# Full wwPDB EM Validation Report ⓘ

May 10, 2022 – 01:35 pm BST

| | | |
|---|---|---|
| PDB ID | : | 7QHM |
| EMDB ID | : | EMD-13976 |
| Title | : | Cytochrome bcc-aa3 supercomplex (respiratory supercomplex III2/IV2) from Corynebacterium glutamicum (stigmatellin and azide bound) |
| Authors | : | Kao, W.-C.; Hunte, C. |
| Deposited on | : | 2021-12-13 |
| Resolution | : | 2.80 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 following versions of software and data (see references ⓘ) were used in the production of this report:

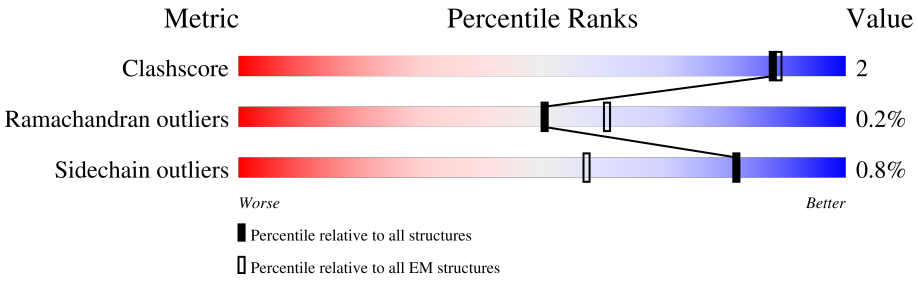
| | | |
|---|---|---|
| EMDB validation analysis | : | 0.0.1.dev8 |
| Mogul | : | 1.8.4, CSD as541be (2020) |
| MolProbity | : | 4.02b-467 |
| buster-report | : | 1.1.7 (2018) |
| Percentile statistics | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | 2.28.1 |

# 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 2.80 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) |
|---|---|---|
| Clashscore | 158937 | 4297 |
| Ramachandran outliers | 154571 | 4023 |
| Sidechain outliers | 154315 | 3826 |

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% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | A | 408 | 94% 5% |
| 1 | N | 408 | 93% 6% |
| 2 | B | 539 | 93% 6% |
| 2 | O | 539 | 94% 5% |
| 3 | C | 283 | 5% 77% 5% 18% |
| 3 | P | 283 | 78% 18% |
| 4 | D | 594 | 93% |
| 4 | Q | 594 | 92% 5% |

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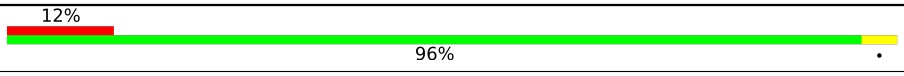
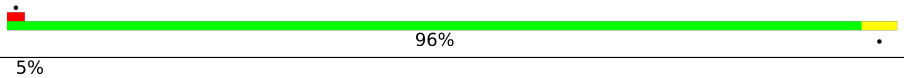
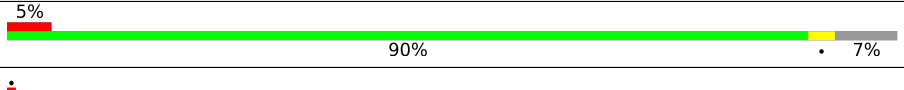
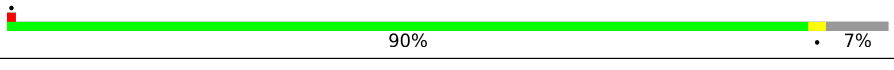
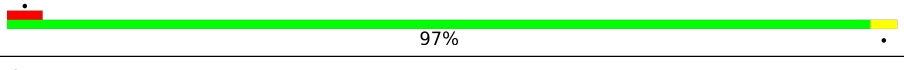
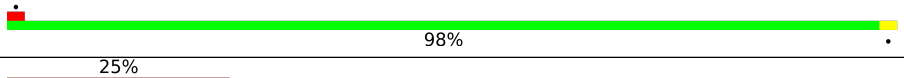
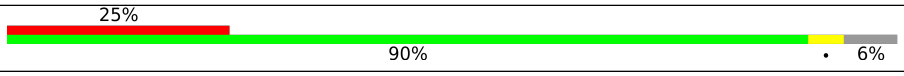
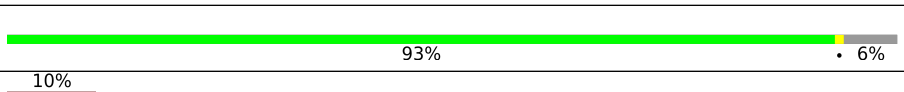
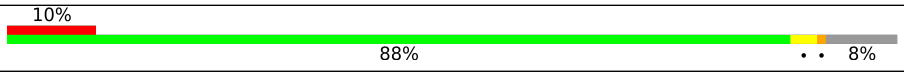
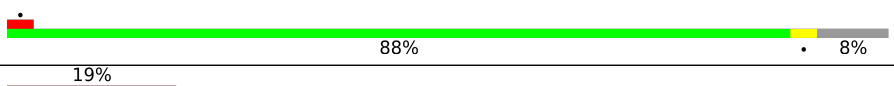
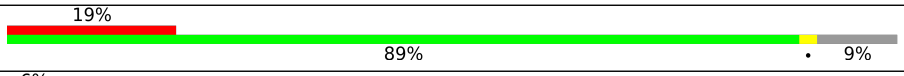
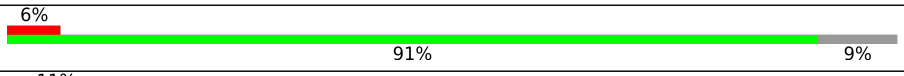
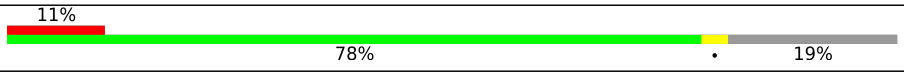
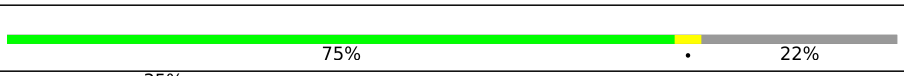
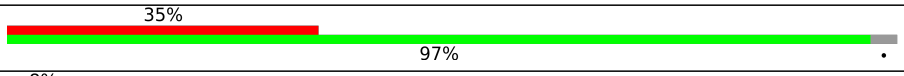
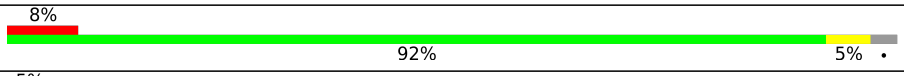
| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 5 | E | 331 |   |
| 5 | R | 331 |   |
| 6 | F | 205 |   |
| 6 | S | 205 |   |
| 7 | G | 143 |   |
| 7 | T | 143 |   |
| 8 | H | 163 |   |
| 8 | U | 163 |   |
| 9 | I | 147 |   |
| 9 | V | 147 |   |
| 10 | J | 112 |   |
| 10 | W | 112 |   |
| 11 | K | 73 |   |
| 11 | X | 73 |   |
| 12 | L | 65 |   |
| 12 | Y | 65 |   |
| 13 | M | 168 |   |
| 13 | Z | 168 |   |

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|---|---|---|---|---|---|---|---|
| 29 | AZI | D | 606 | - | - | X | - |

# 2 Entry composition

There are 35 unique types of molecules in this entry. The entry contains 97775 atoms, of which 48245 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 bc1 complex Rieske iron-sulfur subunit.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 1 | A | 402 | Total | C | H | N | O | S | 2 | 0 |
| | | | 6231 | 2004 | 3084 | 540 | 587 | 16 | | |
| 1 | N | 401 | Total | C | H | N | O | S | 4 | 0 |
| | | | 6224 | 2004 | 3079 | 539 | 586 | 16 | | |

- Molecule 2 is a protein called Cytochrome bc1 complex cytochrome b subunit.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 2 | B | 534 | Total | C | H | N | O | S | 6 | 0 |
| | | | 8485 | 2765 | 4268 | 709 | 721 | 22 | | |
| 2 | O | 534 | Total | C | H | N | O | S | 0 | 0 |
| | | | 8425 | 2746 | 4239 | 703 | 715 | 22 | | |

- Molecule 3 is a protein called Cytochrome bc1 complex cytochrome c subunit.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 3 | C | 233 | Total | C | H | N | O | S | 2 | 0 |
| | | | 3443 | 1089 | 1694 | 306 | 344 | 10 | | |
| 3 | P | 233 | Total | C | H | N | O | S | 0 | 0 |
| | | | 3418 | 1083 | 1680 | 302 | 343 | 10 | | |

- Molecule 4 is a protein called Cytochrome c oxidase subunit 1.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 4 | D | 576 | Total | C | H | N | O | S | 0 | 0 |
| | | | 9018 | 3031 | 4470 | 735 | 750 | 32 | | |
| 4 | Q | 576 | Total | C | H | N | O | S | 2 | 0 |
| | | | 9034 | 3036 | 4477 | 736 | 753 | 32 | | |

There are 20 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| D | 585 | ALA | - | expression tag | UNP Q79VD7 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| D | 586 | ALA | - | expression tag | UNP Q79VD7 |
| D | 587 | TRP | - | expression tag | UNP Q79VD7 |
| D | 588 | SER | - | expression tag | UNP Q79VD7 |
| D | 589 | HIS | - | expression tag | UNP Q79VD7 |
| D | 590 | PRO | - | expression tag | UNP Q79VD7 |
| D | 591 | GLN | - | expression tag | UNP Q79VD7 |
| D | 592 | PHE | - | expression tag | UNP Q79VD7 |
| D | 593 | GLU | - | expression tag | UNP Q79VD7 |
| D | 594 | LYS | - | expression tag | UNP Q79VD7 |
| Q | 585 | ALA | - | expression tag | UNP Q79VD7 |
| Q | 586 | ALA | - | expression tag | UNP Q79VD7 |
| Q | 587 | TRP | - | expression tag | UNP Q79VD7 |
| Q | 588 | SER | - | expression tag | UNP Q79VD7 |
| Q | 589 | HIS | - | expression tag | UNP Q79VD7 |
| Q | 590 | PRO | - | expression tag | UNP Q79VD7 |
| Q | 591 | GLN | - | expression tag | UNP Q79VD7 |
| Q | 592 | PHE | - | expression tag | UNP Q79VD7 |
| Q | 593 | GLU | - | expression tag | UNP Q79VD7 |
| Q | 594 | LYS | - | expression tag | UNP Q79VD7 |

- Molecule 5 is a protein called Cytochrome c oxidase subunit 2.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 5 | E | 331 | Total | C | H | N | O | S | 0 | 0 |
| | | | 5066 | 1660 | 2468 | 429 | 498 | 11 | | |
| 5 | R | 331 | Total | C | H | N | O | S | 2 | 0 |
| | | | 5089 | 1666 | 2482 | 431 | 499 | 11 | | |

- Molecule 6 is a protein called Cytochrome c oxidase subunit 3.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 6 | F | 190 | Total | C | H | N | O | S | 0 | 0 |
| | | | 2981 | 992 | 1495 | 236 | 251 | 7 | | |
| 6 | S | 190 | Total | C | H | N | O | S | 0 | 0 |
| | | | 2980 | 992 | 1494 | 236 | 251 | 7 | | |

- Molecule 7 is a protein called Cytochrome c oxidase polypeptide 4.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 7 | G | 143 | Total | C | H | N | O | S | 0 | 0 |
| | | | 2201 | 728 | 1106 | 167 | 191 | 9 | | |

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| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 7 | T | 143 | Total | C | H | N | O | S | 2 | 0 |
| | | | 2219 | 734 | 1114 | 170 | 192 | 9 | | |

- Molecule 8 is a protein called Uncharacterized protein Cgl2664/cg2949.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 8 | H | 153 | Total | C | H | N | O | S | 0 | 0 |
| | | | 2174 | 684 | 1054 | 184 | 249 | 3 | | |
| 8 | U | 154 | Total | C | H | N | O | S | 0 | 0 |
| | | | 2181 | 686 | 1057 | 185 | 250 | 3 | | |

- Molecule 9 is a protein called Uncharacterized membrane protein Cgl2017/cg2211.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 9 | I | 135 | Total | C | H | N | O | S | 0 | 0 |
| | | | 2144 | 691 | 1071 | 190 | 191 | 1 | | |
| 9 | V | 135 | Total | C | H | N | O | S | 0 | 0 |
| | | | 2144 | 691 | 1071 | 190 | 191 | 1 | | |

- Molecule 10 is a protein called Hypothetical membrane protein.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 10 | J | 102 | Total | C | H | N | O | S | 0 | 0 |
| | | | 1571 | 506 | 792 | 134 | 136 | 3 | | |
| 10 | W | 102 | Total | C | H | N | O | S | 0 | 0 |
| | | | 1571 | 506 | 792 | 134 | 136 | 3 | | |

- Molecule 11 is a protein called Actinobacterial supercomplex, subunit C (AscC).

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 11 | K | 59 | Total | C | H | N | O | 0 | 0 |
| | | | 901 | 297 | 432 | 81 | 91 | | |
| 11 | X | 57 | Total | C | H | N | O | 0 | 0 |
| | | | 864 | 286 | 413 | 78 | 87 | | |

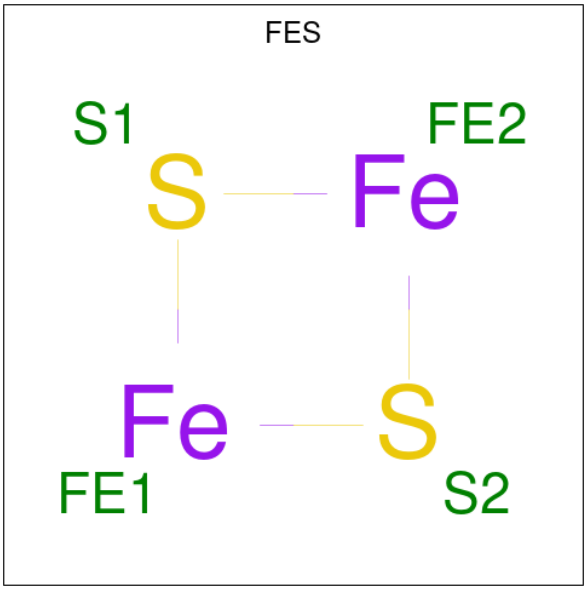
- Molecule 12 is a protein called Hypothetical membrane protein.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 12 | L | 63 | Total | C | H | N | O | S | 0 | 0 |
| | | | 915 | 294 | 470 | 70 | 78 | 3 | | |
| 12 | Y | 63 | Total | C | H | N | O | S | 0 | 0 |
| | | | 915 | 294 | 470 | 70 | 78 | 3 | | |

- Molecule 13 is a protein called Thiamine biosynthesis protein X.

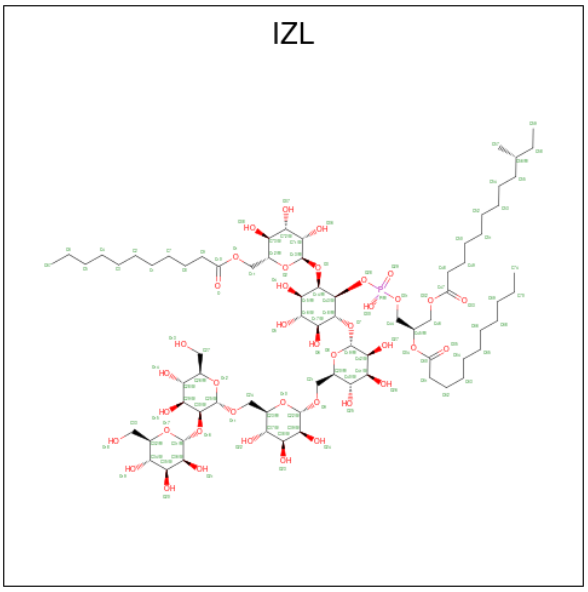
| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 13 | M | 22 | Total | C | H | N | O | S | 0 | 0 |
| | | | 330 | 101 | 159 | 32 | 37 | 1 | | |
| 13 | Z | 24 | Total | C | H | N | O | S | 0 | 0 |
| | | | 358 | 110 | 172 | 35 | 40 | 1 | | |

- Molecule 14 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: $Fe_2S_2$) (labeled as "Ligand of Interest" by depositor).



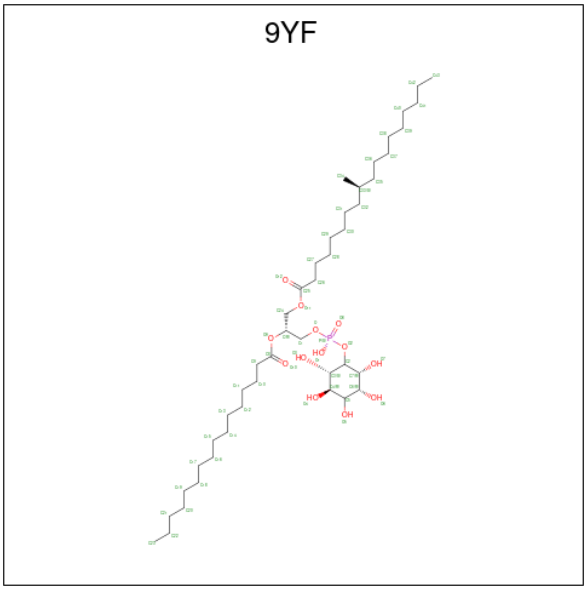

| Mol | Chain | Residues | Atoms | | | | AltConf |
|---|---|---|---|---|---|---|---|
| 14 | A | 1 | Total | Fe | S | | 0 |
| | | | 4 | 2 | 2 | | |
| 14 | N | 1 | Total | Fe | S | | 0 |
| | | | 4 | 2 | 2 | | |

- Molecule 15 is [(2 {R})-3-[[(1 {S},2 {R},3 {S},4 {S},5 {R},6 {R})-2-[(2 {R},3 {S},4 {S},5 {S},6 {R})-6-[[(2 {S},3 {S},4 {S},5 {S},6 {R})-6-[[(2 {S},3 {S},4 {S},5 {S},6 {R})-6-(hydroxymethyl)-3-[(2 {R},3 {S},4 {S},5 {S},6 {R})-6-(hydroxymethyl)-3,4,5-tris(oxidanyl)oxan-2-yl]oxy-4,5-bis(oxidanyl)oxan-2-yl]oxymethyl]-3,4,5-tris(oxidanyl)oxan-2-yl]oxymethyl]-3,4,5-tris(oxidanyl)oxan-2-yl]oxy-3,4,5-tris(oxidanyl)-6-[(2 {R},3 {S},4 {S},5 {S},6 {R})-3,4,5-tris(oxidanyl)-6-(undecanoyloxymethyl)oxan-2-yl]oxy-cyclohexyl]oxy-oxidanyl-phosphoryl]oxy-2-undecanoyloxy-propyl] (10 {R})-10-methyldodecanoate (three-letter code: IZL) (formula: $C_{74}H_{133}O_{39}P$) (labeled as "Ligand of Interest" by depositor).



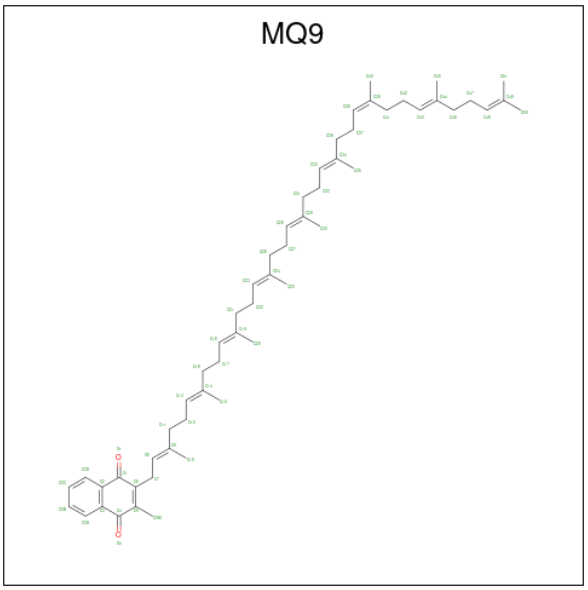

| Mol | Chain | Residues | Atoms | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|
| 15 | A | 1 | Total | C | H | O | P | 0 |
| | | | 212 | 63 | 109 | 39 | 1 | |
| 15 | N | 1 | Total | C | H | O | P | 0 |
| | | | 212 | 63 | 109 | 39 | 1 | |

- Molecule 16 is (2R)-2-(hexadecanoyloxy)-3-{[(S)-hydroxy{[(1R,2R,3R,4R,5R,6S)-2,3,4,5,6-pentahydroxycyclohexyl]oxy}phosphoryl]oxy}propyl (9S)-9-methyloctadecanoate (three-letter code: 9YF) (formula: $C_{44}H_{85}O_{13}P$) (labeled as "Ligand of Interest" by depositor).



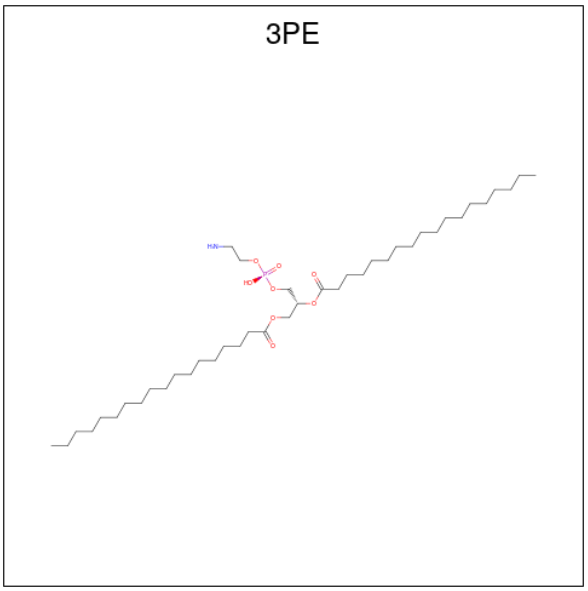
| Mol | Chain | Residues | Atoms | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|
| 16 | A | 1 | Total | C | H | O | P | 0 |
| | | | 66 | 22 | 30 | 13 | 1 | |
| 16 | H | 1 | Total | C | H | O | P | 0 |
| | | | 60 | 20 | 26 | 13 | 1 | |
| 16 | N | 1 | Total | C | H | O | P | 0 |
| | | | 66 | 22 | 30 | 13 | 1 | |
| 16 | U | 1 | Total | C | H | O | P | 0 |
| | | | 75 | 25 | 36 | 13 | 1 | |

- Molecule 17 is MENAQUINONE-9 (three-letter code: MQ9) (formula: $C_{56}H_{80}O_2$) (labeled as "Ligand of Interest" by depositor).




| Mol | Chain | Residues | Atoms | | | | AltConf |
|---|---|---|---|---|---|---|---|
| 17 | A | 1 | Total | C | H | O | 0 |
| | | | 138 | 56 | 80 | 2 | |
| 17 | B | 1 | Total | C | H | O | 0 |
| | | | 46 | 21 | 23 | 2 | |
| 17 | N | 1 | Total | C | H | O | 0 |
| | | | 78 | 34 | 42 | 2 | |
| 17 | O | 1 | Total | C | H | O | 0 |
| | | | 56 | 25 | 29 | 2 | |

- Molecule 18 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (three-letter code: 3PE) (formula: $C_{41}H_{82}NO_8P$) (labeled as "Ligand of Interest" by depositor).




| Mol | Chain | Residues | Atoms | | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|---|
| 18 | A | 1 | Total | C | H | N | O | P | 0 |
| | | | 76 | 30 | 36 | 1 | 8 | 1 | |
| 18 | C | 1 | Total | C | H | N | O | P | 0 |
| | | | 90 | 30 | 40 | 2 | 16 | 2 | |
| 18 | C | 1 | Total | C | H | N | O | P | 0 |
| | | | 90 | 30 | 40 | 2 | 16 | 2 | |
| 18 | D | 1 | Total | C | H | N | O | P | 0 |
| | | | 57 | 21 | 26 | 1 | 8 | 1 | |
| 18 | F | 1 | Total | C | H | N | O | P | 0 |
| | | | 54 | 22 | 22 | 1 | 8 | 1 | |
| 18 | J | 1 | Total | C | H | N | O | P | 0 |
| | | | 111 | 37 | 64 | 1 | 8 | 1 | |
| 18 | L | 1 | Total | C | H | N | O | P | 0 |
| | | | 68 | 20 | 38 | 1 | 8 | 1 | |
| 18 | N | 1 | Total | C | H | N | O | P | 0 |
| | | | 66 | 28 | 28 | 1 | 8 | 1 | |
| 18 | P | 1 | Total | C | H | N | O | P | 0 |
| | | | 45 | 17 | 18 | 1 | 8 | 1 | |
| 18 | Q | 1 | Total | C | H | N | O | P | 0 |
| | | | 71 | 29 | 32 | 1 | 8 | 1 | |
| 18 | R | 1 | Total | C | H | N | O | P | 0 |
| | | | 47 | 21 | 16 | 1 | 8 | 1 | |
| 18 | S | 1 | Total | C | H | N | O | P | 0 |
| | | | 95 | 33 | 52 | 1 | 8 | 1 | |
| 18 | T | 1 | Total | C | H | N | O | P | 0 |
| | | | 294 | 106 | 148 | 4 | 32 | 4 | |
| 18 | T | 1 | Total | C | H | N | O | P | 0 |
| | | | 294 | 106 | 148 | 4 | 32 | 4 | |

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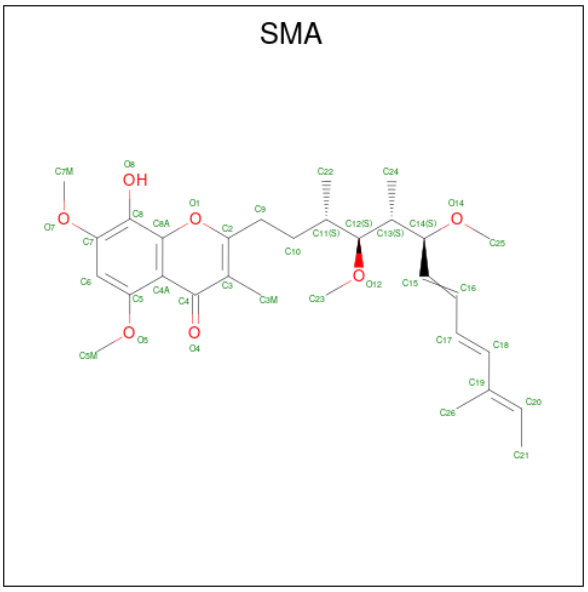
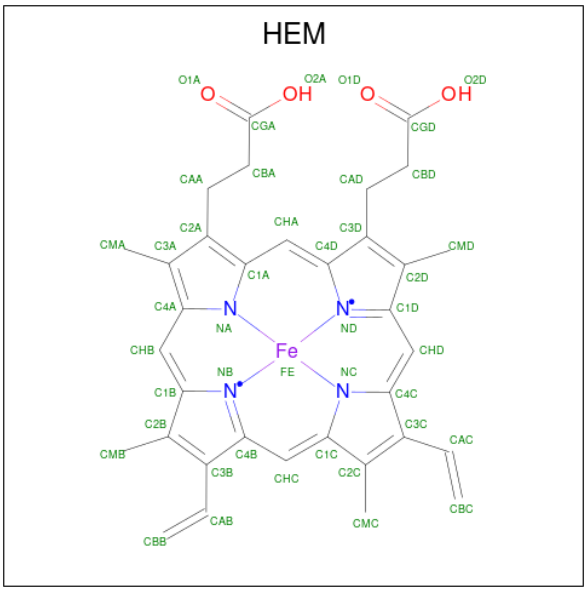
| Mol | Chain | Residues | Atoms | | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|---|
| 18 | T | 1 | Total | C | H | N | O | P | 0 |
| | | | 294 | 106 | 148 | 4 | 32 | 4 | |
| 18 | T | 1 | Total | C | H | N | O | P | 0 |
| | | | 294 | 106 | 148 | 4 | 32 | 4 | |
| 18 | W | 1 | Total | C | H | N | O | P | 0 |
| | | | 115 | 37 | 68 | 1 | 8 | 1 | |

- Molecule 19 is STIGMATELLIN A (three-letter code: SMA) (formula: $C_{30}H_{42}O_7$) (labeled as "Ligand of Interest" by depositor).



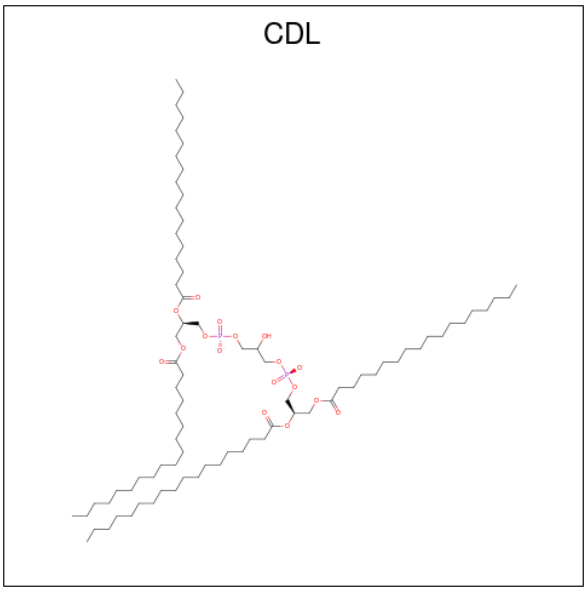

| Mol | Chain | Residues | Atoms | | | | AltConf |
|---|---|---|---|---|---|---|---|
| 19 | B | 1 | Total | C | H | O | 0 |
| | | | 79 | 30 | 42 | 7 | |
| 19 | O | 1 | Total | C | H | O | 0 |
| | | | 79 | 30 | 42 | 7 | |

- Molecule 20 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



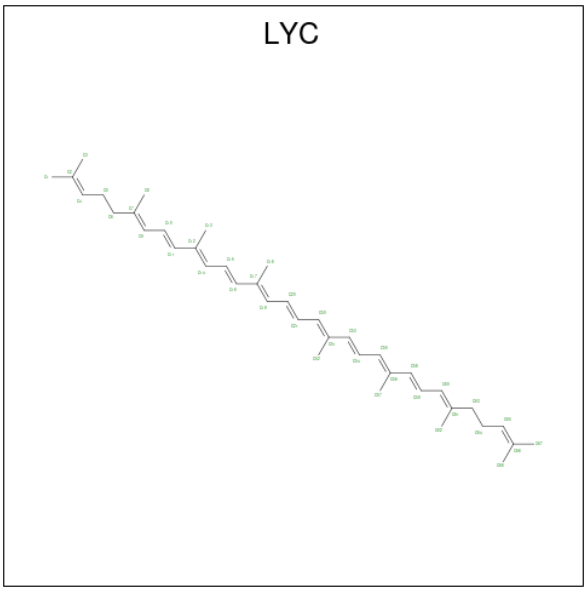

| Mol | Chain | Residues | Atoms | | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|---|
| 20 | B | 1 | Total | C | Fe | H | N | O | 0 |
| | | | 146 | 68 | 2 | 60 | 8 | 8 | |
| 20 | B | 1 | Total | C | Fe | H | N | O | 0 |
| | | | 146 | 68 | 2 | 60 | 8 | 8 | |
| 20 | O | 1 | Total | C | Fe | H | N | O | 0 |
| | | | 146 | 68 | 2 | 60 | 8 | 8 | |
| 20 | O | 1 | Total | C | Fe | H | N | O | 0 |
| | | | 146 | 68 | 2 | 60 | 8 | 8 | |

- Molecule 21 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$) (labeled as "Ligand of Interest" by depositor).



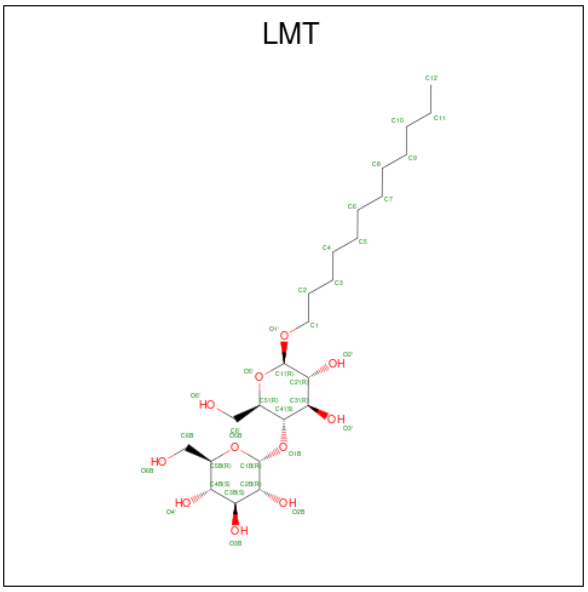
| Mol | Chain | Residues | Atoms | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|
| 21 | B | 1 | Total | C | H | O | P | 0 |
| | | | 293 | 114 | 122 | 51 | 6 | |
| 21 | B | 1 | Total | C | H | O | P | 0 |
| | | | 293 | 114 | 122 | 51 | 6 | |
| 21 | B | 1 | Total | C | H | O | P | 0 |
| | | | 293 | 114 | 122 | 51 | 6 | |
| 21 | D | 1 | Total | C | H | O | P | 0 |
| | | | 289 | 102 | 149 | 34 | 4 | |
| 21 | D | 1 | Total | C | H | O | P | 0 |
| | | | 289 | 102 | 149 | 34 | 4 | |
| 21 | F | 1 | Total | C | H | O | P | 0 |
| | | | 94 | 38 | 37 | 17 | 2 | |
| 21 | G | 1 | Total | C | H | O | P | 0 |
| | | | 279 | 106 | 135 | 34 | 4 | |
| 21 | G | 1 | Total | C | H | O | P | 0 |
| | | | 279 | 106 | 135 | 34 | 4 | |
| 21 | I | 1 | Total | C | H | O | P | 0 |
| | | | 107 | 38 | 50 | 17 | 2 | |
| 21 | O | 1 | Total | C | H | O | P | 0 |
| | | | 145 | 47 | 79 | 17 | 2 | |
| 21 | Q | 1 | Total | C | H | O | P | 0 |
| | | | 328 | 111 | 179 | 34 | 4 | |
| 21 | Q | 1 | Total | C | H | O | P | 0 |
| | | | 328 | 111 | 179 | 34 | 4 | |
| 21 | S | 1 | Total | C | H | O | P | 0 |
| | | | 135 | 46 | 70 | 17 | 2 | |
| 21 | T | 1 | Total | C | H | O | P | 0 |
| | | | 286 | 107 | 141 | 34 | 4 | |
| 21 | T | 1 | Total | C | H | O | P | 0 |
| | | | 286 | 107 | 141 | 34 | 4 | |
| 21 | V | 1 | Total | C | H | O | P | 0 |
| | | | 159 | 50 | 90 | 17 | 2 | |

- Molecule 22 is LYCOPENE (three-letter code: LYC) (formula: $C_{40}H_{56}$) (labeled as "Ligand of Interest" by depositor).




| Mol | Chain | Residues | Atoms | | | AltConf |
|---|---|---|---|---|---|---|
| 22 | B | 1 | Total | C | H | 0 |
| | | | 96 | 40 | 56 | |
| 22 | O | 1 | Total | C | H | 0 |
| | | | 96 | 40 | 56 | |

- Molecule 23 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$).




| Mol | Chain | Residues | Atoms | | | | AltConf |
|---|---|---|---|---|---|---|---|
| 23 | B | 1 | Total | C | H | O | 0 |
| | | | 71 | 21 | 39 | 11 | |

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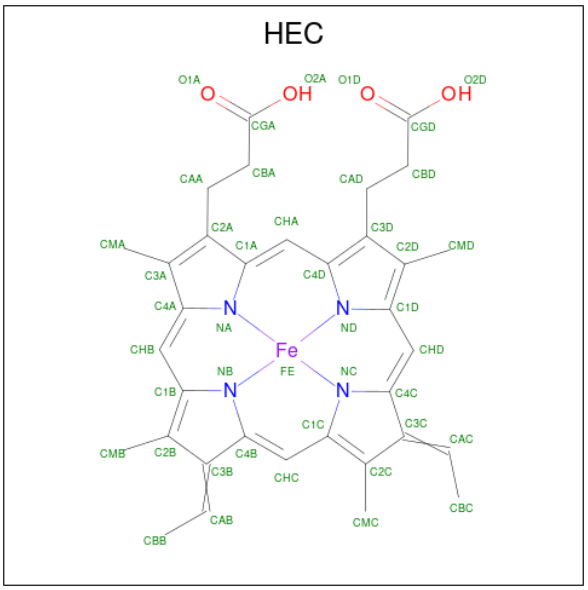
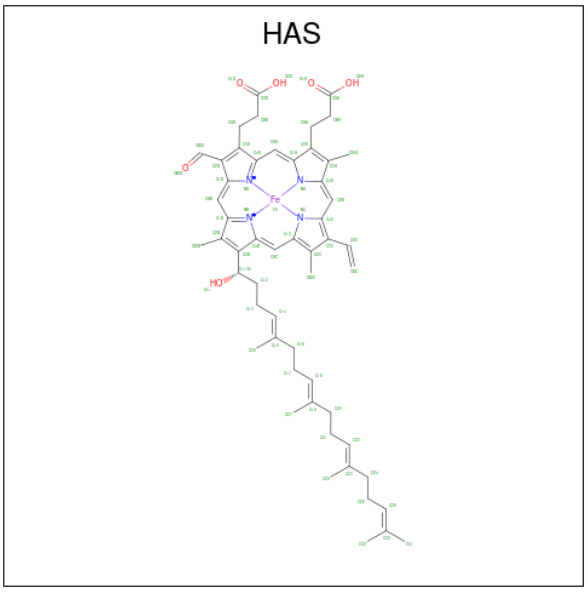
| Mol | Chain | Residues | Atoms | | | | AltConf |
|---|---|---|---|---|---|---|---|
| 23 | O | 1 | Total | C | H | O | 0 |
| | | | 71 | 21 | 39 | 11 | |

- Molecule 24 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).




| Mol | Chain | Residues | Atoms | | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|---|
| 24 | C | 1 | Total | C | Fe | H | N | O | 0 |
| | | | 146 | 68 | 2 | 60 | 8 | 8 | |
| 24 | C | 1 | Total | C | Fe | H | N | O | 0 |
| | | | 146 | 68 | 2 | 60 | 8 | 8 | |
| 24 | P | 1 | Total | C | Fe | H | N | O | 0 |
| | | | 146 | 68 | 2 | 60 | 8 | 8 | |
| 24 | P | 1 | Total | C | Fe | H | N | O | 0 |
| | | | 146 | 68 | 2 | 60 | 8 | 8 | |

- Molecule 25 is HEME-AS (three-letter code: HAS) (formula: $C_{54}H_{64}FeN_4O_6$) (labeled as "Ligand of Interest" by depositor).




| Mol | Chain | Residues | Atoms | | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|---|
| 25 | D | 1 | Total | C | Fe | H | N | O | 0 |
| | | | 254 | 108 | 2 | 124 | 8 | 12 | |
| 25 | D | 1 | Total | C | Fe | H | N | O | 0 |
| | | | 254 | 108 | 2 | 124 | 8 | 12 | |
| 25 | Q | 1 | Total | C | Fe | H | N | O | 0 |
| | | | 254 | 108 | 2 | 124 | 8 | 12 | |
| 25 | Q | 1 | Total | C | Fe | H | N | O | 0 |
| | | | 254 | 108 | 2 | 124 | 8 | 12 | |

- Molecule 26 is COPPER (II) ION (three-letter code: CU) (formula: Cu) (labeled as "Ligand of Interest" by depositor).

| Mol | Chain | Residues | Atoms | | AltConf |
|---|---|---|---|---|---|
| 26 | D | 1 | Total | Cu | 0 |
| | | | 1 | 1 | |
| 26 | Q | 1 | Total | Cu | 0 |
| | | | 1 | 1 | |

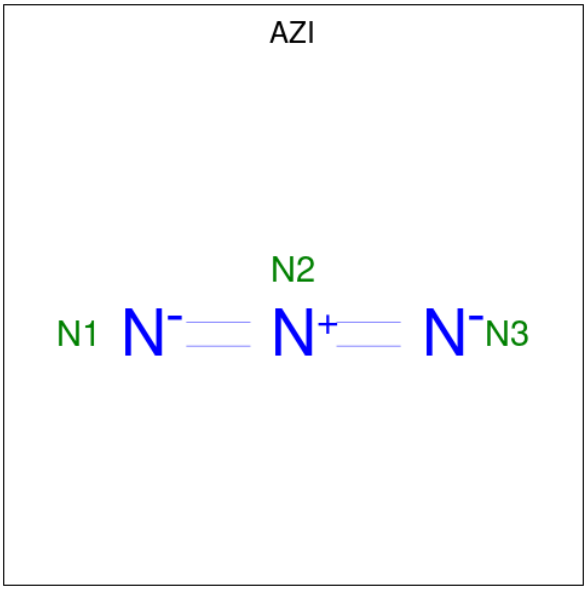
- Molecule 27 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn) (labeled as "Ligand of Interest" by depositor).

| Mol | Chain | Residues | Atoms | | AltConf |
|---|---|---|---|---|---|
| 27 | D | 1 | Total | Mn | 0 |
| | | | 1 | 1 | |
| 27 | R | 1 | Total | Mn | 0 |
| | | | 1 | 1 | |

- Molecule 28 is CALCIUM ION (three-letter code: CA) (formula: Ca).

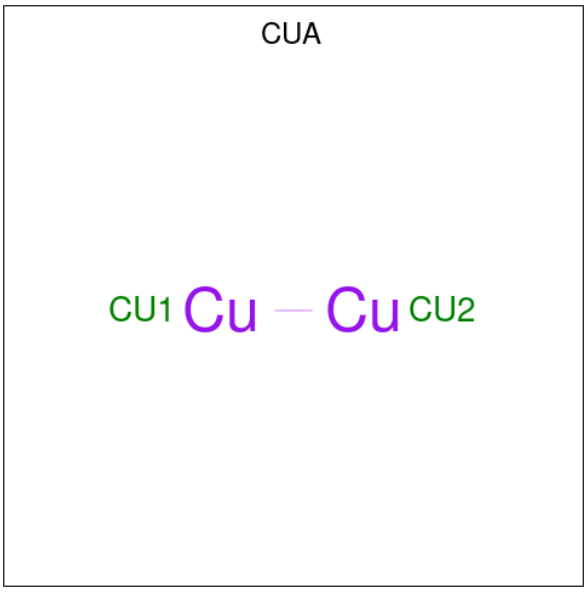
| Mol | Chain | Residues | Atoms | AltConf |
|---|---|---|---|---|
| 28 | D | 1 | Total Ca<br>1 1 | 0 |
| 28 | Q | 1 | Total Ca<br>1 1 | 0 |

- Molecule 29 is AZIDE ION (three-letter code: AZI) (formula: $N_3$) (labeled as "Ligand of Interest" by depositor).



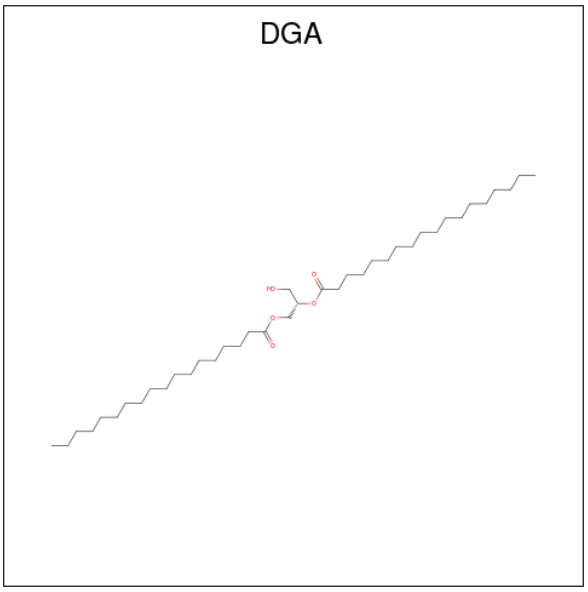

| Mol | Chain | Residues | Atoms | AltConf |
|---|---|---|---|---|
| 29 | D | 1 | Total N<br>3 3 | 0 |
| 29 | Q | 1 | Total N<br>3 3 | 0 |

- Molecule 30 is DINUCLEAR COPPER ION (three-letter code: CUA) (formula: $Cu_2$) (labeled as "Ligand of Interest" by depositor).



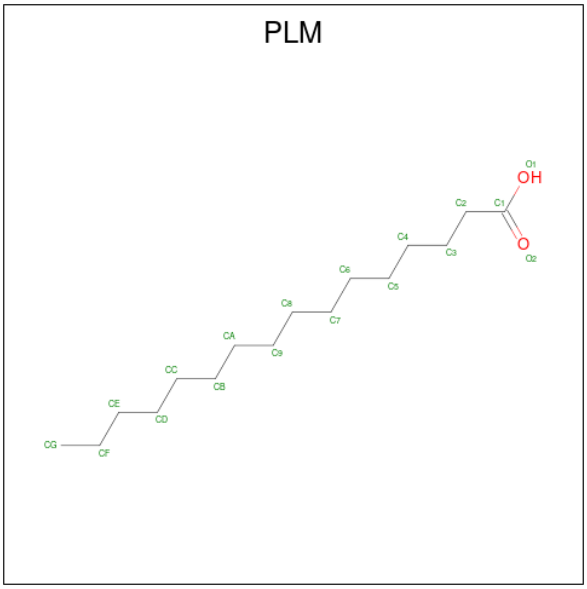

| Mol | Chain | Residues | Atoms | AltConf |
|---|---|---|---|---|
| 30 | E | 1 | Total Cu<br>2 2 | 0 |
| 30 | E | 1 | Total Cu<br>2 2 | 0 |
| 30 | R | 1 | Total Cu<br>2 2 | 0 |
| 30 | R | 1 | Total Cu<br>2 2 | 0 |

- Molecule 31 is DIACYL GLYCEROL (three-letter code: DGA) (formula: $C_{39}H_{76}O_5$) (labeled as "Ligand of Interest" by depositor).



| Mol | Chain | Residues | Atoms | AltConf |
|---|---|---|---|---|
| 31 | E | 1 | Total C O<br>20 16 4 | 0 |
| 31 | H | 1 | Total C O<br>17 13 4 | 0 |
| 31 | M | 1 | Total C O<br>22 18 4 | 0 |
| 31 | R | 1 | Total C O<br>25 21 4 | 0 |
| 31 | U | 1 | Total C O<br>27 23 4 | 0 |
| 31 | Z | 1 | Total C O<br>29 25 4 | 0 |

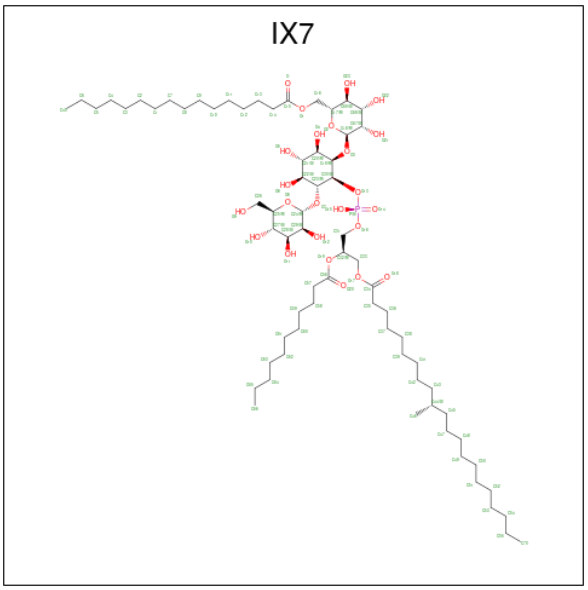
- Molecule 32 is PALMITIC ACID (three-letter code: PLM) (formula: $C_{16}H_{32}O_2$) (labeled as "Ligand of Interest" by depositor).




| Mol | Chain | Residues | Atoms | AltConf |
|---|---|---|---|---|
| 32 | H | 1 | Total C H O<br>41 16 24 1 | 0 |
| 32 | M | 1 | Total C H O<br>9 4 4 1 | 0 |
| 32 | U | 1 | Total C H O<br>45 16 28 1 | 0 |
| 32 | Z | 1 | Total C H O<br>9 4 4 1 | 0 |

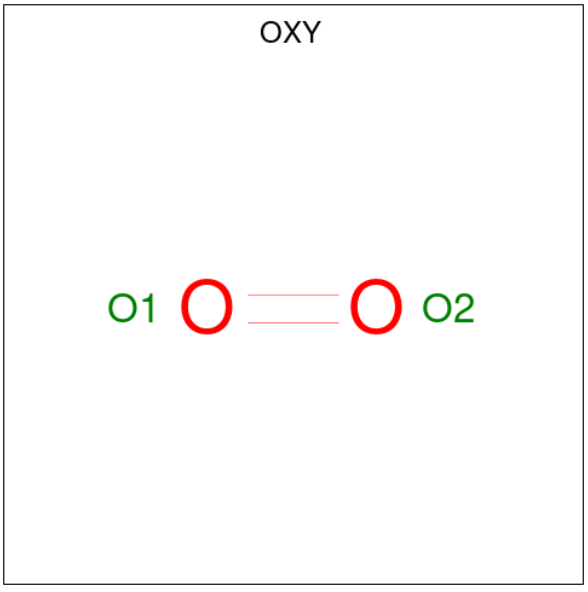
- Molecule 33 is [(2 {R})-3-[[(1 {S},2 {R},3 {R},4 {S},5 {S},6 {R})-2-[(2 {R},3 {S},4 {S},5 {S},6 {R})-6-(hexadecanoyloxymethyl)-3,4,5-tris(oxidanyl)oxan-2-yl]oxy-6-[(2 {R},3 {S},4 {

S},5 {S},6 {R})-6-(hydroxymethyl)-3,4,5-tris(oxidanyl)oxan-2-yl]oxy-3,4,5-tris(oxidanyl)cyclohexyl]oxy-oxidanyl-phosphoryl]oxy-2-undecanoyloxy-propyl] (10 {S})-10-methylhenicosanoate (three-letter code: IX7) (formula: $C_{70}H_{131}O_{24}P$) (labeled as "Ligand of Interest" by depositor).




| Mol | Chain | Residues | Atoms | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|
| 33 | H | 1 | Total | C | H | O | P | 0 |
| | | | 155 | 47 | 83 | 24 | 1 | |
| 33 | U | 1 | Total | C | H | O | P | 0 |
| | | | 155 | 47 | 83 | 24 | 1 | |

- Molecule 34 is OXYGEN MOLECULE (three-letter code: OXY) (formula: $O_2$) (labeled as "Ligand of Interest" by depositor).



| Mol | Chain | Residues | Atoms | AltConf |
|---|---|---|---|---|
| 34 | Q | 1 | Total O<br>2 2 | 0 |

- Molecule 35 is water.

