# Full wwPDB EM Validation Report ⓘ

Aug 27, 2026 – 02:24 pm BST

| | | |
|---|---|---|
| PDB ID | : | 8B6H / pdb_00008b6h |
| EMDB ID | : | EMD-15867 |
| Title | : | Cryo-EM structure of cytochrome c oxidase dimer (complex IV) from respiratory supercomplex of Tetrahymena thermophila |
| Authors | : | Muhleip, A.; Kock Flygaard, R.; Amunts, A. |
| Deposited on | : | 2022-09-27 |
| Resolution | : | 2.60 Å(reported) |

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

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

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

---

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

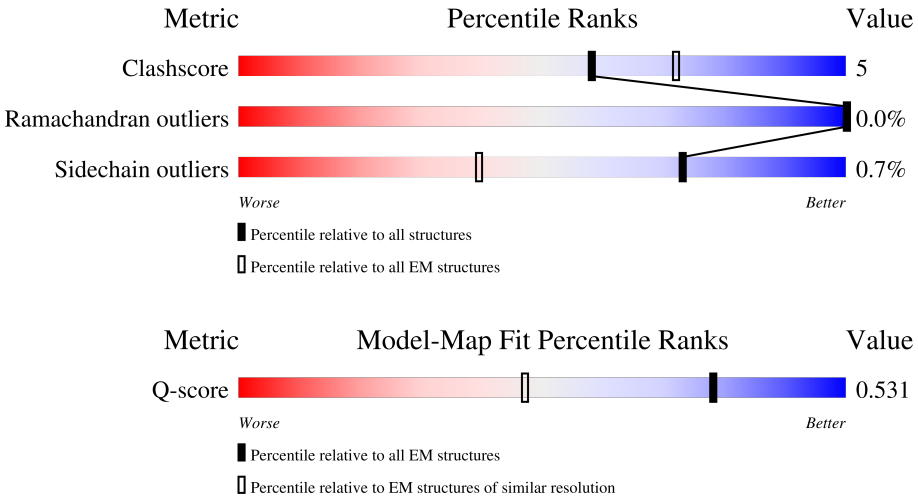
| | | |
|---|---|---|
| EMDB validation analysis | : | 0.0.1.dev133 |
| Mogul | : | 1.8.4, CSD as541be (2020) |
| MolProbity | : | 4-5-2 with Phenix2.0 |
| Buster-report | : | wwPDB partial adaption of 1.1.7 (2018) |
| Percentile statistics | : | 20250101.v01 (using entries in the PDB archive January 1st 2025) |
| EM percentile statistics | : | 202505.v01 (Using data in the EMDB archive up until May 2025) |
| MapQ | : | 1.9.13 |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | 2.50 |

# 1 Overall quality at a glance

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

The reported resolution of this entry is 2.60 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) | Similar EM resolution (#Entries, resolution range(Å)) |
|---|---|---|---|
| Clashscore | 229148 | 23984 | - |
| Ramachandran outliers | 224038 | 23583 | - |
| Sidechain outliers | 223484 | 23102 | - |
| Q-score | - | 25397 | 8728 ( 2.10 - 3.10 ) |

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 | DA | 688 | 83% 15% |
| 1 | Da | 688 | 82% 15% |
| 2 | DB | 604 | 88% 12% |
| 2 | Db | 604 | 86% 14% |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 3 | DC | 594 | 6% 83% 15% |
| 3 | Dc | 594 | 7% 84% 14% |
| 4 | DD | 637 | 76% 12% 12% |
| 4 | Dd | 637 | 76% 11% 12% |
| 5 | DE | 130 | 87% 10% |
| 5 | De | 130 | 82% 14% |
| 6 | DF | 230 | 84% 12% |
| 6 | Df | 230 | 85% 11% |
| 7 | DG | 103 | 83% 12% 5% |
| 7 | Dg | 103 | 87% 8% 5% |
| 8 | DH | 133 | 77% 23% |
| 8 | Dh | 133 | 80% 20% |
| 9 | DI | 236 | 78% 8% 13% |
| 9 | Di | 236 | 78% 9% 13% |
| 10 | DJ | 220 | 83% 16% |
| 10 | Dj | 220 | 87% 13% |
| 11 | DK | 990 | 11% 87% |
| 11 | Dk | 990 | 12% 87% |
| 12 | DM | 490 | 81% 12% 7% |
| 12 | Dm | 490 | 80% 13% 7% |
| 13 | DN | 453 | 6% 90% 9% |
| 13 | Dn | 453 | 8% 88% 12% |
| 14 | DO | 473 | 11% 81% 11% 8% |
| 14 | Do | 473 | 26% 80% 12% 8% |
| 15 | DP | 402 | 65% 7% 28% |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 15 | Dp | 402 | 65% 7% 28% |
| 16 | DQ | 385 | 85% 14% |
| 16 | Dq | 385 | 86% 14% |
| 17 | DR | 348 | 61% 9% 30% |
| 17 | Dr | 348 | 59% 11% 30% |
| 18 | DS | 346 | 85% 14% |
| 18 | Ds | 346 | 84% 16% |
| 19 | DT | 318 | 74% 18% 8% |
| 19 | Dt | 318 | 76% 16% 8% |
| 20 | DU | 330 | 86% 13% |
| 20 | Du | 330 | 81% 18% |
| 21 | DV | 318 | 87% 13% |
| 21 | Dv | 318 | 86% 13% |
| 22 | DW | 318 | 5% 87% 7% 5% |
| 22 | Dw | 318 | 6% 86% 8% 5% |
| 23 | DX | 252 | 88% 12% |
| 23 | Dx | 252 | 87% 12% |
| 24 | DY | 234 | 69% 11% 20% |
| 24 | Dy | 234 | 69% 10% 20% |
| 25 | DZ | 231 | 80% 10% 10% |
| 25 | Dz | 231 | 75% 15% 10% |
| 26 | EA | 215 | 78% 12% 10% |
| 26 | Ea | 215 | 78% 12% 10% |
| 27 | EB | 210 | 91% 9% |
| 27 | Eb | 210 | 86% 14% |

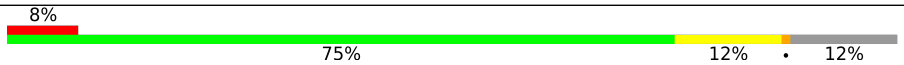
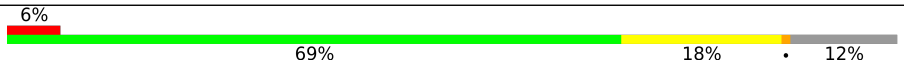
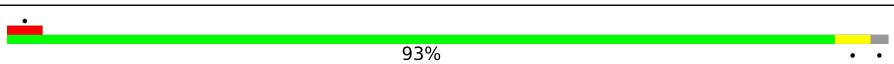
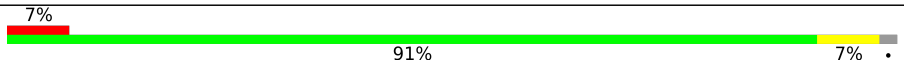
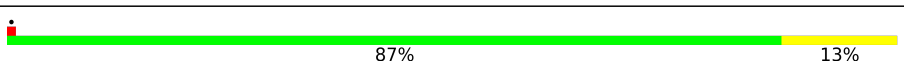
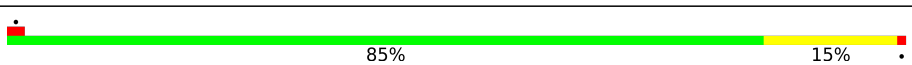
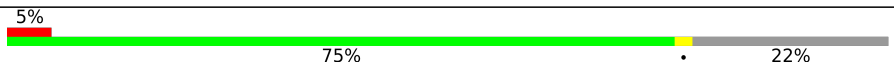
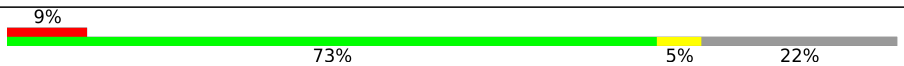
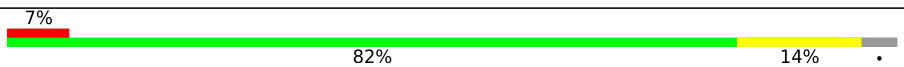
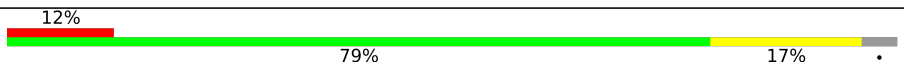
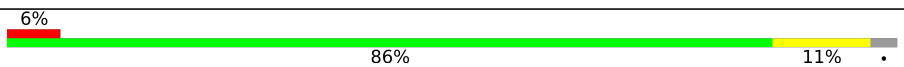
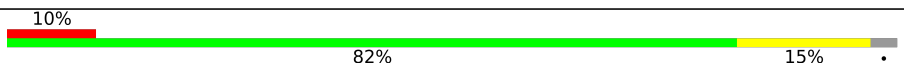
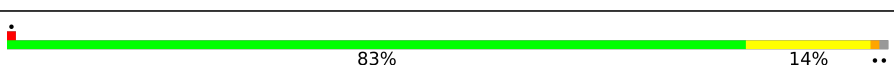
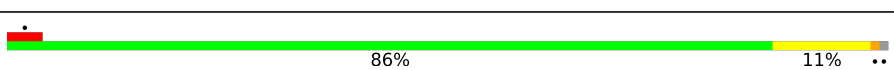
*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 28 | EC | 212 | 21% 87% 13% |
| 28 | Ec | 212 | 38% 87% 13% |
| 29 | ED | 190 | 5% 84% 16% |
| 29 | Ed | 190 | 9% 86% 14% |
| 30 | EE | 193 | 57% 8% 35% |
| 30 | Ee | 193 | 59% 6% 35% |
| 31 | EF | 188 | 88% 12% |
| 31 | Ef | 188 | 90% 10% |
| 32 | EG | 100 | 88% 10% |
| 32 | Eg | 100 | 86% 12% |
| 33 | EH | 173 | 85% 15% |
| 33 | Eh | 173 | 83% 17% |
| 34 | EI | 173 | 91% 9% |
| 34 | Ei | 173 | 89% 10% |
| 35 | EV | 88 | 80% 9% 11% |
| 35 | Ev | 88 | 78% 10% 11% |
| 36 | EK | 170 | 88% 11% |
| 36 | Ek | 170 | 84% 15% |
| 37 | EL | 158 | 84% 13% |
| 37 | El | 158 | 85% 12% |
| 38 | EM | 154 | 87% 12% |
| 38 | Em | 154 | 87% 12% |
| 39 | EN | 149 | 89% 8% |
| 39 | En | 149 | 91% 6% |
| 40 | EO | 124 | 87% 12% |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 40 | Eo | 124 |   |
| 41 | EP | 127 |   |
| 41 | Ep | 127 |   |
| 42 | EQ | 122 |   |
| 42 | Eq | 122 |   |
| 43 | ER | 105 |   |
| 43 | Er | 105 |   |
| 44 | ES | 89 |   |
| 44 | Es | 89 |   |
| 45 | ET | 93 |   |
| 45 | Et | 93 |   |
| 46 | EU | 90 |   |
| 46 | Eu | 90 |   |
| 47 | EJ | 175 |   |
| 47 | Ej | 175 |   |
| 48 | EW | 81 |   |
| 48 | Ew | 81 |   |
| 49 | EX | 72 |   |
| 49 | Ex | 72 |   |
| 50 | EY | 72 |   |
| 50 | Ey | 72 |   |
| 51 | EZ | 68 |   |
| 51 | Ez | 68 |   |
| 52 | FA | 72 |   |
| 52 | Fa | 72 |   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 53 | DL | 536 |   |
| 53 | Dl | 536 |   |

# 2 Entry composition

There are 68 unique types of molecules in this entry. The entry contains 436035 atoms, of which 220788 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 c oxidase subunit 1.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 1 | DA | 671 | Total | C | H | N | O | S | 0 | 0 |
| | | | 11168 | 3720 | 5609 | 907 | 896 | 36 | | |
| 1 | Da | 671 | Total | C | H | N | O | S | 0 | 0 |
| | | | 11167 | 3720 | 5608 | 907 | 896 | 36 | | |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| DA | 288 | ALA | GLY | variant | UNP Q950Y4 |
| Da | 288 | ALA | GLY | variant | UNP Q950Y4 |

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

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 2 | DB | 604 | Total | C | H | N | O | S | 0 | 0 |
| | | | 10232 | 3340 | 5101 | 888 | 892 | 11 | | |
| 2 | Db | 604 | Total | C | H | N | O | S | 0 | 0 |
| | | | 10233 | 3340 | 5102 | 888 | 892 | 11 | | |

- Molecule 3 is a protein called Ymf68.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 3 | DC | 582 | Total | C | H | N | O | S | 0 | 0 |
| | | | 10151 | 3451 | 5067 | 787 | 838 | 8 | | |
| 3 | Dc | 582 | Total | C | H | N | O | S | 0 | 0 |
| | | | 10151 | 3451 | 5067 | 787 | 838 | 8 | | |

- Molecule 4 is a protein called Cytochrome C oxidase subunit Vb protein.

| Mol | Chain | Residues | Atoms | | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 4 | DD | 558 | Total | C | H | N | O | P | S | 0 | 0 |
| | | | 9076 | 2930 | 4424 | 782 | 921 | 2 | 17 | | |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Residues | Atoms | | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 4 | Dd | 558 | Total | C | H | N | O | P | S | 0 | 0 |
| | | | 9076 | 2930 | 4424 | 782 | 921 | 2 | 17 | | |

- Molecule 5 is a protein called Transmembrane protein, putative.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 5 | DE | 126 | Total | C | H | N | O | S | 0 | 0 |
| | | | 2104 | 698 | 1021 | 184 | 199 | 2 | | |
| 5 | De | 126 | Total | C | H | N | O | S | 0 | 0 |
| | | | 2103 | 698 | 1020 | 184 | 199 | 2 | | |

- Molecule 6 is a protein called Structural protein.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 6 | DF | 222 | Total | C | H | N | O | S | 0 | 0 |
| | | | 3681 | 1238 | 1768 | 312 | 350 | 13 | | |
| 6 | Df | 222 | Total | C | H | N | O | S | 0 | 0 |
| | | | 3681 | 1238 | 1768 | 312 | 350 | 13 | | |

- Molecule 7 is a protein called Transmembrane protein, putative.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 7 | DG | 98 | Total | C | H | N | O | S | 0 | 0 |
| | | | 1659 | 567 | 788 | 155 | 147 | 2 | | |
| 7 | Dg | 98 | Total | C | H | N | O | S | 0 | 0 |
| | | | 1659 | 567 | 788 | 155 | 147 | 2 | | |

- Molecule 8 is a protein called Transmembrane protein, putative.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 8 | DH | 133 | Total | C | H | N | O | S | 0 | 0 |
| | | | 2299 | 771 | 1129 | 197 | 201 | 1 | | |
| 8 | Dh | 133 | Total | C | H | N | O | S | 0 | 0 |
| | | | 2299 | 771 | 1129 | 197 | 201 | 1 | | |

- Molecule 9 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 9 | DI | 206 | Total | C | H | N | O | P | S | 0 | 0 |
| | | | 3381 | 1134 | 1604 | 286 | 348 | 1 | 8 | | |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Residues | Atoms | | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 9 | Di | 206 | Total | C | H | N | O | P | S | 0 | 0 |
| | | | 3381 | 1134 | 1604 | 286 | 348 | 1 | 8 | | |

- Molecule 10 is a protein called Transmembrane protein, putative.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 10 | DJ | 220 | Total | C | H | N | O | S | 0 | 0 |
| | | | 3653 | 1223 | 1772 | 316 | 330 | 12 | | |
| 10 | Dj | 220 | Total | C | H | N | O | S | 0 | 0 |
| | | | 3653 | 1223 | 1772 | 316 | 330 | 12 | | |

- Molecule 11 is a protein called CTF/NF-I domain-containing protein.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 11 | DK | 130 | Total | C | H | N | O | S | 0 | 0 |
| | | | 2133 | 693 | 1062 | 174 | 196 | 8 | | |
| 11 | Dk | 130 | Total | C | H | N | O | S | 0 | 0 |
| | | | 2133 | 693 | 1062 | 174 | 196 | 8 | | |

- Molecule 12 is a protein called Transmembrane protein, putative.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 12 | DM | 455 | Total | C | H | N | O | S | 0 | 0 |
| | | | 7385 | 2430 | 3592 | 645 | 709 | 9 | | |
| 12 | Dm | 455 | Total | C | H | N | O | S | 0 | 0 |
| | | | 7385 | 2430 | 3592 | 645 | 709 | 9 | | |

- Molecule 13 is a protein called Ymf67.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 13 | DN | 453 | Total | C | H | N | O | S | 0 | 0 |
| | | | 7849 | 2578 | 3980 | 618 | 666 | 7 | | |
| 13 | Dn | 453 | Total | C | H | N | O | S | 0 | 0 |
| | | | 7849 | 2578 | 3980 | 618 | 666 | 7 | | |

- Molecule 14 is a protein called Protein phosphatase 2C, putative.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 14 | DO | 435 | Total | C | H | N | O | S | 0 | 0 |
| | | | 6956 | 2192 | 3508 | 603 | 650 | 3 | | |
| 14 | Do | 435 | Total | C | H | N | O | S | 0 | 0 |
| | | | 6956 | 2192 | 3508 | 603 | 650 | 3 | | |

- Molecule 15 is a protein called SURF1-like protein.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 15 | DP | 290 | Total | C | H | N | O | S | 0 | 0 |
| | | | 4660 | 1525 | 2291 | 400 | 439 | 5 | | |
| 15 | Dp | 290 | Total | C | H | N | O | S | 0 | 0 |
| | | | 4660 | 1525 | 2291 | 400 | 439 | 5 | | |

- Molecule 16 is a protein called TraB family protein.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 16 | DQ | 383 | Total | C | H | N | O | S | 0 | 0 |
| | | | 6271 | 2041 | 3102 | 546 | 575 | 7 | | |
| 16 | Dq | 383 | Total | C | H | N | O | S | 0 | 0 |
| | | | 6271 | 2041 | 3102 | 546 | 575 | 7 | | |

- Molecule 17 is a protein called Transmembrane protein, putative.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 17 | DR | 243 | Total | C | H | N | O | S | 0 | 0 |
| | | | 3982 | 1304 | 1958 | 335 | 380 | 5 | | |
| 17 | Dr | 243 | Total | C | H | N | O | S | 0 | 0 |
| | | | 3982 | 1304 | 1958 | 335 | 380 | 5 | | |

- Molecule 18 is a protein called Oxoglutarate/malate translocator protein, putative.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 18 | DS | 346 | Total | C | H | N | O | S | 0 | 0 |
| | | | 5636 | 1892 | 2770 | 469 | 492 | 13 | | |
| 18 | Ds | 346 | Total | C | H | N | O | S | 0 | 0 |
| | | | 5636 | 1892 | 2770 | 469 | 492 | 13 | | |

- Molecule 19 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 19 | DT | 293 | Total | C | H | N | O | S | 0 | 0 |
| | | | 4733 | 1555 | 2290 | 410 | 466 | 12 | | |
| 19 | Dt | 293 | Total | C | H | N | O | S | 0 | 0 |
| | | | 4733 | 1555 | 2290 | 410 | 466 | 12 | | |

- Molecule 20 is a protein called Carrier protein.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 20 | DU | 329 | Total | C | H | N | O | S | 0 | 0 |
| | | | 5204 | 1700 | 2584 | 446 | 470 | 4 | | |
| 20 | Du | 329 | Total | C | H | N | O | S | 0 | 0 |
| | | | 5204 | 1700 | 2584 | 446 | 470 | 4 | | |

- Molecule 21 is a protein called 2-oxoglutarate/malate carrier protein.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 21 | DV | 318 | Total | C | H | N | O | S | 0 | 0 |
| | | | 5114 | 1667 | 2552 | 440 | 451 | 4 | | |
| 21 | Dv | 318 | Total | C | H | N | O | S | 0 | 0 |
| | | | 5114 | 1667 | 2552 | 440 | 451 | 4 | | |

- Molecule 22 is a protein called SURF1-like protein.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 22 | DW | 301 | Total | C | H | N | O | S | 0 | 0 |
| | | | 4738 | 1515 | 2344 | 415 | 454 | 10 | | |
| 22 | Dw | 301 | Total | C | H | N | O | S | 0 | 0 |
| | | | 4738 | 1515 | 2344 | 415 | 454 | 10 | | |

- Molecule 23 is a protein called COXTT9.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 23 | DX | 251 | Total | C | H | N | O | S | 0 | 0 |
| | | | 4126 | 1358 | 2018 | 368 | 377 | 5 | | |
| 23 | Dx | 251 | Total | C | H | N | O | S | 0 | 0 |
| | | | 4126 | 1358 | 2018 | 368 | 377 | 5 | | |

- Molecule 24 is a protein called COXTT10.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 24 | DY | 187 | Total | C | H | N | O | S | 0 | 0 |
| | | | 3135 | 1023 | 1562 | 276 | 273 | 1 | | |
| 24 | Dy | 187 | Total | C | H | N | O | S | 0 | 0 |
| | | | 3135 | 1023 | 1562 | 276 | 273 | 1 | | |

- Molecule 25 is a protein called 39S ribosomal protein L9, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 25 | DZ | 208 | Total | C | H | N | O | S | 0 | 0 |
| | | | 3382 | 1089 | 1671 | 302 | 317 | 3 | | |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 25 | Dz | 208 | Total | C | H | N | O | S | 0 | 0 |
| | | | 3383 | 1089 | 1672 | 302 | 317 | 3 | | |

- Molecule 26 is a protein called COXTT12,Transmembrane protein,Transmembrane protein.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 26 | EA | 193 | Total | C | H | N | O | S | 0 | 0 |
| | | | 3296 | 1084 | 1637 | 283 | 290 | 2 | | |
| 26 | Ea | 193 | Total | C | H | N | O | S | 0 | 0 |
| | | | 3296 | 1084 | 1637 | 283 | 290 | 2 | | |

- Molecule 27 is a protein called Transmembrane protein, putative.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 27 | EB | 209 | Total | C | H | N | O | S | 0 | 0 |
| | | | 3417 | 1131 | 1678 | 291 | 310 | 7 | | |
| 27 | Eb | 209 | Total | C | H | N | O | S | 0 | 0 |
| | | | 3417 | 1131 | 1678 | 291 | 310 | 7 | | |

- Molecule 28 is a protein called COXTT27.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 28 | EC | 212 | Total | C | H | N | O | S | 0 | 0 |
| | | | 3307 | 1045 | 1660 | 276 | 324 | 2 | | |
| 28 | Ec | 212 | Total | C | H | N | O | S | 0 | 0 |
| | | | 3307 | 1045 | 1660 | 276 | 324 | 2 | | |

- Molecule 29 is a protein called Ymf75.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 29 | ED | 190 | Total | C | H | N | O | S | 0 | 0 |
| | | | 3384 | 1141 | 1725 | 249 | 265 | 4 | | |
| 29 | Ed | 190 | Total | C | H | N | O | S | 0 | 0 |
| | | | 3384 | 1141 | 1725 | 249 | 265 | 4 | | |

- Molecule 30 is a protein called Mobilization protein.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 30 | EE | 125 | Total | C | H | N | O | S | 0 | 0 |
| | | | 2073 | 656 | 1024 | 186 | 201 | 6 | | |
| 30 | Ee | 125 | Total | C | H | N | O | S | 0 | 0 |
| | | | 2073 | 656 | 1024 | 186 | 201 | 6 | | |

- Molecule 31 is a protein called Iron-binding zinc finger CDGSH type protein.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 31 | EF | 188 | Total | C | H | N | O | S | 0 | 0 |
| | | | 2986 | 978 | 1477 | 260 | 257 | 14 | | |
| 31 | Ef | 188 | Total | C | H | N | O | S | 0 | 0 |
| | | | 2986 | 978 | 1477 | 260 | 257 | 14 | | |

- Molecule 32 is a protein called COXTT28.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 32 | EG | 98 | Total | C | H | N | O | S | 0 | 0 |
| | | | 1523 | 492 | 752 | 136 | 141 | 2 | | |
| 32 | Eg | 98 | Total | C | H | N | O | S | 0 | 0 |
| | | | 1523 | 492 | 752 | 136 | 141 | 2 | | |

- Molecule 33 is a protein called Transmembrane protein, putative.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 33 | EH | 173 | Total | C | H | N | O | S | 0 | 0 |
| | | | 2820 | 929 | 1382 | 243 | 257 | 9 | | |
| 33 | Eh | 173 | Total | C | H | N | O | S | 0 | 0 |
| | | | 2820 | 929 | 1382 | 243 | 257 | 9 | | |

- Molecule 34 is a protein called Transmembrane protein.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 34 | EI | 172 | Total | C | H | N | O | S | 0 | 0 |
| | | | 2827 | 921 | 1419 | 231 | 253 | 3 | | |
| 34 | Ei | 172 | Total | C | H | N | O | S | 0 | 0 |
| | | | 2827 | 921 | 1419 | 231 | 253 | 3 | | |

- Molecule 35 is a protein called Decapping nuclease.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 35 | EV | 78 | Total | C | H | N | O | S | 0 | 0 |
| | | | 1276 | 411 | 633 | 109 | 117 | 6 | | |
| 35 | Ev | 78 | Total | C | H | N | O | S | 0 | 0 |
| | | | 1276 | 411 | 633 | 109 | 117 | 6 | | |

- Molecule 36 is a protein called Complex III subunit VII.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 36 | EK | 169 | Total | C | H | N | O | S | 0 | 0 |
| | | | 2796 | 878 | 1407 | 243 | 264 | 4 | | |
| 36 | Ek | 169 | Total | C | H | N | O | S | 0 | 0 |
| | | | 2796 | 878 | 1407 | 243 | 264 | 4 | | |

- Molecule 37 is a protein called Transmembrane protein, putative.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 37 | EL | 153 | Total | C | H | N | O | S | 0 | 0 |
| | | | 2544 | 841 | 1253 | 226 | 220 | 4 | | |
| 37 | El | 153 | Total | C | H | N | O | S | 0 | 0 |
| | | | 2544 | 841 | 1253 | 226 | 220 | 4 | | |

- Molecule 38 is a protein called Transmembrane protein, putative.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 38 | EM | 153 | Total | C | H | N | O | S | 0 | 0 |
| | | | 2603 | 848 | 1299 | 221 | 230 | 5 | | |
| 38 | Em | 153 | Total | C | H | N | O | S | 0 | 0 |
| | | | 2603 | 848 | 1299 | 221 | 230 | 5 | | |

- Molecule 39 is a protein called COXTT22.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 39 | EN | 145 | Total | C | H | N | O | S | 0 | 0 |
| | | | 2417 | 798 | 1190 | 216 | 211 | 2 | | |
| 39 | En | 145 | Total | C | H | N | O | S | 0 | 0 |
| | | | 2417 | 798 | 1190 | 216 | 211 | 2 | | |

- Molecule 40 is a protein called Transmembrane protein, putative.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 40 | EO | 123 | Total | C | H | N | O | S | 0 | 0 |
| | | | 2128 | 716 | 1031 | 183 | 194 | 4 | | |
| 40 | Eo | 123 | Total | C | H | N | O | S | 0 | 0 |
| | | | 2128 | 716 | 1031 | 183 | 194 | 4 | | |

- Molecule 41 is a protein called Phage protein.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 41 | EP | 100 | Total | C | H | N | O | S | 0 | 0 |
| | | | 1612 | 519 | 795 | 144 | 152 | 2 | | |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 41 | Ep | 100 | Total | C | H | N | O | S | 0 | 0 |
| | | | 1612 | 519 | 795 | 144 | 152 | 2 | | |

- Molecule 42 is a protein called Transmembrane protein, putative.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 42 | EQ | 122 | Total | C | H | N | O | S | 0 | 0 |
| | | | 2004 | 667 | 989 | 171 | 173 | 4 | | |
| 42 | Eq | 122 | Total | C | H | N | O | S | 0 | 0 |
| | | | 2004 | 667 | 989 | 171 | 173 | 4 | | |

- Molecule 43 is a protein called Lysozyme.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 43 | ER | 104 | Total | C | H | N | O | S | 0 | 0 |
| | | | 1651 | 535 | 800 | 156 | 152 | 8 | | |
| 43 | Er | 104 | Total | C | H | N | O | S | 0 | 0 |
| | | | 1651 | 535 | 800 | 156 | 152 | 8 | | |

- Molecule 44 is a protein called Ymf70.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 44 | ES | 89 | Total | C | H | N | O | S | 0 | 0 |
| | | | 1574 | 535 | 798 | 115 | 124 | 2 | | |
| 44 | Es | 89 | Total | C | H | N | O | S | 0 | 0 |
| | | | 1574 | 535 | 798 | 115 | 124 | 2 | | |

- Molecule 45 is a protein called Zf-Tim10_DDP domain-containing protein.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 45 | ET | 82 | Total | C | H | N | O | S | 0 | 0 |
| | | | 1302 | 407 | 655 | 108 | 127 | 5 | | |
| 45 | Et | 82 | Total | C | H | N | O | S | 0 | 0 |
| | | | 1302 | 407 | 655 | 108 | 127 | 5 | | |

- Molecule 46 is a protein called ABC transporter.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 46 | EU | 88 | Total | C | H | N | O | 0 | 0 |
| | | | 1423 | 462 | 699 | 131 | 131 | | |
| 46 | Eu | 88 | Total | C | H | N | O | 0 | 0 |
| | | | 1423 | 462 | 699 | 131 | 131 | | |

- Molecule 47 is a protein called YflT domain-containing protein.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 47 | EJ | 175 | Total | C | H | N | O | S | 0 | 0 |
| | | | 2802 | 889 | 1391 | 247 | 274 | 1 | | |
| 47 | Ej | 175 | Total | C | H | N | O | S | 0 | 0 |
| | | | 2802 | 889 | 1391 | 247 | 274 | 1 | | |

- Molecule 48 is a protein called Cullin domain-containing protein.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 48 | EW | 63 | Total | C | H | N | O | S | 0 | 0 |
| | | | 1025 | 327 | 510 | 90 | 96 | 2 | | |
| 48 | Ew | 63 | Total | C | H | N | O | S | 0 | 0 |
| | | | 1025 | 327 | 510 | 90 | 96 | 2 | | |

- Molecule 49 is a protein called Zf-Tim10_DDP domain-containing protein.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 49 | EX | 69 | Total | C | H | N | O | S | 0 | 0 |
| | | | 1117 | 347 | 559 | 98 | 109 | 4 | | |
| 49 | Ex | 69 | Total | C | H | N | O | S | 0 | 0 |
| | | | 1117 | 347 | 559 | 98 | 109 | 4 | | |

- Molecule 50 is a protein called Annexin.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 50 | EY | 70 | Total | C | H | N | O | S | 0 | 0 |
| | | | 1123 | 362 | 562 | 90 | 105 | 4 | | |
| 50 | Ey | 70 | Total | C | H | N | O | S | 0 | 0 |
| | | | 1123 | 362 | 562 | 90 | 105 | 4 | | |

- Molecule 51 is a protein called Transposase.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 51 | EZ | 58 | Total | C | H | N | O | S | 0 | 0 |
| | | | 966 | 314 | 474 | 84 | 91 | 3 | | |
| 51 | Ez | 58 | Total | C | H | N | O | S | 0 | 0 |
| | | | 966 | 314 | 474 | 84 | 91 | 3 | | |

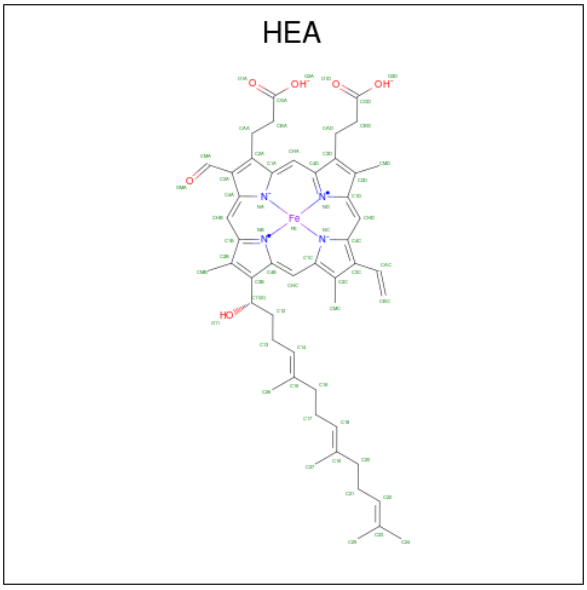
- Molecule 52 is a protein called Tim10/DDP family zinc finger protein.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 52 | FA | 71 | Total | C | H | N | O | S | 0 | 0 |
| | | | 1084 | 333 | 536 | 99 | 112 | 4 | | |
| 52 | Fa | 71 | Total | C | H | N | O | S | 0 | 0 |
| | | | 1084 | 333 | 536 | 99 | 112 | 4 | | |

- Molecule 53 is a protein called COXBP,Chromosome condensation regulator RCC1 repeat protein,Chromosome condensation regulator RCC1 repeat protein.

| Mol | Chain | Residues | Atoms | | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 53 | Dl | 380 | Total | C | H | N | O | S | 0 | 0 |
| | | | 5730 | 1856 | 2814 | 492 | 566 | 2 | | |
| 53 | DL | 380 | Total | C | H | N | O | S | 0 | 0 |
| | | | 5730 | 1856 | 2814 | 492 | 566 | 2 | | |

- Molecule 54 is HEME-A (CCD ID: HEA) (formula: $C_{49}H_{56}FeN_4O_6$) (labeled as "Ligand of Interest" by depositor).




| Mol | Chain | Residues | Atoms | | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|---|
| 54 | DA | 1 | Total | C | Fe | H | N | O | 0 |
| | | | 114 | 49 | 1 | 54 | 4 | 6 | |
| 54 | DA | 1 | Total | C | Fe | H | N | O | 0 |
| | | | 114 | 49 | 1 | 54 | 4 | 6 | |
| 54 | Da | 1 | Total | C | Fe | H | N | O | 0 |
| | | | 114 | 49 | 1 | 54 | 4 | 6 | |
| 54 | Da | 1 | Total | C | Fe | H | N | O | 0 |
| | | | 114 | 49 | 1 | 54 | 4 | 6 | |

- Molecule 55 is COPPER (II) ION (CCD ID: CU) (formula: Cu) (labeled as "Ligand of

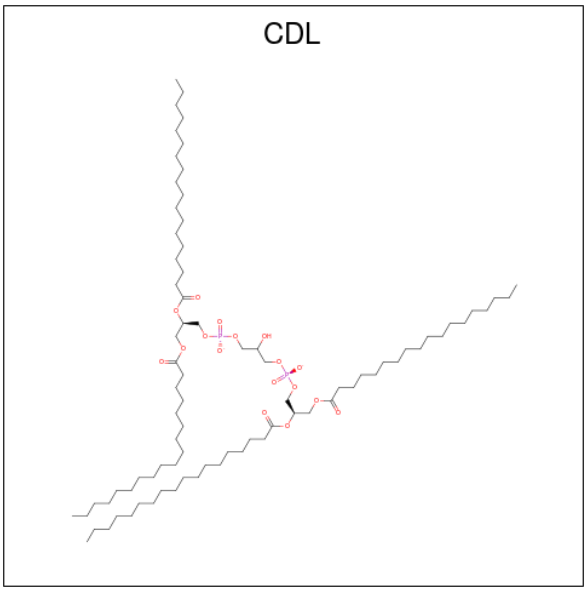
Interest" by depositor).

| Mol | Chain | Residues | Atoms | AltConf |
|---|---|---|---|---|
| 55 | DA | 1 | Total Cu<br>1 1 | 0 |
| 55 | Da | 1 | Total Cu<br>1 1 | 0 |

- Molecule 56 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

| Mol | Chain | Residues | Atoms | AltConf |
|---|---|---|---|---|
| 56 | DA | 1 | Total Mg<br>1 1 | 0 |
| 56 | Da | 1 | Total Mg<br>1 1 | 0 |

- Molecule 57 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$) (labeled as "Ligand of Interest" by depositor).




| Mol | Chain | Residues | Atoms | AltConf |
|---|---|---|---|---|
| 57 | DA | 1 | Total C H O P<br>256 81 156 17 2 | 0 |
| 57 | DA | 1 | Total C H O P<br>256 81 156 17 2 | 0 |
| 57 | DA | 1 | Total C H O P<br>256 81 156 17 2 | 0 |
| 57 | DC | 1 | Total C H O P<br>256 81 156 17 2 | 0 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Residues | Atoms | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|
| 57 | DD | 1 | Total | C | H | O | P | 0 |
| | | | 256 | 81 | 156 | 17 | 2 | |
| 57 | DD | 1 | Total | C | H | O | P | 0 |
| | | | 256 | 81 | 156 | 17 | 2 | |
| 57 | DD | 1 | Total | C | H | O | P | 0 |
| | | | 256 | 81 | 156 | 17 | 2 | |
| 57 | DG | 1 | Total | C | H | O | P | 0 |
| | | | 256 | 81 | 156 | 17 | 2 | |
| 57 | DG | 1 | Total | C | H | O | P | 0 |
| | | | 256 | 81 | 156 | 17 | 2 | |
| 57 | DH | 1 | Total | C | H | O | P | 0 |
| | | | 256 | 81 | 156 | 17 | 2 | |
| 57 | DI | 1 | Total | C | H | O | P | 0 |
| | | | 256 | 81 | 156 | 17 | 2 | |
| 57 | DJ | 1 | Total | C | H | O | P | 0 |
| | | | 256 | 81 | 156 | 17 | 2 | |
| 57 | DJ | 1 | Total | C | H | O | P | 0 |
| | | | 256 | 81 | 156 | 17 | 2 | |
| 57 | DJ | 1 | Total | C | H | O | P | 0 |
| | | | 256 | 81 | 156 | 17 | 2 | |
| 57 | DJ | 1 | Total | C | H | O | P | 0 |
| | | | 256 | 81 | 156 | 17 | 2 | |
| 57 | DJ | 1 | Total | C | H | O | P | 0 |
| | | | 256 | 81 | 156 | 17 | 2 | |
| 57 | DM | 1 | Total | C | H | O | P | 0 |
| | | | 256 | 81 | 156 | 17 | 2 | |
| 57 | DM | 1 | Total | C | H | O | P | 0 |
| | | | 256 | 81 | 156 | 17 | 2 | |
| 57 | DN | 1 | Total | C | H | O | P | 0 |
| | | | 256 | 81 | 156 | 17 | 2 | |
| 57 | DN | 1 | Total | C | H | O | P | 0 |
| | | | 256 | 81 | 156 | 17 | 2 | |
| 57 | DN | 1 | Total | C | H | O | P | 0 |
| | | | 256 | 81 | 156 | 17 | 2 | |
| 57 | DO | 1 | Total | C | H | O | P | 0 |
| | | | 256 | 81 | 156 | 17 | 2 | |
| 57 | DQ | 1 | Total | C | H | O | P | 0 |
| | | | 256 | 81 | 156 | 17 | 2 | |
| 57 | DQ | 1 | Total | C | H | O | P | 0 |
| | | | 256 | 81 | 156 | 17 | 2 | |
| 57 | DQ | 1 | Total | C | H | O | P | 0 |
| | | | 256 | 81 | 156 | 17 | 2 | |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Residues | Atoms | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|
| 57 | DR | 1 | Total | C | H | O | P | 0 |
| | | | 256 | 81 | 156 | 17 | 2 | |
| 57 | DR | 1 | Total | C | H | O | P | 0 |
| | | | 256 | 81 | 156 | 17 | 2 | |
| 57 | DS | 1 | Total | C | H | O | P | 0 |
| | | | 256 | 81 | 156 | 17 | 2 | |
| 57 | DS | 1 | Total | C | H | O | P | 0 |
| | | | 256 | 81 | 156 | 17 | 2 | |
| 57 | DU | 1 | Total | C | H | O | P | 0 |
| | | | 256 | 81 | 156 | 17 | 2 | |
| 57 | DU | 1 | Total | C | H | O | P | 0 |
| | | | 256 | 81 | 156 | 17 | 2 | |
| 57 | DU | 1 | Total | C | H | O | P | 0 |
| | | | 256 | 81 | 156 | 17 | 2 | |
| 57 | DU | 1 | Total | C | H | O | P | 0 |
| | | | 256 | 81 | 156 | 17 | 2 | |
| 57 | DV | 1 | Total | C | H | O | P | 0 |
| | | | 256 | 81 | 156 | 17 | 2 | |
| 57 | DV | 1 | Total | C | H | O | P | 0 |
| | | | 256 | 81 | 156 | 17 | 2 | |
| 57 | DV | 1 | Total | C | H | O | P | 0 |
| | | | 256 | 81 | 156 | 17 | 2 | |
| 57 | DV | 1 | Total | C | H | O | P | 0 |
| | | | 256 | 81 | 156 | 17 | 2 | |
| 57 | DX | 1 | Total | C | H | O | P | 0 |
| | | | 256 | 81 | 156 | 17 | 2 | |
| 57 | DX | 1 | Total | C | H | O | P | 0 |
| | | | 256 | 81 | 156 | 17 | 2 | |
| 57 | DY | 1 | Total | C | H | O | P | 0 |
| | | | 256 | 81 | 156 | 17 | 2 | |
| 57 | DZ | 1 | Total | C | H | O | P | 0 |
| | | | 256 | 81 | 156 | 17 | 2 | |
| 57 | EA | 1 | Total | C | H | O | P | 0 |
| | | | 256 | 81 | 156 | 17 | 2 | |
| 57 | EB | 1 | Total | C | H | O | P | 0 |
| | | | 256 | 81 | 156 | 17 | 2 | |
| 57 | EB | 1 | Total | C | H | O | P | 0 |
| | | | 256 | 81 | 156 | 17 | 2 | |
| 57 | ED | 1 | Total | C | H | O | P | 0 |
| | | | 256 | 81 | 156 | 17 | 2 | |
| 57 | ED | 1 | Total | C | H | O | P | 0 |
| | | | 256 | 81 | 156 | 17 | 2 | |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Residues | Atoms | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|
| 57 | EH | 1 | Total | C | H | O | P | 0 |
| | | | 256 | 81 | 156 | 17 | 2 | |
| 57 | EH | 1 | Total | C | H | O | P | 0 |
| | | | 255 | 81 | 155 | 17 | 2 | |
| 57 | EI | 1 | Total | C | H | O | P | 0 |
| | | | 256 | 81 | 156 | 17 | 2 | |
| 57 | EK | 1 | Total | C | H | O | P | 0 |
| | | | 256 | 81 | 156 | 17 | 2 | |
| 57 | EL | 1 | Total | C | H | O | P | 0 |
| | | | 256 | 81 | 156 | 17 | 2 | |
| 57 | EL | 1 | Total | C | H | O | P | 0 |
| | | | 256 | 81 | 156 | 17 | 2 | |
| 57 | EL | 1 | Total | C | H | O | P | 0 |
| | | | 256 | 81 | 156 | 17 | 2 | |
| 57 | EL | 1 | Total | C | H | O | P | 0 |
| | | | 256 | 81 | 156 | 17 | 2 | |
| 57 | EN | 1 | Total | C | H | O | P | 0 |
| | | | 256 | 81 | 156 | 17 | 2 | |
| 57 | EN | 1 | Total | C | H | O | P | 0 |
| | | | 256 | 81 | 156 | 17 | 2 | |
| 57 | EO | 1 | Total | C | H | O | P | 0 |
| | | | 256 | 81 | 156 | 17 | 2 | |
| 57 | EU | 1 | Total | C | H | O | P | 0 |
| | | | 256 | 81 | 156 | 17 | 2 | |
| 57 | Da | 1 | Total | C | H | O | P | 0 |
| | | | 256 | 81 | 156 | 17 | 2 | |
| 57 | Da | 1 | Total | C | H | O | P | 0 |
| | | | 256 | 81 | 156 | 17 | 2 | |
| 57 | Dc | 1 | Total | C | H | O | P | 0 |
| | | | 256 | 81 | 156 | 17 | 2 | |
| 57 | Dd | 1 | Total | C | H | O | P | 0 |
| | | | 256 | 81 | 156 | 17 | 2 | |
| 57 | Dd | 1 | Total | C | H | O | P | 0 |
| | | | 256 | 81 | 156 | 17 | 2 | |
| 57 | Dd | 1 | Total | C | H | O | P | 0 |
| | | | 256 | 81 | 156 | 17 | 2 | |
| 57 | Dd | 1 | Total | C | H | O | P | 0 |
| | | | 256 | 81 | 156 | 17 | 2 | |
| 57 | Dg | 1 | Total | C | H | O | P | 0 |
| | | | 256 | 81 | 156 | 17 | 2 | |
| 57 | Dg | 1 | Total | C | H | O | P | 0 |
| | | | 256 | 81 | 156 | 17 | 2 | |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Residues | Atoms | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|
| 57 | Dh | 1 | Total | C | H | O | P | 0 |
| | | | 256 | 81 | 156 | 17 | 2 | |
| 57 | Dh | 1 | Total | C | H | O | P | 0 |
| | | | 256 | 81 | 156 | 17 | 2 | |
| 57 | Di | 1 | Total | C | H | O | P | 0 |
| | | | 256 | 81 | 156 | 17 | 2 | |
| 57 | Dj | 1 | Total | C | H | O | P | 0 |
| | | | 256 | 81 | 156 | 17 | 2 | |
| 57 | Dj | 1 | Total | C | H | O | P | 0 |
| | | | 256 | 81 | 156 | 17 | 2 | |
| 57 | Dj | 1 | Total | C | H | O | P | 0 |
| | | | 256 | 81 | 156 | 17 | 2 | |
| 57 | Dj | 1 | Total | C | H | O | P | 0 |
| | | | 256 | 81 | 156 | 17 | 2 | |
| 57 | Dj | 1 | Total | C | H | O | P | 0 |
| | | | 256 | 81 | 156 | 17 | 2 | |
| 57 | Dj | 1 | Total | C | H | O | P | 0 |
| | | | 256 | 81 | 156 | 17 | 2 | |
| 57 | Dm | 1 | Total | C | H | O | P | 0 |
| | | | 256 | 81 | 156 | 17 | 2 | |
| 57 | Dm | 1 | Total | C | H | O | P | 0 |
| | | | 256 | 81 | 156 | 17 | 2 | |
| 57 | Dn | 1 | Total | C | H | O | P | 0 |
| | | | 256 | 81 | 156 | 17 | 2 | |
| 57 | Dn | 1 | Total | C | H | O | P | 0 |
| | | | 256 | 81 | 156 | 17 | 2 | |
| 57 | Dn | 1 | Total | C | H | O | P | 0 |
| | | | 256 | 81 | 156 | 17 | 2 | |
| 57 | Dn | 1 | Total | C | H | O | P | 0 |
| | | | 256 | 81 | 156 | 17 | 2 | |
| 57 | Dn | 1 | Total | C | H | O | P | 0 |
| | | | 256 | 81 | 156 | 17 | 2 | |
| 57 | Do | 1 | Total | C | H | O | P | 0 |
| | | | 256 | 81 | 156 | 17 | 2 | |
| 57 | Dq | 1 | Total | C | H | O | P | 0 |
| | | | 256 | 81 | 156 | 17 | 2 | |
| 57 | Dq | 1 | Total | C | H | O | P | 0 |
| | | | 256 | 81 | 156 | 17 | 2 | |
| 57 | Dq | 1 | Total | C | H | O | P | 0 |
| | | | 256 | 81 | 156 | 17 | 2 | |
| 57 | Dq | 1 | Total | C | H | O | P | 0 |
| | | | 256 | 81 | 156 | 17 | 2 | |

