | 249 | 63 | 70 | | |
| 21 | 3K | 47 | Total | C | N | O | 0 | 0 |
| | | | 382 | 249 | 63 | 70 | | |

- Molecule 22 is a protein called CoxIn.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 22 | 2L | 76 | Total | C | N | O | S | 0 | 0 |
| | | | 605 | 390 | 100 | 111 | 4 | | |
| 22 | 3L | 78 | Total | C | N | O | S | 0 | 0 |
| | | | 627 | 405 | 104 | 114 | 4 | | |

- Molecule 23 is a protein called NADH:ubiquinone oxidoreductase 24 kD subunit.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 23 | A | 239 | Total | C | N | O | S | 0 | 0 |
| | | | 1839 | 1165 | 311 | 352 | 11 | | |

- Molecule 24 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 24 | B | 435 | Total | C | N | O | S | 0 | 0 |
| | | | 3331 | 2099 | 592 | 614 | 26 | | |

- Molecule 25 is a protein called NADH:ubiquinone oxidoreductase 78 kDa subunit.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 25 | C | 688 | Total | C | N | O | S | 0 | 0 |
| | | | 5175 | 3235 | 936 | 972 | 32 | | |

- Molecule 26 is a protein called NADH:ubiquinone oxidoreductase 30kDa subunit domain-containing protein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 26 | D | 216 | Total | C | N | O | S | 0 | 0 |
| | | | 1790 | 1156 | 301 | 325 | 8 | | |

- Molecule 27 is a protein called NADH:ubiquinone oxidoreductase 49 kD subunit.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 27 | E | 383 | Total | C | N | O | S | 0 | 0 |
| | | | 3085 | 1971 | 537 | 554 | 23 | | |

- Molecule 28 is a protein called NADH:ubiquinone oxidoreductase subunit 10.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 28 | F | 157 | Total | C | N | O | S | 0 | 0 |
| | | | 1225 | 787 | 211 | 215 | 12 | | |

- Molecule 29 is a protein called NADH:ubiquinone oxidoreductase subunit 8.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 29 | G | 199 | Total | C | N | O | S | 0 | 0 |
| | | | 1615 | 1007 | 281 | 315 | 12 | | |

- Molecule 30 is a protein called B14.5a.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 30 | H | 90 | Total | C | N | O | S | 0 | 0 |
| | | | 750 | 486 | 129 | 132 | 3 | | |

- Molecule 31 is a protein called Mitochondrial NADH:ubiquinone oxidoreductase 18 kDa subunit.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 31 | I | 135 | Total | C | N | O | S | 0 | 0 |
| | | | 1044 | 661 | 173 | 208 | 2 | | |

- Molecule 32 is a protein called Acyl carrier protein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 32 | J | 84 | Total | C | N | O | S | 0 | 0 |
| | | | 640 | 404 | 100 | 133 | 3 | | |
| 32 | r | 88 | Total | C | N | O | S | 0 | 0 |
| | | | 663 | 419 | 104 | 137 | 3 | | |

- Molecule 33 is a protein called NADH:ubiquinone oxidoreductase B14 subunit.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 33 | K | 119 | Total | C | N | O | S | 0 | 0 |
| | | | 986 | 640 | 173 | 168 | 5 | | |

- Molecule 34 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 34 | L | 164 | Total | C | N | O | S | 0 | 0 |
| | | | 1275 | 803 | 221 | 245 | 6 | | |

- Molecule 35 is a protein called NADH:ubiquinone oxidoreductase 13 kD-like subunit.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 35 | M | 121 | Total | C | N | O | S | 0 | 0 |
| | | | 913 | 582 | 150 | 178 | 3 | | |

- Molecule 36 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 36 | N | 150 | Total | C | N | O | S | 0 | 0 |
| | | | 1235 | 791 | 214 | 227 | 3 | | |

- Molecule 37 is a protein called NADH:ubiquinone oxidoreductase B8 subunit.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 37 | O | 100 | Total | C | N | O | S | 0 | 0 |
| | | | 761 | 471 | 138 | 147 | 5 | | |

- Molecule 38 is a protein called Putative NADH:ubiquinone oxidoreductase 39 kDa subunit.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 38 | P | 363 | Total | C | N | O | S | 0 | 0 |
| | | | 2823 | 1793 | 489 | 527 | 14 | | |

- Molecule 39 is a protein called NADH-ubiquinone oxidoreductase chain 1.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 39 | Q | 286 | Total | C | N | O | S | 0 | 0 |
| | | | 2179 | 1448 | 338 | 374 | 19 | | |

- Molecule 40 is a protein called NADH-ubiquinone oxidoreductase chain 2.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 40 | R | 387 | Total | C | N | O | S | 0 | 0 |
| | | | 3014 | 2026 | 467 | 496 | 25 | | |

- Molecule 41 is a protein called NADH-ubiquinone oxidoreductase chain 3.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 41 | S | 134 | Total | C | N | O | S | 0 | 0 |
| | | | 1071 | 715 | 159 | 192 | 5 | | |

- Molecule 42 is a protein called NADH-ubiquinone oxidoreductase chain 4.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 42 | T | 443 | Total | C | N | O | S | 0 | 0 |
| | | | 3434 | 2321 | 526 | 557 | 30 | | |

- Molecule 43 is a protein called NADH dehydrogenase subunit 4L.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 43 | U | 105 | Total | C | N | O | S | 0 | 0 |
| | | | 805 | 524 | 124 | 146 | 11 | | |

- Molecule 44 is a protein called NADH-ubiquinone oxidoreductase chain 5.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 44 | V | 546 | Total | C | N | O | S | 0 | 0 |
| | | | 4152 | 2731 | 668 | 716 | 37 | | |

- Molecule 45 is a protein called NADH-ubiquinone oxidoreductase chain 6.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 45 | W | 157 | Total | C | N | O | S | 0 | 0 |
| | | | 1210 | 820 | 180 | 201 | 9 | | |

- Molecule 46 is a protein called ASHI.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 46 | X | 125 | Total | C | N | O | S | 0 | 0 |
| | | | 1037 | 685 | 168 | 178 | 6 | | |

- Molecule 47 is a protein called P9.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 47 | Y | 54 | Total | C | N | O | S | 0 | 0 |
| | | | 405 | 256 | 74 | 74 | 1 | | |

- Molecule 48 is a protein called KFYI.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 48 | Z | 107 | Total | C | N | O | S | 0 | 0 |
| | | | 861 | 555 | 149 | 152 | 5 | | |

- Molecule 49 is a protein called AGGG.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 49 | a | 82 | Total | C | N | O | S | 0 | 0 |
| | | | 674 | 440 | 109 | 123 | 2 | | |

- Molecule 50 is a protein called ESSS.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 50 | b | 144 | Total | C | N | O | S | 0 | 0 |
| | | | 1169 | 756 | 192 | 214 | 7 | | |

- Molecule 51 is a protein called B9.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 51 | c | 59 | Total | C | N | O | S | 0 | 0 |
| | | | 453 | 298 | 71 | 79 | 5 | | |

- Molecule 52 is a protein called Mitochondrial NADH:ubiquinone oxidoreductase 10 kDa subunit.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 52 | d | 85 | Total | C | N | O | S | 0 | 0 |
| | | | 699 | 456 | 120 | 120 | 3 | | |

- Molecule 53 is a protein called Mitochondrial NADH:ubiquinone oxidoreductase 23 kDa subunit.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 53 | e | 218 | Total | C | N | O | S | 0 | 0 |
| | | | 1639 | 1055 | 279 | 297 | 8 | | |

- Molecule 54 is a protein called Mitochondrial NADH:ubiquinone oxidoreductase 7.5 kDa subunit.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 54 | f | 64 | Total | C | N | O | S | 0 | 0 |
| | | | 532 | 345 | 93 | 92 | 2 | | |

- Molecule 55 is a protein called Mitochondrial putative NADH:ubiquinone oxidoreductase 6.5

kDa subunit.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 55 | g | 50 | Total | C | N | O | S | 0 | 0 |
| | | | 416 | 277 | 73 | 65 | 1 | | |

- Molecule 56 is a protein called Mitochondrial NADH:ubiquinone oxidoreductase 13 kDa subunit.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 56 | h | 108 | Total | C | N | O | S | 0 | 0 |
| | | | 915 | 597 | 157 | 159 | 2 | | |

- Molecule 57 is a protein called NADH:ubiquinone oxidoreductase 15 kDa subunit-like.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 57 | i | 76 | Total | C | N | O | S | 0 | 0 |
| | | | 633 | 387 | 122 | 116 | 8 | | |

- Molecule 58 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 58 | j | 85 | Total | C | N | O | S | 0 | 0 |
| | | | 712 | 449 | 131 | 125 | 7 | | |

- Molecule 59 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 59 | k | 117 | Total | C | N | O | S | 0 | 0 |
| | | | 984 | 631 | 176 | 173 | 4 | | |

- Molecule 60 is a protein called NADH:ubiquinone oxidoreductase 20,9 kD-like subunit.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 60 | l | 116 | Total | C | N | O | S | 0 | 0 |
| | | | 904 | 589 | 150 | 161 | 4 | | |

- Molecule 61 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 61 | m | 138 | Total | C | N | O | S | 0 | 0 |
| | | | 1126 | 724 | 205 | 193 | 4 | | |

- Molecule 62 is a protein called Putative NADH:ubiquinone oxidoreductase 12.5 kDa subunit.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 62 | n | 104 | Total | C | N | O | S | 0 | 0 |
| | | | 864 | 547 | 152 | 159 | 6 | | |

- Molecule 63 is a protein called Putative NADH:ubiquinone oxidoreductase 17.8 kDa subunit.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 63 | o | 152 | Total | C | N | O | S | 0 | 0 |
| | | | 1240 | 771 | 238 | 228 | 3 | | |

- Molecule 64 is a protein called Mitochondrial NADH:ubiquinone oxidoreductase 16 kDa subunit.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 64 | p | 129 | Total | C | N | O | S | 0 | 0 |
| | | | 1069 | 670 | 192 | 204 | 3 | | |

- Molecule 65 is a protein called Mitochondrial NADH:ubiquinone oxidoreductase 19 kDa subunit.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 65 | q | 157 | Total | C | N | O | S | 0 | 0 |
| | | | 1268 | 818 | 217 | 229 | 4 | | |

- Molecule 66 is a protein called Mitochondrial NADH:ubiquinone oxidoreductase 32 kDa subunit.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 66 | s | 312 | Total | C | N | O | S | 0 | 0 |
| | | | 2302 | 1451 | 407 | 435 | 9 | | |

- Molecule 67 is a protein called CAG2 - CA-like.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 67 | t | 253 | Total | C | N | O | S | 0 | 0 |
| | | | 1997 | 1268 | 357 | 367 | 5 | | |

- Molecule 68 is a protein called CAG1.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 68 | u | 228 | Total | C | N | O | S | 0 | 0 |
| | | | 1698 | 1063 | 300 | 327 | 8 | | |

- Molecule 69 is a protein called P10.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 69 | v | 45 | Total | C | N | O | S | 0 | 0 |
| | | | 361 | 233 | 61 | 66 | 1 | | |

- Molecule 70 is a protein called Mitochondrial NADH:ubiquinone oxidoreductase 9 kDa subunit.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 70 | w | 64 | Total | C | N | O | S | 0 | 0 |
| | | | 508 | 334 | 78 | 91 | 5 | | |

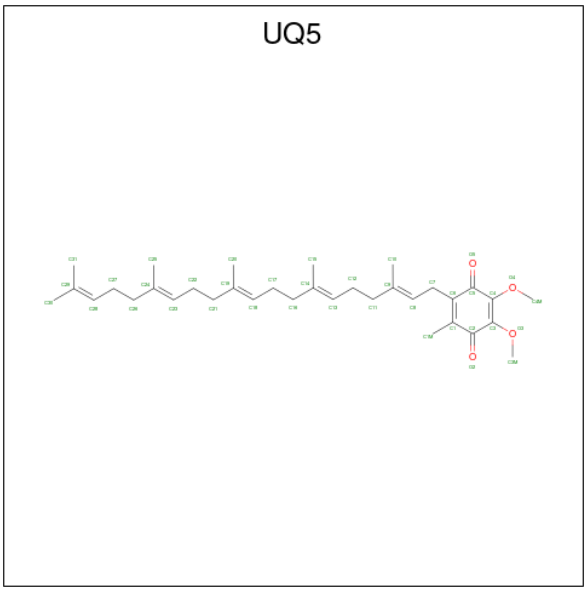
- Molecule 71 is a protein called NUOP8.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 71 | x | 83 | Total | C | N | O | S | 0 | 0 |
| | | | 699 | 467 | 110 | 121 | 1 | | |

- Molecule 72 is a protein called NUOP7.

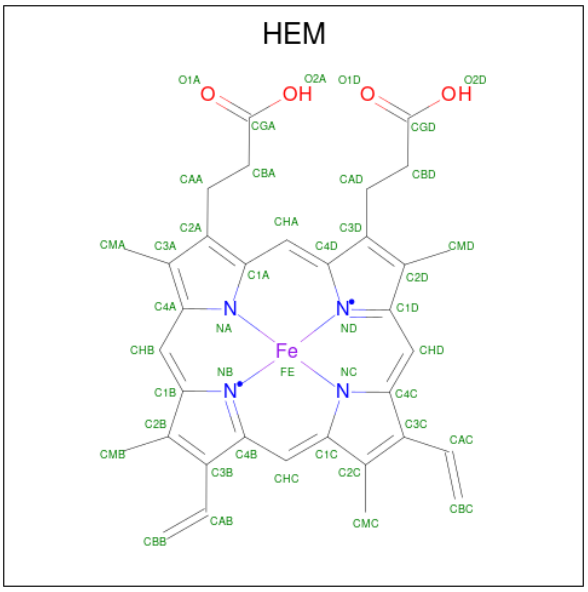
| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 72 | y | 114 | Total | C | N | O | S | 0 | 0 |
| | | | 932 | 615 | 154 | 161 | 2 | | |

- Molecule 73 is 2,3-DIMETHOXY-5-METHYL-6-(3,11,15,19-TETRAMETHYL-EICOSA-2,6,10,14,18-PENTAENYL)-[1,4]BENZOQUINONE (three-letter code: UQ5) (formula: $C_{34}H_{50}O_4$).



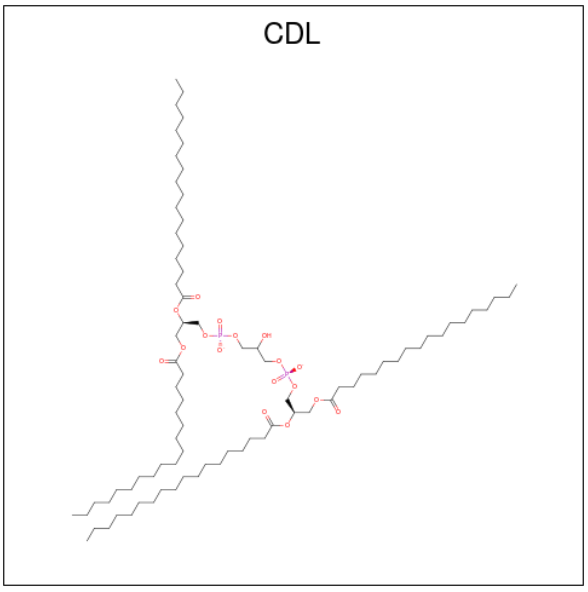

| Mol | Chain | Residues | Atoms | AltConf |
|---|---|---|---|---|
| 73 | 1A | 1 | Total C O<br>38 34 4 | 0 |
| 73 | 1A | 1 | Total C O<br>38 34 4 | 0 |
| 73 | 1B | 1 | Total C O<br>38 34 4 | 0 |
| 73 | 1B | 1 | Total C O<br>38 34 4 | 0 |
| 73 | Q | 1 | Total C O<br>38 34 4 | 0 |

- Molecule 74 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



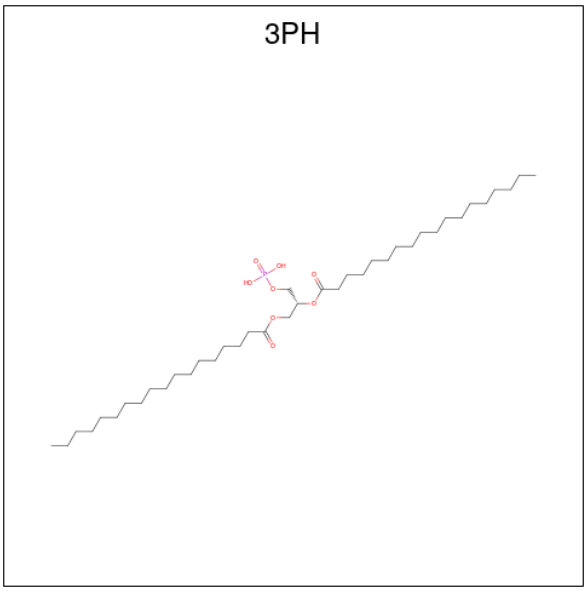

| Mol | Chain | Residues | Atoms | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|
| 74 | 1A | 1 | Total | C | Fe | N | O | 0 |
| | | | 43 | 34 | 1 | 4 | 4 | |
| 74 | 1A | 1 | Total | C | Fe | N | O | 0 |
| | | | 43 | 34 | 1 | 4 | 4 | |
| 74 | 1B | 1 | Total | C | Fe | N | O | 0 |
| | | | 43 | 34 | 1 | 4 | 4 | |
| 74 | 1B | 1 | Total | C | Fe | N | O | 0 |
| | | | 43 | 34 | 1 | 4 | 4 | |

- Molecule 75 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



| Mol | Chain | Residues | Atoms | | | | AltConf |
|---|---|---|---|---|---|---|---|
| 75 | 1A | 1 | Total | C | O | P | 0 |
| | | | 59 | 40 | 17 | 2 | |
| 75 | 1B | 1 | Total | C | O | P | 0 |
| | | | 64 | 45 | 17 | 2 | |
| 75 | 1B | 1 | Total | C | O | P | 0 |
| | | | 71 | 52 | 17 | 2 | |
| 75 | 1E | 1 | Total | C | O | P | 0 |
| | | | 53 | 34 | 17 | 2 | |
| 75 | 1F | 1 | Total | C | O | P | 0 |
| | | | 56 | 37 | 17 | 2 | |
| 75 | 1K | 1 | Total | C | O | P | 0 |
| | | | 79 | 60 | 17 | 2 | |
| 75 | 1L | 1 | Total | C | O | P | 0 |
| | | | 59 | 40 | 17 | 2 | |
| 75 | 1M | 1 | Total | C | O | P | 0 |
| | | | 54 | 35 | 17 | 2 | |
| 75 | R | 1 | Total | C | O | P | 0 |
| | | | 63 | 44 | 17 | 2 | |
| 75 | V | 1 | Total | C | O | P | 0 |
| | | | 64 | 45 | 17 | 2 | |
| 75 | W | 1 | Total | C | O | P | 0 |
| | | | 95 | 76 | 17 | 2 | |
| 75 | h | 1 | Total | C | O | P | 0 |
| | | | 77 | 58 | 17 | 2 | |
| 75 | u | 1 | Total | C | O | P | 0 |
| | | | 83 | 64 | 17 | 2 | |
| 75 | u | 1 | Total | C | O | P | 0 |
| | | | 71 | 52 | 17 | 2 | |
| 75 | x | 1 | Total | C | O | P | 0 |
| | | | 92 | 73 | 17 | 2 | |
| 75 | y | 1 | Total | C | O | P | 0 |
| | | | 55 | 36 | 17 | 2 | |

- Molecule 76 is 1,2-DIACYL-GLYCEROL-3-SN-PHOSPHATE (three-letter code: 3PH) (formula: $C_{39}H_{77}O_8P$).




| Mol | Chain | Residues | Atoms | | | | AltConf |
|---|---|---|---|---|---|---|---|
| 76 | 1A | 1 | Total | C | O | P | 0 |
| | | | 31 | 22 | 8 | 1 | |
| 76 | 1B | 1 | Total | C | O | P | 0 |
| | | | 48 | 39 | 8 | 1 | |
| 76 | 1B | 1 | Total | C | O | P | 0 |
| | | | 48 | 39 | 8 | 1 | |
| 76 | 1E | 1 | Total | C | O | P | 0 |
| | | | 40 | 31 | 8 | 1 | |
| 76 | 1K | 1 | Total | C | O | P | 0 |
| | | | 48 | 39 | 8 | 1 | |
| 76 | 1R | 1 | Total | C | O | P | 0 |
| | | | 37 | 28 | 8 | 1 | |
| 76 | 2D | 1 | Total | C | O | P | 0 |
| | | | 32 | 23 | 8 | 1 | |
| 76 | 2I | 1 | Total | C | O | P | 0 |
| | | | 42 | 33 | 8 | 1 | |
| 76 | 3D | 1 | Total | C | O | P | 0 |
| | | | 32 | 23 | 8 | 1 | |
| 76 | 3I | 1 | Total | C | O | P | 0 |
| | | | 42 | 33 | 8 | 1 | |
| 76 | R | 1 | Total | C | O | P | 0 |
| | | | 32 | 23 | 8 | 1 | |
| 76 | S | 1 | Total | C | O | P | 0 |
| | | | 37 | 28 | 8 | 1 | |
| 76 | V | 1 | Total | C | O | P | 0 |
| | | | 42 | 33 | 8 | 1 | |
| 76 | V | 1 | Total | C | O | P | 0 |
| | | | 41 | 32 | 8 | 1 | |

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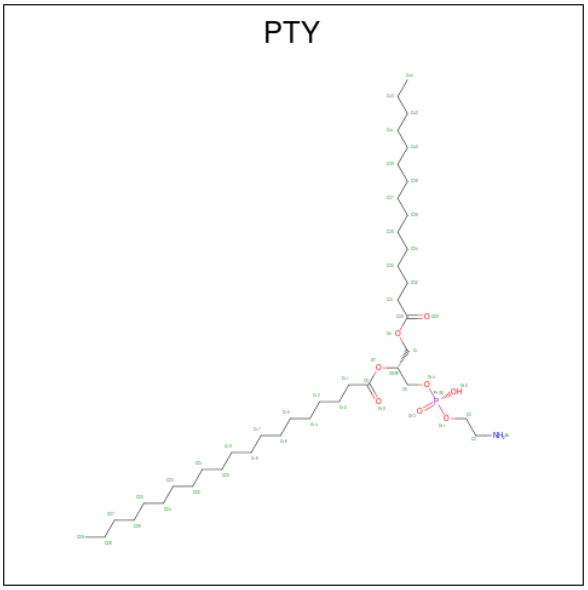
| Mol | Chain | Residues | Atoms | | | | AltConf |
|---|---|---|---|---|---|---|---|
| 76 | c | 1 | Total | C | O | P | 0 |
| | | | 48 | 39 | 8 | 1 | |
| 76 | g | 1 | Total | C | O | P | 0 |
| | | | 37 | 28 | 8 | 1 | |
| 76 | h | 1 | Total | C | O | P | 0 |
| | | | 45 | 36 | 8 | 1 | |
| 76 | w | 1 | Total | C | O | P | 0 |
| | | | 45 | 36 | 8 | 1 | |
| 76 | y | 1 | Total | C | O | P | 0 |
| | | | 32 | 23 | 8 | 1 | |

- Molecule 77 is PHOSPHATIDYLETHANOLAMINE (three-letter code: PTY) (formula: $C_{40}H_{80}NO_8P$).




| Mol | Chain | Residues | Atoms | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|
| 77 | 1E | 1 | Total | C | N | O | P | 0 |
| | | | 34 | 24 | 1 | 8 | 1 | |
| 77 | 1F | 1 | Total | C | N | O | P | 0 |
| | | | 38 | 28 | 1 | 8 | 1 | |
| 77 | 2D | 1 | Total | C | N | O | P | 0 |
| | | | 35 | 25 | 1 | 8 | 1 | |
| 77 | 2F | 1 | Total | C | N | O | P | 0 |
| | | | 34 | 24 | 1 | 8 | 1 | |
| 77 | 3D | 1 | Total | C | N | O | P | 0 |
| | | | 35 | 25 | 1 | 8 | 1 | |
| 77 | 3F | 1 | Total | C | N | O | P | 0 |
| | | | 34 | 24 | 1 | 8 | 1 | |

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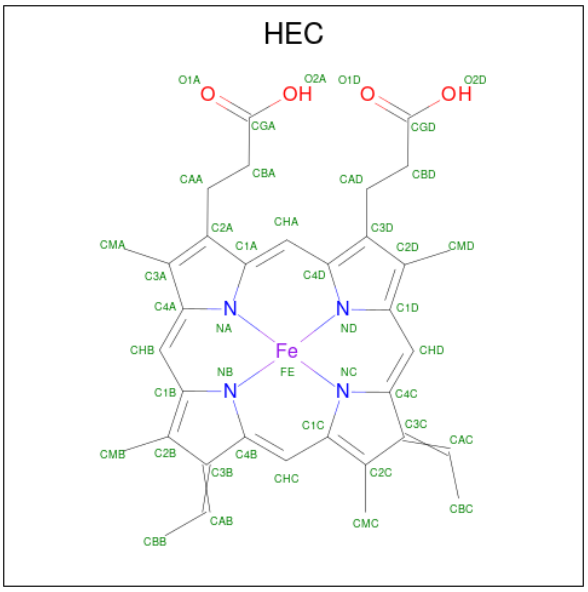
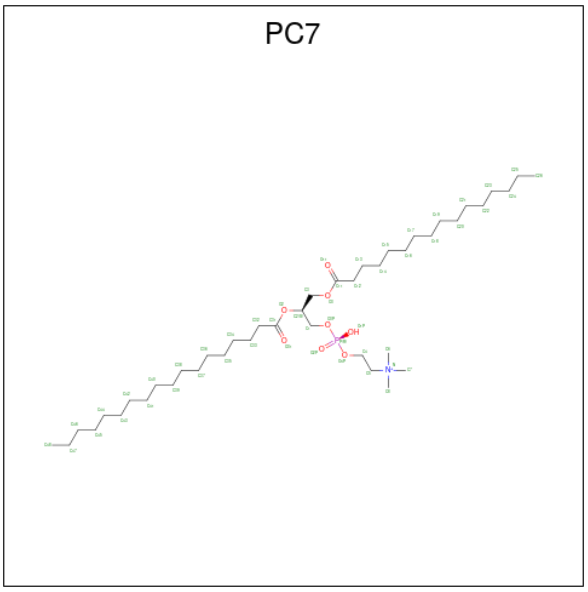
| Mol | Chain | Residues | Atoms | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|
| 77 | G | 1 | Total | C | N | O | P | 0 |
| | | | 43 | 33 | 1 | 8 | 1 | |
| 77 | R | 1 | Total | C | N | O | P | 0 |
| | | | 34 | 24 | 1 | 8 | 1 | |
| 77 | R | 1 | Total | C | N | O | P | 0 |
| | | | 44 | 34 | 1 | 8 | 1 | |
| 77 | R | 1 | Total | C | N | O | P | 0 |
| | | | 40 | 30 | 1 | 8 | 1 | |
| 77 | S | 1 | Total | C | N | O | P | 0 |
| | | | 46 | 36 | 1 | 8 | 1 | |
| 77 | T | 1 | Total | C | N | O | P | 0 |
| | | | 50 | 40 | 1 | 8 | 1 | |
| 77 | T | 1 | Total | C | N | O | P | 0 |
| | | | 28 | 18 | 1 | 8 | 1 | |
| 77 | T | 1 | Total | C | N | O | P | 0 |
| | | | 26 | 16 | 1 | 8 | 1 | |
| 77 | V | 1 | Total | C | N | O | P | 0 |
| | | | 40 | 30 | 1 | 8 | 1 | |
| 77 | V | 1 | Total | C | N | O | P | 0 |
| | | | 50 | 40 | 1 | 8 | 1 | |
| 77 | V | 1 | Total | C | N | O | P | 0 |
| | | | 35 | 25 | 1 | 8 | 1 | |
| 77 | e | 1 | Total | C | N | O | P | 0 |
| | | | 25 | 15 | 1 | 8 | 1 | |
| 77 | e | 1 | Total | C | N | O | P | 0 |
| | | | 43 | 33 | 1 | 8 | 1 | |
| 77 | h | 1 | Total | C | N | O | P | 0 |
| | | | 46 | 36 | 1 | 8 | 1 | |
| 77 | x | 1 | Total | C | N | O | P | 0 |
| | | | 50 | 40 | 1 | 8 | 1 | |

- Molecule 78 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).




| Mol | Chain | Residues | Atoms | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|
| 78 | 1E | 1 | Total | C | Fe | N | O | 0 |
| | | | 43 | 34 | 1 | 4 | 4 | |
| 78 | 1F | 1 | Total | C | Fe | N | O | 0 |
| | | | 43 | 34 | 1 | 4 | 4 | |

- Molecule 79 is (7S)-4-HYDROXY-N,N,N-TRIMETHYL-9-OXO-7-[(PALMITOYLOXY)METHYL]-3,5,8-TRIOXA-4-PHOSPHAHEXACOSAN-1-AMINIUM 4-OXIDE (three-letter code: PC7) (formula: $C_{42}H_{85}NO_8P$).




| Mol | Chain | Residues | Atoms | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|
| 79 | 1G | 1 | Total | C | N | O | P | 0 |
| | | | 36 | 26 | 1 | 8 | 1 | |

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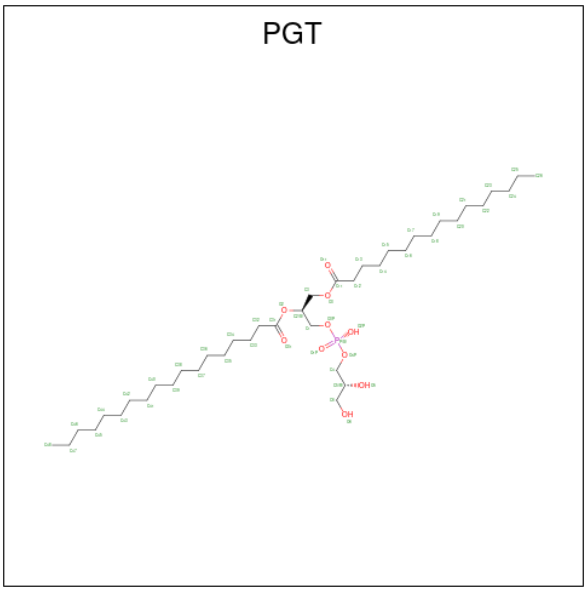
| Mol | Chain | Residues | Atoms | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|
| 79 | 1H | 1 | Total | C | N | O | P | 0 |
| | | | 39 | 29 | 1 | 8 | 1 | |
| 79 | 2A | 1 | Total | C | N | O | P | 0 |
| | | | 27 | 17 | 1 | 8 | 1 | |
| 79 | 3A | 1 | Total | C | N | O | P | 0 |
| | | | 27 | 17 | 1 | 8 | 1 | |
| 79 | Q | 1 | Total | C | N | O | P | 0 |
| | | | 33 | 23 | 1 | 8 | 1 | |
| 79 | R | 1 | Total | C | N | O | P | 0 |
| | | | 44 | 34 | 1 | 8 | 1 | |
| 79 | T | 1 | Total | C | N | O | P | 0 |
| | | | 52 | 42 | 1 | 8 | 1 | |
| 79 | u | 1 | Total | C | N | O | P | 0 |
| | | | 42 | 32 | 1 | 8 | 1 | |

- Molecule 80 is ZINC ION (three-letter code: ZN) (formula: Zn).

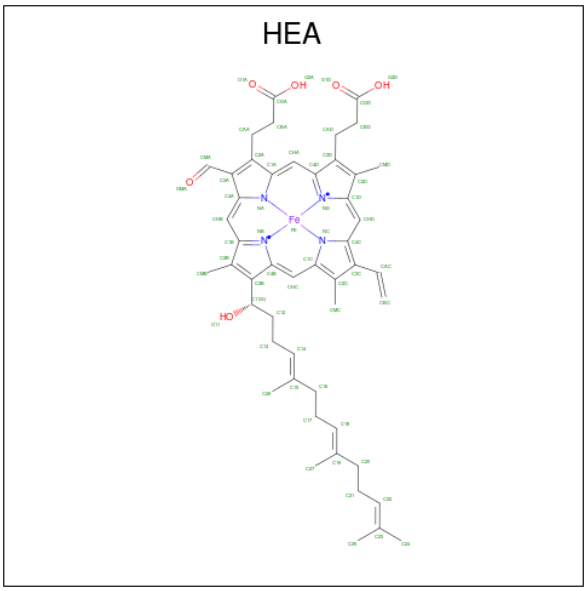
| Mol | Chain | Residues | Atoms | | AltConf |
|---|---|---|---|---|---|
| 80 | 1M | 1 | Total | Zn | 0 |
| | | | 1 | 1 | |
| 80 | 1N | 1 | Total | Zn | 0 |
| | | | 1 | 1 | |
| 80 | s | 1 | Total | Zn | 0 |
| | | | 1 | 1 | |

- Molecule 81 is (1S)-2-{[{[(2R)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL STEARATE (three-letter code: PGT) (formula: $C_{40}H_{79}O_{10}P$).




| Mol | Chain | Residues | Atoms | | | | AltConf |
|---|---|---|---|---|---|---|---|
| 81 | 2A | 1 | Total | C | O | P | 0 |
| | | | 33 | 22 | 10 | 1 | |
| 81 | 3A | 1 | Total | C | O | P | 0 |
| | | | 33 | 22 | 10 | 1 | |
| 81 | T | 1 | Total | C | O | P | 0 |
| | | | 48 | 37 | 10 | 1 | |
| 81 | T | 1 | Total | C | O | P | 0 |
| | | | 40 | 29 | 10 | 1 | |
| 81 | b | 1 | Total | C | O | P | 0 |
| | | | 44 | 33 | 10 | 1 | |
| 81 | l | 1 | Total | C | O | P | 0 |
| | | | 51 | 40 | 10 | 1 | |

- Molecule 82 is HEME-A (three-letter code: HEA) (formula: $C_{49}H_{56}FeN_4O_6$).




| Mol | Chain | Residues | Atoms | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|
| 82 | 2A | 1 | Total | C | Fe | N | O | 0 |
| | | | 60 | 49 | 1 | 4 | 6 | |
| 82 | 2A | 1 | Total | C | Fe | N | O | 0 |
| | | | 60 | 49 | 1 | 4 | 6 | |
| 82 | 3A | 1 | Total | C | Fe | N | O | 0 |
| | | | 60 | 49 | 1 | 4 | 6 | |
| 82 | 3A | 1 | Total | C | Fe | N | O | 0 |
| | | | 60 | 49 | 1 | 4 | 6 | |

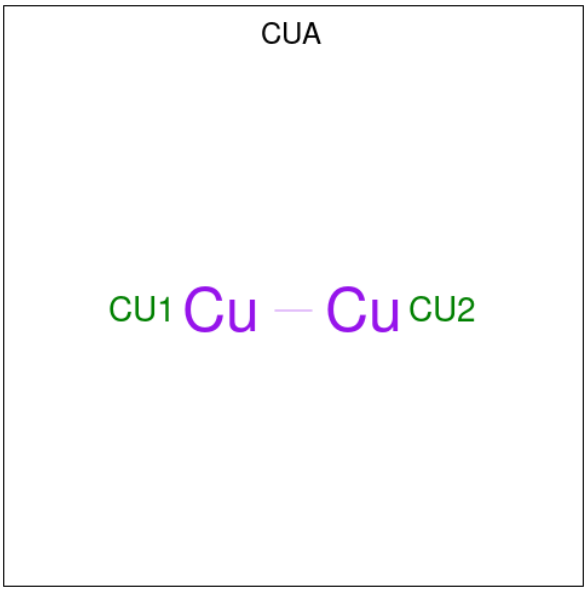
- Molecule 83 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

| Mol | Chain | Residues | Atoms | | AltConf |
|---|---|---|---|---|---|
| 83 | 2A | 1 | Total | Cu | 0 |
| | | | 1 | 1 | |
| 83 | 3A | 1 | Total | Cu | 0 |
| | | | 1 | 1 | |

- Molecule 84 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

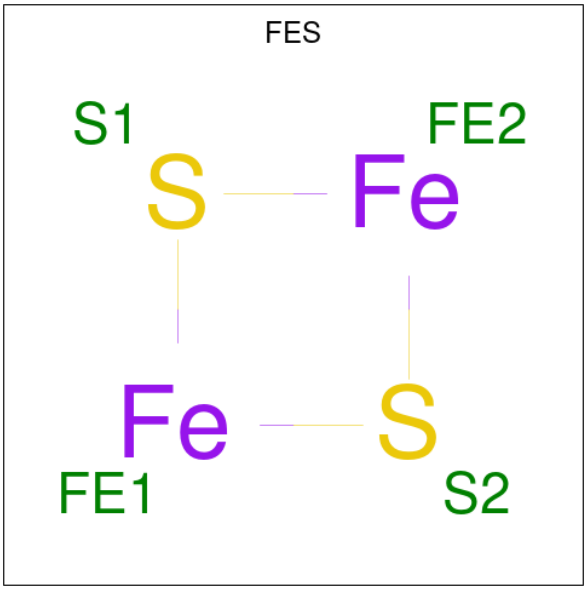
| Mol | Chain | Residues | Atoms | | AltConf |
|---|---|---|---|---|---|
| 84 | 2A | 1 | Total | Mg | 0 |
| | | | 1 | 1 | |
| 84 | 3A | 1 | Total | Mg | 0 |
| | | | 1 | 1 | |

- Molecule 85 is DINUCLEAR COPPER ION (three-letter code: CUA) (formula: $Cu_2$).



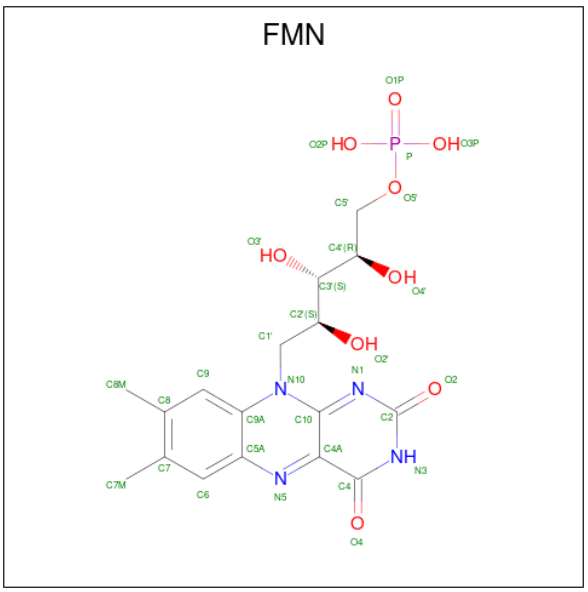

| Mol | Chain | Residues | Atoms | AltConf |
|---|---|---|---|---|
| 85 | 2C | 1 | Total Cu<br>2 2 | 0 |
| 85 | 3C | 1 | Total Cu<br>2 2 | 0 |

- Molecule 86 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: $Fe_2S_2$).



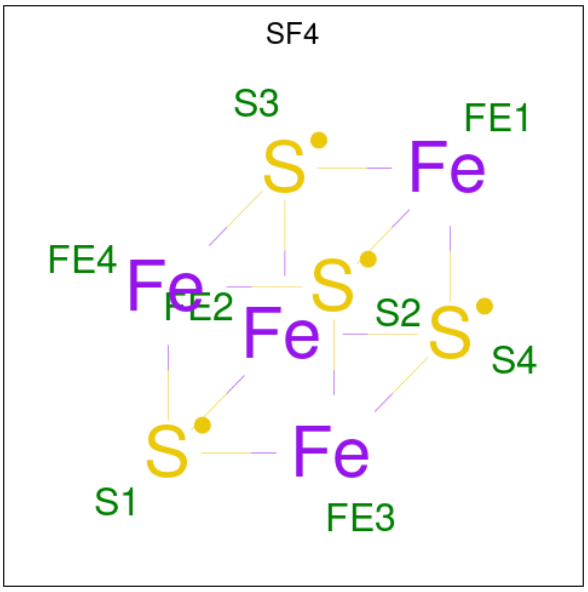

| Mol | Chain | Residues | Atoms | AltConf |
|---|---|---|---|---|
| 86 | A | 1 | Total Fe S<br>4 2 2 | 0 |
| 86 | C | 1 | Total Fe S<br>4 2 2 | 0 |

- Molecule 87 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: $C_{17}H_{21}N_4O_9P$).




| Mol | Chain | Residues | Atoms | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|
| 87 | B | 1 | Total | C | N | O | P | 0 |
| | | | 31 | 17 | 4 | 9 | 1 | |

- Molecule 88 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: $Fe_4S_4$).




| Mol | Chain | Residues | Atoms | | | AltConf |
|---|---|---|---|---|---|---|
| 88 | B | 1 | Total | Fe | S | 0 |
| | | | 8 | 4 | 4 | |
| 88 | C | 1 | Total | Fe | S | 0 |
| | | | 8 | 4 | 4 | |

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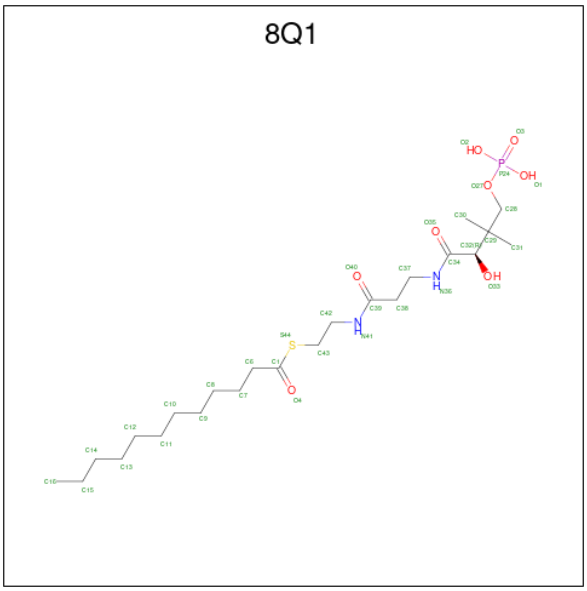
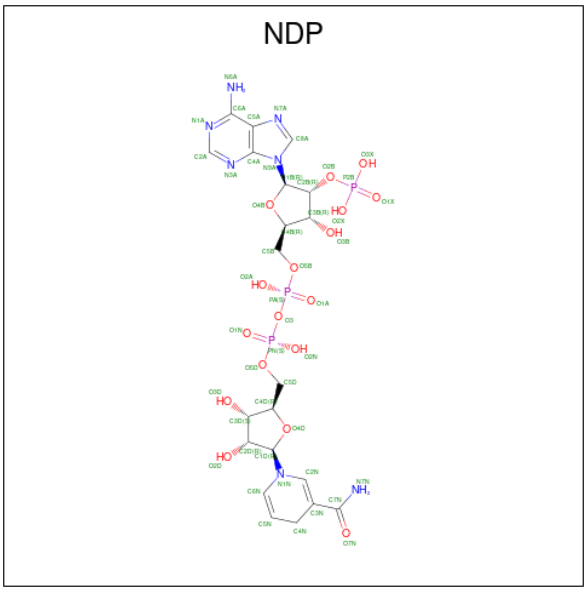
| Mol | Chain | Residues | Atoms | AltConf |
|---|---|---|---|---|
| 88 | C | 1 | Total Fe S<br>8 4 4 | 0 |
| 88 | F | 1 | Total Fe S<br>8 4 4 | 0 |
| 88 | G | 1 | Total Fe S<br>8 4 4 | 0 |
| 88 | G | 1 | Total Fe S<br>8 4 4 | 0 |

- Molecule 89 is S-[2-({N-[(2R)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-beta-alanyl}amino)ethyl] dodecanethioate (three-letter code: 8Q1) (formula: $C_{23}H_{45}N_2O_8PS$).



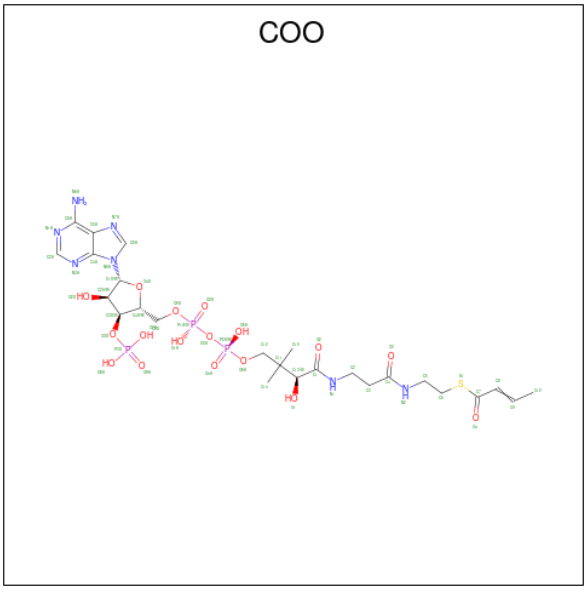

| Mol | Chain | Residues | Atoms | AltConf |
|---|---|---|---|---|
| 89 | J | 1 | Total C N O P S<br>35 23 2 8 1 1 | 0 |
| 89 | r | 1 | Total C N O P S<br>35 23 2 8 1 1 | 0 |

- Molecule 90 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).




| Mol | Chain | Residues | Atoms | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|
| 90 | P | 1 | Total | C | N | O | P | 0 |
| | | | 48 | 21 | 7 | 17 | 3 | |

- Molecule 91 is CROTONYL COENZYME A (three-letter code: COO) (formula: $C_{25}H_{40}N_7O_{17}P_3S$).




| Mol | Chain | Residues | Atoms | | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|---|
| 91 | s | 1 | Total | C | N | O | P | S | 0 |
| | | | 53 | 25 | 7 | 17 | 3 | 1 | |

- Molecule 92 is water.

| Mol | Chain | Residues | Atoms | AltConf |
|---|---|---|---|---|
| 92 | 1A | 48 | Total O<br>48 48 | 0 |
| 92 | 1B | 52 | Total O<br>52 52 | 0 |
| 92 | 1C | 13 | Total O<br>13 13 | 0 |
| 92 | 1D | 12 | Total O<br>12 12 | 0 |
| 92 | 1E | 51 | Total O<br>51 51 | 0 |
| 92 | 1F | 34 | Total O<br>34 34 | 0 |
| 92 | 1G | 7 | Total O<br>7 7 | 0 |
| 92 | 1H | 9 | Total O<br>9 9 | 0 |
| 92 | 1I | 11 | Total O<br>11 11 | 0 |
| 92 | 1J | 3 | Total O<br>3 3 | 0 |
| 92 | 1K | 12 | Total O<br>12 12 | 0 |
| 92 | 1L | 12 | Total O<br>12 12 | 0 |
| 92 | 1M | 76 | Total O<br>76 76 | 0 |
| 92 | 1N | 74 | Total O<br>74 74 | 0 |
| 92 | 1O | 4 | Total O<br>4 4 | 0 |
| 92 | 1P | 6 | Total O<br>6 6 | 0 |
| 92 | 1Q | 27 | Total O<br>27 27 | 0 |
| 92 | 1R | 32 | Total O<br>32 32 | 0 |
| 92 | 1S | 29 | Total O<br>29 29 | 0 |
| 92 | 1T | 28 | Total O<br>28 28 | 0 |
| 92 | A | 24 | Total O<br>24 24 | 0 |
| 92 | B | 66 | Total O<br>66 66 | 0 |

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| Mol | Chain | Residues | Atoms | AltConf |
|---|---|---|---|---|
| 92 | C | 168 | Total O<br>168 168 | 0 |
| 92 | D | 66 | Total O<br>66 66 | 0 |
| 92 | E | 87 | Total O<br>87 87 | 0 |
| 92 | F | 39 | Total O<br>39 39 | 0 |
| 92 | G | 62 | Total O<br>62 62 | 0 |
| 92 | H | 16 | Total O<br>16 16 | 0 |
| 92 | I | 19 | Total O<br>19 19 | 0 |
| 92 | K | 16 | Total O<br>16 16 | 0 |
| 92 | L | 68 | Total O<br>68 68 | 0 |
| 92 | M | 30 | Total O<br>30 30 | 0 |
| 92 | N | 53 | Total O<br>53 53 | 0 |
| 92 | O | 6 | Total O<br>6 6 | 0 |
| 92 | P | 69 | Total O<br>69 69 | 0 |
| 92 | Q | 24 | Total O<br>24 24 | 0 |
| 92 | R | 64 | Total O<br>64 64 | 0 |
| 92 | S | 22 | Total O<br>22 22 | 0 |
| 92 | T | 85 | Total O<br>85 85 | 0 |
| 92 | U | 14 | Total O<br>14 14 | 0 |
| 92 | V | 99 | Total O<br>99 99 | 0 |
| 92 | W | 25 | Total O<br>25 25 | 0 |
| 92 | X | 50 | Total O<br>50 50 | 0 |

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| Mol | Chain | Residues | Atoms | AltConf |
|---|---|---|---|---|
| 92 | Y | 4 | Total O<br>4 4 | 0 |
| 92 | Z | 20 | Total O<br>20 20 | 0 |
| 92 | a | 6 | Total O<br>6 6 | 0 |
| 92 | b | 24 | Total O<br>24 24 | 0 |
| 92 | c | 1 | Total O<br>1 1 | 0 |
| 92 | d | 12 | Total O<br>12 12 | 0 |
| 92 | e | 55 | Total O<br>55 55 | 0 |
| 92 | f | 10 | Total O<br>10 10 | 0 |
| 92 | g | 7 | Total O<br>7 7 | 0 |
| 92 | h | 38 | Total O<br>38 38 | 0 |
| 92 | i | 30 | Total O<br>30 30 | 0 |
| 92 | j | 29 | Total O<br>29 29 | 0 |
| 92 | k | 51 | Total O<br>51 51 | 0 |
| 92 | l | 17 | Total O<br>17 17 | 0 |
| 92 | m | 32 | Total O<br>32 32 | 0 |
| 92 | n | 7 | Total O<br>7 7 | 0 |
| 92 | o | 51 | Total O<br>51 51 | 0 |
| 92 | p | 21 | Total O<br>21 21 | 0 |
| 92 | q | 24 | Total O<br>24 24 | 0 |
| 92 | r | 12 | Total O<br>12 12 | 0 |
| 92 | s | 39 | Total O<br>39 39 | 0 |

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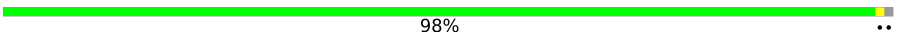
| Mol | Chain | Residues | Atoms | AltConf |
|---|---|---|---|---|
| 92 | t | 55 | Total O<br>55 55 | 0 |
| 92 | u | 41 | Total O<br>41 41 | 0 |
| 92 | v | 2 | Total O<br>2 2 | 0 |
| 92 | w | 16 | Total O<br>16 16 | 0 |
| 92 | x | 22 | Total O<br>22 22 | 0 |
| 92 | y | 29 | Total O<br>29 29 | 0 |

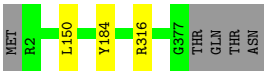
# 3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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: Cytochrome b

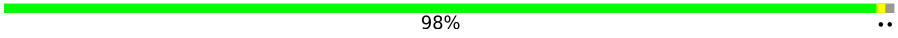
Chain 1A:




• Molecule 1: Cytochrome b

Chain 1B:





• Molecule 2: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain 1C:



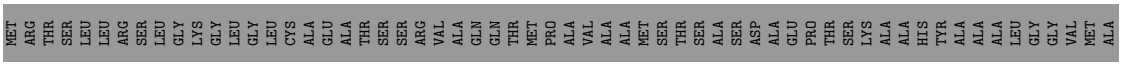
• Molecule 2: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain 1D:



• Molecule 3: Cytochrome c1

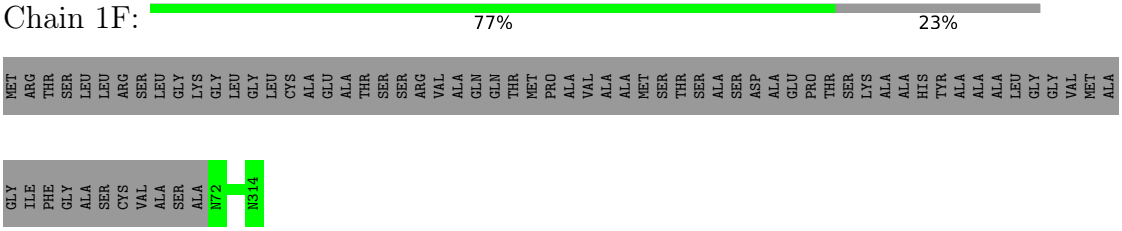
Chain 1E:



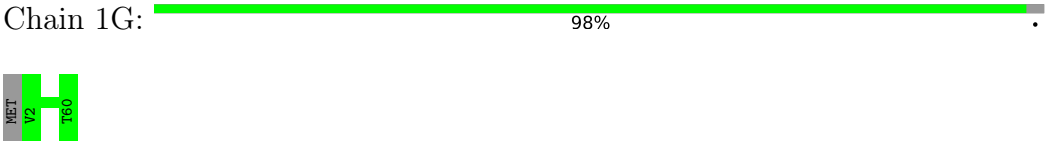
• Molecule 3: Cytochrome c1

Chain 1F:



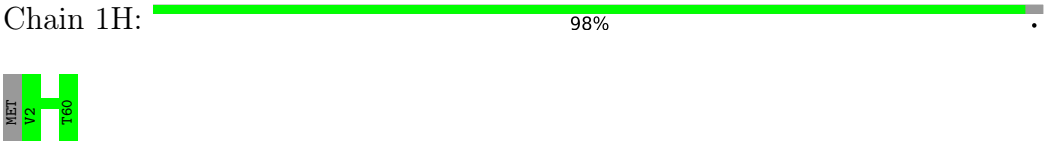

• Molecule 4: Complex III subunit 9

Chain 1G:



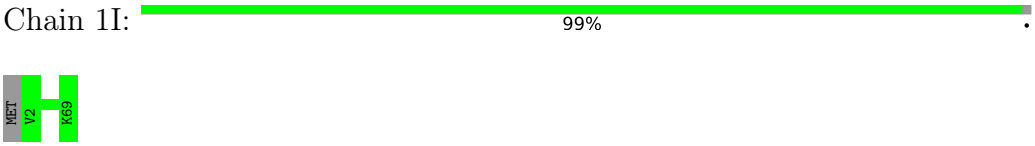

• Molecule 4: Complex III subunit 9

Chain 1H:




• Molecule 5: Cytochrome b-c1 complex subunit 6

Chain 1I:

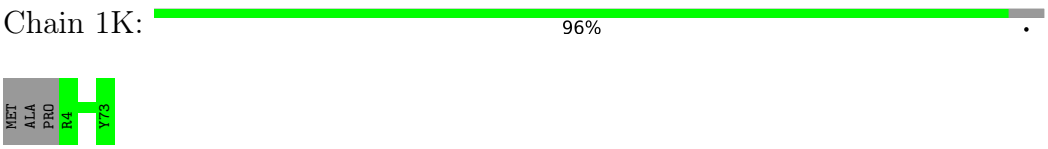



• Molecule 5: Cytochrome b-c1 complex subunit 6

Chain 1J:

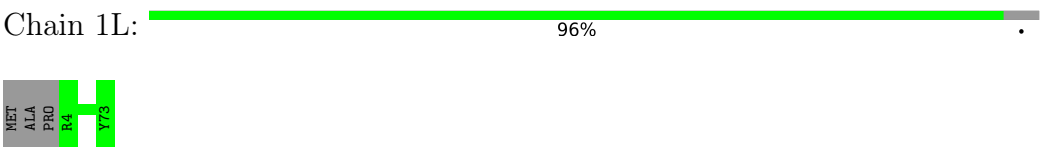

• Molecule 6: Mitochondrial ubiquinol-cytochrome c oxidoreductase subunit 8

Chain 1K:



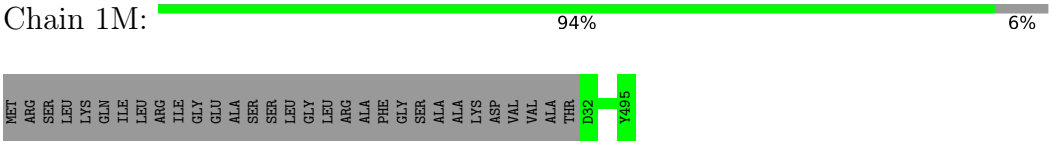

• Molecule 6: Mitochondrial ubiquinol-cytochrome c oxidoreductase subunit 8

Chain 1L:



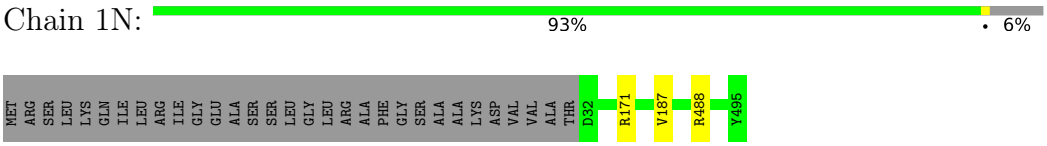
• Molecule 7: MPP-Beta

Chain 1M:



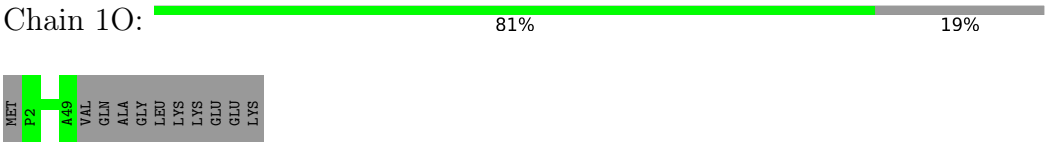

• Molecule 7: MPP-Beta

Chain 1N:



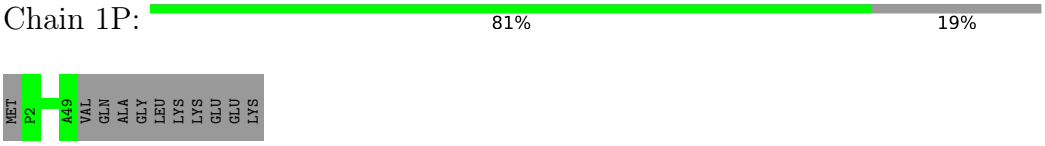

• Molecule 8: Mitochondrial ubiquinol-cytochrome c oxidoreductase subunit 10

Chain 1O:



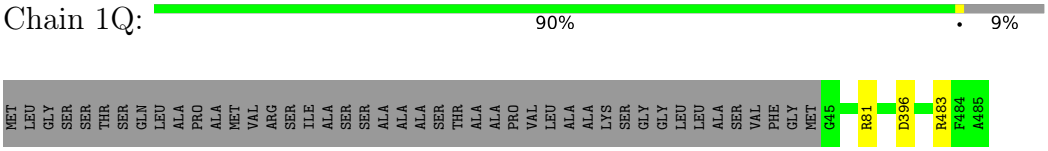

• Molecule 8: Mitochondrial ubiquinol-cytochrome c oxidoreductase subunit 10

Chain 1P:



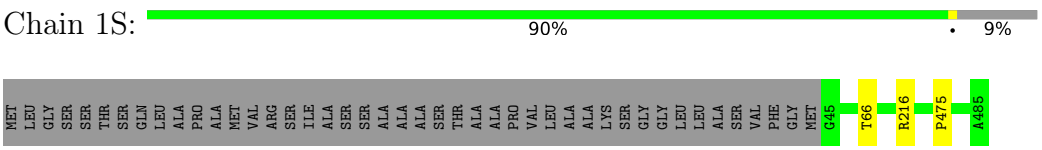

• Molecule 9: Alpha-MPP

Chain 1Q:



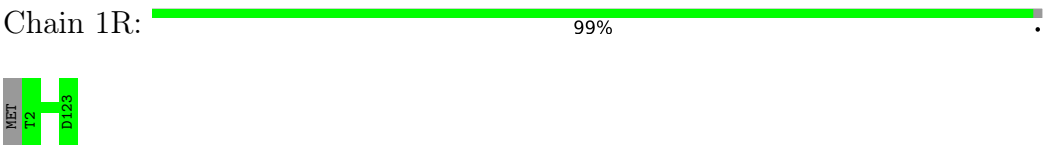

• Molecule 9: Alpha-MPP

Chain 1S:



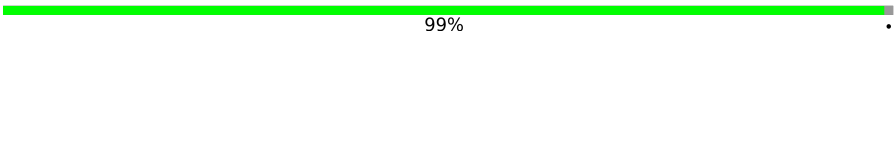

• Molecule 10: Cytochrome b-c1 complex subunit 7

Chain 1R:



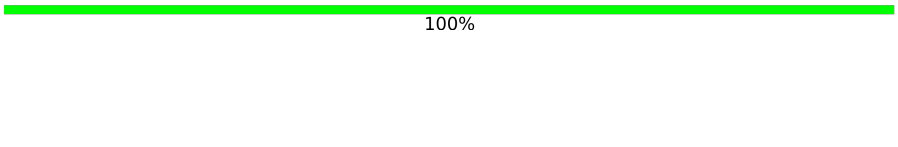

• Molecule 10: Cytochrome b-c1 complex subunit 7

Chain 1T:



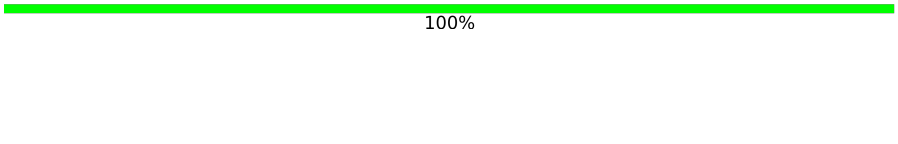

• Molecule 11: Cytochrome c oxidase subunit 1

Chain 2A:



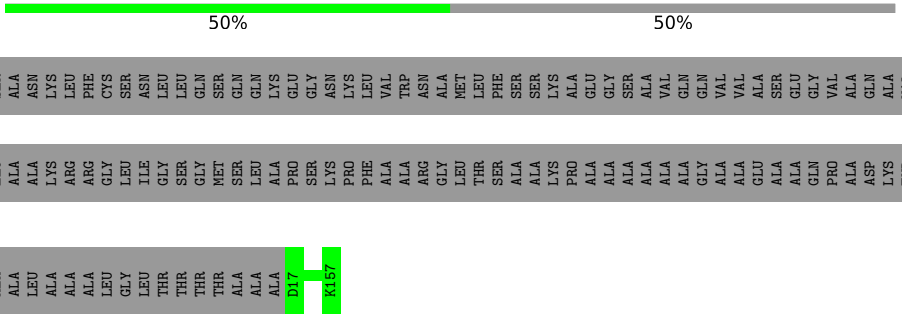

• Molecule 11: Cytochrome c oxidase subunit 1

Chain 3A:



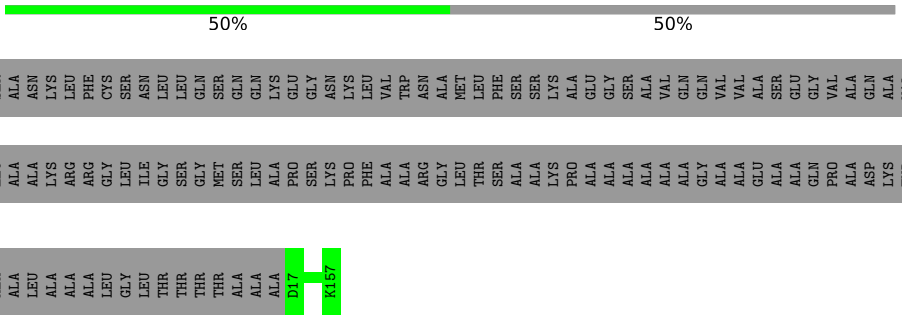

• Molecule 12: Cytochrome c oxidase polypeptide II

Chain 2B:



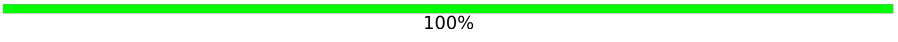

• Molecule 12: Cytochrome c oxidase polypeptide II

Chain 3B:




• Molecule 13: cytochrome-c oxidase

Chain 2C:




There are no outlier residues recorded for this chain.

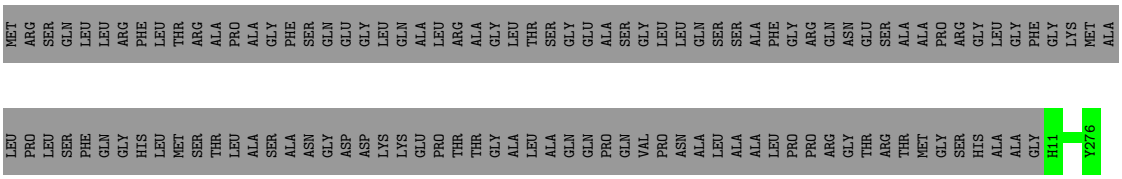
• Molecule 13: cytochrome-c oxidase

Chain 3C:


There are no outlier residues recorded for this chain.

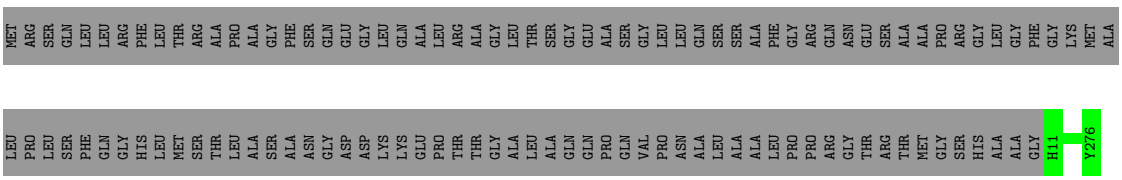
• Molecule 14: Cytochrome c oxidase subunit 3

Chain 2D:

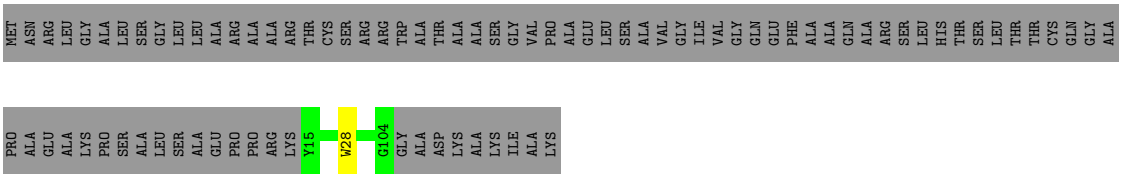

• Molecule 14: Cytochrome c oxidase subunit 3

Chain 3D:

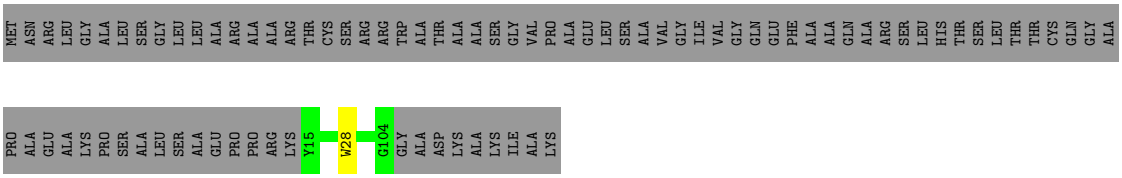

• Molecule 15: Cox5b

Chain 2E:

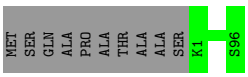

• Molecule 15: Cox5b

Chain 3E:

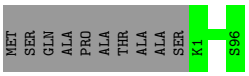

• Molecule 16: Cox5c

Chain 2F:


• Molecule 16: Cox5c

Chain 3F:

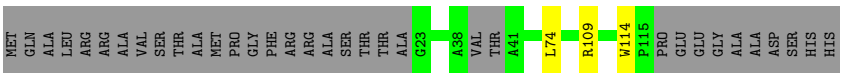

• Molecule 17: Cox6a

Chain 2G:



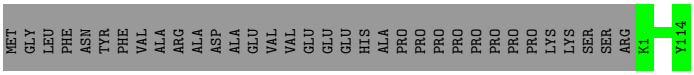
• Molecule 17: Cox6a

Chain 3G:

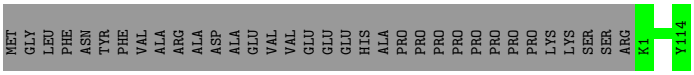

• Molecule 18: Cox6b

Chain 2H:

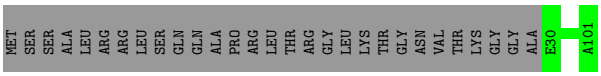

• Molecule 18: Cox6b

Chain 3H:

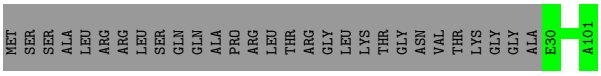

• Molecule 19: Cox7c

Chain 2I:

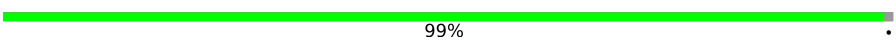

• Molecule 19: Cox7c

Chain 3I:

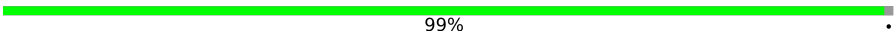

• Molecule 20: Cytochrome c oxidase subunit

Chain 2J:




• Molecule 20: Cytochrome c oxidase subunit

Chain 3J:





• Molecule 21: Cox7a

Chain 2K:



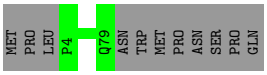
• Molecule 21: Cox7a

Chain 3K:



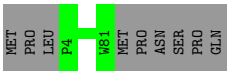
• Molecule 22: CoxIn

Chain 2L:


• Molecule 22: CoxIn

Chain 3L:

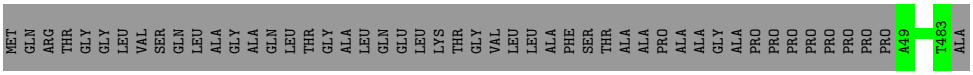

• Molecule 23: NADH:ubiquinone oxidoreductase 24 kD subunit

Chain A:



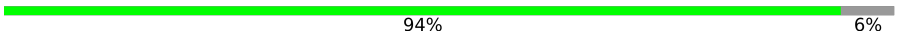
• Molecule 24: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

Chain B:




• Molecule 25: NADH:ubiquinone oxidoreductase 78 kDa subunit

Chain C:

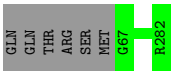




• Molecule 26: NADH:ubiquinone oxidoreductase 30kDa subunit domain-containing protein

Chain D:

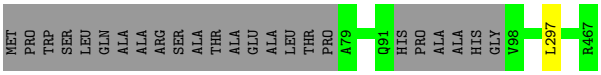





• Molecule 27: NADH:ubiquinone oxidoreductase 49 kD subunit

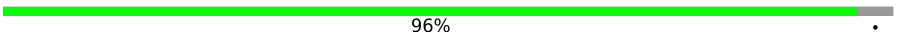
Chain E:

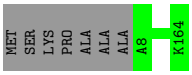





• Molecule 28: NADH:ubiquinone oxidoreductase subunit 10

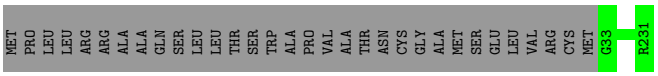
Chain F:



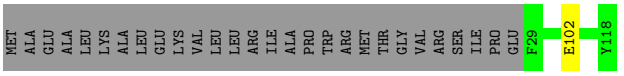

• Molecule 29: NADH:ubiquinone oxidoreductase subunit 8

Chain G:

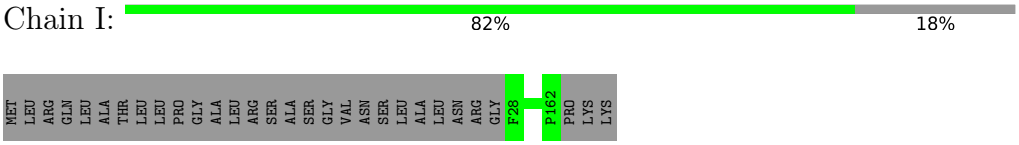

• Molecule 30: B14.5a

Chain H:

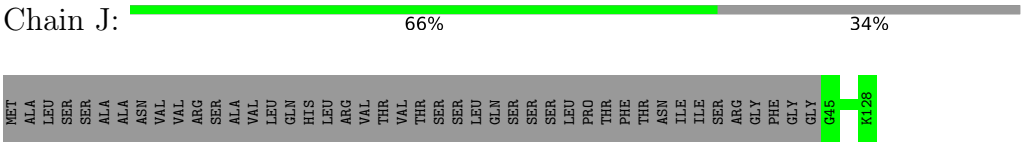
• Molecule 31: Mitochondrial NADH:ubiquinone oxidoreductase 18 kDa subunit

Chain I:



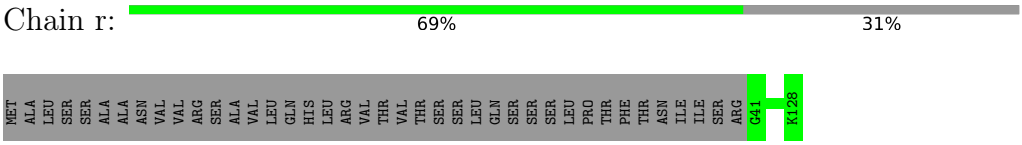

• Molecule 32: Acyl carrier protein

Chain J:



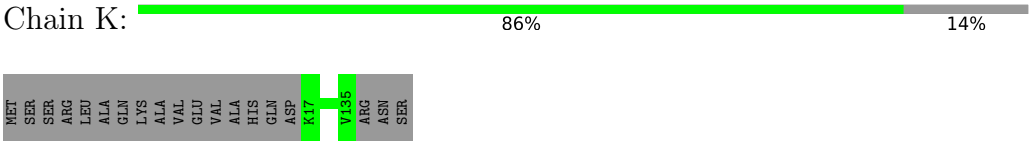

• Molecule 32: Acyl carrier protein

Chain r:



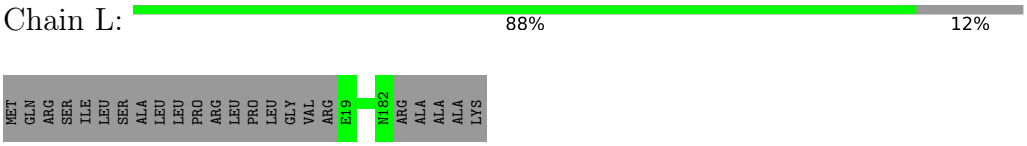

• Molecule 33: NADH:ubiquinone oxidoreductase B14 subunit

Chain K:



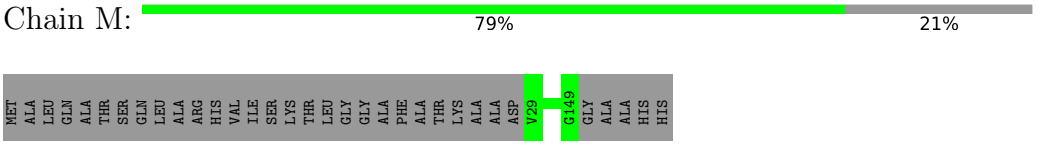

• Molecule 34: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

Chain L:



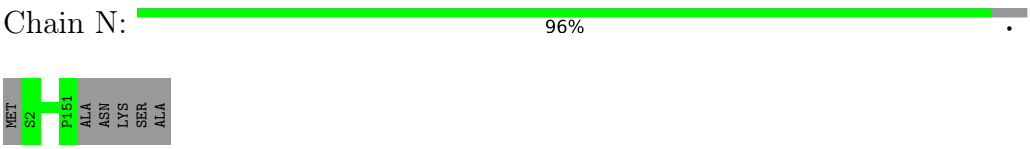

• Molecule 35: NADH:ubiquinone oxidoreductase 13 kD-like subunit

Chain M:



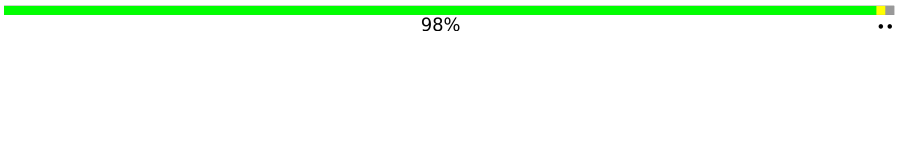

• Molecule 36: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

Chain N:



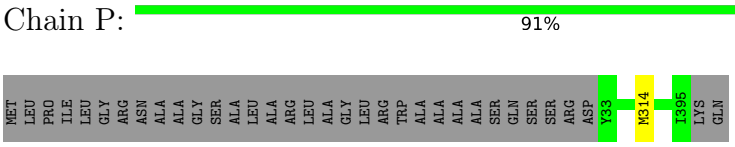

• Molecule 37: NADH:ubiquinone oxidoreductase B8 subunit

Chain O:



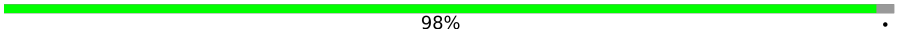

• Molecule 38: Putative NADH:ubiquinone oxidoreductase 39 kDa subunit

Chain P:




• Molecule 39: NADH-ubiquinone oxidoreductase chain 1

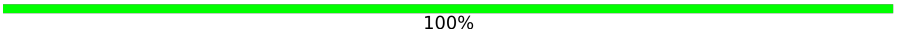
Chain Q:





• Molecule 40: NADH-ubiquinone oxidoreductase chain 2

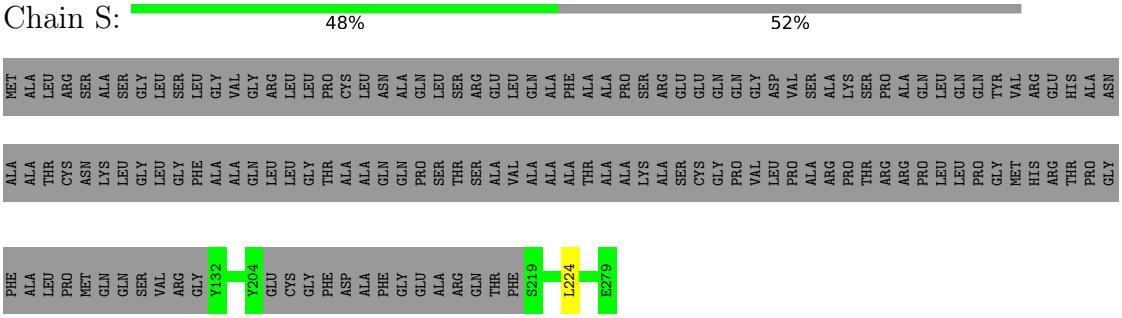
Chain R:




There are no outlier residues recorded for this chain.