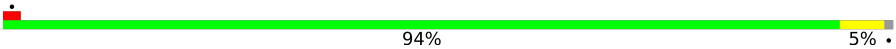
| Mol | Chain | Residues | Atoms | AltConf |
|---|---|---|---|---|
| 35 | A | 31 | Total O<br>31 31 | 0 |
| 35 | B | 56 | Total O<br>56 56 | 0 |
| 35 | C | 26 | Total O<br>26 26 | 0 |
| 35 | D | 21 | Total O<br>21 21 | 0 |
| 35 | E | 13 | Total O<br>13 13 | 0 |
| 35 | F | 3 | Total O<br>3 3 | 0 |
| 35 | G | 6 | Total O<br>6 6 | 0 |
| 35 | K | 3 | Total O<br>3 3 | 0 |
| 35 | N | 31 | Total O<br>31 31 | 0 |
| 35 | O | 46 | Total O<br>46 46 | 0 |
| 35 | P | 49 | Total O<br>49 49 | 0 |
| 35 | Q | 53 | Total O<br>53 53 | 0 |
| 35 | R | 44 | Total O<br>44 44 | 0 |
| 35 | S | 5 | Total O<br>5 5 | 0 |
| 35 | T | 13 | Total O<br>13 13 | 0 |
| 35 | U | 12 | Total O<br>12 12 | 0 |
| 35 | V | 2 | Total O<br>2 2 | 0 |
| 35 | X | 2 | Total O<br>2 2 | 0 |

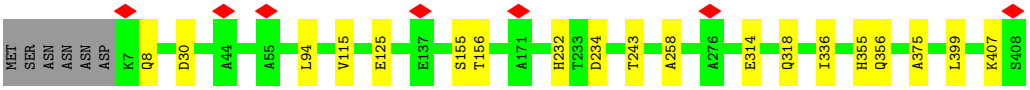
# 3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Cytochrome bc1 complex Rieske iron-sulfur subunit

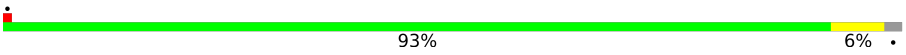
Chain A:

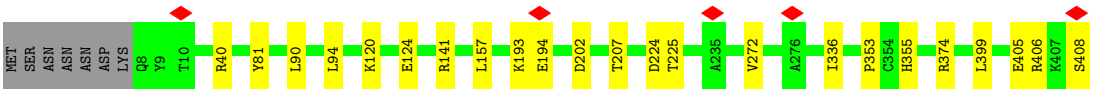



• Molecule 1: Cytochrome bc1 complex Rieske iron-sulfur subunit

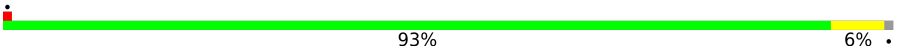
Chain N:

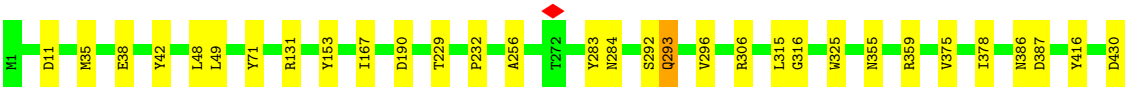



• Molecule 2: Cytochrome bc1 complex cytochrome b subunit

Chain B:

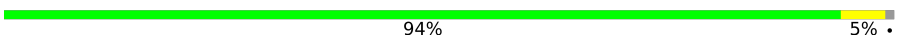


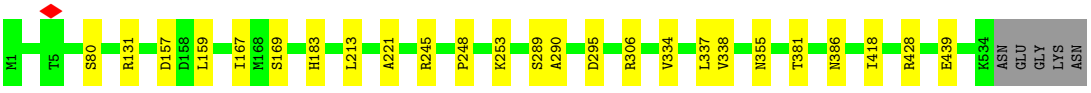





• Molecule 2: Cytochrome bc1 complex cytochrome b subunit

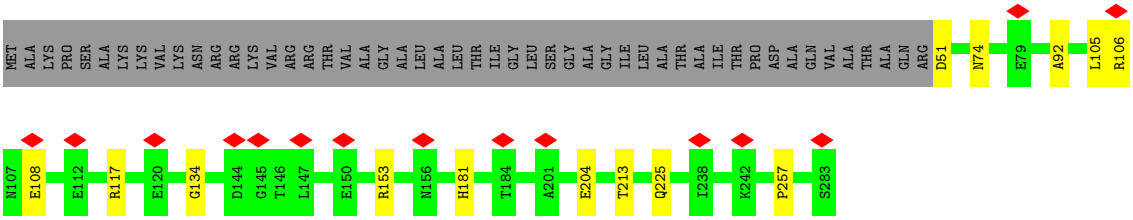
Chain O:



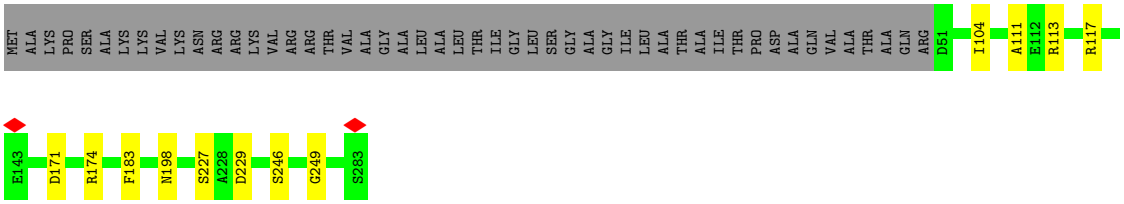

• Molecule 3: Cytochrome bc1 complex cytochrome c subunit

Chain C:



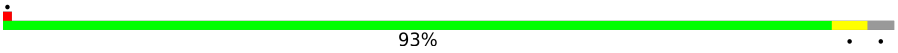

• Molecule 3: Cytochrome bc1 complex cytochrome c subunit

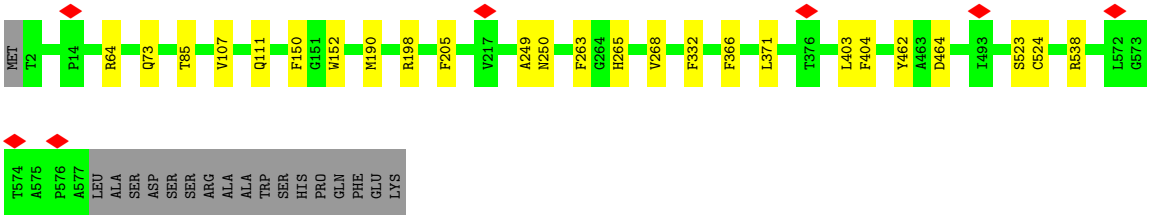
Chain P:


• Molecule 4: Cytochrome c oxidase subunit 1

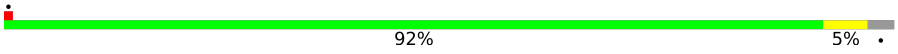
Chain D:

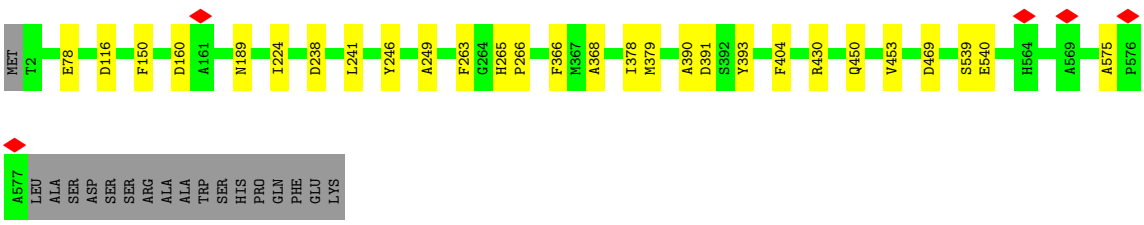



• Molecule 4: Cytochrome c oxidase subunit 1

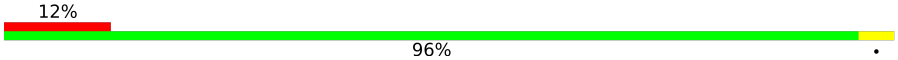
Chain Q:

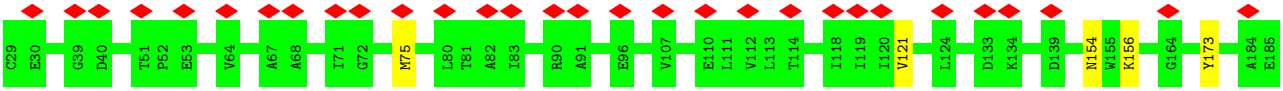


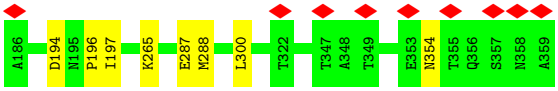




• Molecule 5: Cytochrome c oxidase subunit 2

Chain E:

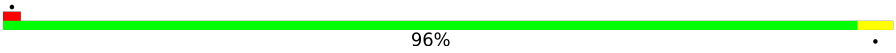


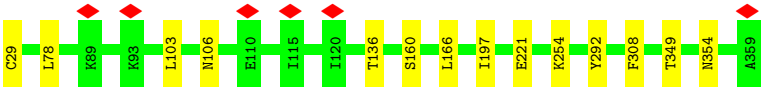






• Molecule 5: Cytochrome c oxidase subunit 2

Chain R:



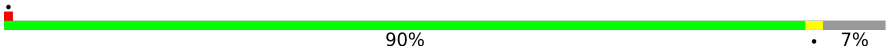

• Molecule 6: Cytochrome c oxidase subunit 3

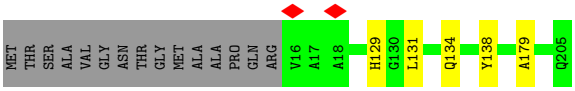
Chain F:



• Molecule 6: Cytochrome c oxidase subunit 3

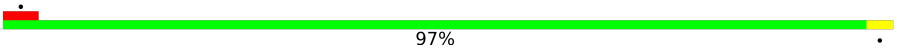
Chain S:

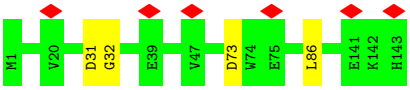



• Molecule 7: Cytochrome c oxidase polypeptide 4

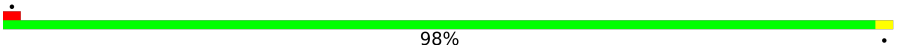
Chain G:

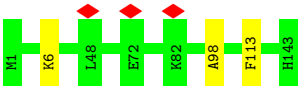



• Molecule 7: Cytochrome c oxidase polypeptide 4

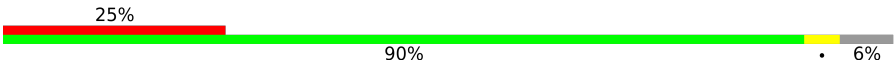
Chain T:

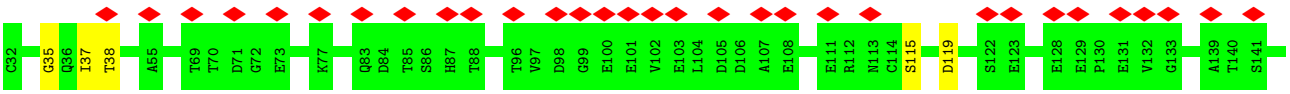


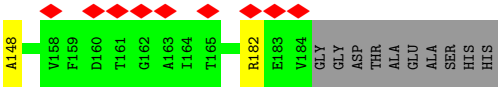




• Molecule 8: Uncharacterized protein Cgl2664/cg2949

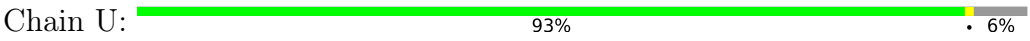
Chain H:

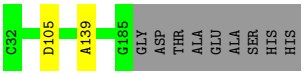


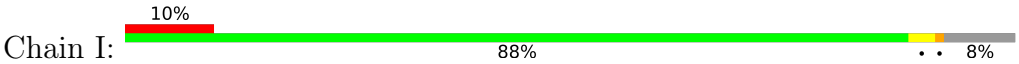


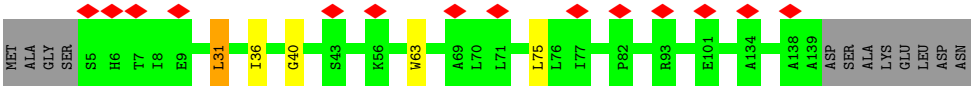

• Molecule 8: Uncharacterized protein Cgl2664/cg2949



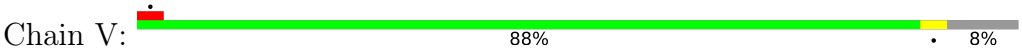



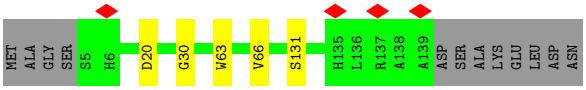

• Molecule 9: Uncharacterized membrane protein Cgl2017/cg2211



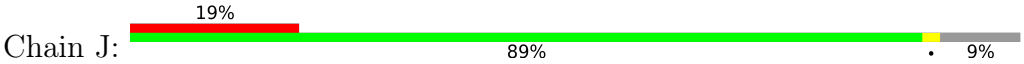



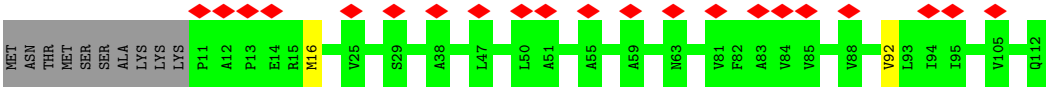

• Molecule 9: Uncharacterized membrane protein Cgl2017/cg2211



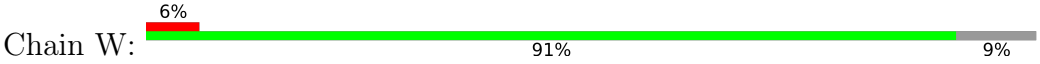



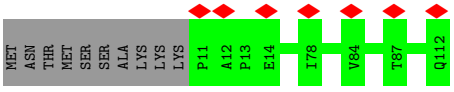

• Molecule 10: Hypothetical membrane protein



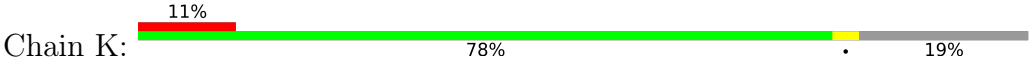



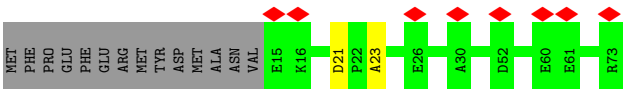

• Molecule 10: Hypothetical membrane protein



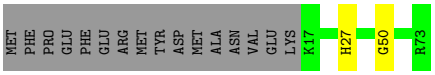

• Molecule 11: Actinobacterial supercomplex, subunit C (AscC)



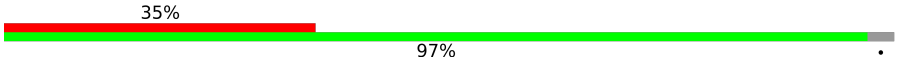

• Molecule 11: Actinobacterial supercomplex, subunit C (AscC)

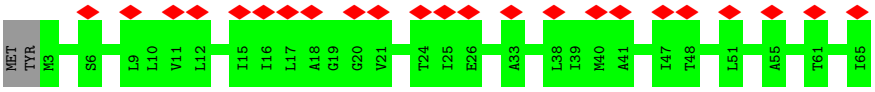
Chain X:


• Molecule 12: Hypothetical membrane protein

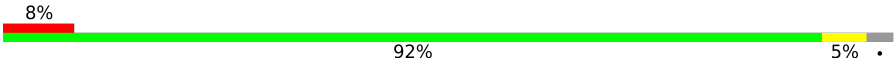
Chain L:

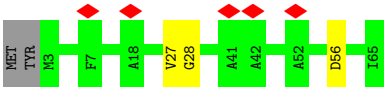



• Molecule 12: Hypothetical membrane protein

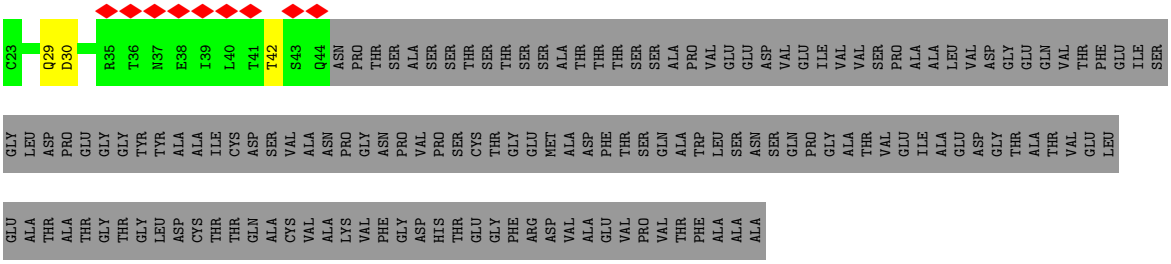
Chain Y:



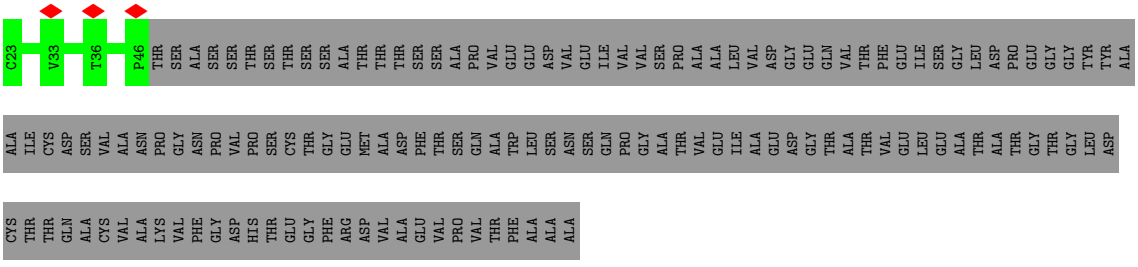

• Molecule 13: Thiamine biosynthesis protein X

Chain M:


• Molecule 13: Thiamine biosynthesis protein X

Chain Z:

# 4 Experimental information (i)

| Property | Value | Source |
|---|---|---|
| EM reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, C1 | Depositor |
| Number of particles used | 200424 | Depositor |
| Resolution determination method | FSC 0.143 CUT-OFF | Depositor |
| CTF correction method | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope | FEI TITAN KRIOS | Depositor |
| Voltage (kV) | 300 | Depositor |
| Electron dose ($e^-/Å^2$) | 40.0 | Depositor |
| Minimum defocus (nm) | 1000 | Depositor |
| Maximum defocus (nm) | 3000 | Depositor |
| Magnification | 75000 | Depositor |
| Image detector | FEI FALCON III (4k x 4k) | Depositor |
| Maximum map value | 2.641 | Depositor |
| Minimum map value | -1.574 | Depositor |
| Average map value | -0.000 | Depositor |
| Map value standard deviation | 0.114 | Depositor |
| Recommended contour level | 0.09 | Depositor |
| Map size (Å) | 281.49, 203.01399, 150.981 | wwPDB |
| Map dimensions | 177, 238, 330 | wwPDB |
| Map angles (°) | 90.0, 90.0, 90.0 | wwPDB |
| Pixel spacing (Å) | 0.853, 0.853, 0.85300004 | Depositor |

# 5 Model quality

## 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: LMT, LYC, IX7, FES, HEM, PLM, HAS, 9YF, MQ9, MN, OXY, IZL, CU, AZI, CDL, HEC, CA, SMA, CUA, 3PE, DGA

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

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | $\#\|Z\| > 5$ | RMSZ | $\#\|Z\| > 5$ |
| 1 | A | 0.39 | 0/3238 | 0.62 | 0/4403 |
| 1 | N | 0.41 | 0/3244 | 0.62 | 0/4414 |
| 2 | B | 0.41 | 0/4359 | 0.62 | 0/5937 |
| 2 | O | 0.44 | 0/4301 | 0.62 | 0/5860 |
| 3 | C | 0.35 | 0/1785 | 0.60 | 0/2413 |
| 3 | P | 0.42 | 0/1770 | 0.60 | 0/2394 |
| 4 | D | 0.40 | 0/4718 | 0.58 | 0/6438 |
| 4 | Q | 0.44 | 0/4734 | 0.60 | 0/6460 |
| 5 | E | 0.36 | 0/2671 | 0.58 | 0/3642 |
| 5 | R | 0.42 | 0/2686 | 0.58 | 0/3661 |
| 6 | F | 0.37 | 0/1528 | 0.56 | 0/2081 |
| 6 | S | 0.42 | 0/1528 | 0.57 | 0/2081 |
| 7 | G | 0.35 | 0/1126 | 0.53 | 0/1529 |
| 7 | T | 0.40 | 0/1144 | 0.52 | 0/1554 |
| 8 | H | 0.32 | 0/1134 | 0.58 | 0/1553 |
| 8 | U | 0.35 | 0/1138 | 0.58 | 0/1558 |
| 9 | I | 0.32 | 0/1103 | 0.58 | 0/1508 |
| 9 | V | 0.35 | 0/1103 | 0.60 | 0/1508 |
| 10 | J | 0.32 | 0/799 | 0.56 | 0/1087 |
| 10 | W | 0.37 | 0/799 | 0.63 | 0/1087 |
| 11 | K | 0.38 | 0/486 | 0.53 | 0/663 |
| 11 | X | 0.41 | 0/468 | 0.56 | 0/640 |
| 12 | L | 0.28 | 0/453 | 0.49 | 0/616 |
| 12 | Y | 0.33 | 0/453 | 0.54 | 0/616 |
| 13 | M | 0.27 | 0/174 | 0.57 | 0/238 |
| 13 | Z | 0.30 | 0/190 | 0.60 | 0/261 |
| All | All | 0.39 | 0/47132 | 0.59 | 0/64202 |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts (i)

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 1 | A | 3147 | 3084 | 3070 | 17 | 0 |
| 1 | N | 3145 | 3079 | 3063 | 16 | 0 |
| 2 | B | 4217 | 4268 | 4238 | 26 | 0 |
| 2 | O | 4186 | 4239 | 4238 | 20 | 0 |
| 3 | C | 1749 | 1694 | 1690 | 7 | 0 |
| 3 | P | 1738 | 1680 | 1680 | 7 | 0 |
| 4 | D | 4548 | 4470 | 4471 | 15 | 0 |
| 4 | Q | 4557 | 4477 | 4468 | 18 | 0 |
| 5 | E | 2598 | 2468 | 2468 | 6 | 0 |
| 5 | R | 2607 | 2482 | 2476 | 10 | 0 |
| 6 | F | 1486 | 1495 | 1494 | 5 | 0 |
| 6 | S | 1486 | 1494 | 1494 | 3 | 0 |
| 7 | G | 1095 | 1106 | 1106 | 2 | 0 |
| 7 | T | 1105 | 1114 | 1104 | 1 | 0 |
| 8 | H | 1120 | 1054 | 1054 | 5 | 0 |
| 8 | U | 1124 | 1057 | 1057 | 1 | 0 |
| 9 | I | 1073 | 1071 | 1071 | 4 | 0 |
| 9 | V | 1073 | 1071 | 1071 | 3 | 0 |
| 10 | J | 779 | 792 | 792 | 1 | 0 |
| 10 | W | 779 | 792 | 792 | 0 | 0 |
| 11 | K | 469 | 432 | 432 | 1 | 0 |
| 11 | X | 451 | 413 | 413 | 0 | 0 |
| 12 | L | 445 | 470 | 469 | 0 | 0 |
| 12 | Y | 445 | 470 | 469 | 2 | 0 |
| 13 | M | 171 | 159 | 159 | 2 | 0 |
| 13 | Z | 186 | 172 | 172 | 0 | 0 |
| 14 | A | 4 | 0 | 0 | 0 | 0 |
| 14 | N | 4 | 0 | 0 | 0 | 0 |
| 15 | A | 103 | 109 | 0 | 3 | 0 |
| 15 | N | 103 | 109 | 0 | 0 | 0 |
| 16 | A | 36 | 30 | 0 | 0 | 0 |
| 16 | H | 34 | 26 | 0 | 0 | 0 |
| 16 | N | 36 | 30 | 0 | 0 | 0 |

*Continued on next page...*

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 16 | U | 39 | 36 | 0 | 2 | 0 |
| 17 | A | 58 | 80 | 80 | 3 | 0 |
| 17 | B | 23 | 23 | 21 | 3 | 0 |
| 17 | N | 36 | 42 | 42 | 2 | 0 |
| 17 | O | 27 | 29 | 29 | 3 | 0 |
| 18 | A | 40 | 36 | 57 | 1 | 0 |
| 18 | C | 50 | 40 | 48 | 2 | 0 |
| 18 | D | 31 | 26 | 36 | 0 | 0 |
| 18 | F | 32 | 22 | 38 | 1 | 0 |
| 18 | J | 47 | 64 | 71 | 0 | 0 |
| 18 | L | 30 | 38 | 34 | 0 | 0 |
| 18 | N | 38 | 28 | 53 | 1 | 0 |
| 18 | P | 27 | 18 | 28 | 2 | 0 |
| 18 | Q | 39 | 32 | 55 | 3 | 0 |
| 18 | R | 31 | 16 | 36 | 3 | 0 |
| 18 | S | 43 | 52 | 60 | 0 | 0 |
| 18 | T | 146 | 148 | 191 | 1 | 0 |
| 18 | W | 47 | 68 | 68 | 0 | 0 |
| 19 | B | 37 | 42 | 41 | 1 | 0 |
| 19 | O | 37 | 42 | 41 | 1 | 0 |
| 20 | B | 86 | 60 | 60 | 3 | 0 |
| 20 | O | 86 | 60 | 60 | 3 | 0 |
| 21 | B | 171 | 122 | 174 | 2 | 0 |
| 21 | D | 140 | 149 | 171 | 1 | 0 |
| 21 | F | 57 | 37 | 58 | 1 | 0 |
| 21 | G | 144 | 135 | 179 | 2 | 0 |
| 21 | I | 57 | 50 | 61 | 0 | 0 |
| 21 | O | 66 | 79 | 79 | 0 | 0 |
| 21 | Q | 149 | 179 | 195 | 4 | 0 |
| 21 | S | 65 | 70 | 74 | 0 | 0 |
| 21 | T | 145 | 141 | 181 | 1 | 0 |
| 21 | V | 69 | 90 | 90 | 0 | 0 |
| 22 | B | 40 | 56 | 56 | 0 | 0 |
| 22 | O | 40 | 56 | 56 | 1 | 0 |
| 23 | B | 32 | 39 | 37 | 0 | 0 |
| 23 | O | 32 | 39 | 37 | 0 | 0 |
| 24 | C | 86 | 60 | 60 | 2 | 0 |
| 24 | P | 86 | 60 | 60 | 1 | 0 |
| 25 | D | 130 | 124 | 124 | 5 | 0 |
| 25 | Q | 130 | 124 | 124 | 4 | 0 |
| 26 | D | 1 | 0 | 0 | 0 | 0 |
| 26 | Q | 1 | 0 | 0 | 0 | 0 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 27 | D | 1 | 0 | 0 | 0 | 0 |
| 27 | R | 1 | 0 | 0 | 0 | 0 |
| 28 | D | 1 | 0 | 0 | 0 | 0 |
| 28 | Q | 1 | 0 | 0 | 0 | 0 |
| 29 | D | 3 | 0 | 0 | 2 | 0 |
| 29 | Q | 3 | 0 | 0 | 0 | 0 |
| 30 | E | 2 | 0 | 0 | 0 | 0 |
| 30 | R | 2 | 0 | 0 | 0 | 0 |
| 31 | E | 20 | 0 | 21 | 0 | 0 |
| 31 | H | 17 | 0 | 15 | 2 | 0 |
| 31 | M | 22 | 0 | 25 | 1 | 0 |
| 31 | R | 25 | 0 | 31 | 0 | 0 |
| 31 | U | 27 | 0 | 35 | 3 | 0 |
| 31 | Z | 29 | 0 | 39 | 0 | 0 |
| 32 | H | 17 | 24 | 31 | 0 | 0 |
| 32 | M | 5 | 4 | 4 | 0 | 0 |
| 32 | U | 17 | 28 | 31 | 0 | 0 |
| 32 | Z | 5 | 4 | 4 | 0 | 0 |
| 33 | H | 72 | 83 | 0 | 2 | 0 |
| 33 | U | 72 | 83 | 0 | 2 | 0 |
| 34 | Q | 2 | 0 | 0 | 0 | 0 |
| 35 | A | 31 | 0 | 0 | 8 | 0 |
| 35 | B | 56 | 0 | 0 | 10 | 0 |
| 35 | C | 26 | 0 | 0 | 1 | 0 |
| 35 | D | 21 | 0 | 0 | 1 | 0 |
| 35 | E | 13 | 0 | 0 | 4 | 0 |
| 35 | F | 3 | 0 | 0 | 1 | 0 |
| 35 | G | 6 | 0 | 0 | 0 | 0 |
| 35 | K | 3 | 0 | 0 | 0 | 0 |
| 35 | N | 31 | 0 | 0 | 5 | 0 |
| 35 | O | 46 | 0 | 0 | 3 | 0 |
| 35 | P | 49 | 0 | 0 | 1 | 0 |
| 35 | Q | 53 | 0 | 0 | 8 | 0 |
| 35 | R | 44 | 0 | 0 | 2 | 0 |
| 35 | S | 5 | 0 | 0 | 0 | 0 |
| 35 | T | 13 | 0 | 0 | 0 | 0 |
| 35 | U | 12 | 0 | 0 | 0 | 0 |
| 35 | V | 2 | 0 | 0 | 0 | 0 |
| 35 | X | 2 | 0 | 0 | 0 | 0 |
| All | All | 49530 | 48245 | 48212 | 187 | 0 |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (187) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 4:Q:238:ASP:OD2 | 35:Q:701:HOH:O | 2.04 | 0.75 |
| 1:N:353:PRO:O | 35:N:601:HOH:O | 2.05 | 0.75 |
| 4:D:205:PHE:O | 35:D:701:HOH:O | 2.04 | 0.74 |
| 6:F:59:SER:O | 35:F:401:HOH:O | 2.07 | 0.73 |
| 3:C:257:PRO:O | 35:C:401:HOH:O | 2.08 | 0.72 |
| 2:B:190:ASP:OD1 | 35:B:701:HOH:O | 2.07 | 0.72 |
| 1:A:399:LEU:O | 35:A:601:HOH:O | 2.08 | 0.72 |
| 2:B:296:VAL:O | 35:B:702:HOH:O | 2.08 | 0.71 |
| 4:Q:469:ASP:O | 35:Q:702:HOH:O | 2.07 | 0.71 |
| 5:R:292:TYR:OH | 35:R:501:HOH:O | 2.08 | 0.71 |
| 4:D:250:ASN:O | 6:F:53:ASN:ND2 | 2.23 | 0.71 |
| 5:E:156:LYS:O | 35:E:501:HOH:O | 2.08 | 0.70 |
| 25:Q:602:HAS:O2A | 35:Q:704:HOH:O | 2.08 | 0.70 |
| 8:U:105:ASP:OD2 | 8:U:139:ALA:N | 2.25 | 0.70 |
| 1:A:318:GLN:O | 35:A:602:HOH:O | 2.09 | 0.70 |
| 2:B:476:ALA:O | 35:B:703:HOH:O | 2.08 | 0.70 |
| 5:E:288:MET:O | 35:E:502:HOH:O | 2.09 | 0.70 |
| 1:A:258:ALA:O | 35:A:603:HOH:O | 2.10 | 0.69 |
| 1:N:225:THR:O | 35:N:603:HOH:O | 2.10 | 0.69 |
| 1:N:224:ASP:OD2 | 35:N:602:HOH:O | 2.08 | 0.69 |
| 4:Q:238:ASP:OD1 | 35:Q:705:HOH:O | 2.10 | 0.69 |
| 15:A:502:IZL:O6 | 15:A:502:IZL:O9 | 2.11 | 0.68 |
| 2:O:439:GLU:OE1 | 35:O:701:HOH:O | 2.12 | 0.68 |
| 1:A:314:GLU:OE1 | 35:A:602:HOH:O | 2.11 | 0.68 |
| 3:P:198:ASN:O | 35:P:401:HOH:O | 2.11 | 0.68 |
| 5:R:221:GLU:OE2 | 35:R:502:HOH:O | 2.12 | 0.67 |
| 1:A:155:SER:O | 1:A:156:THR:OG1 | 2.12 | 0.67 |
| 1:A:30:ASP:O | 35:A:604:HOH:O | 2.13 | 0.67 |
| 1:A:94:LEU:HD21 | 18:C:303:3PE:H222 | 1.76 | 0.67 |
| 2:B:283:TYR:O | 35:B:704:HOH:O | 2.12 | 0.67 |
| 4:Q:160:ASP:OD1 | 35:Q:706:HOH:O | 2.13 | 0.66 |
| 25:Q:601:HAS:HMC1 | 25:Q:601:HAS:HBC1 | 1.78 | 0.66 |
| 9:I:31:LEU:HD23 | 9:I:36:ILE:HD11 | 1.77 | 0.66 |
| 1:A:125:GLU:O | 35:A:605:HOH:O | 2.14 | 0.65 |
| 2:B:229:THR:OG1 | 20:B:603:HEM:O2D | 2.10 | 0.63 |
| 15:A:502:IZL:O6 | 15:A:502:IZL:O8 | 2.18 | 0.62 |
| 1:A:375:ALA:O | 35:A:606:HOH:O | 2.16 | 0.61 |
| 5:E:354:ASN:OD1 | 35:E:503:HOH:O | 2.16 | 0.61 |
| 3:P:227:SER:OG | 3:P:229:ASP:OD1 | 2.15 | 0.61 |
| 2:O:80:SER:OG | 2:O:157:ASP:OD2 | 2.13 | 0.61 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 17:B:604:MQ9:H8 | 17:B:604:MQ9:H5M3 | 1.83 | 0.60 |
| 4:D:198:ARG:NH2 | 7:G:73:ASP:OD1 | 2.33 | 0.60 |
| 17:O:605:MQ9:H5M3 | 17:O:605:MQ9:C8 | 2.30 | 0.60 |
| 1:A:356:GLN:OE1 | 35:A:607:HOH:O | 2.17 | 0.60 |
| 17:A:504:MQ9:H402 | 20:B:602:HEM:HBB1 | 1.84 | 0.59 |
| 19:O:602:SMA:H37 | 19:O:602:SMA:H33 | 1.85 | 0.59 |
| 2:O:418:ILE:CD1 | 21:Q:608:CDL:H712 | 2.33 | 0.59 |
| 2:B:355:ASN:ND2 | 35:B:709:HOH:O | 2.35 | 0.58 |
| 4:Q:241:LEU:O | 6:S:134:GLN:NE2 | 2.36 | 0.58 |
| 25:D:601:HAS:HBC1 | 25:D:601:HAS:HMC1 | 1.86 | 0.58 |
| 31:H:201:DGA:HB32 | 33:H:204:IX7:C7 | 2.34 | 0.58 |
| 2:O:253:LYS:NZ | 35:O:708:HOH:O | 2.34 | 0.58 |
| 25:Q:601:HAS:O2D | 35:Q:707:HOH:O | 2.17 | 0.58 |
| 16:U:203:9YF:O7 | 16:U:203:9YF:O8 | 2.22 | 0.58 |
| 25:D:602:HAS:HMC1 | 25:D:602:HAS:HBC1 | 1.87 | 0.57 |
| 20:O:603:HEM:HBB2 | 20:O:603:HEM:HMB2 | 1.86 | 0.56 |
| 2:B:359:ARG:NH2 | 2:B:430[B]:ASP:OD2 | 2.39 | 0.56 |
| 4:Q:368:ALA:HB2 | 18:Q:609:3PE:H2B1 | 1.88 | 0.56 |
| 18:A:505:3PE:H282 | 2:O:248:PRO:HB3 | 1.88 | 0.55 |
| 17:B:604:MQ9:H5M3 | 17:B:604:MQ9:C8 | 2.36 | 0.55 |
| 2:O:418:ILE:HD12 | 21:Q:608:CDL:H712 | 1.88 | 0.55 |
| 2:B:232:PRO:O | 35:B:705:HOH:O | 2.18 | 0.54 |
| 4:Q:430:ARG:NE | 12:Y:56:ASP:OD2 | 2.38 | 0.54 |
| 1:A:336:ILE:HD12 | 2:B:167:ILE:HG23 | 1.90 | 0.54 |
| 2:B:306:ARG:O | 35:B:706:HOH:O | 2.19 | 0.54 |
| 1:N:40:ARG:NH2 | 1:N:124:GLU:OE1 | 2.41 | 0.54 |
| 8:H:37:ILE:HG12 | 33:H:204:IX7:O9 | 2.08 | 0.53 |
| 2:B:42:TYR:HE1 | 17:B:604:MQ9:H102 | 1.74 | 0.53 |
| 4:D:464:ASP:OD2 | 35:E:503:HOH:O | 2.18 | 0.53 |
| 4:Q:539:SER:OG | 4:Q:540:GLU:N | 2.39 | 0.53 |
| 1:N:90:LEU:HD11 | 18:P:303:3PE:H241 | 1.90 | 0.52 |
| 2:O:337:LEU:HD22 | 22:O:607:LYC:H623 | 1.92 | 0.52 |
| 4:D:371:LEU:HD21 | 5:E:75:MET:HB2 | 1.92 | 0.52 |
| 4:D:332:PHE:HB3 | 5:E:121:VAL:HG13 | 1.93 | 0.51 |
| 2:B:416:TYR:OH | 9:I:31:LEU:HD22 | 2.09 | 0.51 |
| 1:N:336:ILE:HD12 | 2:O:167:ILE:HG23 | 1.93 | 0.51 |
| 10:J:16:MET:SD | 10:J:16:MET:N | 2.83 | 0.51 |
| 4:Q:391:ASP:OD1 | 35:Q:708:HOH:O | 2.19 | 0.51 |
| 17:A:504:MQ9:H401 | 2:B:48:LEU:HD22 | 1.93 | 0.51 |
| 3:C:92:ALA:HA | 3:C:213:THR:HG21 | 1.93 | 0.51 |
| 25:D:602:HAS:C1A | 29:D:606:AZI:N3 | 2.65 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:C:74:ASN:OD1 | 8:H:115:SER:OG | 2.30 | 0.50 |
| 1:N:157:LEU:HD22 | 18:N:502:3PE:H2D1 | 1.93 | 0.50 |
| 4:Q:390:ALA:O | 5:R:254:LYS:NZ | 2.40 | 0.50 |
| 2:B:325:TRP:HB3 | 31:M:201:DGA:HA71 | 1.94 | 0.50 |
| 4:Q:368:ALA:CB | 18:Q:609:3PE:H2B1 | 2.42 | 0.50 |
| 4:D:152:TRP:NE1 | 25:D:602:HAS:O1A | 2.41 | 0.50 |
| 17:O:605:MQ9:H5M3 | 17:O:605:MQ9:C9 | 2.42 | 0.49 |
| 3:C:51:ASP:OD1 | 3:C:51:ASP:N | 2.45 | 0.49 |
| 25:Q:602:HAS:HMC1 | 25:Q:602:HAS:HBC1 | 1.94 | 0.49 |
| 7:G:31:ASP:OD1 | 7:G:32:GLY:N | 2.45 | 0.49 |
| 2:B:35:MET:HA | 2:B:38:GLU:HG3 | 1.94 | 0.49 |
| 11:K:21:ASP:OD1 | 11:K:23:ALA:N | 2.44 | 0.49 |
| 3:C:225:GLN:O | 8:H:182:ARG:NH2 | 2.44 | 0.49 |
| 5:R:166:LEU:HD13 | 5:R:308:PHE:HD2 | 1.77 | 0.49 |
| 24:C:301:HEC:HBB2 | 24:C:301:HEC:HHC | 1.94 | 0.49 |
| 4:Q:249:ALA:HB3 | 5:R:197:ILE:HG21 | 1.95 | 0.49 |
| 2:B:526:ASN:OD1 | 35:B:707:HOH:O | 2.20 | 0.49 |
| 19:B:601:SMA:H36 | 19:B:601:SMA:H31 | 1.95 | 0.48 |
| 1:N:374:ARG:NH1 | 35:N:605:HOH:O | 2.40 | 0.48 |
| 4:D:73:GLN:N | 4:D:73:GLN:OE1 | 2.45 | 0.48 |
| 31:U:201:DGA:HB92 | 9:V:63:TRP:CZ3 | 2.48 | 0.48 |
| 1:N:81:TYR:OH | 35:N:604:HOH:O | 2.19 | 0.48 |
| 3:C:204:GLU:OE1 | 3:C:204:GLU:N | 2.45 | 0.48 |
| 6:F:25:VAL:HG12 | 6:F:182:VAL:HG11 | 1.94 | 0.48 |
| 2:O:169:SER:OG | 2:O:183:HIS:NE2 | 2.40 | 0.48 |
| 4:D:265:HIS:CE1 | 29:D:606:AZI:N1 | 2.82 | 0.48 |
| 1:N:406:ARG:NH1 | 1:N:408:SER:O | 2.47 | 0.48 |
| 2:O:381:THR:HG22 | 18:T:203:3PE:H2C1 | 1.95 | 0.47 |
| 1:N:405:GLU:N | 1:N:405:GLU:OE1 | 2.45 | 0.47 |
| 4:D:265:HIS:O | 4:D:268:VAL:HG22 | 2.14 | 0.47 |
| 8:H:35:GLY:O | 8:H:38:THR:HG23 | 2.14 | 0.47 |
| 1:A:407:LYS:HG3 | 15:A:502:IZL:O23 | 2.14 | 0.47 |
| 4:Q:78:GLU:OE1 | 4:Q:78:GLU:N | 2.46 | 0.47 |
| 6:F:129:HIS:ND1 | 6:F:129:HIS:O | 2.48 | 0.47 |
| 1:N:336:ILE:HD11 | 1:N:355:HIS:CE1 | 2.49 | 0.47 |
| 5:R:106:ASN:ND2 | 18:R:405:3PE:O22 | 2.47 | 0.47 |
| 2:B:315:LEU:N | 2:B:316:GLY:HA2 | 2.29 | 0.47 |
| 1:A:336:ILE:HD11 | 1:A:355:HIS:CE1 | 2.50 | 0.46 |
| 1:N:94:LEU:HD11 | 18:P:303:3PE:H271 | 1.97 | 0.46 |
| 4:D:523:SER:OG | 4:D:524:CYS:N | 2.48 | 0.46 |
| 4:Q:378:ILE:HD12 | 4:Q:379:MET:N | 2.30 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:O:245:ARG:NH1 | 35:O:707:HOH:O | 2.48 | 0.46 |
| 8:H:148:ALA:HB2 | 13:M:42:THR:HB | 1.98 | 0.46 |
| 1:N:193:LYS:N | 1:N:194:GLU:HA | 2.31 | 0.46 |
| 2:B:526:ASN:ND2 | 35:B:716:HOH:O | 2.48 | 0.45 |
| 20:B:602:HEM:HHA | 20:B:602:HEM:HBA2 | 1.97 | 0.45 |
| 5:R:103:LEU:HD23 | 18:R:405:3PE:H222 | 1.97 | 0.45 |
| 1:A:8:GLN:N | 1:A:8:GLN:OE1 | 2.49 | 0.45 |
| 3:P:113:ARG:NH1 | 24:P:302:HEC:O1A | 2.50 | 0.45 |
| 21:D:607:CDL:H781 | 6:F:155:ALA:HB1 | 1.99 | 0.45 |
| 1:A:94:LEU:CD2 | 18:C:303:3PE:H222 | 2.45 | 0.45 |
| 13:M:29:GLN:NE2 | 13:M:30:ASP:OD2 | 2.49 | 0.45 |
| 4:Q:246:TYR:N | 35:Q:701:HOH:O | 2.38 | 0.44 |
| 5:R:78:LEU:CD1 | 18:R:405:3PE:H2B2 | 2.48 | 0.44 |
| 3:P:171:ASP:OD1 | 3:P:174:ARG:NH1 | 2.48 | 0.44 |
| 4:Q:450:GLN:HA | 4:Q:453:VAL:HG12 | 1.99 | 0.44 |
| 6:S:131:LEU:HD11 | 6:S:138:TYR:HD2 | 1.82 | 0.44 |
| 21:Q:607:CDL:OB7 | 6:S:179:ALA:HB1 | 2.18 | 0.44 |
| 17:A:504:MQ9:H302 | 2:O:213:LEU:HD22 | 2.00 | 0.44 |
| 31:U:201:DGA:HB82 | 9:V:66:VAL:HG11 | 1.99 | 0.44 |
| 16:U:203:9YF:O4 | 33:U:204:IX7:O21 | 2.36 | 0.44 |
| 21:G:202:CDL:HB62 | 21:G:202:CDL:H132 | 1.98 | 0.44 |
| 2:O:418:ILE:HD13 | 21:Q:608:CDL:H712 | 2.00 | 0.44 |
| 2:B:293:GLN:NE2 | 2:B:387:ASP:OD1 | 2.51 | 0.43 |
| 21:G:201:CDL:HB62 | 21:G:201:CDL:HB22 | 2.00 | 0.43 |
| 21:B:609:CDL:H711 | 2:O:221:ALA:HB2 | 1.99 | 0.43 |
| 2:B:375:VAL:O | 2:B:378:ILE:HG22 | 2.19 | 0.43 |
| 20:O:604:HEM:HMC2 | 20:O:604:HEM:HBC2 | 2.00 | 0.43 |
| 12:Y:27:VAL:HG23 | 12:Y:28:GLY:HA2 | 2.00 | 0.43 |
| 1:N:202:ASP:OD1 | 1:N:207:THR:OG1 | 2.35 | 0.43 |
| 17:O:605:MQ9:H122 | 17:O:605:MQ9:H103 | 1.81 | 0.43 |
| 31:U:201:DGA:HB61 | 33:U:204:IX7:C66 | 2.48 | 0.43 |
| 4:D:85:THR:OG1 | 4:D:150:PHE:O | 2.26 | 0.43 |
| 5:R:349:THR:HG22 | 5:R:354:ASN:HA | 2.00 | 0.43 |
| 1:A:232:HIS:NE2 | 1:A:234:ASP:OD2 | 2.52 | 0.43 |
| 18:F:301:3PE:H232 | 18:F:301:3PE:H321 | 2.01 | 0.42 |
| 2:B:306:ARG:NH1 | 2:B:386:ASN:OD1 | 2.52 | 0.42 |
| 2:O:289:SER:OG | 2:O:290:ALA:N | 2.51 | 0.42 |
| 2:B:49:LEU:HB2 | 17:N:501:MQ9:H5M3 | 2.01 | 0.42 |
| 21:F:302:CDL:OB7 | 21:F:302:CDL:HB31 | 2.19 | 0.42 |
| 2:O:159:LEU:HD23 | 3:P:183:PHE:HE1 | 1.85 | 0.42 |
| 3:C:106:ARG:NE | 3:C:108:GLU:OE2 | 2.52 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 24:C:302:HEC:HMC1 | 24:C:302:HEC:HBC3 | 2.01 | 0.42 |
| 2:O:131:ARG:NH2 | 2:O:355:ASN:OD1 | 2.48 | 0.42 |
| 2:B:11:ASP:OD2 | 1:N:141:ARG:NH1 | 2.52 | 0.42 |
| 4:Q:224:ILE:HG21 | 4:Q:266:PRO:HB2 | 2.02 | 0.42 |
| 2:B:131:ARG:NH2 | 2:B:355:ASN:OD1 | 2.53 | 0.41 |
| 20:O:603:HEM:HHA | 20:O:603:HEM:HBA2 | 2.01 | 0.41 |
| 2:B:284:ASN:ND2 | 35:B:718:HOH:O | 2.53 | 0.41 |
| 21:B:605:CDL:H112 | 21:B:605:CDL:H512 | 2.02 | 0.41 |
| 4:D:403:LEU:HD23 | 25:D:602:HAS:HBC2 | 2.01 | 0.41 |
| 2:O:334:VAL:O | 2:O:338:VAL:HG23 | 2.21 | 0.41 |
| 2:O:428:ARG:NH2 | 9:V:20:ASP:O | 2.53 | 0.41 |
| 31:H:201:DGA:HB51 | 9:I:63:TRP:CZ2 | 2.55 | 0.41 |
| 3:P:104:ILE:HD11 | 3:P:111:ALA:HB2 | 2.03 | 0.41 |
| 5:R:136:THR:HG22 | 5:R:136:THR:O | 2.21 | 0.41 |
| 7:T:98:ALA:HB1 | 21:T:201:CDL:H152 | 2.03 | 0.41 |
| 17:N:501:MQ9:H5M3 | 17:N:501:MQ9:H72 | 1.90 | 0.40 |
| 1:A:115:VAL:HG23 | 2:B:256:ALA:HB1 | 2.03 | 0.40 |
| 3:P:246:SER:OG | 3:P:249:GLY:O | 2.35 | 0.40 |
| 4:D:107:VAL:HG12 | 4:D:111:GLN:HG3 | 2.03 | 0.40 |
| 4:D:249:ALA:HB3 | 5:E:197:ILE:HG21 | 2.03 | 0.40 |
| 18:Q:609:3PE:H2B2 | 18:Q:609:3PE:H2E1 | 1.94 | 0.40 |
| 9:I:40:GLY:HA3 | 9:I:75:LEU:HD21 | 2.04 | 0.40 |
| 2:O:306:ARG:NH1 | 2:O:386:ASN:OD1 | 2.54 | 0.40 |

There are no symmetry-related clashes.

## 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 | A | 402/408 (98%) | 382 (95%) | 20 (5%) | 0 | 100 | 100 |
| 1 | N | 403/408 (99%) | 388 (96%) | 14 (4%) | 1 (0%) | 47 | 78 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles |
|---|---|---|---|---|---|---|
| 2 | B | 538/539 (100%) | 519 (96%) | 16 (3%) | 3 (1%) | 25 56 |
| 2 | O | 532/539 (99%) | 518 (97%) | 14 (3%) | 0 | 100 100 |
| 3 | C | 233/283 (82%) | 217 (93%) | 13 (6%) | 3 (1%) | 12 36 |
| 3 | P | 231/283 (82%) | 214 (93%) | 17 (7%) | 0 | 100 100 |
| 4 | D | 574/594 (97%) | 553 (96%) | 21 (4%) | 0 | 100 100 |
| 4 | Q | 576/594 (97%) | 553 (96%) | 22 (4%) | 1 (0%) | 47 78 |
| 5 | E | 329/331 (99%) | 313 (95%) | 14 (4%) | 2 (1%) | 25 56 |
| 5 | R | 331/331 (100%) | 318 (96%) | 13 (4%) | 0 | 100 100 |
| 6 | F | 188/205 (92%) | 185 (98%) | 3 (2%) | 0 | 100 100 |
| 6 | S | 188/205 (92%) | 182 (97%) | 6 (3%) | 0 | 100 100 |
| 7 | G | 141/143 (99%) | 135 (96%) | 6 (4%) | 0 | 100 100 |
| 7 | T | 143/143 (100%) | 137 (96%) | 6 (4%) | 0 | 100 100 |
| 8 | H | 151/163 (93%) | 147 (97%) | 4 (3%) | 0 | 100 100 |
| 8 | U | 152/163 (93%) | 146 (96%) | 6 (4%) | 0 | 100 100 |
| 9 | I | 133/147 (90%) | 124 (93%) | 8 (6%) | 1 (1%) | 19 49 |
| 9 | V | 133/147 (90%) | 126 (95%) | 6 (4%) | 1 (1%) | 19 49 |
| 10 | J | 100/112 (89%) | 97 (97%) | 3 (3%) | 0 | 100 100 |
| 10 | W | 100/112 (89%) | 95 (95%) | 5 (5%) | 0 | 100 100 |
| 11 | K | 57/73 (78%) | 55 (96%) | 2 (4%) | 0 | 100 100 |
| 11 | X | 55/73 (75%) | 53 (96%) | 1 (2%) | 1 (2%) | 8 28 |
| 12 | L | 61/65 (94%) | 57 (93%) | 4 (7%) | 0 | 100 100 |
| 12 | Y | 61/65 (94%) | 58 (95%) | 3 (5%) | 0 | 100 100 |
| 13 | M | 20/168 (12%) | 16 (80%) | 4 (20%) | 0 | 100 100 |
| 13 | Z | 22/168 (13%) | 20 (91%) | 2 (9%) | 0 | 100 100 |
| All | All | 5854/6462 (91%) | 5608 (96%) | 233 (4%) | 13 (0%) | 50 78 |

All (13) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | B | 292 | SER |
| 4 | Q | 575 | ALA |
| 9 | V | 30 | GLY |
| 2 | B | 71 | TYR |
| 3 | C | 181 | HIS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 5 | E | 194 | ASP |
| 9 | I | 31 | LEU |
| 2 | B | 293 | GLN |
| 3 | C | 153 | ARG |
| 1 | N | 272 | VAL |
| 3 | C | 134 | GLY |
| 11 | X | 50 | GLY |
| 5 | E | 196 | 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 | A | 328/332 (99%) | 327 (100%) | 1 (0%) | 92 98 |
| 1 | N | 329/332 (99%) | 326 (99%) | 3 (1%) | 78 94 |
| 2 | B | 443/441 (100%) | 440 (99%) | 3 (1%) | 84 95 |
| 2 | O | 437/441 (99%) | 436 (100%) | 1 (0%) | 93 98 |
| 3 | C | 178/212 (84%) | 176 (99%) | 2 (1%) | 73 92 |
| 3 | P | 177/212 (84%) | 176 (99%) | 1 (1%) | 86 96 |
| 4 | D | 473/488 (97%) | 466 (98%) | 7 (2%) | 65 89 |
| 4 | Q | 475/488 (97%) | 468 (98%) | 7 (2%) | 65 89 |
| 5 | E | 274/274 (100%) | 269 (98%) | 5 (2%) | 59 86 |
| 5 | R | 276/274 (101%) | 274 (99%) | 2 (1%) | 84 95 |
| 6 | F | 156/166 (94%) | 156 (100%) | 0 | 100 100 |
| 6 | S | 156/166 (94%) | 155 (99%) | 1 (1%) | 86 96 |
| 7 | G | 114/114 (100%) | 113 (99%) | 1 (1%) | 78 94 |
| 7 | T | 116/114 (102%) | 114 (98%) | 2 (2%) | 60 87 |
| 8 | H | 127/133 (96%) | 126 (99%) | 1 (1%) | 81 94 |
| 8 | U | 127/133 (96%) | 127 (100%) | 0 | 100 100 |
| 9 | I | 116/125 (93%) | 116 (100%) | 0 | 100 100 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles |
|---|---|---|---|---|---|
| 9 | V | 116/125 (93%) | 115 (99%) | 1 (1%) | 78 94 |
| 10 | J | 81/90 (90%) | 80 (99%) | 1 (1%) | 71 92 |
| 10 | W | 81/90 (90%) | 81 (100%) | 0 | 100 100 |
| 11 | K | 50/63 (79%) | 50 (100%) | 0 | 100 100 |
| 11 | X | 48/63 (76%) | 47 (98%) | 1 (2%) | 53 84 |
| 12 | L | 43/45 (96%) | 43 (100%) | 0 | 100 100 |
| 12 | Y | 43/45 (96%) | 43 (100%) | 0 | 100 100 |
| 13 | M | 22/135 (16%) | 22 (100%) | 0 | 100 100 |
| 13 | Z | 24/135 (18%) | 24 (100%) | 0 | 100 100 |
| All | All | 4810/5236 (92%) | 4770 (99%) | 40 (1%) | 82 94 |

All (40) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 243 | THR |
| 2 | B | 153[A] | TYR |
| 2 | B | 153[B] | TYR |
| 2 | B | 518 | GLU |
| 3 | C | 105 | LEU |
| 3 | C | 117 | ARG |
| 4 | D | 64 | ARG |
| 4 | D | 190 | MET |
| 4 | D | 263 | PHE |
| 4 | D | 366 | PHE |
| 4 | D | 404 | PHE |
| 4 | D | 462 | TYR |
| 4 | D | 538 | ARG |
| 5 | E | 154 | ASN |
| 5 | E | 173 | TYR |
| 5 | E | 265 | LYS |
| 5 | E | 287 | GLU |
| 5 | E | 300 | LEU |
| 7 | G | 86 | LEU |
| 8 | H | 119 | ASP |
| 10 | J | 92 | VAL |
| 1 | N | 120[A] | LYS |
| 1 | N | 120[B] | LYS |
| 1 | N | 399 | LEU |
| 2 | O | 295 | ASP |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 3 | P | 117 | ARG |
| 4 | Q | 116 | ASP |
| 4 | Q | 150 | PHE |
| 4 | Q | 189 | ASN |
| 4 | Q | 263 | PHE |
| 4 | Q | 366 | PHE |
| 4 | Q | 393 | TYR |
| 4 | Q | 404 | PHE |
| 5 | R | 29 | CYS |
| 5 | R | 160 | SER |
| 6 | S | 129 | HIS |
| 7 | T | 6 | LYS |
| 7 | T | 113 | PHE |
| 9 | V | 131 | SER |
| 11 | X | 27 | HIS |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 5 | R | 318 | ASN |

### 5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry (i)

Of 88 ligands modelled in this entry, 6 are monoatomic and 4 are modelled with single atom - leaving 78 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 | $\#\|Z\| > 2$ |
| 21 | CDL | B | 606 | - | 44,44,99 | 0.43 | 0 | 50,56,111 | 0.38 | 0 |
| 21 | CDL | T | 201 | - | 79,79,99 | 0.35 | 0 | 85,91,111 | 0.47 | 1 (1%) |
| 21 | CDL | G | 201 | - | 74,74,99 | 0.35 | 0 | 80,86,111 | 0.59 | 1 (1%) |
| 31 | DGA | H | 201 | - | 16,16,43 | 0.30 | 0 | 18,18,45 | 0.19 | 0 |
| 21 | CDL | I | 201 | - | 56,56,99 | 0.39 | 0 | 62,68,111 | 0.45 | 0 |
| 31 | DGA | M | 201 | - | 21,21,43 | 0.26 | 0 | 23,23,45 | 0.24 | 0 |
| 16 | 9YF | H | 203 | - | 34,34,58 | 0.32 | 0 | 44,46,71 | 0.47 | 1 (2%) |
| 17 | MQ9 | N | 501 | - | 37,37,59 | 0.50 | 1 (2%) | 45,48,75 | 0.84 | 3 (6%) |
| 18 | 3PE | T | 202 | - | 25,25,50 | 0.42 | 0 | 28,30,55 | 0.48 | 0 |
| 22 | LYC | O | 607 | - | 39,39,39 | 0.37 | 0 | 44,46,46 | 0.47 | 0 |
| 16 | 9YF | U | 203 | - | 39,39,58 | 0.32 | 0 | 49,51,71 | 0.43 | 0 |
| 24 | HEC | P | 302 | 3 | 26,50,50 | 1.49 | 2 (7%) | 18,82,82 | 1.87 | 7 (38%) |
| 18 | 3PE | L | 101 | - | 29,29,50 | 0.41 | 0 | 32,34,55 | 0.57 | 0 |
| 21 | CDL | S | 302 | - | 64,64,99 | 0.38 | 0 | 70,76,111 | 0.58 | 1 (1%) |
| 18 | 3PE | A | 505 | - | 39,39,50 | 0.33 | 0 | 42,44,55 | 0.55 | 0 |
| 21 | CDL | Q | 607 | - | 82,82,99 | 0.35 | 0 | 88,94,111 | 0.40 | 0 |
| 18 | 3PE | J | 201 | - | 46,46,50 | 0.33 | 0 | 49,51,55 | 0.64 | 1 (2%) |
| 16 | 9YF | A | 503 | - | 36,36,58 | 0.42 | 0 | 46,48,71 | 0.50 | 1 (2%) |
| 21 | CDL | T | 204 | - | 64,64,99 | 0.38 | 0 | 70,76,111 | 0.67 | 1 (1%) |
| 18 | 3PE | N | 502 | - | 37,37,50 | 0.34 | 0 | 40,42,55 | 0.43 | 0 |
| 18 | 3PE | P | 303 | - | 26,26,50 | 0.44 | 0 | 29,31,55 | 0.73 | 2 (6%) |
| 18 | 3PE | Q | 609 | - | 38,38,50 | 0.35 | 0 | 41,43,55 | 0.43 | 0 |
| 20 | HEM | O | 604 | 2 | 27,50,50 | 1.26 | 4 (14%) | 17,82,82 | 1.45 | 3 (17%) |
| 15 | IZL | A | 502 | - | 108,108,119 | 0.34 | 0 | 150,152,163 | 1.04 | 9 (6%) |
| 25 | HAS | Q | 602 | 4 | 56,72,72 | 4.21 | 20 (35%) | 50,109,109 | 4.03 | 27 (54%) |
| 16 | 9YF | N | 505 | - | 36,36,58 | 0.34 | 0 | 46,48,71 | 0.41 | 0 |
| 32 | PLM | U | 202 | 8 | 16,16,17 | 0.16 | 0 | 15,15,17 | 0.21 | 0 |
| 18 | 3PE | R | 405 | - | 30,30,50 | 0.37 | 0 | 33,35,55 | 0.47 | 0 |
| 20 | HEM | B | 602 | 2 | 27,50,50 | 1.32 | 4 (14%) | 17,82,82 | 1.87 | 5 (29%) |
| 18 | 3PE | D | 609 | - | 30,30,50 | 0.39 | 0 | 33,35,55 | 0.38 | 0 |
| 31 | DGA | E | 403 | - | 19,19,43 | 0.28 | 0 | 21,21,45 | 0.18 | 0 |
| 21 | CDL | G | 202 | - | 68,68,99 | 0.36 | 0 | 74,80,111 | 0.64 | 2 (2%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\|>2$ | Counts | RMSZ | $\#\|Z\|>2$ |
| 24 | HEC | P | 301 | 3 | 26,50,50 | 1.54 | 2 (7%) | 18,82,82 | 2.08 | 6 (33%) |
| 18 | 3PE | T | 206 | - | 39,39,50 | 0.35 | 0 | 42,44,55 | 0.72 | 1 (2%) |
| 32 | PLM | M | 202 | 13 | 4,4,17 | 0.33 | 0 | 3,3,17 | 0.27 | 0 |
| 14 | FES | N | 503 | 1 | 0,4,4 | - | - | - | | |
| 20 | HEM | O | 603 | 2 | 27,50,50 | 1.33 | 3 (11%) | 17,82,82 | 1.97 | 5 (29%) |
| 23 | LMT | O | 601 | - | 33,33,36 | 0.16 | 0 | 44,44,47 | 1.04 | 2 (4%) |
| 18 | 3PE | C | 303 | - | 24,24,50 | 0.45 | 0 | 27,29,55 | 0.62 | 0 |
| 15 | IZL | N | 504 | - | 108,108,119 | 0.41 | 0 | 150,152,163 | 1.11 | 15 (10%) |
| 29 | AZI | D | 606 | 25,26 | 0,2,2 | - | - | 0,1,1 | - | - |
| 21 | CDL | D | 607 | - | 76,76,99 | 0.36 | 0 | 82,88,111 | 0.54 | 1 (1%) |
| 20 | HEM | B | 603 | 2 | 27,50,50 | 1.30 | 4 (14%) | 17,82,82 | 1.43 | 3 (17%) |
| 31 | DGA | U | 201 | - | 26,26,43 | 0.29 | 0 | 28,28,45 | 0.34 | 0 |
| 17 | MQ9 | O | 605 | - | 28,28,59 | 0.57 | 1 (3%) | 34,37,75 | 1.21 | 3 (8%) |
| 21 | CDL | D | 608 | - | 62,62,99 | 0.39 | 0 | 68,74,111 | 0.56 | 0 |
| 21 | CDL | V | 201 | - | 68,68,99 | 0.37 | 0 | 72,79,111 | 0.45 | 0 |
| 33 | IX7 | U | 204 | - | 74,74,97 | 0.34 | 0 | 97,99,123 | 0.94 | 4 (4%) |
| 18 | 3PE | T | 203 | - | 41,41,50 | 0.34 | 0 | 44,46,55 | 0.41 | 0 |
| 19 | SMA | O | 602 | - | 35,38,38 | 0.80 | 2 (5%) | 46,52,52 | 1.15 | 4 (8%) |
| 17 | MQ9 | B | 604 | - | 24,24,59 | 0.72 | 1 (4%) | 30,33,75 | 1.36 | 2 (6%) |
| 34 | OXY | Q | 606 | - | 1,1,1 | 0.16 | 0 | - | | |
| 18 | 3PE | C | 304 | - | 24,24,50 | 0.43 | 0 | 27,29,55 | 0.63 | 0 |
| 17 | MQ9 | A | 504 | - | 59,59,59 | 0.55 | 1 (1%) | 72,75,75 | 0.94 | 5 (6%) |
| 22 | LYC | B | 607 | - | 39,39,39 | 0.22 | 0 | 44,46,46 | 0.31 | 0 |
| 33 | IX7 | H | 204 | - | 74,74,97 | 0.39 | 0 | 97,99,123 | 1.07 | 6 (6%) |
| 14 | FES | A | 501 | 1 | 0,4,4 | - | - | - | | |
| 29 | AZI | Q | 605 | 26 | 0,2,2 | - | - | 0,1,1 | - | - |
| 21 | CDL | B | 609 | - | 69,69,99 | 0.37 | 0 | 75,81,111 | 0.46 | 0 |
| 24 | HEC | C | 302 | 3 | 26,50,50 | 1.40 | 2 (7%) | 18,82,82 | 1.78 | 6 (33%) |
| 23 | LMT | B | 608 | - | 33,33,36 | 0.14 | 0 | 44,44,47 | 0.59 | 0 |
| 19 | SMA | B | 601 | - | 35,38,38 | 0.99 | 4 (11%) | 46,52,52 | 1.34 | 5 (10%) |
| 18 | 3PE | F | 301 | - | 31,31,50 | 0.39 | 0 | 34,36,55 | 0.85 | 1 (2%) |
| 25 | HAS | D | 601 | 4 | 56,72,72 | 4.19 | 20 (35%) | 50,109,109 | 3.68 | 24 (48%) |
| 21 | CDL | Q | 608 | - | 65,65,99 | 0.38 | 0 | 71,77,111 | 0.42 | 0 |
| 18 | 3PE | S | 301 | - | 42,42,50 | 0.39 | 0 | 45,47,55 | 0.58 | 1 (2%) |
| 32 | PLM | H | 202 | 8 | 16,16,17 | 0.18 | 0 | 15,15,17 | 0.24 | 0 |
| 18 | 3PE | W | 201 | - | 46,46,50 | 0.34 | 0 | 49,51,55 | 0.93 | 3 (6%) |
| 25 | HAS | Q | 601 | 4 | 56,72,72 | 4.24 | 21 (37%) | 50,109,109 | 3.56 | 22 (44%) |
| 21 | CDL | B | 605 | - | 55,55,99 | 0.40 | 0 | 61,67,111 | 0.53 | 0 |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\|>2$ | Counts | RMSZ | $\#\|Z\|>2$ |
| 25 | HAS | D | 602 | 29,4 | 56,72,72 | 4.20 | 21 (37%) | 50,109,109 | 3.65 | 24 (48%) |
| 31 | DGA | Z | 201 | - | 28,28,43 | 0.24 | 0 | 30,30,45 | 0.35 | 0 |
| 18 | 3PE | T | 205 | - | 37,37,50 | 0.36 | 0 | 40,42,55 | 0.41 | 0 |
| 21 | CDL | F | 302 | - | 56,56,99 | 0.40 | 0 | 62,68,111 | 0.60 | 1 (1%) |
| 32 | PLM | Z | 202 | 13 | 4,4,17 | 0.30 | 0 | 3,3,17 | 0.34 | 0 |
| 31 | DGA | R | 404 | - | 24,24,43 | 0.28 | 0 | 26,26,45 | 0.19 | 0 |
| 24 | HEC | C | 301 | 3 | 26,50,50 | 1.50 | 2 (7%) | 18,82,82 | 1.52 | 3 (16%) |
| 21 | CDL | O | 606 | - | 65,65,99 | 0.39 | 0 | 71,77,111 | 0.59 | 1 (1%) |