*Continued on next page...*

*Continued from previous page...*

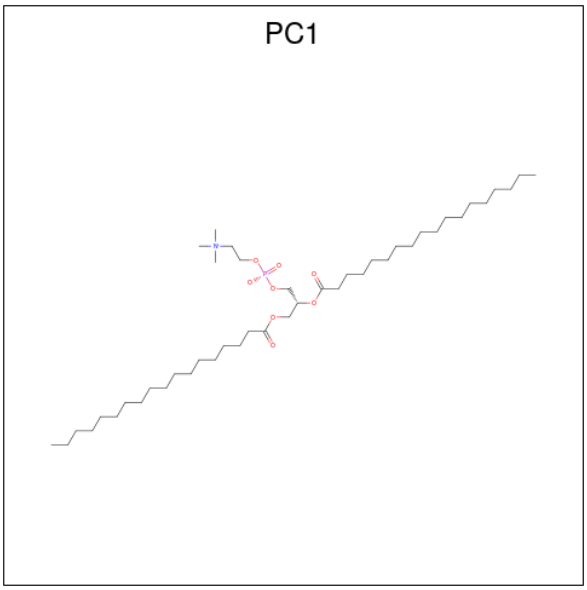
| Mol | Chain | Residues | Atoms | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|
| 57 | Dr | 1 | Total | C | H | O | P | 0 |
| | | | 256 | 81 | 156 | 17 | 2 | |
| 57 | Dr | 1 | Total | C | H | O | P | 0 |
| | | | 256 | 81 | 156 | 17 | 2 | |
| 57 | Ds | 1 | Total | C | H | O | P | 0 |
| | | | 256 | 81 | 156 | 17 | 2 | |
| 57 | Ds | 1 | Total | C | H | O | P | 0 |
| | | | 256 | 81 | 156 | 17 | 2 | |
| 57 | Du | 1 | Total | C | H | O | P | 0 |
| | | | 256 | 81 | 156 | 17 | 2 | |
| 57 | Du | 1 | Total | C | H | O | P | 0 |
| | | | 256 | 81 | 156 | 17 | 2 | |
| 57 | Du | 1 | Total | C | H | O | P | 0 |
| | | | 256 | 81 | 156 | 17 | 2 | |
| 57 | Du | 1 | Total | C | H | O | P | 0 |
| | | | 256 | 81 | 156 | 17 | 2 | |
| 57 | Dv | 1 | Total | C | H | O | P | 0 |
| | | | 256 | 81 | 156 | 17 | 2 | |
| 57 | Dv | 1 | Total | C | H | O | P | 0 |
| | | | 256 | 81 | 156 | 17 | 2 | |
| 57 | Dv | 1 | Total | C | H | O | P | 0 |
| | | | 256 | 81 | 156 | 17 | 2 | |
| 57 | Dv | 1 | Total | C | H | O | P | 0 |
| | | | 256 | 81 | 156 | 17 | 2 | |
| 57 | Dx | 1 | Total | C | H | O | P | 0 |
| | | | 256 | 81 | 156 | 17 | 2 | |
| 57 | Dx | 1 | Total | C | H | O | P | 0 |
| | | | 256 | 81 | 156 | 17 | 2 | |
| 57 | Dy | 1 | Total | C | H | O | P | 0 |
| | | | 256 | 81 | 156 | 17 | 2 | |
| 57 | Dz | 1 | Total | C | H | O | P | 0 |
| | | | 256 | 81 | 156 | 17 | 2 | |
| 57 | Ea | 1 | Total | C | H | O | P | 0 |
| | | | 256 | 81 | 156 | 17 | 2 | |
| 57 | Ed | 1 | Total | C | H | O | P | 0 |
| | | | 255 | 81 | 155 | 17 | 2 | |
| 57 | Ed | 1 | Total | C | H | O | P | 0 |
| | | | 256 | 81 | 156 | 17 | 2 | |
| 57 | Eg | 1 | Total | C | H | O | P | 0 |
| | | | 256 | 81 | 156 | 17 | 2 | |
| 57 | Eh | 1 | Total | C | H | O | P | 0 |
| | | | 256 | 81 | 156 | 17 | 2 | |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Residues | Atoms | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|
| 57 | Ei | 1 | Total | C | H | O | P | 0 |
| | | | 256 | 81 | 156 | 17 | 2 | |
| 57 | Ek | 1 | Total | C | H | O | P | 0 |
| | | | 256 | 81 | 156 | 17 | 2 | |
| 57 | El | 1 | Total | C | H | O | P | 0 |
| | | | 256 | 81 | 156 | 17 | 2 | |
| 57 | El | 1 | Total | C | H | O | P | 0 |
| | | | 256 | 81 | 156 | 17 | 2 | |
| 57 | El | 1 | Total | C | H | O | P | 0 |
| | | | 256 | 81 | 156 | 17 | 2 | |
| 57 | En | 1 | Total | C | H | O | P | 0 |
| | | | 256 | 81 | 156 | 17 | 2 | |
| 57 | En | 1 | Total | C | H | O | P | 0 |
| | | | 256 | 81 | 156 | 17 | 2 | |
| 57 | Ep | 1 | Total | C | H | O | P | 0 |
| | | | 256 | 81 | 156 | 17 | 2 | |
| 57 | Eu | 1 | Total | C | H | O | P | 0 |
| | | | 256 | 81 | 156 | 17 | 2 | |

- Molecule 58 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: $C_{44}H_{88}NO_8P$) (labeled as "Ligand of Interest" by depositor).




| Mol | Chain | Residues | Atoms | | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|---|
| 58 | DA | 1 | Total | C | H | N | O | P | 0 |
| | | | 141 | 44 | 87 | 1 | 8 | 1 | |
| 58 | DA | 1 | Total | C | H | N | O | P | 0 |
| | | | 142 | 44 | 88 | 1 | 8 | 1 | |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Residues | Atoms | | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|---|
| 58 | DB | 1 | Total | C | H | N | O | P | 0 |
| | | | 142 | 44 | 88 | 1 | 8 | 1 | |
| 58 | DC | 1 | Total | C | H | N | O | P | 0 |
| | | | 142 | 44 | 88 | 1 | 8 | 1 | |
| 58 | DC | 1 | Total | C | H | N | O | P | 0 |
| | | | 142 | 44 | 88 | 1 | 8 | 1 | |
| 58 | DC | 1 | Total | C | H | N | O | P | 0 |
| | | | 142 | 44 | 88 | 1 | 8 | 1 | |
| 58 | DC | 1 | Total | C | H | N | O | P | 0 |
| | | | 142 | 44 | 88 | 1 | 8 | 1 | |
| 58 | DC | 1 | Total | C | H | N | O | P | 0 |
| | | | 141 | 44 | 87 | 1 | 8 | 1 | |
| 58 | DG | 1 | Total | C | H | N | O | P | 0 |
| | | | 142 | 44 | 88 | 1 | 8 | 1 | |
| 58 | DI | 1 | Total | C | H | N | O | P | 0 |
| | | | 142 | 44 | 88 | 1 | 8 | 1 | |
| 58 | DJ | 1 | Total | C | H | N | O | P | 0 |
| | | | 142 | 44 | 88 | 1 | 8 | 1 | |
| 58 | DQ | 1 | Total | C | H | N | O | P | 0 |
| | | | 142 | 44 | 88 | 1 | 8 | 1 | |
| 58 | DS | 1 | Total | C | H | N | O | P | 0 |
| | | | 142 | 44 | 88 | 1 | 8 | 1 | |
| 58 | DS | 1 | Total | C | H | N | O | P | 0 |
| | | | 142 | 44 | 88 | 1 | 8 | 1 | |
| 58 | DV | 1 | Total | C | H | N | O | P | 0 |
| | | | 142 | 44 | 88 | 1 | 8 | 1 | |
| 58 | DV | 1 | Total | C | H | N | O | P | 0 |
| | | | 142 | 44 | 88 | 1 | 8 | 1 | |
| 58 | DV | 1 | Total | C | H | N | O | P | 0 |
| | | | 142 | 44 | 88 | 1 | 8 | 1 | |
| 58 | DX | 1 | Total | C | H | N | O | P | 0 |
| | | | 142 | 44 | 88 | 1 | 8 | 1 | |
| 58 | DX | 1 | Total | C | H | N | O | P | 0 |
| | | | 142 | 44 | 88 | 1 | 8 | 1 | |
| 58 | DY | 1 | Total | C | H | N | O | P | 0 |
| | | | 142 | 44 | 88 | 1 | 8 | 1 | |
| 58 | EB | 1 | Total | C | H | N | O | P | 0 |
| | | | 142 | 44 | 88 | 1 | 8 | 1 | |
| 58 | EB | 1 | Total | C | H | N | O | P | 0 |
| | | | 142 | 44 | 88 | 1 | 8 | 1 | |
| 58 | EO | 1 | Total | C | H | N | O | P | 0 |
| | | | 142 | 44 | 88 | 1 | 8 | 1 | |

*Continued on next page...*

*Continued from previous page...*

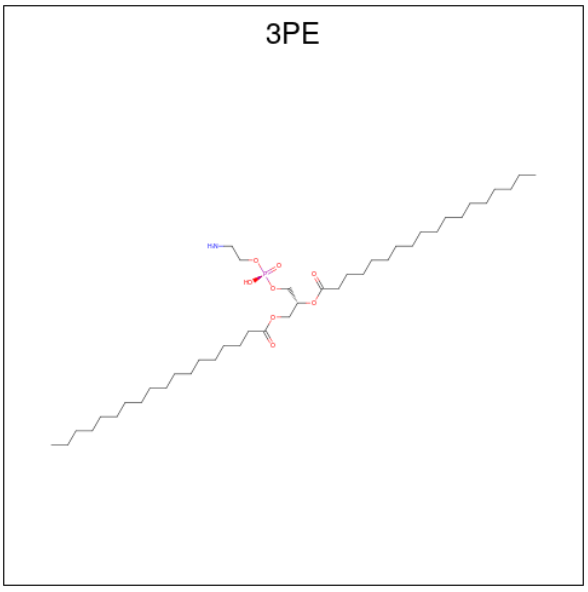
| Mol | Chain | Residues | Atoms | | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|---|
| 58 | EO | 1 | Total | C | H | N | O | P | 0 |
| | | | 142 | 44 | 88 | 1 | 8 | 1 | |
| 58 | EO | 1 | Total | C | H | N | O | P | 0 |
| | | | 142 | 44 | 88 | 1 | 8 | 1 | |
| 58 | EO | 1 | Total | C | H | N | O | P | 0 |
| | | | 142 | 44 | 88 | 1 | 8 | 1 | |
| 58 | Da | 1 | Total | C | H | N | O | P | 0 |
| | | | 141 | 44 | 87 | 1 | 8 | 1 | |
| 58 | Da | 1 | Total | C | H | N | O | P | 0 |
| | | | 142 | 44 | 88 | 1 | 8 | 1 | |
| 58 | Db | 1 | Total | C | H | N | O | P | 0 |
| | | | 142 | 44 | 88 | 1 | 8 | 1 | |
| 58 | Dc | 1 | Total | C | H | N | O | P | 0 |
| | | | 142 | 44 | 88 | 1 | 8 | 1 | |
| 58 | Dc | 1 | Total | C | H | N | O | P | 0 |
| | | | 142 | 44 | 88 | 1 | 8 | 1 | |
| 58 | Dc | 1 | Total | C | H | N | O | P | 0 |
| | | | 142 | 44 | 88 | 1 | 8 | 1 | |
| 58 | Dc | 1 | Total | C | H | N | O | P | 0 |
| | | | 142 | 44 | 88 | 1 | 8 | 1 | |
| 58 | Dc | 1 | Total | C | H | N | O | P | 0 |
| | | | 141 | 44 | 87 | 1 | 8 | 1 | |
| 58 | Dg | 1 | Total | C | H | N | O | P | 0 |
| | | | 142 | 44 | 88 | 1 | 8 | 1 | |
| 58 | Di | 1 | Total | C | H | N | O | P | 0 |
| | | | 142 | 44 | 88 | 1 | 8 | 1 | |
| 58 | Dj | 1 | Total | C | H | N | O | P | 0 |
| | | | 142 | 44 | 88 | 1 | 8 | 1 | |
| 58 | Dq | 1 | Total | C | H | N | O | P | 0 |
| | | | 142 | 44 | 88 | 1 | 8 | 1 | |
| 58 | Ds | 1 | Total | C | H | N | O | P | 0 |
| | | | 142 | 44 | 88 | 1 | 8 | 1 | |
| 58 | Dv | 1 | Total | C | H | N | O | P | 0 |
| | | | 142 | 44 | 88 | 1 | 8 | 1 | |
| 58 | Dv | 1 | Total | C | H | N | O | P | 0 |
| | | | 142 | 44 | 88 | 1 | 8 | 1 | |
| 58 | Dv | 1 | Total | C | H | N | O | P | 0 |
| | | | 142 | 44 | 88 | 1 | 8 | 1 | |
| 58 | Dv | 1 | Total | C | H | N | O | P | 0 |
| | | | 142 | 44 | 88 | 1 | 8 | 1 | |
| 58 | Dx | 1 | Total | C | H | N | O | P | 0 |
| | | | 142 | 44 | 88 | 1 | 8 | 1 | |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Residues | Atoms | | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|---|
| 58 | Dx | 1 | Total | C | H | N | O | P | 0 |
| | | | 142 | 44 | 88 | 1 | 8 | 1 | |
| 58 | Dx | 1 | Total | C | H | N | O | P | 0 |
| | | | 142 | 44 | 88 | 1 | 8 | 1 | |
| 58 | Dy | 1 | Total | C | H | N | O | P | 0 |
| | | | 142 | 44 | 88 | 1 | 8 | 1 | |
| 58 | Eb | 1 | Total | C | H | N | O | P | 0 |
| | | | 142 | 44 | 88 | 1 | 8 | 1 | |
| 58 | Eb | 1 | Total | C | H | N | O | P | 0 |
| | | | 142 | 44 | 88 | 1 | 8 | 1 | |
| 58 | Ef | 1 | Total | C | H | N | O | P | 0 |
| | | | 142 | 44 | 88 | 1 | 8 | 1 | |
| 58 | El | 1 | Total | C | H | N | O | P | 0 |
| | | | 142 | 44 | 88 | 1 | 8 | 1 | |
| 58 | Eo | 1 | Total | C | H | N | O | P | 0 |
| | | | 142 | 44 | 88 | 1 | 8 | 1 | |
| 58 | Eo | 1 | Total | C | H | N | O | P | 0 |
| | | | 142 | 44 | 88 | 1 | 8 | 1 | |
| 58 | Eo | 1 | Total | C | H | N | O | P | 0 |
| | | | 142 | 44 | 88 | 1 | 8 | 1 | |

- Molecule 59 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: $C_{41}H_{82}NO_8P$) (labeled as "Ligand of Interest" by depositor).




| Mol | Chain | Residues | Atoms | | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|---|
| 59 | DA | 1 | Total | C | H | N | O | P | 0 |
| | | | 133 | 41 | 82 | 1 | 8 | 1 | |

*Continued on next page...*

*Continued from previous page...*

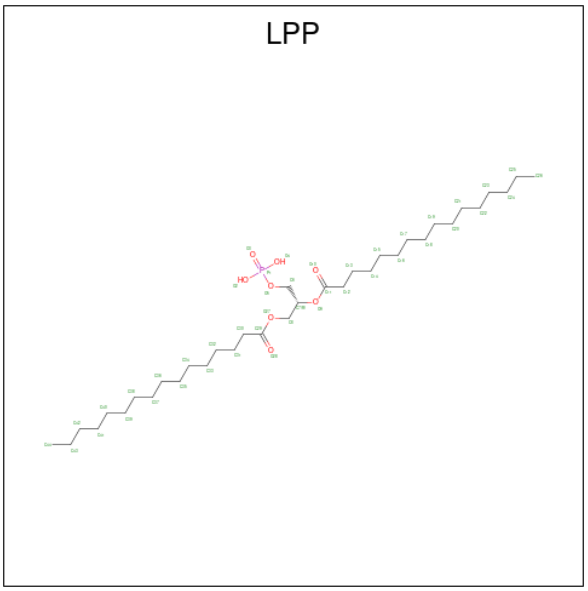
| Mol | Chain | Residues | Atoms | | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|---|
| 59 | DC | 1 | Total | C | H | N | O | P | 0 |
| | | | 133 | 41 | 82 | 1 | 8 | 1 | |
| 59 | DC | 1 | Total | C | H | N | O | P | 0 |
| | | | 133 | 41 | 82 | 1 | 8 | 1 | |
| 59 | DG | 1 | Total | C | H | N | O | P | 0 |
| | | | 133 | 41 | 82 | 1 | 8 | 1 | |
| 59 | DG | 1 | Total | C | H | N | O | P | 0 |
| | | | 133 | 41 | 82 | 1 | 8 | 1 | |
| 59 | DJ | 1 | Total | C | H | N | O | P | 0 |
| | | | 133 | 41 | 82 | 1 | 8 | 1 | |
| 59 | DR | 1 | Total | C | H | N | O | P | 0 |
| | | | 133 | 41 | 82 | 1 | 8 | 1 | |
| 59 | DS | 1 | Total | C | H | N | O | P | 0 |
| | | | 133 | 41 | 82 | 1 | 8 | 1 | |
| 59 | DS | 1 | Total | C | H | N | O | P | 0 |
| | | | 133 | 41 | 82 | 1 | 8 | 1 | |
| 59 | DX | 1 | Total | C | H | N | O | P | 0 |
| | | | 133 | 41 | 82 | 1 | 8 | 1 | |
| 59 | DX | 1 | Total | C | H | N | O | P | 0 |
| | | | 133 | 41 | 82 | 1 | 8 | 1 | |
| 59 | DX | 1 | Total | C | H | N | O | P | 0 |
| | | | 133 | 41 | 82 | 1 | 8 | 1 | |
| 59 | EL | 1 | Total | C | H | N | O | P | 0 |
| | | | 133 | 41 | 82 | 1 | 8 | 1 | |
| 59 | EM | 1 | Total | C | H | N | O | P | 0 |
| | | | 133 | 41 | 82 | 1 | 8 | 1 | |
| 59 | EN | 1 | Total | C | H | N | O | P | 0 |
| | | | 133 | 41 | 82 | 1 | 8 | 1 | |
| 59 | EO | 1 | Total | C | H | N | O | P | 0 |
| | | | 133 | 41 | 82 | 1 | 8 | 1 | |
| 59 | EO | 1 | Total | C | H | N | O | P | 0 |
| | | | 133 | 41 | 82 | 1 | 8 | 1 | |
| 59 | Da | 1 | Total | C | H | N | O | P | 0 |
| | | | 133 | 41 | 82 | 1 | 8 | 1 | |
| 59 | Dc | 1 | Total | C | H | N | O | P | 0 |
| | | | 133 | 41 | 82 | 1 | 8 | 1 | |
| 59 | Dd | 1 | Total | C | H | N | O | P | 0 |
| | | | 133 | 41 | 82 | 1 | 8 | 1 | |
| 59 | Dg | 1 | Total | C | H | N | O | P | 0 |
| | | | 133 | 41 | 82 | 1 | 8 | 1 | |
| 59 | Dj | 1 | Total | C | H | N | O | P | 0 |
| | | | 133 | 41 | 82 | 1 | 8 | 1 | |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Residues | Atoms | | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|---|
| 59 | Dr | 1 | Total | C | H | N | O | P | 0 |
| | | | 133 | 41 | 82 | 1 | 8 | 1 | |
| 59 | Dr | 1 | Total | C | H | N | O | P | 0 |
| | | | 133 | 41 | 82 | 1 | 8 | 1 | |
| 59 | Ds | 1 | Total | C | H | N | O | P | 0 |
| | | | 133 | 41 | 82 | 1 | 8 | 1 | |
| 59 | Ds | 1 | Total | C | H | N | O | P | 0 |
| | | | 133 | 41 | 82 | 1 | 8 | 1 | |
| 59 | Ds | 1 | Total | C | H | N | O | P | 0 |
| | | | 133 | 41 | 82 | 1 | 8 | 1 | |
| 59 | Dx | 1 | Total | C | H | N | O | P | 0 |
| | | | 133 | 41 | 82 | 1 | 8 | 1 | |
| 59 | Dx | 1 | Total | C | H | N | O | P | 0 |
| | | | 133 | 41 | 82 | 1 | 8 | 1 | |
| 59 | Dx | 1 | Total | C | H | N | O | P | 0 |
| | | | 133 | 41 | 82 | 1 | 8 | 1 | |
| 59 | El | 1 | Total | C | H | N | O | P | 0 |
| | | | 133 | 41 | 82 | 1 | 8 | 1 | |
| 59 | Em | 1 | Total | C | H | N | O | P | 0 |
| | | | 133 | 41 | 82 | 1 | 8 | 1 | |
| 59 | Eo | 1 | Total | C | H | N | O | P | 0 |
| | | | 133 | 41 | 82 | 1 | 8 | 1 | |
| 59 | Eo | 1 | Total | C | H | N | O | P | 0 |
| | | | 133 | 41 | 82 | 1 | 8 | 1 | |

- Molecule 60 is 2-(HEXADECANOYLOXY)-1-[(PHOSPHONOOXY)METHYL]ETHYL HEXADECANOATE (CCD ID: LPP) (formula: $C_{35}H_{69}O_8P$) (labeled as "Ligand of Interest" by depositor).

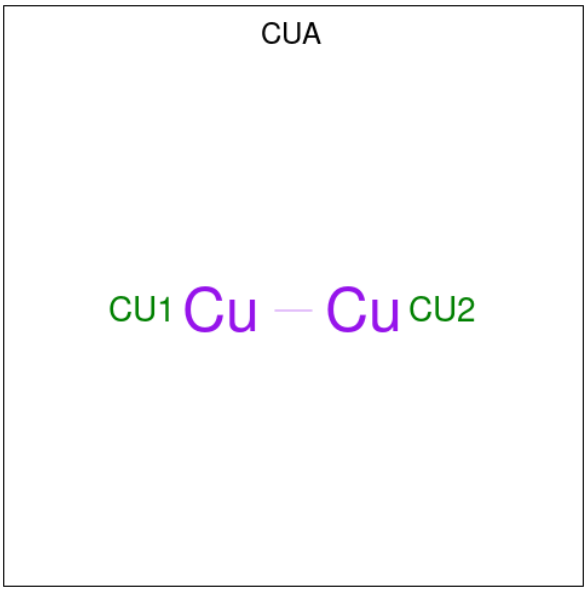



| Mol | Chain | Residues | Atoms | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|
| 60 | DA | 1 | Total | C | H | O | P | 0 |
| | | | 111 | 35 | 67 | 8 | 1 | |
| 60 | DN | 1 | Total | C | H | O | P | 0 |
| | | | 111 | 35 | 67 | 8 | 1 | |
| 60 | DN | 1 | Total | C | H | O | P | 0 |
| | | | 111 | 35 | 67 | 8 | 1 | |
| 60 | EI | 1 | Total | C | H | O | P | 0 |
| | | | 111 | 35 | 67 | 8 | 1 | |
| 60 | Dn | 1 | Total | C | H | O | P | 0 |
| | | | 111 | 35 | 67 | 8 | 1 | |
| 60 | Dn | 1 | Total | C | H | O | P | 0 |
| | | | 111 | 35 | 67 | 8 | 1 | |
| 60 | Ed | 1 | Total | C | H | O | P | 0 |
| | | | 111 | 35 | 67 | 8 | 1 | |
| 60 | Dl | 1 | Total | C | H | O | P | 0 |
| | | | 111 | 35 | 67 | 8 | 1 | |

- Molecule 61 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

| Mol | Chain | Residues | Atoms | | AltConf |
|---|---|---|---|---|---|
| 61 | DA | 1 | Total | Ca | 0 |
| | | | 1 | 1 | |
| 61 | Da | 1 | Total | Ca | 0 |
| | | | 1 | 1 | |

- Molecule 62 is DINUCLEAR COPPER ION (CCD ID: CUA) (formula: $Cu_2$) (labeled as "Ligand of Interest" by depositor).




| Mol | Chain | Residues | Atoms | AltConf |
|---|---|---|---|---|
| 62 | DB | 1 | Total Cu<br>2 2 | 0 |
| 62 | Db | 1 | Total Cu<br>2 2 | 0 |

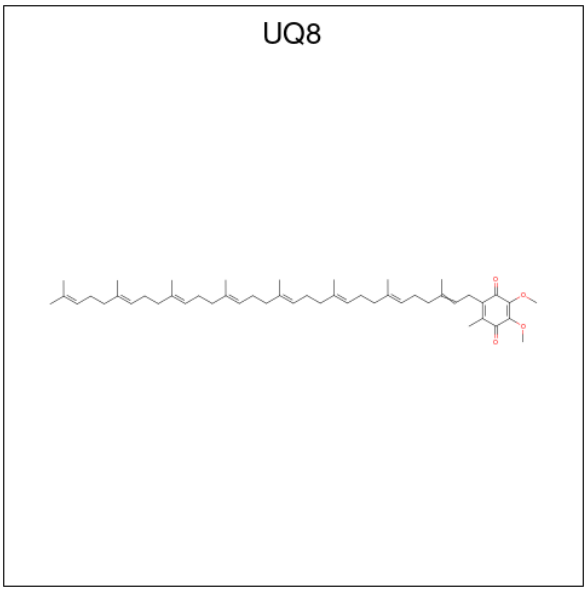
- Molecule 63 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

| Mol | Chain | Residues | Atoms | AltConf |
|---|---|---|---|---|
| 63 | DD | 1 | Total Zn<br>1 1 | 0 |
| 63 | Dd | 1 | Total Zn<br>1 1 | 0 |

- Molecule 64 is POTASSIUM ION (CCD ID: K) (formula: K) (labeled as "Ligand of Interest" by depositor).

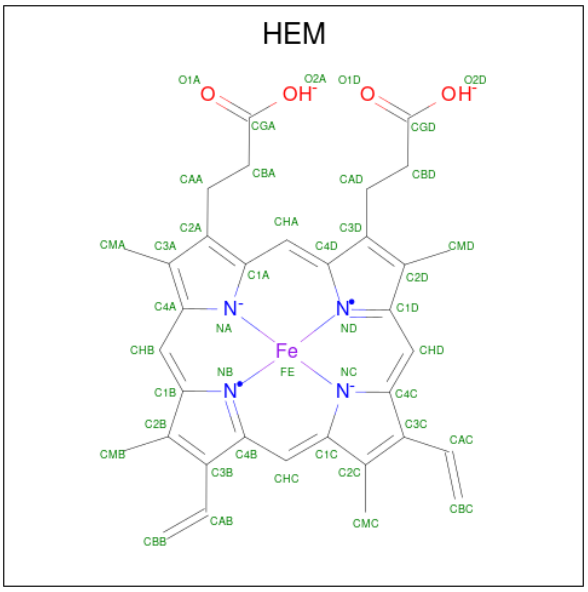
| Mol | Chain | Residues | Atoms | AltConf |
|---|---|---|---|---|
| 64 | DD | 1 | Total K<br>1 1 | 0 |

- Molecule 65 is Ubiquinone-8 (CCD ID: UQ8) (formula: $C_{49}H_{74}O_4$) (labeled as "Ligand of Interest" by depositor).



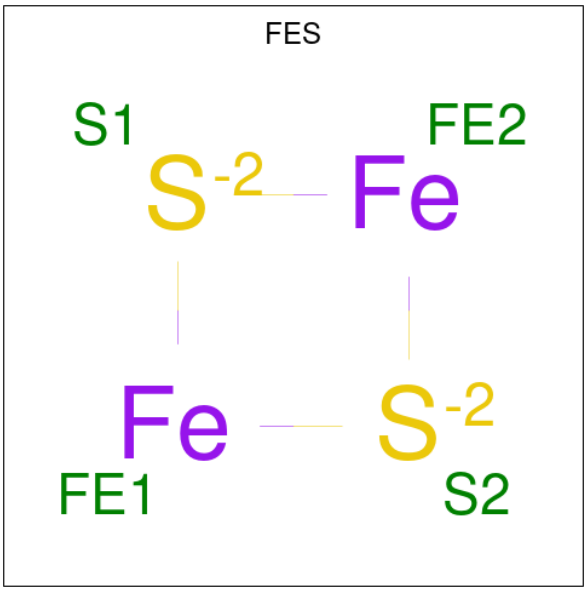

| Mol | Chain | Residues | Atoms | | | | AltConf |
|---|---|---|---|---|---|---|---|
| 65 | DS | 1 | Total | C | H | O | 0 |
| | | | 127 | 49 | 74 | 4 | |
| 65 | ED | 1 | Total | C | H | O | 0 |
| | | | 127 | 49 | 74 | 4 | |
| 65 | EL | 1 | Total | C | H | O | 0 |
| | | | 127 | 49 | 74 | 4 | |
| 65 | EN | 1 | Total | C | H | O | 0 |
| | | | 127 | 49 | 74 | 4 | |
| 65 | Ds | 1 | Total | C | H | O | 0 |
| | | | 127 | 49 | 74 | 4 | |
| 65 | Ed | 1 | Total | C | H | O | 0 |
| | | | 127 | 49 | 74 | 4 | |
| 65 | El | 1 | Total | C | H | O | 0 |
| | | | 127 | 49 | 74 | 4 | |
| 65 | En | 1 | Total | C | H | O | 0 |
| | | | 127 | 49 | 74 | 4 | |

- Molecule 66 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).




| Mol | Chain | Residues | Atoms | | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|---|
| 66 | ED | 1 | Total | C | Fe | H | N | O | 0 |
| | | | 65 | 34 | 1 | 22 | 4 | 4 | |
| 66 | Ed | 1 | Total | C | Fe | H | N | O | 0 |
| | | | 67 | 34 | 1 | 24 | 4 | 4 | |

- Molecule 67 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: $Fe_2S_2$) (labeled as "Ligand of Interest" by depositor).



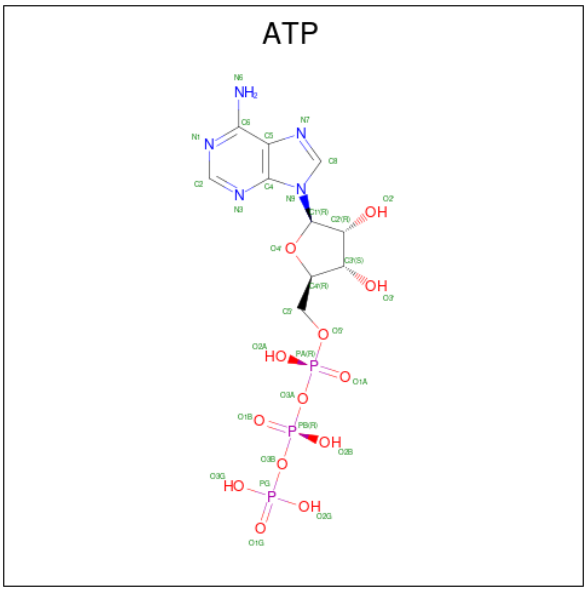

| Mol | Chain | Residues | Atoms | | | AltConf |
|---|---|---|---|---|---|---|
| 67 | EF | 1 | Total | Fe | S | 0 |
| | | | 4 | 2 | 2 | |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Residues | Atoms | | | AltConf |
|---|---|---|---|---|---|---|
| 67 | EF | 1 | Total | Fe | S | 0 |
| | | | 4 | 2 | 2 | |
| 67 | Ef | 1 | Total | Fe | S | 0 |
| | | | 4 | 2 | 2 | |
| 67 | Ef | 1 | Total | Fe | S | 0 |
| | | | 4 | 2 | 2 | |

- Molecule 68 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



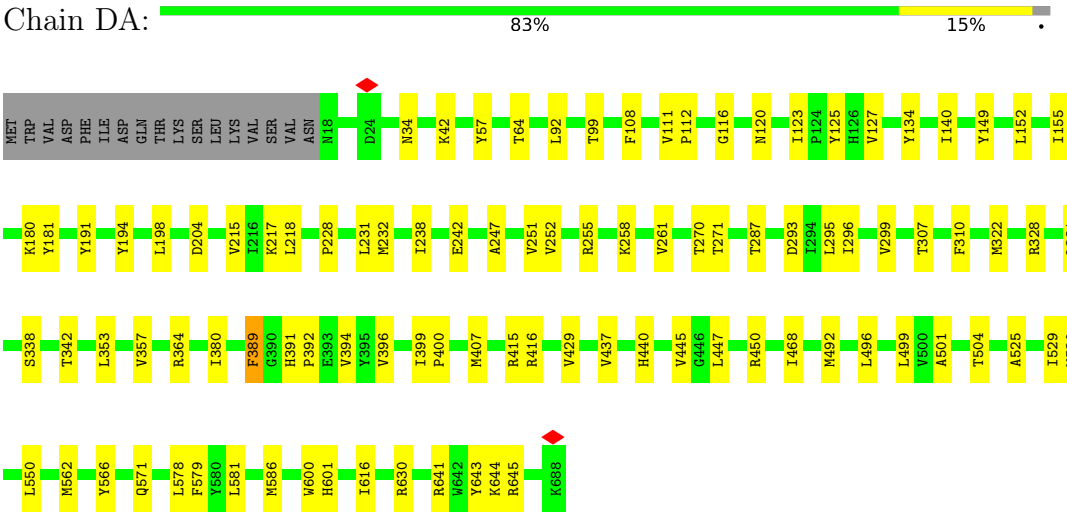

| Mol | Chain | Residues | Atoms | | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|---|
| 68 | ER | 1 | Total | C | H | N | O | P | 0 |
| | | | 43 | 10 | 12 | 5 | 13 | 3 | |
| 68 | Er | 1 | Total | C | H | N | O | P | 0 |
| | | | 43 | 10 | 12 | 5 | 13 | 3 | |

# 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.

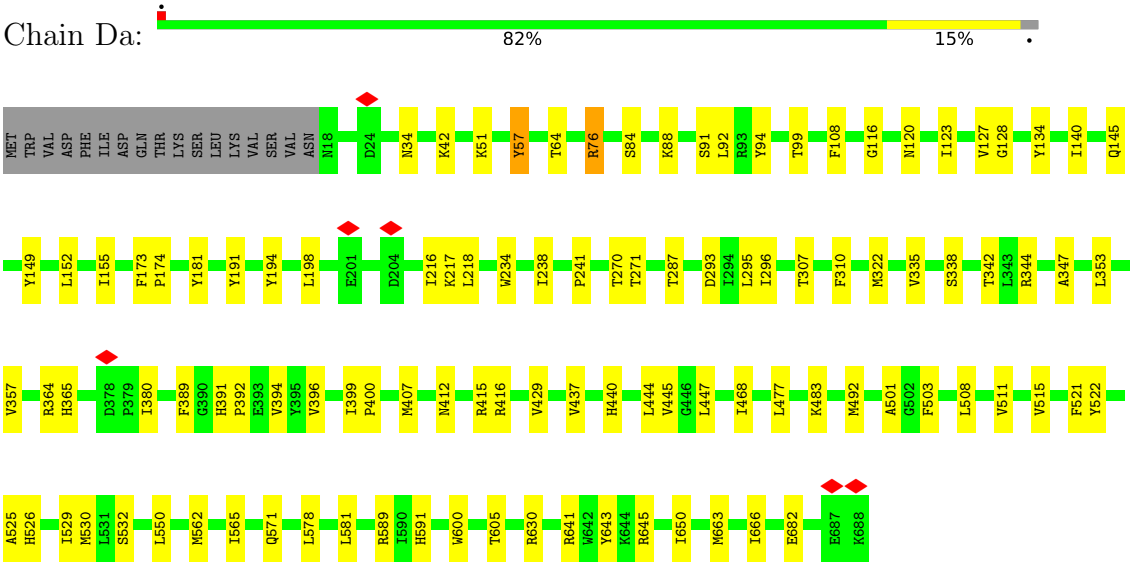
• Molecule 1: Cytochrome c oxidase subunit 1

Chain DA:



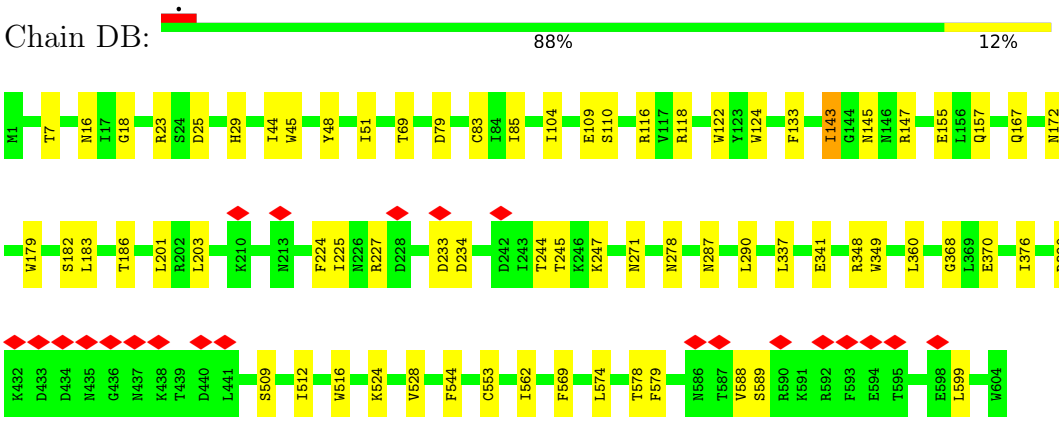

• Molecule 1: Cytochrome c oxidase subunit 1

Chain Da:



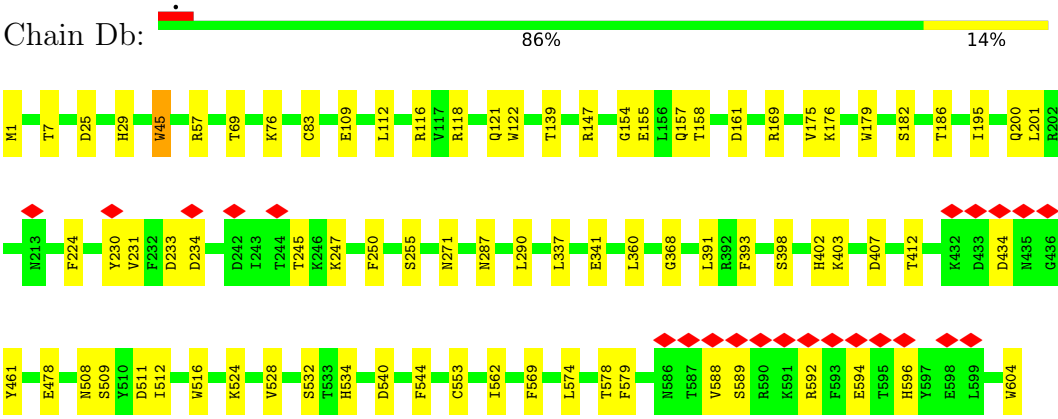

• Molecule 2: Cytochrome c oxidase subunit 2

Chain DB:



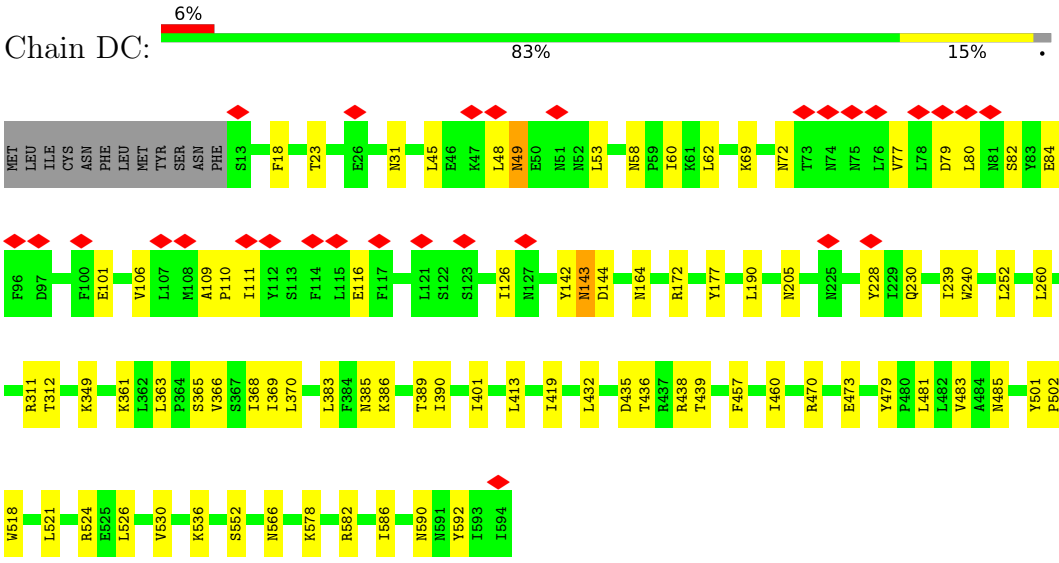

• Molecule 2: Cytochrome c oxidase subunit 2

Chain Db:



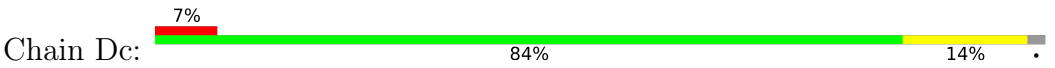

• Molecule 3: Ymf68

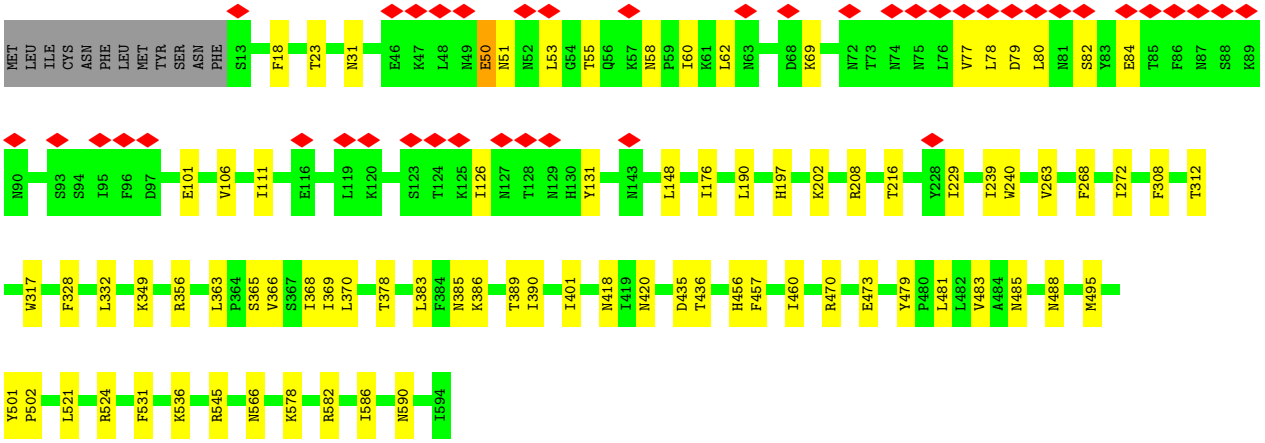
Chain DC:




• Molecule 3: Ymf68

Chain Dc:

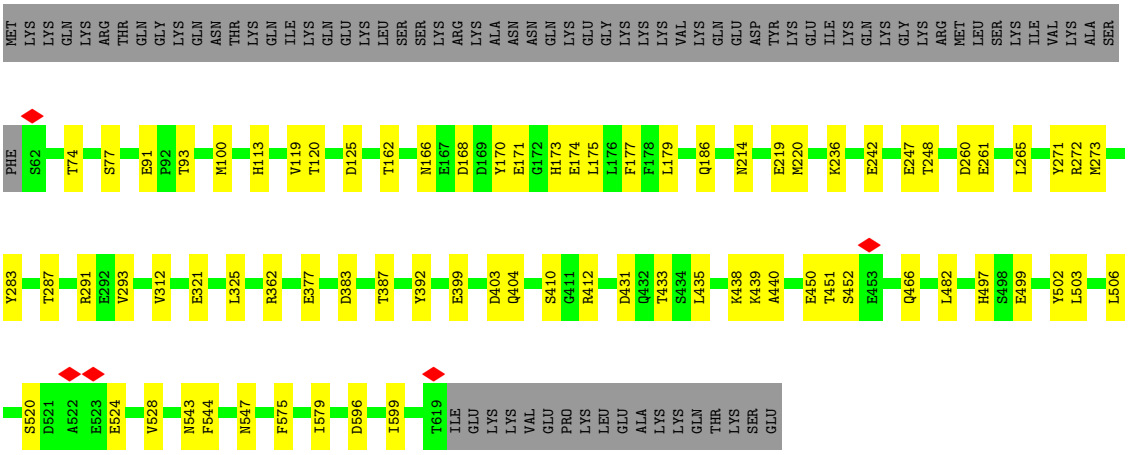




• Molecule 4: Cytochrome C oxidase subunit Vb protein

Chain DD:

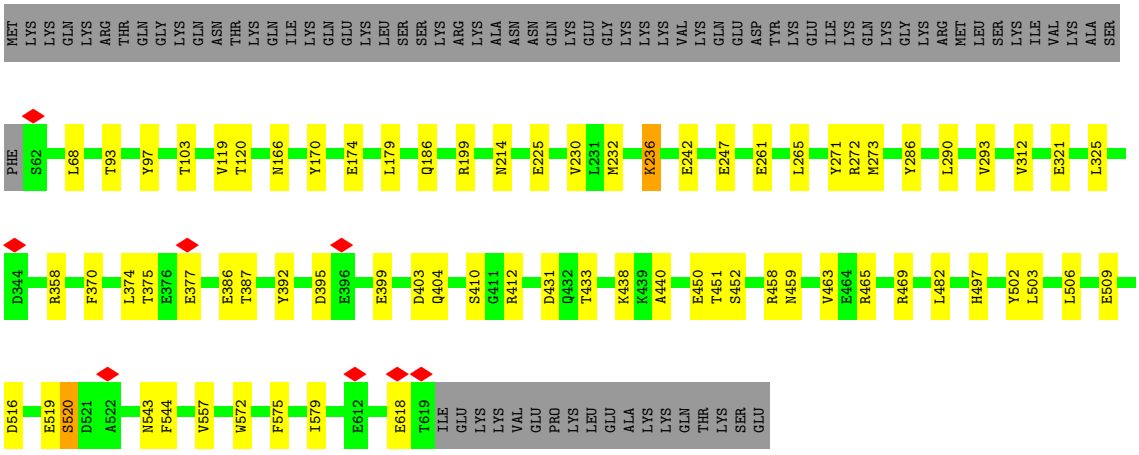


• Molecule 4: Cytochrome C oxidase subunit Vb protein

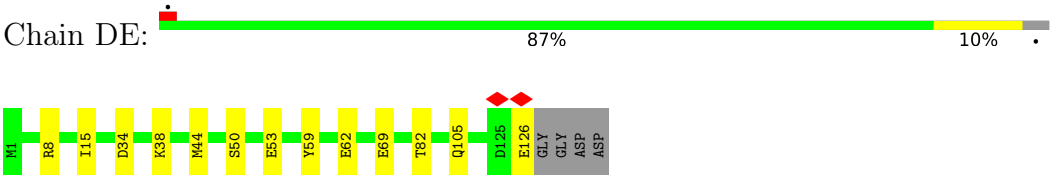
Chain Dd:



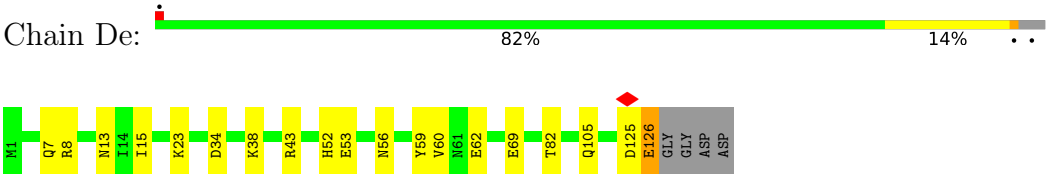
• Molecule 5: Transmembrane protein, putative

Chain DE:



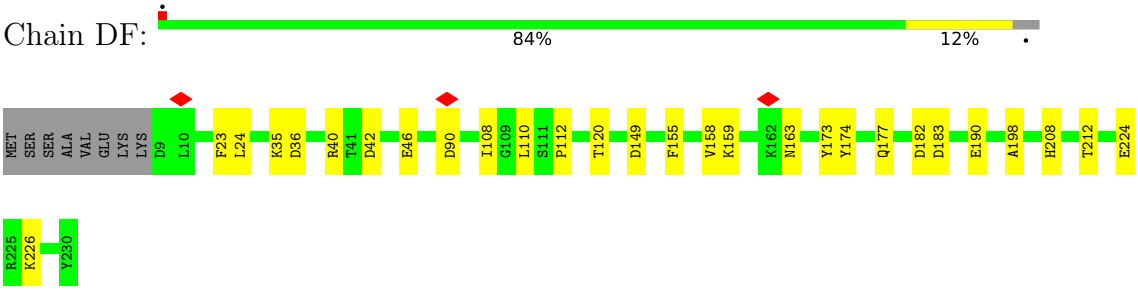

• Molecule 5: Transmembrane protein, putative

Chain De:



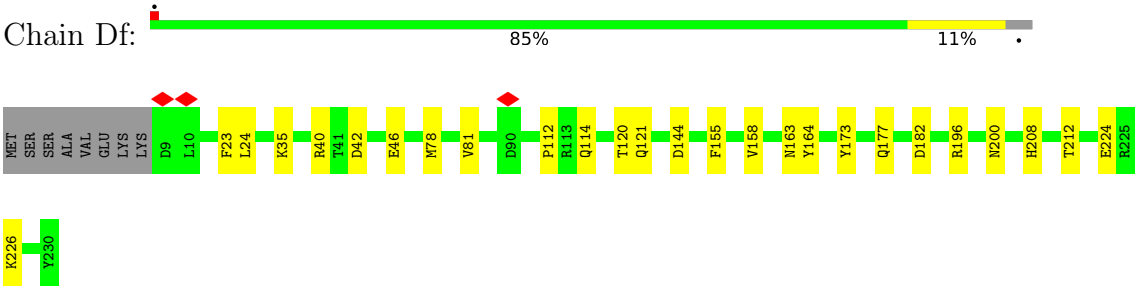

• Molecule 6: Structural protein

Chain DF:



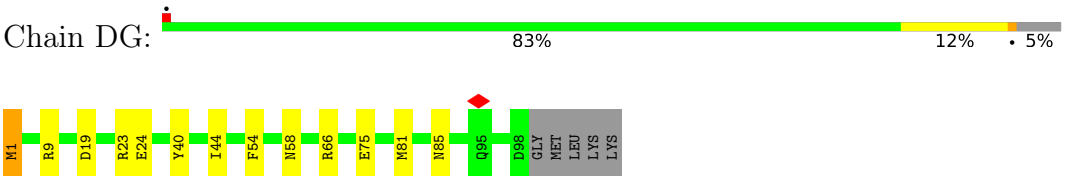

• Molecule 6: Structural protein

Chain Df:



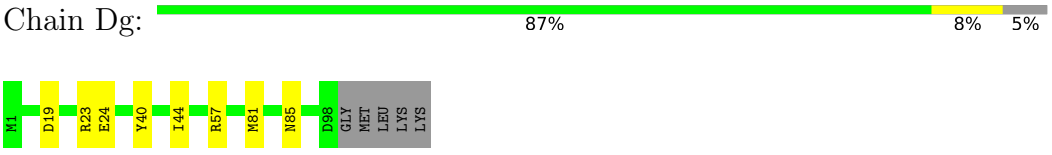

• Molecule 7: Transmembrane protein, putative

Chain DG:



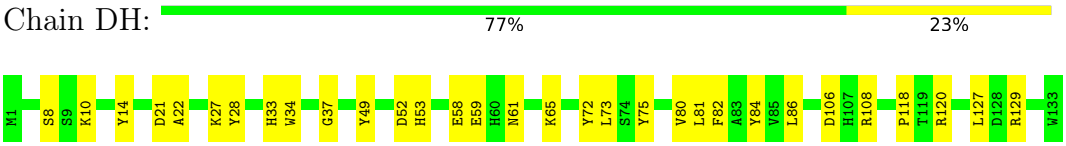

• Molecule 7: Transmembrane protein, putative

Chain Dg:



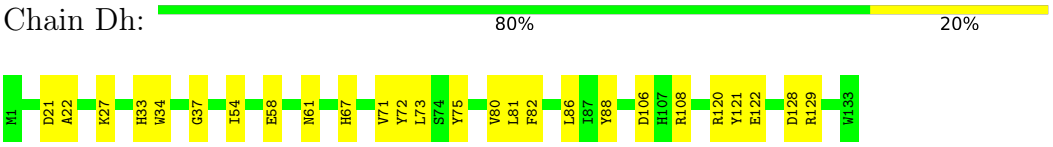

• Molecule 8: Transmembrane protein, putative

Chain DH:



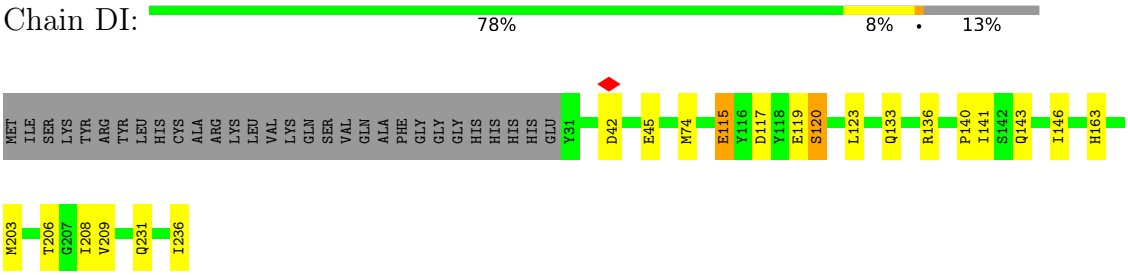

• Molecule 8: Transmembrane protein, putative

Chain Dh:



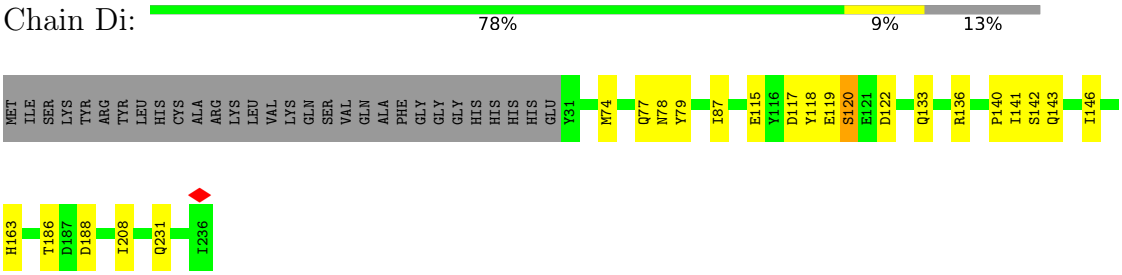

• Molecule 9: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

Chain DI:



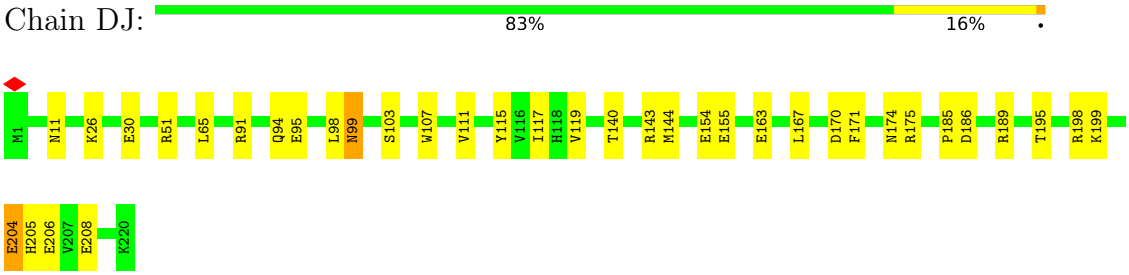

• Molecule 9: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

Chain Di:



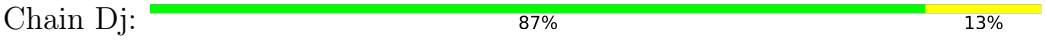

• Molecule 10: Transmembrane protein, putative

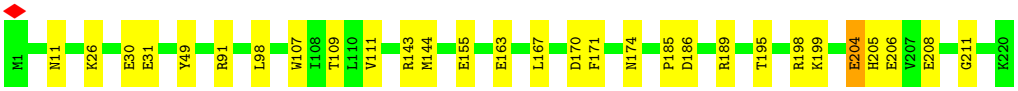
Chain DJ:




• Molecule 10: Transmembrane protein, putative

Chain Dj:

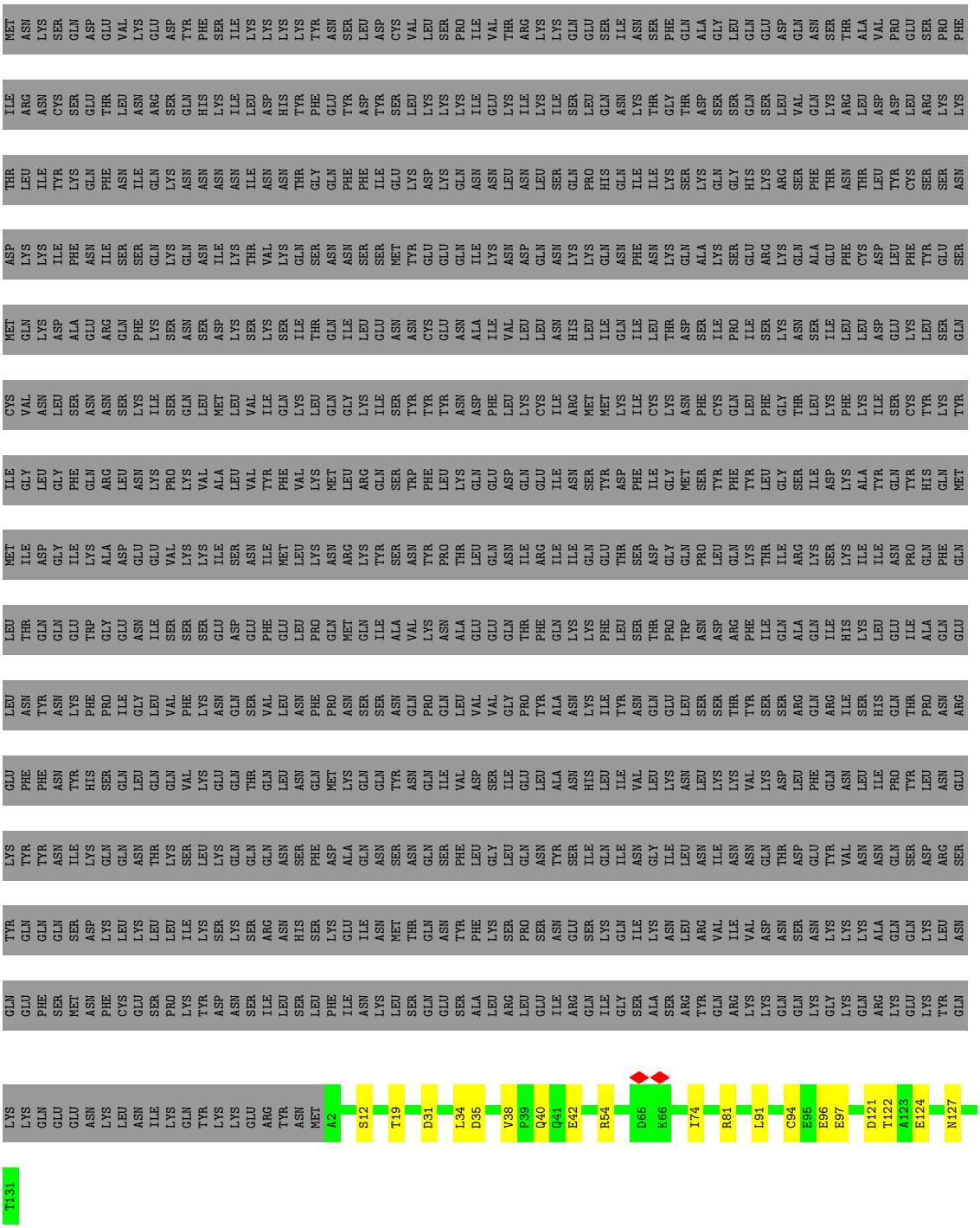





• Molecule 11: CTF/NF-I domain-containing protein

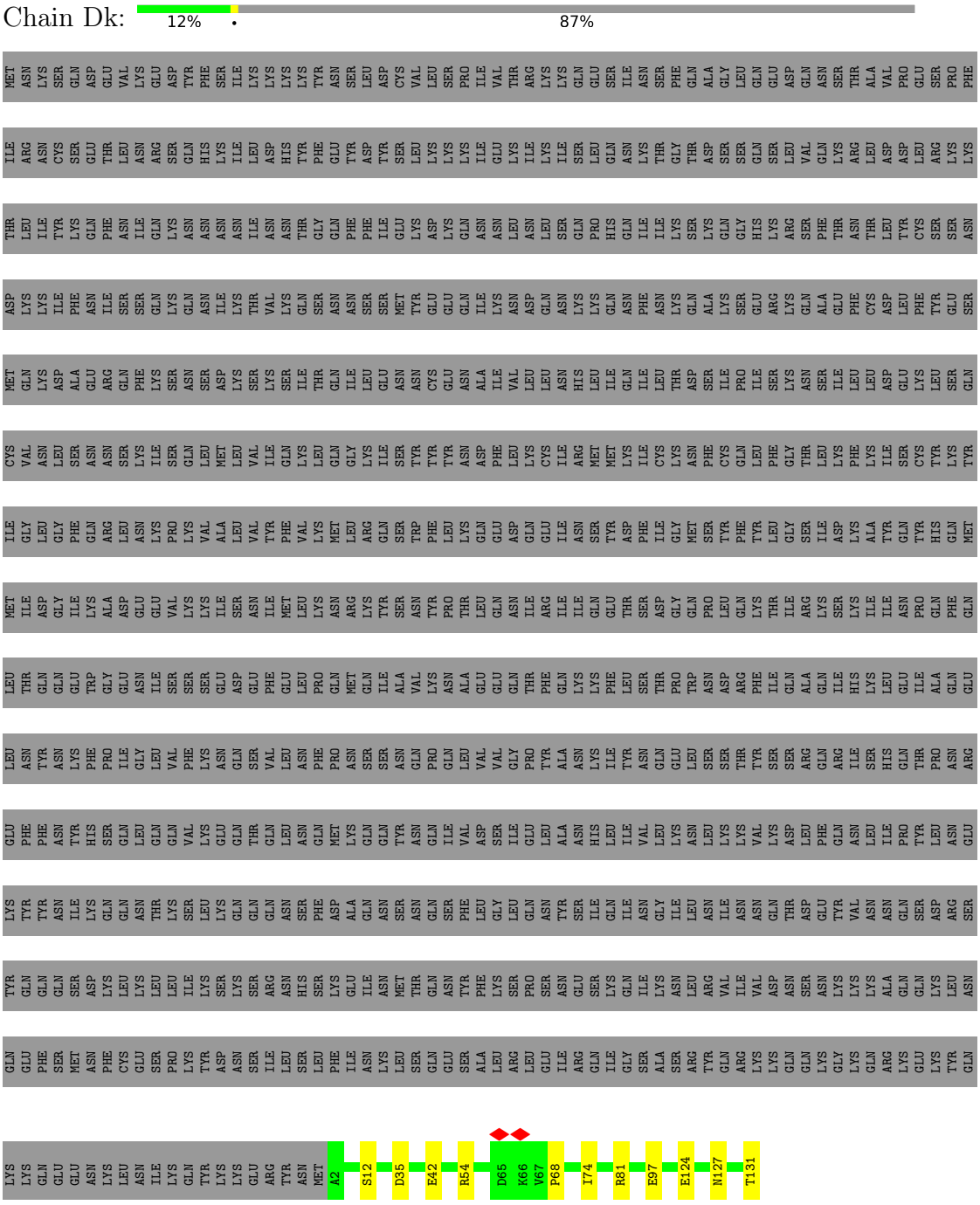
Chain DK:



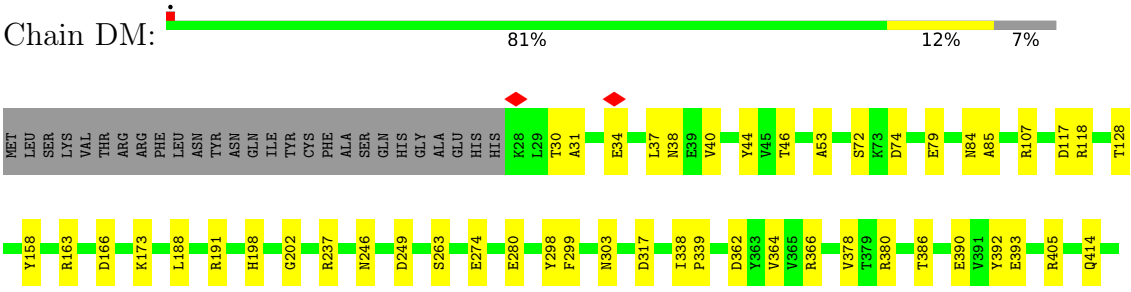

• Molecule 11: CTF/NF-I domain-containing protein

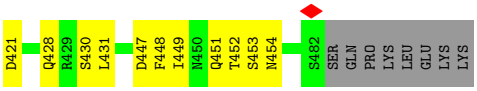
Chain Dk:



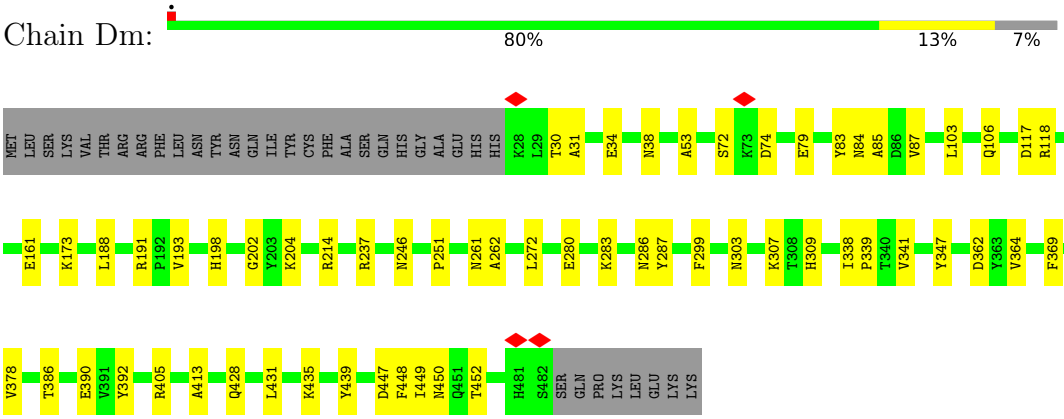

• Molecule 12: Transmembrane protein, putative

Chain DM:

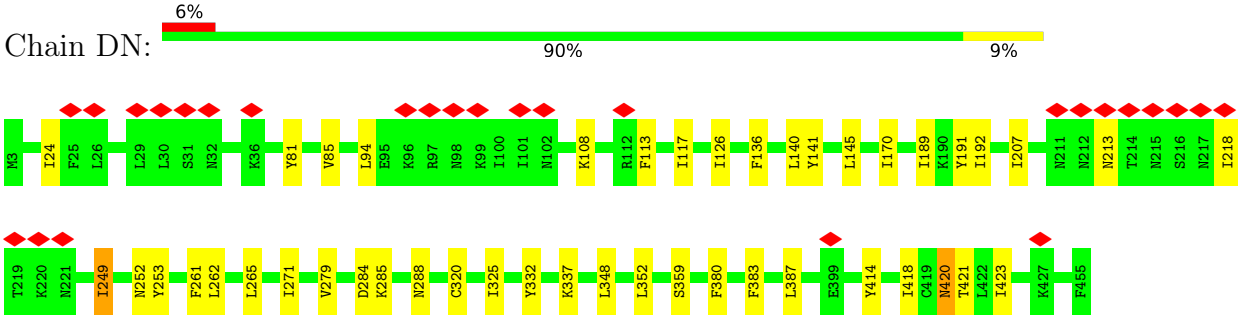




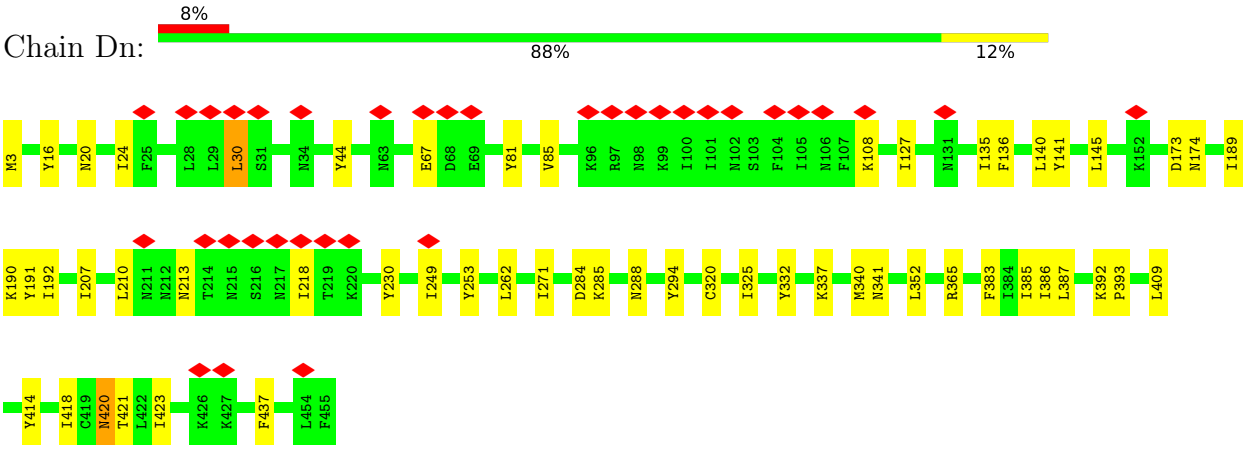

• Molecule 12: Transmembrane protein, putative



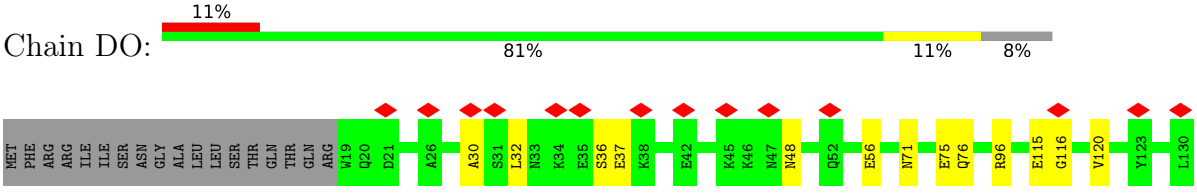

• Molecule 13: Ymf67

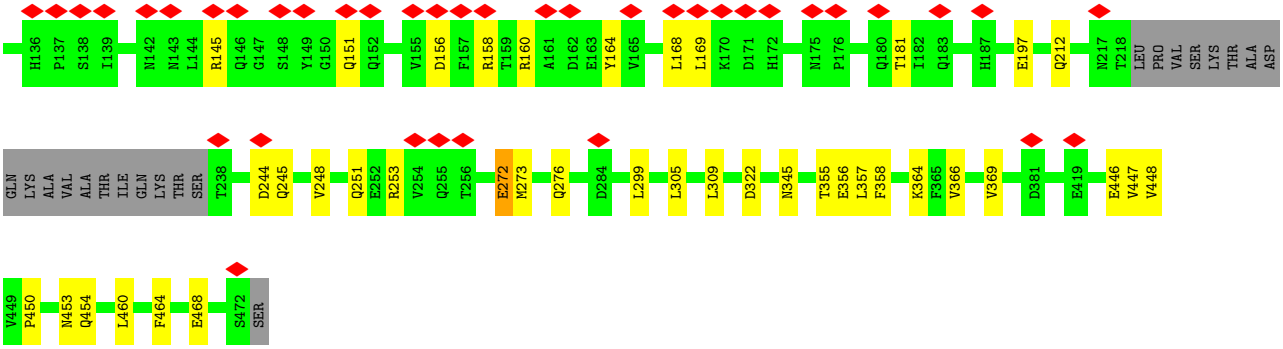



• Molecule 13: Ymf67




• Molecule 14: Protein phosphatase 2C, putative

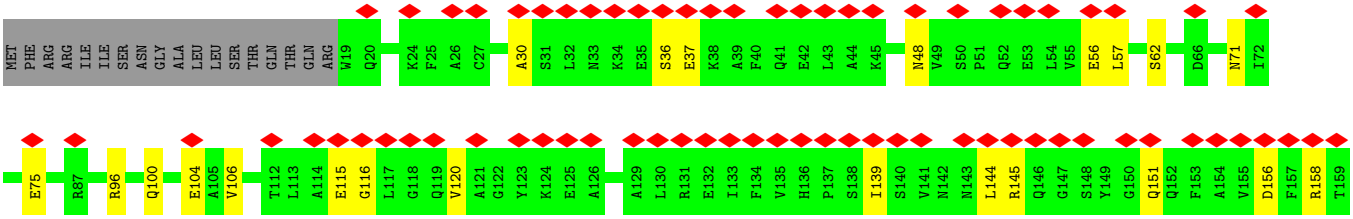





• Molecule 14: Protein phosphatase 2C, putative

Chain Do:

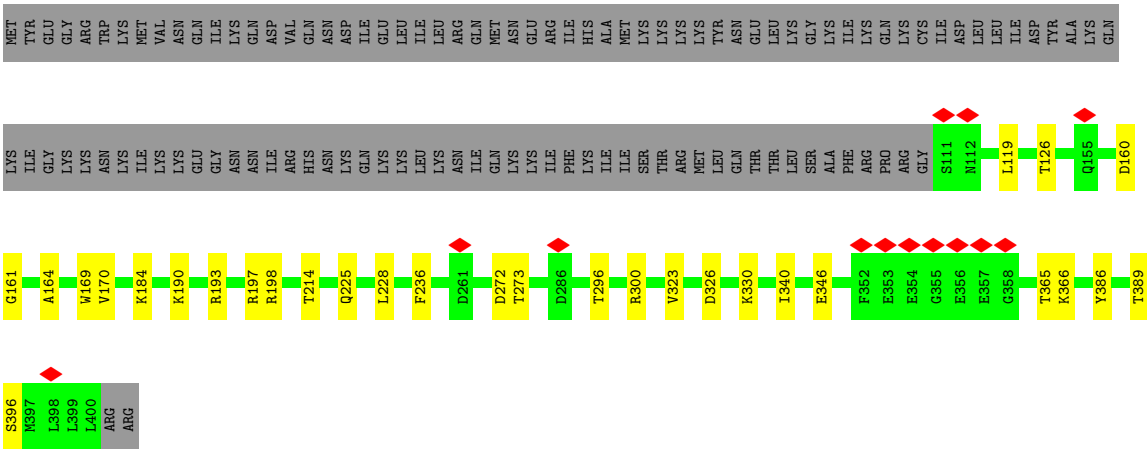



• Molecule 15: SURF1-like protein

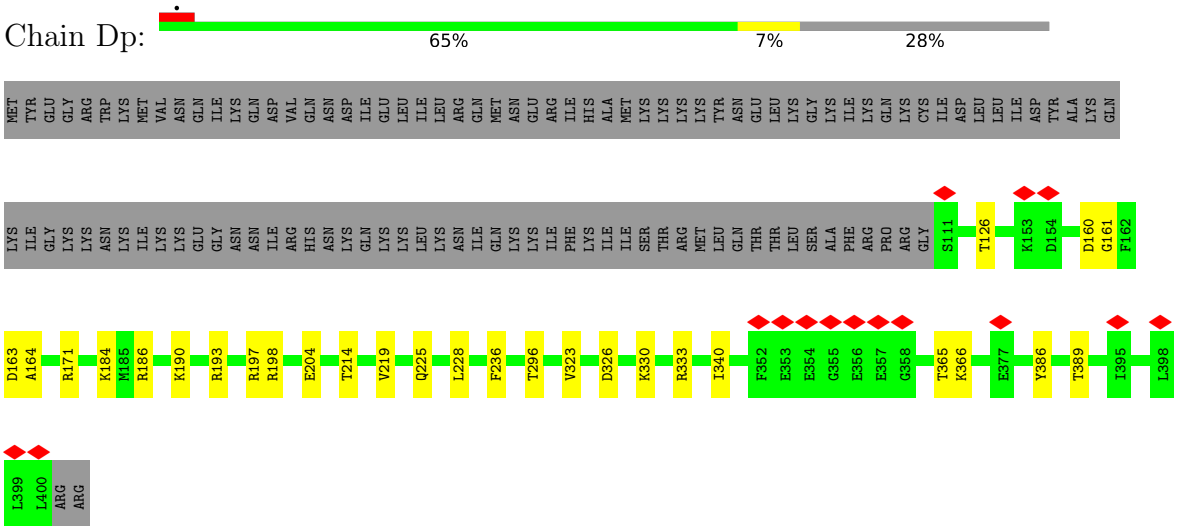
Chain DP:



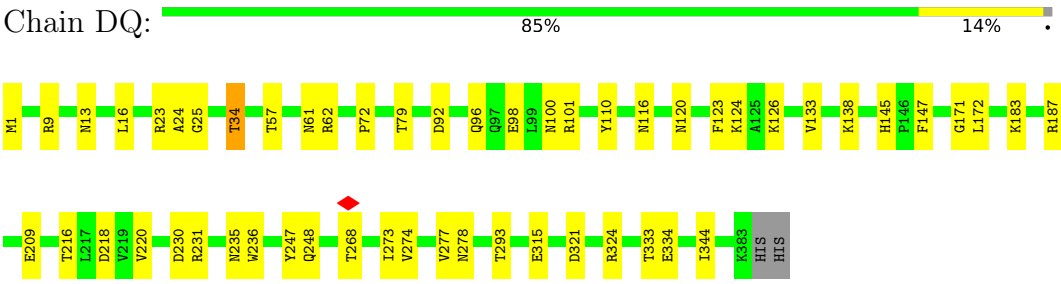
• Molecule 15: SURF1-like protein

Chain Dp:



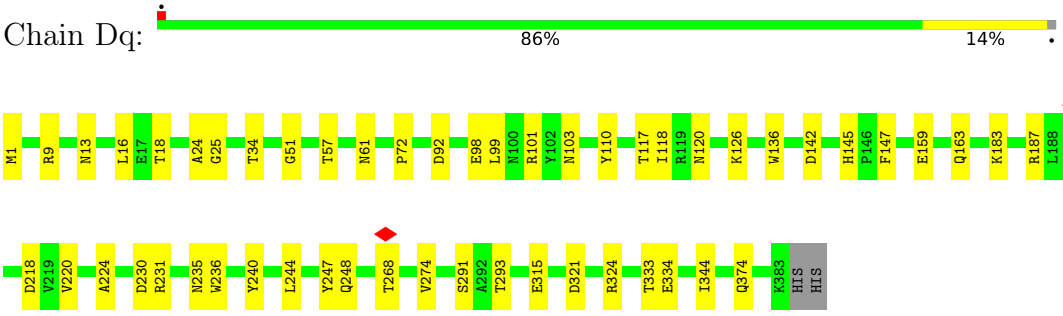

• Molecule 16: TraB family protein

Chain DQ:



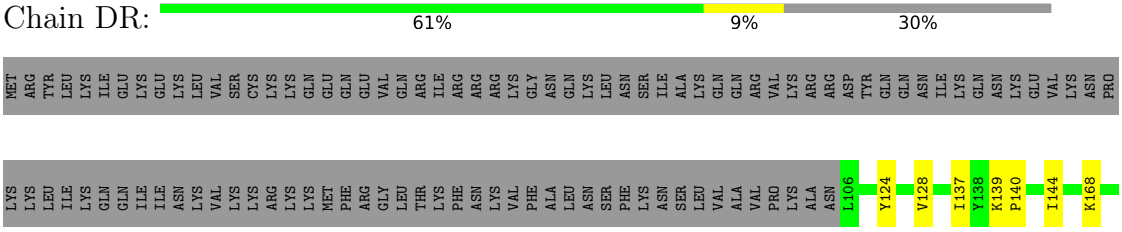

• Molecule 16: TraB family protein

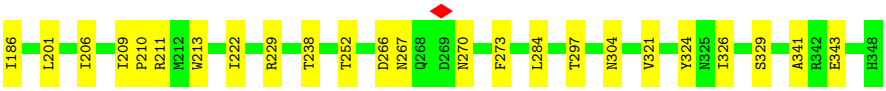
Chain Dq:



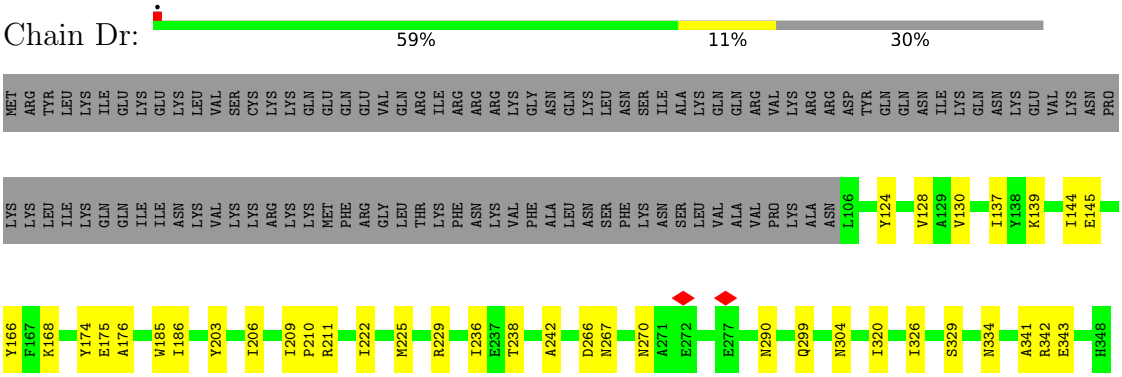

• Molecule 17: Transmembrane protein, putative

Chain DR:

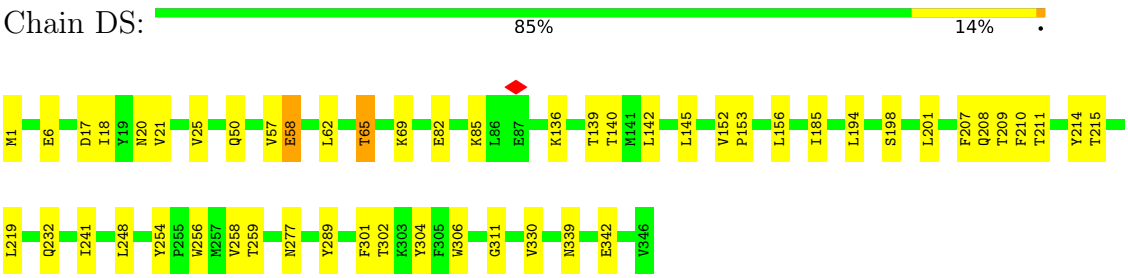




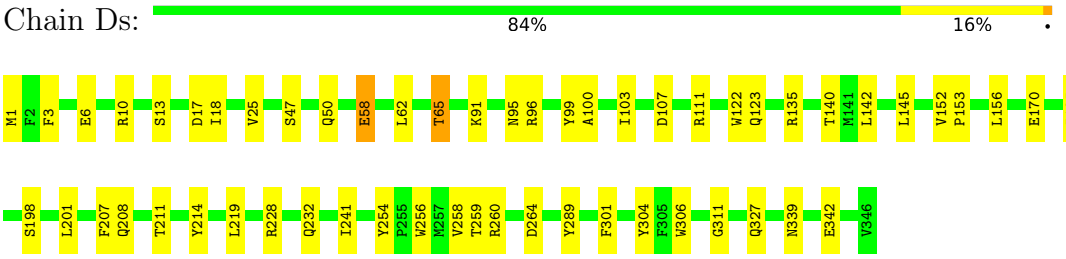

• Molecule 17: Transmembrane protein, putative



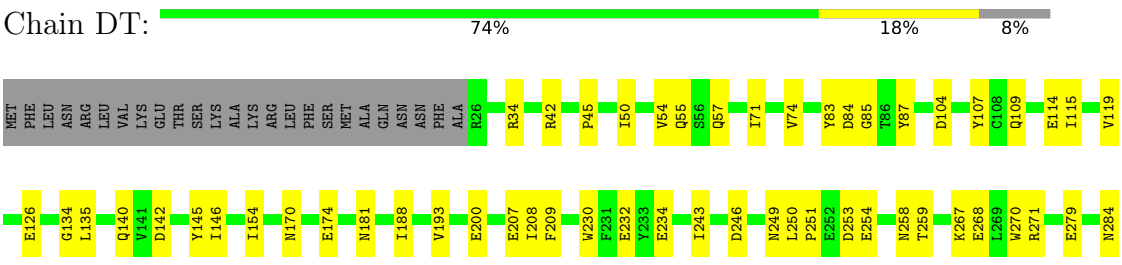

• Molecule 18: Oxoglutarate/malate translocator protein, putative




• Molecule 18: Oxoglutarate/malate translocator protein, putative




• Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8, mitochondrial

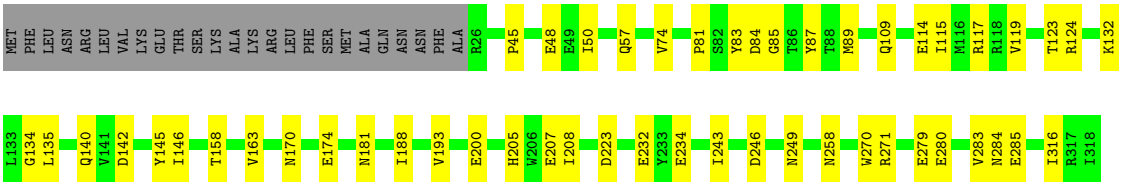





• Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8, mitochondrial

Chain Dt:




• Molecule 20: Carrier protein

Chain DU:



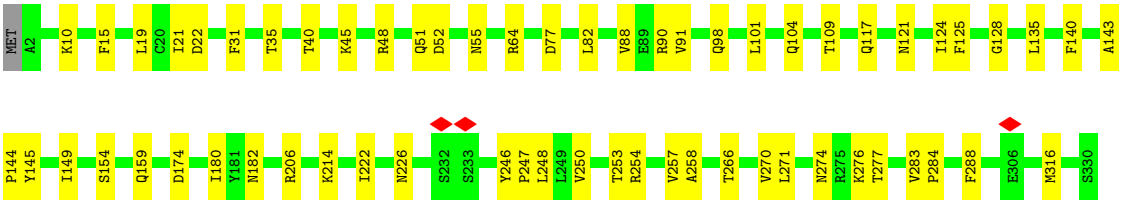




• Molecule 20: Carrier protein

Chain Du:

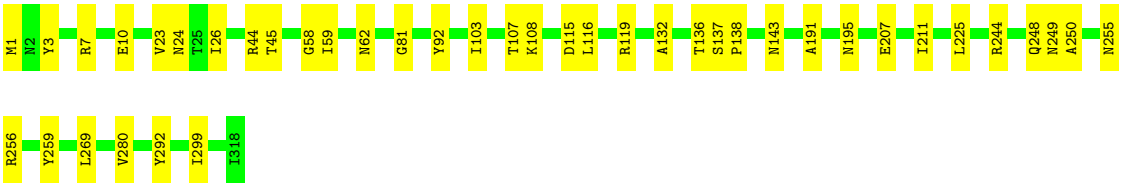



• Molecule 21: 2-oxoglutarate/malate carrier protein

Chain DV:

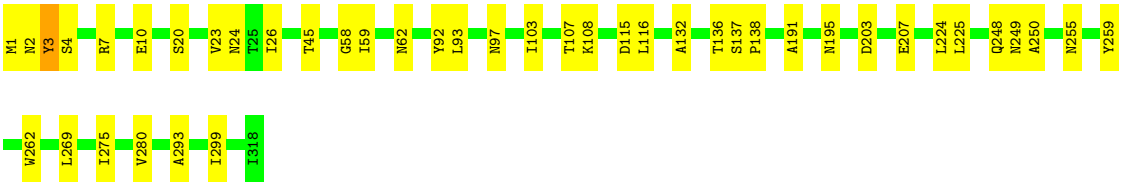


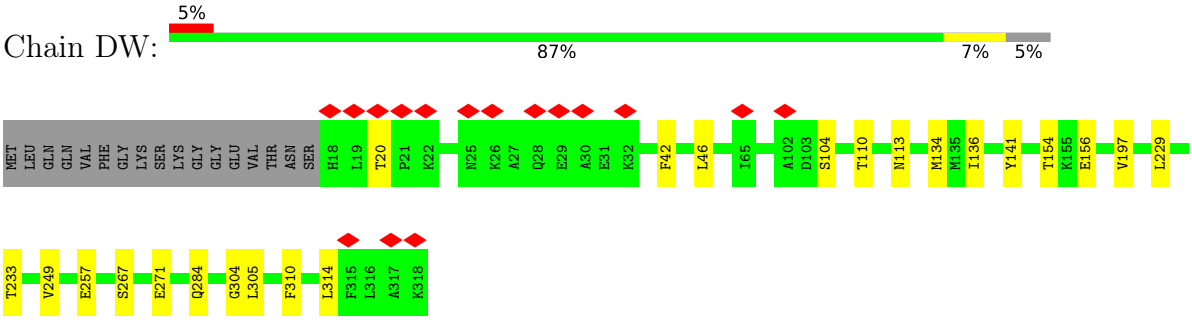

• Molecule 21: 2-oxoglutarate/malate carrier protein

Chain Dv:

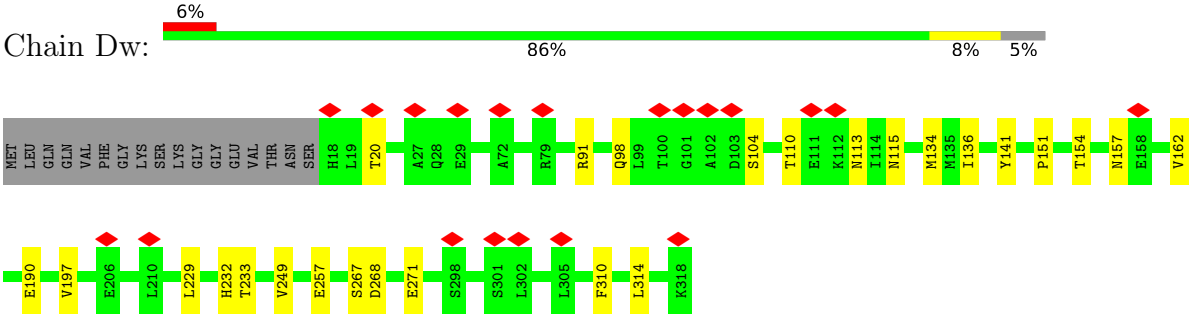




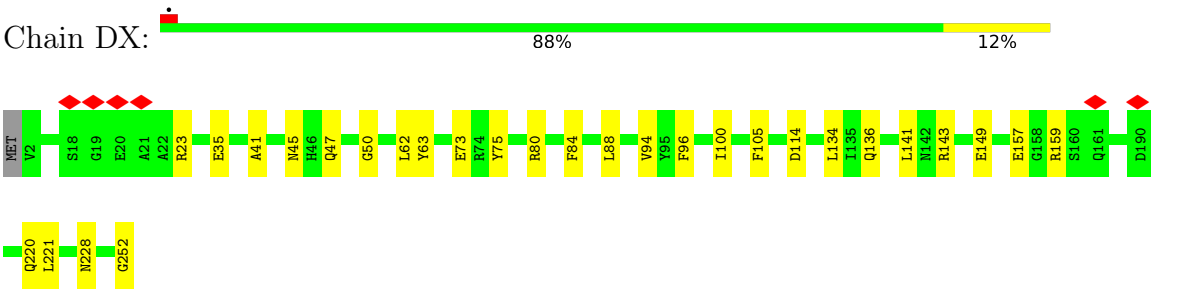

• Molecule 22: SURF1-like protein



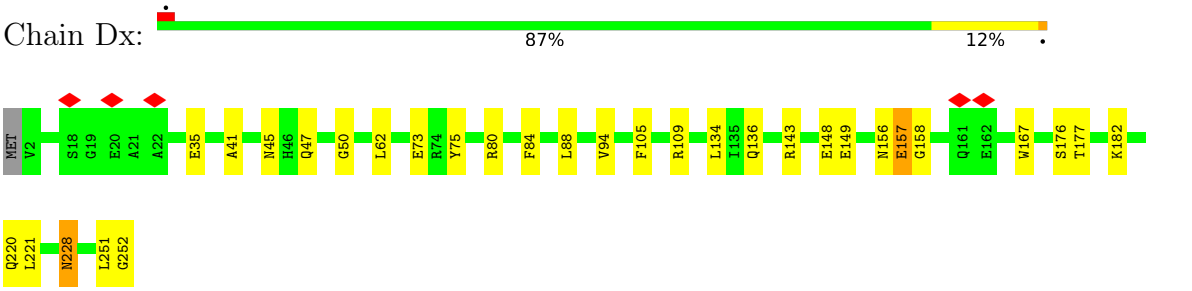

• Molecule 22: SURF1-like protein




• Molecule 23: COXTT9

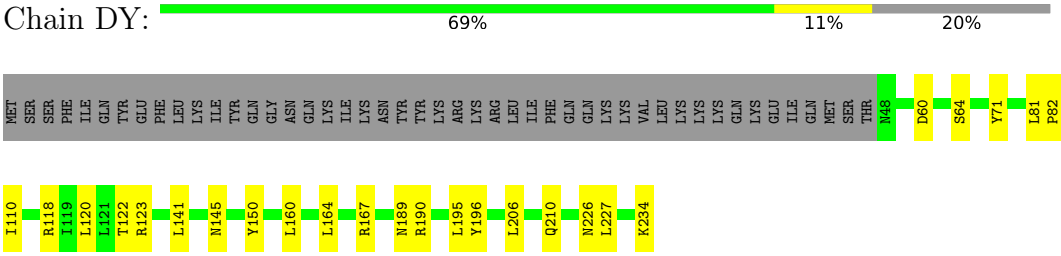



• Molecule 23: COXTT9



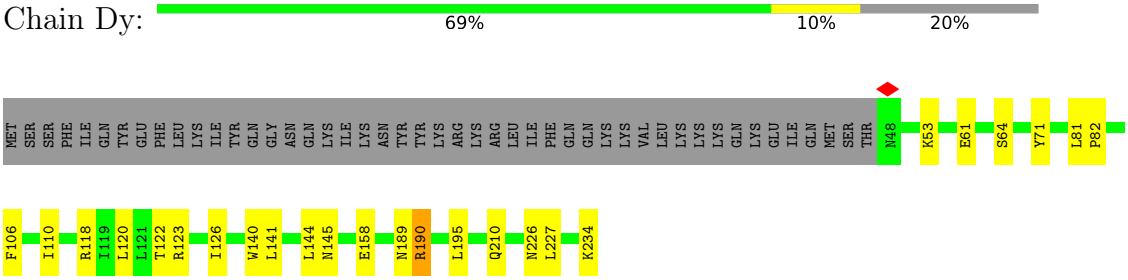
• Molecule 24: COXTT10

Chain DY:



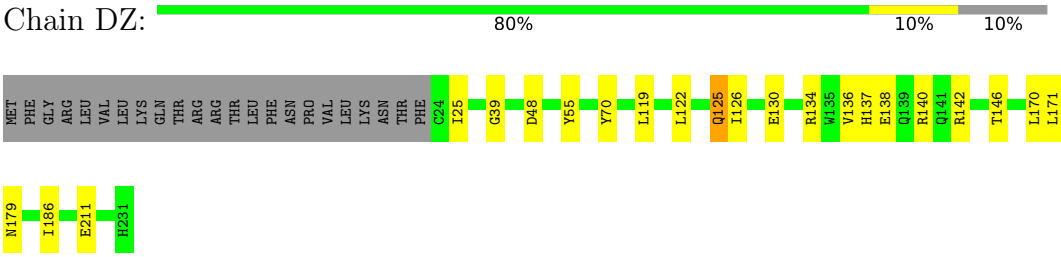

• Molecule 24: COXTT10

Chain Dy:



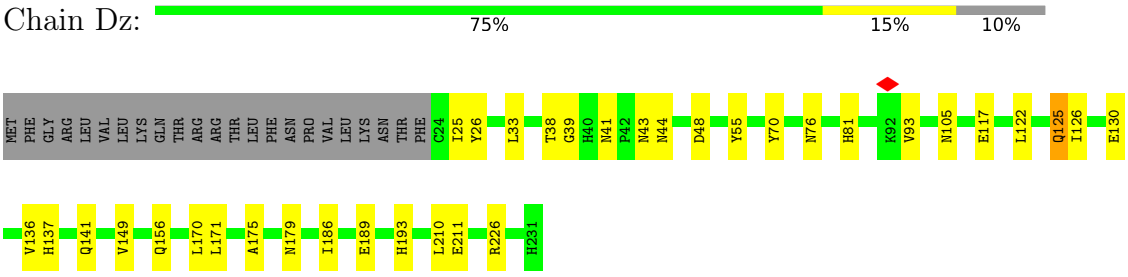

• Molecule 25: 39S ribosomal protein L9, mitochondrial

Chain DZ:



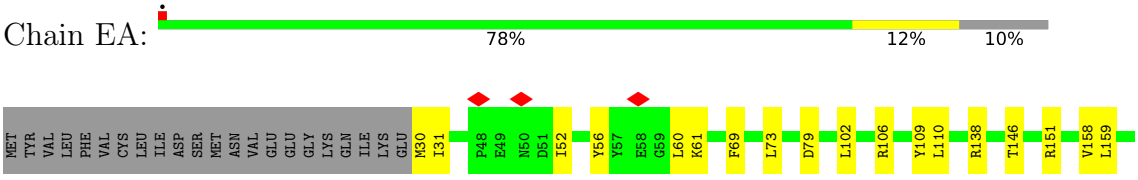

• Molecule 25: 39S ribosomal protein L9, mitochondrial

Chain Dz:




• Molecule 26: COXTT12,Transmembrane protein,Transmembrane protein

Chain EA:

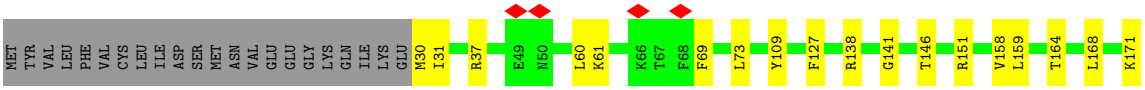





• Molecule 26: COXTT12,Transmembrane protein,Transmembrane protein

Chain Ea:



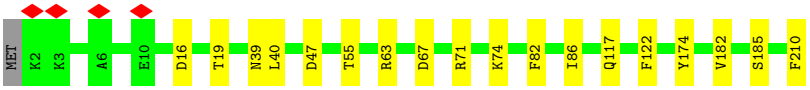




• Molecule 27: Transmembrane protein, putative

Chain EB:




• Molecule 27: Transmembrane protein, putative

Chain Eb:



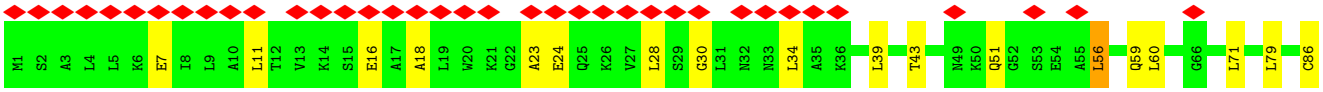


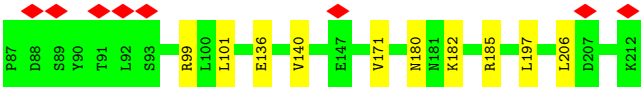


• Molecule 28: COXTT27

Chain EC:



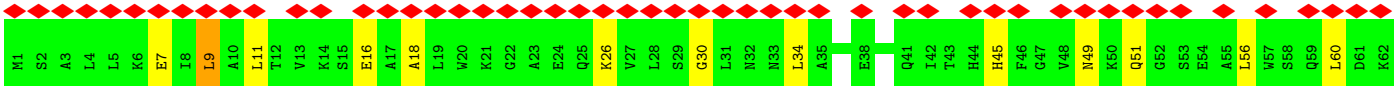



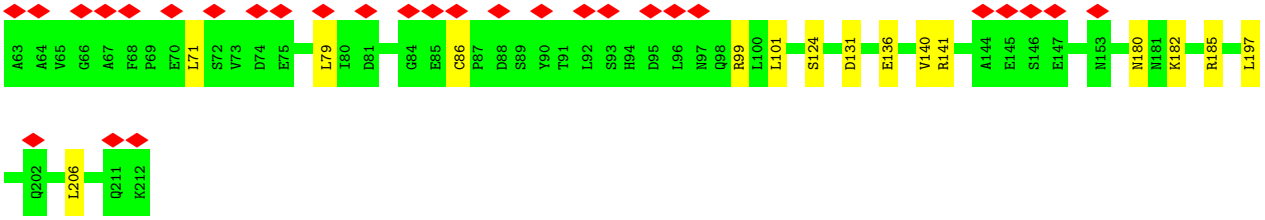




• Molecule 28: COXTT27

Chain Ec:



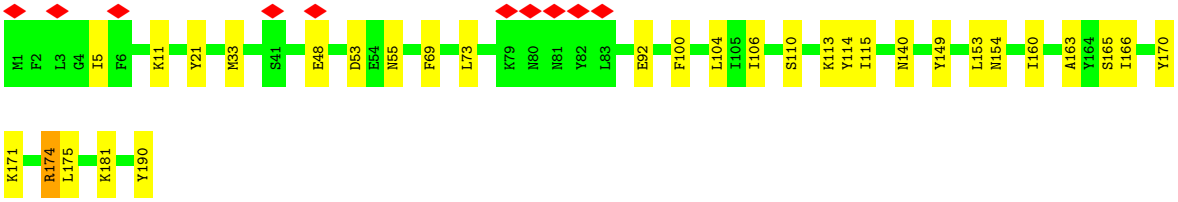






• Molecule 29: Ymf75

Chain ED:

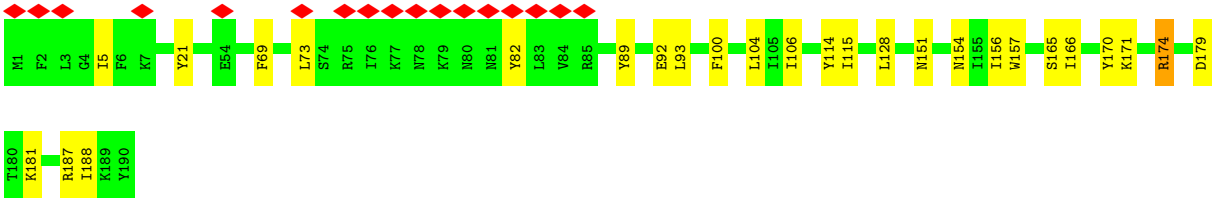



• Molecule 29: Ymf75

Chain Ed:

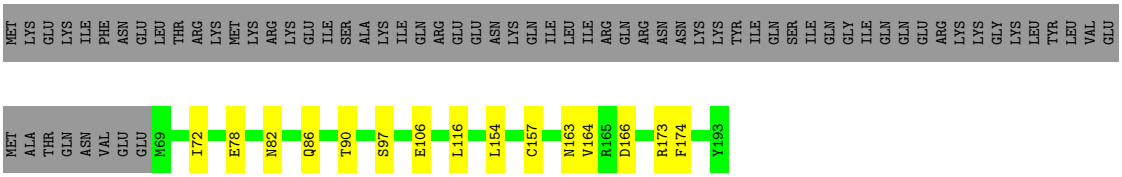



• Molecule 30: Mobilization protein

Chain EE:

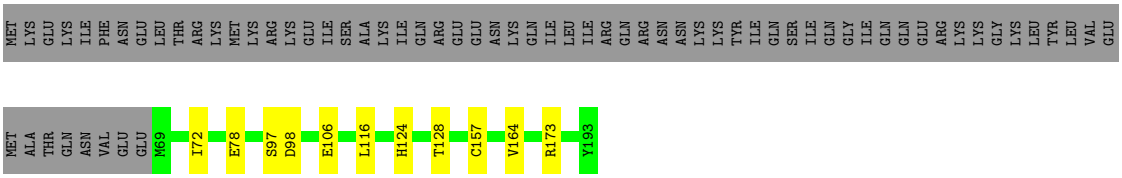



• Molecule 30: Mobilization protein

Chain Ee:




• Molecule 31: Iron-binding zinc finger CDGSH type protein

Chain EF:






• Molecule 31: Iron-binding zinc finger CDGSH type protein

Chain Ef:



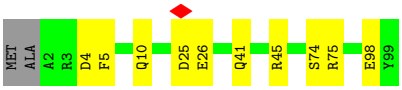




• Molecule 32: COXTT28

Chain EG:

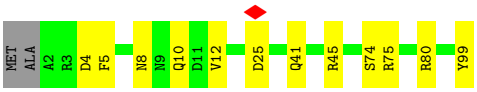



• Molecule 32: COXTT28

Chain Eg:

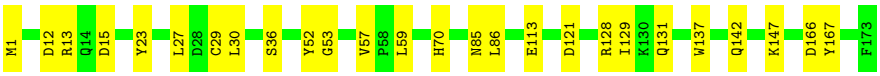



• Molecule 33: Transmembrane protein, putative

Chain EH:




• Molecule 33: Transmembrane protein, putative

Chain Eh:







• Molecule 34: Transmembrane protein

Chain EI:







• Molecule 34: Transmembrane protein

Chain Ei:

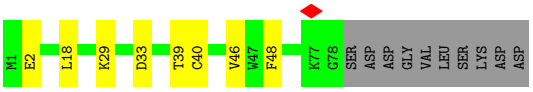





• Molecule 35: Decapping nuclease

Chain EV:

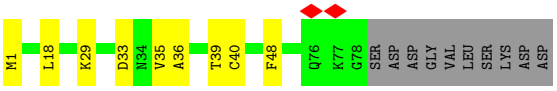



• Molecule 35: Decapping nuclease

Chain Ev:

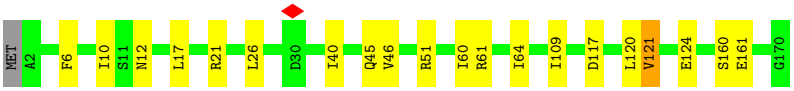



• Molecule 36: Complex III subunit VII

Chain EK:

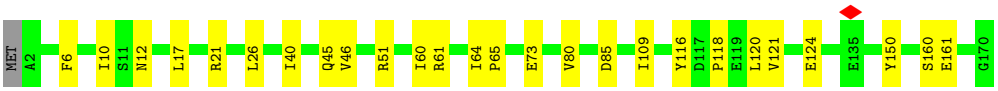



• Molecule 36: Complex III subunit VII

Chain Ek:




• Molecule 37: Transmembrane protein, putative

Chain EL:







• Molecule 37: Transmembrane protein, putative

Chain El:

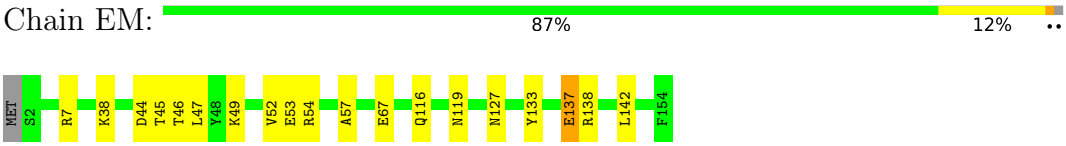






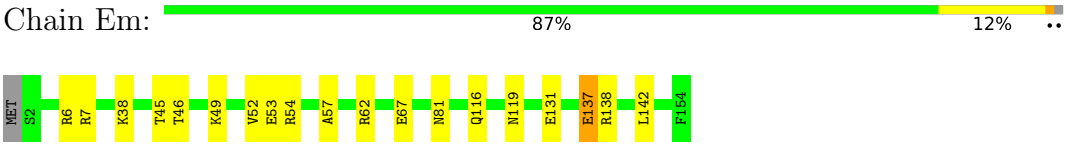
• Molecule 38: Transmembrane protein, putative

Chain EM:



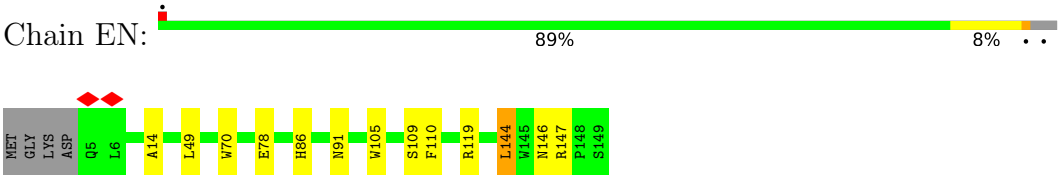

• Molecule 38: Transmembrane protein, putative

Chain Em:



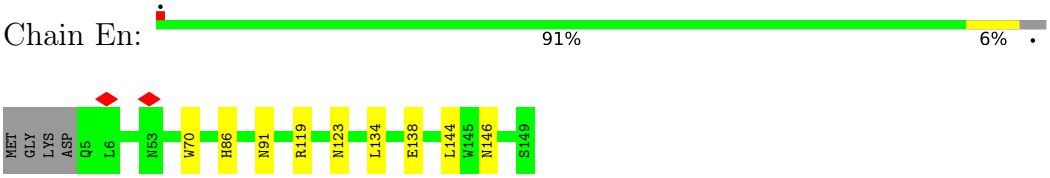

• Molecule 39: COXTT22

Chain EN:



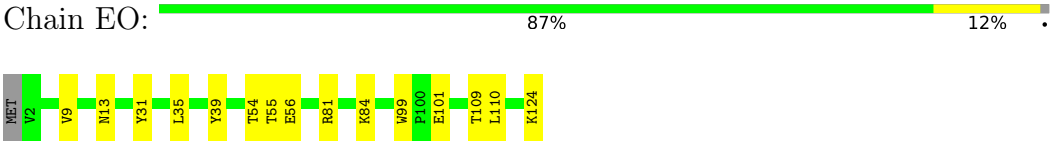

• Molecule 39: COXTT22

Chain En:



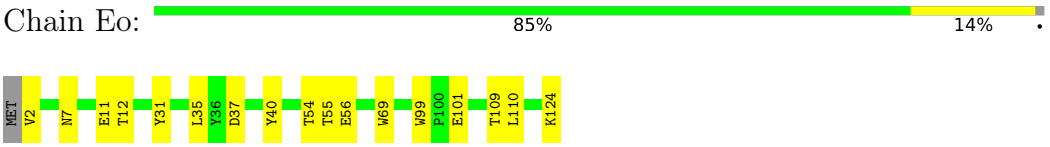

• Molecule 40: Transmembrane protein, putative

Chain EO:



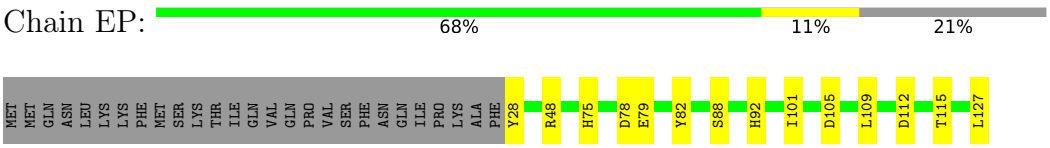

• Molecule 40: Transmembrane protein, putative

Chain Eo:



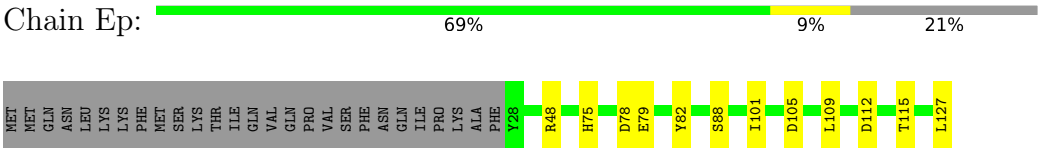

• Molecule 41: Phage protein

Chain EP:



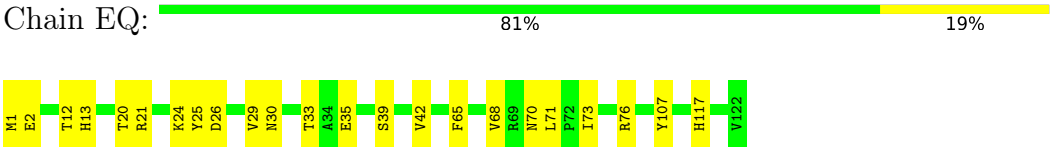

• Molecule 41: Phage protein

Chain Ep:



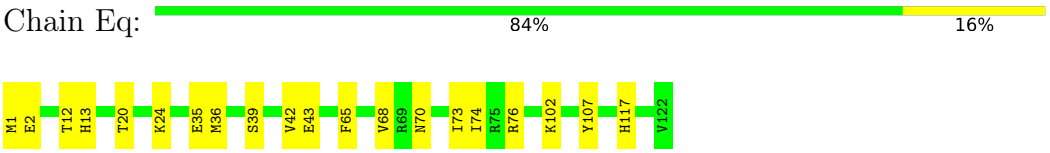

• Molecule 42: Transmembrane protein, putative

Chain EQ:



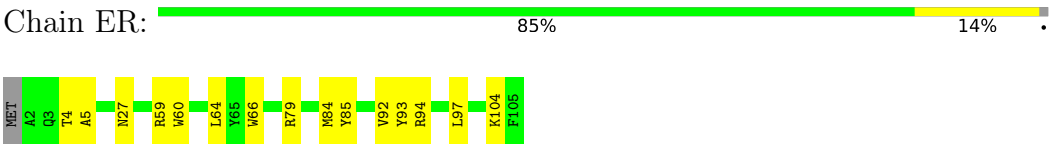

• Molecule 42: Transmembrane protein, putative

Chain Eq:



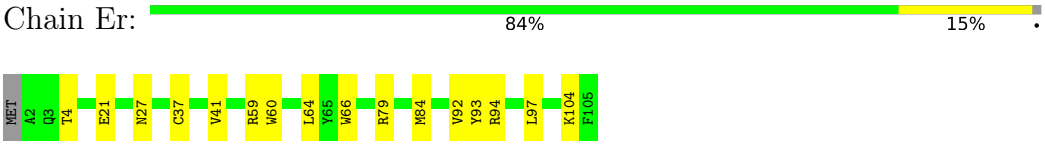

• Molecule 43: Lysozyme

Chain ER:



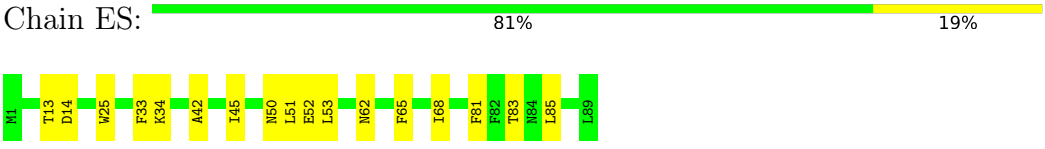

• Molecule 43: Lysozyme

Chain Er:



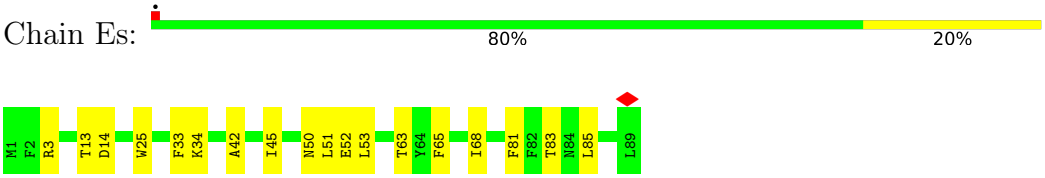

• Molecule 44: Ymf70

Chain ES:



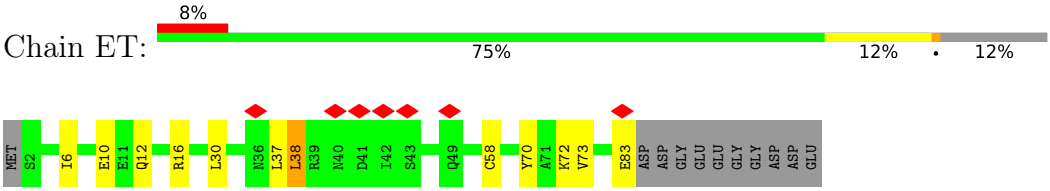

• Molecule 44: Ymf70

Chain Es:



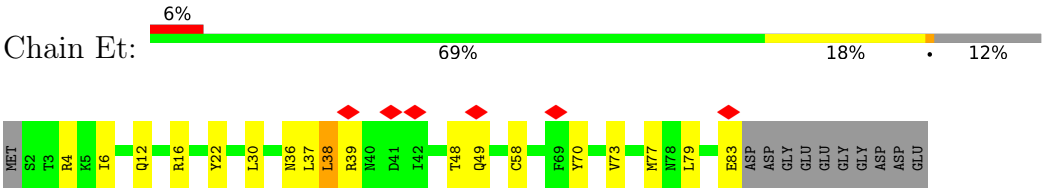

• Molecule 45: Zf-Tim10_DDP domain-containing protein

Chain ET:



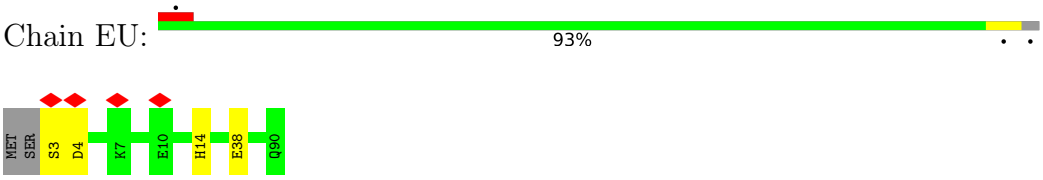

• Molecule 45: Zf-Tim10_DDP domain-containing protein

Chain Et:



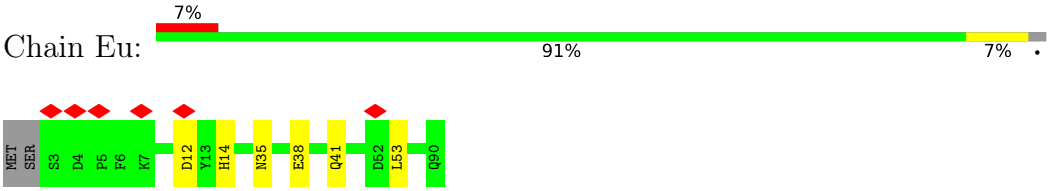

• Molecule 46: ABC transporter

Chain EU:



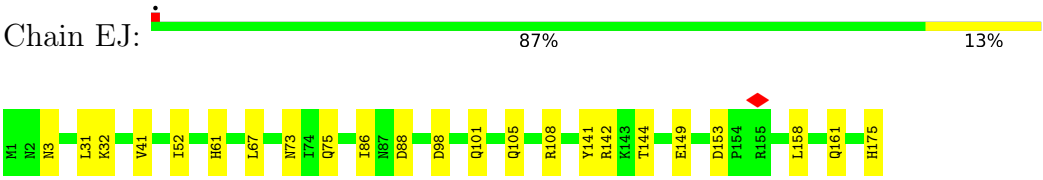

• Molecule 46: ABC transporter

Chain Eu:



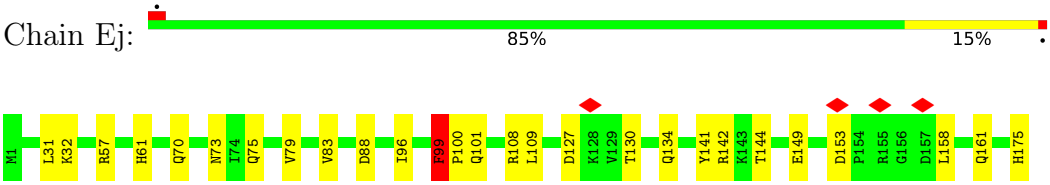

• Molecule 47: YflT domain-containing protein

Chain EJ:



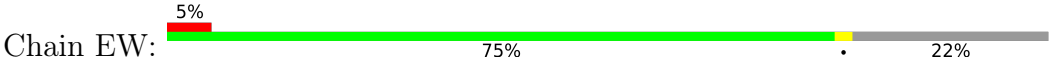

• Molecule 47: YflT domain-containing protein

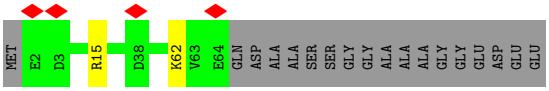
Chain Ej:



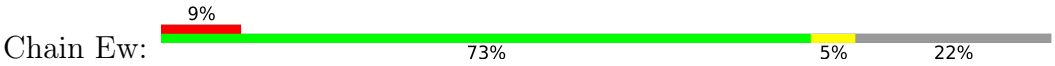

• Molecule 48: Cullin domain-containing protein

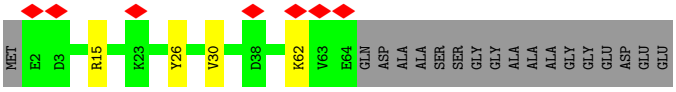
Chain EW:



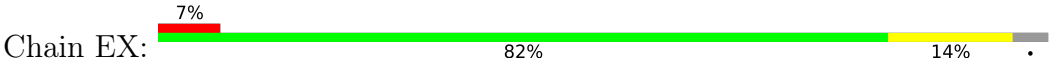


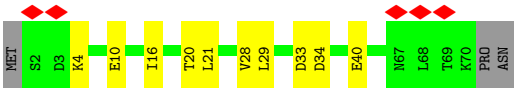

• Molecule 48: Cullin domain-containing protein



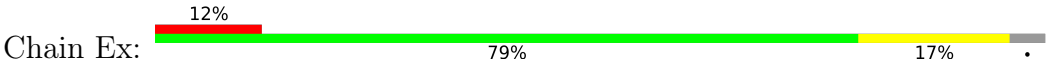



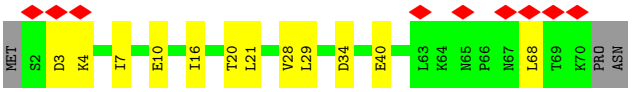

• Molecule 49: Zf-Tim10_DDP domain-containing protein



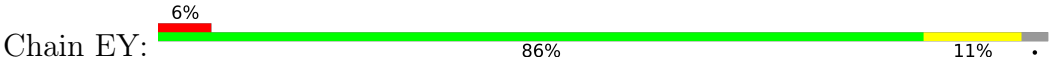



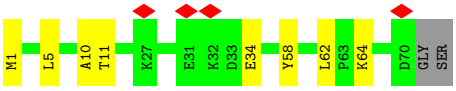

• Molecule 49: Zf-Tim10_DDP domain-containing protein



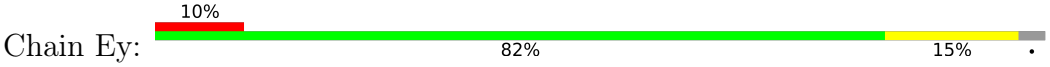



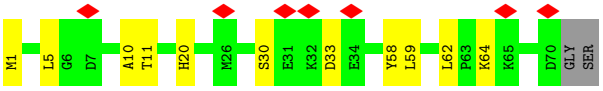

• Molecule 50: Annexin



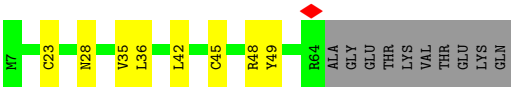

• Molecule 50: Annexin



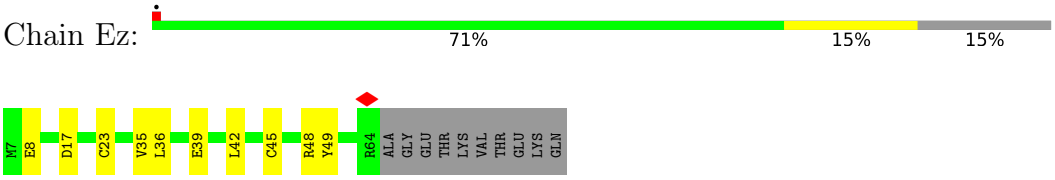

• Molecule 51: Transposase



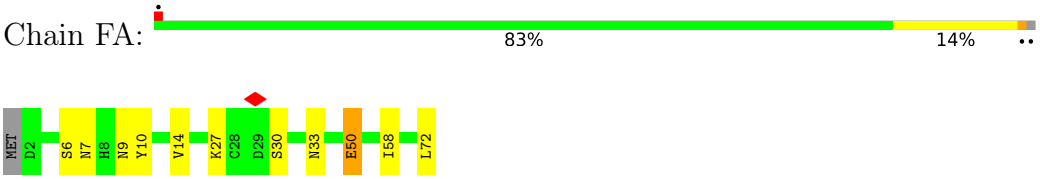

• Molecule 51: Transposase

Chain Ez:



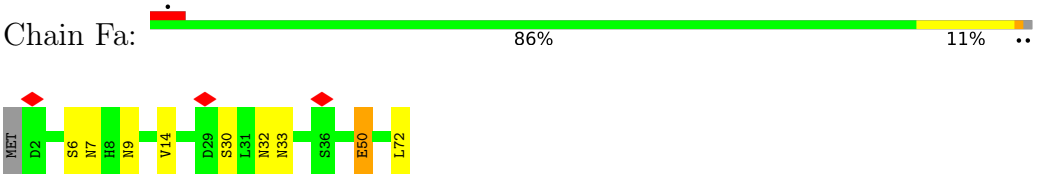

• Molecule 52: Tim10/DDP family zinc finger protein

Chain FA:



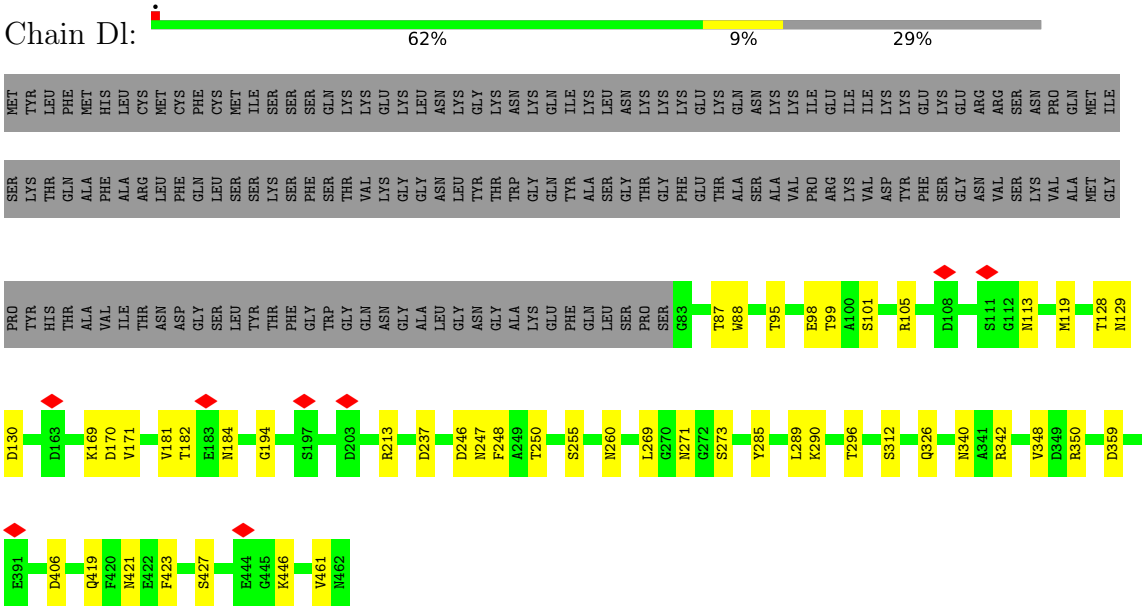

• Molecule 52: Tim10/DDP family zinc finger protein

Chain Fa:



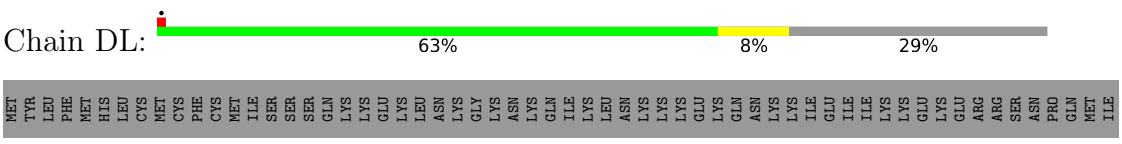

• Molecule 53: COXBP,Chromosome condensation regulator RCC1 repeat protein,Chromosome condensation regulator RCC1 repeat protein

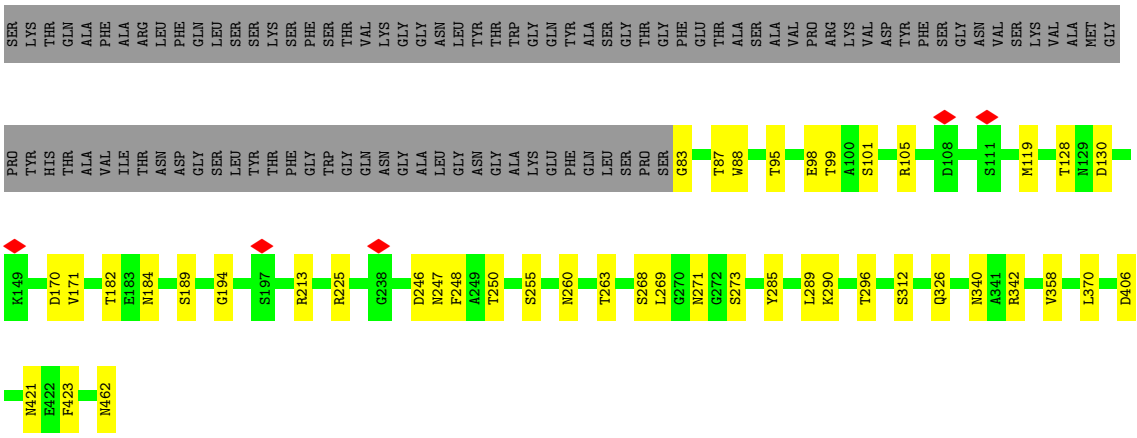
Chain Dl:




• Molecule 53: COXBP,Chromosome condensation regulator RCC1 repeat protein,Chromosome condensation regulator RCC1 repeat protein

Chain DL:




SER LYS THR GLN ALA PHE ALA ARG LEU PHE GLN LEU SER SER LYS SER PHE SER THR VAL LYS GLY GLY ASN LEU TYR THR TRP GLY GLN TYR ALA SER GLY THR GLY PHE GLU THR ALA SER ALA VAL PRO ARG LYS VAL ASP TYR PHE SER GLY ASN VAL SER LYS VAL ALA MET GLY
PRO TYR HIS THR ALA VAL ILE THR ASN ASP GLY SER LEU TYR THR PHE GLY TRP GLY GLN ASN GLY ALA LEU GLY ASN GLY ALA LYS GLU PHE GLN LEU SER PRO SER G83 T87 W88 T95 E98 T99 A100 S101 R105 D108 S111 M119 T128 N129 D130
K149 D170 V171 T182 E183 N184 S189 G194 S197 R213 R225 G238 D246 N247 F248 A249 T250 S255 N260 T263 S268 L269 G270 N271 G272 S273 Y285 L289 K290 T296 S312 Q326 N340 A341 R342 V358 L370 D406
N421 E422 F423 N462

# 4 Experimental information (i)

| Property | Value | Source |
|---|---|---|
| EM reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, C1 | Depositor |
| Number of particles used | 138746 | 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 ($e^-/Å^2$) | 25.66 | Depositor |
| Minimum defocus (nm) | 600 | Depositor |
| Maximum defocus (nm) | 2600 | Depositor |
| Magnification | Not provided | |
| Image detector | GATAN K2 QUANTUM (4k x 4k) | Depositor |
| Maximum map value | 7.005 | Depositor |
| Minimum map value | -3.774 | Depositor |
| Average map value | 0.004 | Depositor |
| Map value standard deviation | 0.539 | Depositor |
| Recommended contour level | 0.85 | Depositor |
| Map size (Å) | 600.912, 600.912, 600.912 | wwPDB |
| Map dimensions | 480, 480, 480 | wwPDB |
| Map angles (°) | 90.0, 90.0, 90.0 | wwPDB |
| Pixel spacing (Å) | 1.2519, 1.2519, 1.2519 | Depositor |

# 5 Model quality

## 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: AME, ATP, CDL, SEP, HEA, MG, LPP, CUA, PC1, K, TPO, HEM, ZN, CU, 3PE, FES, CA, UQ8

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 | DA | 0.09 | 0/5748 | 0.23 | 0/7793 |
| 1 | Da | 0.09 | 0/5748 | 0.23 | 0/7793 |
| 2 | DB | 0.08 | 0/5282 | 0.22 | 0/7159 |
| 2 | Db | 0.07 | 0/5282 | 0.22 | 0/7159 |
| 3 | DC | 0.08 | 0/5256 | 0.22 | 0/7142 |
| 3 | Dc | 0.08 | 0/5256 | 0.22 | 0/7142 |
| 4 | DD | 0.08 | 0/4734 | 0.21 | 0/6387 |
| 4 | Dd | 0.08 | 0/4734 | 0.20 | 0/6387 |
| 5 | DE | 0.08 | 0/1116 | 0.19 | 0/1512 |
| 5 | De | 0.09 | 0/1116 | 0.20 | 0/1512 |
| 6 | DF | 0.08 | 0/1977 | 0.22 | 0/2673 |
| 6 | Df | 0.08 | 0/1977 | 0.22 | 0/2673 |
| 7 | DG | 0.09 | 0/906 | 0.23 | 0/1230 |
| 7 | Dg | 0.09 | 0/906 | 0.20 | 0/1230 |
| 8 | DH | 0.07 | 0/1199 | 0.20 | 0/1621 |
| 8 | Dh | 0.06 | 0/1199 | 0.20 | 0/1621 |
| 9 | DI | 0.07 | 0/1829 | 0.19 | 0/2486 |
| 9 | Di | 0.07 | 0/1829 | 0.19 | 0/2486 |
| 10 | DJ | 0.07 | 0/1950 | 0.20 | 0/2647 |
| 10 | Dj | 0.07 | 0/1950 | 0.19 | 0/2647 |
| 11 | DK | 0.08 | 0/1100 | 0.26 | 0/1495 |
| 11 | Dk | 0.08 | 0/1100 | 0.24 | 0/1495 |
| 12 | DM | 0.07 | 0/3910 | 0.20 | 0/5320 |
| 12 | Dm | 0.07 | 0/3910 | 0.20 | 0/5320 |
| 13 | DN | 0.08 | 0/3963 | 0.20 | 0/5359 |
| 13 | Dn | 0.08 | 0/3963 | 0.21 | 0/5359 |
| 14 | DO | 0.06 | 0/3505 | 0.17 | 0/4745 |
| 14 | Do | 0.06 | 0/3505 | 0.17 | 0/4745 |
| 15 | DP | 0.07 | 0/2433 | 0.19 | 0/3307 |
| 15 | Dp | 0.07 | 0/2433 | 0.18 | 0/3307 |
| 16 | DQ | 0.08 | 0/3247 | 0.21 | 0/4410 |

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | #\|Z\| >5 | RMSZ | #\|Z\| >5 |
| 16 | Dq | 0.07 | 0/3247 | 0.21 | 0/4410 |
| 17 | DR | 0.07 | 0/2077 | 0.23 | 0/2824 |
| 17 | Dr | 0.08 | 0/2077 | 0.23 | 0/2824 |
| 18 | DS | 0.08 | 0/2950 | 0.21 | 0/4003 |
| 18 | Ds | 0.08 | 0/2950 | 0.21 | 0/4003 |
| 19 | DT | 0.07 | 0/2518 | 0.20 | 0/3433 |
| 19 | Dt | 0.07 | 0/2518 | 0.20 | 0/3433 |
| 20 | DU | 0.08 | 0/2689 | 0.21 | 0/3657 |
| 20 | Du | 0.08 | 0/2689 | 0.20 | 0/3657 |
| 21 | DV | 0.09 | 0/2622 | 0.20 | 0/3554 |
| 21 | Dv | 0.09 | 0/2622 | 0.20 | 0/3554 |
| 22 | DW | 0.07 | 0/2449 | 0.19 | 0/3312 |
| 22 | Dw | 0.07 | 0/2449 | 0.19 | 0/3312 |
| 23 | DX | 0.07 | 0/2171 | 0.19 | 0/2930 |
| 23 | Dx | 0.07 | 0/2171 | 0.19 | 0/2930 |
| 24 | DY | 0.07 | 0/1619 | 0.21 | 0/2198 |
| 24 | Dy | 0.07 | 0/1619 | 0.20 | 0/2198 |
| 25 | DZ | 0.07 | 0/1752 | 0.18 | 0/2372 |
| 25 | Dz | 0.07 | 0/1752 | 0.18 | 0/2372 |
| 26 | EA | 0.07 | 0/1709 | 0.18 | 0/2321 |
| 26 | Ea | 0.07 | 0/1709 | 0.18 | 0/2321 |
| 27 | EB | 0.07 | 0/1793 | 0.19 | 0/2418 |
| 27 | Eb | 0.07 | 0/1793 | 0.19 | 0/2418 |
| 28 | EC | 0.08 | 0/1673 | 0.24 | 0/2258 |
| 28 | Ec | 0.08 | 0/1673 | 0.23 | 0/2258 |
| 29 | ED | 0.08 | 0/1708 | 0.18 | 0/2306 |
| 29 | Ed | 0.08 | 0/1708 | 0.18 | 0/2306 |
| 30 | EE | 0.08 | 0/1066 | 0.20 | 0/1432 |
| 30 | Ee | 0.10 | 0/1066 | 0.21 | 0/1432 |
| 31 | EF | 0.09 | 0/1562 | 0.23 | 0/2123 |
| 31 | Ef | 0.08 | 0/1562 | 0.22 | 0/2123 |
| 32 | EG | 0.11 | 0/786 | 0.20 | 0/1060 |
| 32 | Eg | 0.09 | 0/786 | 0.18 | 0/1060 |
| 33 | EH | 0.08 | 0/1471 | 0.21 | 0/1995 |
| 33 | Eh | 0.08 | 0/1471 | 0.21 | 0/1995 |
| 34 | EI | 0.10 | 0/1442 | 0.27 | 0/1952 |
| 34 | Ei | 0.10 | 0/1442 | 0.26 | 0/1952 |
| 35 | EV | 0.07 | 0/645 | 0.20 | 0/866 |
| 35 | Ev | 0.07 | 0/645 | 0.20 | 0/866 |
| 36 | EK | 0.09 | 0/1410 | 0.22 | 0/1900 |
| 36 | Ek | 0.09 | 0/1410 | 0.21 | 0/1900 |
| 37 | EL | 0.08 | 0/1335 | 0.20 | 0/1810 |
| 37 | El | 0.08 | 0/1335 | 0.21 | 0/1810 |

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | #\|Z\| >5 | RMSZ | #\|Z\| >5 |
| 38 | EM | 0.09 | 0/1335 | 0.22 | 0/1794 |
| 38 | Em | 0.09 | 0/1335 | 0.22 | 0/1794 |
| 39 | EN | 0.08 | 0/1270 | 0.25 | 0/1724 |
| 39 | En | 0.08 | 0/1270 | 0.25 | 0/1724 |
| 40 | EO | 0.07 | 0/1137 | 0.20 | 0/1545 |
| 40 | Eo | 0.07 | 0/1137 | 0.21 | 0/1545 |
| 41 | EP | 0.07 | 0/837 | 0.20 | 0/1133 |
| 41 | Ep | 0.07 | 0/837 | 0.19 | 0/1133 |
| 42 | EQ | 0.09 | 0/1035 | 0.20 | 0/1403 |
| 42 | Eq | 0.09 | 0/1035 | 0.20 | 0/1403 |
| 43 | ER | 0.07 | 0/874 | 0.18 | 0/1182 |
| 43 | Er | 0.07 | 0/874 | 0.18 | 0/1182 |
| 44 | ES | 0.07 | 0/802 | 0.20 | 0/1087 |
| 44 | Es | 0.07 | 0/802 | 0.20 | 0/1087 |
| 45 | ET | 0.07 | 0/654 | 0.18 | 0/878 |
| 45 | Et | 0.07 | 0/654 | 0.17 | 0/878 |
| 46 | EU | 0.06 | 0/744 | 0.18 | 0/1003 |
| 46 | Eu | 0.06 | 0/744 | 0.17 | 0/1003 |
| 47 | EJ | 0.07 | 0/1437 | 0.20 | 0/1941 |
| 47 | Ej | 0.08 | 0/1437 | 0.20 | 0/1941 |
| 48 | EW | 0.07 | 0/523 | 0.19 | 0/705 |
| 48 | Ew | 0.09 | 0/523 | 0.21 | 0/705 |
| 49 | EX | 0.07 | 0/564 | 0.18 | 0/757 |
| 49 | Ex | 0.06 | 0/564 | 0.17 | 0/757 |
| 50 | EY | 0.10 | 0/573 | 0.28 | 0/770 |
| 50 | Ey | 0.09 | 0/573 | 0.28 | 0/770 |
| 51 | EZ | 0.08 | 0/502 | 0.20 | 0/676 |
| 51 | Ez | 0.08 | 0/502 | 0.20 | 0/676 |
| 52 | FA | 0.08 | 0/554 | 0.18 | 0/746 |
| 52 | Fa | 0.08 | 0/554 | 0.19 | 0/746 |
| 53 | DL | 0.07 | 0/2984 | 0.22 | 0/4047 |
| 53 | Dl | 0.07 | 0/2984 | 0.22 | 0/4047 |
| All | All | 0.08 | 0/202854 | 0.21 | 0/274802 |

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|---|---|---|---|
| 47 | Ej | 0 | 1 |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 47 | Ej | 99 | PHE | Peptide |