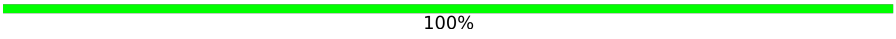
• Molecule 41: NADH-ubiquinone oxidoreductase chain 3

Chain S:




• Molecule 42: NADH-ubiquinone oxidoreductase chain 4

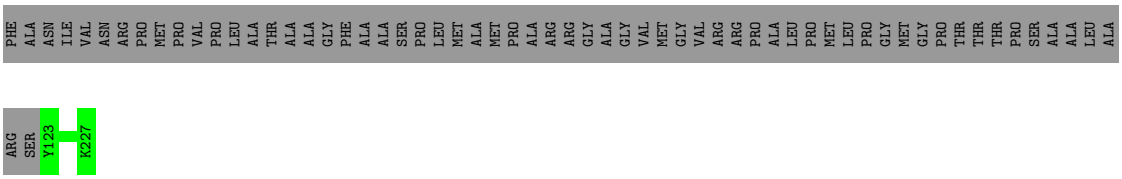
Chain T:





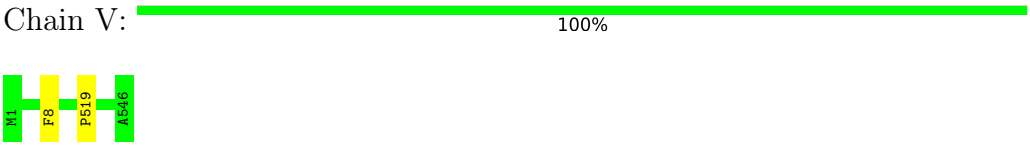
• Molecule 43: NADH dehydrogenase subunit 4L

Chain U:

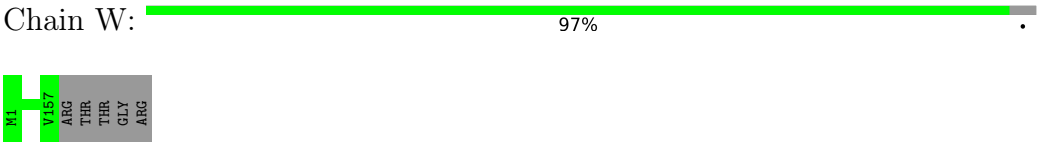

• Molecule 44: NADH-ubiquinone oxidoreductase chain 5

Chain V:



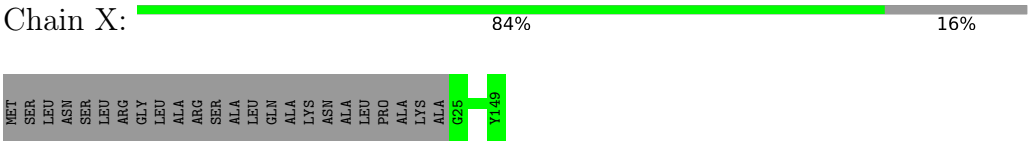

• Molecule 45: NADH-ubiquinone oxidoreductase chain 6

Chain W:



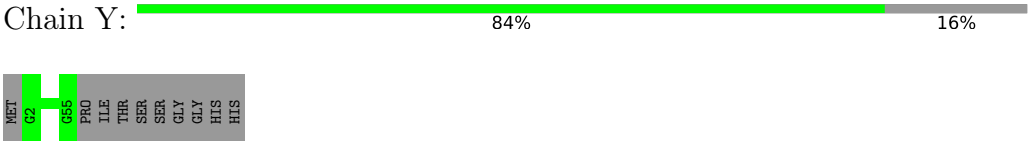

• Molecule 46: ASHI

Chain X:



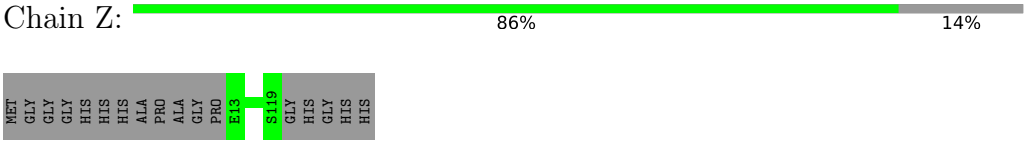

• Molecule 47: P9

Chain Y:



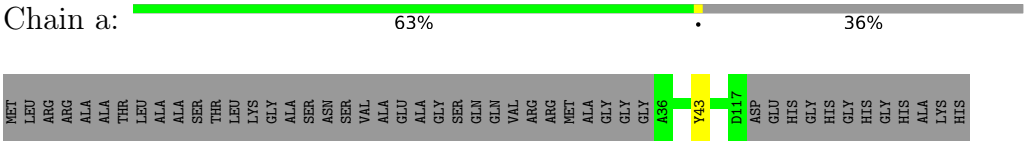

• Molecule 48: KFYI

Chain Z:



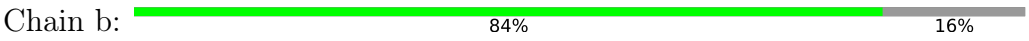

• Molecule 49: AGGG

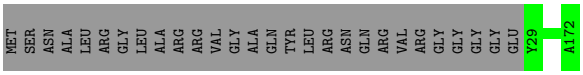
Chain a:




• Molecule 50: ESSS

Chain b:





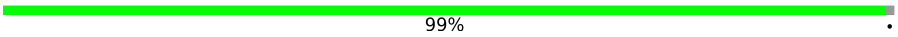

• Molecule 51: B9

Chain c:



• Molecule 52: Mitochondrial NADH:ubiquinone oxidoreductase 10 kDa subunit

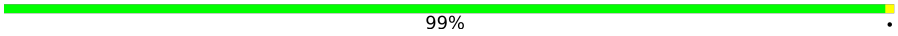
Chain d:

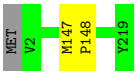




• Molecule 53: Mitochondrial NADH:ubiquinone oxidoreductase 23 kDa subunit

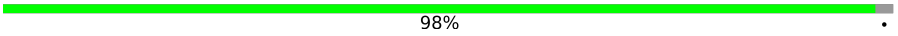
Chain e:




• Molecule 54: Mitochondrial NADH:ubiquinone oxidoreductase 7.5 kDa subunit

Chain f:





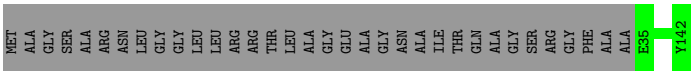
• Molecule 55: Mitochondrial putative NADH:ubiquinone oxidoreductase 6.5 kDa subunit

Chain g:



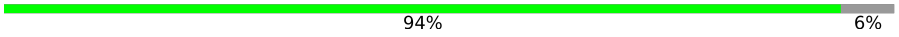
• Molecule 56: Mitochondrial NADH:ubiquinone oxidoreductase 13 kDa subunit

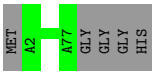
Chain h:


• Molecule 57: NADH:ubiquinone oxidoreductase 15 kDa subunit-like

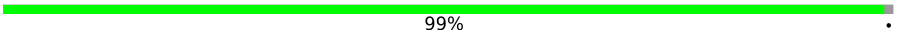
Chain i:






• Molecule 58: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7

Chain j:





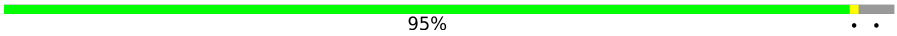
• Molecule 59: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9

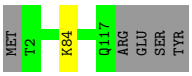
Chain k:


There are no outlier residues recorded for this chain.

• Molecule 60: NADH:ubiquinone oxidoreductase 20,9 kD-like subunit

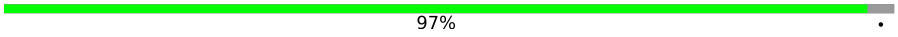
Chain l:




• Molecule 61: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13

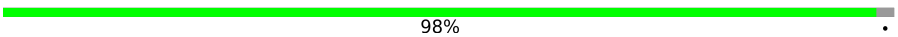
Chain m:





• Molecule 62: Putative NADH:ubiquinone oxidoreductase 12.5 kDa subunit

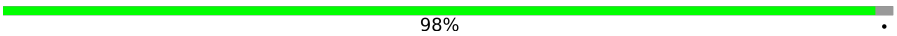
Chain n:

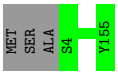




• Molecule 63: Putative NADH:ubiquinone oxidoreductase 17.8 kDa subunit

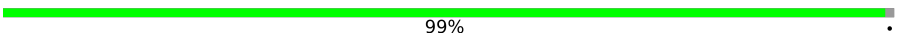
Chain o:



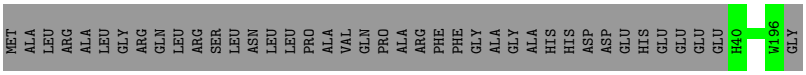

• Molecule 64: Mitochondrial NADH:ubiquinone oxidoreductase 16 kDa subunit

Chain p:



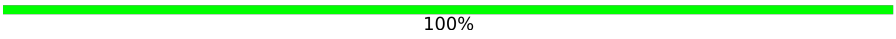

• Molecule 65: Mitochondrial NADH:ubiquinone oxidoreductase 19 kDa subunit

Chain q:


• Molecule 66: Mitochondrial NADH:ubiquinone oxidoreductase 32 kDa subunit

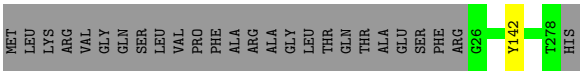
Chain s:





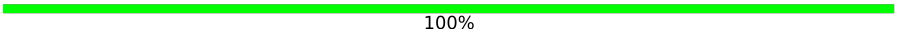
• Molecule 67: CAG2 - CA-like

Chain t:


• Molecule 68: CAG1

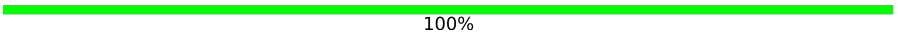
Chain u:





• Molecule 69: P10

Chain v:




There are no outlier residues recorded for this chain.

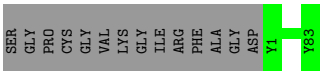
• Molecule 70: Mitochondrial NADH:ubiquinone oxidoreductase 9 kDa subunit

Chain w:



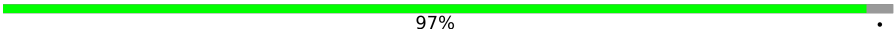
• Molecule 71: NUOP8

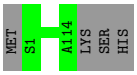
Chain x:


• Molecule 72: NUOP7

Chain y:



# 4 Experimental information (i)

| Property | Value | Source |
|---|---|---|
| EM reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, Not provided | |
| Number of particles used | 83443 | 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 ($e^-/Å^2$) | 40 | Depositor |
| Minimum defocus (nm) | 500 | Depositor |
| Maximum defocus (nm) | 2000 | Depositor |
| Magnification | Not provided | |
| Image detector | TFS FALCON 4i (4k x 4k) | Depositor |

# 5 Model quality

## 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, HEM, CDL, PC7, PTY, SF4, ZN, CU, FMN, FES, HEC, HEA, 3PH, CUA, NDP, UQ5, 8Q1, PGT, COO

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 | 1A | 0.34 | 0/3060 | 0.52 | 1/4187 (0.0%) |
| 1 | 1B | 0.35 | 0/3060 | 0.53 | 0/4187 |
| 2 | 1C | 0.28 | 0/1643 | 0.50 | 0/2233 |
| 2 | 1D | 0.28 | 0/1643 | 0.50 | 0/2233 |
| 3 | 1E | 0.34 | 0/1953 | 0.53 | 1/2654 (0.0%) |
| 3 | 1F | 0.33 | 0/1953 | 0.52 | 0/2654 |
| 4 | 1G | 0.32 | 0/496 | 0.54 | 0/667 |
| 4 | 1H | 0.32 | 0/496 | 0.50 | 0/667 |
| 5 | 1I | 0.31 | 0/567 | 0.50 | 0/766 |
| 5 | 1J | 0.30 | 0/567 | 0.45 | 0/766 |
| 6 | 1K | 0.33 | 0/609 | 0.54 | 0/817 |
| 6 | 1L | 0.31 | 0/609 | 0.54 | 0/817 |
| 7 | 1M | 0.31 | 0/3723 | 0.54 | 0/5046 |
| 7 | 1N | 0.30 | 0/3723 | 0.54 | 0/5046 |
| 8 | 1O | 0.28 | 0/385 | 0.53 | 0/531 |
| 8 | 1P | 0.29 | 0/385 | 0.59 | 0/531 |
| 9 | 1Q | 0.31 | 0/3258 | 0.54 | 0/4439 |
| 9 | 1S | 0.30 | 0/3258 | 0.53 | 0/4439 |
| 10 | 1R | 0.31 | 0/996 | 0.55 | 0/1349 |
| 10 | 1T | 0.33 | 0/996 | 0.57 | 0/1349 |
| 11 | 2A | 0.33 | 0/4011 | 0.54 | 1/5484 (0.0%) |
| 11 | 3A | 0.34 | 0/4011 | 0.56 | 1/5484 (0.0%) |
| 12 | 2B | 0.30 | 0/1204 | 0.51 | 0/1641 |
| 12 | 3B | 0.30 | 0/1204 | 0.52 | 0/1641 |
| 13 | 2C | 0.30 | 0/1237 | 0.53 | 0/1676 |
| 13 | 3C | 0.32 | 0/1237 | 0.55 | 0/1676 |
| 14 | 2D | 0.32 | 0/2152 | 0.49 | 0/2937 |
| 14 | 3D | 0.32 | 0/2152 | 0.50 | 0/2937 |
| 15 | 2E | 0.31 | 0/757 | 0.63 | 0/1029 |
| 15 | 3E | 0.32 | 0/757 | 0.60 | 0/1029 |
| 16 | 2F | 0.30 | 0/726 | 0.46 | 0/974 |

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | $\#\|Z\| > 5$ | RMSZ | $\#\|Z\| > 5$ |
| 16 | 3F | 0.30 | 0/726 | 0.46 | 0/974 |
| 17 | 2G | 0.30 | 0/762 | 0.58 | 1/1038 (0.1%) |
| 17 | 3G | 0.30 | 0/762 | 0.55 | 1/1038 (0.1%) |
| 18 | 2H | 0.30 | 0/980 | 0.51 | 0/1325 |
| 18 | 3H | 0.32 | 0/980 | 0.55 | 0/1325 |
| 19 | 2I | 0.33 | 0/619 | 0.51 | 0/839 |
| 19 | 3I | 0.31 | 0/619 | 0.50 | 0/839 |
| 20 | 2J | 0.30 | 0/839 | 0.51 | 0/1143 |
| 20 | 3J | 0.31 | 0/839 | 0.53 | 0/1143 |
| 21 | 2K | 0.31 | 0/392 | 0.51 | 0/531 |
| 21 | 3K | 0.32 | 0/392 | 0.51 | 0/531 |
| 22 | 2L | 0.31 | 0/621 | 0.56 | 0/841 |
| 22 | 3L | 0.30 | 0/645 | 0.55 | 0/875 |
| 23 | A | 0.31 | 0/1878 | 0.54 | 0/2549 |
| 24 | B | 0.33 | 0/3400 | 0.56 | 0/4573 |
| 25 | C | 0.31 | 0/5272 | 0.56 | 0/7143 |
| 26 | D | 0.36 | 0/1843 | 0.58 | 0/2506 |
| 27 | E | 0.38 | 0/3158 | 0.61 | 1/4270 (0.0%) |
| 28 | F | 0.41 | 0/1258 | 0.57 | 0/1706 |
| 29 | G | 0.32 | 0/1648 | 0.60 | 0/2222 |
| 30 | H | 0.35 | 0/773 | 0.60 | 1/1046 (0.1%) |
| 31 | I | 0.31 | 0/1061 | 0.49 | 0/1441 |
| 32 | J | 0.29 | 0/649 | 0.49 | 0/875 |
| 32 | r | 0.32 | 0/673 | 0.47 | 0/906 |
| 33 | K | 0.34 | 0/1007 | 0.59 | 0/1348 |
| 34 | L | 0.33 | 0/1306 | 0.59 | 0/1769 |
| 35 | M | 0.31 | 0/936 | 0.52 | 0/1276 |
| 36 | N | 0.32 | 0/1277 | 0.52 | 0/1735 |
| 37 | O | 0.28 | 0/772 | 0.60 | 1/1037 (0.1%) |
| 38 | P | 0.30 | 0/2879 | 0.55 | 1/3905 (0.0%) |
| 39 | Q | 0.36 | 0/2234 | 0.58 | 0/3034 |
| 40 | R | 0.36 | 0/3100 | 0.55 | 0/4226 |
| 41 | S | 0.37 | 0/1106 | 0.57 | 1/1512 (0.1%) |
| 42 | T | 0.37 | 1/3533 (0.0%) | 0.56 | 0/4825 |
| 43 | U | 0.34 | 0/819 | 0.53 | 0/1112 |
| 44 | V | 0.36 | 0/4258 | 0.57 | 2/5792 (0.0%) |
| 45 | W | 0.34 | 0/1239 | 0.52 | 0/1686 |
| 46 | X | 0.36 | 0/1081 | 0.55 | 0/1479 |
| 47 | Y | 0.32 | 0/411 | 0.49 | 0/557 |
| 48 | Z | 0.33 | 0/894 | 0.53 | 0/1218 |
| 49 | a | 0.33 | 0/698 | 0.47 | 0/949 |
| 50 | b | 0.35 | 0/1201 | 0.56 | 0/1623 |
| 51 | c | 0.31 | 0/463 | 0.53 | 0/623 |

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | #\|Z\| >5 | RMSZ | #\|Z\| >5 |
| 52 | d | 0.37 | 0/721 | 0.53 | 0/968 |
| 53 | e | 0.34 | 0/1688 | 0.54 | 0/2301 |
| 54 | f | 0.32 | 0/547 | 0.53 | 0/740 |
| 55 | g | 0.30 | 0/433 | 0.55 | 0/587 |
| 56 | h | 0.34 | 0/948 | 0.55 | 0/1285 |
| 57 | i | 0.32 | 0/644 | 0.60 | 0/860 |
| 58 | j | 0.34 | 0/732 | 0.54 | 0/983 |
| 59 | k | 0.32 | 0/1011 | 0.55 | 0/1361 |
| 60 | l | 0.33 | 0/936 | 0.49 | 0/1278 |
| 61 | m | 0.36 | 0/1155 | 0.56 | 0/1558 |
| 62 | n | 0.32 | 0/886 | 0.50 | 0/1188 |
| 63 | o | 0.33 | 0/1265 | 0.59 | 0/1705 |
| 64 | p | 0.32 | 0/1095 | 0.55 | 0/1480 |
| 65 | q | 0.32 | 0/1308 | 0.51 | 0/1779 |
| 66 | s | 0.32 | 0/2353 | 0.53 | 1/3202 (0.0%) |
| 67 | t | 0.32 | 0/2043 | 0.56 | 0/2778 |
| 68 | u | 0.32 | 0/1730 | 0.54 | 0/2341 |
| 69 | v | 0.33 | 0/369 | 0.48 | 0/498 |
| 70 | w | 0.34 | 0/521 | 0.49 | 0/702 |
| 71 | x | 0.34 | 0/727 | 0.49 | 0/994 |
| 72 | y | 0.34 | 0/963 | 0.52 | 0/1313 |
| All | All | 0.33 | 1/134906 (0.0%) | 0.54 | 14/183172 (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 | 1A | 0 | 1 |
| 1 | 1B | 0 | 1 |
| 17 | 3G | 0 | 1 |
| 53 | e | 0 | 1 |
| All | All | 0 | 4 |

All (1) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 42 | T | 195 | VAL | CB-CG1 | -5.47 | 1.41 | 1.52 |

All (14) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 37 | O | 7 | LEU | CA-CB-CG | 7.19 | 131.83 | 115.30 |
| 27 | E | 297 | LEU | CA-CB-CG | 6.98 | 131.35 | 115.30 |
| 17 | 2G | 74 | LEU | CA-CB-CG | 6.55 | 130.36 | 115.30 |
| 17 | 3G | 74 | LEU | CA-CB-CG | 6.43 | 130.10 | 115.30 |
| 11 | 3A | 417 | LEU | CA-CB-CG | 6.25 | 129.68 | 115.30 |
| 41 | S | 224 | LEU | CA-CB-CG | 6.21 | 129.59 | 115.30 |
| 66 | s | 94 | LEU | CA-CB-CG | 5.91 | 128.90 | 115.30 |
| 44 | V | 8 | PHE | CB-CG-CD1 | -5.81 | 116.73 | 120.80 |
| 38 | P | 314 | MET | CA-CB-CG | 5.76 | 123.09 | 113.30 |
| 30 | H | 102 | GLU | C-N-CA | 5.64 | 135.79 | 121.70 |
| 11 | 2A | 417 | LEU | CA-CB-CG | 5.63 | 128.25 | 115.30 |
| 3 | 1E | 110 | CYS | CA-CB-SG | 5.16 | 123.30 | 114.00 |
| 44 | V | 8 | PHE | CB-CG-CD2 | 5.12 | 124.38 | 120.80 |
| 1 | 1A | 150 | LEU | CA-CB-CG | 5.06 | 126.93 | 115.30 |

There are no chirality outliers.

All (4) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 1 | 1A | 184 | TYR | Sidechain |
| 1 | 1B | 184 | TYR | Sidechain |
| 17 | 3G | 114 | TRP | Peptide |
| 53 | e | 147 | 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)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|---|---|---|---|---|---|---|---|
| 1 | 1A | 374/381 (98%) | 363 (97%) | 11 (3%) | 0 | 100 | 100 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|---|---|---|---|---|---|---|---|
| 1 | 1B | 374/381 (98%) | 366 (98%) | 8 (2%) | 0 | 100 | 100 |
| 2 | 1C | 205/262 (78%) | 194 (95%) | 11 (5%) | 0 | 100 | 100 |
| 2 | 1D | 205/262 (78%) | 201 (98%) | 4 (2%) | 0 | 100 | 100 |
| 3 | 1E | 241/314 (77%) | 236 (98%) | 5 (2%) | 0 | 100 | 100 |
| 3 | 1F | 241/314 (77%) | 235 (98%) | 6 (2%) | 0 | 100 | 100 |
| 4 | 1G | 57/60 (95%) | 57 (100%) | 0 | 0 | 100 | 100 |
| 4 | 1H | 57/60 (95%) | 57 (100%) | 0 | 0 | 100 | 100 |
| 5 | 1I | 66/69 (96%) | 66 (100%) | 0 | 0 | 100 | 100 |
| 5 | 1J | 66/69 (96%) | 64 (97%) | 2 (3%) | 0 | 100 | 100 |
| 6 | 1K | 68/73 (93%) | 67 (98%) | 1 (2%) | 0 | 100 | 100 |
| 6 | 1L | 68/73 (93%) | 65 (96%) | 3 (4%) | 0 | 100 | 100 |
| 7 | 1M | 462/495 (93%) | 454 (98%) | 8 (2%) | 0 | 100 | 100 |
| 7 | 1N | 462/495 (93%) | 456 (99%) | 5 (1%) | 1 (0%) | 44 | 71 |
| 8 | 1O | 46/59 (78%) | 43 (94%) | 3 (6%) | 0 | 100 | 100 |
| 8 | 1P | 46/59 (78%) | 44 (96%) | 2 (4%) | 0 | 100 | 100 |
| 9 | 1Q | 439/485 (90%) | 418 (95%) | 20 (5%) | 1 (0%) | 44 | 71 |
| 9 | 1S | 439/485 (90%) | 425 (97%) | 12 (3%) | 2 (0%) | 25 | 54 |
| 10 | 1R | 120/123 (98%) | 119 (99%) | 1 (1%) | 0 | 100 | 100 |
| 10 | 1T | 120/123 (98%) | 118 (98%) | 2 (2%) | 0 | 100 | 100 |
| 11 | 2A | 502/504 (100%) | 489 (97%) | 13 (3%) | 0 | 100 | 100 |
| 11 | 3A | 502/504 (100%) | 490 (98%) | 12 (2%) | 0 | 100 | 100 |
| 12 | 2B | 139/284 (49%) | 136 (98%) | 3 (2%) | 0 | 100 | 100 |
| 12 | 3B | 139/284 (49%) | 135 (97%) | 4 (3%) | 0 | 100 | 100 |
| 13 | 2C | 151/153 (99%) | 144 (95%) | 7 (5%) | 0 | 100 | 100 |
| 13 | 3C | 151/153 (99%) | 145 (96%) | 6 (4%) | 0 | 100 | 100 |
| 14 | 2D | 264/382 (69%) | 255 (97%) | 9 (3%) | 0 | 100 | 100 |
| 14 | 3D | 264/382 (69%) | 254 (96%) | 10 (4%) | 0 | 100 | 100 |
| 15 | 2E | 88/175 (50%) | 85 (97%) | 2 (2%) | 1 (1%) | 12 | 35 |
| 15 | 3E | 88/175 (50%) | 85 (97%) | 2 (2%) | 1 (1%) | 12 | 35 |
| 16 | 2F | 84/96 (88%) | 81 (96%) | 3 (4%) | 0 | 100 | 100 |
| 16 | 3F | 84/96 (88%) | 80 (95%) | 4 (5%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|---|---|---|---|---|---|---|---|
| 17 | 2G | 87/125 (70%) | 78 (90%) | 9 (10%) | 0 | 100 | 100 |
| 17 | 3G | 87/125 (70%) | 80 (92%) | 7 (8%) | 0 | 100 | 100 |
| 18 | 2H | 112/148 (76%) | 108 (96%) | 4 (4%) | 0 | 100 | 100 |
| 18 | 3H | 112/148 (76%) | 108 (96%) | 4 (4%) | 0 | 100 | 100 |
| 19 | 2I | 70/101 (69%) | 67 (96%) | 3 (4%) | 0 | 100 | 100 |
| 19 | 3I | 70/101 (69%) | 67 (96%) | 3 (4%) | 0 | 100 | 100 |
| 20 | 2J | 102/105 (97%) | 100 (98%) | 2 (2%) | 0 | 100 | 100 |
| 20 | 3J | 102/105 (97%) | 100 (98%) | 2 (2%) | 0 | 100 | 100 |
| 21 | 2K | 45/58 (78%) | 44 (98%) | 1 (2%) | 0 | 100 | 100 |
| 21 | 3K | 45/58 (78%) | 44 (98%) | 1 (2%) | 0 | 100 | 100 |
| 22 | 2L | 74/87 (85%) | 70 (95%) | 4 (5%) | 0 | 100 | 100 |
| 22 | 3L | 76/87 (87%) | 72 (95%) | 4 (5%) | 0 | 100 | 100 |
| 23 | A | 237/282 (84%) | 228 (96%) | 9 (4%) | 0 | 100 | 100 |
| 24 | B | 433/484 (90%) | 417 (96%) | 16 (4%) | 0 | 100 | 100 |
| 25 | C | 686/733 (94%) | 667 (97%) | 19 (3%) | 0 | 100 | 100 |
| 26 | D | 214/282 (76%) | 204 (95%) | 10 (5%) | 0 | 100 | 100 |
| 27 | E | 379/467 (81%) | 368 (97%) | 11 (3%) | 0 | 100 | 100 |
| 28 | F | 155/164 (94%) | 149 (96%) | 6 (4%) | 0 | 100 | 100 |
| 29 | G | 197/231 (85%) | 189 (96%) | 8 (4%) | 0 | 100 | 100 |
| 30 | H | 88/118 (75%) | 81 (92%) | 7 (8%) | 0 | 100 | 100 |
| 31 | I | 133/165 (81%) | 130 (98%) | 3 (2%) | 0 | 100 | 100 |
| 32 | J | 82/128 (64%) | 76 (93%) | 6 (7%) | 0 | 100 | 100 |
| 32 | r | 86/128 (67%) | 84 (98%) | 2 (2%) | 0 | 100 | 100 |
| 33 | K | 117/138 (85%) | 115 (98%) | 2 (2%) | 0 | 100 | 100 |
| 34 | L | 162/187 (87%) | 155 (96%) | 7 (4%) | 0 | 100 | 100 |
| 35 | M | 119/154 (77%) | 111 (93%) | 8 (7%) | 0 | 100 | 100 |
| 36 | N | 148/156 (95%) | 145 (98%) | 3 (2%) | 0 | 100 | 100 |
| 37 | O | 98/101 (97%) | 94 (96%) | 4 (4%) | 0 | 100 | 100 |
| 38 | P | 361/397 (91%) | 350 (97%) | 11 (3%) | 0 | 100 | 100 |
| 39 | Q | 282/292 (97%) | 274 (97%) | 8 (3%) | 0 | 100 | 100 |
| 40 | R | 385/387 (100%) | 369 (96%) | 16 (4%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|---|---|---|---|---|---|---|---|
| 41 | S | 130/279 (47%) | 128 (98%) | 2 (2%) | 0 | 100 | 100 |
| 42 | T | 441/443 (100%) | 431 (98%) | 10 (2%) | 0 | 100 | 100 |
| 43 | U | 103/227 (45%) | 102 (99%) | 1 (1%) | 0 | 100 | 100 |
| 44 | V | 544/546 (100%) | 525 (96%) | 18 (3%) | 1 (0%) | 44 | 71 |
| 45 | W | 155/162 (96%) | 151 (97%) | 4 (3%) | 0 | 100 | 100 |
| 46 | X | 123/149 (83%) | 117 (95%) | 6 (5%) | 0 | 100 | 100 |
| 47 | Y | 52/64 (81%) | 52 (100%) | 0 | 0 | 100 | 100 |
| 48 | Z | 105/124 (85%) | 100 (95%) | 5 (5%) | 0 | 100 | 100 |
| 49 | a | 80/129 (62%) | 78 (98%) | 1 (1%) | 1 (1%) | 10 | 30 |
| 50 | b | 142/172 (83%) | 139 (98%) | 3 (2%) | 0 | 100 | 100 |
| 51 | c | 55/67 (82%) | 52 (94%) | 3 (6%) | 0 | 100 | 100 |
| 52 | d | 83/86 (96%) | 82 (99%) | 1 (1%) | 0 | 100 | 100 |
| 53 | e | 216/219 (99%) | 214 (99%) | 1 (0%) | 1 (0%) | 25 | 54 |
| 54 | f | 62/65 (95%) | 59 (95%) | 3 (5%) | 0 | 100 | 100 |
| 55 | g | 48/55 (87%) | 42 (88%) | 6 (12%) | 0 | 100 | 100 |
| 56 | h | 106/142 (75%) | 97 (92%) | 9 (8%) | 0 | 100 | 100 |
| 57 | i | 74/81 (91%) | 73 (99%) | 1 (1%) | 0 | 100 | 100 |
| 58 | j | 83/86 (96%) | 80 (96%) | 3 (4%) | 0 | 100 | 100 |
| 59 | k | 115/117 (98%) | 110 (96%) | 5 (4%) | 0 | 100 | 100 |
| 60 | l | 114/121 (94%) | 110 (96%) | 4 (4%) | 0 | 100 | 100 |
| 61 | m | 134/142 (94%) | 133 (99%) | 1 (1%) | 0 | 100 | 100 |
| 62 | n | 102/106 (96%) | 100 (98%) | 2 (2%) | 0 | 100 | 100 |
| 63 | o | 150/155 (97%) | 145 (97%) | 5 (3%) | 0 | 100 | 100 |
| 64 | p | 127/130 (98%) | 125 (98%) | 2 (2%) | 0 | 100 | 100 |
| 65 | q | 155/197 (79%) | 149 (96%) | 6 (4%) | 0 | 100 | 100 |
| 66 | s | 310/312 (99%) | 303 (98%) | 7 (2%) | 0 | 100 | 100 |
| 67 | t | 251/279 (90%) | 243 (97%) | 8 (3%) | 0 | 100 | 100 |
| 68 | u | 226/229 (99%) | 220 (97%) | 6 (3%) | 0 | 100 | 100 |
| 69 | v | 43/45 (96%) | 43 (100%) | 0 | 0 | 100 | 100 |
| 70 | w | 62/109 (57%) | 61 (98%) | 1 (2%) | 0 | 100 | 100 |
| 71 | x | 81/157 (52%) | 81 (100%) | 0 | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles |
|---|---|---|---|---|---|---|
| 72 | y | 112/118 (95%) | 111 (99%) | 1 (1%) | 0 | 100 100 |
| All | All | 16540/19385 (85%) | 16027 (97%) | 504 (3%) | 9 (0%) | 50 76 |

All (9) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 9 | 1Q | 396 | ASP |
| 15 | 2E | 28 | TRP |
| 15 | 3E | 28 | TRP |
| 49 | a | 43 | TYR |
| 9 | 1S | 66 | THR |
| 44 | V | 519 | PRO |
| 53 | e | 148 | PRO |
| 7 | 1N | 187 | VAL |
| 9 | 1S | 475 | PRO |

### 5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles |
|---|---|---|---|---|---|
| 1 | 1A | 312/317 (98%) | 311 (100%) | 1 (0%) | 91 97 |
| 1 | 1B | 312/317 (98%) | 309 (99%) | 3 (1%) | 73 91 |
| 2 | 1C | 171/213 (80%) | 170 (99%) | 1 (1%) | 84 94 |
| 2 | 1D | 171/213 (80%) | 171 (100%) | 0 | 100 100 |
| 3 | 1E | 191/238 (80%) | 191 (100%) | 0 | 100 100 |
| 3 | 1F | 191/238 (80%) | 191 (100%) | 0 | 100 100 |
| 4 | 1G | 52/53 (98%) | 52 (100%) | 0 | 100 100 |
| 4 | 1H | 52/53 (98%) | 52 (100%) | 0 | 100 100 |
| 5 | 1I | 58/59 (98%) | 58 (100%) | 0 | 100 100 |
| 5 | 1J | 58/59 (98%) | 58 (100%) | 0 | 100 100 |
| 6 | 1K | 62/64 (97%) | 62 (100%) | 0 | 100 100 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|---|---|---|---|---|---|---|
| 6 | 1L | 62/64 (97%) | 62 (100%) | 0 | 100 | 100 |
| 7 | 1M | 390/413 (94%) | 390 (100%) | 0 | 100 | 100 |
| 7 | 1N | 390/413 (94%) | 388 (100%) | 2 (0%) | 86 | 95 |
| 8 | 1O | 38/47 (81%) | 38 (100%) | 0 | 100 | 100 |
| 8 | 1P | 38/47 (81%) | 38 (100%) | 0 | 100 | 100 |
| 9 | 1Q | 333/362 (92%) | 331 (99%) | 2 (1%) | 84 | 94 |
| 9 | 1S | 333/362 (92%) | 332 (100%) | 1 (0%) | 91 | 97 |
| 10 | 1R | 106/107 (99%) | 106 (100%) | 0 | 100 | 100 |
| 10 | 1T | 106/107 (99%) | 106 (100%) | 0 | 100 | 100 |
| 11 | 2A | 408/408 (100%) | 408 (100%) | 0 | 100 | 100 |
| 11 | 3A | 408/408 (100%) | 408 (100%) | 0 | 100 | 100 |
| 12 | 2B | 132/224 (59%) | 132 (100%) | 0 | 100 | 100 |
| 12 | 3B | 132/224 (59%) | 132 (100%) | 0 | 100 | 100 |
| 13 | 2C | 137/137 (100%) | 137 (100%) | 0 | 100 | 100 |
| 13 | 3C | 137/137 (100%) | 137 (100%) | 0 | 100 | 100 |
| 14 | 2D | 211/294 (72%) | 211 (100%) | 0 | 100 | 100 |
| 14 | 3D | 211/294 (72%) | 211 (100%) | 0 | 100 | 100 |
| 15 | 2E | 79/137 (58%) | 79 (100%) | 0 | 100 | 100 |
| 15 | 3E | 79/137 (58%) | 79 (100%) | 0 | 100 | 100 |
| 16 | 2F | 66/72 (92%) | 66 (100%) | 0 | 100 | 100 |
| 16 | 3F | 66/72 (92%) | 66 (100%) | 0 | 100 | 100 |
| 17 | 2G | 75/100 (75%) | 75 (100%) | 0 | 100 | 100 |
| 17 | 3G | 75/100 (75%) | 74 (99%) | 1 (1%) | 65 | 88 |
| 18 | 2H | 103/132 (78%) | 103 (100%) | 0 | 100 | 100 |
| 18 | 3H | 103/132 (78%) | 103 (100%) | 0 | 100 | 100 |
| 19 | 2I | 58/80 (72%) | 58 (100%) | 0 | 100 | 100 |
| 19 | 3I | 58/80 (72%) | 58 (100%) | 0 | 100 | 100 |
| 20 | 2J | 83/84 (99%) | 83 (100%) | 0 | 100 | 100 |
| 20 | 3J | 83/84 (99%) | 83 (100%) | 0 | 100 | 100 |
| 21 | 2K | 39/46 (85%) | 39 (100%) | 0 | 100 | 100 |
| 21 | 3K | 39/46 (85%) | 39 (100%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|---|---|---|---|---|---|---|
| 22 | 2L | 63/74 (85%) | 63 (100%) | 0 | 100 | 100 |
| 22 | 3L | 65/74 (88%) | 65 (100%) | 0 | 100 | 100 |
| 23 | A | 197/228 (86%) | 197 (100%) | 0 | 100 | 100 |
| 24 | B | 344/377 (91%) | 344 (100%) | 0 | 100 | 100 |
| 25 | C | 537/572 (94%) | 536 (100%) | 1 (0%) | 92 | 97 |
| 26 | D | 196/248 (79%) | 196 (100%) | 0 | 100 | 100 |
| 27 | E | 329/388 (85%) | 329 (100%) | 0 | 100 | 100 |
| 28 | F | 129/133 (97%) | 129 (100%) | 0 | 100 | 100 |
| 29 | G | 172/198 (87%) | 172 (100%) | 0 | 100 | 100 |
| 30 | H | 82/105 (78%) | 82 (100%) | 0 | 100 | 100 |
| 31 | I | 111/134 (83%) | 111 (100%) | 0 | 100 | 100 |
| 32 | J | 71/108 (66%) | 71 (100%) | 0 | 100 | 100 |
| 32 | r | 72/108 (67%) | 72 (100%) | 0 | 100 | 100 |
| 33 | K | 106/122 (87%) | 106 (100%) | 0 | 100 | 100 |
| 34 | L | 130/148 (88%) | 130 (100%) | 0 | 100 | 100 |
| 35 | M | 100/121 (83%) | 100 (100%) | 0 | 100 | 100 |
| 36 | N | 128/132 (97%) | 128 (100%) | 0 | 100 | 100 |
| 37 | O | 80/81 (99%) | 80 (100%) | 0 | 100 | 100 |
| 38 | P | 305/327 (93%) | 305 (100%) | 0 | 100 | 100 |
| 39 | Q | 230/234 (98%) | 230 (100%) | 0 | 100 | 100 |
| 40 | R | 321/321 (100%) | 321 (100%) | 0 | 100 | 100 |
| 41 | S | 111/217 (51%) | 111 (100%) | 0 | 100 | 100 |
| 42 | T | 374/374 (100%) | 374 (100%) | 0 | 100 | 100 |
| 43 | U | 84/180 (47%) | 84 (100%) | 0 | 100 | 100 |
| 44 | V | 439/439 (100%) | 439 (100%) | 0 | 100 | 100 |
| 45 | W | 131/135 (97%) | 131 (100%) | 0 | 100 | 100 |
| 46 | X | 105/122 (86%) | 105 (100%) | 0 | 100 | 100 |
| 47 | Y | 38/46 (83%) | 38 (100%) | 0 | 100 | 100 |
| 48 | Z | 93/102 (91%) | 93 (100%) | 0 | 100 | 100 |
| 49 | a | 68/98 (69%) | 68 (100%) | 0 | 100 | 100 |
| 50 | b | 119/138 (86%) | 119 (100%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|---|---|---|---|---|---|---|
| 51 | c | 49/56 (88%) | 49 (100%) | 0 | 100 | 100 |
| 52 | d | 63/64 (98%) | 63 (100%) | 0 | 100 | 100 |
| 53 | e | 163/164 (99%) | 163 (100%) | 0 | 100 | 100 |
| 54 | f | 52/53 (98%) | 52 (100%) | 0 | 100 | 100 |
| 55 | g | 40/45 (89%) | 40 (100%) | 0 | 100 | 100 |
| 56 | h | 91/110 (83%) | 91 (100%) | 0 | 100 | 100 |
| 57 | i | 65/67 (97%) | 65 (100%) | 0 | 100 | 100 |
| 58 | j | 72/73 (99%) | 72 (100%) | 0 | 100 | 100 |
| 59 | k | 102/102 (100%) | 102 (100%) | 0 | 100 | 100 |
| 60 | l | 94/99 (95%) | 93 (99%) | 1 (1%) | 70 | 90 |
| 61 | m | 118/122 (97%) | 118 (100%) | 0 | 100 | 100 |
| 62 | n | 92/94 (98%) | 92 (100%) | 0 | 100 | 100 |
| 63 | o | 130/132 (98%) | 130 (100%) | 0 | 100 | 100 |
| 64 | p | 109/110 (99%) | 109 (100%) | 0 | 100 | 100 |
| 65 | q | 135/165 (82%) | 135 (100%) | 0 | 100 | 100 |
| 66 | s | 243/243 (100%) | 243 (100%) | 0 | 100 | 100 |
| 67 | t | 212/233 (91%) | 211 (100%) | 1 (0%) | 86 | 95 |
| 68 | u | 180/181 (99%) | 180 (100%) | 0 | 100 | 100 |
| 69 | v | 38/38 (100%) | 38 (100%) | 0 | 100 | 100 |
| 70 | w | 55/91 (60%) | 55 (100%) | 0 | 100 | 100 |
| 71 | x | 70/130 (54%) | 70 (100%) | 0 | 100 | 100 |
| 72 | y | 102/106 (96%) | 102 (100%) | 0 | 100 | 100 |
| All | All | 13813/15736 (88%) | 13799 (100%) | 14 (0%) | 92 | 98 |

All (14) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 1A | 316 | ARG |
| 1 | 1B | 79 | ARG |
| 1 | 1B | 261 | ASN |
| 1 | 1B | 316 | ARG |
| 2 | 1C | 230 | HIS |
| 7 | 1N | 171 | ARG |
| 7 | 1N | 488 | ARG |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 9 | 1Q | 81 | ARG |
| 9 | 1Q | 483 | ARG |
| 9 | 1S | 216 | ARG |
| 17 | 3G | 109 | ARG |
| 25 | C | 593 | ARG |
| 60 | l | 84 | LYS |
| 67 | t | 142 | TYR |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 1B | 261 | ASN |
| 25 | C | 279 | ASN |
| 25 | C | 297 | ASN |
| 25 | C | 618 | GLN |
| 60 | l | 41 | ASN |

#### 5.3.3 RNA

There are no RNA molecules in this entry.

### 5.4 Non-standard residues in protein, DNA, RNA chains

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

### 5.5 Carbohydrates

There are no oligosaccharides in this entry.

### 5.6 Ligand geometry

Of 107 ligands modelled in this entry, 7 are monoatomic - leaving 100 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 | $\#\|Z\|>2$ |
| 88 | SF4 | C | 803 | 25 | 0,12,12 | - | - | - | | |
| 74 | HEM | 1A | 403 | 1 | 41,50,50 | 1.42 | 4 (9%) | 45,82,82 | 1.76 | 11 (24%) |
| 81 | PGT | T | 502 | - | 47,47,50 | 0.53 | 0 | 50,53,56 | 0.56 | 1 (2%) |
| 77 | PTY | 1E | 403 | - | 33,33,49 | 0.55 | 0 | 36,38,54 | 0.50 | 0 |
| 77 | PTY | T | 501 | - | 49,49,49 | 0.46 | 0 | 52,54,54 | 0.62 | 1 (1%) |
| 79 | PC7 | 2A | 606 | - | 26,26,51 | 0.66 | 0 | 32,34,59 | 0.70 | 0 |
| 77 | PTY | T | 504 | - | 27,27,49 | 0.65 | 0 | 30,32,54 | 0.48 | 0 |
| 82 | HEA | 3A | 602 | 11 | 57,67,67 | 2.05 | 16 (28%) | 61,103,103 | 2.43 | 25 (40%) |
| 81 | PGT | 2A | 601 | - | 32,32,50 | 0.61 | 0 | 35,38,56 | 0.60 | 0 |
| 79 | PC7 | T | 503 | - | 51,51,51 | 0.50 | 0 | 57,59,59 | 0.59 | 0 |
| 79 | PC7 | 1H | 101 | - | 38,38,51 | 0.57 | 0 | 44,46,59 | 0.56 | 0 |
| 76 | 3PH | R | 401 | - | 31,31,47 | 0.75 | 1 (3%) | 35,36,52 | 0.73 | 2 (5%) |
| 76 | 3PH | 1A | 406 | - | 30,30,47 | 0.78 | 1 (3%) | 34,35,52 | 0.69 | 1 (2%) |
| 77 | PTY | V | 604 | - | 39,39,49 | 0.54 | 0 | 42,44,54 | 0.50 | 0 |
| 77 | PTY | V | 605 | - | 49,49,49 | 0.46 | 0 | 52,54,54 | 0.38 | 0 |
| 82 | HEA | 2A | 602 | 11 | 57,67,67 | 2.06 | 17 (29%) | 61,103,103 | 2.43 | 25 (40%) |
| 86 | FES | C | 801 | 25 | 0,4,4 | - | - | - | | |
| 79 | PC7 | 3A | 606 | - | 26,26,51 | 0.66 | 0 | 32,34,59 | 0.65 | 0 |
| 86 | FES | A | 301 | 23 | 0,4,4 | - | - | - | | |
| 76 | 3PH | y | 201 | - | 31,31,47 | 0.78 | 1 (3%) | 35,36,52 | 0.66 | 1 (2%) |
| 81 | PGT | 3A | 601 | - | 32,32,50 | 0.59 | 0 | 35,38,56 | 0.52 | 0 |
| 78 | HEC | 1E | 404 | 3 | 32,50,50 | 2.19 | 3 (9%) | 24,82,82 | 1.81 | 5 (20%) |
| 75 | CDL | 1K | 101 | - | 78,78,99 | 0.43 | 0 | 84,90,111 | 0.28 | 0 |
| 76 | 3PH | 1R | 201 | - | 36,36,47 | 0.71 | 1 (2%) | 40,41,52 | 0.70 | 1 (2%) |
| 79 | PC7 | u | 601 | - | 41,41,51 | 0.55 | 0 | 47,49,59 | 0.68 | 2 (4%) |
| 77 | PTY | G | 303 | - | 42,42,49 | 0.49 | 0 | 45,47,54 | 0.44 | 0 |
| 75 | CDL | R | 405 | - | 62,62,99 | 0.40 | 0 | 68,74,111 | 0.28 | 0 |
| 75 | CDL | y | 202 | - | 54,54,99 | 0.53 | 1 (1%) | 60,66,111 | 0.32 | 0 |
| 75 | CDL | x | 101 | - | 91,91,99 | 0.40 | 1 (1%) | 97,103,111 | 0.24 | 0 |
| 73 | UQ5 | 1A | 401 | - | 38,38,38 | 0.53 | 0 | 46,49,49 | 1.08 | 4 (8%) |
| 89 | 8Q1 | r | 200 | - | 31,34,34 | 1.76 | 5 (16%) | 40,43,43 | 1.88 | 10 (25%) |
| 75 | CDL | W | 701 | - | 94,94,99 | 0.35 | 0 | 100,106,111 | 0.28 | 0 |
| 77 | PTY | e | 302 | - | 42,42,49 | 0.52 | 0 | 45,47,54 | 0.42 | 0 |
| 73 | UQ5 | 1B | 401 | - | 38,38,38 | 0.46 | 0 | 46,49,49 | 0.73 | 1 (2%) |
| 76 | 3PH | h | 201 | - | 44,44,47 | 0.65 | 1 (2%) | 48,49,52 | 3.77 | 5 (10%) |
| 76 | 3PH | V | 601 | - | 41,41,47 | 0.66 | 1 (2%) | 45,46,52 | 0.63 | 1 (2%) |
| 75 | CDL | 1A | 405 | - | 58,58,99 | 0.44 | 0 | 64,70,111 | 0.27 | 0 |
| 77 | PTY | 2D | 301 | - | 34,34,49 | 0.56 | 0 | 37,39,54 | 0.56 | 0 |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\|>2$ | Counts | RMSZ | $\#\|Z\|>2$ |
| 75 | CDL | 1M | 501 | - | 53,53,99 | 0.49 | 1 (1%) | 59,65,111 | 0.26 | 0 |
| 75 | CDL | 1B | 408 | - | 70,70,99 | 0.34 | 0 | 76,82,111 | 0.34 | 0 |
| 77 | PTY | x | 102 | - | 49,49,49 | 0.46 | 0 | 52,54,54 | 0.40 | 0 |
| 77 | PTY | R | 404 | - | 43,43,49 | 0.51 | 0 | 46,48,54 | 0.46 | 0 |
| 75 | CDL | 1B | 405 | - | 63,63,99 | 0.44 | 1 (1%) | 69,75,111 | 0.25 | 0 |
| 82 | HEA | 2A | 603 | 11 | 57,67,67 | 2.08 | 16 (28%) | 61,103,103 | 2.42 | 23 (37%) |
| 75 | CDL | V | 603 | - | 63,63,99 | 0.41 | 0 | 69,75,111 | 0.25 | 0 |
| 73 | UQ5 | 1B | 402 | - | 38,38,38 | 0.51 | 0 | 46,49,49 | 1.51 | 6 (13%) |
| 76 | 3PH | 2D | 302 | - | 31,31,47 | 0.77 | 1 (3%) | 35,36,52 | 0.72 | 1 (2%) |
| 75 | CDL | u | 602 | - | 82,82,99 | 0.38 | 0 | 88,94,111 | 0.30 | 0 |
| 75 | CDL | 1L | 101 | - | 58,58,99 | 0.43 | 0 | 64,70,111 | 0.35 | 0 |
| 77 | PTY | S | 302 | - | 45,45,49 | 0.49 | 0 | 48,50,54 | 0.41 | 0 |
| 76 | 3PH | w | 201 | - | 44,44,47 | 0.64 | 1 (2%) | 48,49,52 | 0.75 | 3 (6%) |
| 90 | NDP | P | 401 | - | 45,52,52 | 2.24 | 6 (13%) | 53,80,80 | 1.65 | 13 (24%) |
| 74 | HEM | 1B | 404 | 1 | 41,50,50 | 1.45 | 3 (7%) | 45,82,82 | 1.38 | 7 (15%) |
| 76 | 3PH | 1B | 406 | - | 47,47,47 | 0.62 | 1 (2%) | 51,52,52 | 0.60 | 1 (1%) |
| 85 | CUA | 3C | 301 | - | 0,1,1 | - | - | - | | |
| 77 | PTY | T | 506 | - | 25,25,49 | 0.64 | 0 | 28,30,54 | 0.47 | 0 |
| 77 | PTY | 2F | 101 | - | 33,33,49 | 0.55 | 0 | 36,38,54 | 0.45 | 0 |
| 77 | PTY | e | 301 | - | 24,24,49 | 0.64 | 0 | 27,29,54 | 0.52 | 0 |
| 91 | COO | s | 401 | - | 45,55,55 | 0.82 | 1 (2%) | 55,81,81 | 4.26 | 10 (18%) |
| 76 | 3PH | 1E | 402 | - | 39,39,47 | 0.69 | 1 (2%) | 43,44,52 | 0.64 | 0 |
| 88 | SF4 | B | 502 | 24 | 0,12,12 | - | - | - | | |
| 85 | CUA | 2C | 301 | - | 0,1,1 | - | - | - | | |
| 73 | UQ5 | Q | 301 | - | 38,38,38 | 0.51 | 0 | 46,49,49 | 0.83 | 3 (6%) |
| 76 | 3PH | 3D | 302 | - | 31,31,47 | 0.75 | 1 (3%) | 35,36,52 | 0.80 | 1 (2%) |
| 74 | HEM | 1B | 403 | 1 | 41,50,50 | 1.54 | 4 (9%) | 45,82,82 | 1.51 | 7 (15%) |
| 77 | PTY | h | 202 | - | 45,45,49 | 0.47 | 0 | 48,50,54 | 0.46 | 0 |
| 82 | HEA | 3A | 603 | 11 | 57,67,67 | 2.06 | 15 (26%) | 61,103,103 | 2.46 | 23 (37%) |
| 88 | SF4 | G | 302 | 29 | 0,12,12 | - | - | - | | |
| 77 | PTY | V | 606 | - | 34,34,49 | 0.56 | 0 | 37,39,54 | 0.44 | 0 |
| 87 | FMN | B | 501 | - | 33,33,33 | 1.09 | 2 (6%) | 48,50,50 | 1.25 | 8 (16%) |
| 79 | PC7 | R | 403 | - | 43,43,51 | 0.53 | 0 | 49,51,59 | 0.61 | 0 |
| 81 | PGT | T | 505 | - | 39,39,50 | 0.54 | 0 | 42,45,56 | 0.50 | 0 |
| 77 | PTY | R | 402 | - | 33,33,49 | 0.53 | 0 | 36,38,54 | 0.43 | 0 |
| 88 | SF4 | G | 301 | 29 | 0,12,12 | - | - | - | | |
| 77 | PTY | 3D | 301 | - | 34,34,49 | 0.57 | 0 | 37,39,54 | 0.47 | 0 |
| 76 | 3PH | 2I | 201 | - | 41,41,47 | 0.67 | 1 (2%) | 45,46,52 | 0.67 | 1 (2%) |
| 75 | CDL | u | 603 | - | 70,70,99 | 0.43 | 0 | 76,82,111 | 0.28 | 0 |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\|>2$ | Counts | RMSZ | $\#\|Z\|>2$ |
| 77 | PTY | 1F | 403 | - | 37,37,49 | 0.51 | 0 | 40,42,54 | 0.44 | 0 |
| 88 | SF4 | C | 802 | 25 | 0,12,12 | - | - | - | | |
| 76 | 3PH | 1B | 407 | - | 47,47,47 | 0.63 | 1 (2%) | 51,52,52 | 0.60 | 0 |
| 79 | PC7 | 1G | 301 | - | 35,35,51 | 0.61 | 0 | 41,43,59 | 0.60 | 1 (2%) |
| 81 | PGT | l | 701 | - | 50,50,50 | 0.48 | 0 | 53,56,56 | 0.59 | 1 (1%) |
| 76 | 3PH | 3I | 201 | - | 41,41,47 | 0.65 | 1 (2%) | 45,46,52 | 0.66 | 1 (2%) |
| 76 | 3PH | S | 301 | - | 36,36,47 | 0.71 | 1 (2%) | 40,41,52 | 0.70 | 1 (2%) |
| 76 | 3PH | c | 101 | - | 47,47,47 | 0.62 | 1 (2%) | 51,52,52 | 0.63 | 1 (1%) |
| 75 | CDL | 1E | 401 | - | 52,52,99 | 0.44 | 0 | 58,64,111 | 0.25 | 0 |
| 81 | PGT | b | 601 | - | 43,43,50 | 0.53 | 0 | 46,49,56 | 0.51 | 0 |
| 88 | SF4 | F | 201 | 28 | 0,12,12 | - | - | - | | |
| 75 | CDL | h | 203 | - | 76,76,99 | 0.37 | 0 | 82,88,111 | 0.25 | 0 |
| 73 | UQ5 | 1A | 402 | - | 38,38,38 | 0.52 | 0 | 46,49,49 | 0.66 | 1 (2%) |
| 78 | HEC | 1F | 402 | 3 | 32,50,50 | 2.08 | 3 (9%) | 24,82,82 | 1.85 | 6 (25%) |
| 76 | 3PH | V | 602 | - | 40,40,47 | 0.67 | 1 (2%) | 44,45,52 | 0.82 | 1 (2%) |
| 74 | HEM | 1A | 404 | 1 | 41,50,50 | 1.40 | 3 (7%) | 45,82,82 | 1.52 | 7 (15%) |
| 79 | PC7 | Q | 302 | - | 32,32,51 | 0.59 | 0 | 38,40,59 | 0.69 | 0 |
| 76 | 3PH | g | 101 | - | 36,36,47 | 0.71 | 1 (2%) | 40,41,52 | 0.70 | 1 (2%) |
| 77 | PTY | R | 406 | - | 39,39,49 | 0.53 | 0 | 42,44,54 | 0.51 | 0 |
| 89 | 8Q1 | J | 200 | - | 31,34,34 | 1.69 | 5 (16%) | 40,43,43 | 1.71 | 5 (12%) |
| 77 | PTY | 3F | 101 | - | 33,33,49 | 0.55 | 0 | 36,38,54 | 0.47 | 0 |
| 75 | CDL | 1F | 401 | - | 55,55,99 | 0.42 | 0 | 61,67,111 | 0.27 | 0 |
| 76 | 3PH | 1K | 102 | - | 47,47,47 | 0.64 | 1 (2%) | 51,52,52 | 0.60 | 2 (3%) |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 88 | SF4 | C | 803 | 25 | - | - | 0/6/5/5 |
| 74 | HEM | 1A | 403 | 1 | - | 3/12/54/54 | - |
| 81 | PGT | T | 502 | - | - | 20/52/52/55 | - |
| 77 | PTY | 1E | 403 | - | - | 15/37/37/53 | - |
| 77 | PTY | T | 501 | - | - | 19/53/53/53 | - |
| 79 | PC7 | 2A | 606 | - | - | 10/30/30/55 | - |
| 77 | PTY | T | 504 | - | - | 11/31/31/53 | - |
| 82 | HEA | 3A | 602 | 11 | - | 7/32/76/76 | - |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 81 | PGT | 2A | 601 | - | - | 10/37/37/55 | - |
| 79 | PC7 | T | 503 | - | - | 22/55/55/55 | - |
| 79 | PC7 | 1H | 101 | - | - | 19/42/42/55 | - |
| 76 | 3PH | R | 401 | - | - | 13/33/33/49 | - |
| 76 | 3PH | 1A | 406 | - | - | 13/32/32/49 | - |
| 77 | PTY | V | 604 | - | - | 15/43/43/53 | - |
| 77 | PTY | V | 605 | - | - | 25/53/53/53 | - |
| 82 | HEA | 2A | 602 | 11 | - | 7/32/76/76 | - |
| 86 | FES | C | 801 | 25 | - | - | 0/1/1/1 |
| 79 | PC7 | 3A | 606 | - | - | 22/30/30/55 | - |
| 86 | FES | A | 301 | 23 | - | - | 0/1/1/1 |
| 76 | 3PH | y | 201 | - | - | 13/33/33/49 | - |
| 81 | PGT | 3A | 601 | - | - | 12/37/37/55 | - |
| 78 | HEC | 1E | 404 | 3 | - | 0/10/54/54 | - |
| 75 | CDL | 1K | 101 | - | - | 59/89/89/110 | - |
| 76 | 3PH | 1R | 201 | - | - | 13/38/38/49 | - |
| 79 | PC7 | u | 601 | - | - | 15/45/45/55 | - |
| 77 | PTY | G | 303 | - | - | 6/46/46/53 | - |
| 75 | CDL | R | 405 | - | - | 43/73/73/110 | - |
| 75 | CDL | y | 202 | - | - | 30/65/65/110 | - |
| 75 | CDL | x | 101 | - | - | 65/102/102/110 | - |
| 73 | UQ5 | 1A | 401 | - | - | 10/33/57/57 | 0/1/1/1 |
| 89 | 8Q1 | r | 200 | - | - | 19/41/41/41 | - |
| 75 | CDL | W | 701 | - | - | 62/105/105/110 | - |
| 77 | PTY | e | 302 | - | - | 22/46/46/53 | - |
| 73 | UQ5 | 1B | 401 | - | - | 7/33/57/57 | 0/1/1/1 |
| 76 | 3PH | h | 201 | - | - | 19/46/46/49 | - |
| 76 | 3PH | V | 601 | - | - | 18/43/43/49 | - |
| 75 | CDL | 1A | 405 | - | - | 34/69/69/110 | - |
| 77 | PTY | 2D | 301 | - | - | 13/38/38/53 | - |
| 75 | CDL | 1M | 501 | - | - | 31/64/64/110 | - |
| 75 | CDL | 1B | 408 | - | - | 45/81/81/110 | - |
| 77 | PTY | x | 102 | - | - | 18/53/53/53 | - |
| 77 | PTY | R | 404 | - | - | 21/47/47/53 | - |
| 75 | CDL | 1B | 405 | - | - | 49/74/74/110 | - |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 82 | HEA | 2A | 603 | 11 | - | 5/32/76/76 | - |
| 75 | CDL | V | 603 | - | - | 42/74/74/110 | - |
| 73 | UQ5 | 1B | 402 | - | - | 10/33/57/57 | 0/1/1/1 |
| 76 | 3PH | 2D | 302 | - | - | 19/33/33/49 | - |
| 75 | CDL | u | 602 | - | - | 51/93/93/110 | - |
| 75 | CDL | 1L | 101 | - | - | 43/69/69/110 | - |
| 77 | PTY | S | 302 | - | - | 21/49/49/53 | - |
| 76 | 3PH | w | 201 | - | - | 21/46/46/49 | - |
| 90 | NDP | P | 401 | - | - | 11/30/77/77 | 0/5/5/5 |
| 74 | HEM | 1B | 404 | 1 | - | 4/12/54/54 | - |
| 76 | 3PH | 1B | 406 | - | - | 22/49/49/49 | - |
| 77 | PTY | T | 506 | - | - | 15/29/29/53 | - |
| 77 | PTY | 2F | 101 | - | - | 15/37/37/53 | - |
| 77 | PTY | e | 301 | - | - | 9/28/28/53 | - |
| 91 | COO | s | 401 | - | - | 22/50/70/70 | 0/3/3/3 |
| 76 | 3PH | 1E | 402 | - | - | 17/41/41/49 | - |
| 88 | SF4 | B | 502 | 24 | - | - | 0/6/5/5 |
| 73 | UQ5 | Q | 301 | - | - | 4/33/57/57 | 0/1/1/1 |
| 76 | 3PH | 3D | 302 | - | - | 10/33/33/49 | - |
| 74 | HEM | 1B | 403 | 1 | - | 3/12/54/54 | - |
| 77 | PTY | h | 202 | - | - | 20/49/49/53 | - |
| 82 | HEA | 3A | 603 | 11 | - | 4/32/76/76 | - |
| 88 | SF4 | G | 302 | 29 | - | - | 0/6/5/5 |
| 77 | PTY | V | 606 | - | - | 18/38/38/53 | - |
| 87 | FMN | B | 501 | - | - | 4/18/18/18 | 0/3/3/3 |
| 79 | PC7 | R | 403 | - | - | 15/47/47/55 | - |
| 81 | PGT | T | 505 | - | - | 18/44/44/55 | - |
| 77 | PTY | R | 402 | - | - | 11/37/37/53 | - |
| 88 | SF4 | G | 301 | 29 | - | - | 0/6/5/5 |
| 77 | PTY | 3D | 301 | - | - | 15/38/38/53 | - |
| 76 | 3PH | 2I | 201 | - | - | 14/43/43/49 | - |
| 75 | CDL | u | 603 | - | - | 57/81/81/110 | - |
| 77 | PTY | 1F | 403 | - | - | 17/41/41/53 | - |
| 88 | SF4 | C | 802 | 25 | - | - | 0/6/5/5 |
| 76 | 3PH | 1B | 407 | - | - | 18/49/49/49 | - |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 79 | PC7 | 1G | 301 | - | - | 16/39/39/55 | - |
| 81 | PGT | l | 701 | - | - | 27/55/55/55 | - |
| 76 | 3PH | 3I | 201 | - | - | 9/43/43/49 | - |
| 76 | 3PH | S | 301 | - | - | 13/38/38/49 | - |
| 76 | 3PH | c | 101 | - | - | 13/49/49/49 | - |
| 75 | CDL | 1E | 401 | - | - | 41/63/63/110 | - |
| 81 | PGT | b | 601 | - | - | 27/48/48/55 | - |
| 88 | SF4 | F | 201 | 28 | - | - | 0/6/5/5 |
| 75 | CDL | h | 203 | - | - | 58/87/87/110 | - |
| 73 | UQ5 | 1A | 402 | - | - | 9/33/57/57 | 0/1/1/1 |
| 78 | HEC | 1F | 402 | 3 | - | 0/10/54/54 | - |
| 76 | 3PH | V | 602 | - | - | 17/42/42/49 | - |
| 74 | HEM | 1A | 404 | 1 | - | 4/12/54/54 | - |
| 79 | PC7 | Q | 302 | - | - | 14/36/36/55 | - |
| 76 | 3PH | g | 101 | - | - | 10/38/38/49 | - |
| 77 | PTY | R | 406 | - | - | 15/43/43/53 | - |
| 89 | 8Q1 | J | 200 | - | - | 11/41/41/41 | - |
| 77 | PTY | 3F | 101 | - | - | 10/37/37/53 | - |
| 75 | CDL | 1F | 401 | - | - | 32/66/66/110 | - |
| 76 | 3PH | 1K | 102 | - | - | 15/49/49/49 | - |

All (126) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 90 | P | 401 | NDP | P2B-O2B | 12.34 | 1.82 | 1.59 |
| 78 | 1E | 404 | HEC | C3C-C2C | -6.90 | 1.33 | 1.40 |
| 78 | 1F | 402 | HEC | C3C-C2C | -6.31 | 1.34 | 1.40 |
| 78 | 1E | 404 | HEC | C2B-C3B | -6.05 | 1.34 | 1.40 |
| 89 | r | 200 | 8Q1 | C34-N36 | 5.99 | 1.46 | 1.33 |
| 78 | 1F | 402 | HEC | C2B-C3B | -5.79 | 1.34 | 1.40 |
| 82 | 2A | 603 | HEA | C3B-C2B | 5.65 | 1.47 | 1.34 |
| 89 | J | 200 | 8Q1 | C34-N36 | 5.48 | 1.45 | 1.33 |
| 82 | 3A | 603 | HEA | C3B-C2B | 5.46 | 1.47 | 1.34 |
| 82 | 2A | 602 | HEA | C3A-C2A | 5.36 | 1.47 | 1.40 |
| 82 | 3A | 602 | HEA | C3B-C2B | 5.34 | 1.46 | 1.34 |
| 78 | 1E | 404 | HEC | C3D-C2D | 5.30 | 1.53 | 1.37 |
| 78 | 1F | 402 | HEC | C3D-C2D | 5.24 | 1.53 | 1.37 |
| 89 | r | 200 | 8Q1 | C39-N41 | 5.24 | 1.45 | 1.33 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 74 | 1B | 403 | HEM | C3C-C2C | -5.21 | 1.33 | 1.40 |
| 82 | 3A | 603 | HEA | C3C-C2C | 5.15 | 1.47 | 1.40 |
| 89 | J | 200 | 8Q1 | C39-N41 | 5.13 | 1.45 | 1.33 |
| 82 | 2A | 602 | HEA | C3B-C2B | 5.11 | 1.46 | 1.34 |
| 82 | 2A | 603 | HEA | CHC-C4B | 4.98 | 1.47 | 1.35 |
| 82 | 2A | 603 | HEA | C3D-C2D | 4.96 | 1.47 | 1.36 |
| 82 | 3A | 603 | HEA | CHC-C4B | 4.91 | 1.47 | 1.35 |
| 82 | 2A | 602 | HEA | C3D-C2D | 4.88 | 1.47 | 1.36 |
| 82 | 3A | 602 | HEA | C3C-C2C | 4.88 | 1.47 | 1.40 |
| 82 | 3A | 602 | HEA | CHC-C4B | 4.88 | 1.47 | 1.35 |
| 82 | 3A | 602 | HEA | C3A-C2A | 4.83 | 1.47 | 1.40 |
| 82 | 2A | 602 | HEA | CHD-C1D | 4.83 | 1.47 | 1.35 |
| 82 | 3A | 602 | HEA | C3D-C2D | 4.80 | 1.46 | 1.36 |
| 82 | 2A | 603 | HEA | C3C-C2C | 4.79 | 1.47 | 1.40 |
| 82 | 2A | 603 | HEA | C3A-C2A | 4.77 | 1.47 | 1.40 |
| 82 | 3A | 602 | HEA | CHD-C1D | 4.75 | 1.47 | 1.35 |
| 82 | 3A | 603 | HEA | C3A-C2A | 4.73 | 1.46 | 1.40 |
| 82 | 3A | 603 | HEA | C3D-C2D | 4.68 | 1.46 | 1.36 |
| 82 | 2A | 603 | HEA | CHD-C1D | 4.68 | 1.47 | 1.35 |
| 82 | 2A | 602 | HEA | CHC-C4B | 4.68 | 1.47 | 1.35 |
| 82 | 2A | 602 | HEA | C3C-C2C | 4.67 | 1.46 | 1.40 |
| 82 | 3A | 603 | HEA | CHD-C1D | 4.63 | 1.46 | 1.35 |
| 90 | P | 401 | NDP | PN-O5D | 3.82 | 1.74 | 1.59 |
| 74 | 1B | 404 | HEM | C3C-CAC | 3.76 | 1.55 | 1.47 |
| 74 | 1B | 403 | HEM | C3C-CAC | 3.70 | 1.55 | 1.47 |
| 74 | 1A | 404 | HEM | C3C-CAC | 3.70 | 1.55 | 1.47 |
| 74 | 1A | 403 | HEM | C3C-CAC | 3.67 | 1.55 | 1.47 |
| 74 | 1B | 404 | HEM | C3C-C2C | -3.66 | 1.35 | 1.40 |
| 74 | 1A | 403 | HEM | C3C-C2C | -3.64 | 1.35 | 1.40 |
| 74 | 1A | 404 | HEM | C3C-C2C | -3.61 | 1.35 | 1.40 |
| 87 | B | 501 | FMN | C4A-N5 | 3.60 | 1.37 | 1.30 |
| 76 | y | 201 | 3PH | P-O11 | 3.39 | 1.71 | 1.60 |
| 76 | V | 602 | 3PH | P-O11 | 3.38 | 1.71 | 1.60 |
| 76 | 1B | 407 | 3PH | P-O11 | 3.36 | 1.71 | 1.60 |
| 76 | 2D | 302 | 3PH | P-O11 | 3.32 | 1.70 | 1.60 |
| 76 | 1A | 406 | 3PH | P-O11 | 3.31 | 1.70 | 1.60 |
| 76 | 1K | 102 | 3PH | P-O11 | 3.30 | 1.70 | 1.60 |
| 76 | h | 201 | 3PH | P-O11 | 3.30 | 1.70 | 1.60 |
| 76 | c | 101 | 3PH | P-O11 | 3.29 | 1.70 | 1.60 |
| 76 | 1E | 402 | 3PH | P-O11 | 3.28 | 1.70 | 1.60 |
| 90 | P | 401 | NDP | O2B-C2B | -3.28 | 1.32 | 1.44 |
| 76 | 2I | 201 | 3PH | P-O11 | 3.28 | 1.70 | 1.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 76 | V | 601 | 3PH | P-O11 | 3.27 | 1.70 | 1.60 |
| 76 | 3D | 302 | 3PH | P-O11 | 3.25 | 1.70 | 1.60 |
| 76 | w | 201 | 3PH | P-O11 | 3.25 | 1.70 | 1.60 |
| 76 | R | 401 | 3PH | P-O11 | 3.25 | 1.70 | 1.60 |
| 76 | S | 301 | 3PH | P-O11 | 3.24 | 1.70 | 1.60 |
| 74 | 1B | 403 | HEM | CAB-C3B | 3.23 | 1.56 | 1.47 |
| 76 | 1B | 406 | 3PH | P-O11 | 3.22 | 1.70 | 1.60 |
| 76 | 1R | 201 | 3PH | P-O11 | 3.20 | 1.70 | 1.60 |
| 76 | g | 101 | 3PH | P-O11 | 3.19 | 1.70 | 1.60 |
| 76 | 3I | 201 | 3PH | P-O11 | 3.16 | 1.70 | 1.60 |
| 82 | 2A | 602 | HEA | FE-NB | 3.10 | 2.12 | 1.96 |
| 82 | 2A | 603 | HEA | FE-ND | 3.09 | 2.12 | 1.96 |
| 74 | 1B | 404 | HEM | CAB-C3B | 3.07 | 1.55 | 1.47 |
| 74 | 1A | 403 | HEM | CAB-C3B | 3.06 | 1.55 | 1.47 |
| 82 | 2A | 603 | HEA | C4B-C3B | 3.06 | 1.49 | 1.44 |
| 82 | 2A | 602 | HEA | FE-ND | 3.04 | 2.11 | 1.96 |
| 82 | 2A | 603 | HEA | C1D-ND | -3.03 | 1.35 | 1.40 |
| 82 | 3A | 603 | HEA | FE-ND | 3.03 | 2.11 | 1.96 |
| 82 | 3A | 602 | HEA | FE-NB | 3.01 | 2.11 | 1.96 |
| 82 | 3A | 603 | HEA | C1D-ND | -3.00 | 1.35 | 1.40 |
| 82 | 3A | 603 | HEA | C4B-C3B | 2.98 | 1.49 | 1.44 |
| 82 | 2A | 603 | HEA | FE-NB | 2.97 | 2.11 | 1.96 |
| 82 | 3A | 603 | HEA | FE-NB | 2.97 | 2.11 | 1.96 |
| 74 | 1A | 404 | HEM | CAB-C3B | 2.96 | 1.55 | 1.47 |
| 82 | 3A | 602 | HEA | FE-ND | 2.95 | 2.11 | 1.96 |
| 82 | 3A | 602 | HEA | C1D-ND | -2.85 | 1.35 | 1.40 |
| 82 | 3A | 602 | HEA | C4B-C3B | 2.83 | 1.49 | 1.44 |
| 82 | 2A | 602 | HEA | C2A-C1A | 2.80 | 1.48 | 1.42 |
| 82 | 2A | 602 | HEA | C4B-NB | -2.77 | 1.35 | 1.40 |
| 82 | 3A | 603 | HEA | C4B-NB | -2.74 | 1.35 | 1.40 |
| 82 | 2A | 602 | HEA | C1D-ND | -2.70 | 1.35 | 1.40 |
| 82 | 3A | 602 | HEA | C4B-NB | -2.68 | 1.35 | 1.40 |
| 82 | 2A | 603 | HEA | C2A-C1A | 2.64 | 1.48 | 1.42 |
| 89 | r | 200 | 8Q1 | C1-S44 | 2.55 | 1.82 | 1.76 |
| 82 | 3A | 602 | HEA | C2A-C1A | 2.51 | 1.48 | 1.42 |
| 91 | s | 401 | COO | C5A-C4A | 2.43 | 1.47 | 1.40 |
| 82 | 2A | 603 | HEA | C4B-NB | -2.43 | 1.36 | 1.40 |
| 89 | r | 200 | 8Q1 | C6-C1 | 2.42 | 1.53 | 1.50 |
| 82 | 2A | 603 | HEA | C1C-CHC | 2.42 | 1.47 | 1.41 |
| 89 | r | 200 | 8Q1 | O40-C39 | -2.39 | 1.18 | 1.23 |
| 82 | 3A | 603 | HEA | C2A-C1A | 2.37 | 1.47 | 1.42 |
| 82 | 2A | 602 | HEA | C4B-C3B | 2.36 | 1.48 | 1.44 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 89 | J | 200 | 8Q1 | O40-C39 | -2.36 | 1.18 | 1.23 |
| 82 | 2A | 602 | HEA | C4C-CHD | 2.36 | 1.47 | 1.41 |
| 82 | 2A | 603 | HEA | C4D-C3D | 2.35 | 1.49 | 1.45 |
| 82 | 3A | 603 | HEA | C1C-CHC | 2.32 | 1.47 | 1.41 |
| 75 | 1M | 501 | CDL | PB2-OB4 | -2.32 | 1.44 | 1.55 |
| 89 | J | 200 | 8Q1 | C1-S44 | 2.31 | 1.81 | 1.76 |
| 90 | P | 401 | NDP | C7N-C3N | -2.29 | 1.43 | 1.48 |
| 89 | J | 200 | 8Q1 | C6-C1 | 2.25 | 1.53 | 1.50 |
| 82 | 3A | 603 | HEA | C4D-C3D | 2.20 | 1.48 | 1.45 |
| 82 | 3A | 603 | HEA | C4C-CHD | 2.19 | 1.47 | 1.41 |
| 75 | x | 101 | CDL | PB2-OB4 | -2.19 | 1.45 | 1.55 |
| 90 | P | 401 | NDP | O3D-C3D | -2.18 | 1.37 | 1.43 |
| 82 | 2A | 603 | HEA | C4C-CHD | 2.16 | 1.47 | 1.41 |
| 82 | 3A | 602 | HEA | C4C-CHD | 2.15 | 1.47 | 1.41 |
| 82 | 2A | 602 | HEA | C1D-C2D | 2.14 | 1.48 | 1.44 |
| 82 | 3A | 602 | HEA | C1C-CHC | 2.13 | 1.46 | 1.41 |
| 87 | B | 501 | FMN | C10-N1 | 2.13 | 1.37 | 1.33 |
| 90 | P | 401 | NDP | O2D-C2D | -2.12 | 1.38 | 1.43 |
| 82 | 3A | 602 | HEA | C1D-C2D | 2.12 | 1.48 | 1.44 |
| 82 | 2A | 602 | HEA | C1B-C2B | 2.09 | 1.48 | 1.44 |
| 74 | 1B | 403 | HEM | CAA-C2A | 2.08 | 1.55 | 1.52 |
| 74 | 1A | 403 | HEM | CAA-C2A | 2.06 | 1.55 | 1.52 |
| 82 | 2A | 602 | HEA | C1C-CHC | 2.06 | 1.46 | 1.41 |
| 82 | 3A | 602 | HEA | C4D-ND | -2.03 | 1.34 | 1.38 |
| 75 | 1B | 405 | CDL | PA1-OA4 | -2.02 | 1.45 | 1.55 |
| 82 | 2A | 602 | HEA | CHB-C1B | 2.02 | 1.46 | 1.41 |
| 82 | 2A | 603 | HEA | C1D-C2D | 2.02 | 1.48 | 1.44 |
| 75 | y | 202 | CDL | PB2-OB4 | -2.01 | 1.45 | 1.55 |