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 |
|---|---|---|---|---|---|---|---|
| 18 | 3PE | N | 502 | - | - | 8/41/41/54 | - |
| 21 | CDL | B | 606 | - | - | 11/54/54/110 | - |
| 18 | 3PE | P | 303 | - | - | 15/30/30/54 | - |
| 18 | 3PE | Q | 609 | - | - | 15/42/42/54 | - |
| 14 | FES | A | 501 | 1 | - | - | 0/1/1/1 |
| 31 | DGA | U | 201 | - | - | 6/27/27/45 | - |
| 20 | HEM | O | 604 | 2 | - | 0/6/54/54 | - |
| 21 | CDL | B | 609 | - | - | 31/80/80/110 | - |
| 15 | IZL | A | 502 | - | - | 29/73/197/208 | 0/6/6/6 |
| 17 | MQ9 | O | 605 | - | - | 8/16/36/73 | 0/2/2/2 |
| 21 | CDL | T | 201 | - | - | 42/90/90/110 | - |
| 21 | CDL | G | 201 | - | - | 33/85/85/110 | - |
| 25 | HAS | Q | 602 | 4 | - | 8/35/122/122 | - |
| 21 | CDL | D | 608 | - | - | 32/73/73/110 | - |
| 24 | HEC | C | 302 | 3 | - | 0/6/54/54 | - |
| 23 | LMT | B | 608 | - | - | 8/18/58/61 | 0/2/2/2 |
| 19 | SMA | B | 601 | - | - | 9/33/34/34 | 0/2/2/2 |
| 16 | 9YF | N | 505 | - | - | 5/31/55/78 | 0/1/1/1 |
| 21 | CDL | I | 201 | - | - | 27/67/67/110 | - |
| 31 | DGA | H | 201 | - | - | 0/17/17/45 | - |
| 21 | CDL | D | 607 | - | - | 39/87/87/110 | - |
| 31 | DGA | M | 201 | - | - | 3/22/22/45 | - |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 21 | CDL | V | 201 | - | - | 37/78/78/110 | - |
| 16 | 9YF | H | 203 | - | - | 5/29/53/78 | 0/1/1/1 |
| 32 | PLM | U | 202 | 8 | - | 2/13/14/15 | - |
| 18 | 3PE | R | 405 | - | - | 16/34/34/54 | - |
| 33 | IX7 | U | 204 | - | - | 25/58/122/146 | 0/3/3/3 |
| 18 | 3PE | F | 301 | - | - | 20/35/35/54 | - |
| 18 | 3PE | D | 609 | - | - | 13/34/34/54 | - |
| 20 | HEM | B | 602 | 2 | - | 2/6/54/54 | - |
| 31 | DGA | E | 403 | - | - | 2/20/20/45 | - |
| 25 | HAS | D | 601 | 4 | - | 9/35/122/122 | - |
| 18 | 3PE | T | 203 | - | - | 17/45/45/54 | - |
| 17 | MQ9 | N | 501 | - | - | 7/27/47/73 | 0/2/2/2 |
| 17 | MQ9 | B | 604 | - | - | 3/11/31/73 | 0/2/2/2 |
| 19 | SMA | O | 602 | - | - | 9/33/34/34 | 0/2/2/2 |
| 21 | CDL | G | 202 | - | - | 24/79/79/110 | - |
| 18 | 3PE | S | 301 | - | - | 21/46/46/54 | - |
| 21 | CDL | Q | 608 | - | - | 19/76/76/110 | - |
| 24 | HEC | P | 301 | 3 | - | 0/6/54/54 | - |
| 32 | PLM | H | 202 | 8 | - | 1/13/14/15 | - |
| 18 | 3PE | W | 201 | - | - | 25/50/50/54 | - |
| 18 | 3PE | T | 202 | - | - | 13/29/29/54 | - |
| 18 | 3PE | T | 206 | - | - | 23/43/43/54 | - |
| 22 | LYC | O | 607 | - | - | 1/43/43/43 | - |
| 32 | PLM | M | 202 | 13 | - | 0/1/2/15 | - |
| 14 | FES | N | 503 | 1 | - | - | 0/1/1/1 |
| 16 | 9YF | U | 203 | - | - | 3/34/58/78 | 0/1/1/1 |
| 20 | HEM | O | 603 | 2 | - | 3/6/54/54 | - |
| 25 | HAS | Q | 601 | 4 | - | 8/35/122/122 | - |
| 23 | LMT | O | 601 | - | - | 11/18/58/61 | 0/2/2/2 |
| 24 | HEC | P | 302 | 3 | - | 0/6/54/54 | - |
| 18 | 3PE | C | 303 | - | - | 12/28/28/54 | - |
| 33 | IX7 | H | 204 | - | - | 28/58/122/146 | 0/3/3/3 |
| 15 | IZL | N | 504 | - | - | 31/73/197/208 | 0/6/6/6 |
| 21 | CDL | B | 605 | - | - | 25/66/66/110 | - |
| 25 | HAS | D | 602 | 29,4 | - | 11/35/122/122 | - |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 31 | DGA | Z | 201 | - | - | 5/29/29/45 | - |
| 18 | 3PE | T | 205 | - | - | 14/41/41/54 | - |
| 21 | CDL | F | 302 | - | - | 27/67/67/110 | - |
| 18 | 3PE | C | 304 | - | - | 10/28/28/54 | - |
| 18 | 3PE | L | 101 | - | - | 14/33/33/54 | - |
| 21 | CDL | S | 302 | - | - | 37/75/75/110 | - |
| 18 | 3PE | A | 505 | - | - | 16/43/43/54 | - |
| 17 | MQ9 | A | 504 | - | - | 21/53/73/73 | 0/2/2/2 |
| 32 | PLM | Z | 202 | 13 | - | 0/1/2/15 | - |
| 21 | CDL | Q | 607 | - | - | 30/93/93/110 | - |
| 18 | 3PE | J | 201 | - | - | 27/50/50/54 | - |
| 16 | 9YF | A | 503 | - | - | 15/31/55/78 | 0/1/1/1 |
| 22 | LYC | B | 607 | - | - | 4/43/43/43 | - |
| 21 | CDL | T | 204 | - | - | 28/75/75/110 | - |
| 21 | CDL | O | 606 | - | - | 37/76/76/110 | - |
| 31 | DGA | R | 404 | - | - | 2/25/25/45 | - |
| 24 | HEC | C | 301 | 3 | - | 0/6/54/54 | - |
| 20 | HEM | B | 603 | 2 | - | 0/6/54/54 | - |

All (115) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 25 | Q | 601 | HAS | CHD-C4A | -12.83 | 1.38 | 1.51 |
| 25 | Q | 602 | HAS | CHD-C4A | -12.62 | 1.38 | 1.51 |
| 25 | Q | 602 | HAS | CHD-C4C | -12.61 | 1.38 | 1.51 |
| 25 | Q | 601 | HAS | CHD-C4C | -12.36 | 1.38 | 1.51 |
| 25 | D | 601 | HAS | CHD-C4A | -12.33 | 1.38 | 1.51 |
| 25 | D | 602 | HAS | CHD-C4C | -12.18 | 1.38 | 1.51 |
| 25 | D | 601 | HAS | CHD-C4C | -12.14 | 1.38 | 1.51 |
| 25 | D | 602 | HAS | CHD-C4A | -11.97 | 1.39 | 1.51 |
| 25 | Q | 601 | HAS | C1D-ND | -9.14 | 1.37 | 1.49 |
| 25 | Q | 601 | HAS | C1B-NB | -9.12 | 1.37 | 1.49 |
| 25 | D | 601 | HAS | C1B-NB | -9.08 | 1.37 | 1.49 |
| 25 | Q | 602 | HAS | C4D-ND | -8.99 | 1.37 | 1.49 |
| 25 | D | 602 | HAS | C4B-NB | -8.96 | 1.37 | 1.49 |
| 25 | Q | 601 | HAS | CHA-C4D | -8.88 | 1.38 | 1.53 |
| 25 | D | 602 | HAS | CHC-C4B | -8.87 | 1.38 | 1.53 |
| 25 | Q | 602 | HAS | C1D-ND | -8.86 | 1.37 | 1.49 |
| 25 | D | 602 | HAS | C1B-NB | -8.85 | 1.37 | 1.49 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 25 | D | 601 | HAS | C1D-ND | -8.83 | 1.37 | 1.49 |
| 25 | D | 601 | HAS | C4D-ND | -8.80 | 1.37 | 1.49 |
| 25 | D | 602 | HAS | C4D-ND | -8.77 | 1.37 | 1.49 |
| 25 | D | 602 | HAS | C1D-ND | -8.74 | 1.37 | 1.49 |
| 25 | Q | 602 | HAS | C1B-NB | -8.69 | 1.37 | 1.49 |
| 25 | Q | 602 | HAS | CHA-C4D | -8.60 | 1.38 | 1.53 |
| 25 | Q | 601 | HAS | C4B-NB | -8.58 | 1.38 | 1.49 |
| 25 | D | 602 | HAS | CHA-C4D | -8.56 | 1.38 | 1.53 |
| 25 | Q | 601 | HAS | C4D-ND | -8.54 | 1.38 | 1.49 |
| 25 | Q | 602 | HAS | C4B-NB | -8.45 | 1.38 | 1.49 |
| 25 | D | 601 | HAS | CHA-C4D | -8.36 | 1.38 | 1.53 |
| 25 | D | 601 | HAS | CHC-C4B | -8.36 | 1.38 | 1.53 |
| 25 | D | 601 | HAS | C4B-NB | -8.15 | 1.38 | 1.49 |
| 25 | Q | 601 | HAS | CHC-C4B | -8.11 | 1.39 | 1.53 |
| 25 | Q | 602 | HAS | CHC-C4B | -8.04 | 1.39 | 1.53 |
| 25 | Q | 601 | HAS | CHA-C1A | -5.56 | 1.37 | 1.51 |
| 25 | D | 602 | HAS | CHC-C1C | -5.40 | 1.38 | 1.51 |
| 24 | P | 301 | HEC | C2B-C3B | -5.31 | 1.35 | 1.40 |
| 24 | C | 301 | HEC | C2B-C3B | -5.24 | 1.35 | 1.40 |
| 25 | D | 602 | HAS | CHA-C1A | -5.24 | 1.38 | 1.51 |
| 25 | D | 601 | HAS | CHA-C1A | -5.21 | 1.38 | 1.51 |
| 25 | Q | 602 | HAS | CHA-C1A | -5.16 | 1.38 | 1.51 |
| 25 | D | 601 | HAS | OMD-CMD | 5.05 | 1.33 | 1.22 |
| 24 | P | 302 | HEC | C2B-C3B | -5.04 | 1.35 | 1.40 |
| 25 | Q | 601 | HAS | CHC-C1C | -5.01 | 1.39 | 1.51 |
| 25 | D | 601 | HAS | CHC-C1C | -4.95 | 1.39 | 1.51 |
| 24 | P | 301 | HEC | C3C-C2C | -4.88 | 1.35 | 1.40 |
| 25 | Q | 602 | HAS | OMD-CMD | 4.87 | 1.33 | 1.22 |
| 25 | Q | 602 | HAS | CHC-C1C | -4.86 | 1.39 | 1.51 |
| 25 | D | 602 | HAS | OMD-CMD | 4.84 | 1.33 | 1.22 |
| 24 | P | 302 | HEC | C3C-C2C | -4.83 | 1.35 | 1.40 |
| 25 | Q | 601 | HAS | C1D-C2D | -4.76 | 1.43 | 1.51 |
| 25 | Q | 601 | HAS | OMD-CMD | 4.68 | 1.32 | 1.22 |
| 25 | Q | 601 | HAS | C1C-C2C | 4.67 | 1.44 | 1.38 |
| 25 | Q | 602 | HAS | C1D-C2D | -4.66 | 1.44 | 1.51 |
| 25 | D | 602 | HAS | C1D-C2D | -4.56 | 1.44 | 1.51 |
| 24 | C | 302 | HEC | C3C-C2C | -4.53 | 1.36 | 1.40 |
| 24 | C | 302 | HEC | C2B-C3B | -4.53 | 1.36 | 1.40 |
| 25 | D | 601 | HAS | C4A-C3A | 4.48 | 1.44 | 1.38 |
| 25 | D | 602 | HAS | C4A-C3A | 4.44 | 1.44 | 1.38 |
| 24 | C | 301 | HEC | C3C-C2C | -4.44 | 1.36 | 1.40 |
| 25 | D | 601 | HAS | C1D-C2D | -4.38 | 1.44 | 1.51 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 25 | D | 601 | HAS | C1C-C2C | 4.35 | 1.44 | 1.38 |
| 25 | Q | 602 | HAS | C4A-C3A | 4.30 | 1.44 | 1.38 |
| 25 | Q | 602 | HAS | C1C-C2C | 4.27 | 1.44 | 1.38 |
| 25 | Q | 602 | HAS | C1A-C2A | 4.20 | 1.43 | 1.38 |
| 25 | D | 602 | HAS | C1A-C2A | 4.19 | 1.43 | 1.38 |
| 25 | D | 601 | HAS | C1A-C2A | 4.16 | 1.43 | 1.38 |
| 25 | Q | 601 | HAS | CHB-C1B | -4.10 | 1.37 | 1.53 |
| 25 | Q | 602 | HAS | CHB-C1B | -4.10 | 1.37 | 1.53 |
| 25 | D | 601 | HAS | CMD-C2D | 4.00 | 1.52 | 1.44 |
| 25 | D | 602 | HAS | CMD-C2D | 4.00 | 1.52 | 1.44 |
| 25 | D | 602 | HAS | CHB-C1B | -3.97 | 1.37 | 1.53 |
| 25 | Q | 601 | HAS | CHB-C1D | -3.97 | 1.37 | 1.53 |
| 25 | D | 601 | HAS | CHB-C1B | -3.93 | 1.38 | 1.53 |
| 25 | Q | 602 | HAS | CHB-C1D | -3.93 | 1.38 | 1.53 |
| 25 | D | 602 | HAS | CHB-C1D | -3.93 | 1.38 | 1.53 |
| 25 | Q | 601 | HAS | C4A-C3A | 3.91 | 1.43 | 1.38 |
| 20 | B | 602 | HEM | C3B-C2B | -3.87 | 1.35 | 1.40 |
| 25 | D | 601 | HAS | CHB-C1D | -3.86 | 1.38 | 1.53 |
| 25 | D | 602 | HAS | C1C-C2C | 3.85 | 1.43 | 1.38 |
| 25 | Q | 602 | HAS | CMD-C2D | 3.80 | 1.51 | 1.44 |
| 25 | Q | 601 | HAS | CMD-C2D | 3.68 | 1.51 | 1.44 |
| 25 | D | 602 | HAS | C3C-C2C | -3.47 | 1.35 | 1.40 |
| 20 | O | 603 | HEM | C3C-C2C | -3.46 | 1.35 | 1.40 |
| 25 | Q | 601 | HAS | C1A-C2A | 3.45 | 1.42 | 1.38 |
| 20 | O | 603 | HEM | C3B-C2B | -3.42 | 1.35 | 1.40 |
| 25 | Q | 601 | HAS | C3C-C2C | -3.42 | 1.35 | 1.40 |
| 20 | B | 603 | HEM | C3B-C2B | -3.35 | 1.35 | 1.40 |
| 20 | B | 603 | HEM | C3C-C2C | -3.22 | 1.35 | 1.40 |
| 20 | O | 604 | HEM | C3B-C2B | -3.22 | 1.35 | 1.40 |
| 25 | D | 601 | HAS | C3C-C2C | -3.17 | 1.36 | 1.40 |
| 25 | Q | 602 | HAS | C3C-C2C | -3.12 | 1.36 | 1.40 |
| 17 | B | 604 | MQ9 | C6-C5 | 3.11 | 1.40 | 1.35 |
| 20 | B | 602 | HEM | C3C-C2C | -3.08 | 1.36 | 1.40 |
| 19 | B | 601 | SMA | C3-C2 | -3.02 | 1.35 | 1.39 |
| 19 | B | 601 | SMA | C20-C19 | 3.00 | 1.36 | 1.33 |
| 19 | O | 602 | SMA | C3-C2 | -2.98 | 1.35 | 1.39 |
| 17 | A | 504 | MQ9 | C6-C1 | 2.93 | 1.54 | 1.47 |
| 20 | O | 604 | HEM | C3C-C2C | -2.87 | 1.36 | 1.40 |
| 25 | Q | 601 | HAS | C3C-CAC | 2.80 | 1.53 | 1.47 |
| 17 | O | 605 | MQ9 | C6-C5 | 2.62 | 1.40 | 1.35 |
| 20 | O | 603 | HEM | C3B-CAB | 2.61 | 1.53 | 1.47 |
| 25 | Q | 602 | HAS | C3C-CAC | 2.56 | 1.53 | 1.47 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 20 | B | 603 | HEM | C3B-CAB | 2.44 | 1.52 | 1.47 |
| 20 | O | 604 | HEM | C3C-CAC | 2.42 | 1.52 | 1.47 |
| 25 | D | 601 | HAS | C3C-CAC | 2.37 | 1.52 | 1.47 |
| 20 | O | 604 | HEM | C3B-CAB | 2.33 | 1.52 | 1.47 |
| 20 | B | 603 | HEM | C3C-CAC | 2.32 | 1.52 | 1.47 |
| 19 | B | 601 | SMA | C3-C4 | 2.28 | 1.47 | 1.41 |
| 25 | D | 602 | HAS | C3C-CAC | 2.26 | 1.52 | 1.47 |
| 17 | N | 501 | MQ9 | C6-C5 | 2.21 | 1.39 | 1.35 |
| 25 | D | 602 | HAS | C11-C3B | -2.21 | 1.48 | 1.51 |
| 20 | B | 602 | HEM | C3C-CAC | 2.21 | 1.52 | 1.47 |
| 19 | O | 602 | SMA | C13-C14 | 2.19 | 1.62 | 1.54 |
| 19 | B | 601 | SMA | C13-C12 | 2.15 | 1.59 | 1.54 |
| 25 | Q | 601 | HAS | C11-C3B | -2.14 | 1.48 | 1.51 |
| 20 | B | 602 | HEM | C3B-CAB | 2.06 | 1.52 | 1.47 |

All (213) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 25 | D | 602 | HAS | CHB-C1B-NB | 12.96 | 127.06 | 110.94 |
| 25 | D | 601 | HAS | CHB-C1B-NB | 12.81 | 126.87 | 110.94 |
| 25 | Q | 602 | HAS | CAA-C2A-C1A | -12.61 | 118.44 | 127.30 |
| 25 | Q | 601 | HAS | CHB-C1B-NB | 12.60 | 126.60 | 110.94 |
| 25 | Q | 602 | HAS | CHB-C1B-NB | 12.23 | 126.15 | 110.94 |
| 25 | D | 602 | HAS | CHB-C1D-ND | 11.38 | 125.09 | 110.94 |
| 25 | Q | 601 | HAS | CHB-C1D-ND | 11.14 | 124.79 | 110.94 |
| 25 | Q | 602 | HAS | CHB-C1D-ND | 11.07 | 124.71 | 110.94 |
| 25 | D | 601 | HAS | CHB-C1D-ND | 10.99 | 124.60 | 110.94 |
| 25 | D | 601 | HAS | CHA-C4D-ND | 7.87 | 125.58 | 110.75 |
| 25 | Q | 601 | HAS | CHA-C4D-ND | 7.82 | 125.50 | 110.75 |
| 25 | D | 602 | HAS | CHA-C4D-ND | 7.76 | 125.39 | 110.75 |
| 25 | Q | 602 | HAS | CHA-C4D-ND | 7.75 | 125.37 | 110.75 |
| 25 | D | 602 | HAS | CHC-C4B-NB | 7.17 | 124.27 | 110.75 |
| 25 | Q | 602 | HAS | CHC-C4B-NB | 6.68 | 123.34 | 110.75 |
| 25 | Q | 601 | HAS | CHC-C4B-NB | 6.37 | 122.76 | 110.75 |
| 25 | D | 601 | HAS | CHC-C4B-NB | 6.23 | 122.49 | 110.75 |
| 17 | B | 604 | MQ9 | C8-C7-C6 | 6.17 | 128.68 | 112.05 |
| 25 | Q | 602 | HAS | C26-C15-C16 | 6.00 | 125.37 | 115.27 |
| 25 | D | 601 | HAS | C4C-CHD-C4A | 5.47 | 126.20 | 112.87 |
| 25 | Q | 601 | HAS | C4C-CHD-C4A | 5.40 | 126.05 | 112.87 |
| 25 | D | 601 | HAS | C25-C23-C24 | 5.14 | 123.92 | 115.27 |
| 19 | O | 602 | SMA | C9-C2-C3 | 4.92 | 127.36 | 120.39 |
| 25 | D | 601 | HAS | C27-C19-C20 | 4.90 | 123.51 | 115.27 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 17 | O | 605 | MQ9 | C8-C7-C6 | 4.88 | 125.20 | 112.05 |
| 25 | Q | 601 | HAS | CAA-C2A-C1A | -4.84 | 123.90 | 127.30 |
| 25 | Q | 602 | HAS | C4C-CHD-C4A | 4.83 | 124.65 | 112.87 |
| 19 | B | 601 | SMA | C9-C2-C3 | 4.78 | 127.17 | 120.39 |
| 25 | D | 602 | HAS | C26-C15-C16 | 4.78 | 123.31 | 115.27 |
| 25 | D | 602 | HAS | C4C-CHD-C4A | 4.72 | 124.39 | 112.87 |
| 25 | Q | 601 | HAS | C26-C15-C16 | 4.72 | 123.20 | 115.27 |
| 25 | D | 602 | HAS | C27-C19-C20 | 4.61 | 123.02 | 115.27 |
| 25 | D | 601 | HAS | C26-C15-C16 | 4.48 | 122.80 | 115.27 |
| 25 | D | 601 | HAS | C26-C15-C14 | -4.43 | 112.32 | 123.68 |
| 23 | O | 601 | LMT | O1B-C4'-C3' | 4.40 | 118.99 | 107.28 |
| 25 | Q | 601 | HAS | OMD-CMD-C2D | -4.38 | 118.85 | 124.39 |
| 25 | D | 602 | HAS | C12-C11-C3B | -4.33 | 108.51 | 114.11 |
| 25 | D | 602 | HAS | OMD-CMD-C2D | -4.32 | 118.93 | 124.39 |
| 25 | Q | 602 | HAS | C26-C15-C14 | -4.17 | 112.97 | 123.68 |
| 20 | O | 603 | HEM | CBA-CAA-C2A | 4.14 | 120.13 | 112.49 |
| 20 | B | 602 | HEM | CBA-CAA-C2A | 4.12 | 120.08 | 112.49 |
| 25 | Q | 602 | HAS | OMD-CMD-C2D | -4.05 | 119.26 | 124.39 |
| 25 | D | 602 | HAS | C26-C15-C14 | -3.99 | 113.44 | 123.68 |
| 15 | N | 504 | IZL | O36-C71-C13 | 3.98 | 119.70 | 110.05 |
| 25 | D | 601 | HAS | OMD-CMD-C2D | -3.95 | 119.39 | 124.39 |
| 25 | D | 601 | HAS | CAD-CBD-CGD | -3.95 | 106.05 | 112.67 |
| 25 | D | 602 | HAS | CMC-C2C-C3C | 3.93 | 132.02 | 124.68 |
| 25 | Q | 602 | HAS | CMA-C3A-C2A | 3.92 | 132.34 | 124.94 |
| 15 | A | 502 | IZL | O7-C18-C43 | -3.92 | 97.52 | 107.48 |
| 25 | Q | 601 | HAS | C26-C15-C14 | -3.87 | 113.75 | 123.68 |
| 25 | Q | 602 | HAS | CHD-C4C-C3C | -3.79 | 124.63 | 129.61 |
| 25 | Q | 601 | HAS | CBD-CAD-C3D | -3.79 | 107.63 | 114.35 |
| 25 | D | 601 | HAS | CAA-C2A-C1A | -3.78 | 124.64 | 127.30 |
| 18 | W | 201 | 3PE | O21-C2-C3 | -3.77 | 94.73 | 108.40 |
| 21 | G | 201 | CDL | OB8-CB6-CB4 | 3.75 | 119.36 | 108.43 |
| 15 | A | 502 | IZL | O32-C46-C45 | 3.74 | 119.32 | 108.43 |
| 24 | P | 302 | HEC | CMB-C2B-C1B | -3.74 | 122.72 | 128.46 |
| 24 | P | 301 | HEC | CMC-C2C-C1C | -3.68 | 122.81 | 128.46 |
| 15 | N | 504 | IZL | O32-C46-C45 | 3.67 | 119.12 | 108.43 |
| 25 | Q | 601 | HAS | C12-C11-C3B | -3.61 | 109.44 | 114.11 |
| 33 | U | 204 | IX7 | P-O13-C30 | 3.61 | 132.54 | 119.41 |
| 19 | B | 601 | SMA | C4A-C4-C3 | -3.57 | 116.99 | 120.58 |
| 24 | P | 301 | HEC | CMB-C2B-C1B | -3.55 | 123.00 | 128.46 |
| 33 | H | 204 | IX7 | O6-C22-C23 | 3.50 | 119.21 | 109.94 |
| 17 | A | 504 | MQ9 | C7-C8-C9 | 3.49 | 132.61 | 126.79 |
| 17 | N | 501 | MQ9 | C8-C7-C6 | 3.47 | 121.41 | 112.05 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 33 | U | 204 | IX7 | O7-C23-C22 | -3.46 | 98.07 | 107.28 |
| 19 | O | 602 | SMA | C4A-C4-C3 | -3.45 | 117.11 | 120.58 |
| 25 | D | 601 | HAS | C25-C23-C22 | -3.45 | 114.83 | 123.68 |
| 25 | D | 601 | HAS | C1B-CHB-C1D | 3.44 | 126.07 | 116.15 |
| 25 | Q | 601 | HAS | C1B-CHB-C1D | 3.41 | 126.00 | 116.15 |
| 17 | B | 604 | MQ9 | C7-C6-C1 | -3.40 | 114.86 | 118.50 |
| 17 | O | 605 | MQ9 | C7-C6-C1 | -3.40 | 114.86 | 118.50 |
| 15 | N | 504 | IZL | P-O28-C43 | 3.39 | 131.74 | 119.41 |
| 24 | P | 301 | HEC | CMD-C2D-C1D | -3.37 | 123.28 | 128.46 |
| 25 | D | 601 | HAS | C12-C11-C3B | -3.37 | 109.75 | 114.11 |
| 24 | C | 302 | HEC | CMB-C2B-C1B | -3.37 | 123.29 | 128.46 |
| 25 | D | 601 | HAS | CBD-CAD-C3D | -3.36 | 108.40 | 114.35 |
| 18 | F | 301 | 3PE | O21-C2-C1 | 3.32 | 120.43 | 108.40 |
| 25 | Q | 601 | HAS | CHD-C4C-C3C | -3.32 | 125.26 | 129.61 |
| 15 | N | 504 | IZL | O7-C18-C17 | 3.32 | 116.10 | 107.28 |
| 25 | D | 602 | HAS | CHC-C1C-C2C | -3.30 | 123.73 | 129.45 |
| 25 | Q | 602 | HAS | C20-C19-C18 | 3.28 | 127.76 | 121.12 |
| 25 | D | 601 | HAS | CHD-C4C-C3C | -3.24 | 125.35 | 129.61 |
| 25 | Q | 602 | HAS | CBD-CAD-C3D | -3.22 | 108.64 | 114.35 |
| 25 | Q | 602 | HAS | C1B-CHB-C1D | 3.21 | 125.43 | 116.15 |
| 24 | P | 302 | HEC | CMD-C2D-C1D | -3.16 | 123.60 | 128.46 |
| 18 | W | 201 | 3PE | O21-C2-C1 | 3.11 | 119.65 | 108.40 |
| 24 | C | 302 | HEC | CMD-C2D-C1D | -3.09 | 123.71 | 128.46 |
| 24 | P | 301 | HEC | CMB-C2B-C3B | 3.07 | 129.43 | 125.82 |
| 20 | O | 603 | HEM | CMC-C2C-C3C | 3.03 | 130.35 | 124.68 |
| 25 | Q | 602 | HAS | C27-C19-C18 | -3.02 | 115.93 | 123.68 |
| 25 | Q | 602 | HAS | C12-C13-C14 | -3.00 | 104.31 | 112.23 |
| 20 | O | 604 | HEM | CBD-CAD-C3D | -2.99 | 106.97 | 112.48 |
| 25 | Q | 601 | HAS | C27-C19-C20 | 2.98 | 120.29 | 115.27 |
| 24 | C | 301 | HEC | CMB-C2B-C1B | -2.97 | 123.90 | 128.46 |
| 15 | A | 502 | IZL | C17-C18-C43 | -2.96 | 104.91 | 111.66 |
| 25 | D | 602 | HAS | CHD-C4C-C3C | -2.95 | 125.75 | 129.61 |
| 20 | O | 603 | HEM | CAA-C2A-C3A | -2.94 | 118.79 | 127.25 |
| 24 | P | 302 | HEC | CMB-C2B-C3B | 2.93 | 129.27 | 125.82 |
| 25 | D | 602 | HAS | C1B-CHB-C1D | 2.93 | 124.60 | 116.15 |
| 20 | B | 602 | HEM | CMC-C2C-C3C | 2.92 | 130.15 | 124.68 |
| 25 | Q | 602 | HAS | CMC-C2C-C3C | 2.90 | 130.10 | 124.68 |
| 25 | D | 602 | HAS | CHB-C1B-C2B | 2.90 | 123.74 | 114.70 |
| 25 | Q | 602 | HAS | CHB-C1B-C2B | 2.89 | 123.74 | 114.70 |
| 25 | Q | 601 | HAS | C32-C30-C31 | 2.88 | 120.96 | 114.60 |
| 24 | C | 302 | HEC | CMB-C2B-C3B | 2.88 | 129.20 | 125.82 |
| 25 | Q | 602 | HAS | CHD-C4A-C3A | -2.87 | 124.73 | 129.53 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 24 | P | 301 | HEC | CMC-C2C-C3C | 2.86 | 129.18 | 125.82 |
| 25 | Q | 602 | HAS | C20-C21-C22 | -2.86 | 102.49 | 111.88 |
| 20 | O | 603 | HEM | CBD-CAD-C3D | -2.85 | 107.22 | 112.48 |
| 24 | P | 301 | HEC | CBA-CAA-C2A | -2.85 | 107.23 | 112.48 |
| 24 | P | 302 | HEC | CMC-C2C-C1C | -2.85 | 124.09 | 128.46 |
| 25 | D | 602 | HAS | C27-C19-C18 | -2.85 | 116.38 | 123.68 |
| 25 | Q | 602 | HAS | CBA-CAA-C2A | 2.84 | 117.73 | 112.49 |
| 25 | Q | 601 | HAS | CHB-C1B-C2B | 2.84 | 123.58 | 114.70 |
| 25 | Q | 602 | HAS | C28-C24-C23 | -2.80 | 103.76 | 112.98 |
| 24 | C | 302 | HEC | CMC-C2C-C1C | -2.79 | 124.18 | 128.46 |
| 25 | D | 601 | HAS | CHB-C1B-C2B | 2.78 | 123.38 | 114.70 |
| 15 | A | 502 | IZL | C19-C42-C41 | 2.78 | 115.78 | 110.00 |
| 25 | D | 602 | HAS | C25-C23-C24 | 2.78 | 119.94 | 115.27 |
| 33 | H | 204 | IX7 | O6-C22-C21 | -2.77 | 103.94 | 110.35 |
| 25 | D | 602 | HAS | CAA-C2A-C1A | -2.77 | 125.35 | 127.30 |
| 20 | B | 602 | HEM | CBD-CAD-C3D | -2.75 | 107.41 | 112.48 |
| 17 | O | 605 | MQ9 | C12-C11-C9 | 2.72 | 121.91 | 112.98 |
| 23 | O | 601 | LMT | C1B-O1B-C4' | 2.71 | 124.68 | 117.96 |
| 33 | H | 204 | IX7 | O7-C23-C30 | -2.71 | 100.59 | 107.48 |
| 25 | Q | 601 | HAS | CHD-C4A-C3A | -2.70 | 125.02 | 129.53 |
| 33 | H | 204 | IX7 | P-O13-C30 | 2.69 | 129.19 | 119.41 |
| 20 | O | 603 | HEM | C4A-C3A-C2A | 2.69 | 108.87 | 107.00 |
| 20 | B | 602 | HEM | C4A-C3A-C2A | 2.68 | 108.86 | 107.00 |
| 21 | O | 606 | CDL | OB6-CB4-CB6 | -2.66 | 98.76 | 108.40 |
| 25 | D | 602 | HAS | CHD-C4A-C3A | -2.66 | 125.08 | 129.53 |
| 15 | N | 504 | IZL | C49-C48-C47 | 2.65 | 123.26 | 113.62 |
| 25 | Q | 602 | HAS | C13-C12-C11 | -2.63 | 110.39 | 114.35 |
| 33 | H | 204 | IX7 | C24-O7-C23 | 2.63 | 124.46 | 117.96 |
| 18 | W | 201 | 3PE | O31-C3-C2 | 2.62 | 116.07 | 108.43 |
| 20 | B | 602 | HEM | CMA-C3A-C4A | -2.62 | 124.44 | 128.46 |
| 17 | N | 501 | MQ9 | C7-C6-C1 | -2.60 | 115.72 | 118.50 |
| 25 | Q | 602 | HAS | CHC-C1C-C2C | -2.58 | 124.99 | 129.45 |
| 21 | D | 607 | CDL | OA8-CA6-CA4 | 2.58 | 115.94 | 108.43 |
| 19 | O | 602 | SMA | C2-C3-C4 | 2.57 | 119.45 | 116.63 |
| 19 | B | 601 | SMA | C22-C11-C12 | 2.56 | 115.34 | 111.15 |
| 17 | A | 504 | MQ9 | O1-C1-C2 | -2.56 | 117.42 | 121.56 |
| 20 | B | 603 | HEM | CAD-CBD-CGD | -2.54 | 108.41 | 112.67 |
| 19 | B | 601 | SMA | C2-C3-C4 | 2.54 | 119.42 | 116.63 |
| 20 | O | 604 | HEM | CMC-C2C-C3C | 2.53 | 129.41 | 124.68 |
| 25 | D | 602 | HAS | CAA-CBA-CGA | -2.52 | 108.44 | 112.67 |
| 20 | B | 603 | HEM | CMC-C2C-C3C | 2.51 | 129.37 | 124.68 |
| 18 | S | 301 | 3PE | O21-C2-C3 | 2.50 | 117.46 | 108.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 17 | A | 504 | MQ9 | C47-C46-C44 | 2.50 | 121.19 | 112.98 |
| 18 | J | 201 | 3PE | O31-C3-C2 | 2.49 | 115.67 | 108.43 |
| 25 | Q | 601 | HAS | CBA-CAA-C2A | -2.48 | 107.92 | 112.49 |
| 20 | O | 604 | HEM | CMB-C2B-C3B | 2.46 | 129.29 | 124.68 |
| 25 | Q | 602 | HAS | CAA-C2A-C3A | 2.46 | 134.32 | 127.25 |
| 25 | D | 601 | HAS | CHD-C4A-C3A | -2.46 | 125.41 | 129.53 |
| 15 | N | 504 | IZL | O7-C18-C43 | -2.45 | 101.26 | 107.48 |
| 25 | Q | 602 | HAS | C32-C30-C31 | 2.44 | 119.99 | 114.60 |
| 33 | U | 204 | IX7 | O1-C16-C17 | -2.43 | 103.27 | 108.43 |
| 25 | Q | 601 | HAS | C20-C19-C18 | -2.43 | 116.19 | 121.12 |
| 25 | D | 601 | HAS | C32-C30-C31 | 2.41 | 119.93 | 114.60 |
| 21 | S | 302 | CDL | OA6-CA4-CA6 | -2.41 | 99.66 | 108.40 |
| 25 | D | 601 | HAS | CMC-C2C-C3C | 2.40 | 129.17 | 124.68 |
| 18 | P | 303 | 3PE | O31-C3-C2 | 2.38 | 115.35 | 108.43 |
| 24 | C | 301 | HEC | CMD-C2D-C1D | -2.37 | 124.81 | 128.46 |
| 15 | N | 504 | IZL | O31-P-O29 | 2.35 | 118.25 | 109.07 |
| 15 | N | 504 | IZL | O14-C28-C29 | -2.33 | 104.96 | 110.35 |
| 17 | A | 504 | MQ9 | C8-C7-C6 | 2.33 | 118.32 | 112.05 |
| 18 | T | 206 | 3PE | O21-C2-C3 | -2.32 | 100.00 | 108.40 |
| 15 | A | 502 | IZL | C21-O9-C22 | -2.32 | 109.21 | 113.74 |
| 21 | G | 202 | CDL | OA6-CA4-CA6 | -2.31 | 100.03 | 108.40 |
| 33 | U | 204 | IX7 | C18-C67-C68 | 2.31 | 114.80 | 110.00 |
| 15 | A | 502 | IZL | O3-C14-C43 | 2.30 | 113.32 | 107.48 |
| 20 | B | 603 | HEM | CMB-C2B-C3B | 2.29 | 128.96 | 124.68 |
| 24 | C | 302 | HEC | CMD-C2D-C3D | 2.28 | 129.25 | 124.94 |
| 16 | A | 503 | 9YF | P-O2-C2 | 2.27 | 127.66 | 119.41 |
| 25 | D | 602 | HAS | C32-C30-C29 | -2.27 | 116.10 | 122.65 |
| 15 | N | 504 | IZL | O15-C29-C30 | 2.27 | 115.95 | 109.94 |
| 25 | Q | 601 | HAS | CAD-CBD-CGD | -2.26 | 108.87 | 112.67 |
| 24 | C | 301 | HEC | CMC-C2C-C1C | -2.25 | 125.00 | 128.46 |
| 15 | N | 504 | IZL | O12-C25-C30 | -2.25 | 105.06 | 109.51 |
| 15 | N | 504 | IZL | C16-C17-C18 | 2.23 | 114.77 | 109.68 |
| 25 | Q | 602 | HAS | CAA-CBA-CGA | -2.22 | 108.94 | 112.67 |
| 17 | A | 504 | MQ9 | C22-C21-C19 | 2.22 | 120.27 | 112.98 |
| 15 | A | 502 | IZL | C22-C39-C38 | 2.22 | 114.61 | 110.00 |
| 25 | D | 601 | HAS | CHC-C1C-C2C | -2.21 | 125.63 | 129.45 |
| 21 | T | 204 | CDL | OA6-CA4-CA3 | 2.20 | 116.36 | 108.40 |
| 25 | D | 602 | HAS | CAD-CBD-CGD | -2.19 | 108.99 | 112.67 |
| 25 | D | 601 | HAS | C21-C20-C19 | 2.19 | 120.17 | 112.98 |
| 25 | Q | 601 | HAS | CMC-C2C-C3C | 2.18 | 128.76 | 124.68 |
| 15 | A | 502 | IZL | C38-C37-C23 | -2.17 | 106.36 | 110.24 |
| 19 | B | 601 | SMA | C12-C13-C14 | 2.17 | 117.94 | 112.02 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 15 | N | 504 | IZL | C35-C34-C32 | -2.17 | 106.38 | 110.24 |
| 25 | Q | 601 | HAS | CHC-C1C-C2C | -2.15 | 125.72 | 129.45 |
| 15 | A | 502 | IZL | C18-C43-C14 | 2.14 | 115.10 | 110.41 |
| 21 | T | 201 | CDL | OA6-CA4-CA6 | -2.13 | 100.67 | 108.40 |
| 19 | O | 602 | SMA | O1-C2-C9 | -2.13 | 109.38 | 111.91 |
| 24 | P | 302 | HEC | CAA-CBA-CGA | -2.13 | 109.10 | 112.67 |
| 18 | P | 303 | 3PE | O21-C2-C1 | 2.12 | 116.09 | 108.40 |
| 21 | G | 202 | CDL | OA6-CA4-CA3 | 2.10 | 116.00 | 108.40 |
| 15 | N | 504 | IZL | O11-C24-C23 | 2.10 | 112.93 | 109.05 |
| 24 | P | 302 | HEC | CMD-C2D-C3D | 2.10 | 128.89 | 124.94 |
| 25 | D | 602 | HAS | CBD-CAD-C3D | -2.06 | 110.70 | 114.35 |
| 15 | N | 504 | IZL | O16-C30-C29 | -2.05 | 101.82 | 107.28 |
| 24 | P | 302 | HEC | CBD-CAD-C3D | -2.05 | 108.70 | 112.49 |
| 33 | H | 204 | IX7 | O19-C32-C31 | 2.05 | 115.82 | 108.40 |
| 21 | F | 302 | CDL | OA8-CA6-CA4 | -2.04 | 102.50 | 108.43 |
| 15 | N | 504 | IZL | O11-C25-C30 | 2.02 | 112.12 | 108.22 |
| 24 | C | 302 | HEC | CAA-CBA-CGA | -2.02 | 109.29 | 112.67 |
| 25 | D | 601 | HAS | C20-C19-C18 | -2.01 | 117.05 | 121.12 |
| 25 | D | 602 | HAS | C32-C30-C31 | 2.01 | 119.03 | 114.60 |
| 17 | N | 501 | MQ9 | C22-C21-C19 | 2.00 | 119.57 | 112.98 |
| 16 | H | 203 | 9YF | P-O2-C2 | 2.00 | 126.69 | 119.41 |

There are no chirality outliers.