## 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 | DA | 5559 | 5609 | 5607 | 78 | 0 |
| 1 | Da | 5559 | 5608 | 5606 | 82 | 0 |
| 2 | DB | 5131 | 5101 | 5104 | 57 | 0 |
| 2 | Db | 5131 | 5102 | 5104 | 63 | 0 |
| 3 | DC | 5084 | 5067 | 5067 | 78 | 0 |
| 3 | Dc | 5084 | 5067 | 5067 | 74 | 0 |
| 4 | DD | 4652 | 4424 | 4424 | 64 | 0 |
| 4 | Dd | 4652 | 4424 | 4424 | 59 | 0 |
| 5 | DE | 1083 | 1021 | 1020 | 14 | 0 |
| 5 | De | 1083 | 1020 | 1020 | 17 | 0 |
| 6 | DF | 1913 | 1768 | 1768 | 24 | 0 |
| 6 | Df | 1913 | 1768 | 1768 | 20 | 0 |
| 7 | DG | 871 | 788 | 788 | 12 | 0 |
| 7 | Dg | 871 | 788 | 788 | 7 | 0 |
| 8 | DH | 1170 | 1129 | 1130 | 23 | 0 |
| 8 | Dh | 1170 | 1129 | 1130 | 19 | 0 |
| 9 | DI | 1777 | 1604 | 1603 | 16 | 0 |
| 9 | Di | 1777 | 1604 | 1603 | 17 | 0 |
| 10 | DJ | 1881 | 1772 | 1772 | 29 | 0 |
| 10 | Dj | 1881 | 1772 | 1772 | 24 | 0 |
| 11 | DK | 1071 | 1062 | 1062 | 15 | 0 |
| 11 | Dk | 1071 | 1062 | 1062 | 10 | 0 |
| 12 | DM | 3793 | 3592 | 3592 | 42 | 0 |
| 12 | Dm | 3793 | 3592 | 3592 | 41 | 0 |
| 13 | DN | 3869 | 3980 | 3980 | 40 | 0 |
| 13 | Dn | 3869 | 3980 | 3980 | 46 | 0 |
| 14 | DO | 3448 | 3508 | 3508 | 37 | 0 |
| 14 | Do | 3448 | 3508 | 3508 | 40 | 0 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 15 | DP | 2369 | 2291 | 2291 | 18 | 0 |
| 15 | Dp | 2369 | 2291 | 2291 | 19 | 0 |
| 16 | DQ | 3169 | 3102 | 3102 | 41 | 0 |
| 16 | Dq | 3169 | 3102 | 3102 | 43 | 0 |
| 17 | DR | 2024 | 1958 | 1958 | 25 | 0 |
| 17 | Dr | 2024 | 1958 | 1958 | 29 | 0 |
| 18 | DS | 2866 | 2770 | 2782 | 37 | 0 |
| 18 | Ds | 2866 | 2770 | 2782 | 38 | 0 |
| 19 | DT | 2443 | 2290 | 2290 | 46 | 0 |
| 19 | Dt | 2443 | 2290 | 2290 | 42 | 0 |
| 20 | DU | 2620 | 2584 | 2584 | 33 | 0 |
| 20 | Du | 2620 | 2584 | 2584 | 39 | 0 |
| 21 | DV | 2562 | 2552 | 2553 | 28 | 0 |
| 21 | Dv | 2562 | 2552 | 2553 | 28 | 0 |
| 22 | DW | 2394 | 2344 | 2344 | 16 | 0 |
| 22 | Dw | 2394 | 2344 | 2344 | 19 | 0 |
| 23 | DX | 2108 | 2018 | 2018 | 21 | 0 |
| 23 | Dx | 2108 | 2018 | 2018 | 21 | 0 |
| 24 | DY | 1573 | 1562 | 1562 | 19 | 0 |
| 24 | Dy | 1573 | 1562 | 1562 | 18 | 0 |
| 25 | DZ | 1711 | 1671 | 1670 | 19 | 0 |
| 25 | Dz | 1711 | 1672 | 1670 | 29 | 0 |
| 26 | EA | 1659 | 1637 | 1637 | 17 | 0 |
| 26 | Ea | 1659 | 1637 | 1637 | 17 | 0 |
| 27 | EB | 1739 | 1678 | 1677 | 13 | 0 |
| 27 | Eb | 1739 | 1678 | 1677 | 24 | 0 |
| 28 | EC | 1647 | 1660 | 1660 | 18 | 0 |
| 28 | Ec | 1647 | 1660 | 1660 | 18 | 0 |
| 29 | ED | 1659 | 1725 | 1726 | 28 | 0 |
| 29 | Ed | 1659 | 1725 | 1726 | 21 | 0 |
| 30 | EE | 1049 | 1024 | 1026 | 13 | 0 |
| 30 | Ee | 1049 | 1024 | 1026 | 13 | 0 |
| 31 | EF | 1509 | 1477 | 1477 | 22 | 0 |
| 31 | Ef | 1509 | 1477 | 1477 | 18 | 0 |
| 32 | EG | 771 | 752 | 752 | 7 | 0 |
| 32 | Eg | 771 | 752 | 752 | 9 | 0 |
| 33 | EH | 1438 | 1382 | 1394 | 16 | 0 |
| 33 | Eh | 1438 | 1382 | 1394 | 22 | 0 |
| 34 | EI | 1408 | 1419 | 1419 | 11 | 0 |
| 34 | Ei | 1408 | 1419 | 1419 | 10 | 0 |
| 35 | EV | 643 | 633 | 645 | 6 | 0 |
| 35 | Ev | 643 | 633 | 645 | 6 | 0 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 36 | EK | 1389 | 1407 | 1406 | 17 | 0 |
| 36 | Ek | 1389 | 1407 | 1407 | 24 | 0 |
| 37 | EL | 1291 | 1253 | 1253 | 17 | 0 |
| 37 | El | 1291 | 1253 | 1253 | 16 | 0 |
| 38 | EM | 1304 | 1299 | 1299 | 14 | 0 |
| 38 | Em | 1304 | 1299 | 1299 | 14 | 0 |
| 39 | EN | 1227 | 1190 | 1190 | 9 | 0 |
| 39 | En | 1227 | 1190 | 1190 | 8 | 0 |
| 40 | EO | 1097 | 1031 | 1031 | 12 | 0 |
| 40 | Eo | 1097 | 1031 | 1031 | 17 | 0 |
| 41 | EP | 817 | 795 | 795 | 10 | 0 |
| 41 | Ep | 817 | 795 | 795 | 9 | 0 |
| 42 | EQ | 1015 | 989 | 1001 | 15 | 0 |
| 42 | Eq | 1015 | 989 | 1001 | 14 | 0 |
| 43 | ER | 851 | 800 | 800 | 13 | 0 |
| 43 | Er | 851 | 800 | 800 | 13 | 0 |
| 44 | ES | 776 | 798 | 798 | 14 | 0 |
| 44 | Es | 776 | 798 | 798 | 15 | 0 |
| 45 | ET | 647 | 655 | 655 | 10 | 0 |
| 45 | Et | 647 | 655 | 655 | 13 | 0 |
| 46 | EU | 724 | 699 | 699 | 3 | 0 |
| 46 | Eu | 724 | 699 | 699 | 5 | 0 |
| 47 | EJ | 1411 | 1391 | 1391 | 15 | 0 |
| 47 | Ej | 1411 | 1391 | 1391 | 21 | 0 |
| 48 | EW | 515 | 510 | 510 | 1 | 0 |
| 48 | Ew | 515 | 510 | 510 | 2 | 0 |
| 49 | EX | 558 | 559 | 559 | 9 | 0 |
| 49 | Ex | 558 | 559 | 559 | 11 | 0 |
| 50 | EY | 561 | 562 | 562 | 8 | 0 |
| 50 | Ey | 561 | 562 | 562 | 10 | 0 |
| 51 | EZ | 492 | 474 | 473 | 9 | 0 |
| 51 | Ez | 492 | 474 | 473 | 9 | 0 |
| 52 | FA | 548 | 536 | 536 | 8 | 0 |
| 52 | Fa | 548 | 536 | 536 | 6 | 0 |
| 53 | DL | 2916 | 2814 | 2814 | 24 | 0 |
| 53 | Dl | 2916 | 2814 | 2814 | 27 | 0 |
| 54 | DA | 120 | 108 | 108 | 2 | 0 |
| 54 | Da | 120 | 108 | 108 | 3 | 0 |
| 55 | DA | 1 | 0 | 0 | 0 | 0 |
| 55 | Da | 1 | 0 | 0 | 0 | 0 |
| 56 | DA | 1 | 0 | 0 | 0 | 0 |
| 56 | Da | 1 | 0 | 0 | 0 | 0 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 57 | DA | 300 | 468 | 468 | 1 | 0 |
| 57 | DC | 100 | 156 | 156 | 1 | 0 |
| 57 | DD | 300 | 468 | 468 | 3 | 0 |
| 57 | DG | 200 | 312 | 312 | 1 | 0 |
| 57 | DH | 100 | 156 | 156 | 4 | 0 |
| 57 | DI | 100 | 156 | 156 | 1 | 0 |
| 57 | DJ | 500 | 780 | 780 | 5 | 0 |
| 57 | DM | 200 | 312 | 312 | 2 | 0 |
| 57 | DN | 300 | 468 | 468 | 3 | 0 |
| 57 | DO | 100 | 156 | 156 | 1 | 0 |
| 57 | DQ | 300 | 468 | 468 | 6 | 0 |
| 57 | DR | 200 | 312 | 312 | 0 | 0 |
| 57 | DS | 200 | 312 | 312 | 3 | 0 |
| 57 | DU | 400 | 624 | 624 | 0 | 0 |
| 57 | DV | 400 | 624 | 624 | 5 | 0 |
| 57 | DX | 200 | 312 | 312 | 3 | 0 |
| 57 | DY | 100 | 156 | 156 | 1 | 0 |
| 57 | DZ | 100 | 156 | 156 | 1 | 0 |
| 57 | Da | 200 | 312 | 312 | 3 | 0 |
| 57 | Dc | 100 | 156 | 156 | 1 | 0 |
| 57 | Dd | 400 | 624 | 624 | 7 | 0 |
| 57 | Dg | 200 | 312 | 312 | 7 | 0 |
| 57 | Dh | 200 | 312 | 312 | 4 | 0 |
| 57 | Di | 100 | 156 | 156 | 1 | 0 |
| 57 | Dj | 600 | 936 | 936 | 4 | 0 |
| 57 | Dm | 200 | 312 | 312 | 1 | 0 |
| 57 | Dn | 500 | 780 | 780 | 8 | 0 |
| 57 | Do | 100 | 156 | 156 | 1 | 0 |
| 57 | Dq | 400 | 624 | 624 | 1 | 0 |
| 57 | Dr | 200 | 312 | 312 | 3 | 0 |
| 57 | Ds | 200 | 312 | 312 | 2 | 0 |
| 57 | Du | 400 | 624 | 624 | 3 | 0 |
| 57 | Dv | 400 | 624 | 624 | 8 | 0 |
| 57 | Dx | 200 | 312 | 312 | 5 | 0 |
| 57 | Dy | 100 | 156 | 156 | 0 | 0 |
| 57 | Dz | 100 | 156 | 156 | 0 | 0 |
| 57 | EA | 100 | 156 | 156 | 1 | 0 |
| 57 | EB | 200 | 312 | 312 | 4 | 0 |
| 57 | ED | 200 | 312 | 312 | 1 | 0 |
| 57 | EH | 200 | 311 | 312 | 0 | 0 |
| 57 | EI | 100 | 156 | 156 | 0 | 0 |
| 57 | EK | 100 | 156 | 156 | 0 | 0 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 57 | EL | 400 | 624 | 624 | 9 | 0 |
| 57 | EN | 200 | 312 | 312 | 3 | 0 |
| 57 | EO | 100 | 156 | 156 | 0 | 0 |
| 57 | EU | 100 | 156 | 156 | 0 | 0 |
| 57 | Ea | 100 | 156 | 156 | 0 | 0 |
| 57 | Ed | 200 | 311 | 312 | 0 | 0 |
| 57 | Eg | 100 | 156 | 156 | 2 | 0 |
| 57 | Eh | 100 | 156 | 156 | 2 | 0 |
| 57 | Ei | 100 | 156 | 156 | 0 | 0 |
| 57 | Ek | 100 | 156 | 156 | 1 | 0 |
| 57 | El | 300 | 468 | 468 | 4 | 0 |
| 57 | En | 200 | 312 | 312 | 4 | 0 |
| 57 | Ep | 100 | 156 | 156 | 1 | 0 |
| 57 | Eu | 100 | 156 | 156 | 0 | 0 |
| 58 | DA | 108 | 175 | 176 | 1 | 0 |
| 58 | DB | 54 | 88 | 88 | 0 | 0 |
| 58 | DC | 270 | 439 | 440 | 3 | 0 |
| 58 | DG | 54 | 88 | 88 | 2 | 0 |
| 58 | DI | 54 | 88 | 88 | 1 | 0 |
| 58 | DJ | 54 | 88 | 88 | 0 | 0 |
| 58 | DQ | 54 | 88 | 88 | 1 | 0 |
| 58 | DS | 108 | 176 | 176 | 0 | 0 |
| 58 | DV | 162 | 264 | 264 | 0 | 0 |
| 58 | DX | 108 | 176 | 176 | 2 | 0 |
| 58 | DY | 54 | 88 | 88 | 0 | 0 |
| 58 | Da | 108 | 175 | 176 | 1 | 0 |
| 58 | Db | 54 | 88 | 88 | 0 | 0 |
| 58 | Dc | 270 | 439 | 440 | 2 | 0 |
| 58 | Dg | 54 | 88 | 88 | 0 | 0 |
| 58 | Di | 54 | 88 | 88 | 1 | 0 |
| 58 | Dj | 54 | 88 | 88 | 0 | 0 |
| 58 | Dq | 54 | 88 | 88 | 0 | 0 |
| 58 | Ds | 54 | 88 | 88 | 0 | 0 |
| 58 | Dv | 216 | 352 | 352 | 2 | 0 |
| 58 | Dx | 162 | 264 | 264 | 3 | 0 |
| 58 | Dy | 54 | 88 | 88 | 0 | 0 |
| 58 | EB | 108 | 176 | 176 | 1 | 0 |
| 58 | EO | 216 | 352 | 352 | 5 | 0 |
| 58 | Eb | 108 | 176 | 176 | 1 | 0 |
| 58 | Ef | 54 | 88 | 88 | 1 | 0 |
| 58 | El | 54 | 88 | 88 | 0 | 0 |
| 58 | Eo | 162 | 264 | 264 | 6 | 0 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 59 | DA | 51 | 82 | 82 | 0 | 0 |
| 59 | DC | 102 | 164 | 164 | 3 | 0 |
| 59 | DG | 102 | 164 | 164 | 1 | 0 |
| 59 | DJ | 51 | 82 | 82 | 0 | 0 |
| 59 | DR | 51 | 82 | 82 | 2 | 0 |
| 59 | DS | 102 | 164 | 164 | 3 | 0 |
| 59 | DX | 153 | 246 | 246 | 1 | 0 |
| 59 | Da | 51 | 82 | 82 | 0 | 0 |
| 59 | Dc | 51 | 82 | 82 | 0 | 0 |
| 59 | Dd | 51 | 82 | 82 | 0 | 0 |
| 59 | Dg | 51 | 82 | 82 | 1 | 0 |
| 59 | Dj | 51 | 82 | 82 | 2 | 0 |
| 59 | Dr | 102 | 164 | 164 | 1 | 0 |
| 59 | Ds | 153 | 246 | 246 | 1 | 0 |
| 59 | Dx | 153 | 246 | 246 | 3 | 0 |
| 59 | EL | 51 | 82 | 82 | 2 | 0 |
| 59 | EM | 51 | 82 | 82 | 2 | 0 |
| 59 | EN | 51 | 82 | 82 | 0 | 0 |
| 59 | EO | 102 | 164 | 164 | 1 | 0 |
| 59 | El | 51 | 82 | 82 | 1 | 0 |
| 59 | Em | 51 | 82 | 82 | 0 | 0 |
| 59 | Eo | 102 | 164 | 164 | 0 | 0 |
| 60 | DA | 44 | 67 | 67 | 0 | 0 |
| 60 | DN | 88 | 134 | 134 | 0 | 0 |
| 60 | Dl | 44 | 67 | 67 | 0 | 0 |
| 60 | Dn | 88 | 134 | 134 | 0 | 0 |
| 60 | EI | 44 | 67 | 67 | 1 | 0 |
| 60 | Ed | 44 | 67 | 67 | 1 | 0 |
| 61 | DA | 1 | 0 | 0 | 0 | 0 |
| 61 | Da | 1 | 0 | 0 | 0 | 0 |
| 62 | DB | 2 | 0 | 0 | 0 | 0 |
| 62 | Db | 2 | 0 | 0 | 0 | 0 |
| 63 | DD | 1 | 0 | 0 | 0 | 0 |
| 63 | Dd | 1 | 0 | 0 | 0 | 0 |
| 64 | DD | 1 | 0 | 0 | 0 | 0 |
| 65 | DS | 53 | 74 | 74 | 2 | 0 |
| 65 | Ds | 53 | 74 | 74 | 3 | 0 |
| 65 | ED | 53 | 74 | 74 | 5 | 0 |
| 65 | EL | 53 | 74 | 74 | 2 | 0 |
| 65 | EN | 53 | 74 | 74 | 2 | 0 |
| 65 | Ed | 53 | 74 | 74 | 5 | 0 |
| 65 | El | 53 | 74 | 74 | 2 | 0 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 65 | En | 53 | 74 | 74 | 4 | 0 |
| 66 | ED | 43 | 22 | 30 | 5 | 0 |
| 66 | Ed | 43 | 24 | 30 | 4 | 0 |
| 67 | EF | 8 | 0 | 0 | 0 | 0 |
| 67 | Ef | 8 | 0 | 0 | 0 | 0 |
| 68 | ER | 31 | 12 | 12 | 2 | 0 |
| 68 | Er | 31 | 12 | 12 | 2 | 0 |
| All | All | 215247 | 220788 | 220904 | 2060 | 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 5.