All (231) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 91 | s | 401 | COO | C15-C11-C12 | -19.13 | 77.03 | 108.23 |
| 76 | h | 201 | 3PH | O31-C31-O32 | -17.93 | 78.33 | 123.59 |
| 91 | s | 401 | COO | C15-C11-C13 | -16.74 | 79.80 | 108.82 |
| 91 | s | 401 | COO | C15-C11-C14 | -15.18 | 78.23 | 109.17 |
| 76 | h | 201 | 3PH | O31-C31-C32 | 14.35 | 156.94 | 111.91 |
| 76 | h | 201 | 3PH | O32-C31-C32 | -11.56 | 78.63 | 123.73 |
| 82 | 3A | 603 | HEA | C3D-C4D-ND | 6.87 | 117.00 | 110.36 |
| 82 | 2A | 602 | HEA | C3D-C4D-ND | 6.79 | 116.93 | 110.36 |
| 82 | 2A | 603 | HEA | C3D-C4D-ND | 6.75 | 116.90 | 110.36 |
| 89 | J | 200 | 8Q1 | C6-C1-S44 | 6.65 | 121.19 | 113.46 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 90 | P | 401 | NDP | PN-O3-PA | -6.31 | 111.17 | 132.83 |
| 82 | 3A | 602 | HEA | C3D-C4D-ND | 6.19 | 116.35 | 110.36 |
| 82 | 3A | 603 | HEA | C2B-C1B-NB | 5.74 | 116.75 | 109.88 |
| 82 | 3A | 602 | HEA | C2D-C1D-ND | 5.71 | 116.61 | 109.84 |
| 82 | 2A | 603 | HEA | C2B-C1B-NB | 5.66 | 116.66 | 109.88 |
| 82 | 2A | 603 | HEA | C2D-C1D-ND | 5.61 | 116.49 | 109.84 |
| 82 | 2A | 602 | HEA | C3B-C4B-NB | 5.59 | 116.46 | 109.84 |
| 82 | 3A | 602 | HEA | C2B-C1B-NB | 5.51 | 116.48 | 109.88 |
| 89 | r | 200 | 8Q1 | C6-C1-S44 | 5.50 | 119.86 | 113.46 |
| 82 | 3A | 603 | HEA | C2D-C1D-ND | 5.38 | 116.21 | 109.84 |
| 82 | 2A | 602 | HEA | C2D-C1D-ND | 5.27 | 116.08 | 109.84 |
| 73 | 1B | 402 | UQ5 | C7-C6-C5 | 5.15 | 124.67 | 118.48 |
| 82 | 3A | 602 | HEA | C1D-C2D-C3D | -5.13 | 101.56 | 106.96 |
| 82 | 3A | 602 | HEA | C3B-C4B-NB | 5.05 | 115.83 | 109.84 |
| 89 | r | 200 | 8Q1 | C32-C34-N36 | 5.00 | 126.53 | 116.58 |
| 91 | s | 401 | COO | C14-C11-C12 | 4.96 | 116.33 | 108.23 |
| 82 | 2A | 602 | HEA | C2B-C1B-NB | 4.95 | 115.81 | 109.88 |
| 82 | 2A | 603 | HEA | C3B-C4B-NB | 4.92 | 115.67 | 109.84 |
| 82 | 3A | 603 | HEA | C3B-C4B-NB | 4.86 | 115.60 | 109.84 |
| 82 | 2A | 602 | HEA | C13-C12-C11 | -4.45 | 107.67 | 114.35 |
| 73 | 1B | 402 | UQ5 | C6-C1-C2 | 4.42 | 122.67 | 119.18 |
| 74 | 1A | 403 | HEM | C3B-C2B-C1B | 4.35 | 109.71 | 106.49 |
| 82 | 2A | 603 | HEA | C3C-C4C-NC | 4.20 | 114.64 | 109.21 |
| 82 | 3A | 602 | HEA | C3C-C4C-NC | 4.17 | 114.60 | 109.21 |
| 78 | 1F | 402 | HEC | CMB-C2B-C1B | -4.15 | 122.09 | 128.46 |
| 82 | 2A | 602 | HEA | C1D-C2D-C3D | -4.10 | 102.64 | 106.96 |
| 82 | 3A | 603 | HEA | C3C-C4C-NC | 4.10 | 114.51 | 109.21 |
| 91 | s | 401 | COO | C14-C11-C13 | 4.05 | 115.84 | 108.82 |
| 74 | 1A | 403 | HEM | CMB-C2B-C1B | -4.03 | 118.90 | 125.04 |
| 82 | 3A | 603 | HEA | CBA-CAA-C2A | -4.02 | 105.83 | 112.60 |
| 82 | 3A | 603 | HEA | CMC-C2C-C3C | 3.97 | 132.12 | 124.68 |
| 74 | 1A | 404 | HEM | CMC-C2C-C3C | 3.95 | 132.06 | 124.68 |
| 78 | 1E | 404 | HEC | CMB-C2B-C1B | -3.89 | 122.48 | 128.46 |
| 82 | 2A | 602 | HEA | CMC-C2C-C3C | 3.89 | 131.96 | 124.68 |
| 82 | 3A | 602 | HEA | CMC-C2C-C3C | 3.88 | 131.94 | 124.68 |
| 89 | J | 200 | 8Q1 | O4-C1-C6 | -3.86 | 119.43 | 123.99 |
| 82 | 2A | 602 | HEA | C3C-C4C-NC | 3.80 | 114.13 | 109.21 |
| 82 | 2A | 603 | HEA | C1D-C2D-C3D | -3.80 | 102.96 | 106.96 |
| 78 | 1E | 404 | HEC | CMC-C2C-C1C | -3.76 | 122.69 | 128.46 |
| 82 | 3A | 603 | HEA | CHA-C4D-ND | -3.71 | 120.40 | 124.43 |
| 82 | 3A | 603 | HEA | C1D-C2D-C3D | -3.67 | 103.10 | 106.96 |
| 82 | 3A | 602 | HEA | CBA-CAA-C2A | -3.65 | 106.44 | 112.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 82 | 3A | 603 | HEA | C4D-C3D-C2D | -3.65 | 101.57 | 106.90 |
| 82 | 2A | 603 | HEA | C4D-C3D-C2D | -3.65 | 101.58 | 106.90 |
| 82 | 3A | 603 | HEA | C27-C19-C20 | 3.64 | 121.40 | 115.27 |
| 74 | 1A | 404 | HEM | CMA-C3A-C4A | -3.64 | 122.88 | 128.46 |
| 73 | 1B | 402 | UQ5 | C8-C7-C6 | 3.60 | 121.76 | 112.05 |
| 82 | 3A | 603 | HEA | C1B-C2B-C3B | -3.55 | 102.55 | 106.80 |
| 82 | 3A | 602 | HEA | CAD-CBD-CGD | -3.54 | 105.98 | 113.60 |
| 82 | 2A | 603 | HEA | CHA-C4D-ND | -3.54 | 120.58 | 124.43 |
| 78 | 1E | 404 | HEC | CMB-C2B-C3B | 3.54 | 129.98 | 125.82 |
| 73 | 1A | 401 | UQ5 | C8-C7-C6 | 3.53 | 121.55 | 112.05 |
| 73 | 1A | 401 | UQ5 | C7-C6-C5 | 3.47 | 122.65 | 118.48 |
| 82 | 2A | 603 | HEA | CBA-CAA-C2A | -3.47 | 106.76 | 112.60 |
| 74 | 1B | 404 | HEM | CMC-C2C-C3C | 3.47 | 131.16 | 124.68 |
| 82 | 3A | 603 | HEA | CAD-C3D-C4D | 3.43 | 130.64 | 124.66 |
| 76 | V | 602 | 3PH | C2-O21-C21 | 3.35 | 126.03 | 117.79 |
| 82 | 3A | 602 | HEA | C1B-C2B-C3B | -3.33 | 102.82 | 106.80 |
| 82 | 2A | 603 | HEA | C1B-C2B-C3B | -3.33 | 102.82 | 106.80 |
| 82 | 2A | 602 | HEA | C4D-C3D-C2D | -3.32 | 102.06 | 106.90 |
| 89 | r | 200 | 8Q1 | C37-C38-C39 | -3.32 | 106.83 | 112.36 |
| 74 | 1B | 403 | HEM | C4C-CHD-C1D | 3.32 | 126.93 | 122.56 |
| 90 | P | 401 | NDP | O2B-P2B-O1X | -3.28 | 96.73 | 109.39 |
| 74 | 1A | 403 | HEM | C4C-CHD-C1D | 3.28 | 126.88 | 122.56 |
| 82 | 2A | 602 | HEA | CMB-C2B-C1B | 3.25 | 129.98 | 125.04 |
| 89 | r | 200 | 8Q1 | O4-C1-C6 | -3.24 | 120.16 | 123.99 |
| 82 | 3A | 602 | HEA | C13-C12-C11 | -3.22 | 109.52 | 114.35 |
| 74 | 1B | 403 | HEM | C3B-C2B-C1B | 3.21 | 108.87 | 106.49 |
| 78 | 1F | 402 | HEC | CMC-C2C-C1C | -3.18 | 123.58 | 128.46 |
| 91 | s | 401 | COO | N3A-C2A-N1A | -3.17 | 123.72 | 128.68 |
| 74 | 1A | 403 | HEM | CHB-C1B-NB | 3.16 | 128.28 | 124.38 |
| 74 | 1A | 403 | HEM | CMC-C2C-C3C | 3.15 | 130.58 | 124.68 |
| 91 | s | 401 | COO | P1A-O3A-P2A | -3.14 | 122.05 | 132.83 |
| 87 | B | 501 | FMN | C4-N3-C2 | -3.12 | 119.88 | 125.64 |
| 82 | 2A | 603 | HEA | C4B-C3B-C2B | -3.11 | 102.10 | 107.41 |
| 90 | P | 401 | NDP | PA-O5B-C5B | -3.10 | 103.49 | 121.68 |
| 82 | 2A | 602 | HEA | C4B-C3B-C2B | -3.09 | 102.12 | 107.41 |
| 82 | 2A | 602 | HEA | C1B-C2B-C3B | -3.08 | 103.12 | 106.80 |
| 89 | r | 200 | 8Q1 | O35-C34-N36 | -3.06 | 116.42 | 122.99 |
| 77 | T | 501 | PTY | C6-O7-C8 | 3.06 | 125.32 | 117.79 |
| 82 | 3A | 602 | HEA | C4B-C3B-C2B | -3.05 | 102.20 | 107.41 |
| 82 | 2A | 603 | HEA | C27-C19-C20 | 2.98 | 120.29 | 115.27 |
| 82 | 2A | 603 | HEA | CAD-C3D-C4D | 2.98 | 129.87 | 124.66 |
| 82 | 2A | 602 | HEA | CAD-CBD-CGD | -2.98 | 107.19 | 113.60 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 78 | 1F | 402 | HEC | C1D-C2D-C3D | -2.97 | 104.93 | 107.00 |
| 74 | 1A | 404 | HEM | C4D-ND-C1D | 2.97 | 108.14 | 105.07 |
| 91 | s | 401 | COO | C4A-C5A-N7A | -2.94 | 106.33 | 109.40 |
| 82 | 3A | 603 | HEA | C4B-C3B-C2B | -2.94 | 102.39 | 107.41 |
| 91 | s | 401 | COO | C3X-C2X-C1X | 2.93 | 106.37 | 99.89 |
| 74 | 1A | 403 | HEM | C4D-ND-C1D | 2.93 | 108.09 | 105.07 |
| 73 | 1A | 401 | UQ5 | C6-C1-C2 | 2.92 | 121.49 | 119.18 |
| 82 | 2A | 603 | HEA | C1D-ND-C4D | -2.91 | 102.07 | 105.07 |
| 74 | 1B | 403 | HEM | C4D-ND-C1D | 2.89 | 108.06 | 105.07 |
| 82 | 2A | 603 | HEA | CMC-C2C-C3C | 2.89 | 130.09 | 124.68 |
| 73 | 1B | 402 | UQ5 | O5-C5-C4 | -2.89 | 114.80 | 120.93 |
| 91 | s | 401 | COO | C10-C9-C8 | -2.88 | 119.65 | 125.34 |
| 82 | 3A | 603 | HEA | C1D-ND-C4D | -2.87 | 102.11 | 105.07 |
| 82 | 2A | 602 | HEA | C13-C14-C15 | -2.81 | 120.89 | 127.66 |
| 82 | 2A | 603 | HEA | CAD-CBD-CGD | -2.81 | 107.56 | 113.60 |
| 73 | 1A | 402 | UQ5 | C7-C6-C5 | -2.78 | 115.13 | 118.48 |
| 87 | B | 501 | FMN | C4A-C10-N10 | 2.75 | 120.51 | 116.48 |
| 90 | P | 401 | NDP | PN-O5D-C5D | -2.74 | 105.64 | 121.68 |
| 82 | 3A | 602 | HEA | CMD-C2D-C1D | 2.73 | 129.20 | 125.04 |
| 82 | 3A | 603 | HEA | CHB-C1B-C2B | -2.73 | 120.71 | 124.98 |
| 74 | 1B | 403 | HEM | C4B-CHC-C1C | 2.73 | 126.16 | 122.56 |
| 74 | 1B | 404 | HEM | C4D-ND-C1D | 2.71 | 107.87 | 105.07 |
| 78 | 1F | 402 | HEC | CMB-C2B-C3B | 2.71 | 129.01 | 125.82 |
| 78 | 1F | 402 | HEC | CAA-CBA-CGA | -2.71 | 106.17 | 113.76 |
| 87 | B | 501 | FMN | C4A-C4-N3 | 2.71 | 120.06 | 113.19 |
| 82 | 2A | 602 | HEA | C1D-ND-C4D | -2.70 | 102.29 | 105.07 |
| 82 | 3A | 602 | HEA | C27-C19-C20 | 2.68 | 119.78 | 115.27 |
| 82 | 2A | 603 | HEA | C13-C14-C15 | -2.67 | 121.23 | 127.66 |
| 82 | 3A | 603 | HEA | C13-C14-C15 | -2.66 | 121.25 | 127.66 |
| 82 | 3A | 602 | HEA | CHA-C4D-C3D | -2.66 | 120.93 | 124.84 |
| 82 | 3A | 603 | HEA | CAD-CBD-CGD | -2.65 | 107.89 | 113.60 |
| 89 | r | 200 | 8Q1 | C38-C39-N41 | 2.64 | 120.87 | 116.42 |
| 82 | 3A | 602 | HEA | C1D-ND-C4D | -2.64 | 102.34 | 105.07 |
| 89 | r | 200 | 8Q1 | C43-S44-C1 | 2.64 | 110.08 | 101.87 |
| 82 | 2A | 603 | HEA | C26-C15-C16 | 2.63 | 119.69 | 115.27 |
| 82 | 2A | 602 | HEA | C27-C19-C20 | 2.62 | 119.68 | 115.27 |
| 78 | 1E | 404 | HEC | C1D-C2D-C3D | -2.61 | 105.18 | 107.00 |
| 82 | 3A | 602 | HEA | C4D-C3D-C2D | -2.59 | 103.13 | 106.90 |
| 82 | 3A | 603 | HEA | CMD-C2D-C1D | 2.54 | 128.90 | 125.04 |
| 82 | 2A | 602 | HEA | C4B-NB-C1B | -2.52 | 102.47 | 105.07 |
| 90 | P | 401 | NDP | O3X-P2B-O2X | 2.50 | 117.17 | 107.64 |
| 74 | 1A | 403 | HEM | CHD-C1D-ND | 2.49 | 127.14 | 124.43 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 89 | J | 200 | 8Q1 | O4-C1-S44 | -2.49 | 119.38 | 122.61 |
| 82 | 2A | 603 | HEA | CHB-C1B-C2B | -2.49 | 121.09 | 124.98 |
| 87 | B | 501 | FMN | O4-C4-C4A | -2.46 | 120.07 | 126.60 |
| 82 | 3A | 602 | HEA | C13-C14-C15 | -2.45 | 121.77 | 127.66 |
| 82 | 3A | 602 | HEA | C26-C15-C16 | 2.44 | 119.38 | 115.27 |
| 89 | J | 200 | 8Q1 | C38-C39-N41 | 2.44 | 120.53 | 116.42 |
| 73 | 1A | 401 | UQ5 | C7-C8-C9 | -2.44 | 122.73 | 126.79 |
| 74 | 1A | 403 | HEM | CMA-C3A-C4A | -2.44 | 124.72 | 128.46 |
| 82 | 2A | 602 | HEA | CHA-C4D-C3D | -2.43 | 121.26 | 124.84 |
| 90 | P | 401 | NDP | C5B-C4B-C3B | -2.42 | 106.12 | 115.18 |
| 82 | 2A | 602 | HEA | CHA-C4D-ND | -2.42 | 121.81 | 124.43 |
| 76 | w | 201 | 3PH | C2-O21-C21 | 2.42 | 123.74 | 117.79 |
| 73 | Q | 301 | UQ5 | C12-C13-C14 | 2.41 | 133.47 | 127.66 |
| 82 | 2A | 602 | HEA | CBA-CAA-C2A | -2.41 | 108.54 | 112.60 |
| 76 | w | 201 | 3PH | O13-P-O11 | -2.40 | 100.35 | 106.73 |
| 90 | P | 401 | NDP | O4B-C4B-C3B | 2.38 | 109.83 | 105.11 |
| 82 | 3A | 602 | HEA | CMB-C2B-C1B | 2.38 | 128.66 | 125.04 |
| 74 | 1B | 404 | HEM | C1B-NB-C4B | 2.37 | 107.53 | 105.07 |
| 73 | 1B | 402 | UQ5 | C1-C6-C5 | -2.37 | 117.35 | 119.58 |
| 74 | 1A | 403 | HEM | C1B-NB-C4B | 2.37 | 107.52 | 105.07 |
| 74 | 1B | 403 | HEM | CMA-C3A-C4A | -2.36 | 124.83 | 128.46 |
| 79 | u | 601 | PC7 | O3-C3-C2 | 2.36 | 115.29 | 108.43 |
| 73 | Q | 301 | UQ5 | C8-C7-C6 | 2.35 | 118.39 | 112.05 |
| 82 | 2A | 602 | HEA | CHB-C1B-NB | -2.34 | 121.89 | 124.43 |
| 82 | 2A | 603 | HEA | C25-C23-C24 | 2.34 | 119.77 | 114.60 |
| 89 | J | 200 | 8Q1 | C43-S44-C1 | 2.34 | 109.15 | 101.87 |
| 82 | 3A | 602 | HEA | CHB-C1B-C2B | -2.33 | 121.34 | 124.98 |
| 74 | 1B | 404 | HEM | C3D-C4D-ND | -2.33 | 107.57 | 110.17 |
| 76 | 3I | 201 | 3PH | O13-P-O11 | -2.33 | 100.54 | 106.73 |
| 74 | 1A | 404 | HEM | C4C-CHD-C1D | 2.32 | 125.63 | 122.56 |
| 74 | 1B | 404 | HEM | C4B-CHC-C1C | 2.32 | 125.62 | 122.56 |
| 82 | 3A | 602 | HEA | C4B-NB-C1B | -2.32 | 102.67 | 105.07 |
| 76 | 3D | 302 | 3PH | O13-P-O11 | -2.32 | 100.56 | 106.73 |
| 74 | 1A | 404 | HEM | C3D-C4D-ND | -2.30 | 107.61 | 110.17 |
| 82 | 3A | 603 | HEA | C4B-NB-C1B | -2.30 | 102.70 | 105.07 |
| 78 | 1F | 402 | HEC | CBD-CAD-C3D | -2.29 | 108.71 | 112.62 |
| 73 | Q | 301 | UQ5 | C12-C11-C9 | 2.29 | 120.50 | 112.98 |
| 90 | P | 401 | NDP | C3N-C2N-N1N | -2.28 | 119.85 | 123.10 |
| 76 | 1R | 201 | 3PH | O13-P-O11 | -2.27 | 100.68 | 106.73 |
| 89 | r | 200 | 8Q1 | C37-N36-C34 | 2.27 | 126.64 | 122.59 |
| 87 | B | 501 | FMN | C4A-C10-N1 | -2.27 | 119.47 | 124.73 |
| 74 | 1A | 404 | HEM | CMB-C2B-C1B | -2.26 | 121.59 | 125.04 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 82 | 2A | 603 | HEA | C4B-NB-C1B | -2.25 | 102.75 | 105.07 |
| 81 | T | 502 | PGT | C3-C2-C1 | 2.25 | 117.11 | 111.79 |
| 82 | 2A | 603 | HEA | CHD-C1D-C2D | -2.25 | 120.50 | 126.72 |
| 76 | 1B | 406 | 3PH | O13-P-O11 | -2.23 | 100.80 | 106.73 |
| 82 | 3A | 603 | HEA | C25-C23-C24 | 2.23 | 119.53 | 114.60 |
| 87 | B | 501 | FMN | C10-C4A-N5 | -2.22 | 120.14 | 124.86 |
| 74 | 1A | 404 | HEM | C4A-C3A-C2A | 2.22 | 108.54 | 107.00 |
| 90 | P | 401 | NDP | O7N-C7N-C3N | 2.21 | 125.07 | 120.90 |
| 76 | y | 201 | 3PH | O13-P-O11 | -2.21 | 100.84 | 106.73 |
| 74 | 1B | 403 | HEM | CBD-CAD-C3D | -2.20 | 106.52 | 112.63 |
| 76 | 1A | 406 | 3PH | O13-P-O11 | -2.19 | 100.92 | 106.73 |
| 78 | 1E | 404 | HEC | CAA-CBA-CGA | -2.18 | 107.64 | 113.76 |
| 76 | 2I | 201 | 3PH | O13-P-O11 | -2.17 | 100.95 | 106.73 |
| 81 | l | 701 | PGT | C2-O2-C31 | 2.17 | 123.14 | 117.79 |
| 82 | 2A | 602 | HEA | CHD-C1D-C2D | -2.16 | 120.74 | 126.72 |
| 74 | 1B | 404 | HEM | CBD-CAD-C3D | -2.16 | 106.63 | 112.63 |
| 89 | r | 200 | 8Q1 | C31-C29-C32 | 2.15 | 112.55 | 108.82 |
| 74 | 1A | 403 | HEM | C4B-CHC-C1C | 2.15 | 125.40 | 122.56 |
| 90 | P | 401 | NDP | C2A-N1A-C6A | -2.14 | 115.09 | 118.75 |
| 76 | c | 101 | 3PH | O13-P-O11 | -2.14 | 101.03 | 106.73 |
| 82 | 3A | 602 | HEA | CHD-C1D-C2D | -2.14 | 120.80 | 126.72 |
| 73 | 1B | 402 | UQ5 | O5-C5-C6 | 2.13 | 125.29 | 121.55 |
| 76 | h | 201 | 3PH | O14-P-O13 | 2.13 | 115.77 | 107.64 |
| 73 | 1B | 401 | UQ5 | C7-C6-C5 | -2.13 | 115.92 | 118.48 |
| 82 | 3A | 603 | HEA | C26-C15-C16 | 2.12 | 118.84 | 115.27 |
| 74 | 1B | 403 | HEM | C3D-C4D-ND | -2.12 | 107.81 | 110.17 |
| 76 | 1K | 102 | 3PH | O13-P-O11 | -2.11 | 101.12 | 106.73 |
| 82 | 2A | 602 | HEA | C26-C15-C16 | 2.10 | 118.81 | 115.27 |
| 76 | g | 101 | 3PH | O13-P-O11 | -2.10 | 101.14 | 106.73 |
| 76 | R | 401 | 3PH | O13-P-O11 | -2.09 | 101.17 | 106.73 |
| 76 | S | 301 | 3PH | O13-P-O11 | -2.09 | 101.17 | 106.73 |
| 82 | 3A | 602 | HEA | C25-C23-C24 | 2.09 | 119.22 | 114.60 |
| 82 | 3A | 602 | HEA | CHB-C1B-NB | -2.07 | 122.18 | 124.43 |
| 90 | P | 401 | NDP | C3B-C2B-C1B | -2.07 | 99.00 | 102.89 |
| 90 | P | 401 | NDP | O5D-PN-O1N | -2.07 | 100.98 | 109.07 |
| 74 | 1B | 404 | HEM | C4C-CHD-C1D | 2.06 | 125.28 | 122.56 |
| 87 | B | 501 | FMN | C9A-C5A-N5 | -2.06 | 120.19 | 122.43 |
| 76 | h | 201 | 3PH | O13-P-O11 | -2.06 | 101.24 | 106.73 |
| 82 | 3A | 603 | HEA | CHD-C1D-C2D | -2.06 | 121.02 | 126.72 |
| 76 | 2D | 302 | 3PH | O13-P-O11 | -2.05 | 101.28 | 106.73 |
| 82 | 2A | 602 | HEA | C25-C23-C24 | 2.04 | 119.12 | 114.60 |
| 79 | 1G | 301 | PC7 | C3-C2-C1 | 2.04 | 116.62 | 111.79 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 76 | V | 601 | 3PH | O13-P-O11 | -2.04 | 101.31 | 106.73 |
| 79 | u | 601 | PC7 | C3-C2-C1 | 2.03 | 116.59 | 111.79 |
| 89 | r | 200 | 8Q1 | O4-C1-S44 | -2.03 | 119.98 | 122.61 |
| 90 | P | 401 | NDP | O2N-PN-O1N | 2.03 | 122.27 | 112.24 |
| 87 | B | 501 | FMN | C5A-C9A-N10 | 2.02 | 120.04 | 117.95 |
| 76 | 1K | 102 | 3PH | O14-P-O13 | 2.02 | 115.37 | 107.64 |
| 76 | R | 401 | 3PH | O14-P-O13 | 2.02 | 115.35 | 107.64 |
| 76 | w | 201 | 3PH | O14-P-O13 | 2.02 | 115.35 | 107.64 |
| 74 | 1A | 403 | HEM | C2D-C1D-ND | -2.02 | 107.47 | 109.88 |
| 82 | 2A | 602 | HEA | C17-C18-C19 | -2.00 | 122.83 | 127.66 |
| 82 | 2A | 603 | HEA | CHB-C1B-NB | -2.00 | 122.25 | 124.43 |

There are no chirality outliers.