All (1042) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 15 | A | 502 | IZL | C44-O31-P-O30 |
| 15 | N | 504 | IZL | O10-C22-O9-C21 |
| 15 | N | 504 | IZL | C61-C60-O34-C45 |
| 16 | A | 503 | 9YF | C2-O2-P-O1 |
| 16 | A | 503 | 9YF | C1-O-P-O1 |
| 16 | A | 503 | 9YF | C1-O-P-O8 |
| 16 | N | 505 | 9YF | C2-O2-P-O1 |
| 16 | N | 505 | 9YF | C2-O2-P-O8 |
| 17 | A | 504 | MQ9 | C5-C6-C7-C8 |
| 17 | A | 504 | MQ9 | C1-C6-C7-C8 |
| 17 | A | 504 | MQ9 | C19-C21-C22-C23 |
| 17 | B | 604 | MQ9 | C5-C6-C7-C8 |
| 17 | B | 604 | MQ9 | C1-C6-C7-C8 |
| 17 | O | 605 | MQ9 | C5-C6-C7-C8 |
| 17 | O | 605 | MQ9 | C1-C6-C7-C8 |
| 18 | A | 505 | 3PE | C1-O11-P-O13 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 18 | A | 505 | 3PE | C11-O13-P-O14 |
| 18 | A | 505 | 3PE | O13-C11-C12-N |
| 18 | C | 303 | 3PE | C11-O13-P-O14 |
| 18 | C | 303 | 3PE | O13-C11-C12-N |
| 18 | C | 304 | 3PE | C1-O11-P-O12 |
| 18 | D | 609 | 3PE | C1-O11-P-O12 |
| 18 | D | 609 | 3PE | C11-O13-P-O11 |
| 18 | D | 609 | 3PE | C11-O13-P-O14 |
| 18 | D | 609 | 3PE | C2-C1-O11-P |
| 18 | D | 609 | 3PE | O13-C11-C12-N |
| 18 | F | 301 | 3PE | C11-O13-P-O14 |
| 18 | F | 301 | 3PE | O13-C11-C12-N |
| 18 | J | 201 | 3PE | C1-O11-P-O14 |
| 18 | J | 201 | 3PE | O13-C11-C12-N |
| 18 | L | 101 | 3PE | C11-O13-P-O11 |
| 18 | L | 101 | 3PE | C12-C11-O13-P |
| 18 | N | 502 | 3PE | O13-C11-C12-N |
| 18 | P | 303 | 3PE | C1-O11-P-O12 |
| 18 | Q | 609 | 3PE | C11-O13-P-O14 |
| 18 | R | 405 | 3PE | C1-O11-P-O14 |
| 18 | R | 405 | 3PE | C11-O13-P-O12 |
| 18 | R | 405 | 3PE | C11-O13-P-O14 |
| 18 | R | 405 | 3PE | O13-C11-C12-N |
| 18 | S | 301 | 3PE | C11-O13-P-O12 |
| 18 | S | 301 | 3PE | C11-O13-P-O14 |
| 18 | S | 301 | 3PE | O13-C11-C12-N |
| 18 | S | 301 | 3PE | C3-C2-O21-C21 |
| 18 | S | 301 | 3PE | C22-C21-O21-C2 |
| 18 | T | 202 | 3PE | C1-O11-P-O12 |
| 18 | T | 202 | 3PE | C11-O13-P-O14 |
| 18 | T | 202 | 3PE | O13-C11-C12-N |
| 18 | T | 203 | 3PE | C1-O11-P-O12 |
| 18 | T | 203 | 3PE | C1-O11-P-O14 |
| 18 | T | 203 | 3PE | O13-C11-C12-N |
| 18 | T | 205 | 3PE | C12-C11-O13-P |
| 18 | T | 206 | 3PE | C11-O13-P-O14 |
| 18 | T | 206 | 3PE | O13-C11-C12-N |
| 18 | W | 201 | 3PE | O22-C21-O21-C2 |
| 18 | W | 201 | 3PE | C22-C21-O21-C2 |
| 19 | B | 601 | SMA | C11-C10-C9-C2 |
| 19 | B | 601 | SMA | C10-C11-C12-C13 |
| 19 | B | 601 | SMA | C10-C11-C12-O12 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 19 | B | 601 | SMA | C22-C11-C12-C13 |
| 19 | B | 601 | SMA | C22-C11-C12-O12 |
| 19 | O | 602 | SMA | C12-C13-C14-C15 |
| 19 | O | 602 | SMA | C12-C13-C14-O14 |
| 19 | O | 602 | SMA | C24-C13-C14-C15 |
| 19 | O | 602 | SMA | C24-C13-C14-O14 |
| 19 | O | 602 | SMA | O14-C14-C15-C16 |
| 19 | O | 602 | SMA | C15-C16-C17-C18 |
| 20 | B | 602 | HEM | C1A-C2A-CAA-CBA |
| 20 | B | 602 | HEM | C3A-C2A-CAA-CBA |
| 20 | O | 603 | HEM | C1A-C2A-CAA-CBA |
| 20 | O | 603 | HEM | C3A-C2A-CAA-CBA |
| 21 | B | 605 | CDL | CA2-OA2-PA1-OA3 |
| 21 | B | 605 | CDL | CA3-OA5-PA1-OA4 |
| 21 | B | 605 | CDL | CB3-OB5-PB2-OB2 |
| 21 | B | 605 | CDL | CB3-OB5-PB2-OB3 |
| 21 | B | 605 | CDL | CB3-OB5-PB2-OB4 |
| 21 | B | 606 | CDL | OB6-CB4-CB6-OB8 |
| 21 | B | 609 | CDL | CB2-C1-CA2-OA2 |
| 21 | B | 609 | CDL | CA3-OA5-PA1-OA4 |
| 21 | B | 609 | CDL | CB2-OB2-PB2-OB3 |
| 21 | B | 609 | CDL | CB2-OB2-PB2-OB4 |
| 21 | B | 609 | CDL | CB2-OB2-PB2-OB5 |
| 21 | B | 609 | CDL | CB3-OB5-PB2-OB4 |
| 21 | D | 607 | CDL | CA2-OA2-PA1-OA4 |
| 21 | D | 607 | CDL | CA3-OA5-PA1-OA3 |
| 21 | D | 607 | CDL | CA3-OA5-PA1-OA4 |
| 21 | D | 607 | CDL | CB2-OB2-PB2-OB3 |
| 21 | D | 607 | CDL | CB2-OB2-PB2-OB4 |
| 21 | D | 607 | CDL | CB2-OB2-PB2-OB5 |
| 21 | D | 607 | CDL | CB3-OB5-PB2-OB3 |
| 21 | D | 608 | CDL | CA2-OA2-PA1-OA3 |
| 21 | D | 608 | CDL | CB2-OB2-PB2-OB3 |
| 21 | D | 608 | CDL | CB3-OB5-PB2-OB4 |
| 21 | F | 302 | CDL | CA2-OA2-PA1-OA3 |
| 21 | F | 302 | CDL | CA3-OA5-PA1-OA4 |
| 21 | F | 302 | CDL | CB2-OB2-PB2-OB4 |
| 21 | F | 302 | CDL | CB3-OB5-PB2-OB3 |
| 21 | G | 201 | CDL | CA2-OA2-PA1-OA3 |
| 21 | G | 202 | CDL | C1-CA2-OA2-PA1 |
| 21 | G | 202 | CDL | CA2-OA2-PA1-OA3 |
| 21 | G | 202 | CDL | OA7-CA5-OA6-CA4 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 21 | G | 202 | CDL | C11-CA5-OA6-CA4 |
| 21 | I | 201 | CDL | O1-C1-CB2-OB2 |
| 21 | I | 201 | CDL | CA2-C1-CB2-OB2 |
| 21 | I | 201 | CDL | CA2-OA2-PA1-OA3 |
| 21 | I | 201 | CDL | CB4-CB3-OB5-PB2 |
| 21 | O | 606 | CDL | CA2-C1-CB2-OB2 |
| 21 | O | 606 | CDL | CA3-OA5-PA1-OA3 |
| 21 | O | 606 | CDL | CB2-OB2-PB2-OB3 |
| 21 | O | 606 | CDL | CB3-OB5-PB2-OB3 |
| 21 | Q | 607 | CDL | CA3-OA5-PA1-OA4 |
| 21 | Q | 607 | CDL | CB2-OB2-PB2-OB3 |
| 21 | Q | 607 | CDL | CB2-OB2-PB2-OB4 |
| 21 | Q | 607 | CDL | CB2-OB2-PB2-OB5 |
| 21 | Q | 608 | CDL | C1-CA2-OA2-PA1 |
| 21 | S | 302 | CDL | CA3-OA5-PA1-OA3 |
| 21 | S | 302 | CDL | CB2-OB2-PB2-OB3 |
| 21 | S | 302 | CDL | CB2-OB2-PB2-OB4 |
| 21 | T | 201 | CDL | CA2-OA2-PA1-OA5 |
| 21 | T | 201 | CDL | CA3-OA5-PA1-OA3 |
| 21 | T | 201 | CDL | CB2-OB2-PB2-OB3 |
| 21 | T | 201 | CDL | CB2-OB2-PB2-OB4 |
| 21 | T | 201 | CDL | CB3-OB5-PB2-OB4 |
| 21 | T | 204 | CDL | CA3-OA5-PA1-OA2 |
| 21 | T | 204 | CDL | CA3-OA5-PA1-OA3 |
| 21 | T | 204 | CDL | CA3-OA5-PA1-OA4 |
| 21 | T | 204 | CDL | CB2-OB2-PB2-OB3 |
| 21 | T | 204 | CDL | CB3-OB5-PB2-OB3 |
| 21 | V | 201 | CDL | O1-C1-CA2-OA2 |
| 21 | V | 201 | CDL | CB2-C1-CA2-OA2 |
| 21 | V | 201 | CDL | CA2-OA2-PA1-OA4 |
| 21 | V | 201 | CDL | CA2-OA2-PA1-OA5 |
| 21 | V | 201 | CDL | CA3-OA5-PA1-OA4 |
| 23 | B | 608 | LMT | C2-C1-O1'-C1' |
| 23 | O | 601 | LMT | O5'-C1'-O1'-C1 |
| 25 | D | 601 | HAS | C11-C12-C13-C14 |
| 25 | D | 601 | HAS | C14-C15-C16-C17 |
| 25 | D | 601 | HAS | C26-C15-C16-C17 |
| 25 | D | 601 | HAS | C15-C16-C17-C18 |
| 25 | D | 601 | HAS | C27-C19-C20-C21 |
| 25 | D | 601 | HAS | C19-C20-C21-C22 |
| 25 | D | 602 | HAS | C14-C15-C16-C17 |
| 25 | D | 602 | HAS | C26-C15-C16-C17 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 25 | Q | 601 | HAS | C14-C15-C16-C17 |
| 25 | Q | 601 | HAS | C26-C15-C16-C17 |
| 25 | Q | 601 | HAS | C23-C24-C28-C29 |
| 25 | Q | 602 | HAS | C1A-C2A-CAA-CBA |
| 25 | Q | 602 | HAS | C3A-C2A-CAA-CBA |
| 31 | E | 403 | DGA | OG1-CG1-CG2-OG2 |
| 31 | E | 403 | DGA | OG1-CG1-CG2-CG3 |
| 31 | U | 201 | DGA | OG1-CG1-CG2-OG2 |
| 31 | U | 201 | DGA | OG1-CG1-CG2-CG3 |
| 33 | H | 204 | IX7 | O8-C24-O7-C23 |
| 33 | H | 204 | IX7 | O20-C56-O19-C32 |
| 33 | H | 204 | IX7 | C30-O13-P-O15 |
| 33 | H | 204 | IX7 | C31-O16-P-O13 |
| 33 | H | 204 | IX7 | C31-O16-P-O14 |
| 33 | U | 204 | IX7 | C57-C56-O19-C32 |
| 23 | O | 601 | LMT | C3'-C4'-O1B-C1B |
| 15 | A | 502 | IZL | C53-C54-C55-C56 |
| 15 | N | 504 | IZL | O35-C60-O34-C45 |
| 18 | S | 301 | 3PE | O22-C21-O21-C2 |
| 21 | G | 201 | CDL | CB4-CB6-OB8-CB7 |
| 21 | T | 204 | CDL | C11-CA5-OA6-CA4 |
| 33 | H | 204 | IX7 | C57-C56-O19-C32 |
| 17 | A | 504 | MQ9 | C25-C24-C26-C27 |
| 25 | D | 601 | HAS | C18-C19-C20-C21 |
| 15 | N | 504 | IZL | C48-C47-O32-C46 |
| 18 | W | 201 | 3PE | C25-C26-C27-C28 |
| 21 | B | 609 | CDL | O1-C1-CA2-OA2 |
| 21 | O | 606 | CDL | O1-C1-CA2-OA2 |
| 18 | J | 201 | 3PE | C32-C31-O31-C3 |
| 15 | N | 504 | IZL | C17-C18-O7-C19 |
| 15 | A | 502 | IZL | C61-C60-O34-C45 |
| 18 | T | 206 | 3PE | C22-C21-O21-C2 |
| 15 | N | 504 | IZL | C49-C50-C51-C52 |
| 15 | N | 504 | IZL | O1-C11-C12-C73 |
| 23 | O | 601 | LMT | O5'-C5'-C6'-O6' |
| 15 | N | 504 | IZL | C34-C32-C33-O18 |
| 18 | S | 301 | 3PE | C33-C34-C35-C36 |
| 17 | O | 605 | MQ9 | C12-C11-C9-C10 |
| 25 | D | 601 | HAS | C25-C23-C24-C28 |
| 25 | D | 602 | HAS | C27-C19-C20-C21 |
| 25 | Q | 602 | HAS | C26-C15-C16-C17 |
| 17 | O | 605 | MQ9 | C12-C11-C9-C8 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 25 | D | 601 | HAS | C22-C23-C24-C28 |
| 25 | D | 602 | HAS | C18-C19-C20-C21 |
| 25 | Q | 602 | HAS | C14-C15-C16-C17 |
| 15 | N | 504 | IZL | O1-C11-C12-O2 |
| 17 | A | 504 | MQ9 | C29-C31-C32-C33 |
| 17 | A | 504 | MQ9 | C44-C46-C47-C48 |
| 17 | B | 604 | MQ9 | C9-C11-C12-C13 |
| 17 | N | 501 | MQ9 | C9-C11-C12-C13 |
| 17 | O | 605 | MQ9 | C14-C16-C17-C18 |
| 22 | O | 607 | LYC | C61-C63-C64-C65 |
| 25 | D | 602 | HAS | C23-C24-C28-C29 |
| 15 | N | 504 | IZL | C47-C48-C49-C50 |
| 33 | U | 204 | IX7 | C27-C25-C26-O9 |
| 18 | F | 301 | 3PE | C22-C21-O21-C2 |
| 21 | S | 302 | CDL | C11-CA5-OA6-CA4 |
| 21 | B | 605 | CDL | CB2-C1-CA2-OA2 |
| 21 | F | 302 | CDL | CA2-C1-CB2-OB2 |
| 21 | I | 201 | CDL | CB2-C1-CA2-OA2 |
| 21 | S | 302 | CDL | CB2-C1-CA2-OA2 |
| 21 | T | 204 | CDL | OA7-CA5-OA6-CA4 |
| 17 | A | 504 | MQ9 | C7-C8-C9-C11 |
| 15 | N | 504 | IZL | O33-C47-O32-C46 |
| 18 | W | 201 | 3PE | C29-C2A-C2B-C2C |
| 15 | A | 502 | IZL | C48-C47-O32-C46 |
| 18 | P | 303 | 3PE | C32-C31-O31-C3 |
| 18 | W | 201 | 3PE | C32-C31-O31-C3 |
| 23 | O | 601 | LMT | O5B-C5B-C6B-O6B |
| 15 | N | 504 | IZL | C43-O28-P-O31 |
| 15 | N | 504 | IZL | O17-C31-O16-C30 |
| 23 | O | 601 | LMT | C4'-C5'-C6'-O6' |
| 21 | B | 605 | CDL | O1-C1-CA2-OA2 |
| 21 | B | 605 | CDL | O1-C1-CB2-OB2 |
| 21 | F | 302 | CDL | O1-C1-CB2-OB2 |
| 21 | I | 201 | CDL | O1-C1-CA2-OA2 |
| 21 | O | 606 | CDL | O1-C1-CB2-OB2 |
| 21 | S | 302 | CDL | O1-C1-CA2-OA2 |
| 21 | V | 201 | CDL | O1-C1-CB2-OB2 |
| 18 | J | 201 | 3PE | C21-C22-C23-C24 |
| 21 | Q | 607 | CDL | CB5-C51-C52-C53 |
| 15 | A | 502 | IZL | C43-C18-O7-C19 |
| 18 | J | 201 | 3PE | O32-C31-O31-C3 |
| 15 | N | 504 | IZL | O17-C32-C33-O18 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 19 | B | 601 | SMA | C17-C18-C19-C26 |
| 19 | B | 601 | SMA | C17-C18-C19-C20 |
| 15 | A | 502 | IZL | O35-C60-O34-C45 |
| 33 | U | 204 | IX7 | O20-C56-O19-C32 |
| 21 | V | 201 | CDL | C21-C22-C23-C24 |
| 16 | U | 203 | 9YF | C25-C26-C27-C28 |
| 21 | S | 302 | CDL | CA7-C31-C32-C33 |
| 33 | U | 204 | IX7 | C34-C35-C36-C37 |
| 18 | T | 206 | 3PE | C28-C29-C2A-C2B |
| 25 | D | 602 | HAS | C3D-CAD-CBD-CGD |
| 18 | D | 609 | 3PE | C21-C22-C23-C24 |
| 21 | T | 201 | CDL | CB5-C51-C52-C53 |
| 33 | H | 204 | IX7 | C12-C13-C14-C15 |
| 18 | W | 201 | 3PE | C36-C37-C38-C39 |
| 15 | A | 502 | IZL | O1-C11-C12-O2 |
| 16 | H | 203 | 9YF | C25-C26-C27-C28 |
| 18 | C | 303 | 3PE | C31-C32-C33-C34 |
| 18 | L | 101 | 3PE | C21-C22-C23-C24 |
| 18 | T | 203 | 3PE | C31-C32-C33-C34 |
| 21 | D | 607 | CDL | CB7-C71-C72-C73 |
| 21 | F | 302 | CDL | CA7-C31-C32-C33 |
| 33 | H | 204 | IX7 | C56-C57-C58-C59 |
| 33 | U | 204 | IX7 | O8-C25-C26-O9 |
| 16 | A | 503 | 9YF | C25-C26-C27-C28 |
| 21 | G | 202 | CDL | CB7-C71-C72-C73 |
| 31 | U | 201 | DGA | CB1-CB2-CB3-CB4 |
| 15 | A | 502 | IZL | C28-C26-C27-O13 |
| 33 | H | 204 | IX7 | C35-C36-C37-C38 |
| 25 | Q | 602 | HAS | C23-C24-C28-C29 |
| 18 | F | 301 | 3PE | C31-C32-C33-C34 |
| 21 | D | 608 | CDL | O1-C1-CB2-OB2 |
| 15 | A | 502 | IZL | O1-C11-C12-C73 |
| 15 | A | 502 | IZL | O33-C47-O32-C46 |
| 18 | P | 303 | 3PE | O32-C31-O31-C3 |
| 18 | W | 201 | 3PE | O32-C31-O31-C3 |
| 15 | A | 502 | IZL | C44-O31-P-O28 |
| 16 | A | 503 | 9YF | C1-O-P-O2 |
| 18 | C | 304 | 3PE | C1-O11-P-O13 |
| 18 | C | 304 | 3PE | C11-O13-P-O11 |
| 18 | D | 609 | 3PE | C1-O11-P-O13 |
| 18 | F | 301 | 3PE | C1-O11-P-O13 |
| 18 | J | 201 | 3PE | C11-O13-P-O11 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 18 | P | 303 | 3PE | C1-O11-P-O13 |
| 18 | P | 303 | 3PE | C11-O13-P-O11 |
| 18 | R | 405 | 3PE | C11-O13-P-O11 |
| 18 | S | 301 | 3PE | C11-O13-P-O11 |
| 18 | T | 202 | 3PE | C1-O11-P-O13 |
| 18 | T | 203 | 3PE | C1-O11-P-O13 |
| 18 | T | 205 | 3PE | C11-O13-P-O11 |
| 21 | B | 605 | CDL | CA3-OA5-PA1-OA2 |
| 21 | B | 609 | CDL | CA3-OA5-PA1-OA2 |
| 21 | B | 609 | CDL | CB3-OB5-PB2-OB2 |
| 21 | D | 607 | CDL | CA2-OA2-PA1-OA5 |
| 21 | D | 607 | CDL | CA3-OA5-PA1-OA2 |
| 21 | D | 607 | CDL | CB3-OB5-PB2-OB2 |
| 21 | D | 608 | CDL | CA3-OA5-PA1-OA2 |
| 21 | D | 608 | CDL | CB2-OB2-PB2-OB5 |
| 21 | D | 608 | CDL | CB3-OB5-PB2-OB2 |
| 21 | F | 302 | CDL | CA3-OA5-PA1-OA2 |
| 21 | F | 302 | CDL | CB2-OB2-PB2-OB5 |
| 21 | F | 302 | CDL | CB3-OB5-PB2-OB2 |
| 21 | G | 201 | CDL | CA2-OA2-PA1-OA5 |
| 21 | G | 201 | CDL | CA3-OA5-PA1-OA2 |
| 21 | G | 202 | CDL | CA2-OA2-PA1-OA5 |
| 21 | I | 201 | CDL | CA2-OA2-PA1-OA5 |
| 21 | O | 606 | CDL | CB2-OB2-PB2-OB5 |
| 21 | O | 606 | CDL | CB3-OB5-PB2-OB2 |
| 21 | Q | 607 | CDL | CA2-OA2-PA1-OA5 |
| 21 | Q | 608 | CDL | CA2-OA2-PA1-OA5 |
| 21 | S | 302 | CDL | CB2-OB2-PB2-OB5 |
| 21 | T | 201 | CDL | CB2-OB2-PB2-OB5 |
| 21 | T | 204 | CDL | CB2-OB2-PB2-OB5 |
| 21 | V | 201 | CDL | CA3-OA5-PA1-OA2 |
| 21 | V | 201 | CDL | CB2-OB2-PB2-OB5 |
| 21 | D | 607 | CDL | CA7-C31-C32-C33 |
| 21 | G | 201 | CDL | CA5-C11-C12-C13 |
| 21 | T | 204 | CDL | C11-C12-C13-C14 |
| 18 | T | 206 | 3PE | C32-C31-O31-C3 |
| 21 | I | 201 | CDL | C23-C24-C25-C26 |
| 21 | B | 605 | CDL | CA2-C1-CB2-OB2 |
| 21 | D | 608 | CDL | CA2-C1-CB2-OB2 |
| 21 | G | 201 | CDL | CA2-C1-CB2-OB2 |
| 18 | F | 301 | 3PE | O22-C21-O21-C2 |
| 18 | T | 206 | 3PE | O22-C21-O21-C2 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 17 | A | 504 | MQ9 | C45-C44-C46-C47 |
| 21 | G | 201 | CDL | CA7-C31-C32-C33 |
| 15 | A | 502 | IZL | C50-C51-C52-C53 |
| 18 | S | 301 | 3PE | C36-C37-C38-C39 |
| 21 | D | 607 | CDL | C15-C16-C17-C18 |
| 21 | G | 201 | CDL | C19-C20-C21-C22 |
| 21 | O | 606 | CDL | C19-C20-C21-C22 |
| 21 | T | 204 | CDL | C13-C14-C15-C16 |
| 33 | H | 204 | IX7 | C10-C11-C12-C13 |
| 18 | S | 301 | 3PE | C38-C39-C3A-C3B |
| 18 | T | 205 | 3PE | C24-C25-C26-C27 |
| 21 | I | 201 | CDL | C11-C12-C13-C14 |
| 21 | T | 201 | CDL | C18-C19-C20-C21 |
| 21 | V | 201 | CDL | C38-C39-C40-C41 |
| 33 | U | 204 | IX7 | C9-C10-C11-C12 |
| 33 | U | 204 | IX7 | C62-C63-C64-C65 |
| 18 | W | 201 | 3PE | C1-C2-O21-C21 |
| 21 | G | 202 | CDL | CA3-CA4-OA6-CA5 |
| 21 | T | 204 | CDL | CA3-CA4-OA6-CA5 |
| 21 | S | 302 | CDL | OA7-CA5-OA6-CA4 |
| 18 | T | 206 | 3PE | C37-C38-C39-C3A |
| 21 | D | 608 | CDL | C1-CB2-OB2-PB2 |
| 18 | Q | 609 | 3PE | C27-C28-C29-C2A |
| 18 | S | 301 | 3PE | C2A-C2B-C2C-C2D |
| 21 | O | 606 | CDL | C15-C16-C17-C18 |
| 21 | T | 201 | CDL | C34-C35-C36-C37 |
| 21 | F | 302 | CDL | O1-C1-CA2-OA2 |
| 21 | O | 606 | CDL | C35-C36-C37-C38 |
| 21 | Q | 607 | CDL | C11-C12-C13-C14 |
| 21 | Q | 608 | CDL | C12-C13-C14-C15 |
| 21 | S | 302 | CDL | C16-C17-C18-C19 |
| 21 | T | 201 | CDL | C38-C39-C40-C41 |
| 21 | V | 201 | CDL | C41-C42-C43-C44 |
| 23 | O | 601 | LMT | C2'-C1'-O1'-C1 |
| 21 | B | 609 | CDL | OB6-CB4-CB6-OB8 |
| 18 | A | 505 | 3PE | C24-C25-C26-C27 |
| 31 | U | 201 | DGA | CB7-CB8-CB9-CAB |
| 33 | H | 204 | IX7 | O8-C25-C26-O9 |
| 17 | A | 504 | MQ9 | C20-C19-C21-C22 |
| 21 | S | 302 | CDL | C18-C19-C20-C21 |
| 21 | V | 201 | CDL | C42-C43-C44-C45 |
| 31 | U | 201 | DGA | CB6-CB7-CB8-CB9 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 21 | B | 609 | CDL | CB5-C51-C52-C53 |
| 18 | S | 301 | 3PE | C34-C35-C36-C37 |
| 18 | W | 201 | 3PE | C39-C3A-C3B-C3C |
| 21 | G | 202 | CDL | C54-C55-C56-C57 |
| 21 | B | 609 | CDL | C53-C54-C55-C56 |
| 21 | D | 608 | CDL | C18-C19-C20-C21 |
| 18 | D | 609 | 3PE | C33-C34-C35-C36 |
| 18 | J | 201 | 3PE | C24-C25-C26-C27 |
| 21 | B | 609 | CDL | C74-C75-C76-C77 |
| 21 | V | 201 | CDL | C37-C38-C39-C40 |
| 23 | B | 608 | LMT | C3-C4-C5-C6 |
| 15 | A | 502 | IZL | C47-C48-C49-C50 |
| 18 | T | 202 | 3PE | C31-C32-C33-C34 |
| 18 | T | 206 | 3PE | C21-C22-C23-C24 |
| 18 | T | 203 | 3PE | C22-C23-C24-C25 |
| 21 | D | 607 | CDL | C58-C59-C60-C61 |
| 21 | D | 608 | CDL | C21-C22-C23-C24 |
| 21 | G | 201 | CDL | C14-C15-C16-C17 |
| 21 | G | 201 | CDL | C32-C33-C34-C35 |
| 21 | S | 302 | CDL | C36-C37-C38-C39 |
| 25 | D | 602 | HAS | C15-C16-C17-C18 |
| 21 | B | 609 | CDL | C55-C56-C57-C58 |
| 21 | I | 201 | CDL | C22-C23-C24-C25 |
| 18 | C | 304 | 3PE | O13-C11-C12-N |
| 18 | P | 303 | 3PE | O13-C11-C12-N |
| 18 | A | 505 | 3PE | C26-C27-C28-C29 |
| 21 | T | 201 | CDL | C33-C34-C35-C36 |
| 21 | D | 608 | CDL | CA7-C31-C32-C33 |
| 21 | G | 202 | CDL | C71-C72-C73-C74 |
| 21 | O | 606 | CDL | C17-C18-C19-C20 |
| 21 | D | 607 | CDL | C33-C34-C35-C36 |
| 21 | I | 201 | CDL | C15-C16-C17-C18 |
| 21 | Q | 607 | CDL | C31-C32-C33-C34 |
| 21 | S | 302 | CDL | C13-C14-C15-C16 |
| 18 | T | 206 | 3PE | C32-C33-C34-C35 |
| 18 | W | 201 | 3PE | C33-C34-C35-C36 |
| 21 | G | 201 | CDL | C22-C23-C24-C25 |
| 21 | S | 302 | CDL | C33-C34-C35-C36 |
| 33 | U | 204 | IX7 | C35-C36-C37-C38 |
| 18 | T | 206 | 3PE | C31-C32-C33-C34 |
| 17 | N | 501 | MQ9 | C20-C19-C21-C22 |
| 17 | A | 504 | MQ9 | C18-C19-C21-C22 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 17 | A | 504 | MQ9 | C43-C44-C46-C47 |
| 17 | N | 501 | MQ9 | C18-C19-C21-C22 |
| 18 | Q | 609 | 3PE | C22-C23-C24-C25 |
| 18 | L | 101 | 3PE | C32-C33-C34-C35 |
| 18 | T | 203 | 3PE | C2D-C2E-C2F-C2G |
| 33 | U | 204 | IX7 | C58-C59-C60-C61 |
| 15 | A | 502 | IZL | C7-C8-C9-C10 |
| 16 | H | 203 | 9YF | C11-C10-C9-C8 |
| 21 | B | 609 | CDL | C32-C33-C34-C35 |
| 21 | T | 201 | CDL | C17-C18-C19-C20 |
| 21 | T | 201 | CDL | C55-C56-C57-C58 |
| 15 | N | 504 | IZL | C15-C14-O3-C13 |
| 21 | G | 201 | CDL | C13-C14-C15-C16 |
| 21 | V | 201 | CDL | C18-C19-C20-C21 |
| 18 | D | 609 | 3PE | C34-C35-C36-C37 |
| 18 | J | 201 | 3PE | C39-C3A-C3B-C3C |
| 21 | B | 609 | CDL | C73-C74-C75-C76 |
| 21 | D | 607 | CDL | C38-C39-C40-C41 |
| 21 | D | 608 | CDL | C32-C33-C34-C35 |
| 21 | O | 606 | CDL | C14-C15-C16-C17 |
| 21 | Q | 607 | CDL | C60-C61-C62-C63 |
| 21 | S | 302 | CDL | C35-C36-C37-C38 |
| 21 | T | 201 | CDL | C16-C17-C18-C19 |
| 23 | B | 608 | LMT | C1-C2-C3-C4 |
| 21 | O | 606 | CDL | C51-CB5-OB6-CB4 |
| 33 | U | 204 | IX7 | C12-C13-C14-C15 |
| 18 | J | 201 | 3PE | C36-C37-C38-C39 |
| 21 | D | 608 | CDL | C14-C15-C16-C17 |
| 33 | H | 204 | IX7 | C30-O13-P-O16 |
| 15 | N | 504 | IZL | C43-C18-O7-C19 |
| 21 | O | 606 | CDL | OB7-CB5-OB6-CB4 |
| 33 | H | 204 | IX7 | C35-C34-O17-C33 |
| 18 | L | 101 | 3PE | C22-C23-C24-C25 |
| 18 | T | 203 | 3PE | C32-C33-C34-C35 |
| 18 | W | 201 | 3PE | C38-C39-C3A-C3B |
| 21 | D | 607 | CDL | C35-C36-C37-C38 |
| 21 | I | 201 | CDL | C20-C21-C22-C23 |
| 21 | O | 606 | CDL | C34-C35-C36-C37 |
| 18 | T | 206 | 3PE | O32-C31-O31-C3 |
| 23 | O | 601 | LMT | C1-C2-C3-C4 |
| 18 | D | 609 | 3PE | C23-C24-C25-C26 |
| 21 | O | 606 | CDL | C31-C32-C33-C34 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 21 | G | 201 | CDL | CB5-C51-C52-C53 |
| 21 | Q | 607 | CDL | CA5-C11-C12-C13 |
| 21 | T | 201 | CDL | CB7-C71-C72-C73 |
| 18 | J | 201 | 3PE | C22-C21-O21-C2 |
| 18 | L | 101 | 3PE | C22-C21-O21-C2 |
| 18 | N | 502 | 3PE | C22-C21-O21-C2 |
| 18 | P | 303 | 3PE | C22-C21-O21-C2 |
| 21 | T | 204 | CDL | C51-CB5-OB6-CB4 |
| 19 | B | 601 | SMA | C16-C17-C18-C19 |
| 21 | V | 201 | CDL | C32-C33-C34-C35 |
| 15 | N | 504 | IZL | O12-C26-C27-O13 |
| 18 | L | 101 | 3PE | O22-C21-O21-C2 |
| 21 | G | 202 | CDL | CB5-C51-C52-C53 |
| 18 | W | 201 | 3PE | C22-C23-C24-C25 |
| 18 | C | 304 | 3PE | O21-C2-C3-O31 |
| 18 | T | 202 | 3PE | O21-C2-C3-O31 |
| 21 | D | 607 | CDL | OA6-CA4-CA6-OA8 |
| 21 | G | 201 | CDL | OB6-CB4-CB6-OB8 |
| 21 | O | 606 | CDL | OB6-CB4-CB6-OB8 |
| 21 | Q | 607 | CDL | C73-C74-C75-C76 |
| 17 | A | 504 | MQ9 | C23-C24-C26-C27 |
| 21 | D | 607 | CDL | C31-C32-C33-C34 |
| 21 | D | 607 | CDL | C59-C60-C61-C62 |
| 18 | W | 201 | 3PE | C32-C33-C34-C35 |
| 21 | G | 202 | CDL | C11-C12-C13-C14 |
| 21 | B | 609 | CDL | C51-C52-C53-C54 |
| 18 | N | 502 | 3PE | O22-C21-O21-C2 |
| 18 | W | 201 | 3PE | C27-C28-C29-C2A |
| 21 | G | 201 | CDL | C53-C54-C55-C56 |
| 23 | B | 608 | LMT | C5-C6-C7-C8 |
| 18 | Q | 609 | 3PE | C11-O13-P-O11 |
| 21 | G | 202 | CDL | CB3-OB5-PB2-OB2 |
| 21 | Q | 607 | CDL | CA3-OA5-PA1-OA2 |
| 21 | S | 302 | CDL | CA3-OA5-PA1-OA2 |
| 21 | T | 201 | CDL | CA3-OA5-PA1-OA2 |
| 18 | S | 301 | 3PE | C31-C32-C33-C34 |
| 21 | O | 606 | CDL | CA7-C31-C32-C33 |
| 21 | B | 605 | CDL | C1-CA2-OA2-PA1 |
| 18 | W | 201 | 3PE | O11-C1-C2-C3 |
| 18 | S | 301 | 3PE | C24-C25-C26-C27 |
| 33 | H | 204 | IX7 | C7-C8-C9-C10 |
| 33 | H | 204 | IX7 | C62-C63-C64-C65 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 18 | Q | 609 | 3PE | C21-C22-C23-C24 |
| 33 | U | 204 | IX7 | C61-C62-C63-C64 |
| 21 | F | 302 | CDL | C31-CA7-OA8-CA6 |
| 21 | F | 302 | CDL | CB2-C1-CA2-OA2 |
| 18 | P | 303 | 3PE | O22-C21-O21-C2 |
| 21 | G | 202 | CDL | C59-C60-C61-C62 |
| 21 | Q | 608 | CDL | C32-C33-C34-C35 |
| 18 | L | 101 | 3PE | C31-C32-C33-C34 |
| 18 | C | 303 | 3PE | C22-C21-O21-C2 |
| 15 | A | 502 | IZL | C48-C49-C50-C51 |
| 18 | T | 206 | 3PE | C35-C36-C37-C38 |
| 21 | D | 607 | CDL | C51-C52-C53-C54 |
| 18 | C | 304 | 3PE | C1-C2-C3-O31 |
| 21 | B | 605 | CDL | CA3-CA4-CA6-OA8 |
| 21 | B | 609 | CDL | CB3-CB4-CB6-OB8 |
| 21 | B | 609 | CDL | C76-C77-C78-C79 |
| 21 | D | 607 | CDL | CA3-CA4-CA6-OA8 |
| 21 | D | 608 | CDL | CA3-CA4-CA6-OA8 |
| 16 | A | 503 | 9YF | C12-C13-C14-C15 |
| 16 | U | 203 | 9YF | C28-C29-C30-C31 |
| 21 | G | 202 | CDL | C33-C34-C35-C36 |
| 21 | D | 607 | CDL | CB5-C51-C52-C53 |
| 17 | N | 501 | MQ9 | C5-C6-C7-C8 |
| 18 | L | 101 | 3PE | C24-C25-C26-C27 |
| 18 | R | 405 | 3PE | C2A-C2B-C2C-C2D |
| 33 | U | 204 | IX7 | C57-C58-C59-C60 |
| 21 | O | 606 | CDL | C12-C11-CA5-OA6 |
| 18 | J | 201 | 3PE | O22-C21-O21-C2 |
| 21 | B | 605 | CDL | C52-C53-C54-C55 |
| 21 | T | 201 | CDL | C13-C14-C15-C16 |
| 16 | A | 503 | 9YF | C2-O2-P-O |
| 16 | N | 505 | 9YF | C2-O2-P-O |
| 21 | B | 605 | CDL | CA7-C31-C32-C33 |
| 21 | F | 302 | CDL | CA5-C11-C12-C13 |
| 18 | Q | 609 | 3PE | C33-C34-C35-C36 |
| 21 | V | 201 | CDL | C24-C25-C26-C27 |
| 17 | N | 501 | MQ9 | C1-C6-C7-C8 |
| 25 | D | 602 | HAS | C11-C12-C13-C14 |
| 25 | Q | 601 | HAS | C11-C12-C13-C14 |
| 21 | G | 201 | CDL | C24-C25-C26-C27 |
| 32 | H | 202 | PLM | C3-C4-C5-C6 |
| 21 | V | 201 | CDL | CA7-C31-C32-C33 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 15 | A | 502 | IZL | C17-C18-O7-C19 |
| 21 | B | 609 | CDL | C54-C55-C56-C57 |
| 21 | S | 302 | CDL | C51-C52-C53-C54 |
| 15 | N | 504 | IZL | C39-C22-O9-C21 |
| 16 | A | 503 | 9YF | O9-C-C24-O11 |
| 18 | C | 303 | 3PE | O21-C2-C3-O31 |
| 21 | B | 605 | CDL | OA6-CA4-CA6-OA8 |
| 21 | D | 608 | CDL | C33-C34-C35-C36 |
| 15 | A | 502 | IZL | C54-C55-C56-C58 |
| 15 | N | 504 | IZL | C43-C14-O3-C13 |
| 21 | V | 201 | CDL | CA2-C1-CB2-OB2 |
| 21 | T | 204 | CDL | OB7-CB5-OB6-CB4 |
| 18 | S | 301 | 3PE | C26-C27-C28-C29 |
| 21 | I | 201 | CDL | C18-C19-C20-C21 |
| 15 | A | 502 | IZL | C51-C52-C53-C54 |
| 18 | T | 203 | 3PE | O11-C1-C2-C3 |
| 21 | Q | 608 | CDL | OB5-CB3-CB4-CB6 |
| 21 | T | 201 | CDL | OB5-CB3-CB4-CB6 |
| 17 | A | 504 | MQ9 | C34-C36-C37-C38 |
| 17 | O | 605 | MQ9 | C9-C11-C12-C13 |
| 25 | Q | 602 | HAS | C19-C20-C21-C22 |
| 21 | T | 201 | CDL | C35-C36-C37-C38 |
| 18 | W | 201 | 3PE | O13-C11-C12-N |
| 21 | Q | 607 | CDL | C32-C33-C34-C35 |
| 33 | U | 204 | IX7 | C22-C23-O7-C24 |
| 21 | D | 608 | CDL | C16-C17-C18-C19 |
| 21 | D | 607 | CDL | O1-C1-CA2-OA2 |
| 18 | W | 201 | 3PE | C2C-C2D-C2E-C2F |
| 33 | H | 204 | IX7 | C9-C10-C11-C12 |
| 21 | B | 606 | CDL | CB4-CB3-OB5-PB2 |
| 23 | B | 608 | LMT | C4B-C5B-C6B-O6B |
| 18 | A | 505 | 3PE | C32-C31-O31-C3 |
| 21 | G | 201 | CDL | C71-CB7-OB8-CB6 |
| 18 | T | 202 | 3PE | C1-C2-C3-O31 |
| 18 | W | 201 | 3PE | C1-C2-C3-O31 |
| 21 | B | 606 | CDL | CB3-CB4-CB6-OB8 |
| 21 | G | 201 | CDL | CB3-CB4-CB6-OB8 |
| 21 | O | 606 | CDL | CB3-CB4-CB6-OB8 |
| 21 | T | 201 | CDL | CA3-CA4-CA6-OA8 |
| 21 | V | 201 | CDL | CB3-CB4-CB6-OB8 |
| 33 | H | 204 | IX7 | C31-C32-C33-O17 |
| 21 | I | 201 | CDL | C24-C25-C26-C27 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 16 | A | 503 | 9YF | C2-O2-P-O8 |
| 33 | H | 204 | IX7 | C30-O13-P-O14 |
| 15 | A | 502 | IZL | O12-C26-C27-O13 |
| 18 | F | 301 | 3PE | C21-C22-C23-C24 |
| 15 | N | 504 | IZL | C62-C63-C64-C65 |
| 21 | B | 605 | CDL | CA2-OA2-PA1-OA5 |
| 21 | I | 201 | CDL | CA3-OA5-PA1-OA2 |
| 21 | T | 201 | CDL | CB3-OB5-PB2-OB2 |
| 18 | J | 201 | 3PE | C3B-C3C-C3D-C3E |
| 18 | T | 206 | 3PE | C36-C37-C38-C39 |
| 18 | P | 303 | 3PE | O11-C1-C2-O21 |
| 18 | R | 405 | 3PE | O11-C1-C2-O21 |
| 18 | T | 205 | 3PE | O11-C1-C2-O21 |
| 21 | D | 607 | CDL | OB5-CB3-CB4-OB6 |
| 21 | G | 202 | CDL | OB5-CB3-CB4-OB6 |
| 21 | Q | 607 | CDL | OB5-CB3-CB4-OB6 |
| 21 | T | 201 | CDL | OA5-CA3-CA4-OA6 |
| 21 | V | 201 | CDL | OB5-CB3-CB4-OB6 |
| 18 | T | 203 | 3PE | C36-C37-C38-C39 |
| 18 | T | 203 | 3PE | C28-C29-C2A-C2B |
| 21 | G | 201 | CDL | O1-C1-CB2-OB2 |
| 15 | N | 504 | IZL | C52-C53-C54-C55 |
| 31 | M | 201 | DGA | OG1-CG1-CG2-OG2 |
| 18 | N | 502 | 3PE | C29-C2A-C2B-C2C |
| 18 | A | 505 | 3PE | O21-C2-C3-O31 |
| 18 | W | 201 | 3PE | O21-C2-C3-O31 |
| 21 | Q | 608 | CDL | OB6-CB4-CB6-OB8 |
| 21 | T | 201 | CDL | OA6-CA4-CA6-OA8 |
| 16 | H | 203 | 9YF | C26-C25-O11-C24 |
| 18 | N | 502 | 3PE | C22-C23-C24-C25 |
| 21 | V | 201 | CDL | C12-C13-C14-C15 |
| 18 | A | 505 | 3PE | C22-C21-O21-C2 |
| 15 | A | 502 | IZL | C43-C14-O3-C13 |
| 21 | O | 606 | CDL | CB2-C1-CA2-OA2 |
| 18 | D | 609 | 3PE | C24-C25-C26-C27 |
| 18 | C | 303 | 3PE | O22-C21-O21-C2 |
| 33 | U | 204 | IX7 | C59-C60-C61-C62 |
| 21 | Q | 607 | CDL | C36-C37-C38-C39 |
| 23 | O | 601 | LMT | C6-C7-C8-C9 |
| 21 | I | 201 | CDL | C13-C14-C15-C16 |
| 18 | T | 206 | 3PE | C2-C1-O11-P |
| 21 | O | 606 | CDL | C1-CB2-OB2-PB2 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 21 | Q | 608 | CDL | CA4-CA3-OA5-PA1 |
| 21 | Q | 608 | CDL | C1-CB2-OB2-PB2 |
| 21 | Q | 608 | CDL | CB4-CB3-OB5-PB2 |
| 33 | U | 204 | IX7 | C63-C64-C65-C66 |
| 17 | N | 501 | MQ9 | C26-C27-C28-C29 |
| 21 | D | 608 | CDL | C13-C14-C15-C16 |
| 22 | B | 607 | LYC | C55-C56-C58-C59 |
| 21 | S | 302 | CDL | C51-CB5-OB6-CB4 |
| 18 | N | 502 | 3PE | C2F-C2G-C2H-C2I |
| 15 | A | 502 | IZL | C57-C56-C58-C59 |
| 21 | O | 606 | CDL | C32-C33-C34-C35 |
| 21 | B | 605 | CDL | C13-C14-C15-C16 |
| 21 | D | 607 | CDL | C52-C53-C54-C55 |
| 21 | T | 201 | CDL | C20-C21-C22-C23 |
| 18 | T | 205 | 3PE | C32-C33-C34-C35 |
| 18 | F | 301 | 3PE | O11-C1-C2-C3 |
| 18 | J | 201 | 3PE | O11-C1-C2-C3 |
| 21 | B | 605 | CDL | OB5-CB3-CB4-CB6 |
| 21 | B | 606 | CDL | OB5-CB3-CB4-CB6 |
| 21 | B | 609 | CDL | OB5-CB3-CB4-CB6 |
| 21 | G | 202 | CDL | OB5-CB3-CB4-CB6 |
| 21 | I | 201 | CDL | OA5-CA3-CA4-CA6 |
| 21 | I | 201 | CDL | OB5-CB3-CB4-CB6 |
| 21 | Q | 607 | CDL | OB5-CB3-CB4-CB6 |
| 21 | V | 201 | CDL | OB5-CB3-CB4-CB6 |
| 18 | T | 206 | 3PE | C27-C28-C29-C2A |
| 15 | A | 502 | IZL | C43-O28-P-O31 |
| 21 | B | 605 | CDL | C11-C12-C13-C14 |
| 21 | D | 608 | CDL | C11-C12-C13-C14 |
| 21 | F | 302 | CDL | OA9-CA7-OA8-CA6 |
| 21 | T | 201 | CDL | C72-C73-C74-C75 |
| 21 | G | 202 | CDL | C12-C13-C14-C15 |
| 15 | A | 502 | IZL | C55-C56-C58-C59 |
| 21 | Q | 607 | CDL | C52-C53-C54-C55 |
| 18 | C | 303 | 3PE | C1-C2-O21-C21 |
| 18 | F | 301 | 3PE | C1-C2-O21-C21 |
| 18 | S | 301 | 3PE | C2D-C2E-C2F-C2G |
| 18 | A | 505 | 3PE | C1-C2-C3-O31 |
| 18 | C | 303 | 3PE | C1-C2-C3-O31 |
| 21 | B | 609 | CDL | C1-CA2-OA2-PA1 |
| 21 | F | 302 | CDL | CA4-CA3-OA5-PA1 |
| 21 | Q | 608 | CDL | CB3-CB4-CB6-OB8 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 21 | T | 204 | CDL | C1-CA2-OA2-PA1 |
| 33 | H | 204 | IX7 | C32-C31-O16-P |
| 21 | G | 201 | CDL | OB9-CB7-OB8-CB6 |
| 31 | U | 201 | DGA | CB5-CB6-CB7-CB8 |
| 16 | N | 505 | 9YF | O9-C-C1-O |
| 18 | C | 304 | 3PE | O11-C1-C2-O21 |
| 18 | J | 201 | 3PE | O11-C1-C2-O21 |
| 18 | S | 301 | 3PE | O11-C1-C2-O21 |
| 21 | B | 609 | CDL | OB5-CB3-CB4-OB6 |
| 21 | F | 302 | CDL | OB5-CB3-CB4-OB6 |
| 21 | I | 201 | CDL | OA5-CA3-CA4-OA6 |
| 21 | I | 201 | CDL | OB5-CB3-CB4-OB6 |
| 21 | O | 606 | CDL | OA5-CA3-CA4-OA6 |
| 21 | Q | 608 | CDL | OB5-CB3-CB4-OB6 |
| 21 | T | 201 | CDL | OB5-CB3-CB4-OB6 |
| 21 | B | 609 | CDL | C71-C72-C73-C74 |
| 21 | B | 606 | CDL | O1-C1-CA2-OA2 |
| 18 | T | 202 | 3PE | C32-C33-C34-C35 |
| 21 | T | 204 | CDL | C14-C15-C16-C17 |
| 18 | T | 206 | 3PE | O21-C2-C3-O31 |
| 21 | D | 608 | CDL | OA6-CA4-CA6-OA8 |
| 21 | T | 204 | CDL | OA6-CA4-CA6-OA8 |
| 21 | V | 201 | CDL | OB6-CB4-CB6-OB8 |
| 15 | A | 502 | IZL | C9-C10-O1-C11 |
| 18 | J | 201 | 3PE | C22-C23-C24-C25 |
| 21 | F | 302 | CDL | C32-C33-C34-C35 |
| 21 | V | 201 | CDL | CB5-C51-C52-C53 |
| 21 | T | 201 | CDL | C12-C13-C14-C15 |
| 23 | O | 601 | LMT | C4B-C5B-C6B-O6B |
| 16 | N | 505 | 9YF | C10-C11-C12-C13 |
| 16 | U | 203 | 9YF | C10-C11-C12-C13 |
| 18 | T | 206 | 3PE | C26-C27-C28-C29 |
| 19 | O | 602 | SMA | C11-C12-C13-C24 |
| 22 | B | 607 | LYC | C57-C56-C58-C59 |
| 21 | V | 201 | CDL | C19-C20-C21-C22 |
| 18 | F | 301 | 3PE | C32-C33-C34-C35 |
| 21 | S | 302 | CDL | C19-C20-C21-C22 |
| 21 | T | 204 | CDL | C16-C17-C18-C19 |
| 21 | T | 204 | CDL | C73-C74-C75-C76 |
| 23 | B | 608 | LMT | C6-C7-C8-C9 |
| 25 | Q | 601 | HAS | C2D-C3D-CAD-CBD |
| 25 | Q | 602 | HAS | C2D-C3D-CAD-CBD |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 21 | S | 302 | CDL | CB7-C71-C72-C73 |
| 21 | S | 302 | CDL | C31-C32-C33-C34 |
| 18 | F | 301 | 3PE | C11-O13-P-O11 |
| 18 | L | 101 | 3PE | C1-O11-P-O13 |
| 18 | R | 405 | 3PE | C1-O11-P-O13 |
| 18 | T | 202 | 3PE | C11-O13-P-O11 |
| 18 | T | 205 | 3PE | C1-O11-P-O13 |
| 21 | D | 608 | CDL | CA2-OA2-PA1-OA5 |
| 21 | F | 302 | CDL | CA2-OA2-PA1-OA5 |
| 18 | T | 205 | 3PE | C26-C27-C28-C29 |
| 17 | A | 504 | MQ9 | C15-C14-C16-C17 |
| 18 | T | 202 | 3PE | O31-C31-C32-C33 |
| 18 | Q | 609 | 3PE | C2-C1-O11-P |
| 18 | T | 203 | 3PE | C2-C1-O11-P |
| 21 | O | 606 | CDL | CB4-CB3-OB5-PB2 |
| 21 | V | 201 | CDL | C13-C14-C15-C16 |
| 18 | A | 505 | 3PE | O32-C31-O31-C3 |
| 18 | A | 505 | 3PE | C1-O11-P-O12 |
| 18 | C | 304 | 3PE | C11-O13-P-O12 |
| 18 | C | 304 | 3PE | C11-O13-P-O14 |
| 18 | F | 301 | 3PE | C1-O11-P-O12 |
| 18 | F | 301 | 3PE | C1-O11-P-O14 |
| 18 | F | 301 | 3PE | C11-O13-P-O12 |
| 18 | J | 201 | 3PE | C11-O13-P-O14 |
| 18 | L | 101 | 3PE | C1-O11-P-O12 |
| 18 | L | 101 | 3PE | C11-O13-P-O12 |
| 18 | P | 303 | 3PE | C11-O13-P-O14 |
| 18 | Q | 609 | 3PE | C11-O13-P-O12 |
| 18 | T | 202 | 3PE | C1-O11-P-O14 |
| 18 | T | 205 | 3PE | C11-O13-P-O14 |
| 21 | B | 605 | CDL | CA3-OA5-PA1-OA3 |
| 21 | B | 609 | CDL | CA3-OA5-PA1-OA3 |
| 21 | D | 607 | CDL | CA2-OA2-PA1-OA3 |
| 21 | D | 608 | CDL | CA3-OA5-PA1-OA3 |
| 21 | D | 608 | CDL | CA3-OA5-PA1-OA4 |
| 21 | D | 608 | CDL | CB2-OB2-PB2-OB4 |
| 21 | F | 302 | CDL | CB3-OB5-PB2-OB4 |
| 21 | G | 201 | CDL | CA2-OA2-PA1-OA4 |
| 21 | G | 201 | CDL | CA3-OA5-PA1-OA3 |
| 21 | G | 201 | CDL | CA3-OA5-PA1-OA4 |
| 21 | G | 202 | CDL | CA2-OA2-PA1-OA4 |
| 21 | G | 202 | CDL | CB3-OB5-PB2-OB3 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 21 | G | 202 | CDL | CB3-OB5-PB2-OB4 |
| 21 | I | 201 | CDL | CA2-OA2-PA1-OA4 |
| 21 | O | 606 | CDL | CB2-OB2-PB2-OB4 |
| 21 | O | 606 | CDL | CB3-OB5-PB2-OB4 |
| 21 | Q | 607 | CDL | CA2-OA2-PA1-OA3 |
| 21 | Q | 607 | CDL | CA2-OA2-PA1-OA4 |
| 21 | Q | 607 | CDL | CA3-OA5-PA1-OA3 |
| 21 | Q | 608 | CDL | CA2-OA2-PA1-OA3 |
| 21 | S | 302 | CDL | CA3-OA5-PA1-OA4 |
| 21 | T | 201 | CDL | CA2-OA2-PA1-OA4 |
| 21 | T | 201 | CDL | CA3-OA5-PA1-OA4 |
| 21 | T | 201 | CDL | CB3-OB5-PB2-OB3 |
| 21 | T | 204 | CDL | CB2-OB2-PB2-OB4 |
| 21 | T | 204 | CDL | CB3-OB5-PB2-OB4 |
| 21 | V | 201 | CDL | CA2-OA2-PA1-OA3 |
| 21 | V | 201 | CDL | CA3-OA5-PA1-OA3 |
| 21 | V | 201 | CDL | CB2-OB2-PB2-OB3 |
| 21 | V | 201 | CDL | CB2-OB2-PB2-OB4 |
| 21 | V | 201 | CDL | CB3-OB5-PB2-OB3 |
| 16 | A | 503 | 9YF | C24-C-C1-O |
| 18 | C | 304 | 3PE | O11-C1-C2-C3 |
| 18 | P | 303 | 3PE | O11-C1-C2-C3 |
| 18 | R | 405 | 3PE | O11-C1-C2-C3 |
| 18 | T | 205 | 3PE | O11-C1-C2-C3 |
| 21 | D | 608 | CDL | OB5-CB3-CB4-CB6 |
| 21 | F | 302 | CDL | OB5-CB3-CB4-CB6 |
| 21 | Q | 608 | CDL | OA5-CA3-CA4-CA6 |
| 21 | S | 302 | CDL | OA5-CA3-CA4-CA6 |
| 21 | T | 201 | CDL | OA5-CA3-CA4-CA6 |
| 18 | P | 303 | 3PE | C24-C25-C26-C27 |
| 33 | H | 204 | IX7 | C36-C37-C38-C39 |
| 18 | T | 203 | 3PE | C27-C28-C29-C2A |
| 21 | D | 608 | CDL | C51-CB5-OB6-CB4 |
| 18 | W | 201 | 3PE | C2B-C2C-C2D-C2E |
| 18 | F | 301 | 3PE | C12-C11-O13-P |
| 18 | Q | 609 | 3PE | C12-C11-O13-P |
| 18 | R | 405 | 3PE | C12-C11-O13-P |
| 18 | T | 206 | 3PE | C12-C11-O13-P |
| 18 | W | 201 | 3PE | C12-C11-O13-P |
| 21 | G | 202 | CDL | C72-C71-CB7-OB8 |
| 21 | V | 201 | CDL | C14-C15-C16-C17 |
| 16 | A | 503 | 9YF | O9-C-C1-O |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 18 | F | 301 | 3PE | O11-C1-C2-O21 |
| 18 | T | 203 | 3PE | O11-C1-C2-O21 |
| 18 | W | 201 | 3PE | O11-C1-C2-O21 |
| 21 | B | 605 | CDL | OB5-CB3-CB4-OB6 |
| 21 | D | 608 | CDL | OB5-CB3-CB4-OB6 |
| 21 | G | 201 | CDL | CB7-C71-C72-C73 |
| 21 | S | 302 | CDL | OA5-CA3-CA4-OA6 |
| 33 | U | 204 | IX7 | O16-C31-C32-O19 |
| 21 | T | 204 | CDL | C72-C73-C74-C75 |
| 32 | U | 202 | PLM | C5-C6-C7-C8 |
| 18 | J | 201 | 3PE | C33-C34-C35-C36 |
| 21 | V | 201 | CDL | C33-C34-C35-C36 |
| 21 | D | 608 | CDL | CB4-CB6-OB8-CB7 |
| 16 | A | 503 | 9YF | C1-C-C24-O11 |
| 21 | D | 608 | CDL | OB7-CB5-OB6-CB4 |
| 21 | S | 302 | CDL | OA6-CA4-CA6-OA8 |
| 21 | S | 302 | CDL | C32-C33-C34-C35 |
| 23 | B | 608 | LMT | C2-C3-C4-C5 |
| 21 | S | 302 | CDL | C1-CA2-OA2-PA1 |
| 21 | T | 201 | CDL | C1-CA2-OA2-PA1 |
| 17 | A | 504 | MQ9 | C12-C11-C9-C10 |
| 18 | F | 301 | 3PE | C32-C31-O31-C3 |
| 21 | Q | 607 | CDL | C14-C15-C16-C17 |
| 15 | N | 504 | IZL | C63-C64-C65-C66 |
| 21 | V | 201 | CDL | C22-C23-C24-C25 |
| 21 | T | 201 | CDL | C40-C41-C42-C43 |
| 22 | B | 607 | LYC | C62-C61-C63-C64 |
| 17 | A | 504 | MQ9 | C13-C14-C16-C17 |
| 21 | T | 201 | CDL | C72-C71-CB7-OB8 |
| 18 | L | 101 | 3PE | C25-C26-C27-C28 |
| 18 | J | 201 | 3PE | C3-C2-O21-C21 |
| 18 | P | 303 | 3PE | C3-C2-O21-C21 |
| 21 | D | 608 | CDL | CB6-CB4-OB6-CB5 |
| 21 | F | 302 | CDL | CB3-CB4-OB6-CB5 |
| 33 | U | 204 | IX7 | O16-C31-C32-C33 |
| 18 | R | 405 | 3PE | C2-C1-O11-P |
| 21 | B | 606 | CDL | OB5-CB3-CB4-OB6 |
| 18 | A | 505 | 3PE | O22-C21-O21-C2 |
| 15 | A | 502 | IZL | O8-C19-O7-C18 |
| 25 | Q | 602 | HAS | C3D-CAD-CBD-CGD |
| 21 | G | 202 | CDL | C52-C51-CB5-OB6 |
| 18 | S | 301 | 3PE | O21-C2-C3-O31 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 33 | H | 204 | IX7 | O19-C32-C33-O17 |
| 18 | F | 301 | 3PE | C23-C24-C25-C26 |
| 21 | G | 202 | CDL | C72-C73-C74-C75 |
| 18 | A | 505 | 3PE | C11-O13-P-O11 |
| 18 | C | 303 | 3PE | C11-O13-P-O11 |
| 18 | T | 206 | 3PE | C11-O13-P-O11 |
| 21 | B | 605 | CDL | CB2-OB2-PB2-OB5 |
| 21 | B | 606 | CDL | CA3-OA5-PA1-OA2 |
| 21 | B | 609 | CDL | CA2-OA2-PA1-OA5 |
| 21 | O | 606 | CDL | CA3-OA5-PA1-OA2 |
| 21 | S | 302 | CDL | CA2-OA2-PA1-OA5 |
| 21 | T | 204 | CDL | CB3-OB5-PB2-OB2 |
| 33 | H | 204 | IX7 | C61-C62-C63-C64 |
| 19 | O | 602 | SMA | C13-C14-C15-C16 |
| 17 | A | 504 | MQ9 | C30-C29-C31-C32 |
| 21 | T | 201 | CDL | C11-C12-C13-C14 |
| 21 | F | 302 | CDL | C13-C14-C15-C16 |
| 21 | B | 606 | CDL | CA4-CA3-OA5-PA1 |
| 21 | O | 606 | CDL | CA4-CA3-OA5-PA1 |
| 15 | N | 504 | IZL | C55-C56-C58-C59 |
| 21 | G | 201 | CDL | C23-C24-C25-C26 |
| 18 | S | 301 | 3PE | C2C-C2D-C2E-C2F |
| 21 | D | 607 | CDL | C17-C18-C19-C20 |
| 16 | H | 203 | 9YF | O12-C25-O11-C24 |
| 21 | T | 204 | CDL | CB7-C71-C72-C73 |
| 21 | G | 201 | CDL | C16-C17-C18-C19 |
| 15 | N | 504 | IZL | O31-C44-C45-O34 |
| 21 | G | 201 | CDL | OA5-CA3-CA4-OA6 |
| 21 | Q | 608 | CDL | OA5-CA3-CA4-OA6 |
| 23 | O | 601 | LMT | O5B-C1B-O1B-C4' |
| 21 | O | 606 | CDL | C12-C11-CA5-OA7 |
| 33 | U | 204 | IX7 | C60-C61-C62-C63 |
| 21 | D | 607 | CDL | C11-C12-C13-C14 |
| 18 | D | 609 | 3PE | O21-C2-C3-O31 |
| 21 | O | 606 | CDL | OA6-CA4-CA6-OA8 |
| 18 | A | 505 | 3PE | C34-C35-C36-C37 |
| 21 | G | 201 | CDL | C11-C12-C13-C14 |
| 21 | G | 201 | CDL | C72-C73-C74-C75 |
| 33 | U | 204 | IX7 | O8-C24-O7-C23 |
| 21 | D | 607 | CDL | C32-C33-C34-C35 |
| 21 | D | 607 | CDL | C75-C76-C77-C78 |
| 21 | I | 201 | CDL | C21-C22-C23-C24 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 21 | I | 201 | CDL | C19-C20-C21-C22 |
| 21 | T | 204 | CDL | CA3-CA4-CA6-OA8 |
| 21 | T | 204 | CDL | CB3-CB4-CB6-OB8 |
| 21 | S | 302 | CDL | OB7-CB5-OB6-CB4 |
| 18 | A | 505 | 3PE | C22-C23-C24-C25 |
| 15 | N | 504 | IZL | C43-O28-P-O30 |
| 18 | C | 303 | 3PE | C22-C23-C24-C25 |
| 33 | U | 204 | IX7 | C30-C23-O7-C24 |
| 33 | H | 204 | IX7 | C60-C61-C62-C63 |
| 18 | Q | 609 | 3PE | C3-C2-O21-C21 |
| 21 | I | 201 | CDL | CB6-CB4-OB6-CB5 |
| 21 | Q | 608 | CDL | CB6-CB4-OB6-CB5 |
| 21 | V | 201 | CDL | CB3-CB4-OB6-CB5 |
| 18 | A | 505 | 3PE | C21-C22-C23-C24 |
| 18 | R | 405 | 3PE | O31-C31-C32-C33 |
| 21 | B | 609 | CDL | C52-C51-CB5-OB6 |
| 21 | Q | 608 | CDL | CB5-C51-C52-C53 |
| 15 | A | 502 | IZL | O-C10-O1-C11 |
| 18 | F | 301 | 3PE | O32-C31-O31-C3 |
| 21 | B | 605 | CDL | C53-C54-C55-C56 |
| 31 | Z | 201 | DGA | CA3-CA4-CA5-CA6 |
| 21 | B | 609 | CDL | CA4-CA3-OA5-PA1 |
| 33 | H | 204 | IX7 | C11-C12-C13-C14 |
| 18 | J | 201 | 3PE | C25-C26-C27-C28 |
| 18 | R | 405 | 3PE | O32-C31-C32-C33 |
| 21 | Q | 608 | CDL | C23-C24-C25-C26 |
| 21 | D | 607 | CDL | OB5-CB3-CB4-CB6 |
| 16 | H | 203 | 9YF | C27-C28-C29-C30 |
| 17 | A | 504 | MQ9 | C28-C29-C31-C32 |
| 21 | S | 302 | CDL | O1-C1-CB2-OB2 |
| 18 | Q | 609 | 3PE | C2E-C2F-C2G-C2H |
| 21 | B | 605 | CDL | C34-C35-C36-C37 |
| 16 | A | 503 | 9YF | C9-C10-C11-C12 |
| 33 | H | 204 | IX7 | C32-C33-O17-C34 |
| 18 | J | 201 | 3PE | C37-C38-C39-C3A |
| 18 | S | 301 | 3PE | C37-C38-C39-C3A |
| 17 | A | 504 | MQ9 | C9-C11-C12-C13 |
| 21 | Q | 607 | CDL | CA2-C1-CB2-OB2 |
| 18 | T | 203 | 3PE | C21-C22-C23-C24 |
| 25 | Q | 601 | HAS | C27-C19-C20-C21 |
| 18 | J | 201 | 3PE | C29-C2A-C2B-C2C |
| 21 | O | 606 | CDL | C12-C13-C14-C15 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 21 | Q | 607 | CDL | C37-C38-C39-C40 |
| 33 | U | 204 | IX7 | C10-C11-C12-C13 |
| 23 | O | 601 | LMT | C3-C4-C5-C6 |
| 21 | G | 202 | CDL | C35-C36-C37-C38 |
| 33 | H | 204 | IX7 | O18-C34-O17-C33 |
| 18 | D | 609 | 3PE | O21-C21-C22-C23 |
| 21 | B | 609 | CDL | C14-C15-C16-C17 |
| 17 | N | 501 | MQ9 | C15-C14-C16-C17 |
| 25 | D | 602 | HAS | C25-C23-C24-C28 |
| 15 | A | 502 | IZL | C15-C14-O3-C13 |
| 22 | B | 607 | LYC | C60-C61-C63-C64 |
| 18 | W | 201 | 3PE | C34-C35-C36-C37 |
| 33 | U | 204 | IX7 | C29-C24-O7-C23 |
| 18 | C | 303 | 3PE | O11-C1-C2-O21 |
| 15 | N | 504 | IZL | C57-C56-C58-C59 |
| 20 | O | 603 | HEM | C2A-CAA-CBA-CGA |
| 18 | N | 502 | 3PE | O21-C21-C22-C23 |
| 19 | O | 602 | SMA | O12-C12-C13-C24 |
| 33 | H | 204 | IX7 | C59-C60-C61-C62 |
| 32 | U | 202 | PLM | C4-C5-C6-C7 |
| 18 | C | 303 | 3PE | O11-C1-C2-C3 |
| 18 | N | 502 | 3PE | O11-C1-C2-C3 |
| 21 | O | 606 | CDL | OA5-CA3-CA4-CA6 |
| 21 | Q | 607 | CDL | C72-C71-CB7-OB8 |
| 21 | V | 201 | CDL | C20-C21-C22-C23 |
| 33 | U | 204 | IX7 | O2-C18-O3-C19 |
| 18 | P | 303 | 3PE | O21-C21-C22-C23 |
| 18 | T | 205 | 3PE | O21-C21-C22-C23 |
| 21 | G | 201 | CDL | CB3-OB5-PB2-OB2 |
| 25 | Q | 601 | HAS | C18-C19-C20-C21 |
| 16 | A | 503 | 9YF | O9-C8-C9-C10 |
| 18 | J | 201 | 3PE | O31-C31-C32-C33 |
| 15 | A | 502 | IZL | C54-C55-C56-C57 |
| 21 | D | 607 | CDL | C37-C38-C39-C40 |
| 18 | R | 405 | 3PE | O21-C21-C22-C23 |
| 21 | Q | 607 | CDL | C52-C51-CB5-OB6 |
| 17 | O | 605 | MQ9 | C16-C17-C18-C19 |
| 18 | T | 206 | 3PE | C1-C2-O21-C21 |
| 21 | D | 607 | CDL | CB3-CB4-OB6-CB5 |
| 18 | S | 301 | 3PE | C27-C28-C29-C2A |
| 19 | B | 601 | SMA | C15-C16-C17-C18 |
| 21 | F | 302 | CDL | C12-C13-C14-C15 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 21 | V | 201 | CDL | C44-C45-C46-C47 |
| 25 | D | 602 | HAS | C22-C23-C24-C28 |
| 31 | R | 404 | DGA | OG1-CA1-CA2-CA3 |
| 18 | W | 201 | 3PE | C23-C24-C25-C26 |
| 21 | S | 302 | CDL | CA3-CA4-CA6-OA8 |
| 15 | N | 504 | IZL | C71-C13-O3-C14 |
| 21 | F | 302 | CDL | OA5-CA3-CA4-OA6 |
| 17 | O | 605 | MQ9 | C11-C12-C13-C14 |
| 21 | G | 201 | CDL | C72-C71-CB7-OB8 |
| 21 | T | 201 | CDL | C32-C31-CA7-OA8 |
| 21 | I | 201 | CDL | C14-C15-C16-C17 |
| 21 | D | 607 | CDL | C12-C11-CA5-OA6 |
| 18 | T | 206 | 3PE | O31-C31-C32-C33 |
| 31 | Z | 201 | DGA | OG2-CB1-CB2-CB3 |
| 21 | B | 606 | CDL | OA6-CA4-CA6-OA8 |
| 21 | Q | 607 | CDL | OB6-CB4-CB6-OB8 |
| 33 | U | 204 | IX7 | O19-C32-C33-O17 |
| 18 | Q | 609 | 3PE | C2D-C2E-C2F-C2G |
| 18 | J | 201 | 3PE | O21-C21-C22-C23 |
| 21 | T | 204 | CDL | C12-C11-CA5-OA6 |
| 21 | F | 302 | CDL | C71-C72-C73-C74 |
| 21 | D | 608 | CDL | C72-C71-CB7-OB8 |
| 18 | T | 205 | 3PE | C34-C35-C36-C37 |
| 18 | J | 201 | 3PE | C2A-C2B-C2C-C2D |
| 21 | O | 606 | CDL | C31-CA7-OA8-CA6 |
| 18 | T | 206 | 3PE | O32-C31-C32-C33 |
| 21 | T | 201 | CDL | C32-C31-CA7-OA9 |
| 21 | Q | 607 | CDL | C51-CB5-OB6-CB4 |
| 25 | Q | 601 | HAS | C24-C28-C29-C30 |
| 23 | B | 608 | LMT | O5B-C5B-C6B-O6B |
| 18 | P | 303 | 3PE | O22-C21-C22-C23 |
| 18 | R | 405 | 3PE | O22-C21-C22-C23 |
| 21 | G | 201 | CDL | C51-C52-C53-C54 |
| 21 | T | 201 | CDL | C52-C51-CB5-OB6 |
| 31 | M | 201 | DGA | OG2-CB1-CB2-CB3 |
| 21 | T | 204 | CDL | C52-C53-C54-C55 |
| 21 | Q | 608 | CDL | CB2-C1-CA2-OA2 |
| 25 | D | 602 | HAS | C2D-C3D-CAD-CBD |
| 17 | A | 504 | MQ9 | C21-C22-C23-C24 |
| 21 | D | 607 | CDL | C73-C74-C75-C76 |
| 31 | Z | 201 | DGA | OB1-CB1-CB2-CB3 |
| 21 | I | 201 | CDL | C12-C11-CA5-OA6 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 21 | T | 201 | CDL | C23-C24-C25-C26 |
| 31 | Z | 201 | DGA | CA7-CA8-CA9-CAA |
| 33 | H | 204 | IX7 | C63-C64-C65-C66 |
| 21 | T | 201 | CDL | C32-C33-C34-C35 |
| 21 | Q | 607 | CDL | O1-C1-CB2-OB2 |
| 21 | Q | 607 | CDL | C72-C71-CB7-OB9 |
| 21 | B | 609 | CDL | C78-C79-C80-C81 |
| 31 | Z | 201 | DGA | CG1-CG2-OG2-CB1 |
| 18 | F | 301 | 3PE | C2-C1-O11-P |
| 21 | B | 609 | CDL | C1-CB2-OB2-PB2 |
| 18 | W | 201 | 3PE | C3C-C3D-C3E-C3F |
| 18 | J | 201 | 3PE | O32-C31-C32-C33 |
| 15 | N | 504 | IZL | C61-C62-C63-C64 |
| 18 | T | 205 | 3PE | C36-C37-C38-C39 |
| 18 | R | 405 | 3PE | C1-O11-P-O12 |
| 18 | T | 203 | 3PE | C11-O13-P-O14 |
| 18 | T | 205 | 3PE | C1-O11-P-O12 |
| 18 | T | 206 | 3PE | C1-O11-P-O14 |
| 21 | B | 606 | CDL | CA3-OA5-PA1-OA3 |
| 21 | D | 607 | CDL | CB3-OB5-PB2-OB4 |
| 16 | A | 503 | 9YF | O10-C8-C9-C10 |
| 21 | Q | 607 | CDL | C52-C51-CB5-OB7 |
| 31 | R | 404 | DGA | OA1-CA1-CA2-CA3 |
| 18 | Q | 609 | 3PE | O13-C11-C12-N |
| 18 | T | 205 | 3PE | O22-C21-C22-C23 |
| 21 | G | 201 | CDL | C72-C71-CB7-OB9 |
| 21 | T | 204 | CDL | C12-C11-CA5-OA7 |
| 18 | T | 202 | 3PE | O32-C31-C32-C33 |
| 21 | D | 607 | CDL | C12-C11-CA5-OA7 |
| 17 | A | 504 | MQ9 | C36-C37-C38-C39 |
| 15 | A | 502 | IZL | C44-C45-O34-C60 |
| 18 | T | 202 | 3PE | C12-C11-O13-P |
| 18 | T | 203 | 3PE | C12-C11-O13-P |
| 21 | D | 607 | CDL | CB6-CB4-OB6-CB5 |
| 21 | F | 302 | CDL | CB6-CB4-OB6-CB5 |
| 33 | U | 204 | IX7 | C56-C57-C58-C59 |
| 21 | T | 201 | CDL | C52-C51-CB5-OB7 |
| 18 | J | 201 | 3PE | C27-C28-C29-C2A |
| 21 | B | 605 | CDL | CA5-C11-C12-C13 |
| 21 | Q | 608 | CDL | C13-C14-C15-C16 |
| 15 | N | 504 | IZL | O34-C60-C61-C62 |
| 18 | Q | 609 | 3PE | C24-C25-C26-C27 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 15 | N | 504 | IZL | O35-C60-C61-C62 |
| 21 | S | 302 | CDL | C52-C51-CB5-OB6 |
| 21 | I | 201 | CDL | C12-C11-CA5-OA7 |
| 21 | O | 606 | CDL | C52-C51-CB5-OB7 |
| 21 | S | 302 | CDL | C12-C11-CA5-OA7 |
| 18 | Q | 609 | 3PE | C2C-C2D-C2E-C2F |
| 21 | B | 606 | CDL | C52-C51-CB5-OB6 |
| 21 | D | 608 | CDL | C72-C71-CB7-OB9 |
| 31 | M | 201 | DGA | OB1-CB1-CB2-CB3 |
| 15 | N | 504 | IZL | O2-C13-O3-C14 |
| 21 | T | 201 | CDL | C51-C52-C53-C54 |
| 18 | L | 101 | 3PE | O21-C21-C22-C23 |
| 21 | O | 606 | CDL | C52-C51-CB5-OB6 |
| 21 | S | 302 | CDL | C12-C11-CA5-OA6 |
| 21 | S | 302 | CDL | C37-C38-C39-C40 |
| 18 | J | 201 | 3PE | O22-C21-C22-C23 |
| 21 | S | 302 | CDL | C17-C18-C19-C20 |
| 21 | S | 302 | CDL | C52-C51-CB5-OB7 |

There are no ring outliers.