All (2060) 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) |
|---|---|---|---|
| 66:Ed:201:HEM:HBB2 | 66:Ed:201:HEM:HMB1 | 1.53 | 0.91 |
| 4:DD:497:HIS:HD1 | 13:DN:191:TYR:HH | 1.19 | 0.89 |
| 66:ED:602:HEM:HMB2 | 66:ED:602:HEM:HBB2 | 1.54 | 0.89 |
| 26:EA:138:ARG:O | 26:EA:151:ARG:NH2 | 2.09 | 0.86 |
| 20:Du:48:ARG:NH1 | 20:Du:52:ASP:OD2 | 2.11 | 0.84 |
| 10:Dj:195:THR:OG1 | 43:Er:4:THR:O | 1.98 | 0.81 |
| 26:EA:146:THR:O | 26:EA:151:ARG:NH1 | 2.14 | 0.80 |
| 4:DD:482:LEU:HD11 | 36:EK:26:LEU:HD22 | 1.61 | 0.80 |
| 3:DC:349:LYS:NZ | 5:DE:105:GLN:O | 2.15 | 0.80 |
| 6:Df:46:GLU:OE2 | 11:Dk:127:ASN:ND2 | 2.14 | 0.79 |
| 1:DA:238:ILE:O | 27:EB:71:ARG:NH2 | 2.15 | 0.79 |
| 36:EK:160:SER:OG | 17:Dr:304:ASN:OD1 | 1.99 | 0.79 |
| 1:Da:238:ILE:O | 27:Eb:71:ARG:NH2 | 2.15 | 0.79 |
| 6:DF:46:GLU:OE2 | 11:DK:127:ASN:ND2 | 2.16 | 0.79 |
| 14:DO:56:GLU:OE1 | 14:DO:96:ARG:NH2 | 2.16 | 0.78 |
| 57:Dn:503:CDL:O1 | 57:Dn:503:CDL:OB7 | 2.01 | 0.78 |
| 17:DR:304:ASN:OD1 | 36:Ek:160:SER:OG | 2.01 | 0.78 |
| 12:Dm:439:TYR:OH | 25:Dz:189:GLU:OE1 | 2.02 | 0.78 |
| 37:El:15:ASP:OD1 | 37:El:18:ARG:NH2 | 2.16 | 0.78 |
| 10:DJ:195:THR:OG1 | 43:ER:4:THR:O | 2.03 | 0.77 |
| 57:Dr:402:CDL:H472 | 31:Ef:174:LEU:HD12 | 1.66 | 0.77 |
| 3:DC:79:ASP:OD2 | 3:DC:82:SER:OG | 2.01 | 0.77 |
| 3:Dc:23:THR:O | 3:Dc:69:LYS:NZ | 2.16 | 0.77 |
| 2:Db:245:THR:OG1 | 2:Db:247:LYS:NZ | 2.18 | 0.77 |
| 2:DB:145:ASN:O | 7:DG:66:ARG:NH2 | 2.18 | 0.77 |
| 5:De:7:GLN:NE2 | 16:Dq:136:TRP:O | 2.18 | 0.77 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 14:Do:56:GLU:OE1 | 14:Do:96:ARG:NH2 | 2.17 | 0.77 |
| 11:DK:94:CYS:SG | 40:EO:84:LYS:NZ | 2.58 | 0.77 |
| 17:DR:229:ARG:NH1 | 19:DT:114:GLU:OE1 | 2.18 | 0.77 |
| 2:DB:509:SER:OG | 2:DB:512:ILE:O | 2.01 | 0.77 |
| 26:Ea:138:ARG:O | 26:Ea:151:ARG:NH2 | 2.18 | 0.77 |
| 20:DU:90:ARG:NH1 | 20:DU:128:GLY:O | 2.17 | 0.76 |
| 1:DA:293:ASP:OD1 | 1:DA:364:ARG:NE | 2.18 | 0.76 |
| 26:Ea:186:ARG:NH2 | 26:Ea:193:GLU:O | 2.19 | 0.76 |
| 5:DE:62:GLU:OE2 | 13:DN:285:LYS:NZ | 2.17 | 0.76 |
| 23:Dx:157:GLU:OE1 | 23:Dx:158:GLY:N | 2.19 | 0.76 |
| 20:Du:206:ARG:NH2 | 20:Du:258:ALA:O | 2.19 | 0.75 |
| 1:DA:42:LYS:NZ | 9:DI:117:ASP:OD2 | 2.14 | 0.75 |
| 6:DF:226:LYS:NZ | 68:ER:201:ATP:O2A | 2.19 | 0.75 |
| 26:Ea:146:THR:O | 26:Ea:151:ARG:NH1 | 2.19 | 0.75 |
| 48:EW:15:ARG:NH1 | 49:EX:10:GLU:OE2 | 2.20 | 0.75 |
| 57:Dg:201:CDL:H472 | 57:Dg:201:CDL:H272 | 1.68 | 0.75 |
| 22:Dw:104:SER:O | 22:Dw:154:THR:OG1 | 2.03 | 0.75 |
| 29:Ed:187:ARG:NH1 | 29:Ed:188:ILE:O | 2.20 | 0.75 |
| 46:EU:14:HIS:NE2 | 38:Em:38:LYS:O | 2.20 | 0.75 |
| 44:Es:14:ASP:OD2 | 44:Es:34:LYS:NZ | 2.19 | 0.75 |
| 47:EJ:98:ASP:O | 47:EJ:101:GLN:NE2 | 2.20 | 0.75 |
| 29:ED:171:LYS:NZ | 44:ES:33:PHE:O | 2.18 | 0.75 |
| 20:Du:90:ARG:NH1 | 20:Du:128:GLY:O | 2.20 | 0.75 |
| 2:DB:118:ARG:NH1 | 6:DF:182:ASP:OD1 | 2.19 | 0.74 |
| 13:Dn:414:TYR:OH | 14:Do:446:GLU:OE1 | 2.05 | 0.74 |
| 14:Do:30:ALA:O | 14:Do:36:SER:OG | 2.03 | 0.74 |
| 30:Ee:157:CYS:SG | 30:Ee:173:ARG:NH2 | 2.60 | 0.74 |
| 32:Eg:10:GLN:NE2 | 33:Eh:113:GLU:OE2 | 2.20 | 0.74 |
| 1:Da:415:ARG:NH2 | 7:Dg:19:ASP:OD1 | 2.20 | 0.74 |
| 16:Dq:92:ASP:O | 36:Ek:51:ARG:NH1 | 2.20 | 0.74 |
| 1:DA:181:TYR:OH | 27:EB:47:ASP:OD2 | 2.05 | 0.74 |
| 22:DW:257:GLU:O | 22:DW:284:GLN:NE2 | 2.20 | 0.74 |
| 37:EL:15:ASP:OD1 | 37:EL:18:ARG:NH2 | 2.21 | 0.74 |
| 13:Dn:108:LYS:NZ | 28:Ec:86:CYS:SG | 2.55 | 0.74 |
| 6:Df:226:LYS:NZ | 68:Er:201:ATP:O2A | 2.20 | 0.74 |
| 17:Dr:229:ARG:NH1 | 19:Dt:114:GLU:OE1 | 2.20 | 0.74 |
| 20:DU:206:ARG:NH2 | 20:DU:258:ALA:O | 2.21 | 0.74 |
| 13:Dn:3:MET:N | 57:Eg:101:CDL:OA4 | 2.21 | 0.74 |
| 24:Dy:234:LYS:NZ | 42:Eq:35:GLU:OE2 | 2.21 | 0.74 |
| 48:Ew:15:ARG:NH1 | 49:Ex:10:GLU:OE2 | 2.20 | 0.74 |
| 2:DB:368:GLY:O | 68:ER:201:ATP:N6 | 2.20 | 0.74 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:Db:176:LYS:NZ | 30:Ee:78:GLU:OE2 | 2.15 | 0.74 |
| 53:DL:255:SER:O | 53:DL:290:LYS:NZ | 2.20 | 0.73 |
| 22:DW:20:THR:OG1 | 28:Ec:99:ARG:NH1 | 2.21 | 0.73 |
| 16:Dq:13:ASN:ND2 | 16:Dq:24:ALA:O | 2.21 | 0.73 |
| 35:Ev:29:LYS:NZ | 35:Ev:40:CYS:SG | 2.60 | 0.73 |
| 3:Dc:536:LYS:NZ | 33:Eh:1:AME:OT | 2.21 | 0.73 |
| 4:Dd:433:THR:O | 4:Dd:438:LYS:NZ | 2.21 | 0.73 |
| 12:Dm:283:LYS:NZ | 57:Dm:502:CDL:OA4 | 2.22 | 0.73 |
| 57:Eh:1601:CDL:OB4 | 37:El:116:LYS:NZ | 2.18 | 0.73 |
| 20:Du:31:PHE:O | 20:Du:45:LYS:NZ | 2.21 | 0.73 |
| 13:DN:108:LYS:NZ | 28:EC:86:CYS:SG | 2.58 | 0.73 |
| 2:Db:76:LYS:NZ | 40:Eo:11:GLU:O | 2.21 | 0.73 |
| 13:DN:414:TYR:OH | 14:DO:446:GLU:OE1 | 2.07 | 0.73 |
| 35:EV:29:LYS:NZ | 35:EV:40:CYS:SG | 2.62 | 0.73 |
| 16:Dq:126:LYS:NZ | 57:Dq:401:CDL:OB3 | 2.22 | 0.73 |
| 53:DL:87:THR:HG23 | 53:DL:119:MET:HE1 | 1.71 | 0.73 |
| 14:DO:450:PRO:O | 14:DO:453:ASN:ND2 | 2.21 | 0.72 |
| 18:DS:289:TYR:OH | 57:DV:402:CDL:OA9 | 2.06 | 0.72 |
| 21:DV:132:ALA:O | 21:DV:136:THR:HG22 | 1.89 | 0.72 |
| 4:Dd:261:GLU:O | 4:Dd:265:LEU:HD22 | 1.89 | 0.72 |
| 16:Dq:321:ASP:OD1 | 16:Dq:324:ARG:NH2 | 2.22 | 0.72 |
| 21:Dv:132:ALA:O | 21:Dv:136:THR:HG22 | 1.90 | 0.72 |
| 1:DA:550:LEU:O | 9:DI:136:ARG:NH1 | 2.22 | 0.72 |
| 14:DO:30:ALA:O | 14:DO:36:SER:OG | 2.06 | 0.72 |
| 1:Da:181:TYR:OH | 27:Eb:47:ASP:OD2 | 2.08 | 0.72 |
| 38:EM:38:LYS:O | 46:Eu:14:HIS:NE2 | 2.22 | 0.72 |
| 6:DF:40:ARG:NH1 | 6:DF:42:ASP:OD2 | 2.23 | 0.71 |
| 15:Dp:197:ARG:NH1 | 24:Dy:210:GLN:OE1 | 2.22 | 0.71 |
| 20:DU:31:PHE:O | 20:DU:45:LYS:NZ | 2.23 | 0.71 |
| 3:Dc:79:ASP:OD2 | 3:Dc:82:SER:OG | 2.08 | 0.71 |
| 2:Db:255:SER:OG | 51:Ez:17:ASP:OD2 | 2.09 | 0.71 |
| 21:Dv:62:ASN:ND2 | 57:Dv:402:CDL:OB9 | 2.23 | 0.71 |
| 12:DM:53:ALA:O | 12:DM:173:LYS:NZ | 2.23 | 0.71 |
| 44:ES:14:ASP:OD2 | 44:ES:34:LYS:NZ | 2.22 | 0.71 |
| 26:Ea:218:ARG:NH1 | 50:Ey:58:TYR:OH | 2.23 | 0.71 |
| 2:Db:118:ARG:NH1 | 6:Df:182:ASP:OD1 | 2.23 | 0.71 |
| 3:DC:308:PHE:O | 3:DC:312:THR:HG23 | 1.90 | 0.71 |
| 25:DZ:55:TYR:O | 27:EB:117:GLN:NE2 | 2.23 | 0.71 |
| 14:DO:151:GLN:N | 14:DO:151:GLN:OE1 | 2.23 | 0.71 |
| 9:Di:74:MET:SD | 19:Dt:109:GLN:NE2 | 2.64 | 0.71 |
| 9:DI:163:HIS:NE2 | 58:DI:702:PC1:O14 | 2.24 | 0.70 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:DC:536:LYS:NZ | 33:EH:1:AME:OT | 2.24 | 0.70 |
| 7:DG:23:ARG:NH1 | 19:DT:246:ASP:OD1 | 2.24 | 0.70 |
| 9:Di:163:HIS:NE2 | 58:Di:702:PC1:O14 | 2.24 | 0.70 |
| 53:DL:83:GLY:N | 53:DL:462:ASN:OD1 | 2.24 | 0.70 |
| 4:DD:439:LYS:NZ | 4:DD:524:GLU:OE1 | 2.23 | 0.70 |
| 28:EC:51:GLN:OE1 | 28:EC:51:GLN:N | 2.25 | 0.70 |
| 6:DF:40:ARG:NH2 | 38:EM:127:ASN:O | 2.24 | 0.70 |
| 26:EA:186:ARG:NH2 | 26:EA:193:GLU:O | 2.23 | 0.70 |
| 45:ET:12:GLN:OE1 | 45:ET:16:ARG:NH2 | 2.24 | 0.70 |
| 16:DQ:120:ASN:OD1 | 16:DQ:183:LYS:NZ | 2.21 | 0.70 |
| 28:EC:16:GLU:OE1 | 28:EC:18:ALA:N | 2.25 | 0.70 |
| 3:Dc:308:PHE:O | 3:Dc:312:THR:HG23 | 1.91 | 0.70 |
| 12:Dm:53:ALA:O | 12:Dm:173:LYS:NZ | 2.24 | 0.70 |
| 25:Dz:55:TYR:O | 27:Eb:117:GLN:NE2 | 2.24 | 0.70 |
| 51:Ez:39:GLU:N | 51:Ez:39:GLU:OE1 | 2.25 | 0.70 |
| 53:DL:340:ASN:OD1 | 53:DL:342:ARG:NH1 | 2.25 | 0.70 |
| 4:DD:261:GLU:O | 4:DD:265:LEU:HD22 | 1.91 | 0.70 |
| 21:DV:62:ASN:ND2 | 57:DV:402:CDL:OB9 | 2.25 | 0.70 |
| 52:Fa:30:SER:O | 52:Fa:33:ASN:ND2 | 2.24 | 0.70 |
| 18:DS:140:THR:HG21 | 18:DS:214:TYR:HB2 | 1.72 | 0.70 |
| 18:DS:208:GLN:OE1 | 18:DS:304:TYR:OH | 2.08 | 0.70 |
| 57:EL:901:CDL:H871 | 57:EL:901:CDL:H671 | 1.73 | 0.70 |
| 41:EP:28:TYR:N | 16:Dq:291:SER:HG | 1.89 | 0.70 |
| 10:Dj:143:ARG:NH2 | 10:Dj:186:ASP:OD1 | 2.25 | 0.70 |
| 15:DP:197:ARG:NH1 | 24:DY:210:GLN:OE1 | 2.25 | 0.70 |
| 4:Dd:321:GLU:OE1 | 5:De:59:TYR:OH | 2.09 | 0.70 |
| 18:DS:17:ASP:O | 18:DS:339:ASN:ND2 | 2.25 | 0.69 |
| 24:DY:234:LYS:NZ | 42:EQ:35:GLU:OE2 | 2.25 | 0.69 |
| 27:Eb:16:ASP:O | 27:Eb:19:THR:HG22 | 1.92 | 0.69 |
| 8:DH:80:VAL:HG21 | 13:DN:352:LEU:HB2 | 1.74 | 0.69 |
| 19:DT:45:PRO:HG2 | 19:DT:50:ILE:HD11 | 1.74 | 0.69 |
| 1:Da:501:ALA:HB2 | 1:Da:529:ILE:HG22 | 1.75 | 0.69 |
| 28:Ec:16:GLU:OE1 | 28:Ec:18:ALA:N | 2.26 | 0.69 |
| 1:Da:155:ILE:HD13 | 1:Da:295:LEU:HD11 | 1.75 | 0.69 |
| 3:Dc:101:GLU:HG2 | 20:Du:271:LEU:HD21 | 1.74 | 0.69 |
| 8:Dh:80:VAL:HG21 | 13:Dn:352:LEU:HB2 | 1.74 | 0.69 |
| 18:Ds:152:VAL:HG21 | 18:Ds:198:SER:HB2 | 1.73 | 0.69 |
| 29:Ed:171:LYS:NZ | 44:Es:33:PHE:O | 2.25 | 0.69 |
| 32:Eg:25:ASP:OD2 | 32:Eg:74:SER:OG | 2.05 | 0.69 |
| 3:DC:368:ILE:HD12 | 3:DC:401:ILE:HD12 | 1.75 | 0.69 |
| 14:DO:158:ARG:NH2 | 14:DO:197:GLU:OE2 | 2.26 | 0.69 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 50:Ey:5:LEU:HD21 | 52:Fa:14:VAL:HG11 | 1.74 | 0.69 |
| 14:DO:322:ASP:O | 24:DY:190:ARG:NH1 | 2.26 | 0.69 |
| 1:Da:550:LEU:O | 9:Di:136:ARG:NH1 | 2.26 | 0.69 |
| 21:Dv:249:ASN:N | 21:Dv:255:ASN:OD1 | 2.26 | 0.69 |
| 23:Dx:143:ARG:NH1 | 23:Dx:221:LEU:O | 2.26 | 0.69 |
| 23:DX:23:ARG:NH1 | 23:DX:45:ASN:OD1 | 2.26 | 0.69 |
| 18:Ds:140:THR:HG21 | 18:Ds:214:TYR:HB2 | 1.74 | 0.69 |
| 4:DD:74:THR:OG1 | 57:DD:702:CDL:OA3 | 2.04 | 0.68 |
| 18:DS:152:VAL:HG21 | 18:DS:198:SER:HB2 | 1.75 | 0.68 |
| 31:EF:174:LEU:HD22 | 58:Dx:1202:PC1:H2I2 | 1.73 | 0.68 |
| 1:Da:84:SER:OG | 1:Da:591:HIS:ND1 | 2.26 | 0.68 |
| 16:Dq:98:GLU:OE2 | 36:Ek:51:ARG:NE | 2.26 | 0.68 |
| 19:Dt:57:GLN:NE2 | 44:Es:13:THR:O | 2.25 | 0.68 |
| 20:Du:154:SER:O | 20:Du:159:GLN:NE2 | 2.26 | 0.68 |
| 1:Da:84:SER:HG | 1:Da:591:HIS:HD1 | 1.40 | 0.68 |
| 14:Do:322:ASP:O | 24:Dy:190:ARG:NH1 | 2.26 | 0.68 |
| 18:Ds:208:GLN:OE1 | 18:Ds:304:TYR:OH | 2.12 | 0.68 |
| 32:Eg:41:GLN:OE1 | 32:Eg:45:ARG:NH1 | 2.27 | 0.68 |
| 27:EB:16:ASP:O | 27:EB:19:THR:HG22 | 1.93 | 0.68 |
| 1:Da:501:ALA:HB1 | 1:Da:530:MET:HG2 | 1.75 | 0.68 |
| 14:DO:37:GLU:OE1 | 14:DO:37:GLU:N | 2.26 | 0.68 |
| 20:DU:266:THR:O | 20:DU:270:VAL:HG23 | 1.94 | 0.68 |
| 9:Di:142:SER:OG | 57:Di:701:CDL:OB4 | 2.08 | 0.68 |
| 12:DM:274:GLU:OE2 | 12:DM:366:ARG:NH1 | 2.26 | 0.68 |
| 14:DO:116:GLY:O | 14:DO:120:VAL:HG23 | 1.93 | 0.68 |
| 17:DR:124:TYR:O | 17:DR:128:VAL:HG22 | 1.94 | 0.68 |
| 30:EE:157:CYS:SG | 30:EE:173:ARG:NH2 | 2.66 | 0.68 |
| 12:Dm:299:PHE:O | 12:Dm:303:ASN:ND2 | 2.27 | 0.68 |
| 2:DB:245:THR:OG1 | 2:DB:247:LYS:NZ | 2.27 | 0.68 |
| 16:DQ:101:ARG:NH1 | 36:EK:45:GLN:OE1 | 2.27 | 0.68 |
| 18:Ds:50:GLN:OE1 | 18:Ds:311:GLY:N | 2.27 | 0.68 |
| 14:Do:151:GLN:OE1 | 14:Do:151:GLN:N | 2.26 | 0.68 |
| 57:Dx:1203:CDL:H872 | 57:Dx:1203:CDL:H831 | 1.75 | 0.68 |
| 25:Dz:210:LEU:HD23 | 25:Dz:226:ARG:HA | 1.76 | 0.68 |
| 8:DH:58:GLU:N | 8:DH:58:GLU:OE1 | 2.27 | 0.67 |
| 21:DV:7:ARG:NH1 | 21:DV:10:GLU:OE2 | 2.27 | 0.67 |
| 3:Dc:84:GLU:OE1 | 20:Du:266:THR:OG1 | 2.11 | 0.67 |
| 4:DD:392:TYR:OH | 4:DD:399:GLU:OE2 | 2.11 | 0.67 |
| 4:DD:433:THR:O | 4:DD:438:LYS:NZ | 2.28 | 0.67 |
| 31:EF:174:LEU:HD23 | 31:EF:177:LEU:HD12 | 1.75 | 0.67 |
| 12:Dm:34:GLU:O | 12:Dm:38:ASN:ND2 | 2.27 | 0.67 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 12:Dm:72:SER:OG | 12:Dm:74:ASP:OD1 | 2.13 | 0.67 |
| 1:DA:437:VAL:O | 1:DA:440:HIS:ND1 | 2.28 | 0.67 |
| 2:DB:271:ASN:ND2 | 52:FA:7:ASN:OD1 | 2.28 | 0.67 |
| 30:EE:106:GLU:OE1 | 30:EE:106:GLU:N | 2.28 | 0.67 |
| 3:Dc:349:LYS:NZ | 5:De:105:GLN:O | 2.27 | 0.67 |
| 18:Ds:58:GLU:OE1 | 18:Ds:58:GLU:N | 2.28 | 0.67 |
| 9:DI:203:MET:O | 9:DI:206:THR:OG1 | 2.12 | 0.67 |
| 4:Dd:482:LEU:HD11 | 36:Ek:26:LEU:HD22 | 1.76 | 0.67 |
| 4:DD:431:ASP:OD2 | 4:DD:433:THR:OG1 | 2.10 | 0.67 |
| 33:EH:53:GLY:O | 33:EH:57:VAL:HG23 | 1.94 | 0.67 |
| 3:DC:435:ASP:OD1 | 3:DC:436:THR:N | 2.28 | 0.67 |
| 14:DO:244:ASP:O | 14:DO:248:VAL:HG13 | 1.95 | 0.67 |
| 16:DQ:57:THR:O | 16:DQ:61:ASN:ND2 | 2.28 | 0.67 |
| 3:Dc:524:ARG:NH2 | 37:El:140:ASP:O | 2.27 | 0.67 |
| 23:DX:220:GLN:N | 23:DX:220:GLN:OE1 | 2.28 | 0.67 |
| 24:DY:167:ARG:NH1 | 27:EB:210:PHE:O | 2.27 | 0.67 |
| 36:EK:109:ILE:HG21 | 36:EK:124:GLU:HG3 | 1.77 | 0.67 |
| 3:Dc:435:ASP:OD1 | 3:Dc:436:THR:N | 2.28 | 0.67 |
| 37:El:102:LYS:NZ | 57:El:901:CDL:OB4 | 2.27 | 0.66 |
| 6:DF:224:GLU:OE1 | 6:DF:224:GLU:N | 2.29 | 0.66 |
| 4:Dd:236:LYS:NZ | 57:Dd:704:CDL:OB4 | 2.29 | 0.66 |
| 4:Dd:503:LEU:HB3 | 36:Ek:40:ILE:HD11 | 1.76 | 0.66 |
| 17:Dr:242:ALA:O | 31:Ef:164:ARG:NH1 | 2.28 | 0.66 |
| 66:Ed:201:HEM:HBC2 | 66:Ed:201:HEM:HMC1 | 1.77 | 0.66 |
| 53:Dl:87:THR:HG23 | 53:Dl:119:MET:HE1 | 1.77 | 0.66 |
| 39:En:123:ASN:ND2 | 39:En:138:GLU:O | 2.29 | 0.66 |
| 44:Es:50:ASN:OD1 | 44:Es:51:LEU:N | 2.28 | 0.66 |
| 23:DX:143:ARG:NH1 | 23:DX:221:LEU:O | 2.27 | 0.66 |
| 33:Eh:53:GLY:O | 33:Eh:57:VAL:HG23 | 1.96 | 0.66 |
| 53:Dl:170:ASP:OD1 | 53:Dl:171:VAL:N | 2.28 | 0.66 |
| 58:DG:203:PC1:O12 | 31:EF:86:TYR:OH | 2.12 | 0.66 |
| 18:Ds:10:ARG:NH1 | 21:Dv:4:SER:OG | 2.29 | 0.66 |
| 40:Eo:101:GLU:N | 40:Eo:101:GLU:OE1 | 2.27 | 0.66 |
| 1:DA:496:LEU:HG | 65:EN:1204:UQ8:H10A | 1.78 | 0.66 |
| 20:DU:145:TYR:CE2 | 20:DU:149:ILE:HD11 | 2.31 | 0.66 |
| 66:Ed:201:HEM:HBB2 | 66:Ed:201:HEM:CMB | 2.24 | 0.66 |
| 26:EA:218:ARG:NH1 | 50:EY:58:TYR:OH | 2.29 | 0.66 |
| 66:ED:602:HEM:HBC2 | 66:ED:602:HEM:HMC2 | 1.77 | 0.66 |
| 11:DK:124:GLU:OE1 | 22:DW:267:SER:OG | 2.14 | 0.66 |
| 52:FA:6:SER:OG | 52:FA:9:ASN:OD1 | 2.14 | 0.66 |
| 2:Db:271:ASN:ND2 | 52:Fa:7:ASN:OD1 | 2.29 | 0.66 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 36:Ek:109:ILE:HG21 | 36:Ek:124:GLU:HG3 | 1.77 | 0.66 |
| 21:DV:249:ASN:N | 21:DV:255:ASN:OD1 | 2.28 | 0.66 |
| 32:EG:41:GLN:OE1 | 32:EG:45:ARG:NH1 | 2.29 | 0.66 |
| 2:Db:7:THR:O | 2:Db:544:PHE:N | 2.28 | 0.66 |
| 10:DJ:175:ARG:NH2 | 10:DJ:204:GLU:OE2 | 2.29 | 0.65 |
| 18:DS:156:LEU:HD12 | 18:DS:194:LEU:C | 2.21 | 0.65 |
| 1:Da:437:VAL:O | 1:Da:440:HIS:ND1 | 2.29 | 0.65 |
| 10:Dj:167:LEU:O | 10:Dj:171:PHE:N | 2.26 | 0.65 |
| 2:DB:7:THR:O | 2:DB:544:PHE:N | 2.29 | 0.65 |
| 51:EZ:28:ASN:O | 52:FA:27:LYS:NZ | 2.28 | 0.65 |
| 18:Ds:289:TYR:OH | 57:Dv:402:CDL:OA9 | 2.06 | 0.65 |
| 9:DI:120:SEP:O | 12:DM:246:ASN:ND2 | 2.30 | 0.65 |
| 15:DP:160:ASP:OD1 | 15:DP:161:GLY:N | 2.30 | 0.65 |
| 32:Eg:74:SER:OG | 33:Eh:13:ARG:NH2 | 2.30 | 0.65 |
| 52:Fa:6:SER:OG | 52:Fa:9:ASN:OD1 | 2.15 | 0.65 |
| 53:DL:170:ASP:OD1 | 53:DL:171:VAL:N | 2.28 | 0.65 |
| 11:Dk:124:GLU:OE1 | 22:Dw:267:SER:OG | 2.14 | 0.65 |
| 12:Dm:272:LEU:HD22 | 12:Dm:369:PHE:CE2 | 2.32 | 0.65 |
| 57:DN:505:CDL:O1 | 29:ED:92:GLU:OE1 | 2.13 | 0.65 |
| 14:Do:355:THR:OG1 | 14:Do:369:VAL:O | 2.13 | 0.65 |
| 14:Do:116:GLY:O | 14:Do:120:VAL:HG23 | 1.97 | 0.65 |
| 15:Dp:190:LYS:O | 15:Dp:193:ARG:NH1 | 2.29 | 0.65 |
| 32:EG:10:GLN:NE2 | 33:EH:113:GLU:OE2 | 2.29 | 0.65 |
| 14:Do:244:ASP:O | 14:Do:248:VAL:HG13 | 1.97 | 0.65 |
| 28:Ec:51:GLN:OE1 | 28:Ec:51:GLN:N | 2.30 | 0.65 |
| 53:Dl:406:ASP:O | 53:Dl:421:ASN:ND2 | 2.29 | 0.65 |
| 50:EY:5:LEU:HD21 | 52:FA:14:VAL:HG11 | 1.78 | 0.65 |
| 52:FA:50:GLU:OE1 | 52:FA:50:GLU:N | 2.30 | 0.65 |
| 1:DA:501:ALA:HB1 | 1:DA:530:MET:HG2 | 1.79 | 0.65 |
| 9:DI:74:MET:SD | 19:DT:109:GLN:NE2 | 2.70 | 0.64 |
| 2:Db:122:TRP:CD1 | 2:Db:553:CYS:HG | 2.15 | 0.64 |
| 20:Du:266:THR:O | 20:Du:270:VAL:HG23 | 1.97 | 0.64 |
| 18:DS:58:GLU:N | 18:DS:58:GLU:OE1 | 2.29 | 0.64 |
| 20:DU:41:ASP:OD1 | 20:DU:44:SER:OG | 2.13 | 0.64 |
| 33:EH:166:ASP:OD1 | 33:EH:167:TYR:N | 2.31 | 0.64 |
| 1:Da:241:PRO:O | 27:Eb:74:LYS:NZ | 2.30 | 0.64 |
| 40:EO:101:GLU:OE1 | 40:EO:101:GLU:N | 2.29 | 0.64 |
| 3:Dc:368:ILE:HD12 | 3:Dc:401:ILE:HD12 | 1.79 | 0.64 |
| 40:Eo:56:GLU:OE1 | 40:Eo:56:GLU:N | 2.31 | 0.64 |
| 8:DH:33:HIS:O | 8:DH:37:GLY:N | 2.30 | 0.64 |
| 66:ED:602:HEM:HBB2 | 66:ED:602:HEM:CMB | 2.24 | 0.64 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 34:EI:49:LEU:O | 34:EI:54:ARG:NE | 2.30 | 0.64 |
| 4:Dd:403:ASP:OD1 | 4:Dd:404:GLN:N | 2.29 | 0.64 |
| 16:DQ:321:ASP:OD1 | 16:DQ:324:ARG:NH2 | 2.31 | 0.64 |
| 34:EI:25:LEU:O | 34:EI:33:ARG:NH1 | 2.31 | 0.64 |
| 13:Dn:409:LEU:HD11 | 13:Dn:437:PHE:CD1 | 2.33 | 0.64 |
| 4:DD:321:GLU:OE1 | 5:DE:59:TYR:OH | 2.12 | 0.64 |
| 3:DC:205:ASN:O | 3:DC:228:TYR:OH | 2.09 | 0.64 |
| 6:DF:36:ASP:OD2 | 40:EO:81:ARG:NH2 | 2.31 | 0.64 |
| 12:DM:79:GLU:N | 12:DM:79:GLU:OE1 | 2.31 | 0.64 |
| 19:DT:104:ASP:OD1 | 19:DT:107:TYR:OH | 2.16 | 0.64 |
| 19:DT:135:LEU:O | 19:DT:140:GLN:NE2 | 2.31 | 0.64 |
| 3:Dc:268:PHE:O | 3:Dc:272:ILE:HG23 | 1.98 | 0.64 |
| 19:DT:232:GLU:OE1 | 19:DT:232:GLU:N | 2.31 | 0.64 |
| 32:EG:75:ARG:NH2 | 46:EU:38:GLU:OE2 | 2.31 | 0.64 |
| 29:ED:115:ILE:HG12 | 65:ED:603:UQ8:H4MB | 1.80 | 0.64 |
| 15:Dp:160:ASP:OD1 | 15:Dp:161:GLY:N | 2.31 | 0.64 |
| 4:DD:287:THR:HG22 | 13:DN:279:VAL:CG1 | 2.28 | 0.63 |
| 3:Dc:202:LYS:NZ | 53:Dl:427:SER:O | 2.27 | 0.63 |
| 6:Df:208:HIS:O | 6:Df:212:THR:HG23 | 1.98 | 0.63 |
| 19:Dt:45:PRO:HG2 | 19:Dt:50:ILE:HD11 | 1.80 | 0.63 |
| 33:Eh:36:SER:OG | 33:Eh:121:ASP:OD2 | 2.08 | 0.63 |
| 34:Ei:49:LEU:O | 34:Ei:54:ARG:NE | 2.30 | 0.63 |
| 57:DJ:304:CDL:H832 | 57:EL:901:CDL:H873 | 1.80 | 0.63 |
| 16:DQ:199:ARG:NH1 | 57:DQ:1501:CDL:O1 | 2.30 | 0.63 |
| 38:EM:49:LYS:O | 38:EM:54:ARG:NH1 | 2.31 | 0.63 |
| 10:DJ:199:LYS:NZ | 23:Dx:252:GLY:O | 2.31 | 0.63 |
| 19:DT:271:ARG:NH1 | 19:DT:279:GLU:OE1 | 2.31 | 0.63 |
| 1:Da:643:TYR:O | 2:Db:69:THR:HG23 | 1.98 | 0.63 |
| 10:DJ:167:LEU:O | 10:DJ:171:PHE:N | 2.27 | 0.63 |
| 40:EO:9:VAL:O | 40:EO:13:ASN:ND2 | 2.31 | 0.63 |
| 28:Ec:56:LEU:O | 28:Ec:60:LEU:HG | 1.97 | 0.63 |
| 12:DM:46:THR:HG21 | 12:DM:107:ARG:HG2 | 1.79 | 0.63 |
| 49:EX:20:THR:HG22 | 51:EZ:49:TYR:CE1 | 2.33 | 0.63 |
| 1:Da:562:MET:HE1 | 65:Ds:404:UQ8:H30 | 1.80 | 0.63 |
| 33:Eh:166:ASP:OD1 | 33:Eh:167:TYR:N | 2.31 | 0.63 |
| 2:DB:225:ILE:O | 2:DB:227:ARG:NH1 | 2.31 | 0.63 |
| 24:DY:64:SER:OG | 24:DY:189:ASN:OD1 | 2.11 | 0.63 |
| 21:Dv:92:TYR:HB2 | 21:Dv:136:THR:HG21 | 1.80 | 0.63 |
| 22:Dw:98:GLN:OE1 | 22:Dw:98:GLN:N | 2.32 | 0.63 |
| 14:DO:355:THR:OG1 | 14:DO:369:VAL:O | 2.13 | 0.63 |
| 19:DT:170:ASN:ND2 | 19:DT:174:GLU:O | 2.32 | 0.63 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 12:Dm:286:ASN:OD1 | 12:Dm:287:TYR:N | 2.32 | 0.63 |
| 25:Dz:130:GLU:OE1 | 25:Dz:130:GLU:N | 2.32 | 0.63 |
| 16:Dq:120:ASN:OD1 | 16:Dq:183:LYS:NZ | 2.28 | 0.63 |
| 19:Dt:81:PRO:HG2 | 19:Dt:89:MET:HE3 | 1.81 | 0.63 |
| 49:Ex:20:THR:HG22 | 51:Ez:49:TYR:CE1 | 2.34 | 0.63 |
| 58:Da:707:PC1:H2E1 | 58:Da:707:PC1:H2I3 | 1.80 | 0.62 |
| 19:Dt:117:ARG:HA | 31:Ef:51:THR:HG21 | 1.81 | 0.62 |
| 1:DA:415:ARG:NH2 | 7:DG:19:ASP:OD1 | 2.32 | 0.62 |
| 13:DN:253:TYR:N | 13:DN:284:ASP:OD2 | 2.32 | 0.62 |
| 49:EX:20:THR:HG22 | 51:EZ:49:TYR:HE1 | 1.64 | 0.62 |
| 3:DC:23:THR:O | 3:DC:69:LYS:NZ | 2.27 | 0.62 |
| 8:DH:10:LYS:NZ | 12:DM:263:SER:OG | 2.32 | 0.62 |
| 21:Dv:7:ARG:NH1 | 21:Dv:10:GLU:OE2 | 2.32 | 0.62 |
| 47:EJ:153:ASP:OD1 | 47:EJ:161:GLN:NE2 | 2.32 | 0.62 |
| 17:Dr:175:GLU:OE1 | 17:Dr:211:ARG:NH1 | 2.33 | 0.62 |
| 19:Dt:135:LEU:O | 19:Dt:140:GLN:NE2 | 2.31 | 0.62 |
| 3:DC:385:ASN:ND2 | 12:DM:362:ASP:OD1 | 2.32 | 0.62 |
| 4:DD:119:VAL:HG23 | 4:DD:120:THR:HG23 | 1.82 | 0.62 |
| 4:DD:403:ASP:OD1 | 4:DD:404:GLN:N | 2.32 | 0.62 |
| 28:EC:136:GLU:O | 28:EC:140:VAL:HG23 | 2.00 | 0.62 |
| 21:Dv:2:ASN:ND2 | 27:Eb:25:ASP:OD1 | 2.32 | 0.62 |
| 25:DZ:130:GLU:OE1 | 25:DZ:130:GLU:N | 2.31 | 0.62 |
| 4:Dd:575:PHE:CE2 | 4:Dd:579:ILE:HD11 | 2.35 | 0.62 |
| 14:DO:115:GLU:N | 14:DO:115:GLU:OE1 | 2.33 | 0.62 |
| 7:Dg:81:MET:O | 7:Dg:85:ASN:ND2 | 2.33 | 0.62 |
| 49:Ex:20:THR:HG22 | 51:Ez:49:TYR:HE1 | 1.63 | 0.62 |
| 18:DS:152:VAL:HG21 | 18:DS:198:SER:CB | 2.29 | 0.62 |
| 22:DW:141:TYR:O | 38:EM:7:ARG:NH1 | 2.31 | 0.62 |
| 22:DW:257:GLU:N | 22:DW:257:GLU:OE1 | 2.33 | 0.62 |
| 12:Dm:413:ALA:O | 12:Dm:435:LYS:NZ | 2.33 | 0.62 |
| 2:Db:592:ARG:O | 2:Db:596:HIS:ND1 | 2.33 | 0.62 |
| 3:Dc:80:LEU:HD13 | 14:Do:273:MET:SD | 2.40 | 0.62 |
| 13:Dn:44:TYR:OH | 57:Dn:503:CDL:OB5 | 2.18 | 0.62 |
| 5:DE:8:ARG:NH1 | 16:DQ:218:ASP:OD1 | 2.33 | 0.62 |
| 2:Db:112:LEU:HD11 | 2:Db:139:THR:HG22 | 1.82 | 0.62 |
| 11:Dk:97:GLU:N | 11:Dk:97:GLU:OE1 | 2.31 | 0.62 |
| 4:DD:502:TYR:CE1 | 4:DD:506:LEU:HD21 | 2.35 | 0.61 |
| 15:DP:197:ARG:O | 15:DP:198:ARG:NH1 | 2.33 | 0.61 |
| 12:Dm:79:GLU:OE1 | 12:Dm:79:GLU:N | 2.33 | 0.61 |
| 14:Do:37:GLU:OE1 | 14:Do:37:GLU:N | 2.32 | 0.61 |
| 28:Ec:7:GLU:OE2 | 28:Ec:26:LYS:NZ | 2.33 | 0.61 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 52:Fa:50:GLU:OE1 | 52:Fa:50:GLU:N | 2.33 | 0.61 |
| 13:Dn:253:TYR:N | 13:Dn:284:ASP:OD2 | 2.33 | 0.61 |
| 4:Dd:265:LEU:HD12 | 4:Dd:272:ARG:HA | 1.81 | 0.61 |
| 18:Ds:152:VAL:HG21 | 18:Ds:198:SER:CB | 2.30 | 0.61 |
| 21:Dv:249:ASN:OD1 | 21:Dv:250:ALA:N | 2.32 | 0.61 |
| 53:Dl:255:SER:O | 53:Dl:290:LYS:NZ | 2.32 | 0.61 |
| 28:EC:56:LEU:O | 28:EC:60:LEU:HG | 1.99 | 0.61 |
| 4:Dd:392:TYR:OH | 4:Dd:399:GLU:OE2 | 2.13 | 0.61 |
| 4:Dd:503:LEU:CB | 36:Ek:40:ILE:HD11 | 2.29 | 0.61 |
| 37:El:13:ARG:NH2 | 43:Er:104:LYS:O | 2.32 | 0.61 |
| 47:Ej:79:VAL:HG11 | 47:Ej:99:PHE:CZ | 2.36 | 0.61 |
| 53:Dl:182:THR:OG1 | 53:Dl:184:ASN:OD1 | 2.16 | 0.61 |
| 3:DC:268:PHE:O | 3:DC:272:ILE:HG23 | 1.99 | 0.61 |
| 5:DE:53:GLU:OE1 | 29:ED:170:TYR:OH | 2.17 | 0.61 |
| 40:EO:56:GLU:N | 40:EO:56:GLU:OE1 | 2.33 | 0.61 |
| 34:Ei:25:LEU:O | 34:Ei:33:ARG:NH1 | 2.34 | 0.61 |
| 28:EC:99:ARG:NH1 | 22:Dw:20:THR:OG1 | 2.33 | 0.61 |
| 14:Do:75:GLU:OE1 | 14:Do:145:ARG:NH2 | 2.34 | 0.61 |
| 2:DB:145:ASN:ND2 | 11:DK:31:ASP:OD2 | 2.34 | 0.61 |
| 16:DQ:98:GLU:OE2 | 36:EK:51:ARG:NE | 2.34 | 0.61 |
| 20:DU:64:ARG:NE | 20:DU:77:ASP:OD2 | 2.30 | 0.61 |
| 21:DV:249:ASN:OD1 | 21:DV:250:ALA:N | 2.33 | 0.61 |
| 6:DF:208:HIS:O | 6:DF:212:THR:HG23 | 2.01 | 0.61 |
| 10:DJ:51:ARG:NH2 | 57:DJ:303:CDL:OB7 | 2.34 | 0.61 |
| 4:DD:506:LEU:HD22 | 4:DD:544:PHE:CZ | 2.36 | 0.61 |
| 12:DM:34:GLU:O | 12:DM:38:ASN:ND2 | 2.32 | 0.61 |
| 30:EE:154:LEU:HD22 | 30:EE:174:PHE:CG | 2.36 | 0.61 |
| 3:Dc:263:VAL:O | 8:Dh:108:ARG:NH1 | 2.34 | 0.61 |
| 52:FA:30:SER:O | 52:FA:33:ASN:ND2 | 2.33 | 0.61 |
| 2:Db:508:ASN:OD1 | 2:Db:509:SER:N | 2.33 | 0.61 |
| 45:Et:12:GLN:OE1 | 45:Et:16:ARG:NH2 | 2.34 | 0.61 |
| 4:DD:265:LEU:HD12 | 4:DD:272:ARG:HA | 1.83 | 0.60 |
| 4:Dd:242:GLU:N | 4:Dd:242:GLU:OE1 | 2.34 | 0.60 |
| 1:DA:643:TYR:O | 2:DB:69:THR:HG23 | 2.01 | 0.60 |
| 25:DZ:138:GLU:OE1 | 25:DZ:142:ARG:NH2 | 2.35 | 0.60 |
| 4:Dd:232:MET:N | 57:Dd:706:CDL:OB4 | 2.34 | 0.60 |
| 23:DX:41:ALA:O | 23:DX:45:ASN:ND2 | 2.33 | 0.60 |
| 5:De:34:ASP:OD1 | 5:De:38:LYS:NZ | 2.33 | 0.60 |
| 58:DX:302:PC1:H282 | 31:Ef:180:VAL:HG21 | 1.84 | 0.60 |
| 8:Dh:72:TYR:OH | 25:Dz:39:GLY:O | 2.10 | 0.60 |
| 12:Dm:390:GLU:OE1 | 12:Dm:392:TYR:OH | 2.18 | 0.60 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 21:Dv:20:SER:O | 21:Dv:24:ASN:ND2 | 2.34 | 0.60 |
| 3:DC:230:GLN:NE2 | 47:EJ:3:ASN:OD1 | 2.35 | 0.60 |
| 17:DR:139:LYS:NZ | 17:DR:329:SER:OG | 2.33 | 0.60 |
| 1:Da:116:GLY:O | 1:Da:120:ASN:ND2 | 2.34 | 0.60 |
| 2:Db:69:THR:HG21 | 19:Dt:234:GLU:O | 2.00 | 0.60 |
| 8:Dh:54:ILE:O | 8:Dh:54:ILE:HG22 | 2.01 | 0.60 |
| 17:Dr:124:TYR:O | 17:Dr:128:VAL:HG22 | 2.01 | 0.60 |
| 39:En:70:TRP:N | 57:En:1202:CDL:OA3 | 2.34 | 0.60 |
| 3:DC:53:LEU:HD23 | 3:DC:58:ASN:OD1 | 2.01 | 0.60 |
| 16:DQ:23:ARG:NH1 | 16:DQ:25:GLY:O | 2.35 | 0.60 |
| 1:Da:682:GLU:OE1 | 18:Ds:96:ARG:NH2 | 2.34 | 0.60 |
| 23:Dx:228:ASN:ND2 | 23:Dx:228:ASN:O | 2.34 | 0.60 |
| 53:Dl:98:GLU:OE1 | 53:Dl:98:GLU:N | 2.35 | 0.60 |
| 58:DA:707:PC1:H2I3 | 58:DA:707:PC1:H2E1 | 1.82 | 0.60 |
| 3:DC:566:ASN:ND2 | 26:EA:30:MET:SD | 2.73 | 0.60 |
| 16:DQ:126:LYS:NZ | 57:Dj:401:CDL:OB3 | 2.35 | 0.60 |
| 1:Da:353:LEU:HD22 | 1:Da:389:PHE:CE2 | 2.37 | 0.60 |
| 53:Dl:128:THR:OG1 | 53:Dl:130:ASP:OD1 | 2.13 | 0.60 |
| 53:Dl:419:GLN:OE1 | 53:Dl:427:SER:OG | 2.19 | 0.60 |
| 2:DB:233:ASP:OD1 | 2:DB:234:ASP:N | 2.35 | 0.60 |
| 2:DB:574:LEU:O | 2:DB:578:THR:HG22 | 2.01 | 0.60 |
| 8:DH:21:ASP:OD1 | 8:DH:22:ALA:N | 2.35 | 0.60 |
| 57:DV:403:CDL:H432 | 57:DV:403:CDL:H471 | 1.83 | 0.60 |
| 8:DH:49:TYR:O | 8:DH:53:HIS:ND1 | 2.34 | 0.60 |
| 3:Dc:481:LEU:O | 3:Dc:485:ASN:ND2 | 2.34 | 0.60 |
| 53:DL:128:THR:OG1 | 53:DL:130:ASP:OD1 | 2.15 | 0.60 |
| 18:Ds:342:GLU:OE1 | 18:Ds:342:GLU:N | 2.34 | 0.59 |
| 4:Dd:618:GLU:OE1 | 4:Dd:618:GLU:N | 2.34 | 0.59 |
| 3:DC:31:ASN:ND2 | 47:EJ:61:HIS:O | 2.36 | 0.59 |
| 7:DG:81:MET:O | 7:DG:85:ASN:ND2 | 2.35 | 0.59 |
| 10:DJ:208:GLU:OE1 | 10:DJ:208:GLU:N | 2.35 | 0.59 |
| 19:DT:83:TYR:OH | 31:EF:27:ASP:OD2 | 2.20 | 0.59 |
| 1:Da:296:ILE:HG23 | 1:Da:357:VAL:CG1 | 2.32 | 0.59 |
| 5:De:62:GLU:OE2 | 13:Dn:285:LYS:NZ | 2.22 | 0.59 |
| 25:Dz:122:LEU:O | 25:Dz:126:ILE:HG22 | 2.02 | 0.59 |
| 27:Eb:82:PHE:CE2 | 27:Eb:86:ILE:HD11 | 2.37 | 0.59 |
| 47:Ej:73:ASN:OD1 | 47:Ej:108:ARG:NH2 | 2.35 | 0.59 |
| 53:DL:406:ASP:O | 53:DL:421:ASN:ND2 | 2.34 | 0.59 |
| 41:EP:78:ASP:OD1 | 41:EP:82:TYR:N | 2.35 | 0.59 |
| 42:EQ:1:AME:HB1 | 42:EQ:107:TYR:OH | 2.01 | 0.59 |
| 23:Dx:41:ALA:O | 23:Dx:45:ASN:ND2 | 2.34 | 0.59 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:DA:252:VAL:O | 1:DA:255:ARG:NH1 | 2.35 | 0.59 |
| 3:DC:80:LEU:HD13 | 14:DO:273:MET:SD | 2.43 | 0.59 |
| 18:DS:306:TRP:NE1 | 57:EN:1202:CDL:OB7 | 2.33 | 0.59 |
| 27:EB:39:ASN:C | 27:EB:40:LEU:HD12 | 2.28 | 0.59 |
| 1:DA:116:GLY:O | 1:DA:120:ASN:ND2 | 2.36 | 0.59 |
| 37:EL:23:THR:HG22 | 37:EL:151:PRO:HG2 | 1.85 | 0.59 |
| 1:Da:565:ILE:HD11 | 57:En:1201:CDL:H342 | 1.85 | 0.59 |
| 2:Db:155:GLU:OE1 | 2:Db:157:GLN:N | 2.34 | 0.59 |
| 4:Dd:119:VAL:HG23 | 4:Dd:120:THR:HG23 | 1.84 | 0.59 |
| 3:DC:101:GLU:HG2 | 20:DU:271:LEU:HD21 | 1.85 | 0.59 |
| 38:EM:67:GLU:OE1 | 38:EM:67:GLU:N | 2.35 | 0.59 |
| 3:Dc:566:ASN:ND2 | 26:Ea:30:MET:SD | 2.76 | 0.59 |
| 41:Ep:88:SER:OG | 41:Ep:109:LEU:HD11 | 2.01 | 0.59 |
| 57:Dd:705:CDL:H231 | 57:Dd:705:CDL:H271 | 1.84 | 0.59 |
| 14:Do:158:ARG:NH2 | 14:Do:197:GLU:OE2 | 2.35 | 0.59 |
| 57:Dv:401:CDL:H431 | 57:Dv:401:CDL:H471 | 1.84 | 0.59 |
| 23:Dx:75:TYR:OH | 58:Dx:1202:PC1:O12 | 2.18 | 0.59 |
| 24:Dy:106:PHE:CD1 | 24:Dy:110:ILE:HD12 | 2.38 | 0.59 |
| 2:DB:69:THR:HG21 | 19:DT:234:GLU:O | 2.03 | 0.59 |
| 4:DD:575:PHE:CE2 | 4:DD:579:ILE:HD11 | 2.38 | 0.58 |
| 19:DT:200:GLU:N | 19:DT:200:GLU:OE1 | 2.36 | 0.58 |
| 22:DW:197:VAL:HG23 | 22:DW:249:VAL:HG11 | 1.85 | 0.58 |
| 23:DX:96:PHE:CE2 | 23:DX:100:ILE:HD11 | 2.38 | 0.58 |
| 36:EK:6:PHE:CE2 | 36:EK:10:ILE:HD11 | 2.38 | 0.58 |
| 4:Dd:312:VAL:HG21 | 5:De:15:ILE:HD11 | 1.83 | 0.58 |
| 4:Dd:377:GLU:N | 4:Dd:377:GLU:OE1 | 2.36 | 0.58 |
| 4:Dd:431:ASP:OD2 | 4:Dd:433:THR:OG1 | 2.10 | 0.58 |
| 10:Dj:91:ARG:NH1 | 40:Eo:7:ASN:OD1 | 2.36 | 0.58 |
| 37:El:23:THR:HG22 | 37:El:151:PRO:HG2 | 1.84 | 0.58 |
| 1:DA:562:MET:HE1 | 65:DS:404:UQ8:H30 | 1.84 | 0.58 |
| 57:DG:201:CDL:H222 | 31:EF:177:LEU:HD11 | 1.85 | 0.58 |
| 12:DM:44:TYR:OH | 16:DQ:315:GLU:OE2 | 2.21 | 0.58 |
| 57:Dv:403:CDL:H471 | 57:Dv:403:CDL:H432 | 1.85 | 0.58 |
| 3:DC:263:VAL:O | 8:DH:108:ARG:NH1 | 2.36 | 0.58 |
| 4:DD:440:ALA:O | 4:DD:543:ASN:ND2 | 2.37 | 0.58 |
| 9:Di:120:SEP:O | 12:Dm:246:ASN:ND2 | 2.37 | 0.58 |
| 29:ED:114:TYR:CD2 | 65:ED:603:UQ8:H4M | 2.38 | 0.58 |
| 20:Du:145:TYR:CE2 | 20:Du:149:ILE:HD11 | 2.38 | 0.58 |
| 1:DA:353:LEU:HD22 | 1:DA:389:PHE:CE2 | 2.39 | 0.58 |
| 3:DC:18:PHE:HD2 | 3:DC:62:LEU:HD11 | 1.69 | 0.58 |
| 57:DJ:302:CDL:H872 | 57:EL:901:CDL:H273 | 1.85 | 0.58 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 37:EL:57:ALA:O | 44:ES:83:THR:HG21 | 2.02 | 0.58 |
| 57:Dh:201:CDL:H673 | 57:Dh:202:CDL:CB5 | 2.34 | 0.58 |
| 1:DA:353:LEU:O | 1:DA:357:VAL:HG23 | 2.04 | 0.58 |
| 3:DC:521:LEU:HD21 | 10:DJ:144:MET:HE1 | 1.86 | 0.58 |
| 39:EN:70:TRP:N | 57:EN:1202:CDL:OA3 | 2.37 | 0.58 |
| 57:Dg:201:CDL:H272 | 57:Dg:201:CDL:C47 | 2.33 | 0.58 |
| 11:Dk:12:SER:OG | 31:Ef:188:THR:O | 2.07 | 0.58 |
| 9:DI:115:GLU:OE1 | 9:DI:115:GLU:N | 2.37 | 0.58 |
| 18:Ds:207:PHE:O | 18:Ds:211:THR:HG22 | 2.02 | 0.58 |
| 1:DA:501:ALA:HB2 | 1:DA:529:ILE:HG22 | 1.85 | 0.58 |
| 27:EB:63:ARG:NH1 | 27:EB:67:ASP:OD2 | 2.37 | 0.58 |
| 28:EC:180:ASN:O | 28:EC:185:ARG:NH1 | 2.37 | 0.58 |
| 36:Ek:6:PHE:CE2 | 36:Ek:10:ILE:HD11 | 2.39 | 0.58 |
| 47:Ej:153:ASP:OD1 | 47:Ej:161:GLN:NE2 | 2.36 | 0.58 |
| 5:DE:53:GLU:OE2 | 29:ED:181:LYS:NZ | 2.35 | 0.58 |
| 57:EL:903:CDL:H431 | 57:EL:903:CDL:H471 | 1.86 | 0.58 |
| 2:Db:461:TYR:OH | 22:Dw:190:GLU:OE2 | 2.19 | 0.58 |
| 6:Df:144:ASP:OD2 | 6:Df:196:ARG:NH2 | 2.35 | 0.58 |
| 13:Dn:385:ILE:HD11 | 24:Dy:126:ILE:CD1 | 2.33 | 0.58 |
| 24:Dy:141:LEU:O | 24:Dy:145:ASN:ND2 | 2.36 | 0.58 |
| 47:Ej:142:ARG:NH2 | 47:Ej:149:GLU:OE2 | 2.36 | 0.58 |
| 2:Db:233:ASP:OD1 | 2:Db:234:ASP:N | 2.37 | 0.58 |
| 3:Dc:197:HIS:CE1 | 3:Dc:229:ILE:HG21 | 2.39 | 0.58 |
| 12:DM:237:ARG:NH2 | 25:DZ:48:ASP:OD2 | 2.37 | 0.57 |
| 18:DS:207:PHE:O | 18:DS:211:THR:HG22 | 2.04 | 0.57 |
| 57:DZ:501:CDL:H431 | 57:DZ:501:CDL:H471 | 1.85 | 0.57 |
| 3:Dc:470:ARG:NH1 | 3:Dc:473:GLU:OE2 | 2.37 | 0.57 |
| 38:Em:116:GLN:O | 38:Em:119:ASN:ND2 | 2.36 | 0.57 |
| 21:DV:191:ALA:O | 21:DV:195:ASN:ND2 | 2.37 | 0.57 |
| 29:ED:154:ASN:OD1 | 37:EL:86:ARG:NH1 | 2.37 | 0.57 |
| 41:EP:88:SER:OG | 41:EP:109:LEU:HD11 | 2.03 | 0.57 |
| 49:EX:40:GLU:OE1 | 51:EZ:48:ARG:NH2 | 2.37 | 0.57 |
| 4:Dd:395:ASP:N | 13:Dn:230:TYR:OH | 2.35 | 0.57 |
| 17:Dr:139:LYS:NZ | 17:Dr:329:SER:OG | 2.37 | 0.57 |
| 22:Dw:197:VAL:HG23 | 22:Dw:249:VAL:HG21 | 1.85 | 0.57 |
| 28:Ec:136:GLU:O | 28:Ec:140:VAL:HG23 | 2.04 | 0.57 |
| 32:Eg:75:ARG:NH2 | 46:Eu:38:GLU:OE2 | 2.36 | 0.57 |
| 33:Eh:15:ASP:O | 33:Eh:147:LYS:NZ | 2.38 | 0.57 |
| 2:DB:155:GLU:OE1 | 2:DB:157:GLN:N | 2.37 | 0.57 |
| 2:DB:360:LEU:HD23 | 30:EE:154:LEU:HD23 | 1.84 | 0.57 |
| 3:DC:386:LYS:O | 3:DC:389:THR:HG22 | 2.03 | 0.57 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:DE:50:SER:O | 29:ED:174:ARG:NH2 | 2.37 | 0.57 |
| 1:Da:296:ILE:HG23 | 1:Da:357:VAL:HG13 | 1.86 | 0.57 |
| 23:DX:35:GLU:OE1 | 23:DX:35:GLU:N | 2.37 | 0.57 |
| 57:EL:902:CDL:H272 | 57:EL:902:CDL:H172 | 1.87 | 0.57 |
| 15:DP:119:LEU:HD21 | 15:DP:396:SER:HB2 | 1.86 | 0.57 |
| 25:DZ:122:LEU:O | 25:DZ:126:ILE:HG22 | 2.04 | 0.57 |
| 8:Dh:58:GLU:OE2 | 8:Dh:75:TYR:OH | 2.23 | 0.57 |
| 53:DL:101:SER:OG | 53:DL:105:ARG:NE | 2.38 | 0.57 |
| 2:DB:341:GLU:OE1 | 30:EE:97:SER:N | 2.37 | 0.57 |
| 1:DA:64:THR:HG22 | 1:DA:149:TYR:CD1 | 2.40 | 0.57 |
| 21:DV:92:TYR:HB2 | 21:DV:136:THR:HG21 | 1.85 | 0.57 |
| 59:EL:905:3PE:H2E2 | 59:EL:905:3PE:H2I2 | 1.87 | 0.57 |
| 1:Da:42:LYS:NZ | 9:Di:117:ASP:OD2 | 2.28 | 0.57 |
| 24:Dy:118:ARG:O | 24:Dy:122:THR:HG22 | 2.04 | 0.57 |