All (1751) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 73 | 1A | 401 | UQ5 | C1-C6-C7-C8 |
| 73 | 1A | 401 | UQ5 | C5-C6-C7-C8 |
| 73 | 1A | 401 | UQ5 | C9-C11-C12-C13 |
| 73 | 1A | 401 | UQ5 | C24-C26-C27-C28 |
| 73 | 1A | 402 | UQ5 | C14-C16-C17-C18 |
| 73 | 1B | 401 | UQ5 | C9-C11-C12-C13 |
| 73 | 1B | 401 | UQ5 | C20-C19-C21-C22 |
| 73 | 1B | 401 | UQ5 | C19-C21-C22-C23 |
| 73 | 1B | 402 | UQ5 | C1-C6-C7-C8 |
| 73 | 1B | 402 | UQ5 | C5-C6-C7-C8 |
| 73 | 1B | 402 | UQ5 | C13-C14-C16-C17 |
| 73 | 1B | 402 | UQ5 | C15-C14-C16-C17 |
| 73 | 1B | 402 | UQ5 | C14-C16-C17-C18 |
| 73 | 1B | 402 | UQ5 | C19-C21-C22-C23 |
| 73 | 1B | 402 | UQ5 | C24-C26-C27-C28 |
| 73 | Q | 301 | UQ5 | C19-C21-C22-C23 |
| 74 | 1B | 404 | HEM | C2A-CAA-CBA-CGA |
| 75 | 1A | 405 | CDL | O1-C1-CB2-OB2 |
| 75 | 1A | 405 | CDL | CA3-OA5-PA1-OA3 |
| 75 | 1A | 405 | CDL | CA3-OA5-PA1-OA4 |
| 75 | 1A | 405 | CDL | CB2-OB2-PB2-OB3 |
| 75 | 1A | 405 | CDL | CB2-OB2-PB2-OB4 |
| 75 | 1A | 405 | CDL | CB2-OB2-PB2-OB5 |
| 75 | 1A | 405 | CDL | CB3-OB5-PB2-OB4 |
| 75 | 1A | 405 | CDL | C51-CB5-OB6-CB4 |
| 75 | 1B | 405 | CDL | CA3-OA5-PA1-OA4 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 75 | 1B | 405 | CDL | C11-CA5-OA6-CA4 |
| 75 | 1B | 405 | CDL | CB3-OB5-PB2-OB3 |
| 75 | 1B | 405 | CDL | OB7-CB5-OB6-CB4 |
| 75 | 1B | 405 | CDL | C51-CB5-OB6-CB4 |
| 75 | 1B | 408 | CDL | CA2-OA2-PA1-OA3 |
| 75 | 1B | 408 | CDL | CA2-OA2-PA1-OA4 |
| 75 | 1B | 408 | CDL | CA2-OA2-PA1-OA5 |
| 75 | 1B | 408 | CDL | OA6-CA4-CA6-OA8 |
| 75 | 1B | 408 | CDL | OA7-CA5-OA6-CA4 |
| 75 | 1E | 401 | CDL | O1-C1-CB2-OB2 |
| 75 | 1E | 401 | CDL | CA2-OA2-PA1-OA3 |
| 75 | 1E | 401 | CDL | CA2-OA2-PA1-OA4 |
| 75 | 1E | 401 | CDL | CA3-OA5-PA1-OA3 |
| 75 | 1E | 401 | CDL | C11-CA5-OA6-CA4 |
| 75 | 1E | 401 | CDL | CB2-OB2-PB2-OB3 |
| 75 | 1E | 401 | CDL | CB2-OB2-PB2-OB4 |
| 75 | 1E | 401 | CDL | OB7-CB5-OB6-CB4 |
| 75 | 1E | 401 | CDL | C51-CB5-OB6-CB4 |
| 75 | 1F | 401 | CDL | CA3-OA5-PA1-OA2 |
| 75 | 1F | 401 | CDL | CA3-OA5-PA1-OA3 |
| 75 | 1F | 401 | CDL | CA3-OA5-PA1-OA4 |
| 75 | 1F | 401 | CDL | CB2-OB2-PB2-OB3 |
| 75 | 1F | 401 | CDL | CB2-OB2-PB2-OB4 |
| 75 | 1F | 401 | CDL | CB2-OB2-PB2-OB5 |
| 75 | 1F | 401 | CDL | OB5-CB3-CB4-OB6 |
| 75 | 1F | 401 | CDL | C51-CB5-OB6-CB4 |
| 75 | 1K | 101 | CDL | CA3-OA5-PA1-OA2 |
| 75 | 1K | 101 | CDL | CB2-OB2-PB2-OB3 |
| 75 | 1K | 101 | CDL | CB2-OB2-PB2-OB4 |
| 75 | 1K | 101 | CDL | CB3-OB5-PB2-OB3 |
| 75 | 1L | 101 | CDL | CA2-OA2-PA1-OA4 |
| 75 | 1L | 101 | CDL | CA3-OA5-PA1-OA3 |
| 75 | 1L | 101 | CDL | OA7-CA5-OA6-CA4 |
| 75 | 1L | 101 | CDL | CB2-OB2-PB2-OB3 |
| 75 | 1L | 101 | CDL | CB2-OB2-PB2-OB4 |
| 75 | 1L | 101 | CDL | CB3-OB5-PB2-OB2 |
| 75 | 1L | 101 | CDL | CB3-OB5-PB2-OB3 |
| 75 | 1L | 101 | CDL | CB3-OB5-PB2-OB4 |
| 75 | 1M | 501 | CDL | CA2-OA2-PA1-OA3 |
| 75 | 1M | 501 | CDL | CA2-OA2-PA1-OA4 |
| 75 | 1M | 501 | CDL | CA2-OA2-PA1-OA5 |
| 75 | 1M | 501 | CDL | OB6-CB4-CB6-OB8 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 75 | 1M | 501 | CDL | C51-CB5-OB6-CB4 |
| 75 | R | 405 | CDL | CA2-OA2-PA1-OA3 |
| 75 | R | 405 | CDL | CA2-OA2-PA1-OA4 |
| 75 | R | 405 | CDL | CA3-OA5-PA1-OA2 |
| 75 | R | 405 | CDL | CA3-OA5-PA1-OA3 |
| 75 | R | 405 | CDL | CA3-OA5-PA1-OA4 |
| 75 | R | 405 | CDL | CB2-OB2-PB2-OB3 |
| 75 | R | 405 | CDL | CB2-OB2-PB2-OB4 |
| 75 | R | 405 | CDL | CB2-OB2-PB2-OB5 |
| 75 | R | 405 | CDL | CB3-OB5-PB2-OB3 |
| 75 | R | 405 | CDL | OB5-CB3-CB4-OB6 |
| 75 | R | 405 | CDL | C51-CB5-OB6-CB4 |
| 75 | V | 603 | CDL | CA2-OA2-PA1-OA3 |
| 75 | V | 603 | CDL | C11-CA5-OA6-CA4 |
| 75 | V | 603 | CDL | CB2-OB2-PB2-OB4 |
| 75 | V | 603 | CDL | CB3-OB5-PB2-OB3 |
| 75 | V | 603 | CDL | CB3-OB5-PB2-OB4 |
| 75 | W | 701 | CDL | CA2-OA2-PA1-OA3 |
| 75 | W | 701 | CDL | CA3-OA5-PA1-OA2 |
| 75 | W | 701 | CDL | CA3-OA5-PA1-OA3 |
| 75 | W | 701 | CDL | CA3-OA5-PA1-OA4 |
| 75 | W | 701 | CDL | OA7-CA5-OA6-CA4 |
| 75 | W | 701 | CDL | C11-CA5-OA6-CA4 |
| 75 | h | 203 | CDL | CA2-C1-CB2-OB2 |
| 75 | h | 203 | CDL | CA2-OA2-PA1-OA3 |
| 75 | h | 203 | CDL | CA2-OA2-PA1-OA4 |
| 75 | h | 203 | CDL | CA2-OA2-PA1-OA5 |
| 75 | h | 203 | CDL | CA3-OA5-PA1-OA3 |
| 75 | h | 203 | CDL | CA3-OA5-PA1-OA4 |
| 75 | h | 203 | CDL | CB2-OB2-PB2-OB3 |
| 75 | h | 203 | CDL | CB2-OB2-PB2-OB5 |
| 75 | h | 203 | CDL | CB3-OB5-PB2-OB3 |
| 75 | u | 602 | CDL | CA2-C1-CB2-OB2 |
| 75 | u | 602 | CDL | CA2-OA2-PA1-OA3 |
| 75 | u | 602 | CDL | CA2-OA2-PA1-OA4 |
| 75 | u | 602 | CDL | CA2-OA2-PA1-OA5 |
| 75 | u | 602 | CDL | CA3-OA5-PA1-OA2 |
| 75 | u | 602 | CDL | CA3-OA5-PA1-OA3 |
| 75 | u | 602 | CDL | CA3-OA5-PA1-OA4 |
| 75 | u | 602 | CDL | C51-CB5-OB6-CB4 |
| 75 | u | 603 | CDL | O1-C1-CB2-OB2 |
| 75 | u | 603 | CDL | CA2-OA2-PA1-OA4 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 75 | u | 603 | CDL | CA3-OA5-PA1-OA3 |
| 75 | u | 603 | CDL | CB2-OB2-PB2-OB4 |
| 75 | u | 603 | CDL | CB3-OB5-PB2-OB3 |
| 75 | x | 101 | CDL | CA3-OA5-PA1-OA4 |
| 75 | x | 101 | CDL | CB2-OB2-PB2-OB3 |
| 75 | y | 202 | CDL | O1-C1-CB2-OB2 |
| 75 | y | 202 | CDL | CA2-C1-CB2-OB2 |
| 75 | y | 202 | CDL | CA3-OA5-PA1-OA3 |
| 75 | y | 202 | CDL | CA3-OA5-PA1-OA4 |
| 76 | 1A | 406 | 3PH | C22-C21-O21-C2 |
| 76 | 1B | 406 | 3PH | C1-O11-P-O13 |
| 76 | 1B | 406 | 3PH | C1-O11-P-O14 |
| 76 | 1B | 406 | 3PH | C1-O11-P-O12 |
| 76 | 1B | 407 | 3PH | C1-O11-P-O13 |
| 76 | 1B | 407 | 3PH | C1-O11-P-O14 |
| 76 | 1B | 407 | 3PH | C1-O11-P-O12 |
| 76 | 1E | 402 | 3PH | C1-O11-P-O13 |
| 76 | 1E | 402 | 3PH | C1-O11-P-O14 |
| 76 | 1E | 402 | 3PH | C1-O11-P-O12 |
| 76 | 1E | 402 | 3PH | O21-C2-C3-O31 |
| 76 | 2D | 302 | 3PH | C1-O11-P-O13 |
| 76 | 2D | 302 | 3PH | C1-O11-P-O14 |
| 76 | 2D | 302 | 3PH | C1-O11-P-O12 |
| 76 | 2D | 302 | 3PH | C22-C21-O21-C2 |
| 76 | 2I | 201 | 3PH | C1-O11-P-O13 |
| 76 | 2I | 201 | 3PH | C1-O11-P-O14 |
| 76 | 3D | 302 | 3PH | C1-O11-P-O13 |
| 76 | 3D | 302 | 3PH | C1-O11-P-O14 |
| 76 | 3D | 302 | 3PH | C1-O11-P-O12 |
| 76 | 3D | 302 | 3PH | O22-C21-O21-C2 |
| 76 | 3D | 302 | 3PH | C22-C21-O21-C2 |
| 76 | R | 401 | 3PH | C1-O11-P-O13 |
| 76 | R | 401 | 3PH | C1-O11-P-O14 |
| 76 | S | 301 | 3PH | C1-O11-P-O13 |
| 76 | S | 301 | 3PH | C1-O11-P-O14 |
| 76 | S | 301 | 3PH | C1-O11-P-O12 |
| 76 | V | 601 | 3PH | C1-O11-P-O13 |
| 76 | V | 601 | 3PH | C1-O11-P-O14 |
| 76 | V | 601 | 3PH | O22-C21-O21-C2 |
| 76 | V | 601 | 3PH | C22-C21-O21-C2 |
| 76 | V | 602 | 3PH | C1-O11-P-O13 |
| 76 | V | 602 | 3PH | C1-O11-P-O14 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 76 | V | 602 | 3PH | C1-O11-P-O12 |
| 76 | V | 602 | 3PH | C22-C21-O21-C2 |
| 76 | c | 101 | 3PH | C1-O11-P-O13 |
| 76 | c | 101 | 3PH | C1-O11-P-O14 |
| 76 | c | 101 | 3PH | C1-O11-P-O12 |
| 76 | h | 201 | 3PH | C1-O11-P-O13 |
| 76 | h | 201 | 3PH | C1-O11-P-O14 |
| 76 | h | 201 | 3PH | O11-C1-C2-O21 |
| 76 | h | 201 | 3PH | C22-C21-O21-C2 |
| 76 | y | 201 | 3PH | C1-O11-P-O13 |
| 76 | y | 201 | 3PH | C1-O11-P-O14 |
| 76 | y | 201 | 3PH | C1-O11-P-O12 |
| 77 | 1F | 403 | PTY | C3-O11-P1-O12 |
| 77 | 2D | 301 | PTY | C11-C8-O7-C6 |
| 77 | 2F | 101 | PTY | C3-O11-P1-O12 |
| 77 | 2F | 101 | PTY | C5-O14-P1-O11 |
| 77 | 2F | 101 | PTY | C5-O14-P1-O13 |
| 77 | 3D | 301 | PTY | N1-C2-C3-O11 |
| 77 | 3D | 301 | PTY | C11-C8-O7-C6 |
| 77 | 3F | 101 | PTY | N1-C2-C3-O11 |
| 77 | 3F | 101 | PTY | C11-C8-O7-C6 |
| 77 | 3F | 101 | PTY | C3-O11-P1-O14 |
| 77 | 3F | 101 | PTY | C5-O14-P1-O11 |
| 77 | G | 303 | PTY | C3-O11-P1-O13 |
| 77 | R | 402 | PTY | C2-C3-O11-P1 |
| 77 | R | 402 | PTY | C6-C5-O14-P1 |
| 77 | R | 402 | PTY | C3-O11-P1-O12 |
| 77 | R | 404 | PTY | C11-C8-O7-C6 |
| 77 | R | 404 | PTY | C5-O14-P1-O12 |
| 77 | R | 406 | PTY | O14-C5-C6-O7 |
| 77 | R | 406 | PTY | C11-C8-O7-C6 |
| 77 | R | 406 | PTY | C5-O14-P1-O11 |
| 77 | S | 302 | PTY | C3-O11-P1-O12 |
| 77 | S | 302 | PTY | C5-O14-P1-O13 |
| 77 | T | 501 | PTY | N1-C2-C3-O11 |
| 77 | T | 501 | PTY | C3-O11-P1-O12 |
| 77 | T | 501 | PTY | C5-O14-P1-O11 |
| 77 | T | 504 | PTY | N1-C2-C3-O11 |
| 77 | T | 504 | PTY | C5-O14-P1-O12 |
| 77 | V | 604 | PTY | N1-C2-C3-O11 |
| 77 | V | 604 | PTY | C3-O11-P1-O12 |
| 77 | V | 604 | PTY | C3-O11-P1-O13 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 77 | V | 605 | PTY | N1-C2-C3-O11 |
| 77 | V | 605 | PTY | C3-O11-P1-O13 |
| 77 | V | 605 | PTY | C5-O14-P1-O12 |
| 77 | e | 301 | PTY | N1-C2-C3-O11 |
| 77 | e | 301 | PTY | C3-O11-P1-O13 |
| 77 | e | 301 | PTY | C3-O11-P1-O14 |
| 77 | e | 302 | PTY | O14-C5-C6-O7 |
| 77 | e | 302 | PTY | O10-C8-O7-C6 |
| 77 | e | 302 | PTY | C11-C8-O7-C6 |
| 77 | e | 302 | PTY | C5-O14-P1-O12 |
| 77 | h | 202 | PTY | O10-C8-O7-C6 |
| 77 | h | 202 | PTY | C3-O11-P1-O14 |
| 77 | h | 202 | PTY | C5-O14-P1-O12 |
| 77 | x | 102 | PTY | O10-C8-O7-C6 |
| 77 | x | 102 | PTY | C3-O11-P1-O13 |
| 79 | 1G | 301 | PC7 | C4-O4P-P-O2P |
| 79 | 1H | 101 | PC7 | C1-O3P-P-O2P |
| 79 | 1H | 101 | PC7 | C4-O4P-P-O2P |
| 79 | 1H | 101 | PC7 | O4P-C4-C5-N |
| 79 | 3A | 606 | PC7 | C2-C1-O3P-P |
| 79 | 3A | 606 | PC7 | C1-O3P-P-O1P |
| 79 | 3A | 606 | PC7 | C1-O3P-P-O2P |
| 79 | 3A | 606 | PC7 | C1-O3P-P-O4P |
| 79 | 3A | 606 | PC7 | C4-O4P-P-O2P |
| 79 | Q | 302 | PC7 | C4-O4P-P-O3P |
| 79 | Q | 302 | PC7 | C4-O4P-P-O1P |
| 79 | Q | 302 | PC7 | C4-O4P-P-O2P |
| 79 | R | 403 | PC7 | C1-O3P-P-O1P |
| 79 | R | 403 | PC7 | C1-O3P-P-O2P |
| 79 | R | 403 | PC7 | C1-O3P-P-O4P |
| 79 | R | 403 | PC7 | O4P-C4-C5-N |
| 79 | T | 503 | PC7 | C32-C31-O2-C2 |
| 79 | T | 503 | PC7 | C4-O4P-P-O2P |
| 79 | T | 503 | PC7 | O4P-C4-C5-N |
| 79 | u | 601 | PC7 | C32-C31-O2-C2 |
| 79 | u | 601 | PC7 | C4-O4P-P-O1P |
| 81 | 3A | 601 | PGT | C1-O3P-P-O1P |
| 81 | T | 502 | PGT | C4-O4P-P-O1P |
| 81 | T | 505 | PGT | C1-O3P-P-O4P |
| 81 | b | 601 | PGT | C2-C1-O3P-P |
| 81 | b | 601 | PGT | C1-O3P-P-O2P |
| 81 | b | 601 | PGT | C4-O4P-P-O1P |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 81 | l | 701 | PGT | O3P-C1-C2-O2 |
| 81 | l | 701 | PGT | C4-O4P-P-O1P |
| 82 | 2A | 603 | HEA | C3B-C11-C12-C13 |
| 82 | 2A | 603 | HEA | O11-C11-C12-C13 |
| 82 | 2A | 603 | HEA | C15-C16-C17-C18 |
| 82 | 3A | 603 | HEA | C3B-C11-C12-C13 |
| 82 | 3A | 603 | HEA | O11-C11-C12-C13 |
| 82 | 3A | 603 | HEA | C15-C16-C17-C18 |
| 82 | 3A | 603 | HEA | C19-C20-C21-C22 |
| 87 | B | 501 | FMN | C5'-O5'-P-O1P |
| 87 | B | 501 | FMN | C5'-O5'-P-O2P |
| 87 | B | 501 | FMN | C5'-O5'-P-O3P |
| 89 | J | 200 | 8Q1 | C1-C6-C7-C8 |
| 89 | J | 200 | 8Q1 | O27-C28-C29-C32 |
| 89 | r | 200 | 8Q1 | C1-C6-C7-C8 |
| 89 | r | 200 | 8Q1 | O4-C1-S44-C43 |
| 89 | r | 200 | 8Q1 | C6-C1-S44-C43 |
| 89 | r | 200 | 8Q1 | C28-C29-C32-C34 |
| 89 | r | 200 | 8Q1 | C28-C29-C32-O33 |
| 89 | r | 200 | 8Q1 | C30-C29-C32-C34 |
| 89 | r | 200 | 8Q1 | C30-C29-C32-O33 |
| 89 | r | 200 | 8Q1 | C31-C29-C32-C34 |
| 89 | r | 200 | 8Q1 | C31-C29-C32-O33 |
| 89 | r | 200 | 8Q1 | O33-C32-C34-N36 |
| 89 | r | 200 | 8Q1 | C32-C34-N36-C37 |
| 89 | r | 200 | 8Q1 | C28-O27-P24-O1 |
| 90 | P | 401 | NDP | C5B-O5B-PA-O2A |
| 90 | P | 401 | NDP | C5B-O5B-PA-O3 |
| 90 | P | 401 | NDP | O4B-C4B-C5B-O5B |
| 90 | P | 401 | NDP | C3B-C4B-C5B-O5B |
| 90 | P | 401 | NDP | C5D-O5D-PN-O3 |
| 90 | P | 401 | NDP | C5D-O5D-PN-O1N |
| 91 | s | 401 | COO | C14-C11-C13-O1 |
| 91 | s | 401 | COO | C12-C11-C13-O1 |
| 91 | s | 401 | COO | C14-C11-C13-C1 |
| 91 | s | 401 | COO | C12-C11-C13-C1 |
| 91 | s | 401 | COO | C13-C11-C12-O6A |
| 91 | s | 401 | COO | C13-C1-N1-C2 |
| 91 | s | 401 | COO | O2-C1-N1-C2 |
| 91 | s | 401 | COO | C3-C4-N2-C5 |
| 91 | s | 401 | COO | O3-C4-N2-C5 |
| 91 | s | 401 | COO | O4-C7-S1-C6 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 91 | s | 401 | COO | C8-C7-S1-C6 |
| 91 | s | 401 | COO | S1-C7-C8-C9 |
| 75 | 1M | 501 | CDL | OA9-CA7-OA8-CA6 |
| 75 | V | 603 | CDL | OB9-CB7-OB8-CB6 |
| 75 | W | 701 | CDL | OB9-CB7-OB8-CB6 |
| 75 | u | 602 | CDL | OA9-CA7-OA8-CA6 |
| 76 | g | 101 | 3PH | O32-C31-O31-C3 |
| 77 | R | 404 | PTY | O30-C30-O4-C1 |
| 77 | V | 606 | PTY | O30-C30-O4-C1 |
| 81 | l | 701 | PGT | O11-C11-O3-C3 |
| 75 | V | 603 | CDL | C71-CB7-OB8-CB6 |
| 75 | u | 602 | CDL | C31-CA7-OA8-CA6 |
| 77 | R | 404 | PTY | C31-C30-O4-C1 |
| 77 | V | 606 | PTY | C31-C30-O4-C1 |
| 81 | b | 601 | PGT | C12-C11-O3-C3 |
| 75 | 1F | 401 | CDL | OB9-CB7-OB8-CB6 |
| 75 | 1K | 101 | CDL | OB9-CB7-OB8-CB6 |
| 76 | 1B | 406 | 3PH | O32-C31-O31-C3 |
| 76 | 1B | 407 | 3PH | O32-C31-O31-C3 |
| 76 | h | 201 | 3PH | O32-C31-O31-C3 |
| 77 | h | 202 | PTY | O30-C30-O4-C1 |
| 79 | 2A | 606 | PC7 | O11-C11-O3-C3 |
| 81 | b | 601 | PGT | O11-C11-O3-C3 |
| 75 | 1A | 405 | CDL | OB7-CB5-OB6-CB4 |
| 75 | 1B | 405 | CDL | OA7-CA5-OA6-CA4 |
| 75 | 1E | 401 | CDL | OA7-CA5-OA6-CA4 |
| 75 | 1F | 401 | CDL | OB7-CB5-OB6-CB4 |
| 75 | 1K | 101 | CDL | OB7-CB5-OB6-CB4 |
| 75 | 1M | 501 | CDL | OB7-CB5-OB6-CB4 |
| 75 | R | 405 | CDL | OB7-CB5-OB6-CB4 |
| 75 | V | 603 | CDL | OA7-CA5-OA6-CA4 |
| 75 | W | 701 | CDL | OB7-CB5-OB6-CB4 |
| 75 | u | 602 | CDL | OB7-CB5-OB6-CB4 |
| 76 | 1A | 406 | 3PH | O22-C21-O21-C2 |
| 76 | V | 602 | 3PH | O22-C21-O21-C2 |
| 77 | 2D | 301 | PTY | O10-C8-O7-C6 |
| 77 | 3D | 301 | PTY | O10-C8-O7-C6 |
| 77 | 3F | 101 | PTY | O10-C8-O7-C6 |
| 77 | R | 404 | PTY | O10-C8-O7-C6 |
| 77 | R | 406 | PTY | O10-C8-O7-C6 |
| 79 | T | 503 | PC7 | O31-C31-O2-C2 |
| 79 | u | 601 | PC7 | O31-C31-O2-C2 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 77 | 1E | 403 | PTY | O30-C30-O4-C1 |
| 75 | 1E | 401 | CDL | C71-CB7-OB8-CB6 |
| 75 | 1F | 401 | CDL | C71-CB7-OB8-CB6 |
| 75 | 1M | 501 | CDL | C31-CA7-OA8-CA6 |
| 75 | W | 701 | CDL | C71-CB7-OB8-CB6 |
| 76 | 1B | 407 | 3PH | C32-C31-O31-C3 |
| 76 | g | 101 | 3PH | C32-C31-O31-C3 |
| 79 | 2A | 606 | PC7 | C12-C11-O3-C3 |
| 81 | T | 505 | PGT | C12-C11-O3-C3 |
| 81 | l | 701 | PGT | C12-C11-O3-C3 |
| 75 | 1B | 408 | CDL | C11-CA5-OA6-CA4 |
| 75 | 1K | 101 | CDL | C51-CB5-OB6-CB4 |
| 75 | 1L | 101 | CDL | C11-CA5-OA6-CA4 |
| 77 | h | 202 | PTY | C11-C8-O7-C6 |
| 77 | x | 102 | PTY | C11-C8-O7-C6 |
| 79 | 3A | 606 | PC7 | O11-C11-O3-C3 |
| 73 | 1B | 401 | UQ5 | C15-C14-C16-C17 |
| 73 | 1B | 401 | UQ5 | C18-C19-C21-C22 |
| 75 | 1B | 405 | CDL | C31-CA7-OA8-CA6 |
| 75 | 1K | 101 | CDL | C71-CB7-OB8-CB6 |
| 76 | 1B | 406 | 3PH | C32-C31-O31-C3 |
| 76 | 1R | 201 | 3PH | C32-C31-O31-C3 |
| 76 | h | 201 | 3PH | C32-C31-O31-C3 |
| 77 | 1E | 403 | PTY | C31-C30-O4-C1 |
| 77 | h | 202 | PTY | C31-C30-O4-C1 |
| 81 | 2A | 601 | PGT | C12-C11-O3-C3 |
| 76 | 2D | 302 | 3PH | O22-C21-O21-C2 |
| 76 | h | 201 | 3PH | O22-C21-O21-C2 |
| 75 | 1E | 401 | CDL | OB9-CB7-OB8-CB6 |
| 77 | e | 302 | PTY | O30-C30-O4-C1 |
| 79 | R | 403 | PC7 | O11-C11-O3-C3 |
| 81 | T | 505 | PGT | O11-C11-O3-C3 |
| 75 | 1B | 405 | CDL | O1-C1-CA2-OA2 |
| 75 | 1F | 401 | CDL | O1-C1-CB2-OB2 |
| 75 | 1K | 101 | CDL | O1-C1-CA2-OA2 |
| 75 | 1L | 101 | CDL | O1-C1-CB2-OB2 |
| 75 | R | 405 | CDL | O1-C1-CA2-OA2 |
| 75 | h | 203 | CDL | O1-C1-CB2-OB2 |
| 75 | u | 602 | CDL | O1-C1-CB2-OB2 |
| 75 | x | 101 | CDL | O1-C1-CB2-OB2 |
| 75 | y | 202 | CDL | O1-C1-CA2-OA2 |
| 81 | b | 601 | PGT | O4P-C4-C5-O5 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 75 | u | 603 | CDL | C31-CA7-OA8-CA6 |
| 77 | e | 301 | PTY | C31-C30-O4-C1 |
| 77 | e | 302 | PTY | C31-C30-O4-C1 |
| 81 | T | 502 | PGT | C12-C11-O3-C3 |
| 75 | h | 203 | CDL | C71-C72-C73-C74 |
| 76 | 1R | 201 | 3PH | O32-C31-O31-C3 |
| 89 | r | 200 | 8Q1 | O35-C34-N36-C37 |
| 75 | 1L | 101 | CDL | C51-CB5-OB6-CB4 |
| 75 | W | 701 | CDL | C51-CB5-OB6-CB4 |
| 77 | T | 501 | PTY | C11-C8-O7-C6 |
| 75 | h | 203 | CDL | C75-C76-C77-C78 |
| 81 | T | 502 | PGT | O11-C11-O3-C3 |
| 75 | x | 101 | CDL | C72-C73-C74-C75 |
| 75 | u | 603 | CDL | C13-C14-C15-C16 |
| 90 | P | 401 | NDP | O4D-C4D-C5D-O5D |
| 79 | 3A | 606 | PC7 | C12-C11-O3-C3 |
| 79 | R | 403 | PC7 | C12-C11-O3-C3 |
| 77 | T | 501 | PTY | O10-C8-O7-C6 |
| 75 | 1B | 405 | CDL | OA9-CA7-OA8-CA6 |
| 75 | u | 603 | CDL | OA9-CA7-OA8-CA6 |
| 81 | 2A | 601 | PGT | O11-C11-O3-C3 |
| 77 | e | 301 | PTY | O30-C30-O4-C1 |
| 76 | h | 201 | 3PH | C3B-C3C-C3D-C3E |
| 81 | T | 502 | PGT | C17-C18-C19-C20 |
| 75 | R | 405 | CDL | C71-CB7-OB8-CB6 |
| 79 | 1H | 101 | PC7 | C12-C11-O3-C3 |
| 75 | W | 701 | CDL | C63-C64-C65-C66 |
| 75 | 1A | 405 | CDL | C11-CA5-OA6-CA4 |
| 76 | 2I | 201 | 3PH | C22-C21-O21-C2 |
| 76 | S | 301 | 3PH | C22-C21-O21-C2 |
| 75 | 1F | 401 | CDL | CA2-C1-CB2-OB2 |
| 75 | 1L | 101 | CDL | CA2-C1-CB2-OB2 |
| 75 | W | 701 | CDL | CA2-C1-CB2-OB2 |
| 75 | u | 603 | CDL | CA2-C1-CB2-OB2 |
| 75 | y | 202 | CDL | CB2-C1-CA2-OA2 |
| 75 | 1L | 101 | CDL | OB7-CB5-OB6-CB4 |
| 75 | R | 405 | CDL | OB9-CB7-OB8-CB6 |
| 79 | Q | 302 | PC7 | C4-C5-N-C7 |
| 75 | 1L | 101 | CDL | C31-CA7-OA8-CA6 |
| 75 | x | 101 | CDL | C31-CA7-OA8-CA6 |
| 76 | 1E | 402 | 3PH | C32-C31-O31-C3 |
| 76 | 1K | 102 | 3PH | C32-C31-O31-C3 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 76 | R | 401 | 3PH | C32-C31-O31-C3 |
| 75 | h | 203 | CDL | CB7-C71-C72-C73 |
| 79 | 1H | 101 | PC7 | O11-C11-O3-C3 |
| 75 | h | 203 | CDL | C12-C13-C14-C15 |
| 75 | u | 603 | CDL | OB6-CB4-CB6-OB8 |
| 75 | y | 202 | CDL | OA6-CA4-CA6-OA8 |
| 79 | T | 503 | PC7 | O2-C2-C3-O3 |
| 76 | R | 401 | 3PH | O32-C31-O31-C3 |
| 75 | h | 203 | CDL | C15-C16-C17-C18 |
| 75 | 1F | 401 | CDL | C55-C56-C57-C58 |
| 75 | 1K | 101 | CDL | C76-C77-C78-C79 |
| 75 | u | 603 | CDL | C39-C40-C41-C42 |
| 75 | R | 405 | CDL | CA7-C31-C32-C33 |
| 76 | S | 301 | 3PH | C21-C22-C23-C24 |
| 77 | 1E | 403 | PTY | C8-C11-C12-C13 |
| 79 | 1H | 101 | PC7 | C31-C32-C33-C34 |
| 79 | T | 503 | PC7 | C11-C12-C13-C14 |
| 75 | 1L | 101 | CDL | OA9-CA7-OA8-CA6 |
| 74 | 1B | 403 | HEM | C2A-CAA-CBA-CGA |
| 82 | 3A | 602 | HEA | C2A-CAA-CBA-CGA |
| 75 | V | 603 | CDL | CB7-C71-C72-C73 |
| 75 | h | 203 | CDL | CA7-C31-C32-C33 |
| 76 | c | 101 | 3PH | C31-C32-C33-C34 |
| 77 | S | 302 | PTY | C30-C31-C32-C33 |
| 81 | l | 701 | PGT | C31-C32-C33-C34 |
| 77 | V | 605 | PTY | C13-C14-C15-C16 |
| 75 | 1K | 101 | CDL | C52-C53-C54-C55 |
| 81 | b | 601 | PGT | O5-C5-C6-O6 |
| 75 | 1B | 408 | CDL | CA7-C31-C32-C33 |
| 75 | 1E | 401 | CDL | CB7-C71-C72-C73 |
| 75 | R | 405 | CDL | CB7-C71-C72-C73 |
| 75 | V | 603 | CDL | CA7-C31-C32-C33 |
| 75 | W | 701 | CDL | CB5-C51-C52-C53 |
| 75 | u | 602 | CDL | CB7-C71-C72-C73 |
| 75 | x | 101 | CDL | CB5-C51-C52-C53 |
| 75 | y | 202 | CDL | CB7-C71-C72-C73 |
| 77 | R | 404 | PTY | C30-C31-C32-C33 |
| 77 | x | 102 | PTY | C8-C11-C12-C13 |
| 79 | u | 601 | PC7 | C31-C32-C33-C34 |
| 75 | W | 701 | CDL | C74-C75-C76-C77 |
| 75 | x | 101 | CDL | C13-C14-C15-C16 |
| 79 | Q | 302 | PC7 | C4-C5-N-C8 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 75 | 1B | 405 | CDL | CB5-C51-C52-C53 |
| 75 | 1M | 501 | CDL | CB5-C51-C52-C53 |
| 75 | u | 603 | CDL | CB7-C71-C72-C73 |
| 77 | V | 605 | PTY | C30-C31-C32-C33 |
| 76 | R | 401 | 3PH | C22-C21-O21-C2 |
| 75 | 1K | 101 | CDL | C33-C34-C35-C36 |
| 75 | x | 101 | CDL | OA9-CA7-OA8-CA6 |
| 73 | 1A | 401 | UQ5 | C14-C16-C17-C18 |
| 73 | 1A | 402 | UQ5 | C9-C11-C12-C13 |
| 82 | 2A | 603 | HEA | C19-C20-C21-C22 |
| 77 | V | 605 | PTY | C19-C20-C21-C22 |
| 75 | 1B | 408 | CDL | O1-C1-CB2-OB2 |
| 75 | W | 701 | CDL | O1-C1-CB2-OB2 |
| 81 | T | 505 | PGT | O4P-C4-C5-O5 |
| 76 | 2I | 201 | 3PH | O22-C21-O21-C2 |
| 76 | S | 301 | 3PH | O22-C21-O21-C2 |
| 76 | 1K | 102 | 3PH | O32-C31-O31-C3 |
| 75 | u | 603 | CDL | CA7-C31-C32-C33 |
| 76 | 1E | 402 | 3PH | O32-C31-O31-C3 |
| 75 | 1F | 401 | CDL | C11-CA5-OA6-CA4 |
| 75 | u | 603 | CDL | C11-CA5-OA6-CA4 |
| 79 | 1G | 301 | PC7 | C32-C31-O2-C2 |
| 75 | 1A | 405 | CDL | CA3-OA5-PA1-OA2 |
| 75 | 1B | 405 | CDL | CA3-OA5-PA1-OA2 |
| 75 | 1B | 405 | CDL | CB2-OB2-PB2-OB5 |
| 75 | 1B | 405 | CDL | CB3-OB5-PB2-OB2 |
| 75 | 1B | 408 | CDL | CA3-OA5-PA1-OA2 |
| 75 | 1E | 401 | CDL | CA2-OA2-PA1-OA5 |
| 75 | 1E | 401 | CDL | CB2-OB2-PB2-OB5 |
| 75 | 1E | 401 | CDL | CB3-OB5-PB2-OB2 |
| 75 | 1K | 101 | CDL | CB2-OB2-PB2-OB5 |
| 75 | 1K | 101 | CDL | CB3-OB5-PB2-OB2 |
| 75 | 1L | 101 | CDL | CA2-OA2-PA1-OA5 |
| 75 | 1L | 101 | CDL | CA3-OA5-PA1-OA2 |
| 75 | 1L | 101 | CDL | CB2-OB2-PB2-OB5 |
| 75 | 1M | 501 | CDL | CB3-OB5-PB2-OB2 |
| 75 | R | 405 | CDL | CA2-OA2-PA1-OA5 |
| 75 | V | 603 | CDL | CB2-OB2-PB2-OB5 |
| 75 | V | 603 | CDL | CB3-OB5-PB2-OB2 |
| 75 | W | 701 | CDL | CA2-OA2-PA1-OA5 |
| 75 | W | 701 | CDL | CB3-OB5-PB2-OB2 |
| 75 | h | 203 | CDL | CA3-OA5-PA1-OA2 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 75 | h | 203 | CDL | CB3-OB5-PB2-OB2 |
| 75 | u | 602 | CDL | CB2-OB2-PB2-OB5 |
| 75 | u | 603 | CDL | CA2-OA2-PA1-OA5 |
| 75 | u | 603 | CDL | CB2-OB2-PB2-OB5 |
| 75 | u | 603 | CDL | CB3-OB5-PB2-OB2 |
| 75 | x | 101 | CDL | CA3-OA5-PA1-OA2 |
| 75 | y | 202 | CDL | CA3-OA5-PA1-OA2 |
| 75 | y | 202 | CDL | CB2-OB2-PB2-OB5 |
| 77 | 1E | 403 | PTY | C3-O11-P1-O14 |
| 77 | 1F | 403 | PTY | C3-O11-P1-O14 |
| 77 | 2F | 101 | PTY | C3-O11-P1-O14 |
| 77 | R | 402 | PTY | C3-O11-P1-O14 |
| 77 | R | 402 | PTY | C5-O14-P1-O11 |
| 77 | R | 404 | PTY | C5-O14-P1-O11 |
| 77 | S | 302 | PTY | C3-O11-P1-O14 |
| 77 | T | 501 | PTY | C3-O11-P1-O14 |
| 77 | T | 504 | PTY | C5-O14-P1-O11 |
| 77 | T | 506 | PTY | C3-O11-P1-O14 |
| 77 | V | 604 | PTY | C3-O11-P1-O14 |
| 77 | V | 604 | PTY | C5-O14-P1-O11 |
| 77 | V | 605 | PTY | C5-O14-P1-O11 |
| 77 | e | 302 | PTY | C5-O14-P1-O11 |
| 77 | h | 202 | PTY | C5-O14-P1-O11 |
| 79 | 1G | 301 | PC7 | C4-O4P-P-O3P |
| 79 | 1H | 101 | PC7 | C4-O4P-P-O3P |
| 79 | 2A | 606 | PC7 | C4-O4P-P-O3P |
| 79 | u | 601 | PC7 | C4-O4P-P-O3P |
| 81 | T | 502 | PGT | C4-O4P-P-O3P |
| 81 | b | 601 | PGT | C1-O3P-P-O4P |
| 81 | l | 701 | PGT | C4-O4P-P-O3P |
| 75 | W | 701 | CDL | C18-C19-C20-C21 |
| 76 | w | 201 | 3PH | C21-C22-C23-C24 |
| 75 | 1A | 405 | CDL | CA2-C1-CB2-OB2 |
| 75 | 1B | 405 | CDL | CB2-C1-CA2-OA2 |
| 75 | 1B | 408 | CDL | CA2-C1-CB2-OB2 |
| 75 | 1E | 401 | CDL | CA2-C1-CB2-OB2 |
| 75 | x | 101 | CDL | CA2-C1-CB2-OB2 |
| 81 | T | 505 | PGT | O4P-C4-C5-C6 |
| 75 | 1A | 405 | CDL | OA7-CA5-OA6-CA4 |
| 75 | 1F | 401 | CDL | OA7-CA5-OA6-CA4 |
| 75 | u | 603 | CDL | OA7-CA5-OA6-CA4 |
| 76 | R | 401 | 3PH | O22-C21-O21-C2 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 76 | w | 201 | 3PH | C32-C31-O31-C3 |
| 75 | 1B | 405 | CDL | C32-C33-C34-C35 |
| 75 | u | 603 | CDL | C20-C21-C22-C23 |
| 75 | u | 603 | CDL | C31-C32-C33-C34 |
| 75 | u | 603 | CDL | C36-C37-C38-C39 |
| 75 | x | 101 | CDL | C77-C78-C79-C80 |
| 76 | V | 602 | 3PH | C26-C27-C28-C29 |
| 81 | T | 502 | PGT | C14-C15-C16-C17 |
| 76 | 1R | 201 | 3PH | C22-C21-O21-C2 |
| 77 | V | 605 | PTY | C11-C8-O7-C6 |
| 81 | 3A | 601 | PGT | C32-C31-O2-C2 |
| 81 | T | 505 | PGT | C32-C31-O2-C2 |
| 75 | 1K | 101 | CDL | C81-C82-C83-C84 |
| 75 | W | 701 | CDL | C83-C84-C85-C86 |
| 75 | h | 203 | CDL | C19-C20-C21-C22 |
| 75 | u | 602 | CDL | C36-C37-C38-C39 |
| 75 | u | 603 | CDL | C14-C15-C16-C17 |
| 75 | u | 603 | CDL | C33-C34-C35-C36 |
| 77 | S | 302 | PTY | C11-C12-C13-C14 |
| 77 | e | 302 | PTY | C34-C35-C36-C37 |
| 89 | J | 200 | 8Q1 | O27-C28-C29-C30 |
| 89 | J | 200 | 8Q1 | O27-C28-C29-C31 |
| 91 | s | 401 | COO | C15-C11-C12-O6A |
| 75 | 1A | 405 | CDL | C32-C33-C34-C35 |
| 75 | 1L | 101 | CDL | C51-C52-C53-C54 |
| 75 | R | 405 | CDL | C72-C73-C74-C75 |
| 75 | W | 701 | CDL | C77-C78-C79-C80 |
| 75 | x | 101 | CDL | C23-C24-C25-C26 |
| 76 | 2I | 201 | 3PH | C24-C25-C26-C27 |
| 77 | T | 501 | PTY | C37-C38-C39-C40 |
| 79 | T | 503 | PC7 | C32-C33-C34-C35 |
| 79 | 1G | 301 | PC7 | O31-C31-O2-C2 |
| 81 | 3A | 601 | PGT | O31-C31-O2-C2 |
| 75 | 1K | 101 | CDL | C57-C58-C59-C60 |
| 75 | 1L | 101 | CDL | C11-C12-C13-C14 |
| 75 | W | 701 | CDL | C61-C62-C63-C64 |
| 76 | V | 601 | 3PH | C2C-C2D-C2E-C2F |
| 75 | 1B | 408 | CDL | C1-CA2-OA2-PA1 |
| 75 | 1B | 408 | CDL | C51-C52-C53-C54 |
| 75 | 1B | 408 | CDL | C72-C73-C74-C75 |
| 75 | W | 701 | CDL | C34-C35-C36-C37 |
| 75 | h | 203 | CDL | C11-C12-C13-C14 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 75 | h | 203 | CDL | C72-C73-C74-C75 |
| 75 | u | 603 | CDL | C12-C13-C14-C15 |
| 75 | y | 202 | CDL | C72-C73-C74-C75 |
| 76 | 1K | 102 | 3PH | C36-C37-C38-C39 |
| 76 | g | 101 | 3PH | C3E-C3F-C3G-C3H |
| 77 | 3F | 101 | PTY | C35-C36-C37-C38 |
| 77 | V | 605 | PTY | C32-C33-C34-C35 |
| 77 | V | 606 | PTY | C13-C14-C15-C16 |
| 81 | b | 601 | PGT | C37-C38-C39-C40 |
| 81 | l | 701 | PGT | C39-C40-C41-C42 |
| 75 | 1K | 101 | CDL | O1-C1-CB2-OB2 |
| 75 | 1K | 101 | CDL | C32-C33-C34-C35 |
| 75 | R | 405 | CDL | C11-C12-C13-C14 |
| 75 | u | 603 | CDL | C40-C41-C42-C43 |
| 76 | h | 201 | 3PH | C2A-C2B-C2C-C2D |
| 77 | S | 302 | PTY | C33-C34-C35-C36 |
| 79 | 1H | 101 | PC7 | C18-C19-C20-C21 |
| 81 | b | 601 | PGT | C36-C37-C38-C39 |
| 89 | r | 200 | 8Q1 | C12-C13-C14-C15 |
| 77 | R | 402 | PTY | C8-C11-C12-C13 |
| 77 | e | 302 | PTY | C30-C31-C32-C33 |
| 75 | W | 701 | CDL | C72-C73-C74-C75 |
| 75 | u | 602 | CDL | C57-C58-C59-C60 |
| 79 | T | 503 | PC7 | C13-C14-C15-C16 |
| 73 | 1A | 401 | UQ5 | C20-C19-C21-C22 |
| 73 | 1A | 402 | UQ5 | C25-C24-C26-C27 |
| 75 | W | 701 | CDL | C51-C52-C53-C54 |
| 75 | W | 701 | CDL | C59-C60-C61-C62 |
| 75 | u | 602 | CDL | C62-C63-C64-C65 |
| 76 | 1B | 406 | 3PH | C38-C39-C3A-C3B |
| 76 | 3I | 201 | 3PH | C29-C2A-C2B-C2C |
| 76 | S | 301 | 3PH | C37-C38-C39-C3A |
| 77 | x | 102 | PTY | C16-C17-C18-C19 |
| 79 | T | 503 | PC7 | C33-C34-C35-C36 |
| 73 | 1B | 401 | UQ5 | C13-C14-C16-C17 |
| 75 | 1L | 101 | CDL | CA5-C11-C12-C13 |
| 75 | u | 603 | CDL | CA5-C11-C12-C13 |
| 81 | 2A | 601 | PGT | C11-C12-C13-C14 |
| 75 | 1B | 408 | CDL | C32-C33-C34-C35 |
| 75 | R | 405 | CDL | C75-C76-C77-C78 |
| 75 | W | 701 | CDL | C35-C36-C37-C38 |
| 76 | 1R | 201 | 3PH | C33-C34-C35-C36 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 76 | 3D | 302 | 3PH | C25-C26-C27-C28 |
| 75 | h | 203 | CDL | C20-C21-C22-C23 |
| 75 | u | 602 | CDL | C63-C64-C65-C66 |
| 75 | u | 603 | CDL | C16-C17-C18-C19 |
| 75 | u | 603 | CDL | C38-C39-C40-C41 |
| 75 | u | 603 | CDL | C42-C43-C44-C45 |
| 75 | x | 101 | CDL | C79-C80-C81-C82 |
| 77 | T | 504 | PTY | C32-C33-C34-C35 |
| 81 | 3A | 601 | PGT | C4-C5-C6-O6 |
| 81 | T | 502 | PGT | C4-C5-C6-O6 |
| 81 | b | 601 | PGT | C4-C5-C6-O6 |
| 81 | l | 701 | PGT | C4-C5-C6-O6 |
| 76 | 1R | 201 | 3PH | O22-C21-O21-C2 |
| 77 | V | 605 | PTY | O10-C8-O7-C6 |
| 81 | T | 505 | PGT | O31-C31-O2-C2 |
| 81 | l | 701 | PGT | O31-C31-O2-C2 |
| 81 | l | 701 | PGT | C32-C31-O2-C2 |
| 75 | 1B | 408 | CDL | C52-C53-C54-C55 |
| 75 | V | 603 | CDL | C71-C72-C73-C74 |
| 75 | W | 701 | CDL | C32-C33-C34-C35 |
| 75 | h | 203 | CDL | C73-C74-C75-C76 |
| 75 | x | 101 | CDL | C16-C17-C18-C19 |
| 76 | V | 602 | 3PH | C2B-C2C-C2D-C2E |
| 75 | 1A | 405 | CDL | CB5-C51-C52-C53 |
| 75 | 1F | 401 | CDL | CA5-C11-C12-C13 |
| 76 | g | 101 | 3PH | C21-C22-C23-C24 |
| 81 | 3A | 601 | PGT | C11-C12-C13-C14 |
| 75 | 1K | 101 | CDL | C72-C73-C74-C75 |
| 75 | 1L | 101 | CDL | C52-C53-C54-C55 |
| 75 | h | 203 | CDL | C57-C58-C59-C60 |
| 75 | x | 101 | CDL | C21-C22-C23-C24 |
| 76 | 1B | 406 | 3PH | C34-C35-C36-C37 |
| 76 | c | 101 | 3PH | C33-C34-C35-C36 |
| 76 | y | 201 | 3PH | C37-C38-C39-C3A |
| 77 | V | 605 | PTY | C33-C34-C35-C36 |
| 77 | x | 102 | PTY | C22-C23-C24-C25 |
| 79 | Q | 302 | PC7 | C12-C13-C14-C15 |
| 79 | T | 503 | PC7 | C40-C41-C42-C43 |
| 81 | T | 505 | PGT | C32-C33-C34-C35 |
| 81 | T | 505 | PGT | C19-C20-C21-C22 |
| 89 | r | 200 | 8Q1 | C11-C10-C9-C8 |
| 75 | 1K | 101 | CDL | C75-C76-C77-C78 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 75 | x | 101 | CDL | C15-C16-C17-C18 |
| 76 | 2I | 201 | 3PH | C29-C2A-C2B-C2C |
| 81 | b | 601 | PGT | C16-C17-C18-C19 |
| 77 | 1E | 403 | PTY | N1-C2-C3-O11 |
| 77 | 2F | 101 | PTY | N1-C2-C3-O11 |
| 75 | 1K | 101 | CDL | C11-C12-C13-C14 |
| 75 | W | 701 | CDL | C11-C12-C13-C14 |
| 75 | h | 203 | CDL | C32-C33-C34-C35 |
| 76 | c | 101 | 3PH | C35-C36-C37-C38 |
| 81 | 3A | 601 | PGT | C15-C16-C17-C18 |
| 81 | b | 601 | PGT | C32-C33-C34-C35 |
| 76 | w | 201 | 3PH | O32-C31-O31-C3 |
| 75 | 1A | 405 | CDL | C52-C53-C54-C55 |
| 75 | h | 203 | CDL | C31-C32-C33-C34 |
| 75 | h | 203 | CDL | C80-C81-C82-C83 |
| 77 | R | 404 | PTY | C25-C26-C27-C28 |
| 77 | S | 302 | PTY | C37-C38-C39-C40 |
| 79 | T | 503 | PC7 | C39-C40-C41-C42 |
| 81 | T | 502 | PGT | C16-C17-C18-C19 |
| 75 | 1E | 401 | CDL | C31-CA7-OA8-CA6 |
| 75 | V | 603 | CDL | C11-C12-C13-C14 |
| 75 | x | 101 | CDL | C11-C12-C13-C14 |
| 91 | s | 401 | COO | N2-C5-C6-S1 |
| 75 | 1B | 408 | CDL | C73-C74-C75-C76 |
| 75 | V | 603 | CDL | C13-C14-C15-C16 |
| 75 | x | 101 | CDL | C62-C63-C64-C65 |
| 75 | x | 101 | CDL | C63-C64-C65-C66 |
| 77 | T | 506 | PTY | C12-C13-C14-C15 |
| 77 | e | 302 | PTY | C13-C14-C15-C16 |
| 79 | T | 503 | PC7 | C38-C39-C40-C41 |
| 75 | 1L | 101 | CDL | C74-C75-C76-C77 |
| 75 | V | 603 | CDL | C34-C35-C36-C37 |
| 75 | u | 602 | CDL | C16-C17-C18-C19 |
| 75 | x | 101 | CDL | C57-C58-C59-C60 |
| 76 | 1E | 402 | 3PH | C2B-C2C-C2D-C2E |
| 76 | g | 101 | 3PH | C37-C38-C39-C3A |
| 75 | 1B | 408 | CDL | C71-C72-C73-C74 |
| 81 | b | 601 | PGT | C17-C18-C19-C20 |
| 79 | Q | 302 | PC7 | C11-C12-C13-C14 |
| 75 | 1F | 401 | CDL | C51-C52-C53-C54 |
| 75 | x | 101 | CDL | C54-C55-C56-C57 |
| 79 | T | 503 | PC7 | C17-C18-C19-C20 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 73 | 1A | 401 | UQ5 | C18-C19-C21-C22 |
| 75 | h | 203 | CDL | C11-CA5-OA6-CA4 |
| 75 | h | 203 | CDL | C51-CB5-OB6-CB4 |
| 77 | 2F | 101 | PTY | C11-C8-O7-C6 |
| 79 | 3A | 606 | PC7 | C32-C31-O2-C2 |
| 76 | 1A | 406 | 3PH | C2A-C2B-C2C-C2D |
| 75 | W | 701 | CDL | C17-C18-C19-C20 |
| 77 | R | 406 | PTY | C14-C15-C16-C17 |
| 79 | 3A | 606 | PC7 | C11-C12-C13-C14 |
| 75 | 1B | 405 | CDL | O1-C1-CB2-OB2 |
| 81 | T | 505 | PGT | C18-C19-C20-C21 |
| 75 | 1B | 408 | CDL | C16-C17-C18-C19 |
| 75 | u | 603 | CDL | C34-C35-C36-C37 |
| 75 | h | 203 | CDL | OA7-CA5-OA6-CA4 |
| 75 | h | 203 | CDL | OB7-CB5-OB6-CB4 |
| 76 | w | 201 | 3PH | O22-C21-O21-C2 |
| 77 | 2F | 101 | PTY | O10-C8-O7-C6 |
| 79 | 3A | 606 | PC7 | O31-C31-O2-C2 |
| 75 | x | 101 | CDL | C80-C81-C82-C83 |
| 76 | R | 401 | 3PH | C36-C37-C38-C39 |
| 77 | 1F | 403 | PTY | C34-C35-C36-C37 |
| 76 | 1B | 406 | 3PH | C33-C34-C35-C36 |
| 77 | 2F | 101 | PTY | C34-C35-C36-C37 |
| 75 | 1L | 101 | CDL | CB7-C71-C72-C73 |
| 75 | 1M | 501 | CDL | CA5-C11-C12-C13 |
| 75 | W | 701 | CDL | C62-C63-C64-C65 |
| 75 | W | 701 | CDL | C76-C77-C78-C79 |
| 75 | W | 701 | CDL | C81-C82-C83-C84 |
| 76 | 1K | 102 | 3PH | C23-C24-C25-C26 |
| 76 | h | 201 | 3PH | C33-C34-C35-C36 |
| 77 | T | 504 | PTY | C11-C8-O7-C6 |
| 75 | W | 701 | CDL | C14-C15-C16-C17 |
| 76 | w | 201 | 3PH | C38-C39-C3A-C3B |
| 77 | R | 404 | PTY | C24-C25-C26-C27 |
| 81 | T | 505 | PGT | C15-C16-C17-C18 |
| 81 | l | 701 | PGT | C11-C12-C13-C14 |
| 77 | 1F | 403 | PTY | C31-C32-C33-C34 |
| 77 | T | 501 | PTY | C19-C20-C21-C22 |
| 79 | T | 503 | PC7 | C44-C45-C46-C47 |
| 73 | 1A | 401 | UQ5 | C13-C14-C16-C17 |
| 73 | 1A | 402 | UQ5 | C23-C24-C26-C27 |
| 75 | 1E | 401 | CDL | OA9-CA7-OA8-CA6 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 75 | y | 202 | CDL | OB7-CB5-OB6-CB4 |
| 76 | 1K | 102 | 3PH | O22-C21-O21-C2 |
| 75 | u | 603 | CDL | C71-CB7-OB8-CB6 |
| 76 | 2D | 302 | 3PH | C32-C31-O31-C3 |
| 76 | y | 201 | 3PH | C32-C31-O31-C3 |
| 75 | 1M | 501 | CDL | C32-C33-C34-C35 |
| 75 | u | 603 | CDL | C71-C72-C73-C74 |
| 91 | s | 401 | COO | O4-C7-C8-C9 |
| 75 | 1L | 101 | CDL | C72-C73-C74-C75 |
| 77 | V | 604 | PTY | C34-C35-C36-C37 |
| 79 | T | 503 | PC7 | C15-C16-C17-C18 |
| 75 | 1M | 501 | CDL | C33-C34-C35-C36 |
| 75 | W | 701 | CDL | C80-C81-C82-C83 |
| 75 | u | 602 | CDL | C13-C14-C15-C16 |
| 75 | u | 602 | CDL | C33-C34-C35-C36 |
| 81 | l | 701 | PGT | C40-C41-C42-C43 |
| 89 | J | 200 | 8Q1 | C10-C11-C12-C13 |
| 77 | T | 501 | PTY | C6-C1-O4-C30 |
| 75 | 1K | 101 | CDL | C13-C14-C15-C16 |
| 73 | 1B | 401 | UQ5 | C24-C26-C27-C28 |
| 75 | 1F | 401 | CDL | C54-C55-C56-C57 |
| 75 | u | 602 | CDL | C54-C55-C56-C57 |
| 79 | u | 601 | PC7 | C39-C40-C41-C42 |
| 75 | R | 405 | CDL | C11-CA5-OA6-CA4 |
| 75 | u | 602 | CDL | C11-CA5-OA6-CA4 |
| 75 | y | 202 | CDL | C51-CB5-OB6-CB4 |
| 76 | 1B | 406 | 3PH | C22-C21-O21-C2 |
| 76 | 1K | 102 | 3PH | C22-C21-O21-C2 |
| 76 | w | 201 | 3PH | C22-C21-O21-C2 |
| 79 | Q | 302 | PC7 | C32-C31-O2-C2 |
| 75 | 1M | 501 | CDL | OB5-CB3-CB4-OB6 |
| 76 | y | 201 | 3PH | O11-C1-C2-O21 |
| 76 | 1A | 406 | 3PH | C24-C25-C26-C27 |
| 76 | V | 602 | 3PH | C2A-C2B-C2C-C2D |
| 75 | x | 101 | CDL | C55-C56-C57-C58 |
| 77 | T | 504 | PTY | O10-C8-O7-C6 |
| 79 | Q | 302 | PC7 | O31-C31-O2-C2 |
| 76 | 2D | 302 | 3PH | O21-C2-C3-O31 |
| 77 | R | 402 | PTY | O4-C1-C6-O7 |
| 77 | T | 506 | PTY | O4-C1-C6-O7 |
| 75 | 1F | 401 | CDL | C11-C12-C13-C14 |
| 75 | 1K | 101 | CDL | C78-C79-C80-C81 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 75 | R | 405 | CDL | C32-C33-C34-C35 |
| 77 | R | 404 | PTY | C16-C17-C18-C19 |
| 79 | Q | 302 | PC7 | C4-C5-N-C6 |
| 75 | 1B | 408 | CDL | C11-C12-C13-C14 |
| 75 | 1B | 408 | CDL | C36-C37-C38-C39 |
| 75 | V | 603 | CDL | C33-C34-C35-C36 |
| 73 | 1A | 401 | UQ5 | C15-C14-C16-C17 |
| 75 | 1A | 405 | CDL | C15-C16-C17-C18 |
| 75 | x | 101 | CDL | C51-C52-C53-C54 |
| 75 | 1A | 405 | CDL | C34-C35-C36-C37 |
| 76 | 2D | 302 | 3PH | C23-C24-C25-C26 |
| 76 | 3I | 201 | 3PH | C32-C33-C34-C35 |
| 77 | x | 102 | PTY | C20-C21-C22-C23 |
| 76 | 1B | 406 | 3PH | O22-C21-O21-C2 |
| 75 | V | 603 | CDL | C51-CB5-OB6-CB4 |
| 75 | x | 101 | CDL | C60-C61-C62-C63 |
| 75 | x | 101 | CDL | C83-C84-C85-C86 |
| 75 | 1A | 405 | CDL | CB3-OB5-PB2-OB2 |
| 75 | u | 603 | CDL | CA3-OA5-PA1-OA2 |
| 77 | T | 506 | PTY | C5-O14-P1-O11 |
| 77 | V | 605 | PTY | C3-O11-P1-O14 |
| 79 | 1H | 101 | PC7 | C1-O3P-P-O4P |
| 79 | 3A | 606 | PC7 | C4-O4P-P-O3P |
| 75 | 1L | 101 | CDL | C75-C76-C77-C78 |
| 75 | u | 603 | CDL | C15-C16-C17-C18 |
| 76 | h | 201 | 3PH | C36-C37-C38-C39 |
| 77 | T | 504 | PTY | C30-C31-C32-C33 |
| 75 | 1B | 408 | CDL | CB4-CB3-OB5-PB2 |
| 75 | h | 203 | CDL | CB4-CB3-OB5-PB2 |
| 77 | V | 605 | PTY | C6-C5-O14-P1 |
| 75 | h | 203 | CDL | C16-C17-C18-C19 |
| 76 | 2D | 302 | 3PH | C22-C23-C24-C25 |
| 81 | T | 502 | PGT | C36-C37-C38-C39 |
| 75 | x | 101 | CDL | C71-CB7-OB8-CB6 |
| 77 | 3D | 301 | PTY | C31-C30-O4-C1 |
| 76 | 3D | 302 | 3PH | O11-C1-C2-C3 |
| 76 | V | 601 | 3PH | O11-C1-C2-C3 |
| 76 | c | 101 | 3PH | O11-C1-C2-C3 |
| 76 | h | 201 | 3PH | O11-C1-C2-C3 |
| 81 | l | 701 | PGT | O3P-C1-C2-C3 |
| 75 | u | 602 | CDL | C11-C12-C13-C14 |
| 75 | x | 101 | CDL | C19-C20-C21-C22 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 79 | 1H | 101 | PC7 | C12-C13-C14-C15 |
| 75 | 1A | 405 | CDL | CA5-C11-C12-C13 |
| 75 | u | 602 | CDL | C18-C19-C20-C21 |
| 76 | 1E | 402 | 3PH | C28-C29-C2A-C2B |
| 76 | 1K | 102 | 3PH | C27-C28-C29-C2A |
| 75 | 1F | 401 | CDL | C12-C13-C14-C15 |
| 77 | T | 501 | PTY | C21-C22-C23-C24 |
| 75 | x | 101 | CDL | C12-C13-C14-C15 |
| 76 | 1A | 406 | 3PH | C23-C24-C25-C26 |
| 76 | 3I | 201 | 3PH | C36-C37-C38-C39 |
| 76 | V | 602 | 3PH | C34-C35-C36-C37 |
| 76 | w | 201 | 3PH | C2A-C2B-C2C-C2D |
| 77 | e | 302 | PTY | C31-C32-C33-C34 |
| 79 | T | 503 | PC7 | C42-C43-C44-C45 |
| 75 | 1K | 101 | CDL | CA2-C1-CB2-OB2 |
| 75 | W | 701 | CDL | CB2-C1-CA2-OA2 |
| 75 | u | 602 | CDL | OA7-CA5-OA6-CA4 |
| 75 | 1B | 405 | CDL | C52-C53-C54-C55 |
| 75 | x | 101 | CDL | C74-C75-C76-C77 |
| 75 | V | 603 | CDL | C21-C22-C23-C24 |
| 77 | e | 302 | PTY | C8-C11-C12-C13 |
| 76 | 1B | 407 | 3PH | C22-C21-O21-C2 |
| 75 | u | 603 | CDL | OB9-CB7-OB8-CB6 |
| 76 | y | 201 | 3PH | O32-C31-O31-C3 |
| 76 | 3D | 302 | 3PH | C24-C25-C26-C27 |
| 77 | R | 404 | PTY | C33-C34-C35-C36 |
| 75 | 1B | 405 | CDL | CB3-CB4-CB6-OB8 |
| 75 | 1B | 408 | CDL | CA3-CA4-CA6-OA8 |
| 75 | 1K | 101 | CDL | CA3-CA4-CA6-OA8 |
| 75 | 1K | 101 | CDL | CB3-CB4-CB6-OB8 |
| 75 | R | 405 | CDL | C77-C78-C79-C80 |
| 75 | V | 603 | CDL | C32-C33-C34-C35 |
| 75 | h | 203 | CDL | CB3-CB4-CB6-OB8 |
| 75 | h | 203 | CDL | C76-C77-C78-C79 |
| 75 | u | 603 | CDL | CB3-CB4-CB6-OB8 |
| 75 | x | 101 | CDL | CA3-CA4-CA6-OA8 |
| 75 | y | 202 | CDL | CA3-CA4-CA6-OA8 |
| 76 | 1B | 406 | 3PH | C1-C2-C3-O31 |
| 76 | 1E | 402 | 3PH | C1-C2-C3-O31 |
| 76 | 2D | 302 | 3PH | C1-C2-C3-O31 |
| 77 | 1E | 403 | PTY | O4-C1-C6-C5 |
| 77 | 3F | 101 | PTY | O4-C1-C6-C5 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 77 | R | 404 | PTY | O4-C1-C6-C5 |
| 81 | 2A | 601 | PGT | C1-C2-C3-O3 |
| 81 | l | 701 | PGT | C41-C42-C43-C44 |
| 76 | 1E | 402 | 3PH | C25-C26-C27-C28 |
| 77 | R | 402 | PTY | C13-C14-C15-C16 |
| 75 | u | 603 | CDL | C37-C38-C39-C40 |
| 75 | 1B | 405 | CDL | C11-C12-C13-C14 |
| 75 | 1B | 408 | CDL | C74-C75-C76-C77 |
| 75 | V | 603 | CDL | C23-C24-C25-C26 |
| 75 | u | 603 | CDL | C44-C45-C46-C47 |
| 77 | 2D | 301 | PTY | C17-C18-C19-C20 |
| 75 | x | 101 | CDL | CB7-C71-C72-C73 |
| 76 | 1B | 407 | 3PH | C21-C22-C23-C24 |
| 79 | 2A | 606 | PC7 | C31-C32-C33-C34 |
| 76 | 2D | 302 | 3PH | O32-C31-O31-C3 |
| 75 | 1K | 101 | CDL | C59-C60-C61-C62 |
| 77 | 1F | 403 | PTY | C11-C12-C13-C14 |
| 79 | 1H | 101 | PC7 | C13-C14-C15-C16 |
| 89 | r | 200 | 8Q1 | O33-C32-C34-O35 |
| 75 | u | 602 | CDL | C37-C38-C39-C40 |
| 75 | u | 602 | CDL | C61-C62-C63-C64 |
| 77 | V | 605 | PTY | C35-C36-C37-C38 |
| 75 | 1B | 405 | CDL | C76-C77-C78-C79 |
| 76 | 1A | 406 | 3PH | C29-C2A-C2B-C2C |
| 76 | 1B | 406 | 3PH | C27-C28-C29-C2A |
| 76 | V | 601 | 3PH | C37-C38-C39-C3A |
| 75 | 1M | 501 | CDL | CB7-C71-C72-C73 |
| 75 | 1B | 405 | CDL | CA7-C31-C32-C33 |
| 77 | 1E | 403 | PTY | C32-C33-C34-C35 |
| 77 | T | 501 | PTY | C32-C33-C34-C35 |
| 79 | T | 503 | PC7 | C45-C46-C47-C48 |
| 75 | 1B | 405 | CDL | C84-C85-C86-C87 |
| 75 | 1K | 101 | CDL | C73-C74-C75-C76 |
| 77 | G | 303 | PTY | C8-C11-C12-C13 |
| 77 | T | 506 | PTY | C31-C30-O4-C1 |
| 75 | 1B | 408 | CDL | C18-C19-C20-C21 |
| 75 | 1L | 101 | CDL | C76-C77-C78-C79 |
| 77 | e | 302 | PTY | C17-C18-C19-C20 |
| 81 | T | 502 | PGT | C20-C21-C22-C23 |
| 75 | 1E | 401 | CDL | C11-C12-C13-C14 |
| 75 | W | 701 | CDL | C19-C20-C21-C22 |
| 75 | x | 101 | CDL | C36-C37-C38-C39 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 79 | T | 503 | PC7 | C23-C24-C25-C26 |
| 75 | W | 701 | CDL | CB6-CB4-OB6-CB5 |
| 75 | R | 405 | CDL | OA7-CA5-OA6-CA4 |
| 75 | u | 602 | CDL | C74-C75-C76-C77 |
| 76 | 2I | 201 | 3PH | C1-O11-P-O12 |
| 76 | h | 201 | 3PH | C1-O11-P-O12 |
| 79 | R | 403 | PC7 | C2-C1-O3P-P |
| 75 | 1B | 408 | CDL | C37-C38-C39-C40 |
| 75 | W | 701 | CDL | C54-C55-C56-C57 |
| 75 | W | 701 | CDL | C75-C76-C77-C78 |
| 77 | T | 501 | PTY | C31-C30-O4-C1 |
| 75 | 1A | 405 | CDL | OA5-CA3-CA4-OA6 |
| 77 | 3D | 301 | PTY | O14-C5-C6-O7 |
| 77 | S | 302 | PTY | O14-C5-C6-O7 |
| 77 | V | 605 | PTY | C12-C11-C8-O7 |
| 81 | b | 601 | PGT | C11-C12-C13-C14 |
| 81 | b | 601 | PGT | C18-C19-C20-C21 |
| 77 | 3D | 301 | PTY | O30-C30-O4-C1 |
| 76 | g | 101 | 3PH | C38-C39-C3A-C3B |
| 77 | V | 605 | PTY | C39-C40-C41-C42 |
| 75 | u | 603 | CDL | C51-C52-C53-C54 |
| 76 | 1B | 406 | 3PH | O21-C2-C3-O31 |
| 77 | S | 302 | PTY | O4-C1-C6-O7 |
| 75 | 1M | 501 | CDL | C51-C52-C53-C54 |
| 76 | 1R | 201 | 3PH | C2D-C2E-C2F-C2G |
| 75 | x | 101 | CDL | OB9-CB7-OB8-CB6 |
| 77 | S | 302 | PTY | C8-C11-C12-C13 |
| 75 | 1L | 101 | CDL | C12-C13-C14-C15 |
| 75 | x | 101 | CDL | C32-C33-C34-C35 |
| 75 | x | 101 | CDL | C61-C62-C63-C64 |
| 75 | y | 202 | CDL | C12-C13-C14-C15 |
| 76 | h | 201 | 3PH | C3D-C3E-C3F-C3G |
| 91 | s | 401 | COO | P1A-O3A-P2A-O4A |
| 75 | 1M | 501 | CDL | C37-C38-C39-C40 |
| 75 | 1M | 501 | CDL | C52-C53-C54-C55 |
| 75 | y | 202 | CDL | C73-C74-C75-C76 |
| 76 | S | 301 | 3PH | C32-C33-C34-C35 |
| 75 | R | 405 | CDL | C12-C13-C14-C15 |
| 76 | S | 301 | 3PH | C38-C39-C3A-C3B |
| 76 | S | 301 | 3PH | C39-C3A-C3B-C3C |
| 75 | 1B | 408 | CDL | C12-C13-C14-C15 |
| 75 | 1L | 101 | CDL | C32-C33-C34-C35 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 75 | V | 603 | CDL | C19-C20-C21-C22 |
| 77 | 2D | 301 | PTY | C19-C20-C21-C22 |
| 75 | W | 701 | CDL | C31-CA7-OA8-CA6 |
| 77 | 1F | 403 | PTY | C31-C30-O4-C1 |
| 81 | 3A | 601 | PGT | C12-C11-O3-C3 |
| 75 | 1F | 401 | CDL | C32-C33-C34-C35 |
| 76 | 1K | 102 | 3PH | C35-C36-C37-C38 |
| 79 | Q | 302 | PC7 | C14-C15-C16-C17 |
| 76 | 1B | 407 | 3PH | C37-C38-C39-C3A |
| 75 | 1F | 401 | CDL | C71-C72-C73-C74 |
| 75 | h | 203 | CDL | C56-C57-C58-C59 |
| 75 | 1B | 408 | CDL | OA5-CA3-CA4-CA6 |
| 75 | 1E | 401 | CDL | OB5-CB3-CB4-CB6 |
| 75 | 1F | 401 | CDL | OB5-CB3-CB4-CB6 |
| 75 | 1M | 501 | CDL | OA5-CA3-CA4-CA6 |
| 75 | 1M | 501 | CDL | OB5-CB3-CB4-CB6 |
| 75 | R | 405 | CDL | OB5-CB3-CB4-CB6 |
| 75 | V | 603 | CDL | OA5-CA3-CA4-CA6 |
| 75 | y | 202 | CDL | OB5-CB3-CB4-CB6 |
| 77 | 3D | 301 | PTY | O14-C5-C6-C1 |
| 77 | R | 404 | PTY | O14-C5-C6-C1 |
| 77 | R | 406 | PTY | O14-C5-C6-C1 |
| 77 | e | 302 | PTY | O14-C5-C6-C1 |
| 75 | 1B | 405 | CDL | C81-C82-C83-C84 |
| 75 | 1B | 405 | CDL | CB7-C71-C72-C73 |
| 75 | 1L | 101 | CDL | CB5-C51-C52-C53 |
| 75 | 1K | 101 | CDL | C83-C84-C85-C86 |
| 75 | W | 701 | CDL | C40-C41-C42-C43 |
| 79 | 3A | 606 | PC7 | C32-C33-C34-C35 |
| 75 | u | 602 | CDL | C71-CB7-OB8-CB6 |
| 75 | x | 101 | CDL | C18-C19-C20-C21 |
| 76 | h | 201 | 3PH | C26-C27-C28-C29 |
| 75 | x | 101 | CDL | C56-C57-C58-C59 |
| 81 | T | 502 | PGT | C18-C19-C20-C21 |
| 75 | 1E | 401 | CDL | O1-C1-CA2-OA2 |
| 75 | V | 603 | CDL | OB7-CB5-OB6-CB4 |
| 75 | W | 701 | CDL | C52-C53-C54-C55 |
| 75 | W | 701 | CDL | C82-C83-C84-C85 |
| 76 | V | 601 | 3PH | C2B-C2C-C2D-C2E |
| 75 | 1M | 501 | CDL | C11-CA5-OA6-CA4 |
| 75 | 1K | 101 | CDL | C71-C72-C73-C74 |
| 77 | e | 302 | PTY | C39-C40-C41-C42 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 81 | l | 701 | PGT | C34-C35-C36-C37 |
| 75 | 1L | 101 | CDL | C1-CB2-OB2-PB2 |
| 75 | u | 603 | CDL | CA4-CA3-OA5-PA1 |
| 76 | 2I | 201 | 3PH | C2-C1-O11-P |
| 79 | 2A | 606 | PC7 | C2-C1-O3P-P |
| 74 | 1A | 403 | HEM | C2A-CAA-CBA-CGA |
| 75 | h | 203 | CDL | C33-C34-C35-C36 |
| 77 | h | 202 | PTY | C31-C32-C33-C34 |
| 75 | h | 203 | CDL | C77-C78-C79-C80 |
| 77 | V | 604 | PTY | C37-C38-C39-C40 |
| 75 | 1B | 405 | CDL | C71-CB7-OB8-CB6 |
| 75 | 1F | 401 | CDL | CB3-CB4-CB6-OB8 |
| 75 | 1L | 101 | CDL | CA3-CA4-CA6-OA8 |
| 75 | V | 603 | CDL | CA3-CA4-CA6-OA8 |
| 75 | h | 203 | CDL | CA3-CA4-CA6-OA8 |
| 75 | y | 202 | CDL | CB3-CB4-CB6-OB8 |
| 76 | 1R | 201 | 3PH | C1-C2-C3-O31 |
| 77 | 1F | 403 | PTY | O4-C1-C6-C5 |
| 77 | 3D | 301 | PTY | O4-C1-C6-C5 |
| 77 | R | 402 | PTY | O4-C1-C6-C5 |
| 77 | S | 302 | PTY | O4-C1-C6-C5 |
| 77 | T | 506 | PTY | O4-C1-C6-C5 |
| 77 | V | 604 | PTY | O4-C1-C6-C5 |
| 79 | T | 503 | PC7 | C1-C2-C3-O3 |
| 81 | T | 505 | PGT | C1-C2-C3-O3 |
| 75 | V | 603 | CDL | C14-C15-C16-C17 |
| 77 | S | 302 | PTY | C12-C13-C14-C15 |
| 77 | T | 501 | PTY | O30-C30-O4-C1 |
| 77 | T | 506 | PTY | O30-C30-O4-C1 |
| 76 | w | 201 | 3PH | C3C-C3D-C3E-C3F |
| 75 | W | 701 | CDL | C60-C61-C62-C63 |
| 77 | 2D | 301 | PTY | C16-C17-C18-C19 |
| 77 | V | 606 | PTY | C14-C15-C16-C17 |
| 81 | T | 505 | PGT | C14-C15-C16-C17 |
| 75 | 1K | 101 | CDL | C34-C35-C36-C37 |
| 76 | 2I | 201 | 3PH | C26-C27-C28-C29 |
| 75 | 1E | 401 | CDL | C31-C32-C33-C34 |
| 77 | 1E | 403 | PTY | C31-C32-C33-C34 |
| 79 | T | 503 | PC7 | C16-C17-C18-C19 |
| 75 | 1M | 501 | CDL | CA3-OA5-PA1-OA2 |
| 75 | x | 101 | CDL | CB3-OB5-PB2-OB2 |
| 77 | S | 302 | PTY | C5-O14-P1-O11 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 76 | 1E | 402 | 3PH | C27-C28-C29-C2A |
| 75 | 1B | 405 | CDL | C31-C32-C33-C34 |
| 75 | 1B | 408 | CDL | C17-C18-C19-C20 |
| 76 | 1B | 406 | 3PH | O11-C1-C2-O21 |
| 77 | T | 504 | PTY | O14-C5-C6-O7 |
| 79 | 1G | 301 | PC7 | O3P-C1-C2-O2 |
| 77 | 3D | 301 | PTY | C30-C31-C32-C33 |
| 79 | u | 601 | PC7 | C16-C17-C18-C19 |
| 75 | V | 603 | CDL | O1-C1-CA2-OA2 |
| 75 | u | 602 | CDL | C22-C23-C24-C25 |
| 77 | R | 404 | PTY | C23-C24-C25-C26 |
| 76 | c | 101 | 3PH | C22-C23-C24-C25 |
| 77 | S | 302 | PTY | C13-C14-C15-C16 |
| 77 | S | 302 | PTY | C38-C39-C40-C41 |
| 75 | 1F | 401 | CDL | OB6-CB4-CB6-OB8 |
| 75 | 1K | 101 | CDL | OB6-CB4-CB6-OB8 |
| 75 | y | 202 | CDL | OB6-CB4-CB6-OB8 |
| 76 | 1B | 407 | 3PH | O21-C2-C3-O31 |
| 76 | h | 201 | 3PH | O21-C2-C3-O31 |
| 77 | V | 604 | PTY | O4-C1-C6-O7 |
| 79 | 1H | 101 | PC7 | O2-C2-C3-O3 |
| 79 | R | 403 | PC7 | O2-C2-C3-O3 |
| 79 | u | 601 | PC7 | O2-C2-C3-O3 |
| 81 | T | 505 | PGT | O2-C2-C3-O3 |
| 81 | b | 601 | PGT | O2-C2-C3-O3 |
| 81 | T | 502 | PGT | O2-C31-C32-C33 |
| 79 | u | 601 | PC7 | C32-C33-C34-C35 |
| 75 | 1K | 101 | CDL | C11-CA5-OA6-CA4 |
| 75 | h | 203 | CDL | CA5-C11-C12-C13 |
| 73 | 1A | 402 | UQ5 | C24-C26-C27-C28 |
| 75 | 1K | 101 | CDL | CB2-C1-CA2-OA2 |
| 75 | R | 405 | CDL | CB2-C1-CA2-OA2 |
| 75 | u | 603 | CDL | CB2-C1-CA2-OA2 |
| 75 | 1M | 501 | CDL | C11-C12-C13-C14 |
| 77 | x | 102 | PTY | C26-C27-C28-C29 |
| 81 | l | 701 | PGT | C20-C21-C22-C23 |
| 75 | 1M | 501 | CDL | OA7-CA5-OA6-CA4 |
| 75 | u | 602 | CDL | C24-C25-C26-C27 |
| 76 | 1A | 406 | 3PH | C25-C26-C27-C28 |
| 75 | u | 602 | CDL | CA5-C11-C12-C13 |
| 75 | h | 203 | CDL | C55-C56-C57-C58 |
| 77 | V | 606 | PTY | C11-C12-C13-C14 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 75 | 1A | 405 | CDL | C51-C52-C53-C54 |
| 75 | 1B | 405 | CDL | C73-C74-C75-C76 |
| 75 | u | 602 | CDL | C51-C52-C53-C54 |
| 75 | u | 603 | CDL | C21-C22-C23-C24 |
| 75 | y | 202 | CDL | C51-C52-C53-C54 |
| 76 | 1E | 402 | 3PH | C32-C33-C34-C35 |
| 75 | 1A | 405 | CDL | C1-CA2-OA2-PA1 |
| 75 | 1A | 405 | CDL | CB4-CB3-OB5-PB2 |
| 75 | 1E | 401 | CDL | C1-CB2-OB2-PB2 |
| 75 | 1F | 401 | CDL | CB4-CB3-OB5-PB2 |
| 76 | R | 401 | 3PH | C2-C1-O11-P |
| 76 | y | 201 | 3PH | C2-C1-O11-P |
| 77 | V | 604 | PTY | C6-C5-O14-P1 |
| 75 | R | 405 | CDL | C74-C75-C76-C77 |
| 77 | 2F | 101 | PTY | C35-C36-C37-C38 |
| 77 | T | 501 | PTY | C11-C12-C13-C14 |
| 79 | 1H | 101 | PC7 | C4-C5-N-C6 |
| 75 | 1F | 401 | CDL | C31-C32-C33-C34 |
| 76 | 1B | 407 | 3PH | C2D-C2E-C2F-C2G |
| 77 | G | 303 | PTY | C37-C38-C39-C40 |
| 77 | R | 406 | PTY | C39-C40-C41-C42 |
| 75 | 1M | 501 | CDL | C34-C35-C36-C37 |
| 79 | 2A | 606 | PC7 | C32-C33-C34-C35 |
| 75 | 1F | 401 | CDL | CB7-C71-C72-C73 |
| 77 | e | 301 | PTY | C30-C31-C32-C33 |
| 75 | 1K | 101 | CDL | OA7-CA5-OA6-CA4 |
| 76 | 1B | 407 | 3PH | O22-C21-O21-C2 |
| 77 | V | 606 | PTY | C11-C8-O7-C6 |
| 75 | 1B | 405 | CDL | C75-C76-C77-C78 |
| 75 | 1A | 405 | CDL | CB7-C71-C72-C73 |
| 90 | P | 401 | NDP | PN-O3-PA-O5B |
| 75 | 1E | 401 | CDL | C71-C72-C73-C74 |
| 75 | 1E | 401 | CDL | C73-C74-C75-C76 |
| 75 | 1K | 101 | CDL | OA5-CA3-CA4-CA6 |
| 75 | u | 602 | CDL | OB5-CB3-CB4-CB6 |
| 76 | 1A | 406 | 3PH | O11-C1-C2-C3 |
| 76 | 1K | 102 | 3PH | O11-C1-C2-C3 |
| 76 | 2D | 302 | 3PH | O11-C1-C2-C3 |
| 76 | y | 201 | 3PH | O11-C1-C2-C3 |
| 77 | S | 302 | PTY | O14-C5-C6-C1 |
| 77 | T | 506 | PTY | O14-C5-C6-C1 |
| 79 | u | 601 | PC7 | O3P-C1-C2-C3 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 81 | T | 502 | PGT | O3P-C1-C2-C3 |
| 81 | T | 505 | PGT | O3P-C1-C2-C3 |
| 75 | 1L | 101 | CDL | O1-C1-CA2-OA2 |
| 75 | u | 602 | CDL | C15-C16-C17-C18 |
| 75 | x | 101 | CDL | C75-C76-C77-C78 |
| 77 | T | 501 | PTY | C33-C34-C35-C36 |
| 75 | u | 602 | CDL | C59-C60-C61-C62 |
| 89 | J | 200 | 8Q1 | C7-C8-C9-C10 |
| 75 | 1K | 101 | CDL | C31-CA7-OA8-CA6 |
| 79 | Q | 302 | PC7 | C12-C11-O3-C3 |
| 76 | 2D | 302 | 3PH | C28-C29-C2A-C2B |
| 75 | u | 602 | CDL | C20-C21-C22-C23 |
| 77 | T | 501 | PTY | C40-C41-C42-C43 |
| 89 | r | 200 | 8Q1 | C28-O27-P24-O2 |
| 75 | V | 603 | CDL | C72-C73-C74-C75 |
| 77 | x | 102 | PTY | C31-C30-O4-C1 |
| 77 | G | 303 | PTY | C32-C33-C34-C35 |
| 76 | R | 401 | 3PH | C3-C2-O21-C21 |
| 76 | w | 201 | 3PH | C3-C2-O21-C21 |
| 81 | l | 701 | PGT | C3-C2-O2-C31 |
| 75 | W | 701 | CDL | C64-C65-C66-C67 |
| 76 | c | 101 | 3PH | C29-C2A-C2B-C2C |
| 76 | g | 101 | 3PH | C32-C33-C34-C35 |
| 73 | 1A | 402 | UQ5 | C12-C11-C9-C10 |
| 75 | 1K | 101 | CDL | C31-C32-C33-C34 |
| 76 | R | 401 | 3PH | C26-C27-C28-C29 |
| 75 | h | 203 | CDL | C17-C18-C19-C20 |
| 75 | u | 602 | CDL | C58-C59-C60-C61 |
| 76 | 1A | 406 | 3PH | C27-C28-C29-C2A |
| 75 | 1B | 408 | CDL | CA4-CA3-OA5-PA1 |
| 75 | 1L | 101 | CDL | CB4-CB3-OB5-PB2 |
| 75 | 1M | 501 | CDL | CB3-CB4-CB6-OB8 |
| 75 | R | 405 | CDL | CB3-CB4-CB6-OB8 |
| 76 | 1B | 407 | 3PH | C1-C2-C3-O31 |
| 76 | h | 201 | 3PH | C1-C2-C3-O31 |
| 79 | 1H | 101 | PC7 | C1-C2-C3-O3 |
| 79 | u | 601 | PC7 | C1-C2-C3-O3 |
| 81 | b | 601 | PGT | C1-C2-C3-O3 |
| 77 | 1F | 403 | PTY | O30-C30-O4-C1 |
| 75 | 1B | 405 | CDL | OB5-CB3-CB4-OB6 |
| 75 | 1B | 408 | CDL | OA5-CA3-CA4-OA6 |
| 75 | 1E | 401 | CDL | OB5-CB3-CB4-OB6 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 75 | 1K | 101 | CDL | OB5-CB3-CB4-OB6 |
| 75 | 1M | 501 | CDL | OA5-CA3-CA4-OA6 |
| 75 | V | 603 | CDL | OA5-CA3-CA4-OA6 |
| 75 | h | 203 | CDL | OB5-CB3-CB4-OB6 |
| 76 | 1E | 402 | 3PH | O11-C1-C2-O21 |
| 76 | 1K | 102 | 3PH | O11-C1-C2-O21 |
| 76 | 3I | 201 | 3PH | O11-C1-C2-O21 |
| 76 | c | 101 | 3PH | O11-C1-C2-O21 |
| 76 | w | 201 | 3PH | O11-C1-C2-O21 |
| 77 | R | 404 | PTY | O14-C5-C6-O7 |
| 77 | T | 506 | PTY | O14-C5-C6-O7 |
| 79 | u | 601 | PC7 | O3P-C1-C2-O2 |
| 76 | w | 201 | 3PH | C29-C2A-C2B-C2C |
| 75 | 1K | 101 | CDL | OA9-CA7-OA8-CA6 |
| 75 | y | 202 | CDL | C11-C12-C13-C14 |
| 77 | V | 606 | PTY | O10-C8-O7-C6 |
| 75 | V | 603 | CDL | C12-C13-C14-C15 |
| 75 | W | 701 | CDL | OA9-CA7-OA8-CA6 |
| 81 | 3A | 601 | PGT | O11-C11-O3-C3 |
| 75 | 1L | 101 | CDL | OA6-CA4-CA6-OA8 |
| 75 | R | 405 | CDL | OB6-CB4-CB6-OB8 |
| 75 | V | 603 | CDL | OA6-CA4-CA6-OA8 |
| 75 | W | 701 | CDL | OB6-CB4-CB6-OB8 |
| 75 | h | 203 | CDL | OA6-CA4-CA6-OA8 |
| 76 | 1A | 406 | 3PH | O21-C2-C3-O31 |
| 76 | 1R | 201 | 3PH | O21-C2-C3-O31 |
| 76 | w | 201 | 3PH | O21-C2-C3-O31 |
| 77 | 1E | 403 | PTY | O4-C1-C6-O7 |
| 77 | 2F | 101 | PTY | O4-C1-C6-O7 |
| 77 | 3D | 301 | PTY | O4-C1-C6-O7 |
| 77 | R | 404 | PTY | O4-C1-C6-O7 |
| 77 | R | 406 | PTY | O4-C1-C6-O7 |
| 77 | V | 605 | PTY | O4-C1-C6-O7 |
| 77 | V | 606 | PTY | O4-C1-C6-O7 |
| 81 | l | 701 | PGT | O2-C2-C3-O3 |
| 75 | 1B | 405 | CDL | OB9-CB7-OB8-CB6 |
| 75 | u | 602 | CDL | OB9-CB7-OB8-CB6 |
| 75 | 1B | 405 | CDL | C72-C71-CB7-OB8 |
| 75 | V | 603 | CDL | C32-C31-CA7-OA8 |
| 75 | W | 701 | CDL | C44-C45-C46-C47 |
| 75 | h | 203 | CDL | C51-C52-C53-C54 |
| 75 | h | 203 | CDL | C78-C79-C80-C81 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 81 | T | 502 | PGT | O5-C5-C6-O6 |
| 75 | 1A | 405 | CDL | C31-C32-C33-C34 |
| 76 | 1K | 102 | 3PH | C28-C29-C2A-C2B |
| 77 | V | 604 | PTY | C11-C8-O7-C6 |
| 77 | x | 102 | PTY | C32-C33-C34-C35 |
| 75 | W | 701 | CDL | C71-C72-C73-C74 |
| 77 | V | 604 | PTY | O10-C8-O7-C6 |
| 77 | x | 102 | PTY | O30-C30-O4-C1 |
| 79 | Q | 302 | PC7 | O11-C11-O3-C3 |
| 75 | R | 405 | CDL | C31-CA7-OA8-CA6 |
| 75 | 1K | 101 | CDL | C37-C38-C39-C40 |
| 75 | h | 203 | CDL | C74-C75-C76-C77 |
| 75 | x | 101 | CDL | C84-C85-C86-C87 |
| 76 | R | 401 | 3PH | C25-C26-C27-C28 |
| 79 | 1G | 301 | PC7 | C12-C11-O3-C3 |
| 77 | R | 404 | PTY | C13-C14-C15-C16 |
| 77 | 3D | 301 | PTY | C3-O11-P1-O14 |
| 77 | R | 404 | PTY | C3-O11-P1-O14 |
| 77 | V | 606 | PTY | C5-O14-P1-O11 |
| 77 | e | 301 | PTY | C5-O14-P1-O11 |
| 79 | R | 403 | PC7 | C4-O4P-P-O3P |
| 75 | V | 603 | CDL | C35-C36-C37-C38 |
| 75 | W | 701 | CDL | C43-C44-C45-C46 |
| 73 | 1A | 402 | UQ5 | C20-C19-C21-C22 |
| 75 | 1M | 501 | CDL | C1-CB2-OB2-PB2 |
| 75 | V | 603 | CDL | C1-CA2-OA2-PA1 |
| 75 | W | 701 | CDL | CB4-CB3-OB5-PB2 |
| 76 | 1B | 406 | 3PH | C2-C1-O11-P |
| 77 | 2D | 301 | PTY | C6-C5-O14-P1 |
| 79 | 1H | 101 | PC7 | C2-C1-O3P-P |
| 75 | 1A | 405 | CDL | CB3-OB5-PB2-OB3 |
| 75 | 1B | 405 | CDL | CA3-OA5-PA1-OA3 |
| 75 | 1B | 405 | CDL | CB2-OB2-PB2-OB3 |
| 75 | 1B | 405 | CDL | CB3-OB5-PB2-OB4 |
| 75 | 1B | 408 | CDL | CA3-OA5-PA1-OA3 |
| 75 | 1B | 408 | CDL | CA3-OA5-PA1-OA4 |
| 75 | 1E | 401 | CDL | CB3-OB5-PB2-OB3 |
| 75 | 1E | 401 | CDL | CB3-OB5-PB2-OB4 |
| 75 | 1K | 101 | CDL | CA3-OA5-PA1-OA4 |
| 75 | 1K | 101 | CDL | CB3-OB5-PB2-OB4 |
| 75 | 1L | 101 | CDL | CA2-OA2-PA1-OA3 |
| 75 | 1M | 501 | CDL | CB3-OB5-PB2-OB4 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 75 | R | 405 | CDL | CB3-OB5-PB2-OB4 |
| 75 | V | 603 | CDL | CA2-OA2-PA1-OA4 |
| 75 | V | 603 | CDL | CA3-OA5-PA1-OA3 |
| 75 | W | 701 | CDL | CA2-OA2-PA1-OA4 |
| 75 | W | 701 | CDL | CB3-OB5-PB2-OB3 |
| 75 | h | 203 | CDL | CB3-OB5-PB2-OB4 |
| 75 | u | 602 | CDL | CB2-OB2-PB2-OB3 |
| 75 | u | 602 | CDL | CB2-OB2-PB2-OB4 |
| 75 | u | 603 | CDL | CA3-OA5-PA1-OA4 |
| 75 | u | 603 | CDL | CB2-OB2-PB2-OB3 |
| 75 | u | 603 | CDL | CB3-OB5-PB2-OB4 |
| 75 | x | 101 | CDL | CA3-OA5-PA1-OA3 |
| 75 | y | 202 | CDL | CB2-OB2-PB2-OB3 |
| 75 | y | 202 | CDL | CB2-OB2-PB2-OB4 |
| 77 | 1E | 403 | PTY | C3-O11-P1-O13 |
| 77 | 3D | 301 | PTY | C3-O11-P1-O12 |
| 77 | 3F | 101 | PTY | C3-O11-P1-O12 |
| 77 | 3F | 101 | PTY | C5-O14-P1-O12 |
| 77 | R | 402 | PTY | C5-O14-P1-O13 |
| 77 | R | 406 | PTY | C5-O14-P1-O12 |
| 77 | T | 501 | PTY | C3-O11-P1-O13 |
| 77 | T | 501 | PTY | C5-O14-P1-O12 |
| 77 | T | 506 | PTY | C3-O11-P1-O13 |
| 77 | T | 506 | PTY | C5-O14-P1-O12 |
| 77 | T | 506 | PTY | C5-O14-P1-O13 |
| 77 | V | 604 | PTY | C5-O14-P1-O13 |
| 77 | V | 605 | PTY | C3-O11-P1-O12 |
| 77 | h | 202 | PTY | C3-O11-P1-O12 |
| 79 | 1G | 301 | PC7 | C4-O4P-P-O1P |
| 79 | 1H | 101 | PC7 | C1-O3P-P-O1P |
| 79 | 1H | 101 | PC7 | C4-O4P-P-O1P |
| 79 | 2A | 606 | PC7 | C4-O4P-P-O2P |
| 79 | 3A | 606 | PC7 | C4-O4P-P-O1P |
| 81 | 3A | 601 | PGT | C1-O3P-P-O2P |
| 81 | T | 502 | PGT | C4-O4P-P-O2P |
| 81 | T | 505 | PGT | C1-O3P-P-O2P |
| 75 | 1K | 101 | CDL | CA7-C31-C32-C33 |
| 75 | 1A | 405 | CDL | OA5-CA3-CA4-CA6 |
| 75 | 1B | 405 | CDL | OA5-CA3-CA4-CA6 |
| 75 | 1B | 405 | CDL | OB5-CB3-CB4-CB6 |
| 75 | V | 603 | CDL | OB5-CB3-CB4-CB6 |
| 75 | h | 203 | CDL | OA5-CA3-CA4-CA6 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 75 | h | 203 | CDL | OB5-CB3-CB4-CB6 |
| 75 | y | 202 | CDL | OA5-CA3-CA4-CA6 |
| 76 | 1B | 406 | 3PH | O11-C1-C2-C3 |
| 76 | 1E | 402 | 3PH | O11-C1-C2-C3 |
| 76 | 1R | 201 | 3PH | O11-C1-C2-C3 |
| 76 | 3I | 201 | 3PH | O11-C1-C2-C3 |
| 77 | V | 605 | PTY | O14-C5-C6-C1 |
| 79 | 1G | 301 | PC7 | O3P-C1-C2-C3 |
| 81 | T | 502 | PGT | C35-C36-C37-C38 |
| 77 | 1F | 403 | PTY | N1-C2-C3-O11 |
| 75 | 1B | 408 | CDL | OB7-CB5-OB6-CB4 |
| 75 | 1B | 405 | CDL | C77-C78-C79-C80 |
| 76 | 1R | 201 | 3PH | C2F-C2G-C2H-C2I |
| 75 | 1E | 401 | CDL | C51-C52-C53-C54 |
| 75 | 1K | 101 | CDL | C12-C13-C14-C15 |
| 76 | w | 201 | 3PH | C3A-C3B-C3C-C3D |
| 77 | e | 302 | PTY | C18-C19-C20-C21 |
| 76 | y | 201 | 3PH | C22-C21-O21-C2 |
| 75 | W | 701 | CDL | C36-C37-C38-C39 |
| 76 | 1B | 406 | 3PH | C2E-C2F-C2G-C2H |
| 81 | T | 502 | PGT | C41-C42-C43-C44 |
| 77 | 2F | 101 | PTY | C2-C3-O11-P1 |
| 77 | S | 302 | PTY | C2-C3-O11-P1 |
| 77 | V | 606 | PTY | C2-C3-O11-P1 |
| 79 | 1G | 301 | PC7 | C5-C4-O4P-P |
| 75 | W | 701 | CDL | C31-C32-C33-C34 |
| 76 | 1B | 406 | 3PH | C2D-C2E-C2F-C2G |
| 81 | l | 701 | PGT | C38-C39-C40-C41 |
| 75 | 1L | 101 | CDL | C73-C74-C75-C76 |
| 75 | x | 101 | CDL | C58-C59-C60-C61 |
| 81 | 3A | 601 | PGT | C31-C32-C33-C34 |
| 81 | b | 601 | PGT | O4P-C4-C5-C6 |
| 75 | 1K | 101 | CDL | C80-C81-C82-C83 |
| 76 | S | 301 | 3PH | C22-C23-C24-C25 |
| 75 | 1B | 405 | CDL | OA5-CA3-CA4-OA6 |
| 75 | 1K | 101 | CDL | OA5-CA3-CA4-OA6 |
| 75 | V | 603 | CDL | OB5-CB3-CB4-OB6 |
| 75 | u | 602 | CDL | OB5-CB3-CB4-OB6 |
| 75 | u | 603 | CDL | OB5-CB3-CB4-OB6 |
| 75 | x | 101 | CDL | CA7-C31-C32-C33 |
| 75 | y | 202 | CDL | OB5-CB3-CB4-OB6 |
| 76 | 1A | 406 | 3PH | O11-C1-C2-O21 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 76 | 1B | 406 | 3PH | C31-C32-C33-C34 |
| 76 | 1R | 201 | 3PH | O11-C1-C2-O21 |
| 76 | 2D | 302 | 3PH | O11-C1-C2-O21 |
| 76 | V | 601 | 3PH | O11-C1-C2-O21 |
| 81 | T | 502 | PGT | O3P-C1-C2-O2 |
| 87 | B | 501 | FMN | N10-C1'-C2'-O2' |
| 79 | R | 403 | PC7 | C12-C13-C14-C15 |
| 81 | b | 601 | PGT | C40-C41-C42-C43 |
| 75 | x | 101 | CDL | C78-C79-C80-C81 |
| 76 | 1B | 407 | 3PH | C39-C3A-C3B-C3C |
| 77 | V | 606 | PTY | C32-C33-C34-C35 |
| 75 | W | 701 | CDL | O1-C1-CA2-OA2 |
| 79 | 2A | 606 | PC7 | C4-C5-N-C6 |
| 75 | x | 101 | CDL | C82-C83-C84-C85 |
| 75 | 1A | 405 | CDL | CB3-CB4-CB6-OB8 |
| 77 | R | 406 | PTY | O4-C1-C6-C5 |
| 77 | V | 605 | PTY | O4-C1-C6-C5 |
| 79 | 1G | 301 | PC7 | O4P-C4-C5-N |
| 75 | 1A | 405 | CDL | OB6-CB4-CB6-OB8 |
| 75 | 1B | 405 | CDL | OB6-CB4-CB6-OB8 |
| 75 | 1E | 401 | CDL | OA6-CA4-CA6-OA8 |
| 75 | 1K | 101 | CDL | OA6-CA4-CA6-OA8 |
| 75 | h | 203 | CDL | OB6-CB4-CB6-OB8 |
| 75 | u | 603 | CDL | OA6-CA4-CA6-OA8 |
| 77 | 1F | 403 | PTY | O4-C1-C6-O7 |
| 77 | 3F | 101 | PTY | O4-C1-C6-O7 |
| 77 | S | 302 | PTY | C15-C16-C17-C18 |
| 77 | V | 604 | PTY | C11-C12-C13-C14 |
| 75 | R | 405 | CDL | OA9-CA7-OA8-CA6 |
| 75 | u | 602 | CDL | C17-C18-C19-C20 |
| 75 | x | 101 | CDL | C52-C53-C54-C55 |
| 76 | y | 201 | 3PH | C38-C39-C3A-C3B |
| 77 | h | 202 | PTY | C36-C37-C38-C39 |
| 76 | 1K | 102 | 3PH | C3A-C3B-C3C-C3D |
| 76 | g | 101 | 3PH | C39-C3A-C3B-C3C |
| 77 | h | 202 | PTY | C33-C34-C35-C36 |
| 81 | b | 601 | PGT | C38-C39-C40-C41 |
| 75 | 1B | 408 | CDL | C34-C35-C36-C37 |
| 77 | V | 605 | PTY | C34-C35-C36-C37 |
| 79 | 1G | 301 | PC7 | O11-C11-O3-C3 |
| 77 | e | 302 | PTY | C33-C34-C35-C36 |
| 75 | y | 202 | CDL | C15-C16-C17-C18 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 76 | V | 601 | 3PH | C29-C2A-C2B-C2C |
| 77 | e | 302 | PTY | C40-C41-C42-C43 |
| 77 | V | 606 | PTY | C15-C16-C17-C18 |
| 79 | 2A | 606 | PC7 | C4-C5-N-C8 |
| 75 | 1K | 101 | CDL | C77-C78-C79-C80 |
| 76 | 2I | 201 | 3PH | C33-C34-C35-C36 |
| 77 | S | 302 | PTY | C17-C18-C19-C20 |
| 77 | 1F | 403 | PTY | C32-C33-C34-C35 |
| 81 | b | 601 | PGT | C32-C31-O2-C2 |
| 77 | 3D | 301 | PTY | C8-C11-C12-C13 |
| 91 | s | 401 | COO | C2X-C3X-O3X-P3X |
| 75 | u | 603 | CDL | C32-C33-C34-C35 |
| 77 | V | 606 | PTY | C36-C37-C38-C39 |
| 75 | x | 101 | CDL | C17-C18-C19-C20 |
| 75 | 1B | 405 | CDL | CB6-CB4-OB6-CB5 |
| 75 | 1L | 101 | CDL | CB6-CB4-OB6-CB5 |
| 75 | R | 405 | CDL | CB6-CB4-OB6-CB5 |
| 75 | u | 602 | CDL | CB6-CB4-OB6-CB5 |
| 76 | V | 602 | 3PH | C1-C2-O21-C21 |
| 77 | R | 404 | PTY | C1-C6-O7-C8 |
| 77 | T | 501 | PTY | C1-C6-O7-C8 |
| 75 | 1K | 101 | CDL | OB5-CB3-CB4-CB6 |
| 81 | l | 701 | PGT | C21-C22-C23-C24 |
| 76 | y | 201 | 3PH | O22-C21-O21-C2 |
| 82 | 2A | 603 | HEA | C11-C12-C13-C14 |
| 76 | 1E | 402 | 3PH | C23-C24-C25-C26 |
| 75 | 1B | 405 | CDL | C1-CA2-OA2-PA1 |
| 89 | r | 200 | 8Q1 | C28-O27-P24-O3 |
| 79 | u | 601 | PC7 | C38-C39-C40-C41 |
| 76 | 3D | 302 | 3PH | O11-C1-C2-O21 |
| 81 | T | 505 | PGT | O3P-C1-C2-O2 |
| 79 | 2A | 606 | PC7 | C4-C5-N-C7 |
| 73 | 1A | 402 | UQ5 | C12-C11-C9-C8 |
| 81 | b | 601 | PGT | O31-C31-O2-C2 |
| 76 | 2I | 201 | 3PH | C31-C32-C33-C34 |
| 75 | 1B | 408 | CDL | C31-C32-C33-C34 |
| 75 | W | 701 | CDL | C84-C85-C86-C87 |
| 76 | 3I | 201 | 3PH | C2A-C2B-C2C-C2D |
| 76 | h | 201 | 3PH | C3A-C3B-C3C-C3D |
| 82 | 2A | 602 | HEA | C2A-CAA-CBA-CGA |
| 75 | 1B | 408 | CDL | C51-CB5-OB6-CB4 |
| 75 | x | 101 | CDL | OA6-CA4-CA6-OA8 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 81 | 2A | 601 | PGT | O2-C2-C3-O3 |
| 76 | 3D | 302 | 3PH | C27-C28-C29-C2A |
| 77 | V | 604 | PTY | C32-C33-C34-C35 |
| 75 | 1B | 405 | CDL | CA2-OA2-PA1-OA5 |
| 75 | 1B | 408 | CDL | CB2-OB2-PB2-OB5 |
| 75 | 1E | 401 | CDL | CA3-OA5-PA1-OA2 |
| 75 | u | 602 | CDL | CB3-OB5-PB2-OB2 |
| 75 | y | 202 | CDL | CB3-OB5-PB2-OB2 |
| 77 | 2D | 301 | PTY | C3-O11-P1-O14 |
| 77 | G | 303 | PTY | C3-O11-P1-O14 |
| 77 | R | 406 | PTY | C3-O11-P1-O14 |
| 77 | T | 504 | PTY | C3-O11-P1-O14 |
| 77 | V | 606 | PTY | C3-O11-P1-O14 |
| 77 | e | 302 | PTY | C3-O11-P1-O14 |
| 77 | x | 102 | PTY | C3-O11-P1-O14 |
| 79 | 1G | 301 | PC7 | C1-O3P-P-O4P |
| 79 | Q | 302 | PC7 | C1-O3P-P-O4P |
| 79 | T | 503 | PC7 | C4-O4P-P-O3P |
| 81 | 3A | 601 | PGT | C1-O3P-P-O4P |
| 81 | b | 601 | PGT | C4-O4P-P-O3P |
| 75 | 1A | 405 | CDL | C36-C37-C38-C39 |
| 75 | R | 405 | CDL | C52-C53-C54-C55 |
| 76 | V | 601 | 3PH | C2D-C2E-C2F-C2G |
| 75 | W | 701 | CDL | CB3-CB4-CB6-OB8 |
| 79 | R | 403 | PC7 | C1-C2-C3-O3 |
| 76 | 1B | 406 | 3PH | C25-C26-C27-C28 |
| 76 | V | 601 | 3PH | C23-C24-C25-C26 |
| 76 | 1B | 407 | 3PH | C2C-C2D-C2E-C2F |
| 90 | P | 401 | NDP | O4D-C1D-N1N-C6N |
| 75 | x | 101 | CDL | CA5-C11-C12-C13 |
| 76 | V | 601 | 3PH | C33-C34-C35-C36 |
| 91 | s | 401 | COO | P1A-O3A-P2A-O5A |
| 77 | 2D | 301 | PTY | C13-C14-C15-C16 |
| 77 | R | 406 | PTY | C35-C36-C37-C38 |
| 76 | 2I | 201 | 3PH | C32-C33-C34-C35 |
| 77 | 1E | 403 | PTY | C35-C36-C37-C38 |
| 75 | 1B | 405 | CDL | C80-C81-C82-C83 |
| 75 | u | 603 | CDL | C17-C18-C19-C20 |
| 89 | J | 200 | 8Q1 | C11-C12-C13-C14 |
| 75 | u | 602 | CDL | CA4-CA3-OA5-PA1 |
| 76 | S | 301 | 3PH | C2-C1-O11-P |
| 79 | 1G | 301 | PC7 | C2-C1-O3P-P |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 75 | 1B | 405 | CDL | CA2-C1-CB2-OB2 |
| 75 | 1E | 401 | CDL | CB2-C1-CA2-OA2 |
| 75 | 1L | 101 | CDL | CB2-C1-CA2-OA2 |
| 75 | x | 101 | CDL | C14-C15-C16-C17 |
| 76 | V | 602 | 3PH | C33-C34-C35-C36 |
| 81 | l | 701 | PGT | C37-C38-C39-C40 |
| 75 | u | 602 | CDL | CA7-C31-C32-C33 |
| 90 | P | 401 | NDP | C2D-C1D-N1N-C6N |
| 77 | G | 303 | PTY | C33-C34-C35-C36 |
| 77 | x | 102 | PTY | C31-C32-C33-C34 |
| 75 | 1M | 501 | CDL | C36-C37-C38-C39 |
| 77 | R | 404 | PTY | C22-C23-C24-C25 |
| 79 | 1H | 101 | PC7 | C4-C5-N-C7 |
| 77 | x | 102 | PTY | C40-C41-C42-C43 |
| 75 | 1L | 101 | CDL | OB5-CB3-CB4-OB6 |
| 75 | W | 701 | CDL | C42-C43-C44-C45 |
| 76 | 1A | 406 | 3PH | C28-C29-C2A-C2B |
| 77 | h | 202 | PTY | C8-C11-C12-C13 |
| 76 | V | 601 | 3PH | C34-C35-C36-C37 |
| 76 | 3I | 201 | 3PH | C22-C23-C24-C25 |
| 77 | V | 605 | PTY | C17-C18-C19-C20 |
| 91 | s | 401 | COO | O2-C1-C13-C11 |
| 76 | R | 401 | 3PH | C37-C38-C39-C3A |
| 81 | 2A | 601 | PGT | O31-C31-O2-C2 |
| 77 | x | 102 | PTY | C38-C39-C40-C41 |
| 75 | y | 202 | CDL | C32-C33-C34-C35 |
| 75 | 1E | 401 | CDL | C72-C73-C74-C75 |
| 77 | h | 202 | PTY | C41-C42-C43-C44 |
| 77 | e | 301 | PTY | O4-C1-C6-O7 |
| 79 | 1G | 301 | PC7 | O2-C2-C3-O3 |
| 75 | R | 405 | CDL | C1-CB2-OB2-PB2 |
| 77 | 3D | 301 | PTY | C6-C5-O14-P1 |
| 77 | V | 605 | PTY | C12-C11-C8-O10 |
| 77 | 1F | 403 | PTY | C35-C36-C37-C38 |
| 77 | e | 302 | PTY | C14-C15-C16-C17 |
| 75 | 1L | 101 | CDL | C13-C14-C15-C16 |
| 75 | 1K | 101 | CDL | C79-C80-C81-C82 |
| 75 | x | 101 | CDL | C71-C72-C73-C74 |
| 75 | 1L | 101 | CDL | C31-C32-C33-C34 |
| 76 | 2D | 302 | 3PH | C35-C36-C37-C38 |
| 90 | P | 401 | NDP | C3D-C4D-C5D-O5D |
| 77 | R | 402 | PTY | C11-C12-C13-C14 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 76 | V | 602 | 3PH | C1-C2-C3-O31 |
| 76 | w | 201 | 3PH | C1-C2-C3-O31 |
| 77 | x | 102 | PTY | O4-C1-C6-C5 |
| 75 | V | 603 | CDL | C17-C18-C19-C20 |
| 79 | u | 601 | PC7 | C35-C36-C37-C38 |
| 77 | V | 606 | PTY | C16-C17-C18-C19 |
| 77 | h | 202 | PTY | C38-C39-C40-C41 |
| 75 | W | 701 | CDL | CA7-C31-C32-C33 |
| 75 | 1B | 408 | CDL | C15-C16-C17-C18 |
| 81 | b | 601 | PGT | C34-C35-C36-C37 |
| 91 | s | 401 | COO | N1-C1-C13-C11 |
| 79 | 3A | 606 | PC7 | C1-C2-O2-C31 |
| 77 | 3D | 301 | PTY | C18-C19-C20-C21 |
| 79 | 1H | 101 | PC7 | C4-C5-N-C8 |
| 75 | h | 203 | CDL | C72-C71-CB7-OB8 |
| 74 | 1A | 404 | HEM | CAD-CBD-CGD-O1D |
| 76 | y | 201 | 3PH | C32-C33-C34-C35 |
| 75 | 1B | 408 | CDL | CB3-OB5-PB2-OB2 |
| 77 | R | 406 | PTY | C32-C33-C34-C35 |
| 75 | 1B | 405 | CDL | C1-CB2-OB2-PB2 |
| 75 | 1E | 401 | CDL | CB4-CB3-OB5-PB2 |
| 81 | l | 701 | PGT | O5-C5-C6-O6 |
| 75 | 1B | 408 | CDL | C56-C57-C58-C59 |
| 76 | 1A | 406 | 3PH | C26-C27-C28-C29 |
| 75 | y | 202 | CDL | CA5-C11-C12-C13 |
| 81 | 2A | 601 | PGT | O3P-C1-C2-O2 |
| 75 | 1B | 405 | CDL | C71-C72-C73-C74 |
| 76 | 1B | 407 | 3PH | C28-C29-C2A-C2B |
| 89 | J | 200 | 8Q1 | C13-C14-C15-C16 |
| 76 | w | 201 | 3PH | C22-C23-C24-C25 |
| 81 | 2A | 601 | PGT | C32-C31-O2-C2 |
| 76 | 2I | 201 | 3PH | C34-C35-C36-C37 |
| 73 | 1B | 402 | UQ5 | C12-C11-C9-C10 |
| 79 | u | 601 | PC7 | C37-C38-C39-C40 |
| 74 | 1B | 404 | HEM | CAA-CBA-CGA-O1A |
| 76 | 1K | 102 | 3PH | O21-C2-C3-O31 |
| 75 | h | 203 | CDL | C13-C14-C15-C16 |
| 76 | 1B | 407 | 3PH | C27-C28-C29-C2A |
| 77 | 1E | 403 | PTY | C11-C12-C13-C14 |
| 79 | R | 403 | PC7 | C36-C37-C38-C39 |
| 75 | h | 203 | CDL | C54-C55-C56-C57 |
| 76 | c | 101 | 3PH | C34-C35-C36-C37 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 73 | Q | 301 | UQ5 | C14-C16-C17-C18 |
| 74 | 1B | 404 | HEM | CAA-CBA-CGA-O2A |
| 77 | T | 506 | PTY | C14-C15-C16-C17 |
| 75 | u | 602 | CDL | C72-C71-CB7-OB8 |
| 89 | r | 200 | 8Q1 | C6-C7-C8-C9 |
| 77 | V | 606 | PTY | C31-C32-C33-C34 |
| 75 | 1B | 408 | CDL | C54-C55-C56-C57 |
| 75 | W | 701 | CDL | C55-C56-C57-C58 |
| 75 | 1E | 401 | CDL | CA3-CA4-CA6-OA8 |
| 77 | V | 606 | PTY | O4-C1-C6-C5 |
| 75 | 1B | 408 | CDL | CB7-C71-C72-C73 |
| 75 | 1K | 101 | CDL | CA5-C11-C12-C13 |
| 82 | 2A | 602 | HEA | CAA-CBA-CGA-O2A |
| 77 | T | 504 | PTY | C33-C34-C35-C36 |
| 89 | J | 200 | 8Q1 | O4-C1-S44-C43 |
| 76 | g | 101 | 3PH | C24-C25-C26-C27 |
| 74 | 1A | 404 | HEM | CAA-CBA-CGA-O2A |
| 76 | V | 602 | 3PH | C3A-C3B-C3C-C3D |
| 75 | h | 203 | CDL | OA5-CA3-CA4-OA6 |
| 77 | V | 605 | PTY | O14-C5-C6-O7 |
| 76 | V | 602 | 3PH | C23-C24-C25-C26 |
| 74 | 1A | 404 | HEM | CAA-CBA-CGA-O1A |
| 75 | u | 603 | CDL | C43-C44-C45-C46 |
| 76 | w | 201 | 3PH | C35-C36-C37-C38 |
| 75 | R | 405 | CDL | C33-C34-C35-C36 |
| 81 | 2A | 601 | PGT | C15-C16-C17-C18 |
| 77 | 2F | 101 | PTY | O14-C5-C6-C1 |
| 77 | T | 504 | PTY | O14-C5-C6-C1 |
| 82 | 2A | 602 | HEA | C26-C15-C16-C17 |
| 73 | 1A | 402 | UQ5 | C18-C19-C21-C22 |
| 74 | 1B | 403 | HEM | CAD-CBD-CGD-O2D |
| 75 | x | 101 | CDL | C35-C36-C37-C38 |
| 81 | 3A | 601 | PGT | O5-C5-C6-O6 |
| 81 | l | 701 | PGT | C33-C34-C35-C36 |
| 77 | h | 202 | PTY | O4-C1-C6-O7 |
| 76 | 1B | 406 | 3PH | C2C-C2D-C2E-C2F |
| 74 | 1B | 403 | HEM | CAD-CBD-CGD-O1D |
| 76 | 1E | 402 | 3PH | O21-C21-C22-C23 |
| 77 | 2D | 301 | PTY | C12-C11-C8-O7 |
| 76 | 1R | 201 | 3PH | C1-O11-P-O13 |
| 76 | 2D | 302 | 3PH | C24-C25-C26-C27 |
| 91 | s | 401 | COO | C3X-O3X-P3X-O9A |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 77 | e | 302 | PTY | C12-C11-C8-O7 |
| 76 | w | 201 | 3PH | C34-C35-C36-C37 |
| 82 | 3A | 602 | HEA | C26-C15-C16-C17 |
| 73 | 1B | 402 | UQ5 | C12-C11-C9-C8 |
| 79 | R | 403 | PC7 | C44-C45-C46-C47 |
| 77 | 1F | 403 | PTY | O4-C30-C31-C32 |
| 79 | 3A | 606 | PC7 | O2-C31-C32-C33 |
| 75 | 1B | 408 | CDL | C14-C15-C16-C17 |
| 76 | h | 201 | 3PH | C24-C25-C26-C27 |
| 76 | w | 201 | 3PH | C2B-C2C-C2D-C2E |
| 75 | 1K | 101 | CDL | C53-C54-C55-C56 |
| 75 | x | 101 | CDL | C33-C34-C35-C36 |
| 75 | 1F | 401 | CDL | O1-C1-CA2-OA2 |
| 75 | u | 603 | CDL | C12-C11-CA5-OA6 |
| 79 | 3A | 606 | PC7 | O3-C11-C12-C13 |
| 75 | 1E | 401 | CDL | CB3-CB4-OB6-CB5 |
| 75 | 1E | 401 | CDL | CB6-CB4-OB6-CB5 |
| 75 | 1B | 408 | CDL | CA5-C11-C12-C13 |
| 73 | Q | 301 | UQ5 | C11-C12-C13-C14 |
| 89 | J | 200 | 8Q1 | C9-C10-C11-C12 |
| 77 | T | 506 | PTY | O10-C8-O7-C6 |
| 79 | T | 503 | PC7 | C37-C38-C39-C40 |
| 74 | 1A | 403 | HEM | CAD-CBD-CGD-O2D |
| 82 | 2A | 602 | HEA | CAD-CBD-CGD-O2D |
| 76 | S | 301 | 3PH | C27-C28-C29-C2A |
| 75 | x | 101 | CDL | C52-C51-CB5-OB6 |
| 75 | x | 101 | CDL | C72-C71-CB7-OB8 |
| 76 | 1K | 102 | 3PH | O21-C21-C22-C23 |
| 76 | w | 201 | 3PH | C32-C33-C34-C35 |
| 77 | 1F | 403 | PTY | C17-C18-C19-C20 |
| 77 | S | 302 | PTY | C12-C11-C8-O7 |
| 77 | 2F | 101 | PTY | C11-C12-C13-C14 |
| 73 | Q | 301 | UQ5 | C5-C4-O4-C4M |
| 76 | R | 401 | 3PH | C1-O11-P-O12 |
| 76 | V | 601 | 3PH | C1-O11-P-O12 |
| 77 | 2F | 101 | PTY | O4-C1-C6-C5 |
| 81 | l | 701 | PGT | C1-C2-C3-O3 |
| 82 | 2A | 602 | HEA | CAA-CBA-CGA-O1A |
| 79 | 3A | 606 | PC7 | O3P-C1-C2-O2 |
| 74 | 1A | 404 | HEM | CAD-CBD-CGD-O2D |
| 82 | 2A | 602 | HEA | CAD-CBD-CGD-O1D |
| 82 | 3A | 602 | HEA | CAD-CBD-CGD-O1D |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 82 | 3A | 602 | HEA | CAD-CBD-CGD-O2D |
| 77 | R | 406 | PTY | C16-C17-C18-C19 |
| 77 | h | 202 | PTY | O4-C30-C31-C32 |
| 76 | V | 601 | 3PH | C2A-C2B-C2C-C2D |
| 81 | l | 701 | PGT | C35-C36-C37-C38 |
| 74 | 1A | 403 | HEM | CAD-CBD-CGD-O1D |
| 75 | 1E | 401 | CDL | C72-C71-CB7-OB8 |
| 75 | x | 101 | CDL | C76-C77-C78-C79 |
| 77 | 2D | 301 | PTY | C15-C16-C17-C18 |
| 75 | 1L | 101 | CDL | OB5-CB3-CB4-CB6 |
| 75 | u | 603 | CDL | OB5-CB3-CB4-CB6 |
| 77 | 1E | 403 | PTY | O14-C5-C6-C1 |
| 81 | 2A | 601 | PGT | O3P-C1-C2-C3 |
| 75 | 1K | 101 | CDL | C52-C51-CB5-OB6 |
| 75 | R | 405 | CDL | C72-C71-CB7-OB8 |
| 76 | 2D | 302 | 3PH | O21-C21-C22-C23 |
| 79 | 1G | 301 | PC7 | O3-C11-C12-C13 |
| 79 | 3A | 606 | PC7 | C4-C5-N-C7 |
| 91 | s | 401 | COO | C3X-O3X-P3X-O8A |
| 76 | w | 201 | 3PH | C39-C3A-C3B-C3C |
| 75 | 1K | 101 | CDL | C12-C11-CA5-OA6 |
| 73 | 1A | 401 | UQ5 | C12-C11-C9-C10 |
| 77 | R | 404 | PTY | C17-C18-C19-C20 |
| 81 | T | 502 | PGT | C31-C32-C33-C34 |
| 77 | h | 202 | PTY | C14-C15-C16-C17 |
| 77 | x | 102 | PTY | C21-C22-C23-C24 |
| 75 | u | 603 | CDL | C52-C51-CB5-OB6 |
| 75 | x | 101 | CDL | C81-C82-C83-C84 |
| 77 | e | 302 | PTY | C12-C11-C8-O10 |
| 76 | V | 601 | 3PH | C27-C28-C29-C2A |
| 75 | 1B | 405 | CDL | C12-C11-CA5-OA6 |
| 77 | 2D | 301 | PTY | C12-C11-C8-O10 |
| 81 | T | 502 | PGT | O31-C31-C32-C33 |
| 77 | T | 506 | PTY | C11-C8-O7-C6 |
| 82 | 3A | 602 | HEA | CAA-CBA-CGA-O2A |
| 77 | S | 302 | PTY | C12-C11-C8-O10 |
| 76 | 3I | 201 | 3PH | C38-C39-C3A-C3B |
| 76 | g | 101 | 3PH | C23-C24-C25-C26 |
| 75 | 1F | 401 | CDL | C72-C71-CB7-OB8 |
| 75 | u | 602 | CDL | C32-C33-C34-C35 |
| 79 | 3A | 606 | PC7 | C4-C5-N-C6 |
| 76 | 3I | 201 | 3PH | C35-C36-C37-C38 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 76 | 1E | 402 | 3PH | O22-C21-C22-C23 |
| 79 | 3A | 606 | PC7 | O31-C31-C32-C33 |
| 75 | V | 603 | CDL | CA2-C1-CB2-OB2 |
| 76 | V | 602 | 3PH | C35-C36-C37-C38 |
| 76 | 1R | 201 | 3PH | C28-C29-C2A-C2B |
| 76 | 2D | 302 | 3PH | C25-C26-C27-C28 |
| 73 | 1B | 402 | UQ5 | C11-C12-C13-C14 |
| 89 | J | 200 | 8Q1 | C6-C7-C8-C9 |
| 75 | x | 101 | CDL | C52-C51-CB5-OB7 |
| 77 | h | 202 | PTY | O30-C30-C31-C32 |
| 75 | u | 603 | CDL | CA3-CA4-CA6-OA8 |
| 77 | e | 301 | PTY | O4-C1-C6-C5 |
| 79 | R | 403 | PC7 | C16-C17-C18-C19 |
| 75 | R | 405 | CDL | CB3-OB5-PB2-OB2 |
| 75 | V | 603 | CDL | CA2-OA2-PA1-OA5 |
| 75 | x | 101 | CDL | CB2-OB2-PB2-OB5 |
| 81 | l | 701 | PGT | O4P-C4-C5-O5 |
| 75 | 1B | 405 | CDL | C12-C11-CA5-OA7 |
| 77 | 1F | 403 | PTY | O30-C30-C31-C32 |
| 75 | R | 405 | CDL | C34-C35-C36-C37 |
| 75 | W | 701 | CDL | C41-C42-C43-C44 |
| 76 | V | 602 | 3PH | C32-C33-C34-C35 |
| 75 | 1A | 405 | CDL | CA4-CA3-OA5-PA1 |
| 76 | 2I | 201 | 3PH | C36-C37-C38-C39 |
| 75 | 1K | 101 | CDL | C52-C51-CB5-OB7 |
| 75 | 1B | 408 | CDL | CB3-OB5-PB2-OB3 |
| 75 | 1M | 501 | CDL | CA3-OA5-PA1-OA3 |
| 75 | V | 603 | CDL | CA3-OA5-PA1-OA4 |
| 75 | u | 602 | CDL | CB3-OB5-PB2-OB3 |
| 75 | x | 101 | CDL | CB2-OB2-PB2-OB4 |
| 75 | x | 101 | CDL | CB3-OB5-PB2-OB3 |
| 75 | y | 202 | CDL | CB3-OB5-PB2-OB3 |
| 77 | 2D | 301 | PTY | C3-O11-P1-O13 |
| 77 | R | 406 | PTY | C3-O11-P1-O13 |
| 81 | T | 505 | PGT | C4-O4P-P-O1P |
| 81 | b | 601 | PGT | C4-O4P-P-O2P |
| 81 | l | 701 | PGT | C4-O4P-P-O2P |
| 75 | 1E | 401 | CDL | C72-C71-CB7-OB9 |
| 75 | u | 603 | CDL | C52-C51-CB5-OB7 |
| 75 | x | 101 | CDL | C72-C71-CB7-OB9 |
| 76 | 1K | 102 | 3PH | O22-C21-C22-C23 |
| 75 | 1K | 101 | CDL | C32-C31-CA7-OA8 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 82 | 2A | 602 | HEA | C19-C20-C21-C22 |
| 76 | V | 602 | 3PH | C25-C26-C27-C28 |
| 76 | 2D | 302 | 3PH | O22-C21-C22-C23 |
| 79 | 3A | 606 | PC7 | O11-C11-C12-C13 |
| 76 | c | 101 | 3PH | C37-C38-C39-C3A |
| 77 | 1F | 403 | PTY | C15-C16-C17-C18 |
| 75 | 1E | 401 | CDL | C52-C51-CB5-OB6 |
| 76 | c | 101 | 3PH | C2D-C2E-C2F-C2G |
| 79 | R | 403 | PC7 | C13-C14-C15-C16 |
| 75 | 1B | 405 | CDL | C82-C83-C84-C85 |
| 81 | b | 601 | PGT | C31-C32-C33-C34 |
| 76 | w | 201 | 3PH | C36-C37-C38-C39 |
| 77 | 1F | 403 | PTY | C2-C3-O11-P1 |
| 77 | h | 202 | PTY | C2-C3-O11-P1 |
| 79 | 3A | 606 | PC7 | C5-C4-O4P-P |
| 82 | 3A | 602 | HEA | C3B-C11-C12-C13 |
| 75 | u | 603 | CDL | C35-C36-C37-C38 |
| 75 | 1A | 405 | CDL | C32-C31-CA7-OA8 |
| 77 | V | 606 | PTY | C33-C34-C35-C36 |
| 82 | 3A | 602 | HEA | CAA-CBA-CGA-O1A |
| 79 | 1G | 301 | PC7 | O11-C11-C12-C13 |
| 75 | h | 203 | CDL | C12-C11-CA5-OA6 |
| 77 | 1E | 403 | PTY | C12-C11-C8-O7 |
| 75 | 1A | 405 | CDL | C35-C36-C37-C38 |
| 76 | 1B | 406 | 3PH | C2B-C2C-C2D-C2E |
| 74 | 1B | 404 | HEM | CAD-CBD-CGD-O1D |
| 75 | R | 405 | CDL | C35-C36-C37-C38 |
| 75 | h | 203 | CDL | C52-C51-CB5-OB6 |
| 77 | V | 605 | PTY | O4-C30-C31-C32 |
| 77 | x | 102 | PTY | C23-C24-C25-C26 |
| 77 | 1E | 403 | PTY | O14-C5-C6-O7 |
| 77 | 2D | 301 | PTY | O14-C5-C6-O7 |
| 77 | 2F | 101 | PTY | O14-C5-C6-O7 |
| 75 | 1F | 401 | CDL | C72-C71-CB7-OB9 |
| 75 | 1K | 101 | CDL | C12-C11-CA5-OA7 |
| 75 | x | 101 | CDL | C12-C11-CA5-OA7 |
| 75 | x | 101 | CDL | C12-C11-CA5-OA6 |
| 75 | h | 203 | CDL | C52-C51-CB5-OB7 |
| 75 | u | 603 | CDL | O1-C1-CA2-OA2 |
| 76 | 1B | 407 | 3PH | C34-C35-C36-C37 |
| 76 | V | 601 | 3PH | C2F-C2G-C2H-C2I |
| 75 | 1K | 101 | CDL | C32-C31-CA7-OA9 |