43 monomers are involved in 69 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 21 | T | 201 | CDL | 1 | 0 |
| 21 | G | 201 | CDL | 1 | 0 |
| 31 | H | 201 | DGA | 2 | 0 |
| 31 | M | 201 | DGA | 1 | 0 |
| 17 | N | 501 | MQ9 | 2 | 0 |
| 22 | O | 607 | LYC | 1 | 0 |
| 16 | U | 203 | 9YF | 2 | 0 |
| 24 | P | 302 | HEC | 1 | 0 |
| 18 | A | 505 | 3PE | 1 | 0 |
| 21 | Q | 607 | CDL | 1 | 0 |
| 18 | N | 502 | 3PE | 1 | 0 |
| 18 | P | 303 | 3PE | 2 | 0 |
| 18 | Q | 609 | 3PE | 3 | 0 |
| 20 | O | 604 | HEM | 1 | 0 |
| 15 | A | 502 | IZL | 3 | 0 |
| 25 | Q | 602 | HAS | 2 | 0 |
| 18 | R | 405 | 3PE | 3 | 0 |
| 20 | B | 602 | HEM | 2 | 0 |
| 21 | G | 202 | CDL | 1 | 0 |

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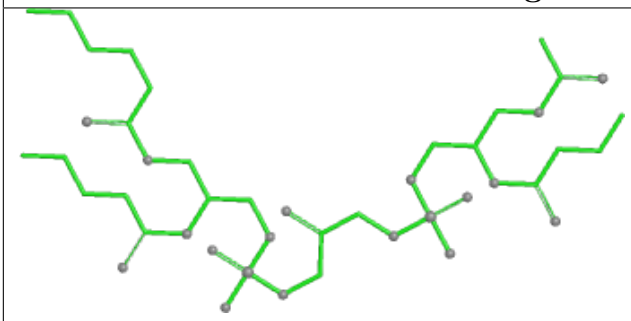
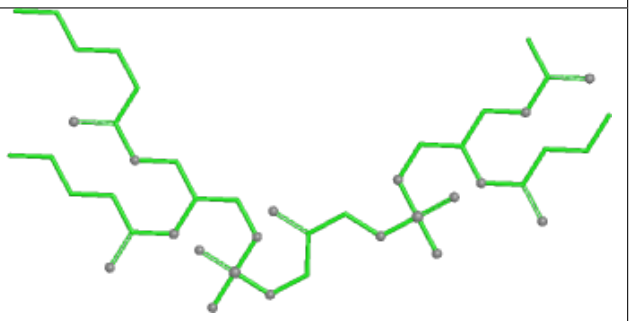
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 20 | O | 603 | HEM | 2 | 0 |
| 18 | C | 303 | 3PE | 2 | 0 |
| 29 | D | 606 | AZI | 2 | 0 |
| 21 | D | 607 | CDL | 1 | 0 |
| 20 | B | 603 | HEM | 1 | 0 |
| 31 | U | 201 | DGA | 3 | 0 |
| 17 | O | 605 | MQ9 | 3 | 0 |
| 33 | U | 204 | IX7 | 2 | 0 |
| 18 | T | 203 | 3PE | 1 | 0 |
| 19 | O | 602 | SMA | 1 | 0 |
| 17 | B | 604 | MQ9 | 3 | 0 |
| 17 | A | 504 | MQ9 | 3 | 0 |
| 33 | H | 204 | IX7 | 2 | 0 |
| 21 | B | 609 | CDL | 1 | 0 |
| 24 | C | 302 | HEC | 1 | 0 |
| 19 | B | 601 | SMA | 1 | 0 |
| 18 | F | 301 | 3PE | 1 | 0 |
| 25 | D | 601 | HAS | 1 | 0 |
| 21 | Q | 608 | CDL | 3 | 0 |
| 25 | Q | 601 | HAS | 2 | 0 |
| 21 | B | 605 | CDL | 1 | 0 |
| 25 | D | 602 | HAS | 4 | 0 |
| 21 | F | 302 | CDL | 1 | 0 |
| 24 | C | 301 | HEC | 1 | 0 |

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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.

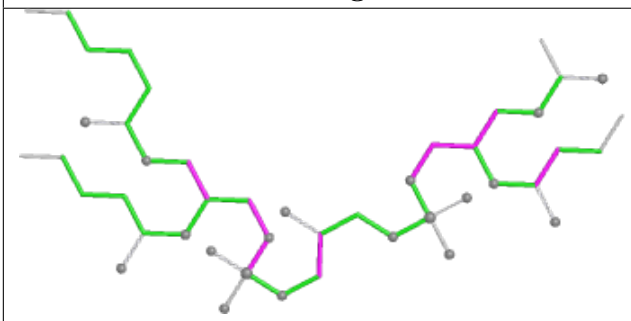
## Ligand CDL B 606



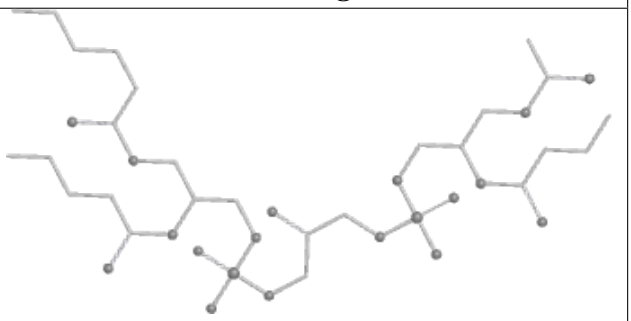
Bond lengths



Bond angles

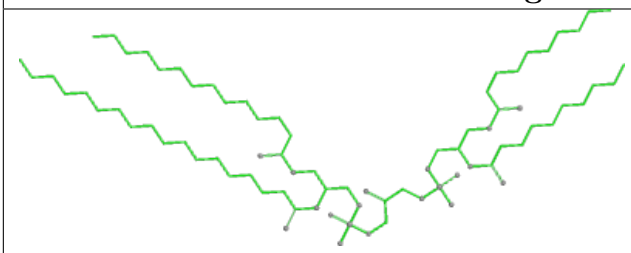


Torsions

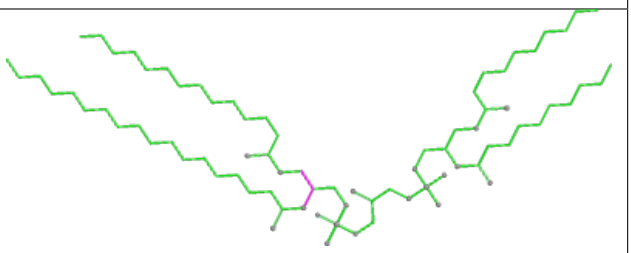


Rings

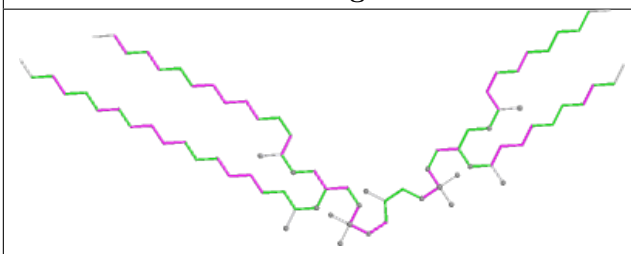
## Ligand CDL T 201



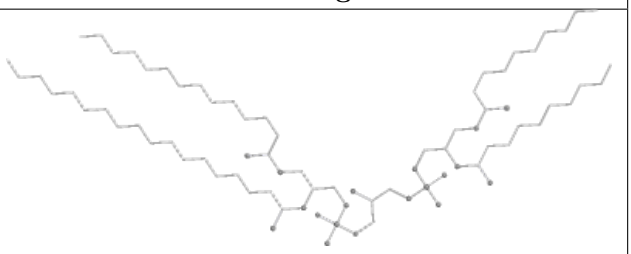
Bond lengths



Bond angles

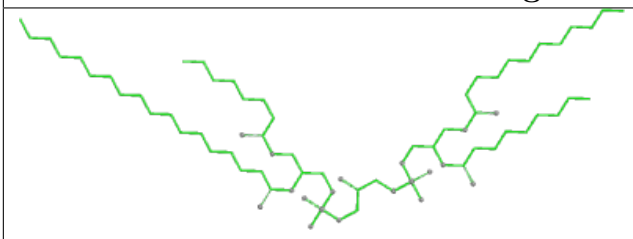


Torsions

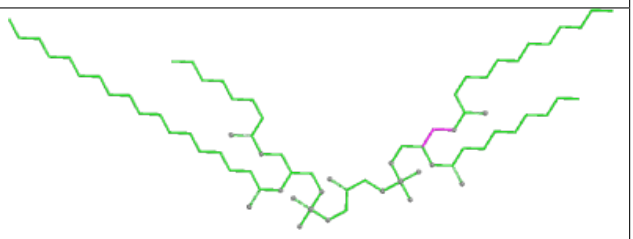


Rings

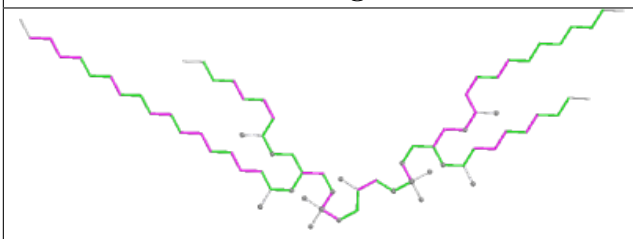
## Ligand CDL G 201



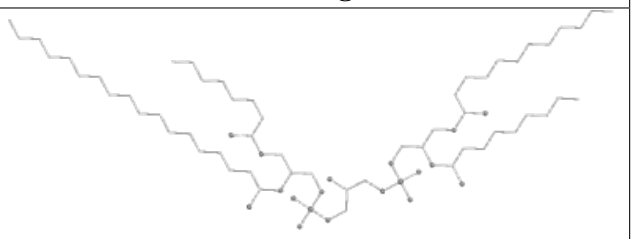
Bond lengths



Bond angles

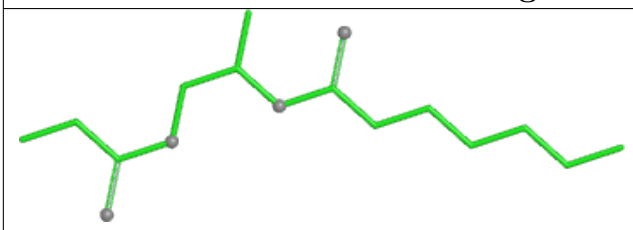


Torsions

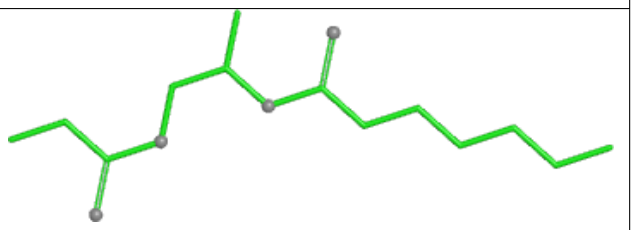


Rings

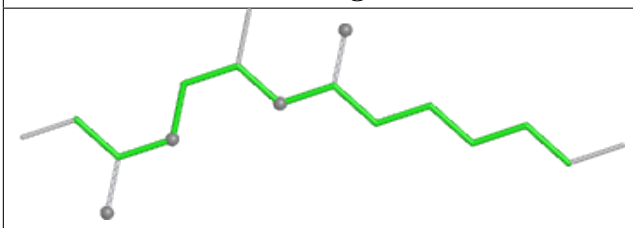
## Ligand DGA H 201



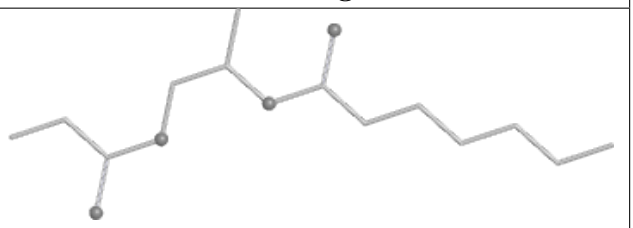
Bond lengths



Bond angles

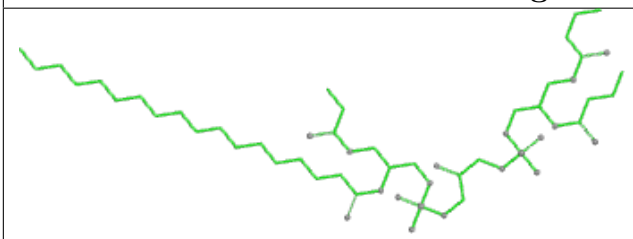


Torsions

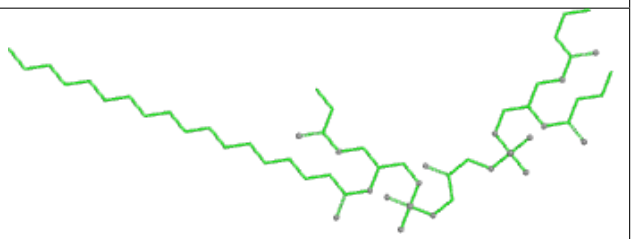


Rings

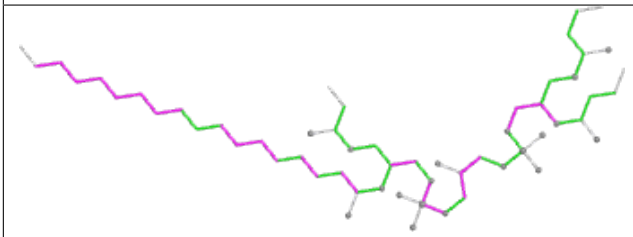
## Ligand CDL I 201



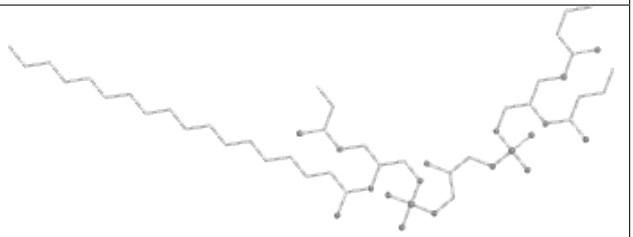
Bond lengths



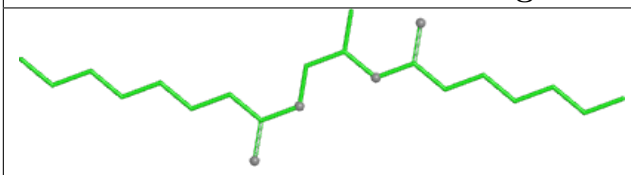
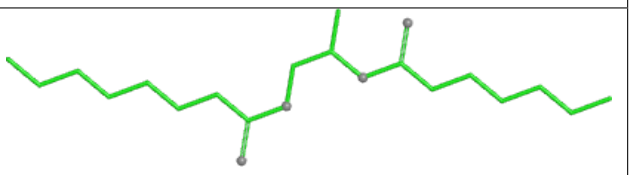
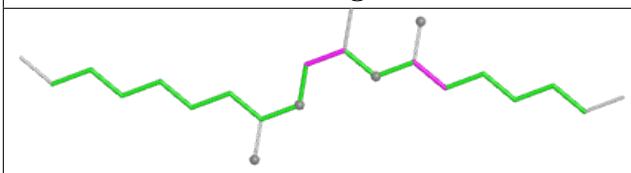
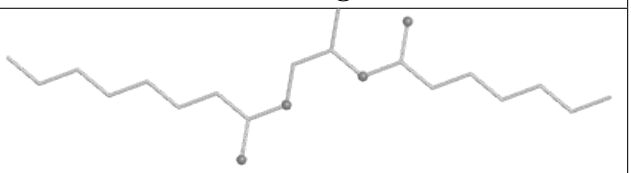
Bond angles

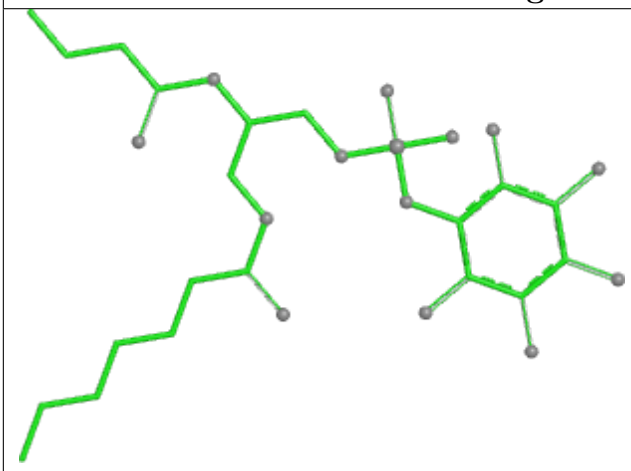
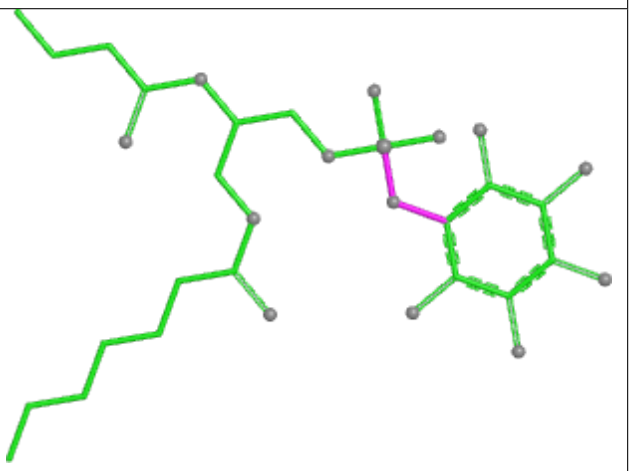
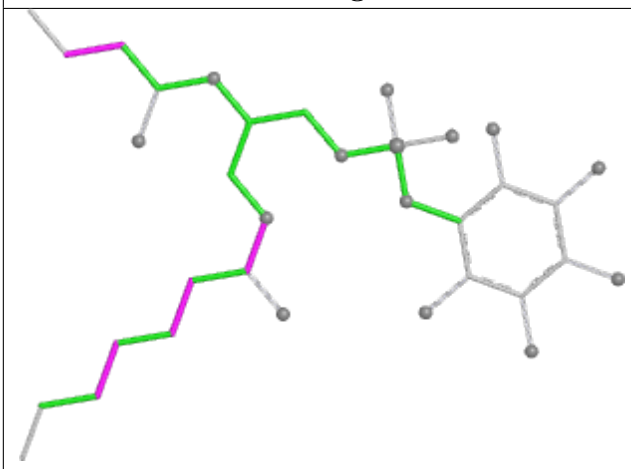
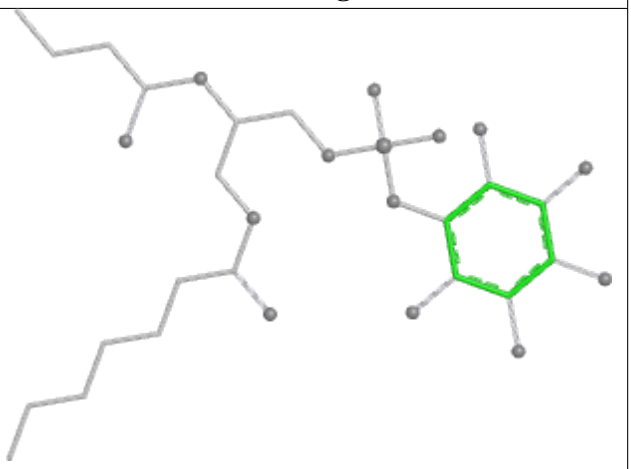


Torsions

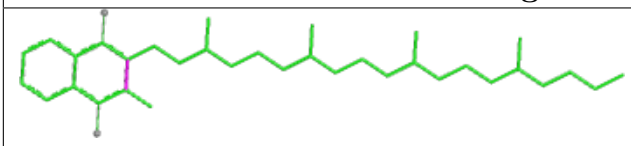


Rings

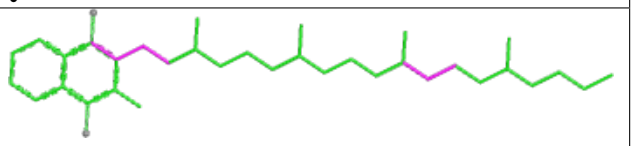
| Ligand DGA M 201 | |
|---|---|
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

| Ligand 9YF H 203 | |
|---|---|
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

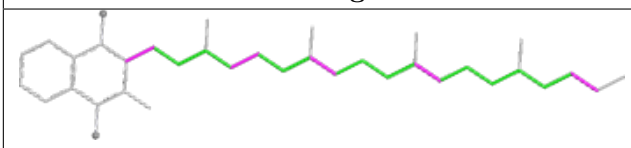
## Ligand MQ9 N 501



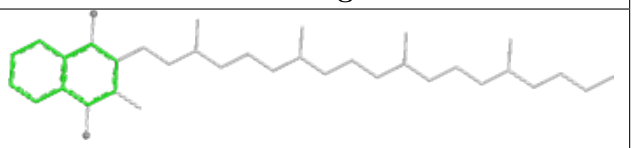
Bond lengths



Bond angles

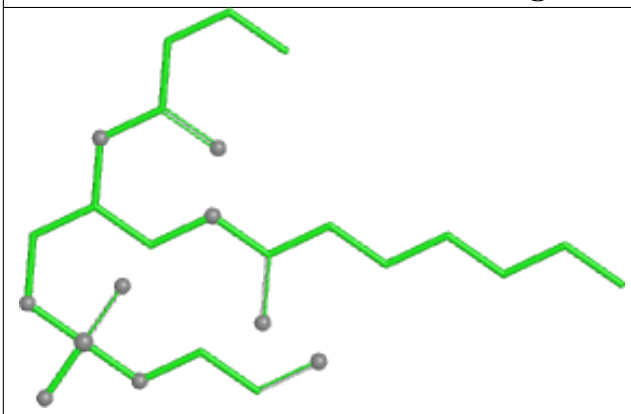


Torsions

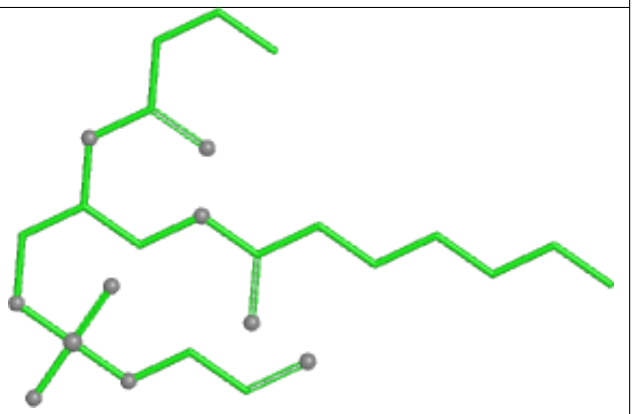


Rings

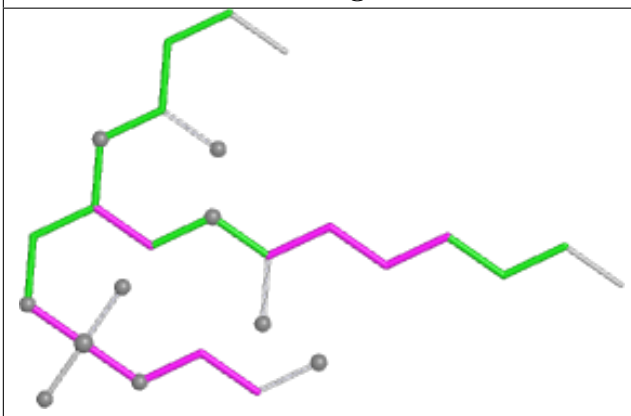
## Ligand 3PE T 202



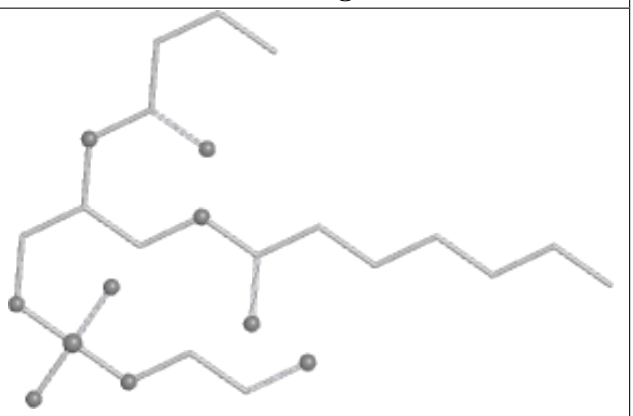
Bond lengths



Bond angles

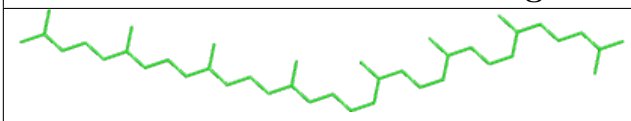


Torsions

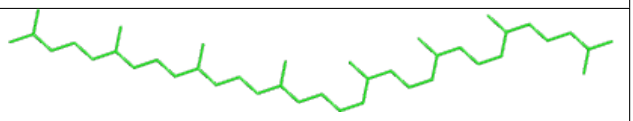


Rings

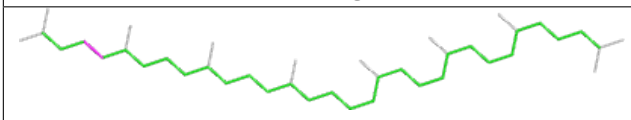
## Ligand LYC O 607



Bond lengths



Bond angles



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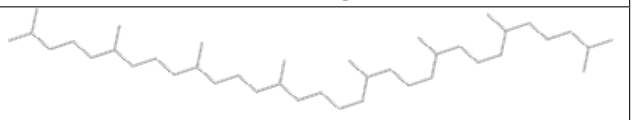
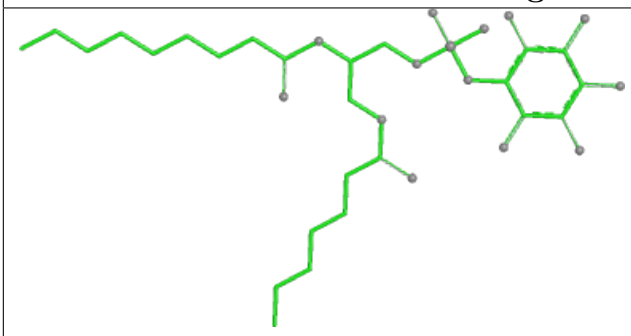
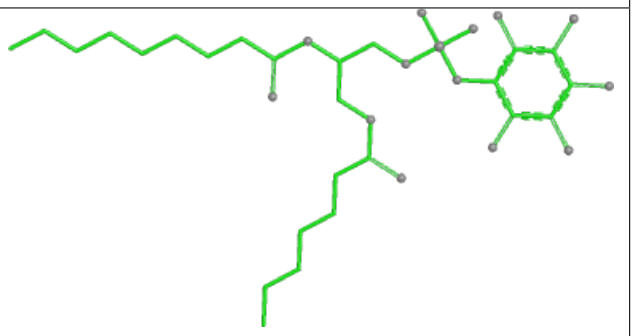


Rings

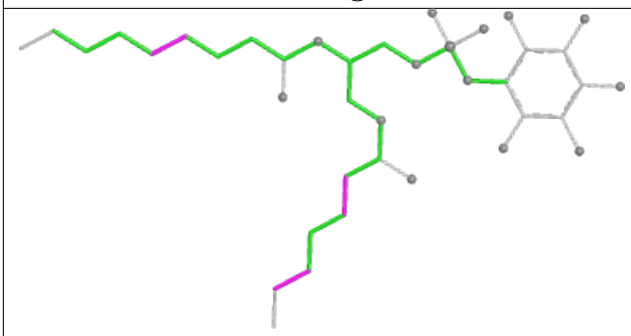
**Ligand 9YF U 203**



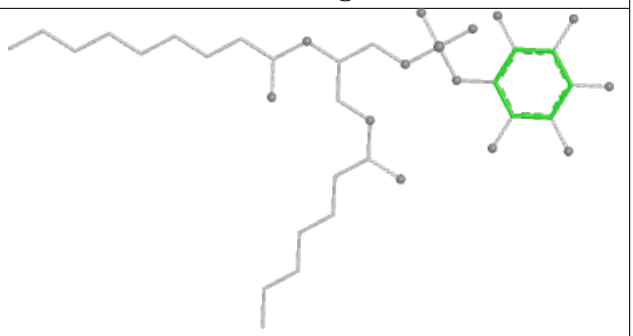
**Bond lengths**



**Bond angles**

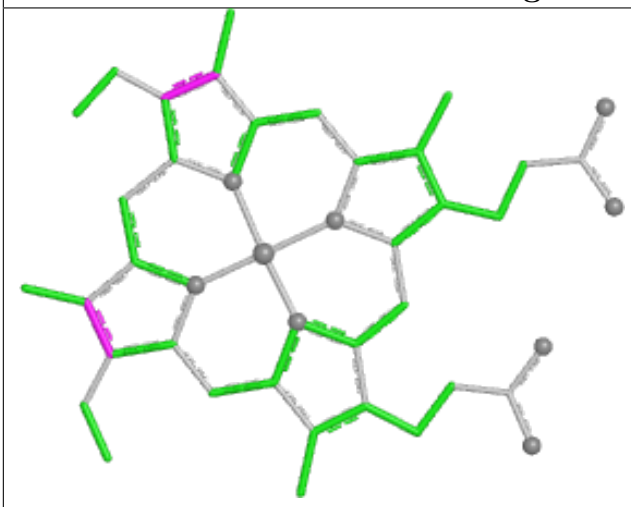


**Torsions**

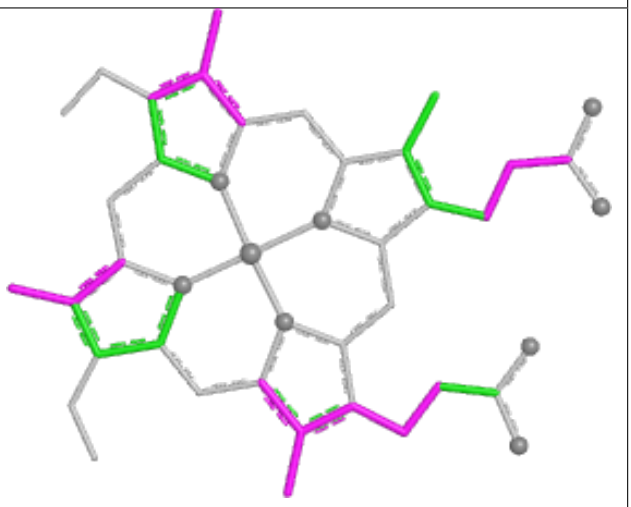


**Rings**

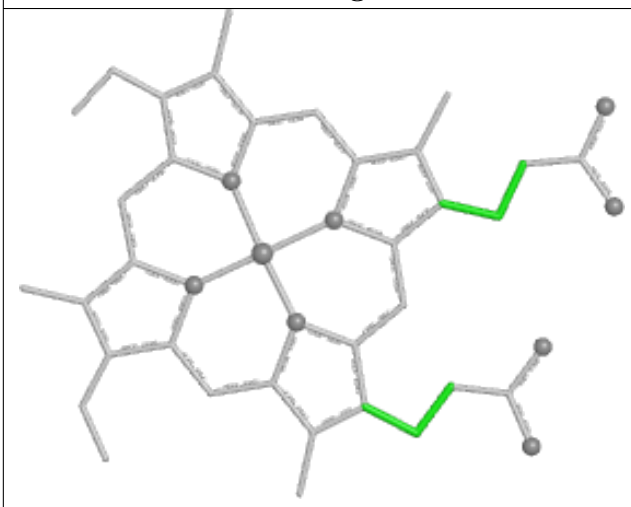
**Ligand HEC P 302**



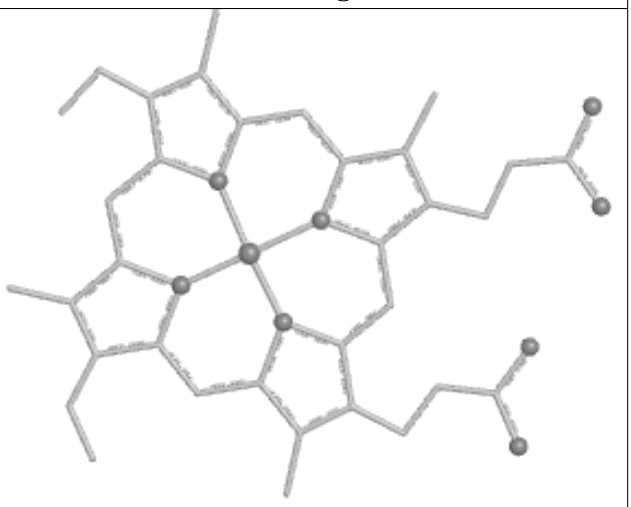
**Bond lengths**



**Bond angles**

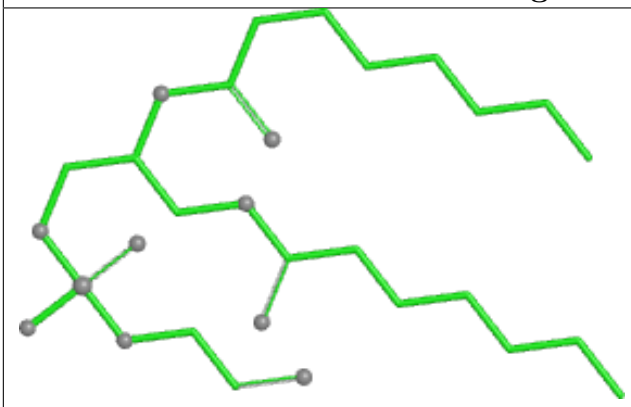


**Torsions**

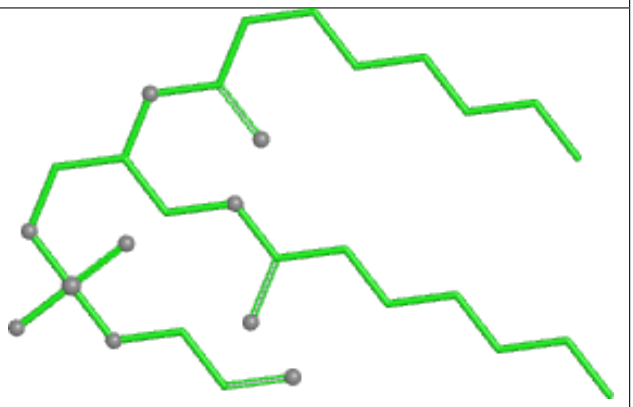


**Rings**

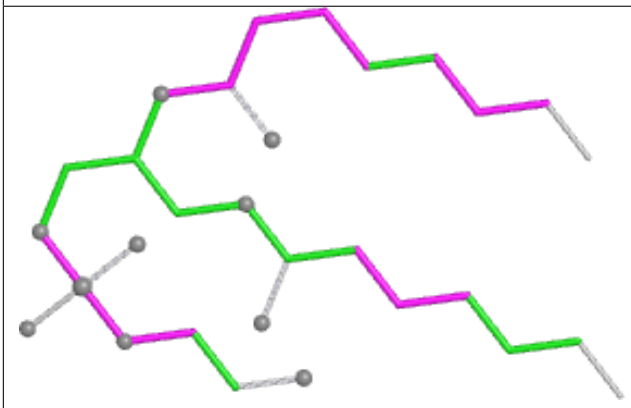
**Ligand 3PE L 101**



Bond lengths



Bond angles



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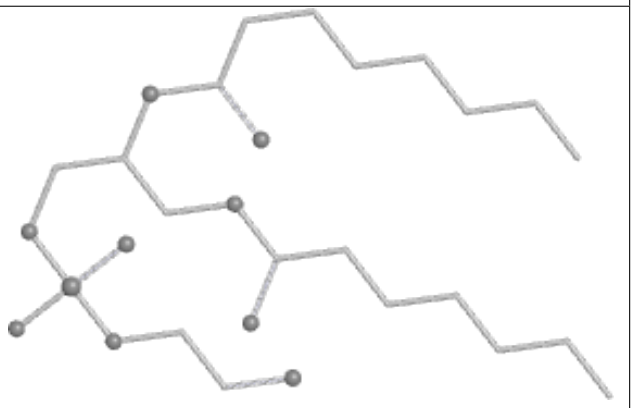
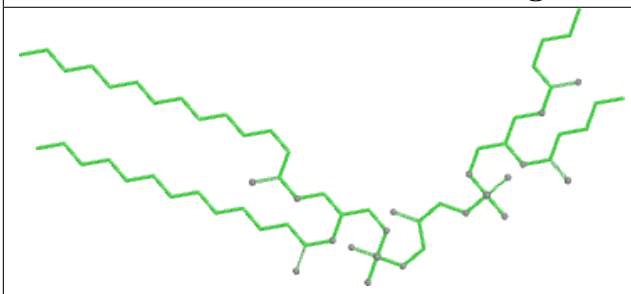


Rings

**Ligand CDL S 302**



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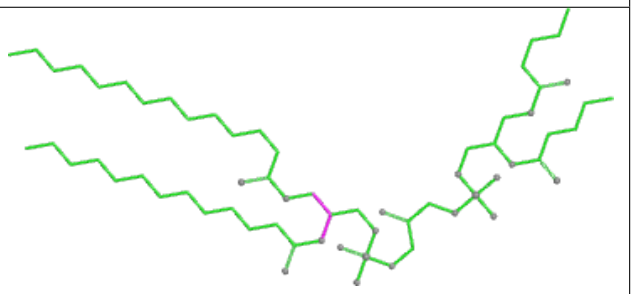
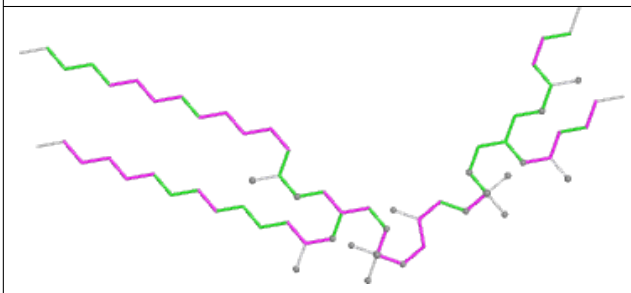


Bond angles



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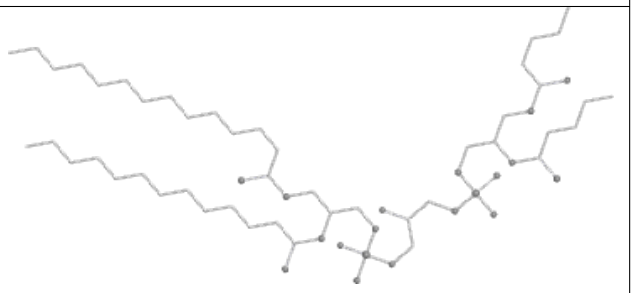
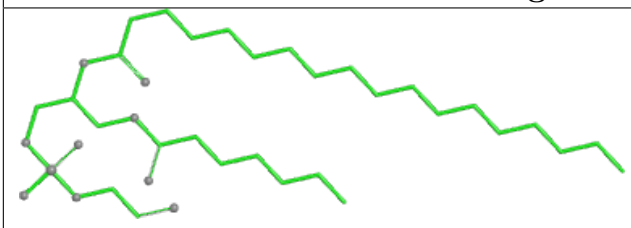


Rings

## Ligand 3PE A 505



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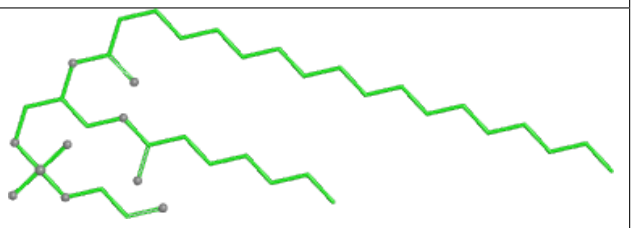
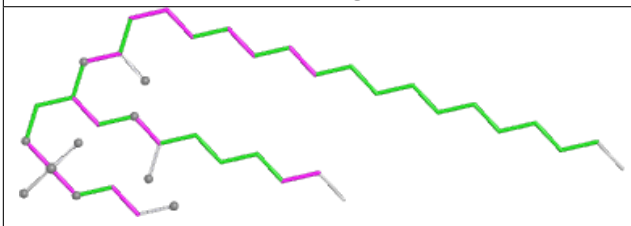
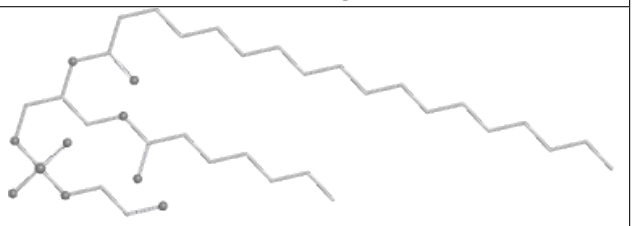


Bond angles

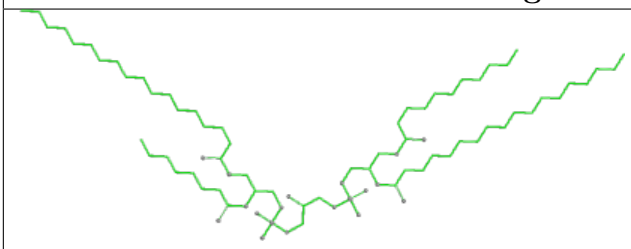


Torsions



Rings

## Ligand CDL Q 607



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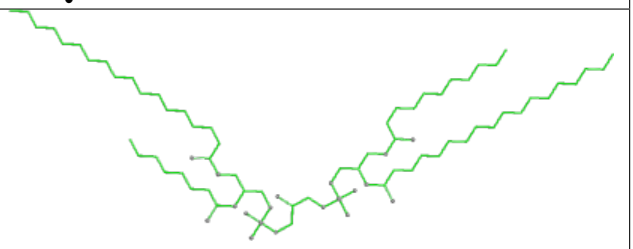
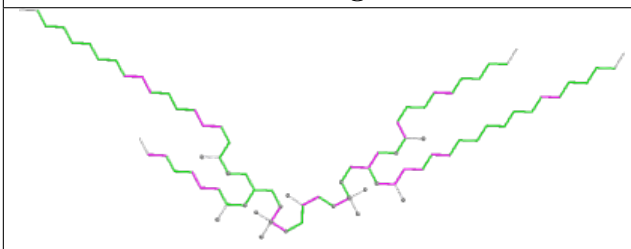
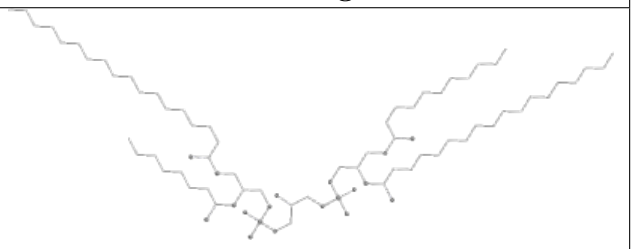


Bond angles

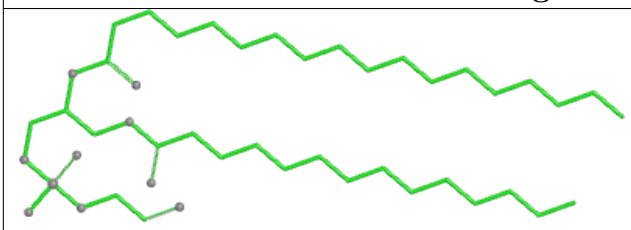


Torsions



Rings

## Ligand 3PE J 201



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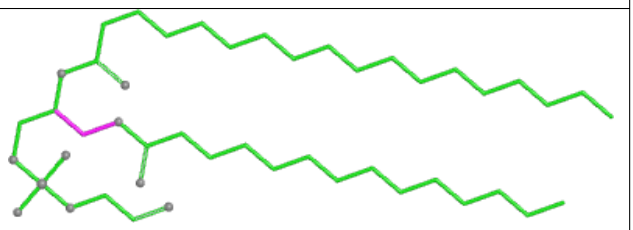
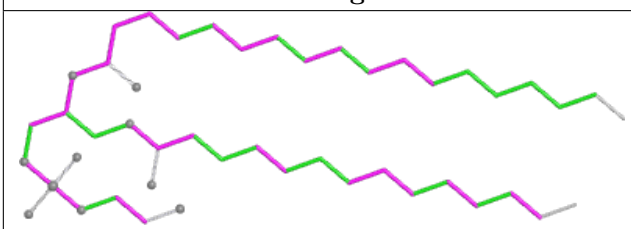
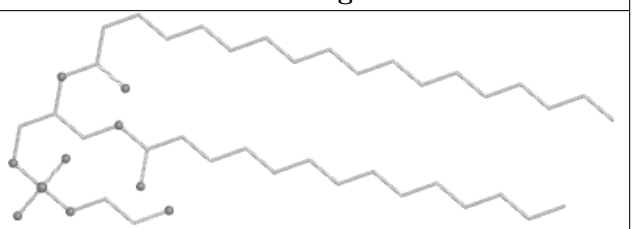


Bond angles

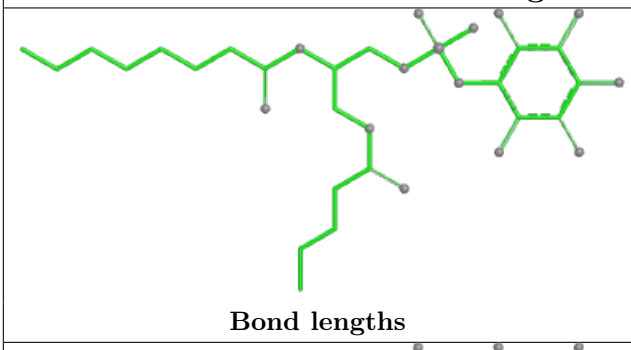


Torsions

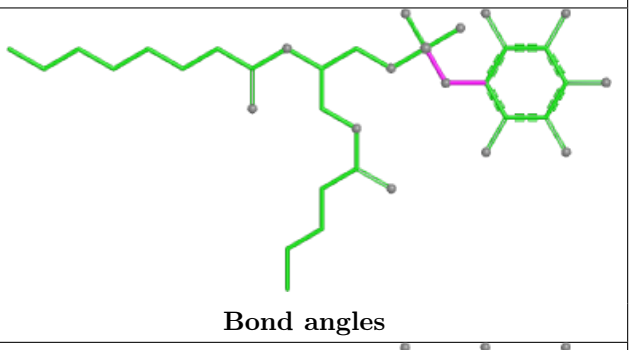


Rings

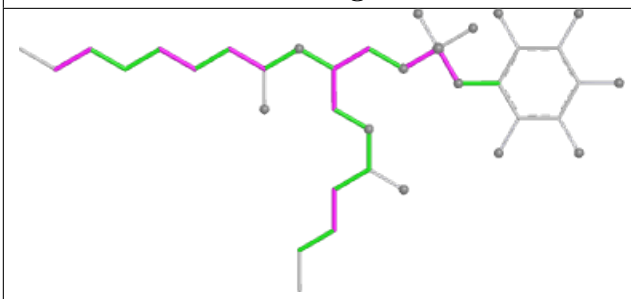
**Ligand 9YF A 503**



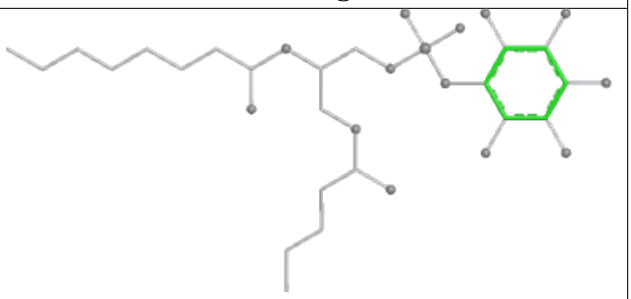
Bond lengths



Bond angles

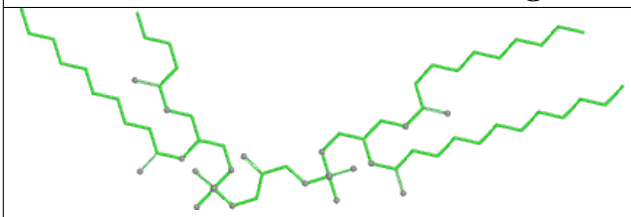


Torsions

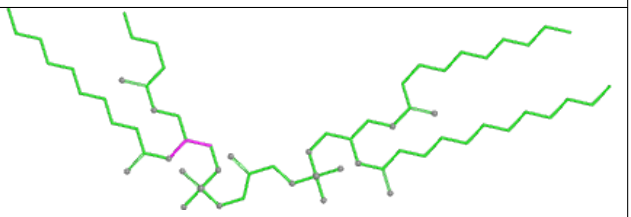


Rings

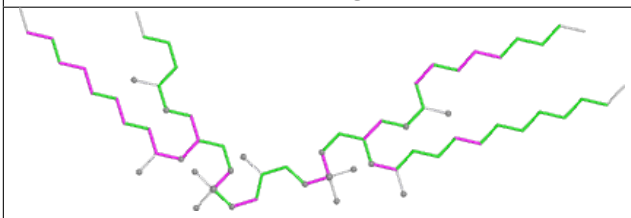
**Ligand CDL T 204**



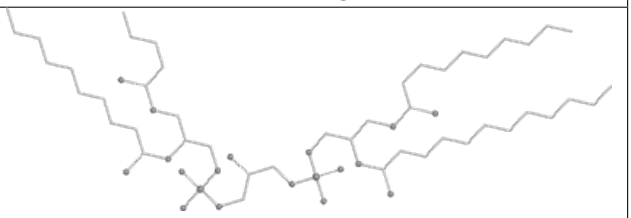
Bond lengths



Bond angles

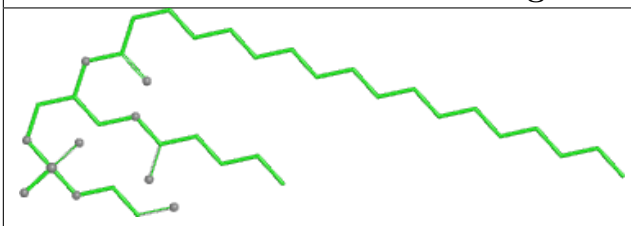


Torsions

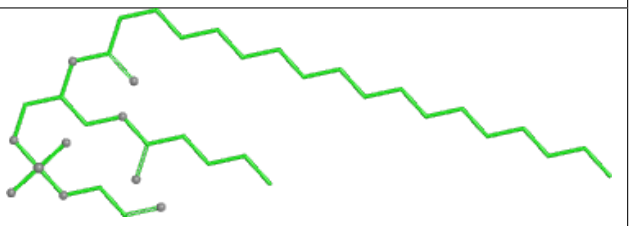


Rings

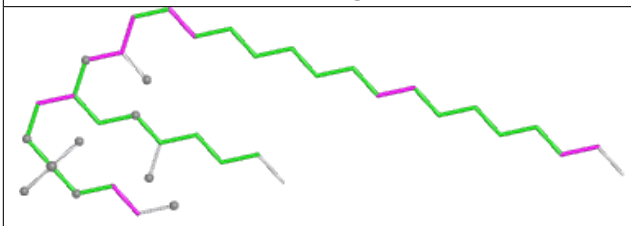
**Ligand 3PE N 502**



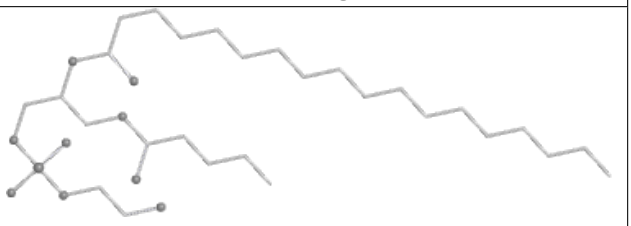
Bond lengths



Bond angles

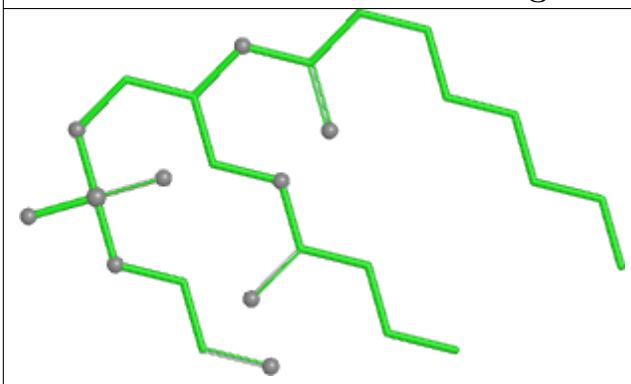


Torsions

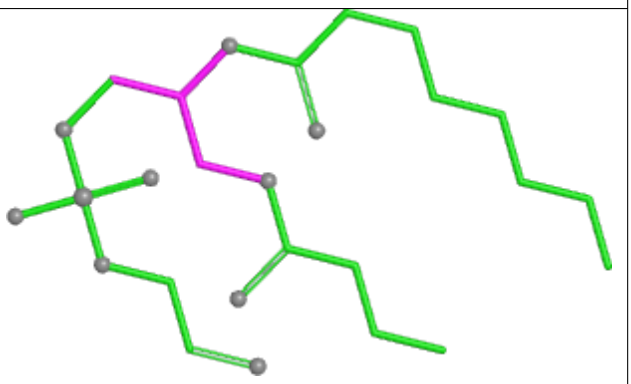


Rings

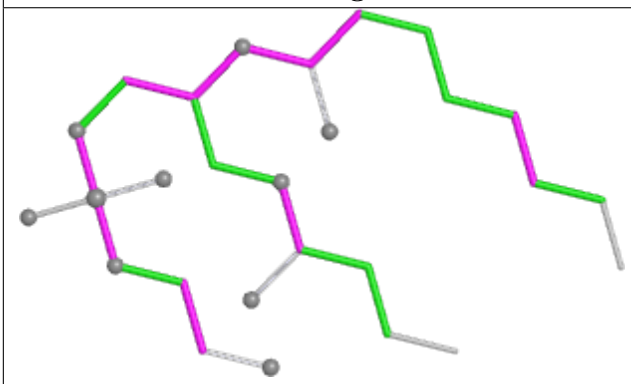
**Ligand 3PE P 303**



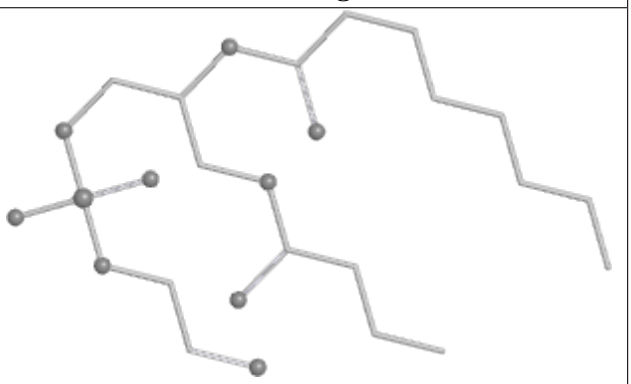
Bond lengths



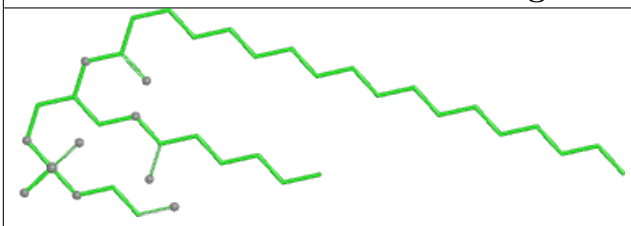
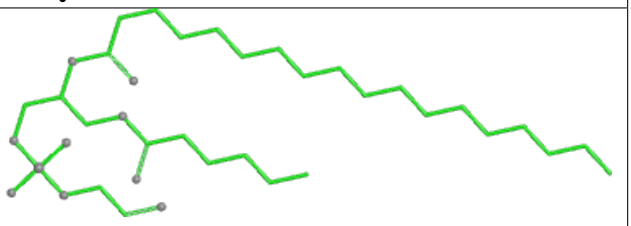
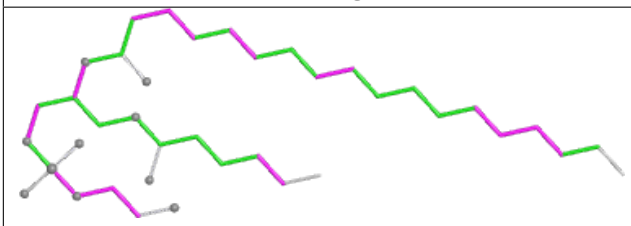
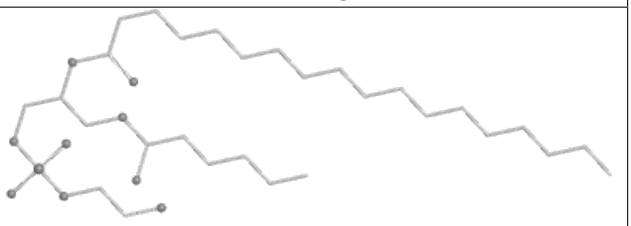
Bond angles