| 38:Em:67:GLU:OE1 | 38:Em:67:GLU:N | 2.38 | 0.57 |
| 1:DA:641:ARG:NE | 4:DD:174:GLU:OE2 | 2.38 | 0.57 |
| 2:DB:167:GLN:OE1 | 6:DF:174:TYR:OH | 2.22 | 0.57 |
| 59:DC:607:3PE:H2E2 | 59:DC:607:3PE:H2I3 | 1.86 | 0.57 |
| 23:Dx:220:GLN:OE1 | 23:Dx:220:GLN:N | 2.38 | 0.57 |
| 41:Ep:78:ASP:OD1 | 41:Ep:82:TYR:N | 2.38 | 0.57 |
| 47:Ej:99:PHE:O | 47:Ej:134:GLN:NE2 | 2.37 | 0.57 |
| 20:DU:222:ILE:O | 20:DU:226:ASN:ND2 | 2.37 | 0.56 |
| 12:Dm:237:ARG:NH2 | 25:Dz:48:ASP:OD2 | 2.37 | 0.56 |
| 12:Dm:449:ILE:HD12 | 12:Dm:450:ASN:N | 2.19 | 0.56 |
| 37:El:57:ALA:O | 44:Es:83:THR:HG21 | 2.05 | 0.56 |
| 43:Er:60:TRP:NE1 | 43:Er:64:LEU:HD11 | 2.20 | 0.56 |
| 1:DA:468:ILE:HD11 | 2:DB:83:CYS:SG | 2.44 | 0.56 |
| 2:DB:407:ASP:OD1 | 6:DF:173:TYR:OH | 2.18 | 0.56 |
| 12:DM:390:GLU:OE1 | 12:DM:392:TYR:OH | 2.15 | 0.56 |
| 20:DU:88:VAL:HG11 | 20:DU:288:PHE:CD1 | 2.40 | 0.56 |
| 27:EB:82:PHE:CE2 | 27:EB:86:ILE:HD11 | 2.40 | 0.56 |
| 5:De:23:LYS:NZ | 29:Ed:151:ASN:OD1 | 2.37 | 0.56 |
| 16:Dq:101:ARG:NH1 | 36:Ek:45:GLN:OE1 | 2.37 | 0.56 |
| 57:DJ:302:CDL:H872 | 57:DJ:302:CDL:H831 | 1.88 | 0.56 |
| 16:DQ:116:ASN:ND2 | 57:DX:301:CDL:OB3 | 2.38 | 0.56 |
| 19:DT:57:GLN:NE2 | 44:ES:13:THR:O | 2.37 | 0.56 |
| 23:DX:228:ASN:O | 23:DX:228:ASN:ND2 | 2.38 | 0.56 |
| 8:Dh:21:ASP:OD1 | 8:Dh:22:ALA:N | 2.38 | 0.56 |
| 24:Dy:226:ASN:C | 24:Dy:227:LEU:HD12 | 2.31 | 0.56 |
| 4:Dd:293:VAL:HG13 | 13:Dn:271:ILE:HD13 | 1.86 | 0.56 |
| 8:Dh:27:LYS:NZ | 13:Dn:288:ASN:O | 2.38 | 0.56 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 9:Di:87:ILE:HG23 | 17:Dr:130:VAL:HG12 | 1.86 | 0.56 |
| 16:Dq:220:VAL:HG22 | 16:Dq:224:ALA:CB | 2.35 | 0.56 |
| 13:DN:192:ILE:HD11 | 36:EK:46:VAL:HG11 | 1.88 | 0.56 |
| 22:Dw:134:MET:HE3 | 22:Dw:232:HIS:HD2 | 1.69 | 0.56 |
| 1:DA:380:ILE:HD12 | 1:DA:445:VAL:CG1 | 2.35 | 0.56 |
| 29:ED:33:MET:HE2 | 34:EI:67:THR:HG22 | 1.87 | 0.56 |
| 2:Db:368:GLY:O | 68:Er:201:ATP:N6 | 2.38 | 0.56 |
| 6:Df:40:ARG:NH1 | 6:Df:42:ASP:OD2 | 2.38 | 0.56 |
| 1:DA:296:ILE:HG23 | 1:DA:357:VAL:CG1 | 2.36 | 0.56 |
| 10:DJ:91:ARG:NH2 | 10:DJ:95:GLU:OE2 | 2.38 | 0.56 |
| 2:Db:578:THR:HG23 | 2:Db:579:PHE:CD2 | 2.41 | 0.56 |
| 6:Df:224:GLU:OE1 | 6:Df:224:GLU:N | 2.37 | 0.56 |
| 13:Dn:340:MET:O | 57:Dn:507:CDL:O1 | 2.24 | 0.56 |
| 19:Dt:232:GLU:OE1 | 19:Dt:232:GLU:N | 2.36 | 0.56 |
| 23:Dx:35:GLU:OE1 | 23:Dx:35:GLU:N | 2.38 | 0.56 |
| 33:Eh:85:ASN:OD1 | 33:Eh:86:LEU:N | 2.39 | 0.56 |
| 21:DV:1:AME:HE2 | 21:DV:207:GLU:HG3 | 1.88 | 0.56 |
| 2:Db:574:LEU:O | 2:Db:578:THR:HG22 | 2.06 | 0.56 |
| 4:Dd:458:ARG:NE | 4:Dd:520:SEP:O2P | 2.38 | 0.56 |
| 7:Dg:40:TYR:CE2 | 7:Dg:44:ILE:HD11 | 2.40 | 0.56 |
| 45:ET:72:LYS:NZ | 50:EY:34:GLU:OE2 | 2.38 | 0.55 |
| 9:Di:115:GLU:OE1 | 9:Di:115:GLU:N | 2.38 | 0.55 |
| 12:Dm:84:ASN:OD1 | 12:Dm:85:ALA:N | 2.40 | 0.55 |
| 13:Dn:16:TYR:O | 13:Dn:20:ASN:ND2 | 2.38 | 0.55 |
| 1:DA:123:ILE:O | 1:DA:127:VAL:HG22 | 2.06 | 0.55 |
| 1:DA:296:ILE:HG23 | 1:DA:357:VAL:HG13 | 1.88 | 0.55 |
| 8:DH:106:ASP:O | 8:DH:129:ARG:NH2 | 2.39 | 0.55 |
| 20:DU:182:ASN:ND2 | 20:DU:257:VAL:HG21 | 2.21 | 0.55 |
| 18:Ds:306:TRP:NE1 | 57:En:1202:CDL:OB7 | 2.37 | 0.55 |
| 20:Du:182:ASN:ND2 | 20:Du:257:VAL:HG21 | 2.22 | 0.55 |
| 2:DB:348:ARG:NH1 | 6:DF:190:GLU:OE2 | 2.38 | 0.55 |
| 7:DG:40:TYR:CE2 | 7:DG:44:ILE:HD11 | 2.41 | 0.55 |
| 59:DS:403:3PE:H3I3 | 59:DS:403:3PE:H3E2 | 1.89 | 0.55 |
| 21:DV:24:ASN:ND2 | 21:DV:292:TYR:OH | 2.39 | 0.55 |
| 10:Dj:170:ASP:OD1 | 10:Dj:174:ASN:ND2 | 2.39 | 0.55 |
| 32:Eg:4:ASP:OD1 | 32:Eg:5:PHE:N | 2.40 | 0.55 |
| 47:Ej:79:VAL:HG11 | 47:Ej:99:PHE:CE2 | 2.41 | 0.55 |
| 2:Db:182:SER:O | 2:Db:186:THR:HG22 | 2.06 | 0.55 |
| 34:Ei:66:SER:OG | 34:Ei:70:ARG:NH1 | 2.38 | 0.55 |
| 53:Dl:340:ASN:OD1 | 53:Dl:342:ARG:NH1 | 2.39 | 0.55 |
| 11:Dk:42:GLU:OE1 | 11:Dk:42:GLU:N | 2.38 | 0.55 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 21:Dv:1:AME:HE2 | 21:Dv:207:GLU:HG3 | 1.88 | 0.55 |
| 17:DR:124:TYR:CZ | 17:DR:128:VAL:HG21 | 2.41 | 0.55 |
| 17:DR:273:PHE:CD1 | 17:DR:284:LEU:HD22 | 2.42 | 0.55 |
| 18:DS:152:VAL:HG23 | 18:DS:201:LEU:HD22 | 1.87 | 0.55 |
| 24:DY:226:ASN:C | 24:DY:227:LEU:HD12 | 2.31 | 0.55 |
| 22:Dw:134:MET:HE3 | 22:Dw:232:HIS:CD2 | 2.42 | 0.55 |
| 47:Ej:70:GLN:O | 47:Ej:75:GLN:NE2 | 2.40 | 0.55 |
| 14:DO:71:ASN:ND2 | 14:DO:212:GLN:OE1 | 2.40 | 0.55 |
| 10:Dj:163:GLU:OE2 | 10:Dj:198:ARG:NH1 | 2.39 | 0.55 |
| 18:Ds:17:ASP:O | 18:Ds:339:ASN:ND2 | 2.39 | 0.55 |
| 18:Ds:152:VAL:HG23 | 18:Ds:201:LEU:HD22 | 1.89 | 0.55 |
| 57:Ep:701:CDL:H831 | 57:Ep:701:CDL:H872 | 1.89 | 0.55 |
| 36:EK:117:ASP:O | 36:EK:121:VAL:HG13 | 2.06 | 0.55 |
| 1:Da:532:SER:OG | 1:Da:571:GLN:NE2 | 2.35 | 0.55 |
| 15:Dp:326:ASP:OD1 | 15:Dp:330:LYS:NZ | 2.37 | 0.55 |
| 16:Dq:16:LEU:O | 41:Ep:75:HIS:NE2 | 2.38 | 0.55 |
| 12:DM:84:ASN:OD1 | 12:DM:85:ALA:N | 2.40 | 0.55 |
| 15:DP:326:ASP:OD1 | 15:DP:330:LYS:NZ | 2.39 | 0.55 |
| 1:Da:123:ILE:O | 1:Da:127:VAL:HG22 | 2.06 | 0.55 |
| 13:Dn:213:ASN:OD1 | 28:Ec:182:LYS:NZ | 2.40 | 0.55 |
| 14:Do:100:GLN:NE2 | 14:Do:104:GLU:OE2 | 2.38 | 0.55 |
| 2:DB:578:THR:HG23 | 2:DB:579:PHE:CD2 | 2.42 | 0.55 |
| 11:DK:74:ILE:O | 11:DK:81:ARG:NH1 | 2.39 | 0.55 |
| 16:DQ:216:THR:O | 16:DQ:220:VAL:HG22 | 2.07 | 0.55 |
| 16:DQ:230:ASP:OD1 | 16:DQ:231:ARG:N | 2.40 | 0.55 |
| 24:DY:71:TYR:CD2 | 24:DY:195:LEU:HD23 | 2.41 | 0.55 |
| 6:Df:112:PRO:O | 43:Er:66:TRP:NE1 | 2.40 | 0.55 |
| 38:EM:46:THR:O | 23:Dx:136:GLN:NE2 | 2.39 | 0.54 |
| 47:EJ:73:ASN:OD1 | 47:EJ:108:ARG:NH2 | 2.40 | 0.54 |
| 29:Ed:92:GLU:OE1 | 57:Eg:101:CDL:O1 | 2.24 | 0.54 |
| 24:DY:118:ARG:O | 24:DY:122:THR:HG22 | 2.07 | 0.54 |
| 24:DY:141:LEU:O | 24:DY:145:ASN:ND2 | 2.39 | 0.54 |
| 17:Dr:174:TYR:O | 17:Dr:203:TYR:OH | 2.20 | 0.54 |
| 14:Do:62:SER:OG | 14:Do:214:ARG:NH2 | 2.40 | 0.54 |
| 14:Do:454:GLN:OE1 | 14:Do:454:GLN:N | 2.40 | 0.54 |
| 3:DC:84:GLU:OE1 | 20:DU:266:THR:OG1 | 2.26 | 0.54 |
| 12:DM:421:ASP:OD1 | 12:DM:430:SER:OG | 2.26 | 0.54 |
| 29:ED:21:TYR:HE1 | 34:EI:79:ILE:HD11 | 1.72 | 0.54 |
| 16:Dq:220:VAL:HG22 | 16:Dq:224:ALA:HB3 | 1.90 | 0.54 |
| 58:Eo:204:PC1:H2E2 | 58:Eo:204:PC1:H2I3 | 1.90 | 0.54 |
| 53:DL:250:THR:OG1 | 53:DL:260:ASN:ND2 | 2.40 | 0.54 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 4:DD:120:THR:HG22 | 44:ES:25:TRP:CD2 | 2.43 | 0.54 |
| 22:DW:104:SER:O | 22:DW:154:THR:OG1 | 2.26 | 0.54 |
| 47:EJ:67:LEU:O | 47:EJ:75:GLN:NE2 | 2.40 | 0.54 |
| 57:Dn:502:CDL:H832 | 57:Dn:502:CDL:H872 | 1.89 | 0.54 |
| 15:Dp:333:ARG:HB3 | 20:Du:40:THR:HG21 | 1.88 | 0.54 |
| 19:Dt:170:ASN:ND2 | 19:Dt:174:GLU:O | 2.40 | 0.54 |
| 22:Dw:141:TYR:O | 38:Em:7:ARG:NH1 | 2.39 | 0.54 |
| 38:Em:49:LYS:O | 38:Em:54:ARG:NH1 | 2.40 | 0.54 |
| 8:DH:52:ASP:O | 9:DI:123:LEU:HD12 | 2.07 | 0.54 |
| 38:EM:133:TYR:OH | 46:Eu:12:ASP:OD1 | 2.25 | 0.54 |
| 20:Du:143:ALA:HB3 | 20:Du:144:PRO:HD3 | 1.90 | 0.54 |
| 21:Dv:262:TRP:N | 57:Dv:403:CDL:OB3 | 2.40 | 0.54 |
| 23:Dx:148:GLU:OE1 | 23:Dx:148:GLU:N | 2.39 | 0.54 |
| 22:DW:134:MET:N | 22:DW:134:MET:SD | 2.81 | 0.54 |
| 41:EP:79:GLU:OE1 | 41:EP:79:GLU:N | 2.41 | 0.54 |
| 13:Dn:173:ASP:OD1 | 13:Dn:174:ASN:N | 2.40 | 0.54 |
| 50:Ey:20:HIS:NE2 | 52:Fa:32:ASN:OD1 | 2.40 | 0.54 |
| 53:Dl:194:GLY:O | 53:Dl:213:ARG:NH1 | 2.40 | 0.54 |
| 13:DN:141:TYR:CE2 | 13:DN:145:LEU:HD11 | 2.43 | 0.54 |
| 1:Da:342:THR:HG21 | 1:Da:400:PRO:HD3 | 1.89 | 0.54 |
| 20:Du:222:ILE:O | 20:Du:226:ASN:ND2 | 2.40 | 0.54 |
| 8:DH:34:TRP:O | 12:DM:428:GLN:NE2 | 2.41 | 0.54 |
| 20:DU:50:GLU:OE1 | 42:EQ:25:TYR:OH | 2.25 | 0.54 |
| 35:EV:18:LEU:HD13 | 35:EV:48:PHE:HA | 1.89 | 0.54 |
| 14:Do:325:TYR:N | 57:Do:501:CDL:OA3 | 2.41 | 0.54 |
| 16:Dq:1:AME:SD | 16:Dq:1:AME:N | 2.81 | 0.54 |
| 26:Ea:60:LEU:HD23 | 26:Ea:61:LYS:N | 2.23 | 0.54 |
| 2:DB:147:ARG:NH1 | 11:DK:35:ASP:OD1 | 2.40 | 0.54 |
| 57:EL:902:CDL:H632 | 57:EL:902:CDL:H671 | 1.90 | 0.54 |
| 10:Dj:206:GLU:OE1 | 10:Dj:206:GLU:N | 2.41 | 0.54 |
| 27:Eb:39:ASN:C | 27:Eb:40:LEU:HD12 | 2.33 | 0.54 |
| 4:DD:265:LEU:HD13 | 4:DD:271:TYR:CD2 | 2.42 | 0.53 |
| 21:DV:248:GLN:NE2 | 21:DV:259:TYR:O | 2.39 | 0.53 |
| 26:EA:60:LEU:HD23 | 26:EA:61:LYS:N | 2.23 | 0.53 |
| 38:EM:137:GLU:OE1 | 38:EM:137:GLU:N | 2.41 | 0.53 |
| 7:Dg:23:ARG:NH1 | 19:Dt:246:ASP:OD1 | 2.39 | 0.53 |
| 38:Em:137:GLU:N | 38:Em:137:GLU:OE1 | 2.41 | 0.53 |
| 58:DG:203:PC1:H3H1 | 57:Dx:1201:CDL:H473 | 1.91 | 0.53 |
| 16:DQ:9:ARG:O | 16:DQ:235:ASN:ND2 | 2.38 | 0.53 |
| 38:EM:116:GLN:O | 38:EM:119:ASN:ND2 | 2.40 | 0.53 |
| 43:ER:60:TRP:NE1 | 43:ER:64:LEU:HD11 | 2.24 | 0.53 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 51:EZ:35:VAL:HG22 | 51:EZ:36:LEU:H | 1.74 | 0.53 |
| 3:Dc:239:ILE:HD11 | 27:Eb:122:PHE:CE1 | 2.43 | 0.53 |
| 57:Dg:202:CDL:H631 | 57:Dg:202:CDL:H671 | 1.90 | 0.53 |
| 37:El:34:LYS:NZ | 37:El:50:ASP:OD1 | 2.42 | 0.53 |
| 37:El:108:ASP:OD1 | 37:El:109:ARG:N | 2.42 | 0.53 |
| 42:Eq:36:MET:O | 42:Eq:102:LYS:NZ | 2.41 | 0.53 |
| 50:Ey:1:MET:HG3 | 50:Ey:5:LEU:HD23 | 1.89 | 0.53 |
| 5:DE:126:GLU:OE1 | 5:DE:126:GLU:N | 2.41 | 0.53 |
| 16:DQ:13:ASN:ND2 | 16:DQ:24:ALA:O | 2.41 | 0.53 |
| 17:DR:168:LYS:NZ | 36:Ek:161:GLU:OE1 | 2.41 | 0.53 |
| 33:EH:12:ASP:OD1 | 33:EH:13:ARG:N | 2.39 | 0.53 |
| 37:EL:131:TRP:CH2 | 65:EL:906:UQ8:H3MB | 2.43 | 0.53 |
| 3:Dc:208:ARG:NH2 | 27:Eb:101:GLN:O | 2.41 | 0.53 |
| 17:Dr:222:ILE:HD12 | 17:Dr:236:ILE:HB | 1.90 | 0.53 |
| 23:DX:143:ARG:NH2 | 23:DX:149:GLU:OE2 | 2.39 | 0.53 |
| 1:Da:650:ILE:HG21 | 19:Dt:163:VAL:HG22 | 1.90 | 0.53 |
| 4:Dd:265:LEU:HD13 | 4:Dd:271:TYR:CD2 | 2.42 | 0.53 |
| 4:Dd:273:MET:HE2 | 4:Dd:273:MET:HA | 1.90 | 0.53 |
| 12:Dm:280:GLU:OE2 | 42:Eq:70:ASN:ND2 | 2.40 | 0.53 |
| 20:Du:254:ARG:NH2 | 20:Du:277:THR:O | 2.42 | 0.53 |
| 3:DC:126:ILE:HD12 | 25:DZ:211:GLU:O | 2.09 | 0.53 |
| 3:Dc:363:LEU:C | 3:Dc:363:LEU:HD23 | 2.34 | 0.53 |
| 8:DH:27:LYS:NZ | 13:DN:288:ASN:O | 2.41 | 0.53 |
| 16:DQ:16:LEU:O | 41:EP:75:HIS:NE2 | 2.38 | 0.53 |
| 38:EM:45:THR:HG23 | 38:EM:57:ALA:HB3 | 1.90 | 0.53 |
| 4:Dd:450:GLU:OE1 | 4:Dd:450:GLU:N | 2.41 | 0.53 |
| 53:Dl:87:THR:HG21 | 53:Dl:95:THR:HA | 1.90 | 0.53 |
| 1:DA:586:MET:SD | 1:DA:601:HIS:NE2 | 2.78 | 0.53 |
| 32:EG:4:ASP:OD1 | 32:EG:5:PHE:N | 2.40 | 0.53 |
| 3:Dc:31:ASN:ND2 | 47:Ej:61:HIS:O | 2.42 | 0.53 |
| 27:Eb:159:GLN:OE1 | 27:Eb:161:ARG:NH2 | 2.42 | 0.53 |
| 5:DE:69:GLU:OE2 | 12:DM:405:ARG:N | 2.41 | 0.53 |
| 14:DO:253:ARG:NH2 | 47:EJ:88:ASP:O | 2.40 | 0.53 |
| 5:De:53:GLU:OE1 | 29:Ed:170:TYR:OH | 2.16 | 0.53 |
| 3:DC:481:LEU:O | 3:DC:485:ASN:ND2 | 2.36 | 0.53 |
| 13:Dn:414:TYR:CE2 | 13:Dn:418:ILE:HD11 | 2.43 | 0.53 |
| 16:Dq:18:THR:OG1 | 41:Ep:79:GLU:O | 2.19 | 0.53 |
| 19:Dt:258:ASN:ND2 | 19:Dt:258:ASN:O | 2.38 | 0.53 |
| 23:Dx:47:GLN:NE2 | 34:Ei:165:ASP:OD1 | 2.42 | 0.53 |
| 14:DO:356:GLU:HB2 | 14:DO:369:VAL:HG22 | 1.91 | 0.53 |
| 16:DQ:344:ILE:O | 16:DQ:344:ILE:HG22 | 2.09 | 0.53 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 17:DR:186:ILE:O | 39:EN:119:ARG:NH2 | 2.42 | 0.53 |
| 1:Da:64:THR:HG22 | 1:Da:149:TYR:CD1 | 2.43 | 0.53 |
| 1:Da:76:ARG:NH1 | 1:Da:605:THR:OG1 | 2.42 | 0.53 |
| 22:Dw:151:PRO:HG3 | 22:Dw:233:THR:HG22 | 1.91 | 0.53 |
| 12:Dm:117:ASP:OD1 | 12:Dm:118:ARG:N | 2.42 | 0.52 |
| 29:Ed:21:TYR:HE2 | 34:Ei:79:ILE:HD11 | 1.74 | 0.52 |
| 43:Er:79:ARG:O | 43:Er:94:ARG:NH2 | 2.38 | 0.52 |
| 53:DL:248:PHE:HB2 | 53:DL:269:LEU:HD21 | 1.90 | 0.52 |
| 18:DS:62:LEU:O | 18:DS:65:THR:HG22 | 2.09 | 0.52 |
| 33:EH:85:ASN:OD1 | 33:EH:86:LEU:N | 2.42 | 0.52 |
| 57:Dh:201:CDL:H671 | 57:Dn:507:CDL:H822 | 1.91 | 0.52 |
| 53:DL:194:GLY:O | 53:DL:213:ARG:NH1 | 2.42 | 0.52 |
| 29:ED:106:ILE:HG21 | 65:ED:603:UQ8:C6 | 2.39 | 0.52 |
| 29:ED:140:ASN:OD1 | 36:EK:21:ARG:NH2 | 2.41 | 0.52 |
| 44:ES:50:ASN:OD1 | 44:ES:51:LEU:N | 2.36 | 0.52 |
| 3:Dc:370:LEU:HD13 | 5:De:82:THR:HG23 | 1.91 | 0.52 |
| 16:Dq:230:ASP:OD1 | 16:Dq:231:ARG:N | 2.41 | 0.52 |
| 17:Dr:206:ILE:HG13 | 17:Dr:209:ILE:HD12 | 1.92 | 0.52 |
| 59:Ds:403:3PE:H3E2 | 59:Ds:403:3PE:H3I3 | 1.90 | 0.52 |
| 1:DA:99:THR:HG21 | 1:DA:271:THR:HG21 | 1.91 | 0.52 |
| 3:DC:365:SER:O | 3:DC:369:ILE:HG23 | 2.09 | 0.52 |
| 3:DC:586:ILE:O | 3:DC:590:ASN:ND2 | 2.40 | 0.52 |
| 12:DM:117:ASP:OD1 | 12:DM:118:ARG:N | 2.42 | 0.52 |
| 33:EH:128:ARG:NH1 | 33:EH:131:GLN:OE1 | 2.42 | 0.52 |
| 57:Dv:402:CDL:OA5 | 57:Dv:402:CDL:O1 | 2.24 | 0.52 |
| 25:Dz:186:ILE:O | 47:Ej:32:LYS:NZ | 2.42 | 0.52 |
| 1:Da:307:THR:HA | 1:Da:310:PHE:CE2 | 2.44 | 0.52 |
| 8:Dh:121:TYR:OH | 27:Eb:72:ASP:OD1 | 2.22 | 0.52 |
| 65:Ed:202:UQ8:H45B | 36:Ek:65:PRO:HG3 | 1.91 | 0.52 |
| 57:El:902:CDL:H431 | 57:El:902:CDL:H471 | 1.91 | 0.52 |
| 45:Et:4:ARG:N | 50:Ey:1:MET:O | 2.38 | 0.52 |
| 53:Dl:99:THR:O | 53:Dl:105:ARG:NH2 | 2.41 | 0.52 |
| 53:Dl:246:ASP:OD1 | 53:Dl:247:ASN:N | 2.42 | 0.52 |
| 1:DA:307:THR:HA | 1:DA:310:PHE:CE2 | 2.45 | 0.52 |
| 8:DH:61:ASN:ND2 | 57:DH:201:CDL:OB2 | 2.42 | 0.52 |
| 13:Dn:141:TYR:CE2 | 13:Dn:145:LEU:HD11 | 2.45 | 0.52 |
| 16:Dq:159:GLU:OE2 | 16:Dq:163:GLN:NE2 | 2.41 | 0.52 |
| 22:Dw:134:MET:N | 22:Dw:134:MET:SD | 2.83 | 0.52 |
| 53:DL:98:GLU:N | 53:DL:98:GLU:OE1 | 2.42 | 0.52 |
| 2:DB:278:ASN:O | 52:FA:10:TYR:OH | 2.28 | 0.52 |
| 4:DD:435:LEU:HD21 | 4:DD:439:LYS:HE2 | 1.91 | 0.52 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 16:DQ:145:HIS:ND1 | 16:DQ:145:HIS:O | 2.43 | 0.52 |
| 16:DQ:187:ARG:O | 16:DQ:248:GLN:NE2 | 2.39 | 0.52 |
| 21:DV:115:ASP:OD1 | 21:DV:116:LEU:N | 2.42 | 0.52 |
| 28:EC:30:GLY:O | 28:EC:34:LEU:HD22 | 2.09 | 0.52 |
| 42:EQ:20:THR:OG1 | 42:EQ:24:LYS:NZ | 2.43 | 0.52 |
| 2:Db:116:ARG:NH2 | 6:Df:177:GLN:O | 2.40 | 0.52 |
| 8:Dh:128:ASP:OD1 | 8:Dh:129:ARG:N | 2.40 | 0.52 |
| 10:Dj:155:GLU:O | 10:Dj:189:ARG:NH2 | 2.40 | 0.52 |
| 59:Dj:407:3PE:H3I3 | 59:Dj:407:3PE:H3E2 | 1.92 | 0.52 |
| 14:Do:450:PRO:O | 14:Do:453:ASN:ND2 | 2.41 | 0.52 |
| 35:Ev:18:LEU:HD13 | 35:Ev:48:PHE:HA | 1.90 | 0.52 |
| 16:DQ:138:LYS:NZ | 57:DQ:1502:CDL:OB3 | 2.30 | 0.52 |
| 57:DV:401:CDL:H431 | 57:DV:401:CDL:H471 | 1.90 | 0.52 |
| 40:EO:31:TYR:CZ | 40:EO:35:LEU:HD11 | 2.44 | 0.52 |
| 2:Db:341:GLU:OE1 | 30:Ee:97:SER:N | 2.39 | 0.52 |
| 13:Dn:67:GLU:OE1 | 13:Dn:67:GLU:N | 2.40 | 0.52 |
| 18:Ds:142:LEU:HD23 | 57:Ds:405:CDL:H851 | 1.92 | 0.52 |
| 19:Dt:271:ARG:NH1 | 19:Dt:279:GLU:OE1 | 2.42 | 0.52 |
| 12:DM:72:SER:OG | 12:DM:74:ASP:OD1 | 2.24 | 0.52 |
| 14:DO:156:ASP:OD1 | 14:DO:160:ARG:NE | 2.42 | 0.52 |
| 19:DT:115:ILE:O | 19:DT:119:VAL:HG22 | 2.10 | 0.52 |
| 2:Db:231:VAL:HG21 | 49:Ex:68:LEU:HD12 | 1.92 | 0.52 |
| 8:Dh:128:ASP:OD2 | 27:Eb:51:TYR:OH | 2.25 | 0.52 |
| 4:DD:166:ASN:O | 4:DD:170:TYR:N | 2.38 | 0.52 |
| 4:DD:293:VAL:HG13 | 13:DN:271:ILE:HD13 | 1.92 | 0.52 |
| 37:EL:108:ASP:OD1 | 37:EL:109:ARG:N | 2.42 | 0.52 |
| 3:Dc:240:TRP:NE1 | 57:Dc:601:CDL:OA4 | 2.40 | 0.52 |
| 17:Dr:266:ASP:OD1 | 17:Dr:267:ASN:N | 2.43 | 0.52 |
| 30:Ee:106:GLU:N | 30:Ee:106:GLU:OE1 | 2.43 | 0.52 |
| 49:Ex:28:VAL:HG23 | 49:Ex:29:LEU:HD12 | 1.92 | 0.52 |
| 3:DC:363:LEU:HD23 | 3:DC:363:LEU:C | 2.35 | 0.51 |
| 23:DX:136:GLN:NE2 | 38:Em:46:THR:O | 2.42 | 0.51 |
| 45:ET:38:LEU:N | 45:ET:38:LEU:HD23 | 2.26 | 0.51 |
| 40:Eo:31:TYR:CE2 | 40:Eo:35:LEU:HD11 | 2.45 | 0.51 |
| 53:DL:246:ASP:OD1 | 53:DL:247:ASN:N | 2.43 | 0.51 |
| 1:DA:228:PRO:HG2 | 1:DA:231:LEU:HD12 | 1.91 | 0.51 |
| 2:DB:186:THR:HG21 | 2:DB:349:TRP:HB2 | 1.91 | 0.51 |
| 8:DH:118:PRO:HD3 | 8:DH:127:LEU:HD22 | 1.93 | 0.51 |
| 59:EO:204:3PE:H2I3 | 59:EO:204:3PE:H2E2 | 1.92 | 0.51 |
| 14:Do:204:TYR:CE2 | 14:Do:208:LEU:HD11 | 2.45 | 0.51 |
| 16:Dq:333:THR:OG1 | 16:Dq:334:GLU:N | 2.43 | 0.51 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 21:Dv:1:AME:HT22 | 21:Dv:3:TYR:CE1 | 2.46 | 0.51 |
| 12:DM:166:ASP:OD1 | 29:ED:190:TYR:OH | 2.23 | 0.51 |
| 14:DO:245:GLN:O | 14:DO:248:VAL:HG22 | 2.11 | 0.51 |
| 14:DO:454:GLN:OE1 | 14:DO:454:GLN:N | 2.43 | 0.51 |
| 38:EM:138:ARG:NH1 | 38:EM:142:LEU:HD22 | 2.24 | 0.51 |
| 53:Dl:113:ASN:O | 53:Dl:129:ASN:N | 2.41 | 0.51 |
| 3:DC:311:ARG:NE | 58:DC:605:PC1:O14 | 2.42 | 0.51 |
| 6:DF:163:ASN:ND2 | 6:DF:163:ASN:O | 2.43 | 0.51 |
| 17:DR:222:ILE:HA | 17:DR:238:THR:HG22 | 1.92 | 0.51 |
| 37:EL:13:ARG:NH2 | 43:ER:104:LYS:O | 2.41 | 0.51 |
| 13:Dn:383:PHE:CE2 | 13:Dn:387:LEU:HD11 | 2.46 | 0.51 |
| 41:Ep:79:GLU:OE1 | 41:Ep:79:GLU:N | 2.40 | 0.51 |
| 14:DO:272:GLU:OE1 | 14:DO:272:GLU:N | 2.44 | 0.51 |
| 16:DQ:1:AME:HE3 | 19:Dt:280:GLU:HG3 | 1.92 | 0.51 |
| 58:DQ:1503:PC1:O12 | 23:DX:63:TYR:OH | 2.27 | 0.51 |
| 33:EH:129:ILE:HG22 | 33:EH:137:TRP:HB2 | 1.91 | 0.51 |
| 18:Ds:62:LEU:O | 18:Ds:65:THR:HG22 | 2.09 | 0.51 |
| 12:DM:280:GLU:OE2 | 42:EQ:70:ASN:ND2 | 2.40 | 0.51 |
| 17:DR:343:GLU:HA | 31:EF:77:ILE:HD11 | 1.92 | 0.51 |
| 1:Da:477:LEU:HD11 | 1:Da:492:MET:HE1 | 1.93 | 0.51 |
| 3:Dc:148:LEU:O | 47:Ej:57:ARG:NH2 | 2.42 | 0.51 |
| 8:Dh:33:HIS:O | 8:Dh:37:GLY:N | 2.44 | 0.51 |
| 10:Dj:185:PRO:HG3 | 43:Er:64:LEU:HD13 | 1.92 | 0.51 |
| 1:Da:663:MET:HG3 | 1:Da:666:ILE:HD11 | 1.93 | 0.51 |
| 3:Dc:385:ASN:ND2 | 12:Dm:362:ASP:OD1 | 2.38 | 0.51 |
| 13:Dn:218:ILE:O | 13:Dn:218:ILE:HG22 | 2.11 | 0.51 |
| 25:Dz:105:ASN:OD1 | 25:Dz:156:GLN:NE2 | 2.43 | 0.51 |
| 6:DF:23:PHE:C | 6:DF:24:LEU:HD12 | 2.35 | 0.51 |
| 14:DO:75:GLU:OE1 | 14:DO:145:ARG:NH2 | 2.44 | 0.51 |
| 23:DX:75:TYR:OH | 58:Ef:1001:PC1:O12 | 2.22 | 0.51 |
| 26:EA:146:THR:OG1 | 57:EA:301:CDL:OB4 | 2.14 | 0.51 |
| 1:Da:335:VAL:HG21 | 1:Da:407:MET:HE2 | 1.92 | 0.51 |
| 57:Dd:705:CDL:HA61 | 13:Dn:30:LEU:HD11 | 1.93 | 0.51 |
| 13:Dn:136:PHE:CE2 | 13:Dn:140:LEU:HD11 | 2.46 | 0.51 |
| 18:Ds:13:SER:OG | 27:Eb:178:PHE:N | 2.43 | 0.51 |
| 21:DV:103:ILE:O | 21:DV:107:THR:HG22 | 2.11 | 0.51 |
| 1:Da:344:ARG:NH1 | 57:Da:709:CDL:OA4 | 2.43 | 0.51 |
| 2:Db:540:ASP:OD2 | 7:Dg:57:ARG:NH1 | 2.42 | 0.51 |
| 4:Dd:440:ALA:O | 4:Dd:543:ASN:ND2 | 2.44 | 0.51 |
| 25:Dz:70:TYR:HB3 | 25:Dz:126:ILE:HD11 | 1.91 | 0.51 |
| 57:El:902:CDL:H832 | 57:El:902:CDL:H872 | 1.93 | 0.51 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 49:Ex:16:ILE:O | 49:Ex:20:THR:HG23 | 2.11 | 0.51 |
| 7:DG:1:MET:CE | 57:Dx:1201:CDL:H472 | 2.41 | 0.51 |
| 1:Da:217:LYS:O | 1:Da:218:LEU:HD12 | 2.10 | 0.51 |
| 1:Da:293:ASP:OD2 | 1:Da:365:HIS:NE2 | 2.44 | 0.51 |
| 4:Dd:166:ASN:O | 4:Dd:170:TYR:N | 2.38 | 0.51 |
| 8:Dh:73:LEU:HD23 | 8:Dh:73:LEU:C | 2.35 | 0.51 |
| 14:Do:115:GLU:OE1 | 14:Do:115:GLU:N | 2.41 | 0.51 |
| 16:Dq:57:THR:O | 16:Dq:61:ASN:ND2 | 2.44 | 0.51 |
| 31:Ef:117:VAL:HG13 | 31:Ef:119:THR:HG22 | 1.93 | 0.51 |
| 40:Eo:12:THR:O | 40:Eo:12:THR:HG22 | 2.11 | 0.51 |
| 4:DD:410:SER:OG | 4:DD:412:ARG:NH1 | 2.44 | 0.50 |
| 17:DR:270:ASN:O | 17:DR:270:ASN:ND2 | 2.44 | 0.50 |
| 18:DS:50:GLN:OE1 | 18:DS:311:GLY:N | 2.42 | 0.50 |
| 18:DS:301:PHE:N | 57:DS:402:CDL:OA3 | 2.44 | 0.50 |
| 22:DW:229:LEU:O | 22:DW:233:THR:HG23 | 2.11 | 0.50 |
| 3:Dc:216:THR:HG23 | 25:Dz:33:LEU:HD22 | 1.93 | 0.50 |
| 12:Dm:106:GLN:NE2 | 12:Dm:161:GLU:O | 2.44 | 0.50 |
| 12:Dm:341:VAL:HG21 | 57:Du:402:CDL:H271 | 1.93 | 0.50 |
| 15:Dp:197:ARG:O | 15:Dp:198:ARG:NH1 | 2.44 | 0.50 |
| 20:Du:117:GLN:NE2 | 20:Du:121:ASN:OD1 | 2.43 | 0.50 |
| 53:Dl:101:SER:OG | 53:Dl:105:ARG:NE | 2.44 | 0.50 |
| 57:DH:201:CDL:H671 | 57:DN:504:CDL:H822 | 1.92 | 0.50 |
| 16:DQ:110:TYR:CE1 | 16:DQ:172:LEU:HD23 | 2.47 | 0.50 |
| 1:Da:108:PHE:CE2 | 1:Da:152:LEU:HD12 | 2.46 | 0.50 |
| 5:De:8:ARG:NH1 | 16:Dq:218:ASP:OD1 | 2.44 | 0.50 |
| 14:Do:71:ASN:ND2 | 14:Do:212:GLN:OE1 | 2.43 | 0.50 |
| 17:Dr:341:ALA:O | 31:Ef:77:ILE:HD12 | 2.11 | 0.50 |
| 19:Dt:84:ASP:OD1 | 19:Dt:85:GLY:N | 2.44 | 0.50 |
| 29:Ed:179:ASP:OD2 | 44:Es:3:ARG:NH1 | 2.43 | 0.50 |
| 53:DL:182:THR:OG1 | 53:DL:184:ASN:OD1 | 2.24 | 0.50 |
| 7:DG:75:GLU:HG3 | 35:EV:46:VAL:HG13 | 1.92 | 0.50 |
| 15:DP:126:THR:HG23 | 15:DP:386:TYR:HD1 | 1.75 | 0.50 |
| 1:Da:525:ALA:HB2 | 1:Da:578:LEU:HB2 | 1.92 | 0.50 |
| 9:Di:231:GLN:N | 9:Di:231:GLN:OE1 | 2.45 | 0.50 |
| 20:Du:174:ASP:OD2 | 20:Du:214:LYS:NZ | 2.43 | 0.50 |
| 33:Eh:46:LEU:HA | 33:Eh:110:LEU:HD13 | 1.92 | 0.50 |
| 39:En:146:ASN:HB2 | 65:En:1203:UQ8:H4M | 1.92 | 0.50 |
| 3:DC:239:ILE:HD11 | 27:EB:122:PHE:CE1 | 2.46 | 0.50 |
| 11:DK:12:SER:OG | 31:EF:188:THR:O | 2.17 | 0.50 |
| 17:DR:266:ASP:OD1 | 17:DR:267:ASN:N | 2.44 | 0.50 |
| 23:DX:47:GLN:NE2 | 34:EI:165:ASP:OD1 | 2.45 | 0.50 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 45:ET:73:VAL:HG11 | 50:EY:10:ALA:HA | 1.92 | 0.50 |
| 2:Db:45:TRP:CE2 | 65:En:1203:UQ8:H3MA | 2.46 | 0.50 |
| 39:En:86:HIS:NE2 | 39:En:91:ASN:OD1 | 2.41 | 0.50 |
| 16:DQ:248:GLN:N | 16:DQ:248:GLN:OE1 | 2.44 | 0.50 |
| 18:DS:136:LYS:O | 18:DS:139:THR:OG1 | 2.30 | 0.50 |
| 19:DT:134:GLY:C | 19:DT:135:LEU:HD12 | 2.37 | 0.50 |
| 21:DV:81:GLY:O | 21:DV:143:ASN:ND2 | 2.44 | 0.50 |
| 3:Dc:190:LEU:HD11 | 25:Dz:170:LEU:HD11 | 1.92 | 0.50 |
| 15:Dp:197:ARG:NE | 15:Dp:204:GLU:OE2 | 2.44 | 0.50 |
| 18:Ds:170:GLU:OE1 | 18:Ds:170:GLU:N | 2.40 | 0.50 |
| 45:Et:36:ASN:O | 45:Et:39:ARG:NH1 | 2.44 | 0.50 |
| 53:Dl:169:LYS:N | 53:Dl:181:VAL:O | 2.43 | 0.50 |
| 2:DB:116:ARG:NH2 | 6:DF:177:GLN:O | 2.42 | 0.50 |
| 9:DI:231:GLN:OE1 | 9:DI:231:GLN:N | 2.44 | 0.50 |
| 18:DS:342:GLU:N | 18:DS:342:GLU:OE1 | 2.44 | 0.50 |
| 33:EH:15:ASP:O | 33:EH:147:LYS:NZ | 2.44 | 0.50 |
| 41:EP:48:ARG:NH2 | 41:EP:127:LEU:OXT | 2.42 | 0.50 |
| 1:Da:641:ARG:NE | 4:Dd:174:GLU:OE2 | 2.44 | 0.50 |
| 16:Dq:103:ASN:ND2 | 16:Dq:142:ASP:OD1 | 2.44 | 0.50 |
| 26:EA:52:ILE:HG22 | 26:EA:56:TYR:CE2 | 2.47 | 0.50 |
| 37:EL:114:MET:CE | 44:ES:68:ILE:HD12 | 2.42 | 0.50 |
| 47:EJ:142:ARG:NH2 | 47:EJ:149:GLU:OE2 | 2.43 | 0.50 |
| 2:Db:200:GLN:OE1 | 2:Db:208:GLN:NE2 | 2.45 | 0.50 |
| 3:Dc:456:HIS:ND1 | 3:Dc:495:MET:SD | 2.81 | 0.50 |
| 10:Dj:204:GLU:OE1 | 10:Dj:206:GLU:N | 2.43 | 0.50 |
| 12:Dm:347:TYR:CE2 | 57:Du:401:CDL:H873 | 2.47 | 0.50 |
| 19:Dt:115:ILE:O | 19:Dt:119:VAL:HG22 | 2.11 | 0.50 |
| 21:Dv:58:GLY:C | 21:Dv:59:ILE:HD12 | 2.37 | 0.50 |
| 53:DL:189:SER:OG | 53:DL:225:ARG:NH1 | 2.44 | 0.50 |
| 13:DN:423:ILE:O | 13:DN:423:ILE:HG22 | 2.12 | 0.50 |
| 1:Da:51:LYS:NZ | 19:Dt:205:HIS:O | 2.27 | 0.50 |
| 57:Dd:702:CDL:H231 | 57:Dd:702:CDL:H272 | 1.94 | 0.50 |
| 17:Dr:343:GLU:HA | 31:Ef:77:ILE:HD11 | 1.93 | 0.50 |
| 25:Dz:175:ALA:O | 25:Dz:179:ASN:ND2 | 2.43 | 0.50 |
| 29:Ed:170:TYR:O | 29:Ed:174:ARG:NH1 | 2.44 | 0.50 |
| 3:DC:361:LYS:NZ | 12:DM:317:ASP:OD2 | 2.43 | 0.50 |
| 13:DN:213:ASN:OD1 | 28:EC:182:LYS:NZ | 2.40 | 0.50 |
| 5:De:56:ASN:O | 5:De:60:VAL:N | 2.44 | 0.50 |
| 26:Ea:37:ARG:NH2 | 26:Ea:204:LEU:O | 2.43 | 0.50 |
| 28:Ec:197:LEU:HD11 | 28:Ec:206:LEU:HG | 1.93 | 0.50 |
| 43:Er:27:ASN:ND2 | 43:Er:84:MET:O | 2.41 | 0.50 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:DB:182:SER:O | 2:DB:186:THR:HG22 | 2.11 | 0.49 |
| 3:DC:240:TRP:NE1 | 57:DC:601:CDL:OA4 | 2.41 | 0.49 |
| 15:DP:126:THR:HG22 | 15:DP:386:TYR:O | 2.12 | 0.49 |
| 39:EN:110:PHE:CD2 | 39:EN:144:LEU:HD13 | 2.47 | 0.49 |
| 1:Da:155:ILE:HG21 | 1:Da:295:LEU:HD11 | 1.93 | 0.49 |
| 34:Ei:79:ILE:O | 34:Ei:82:VAL:HG12 | 2.11 | 0.49 |
| 37:El:114:MET:CE | 44:Es:68:ILE:HD12 | 2.41 | 0.49 |
| 53:DL:285:TYR:CE2 | 53:DL:289:LEU:HD11 | 2.46 | 0.49 |
| 1:DA:287:THR:O | 1:DA:364:ARG:NH2 | 2.43 | 0.49 |
| 1:DA:342:THR:HG21 | 1:DA:400:PRO:HD3 | 1.94 | 0.49 |
| 10:DJ:111:VAL:HG21 | 58:EO:201:PC1:H2A1 | 1.94 | 0.49 |
| 26:EA:69:PHE:CE2 | 26:EA:73:LEU:HD11 | 2.47 | 0.49 |
| 41:EP:112:ASP:OD1 | 41:EP:115:THR:OG1 | 2.26 | 0.49 |
| 2:Db:147:ARG:NH1 | 11:Dk:35:ASP:OD1 | 2.43 | 0.49 |
| 11:Dk:68:PRO:HG3 | 30:Ee:72:ILE:HD13 | 1.95 | 0.49 |
| 40:Eo:40:TYR:OH | 58:Eo:204:PC1:O32 | 2.19 | 0.49 |
| 1:DA:155:ILE:HD13 | 1:DA:295:LEU:HD11 | 1.94 | 0.49 |
| 21:DV:58:GLY:C | 21:DV:59:ILE:HD12 | 2.37 | 0.49 |
| 26:EA:31:ILE:HD13 | 26:EA:200:TYR:CE2 | 2.47 | 0.49 |
| 27:EB:55:THR:O | 27:EB:55:THR:HG22 | 2.12 | 0.49 |
| 13:Dn:420:ASN:OD1 | 13:Dn:421:THR:N | 2.46 | 0.49 |
| 18:Ds:107:ASP:OD1 | 18:Ds:111:ARG:NE | 2.46 | 0.49 |
| 2:DB:391:LEU:HG | 30:EE:116:LEU:HD22 | 1.94 | 0.49 |
| 3:DC:582:ARG:HD2 | 42:EQ:1:AME:HG2 | 1.94 | 0.49 |
| 23:DX:114:ASP:OD2 | 57:DX:307:CDL:O1 | 2.30 | 0.49 |
| 28:EC:197:LEU:HD11 | 28:EC:206:LEU:HG | 1.94 | 0.49 |
| 59:EM:901:3PE:H2I2 | 59:Dx:1205:3PE:H2E1 | 1.94 | 0.49 |
| 45:ET:70:TYR:OH | 50:EY:11:THR:OG1 | 2.21 | 0.49 |
| 1:Da:380:ILE:HD12 | 1:Da:445:VAL:CG1 | 2.42 | 0.49 |
| 3:Dc:501:TYR:N | 3:Dc:502:PRO:CD | 2.75 | 0.49 |
| 3:Dc:586:ILE:O | 3:Dc:590:ASN:ND2 | 2.43 | 0.49 |
| 6:Df:23:PHE:C | 6:Df:24:LEU:HD12 | 2.38 | 0.49 |
| 8:Dh:106:ASP:O | 8:Dh:129:ARG:NH2 | 2.42 | 0.49 |
| 17:Dr:290:ASN:OD1 | 17:Dr:299:GLN:NE2 | 2.43 | 0.49 |
| 19:Dt:119:VAL:HG11 | 19:Dt:145:TYR:HA | 1.94 | 0.49 |
| 20:Du:257:VAL:O | 20:Du:257:VAL:HG12 | 2.11 | 0.49 |
| 51:Ez:8:GLU:N | 51:Ez:8:GLU:OE1 | 2.45 | 0.49 |
| 2:DB:122:TRP:CD1 | 2:DB:553:CYS:HG | 2.29 | 0.49 |
| 3:DC:370:LEU:HD13 | 5:DE:82:THR:HG23 | 1.95 | 0.49 |
| 3:DC:501:TYR:N | 3:DC:502:PRO:CD | 2.75 | 0.49 |
| 1:Da:353:LEU:O | 1:Da:357:VAL:HG23 | 2.13 | 0.49 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 12:Dm:118:ARG:NH1 | 16:Dq:315:GLU:OE2 | 2.42 | 0.49 |
| 13:Dn:218:ILE:HD12 | 13:Dn:218:ILE:N | 2.28 | 0.49 |
| 17:Dr:124:TYR:CZ | 17:Dr:128:VAL:HG21 | 2.48 | 0.49 |
| 17:Dr:185:TRP:O | 39:En:119:ARG:NH2 | 2.41 | 0.49 |
| 4:DD:291:ARG:NH1 | 13:DN:252:ASN:OD1 | 2.46 | 0.49 |
| 10:DJ:170:ASP:OD1 | 10:DJ:174:ASN:ND2 | 2.46 | 0.49 |
| 23:DX:141:LEU:N | 34:EI:152:GLU:OE2 | 2.44 | 0.49 |
| 1:Da:91:SER:OG | 1:Da:591:HIS:NE2 | 2.45 | 0.49 |
| 25:Dz:210:LEU:HD23 | 25:Dz:226:ARG:CA | 2.42 | 0.49 |
| 1:DA:353:LEU:HD22 | 1:DA:389:PHE:CZ | 2.47 | 0.49 |
| 4:DD:435:LEU:HD22 | 4:DD:528:VAL:HG11 | 1.94 | 0.49 |
| 10:DJ:51:ARG:NH1 | 57:DJ:303:CDL:OB3 | 2.44 | 0.49 |
| 10:DJ:94:GLN:OE1 | 10:DJ:94:GLN:N | 2.46 | 0.49 |
| 16:DQ:110:TYR:OH | 16:DQ:147:PHE:O | 2.29 | 0.49 |
| 45:ET:38:LEU:HD23 | 45:ET:38:LEU:H | 1.78 | 0.49 |
| 47:Ej:31:LEU:O | 47:Ej:175:HIS:NE2 | 2.44 | 0.49 |
| 4:DD:451:THR:HG22 | 4:DD:452:SER:H | 1.78 | 0.49 |
| 57:DH:201:CDL:H673 | 57:EB:304:CDL:CB5 | 2.42 | 0.49 |
| 14:DO:48:ASN:ND2 | 14:DO:48:ASN:O | 2.46 | 0.49 |
| 14:DO:299:LEU:O | 14:DO:345:ASN:ND2 | 2.42 | 0.49 |
| 1:Da:128:GLY:HA3 | 1:Da:322:MET:HE2 | 1.93 | 0.49 |
| 20:Du:35:THR:O | 20:Du:35:THR:HG22 | 2.12 | 0.49 |
| 27:Eb:55:THR:HG22 | 27:Eb:55:THR:O | 2.13 | 0.49 |
| 1:DA:217:LYS:O | 1:DA:218:LEU:HD12 | 2.13 | 0.49 |
| 1:DA:525:ALA:HB2 | 1:DA:578:LEU:HB2 | 1.95 | 0.49 |
| 1:Da:338:SER:HB2 | 1:Da:399:ILE:HG22 | 1.93 | 0.49 |
| 3:Dc:176:ILE:O | 25:Dz:141:GLN:NE2 | 2.46 | 0.49 |
| 24:Dy:64:SER:OG | 24:Dy:189:ASN:OD1 | 2.22 | 0.49 |
| 28:Ec:30:GLY:O | 28:Ec:34:LEU:HD22 | 2.13 | 0.49 |
| 33:Eh:156:GLN:OE1 | 33:Eh:156:GLN:N | 2.46 | 0.49 |
| 37:El:42:ARG:NE | 43:Er:21:GLU:OE2 | 2.38 | 0.49 |
| 7:DG:40:TYR:CZ | 7:DG:44:ILE:HD11 | 2.48 | 0.49 |
| 15:DP:300:ARG:NH1 | 15:DP:346:GLU:OE1 | 2.40 | 0.49 |
| 25:DZ:175:ALA:O | 25:DZ:179:ASN:ND2 | 2.43 | 0.49 |
| 57:Dj:403:CDL:HB61 | 44:Es:63:THR:HG21 | 1.94 | 0.49 |
| 13:Dn:423:ILE:O | 13:Dn:423:ILE:HG22 | 2.13 | 0.49 |
| 53:DL:263:THR:O | 53:DL:268:SER:OG | 2.31 | 0.49 |
| 36:EK:61:ARG:O | 36:EK:64:ILE:HG22 | 2.13 | 0.48 |
| 49:EX:16:ILE:O | 49:EX:20:THR:HG23 | 2.13 | 0.48 |
| 3:Dc:386:LYS:O | 3:Dc:389:THR:HG22 | 2.13 | 0.48 |
| 17:Dr:270:ASN:ND2 | 17:Dr:270:ASN:O | 2.46 | 0.48 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:DB:23:ARG:NH2 | 35:EV:2:GLU:OE2 | 2.46 | 0.48 |
| 2:DB:201:LEU:HD13 | 20:DU:55:ASN:HB2 | 1.93 | 0.48 |
| 8:DH:58:GLU:OE2 | 8:DH:75:TYR:OH | 2.29 | 0.48 |
| 24:DY:60:ASP:OD2 | 24:DY:150:TYR:OH | 2.28 | 0.48 |
| 33:EH:23:TYR:CZ | 33:EH:27:LEU:HD11 | 2.48 | 0.48 |
| 3:Dc:78:LEU:HD23 | 3:Dc:79:ASP:N | 2.27 | 0.48 |
| 13:Dn:192:ILE:HD11 | 36:Ek:46:VAL:HG11 | 1.95 | 0.48 |
| 16:Dq:117:THR:HG22 | 16:Dq:118:ILE:H | 1.78 | 0.48 |
| 21:Dv:93:LEU:O | 21:Dv:97:ASN:ND2 | 2.42 | 0.48 |
| 21:Dv:115:ASP:OD1 | 21:Dv:116:LEU:N | 2.46 | 0.48 |
| 1:DA:140:ILE:HA | 13:DN:320:CYS:SG | 2.52 | 0.48 |
| 2:DB:287:ASN:O | 2:DB:290:LEU:N | 2.46 | 0.48 |
| 13:DN:420:ASN:OD1 | 13:DN:421:THR:N | 2.46 | 0.48 |
| 19:DT:253:ASP:OD1 | 19:DT:254:GLU:N | 2.45 | 0.48 |
| 17:Dr:144:ILE:HD12 | 17:Dr:144:ILE:N | 2.28 | 0.48 |
| 18:Ds:185:ILE:HG21 | 18:Ds:194:LEU:HD21 | 1.95 | 0.48 |
| 19:Dt:134:GLY:C | 19:Dt:135:LEU:HD12 | 2.38 | 0.48 |
| 36:Ek:150:TYR:N | 57:Ek:201:CDL:OA4 | 2.44 | 0.48 |
| 1:DA:532:SER:OG | 1:DA:571:GLN:NE2 | 2.38 | 0.48 |
| 2:DB:569:PHE:CD2 | 6:DF:108:ILE:HG21 | 2.49 | 0.48 |
| 59:DR:401:3PE:O12 | 36:Ek:116:TYR:OH | 2.28 | 0.48 |
| 29:ED:114:TYR:HD2 | 65:ED:603:UQ8:H4M | 1.76 | 0.48 |
| 42:EQ:1:AME:O | 42:EQ:1:AME:HG1 | 2.13 | 0.48 |
| 2:Db:391:LEU:HG | 30:Ee:116:LEU:HD22 | 1.95 | 0.48 |
| 4:Dd:502:TYR:CE1 | 4:Dd:506:LEU:HD21 | 2.47 | 0.48 |
| 19:Dt:223:ASP:OD1 | 40:Eo:2:VAL:HG23 | 2.14 | 0.48 |
| 25:Dz:76:ASN:HA | 25:Dz:93:VAL:HG22 | 1.95 | 0.48 |
| 28:Ec:7:GLU:O | 28:Ec:11:LEU:HD13 | 2.12 | 0.48 |
| 28:Ec:131:ASP:OD2 | 28:Ec:141:ARG:NH2 | 2.44 | 0.48 |
| 57:El:903:CDL:H872 | 57:El:903:CDL:H831 | 1.95 | 0.48 |
| 1:DA:134:TYR:OH | 3:DC:312:THR:HG22 | 2.14 | 0.48 |
| 3:DC:512:LEU:HD21 | 59:DC:606:3PE:H272 | 1.95 | 0.48 |
| 17:DR:144:ILE:HD12 | 17:DR:144:ILE:N | 2.28 | 0.48 |
| 17:DR:206:ILE:HG13 | 17:DR:209:ILE:HD12 | 1.94 | 0.48 |
| 20:DU:24:HIS:NE2 | 20:DU:52:ASP:OD2 | 2.44 | 0.48 |
| 31:EF:20:GLU:OE1 | 31:EF:20:GLU:N | 2.43 | 0.48 |
| 39:EN:86:HIS:NE2 | 39:EN:91:ASN:OD1 | 2.42 | 0.48 |
| 2:Db:161:ASP:OD1 | 6:Df:164:TYR:OH | 2.31 | 0.48 |
| 11:Dk:54:ARG:NH2 | 35:Ev:33:ASP:O | 2.46 | 0.48 |
| 16:Dq:118:ILE:HD11 | 57:Dx:1203:CDL:H732 | 1.96 | 0.48 |
| 19:Dt:83:TYR:N | 31:Ef:59:ILE:O | 2.45 | 0.48 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 33:Eh:23:TYR:CZ | 33:Eh:27:LEU:HD11 | 2.48 | 0.48 |
| 1:DA:108:PHE:CE2 | 1:DA:152:LEU:HD12 | 2.49 | 0.48 |
| 1:DA:335:VAL:HG21 | 1:DA:407:MET:HE2 | 1.96 | 0.48 |
| 1:DA:338:SER:HB2 | 1:DA:399:ILE:HG22 | 1.95 | 0.48 |
| 18:DS:142:LEU:HD23 | 57:DS:405:CDL:H851 | 1.94 | 0.48 |
| 2:Db:478:GLU:OE2 | 18:Ds:228:ARG:NE | 2.39 | 0.48 |
| 23:Dx:84:PHE:CE2 | 23:Dx:88:LEU:HD11 | 2.49 | 0.48 |
| 3:DC:470:ARG:NH1 | 3:DC:473:GLU:OE2 | 2.47 | 0.48 |
| 8:DH:72:TYR:OH | 25:DZ:39:GLY:O | 2.16 | 0.48 |
| 17:DR:297:THR:OG1 | 39:EN:78:GLU:OE1 | 2.29 | 0.48 |
| 19:DT:243:ILE:HG21 | 31:EF:79:MET:SD | 2.54 | 0.48 |