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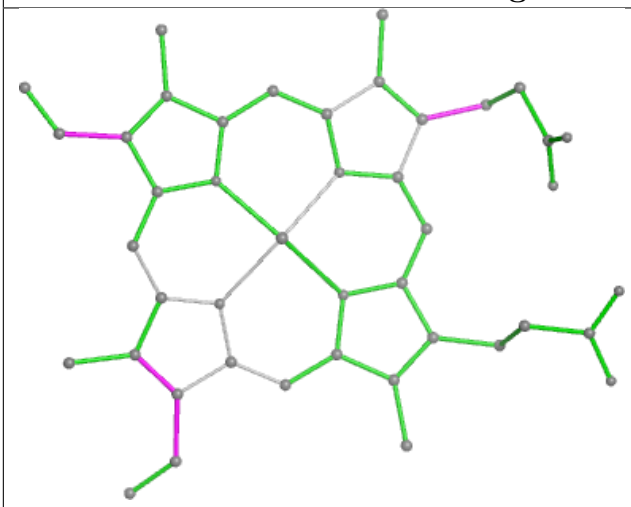
| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 75 | R | 405 | CDL | C72-C71-CB7-OB9 |
| 76 | 1B | 407 | 3PH | C26-C27-C28-C29 |
| 77 | h | 202 | PTY | C37-C38-C39-C40 |

There are no ring outliers.

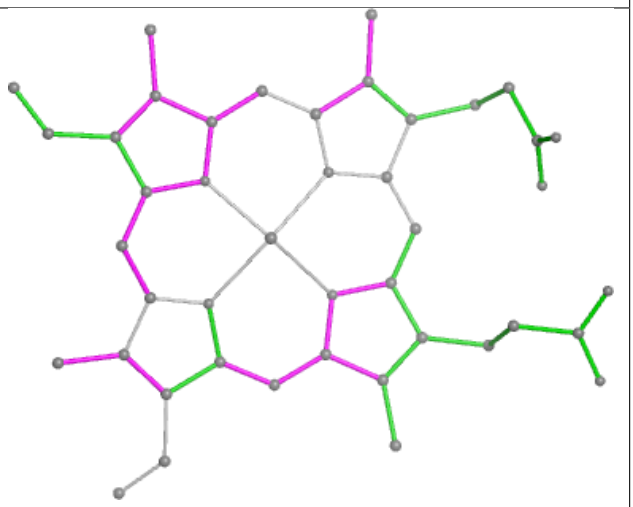
No monomer is involved in short contacts.

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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

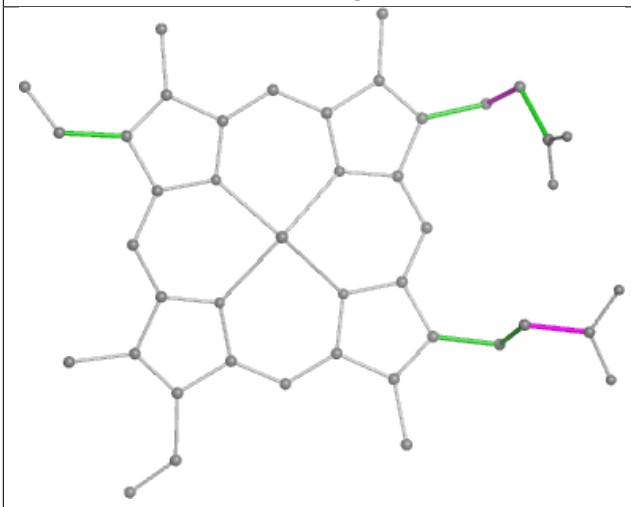
**Ligand HEM 1A 403**



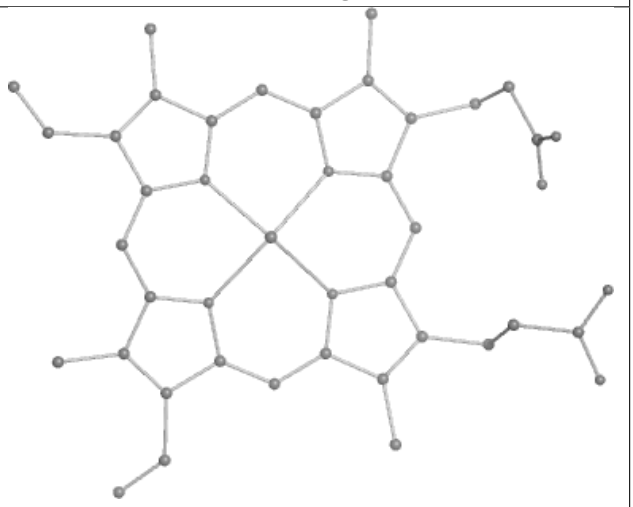
**Bond lengths**



**Bond angles**

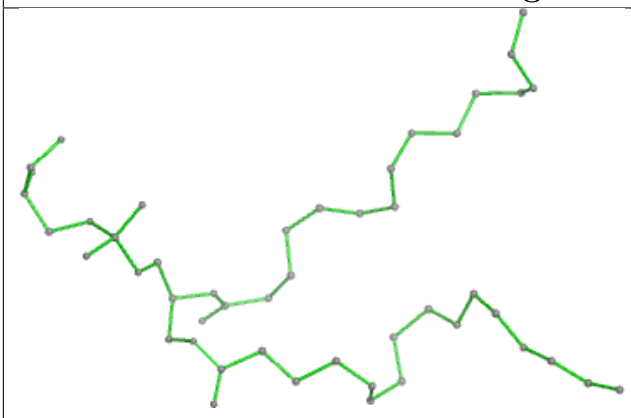


**Torsions**

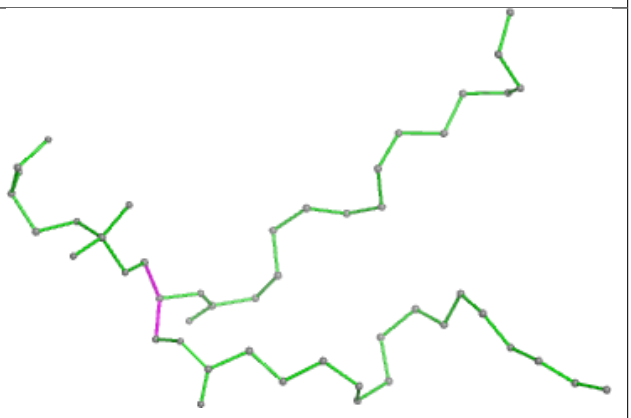


**Rings**

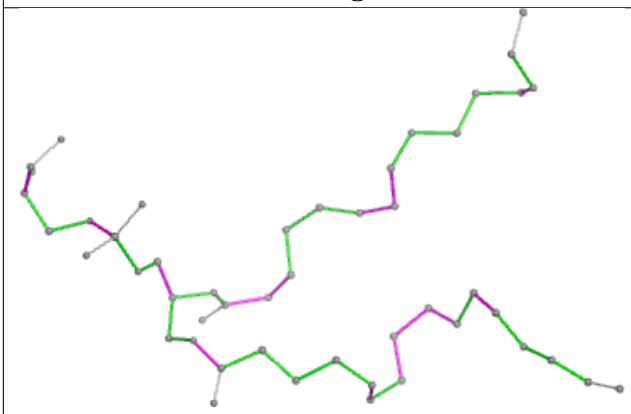
## Ligand PGT T 502



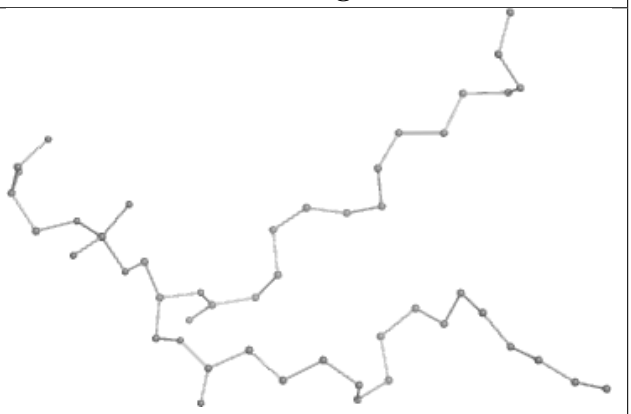
Bond lengths



Bond angles

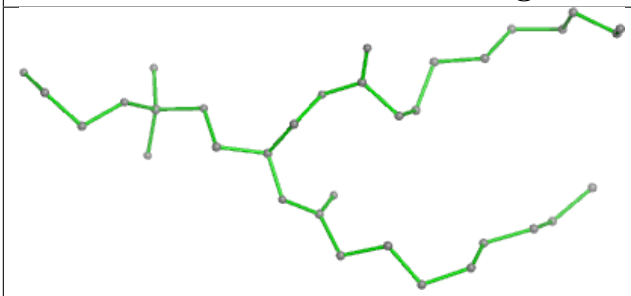


Torsions

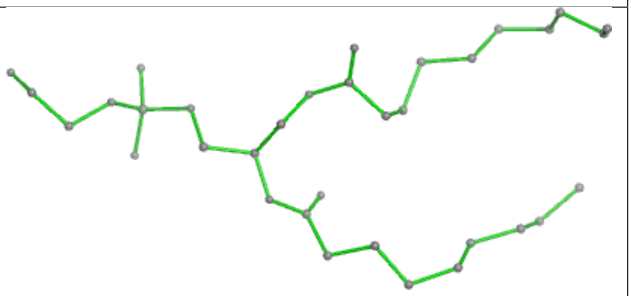


Rings

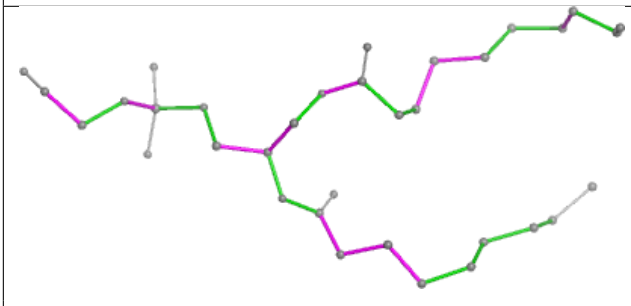
## Ligand PTY 1E 403



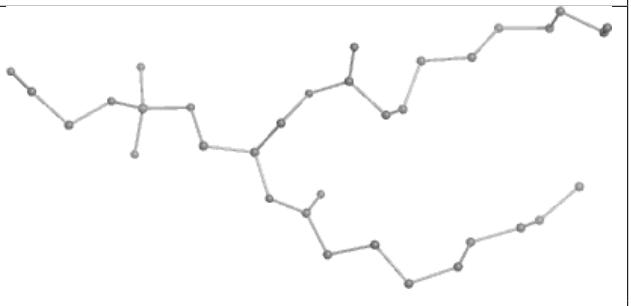
Bond lengths



Bond angles

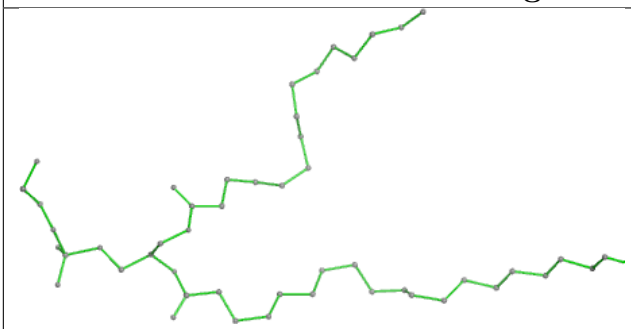


Torsions

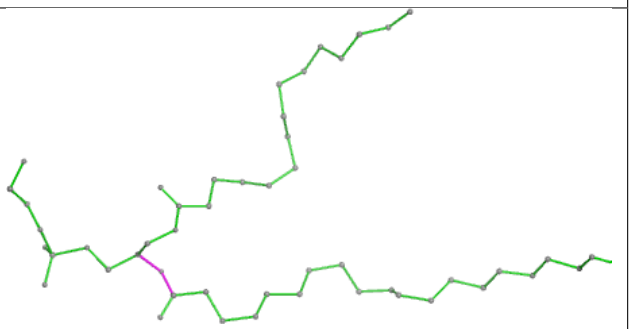


Rings

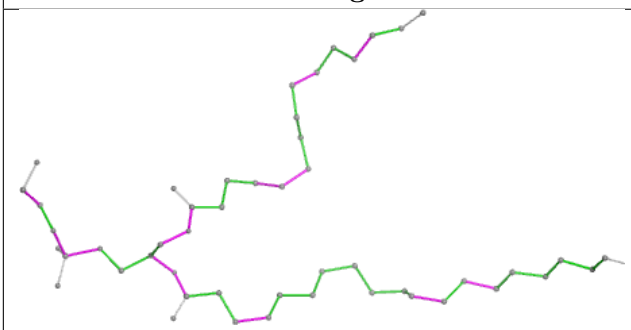
## Ligand PTY T 501



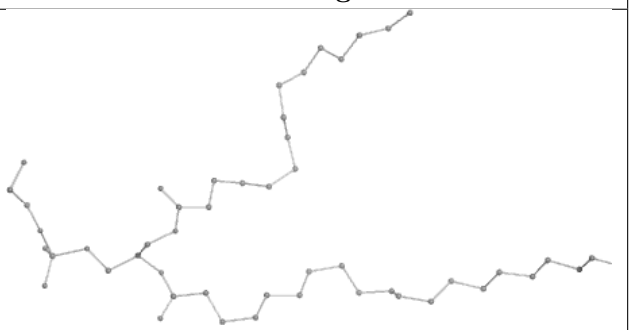
Bond lengths



Bond angles

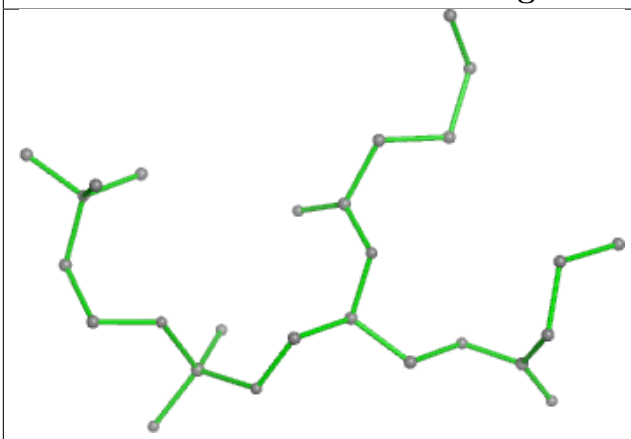


Torsions



Rings

## Ligand PC7 2A 606



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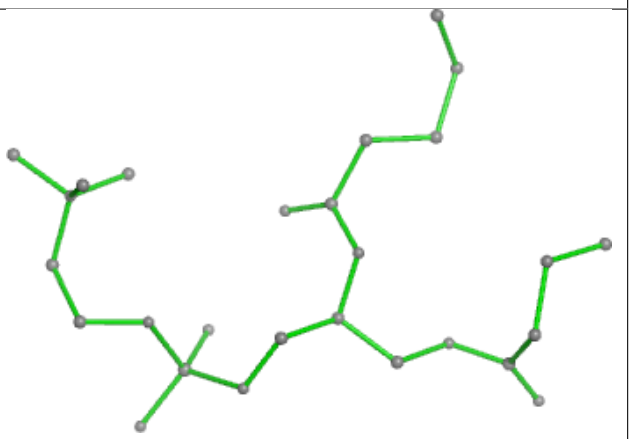
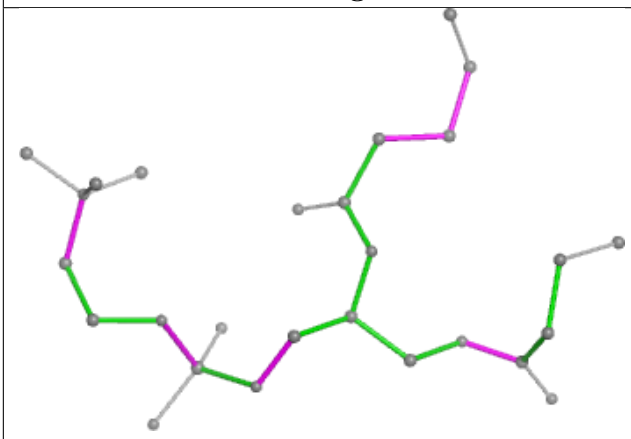
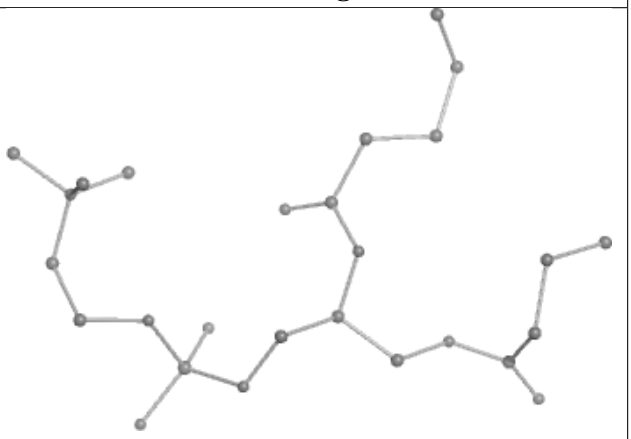


Bond angles

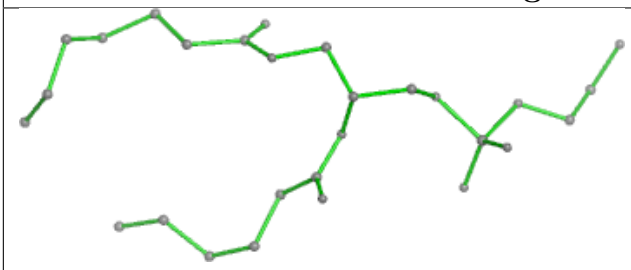


Torsions

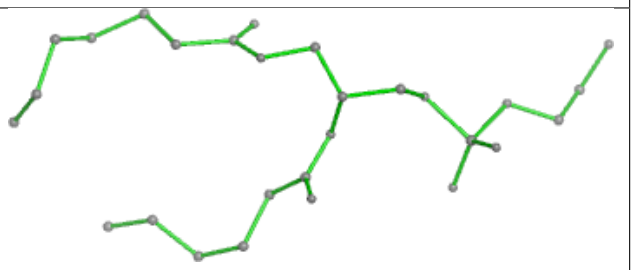


Rings

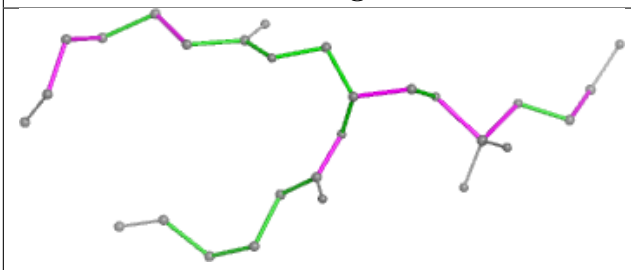
## Ligand PTY T 504



Bond lengths



Bond angles



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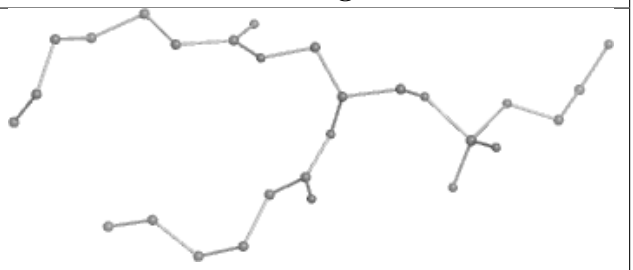
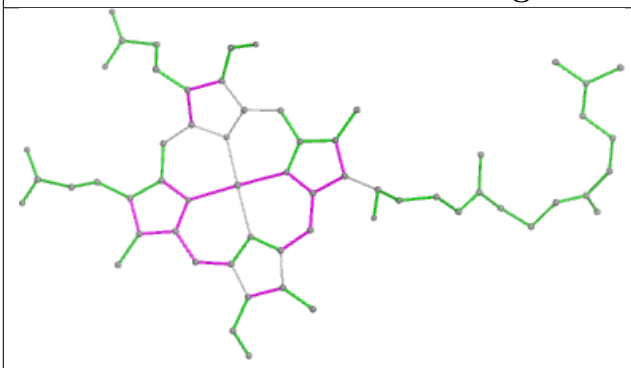
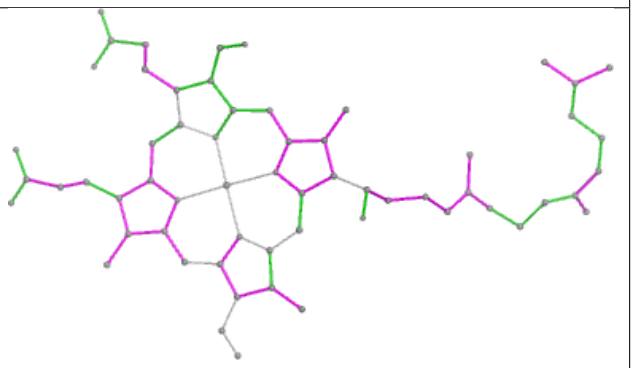


Rings

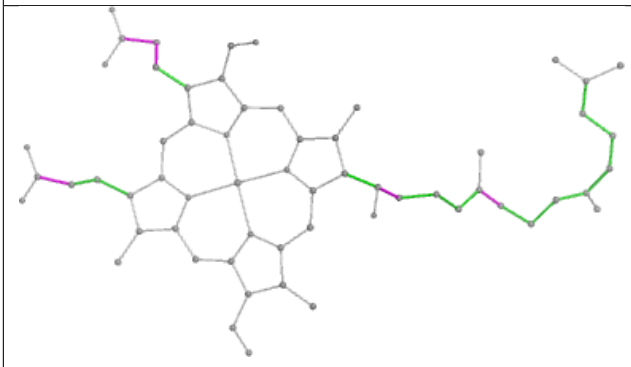
## Ligand HEA 3A 602



Bond lengths



Bond angles



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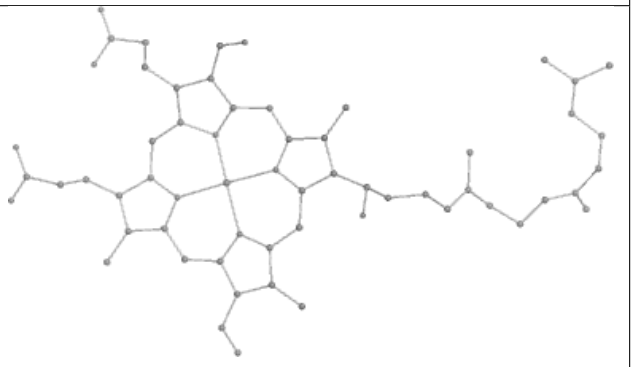
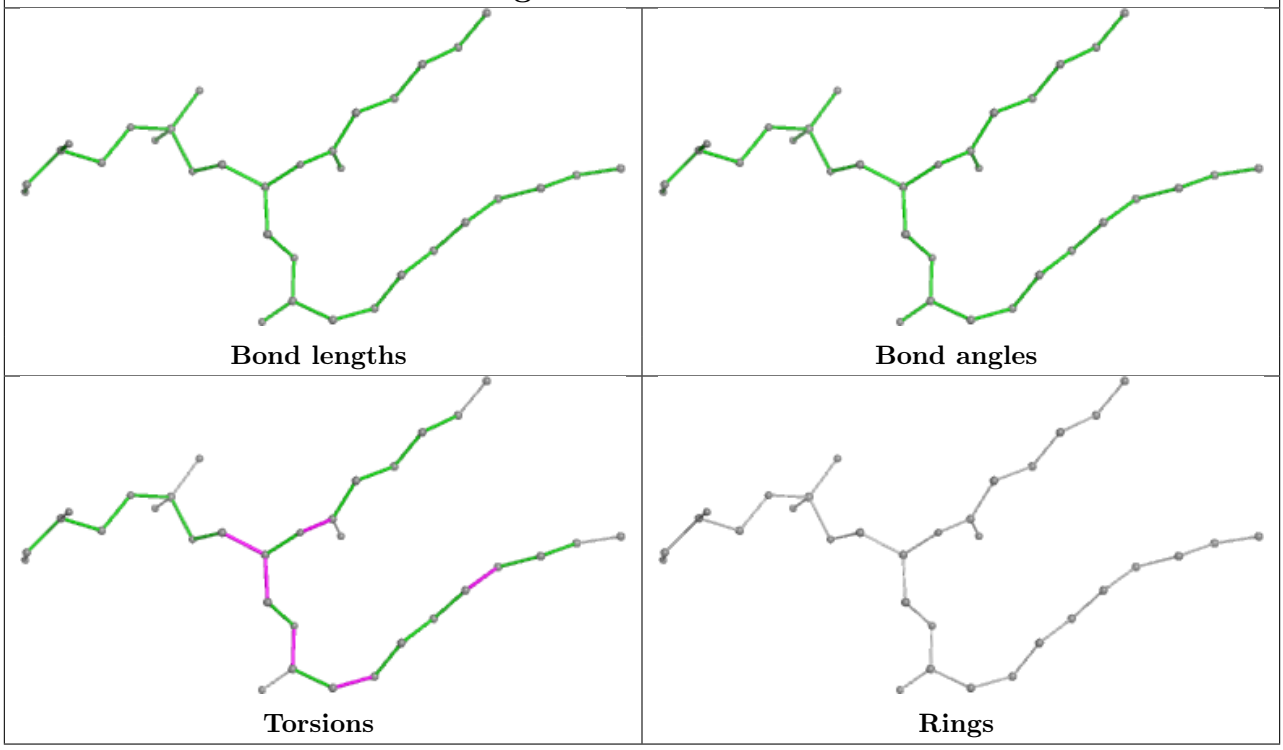
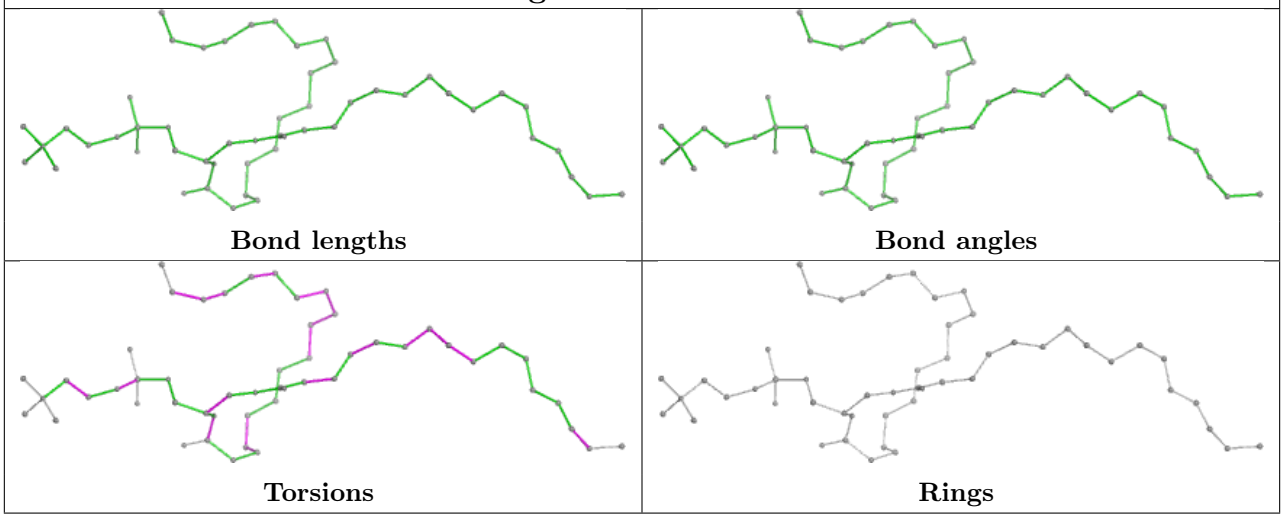


Rings

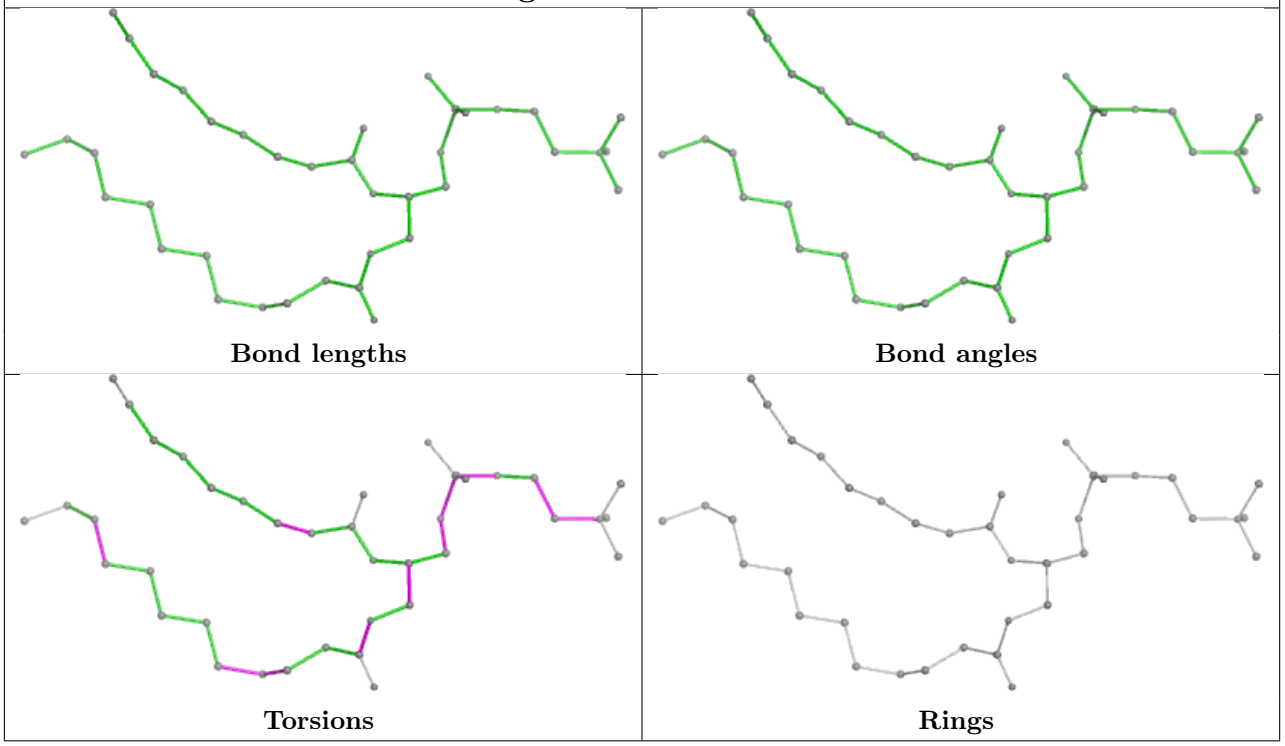
**Ligand PGT 2A 601**



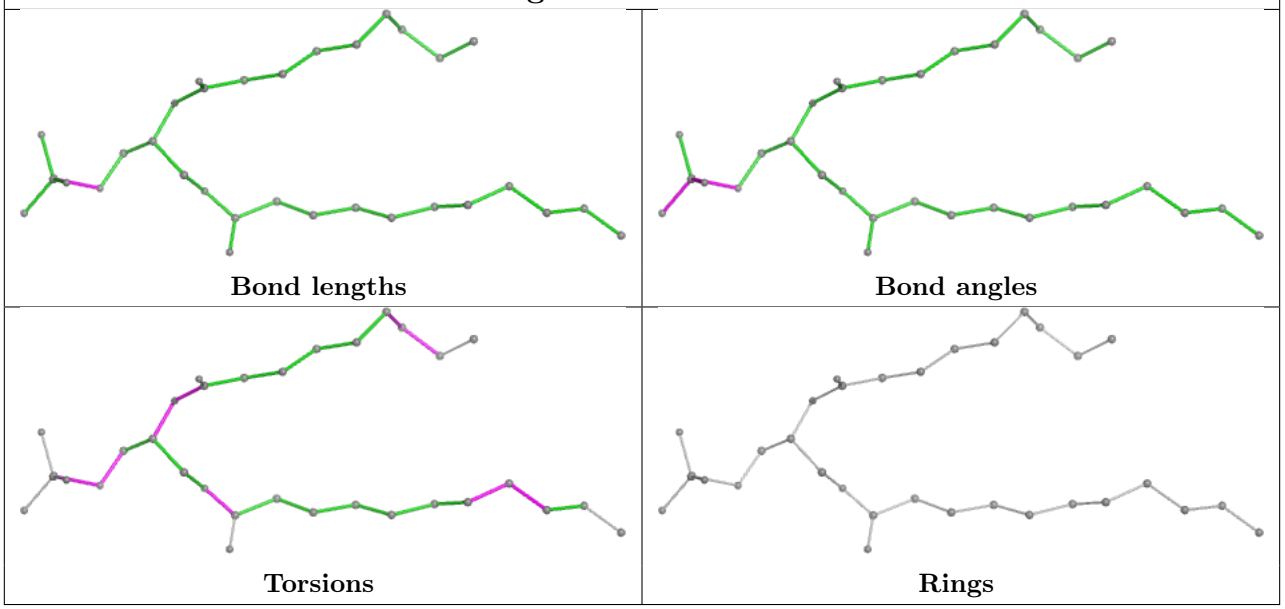

**Ligand PC7 T 503**



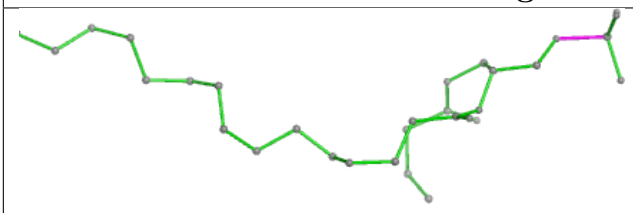
## Ligand PC7 1H 101



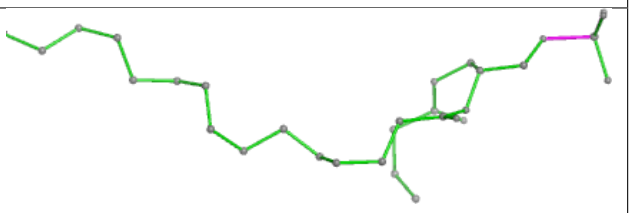

## Ligand 3PH R 401



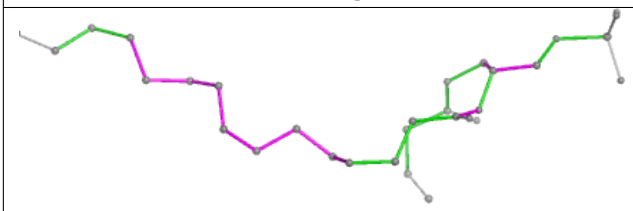
## Ligand 3PH 1A 406



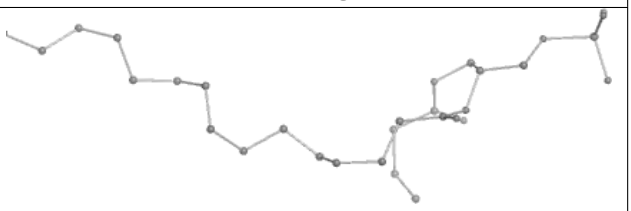
Bond lengths



Bond angles

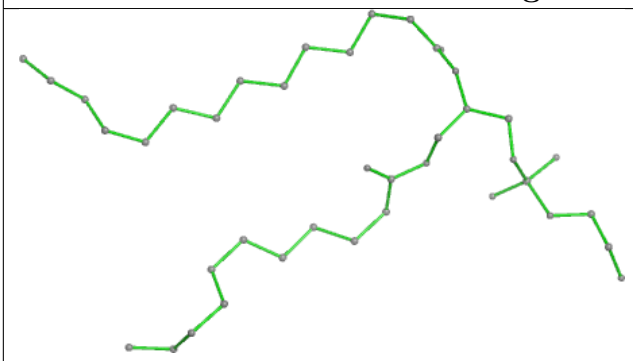


Torsions



Rings

## Ligand PTY V 604



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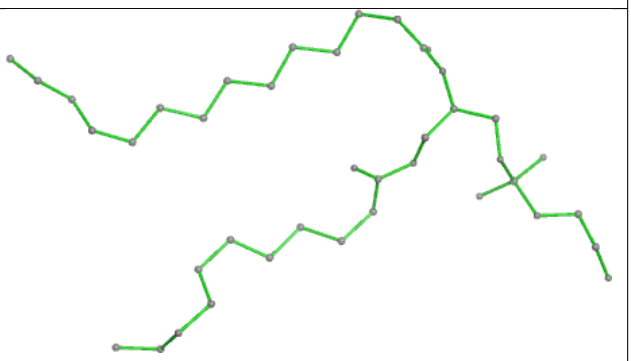
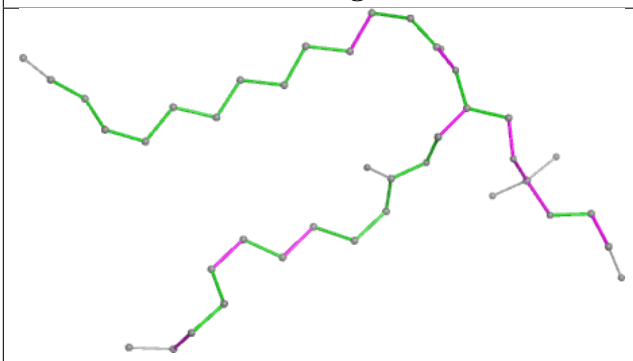


Bond angles



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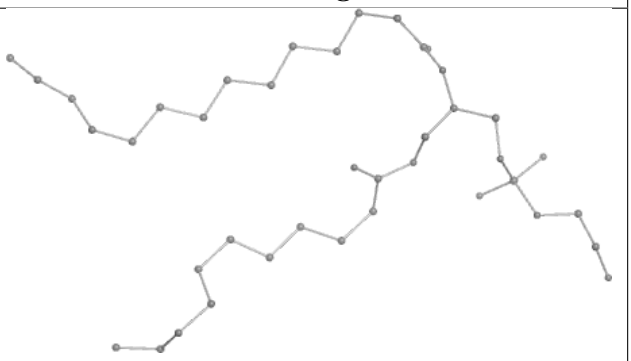
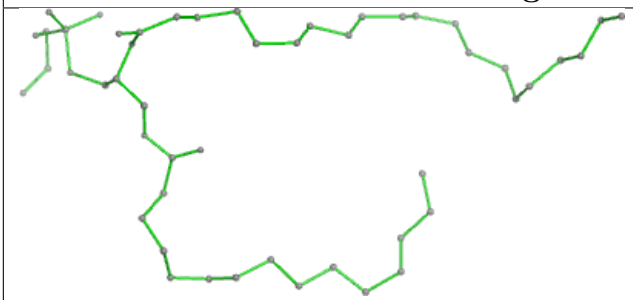


Rings

## Ligand PTY V 605



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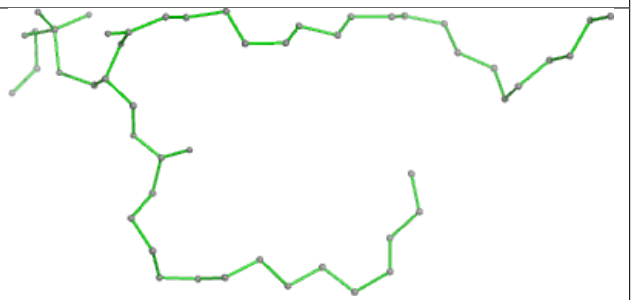
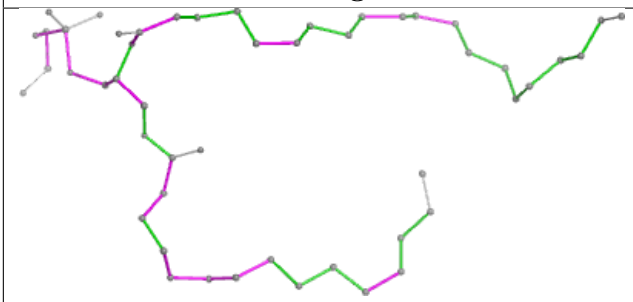


Bond angles



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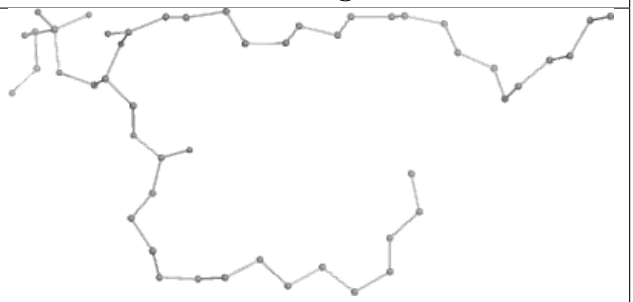
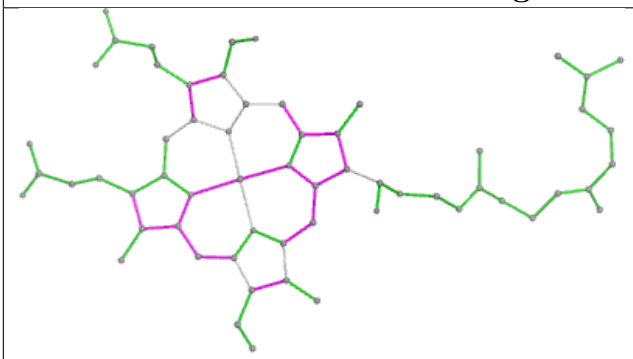


Rings

## Ligand HEA 2A 602



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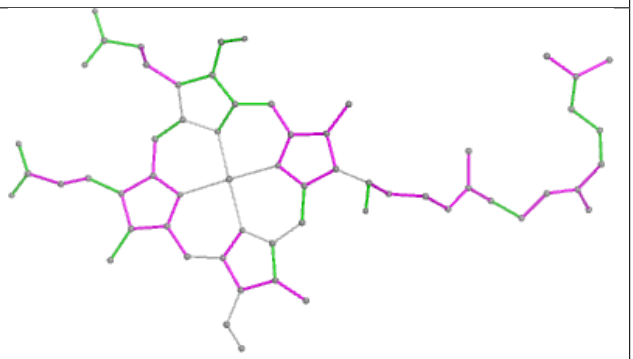
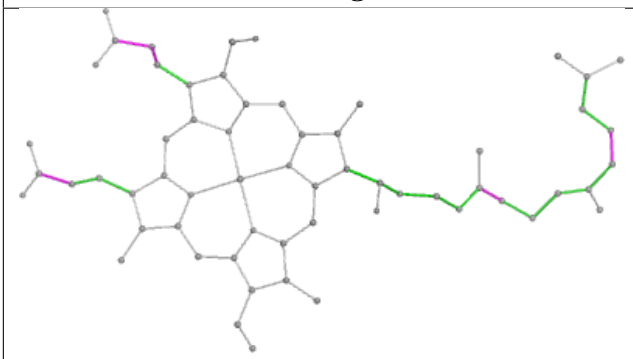


Bond angles



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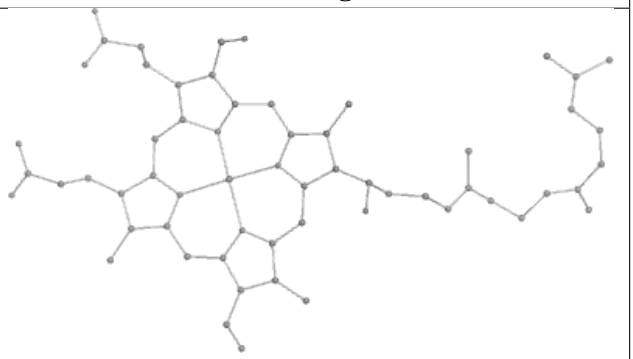
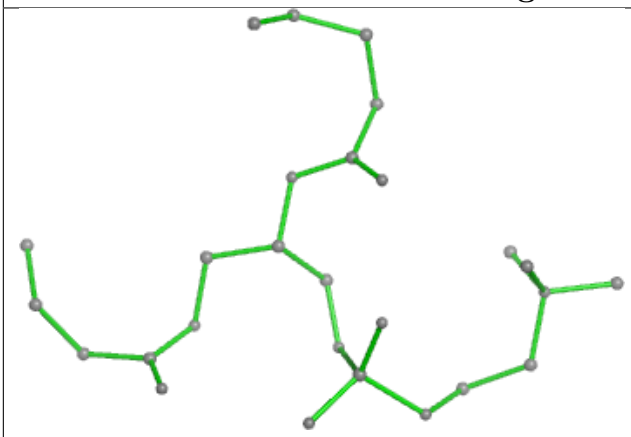
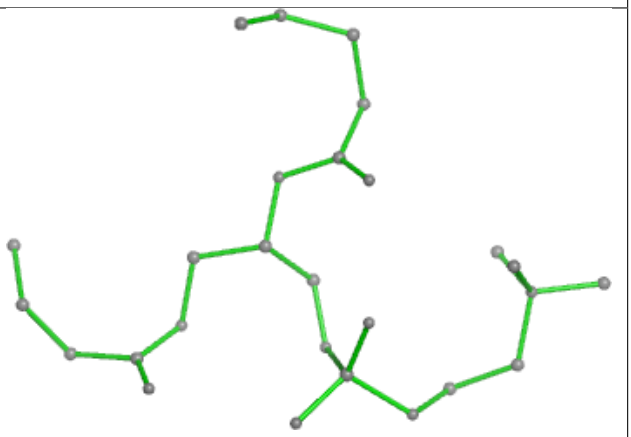


Rings

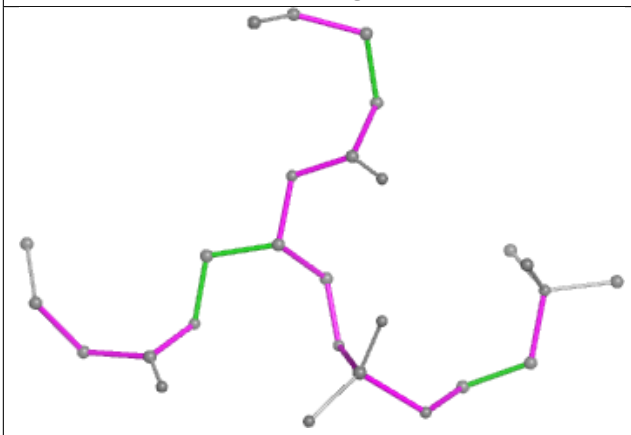
**Ligand PC7 3A 606**



**Bond lengths**



**Bond angles**



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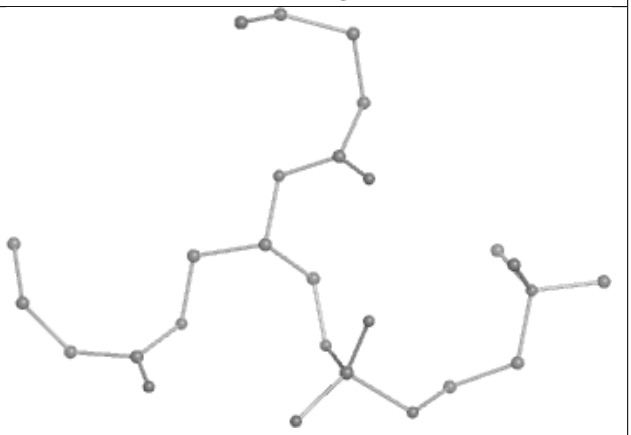
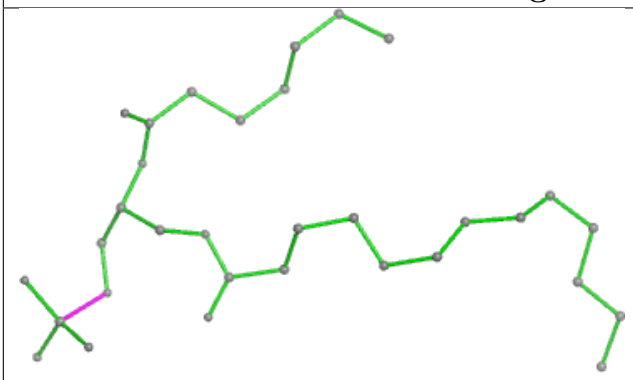
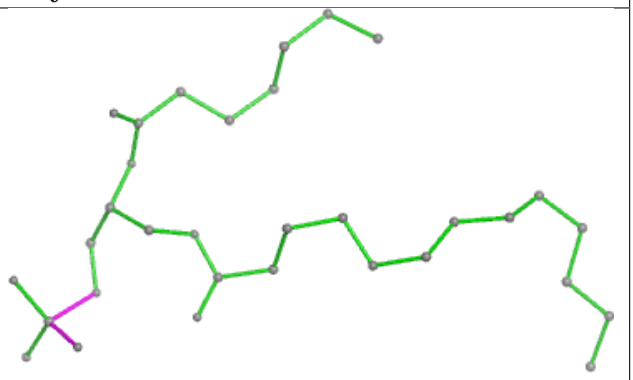


**Rings**

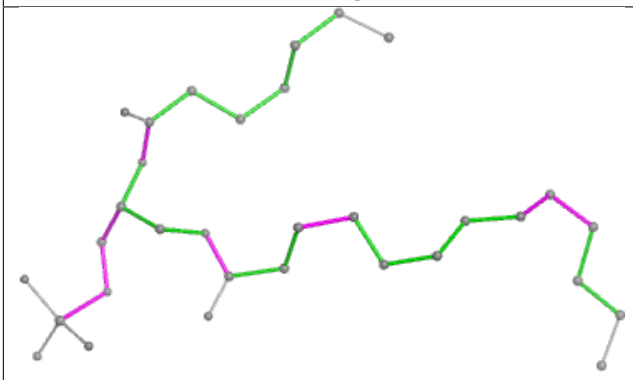
**Ligand 3PH y 201**



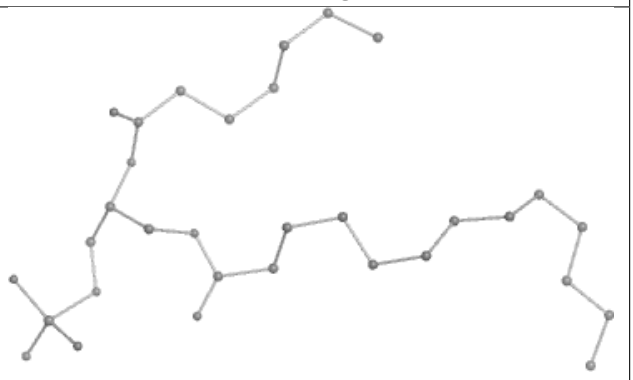
Bond lengths



Bond angles

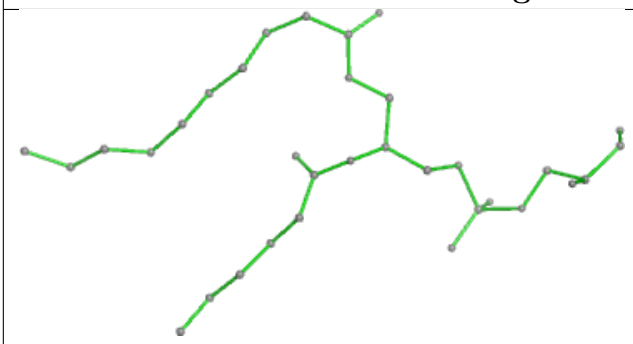


Torsions



Rings

**Ligand PGT 3A 601**



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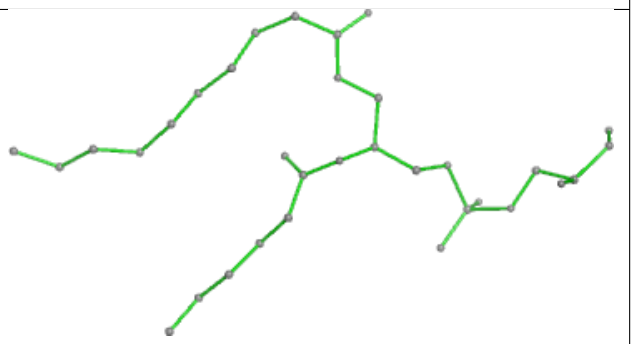
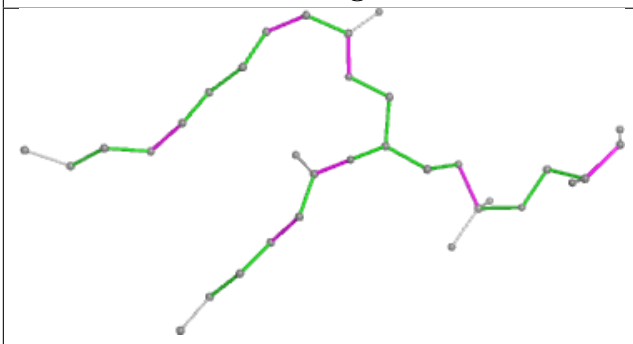


Bond angles



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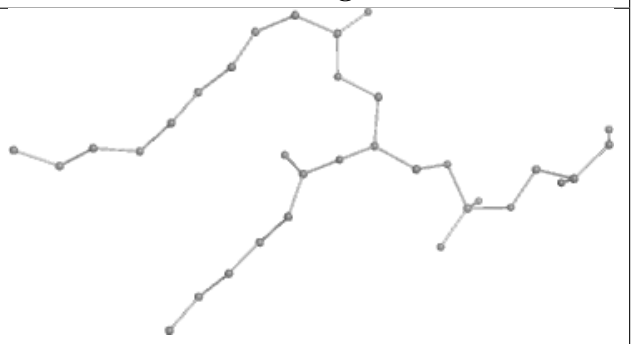
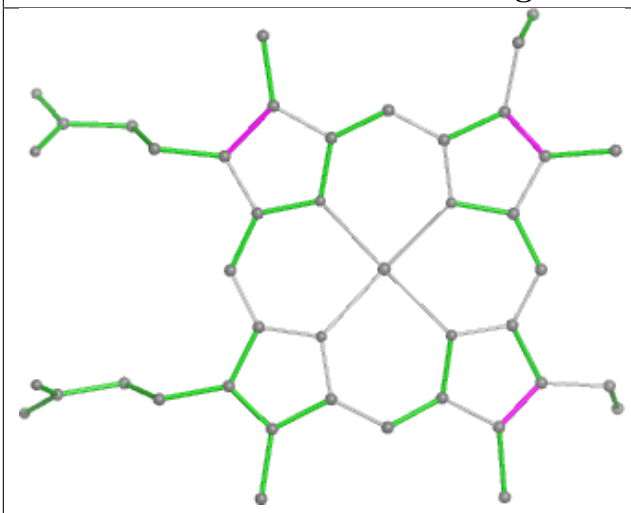
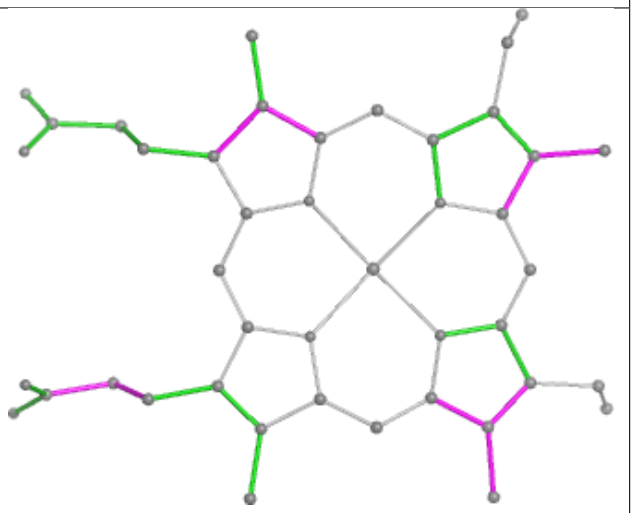