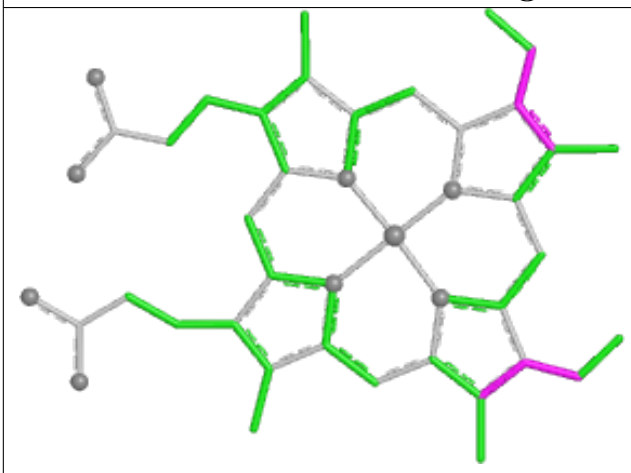
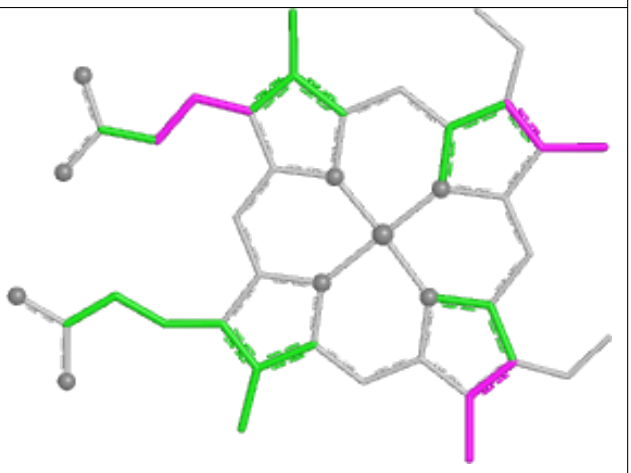
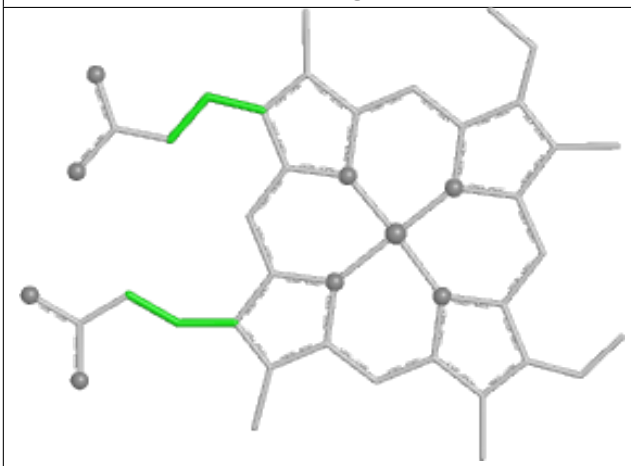
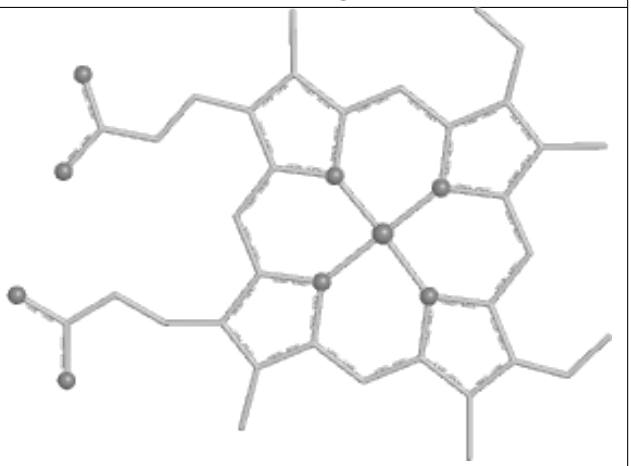


Torsions

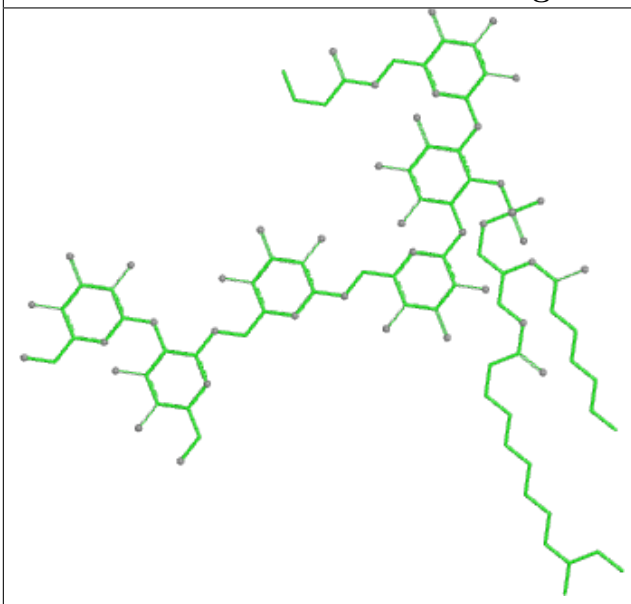


Rings

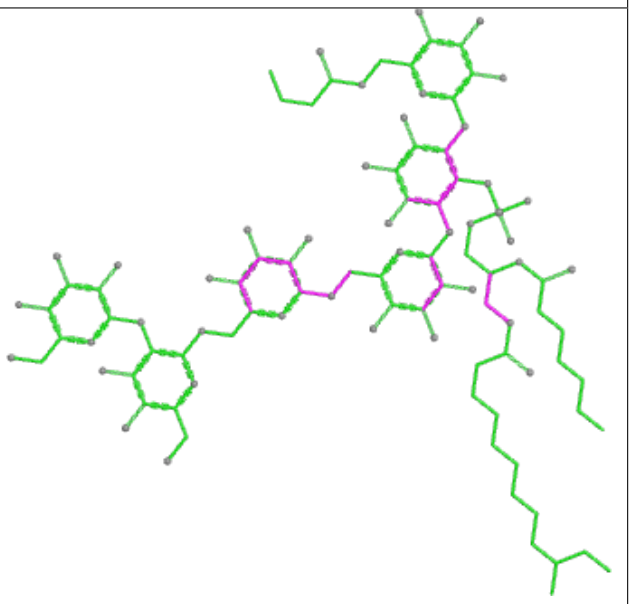
| Ligand 3PE Q 609 | |
|---|---|
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

| Ligand HEM O 604 | |
|---|---|
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

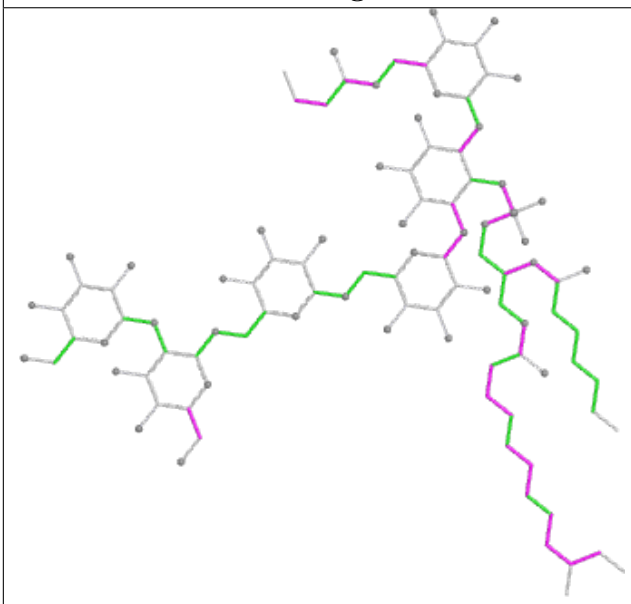
**Ligand IZL A 502**



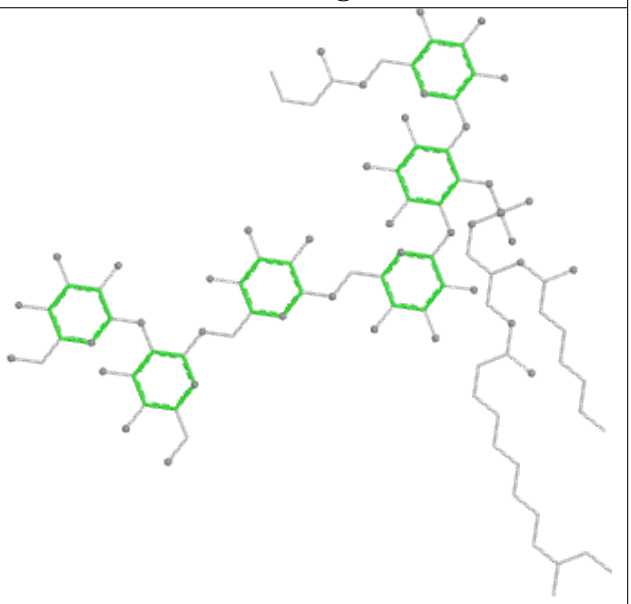
**Bond lengths**



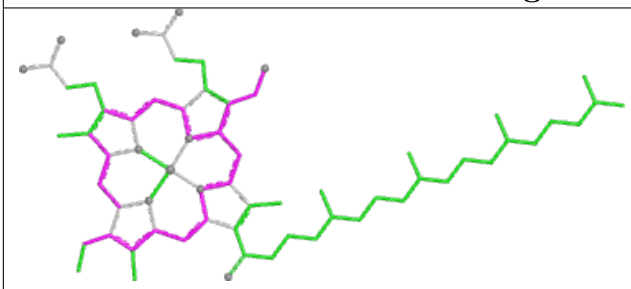
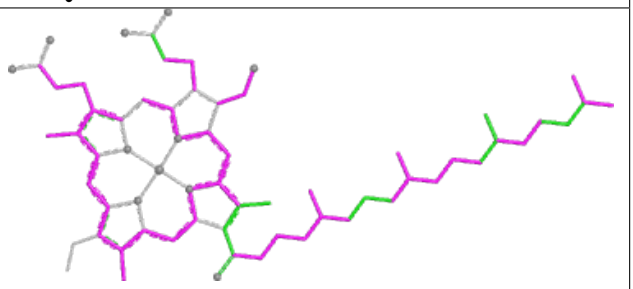
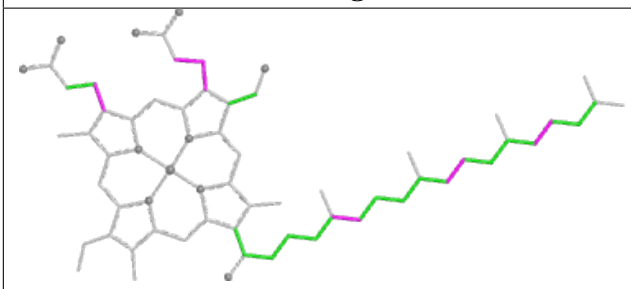
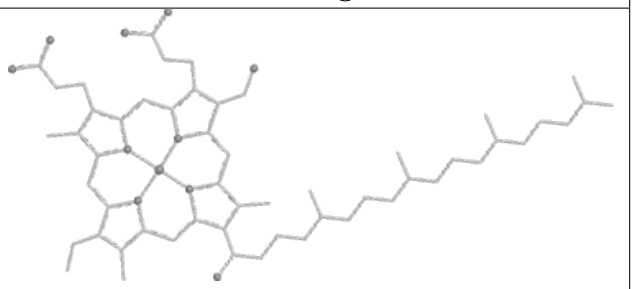
**Bond angles**

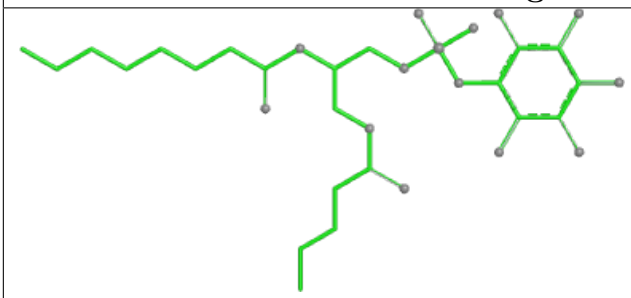
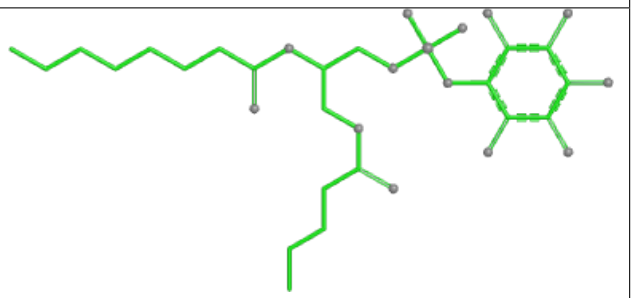
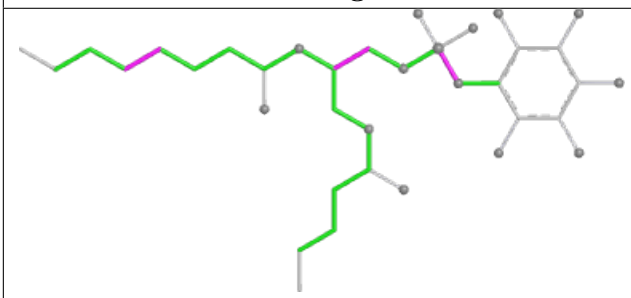
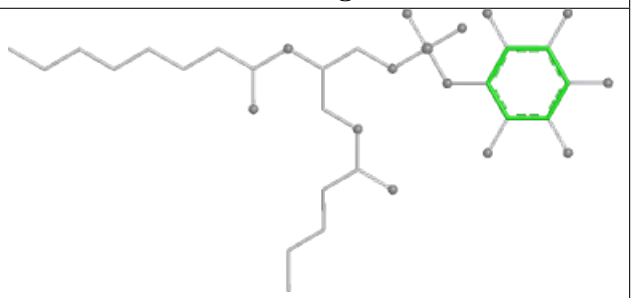


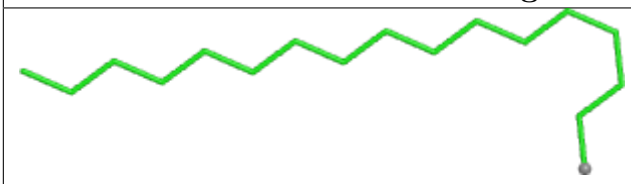
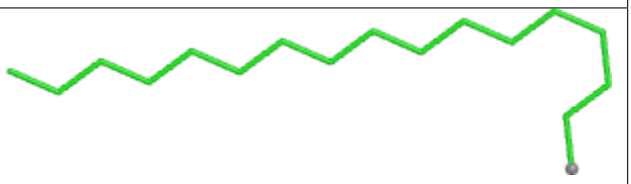
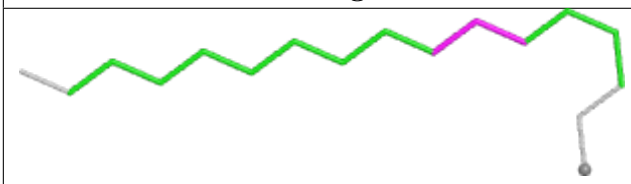
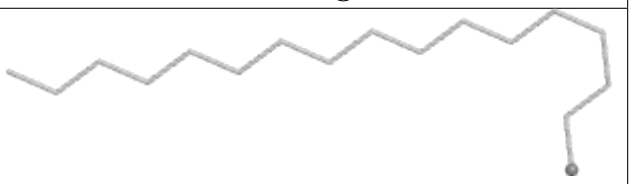
**Torsions**

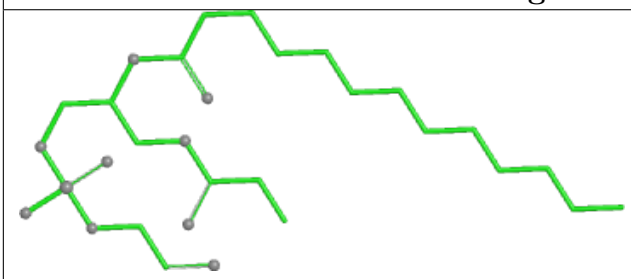
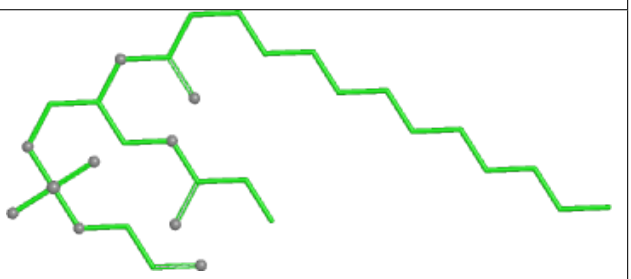
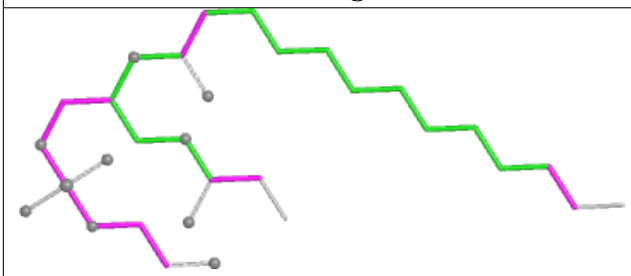
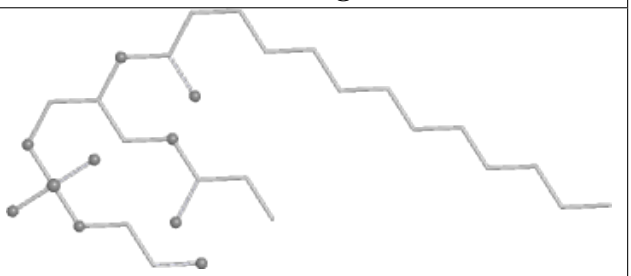


**Rings**

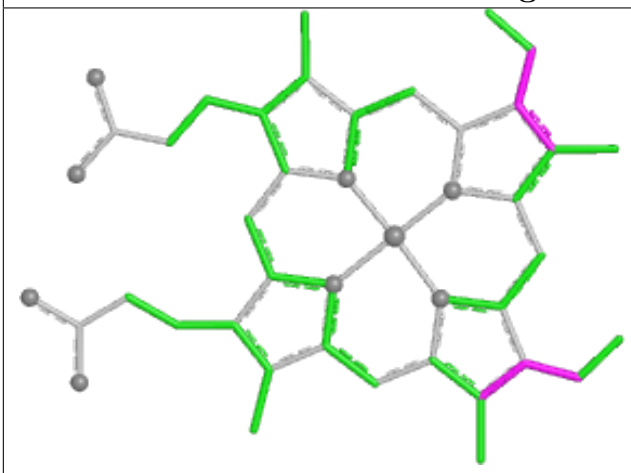
| Ligand HAS Q 602 | |
|---|---|
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

| Ligand 9YF N 505 | |
|---|---|
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

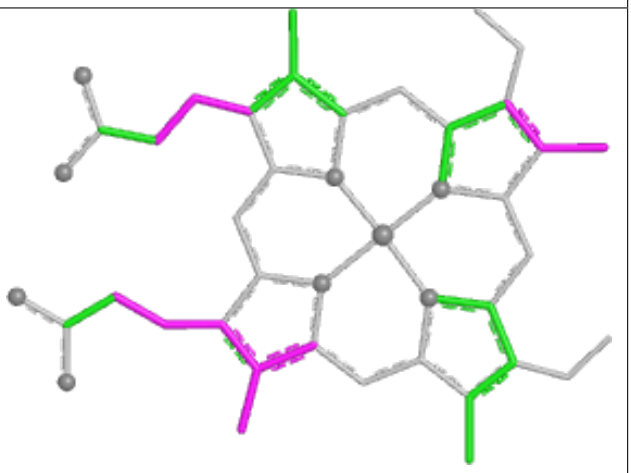
| Ligand PLM U 202 | |
|---|---|
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

| Ligand 3PE R 405 | |
|---|---|
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

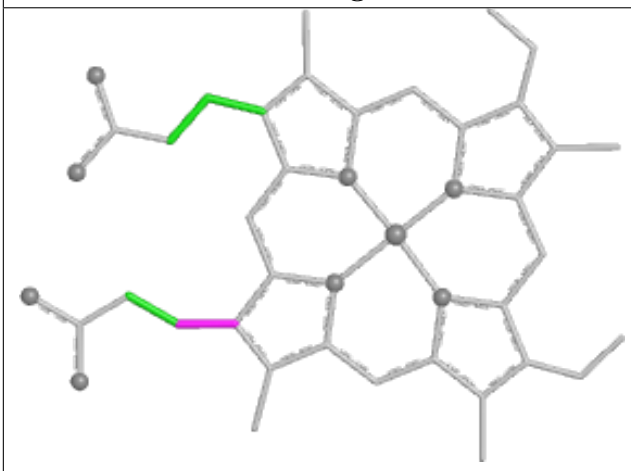
**Ligand HEM B 602**



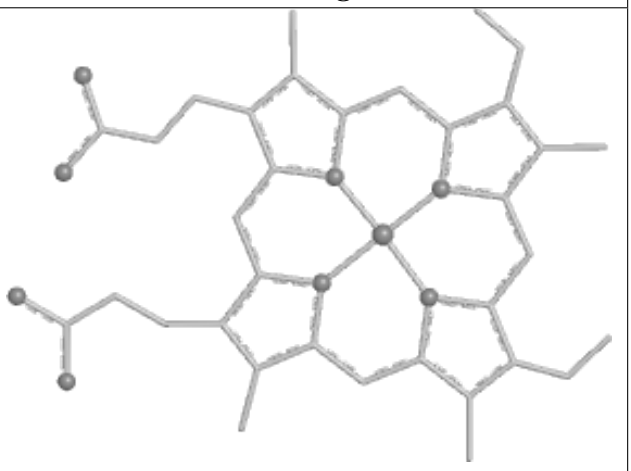
**Bond lengths**



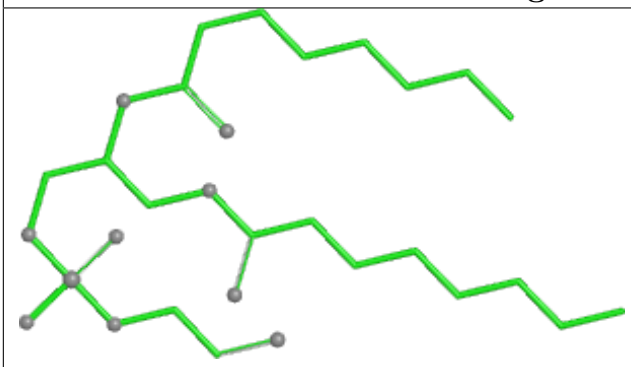
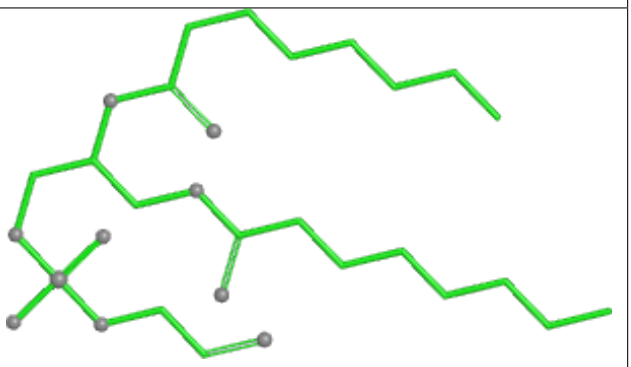
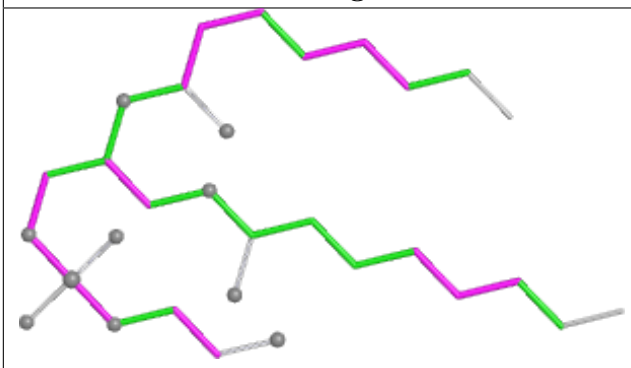
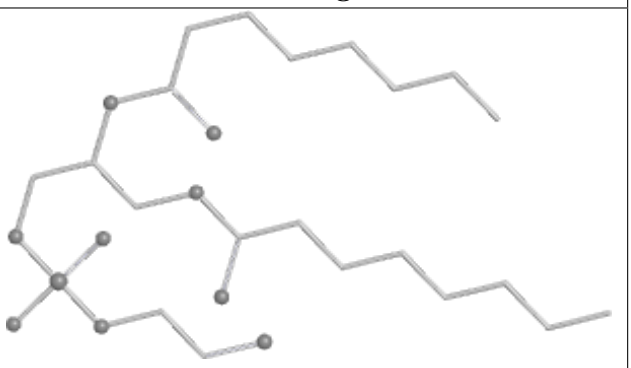
**Bond angles**

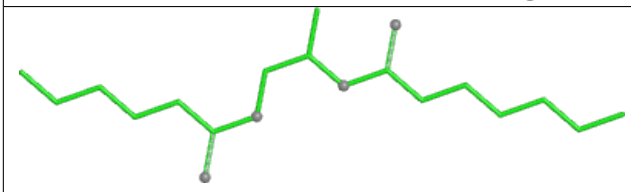
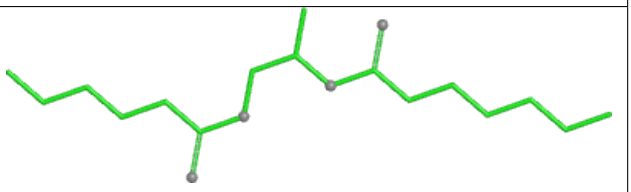
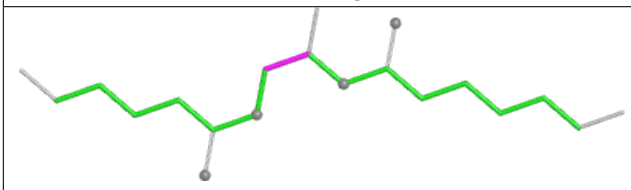
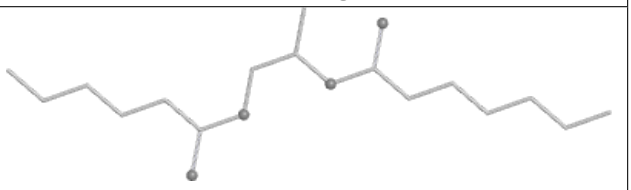


**Torsions**

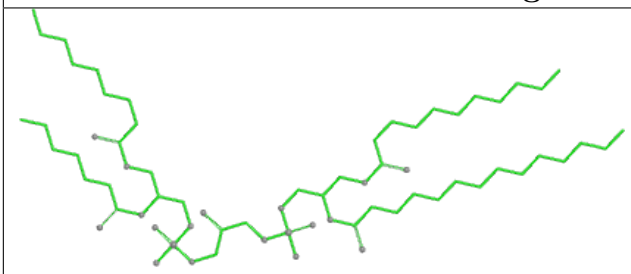


**Rings**

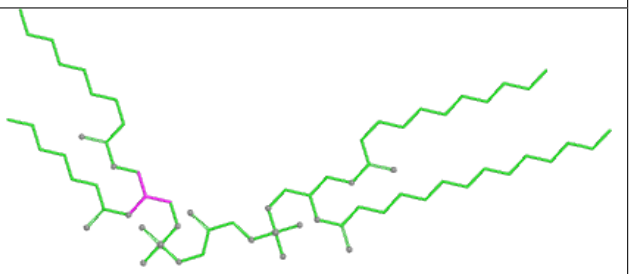
| Ligand 3PE D 609 | |
|---|---|
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

| Ligand DGA E 403 | |
|---|---|
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

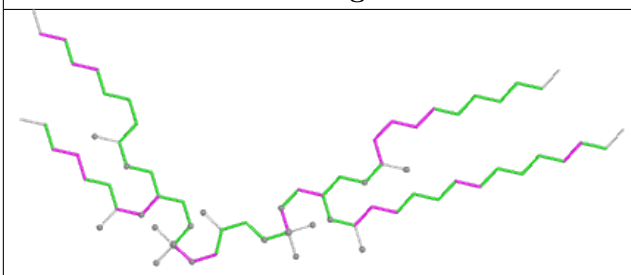
## Ligand CDL G 202



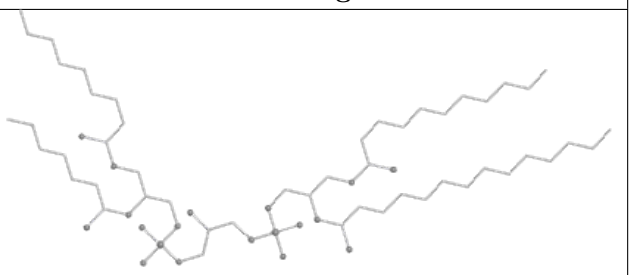
Bond lengths



Bond angles

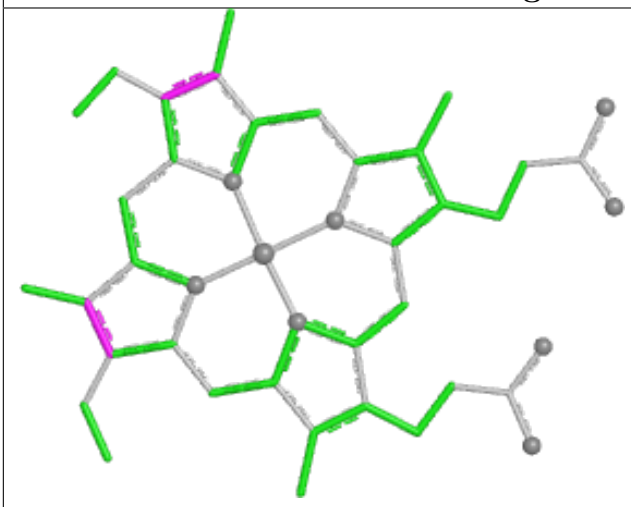


Torsions

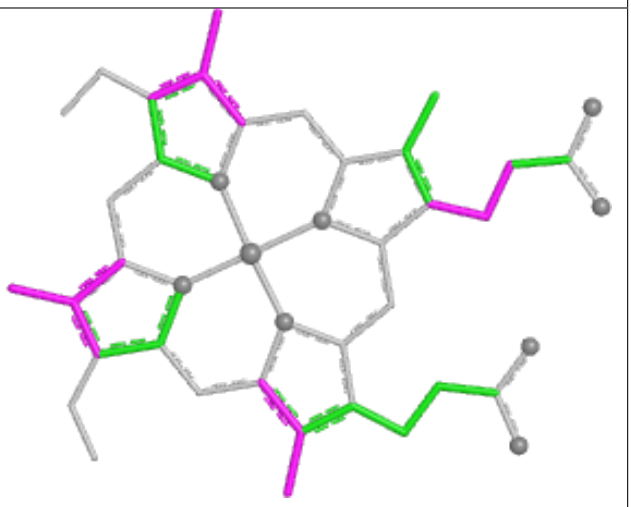


Rings

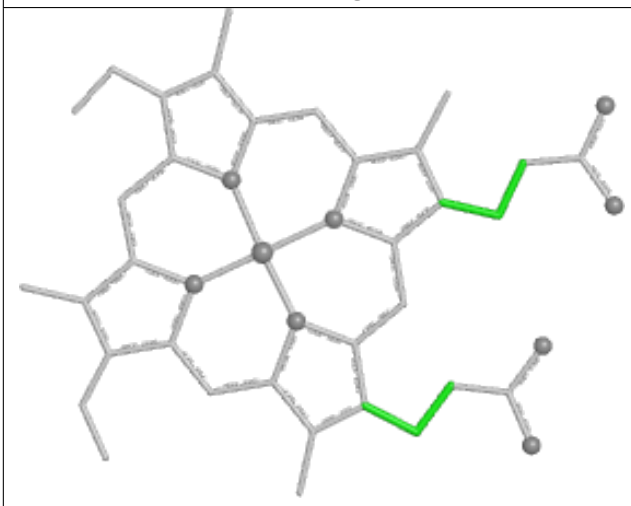
## Ligand HEC P 301



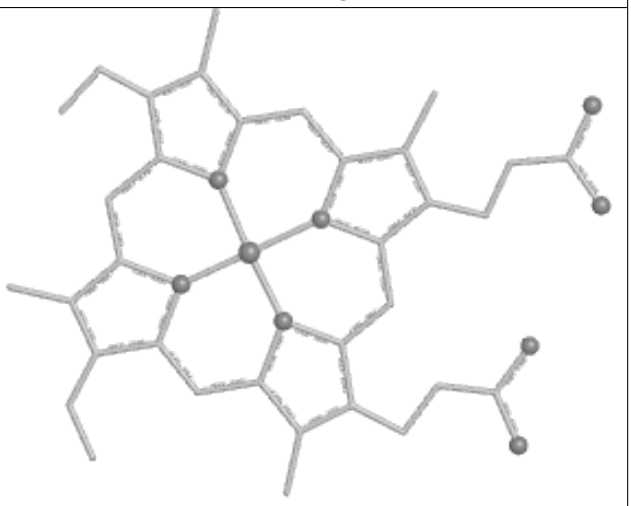
Bond lengths



Bond angles

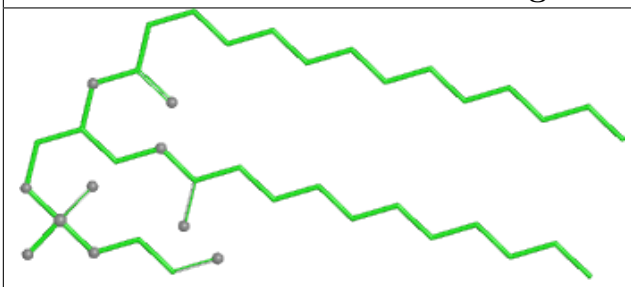


Torsions

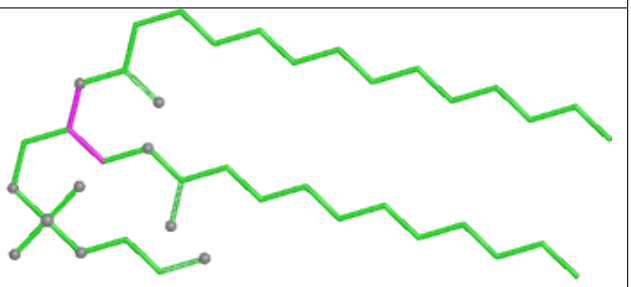


Rings

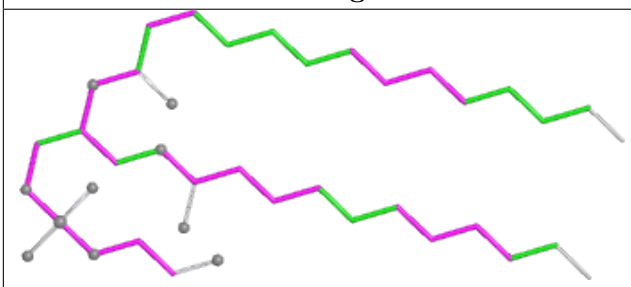
**Ligand 3PE T 206**



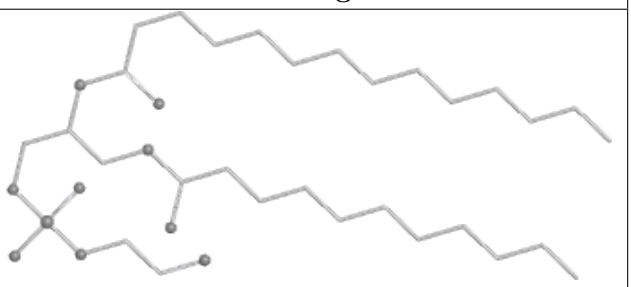
Bond lengths



Bond angles

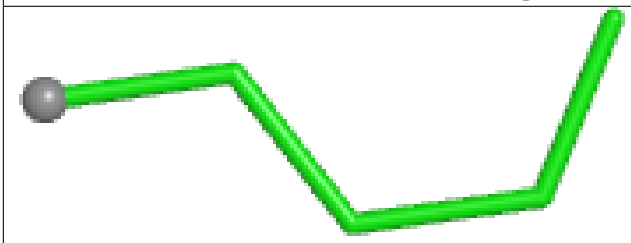


Torsions

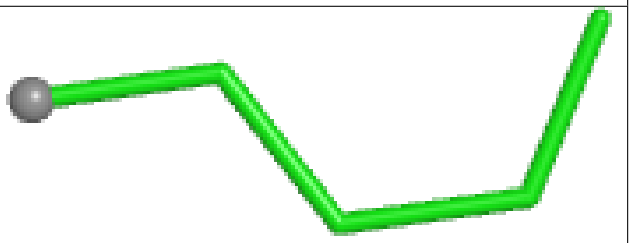


Rings

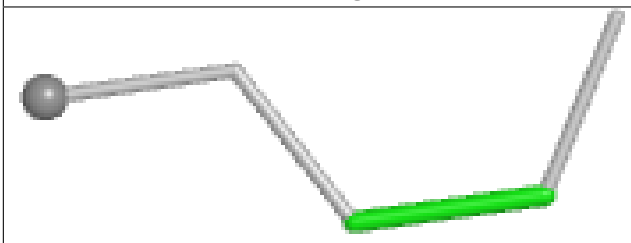
**Ligand PLM M 202**



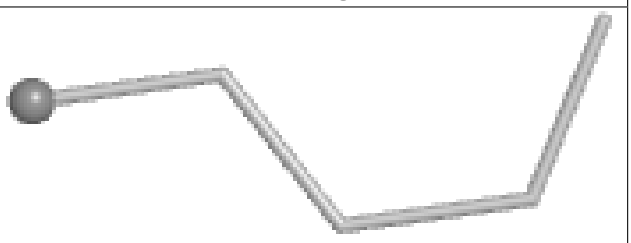
Bond lengths



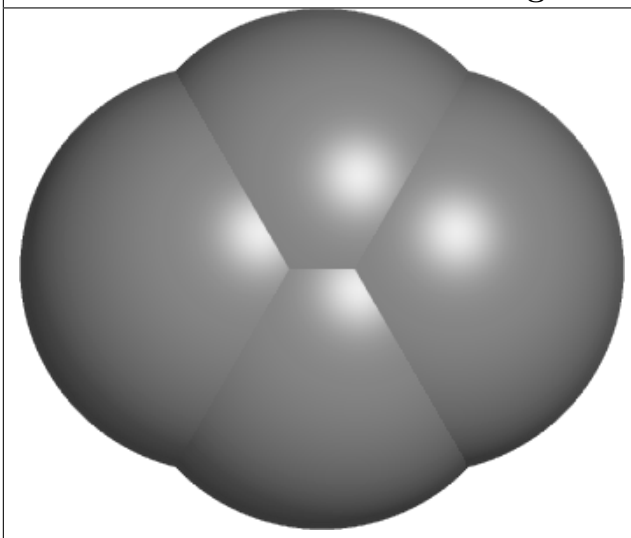
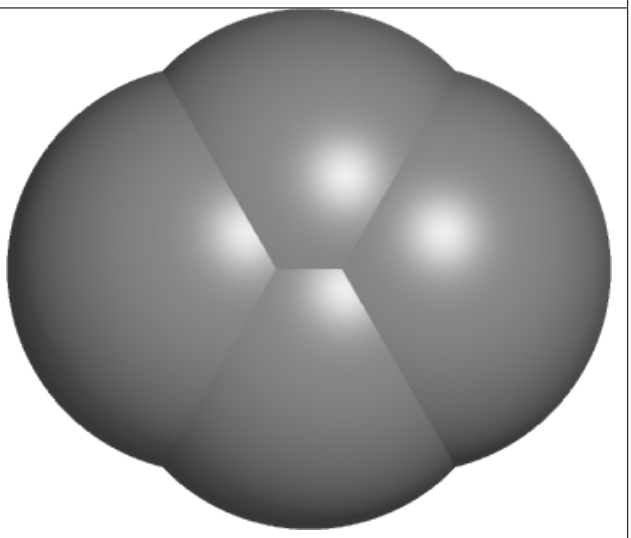
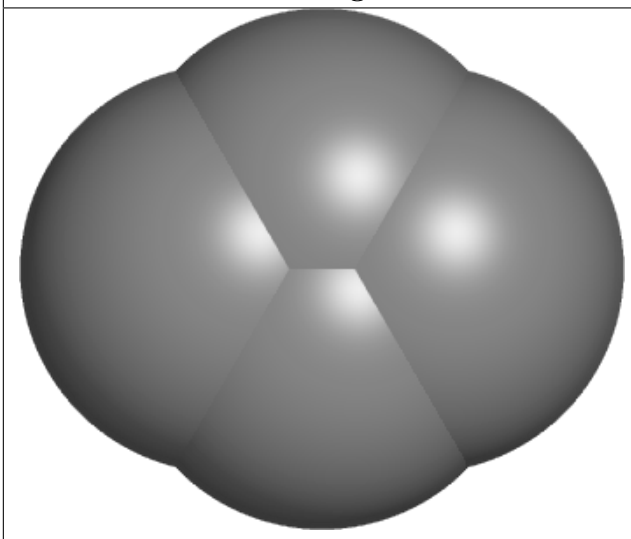
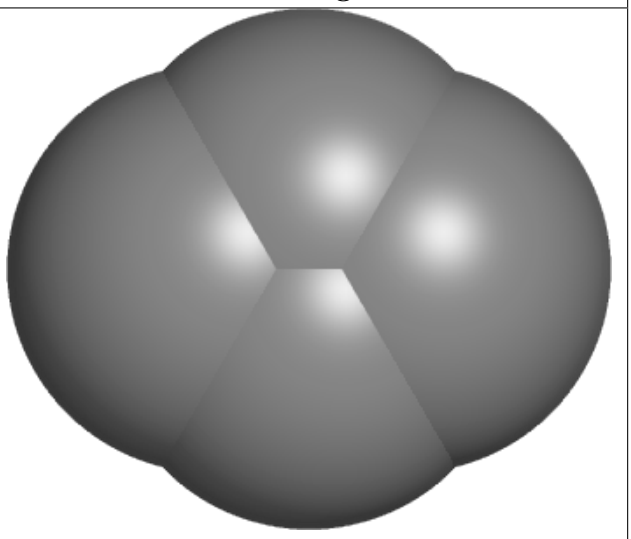
Bond angles



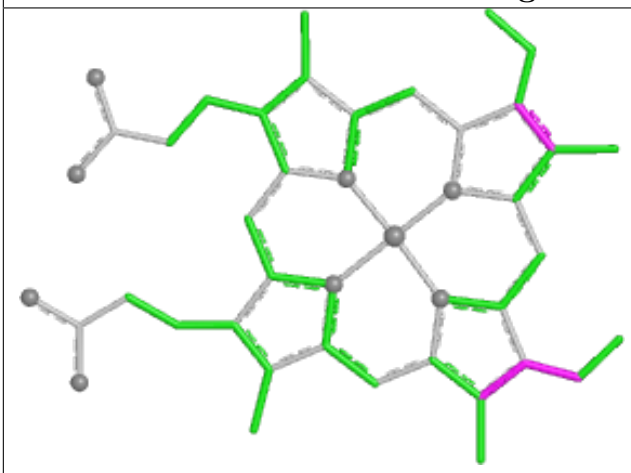
Torsions



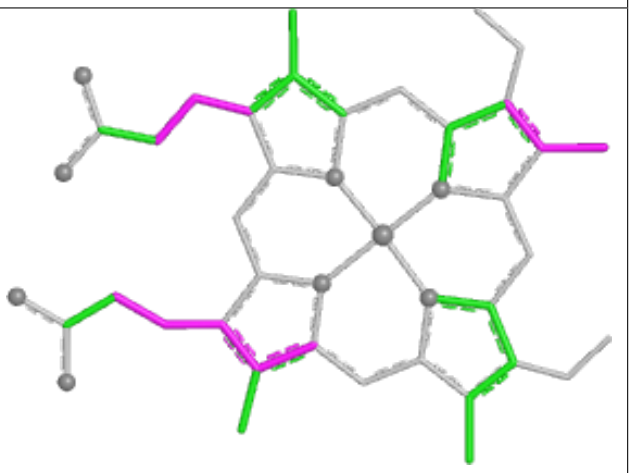
Rings

| Ligand FES N 503 | |
|---|---|
|  |  |
| **Bond lengths** | **Bond angles** |
|  |  |
| **Torsions** | **Rings** |