Rings

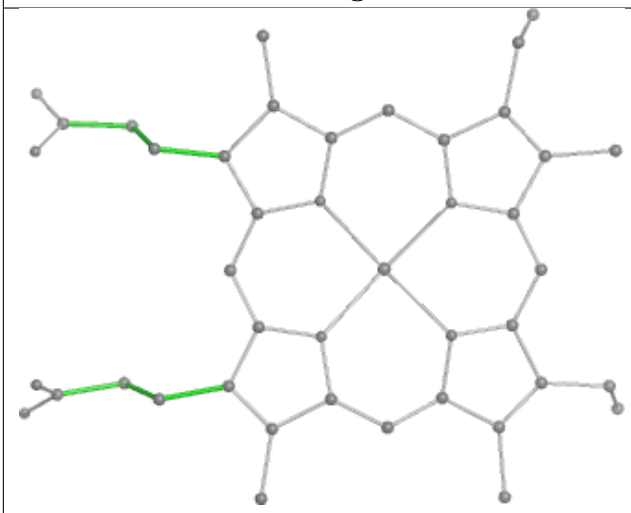
**Ligand HEC 1E 404**



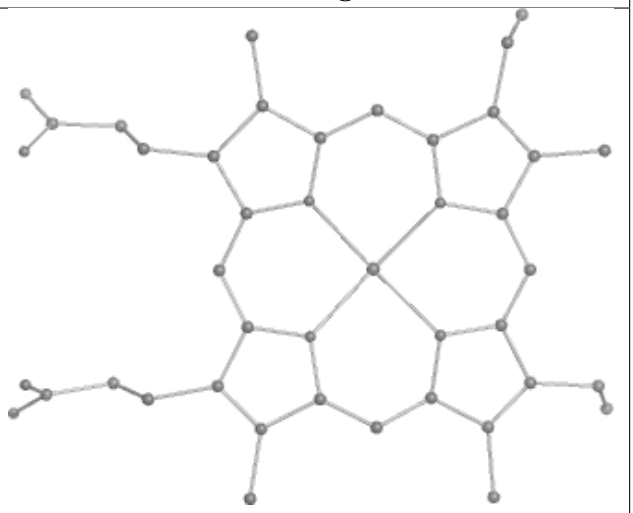
**Bond lengths**



**Bond angles**

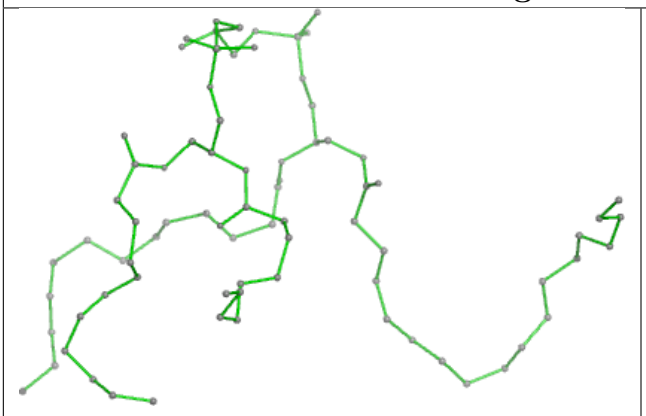


**Torsions**

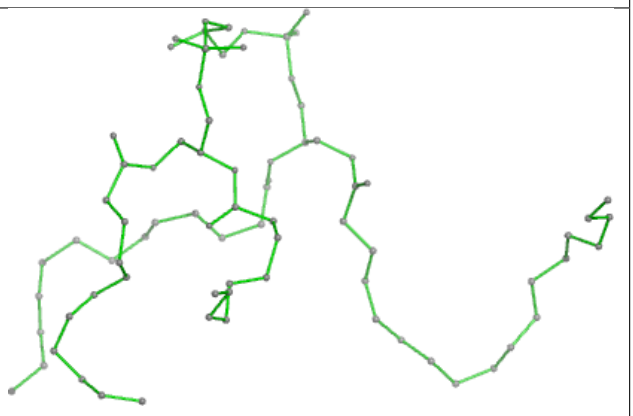


**Rings**

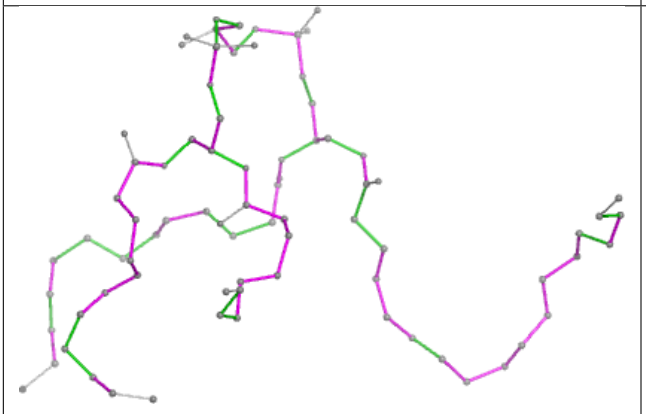
## Ligand CDL 1K 101



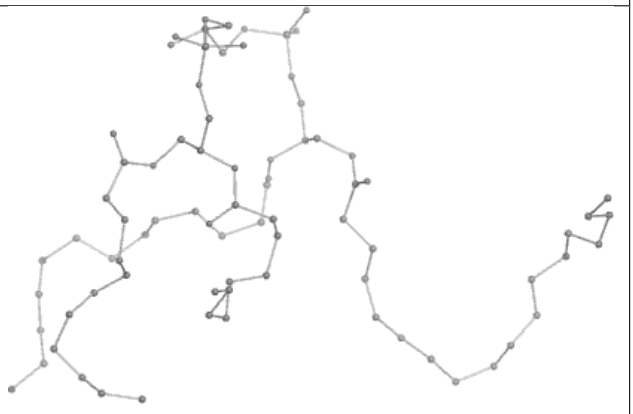
Bond lengths



Bond angles

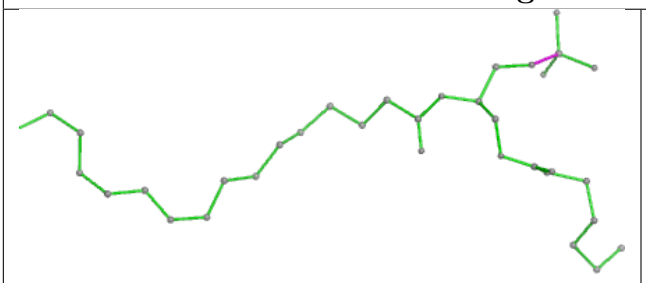


Torsions

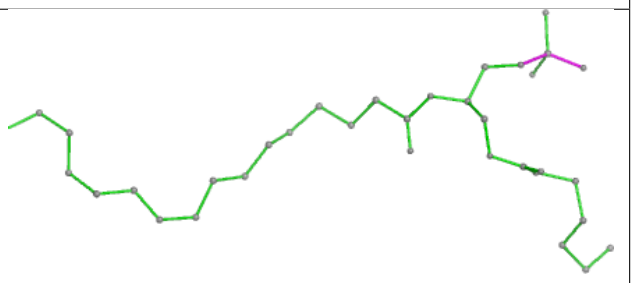


Rings

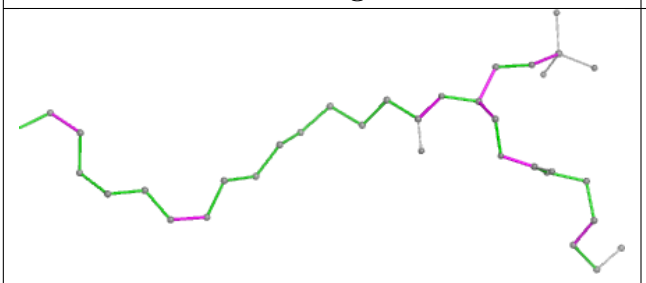
## Ligand 3PH 1R 201



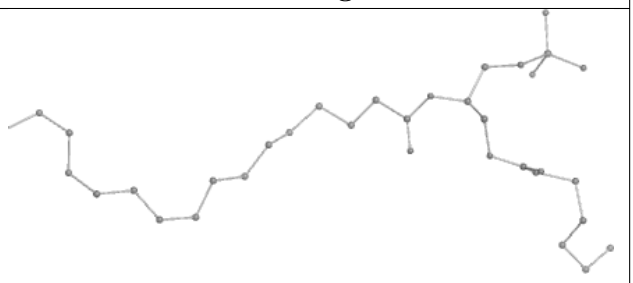
Bond lengths



Bond angles

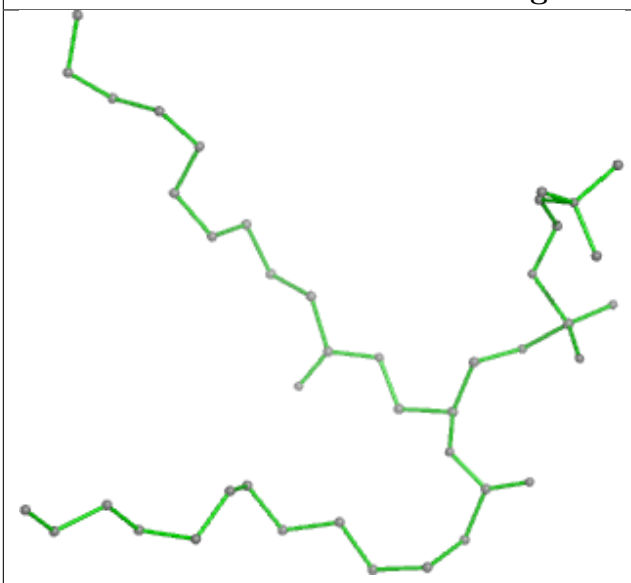


Torsions

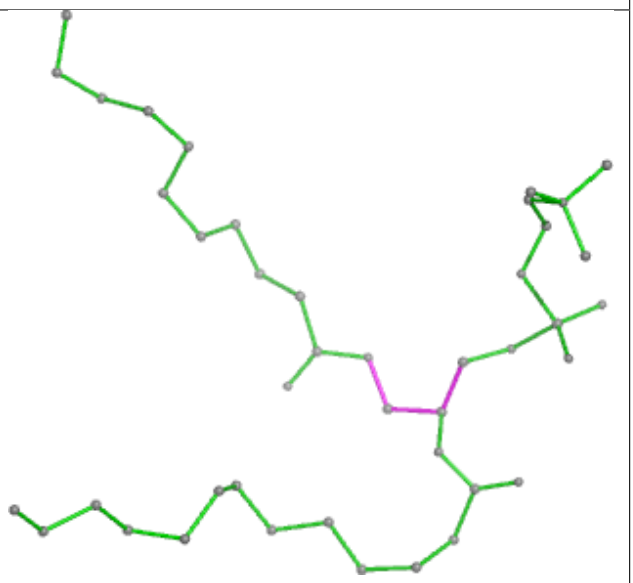


Rings

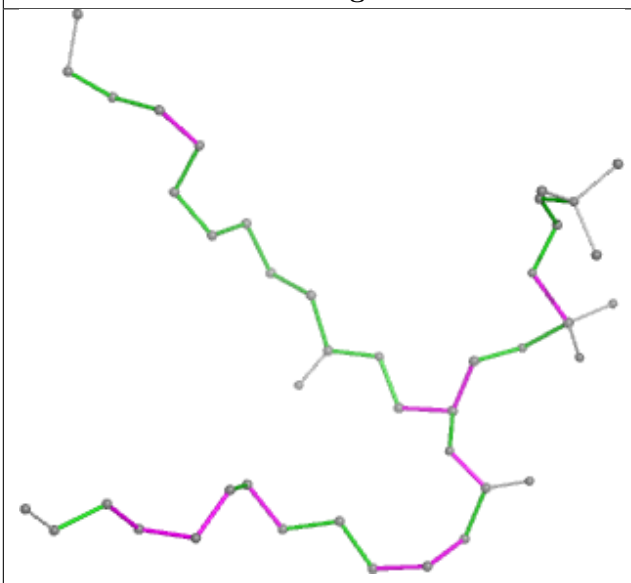
**Ligand PC7 u 601**



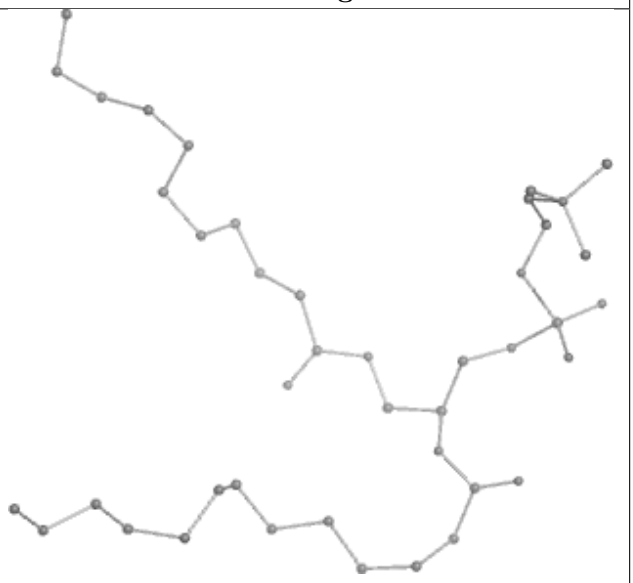
**Bond lengths**



**Bond angles**

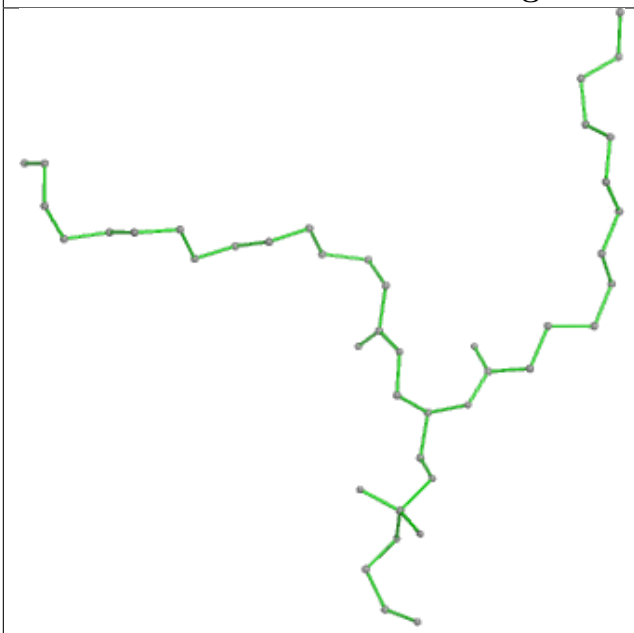


**Torsions**

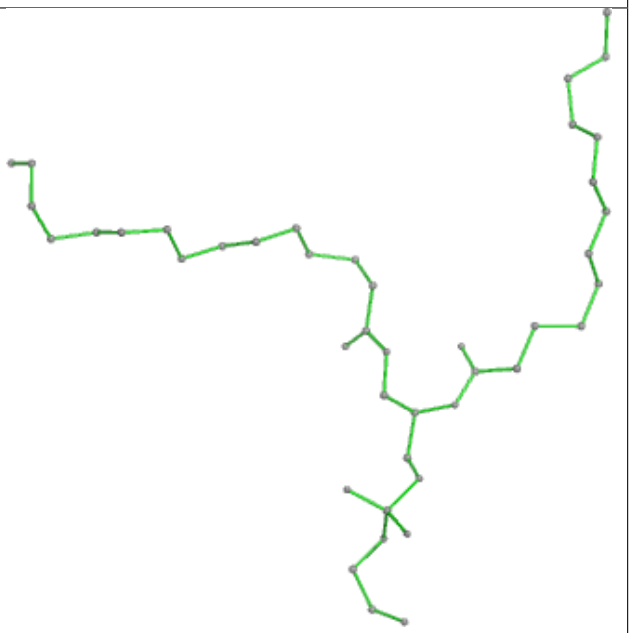


**Rings**

**Ligand PTY G 303**

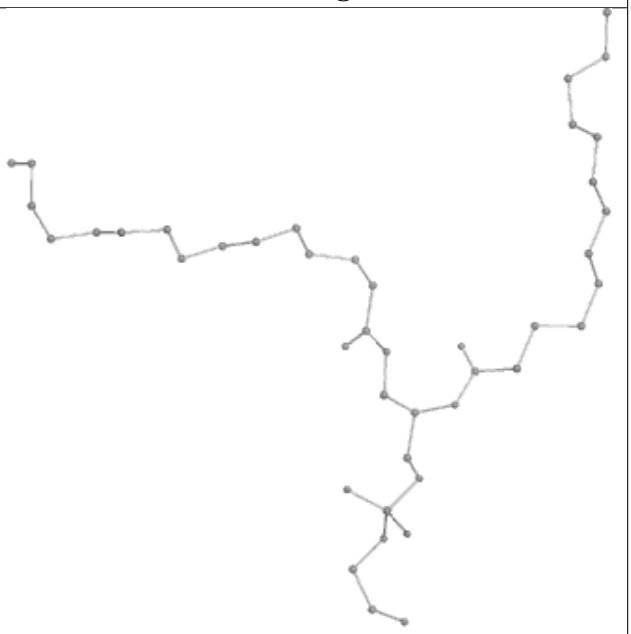


**Bond lengths**



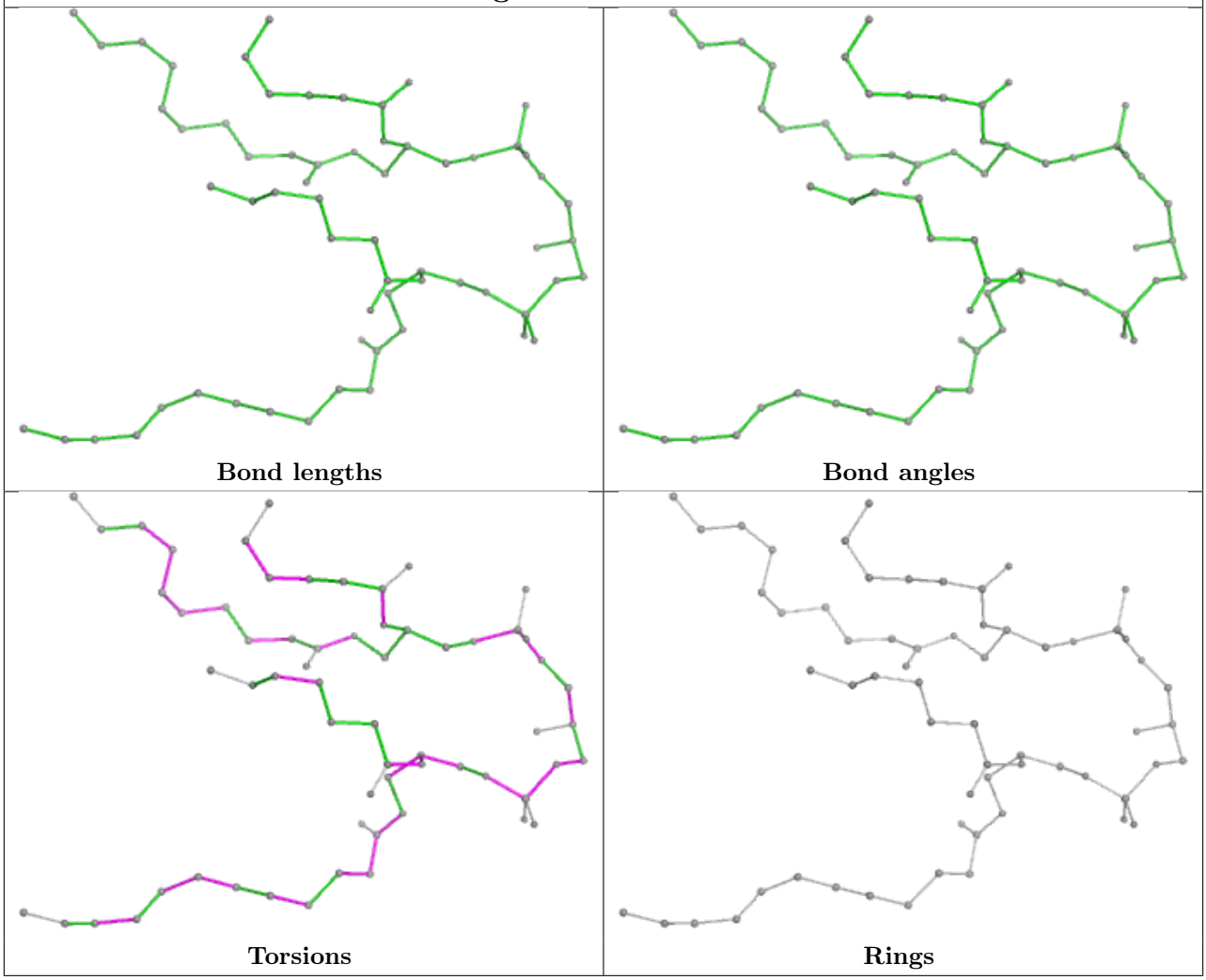
**Bond angles**

**Torsions**

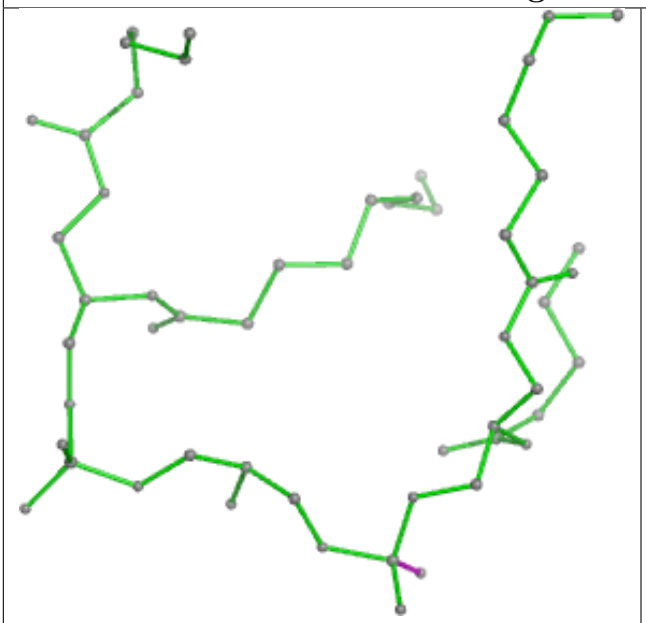


**Rings**

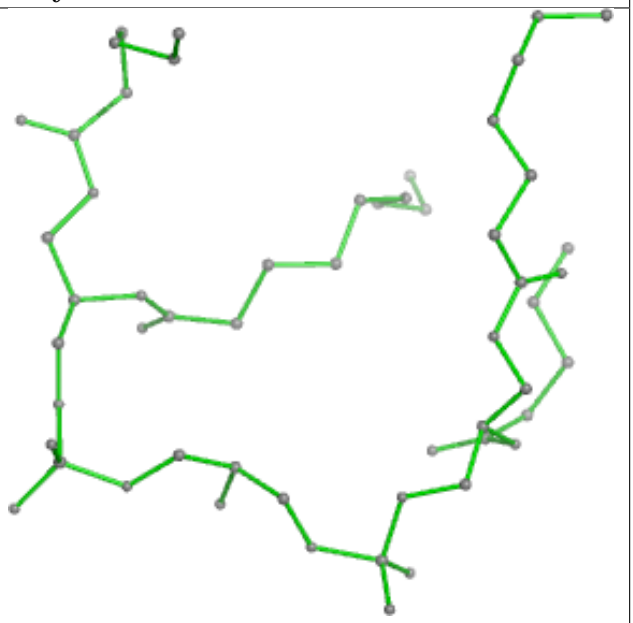
**Ligand CDL R 405**



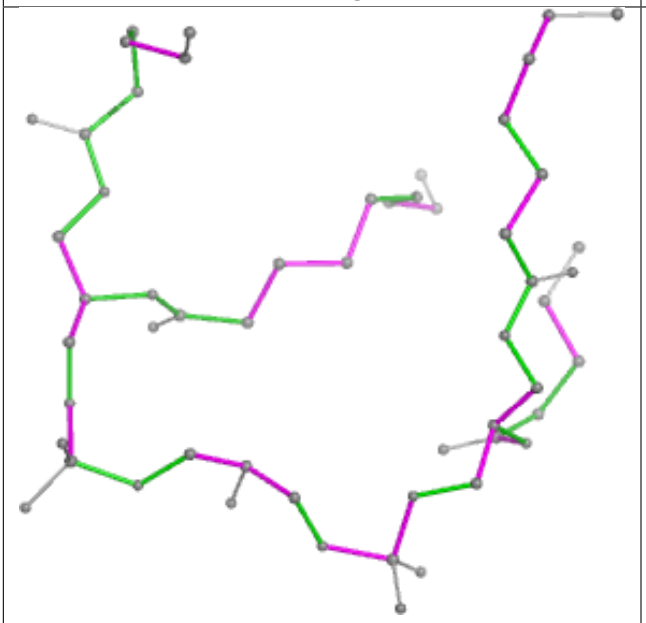
**Ligand CDL y 202**



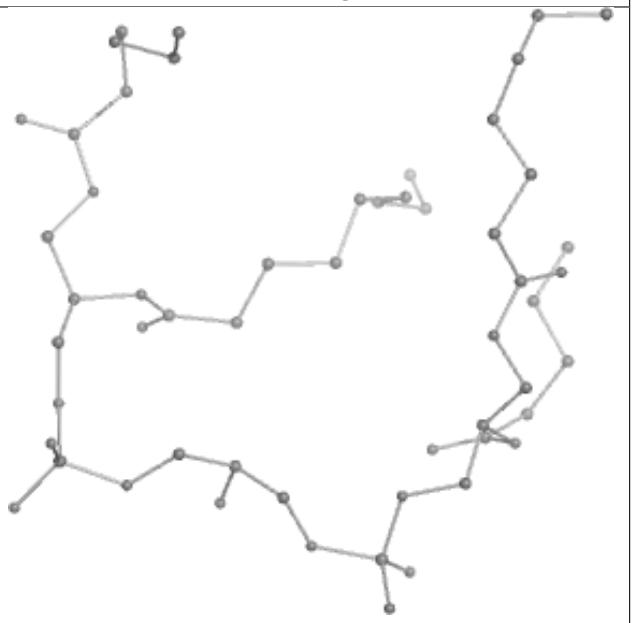
**Bond lengths**



**Bond angles**

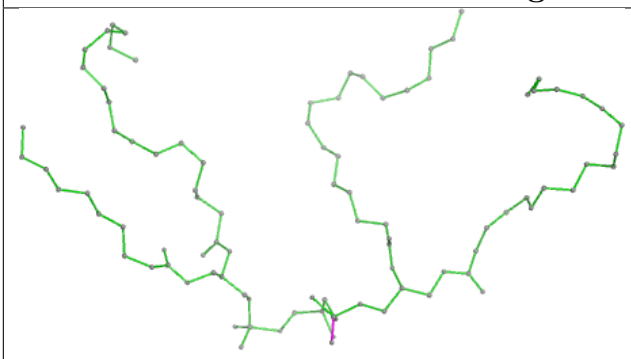


**Torsions**

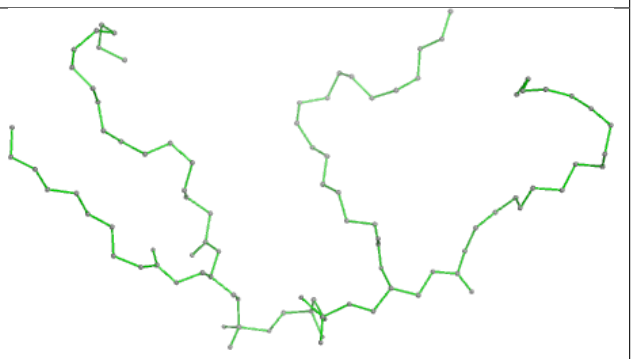


**Rings**

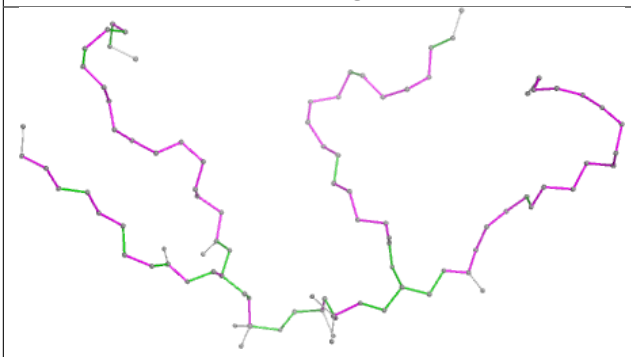
## Ligand CDL x 101



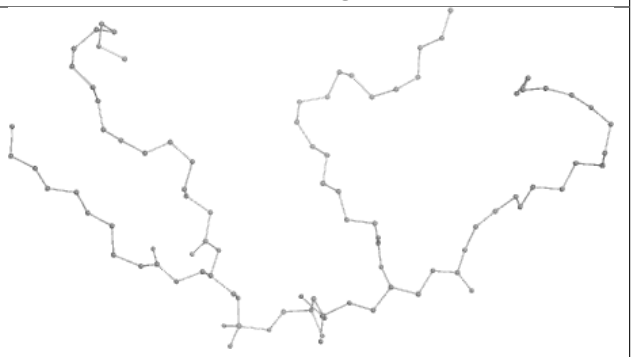
Bond lengths



Bond angles

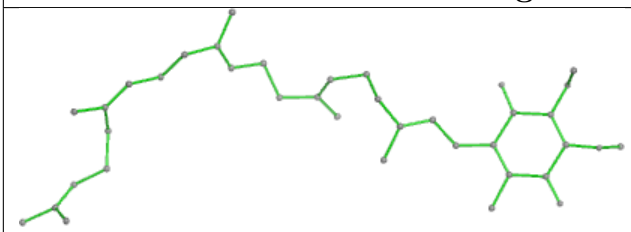


Torsions

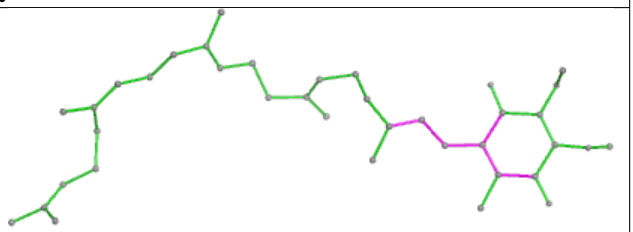


Rings

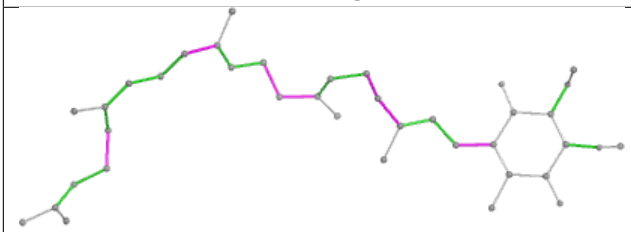
## Ligand UQ5 1A 401



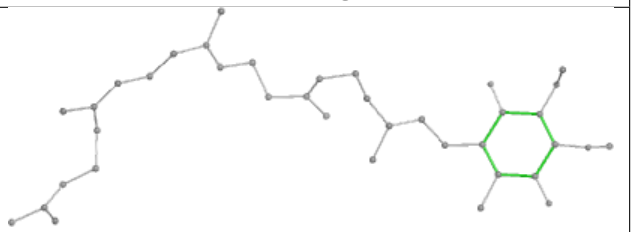
Bond lengths



Bond angles

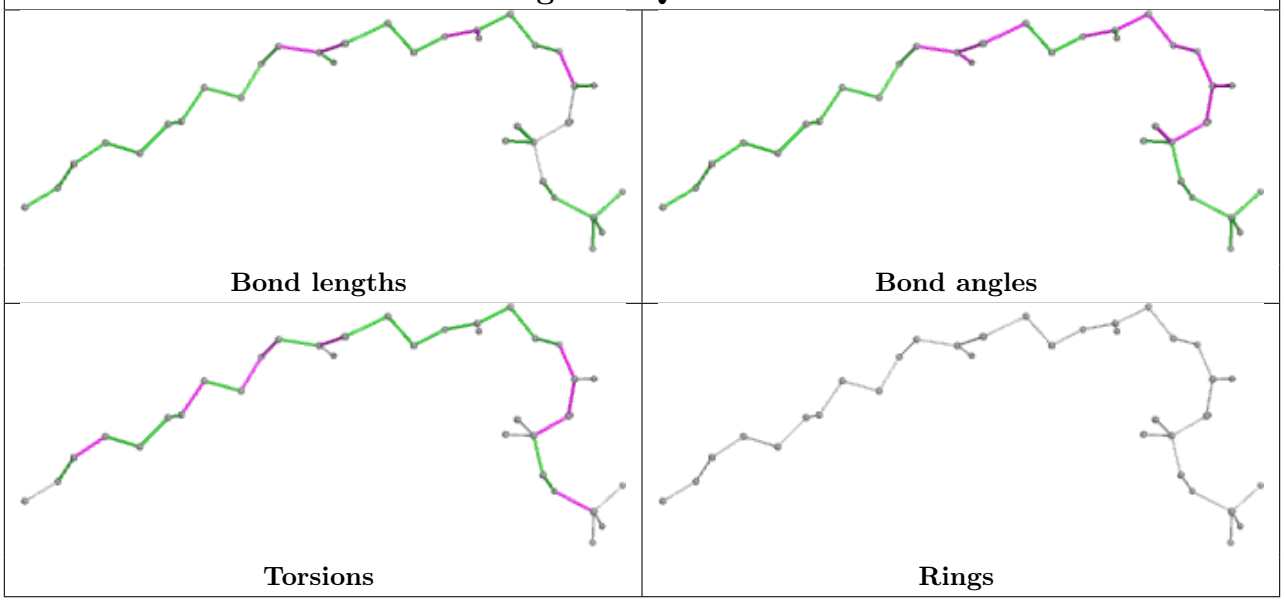


Torsions

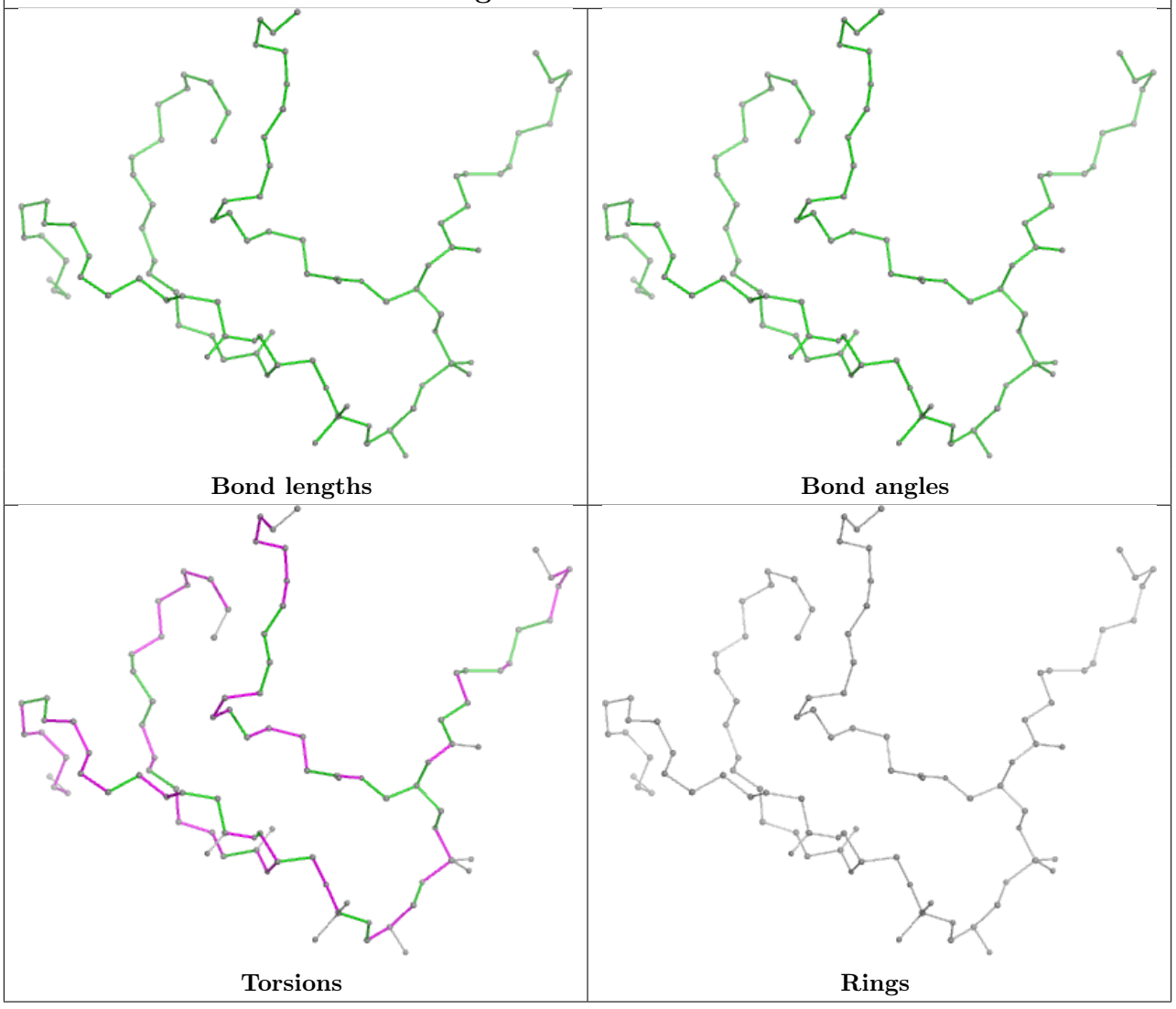


Rings

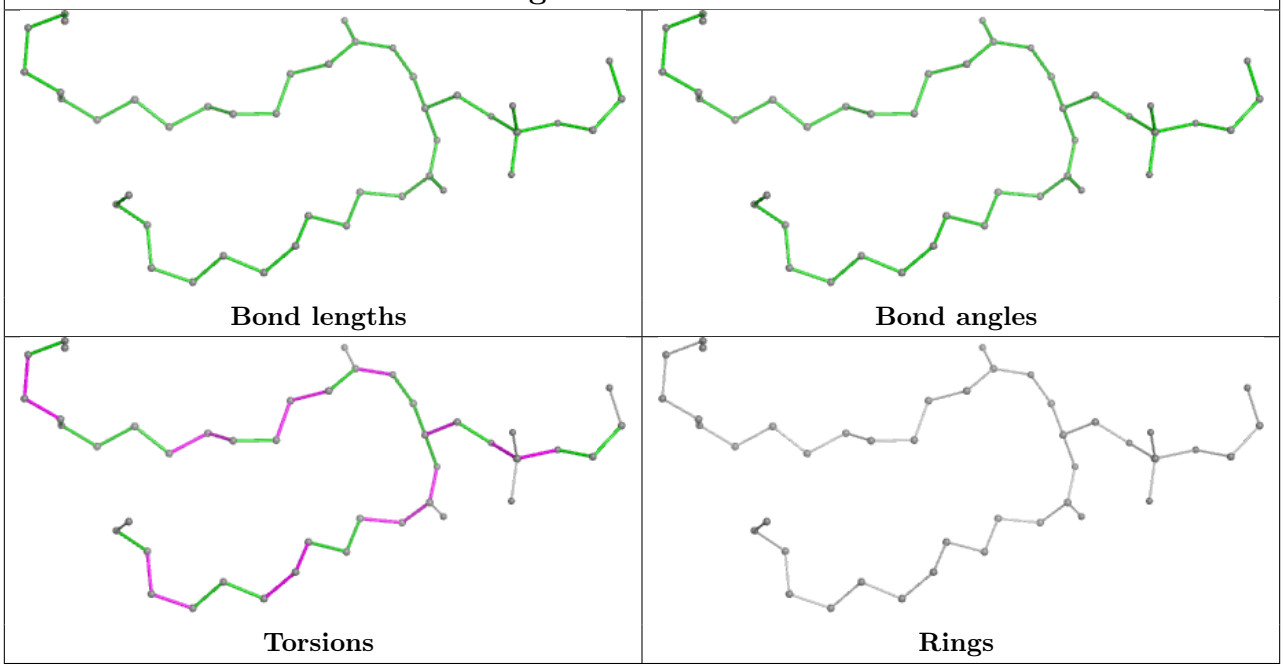
## Ligand 8Q1 r 200



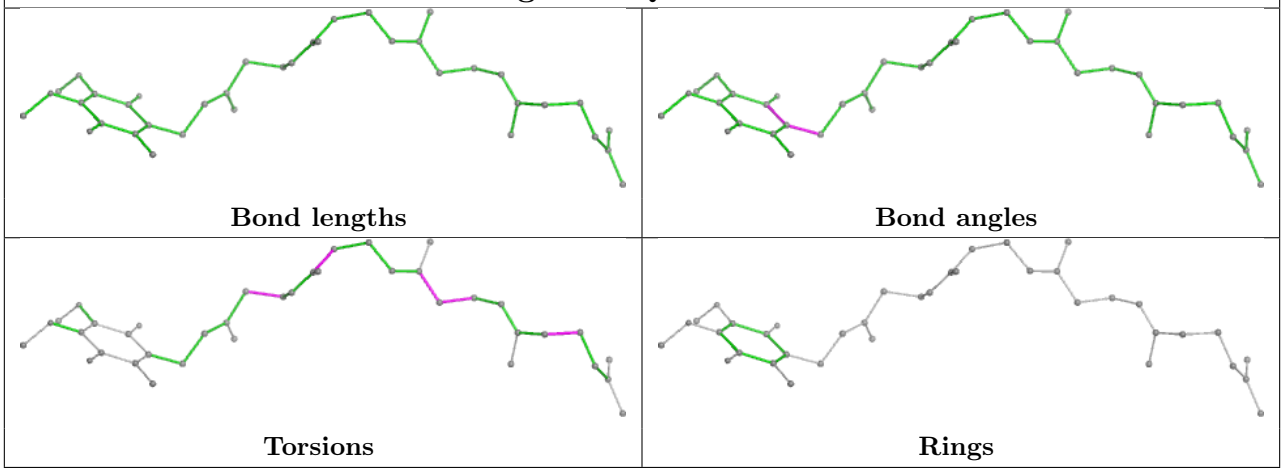

## Ligand CDL W 701



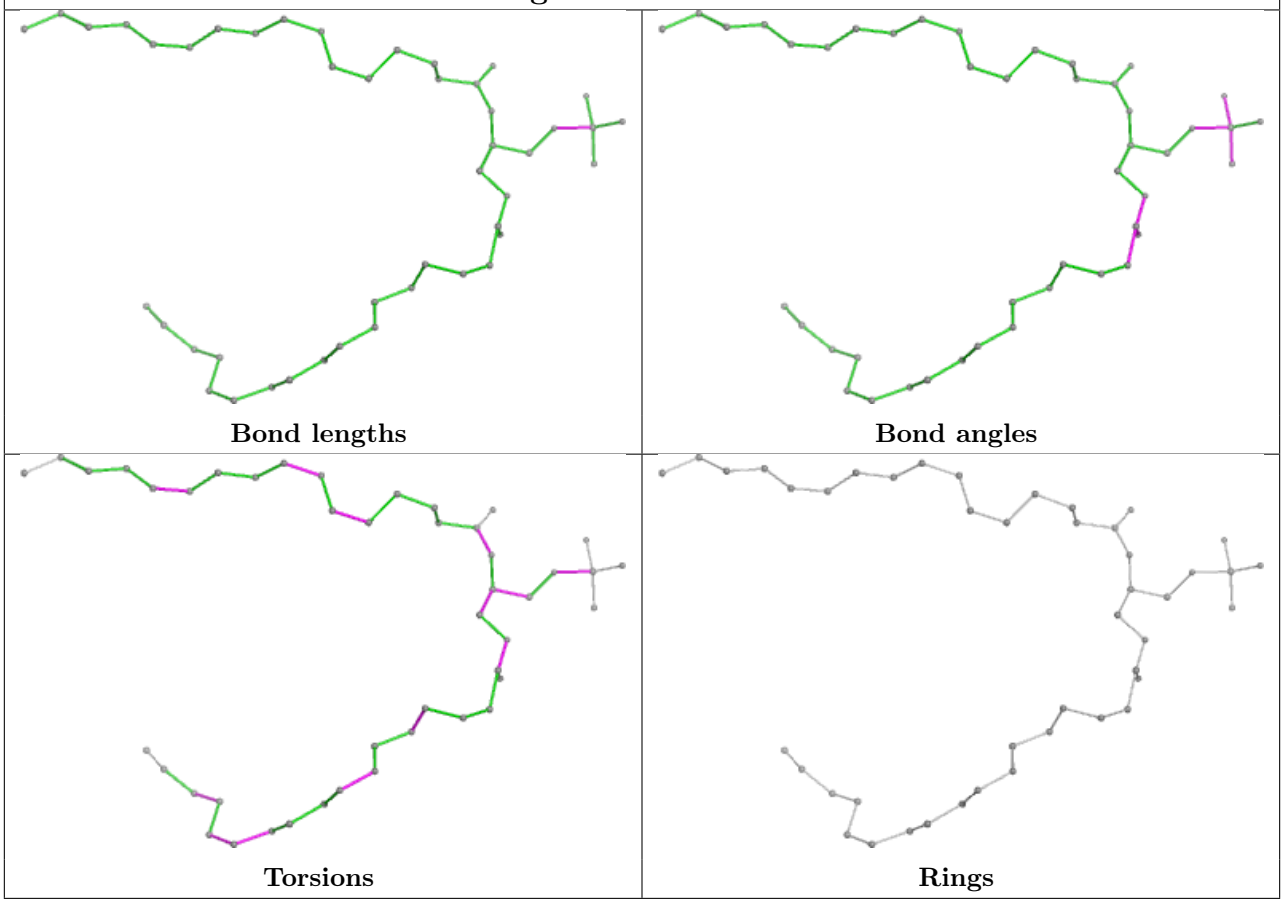
**Ligand PTY e 302**



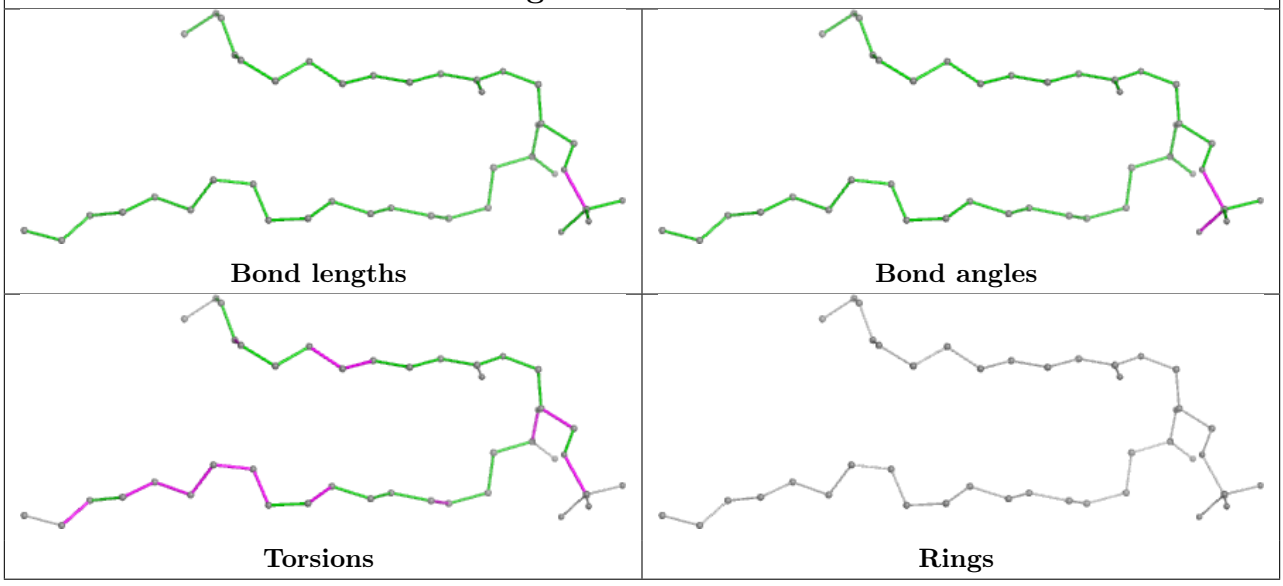

**Ligand UQ5 1B 401**



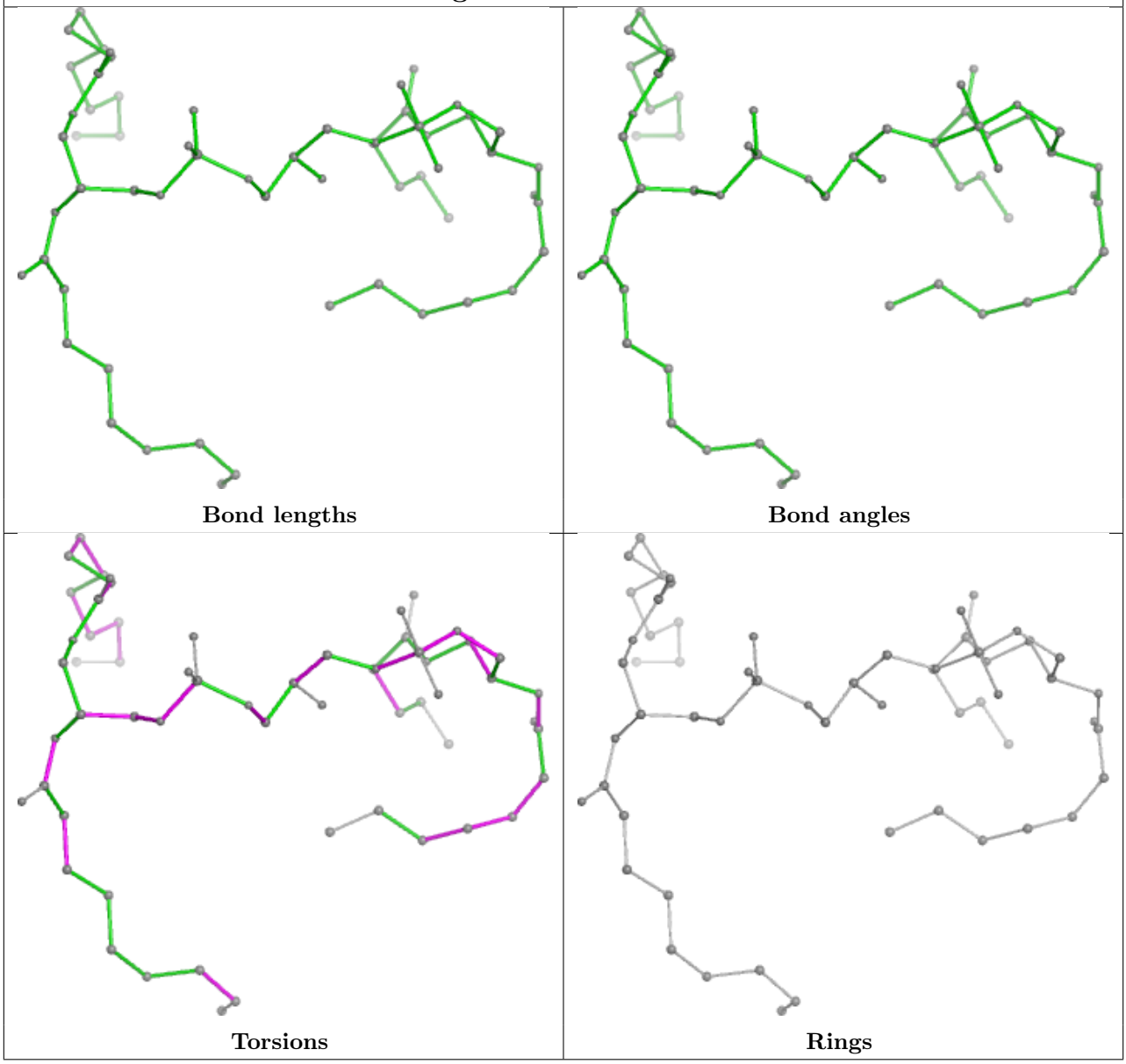
**Ligand 3PH h 201**



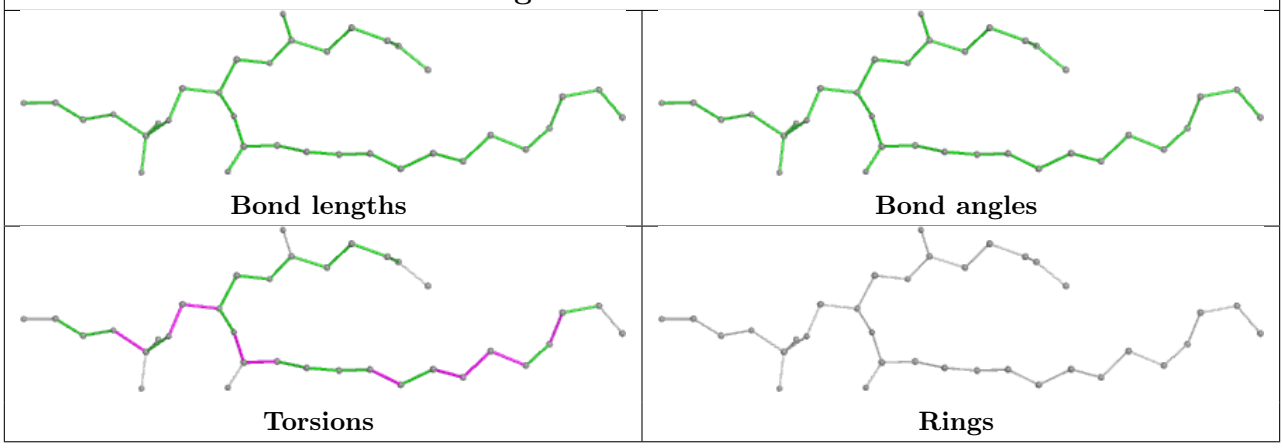

**Ligand 3PH V 601**



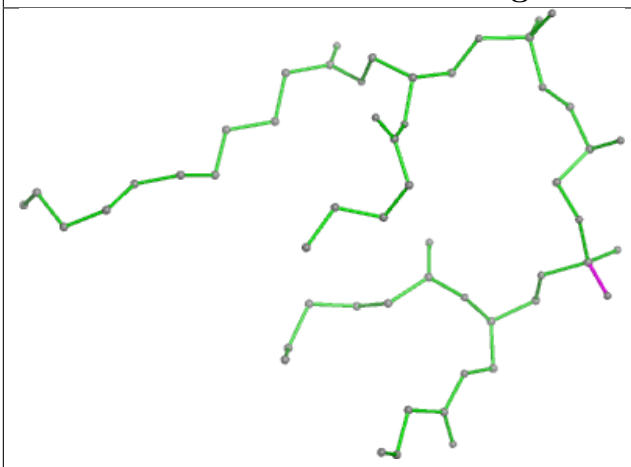
## Ligand CDL 1A 405



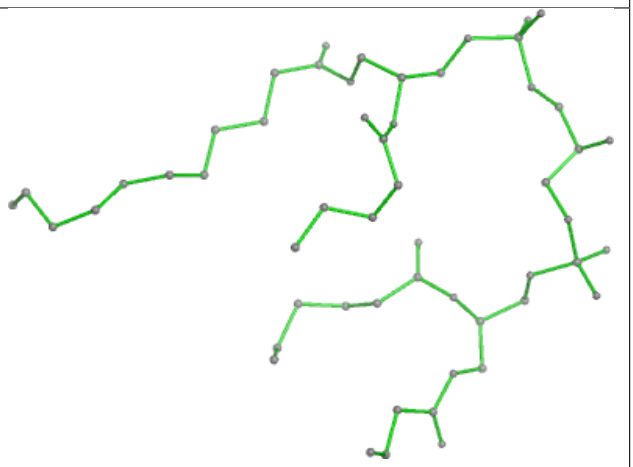

## Ligand PTY 2D 301



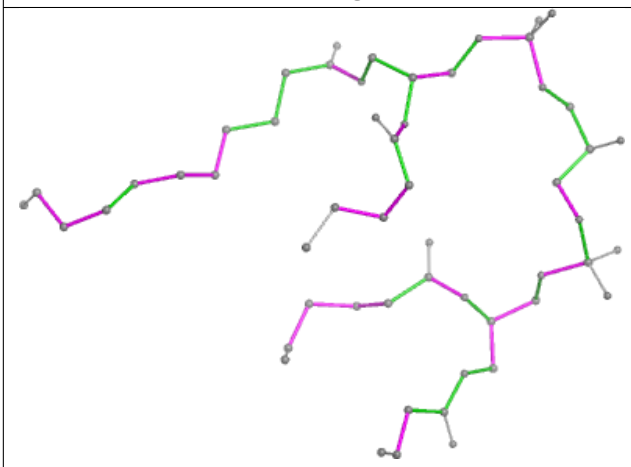
**Ligand CDL 1M 501**



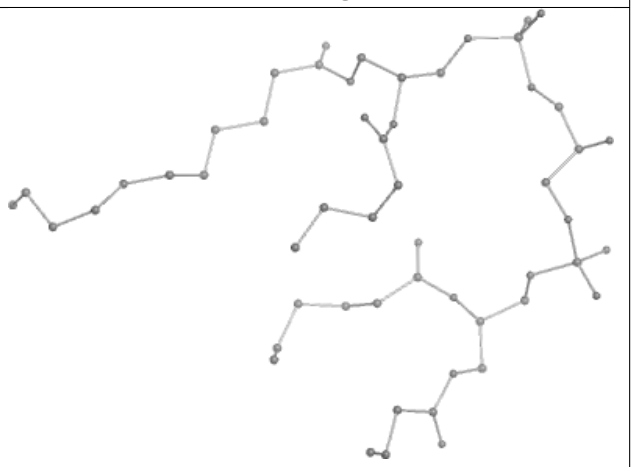
**Bond lengths**



**Bond angles**

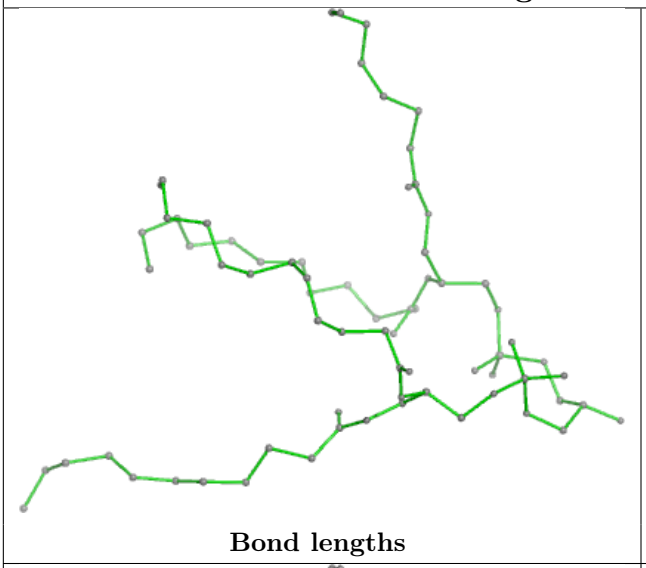


**Torsions**

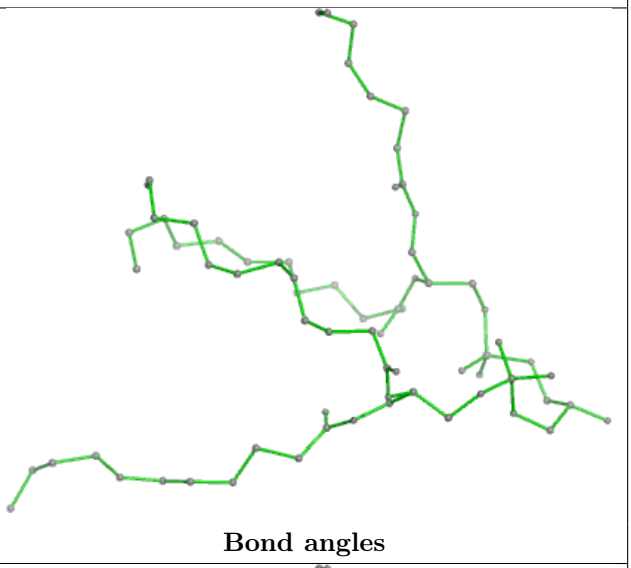


**Rings**

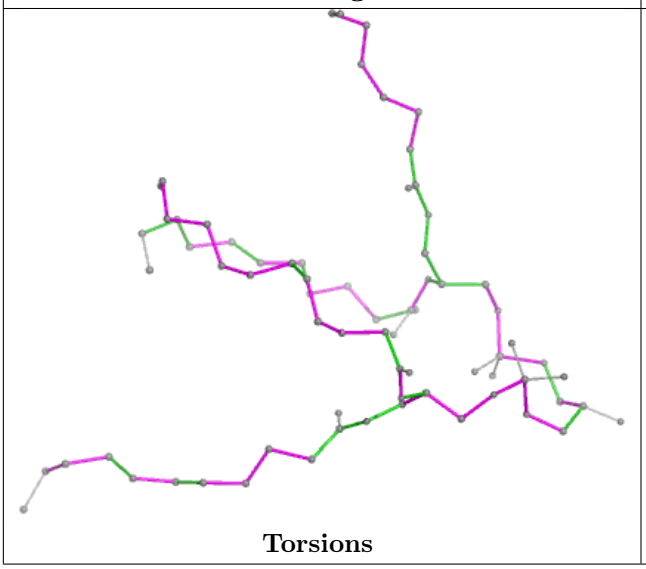
## Ligand CDL 1B 408



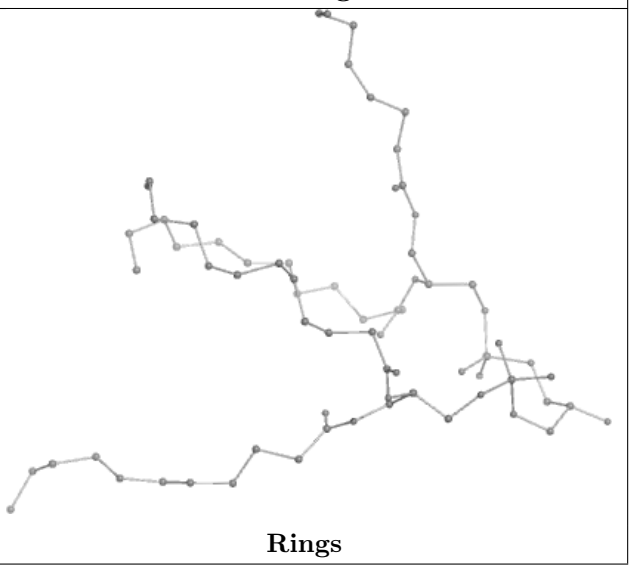
Bond lengths



Bond angles

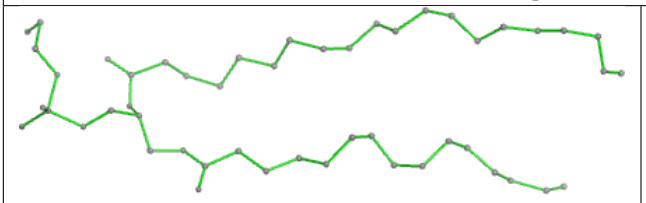


Torsions

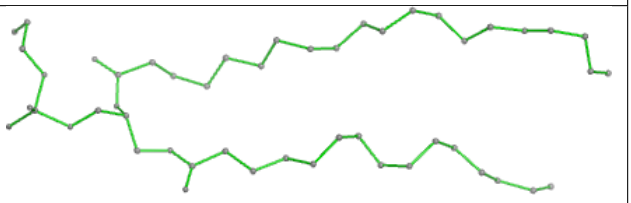


Rings

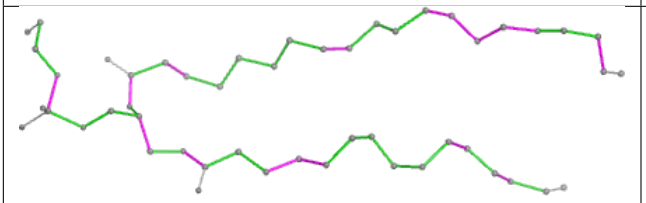
## Ligand PTY x 102



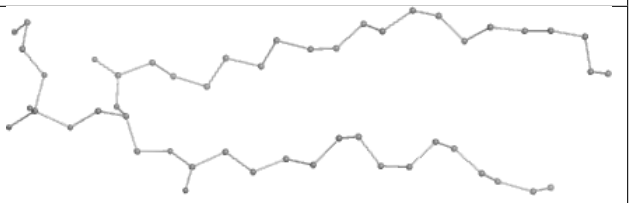
Bond lengths



Bond angles

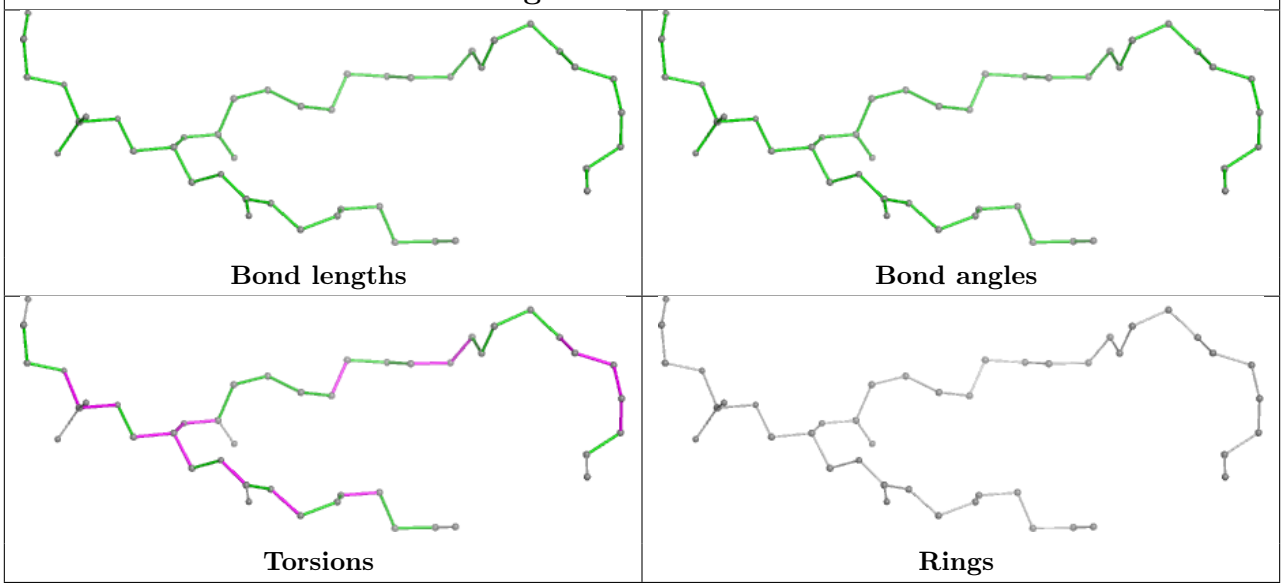


Torsions

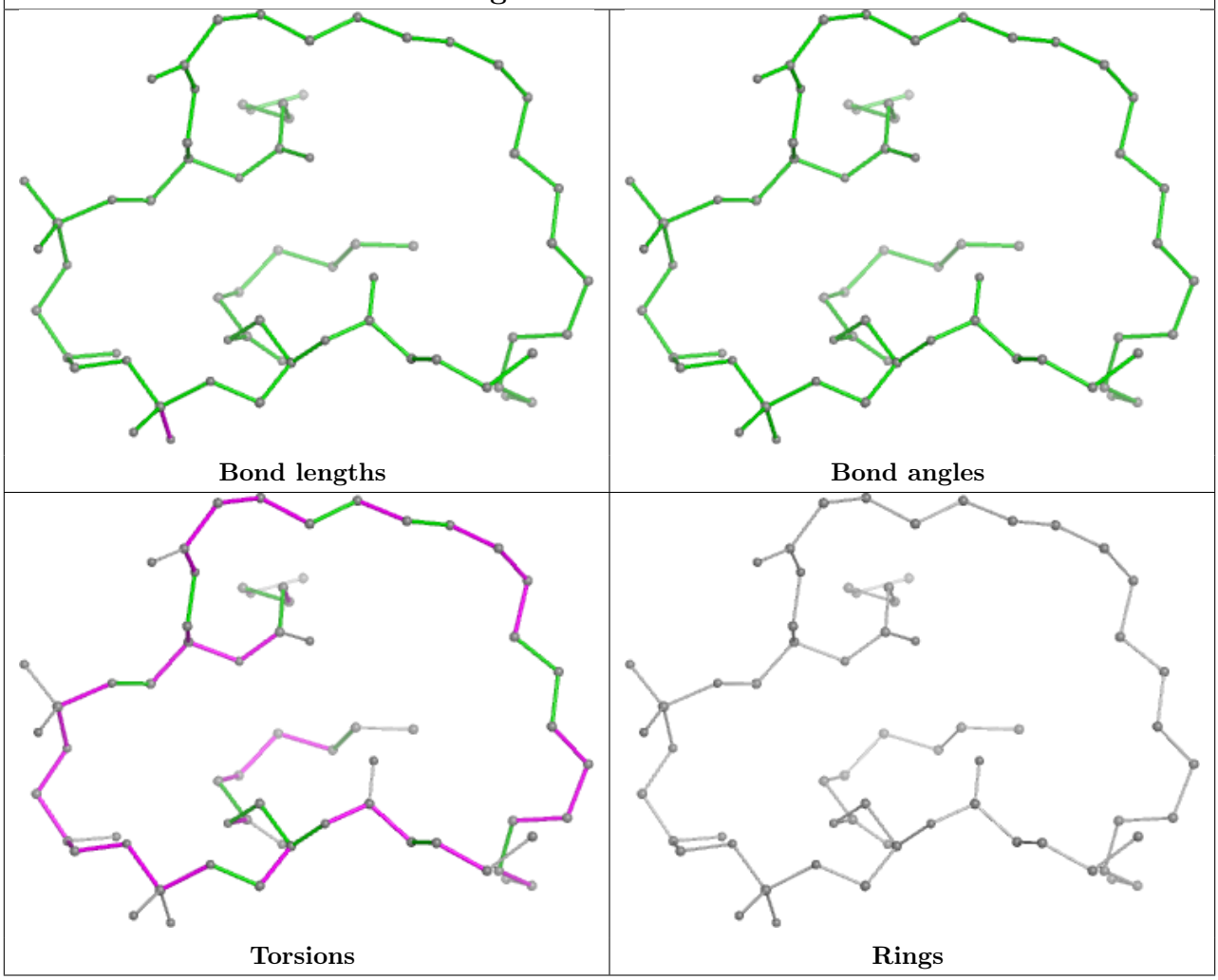


Rings

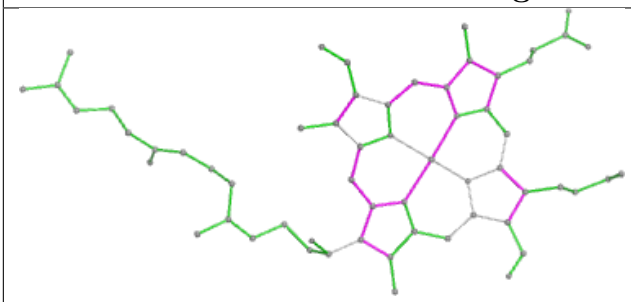
## Ligand PTY R 404



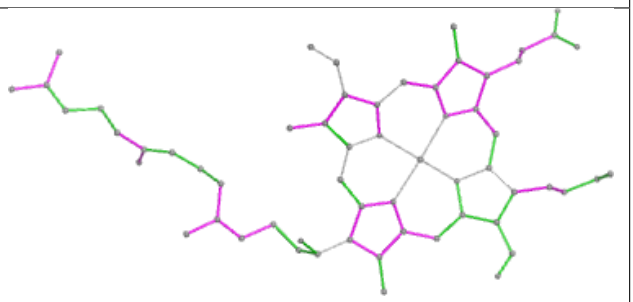

## Ligand CDL 1B 405



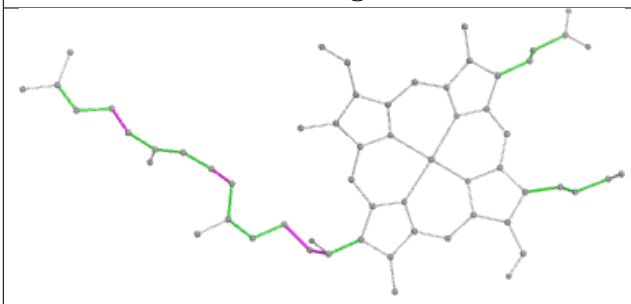
**Ligand HEA 2A 603**



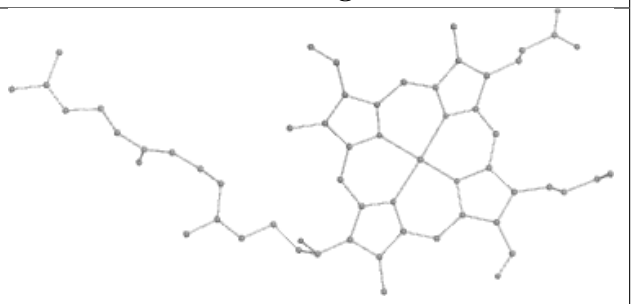
Bond lengths



Bond angles

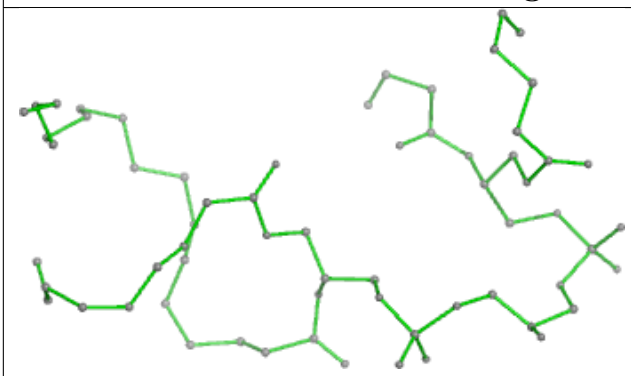


Torsions

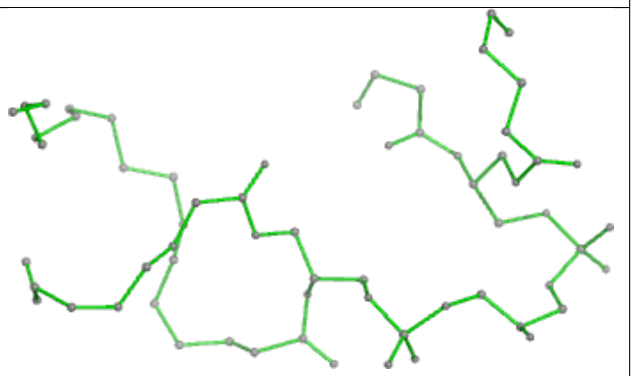


Rings

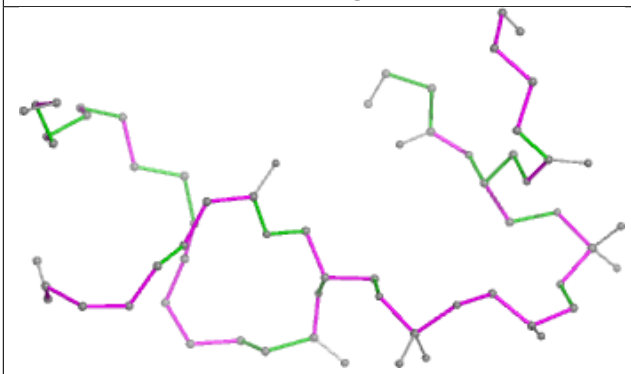
**Ligand CDL V 603**



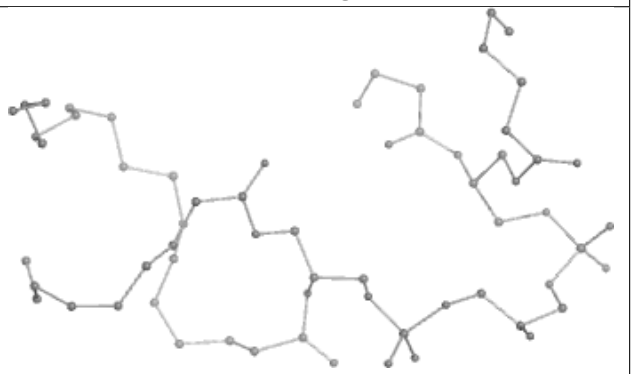
Bond lengths



Bond angles

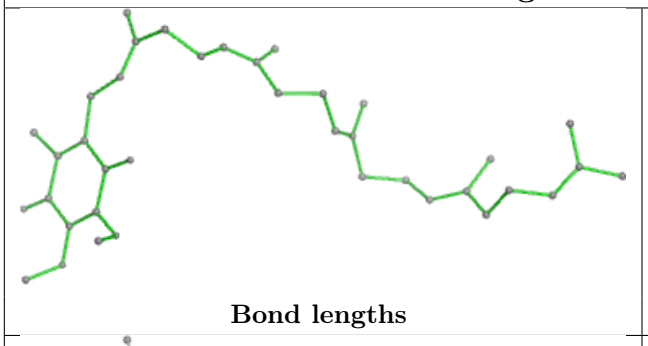


Torsions

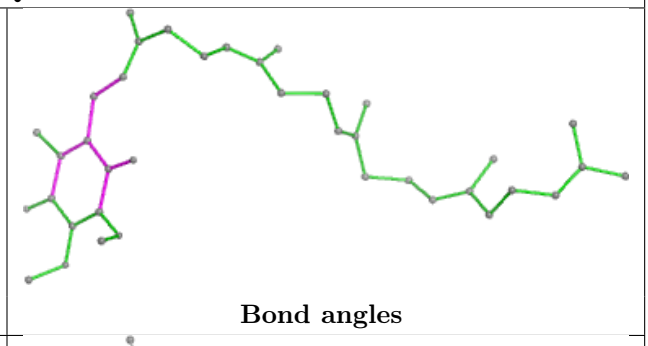


Rings

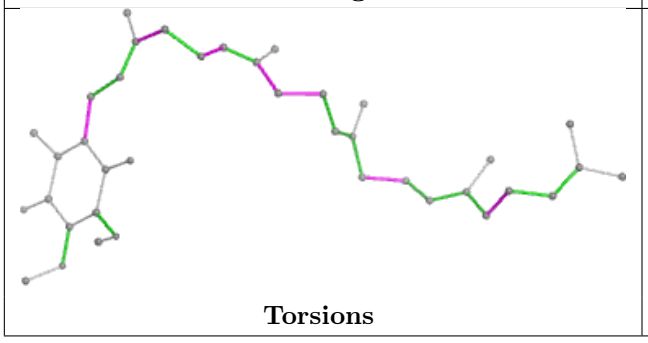
## Ligand UQ5 1B 402



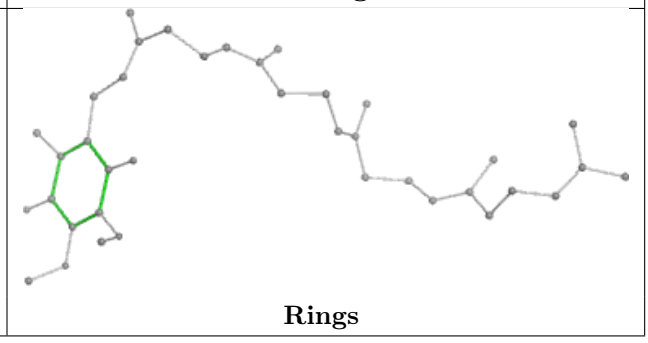
Bond lengths



Bond angles

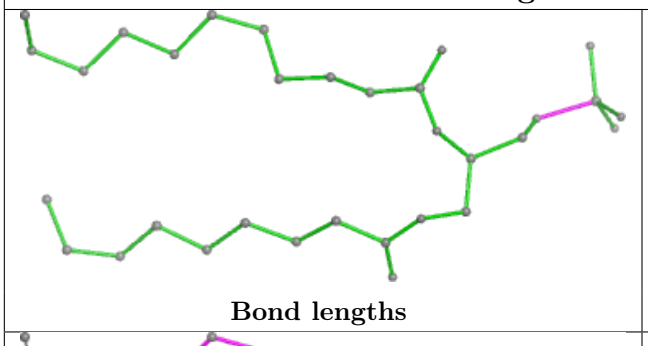


Torsions

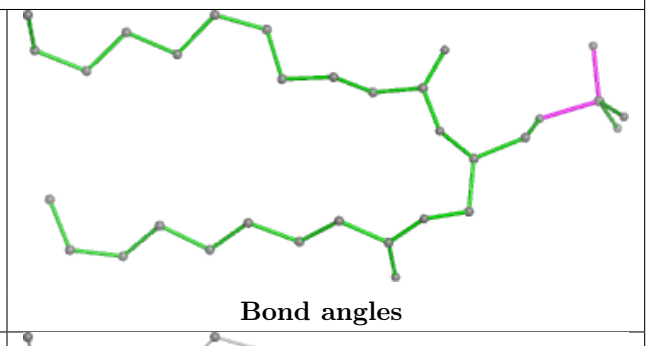


Rings

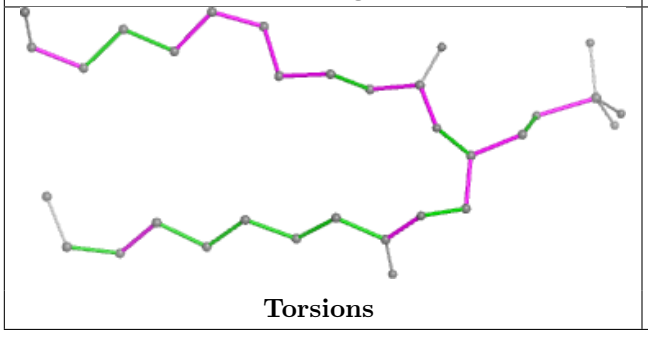
## Ligand 3PH 2D 302



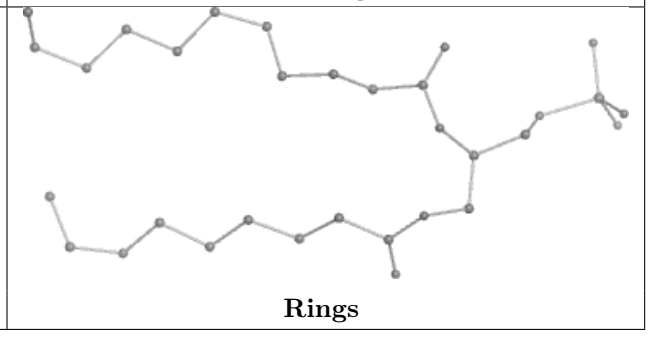
Bond lengths



Bond angles

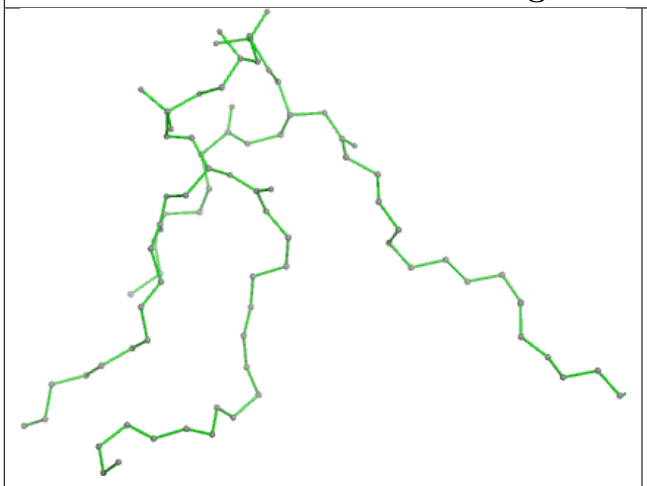


Torsions



Rings

**Ligand CDL u 602**



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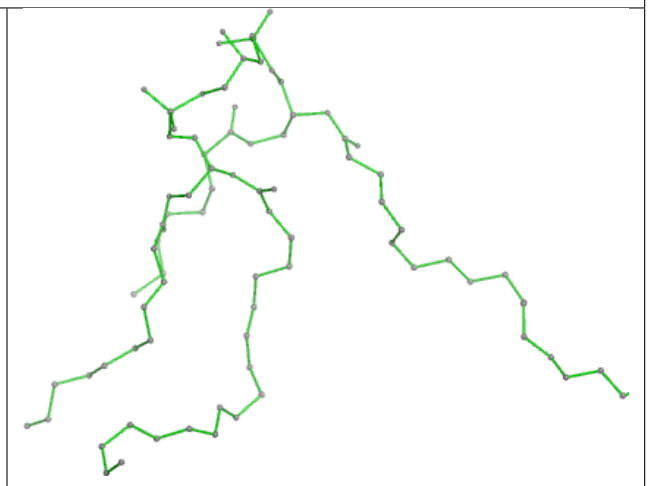