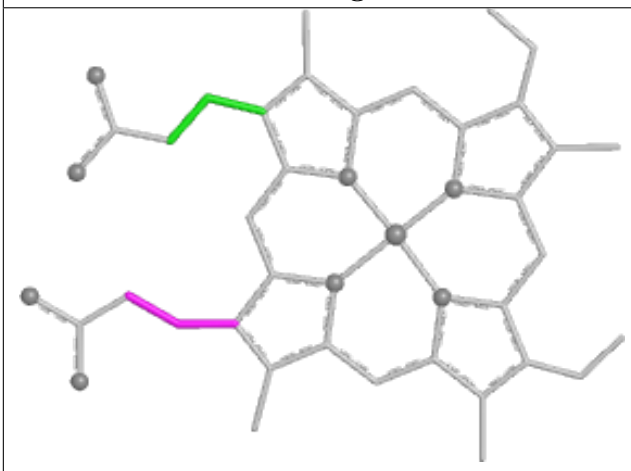
**Ligand HEM O 603**



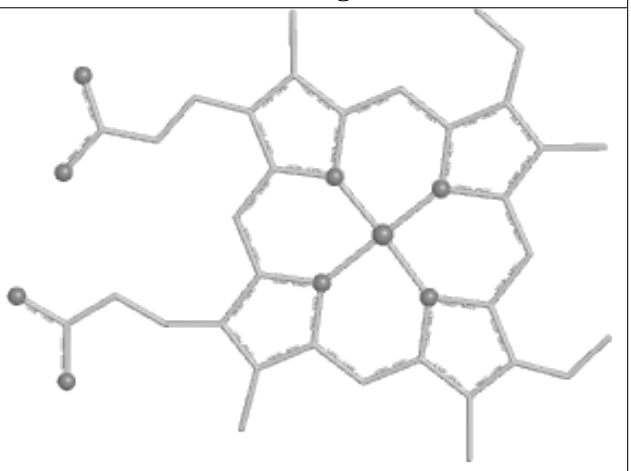
Bond lengths



Bond angles

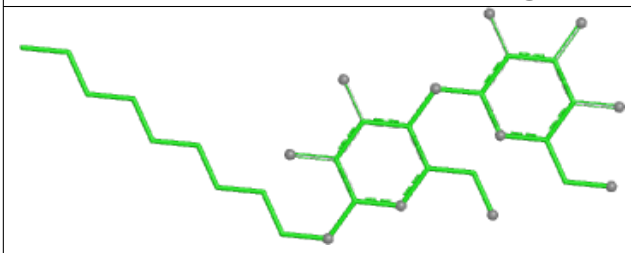


Torsions

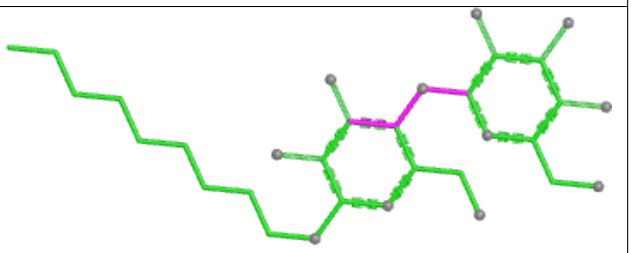


Rings

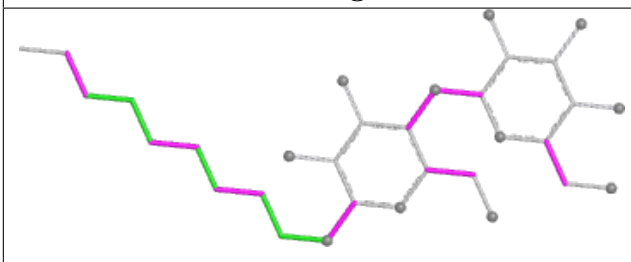
**Ligand LMT O 601**



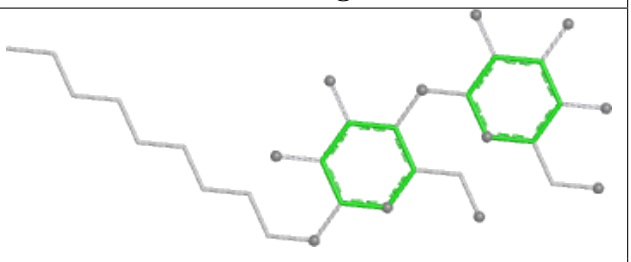
Bond lengths



Bond angles

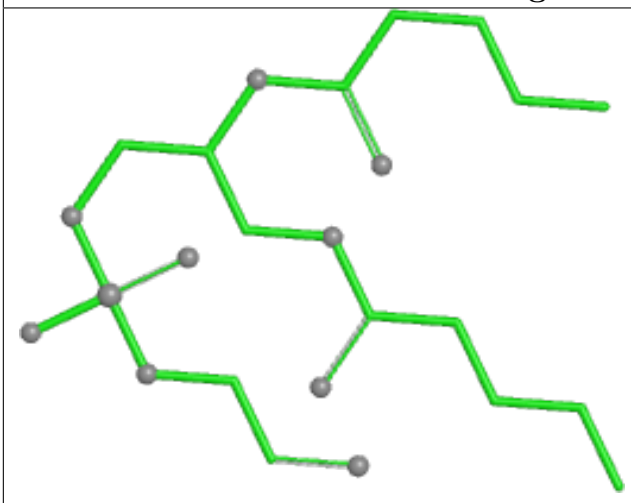


Torsions

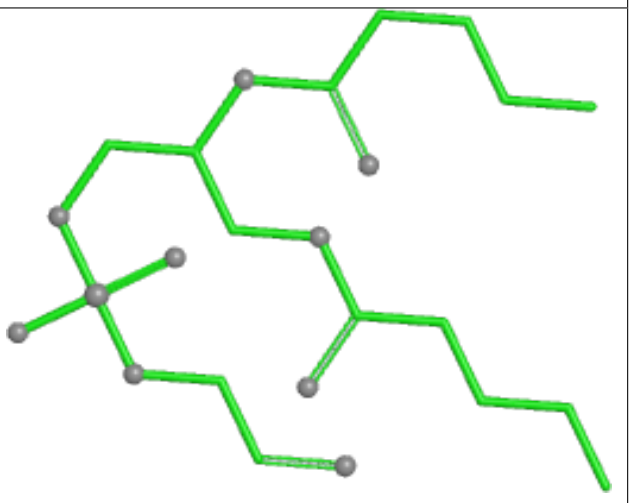


Rings

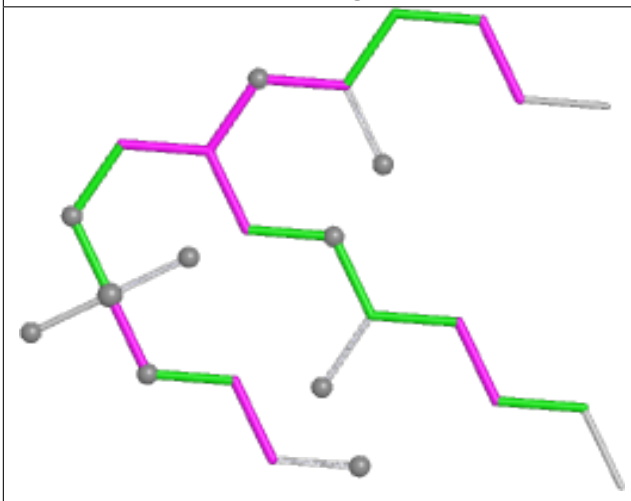
**Ligand 3PE C 303**



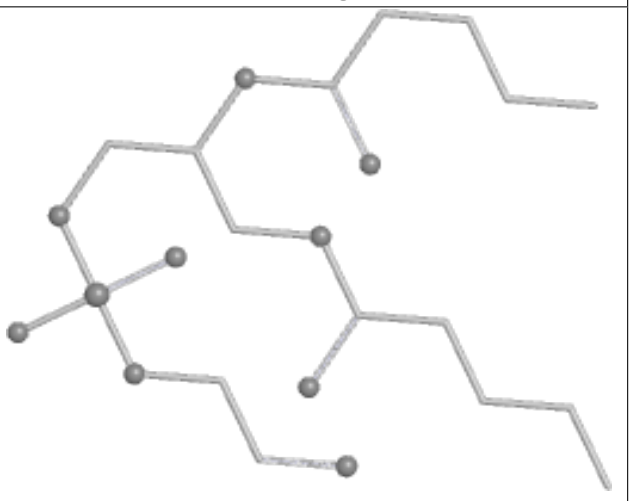
**Bond lengths**



**Bond angles**

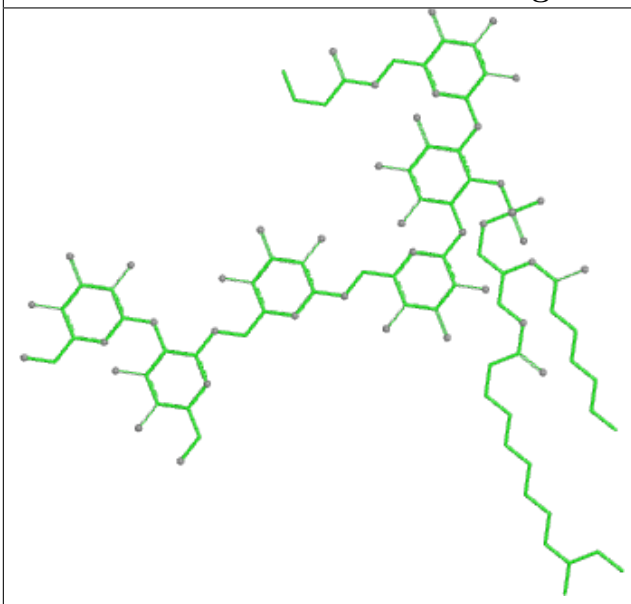


**Torsions**

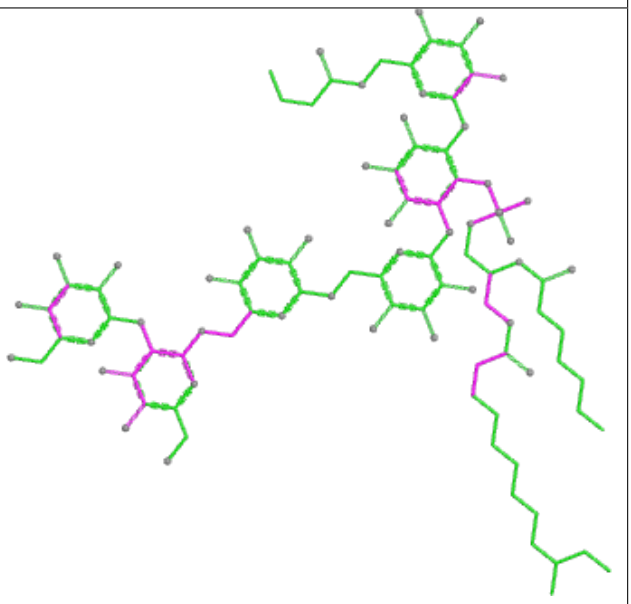


**Rings**

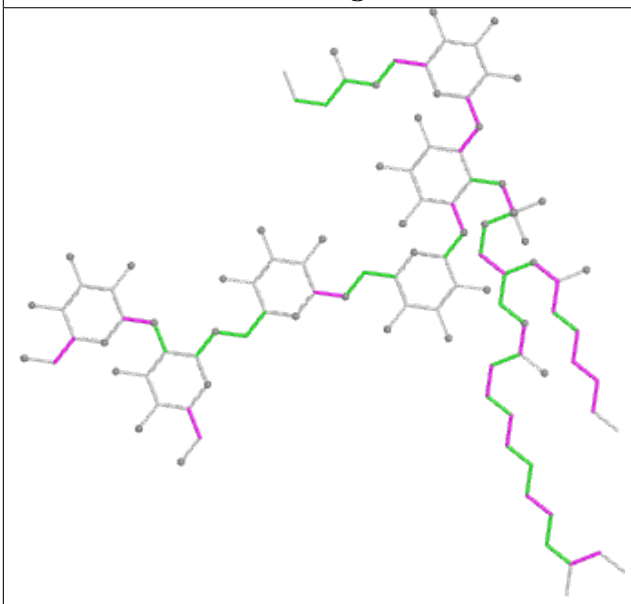
**Ligand IZL N 504**



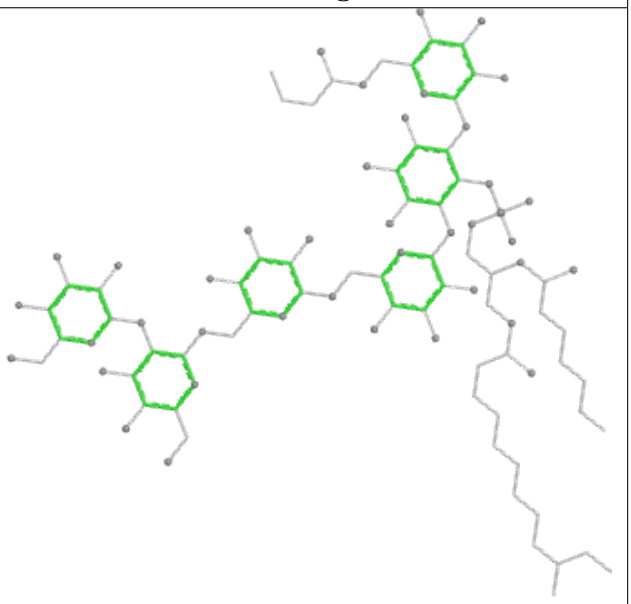
**Bond lengths**



**Bond angles**

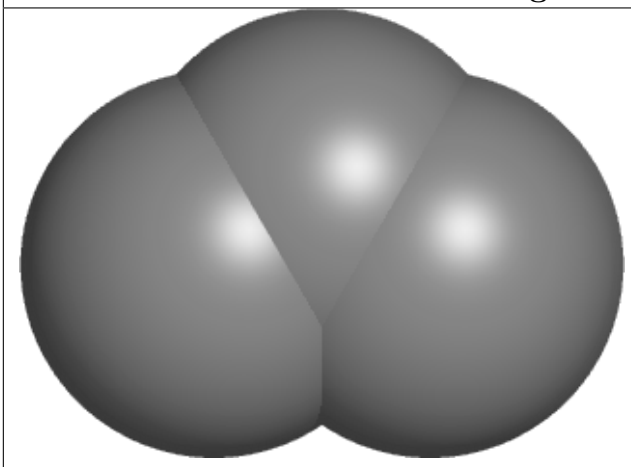


**Torsions**

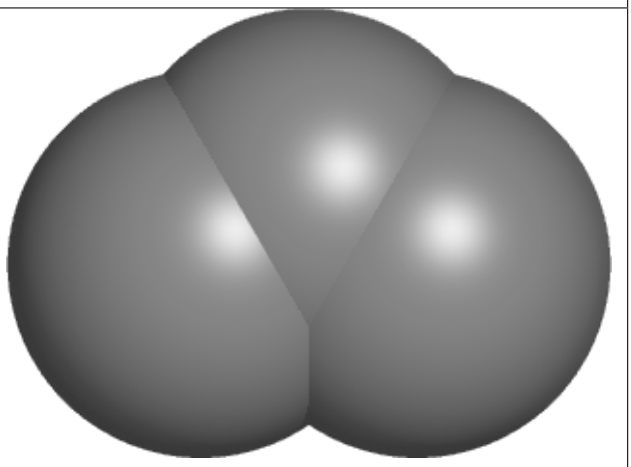


**Rings**

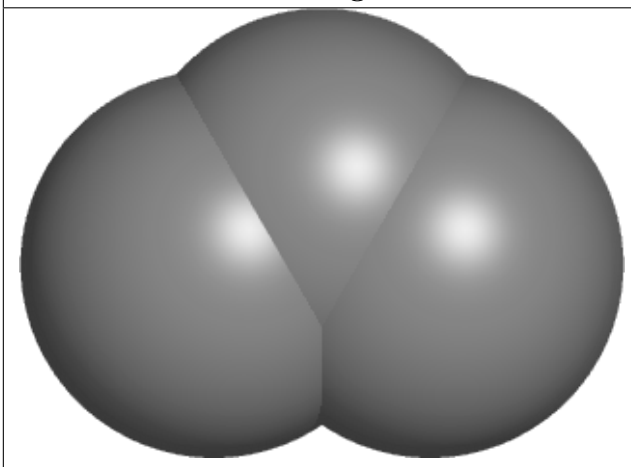
## Ligand AZI D 606



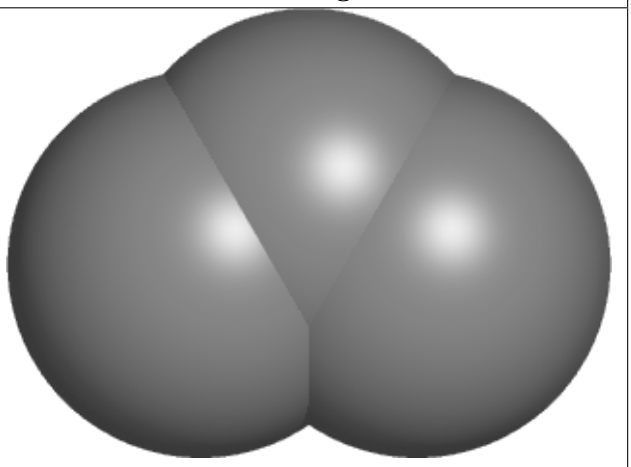
Bond lengths



Bond angles

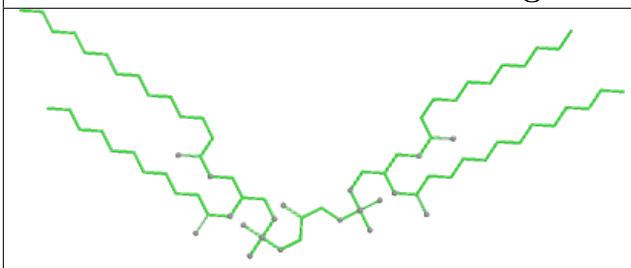


Torsions

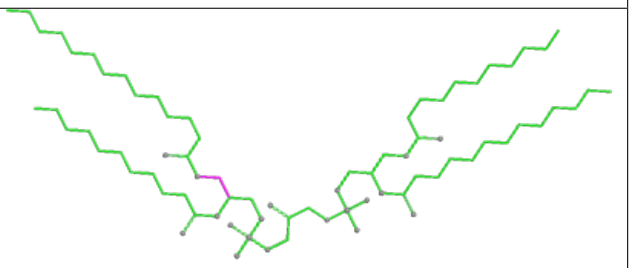


Rings

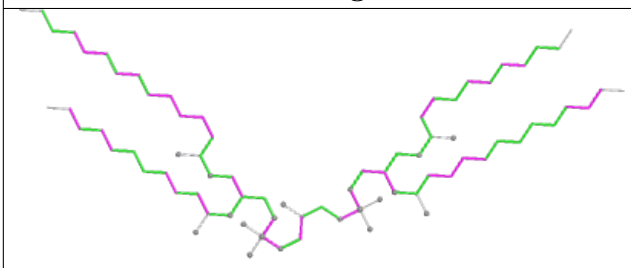
## Ligand CDL D 607



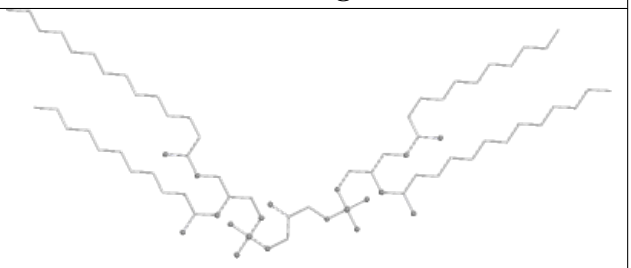
Bond lengths



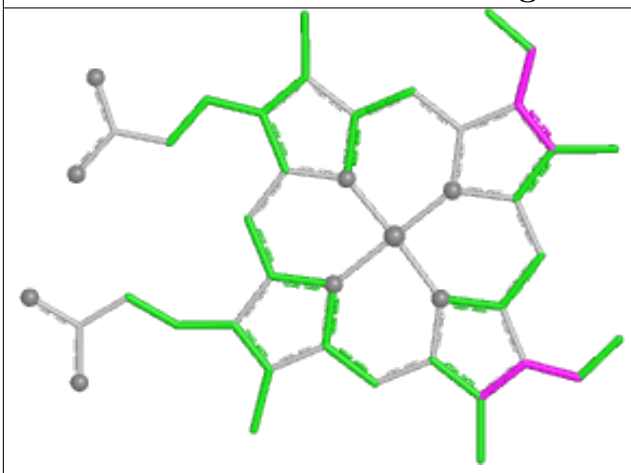
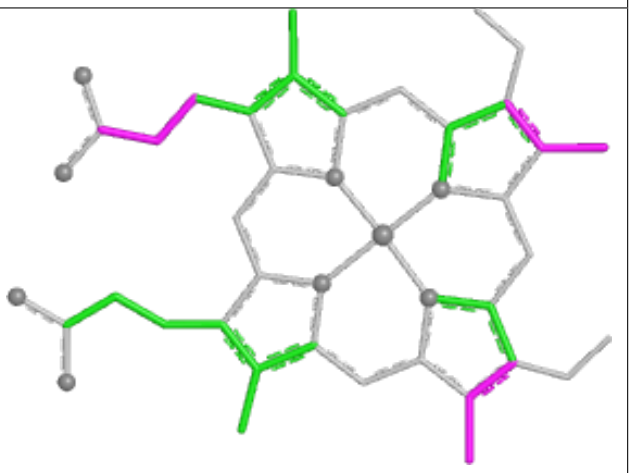
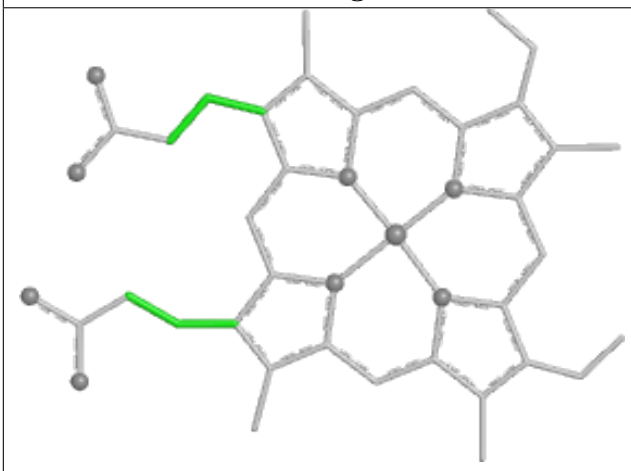
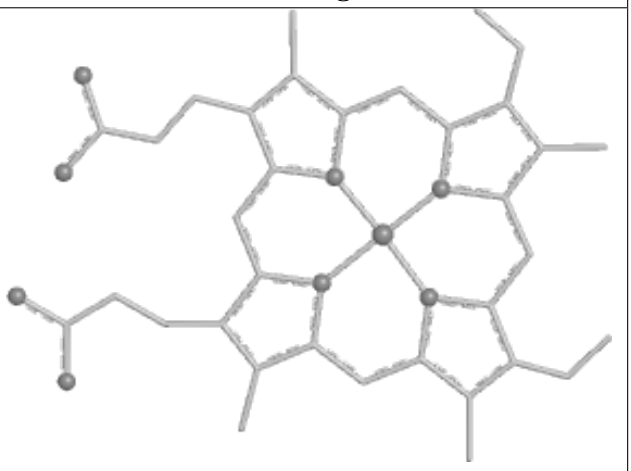
Bond angles

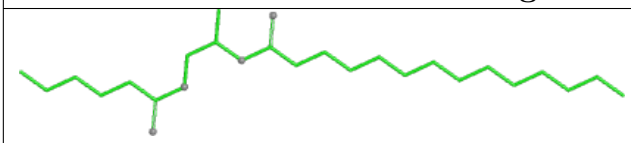
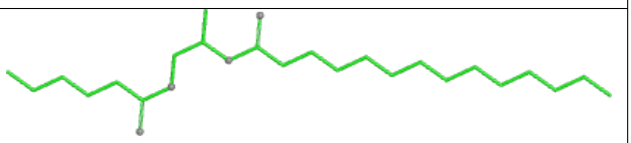
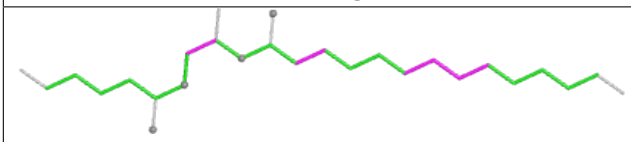
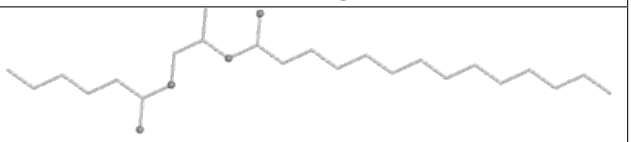


Torsions

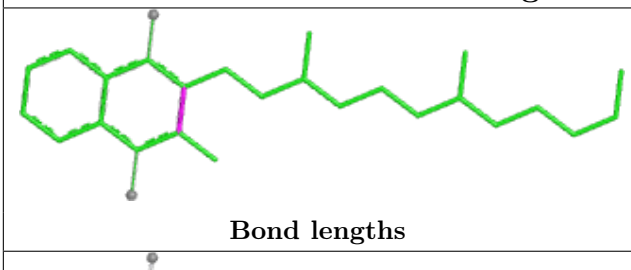


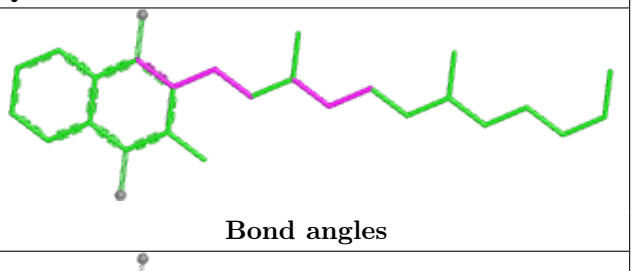
Rings

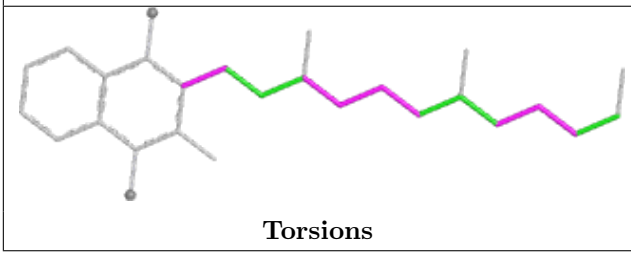
| Ligand HEM B 603 | |
|---|---|
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

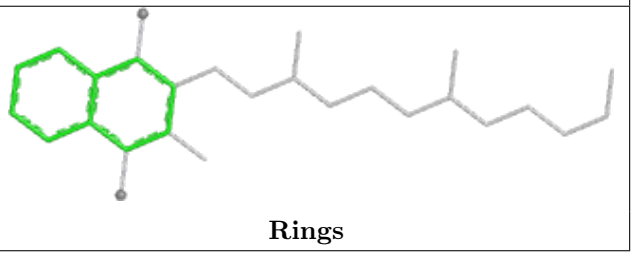
| Ligand DGA U 201 | |
|---|---|
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

## Ligand MQ9 O 605

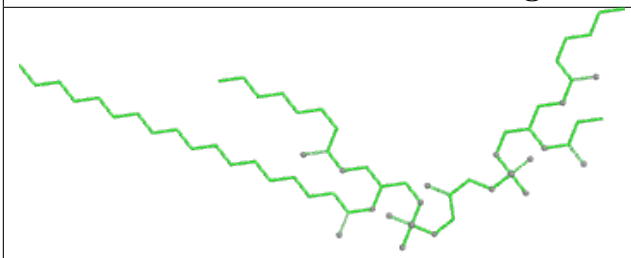

Bond lengths

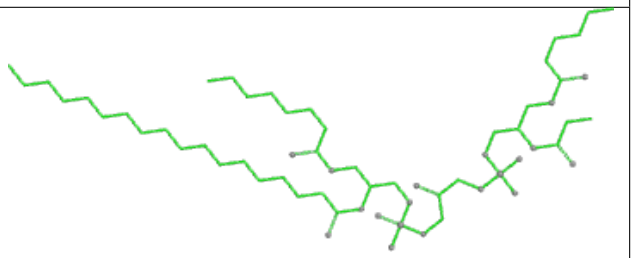

Bond angles

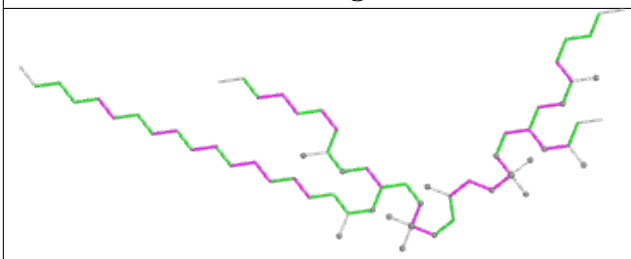

Torsions

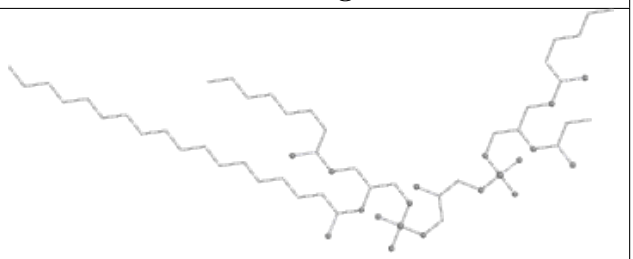

Rings

## Ligand CDL D 608

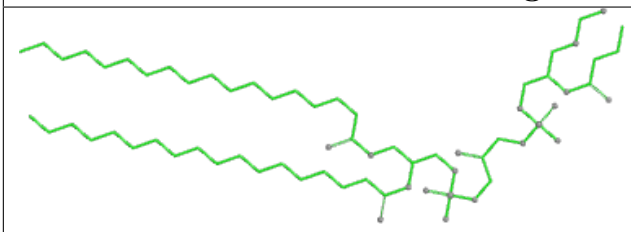

Bond lengths

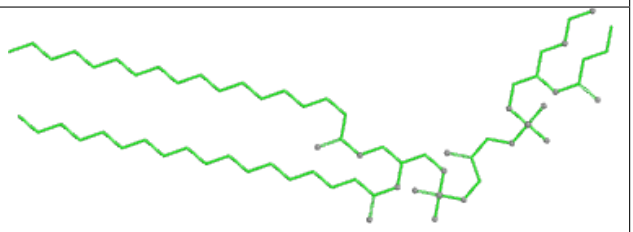

Bond angles

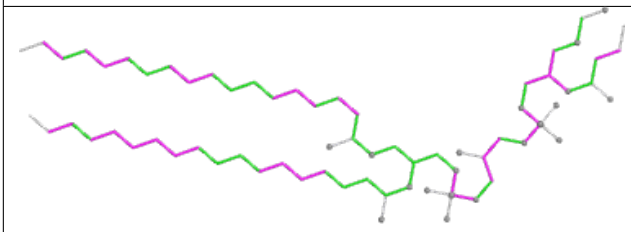

Torsions

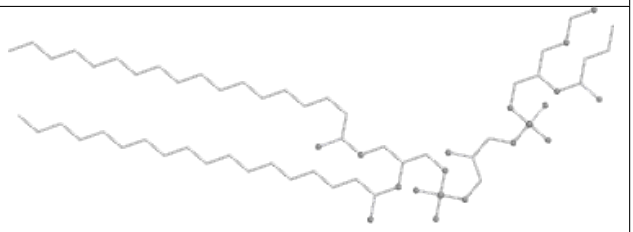

Rings

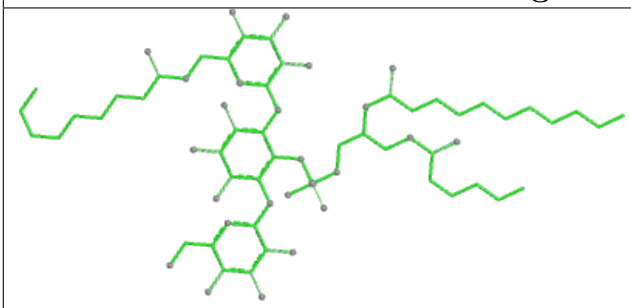
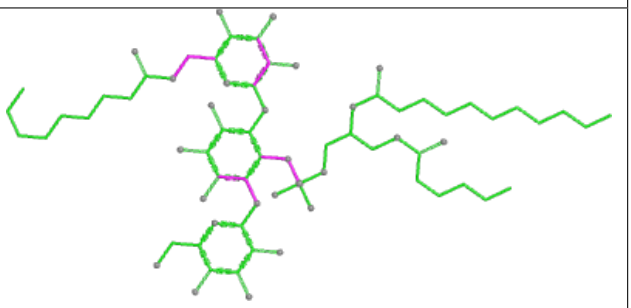
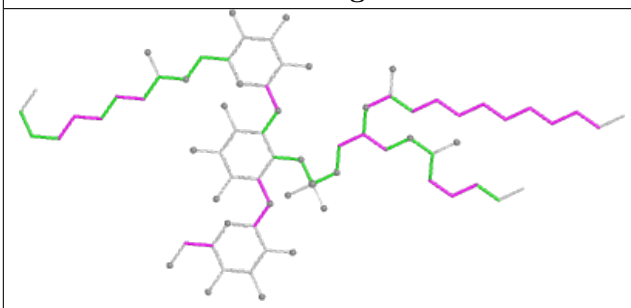
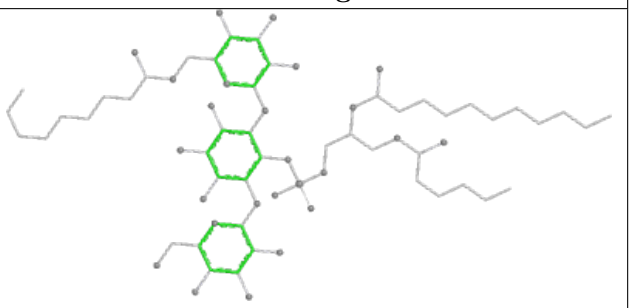
## Ligand CDL V 201

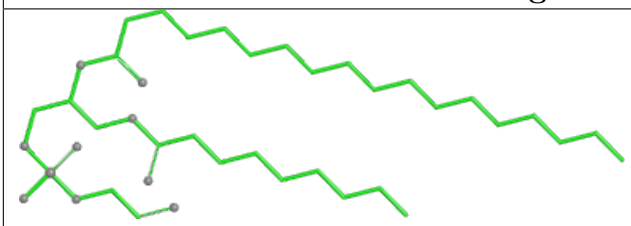
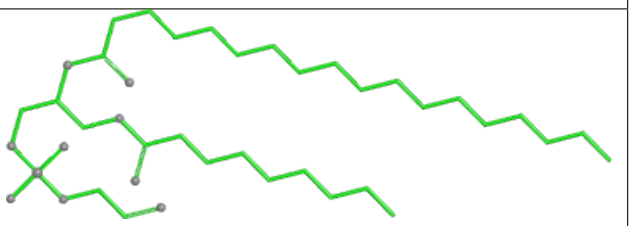
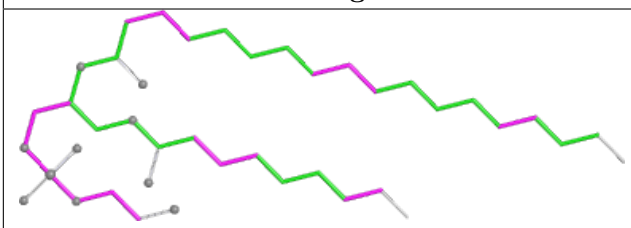
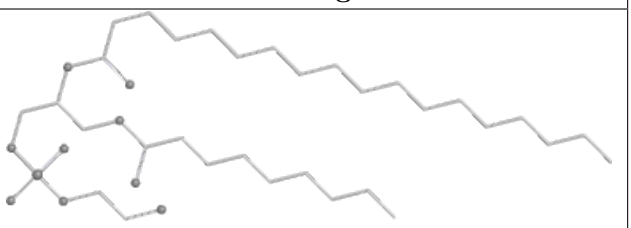

Bond lengths

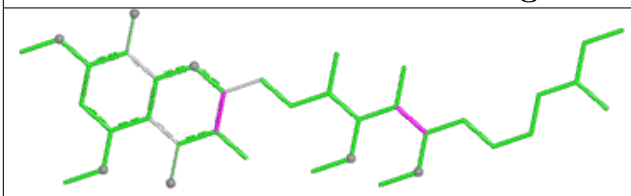
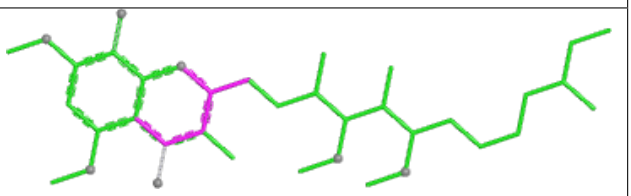
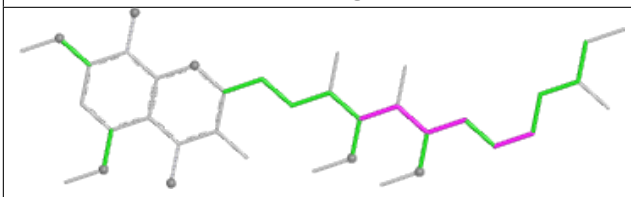
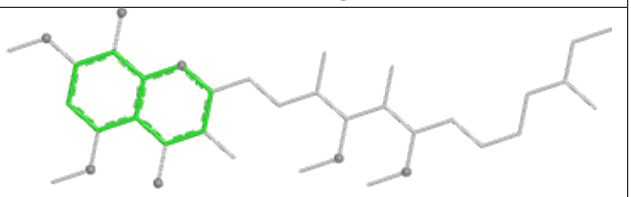

Bond angles

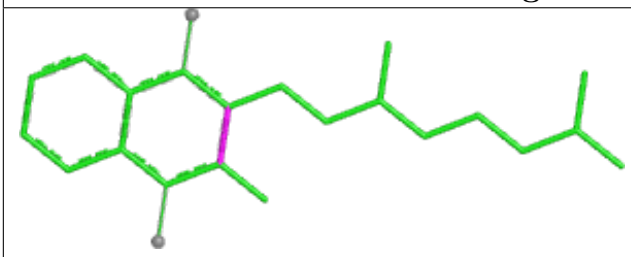
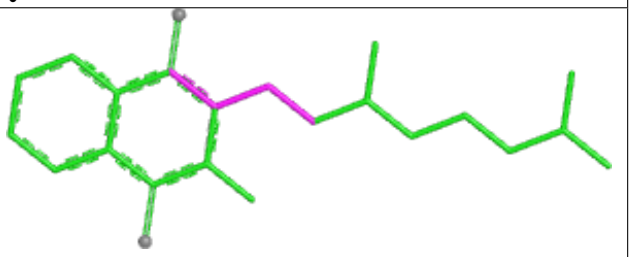
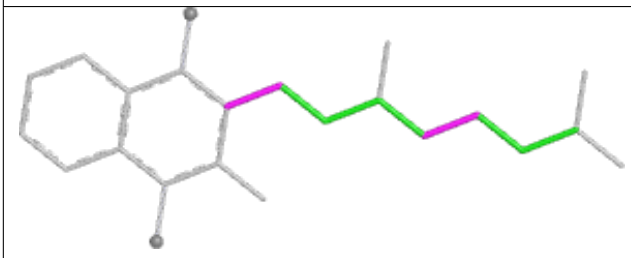
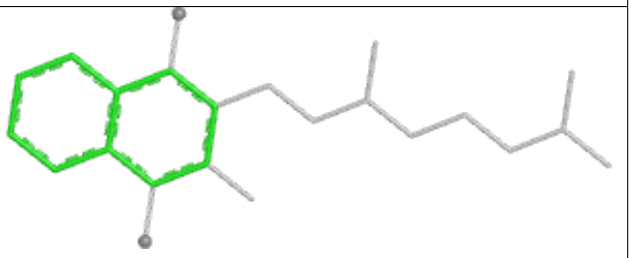

Torsions

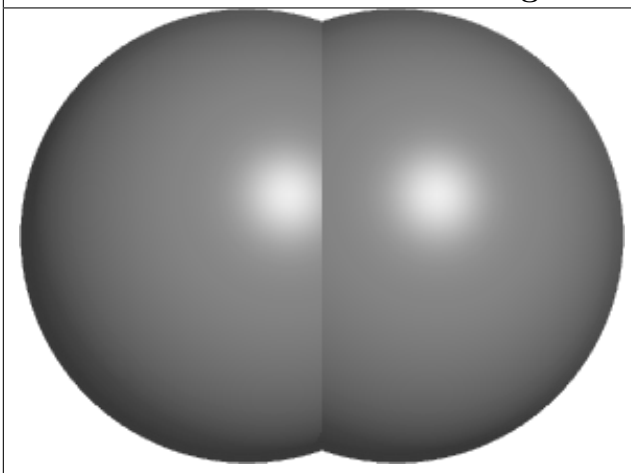
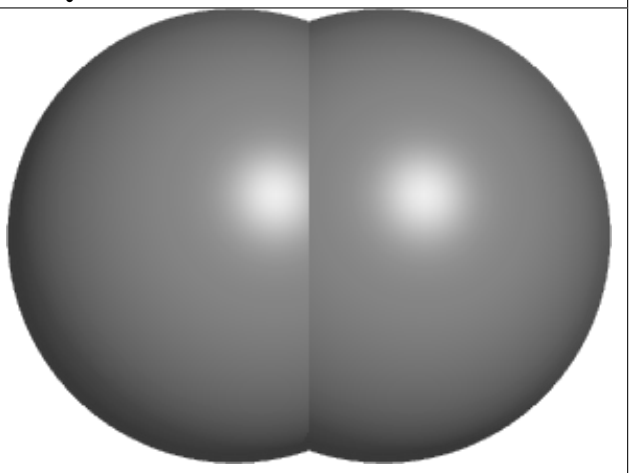
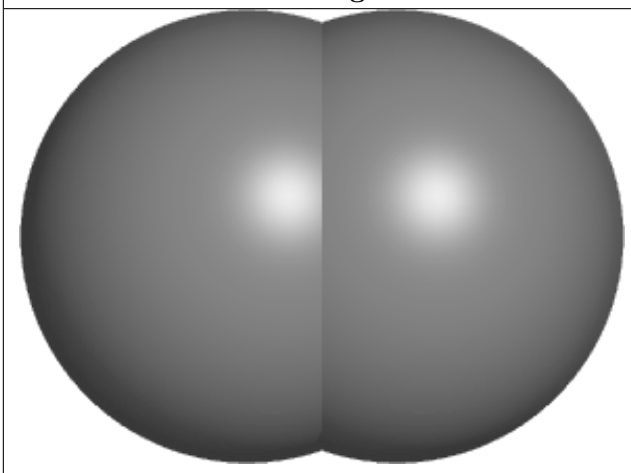
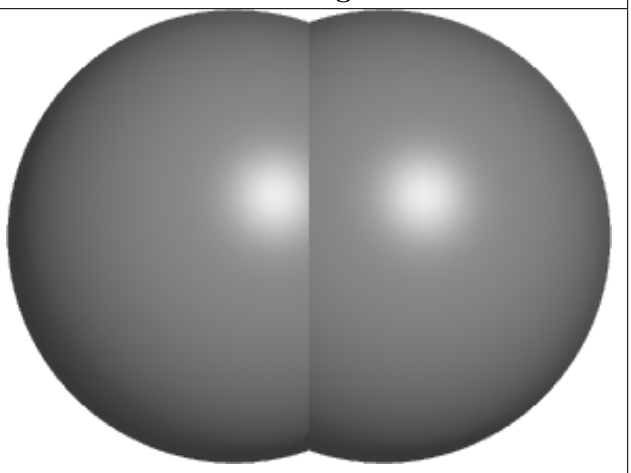

Rings

| Ligand IX7 U 204 | |
|---|---|
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

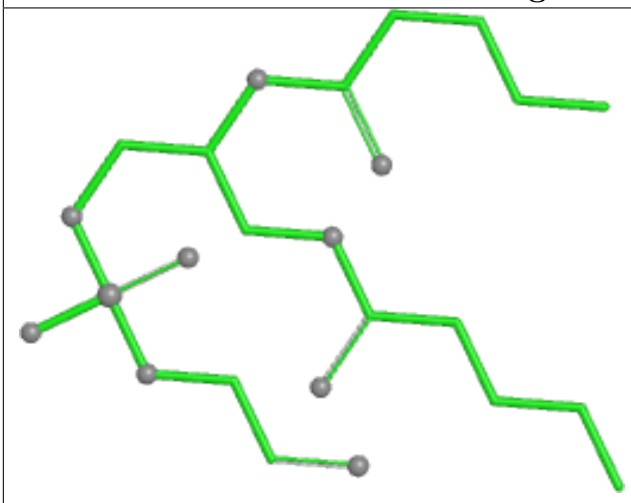
| Ligand 3PE T 203 | |
|---|---|
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

| Ligand SMA O 602 | |
|---|---|
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

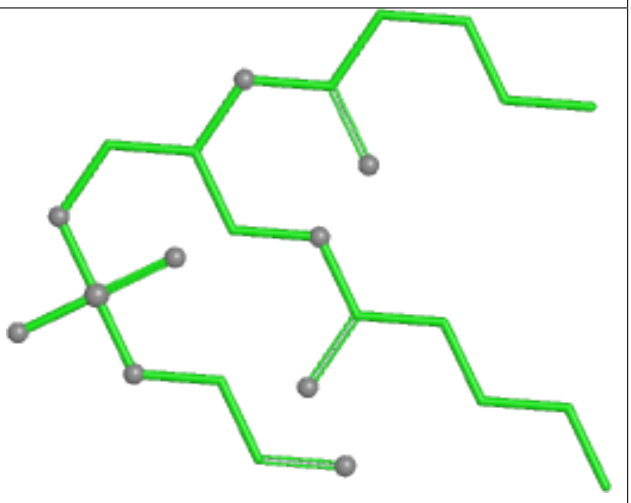
| Ligand MQ9 B 604 | |
|---|---|
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

| Ligand OXY Q 606 | |
|---|---|
|  |  |
| **Bond lengths** | **Bond angles** |
|  |  |
| **Torsions** | **Rings** |

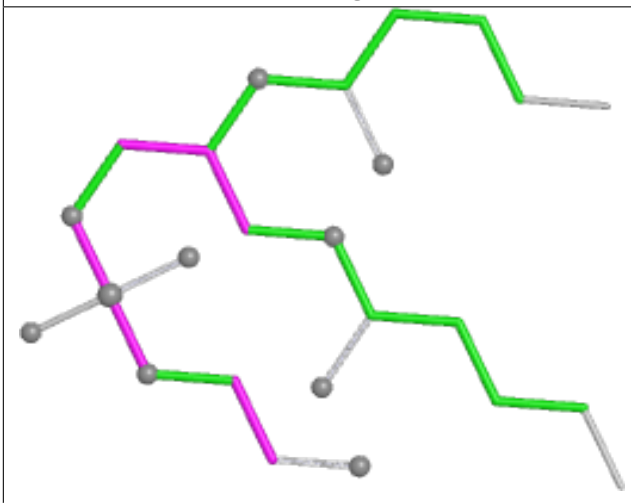
**Ligand 3PE C 304**



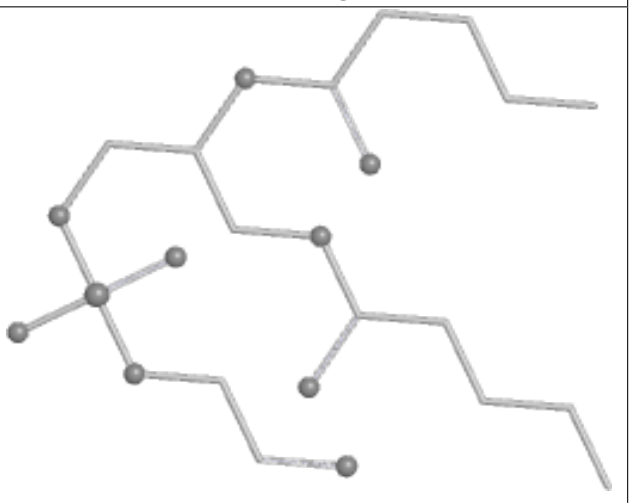
Bond lengths



Bond angles

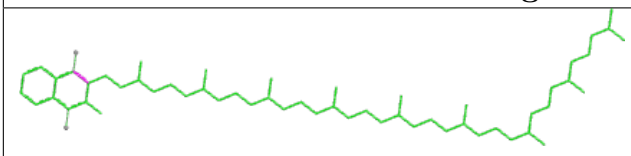


Torsions

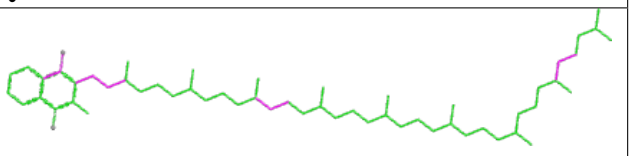


Rings

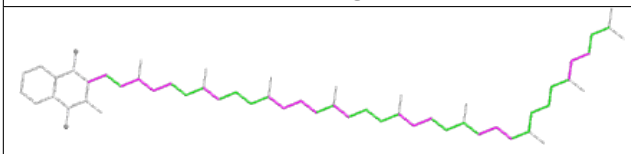
**Ligand MQ9 A 504**



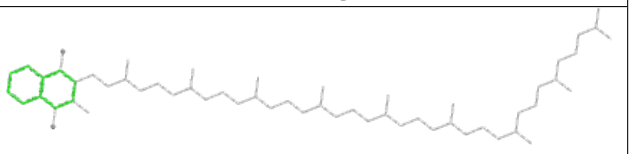
Bond lengths



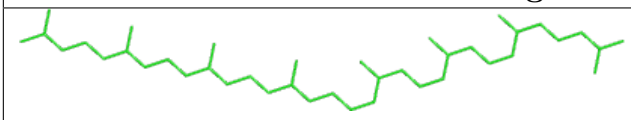
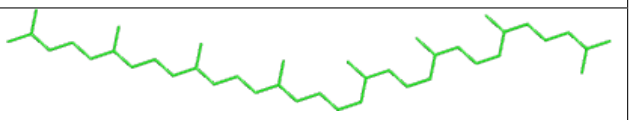
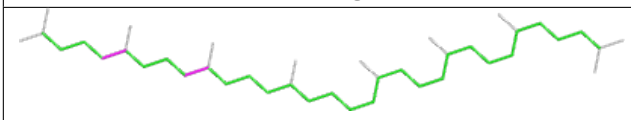
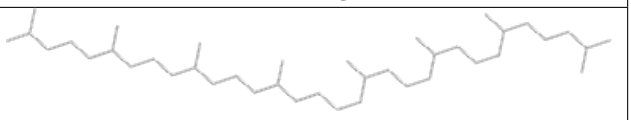
Bond angles

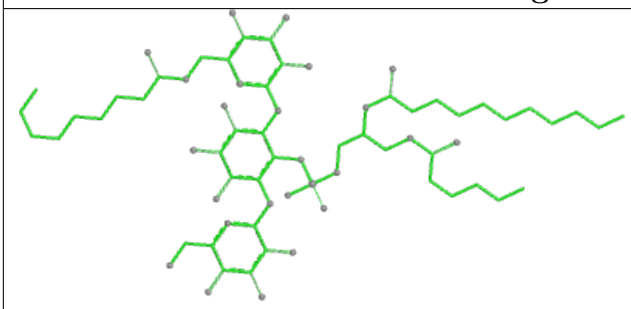
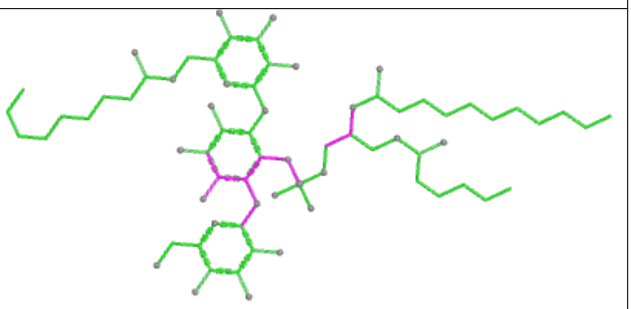
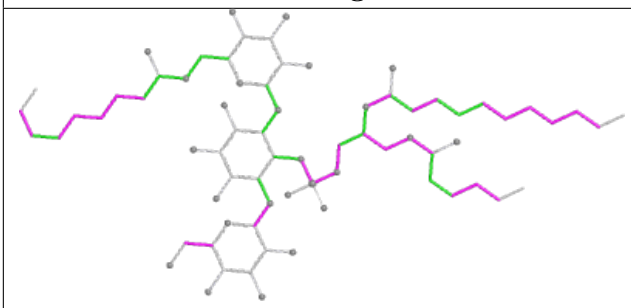
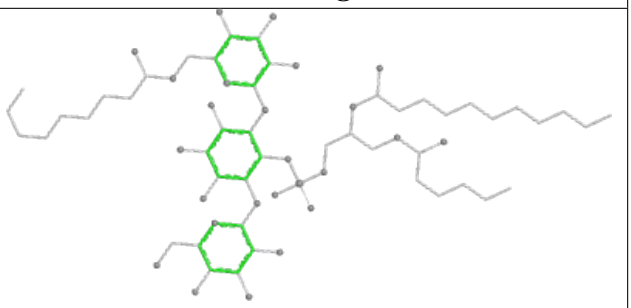


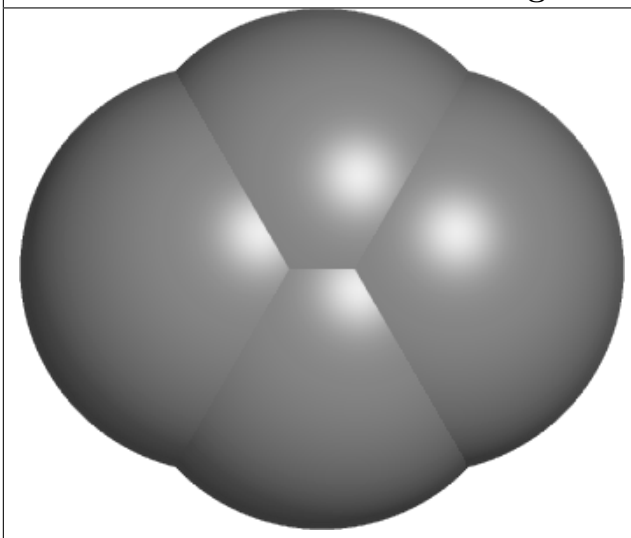
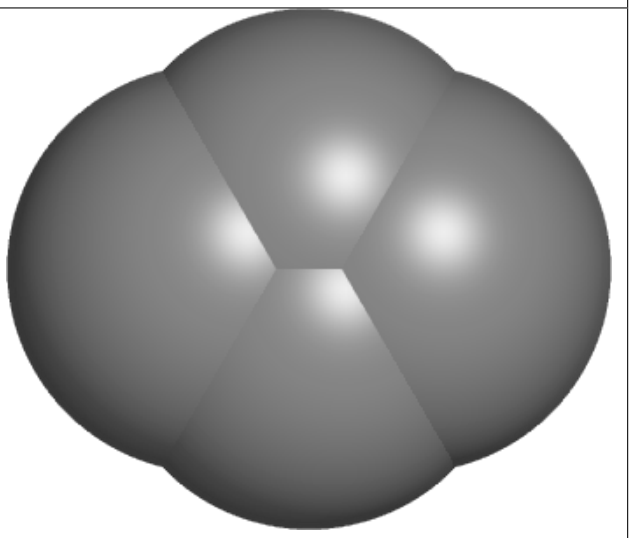
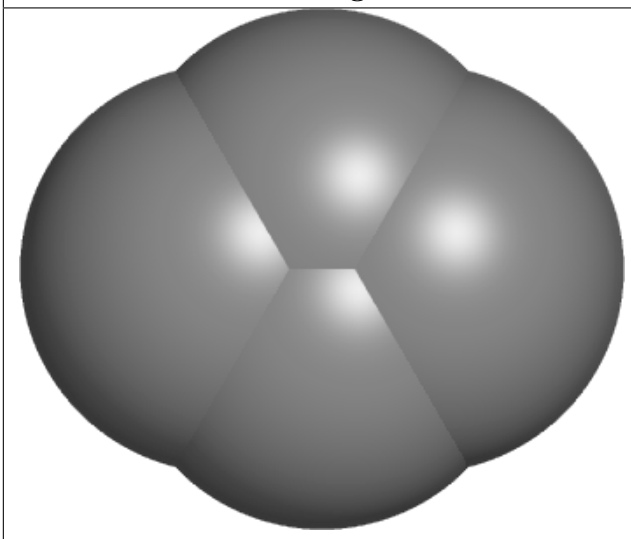
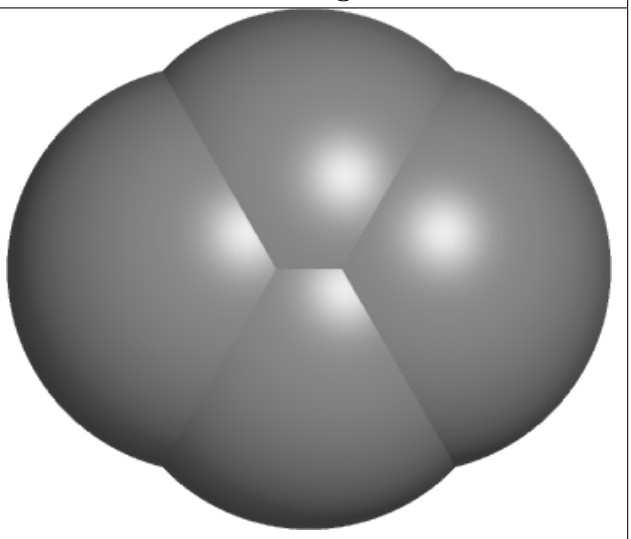
Torsions



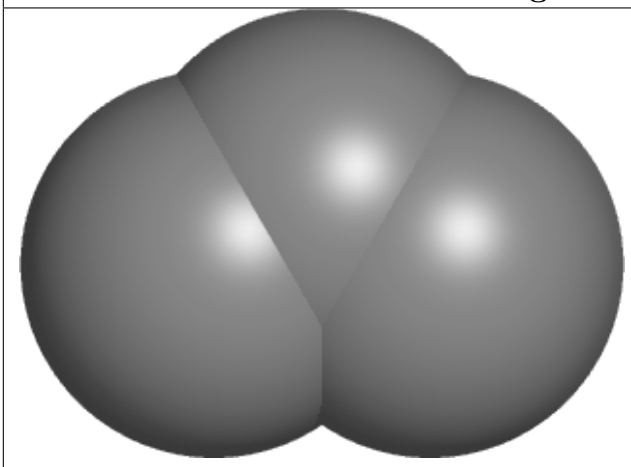
Rings

| Ligand LYC B 607 | |
|---|---|
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

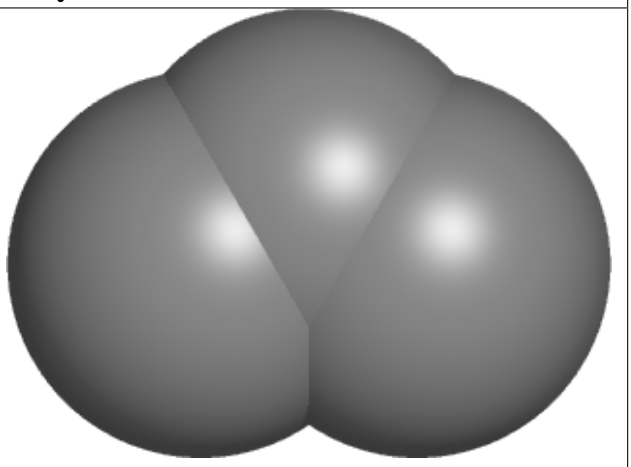
| Ligand IX7 H 204 | |
|---|---|
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

| Ligand FES A 501 | |
|---|---|
|  |  |
| **Bond lengths** | **Bond angles** |
|  |  |
| **Torsions** | **Rings** |

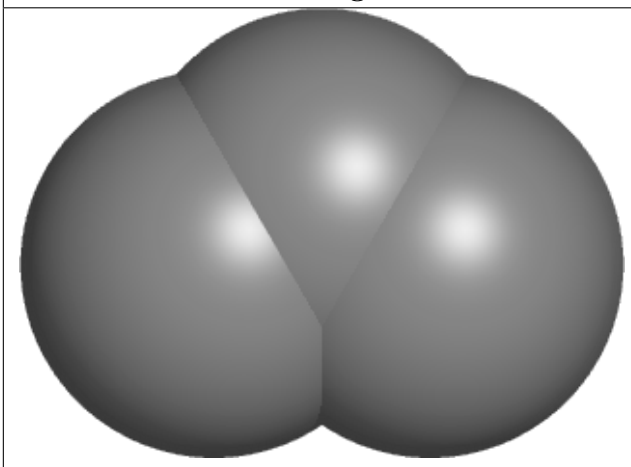
## Ligand AZI Q 605



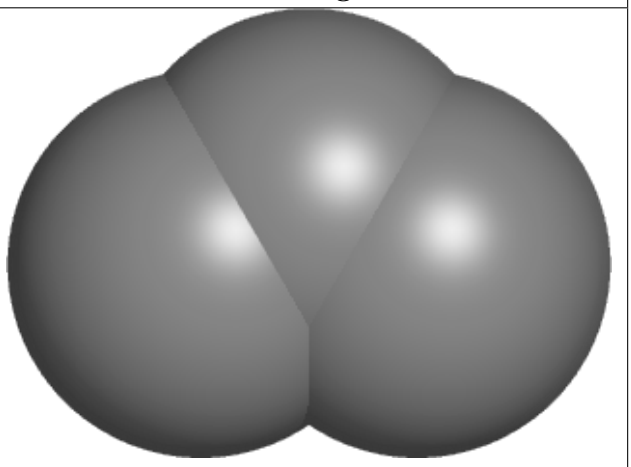
Bond lengths



Bond angles

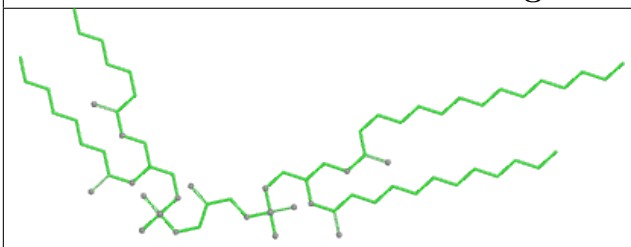


Torsions

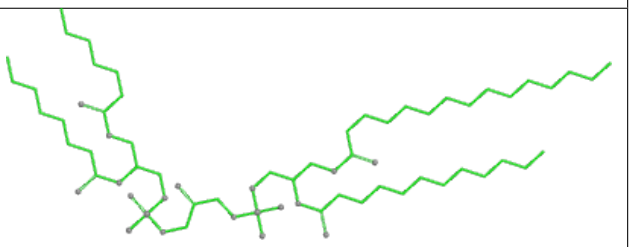


Rings

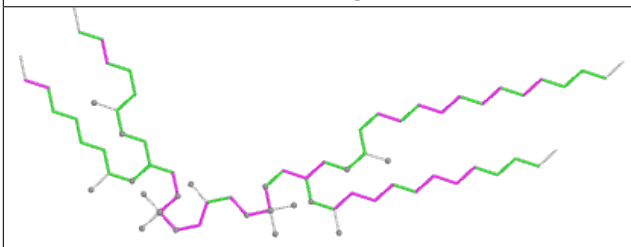
## Ligand CDL B 609



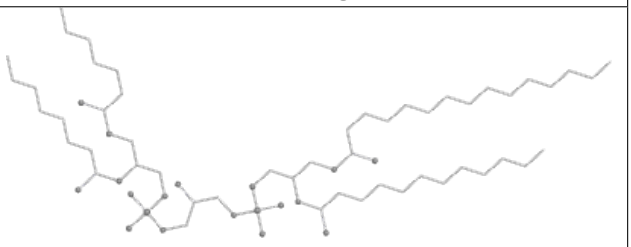
Bond lengths



Bond angles

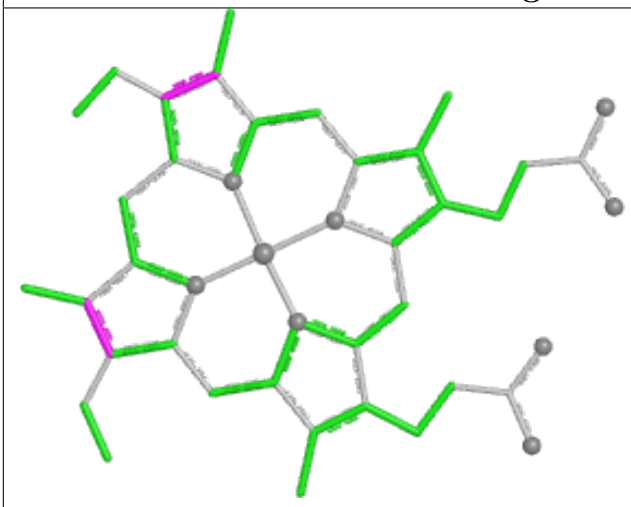


Torsions

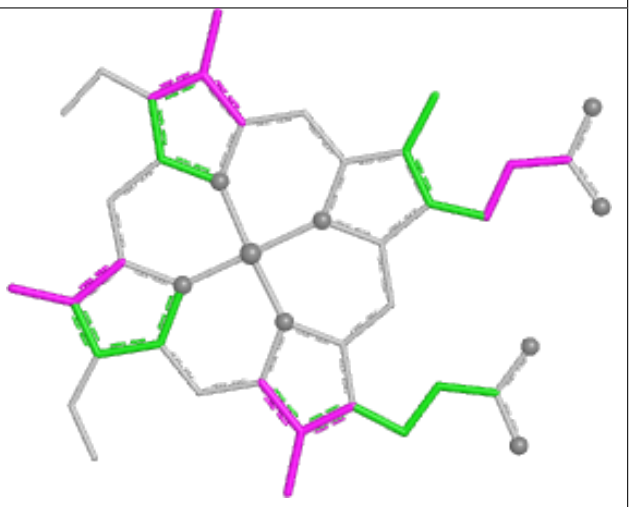


Rings

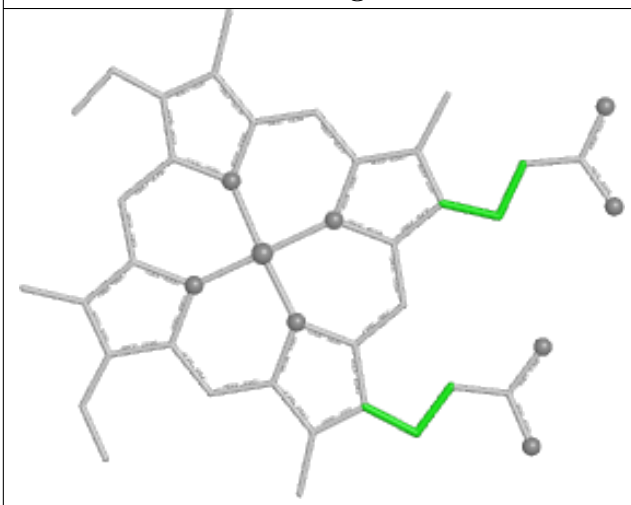
## Ligand HEC C 302



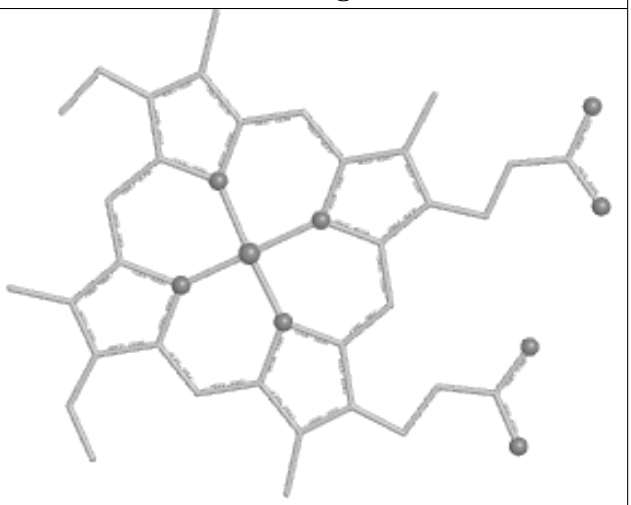
Bond lengths



Bond angles

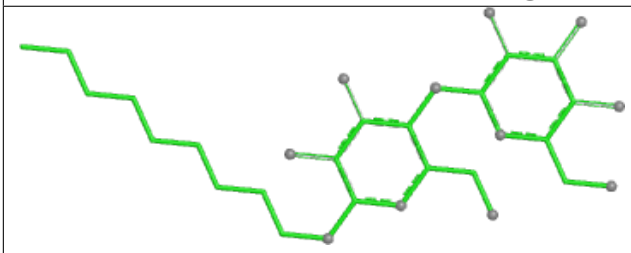


Torsions

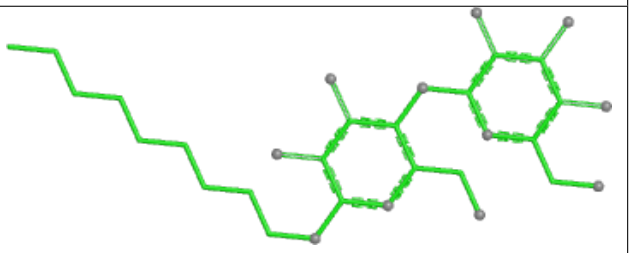


Rings

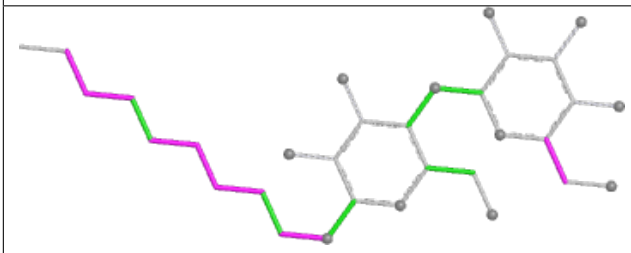
## Ligand LMT B 608



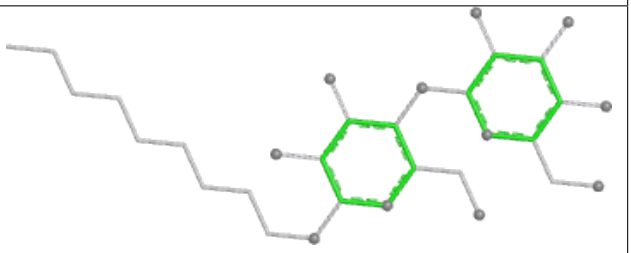
Bond lengths



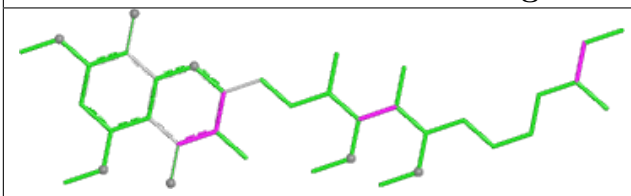
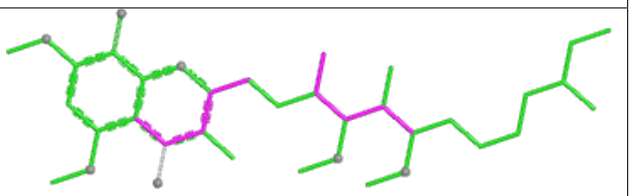
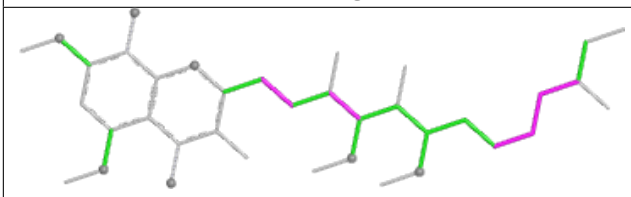
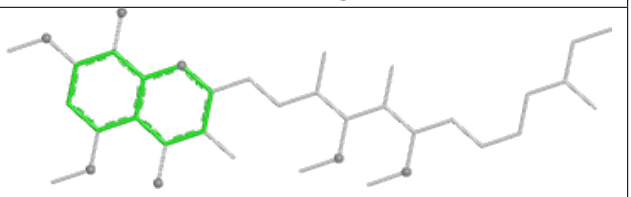
Bond angles