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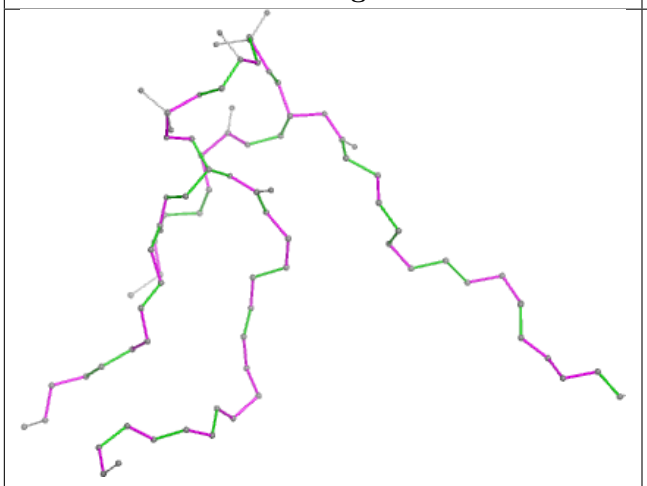

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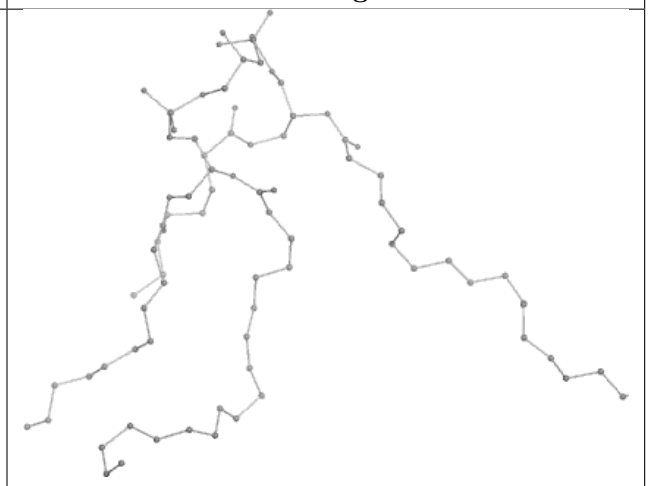
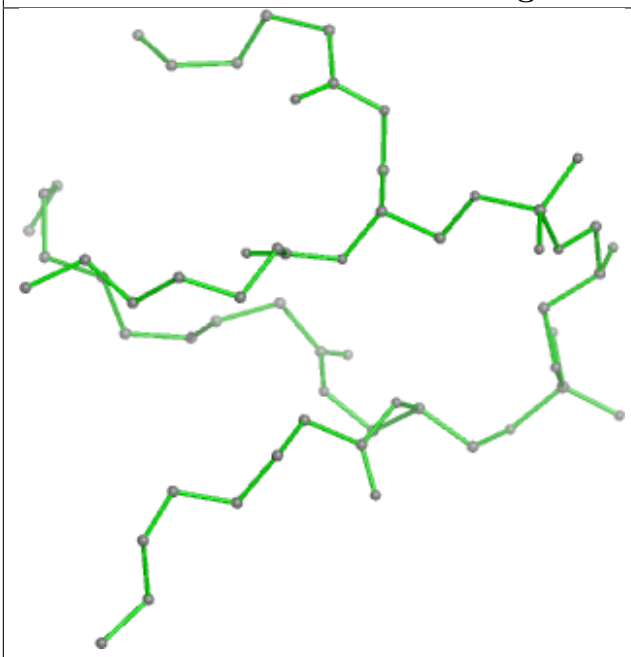


**Rings**

**Ligand CDL 1L 101**



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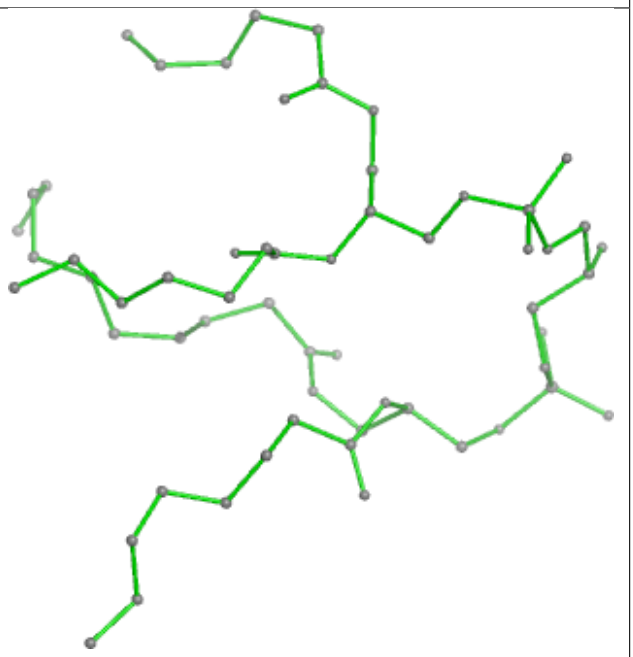

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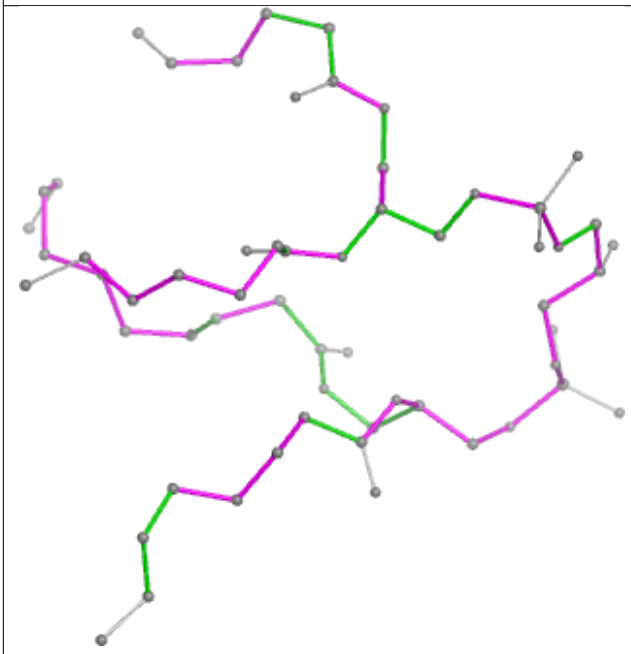

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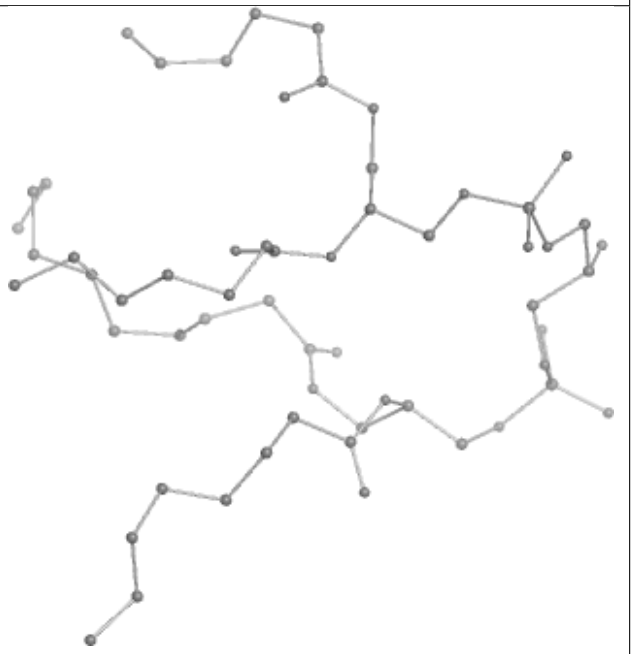
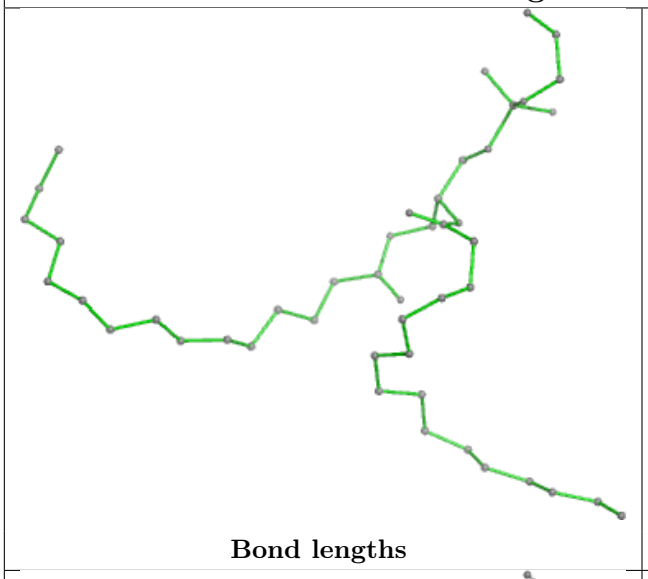


**Rings**

**Ligand PTY S 302**



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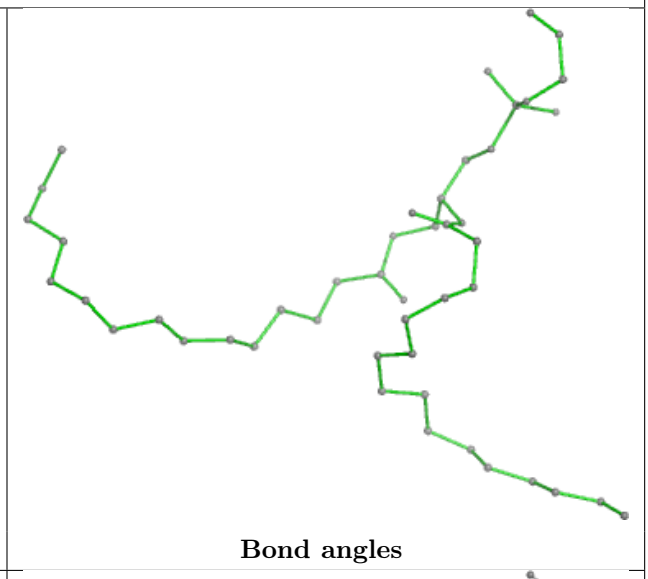

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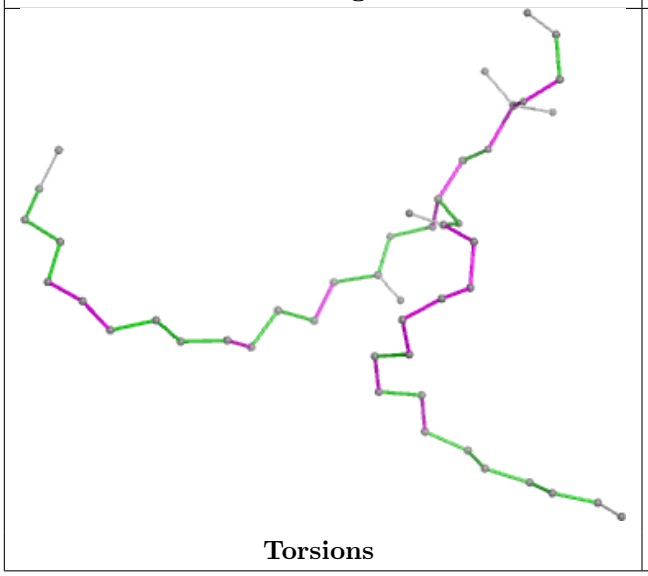

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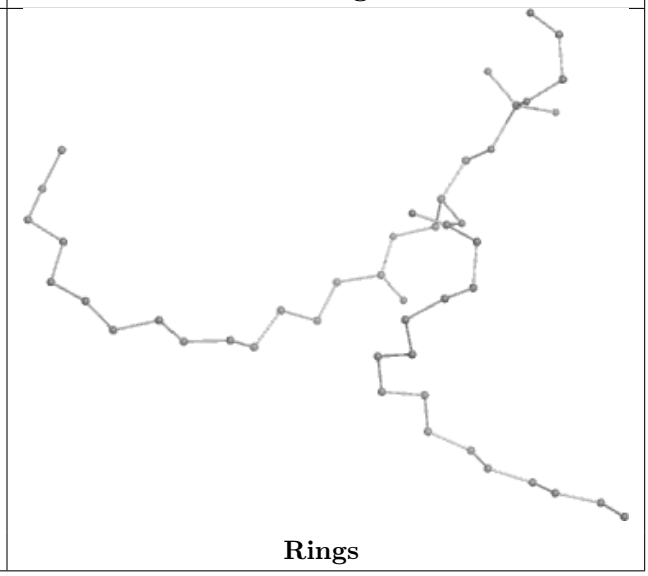
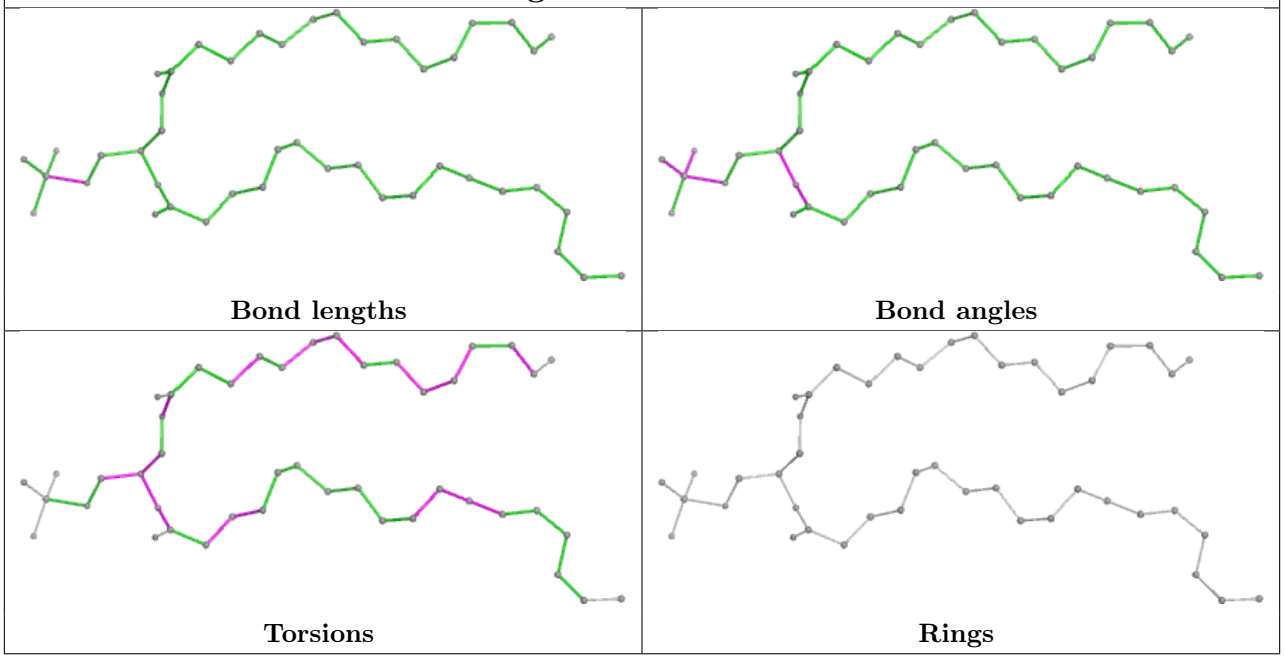
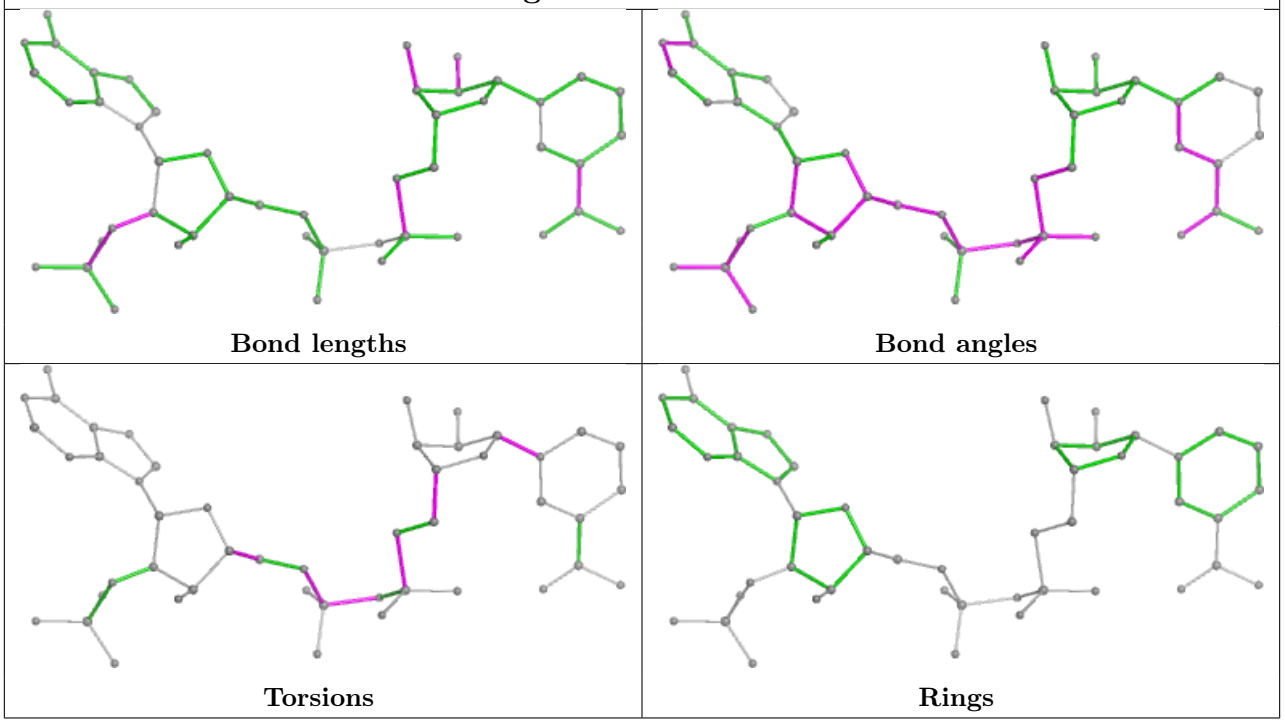


**Rings**

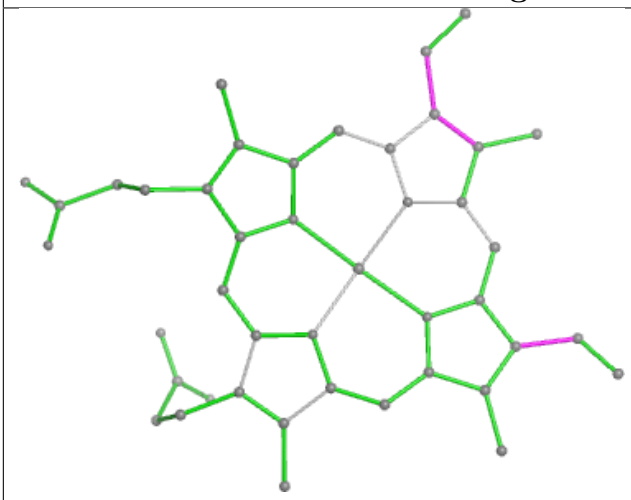
**Ligand 3PH w 201**




**Ligand NDP P 401**



**Ligand HEM 1B 404**



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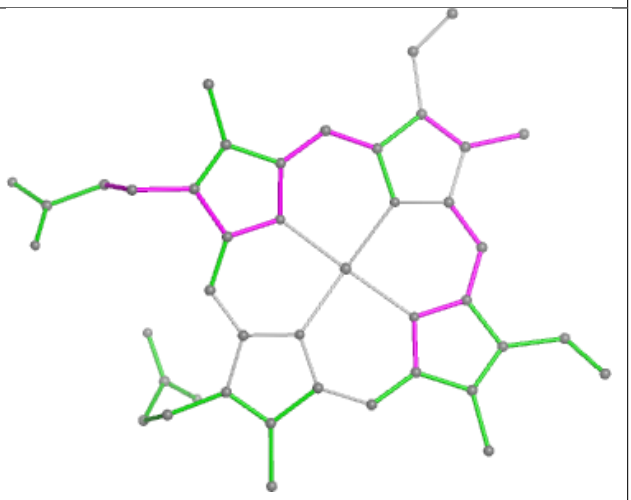

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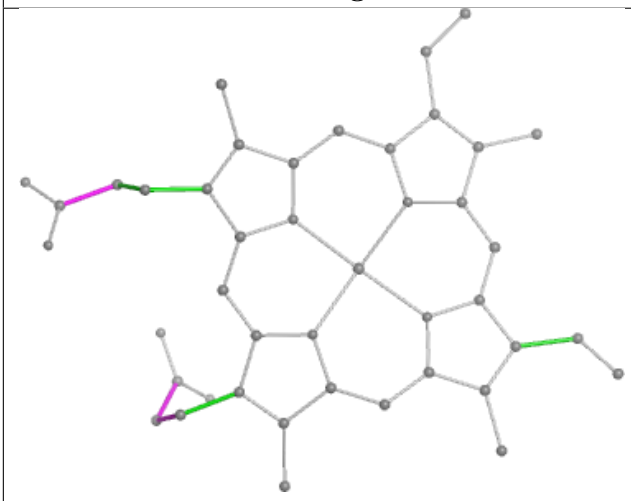

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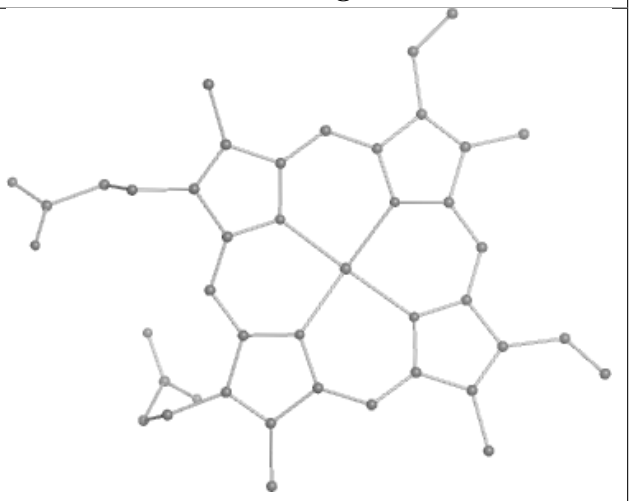
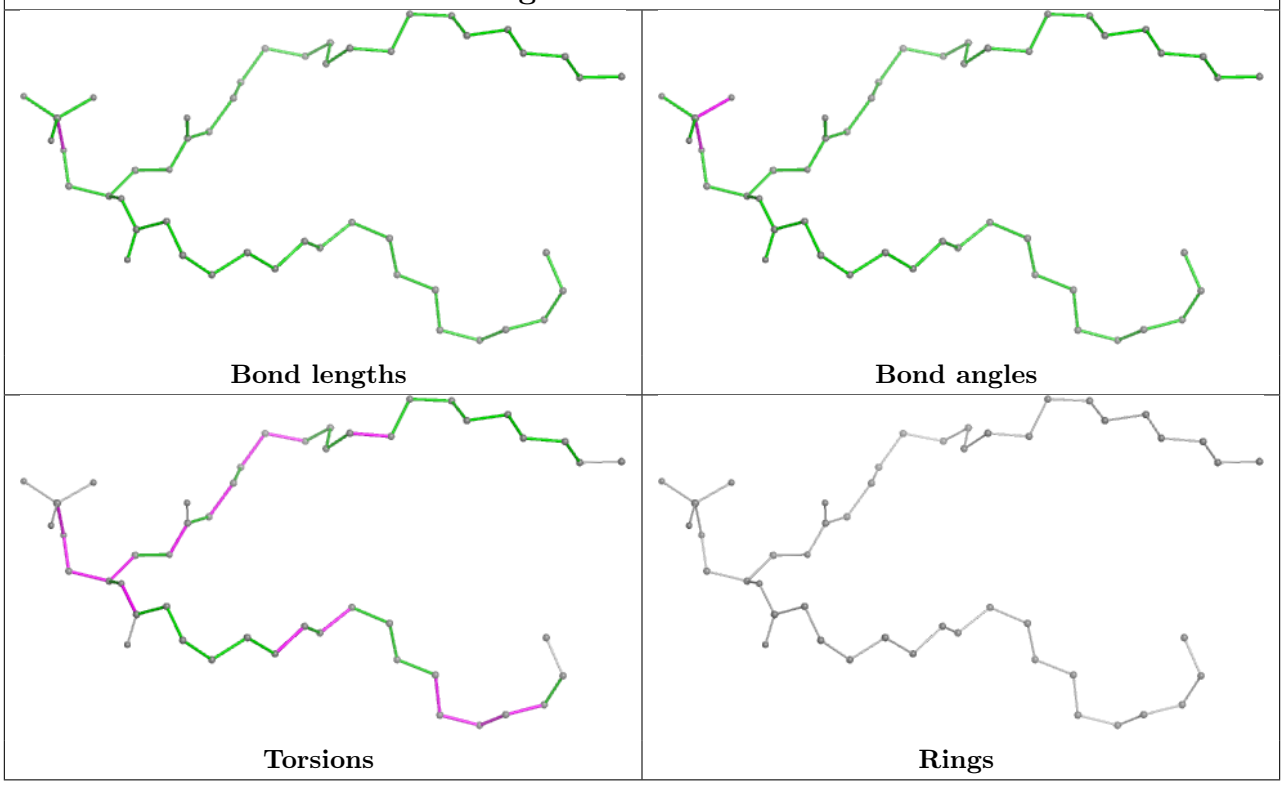
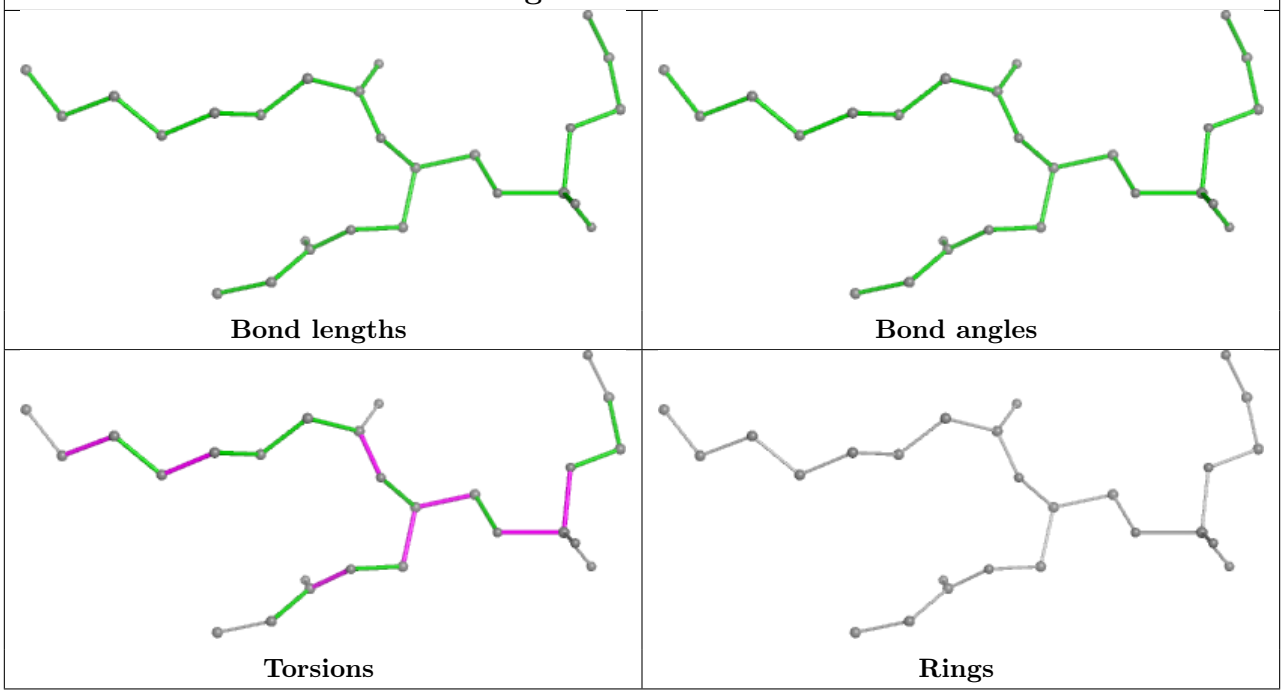


**Rings**

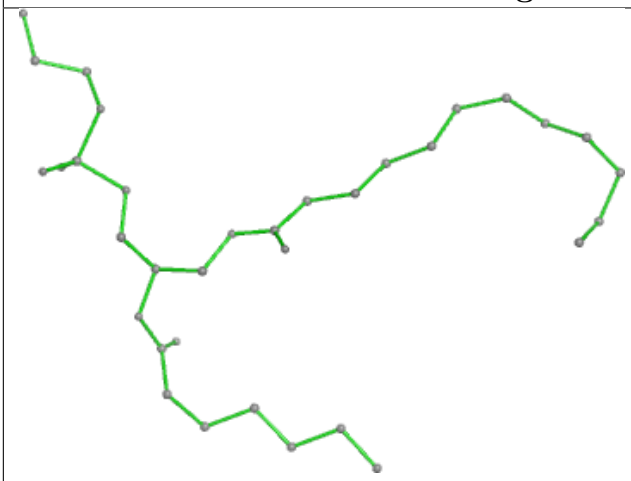
## Ligand 3PH 1B 406



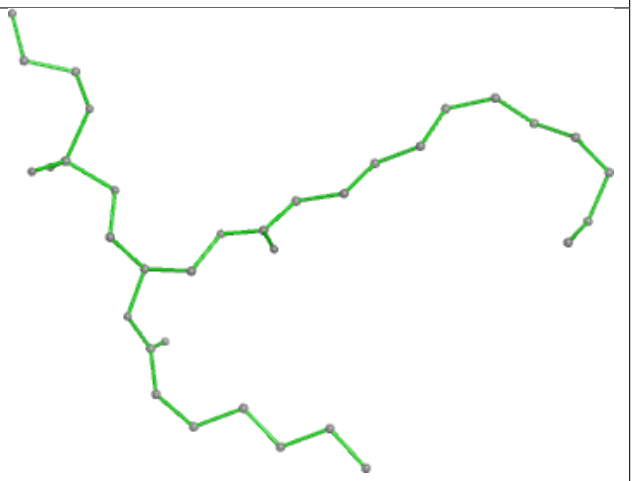

## Ligand PTY T 506



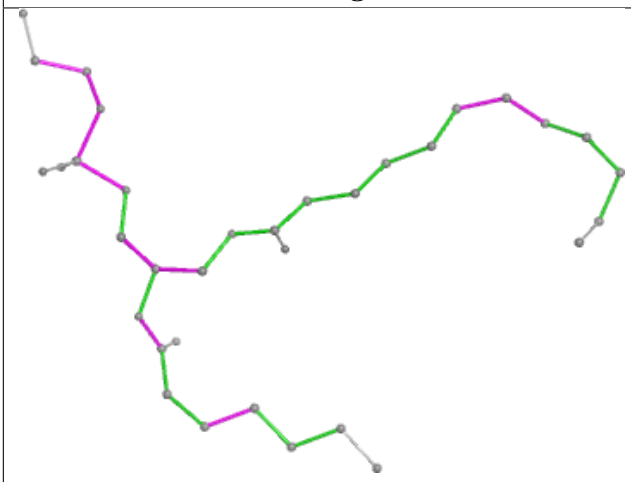
**Ligand PTY 2F 101**



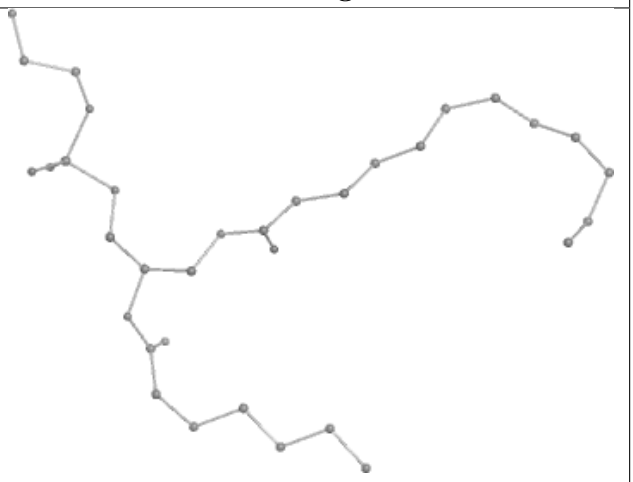
**Bond lengths**



**Bond angles**

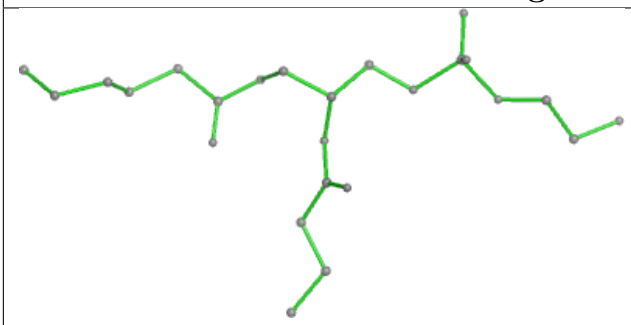


**Torsions**



**Rings**

## Ligand PTY e 301



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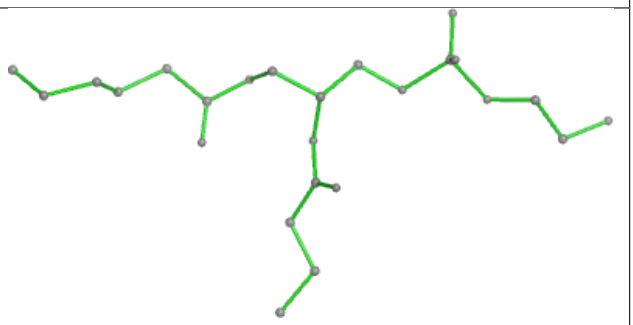
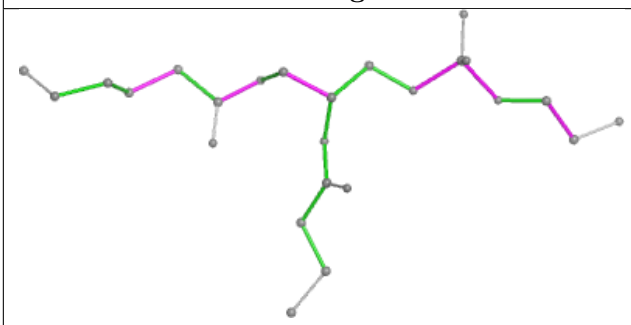


Bond angles



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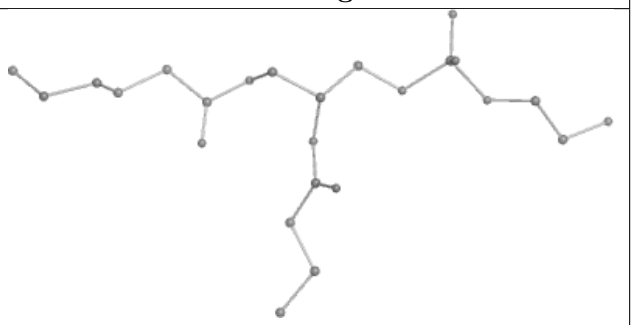
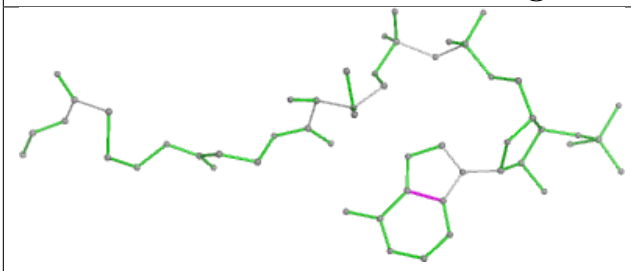


Rings

## Ligand COO s 401



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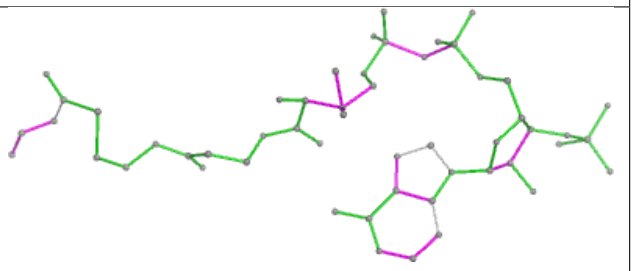
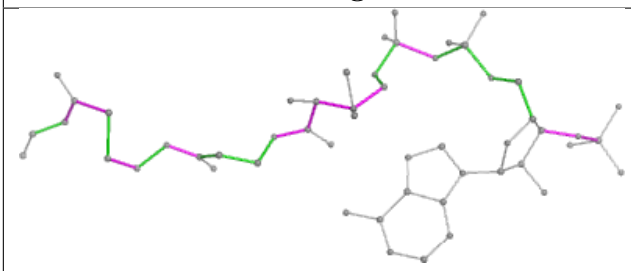
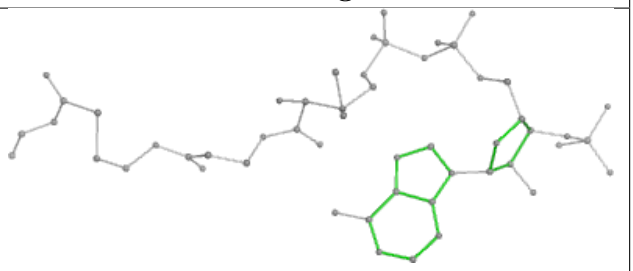


Bond angles

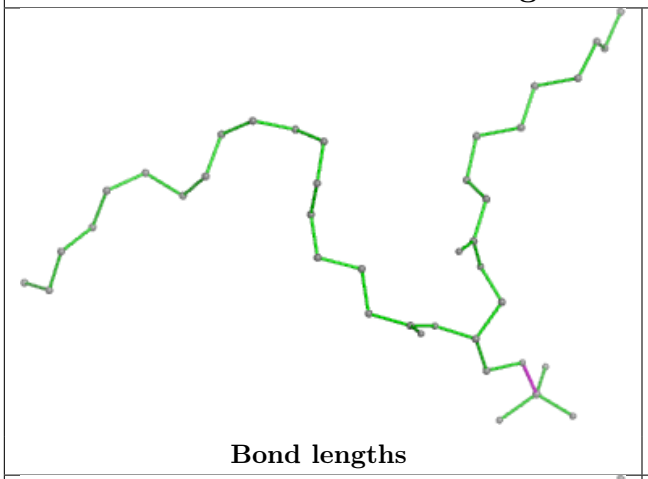


Torsions



Rings

**Ligand 3PH 1E 402**



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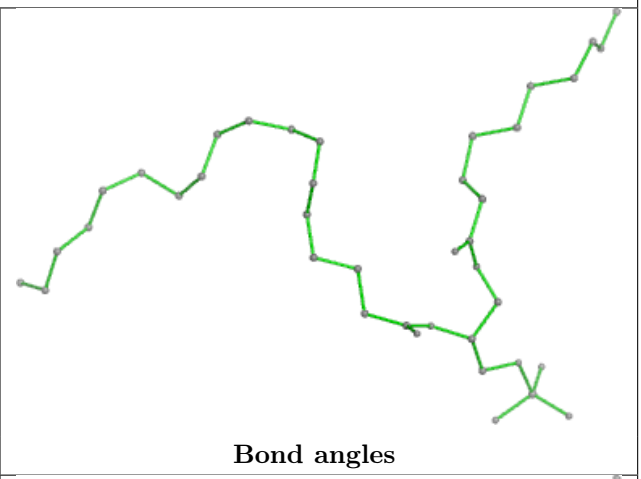
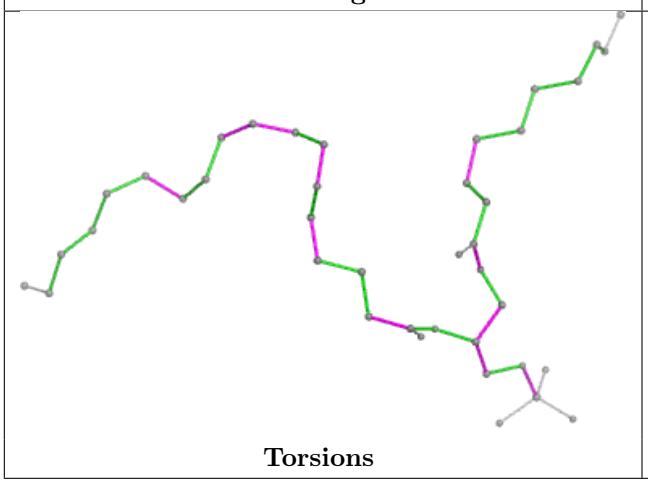


Bond angles



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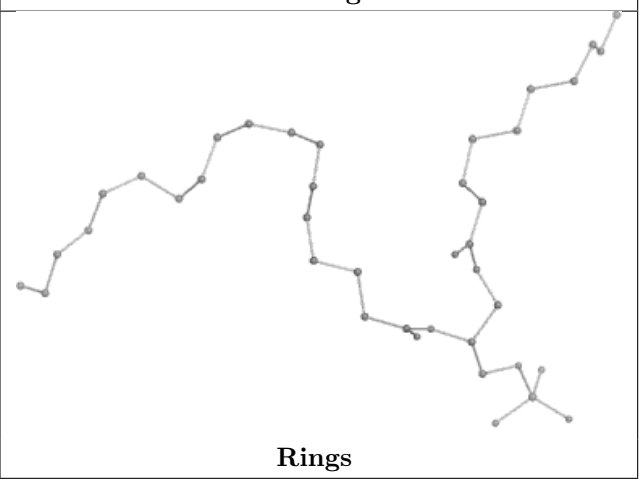
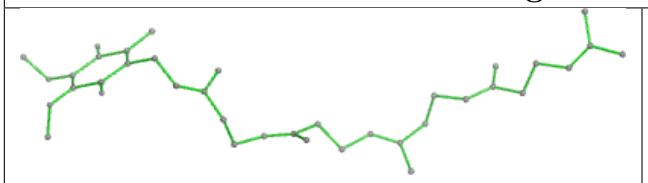


Rings

**Ligand UQ5 Q 301**



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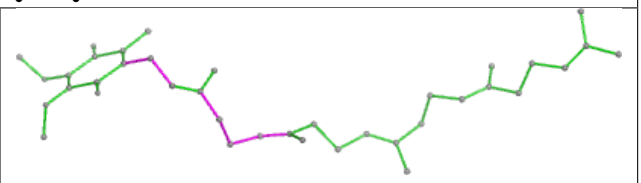
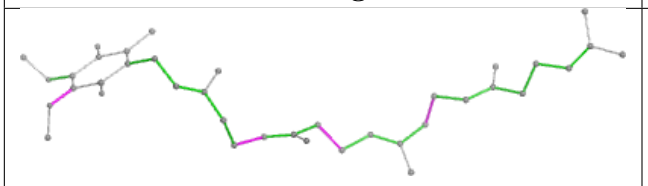


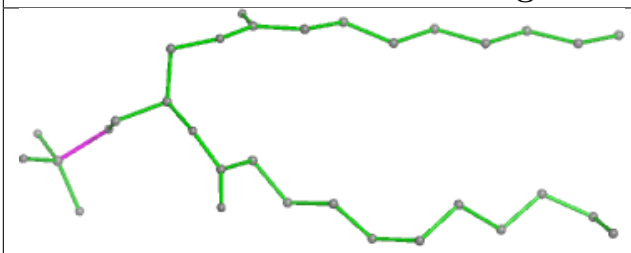
Bond angles



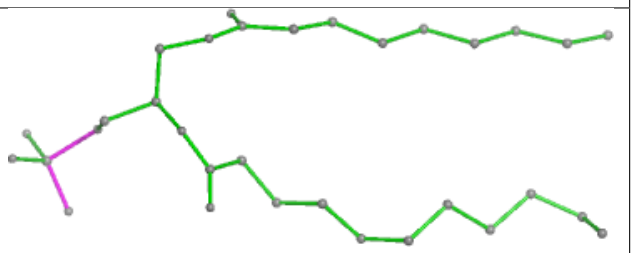
Torsions

Rings

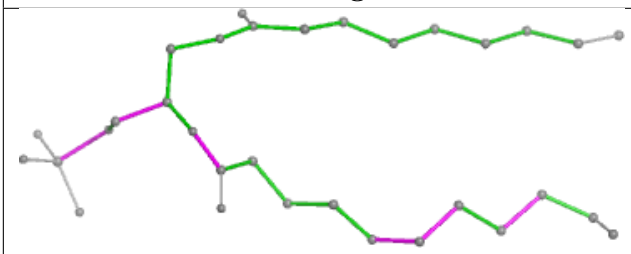
## Ligand 3PH 3D 302



Bond lengths



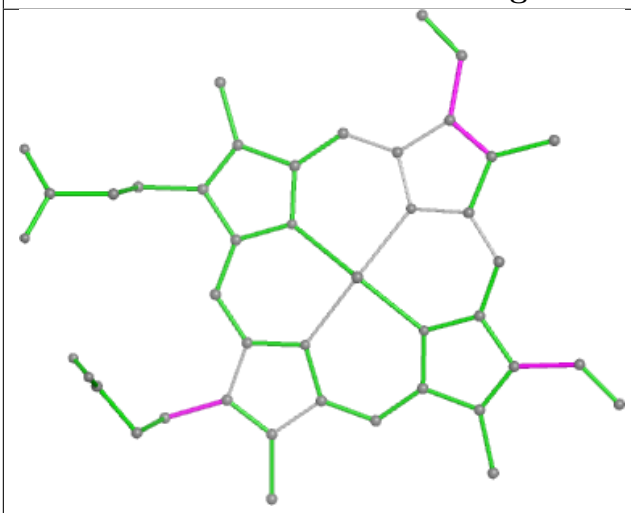
Bond angles



Torsions

Rings

## Ligand HEM 1B 403



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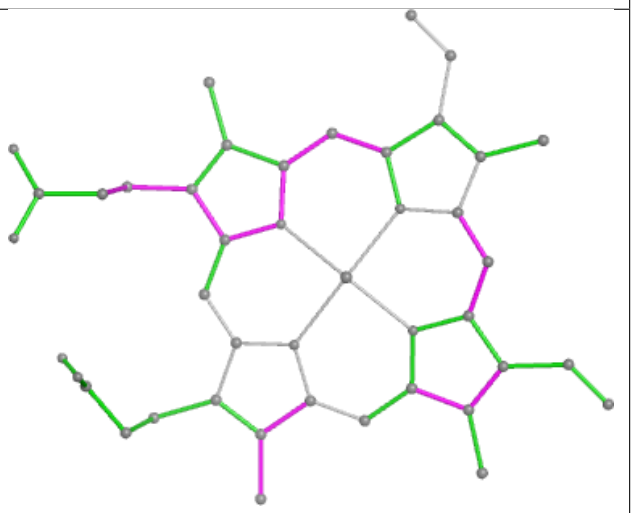
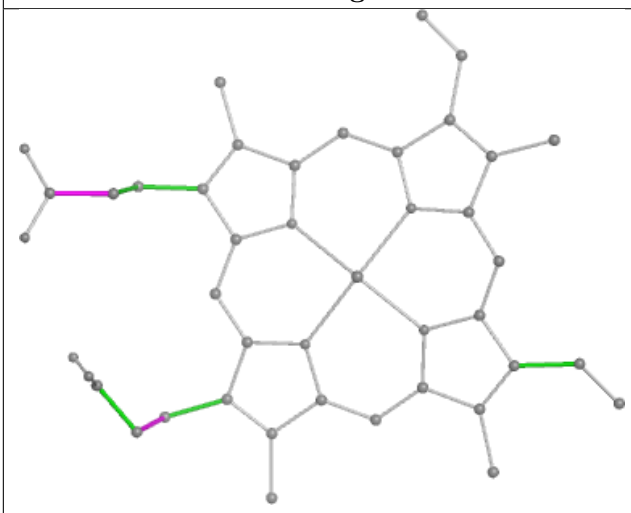
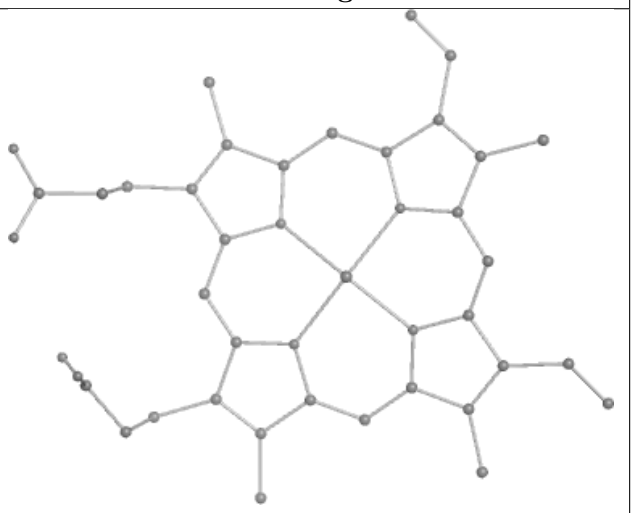


Bond angles

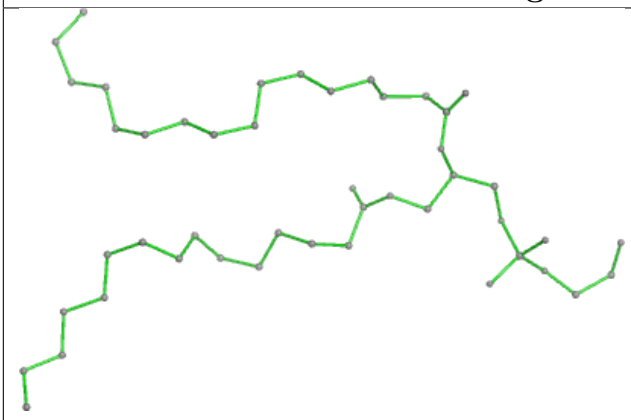


Torsions



Rings

## Ligand PTY h 202



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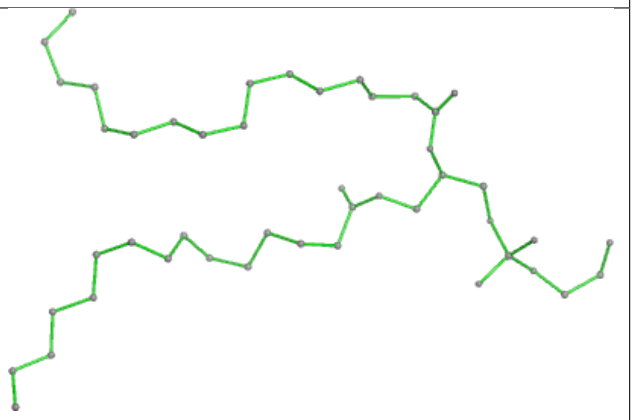
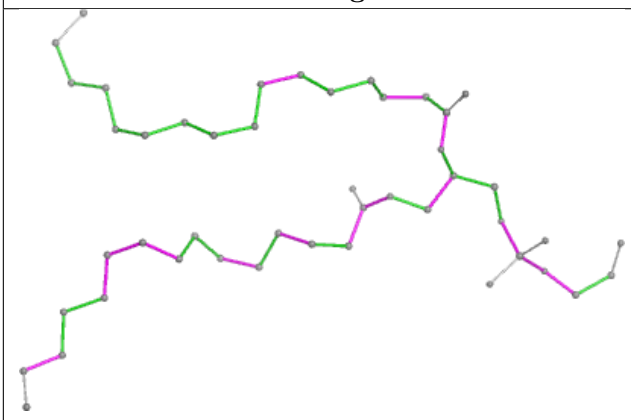
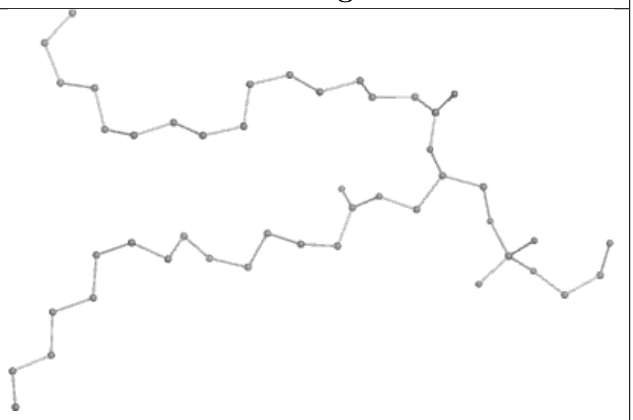