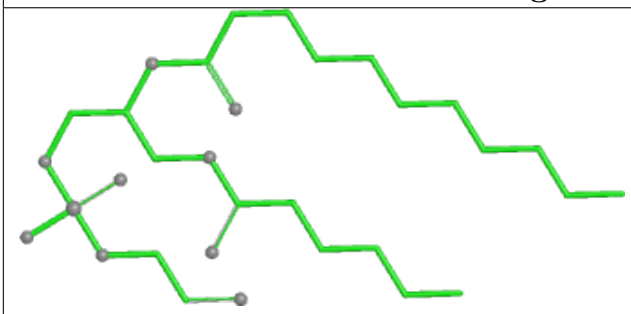
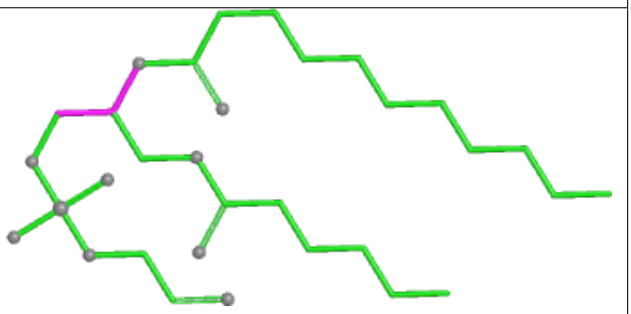
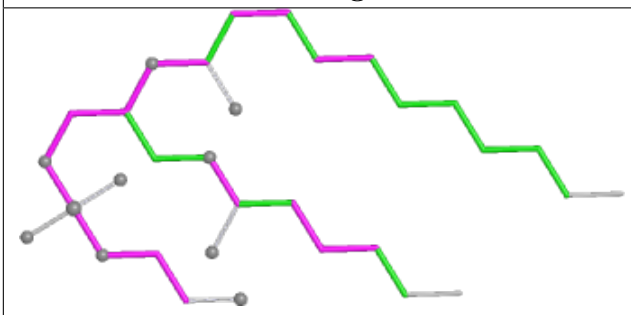
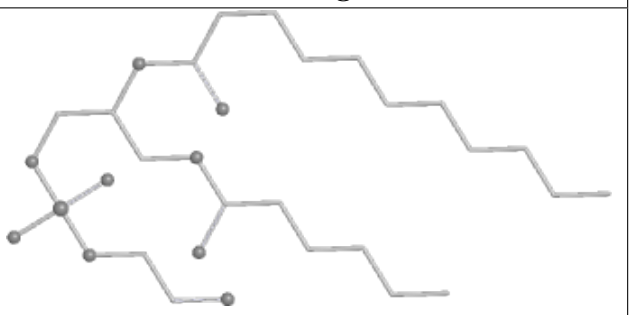


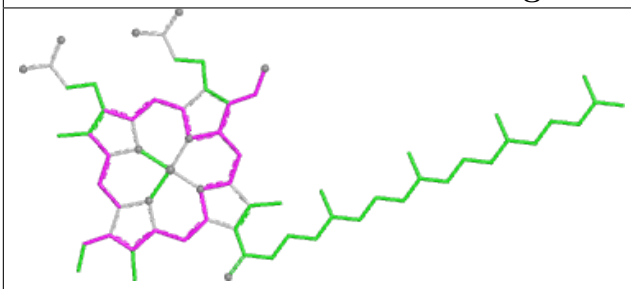
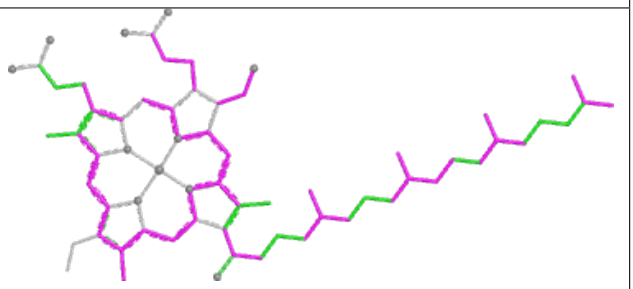
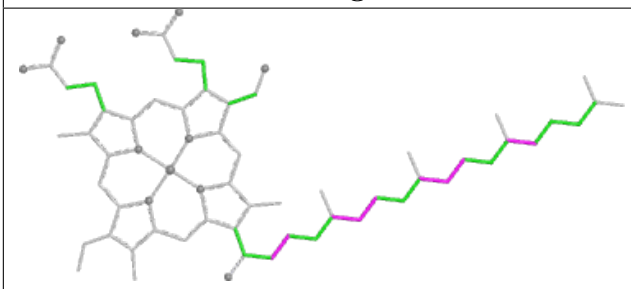
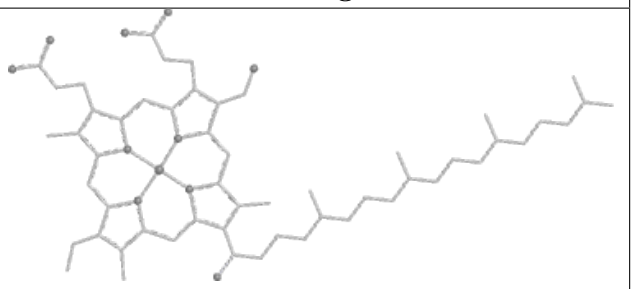
Torsions

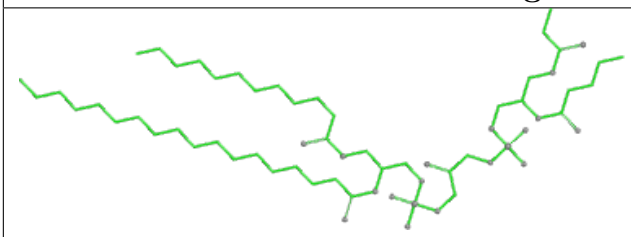
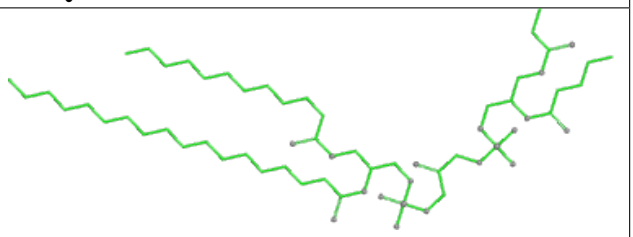
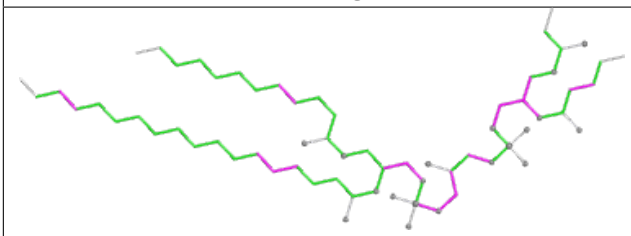
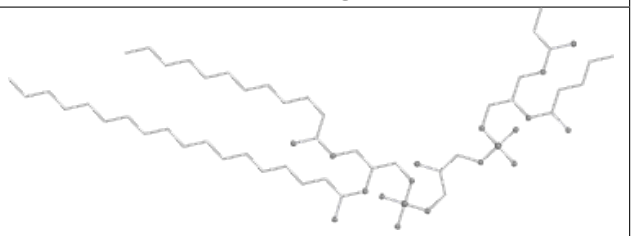


Rings

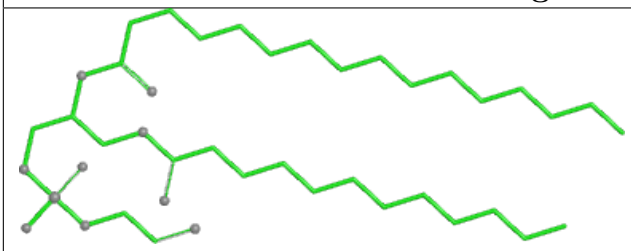
| Ligand SMA B 601 | |
|---|---|
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

| Ligand 3PE F 301 | |
|---|---|
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

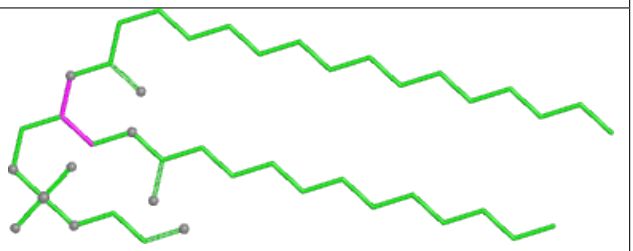
| Ligand HAS D 601 | |
|---|---|
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

| Ligand CDL Q 608 | |
|---|---|
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

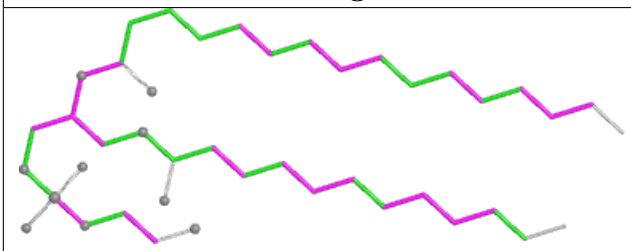
## Ligand 3PE S 301



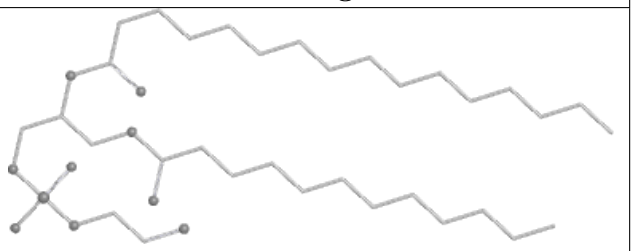
Bond lengths



Bond angles

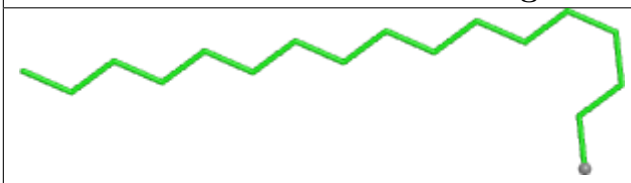


Torsions

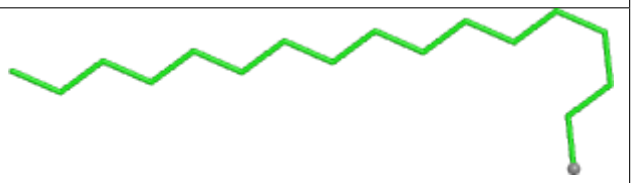


Rings

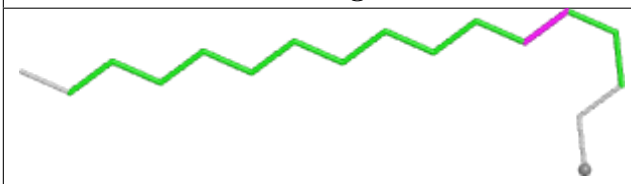
## Ligand PLM H 202



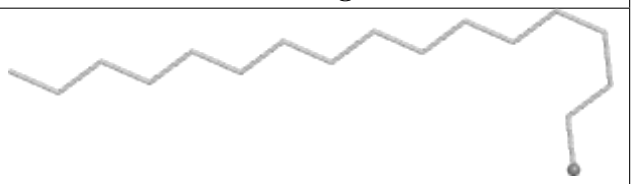
Bond lengths



Bond angles

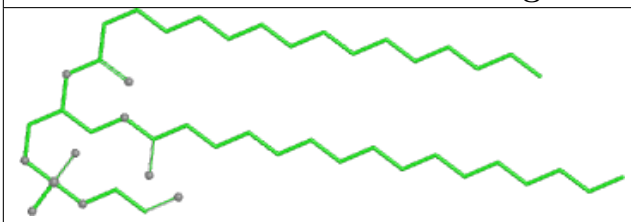


Torsions

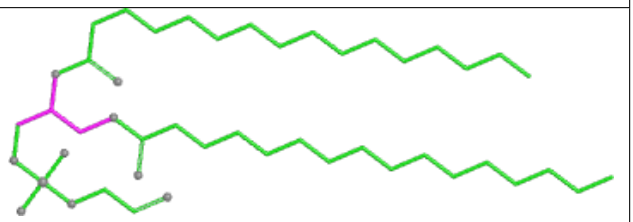


Rings

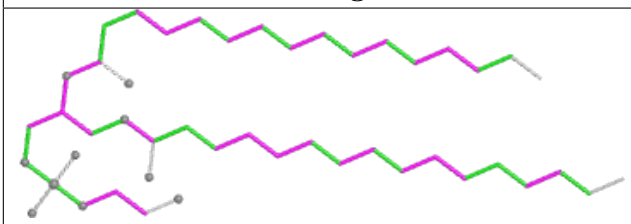
## Ligand 3PE W 201



Bond lengths



Bond angles



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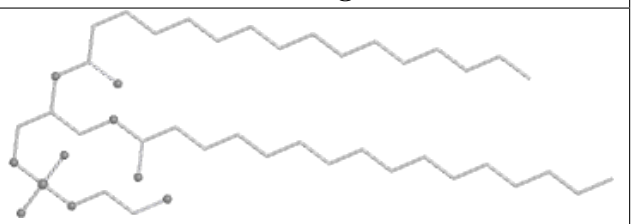
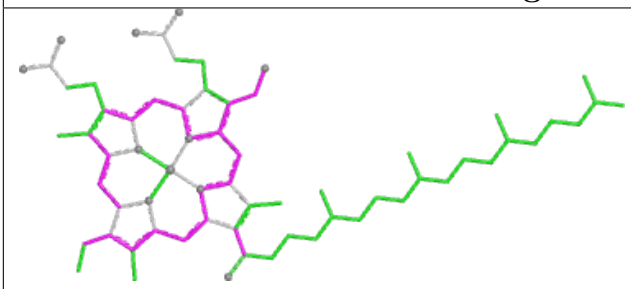
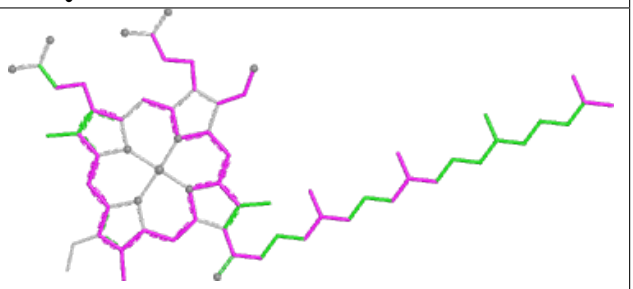
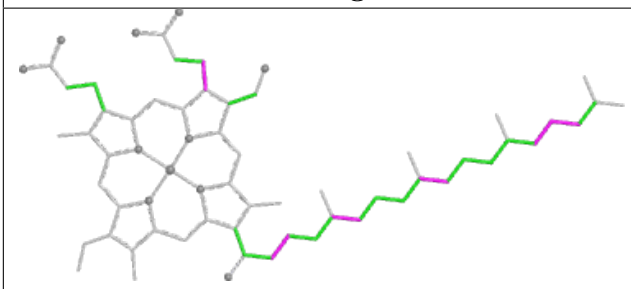
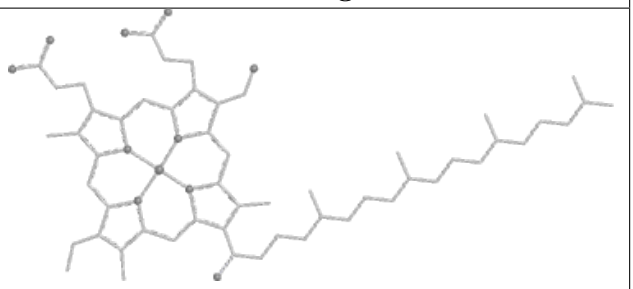
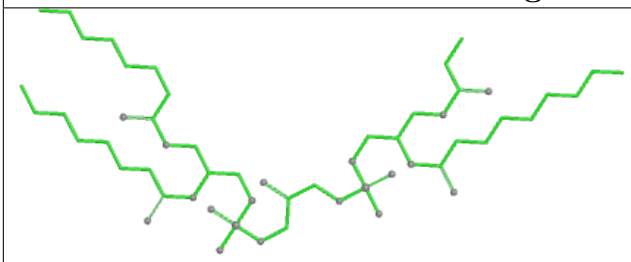
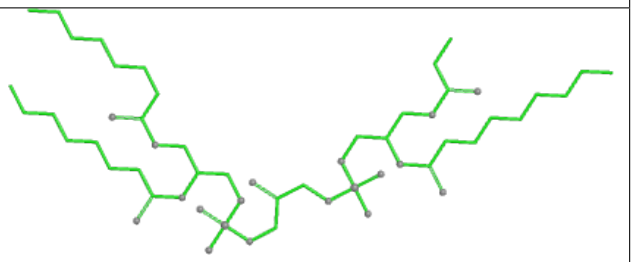
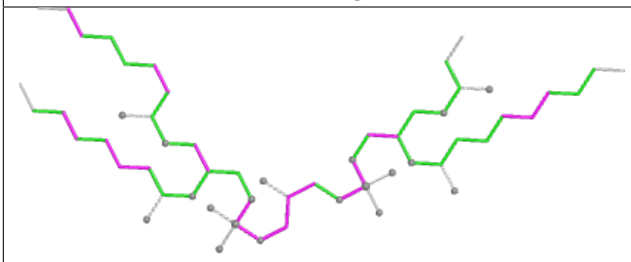
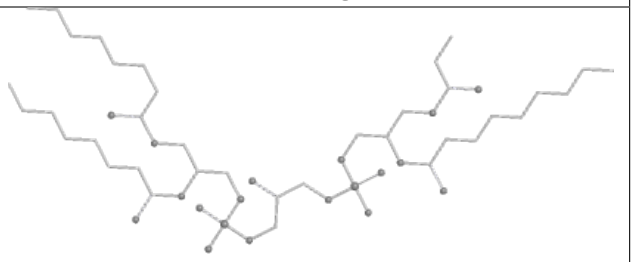
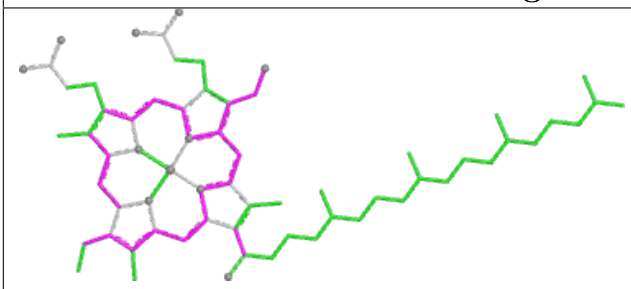


Rings

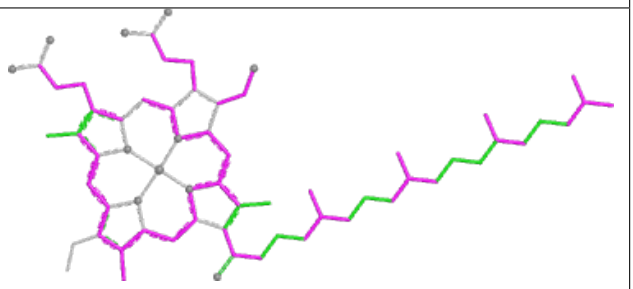
| Ligand HAS Q 601 | |
|---|---|
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

| Ligand CDL B 605 | |
|---|---|
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

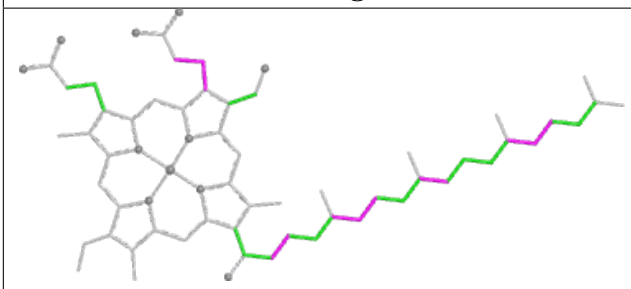
## Ligand HAS D 602



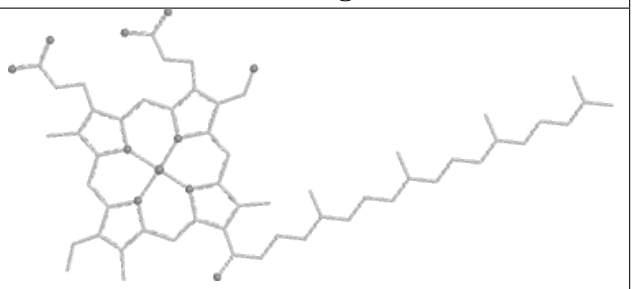
Bond lengths



Bond angles

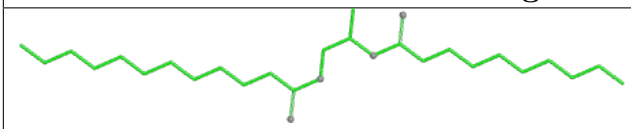


Torsions

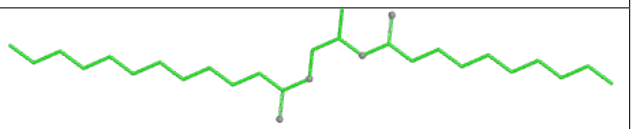


Rings

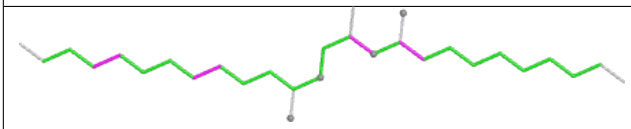
## Ligand DGA Z 201



Bond lengths



Bond angles



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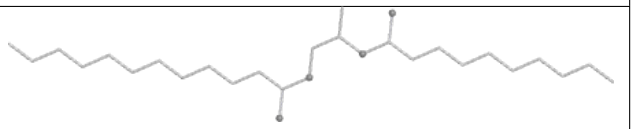
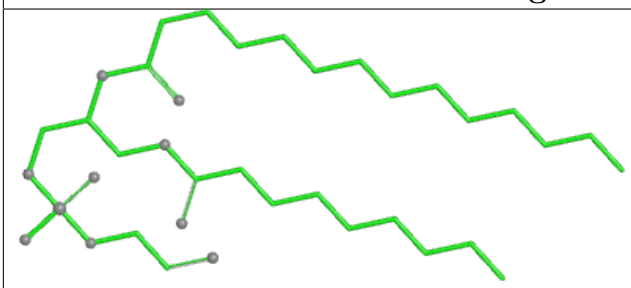
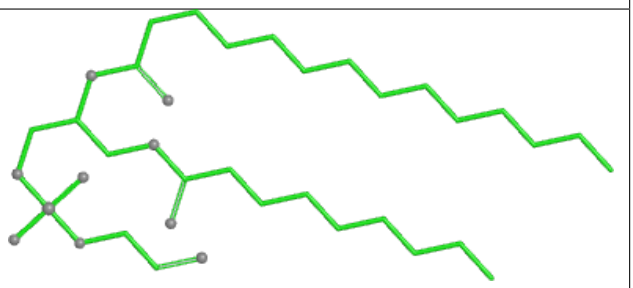


Rings

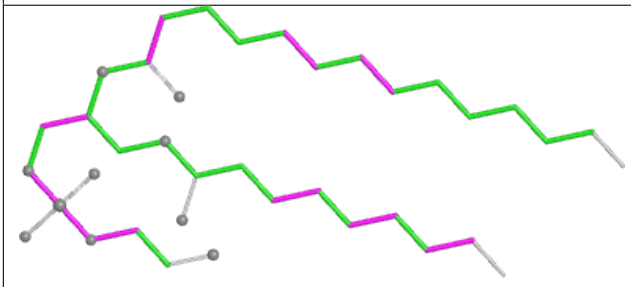
## Ligand 3PE T 205



Bond lengths



Bond angles



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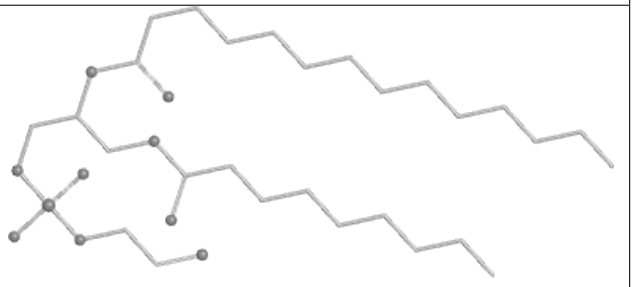
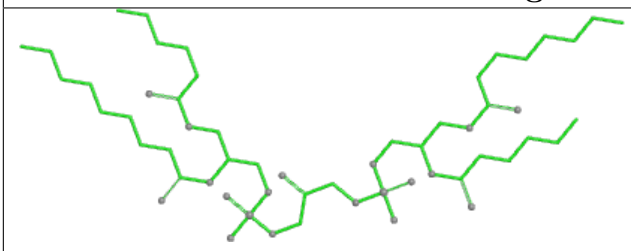
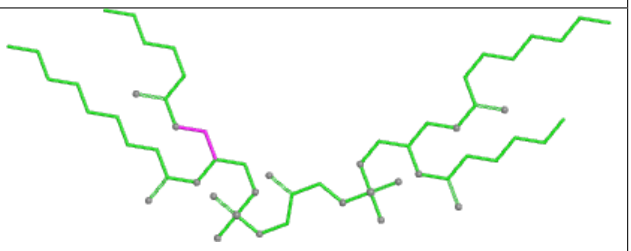
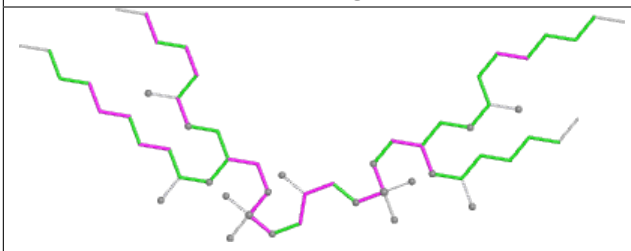


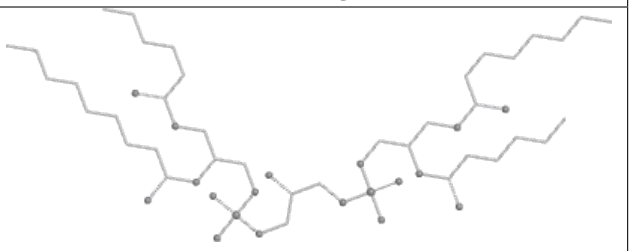
Rings

## Ligand CDL F 302

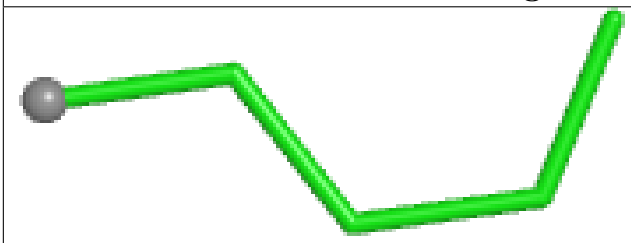

Bond lengths

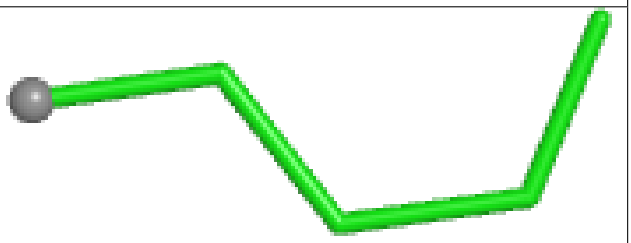

Bond angles

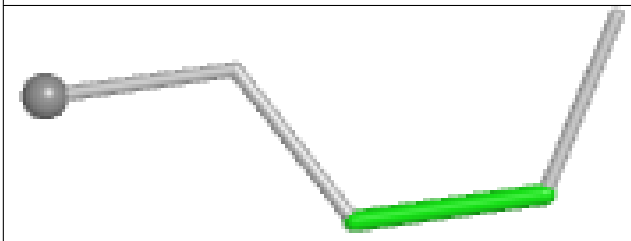

Torsions

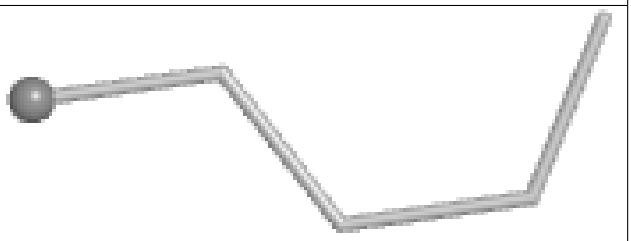

Rings

## Ligand PLM Z 202

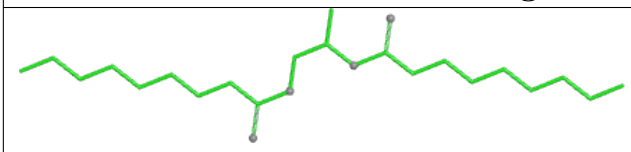

Bond lengths

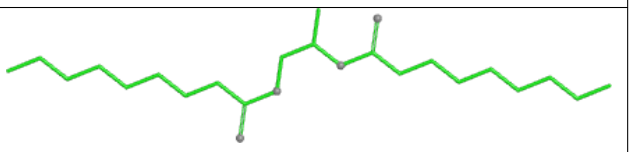

Bond angles

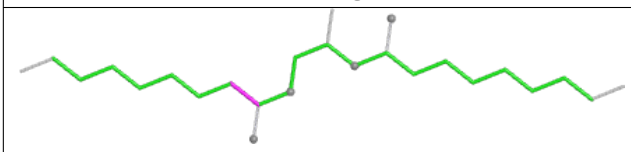

Torsions

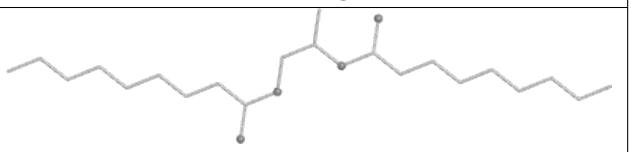

Rings

## Ligand DGA R 404

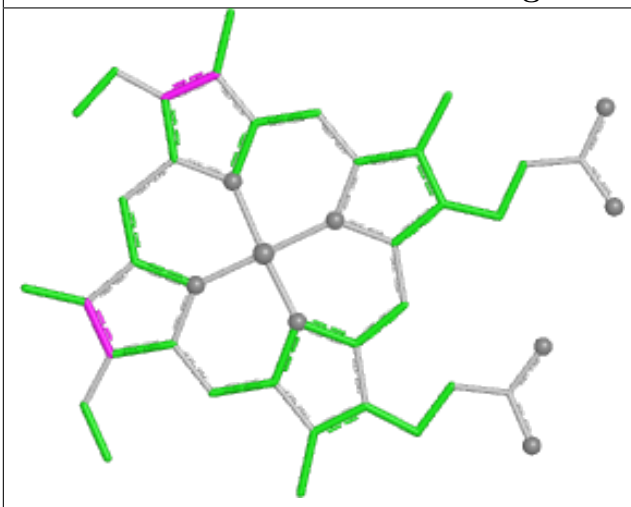

Bond lengths


Bond angles

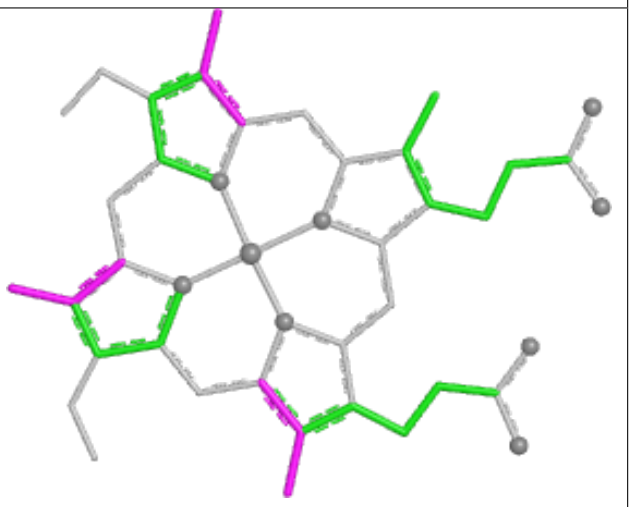

Torsions


Rings

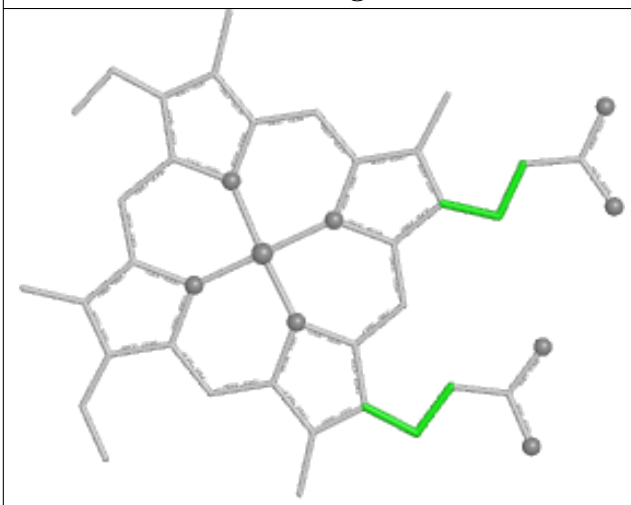
## Ligand HEC C 301



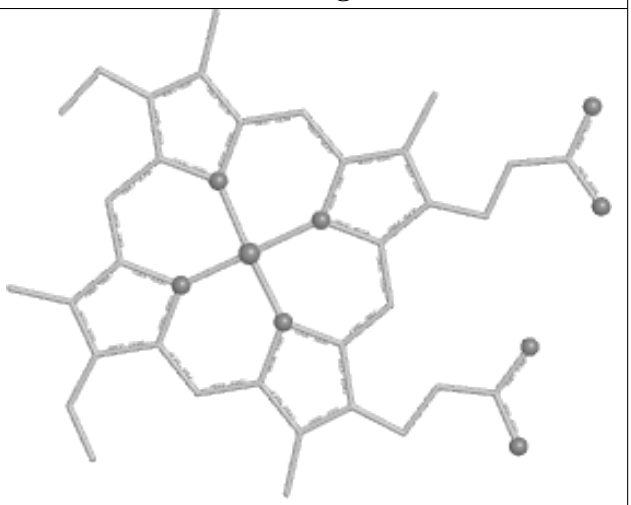
Bond lengths



Bond angles

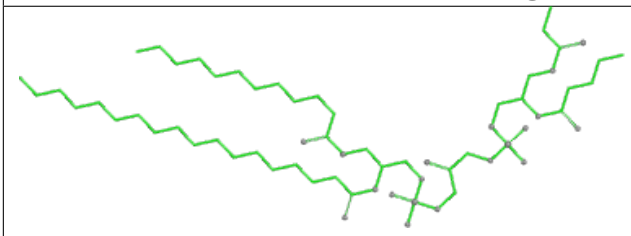


Torsions

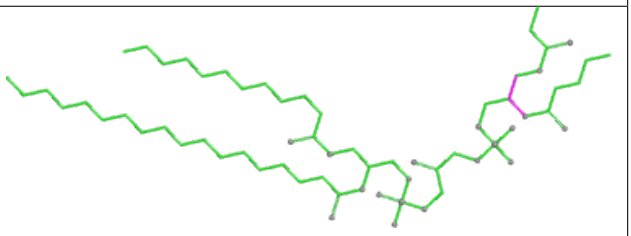


Rings

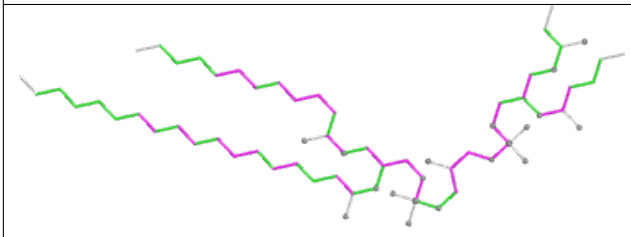
## Ligand CDL O 606



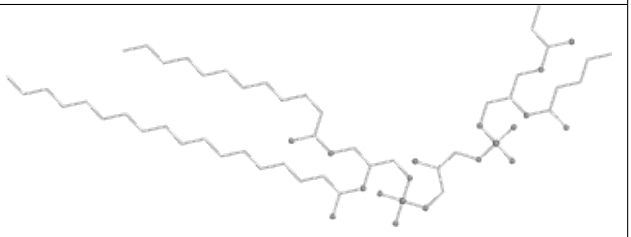
Bond lengths



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.

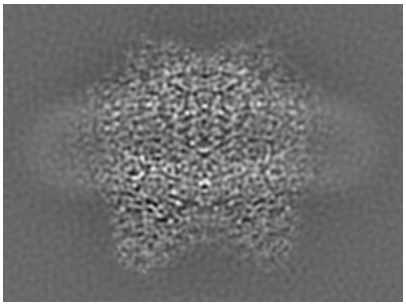
# 6 Map visualisation

This section contains visualisations of the EMDB entry EMD-13976. These allow visual inspection of the internal detail of the map and identification of artifacts.

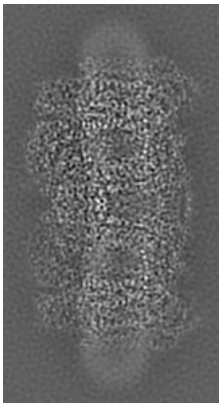
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

## 6.1 Orthogonal projections

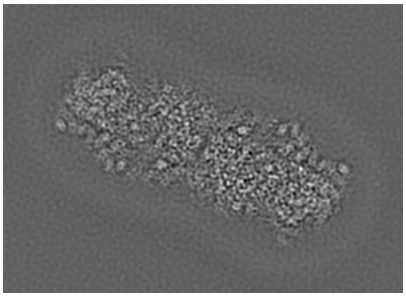
### 6.1.1 Primary map



X



Y

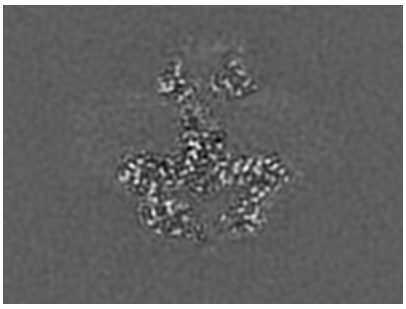


Z

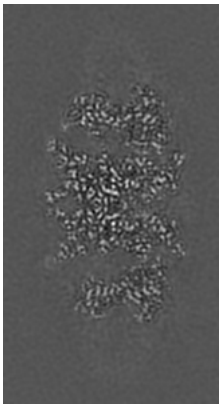
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices

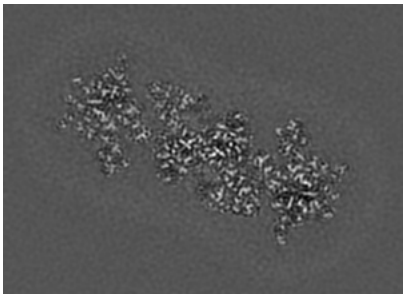
### 6.2.1 Primary map



X Index: 165



Y Index: 119

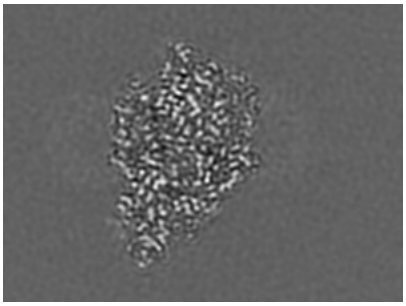


Z Index: 88

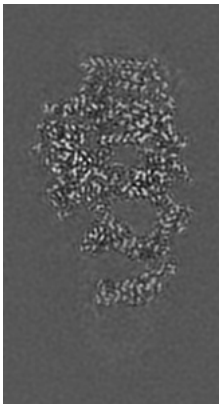
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices (i)

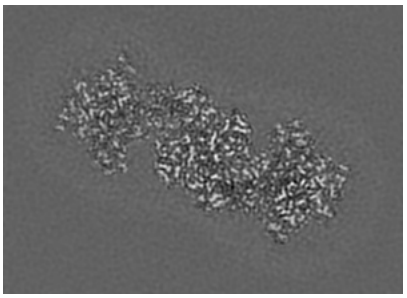
### 6.3.1 Primary map



X Index: 190



Y Index: 102



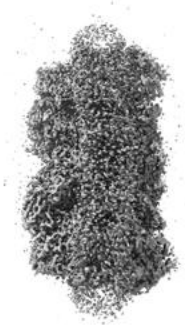
Z Index: 80

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

## 6.4 Orthogonal surface views (i)

### 6.4.1 Primary map

X



Y

Z

The images above show the 3D surface view of the map at the recommended contour level 0.09. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

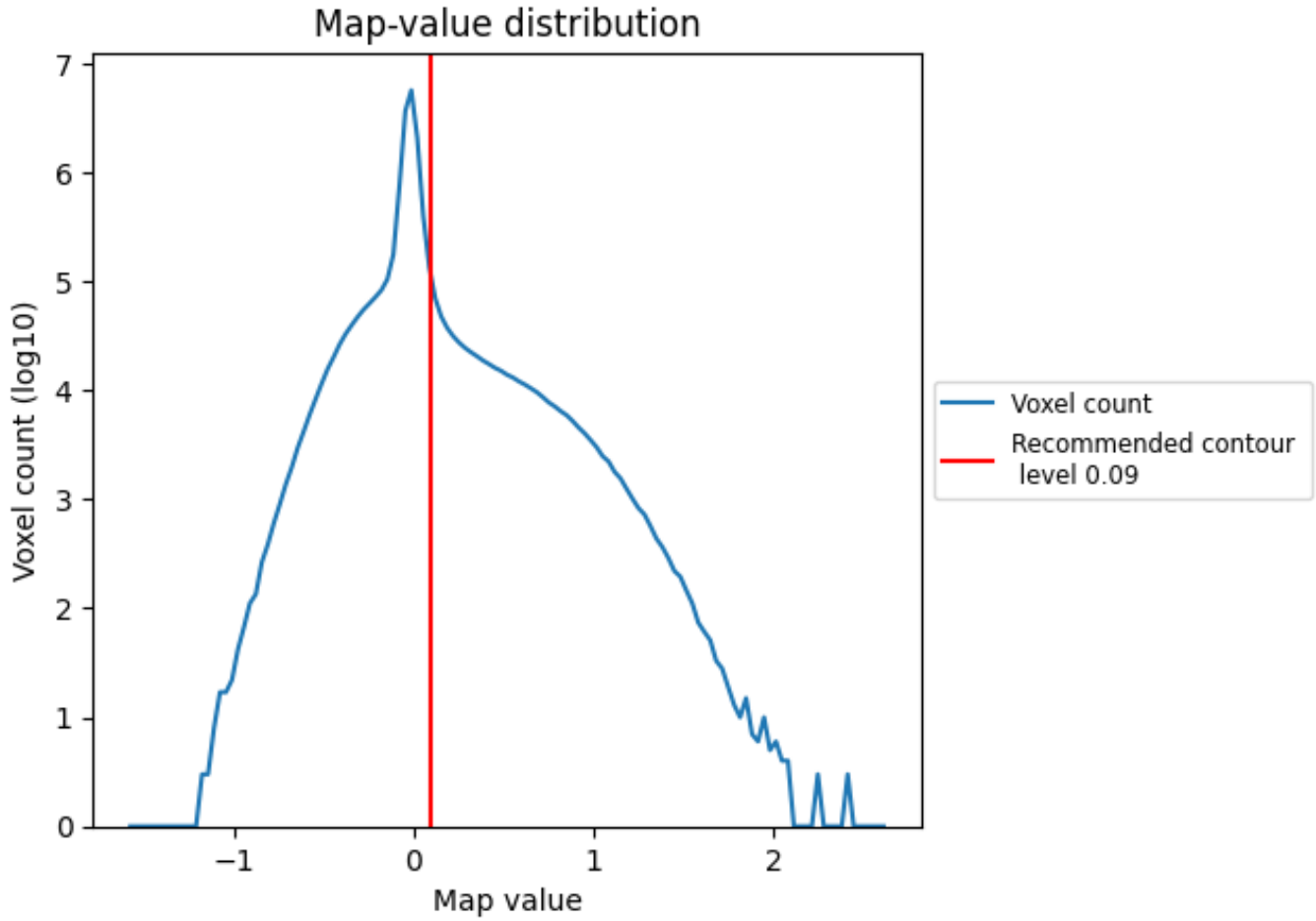
## 6.5 Mask visualisation (i)

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

# 7 Map analysis

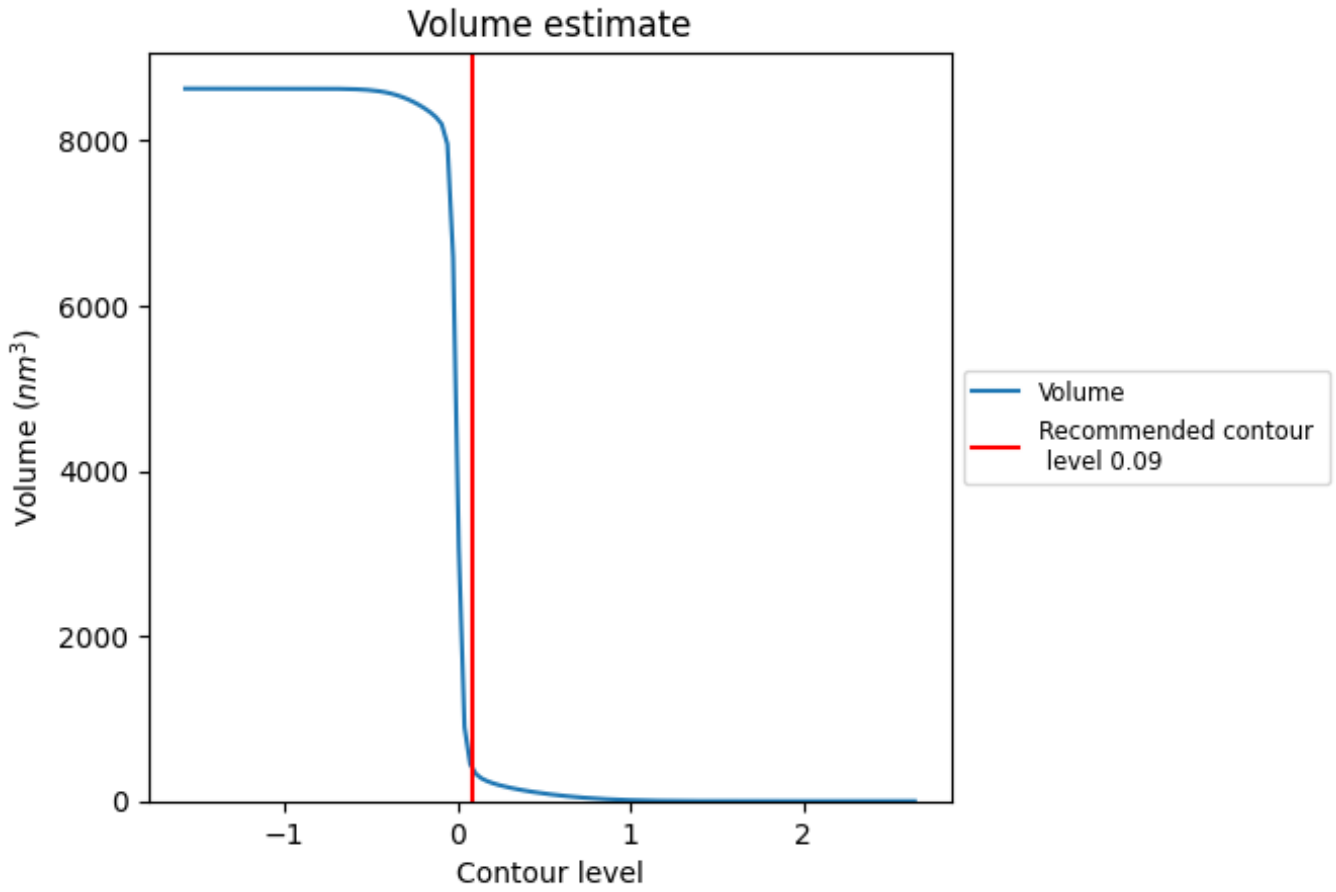
This section contains the results of statistical analysis of the map.

## 7.1 Map-value distribution




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

## 7.2 Volume estimate




The volume at the recommended contour level is 385 $nm^3$; this corresponds to an approximate mass of 348 kDa.

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

## 7.3 Rotationally averaged power spectrum

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

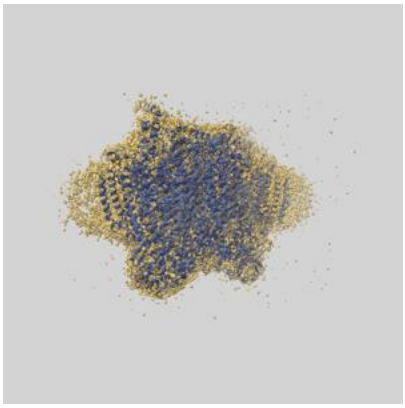
# 8 Fourier-Shell correlation

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

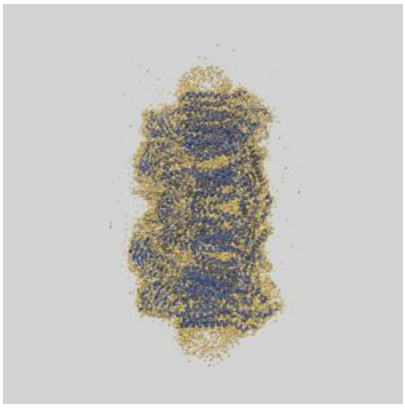
# 9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-13976 and PDB model 7QHM. Per-residue inclusion information can be found in section 3 on page 22.

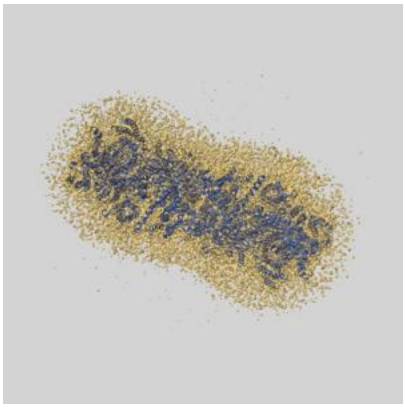
## 9.1 Map-model overlay



X



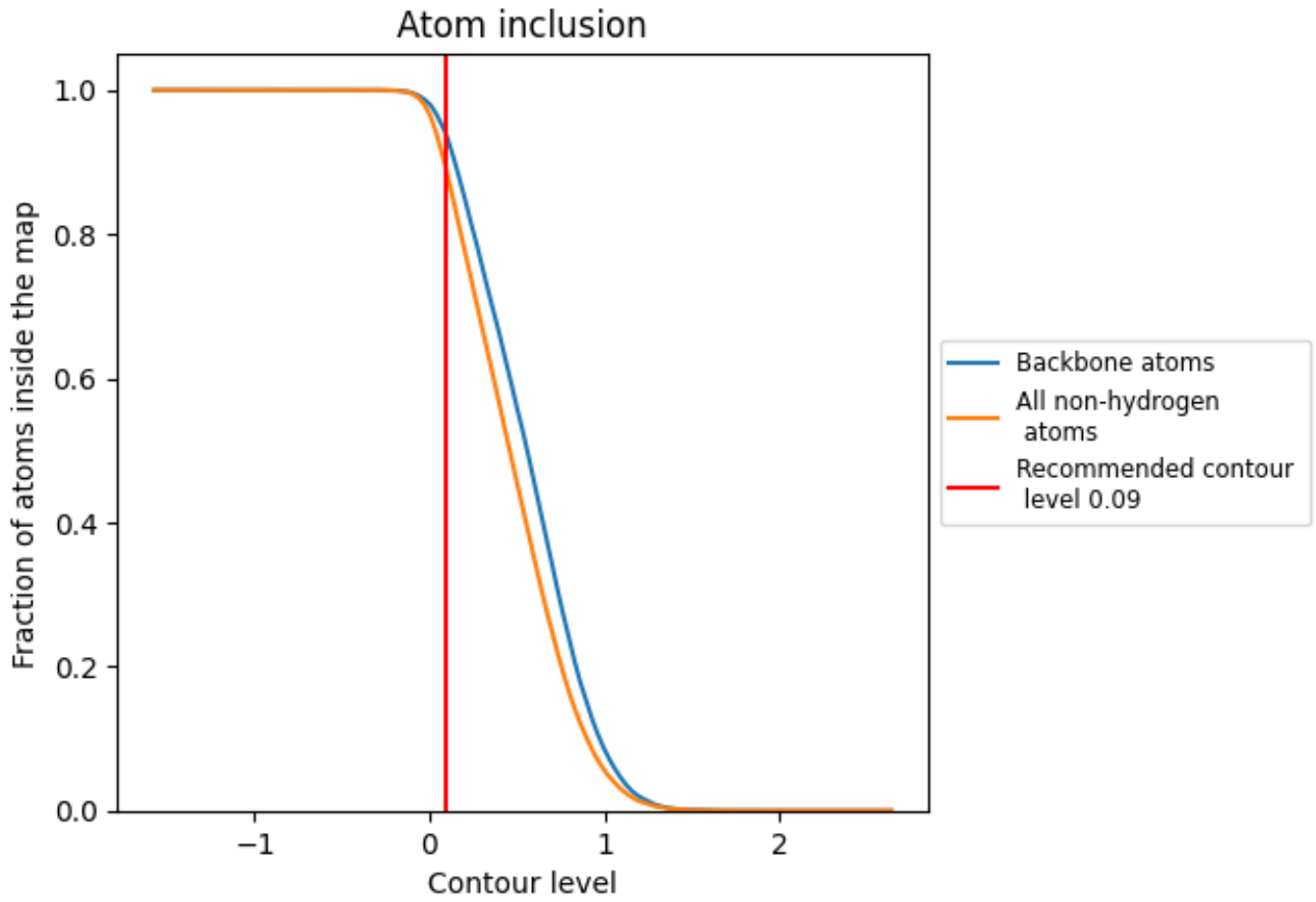
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.09 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 9.2 Atom inclusion (i)




At the recommended contour level, 94% of all backbone atoms, 90% of all non-hydrogen atoms, are inside the map.