Bond angles

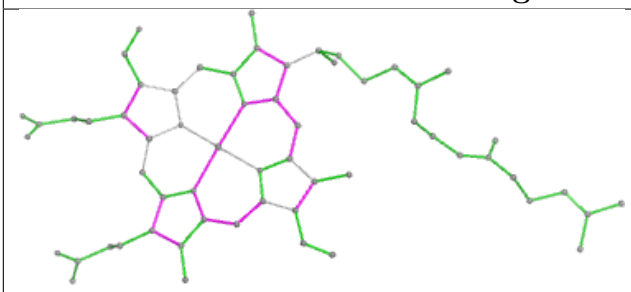


Torsions

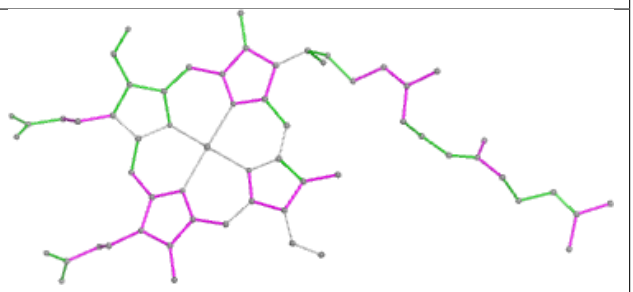


Rings

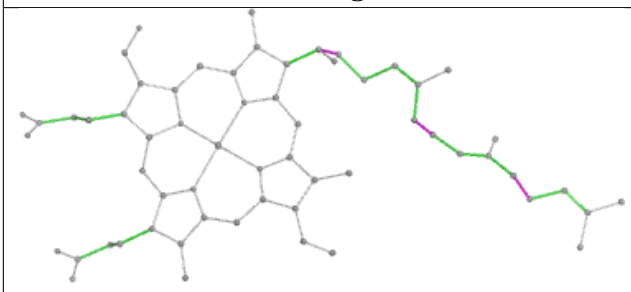
## Ligand HEA 3A 603



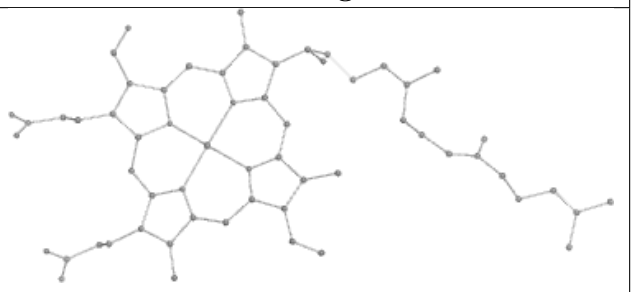
Bond lengths



Bond angles

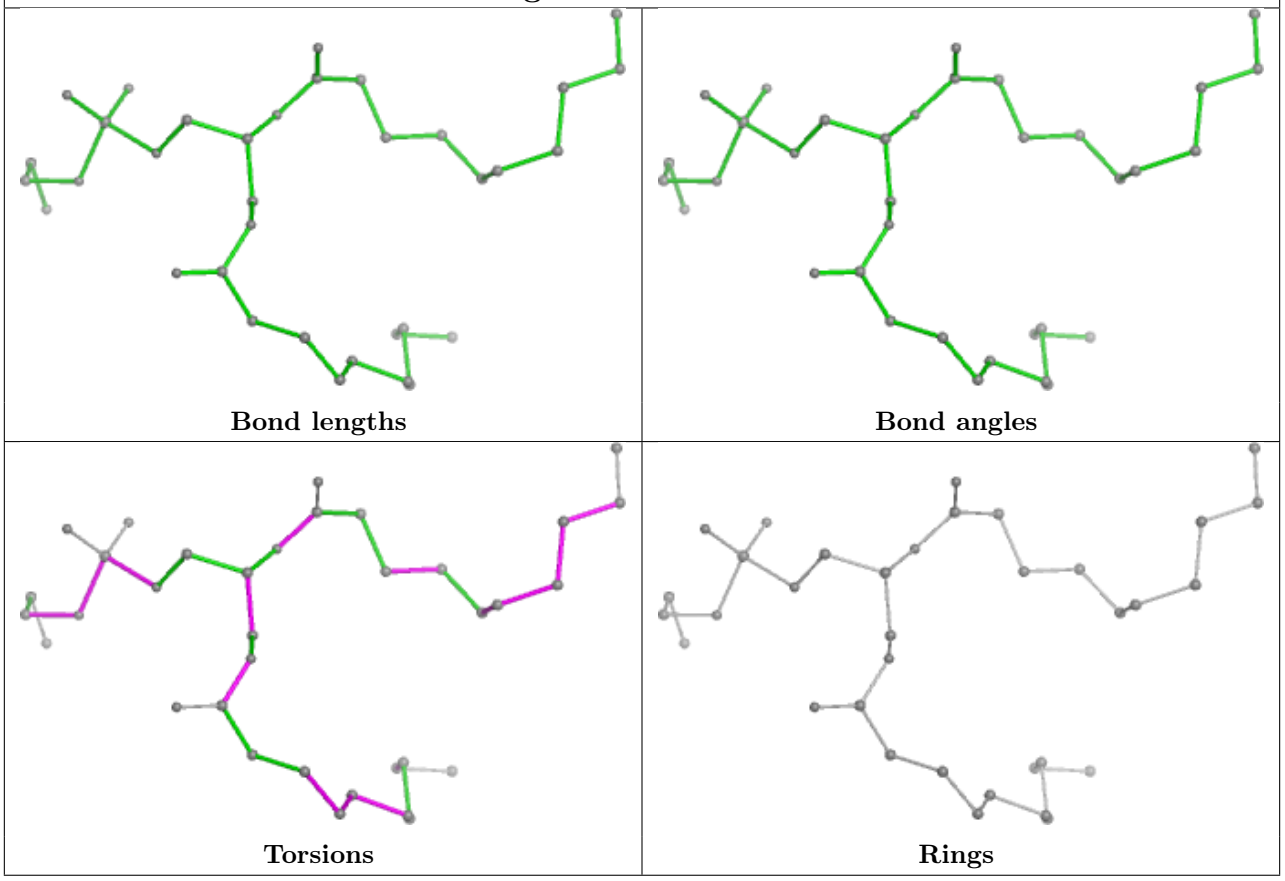


Torsions

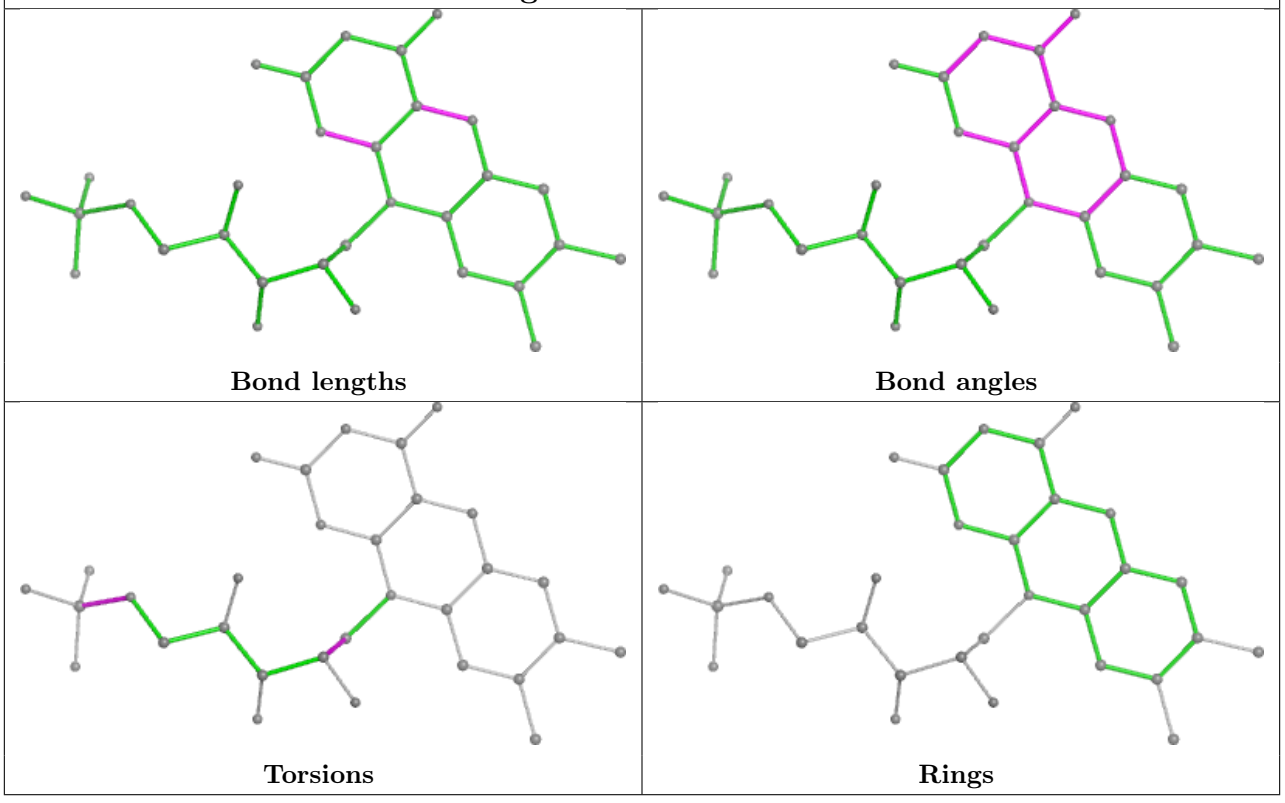


Rings

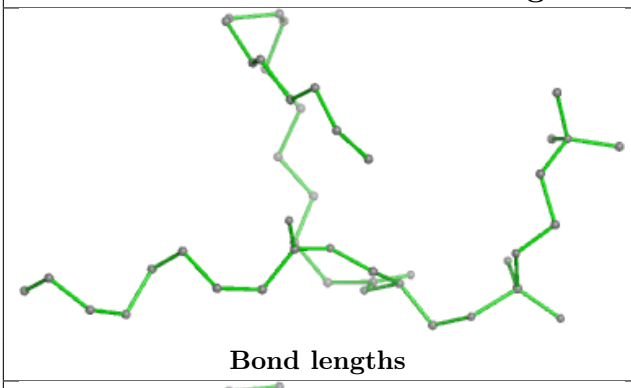
## Ligand PTY V 606



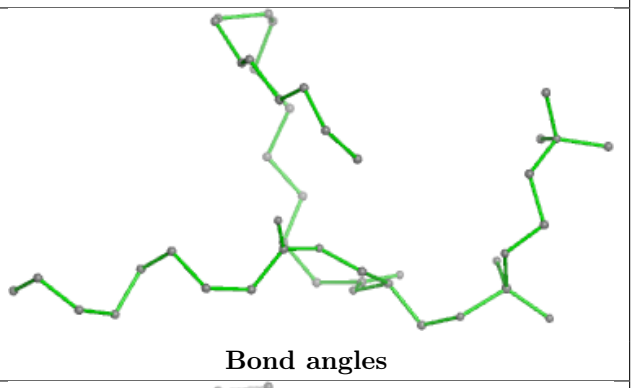

## Ligand FMN B 501



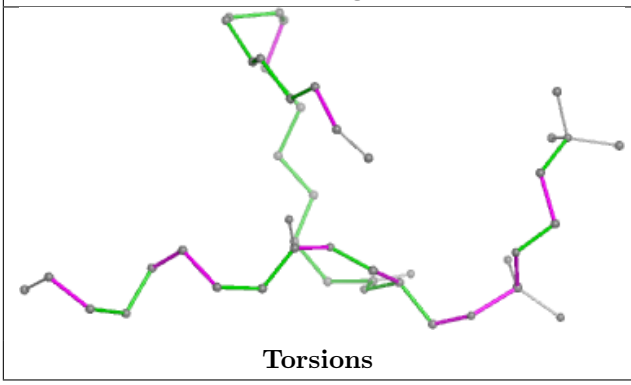
## Ligand PC7 R 403



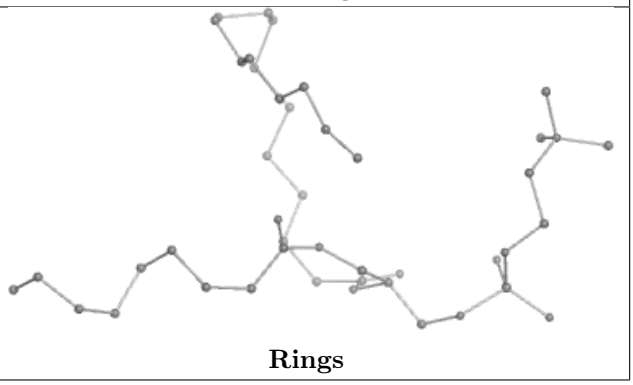
Bond lengths



Bond angles

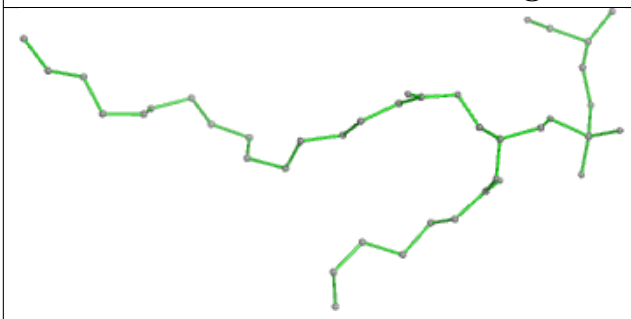


Torsions

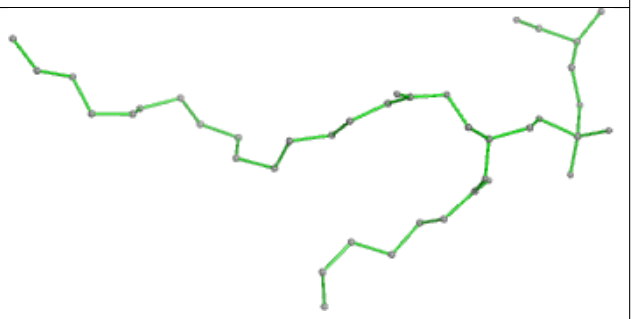


Rings

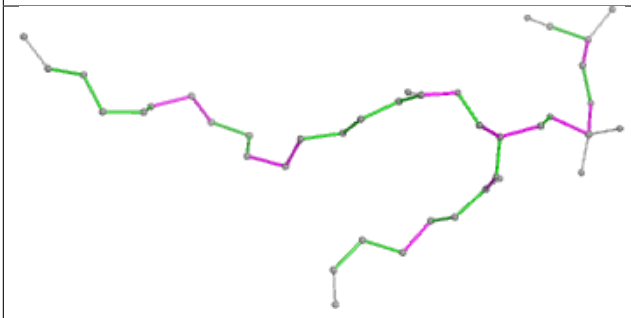
## Ligand PGT T 505



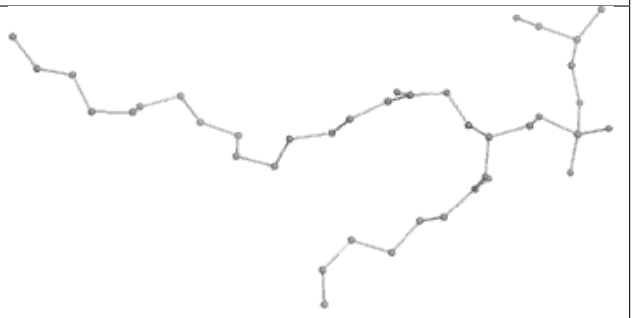
Bond lengths



Bond angles

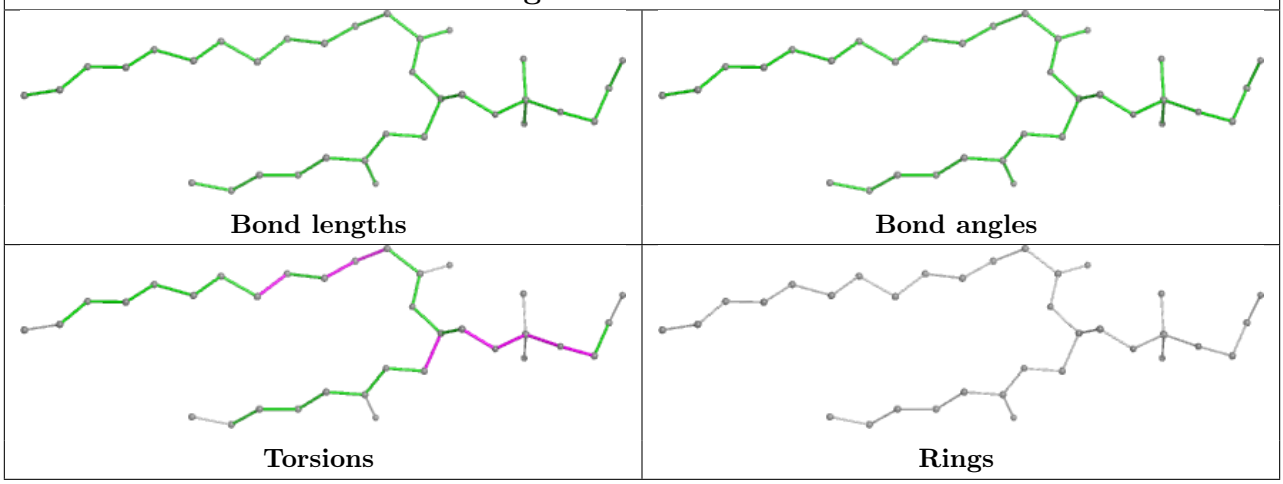


Torsions

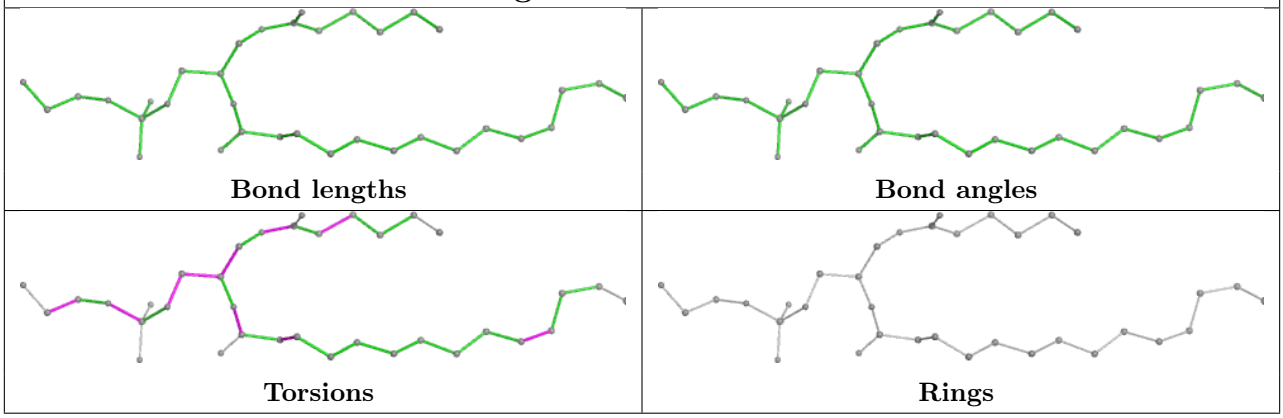


Rings

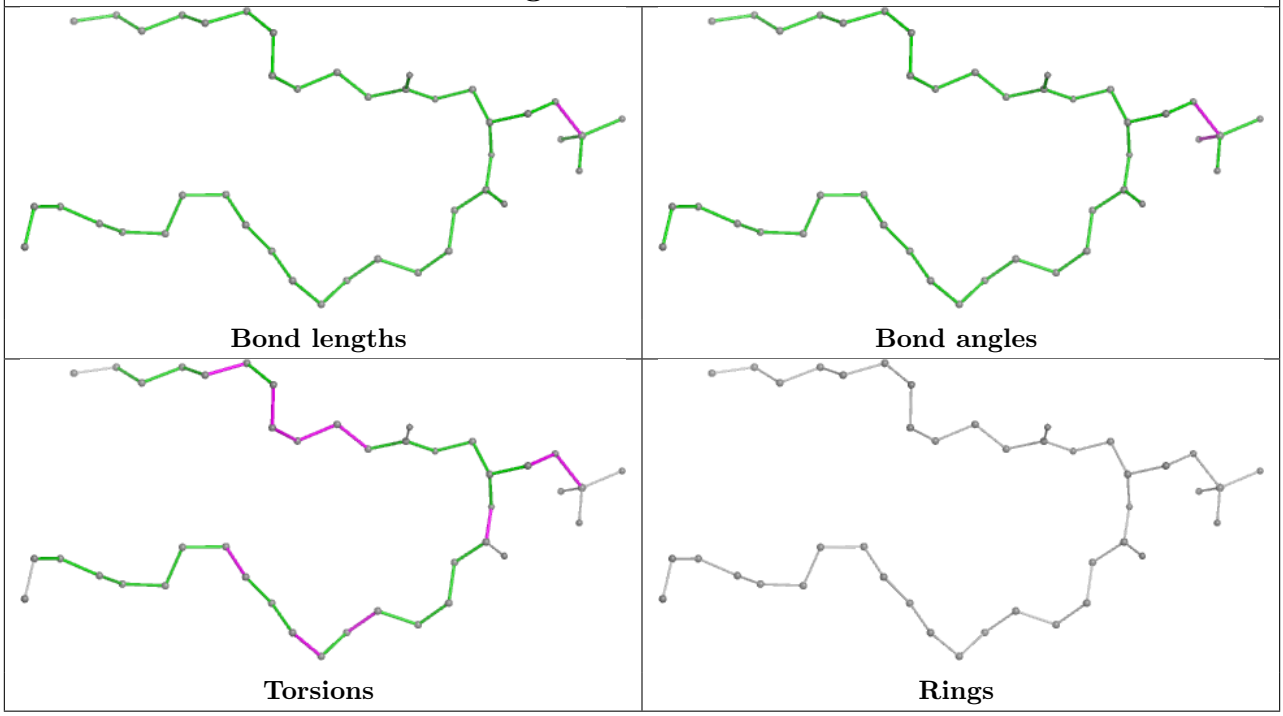
## Ligand PTY R 402



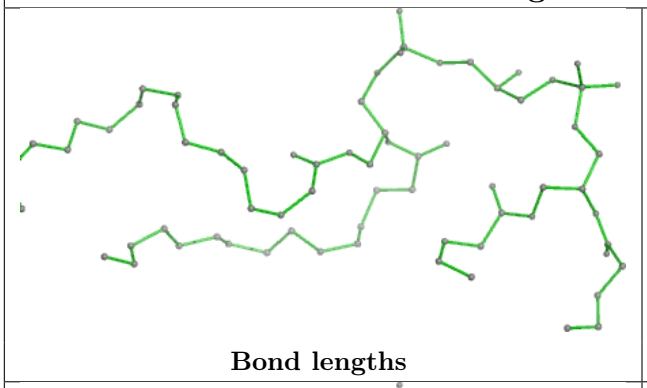

## Ligand PTY 3D 301



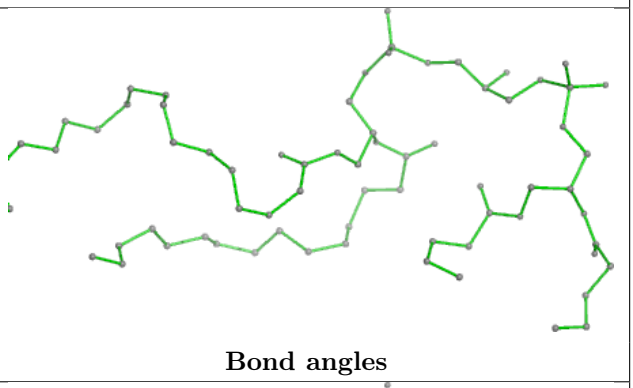

## Ligand 3PH 2I 201



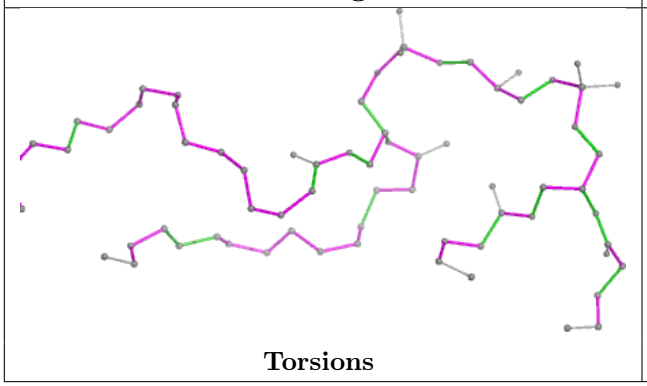
## Ligand CDL u 603



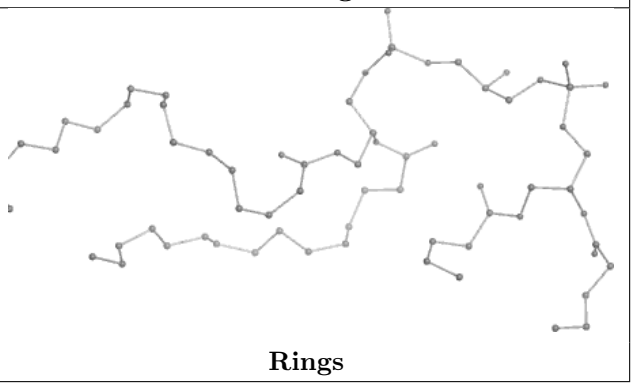
Bond lengths



Bond angles

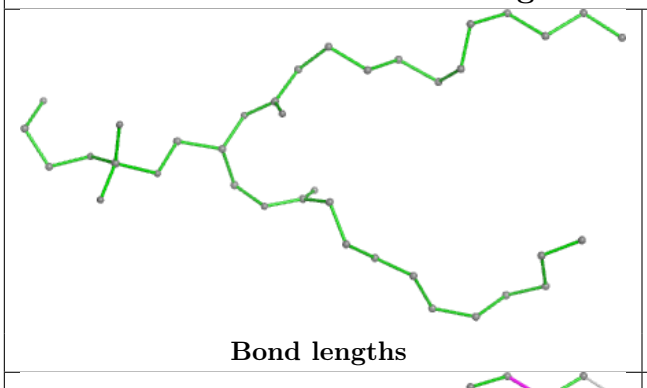


Torsions

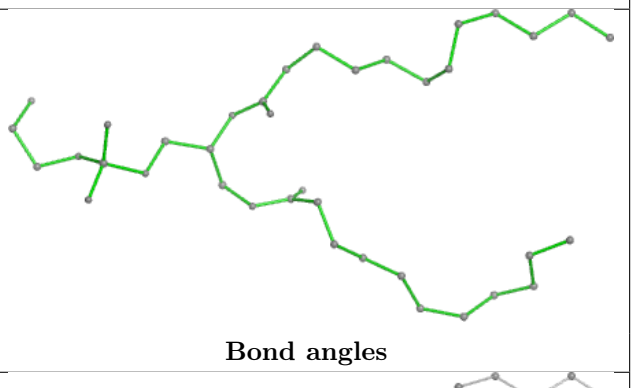


Rings

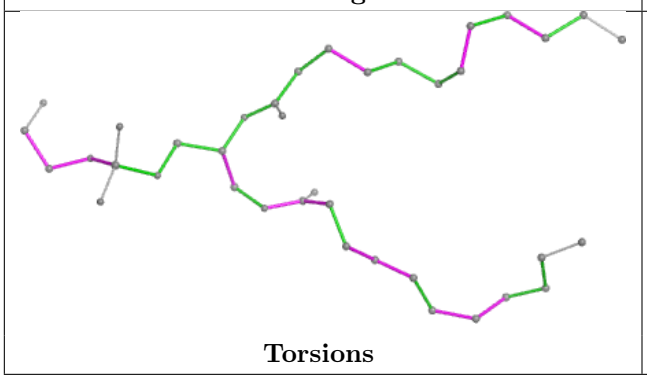
## Ligand PTY 1F 403



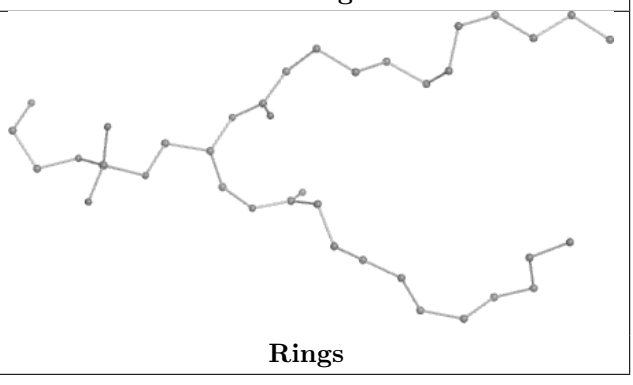
Bond lengths



Bond angles

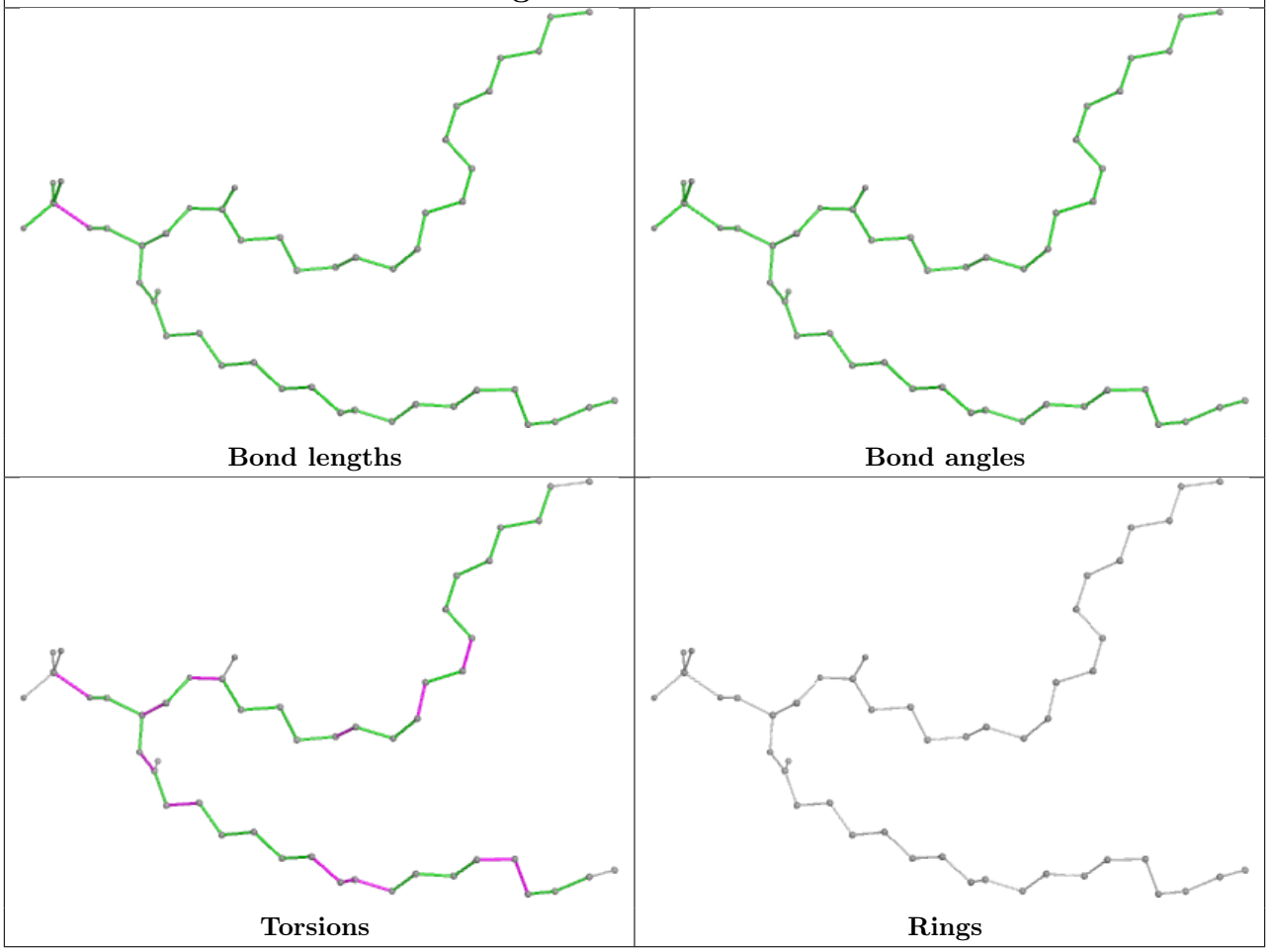


Torsions

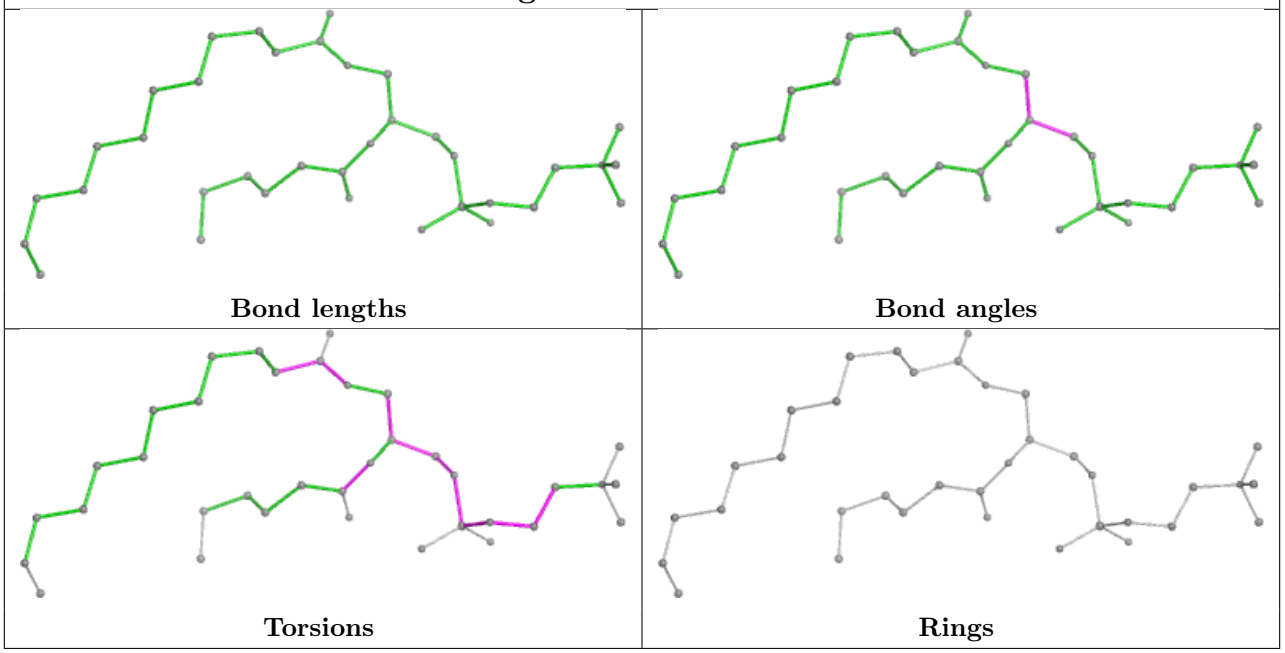


Rings

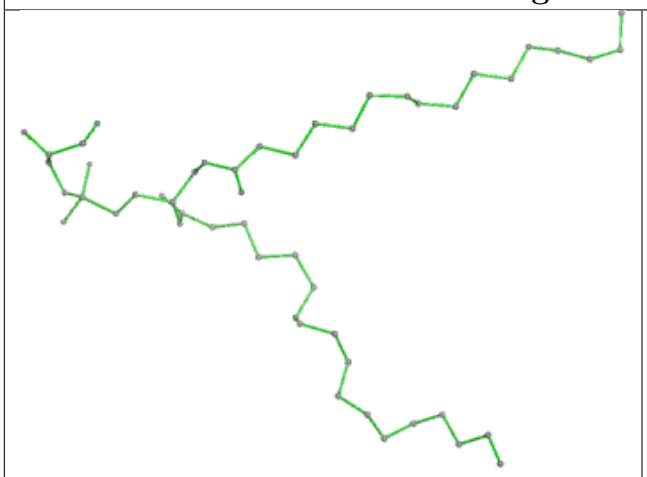
## Ligand 3PH 1B 407



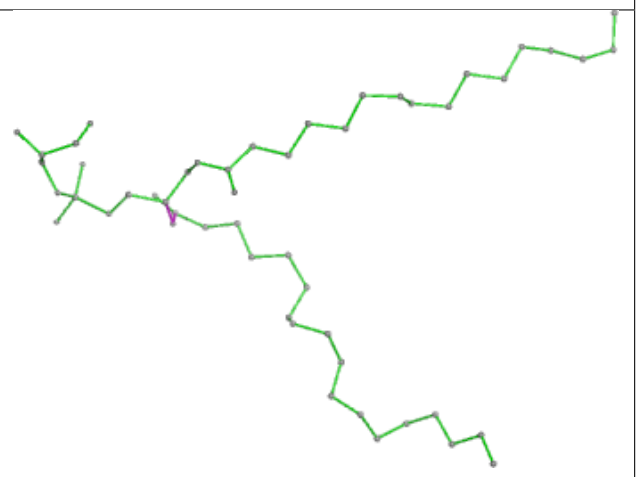

## Ligand PC7 1G 301



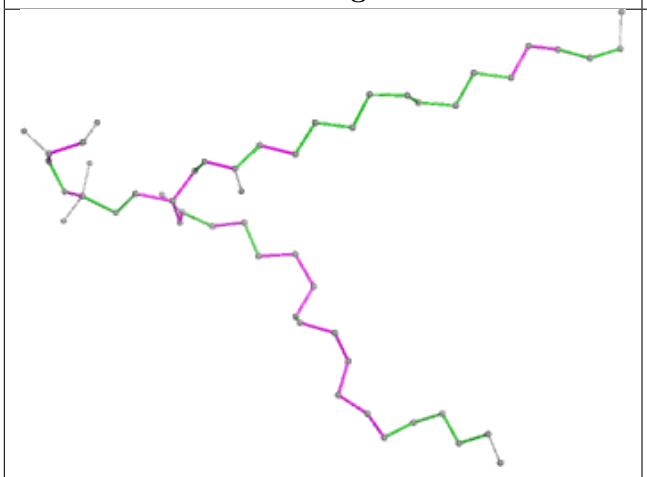
**Ligand PGT l 701**



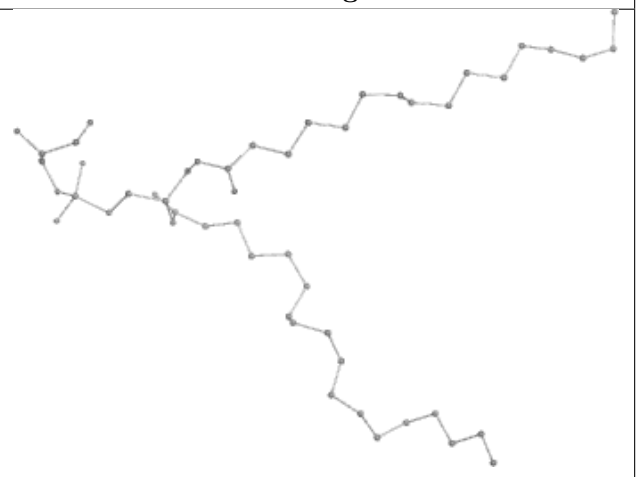
**Bond lengths**



**Bond angles**

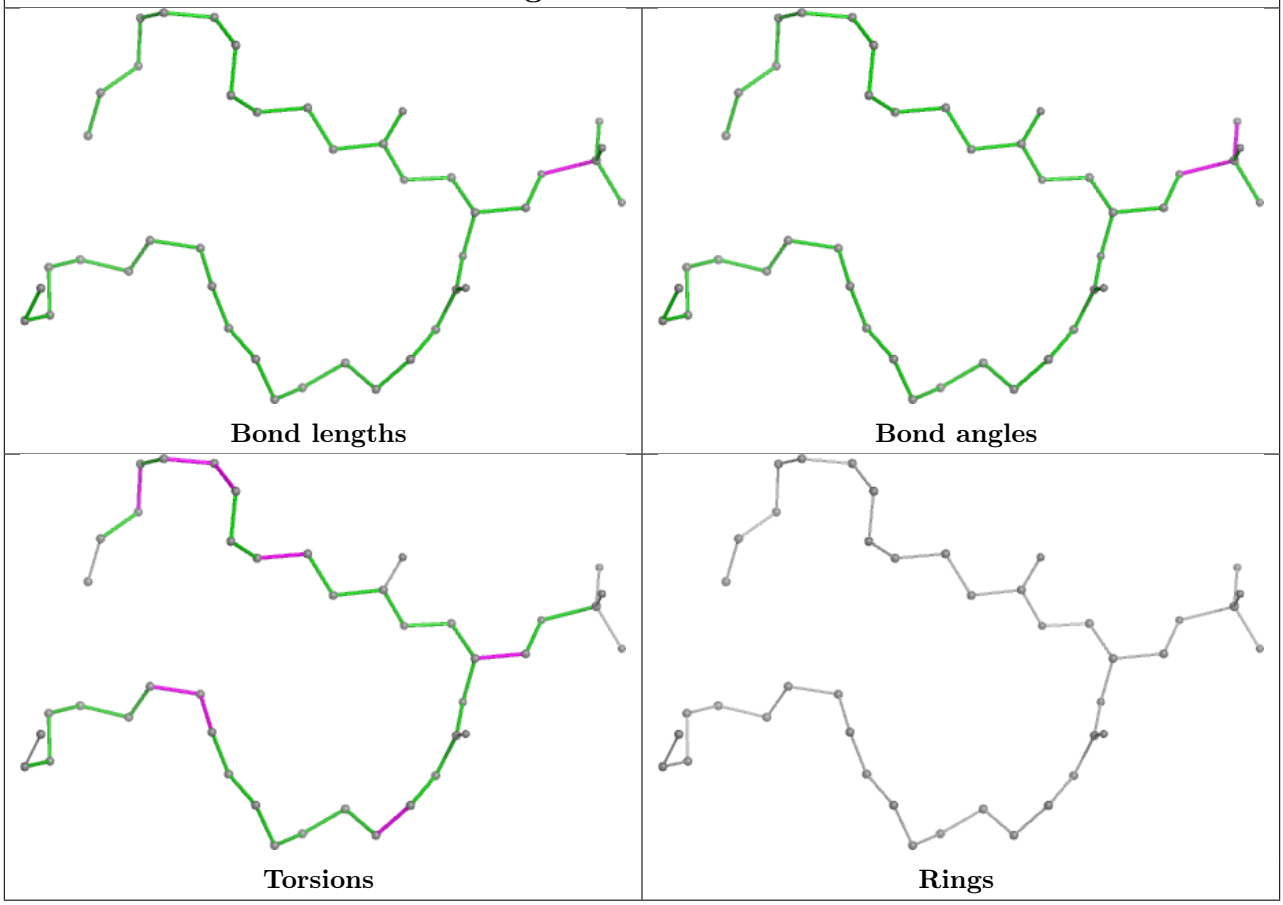


**Torsions**

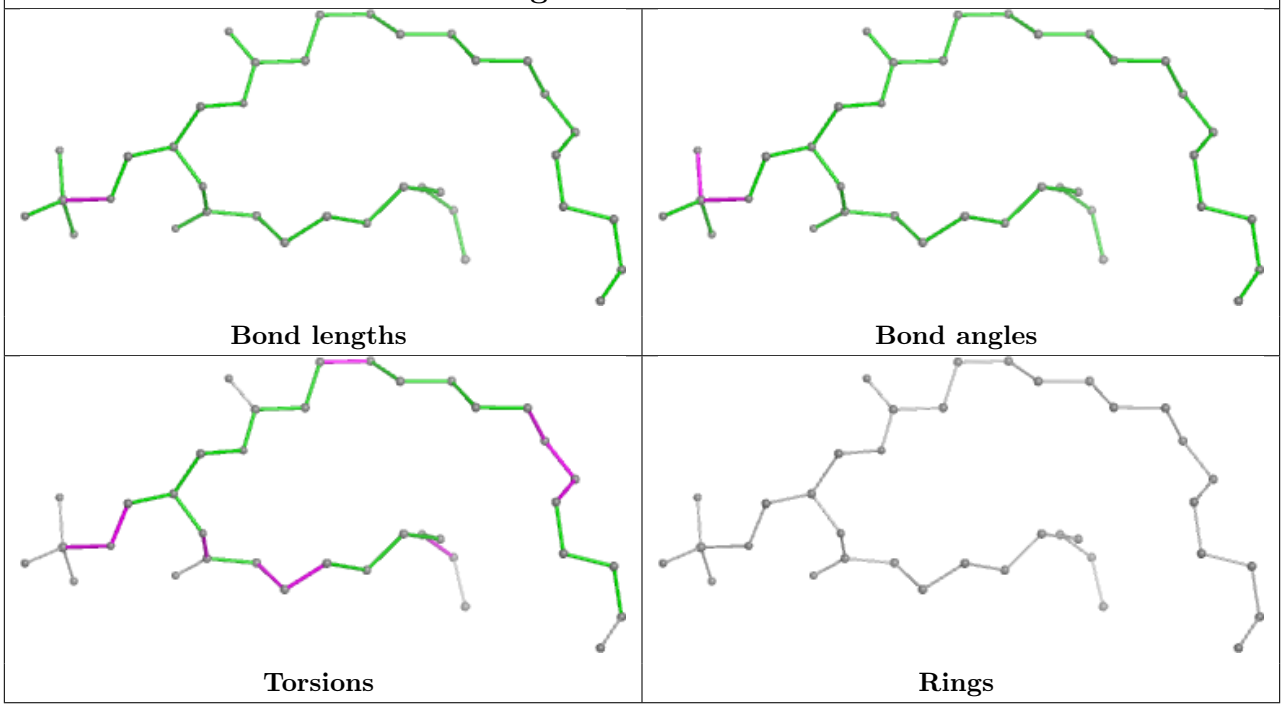


**Rings**

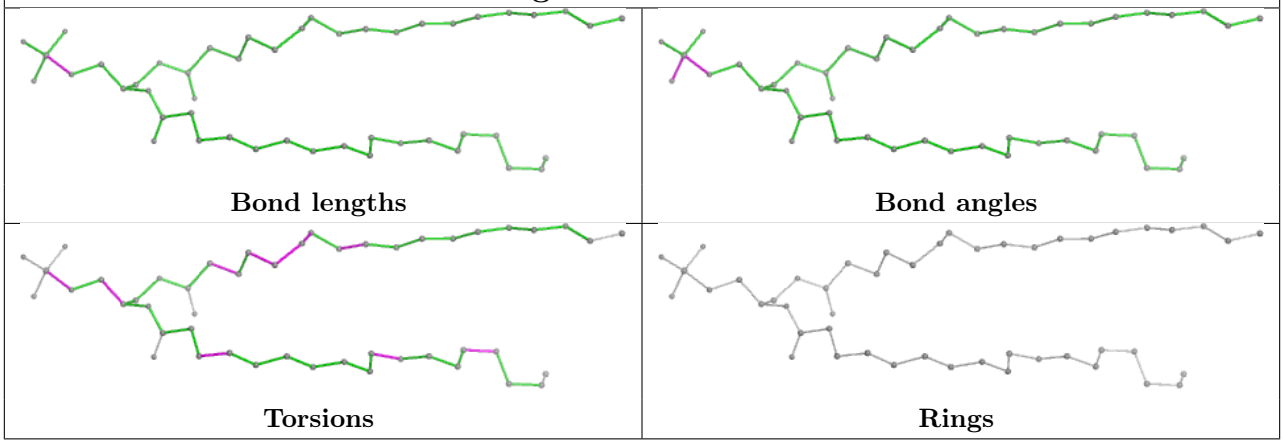
## Ligand 3PH 3I 201



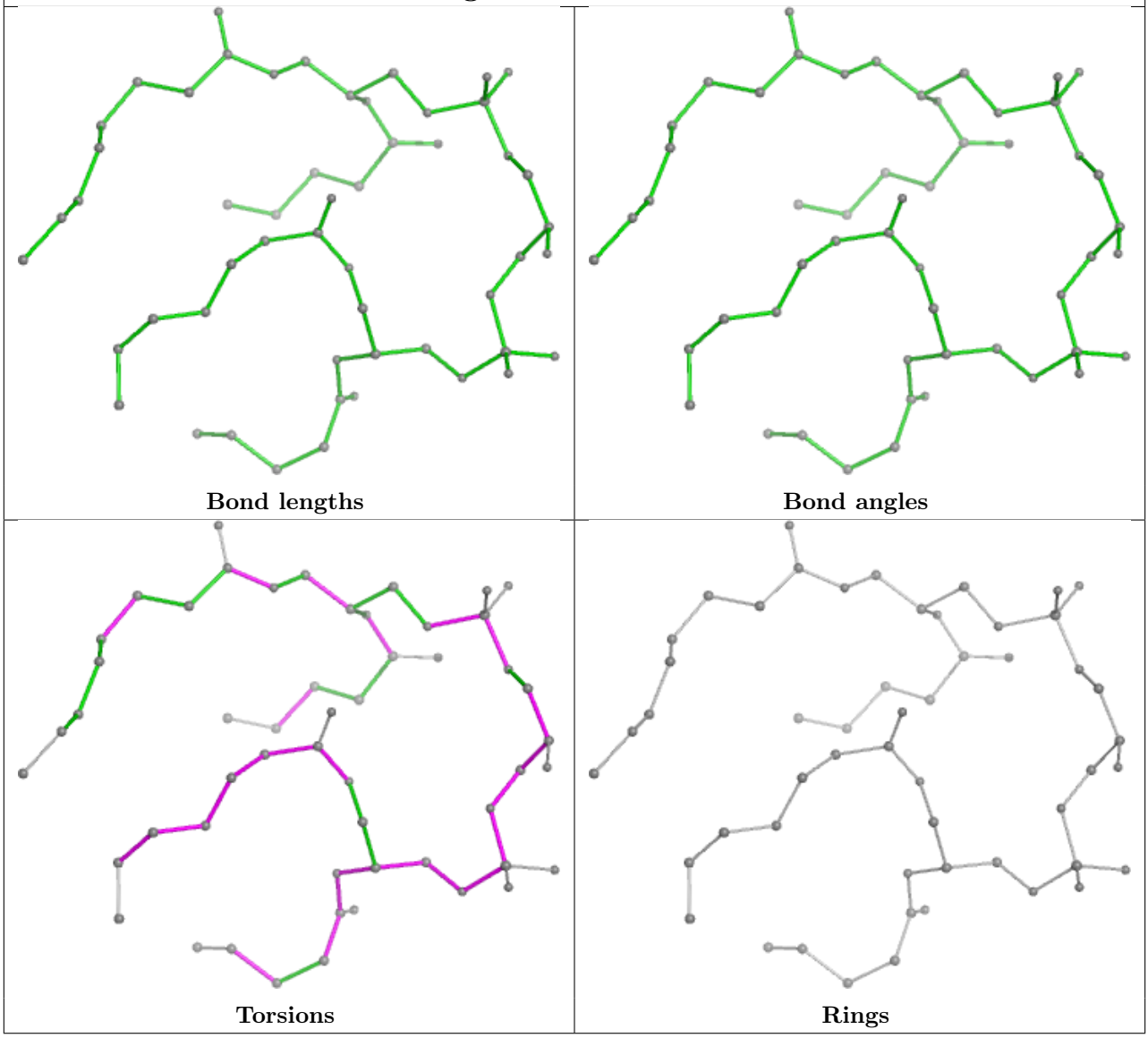

## Ligand 3PH S 301



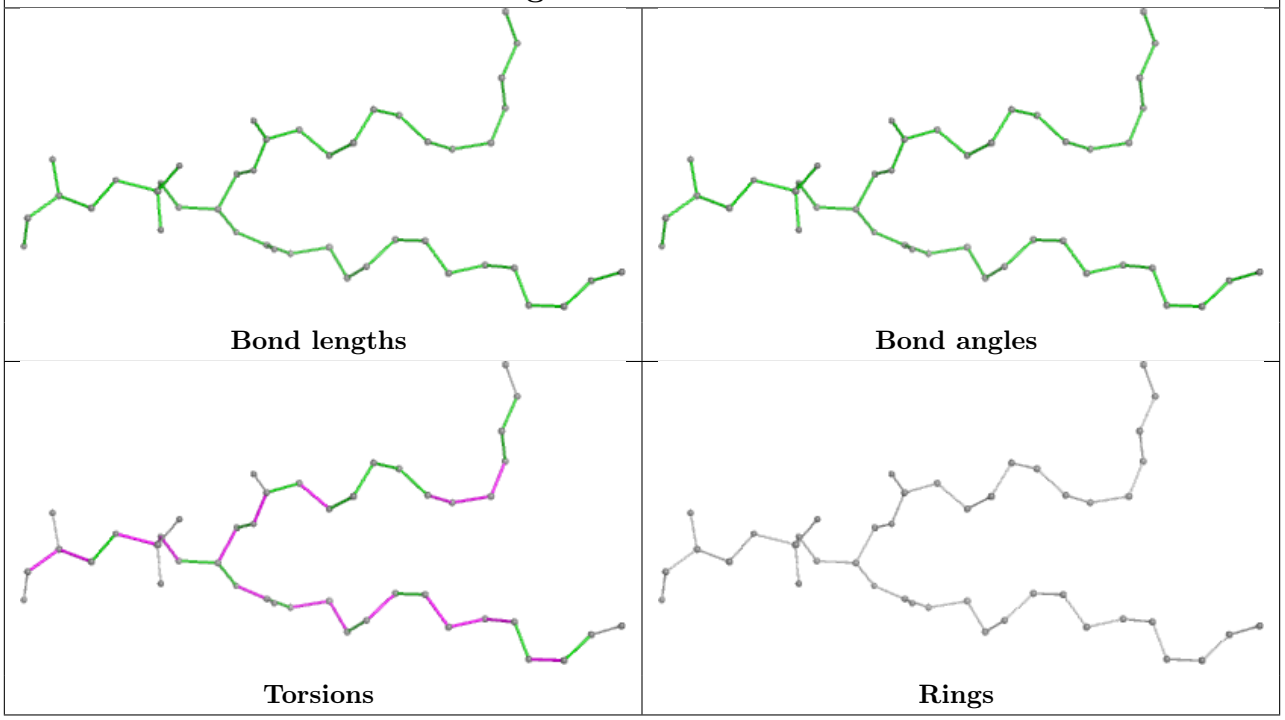
**Ligand 3PH c 101**



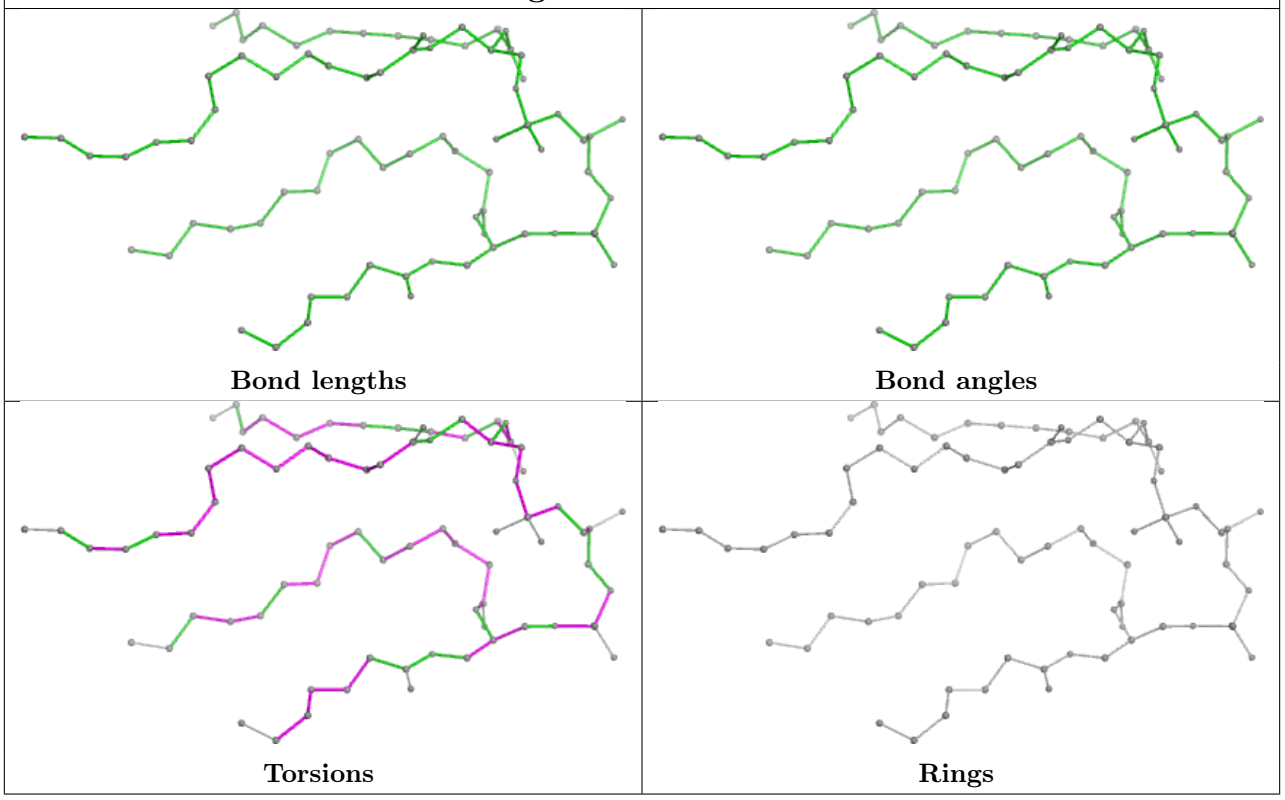

**Ligand CDL 1E 401**



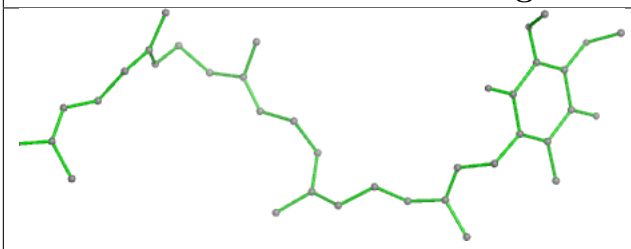
## Ligand PGT b 601



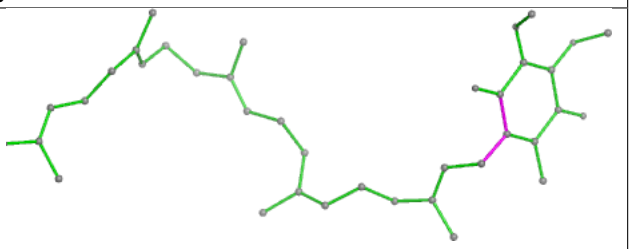

## Ligand CDL h 203



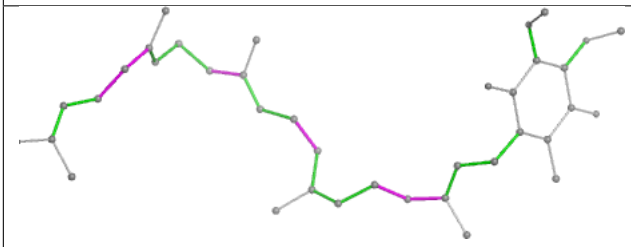
## Ligand UQ5 1A 402



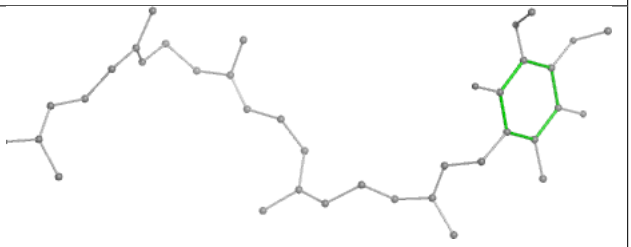
Bond lengths



Bond angles

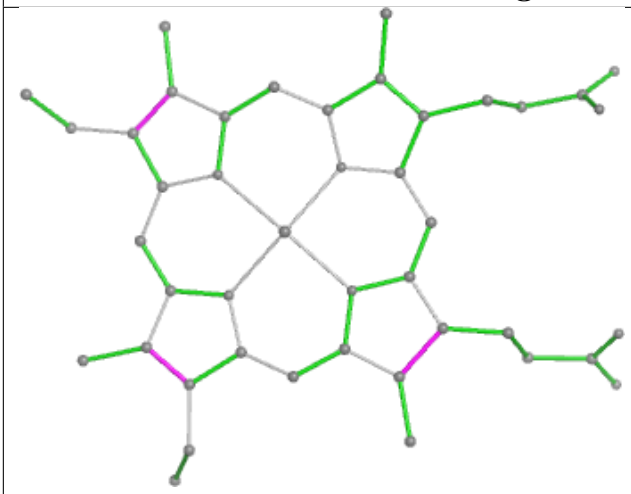


Torsions

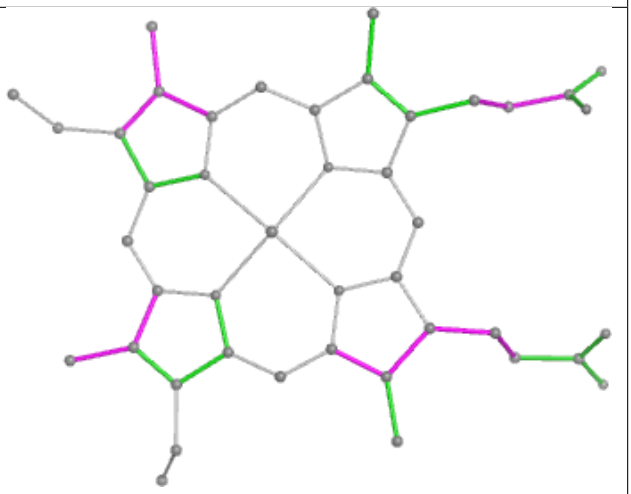


Rings

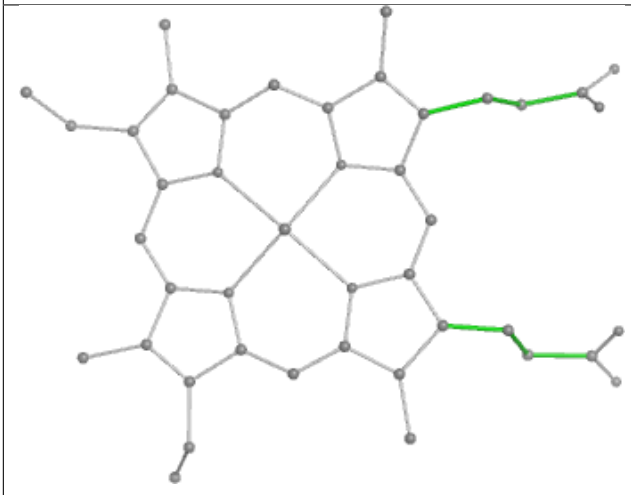
## Ligand HEC 1F 402



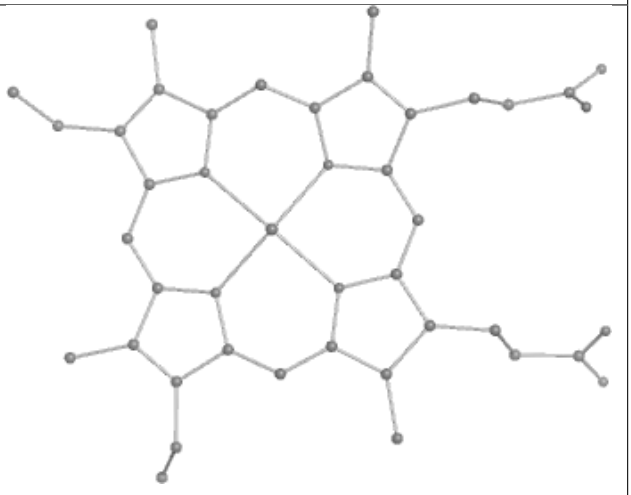
Bond lengths



Bond angles

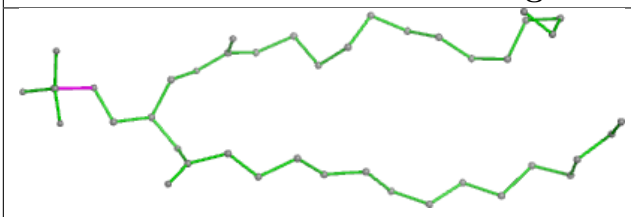


Torsions

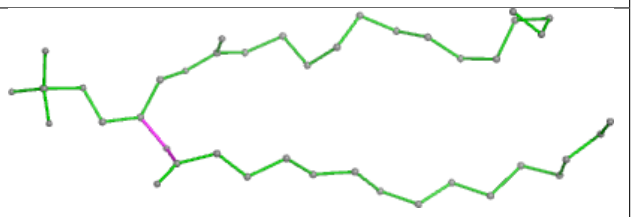


Rings

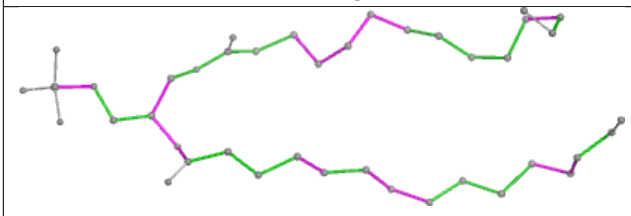
## Ligand 3PH V 602



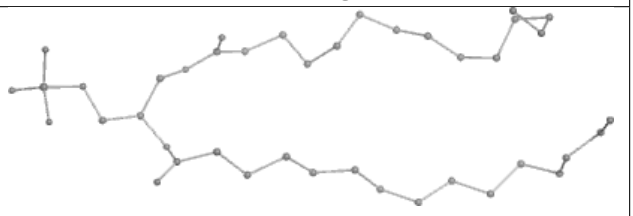
Bond lengths



Bond angles

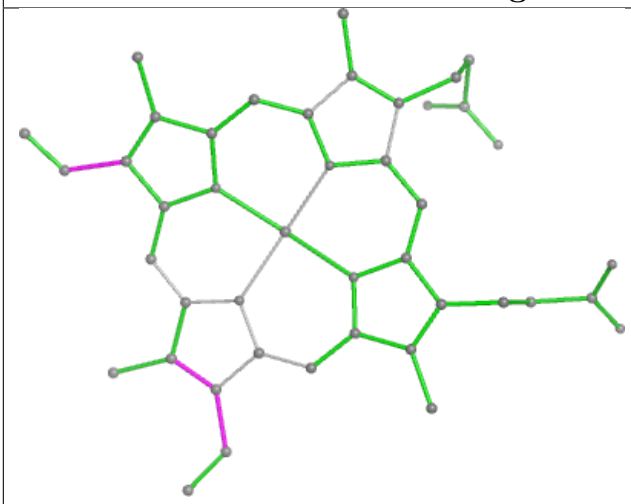


Torsions

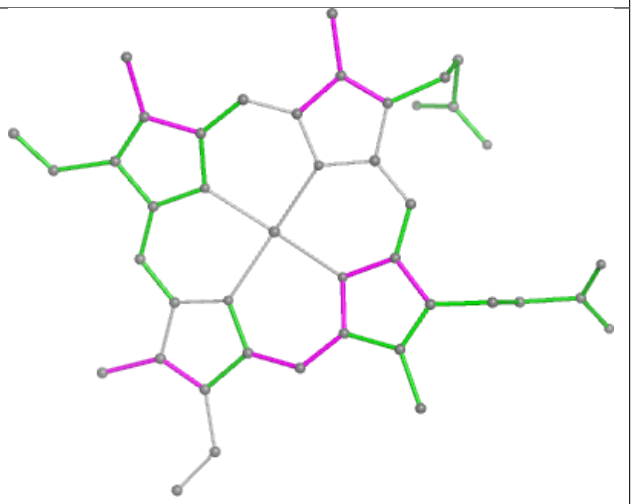


Rings

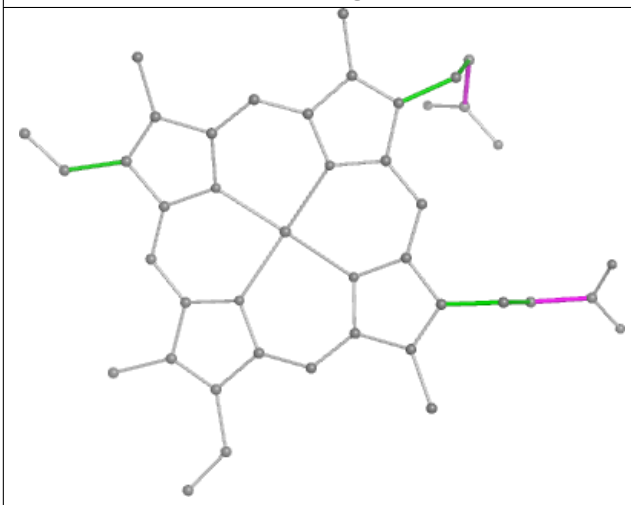
## Ligand HEM 1A 404



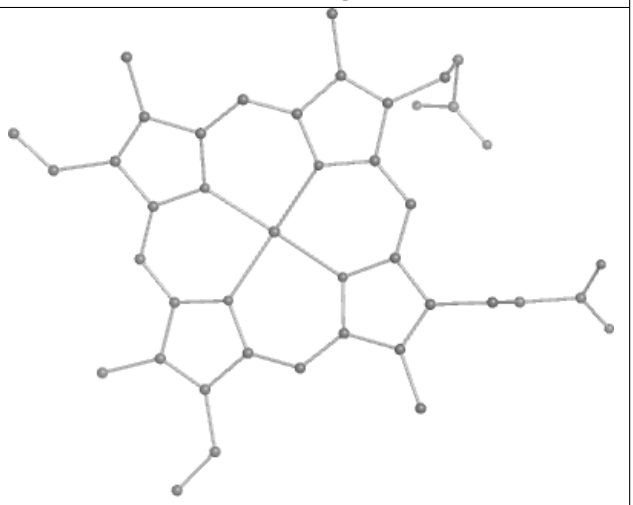
Bond lengths



Bond angles

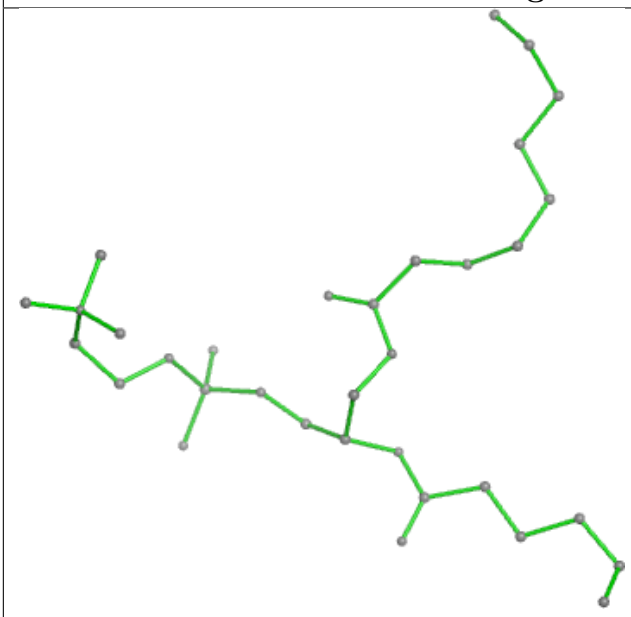


Torsions

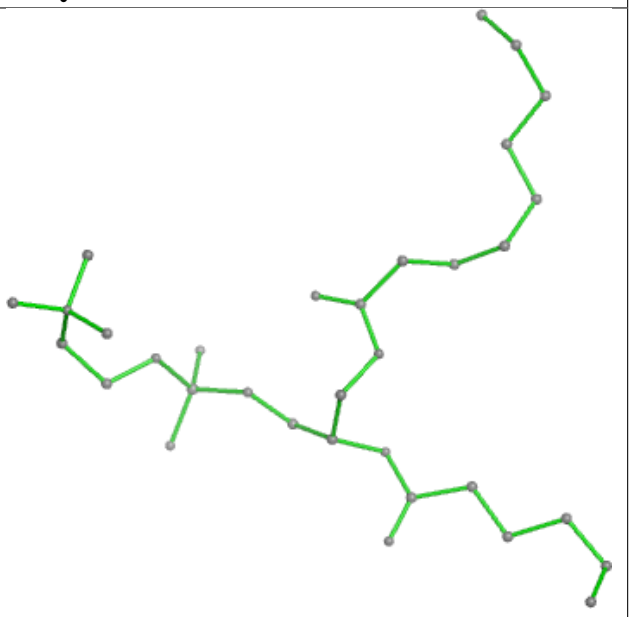


Rings

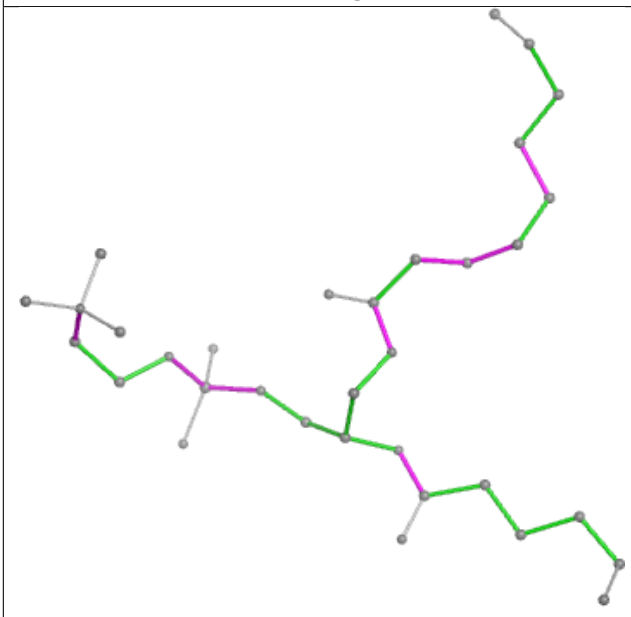
**Ligand PC7 Q 302**



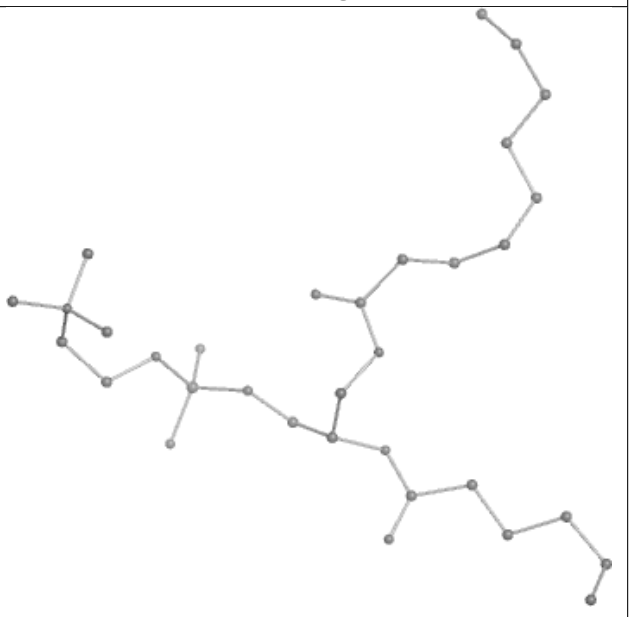
**Bond lengths**



**Bond angles**

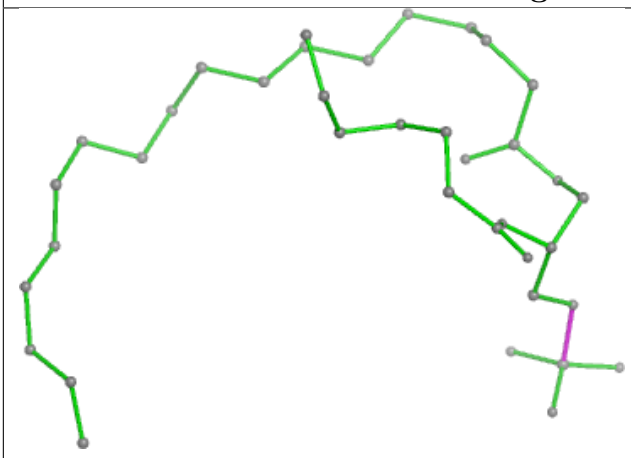


**Torsions**

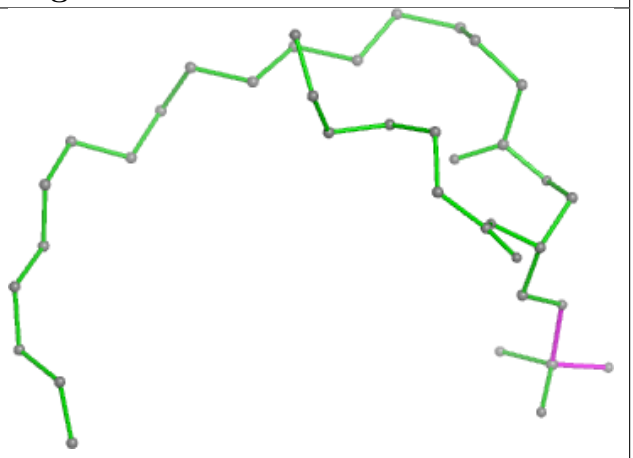


**Rings**

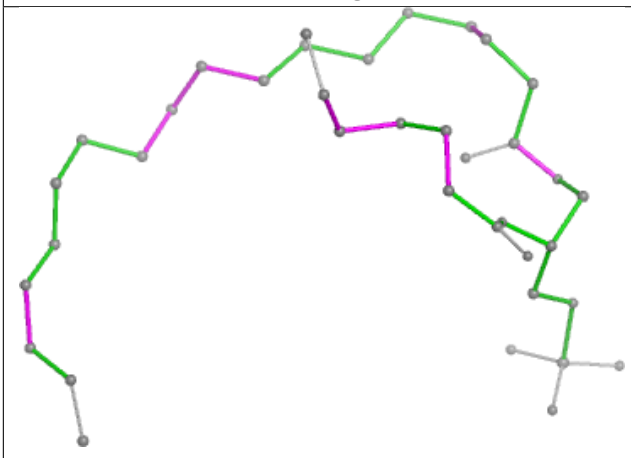
**Ligand 3PH g 101**



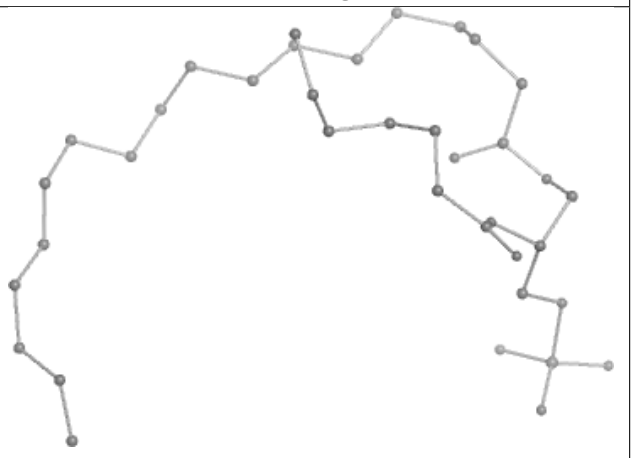
**Bond lengths**



**Bond angles**

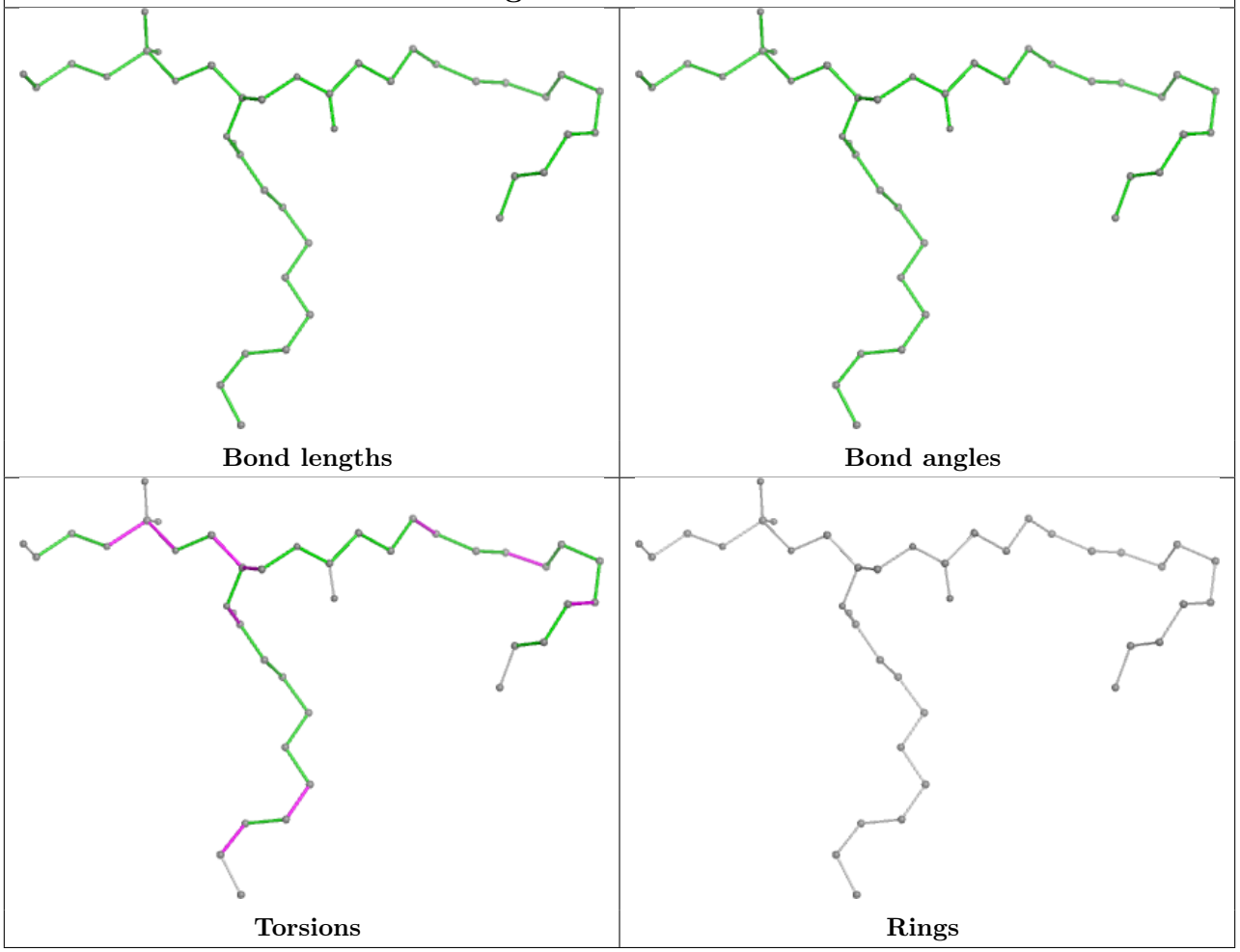


**Torsions**

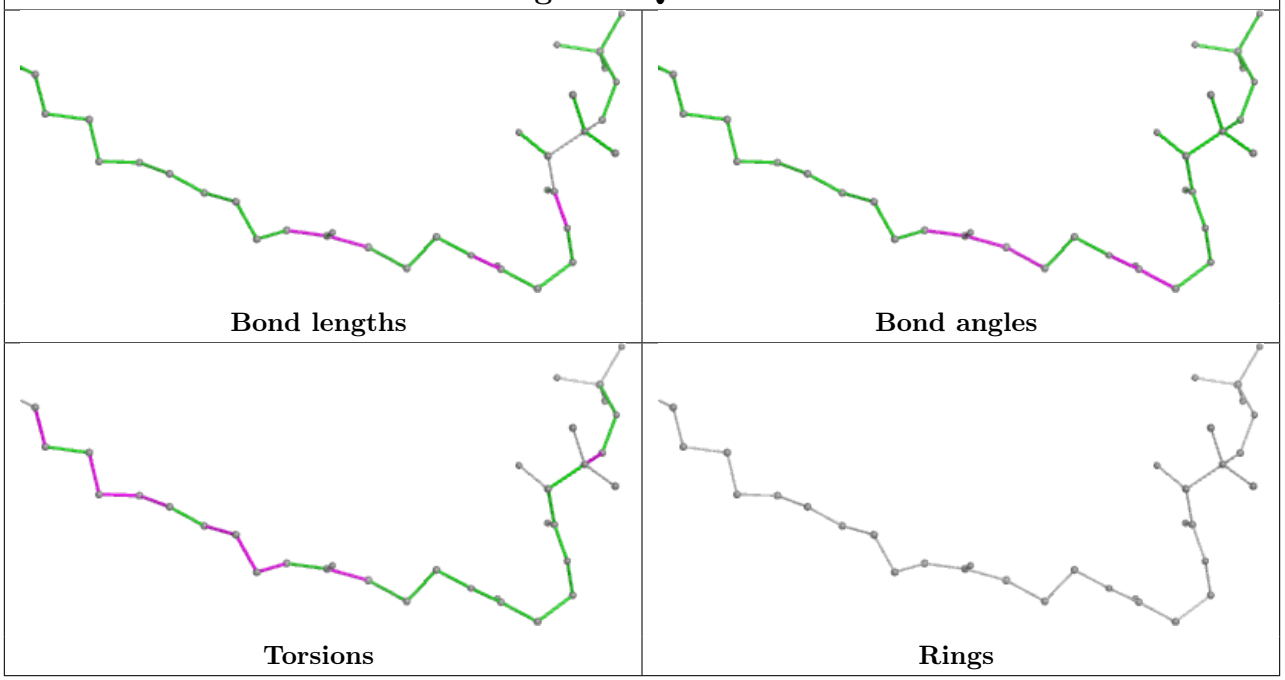


**Rings**

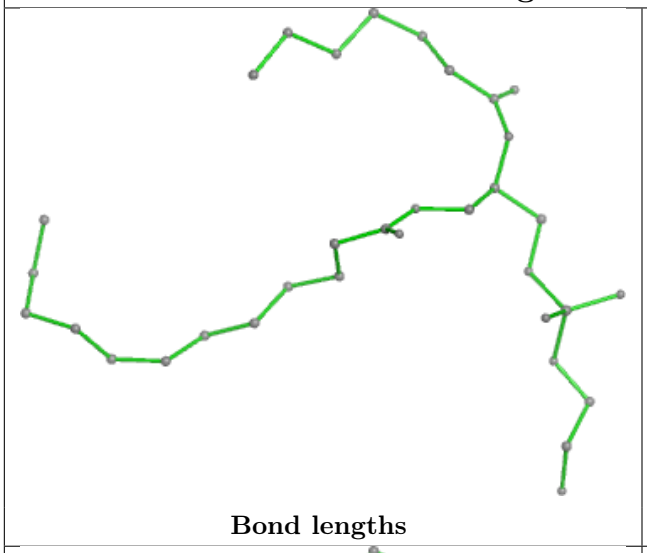
## Ligand PTY R 406



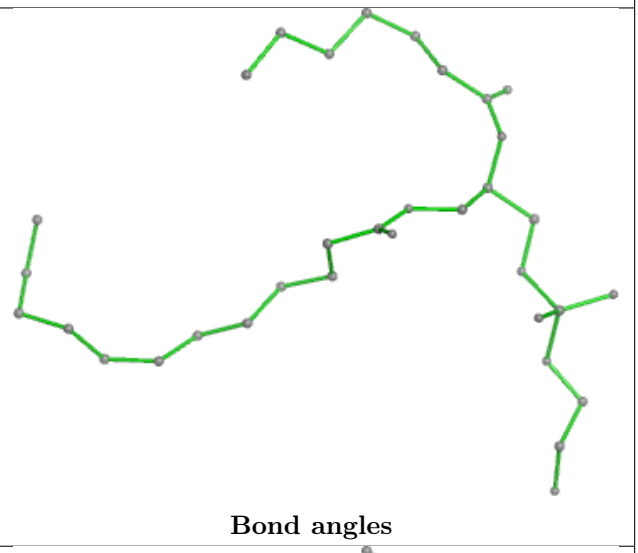

## Ligand 8Q1 J 200



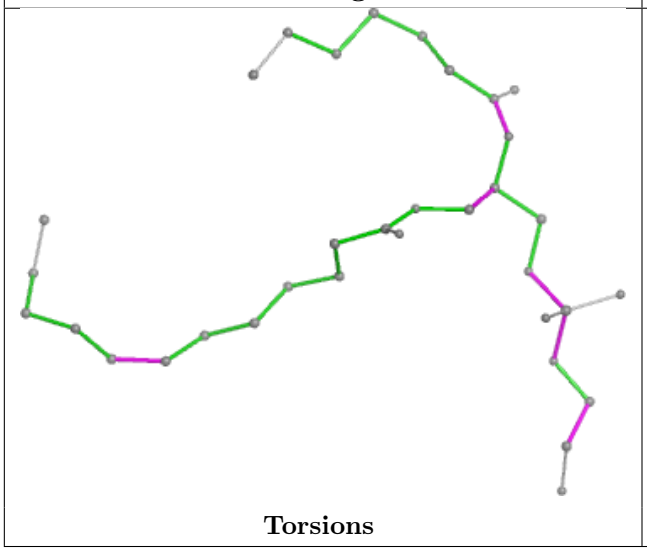
**Ligand PTY 3F 101**



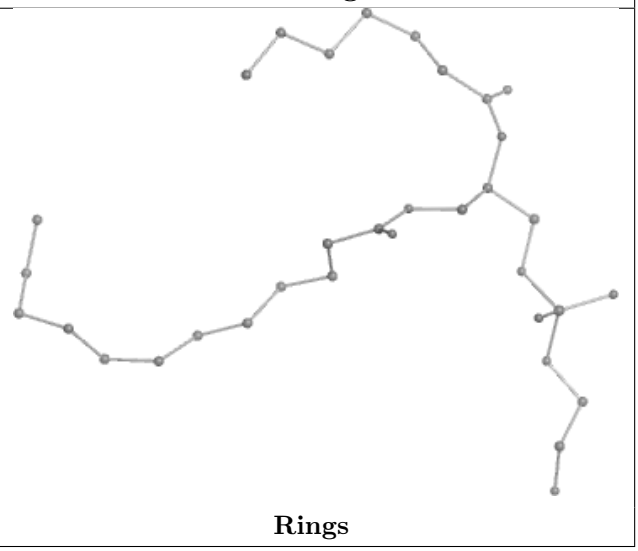
**Bond lengths**



**Bond angles**

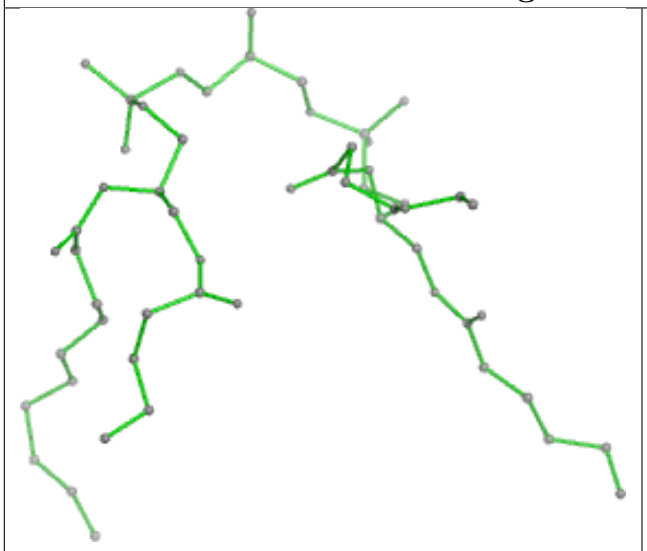


**Torsions**

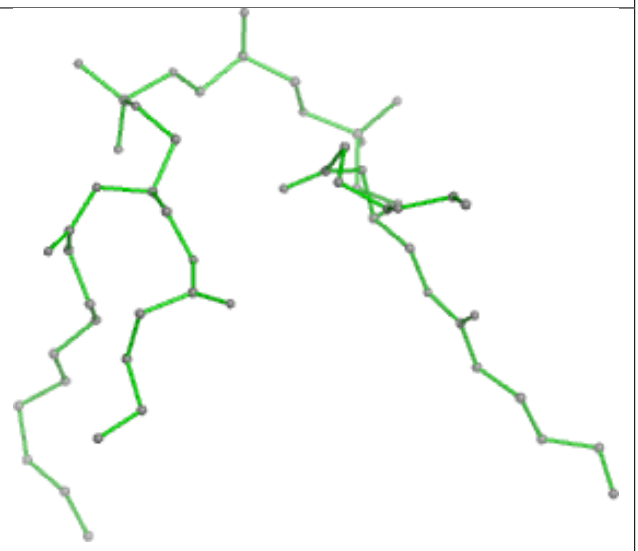


**Rings**

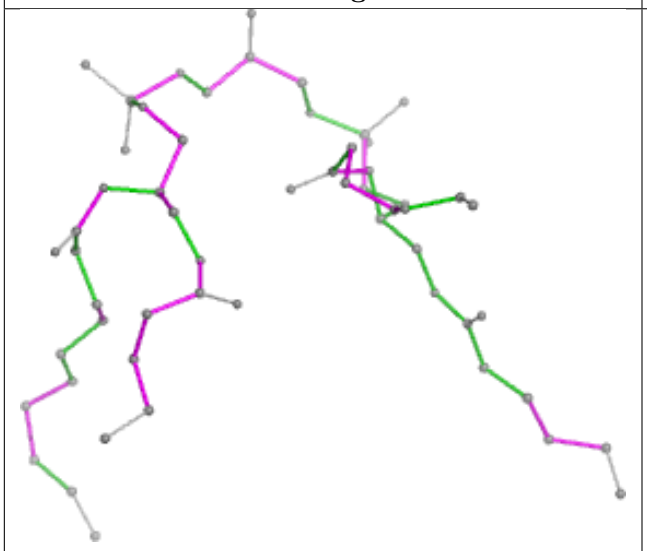
**Ligand CDL 1F 401**



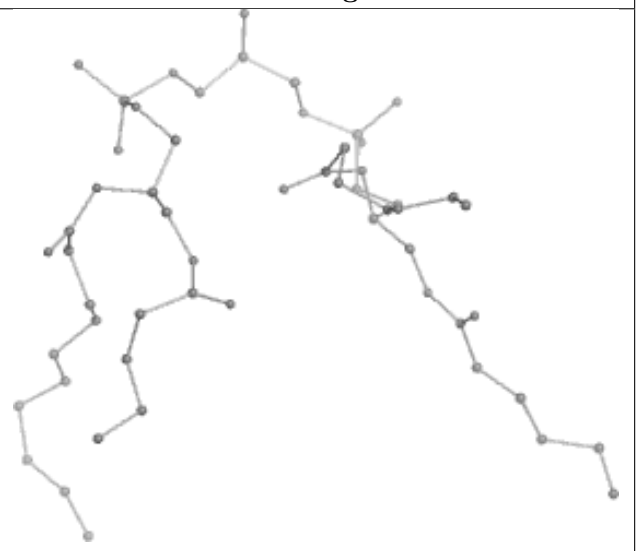
**Bond lengths**



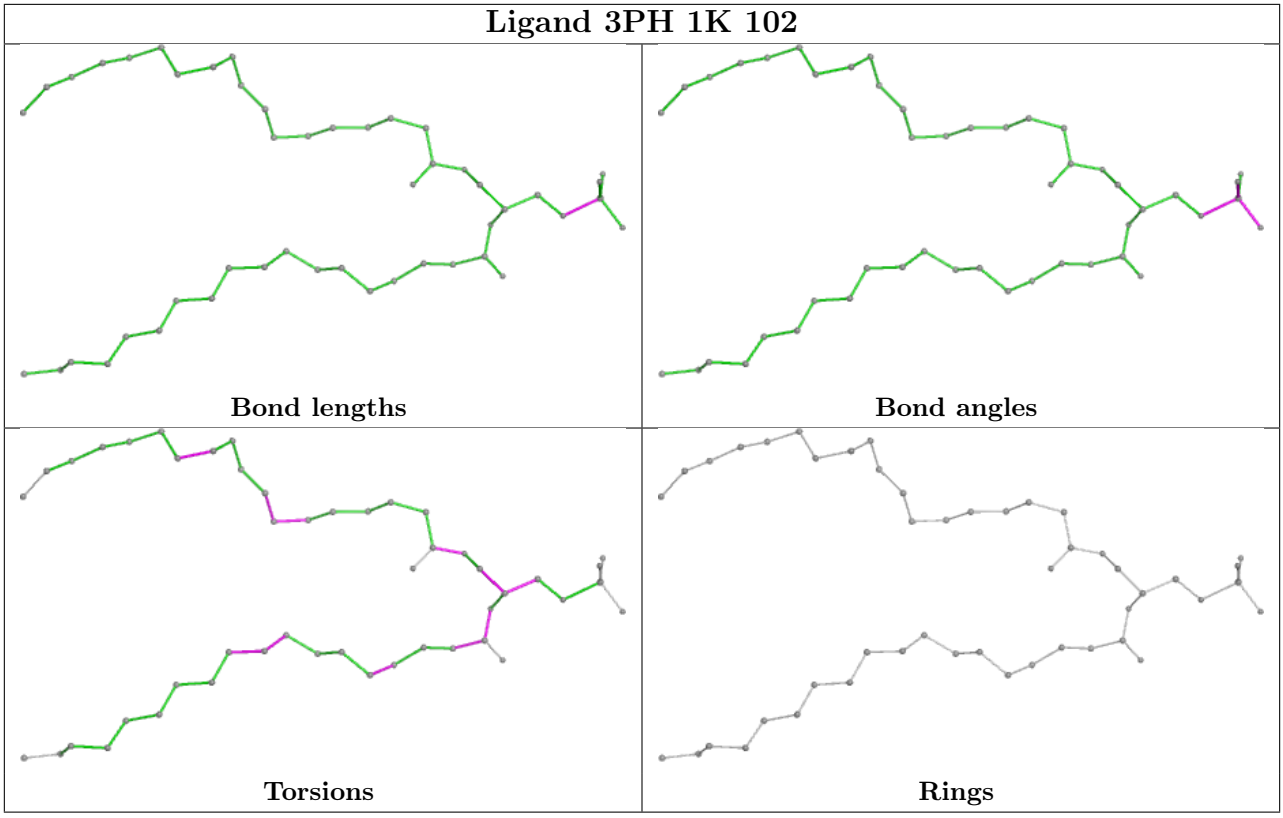
**Bond angles**



**Torsions**



**Rings**




## 5.7 Other polymers (i)

There are no such residues in this entry.

## 5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

# 6 Map visualisation

This section contains visualisations of the EMDB entry EMD-50202. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

## 6.1 Orthogonal projections

This section was not generated.

## 6.2 Central slices

This section was not generated.

## 6.3 Largest variance slices

This section was not generated.

## 6.4 Orthogonal standard-deviation projections (False-color)

This section was not generated.

## 6.5 Orthogonal surface views

This section was not generated.

## 6.6 Mask visualisation

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

# 7 Map analysis

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

## 7.1 Map-value distribution

This section was not generated.

## 7.2 Volume estimate versus contour level

This section was not generated.

## 7.3 Rotationally averaged power spectrum

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

# 8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

# 9 Map-model fit

This section was not generated.