| 36:EK:161:GLU:OE1 | 17:Dr:168:LYS:NZ | 2.46 | 0.48 |
| 1:Da:99:THR:HG21 | 1:Da:271:THR:HG21 | 1.95 | 0.48 |
| 5:De:43:ARG:NE | 5:De:62:GLU:OE1 | 2.41 | 0.48 |
| 15:Dp:126:THR:HG22 | 15:Dp:386:TYR:O | 2.12 | 0.48 |
| 17:Dr:176:ALA:O | 38:Em:81:ASN:ND2 | 2.41 | 0.48 |
| 17:Dr:225:MET:HE2 | 17:Dr:320:ILE:HG21 | 1.96 | 0.48 |
| 20:Du:124:ILE:HD12 | 20:Du:124:ILE:N | 2.29 | 0.48 |
| 24:Dy:71:TYR:CE1 | 24:Dy:81:LEU:HD11 | 2.49 | 0.48 |
| 2:DB:69:THR:HG22 | 2:DB:69:THR:O | 2.14 | 0.48 |
| 28:EC:7:GLU:O | 28:EC:11:LEU:HD13 | 2.14 | 0.48 |
| 33:EH:36:SER:OG | 33:EH:121:ASP:OD2 | 2.19 | 0.48 |
| 42:EQ:68:VAL:HG12 | 42:EQ:76:ARG:HG3 | 1.96 | 0.48 |
| 43:ER:60:TRP:CE2 | 43:ER:64:LEU:HD11 | 2.48 | 0.48 |
| 57:Da:709:CDL:C16 | 10:Dj:109:THR:HG21 | 2.43 | 0.48 |
| 8:Dh:82:PHE:CE2 | 8:Dh:86:LEU:HD11 | 2.49 | 0.48 |
| 18:Ds:256:TRP:O | 18:Ds:259:THR:HG22 | 2.14 | 0.48 |
| 21:Dv:59:ILE:HD13 | 21:Dv:280:VAL:HG13 | 1.96 | 0.48 |
| 25:Dz:41:ASN:O | 25:Dz:43:ASN:ND2 | 2.47 | 0.48 |
| 53:Dl:285:TYR:CE2 | 53:Dl:289:LEU:HD11 | 2.49 | 0.48 |
| 3:DC:48:LEU:O | 3:DC:49:ASN:CB | 2.62 | 0.48 |
| 4:DD:219:GLU:OE1 | 4:DD:220:MET:N | 2.46 | 0.48 |
| 10:DJ:204:GLU:OE1 | 10:DJ:206:GLU:N | 2.46 | 0.48 |
| 19:DT:284:ASN:OD1 | 19:DT:285:GLU:N | 2.47 | 0.48 |
| 25:DZ:186:ILE:O | 47:EJ:32:LYS:NZ | 2.46 | 0.48 |
| 59:EM:901:3PE:H2I2 | 59:Dx:1205:3PE:C2E | 2.44 | 0.48 |
| 4:Dd:230:VAL:O | 33:Eh:84:ARG:NH2 | 2.46 | 0.48 |
| 22:Dw:229:LEU:O | 22:Dw:233:THR:HG23 | 2.14 | 0.48 |
| 53:Dl:271:ASN:ND2 | 53:Dl:273:SER:OG | 2.47 | 0.48 |
| 3:DC:106:VAL:HG21 | 20:DU:248:LEU:CD2 | 2.44 | 0.48 |
| 9:DI:140:PRO:O | 9:DI:143:GLN:NE2 | 2.46 | 0.48 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:Dc:239:ILE:HD13 | 57:Dh:202:CDL:H221 | 1.96 | 0.48 |
| 29:Ed:100:PHE:CE2 | 29:Ed:104:LEU:HD11 | 2.49 | 0.48 |
| 37:El:140:ASP:OD2 | 37:El:144:GLU:N | 2.47 | 0.48 |
| 41:Ep:112:ASP:OD1 | 41:Ep:115:THR:OG1 | 2.19 | 0.48 |
| 2:DB:44:ILE:HD11 | 2:DB:85:ILE:HD13 | 1.95 | 0.47 |
| 3:DC:252:LEU:HD23 | 12:DM:298:TYR:CZ | 2.49 | 0.47 |
| 7:DG:54:PHE:O | 7:DG:58:ASN:ND2 | 2.45 | 0.47 |
| 16:DQ:333:THR:OG1 | 16:DQ:334:GLU:N | 2.44 | 0.47 |
| 29:ED:33:MET:HE2 | 34:EI:67:THR:CG2 | 2.44 | 0.47 |
| 10:Dj:31:GLU:OE1 | 10:Dj:31:GLU:N | 2.45 | 0.47 |
| 14:Do:139:ILE:CG2 | 14:Do:144:LEU:HD11 | 2.44 | 0.47 |
| 15:Dp:225:GLN:N | 15:Dp:225:GLN:OE1 | 2.47 | 0.47 |
| 20:Du:88:VAL:HG11 | 20:Du:288:PHE:CD1 | 2.49 | 0.47 |
| 1:DA:92:LEU:HD22 | 1:DA:270:THR:HB | 1.95 | 0.47 |
| 10:DJ:185:PRO:HG3 | 43:ER:64:LEU:HD13 | 1.96 | 0.47 |
| 59:DX:304:3PE:H3I3 | 59:DX:304:3PE:H3E2 | 1.96 | 0.47 |
| 14:Do:156:ASP:OD1 | 14:Do:160:ARG:NE | 2.47 | 0.47 |
| 19:Dt:48:GLU:OE1 | 19:Dt:48:GLU:N | 2.44 | 0.47 |
| 22:Dw:110:THR:OG1 | 22:Dw:113:ASN:OD1 | 2.33 | 0.47 |
| 16:DQ:1:AME:N | 16:DQ:1:AME:SD | 2.87 | 0.47 |
| 20:DU:123:GLY:C | 20:DU:124:ILE:HD12 | 2.40 | 0.47 |
| 43:ER:5:ALA:HB1 | 23:Dx:251:LEU:HD22 | 1.96 | 0.47 |
| 8:Dh:61:ASN:ND2 | 57:Dh:201:CDL:OB2 | 2.47 | 0.47 |
| 22:Dw:271:GLU:OE1 | 22:Dw:271:GLU:N | 2.42 | 0.47 |
| 40:Eo:31:TYR:CZ | 40:Eo:35:LEU:HD11 | 2.49 | 0.47 |
| 1:DA:450:ARG:CZ | 10:DJ:119:VAL:HG22 | 2.45 | 0.47 |
| 4:DD:325:LEU:HD13 | 4:DD:403:ASP:HB2 | 1.96 | 0.47 |
| 4:DD:450:GLU:OE1 | 4:DD:450:GLU:N | 2.48 | 0.47 |
| 12:DM:46:THR:HG21 | 12:DM:107:ARG:CG | 2.44 | 0.47 |
| 12:DM:451:GLN:O | 12:DM:454:ASN:ND2 | 2.47 | 0.47 |
| 15:DP:126:THR:HG21 | 15:DP:389:THR:HB | 1.97 | 0.47 |
| 1:Da:94:TYR:OH | 54:Da:701:HEA:O1A | 2.19 | 0.47 |
| 1:Da:562:MET:SD | 65:Ds:404:UQ8:H25A | 2.55 | 0.47 |
| 13:Dn:207:ILE:HD12 | 13:Dn:207:ILE:N | 2.29 | 0.47 |
| 14:Do:357:LEU:HD21 | 14:Do:366:VAL:HG13 | 1.97 | 0.47 |
| 26:Ea:69:PHE:CE2 | 26:Ea:73:LEU:HD11 | 2.49 | 0.47 |
| 28:Ec:180:ASN:O | 28:Ec:185:ARG:NH1 | 2.48 | 0.47 |
| 36:Ek:120:LEU:O | 36:Ek:120:LEU:HD23 | 2.14 | 0.47 |
| 10:DJ:103:SER:OG | 58:EO:201:PC1:O12 | 2.32 | 0.47 |
| 13:DN:218:ILE:O | 13:DN:218:ILE:HG22 | 2.14 | 0.47 |
| 1:Da:140:ILE:HA | 13:Dn:320:CYS:SG | 2.54 | 0.47 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 18:Ds:1:AME:HT22 | 18:Ds:3:PHE:O | 2.15 | 0.47 |
| 43:Er:60:TRP:CE2 | 43:Er:64:LEU:HD11 | 2.49 | 0.47 |
| 1:DA:380:ILE:HG23 | 1:DA:445:VAL:HG11 | 1.97 | 0.47 |
| 6:DF:112:PRO:O | 43:ER:66:TRP:NE1 | 2.48 | 0.47 |
| 13:DN:81:TYR:O | 13:DN:85:VAL:HG23 | 2.15 | 0.47 |
| 20:DU:257:VAL:O | 20:DU:257:VAL:HG12 | 2.15 | 0.47 |
| 22:DW:110:THR:OG1 | 22:DW:113:ASN:OD1 | 2.32 | 0.47 |
| 29:ED:69:PHE:CE2 | 29:ED:73:LEU:HD11 | 2.49 | 0.47 |
| 10:Dj:208:GLU:OE1 | 10:Dj:208:GLU:N | 2.47 | 0.47 |
| 36:Ek:61:ARG:NH1 | 36:Ek:73:GLU:OE2 | 2.48 | 0.47 |
| 50:Ey:59:LEU:O | 50:Ey:64:LYS:NZ | 2.46 | 0.47 |
| 2:DB:516:TRP:CD1 | 2:DB:562:ILE:HD13 | 2.49 | 0.47 |
| 4:DD:186:GLN:OE1 | 19:DT:181:ASN:ND2 | 2.44 | 0.47 |
| 4:DD:502:TYR:CZ | 4:DD:506:LEU:HD21 | 2.49 | 0.47 |
| 11:DK:19:THR:O | 11:DK:19:THR:HG22 | 2.15 | 0.47 |
| 16:DQ:79:THR:O | 16:DQ:171:GLY:N | 2.44 | 0.47 |
| 19:DT:119:VAL:HG11 | 19:DT:145:TYR:HA | 1.95 | 0.47 |
| 23:DX:62:LEU:HD11 | 23:DX:94:VAL:CG2 | 2.45 | 0.47 |
| 47:EJ:75:GLN:OE1 | 47:EJ:105:GLN:NE2 | 2.48 | 0.47 |
| 2:Db:434:ASP:OD2 | 2:Db:439:THR:OG1 | 2.22 | 0.47 |
| 3:Dc:126:ILE:HD12 | 25:Dz:211:GLU:O | 2.15 | 0.47 |
| 16:Dq:34:THR:OG1 | 16:Dq:51:GLY:O | 2.31 | 0.47 |
| 17:Dr:145:GLU:OE2 | 17:Dr:334:ASN:ND2 | 2.45 | 0.47 |
| 19:Dt:249:ASN:ND2 | 31:Ef:77:ILE:HD13 | 2.30 | 0.47 |
| 32:Eg:80:ARG:NH2 | 33:Eh:1:AME:HB2 | 2.30 | 0.47 |
| 42:Eq:1:AME:HB1 | 42:Eq:107:TYR:OH | 2.14 | 0.47 |
| 47:Ej:141:TYR:HA | 47:Ej:144:THR:HG22 | 1.97 | 0.47 |
| 14:DO:76:GLN:NE2 | 14:DO:145:ARG:O | 2.48 | 0.47 |
| 19:DT:84:ASP:OD1 | 19:DT:85:GLY:N | 2.48 | 0.47 |
| 4:Dd:358:ARG:NH2 | 4:Dd:386:GLU:OE1 | 2.48 | 0.47 |
| 18:Ds:10:ARG:NH2 | 21:Dv:203:ASP:OD2 | 2.40 | 0.47 |
| 28:Ec:71:LEU:HD13 | 28:Ec:79:LEU:HD12 | 1.95 | 0.47 |
| 53:Dl:88:TRP:NE1 | 53:Dl:423:PHE:O | 2.42 | 0.47 |
| 3:DC:389:THR:HG23 | 3:DC:390:ILE:N | 2.30 | 0.47 |
| 10:DJ:155:GLU:O | 10:DJ:189:ARG:NH2 | 2.47 | 0.47 |
| 25:DZ:119:LEU:HD22 | 25:DZ:146:THR:HB | 1.97 | 0.47 |
| 38:EM:138:ARG:HH12 | 38:EM:142:LEU:HD22 | 1.80 | 0.47 |
| 2:Db:398:SER:OG | 30:Ee:98:ASP:OD2 | 2.25 | 0.47 |
| 2:Db:532:SER:O | 2:Db:534:HIS:ND1 | 2.46 | 0.47 |
| 8:Dh:81:LEU:HB2 | 13:Dn:325:ILE:HD13 | 1.96 | 0.47 |
| 16:Dq:145:HIS:ND1 | 16:Dq:145:HIS:O | 2.48 | 0.47 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 29:Ed:69:PHE:CE2 | 29:Ed:73:LEU:HD11 | 2.50 | 0.47 |
| 3:DC:592:TYR:OH | 42:EQ:21:ARG:NH2 | 2.47 | 0.47 |
| 17:DR:341:ALA:O | 31:EF:77:ILE:HD12 | 2.14 | 0.47 |
| 51:EZ:35:VAL:HG22 | 51:EZ:36:LEU:N | 2.30 | 0.47 |
| 4:Dd:120:THR:HG22 | 44:Es:25:TRP:CD2 | 2.50 | 0.47 |
| 4:Dd:120:THR:HG22 | 44:Es:25:TRP:CE3 | 2.50 | 0.47 |
| 59:Dx:1206:3PE:H3E2 | 59:Dx:1206:3PE:H3I3 | 1.96 | 0.47 |
| 33:Eh:32:ASP:OD1 | 33:Eh:33:GLU:N | 2.48 | 0.47 |
| 45:Et:38:LEU:N | 45:Et:38:LEU:HD23 | 2.29 | 0.47 |
| 3:Dc:268:PHE:CZ | 3:Dc:272:ILE:HG21 | 2.50 | 0.46 |
| 4:Dd:186:GLN:OE1 | 19:Dt:181:ASN:ND2 | 2.45 | 0.46 |
| 4:Dd:451:THR:HG22 | 4:Dd:452:SER:H | 1.79 | 0.46 |
| 21:Dv:225:LEU:HD21 | 57:Dv:401:CDL:H202 | 1.97 | 0.46 |
| 36:Ek:118:PRO:HA | 36:Ek:121:VAL:HG22 | 1.98 | 0.46 |
| 38:Em:45:THR:HG23 | 38:Em:57:ALA:HB3 | 1.97 | 0.46 |
| 49:Ex:40:GLU:OE1 | 51:Ez:48:ARG:NH2 | 2.49 | 0.46 |
| 50:Ey:62:LEU:O | 50:Ey:64:LYS:NZ | 2.49 | 0.46 |
| 53:Dl:250:THR:OG1 | 53:Dl:260:ASN:ND2 | 2.48 | 0.46 |
| 5:DE:44:MET:CE | 29:ED:160:ILE:HD11 | 2.45 | 0.46 |
| 13:DN:414:TYR:CE2 | 13:DN:418:ILE:HD11 | 2.51 | 0.46 |
| 16:DQ:268:THR:HG23 | 16:DQ:268:THR:O | 2.15 | 0.46 |
| 17:DR:252:THR:HG21 | 17:DR:324:TYR:O | 2.14 | 0.46 |
| 18:DS:17:ASP:OD1 | 18:DS:18:ILE:N | 2.46 | 0.46 |
| 27:EB:182:VAL:HG23 | 27:EB:185:SER:HB2 | 1.97 | 0.46 |
| 32:EG:25:ASP:O | 32:EG:26:GLU:C | 2.58 | 0.46 |
| 40:EO:31:TYR:CE2 | 40:EO:35:LEU:HD11 | 2.51 | 0.46 |
| 1:Da:194:TYR:CE2 | 1:Da:198:LEU:HD11 | 2.50 | 0.46 |
| 1:Da:415:ARG:NH1 | 1:Da:416:ARG:O | 2.48 | 0.46 |
| 1:Da:511:VAL:O | 1:Da:515:VAL:HG23 | 2.15 | 0.46 |
| 1:Da:645:ARG:NE | 19:Dt:146:ILE:HD11 | 2.30 | 0.46 |
| 14:Do:164:TYR:CE2 | 14:Do:168:LEU:HD11 | 2.49 | 0.46 |
| 15:Dp:126:THR:HG23 | 15:Dp:386:TYR:HD1 | 1.81 | 0.46 |
| 15:Dp:126:THR:HG21 | 15:Dp:389:THR:HB | 1.96 | 0.46 |
| 16:Dq:9:ARG:O | 16:Dq:235:ASN:ND2 | 2.41 | 0.46 |
| 59:Dr:401:3PE:H3I1 | 57:Dr:402:CDL:H251 | 1.96 | 0.46 |
| 19:Dt:243:ILE:HG21 | 31:Ef:79:MET:SD | 2.55 | 0.46 |
| 43:Er:64:LEU:HD12 | 43:Er:92:VAL:HG11 | 1.97 | 0.46 |
| 45:Et:38:LEU:HD23 | 45:Et:38:LEU:H | 1.81 | 0.46 |
| 13:DN:126:ILE:HD12 | 13:DN:126:ILE:N | 2.30 | 0.46 |
| 13:DN:189:ILE:HB | 36:EK:46:VAL:HG13 | 1.97 | 0.46 |
| 17:DR:284:LEU:HD21 | 17:DR:321:VAL:HG11 | 1.97 | 0.46 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 18:DS:248:LEU:HD21 | 57:DS:402:CDL:H271 | 1.97 | 0.46 |
| 2:Db:69:THR:O | 2:Db:69:THR:HG22 | 2.15 | 0.46 |
| 6:Df:163:ASN:O | 6:Df:163:ASN:ND2 | 2.48 | 0.46 |
| 12:Dm:449:ILE:HA | 12:Dm:452:THR:HG22 | 1.98 | 0.46 |
| 30:Ee:164:VAL:HG22 | 49:Ex:34:ASP:CG | 2.40 | 0.46 |
| 53:Dl:296:THR:O | 53:Dl:312:SER:N | 2.49 | 0.46 |
| 11:DK:97:GLU:OE1 | 11:DK:97:GLU:N | 2.45 | 0.46 |
| 14:DO:357:LEU:HD21 | 14:DO:366:VAL:HG13 | 1.96 | 0.46 |
| 20:DU:270:VAL:O | 20:DU:273:VAL:HG23 | 2.16 | 0.46 |
| 31:EF:117:VAL:HG13 | 31:EF:119:THR:HG22 | 1.96 | 0.46 |
| 47:EJ:141:TYR:HA | 47:EJ:144:THR:HG22 | 1.98 | 0.46 |
| 1:Da:581:LEU:HD21 | 1:Da:600:TRP:HB2 | 1.97 | 0.46 |
| 57:Dj:404:CDL:OA9 | 40:Eo:31:TYR:OH | 2.31 | 0.46 |
| 13:Dn:136:PHE:CZ | 13:Dn:140:LEU:HD11 | 2.51 | 0.46 |
| 14:Do:48:ASN:O | 14:Do:48:ASN:ND2 | 2.48 | 0.46 |
| 1:DA:581:LEU:HD21 | 1:DA:600:TRP:HB2 | 1.97 | 0.46 |
| 6:DF:155:PHE:O | 6:DF:158:VAL:HG13 | 2.15 | 0.46 |
| 8:DH:59:GLU:OE2 | 8:DH:65:LYS:NZ | 2.49 | 0.46 |
| 12:DM:128:THR:O | 12:DM:128:THR:HG22 | 2.16 | 0.46 |
| 49:EX:28:VAL:HG23 | 49:EX:29:LEU:HD12 | 1.98 | 0.46 |
| 1:Da:92:LEU:HD22 | 1:Da:270:THR:HB | 1.97 | 0.46 |
| 2:Db:250:PHE:O | 45:Et:22:TYR:OH | 2.31 | 0.46 |
| 59:Dg:204:3PE:O12 | 38:Em:62:ARG:NH1 | 2.43 | 0.46 |
| 12:Dm:193:VAL:HG13 | 12:Dm:204:LYS:HG2 | 1.96 | 0.46 |
| 19:Dt:45:PRO:CG | 19:Dt:50:ILE:HD11 | 2.45 | 0.46 |
| 27:Eb:166:GLU:OE1 | 27:Eb:169:ARG:NH1 | 2.49 | 0.46 |
| 58:Eb:302:PC1:H2E1 | 58:Eb:302:PC1:H2I2 | 1.96 | 0.46 |
| 47:Ej:99:PHE:CE2 | 47:Ej:109:LEU:HD22 | 2.50 | 0.46 |
| 47:Ej:127:ASP:OD2 | 47:Ej:130:THR:OG1 | 2.27 | 0.46 |
| 50:Ey:30:SER:N | 50:Ey:33:ASP:OD2 | 2.48 | 0.46 |
| 14:DO:169:LEU:C | 14:DO:169:LEU:HD12 | 2.41 | 0.46 |
| 31:EF:128:VAL:HG12 | 31:EF:130:GLN:H | 1.81 | 0.46 |
| 1:Da:42:LYS:NZ | 9:Di:115:GLU:O | 2.48 | 0.46 |
| 10:Dj:49:TYR:OH | 41:Ep:105:ASP:O | 2.30 | 0.46 |
| 24:Dy:120:LEU:HD23 | 24:Dy:120:LEU:O | 2.16 | 0.46 |
| 40:Eo:99:TRP:O | 43:Er:59:ARG:NH1 | 2.49 | 0.46 |
| 47:Ej:101:GLN:OE1 | 47:Ej:101:GLN:N | 2.48 | 0.46 |
| 1:DA:492:MET:N | 1:DA:492:MET:SD | 2.89 | 0.46 |
| 2:DB:390:ARG:NH2 | 6:DF:149:ASP:OD2 | 2.48 | 0.46 |
| 10:DJ:107:TRP:O | 10:DJ:111:VAL:HG23 | 2.15 | 0.46 |
| 14:DO:309:LEU:HD23 | 14:DO:309:LEU:O | 2.16 | 0.46 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 16:DQ:72:PRO:HB3 | 16:DQ:274:VAL:HG23 | 1.97 | 0.46 |
| 17:DR:326:ILE:N | 17:DR:326:ILE:HD12 | 2.31 | 0.46 |
| 23:DX:252:GLY:O | 10:Dj:199:LYS:NZ | 2.48 | 0.46 |
| 30:EE:86:GLN:O | 30:EE:90:THR:HG23 | 2.16 | 0.46 |
| 36:EK:120:LEU:HD23 | 36:EK:120:LEU:O | 2.15 | 0.46 |
| 2:Db:139:THR:OG1 | 2:Db:604:TRP:NE1 | 2.49 | 0.46 |
| 2:Db:516:TRP:CD1 | 2:Db:562:ILE:HD13 | 2.50 | 0.46 |
| 12:Dm:128:THR:O | 12:Dm:128:THR:HG22 | 2.15 | 0.46 |
| 16:Dq:344:ILE:HG22 | 16:Dq:344:ILE:O | 2.15 | 0.46 |
| 20:Du:98:GLN:NE2 | 20:Du:109:THR:O | 2.49 | 0.46 |
| 1:DA:501:ALA:HB1 | 1:DA:530:MET:CG | 2.46 | 0.46 |
| 3:DC:386:LYS:NZ | 4:DD:91:GLU:O | 2.49 | 0.46 |
| 3:DC:530:VAL:HG11 | 33:EH:52:TYR:HB2 | 1.98 | 0.46 |
| 4:DD:273:MET:HE2 | 4:DD:273:MET:HA | 1.97 | 0.46 |
| 6:DF:159:LYS:NZ | 26:EA:220:THR:O | 2.48 | 0.46 |
| 13:DN:136:PHE:CE2 | 13:DN:140:LEU:HD11 | 2.51 | 0.46 |
| 29:ED:48:GLU:O | 29:ED:55:ASN:ND2 | 2.49 | 0.46 |
| 37:EL:75:ILE:N | 37:EL:75:ILE:HD12 | 2.31 | 0.46 |
| 3:Dc:365:SER:O | 3:Dc:369:ILE:HG23 | 2.16 | 0.46 |
| 4:Dd:103:THR:HG22 | 13:Dn:294:TYR:O | 2.16 | 0.46 |
| 7:Dg:24:GLU:OE1 | 7:Dg:24:GLU:N | 2.45 | 0.46 |
| 10:Dj:11:ASN:ND2 | 10:Dj:30:GLU:OE1 | 2.44 | 0.46 |
| 16:Dq:268:THR:HG23 | 16:Dq:268:THR:O | 2.16 | 0.46 |
| 23:Dx:73:GLU:OE1 | 23:Dx:80:ARG:NH2 | 2.49 | 0.46 |
| 30:Ee:72:ILE:HD12 | 30:Ee:72:ILE:N | 2.30 | 0.46 |
| 33:Eh:18:LEU:HD11 | 33:Eh:140:LEU:HD13 | 1.98 | 0.46 |
| 37:El:114:MET:HE1 | 44:Es:65:PHE:N | 2.31 | 0.46 |
| 42:Eq:1:AME:O | 42:Eq:1:AME:HG1 | 2.16 | 0.46 |
| 53:DL:99:THR:O | 53:DL:105:ARG:NH2 | 2.48 | 0.46 |
| 53:DL:260:ASN:HB3 | 53:DL:269:LEU:HD22 | 1.98 | 0.46 |
| 3:DC:268:PHE:CZ | 3:DC:272:ILE:HG21 | 2.51 | 0.46 |
| 12:DM:447:ASP:OD1 | 12:DM:448:PHE:N | 2.49 | 0.46 |
| 19:DT:188:ILE:HG21 | 19:DT:208:ILE:HD11 | 1.98 | 0.46 |
| 31:EF:95:VAL:CG2 | 41:EP:127:LEU:HD12 | 2.46 | 0.46 |
| 37:EL:34:LYS:NZ | 37:EL:50:ASP:OD1 | 2.48 | 0.46 |
| 51:EZ:42:LEU:HD23 | 52:FA:58:ILE:HB | 1.97 | 0.46 |
| 3:Dc:383:LEU:HD13 | 4:Dd:93:THR:HG21 | 1.97 | 0.46 |
| 12:Dm:188:LEU:O | 12:Dm:191:ARG:NE | 2.49 | 0.46 |
| 53:DL:296:THR:O | 53:DL:312:SER:N | 2.49 | 0.46 |
| 3:DC:84:GLU:OE2 | 20:DU:267:SER:OG | 2.34 | 0.46 |
| 3:DC:260:LEU:HB3 | 12:DM:338:ILE:HD12 | 1.98 | 0.46 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 26:EA:218:ARG:HH12 | 50:EY:58:TYR:HH | 1.64 | 0.46 |
| 29:ED:100:PHE:CE2 | 29:ED:104:LEU:HD11 | 2.51 | 0.46 |
| 40:EO:109:THR:HG22 | 40:EO:110:LEU:N | 2.30 | 0.46 |
| 3:Dc:18:PHE:HD2 | 3:Dc:62:LEU:HD11 | 1.80 | 0.46 |
| 3:Dc:80:LEU:HD11 | 14:Do:272:GLU:HB3 | 1.98 | 0.46 |
| 3:Dc:389:THR:HG23 | 3:Dc:390:ILE:N | 2.31 | 0.46 |
| 17:Dr:186:ILE:O | 39:En:119:ARG:NH2 | 2.49 | 0.46 |
| 31:Ef:51:THR:HG22 | 31:Ef:53:PHE:H | 1.81 | 0.46 |
| 3:DC:106:VAL:HG21 | 20:DU:248:LEU:HD23 | 1.97 | 0.45 |
| 57:DQ:1504:CDL:H271 | 57:Dg:202:CDL:H322 | 1.98 | 0.45 |
| 1:Da:173:PHE:N | 1:Da:174:PRO:HD2 | 2.31 | 0.45 |
| 3:Dc:80:LEU:HD12 | 14:Do:276:GLN:CD | 2.41 | 0.45 |
| 3:Dc:521:LEU:HD21 | 10:Dj:144:MET:HE1 | 1.97 | 0.45 |
| 14:Do:299:LEU:O | 14:Do:345:ASN:ND2 | 2.46 | 0.45 |
| 30:Ee:164:VAL:HG22 | 49:Ex:34:ASP:OD1 | 2.16 | 0.45 |
| 12:DM:249:ASP:O | 19:DT:34:ARG:NH2 | 2.47 | 0.45 |
| 20:DU:35:THR:HG22 | 20:DU:35:THR:O | 2.16 | 0.45 |
| 20:DU:253:THR:O | 20:DU:257:VAL:HG23 | 2.16 | 0.45 |
| 21:DV:119:ARG:NH2 | 57:EB:302:CDL:O1 | 2.49 | 0.45 |
| 58:EB:303:PC1:H2I2 | 58:EB:303:PC1:H2E1 | 1.98 | 0.45 |
| 1:Da:88:LYS:HG3 | 18:Ds:18:ILE:HD12 | 1.97 | 0.45 |
| 1:Da:134:TYR:OH | 3:Dc:312:THR:HG22 | 2.16 | 0.45 |
| 3:Dc:418:ASN:OD1 | 3:Dc:420:ASN:ND2 | 2.46 | 0.45 |
| 4:Dd:325:LEU:HD13 | 4:Dd:403:ASP:HB2 | 1.97 | 0.45 |
| 57:Dg:201:CDL:H472 | 57:Dg:201:CDL:C27 | 2.42 | 0.45 |
| 57:Dg:201:CDL:H272 | 57:Dg:201:CDL:C46 | 2.47 | 0.45 |
| 14:Do:356:GLU:HB2 | 14:Do:369:VAL:HG22 | 1.97 | 0.45 |
| 20:Du:125:PHE:O | 20:Du:128:GLY:N | 2.40 | 0.45 |
| 51:Ez:35:VAL:HG22 | 51:Ez:36:LEU:N | 2.31 | 0.45 |
| 4:DD:503:LEU:HB3 | 36:EK:40:ILE:HD11 | 1.99 | 0.45 |
| 57:DD:702:CDL:H272 | 57:DD:702:CDL:H231 | 1.98 | 0.45 |
| 9:DI:208:ILE:HG23 | 9:DI:209:VAL:HG23 | 1.97 | 0.45 |
| 20:DU:258:ALA:HB2 | 20:DU:270:VAL:HG21 | 1.99 | 0.45 |
| 32:EG:25:ASP:OD2 | 32:EG:74:SER:OG | 2.30 | 0.45 |
| 44:ES:81:PHE:CE2 | 44:ES:85:LEU:HD11 | 2.52 | 0.45 |
| 51:EZ:42:LEU:O | 51:EZ:45:CYS:SG | 2.74 | 0.45 |
| 2:Db:109:GLU:OE2 | 6:Df:120:THR:OG1 | 2.33 | 0.45 |
| 9:Di:118:TYR:N | 9:Di:122:ASP:OD2 | 2.47 | 0.45 |
| 12:Dm:214:ARG:NH1 | 12:Dm:251:PRO:O | 2.41 | 0.45 |
| 22:Dw:91:ARG:NH2 | 22:Dw:115:ASN:O | 2.48 | 0.45 |
| 53:DL:88:TRP:NE1 | 53:DL:423:PHE:O | 2.41 | 0.45 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:DC:177:TYR:OH | 25:DZ:140:ARG:NE | 2.45 | 0.45 |
| 4:DD:220:MET:HE1 | 29:ED:163:ALA:O | 2.15 | 0.45 |
| 18:DS:20:ASN:ND2 | 18:DS:339:ASN:OD1 | 2.47 | 0.45 |
| 18:DS:219:LEU:HB3 | 18:DS:241:ILE:HD12 | 1.97 | 0.45 |
| 23:DX:50:GLY:HA3 | 23:DX:105:PHE:HB2 | 1.99 | 0.45 |
| 28:EC:28:LEU:HD11 | 28:EC:59:GLN:OE1 | 2.16 | 0.45 |
| 2:Db:45:TRP:NE1 | 65:En:1203:UQ8:H3MA | 2.31 | 0.45 |
| 12:Dm:198:HIS:O | 12:Dm:202:GLY:N | 2.46 | 0.45 |
| 16:Dq:117:THR:HG22 | 16:Dq:118:ILE:N | 2.31 | 0.45 |
| 18:Ds:260:ARG:NH1 | 18:Ds:264:ASP:OD2 | 2.49 | 0.45 |
| 19:Dt:188:ILE:HG21 | 19:Dt:208:ILE:HD11 | 1.98 | 0.45 |
| 22:Dw:310:PHE:CE2 | 22:Dw:314:LEU:HD11 | 2.51 | 0.45 |
| 23:Dx:167:TRP:O | 23:Dx:182:LYS:NZ | 2.49 | 0.45 |
| 26:Ea:31:ILE:HD13 | 26:Ea:200:TYR:CE2 | 2.51 | 0.45 |
| 26:Ea:171:LYS:O | 33:Eh:167:TYR:OH | 2.29 | 0.45 |
| 1:DA:180:LYS:NZ | 1:DA:204:ASP:O | 2.48 | 0.45 |
| 4:DD:113:HIS:NE2 | 4:DD:125:ASP:OD1 | 2.45 | 0.45 |
| 10:DJ:204:GLU:OE1 | 10:DJ:205:HIS:N | 2.50 | 0.45 |
| 13:DN:218:ILE:H | 13:DN:218:ILE:HD12 | 1.80 | 0.45 |
| 19:DT:246:ASP:O | 31:EF:164:ARG:NH2 | 2.47 | 0.45 |
| 2:Db:402:HIS:ND1 | 2:Db:403:LYS:O | 2.50 | 0.45 |
| 22:Dw:257:GLU:OE1 | 22:Dw:257:GLU:N | 2.41 | 0.45 |
| 25:Dz:125:GLN:OE1 | 25:Dz:125:GLN:N | 2.49 | 0.45 |
| 3:DC:190:LEU:HD11 | 25:DZ:170:LEU:CD1 | 2.46 | 0.45 |
| 17:DR:137:ILE:N | 17:DR:137:ILE:HD12 | 2.31 | 0.45 |
| 19:DT:267:LYS:NZ | 19:DT:268:GLU:OE2 | 2.34 | 0.45 |
| 22:DW:310:PHE:CE2 | 22:DW:314:LEU:HD11 | 2.51 | 0.45 |
| 24:DY:120:LEU:O | 24:DY:120:LEU:HD23 | 2.16 | 0.45 |
| 41:EP:92:HIS:ND1 | 41:EP:105:ASP:OD1 | 2.49 | 0.45 |
| 9:Di:133:GLN:NE2 | 19:Dt:207:GLU:O | 2.46 | 0.45 |
| 51:Ez:35:VAL:HG22 | 51:Ez:36:LEU:H | 1.81 | 0.45 |
| 51:Ez:42:LEU:O | 51:Ez:45:CYS:SG | 2.75 | 0.45 |
| 2:DB:599:LEU:C | 2:DB:599:LEU:HD12 | 2.42 | 0.45 |
| 3:DC:72:ASN:ND2 | 47:EJ:86:ILE:O | 2.50 | 0.45 |
| 3:DC:77:VAL:HG22 | 3:DC:77:VAL:O | 2.16 | 0.45 |
| 4:DD:242:GLU:OE1 | 4:DD:242:GLU:N | 2.44 | 0.45 |
| 15:DP:323:VAL:HG23 | 15:DP:323:VAL:O | 2.16 | 0.45 |
| 24:DY:106:PHE:CD1 | 24:DY:110:ILE:HD12 | 2.52 | 0.45 |
| 66:ED:602:HEM:HMB2 | 66:ED:602:HEM:CBB | 2.37 | 0.45 |
| 33:EH:59:LEU:HD22 | 57:EL:902:CDL:H271 | 1.99 | 0.45 |
| 49:EX:33:ASP:OD1 | 51:EZ:48:ARG:NH1 | 2.50 | 0.45 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:Dc:268:PHE:CE2 | 3:Dc:272:ILE:HD13 | 2.51 | 0.45 |
| 14:Do:253:ARG:NH2 | 47:Ej:88:ASP:O | 2.49 | 0.45 |
| 15:Dp:236:PHE:HD2 | 15:Dp:340:ILE:HG23 | 1.82 | 0.45 |
| 18:Ds:25:VAL:O | 18:Ds:25:VAL:HG23 | 2.17 | 0.45 |
| 20:Du:101:LEU:O | 20:Du:104:GLN:NE2 | 2.48 | 0.45 |
| 20:Du:283:VAL:HB | 20:Du:284:PRO:HD3 | 1.99 | 0.45 |
| 21:Dv:103:ILE:O | 21:Dv:107:THR:HG22 | 2.17 | 0.45 |
| 24:Dy:61:GLU:OE1 | 24:Dy:61:GLU:N | 2.46 | 0.45 |
| 34:Ei:105:ILE:HG23 | 34:Ei:106:CYS:N | 2.31 | 0.45 |
| 7:DG:1:MET:HE1 | 57:Dx:1201:CDL:H472 | 1.99 | 0.45 |
| 18:DS:254:TYR:O | 18:DS:258:VAL:HG23 | 2.17 | 0.45 |
| 25:DZ:136:VAL:HG23 | 25:DZ:137:HIS:N | 2.32 | 0.45 |
| 3:Dc:328:PHE:CE2 | 3:Dc:332:LEU:HD11 | 2.52 | 0.45 |
| 4:Dd:497:HIS:CE1 | 13:Dn:191:TYR:HH | 2.34 | 0.45 |
| 29:Ed:115:ILE:HG12 | 65:Ed:202:UQ8:H4MB | 1.98 | 0.45 |
| 1:DA:127:VAL:O | 1:DA:322:MET:N | 2.44 | 0.45 |
| 3:DC:45:LEU:HD22 | 3:DC:60:ILE:HD11 | 1.97 | 0.45 |
| 4:DD:312:VAL:HG21 | 5:DE:15:ILE:HD11 | 1.97 | 0.45 |
| 8:DH:8:SER:OG | 12:DM:451:GLN:OE1 | 2.35 | 0.45 |
| 10:DJ:206:GLU:N | 10:DJ:206:GLU:OE1 | 2.50 | 0.45 |
| 13:DN:170:ILE:HG21 | 28:EC:171:VAL:HG11 | 1.99 | 0.45 |
| 58:DX:306:PC1:H143 | 58:DX:306:PC1:O13 | 2.17 | 0.45 |
| 16:Dq:209:GLU:OE1 | 16:Dq:236:TRP:NE1 | 2.48 | 0.45 |
| 19:Dt:158:THR:HG22 | 19:Dt:163:VAL:O | 2.17 | 0.45 |
| 19:Dt:284:ASN:OD1 | 19:Dt:285:GLU:N | 2.50 | 0.45 |
| 27:Eb:188:GLU:OE1 | 27:Eb:188:GLU:N | 2.47 | 0.45 |
| 28:Ec:124:SER:OG | 36:Ek:85:ASP:OD2 | 2.23 | 0.45 |
| 44:Es:81:PHE:CE2 | 44:Es:85:LEU:HD11 | 2.52 | 0.45 |
| 9:DI:42:ASP:OD1 | 21:DV:44:ARG:NH1 | 2.50 | 0.45 |
| 10:DJ:11:ASN:ND2 | 10:DJ:30:GLU:OE1 | 2.43 | 0.45 |
| 21:DV:45:THR:O | 21:DV:45:THR:HG22 | 2.17 | 0.45 |
| 28:EC:101:LEU:HD23 | 28:EC:101:LEU:C | 2.42 | 0.45 |
| 33:EH:29:CYS:O | 33:EH:30:LEU:HD12 | 2.17 | 0.45 |
| 1:Da:155:ILE:HG21 | 1:Da:295:LEU:CD1 | 2.47 | 0.45 |
| 4:Dd:497:HIS:ND1 | 13:Dn:191:TYR:OH | 2.38 | 0.45 |
| 13:Dn:81:TYR:O | 13:Dn:85:VAL:HG23 | 2.17 | 0.45 |
| 57:Dn:502:CDL:H872 | 57:Dn:502:CDL:C83 | 2.46 | 0.45 |
| 16:Dq:99:LEU:O | 16:Dq:99:LEU:HD23 | 2.17 | 0.45 |
| 17:Dr:166:TYR:O | 17:Dr:211:ARG:NH2 | 2.50 | 0.45 |
| 25:Dz:38:THR:OG1 | 25:Dz:48:ASP:OD1 | 2.31 | 0.45 |
| 40:Eo:109:THR:HG22 | 40:Eo:110:LEU:N | 2.32 | 0.45 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:DA:34:ASN:HB2 | 25:DZ:25:ILE:HD12 | 1.99 | 0.44 |
| 2:DB:109:GLU:OE2 | 6:DF:120:THR:OG1 | 2.35 | 0.44 |
| 2:DB:124:TRP:CZ2 | 2:DB:562:ILE:HD11 | 2.52 | 0.44 |
| 3:DC:383:LEU:HD13 | 4:DD:93:THR:HG21 | 1.98 | 0.44 |
| 4:DD:179:LEU:HD11 | 19:DT:193:VAL:HG13 | 1.99 | 0.44 |
| 12:DM:448:PHE:O | 12:DM:452:THR:HG22 | 2.16 | 0.44 |
| 16:DQ:209:GLU:OE1 | 16:DQ:236:TRP:NE1 | 2.49 | 0.44 |
| 57:DX:307:CDL:H671 | 58:Eo:201:PC1:H222 | 1.99 | 0.44 |
| 30:EE:72:ILE:N | 30:EE:72:ILE:HD12 | 2.32 | 0.44 |
| 46:EU:3:SER:OG | 46:EU:4:ASP:N | 2.51 | 0.44 |
| 1:Da:444:LEU:HD21 | 1:Da:515:VAL:HG22 | 1.99 | 0.44 |
| 9:Di:78:ASN:OD1 | 19:Dt:132:LYS:NZ | 2.29 | 0.44 |
| 57:Dn:502:CDL:OA5 | 57:Dn:502:CDL:O1 | 2.31 | 0.44 |
| 14:Do:169:LEU:C | 14:Do:169:LEU:HD12 | 2.42 | 0.44 |
| 21:Dv:191:ALA:O | 21:Dv:195:ASN:ND2 | 2.44 | 0.44 |
| 38:Em:131:GLU:OE1 | 38:Em:131:GLU:N | 2.46 | 0.44 |
| 1:DA:173:PHE:N | 1:DA:174:PRO:HD2 | 2.32 | 0.44 |
| 1:DA:342:THR:HB | 1:DA:396:VAL:HG13 | 1.99 | 0.44 |
| 2:DB:143:ILE:HB | 11:DK:34:LEU:HD11 | 1.99 | 0.44 |
| 2:DB:569:PHE:CG | 6:DF:108:ILE:HG21 | 2.53 | 0.44 |
| 10:DJ:163:GLU:OE2 | 10:DJ:198:ARG:NH1 | 2.43 | 0.44 |
| 12:DM:364:VAL:HG13 | 12:DM:378:VAL:HG13 | 1.99 | 0.44 |
| 13:DN:207:ILE:N | 13:DN:207:ILE:HD12 | 2.32 | 0.44 |
| 14:DO:460:LEU:HD11 | 14:DO:464:PHE:CZ | 2.52 | 0.44 |
| 19:DT:87:TYR:OH | 19:DT:142:ASP:OD1 | 2.22 | 0.44 |
| 34:EI:79:ILE:O | 34:EI:82:VAL:HG12 | 2.17 | 0.44 |
| 1:Da:34:ASN:HB2 | 25:Dz:25:ILE:HD12 | 2.00 | 0.44 |
| 1:Da:565:ILE:HD11 | 57:En:1201:CDL:C34 | 2.46 | 0.44 |
| 2:Db:1:MET:HE3 | 6:Df:78:MET:HG3 | 1.99 | 0.44 |
| 4:Dd:68:LEU:HD12 | 26:Ea:127:PHE:CE2 | 2.52 | 0.44 |
| 4:Dd:199:ARG:NH1 | 12:Dm:83:TYR:OH | 2.50 | 0.44 |
| 12:Dm:338:ILE:HB | 12:Dm:339:PRO:HD3 | 1.99 | 0.44 |
| 16:Dq:187:ARG:O | 16:Dq:248:GLN:NE2 | 2.41 | 0.44 |
| 16:Dq:344:ILE:HB | 40:Eo:2:VAL:HG21 | 2.00 | 0.44 |
| 21:Dv:248:GLN:NE2 | 21:Dv:259:TYR:O | 2.46 | 0.44 |
| 29:Ed:154:ASN:OD1 | 37:El:86:ARG:NH1 | 2.50 | 0.44 |
| 44:Es:42:ALA:HB1 | 44:Es:53:LEU:HD11 | 1.99 | 0.44 |
| 44:Es:45:ILE:HD11 | 44:Es:52:GLU:OE2 | 2.17 | 0.44 |
| 1:DA:504:THR:HG21 | 1:DA:579:PHE:CE1 | 2.53 | 0.44 |
| 4:DD:220:MET:HE3 | 4:DD:248:THR:HG21 | 2.00 | 0.44 |
| 14:DO:364:LYS:NZ | 14:DO:468:GLU:OE1 | 2.40 | 0.44 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 24:DY:206:LEU:HD23 | 24:DY:206:LEU:C | 2.43 | 0.44 |
| 2:Db:25:ASP:OD1 | 2:Db:29:HIS:NE2 | 2.51 | 0.44 |
| 2:Db:407:ASP:OD1 | 6:Df:173:TYR:OH | 2.22 | 0.44 |
| 5:De:53:GLU:OE2 | 29:Ed:181:LYS:NZ | 2.40 | 0.44 |
| 7:Dg:40:TYR:CZ | 7:Dg:44:ILE:HD11 | 2.52 | 0.44 |
| 12:Dm:30:THR:HG22 | 12:Dm:31:ALA:N | 2.33 | 0.44 |
| 23:Dx:50:GLY:HA3 | 23:Dx:105:PHE:HB2 | 1.99 | 0.44 |
| 3:DC:526:LEU:O | 3:DC:530:VAL:HG23 | 2.18 | 0.44 |
| 8:DH:82:PHE:CE2 | 8:DH:86:LEU:HD11 | 2.52 | 0.44 |
| 22:DW:42:PHE:CE2 | 22:DW:46:LEU:HD11 | 2.53 | 0.44 |
| 26:EA:31:ILE:HD11 | 26:EA:198:THR:O | 2.18 | 0.44 |
| 3:Dc:106:VAL:HG22 | 20:Du:247:PRO:HB2 | 1.99 | 0.44 |
| 3:Dc:531:PHE:O | 33:Eh:60:TYR:OH | 2.24 | 0.44 |
| 4:Dd:451:THR:HG22 | 4:Dd:452:SER:N | 2.33 | 0.44 |
| 57:Dg:201:CDL:H831 | 57:Dg:201:CDL:H871 | 1.99 | 0.44 |
| 14:Do:309:LEU:HD23 | 14:Do:309:LEU:C | 2.43 | 0.44 |
| 17:Dr:326:ILE:HD12 | 17:Dr:326:ILE:N | 2.33 | 0.44 |
| 1:DA:499:LEU:HD22 | 54:DA:702:HEA:H202 | 1.99 | 0.44 |
| 12:DM:198:HIS:O | 12:DM:202:GLY:N | 2.50 | 0.44 |
| 57:DQ:1502:CDL:OA3 | 29:ED:113:LYS:NZ | 2.51 | 0.44 |
| 18:DS:69:LYS:NZ | 57:EN:1202:CDL:OA4 | 2.40 | 0.44 |
| 23:DX:73:GLU:OE1 | 23:DX:80:ARG:NE | 2.51 | 0.44 |
| 25:DZ:171:LEU:C | 25:DZ:171:LEU:HD23 | 2.42 | 0.44 |
| 37:EL:114:MET:HE1 | 44:ES:65:PHE:N | 2.33 | 0.44 |
| 1:Da:589:ARG:NH2 | 54:Da:701:HEA:O1D | 2.50 | 0.44 |
| 4:Dd:68:LEU:C | 4:Dd:68:LEU:HD13 | 2.43 | 0.44 |
| 59:Dj:407:3PE:H3I3 | 59:Dj:407:3PE:C3E | 2.48 | 0.44 |
| 15:Dp:163:ASP:OD1 | 15:Dp:171:ARG:NH2 | 2.45 | 0.44 |
| 19:Dt:270:TRP:O | 31:Ef:127:ASN:ND2 | 2.50 | 0.44 |
| 25:Dz:136:VAL:HG23 | 25:Dz:137:HIS:N | 2.33 | 0.44 |
| 29:Ed:106:ILE:HD13 | 36:Ek:60:ILE:CD1 | 2.47 | 0.44 |
| 42:Eq:20:THR:OG1 | 42:Eq:24:LYS:NZ | 2.50 | 0.44 |
| 3:DC:419:ILE:HG22 | 3:DC:432:LEU:HD11 | 2.00 | 0.44 |
| 3:DC:518:TRP:CZ2 | 58:EO:205:PC1:H142 | 2.52 | 0.44 |
| 10:DJ:143:ARG:NH2 | 10:DJ:186:ASP:OD1 | 2.50 | 0.44 |
| 11:DK:42:GLU:OE1 | 11:DK:42:GLU:N | 2.45 | 0.44 |
| 11:DK:54:ARG:NH2 | 35:EV:33:ASP:O | 2.50 | 0.44 |
| 16:DQ:96:GLN:NE2 | 16:DQ:100:ASN:OD1 | 2.50 | 0.44 |
| 16:DQ:333:THR:HG23 | 19:DT:74:VAL:HG21 | 1.99 | 0.44 |
| 19:DT:126:GLU:HA | 19:DT:154:ILE:HD11 | 2.00 | 0.44 |
| 16:Dq:98:GLU:OE1 | 36:Ek:51:ARG:NH2 | 2.51 | 0.44 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 21:Dv:26:ILE:HD11 | 21:Dv:299:ILE:HD12 | 1.98 | 0.44 |
| 47:Ej:99:PHE:CG | 47:Ej:100:PRO:HD3 | 2.53 | 0.44 |
| 7:DG:24:GLU:OE1 | 7:DG:24:GLU:N | 2.48 | 0.44 |
| 21:DV:1:AME:HT22 | 21:DV:3:TYR:CZ | 2.52 | 0.44 |
| 40:EO:54:THR:HG22 | 40:EO:55:THR:N | 2.32 | 0.44 |
| 40:EO:99:TRP:O | 43:ER:59:ARG:NH1 | 2.50 | 0.44 |
| 1:Da:391:HIS:O | 1:Da:394:VAL:HG22 | 2.18 | 0.44 |
| 4:Dd:459:ASN:O | 4:Dd:463:VAL:HG23 | 2.17 | 0.44 |
| 5:De:52:HIS:O | 5:De:56:ASN:ND2 | 2.51 | 0.44 |
| 10:Dj:204:GLU:OE1 | 10:Dj:205:HIS:N | 2.51 | 0.44 |
| 12:Dm:364:VAL:HG13 | 12:Dm:378:VAL:HG13 | 1.99 | 0.44 |
| 13:Dn:190:LYS:NZ | 36:Ek:80:VAL:O | 2.50 | 0.44 |
| 18:Ds:17:ASP:OD1 | 18:Ds:18:ILE:N | 2.49 | 0.44 |
| 31:Ef:35:ILE:N | 31:Ef:35:ILE:HD12 | 2.33 | 0.44 |
| 33:Eh:129:ILE:HG22 | 33:Eh:137:TRP:HB2 | 2.00 | 0.44 |
| 53:Dl:446:LYS:O | 53:Dl:461:VAL:HG13 | 2.17 | 0.44 |
| 1:DA:328:ARG:HA | 1:DA:328:ARG:HE | 1.83 | 0.44 |
| 1:DA:380:ILE:HD11 | 2:DB:528:VAL:HG11 | 1.99 | 0.44 |
| 3:DC:106:VAL:HG22 | 20:DU:247:PRO:HB2 | 2.00 | 0.44 |
| 13:DN:261:PHE:CE2 | 13:DN:265:LEU:HD11 | 2.53 | 0.44 |
| 14:DO:299:LEU:N | 14:DO:299:LEU:HD12 | 2.33 | 0.44 |
| 18:DS:215:THR:OG1 | 65:EN:1204:UQ8:H30B | 2.18 | 0.44 |
| 19:DT:208:ILE:HG23 | 19:DT:209:PHE:CD2 | 2.52 | 0.44 |
| 25:DZ:125:GLN:OE1 | 25:DZ:125:GLN:N | 2.51 | 0.44 |
| 1:Da:468:ILE:HD11 | 2:Db:83:CYS:SG | 2.57 | 0.44 |
| 1:DA:295:LEU:O | 1:DA:299:VAL:HG23 | 2.18 | 0.44 |
| 14:DO:164:TYR:CE2 | 14:DO:168:LEU:HD11 | 2.53 | 0.44 |
| 16:DQ:247:TYR:CD1 | 19:DT:316:ILE:HD11 | 2.53 | 0.44 |
| 18:DS:185:ILE:HG21 | 18:DS:194:LEU:HD21 | 2.00 | 0.44 |
| 18:DS:256:TRP:O | 18:DS:259:THR:HG22 | 2.18 | 0.44 |
| 19:DT:83:TYR:N | 31:EF:59:ILE:O | 2.50 | 0.44 |
| 20:DU:254:ARG:NH2 | 20:DU:277:THR:O | 2.50 | 0.44 |
| 21:DV:225:LEU:HD21 | 57:DV:401:CDL:H202 | 1.99 | 0.44 |
| 1:Da:562:MET:HE2 | 65:Ds:404:UQ8:O2 | 2.18 | 0.44 |
| 15:Dp:184:LYS:HG2 | 15:Dp:296:THR:HG22 | 1.99 | 0.44 |
| 18:Ds:123:GLN:O | 18:Ds:135:ARG:NH2 | 2.51 | 0.44 |
| 18:Ds:254:TYR:O | 18:Ds:258:VAL:HG23 | 2.18 | 0.44 |
| 13:DN:24:ILE:HD12 | 29:ED:5:ILE:HD12 | 2.00 | 0.43 |
| 16:DQ:92:ASP:O | 36:EK:51:ARG:NH1 | 2.51 | 0.43 |
| 19:DT:250:LEU:HD12 | 19:DT:251:PRO:HD2 | 2.00 | 0.43 |
| 23:DX:159:ARG:NH2 | 32:EG:98:GLU:O | 2.43 | 0.43 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 25:DZ:134:ARG:NE | 47:EJ:175:HIS:O | 2.51 | 0.43 |
| 1:Da:342:THR:HB | 1:Da:396:VAL:HG13 | 1.99 | 0.43 |
| 2:Db:594:GLU:OE1 | 30:Ee:72:ILE:HD11 | 2.18 | 0.43 |
| 4:Dd:179:LEU:HD11 | 19:Dt:193:VAL:HG13 | 2.00 | 0.43 |
| 4:Dd:469:ARG:NH1 | 4:Dd:516:ASP:OD2 | 2.48 | 0.43 |
| 5:De:69:GLU:OE2 | 12:Dm:405:ARG:N | 2.46 | 0.43 |
| 24:Dy:53:LYS:NZ | 24:Dy:158:GLU:OE2 | 2.41 | 0.43 |
| 29:Ed:106:ILE:HG21 | 65:Ed:202:UQ8:C6 | 2.48 | 0.43 |
| 43:Er:37:CYS:O | 43:Er:41:VAL:HG23 | 2.18 | 0.43 |
| 47:Ej:99:PHE:CG | 47:Ej:100:PRO:CD | 3.00 | 0.43 |
| 2:DB:16:ASN:ND2 | 2:DB:18:GLY:O | 2.45 | 0.43 |
| 8:DH:73:LEU:HD23 | 8:DH:73:LEU:C | 2.43 | 0.43 |
| 29:ED:149:TYR:CE2 | 29:ED:153:LEU:HD11 | 2.54 | 0.43 |
| 35:EV:39:THR:O | 35:EV:39:THR:HG22 | 2.17 | 0.43 |
| 59:EL:905:3PE:O13 | 58:EO:205:PC1:H141 | 2.18 | 0.43 |
| 2:Db:57:ARG:NH2 | 57:Dr:402:CDL:OA4 | 2.44 | 0.43 |
| 6:Df:121:GLN:NE2 | 10:Dj:186:ASP:O | 2.51 | 0.43 |
| 16:Dq:240:TYR:CE2 | 16:Dq:244:LEU:HD11 | 2.54 | 0.43 |
| 20:Du:253:THR:O | 20:Du:257:VAL:HG23 | 2.18 | 0.43 |
| 22:Dw:157:ASN:ND2 | 22:Dw:162:VAL:O | 2.51 | 0.43 |
| 23:Dx:176:SER:OG | 23:Dx:177:THR:N | 2.50 | 0.43 |
| 1:DA:468:ILE:HD12 | 2:DB:79:ASP:HA | 1.99 | 0.43 |
| 7:DG:9:ARG:NH1 | 31:EF:79:MET:HE1 | 2.33 | 0.43 |
| 13:DN:383:PHE:CE2 | 13:DN:387:LEU:HD11 | 2.52 | 0.43 |
| 24:DY:71:TYR:CE1 | 24:DY:81:LEU:HD11 | 2.54 | 0.43 |
| 26:EA:109:TYR:HB3 | 26:EA:164:THR:HG23 | 2.00 | 0.43 |
| 43:ER:64:LEU:HD12 | 43:ER:92:VAL:HG11 | 1.99 | 0.43 |
| 1:Da:310:PHE:CD1 | 1:Da:310:PHE:C | 2.96 | 0.43 |
| 3:Dc:190:LEU:HD11 | 25:Dz:170:LEU:CD1 | 2.48 | 0.43 |
| 16:Dq:110:TYR:OH | 16:Dq:147:PHE:O | 2.31 | 0.43 |
| 18:Ds:1:AME:HT23 | 18:Ds:6:GLU:HB2 | 2.00 | 0.43 |
| 18:Ds:122:TRP:O | 18:Ds:327:GLN:NE2 | 2.51 | 0.43 |
| 27:Eb:182:VAL:HG23 | 27:Eb:185:SER:HB2 | 2.00 | 0.43 |
| 60:Ed:203:LPP:H261 | 34:Ei:103:LEU:HD21 | 2.01 | 0.43 |
| 31:Ef:42:ARG:NH2 | 31:Ef:50:ILE:O | 2.51 | 0.43 |
| 37:El:32:ARG:NH2 | 40:Eo:37:ASP:OD2 | 2.52 | 0.43 |
| 42:Eq:1:AME:HT21 | 42:Eq:117:HIS:CD2 | 2.53 | 0.43 |
| 1:DA:391:HIS:O | 1:DA:394:VAL:HG22 | 2.19 | 0.43 |
| 3:DC:368:ILE:HD12 | 3:DC:401:ILE:CD1 | 2.45 | 0.43 |
| 17:DR:209:ILE:N | 17:DR:210:PRO:HD2 | 2.33 | 0.43 |
| 36:EK:17:LEU:O | 36:EK:17:LEU:HD23 | 2.18 | 0.43 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 54:Da:701:HEA:HBC1 | 54:Da:701:HEA:HMC3 | 2.01 | 0.43 |
| 57:Da:709:CDL:H162 | 10:Dj:109:THR:HG21 | 2.00 | 0.43 |
| 3:Dc:190:LEU:HD12 | 25:Dz:149:VAL:HG11 | 2.01 | 0.43 |
| 4:Dd:374:LEU:HD23 | 4:Dd:375:THR:N | 2.34 | 0.43 |
| 8:Dh:34:TRP:O | 12:Dm:428:GLN:NE2 | 2.51 | 0.43 |
| 11:Dk:131:THR:O | 38:Em:6:ARG:NH2 | 2.51 | 0.43 |
| 13:Dn:249:ILE:HD12 | 13:Dn:249:ILE:O | 2.18 | 0.43 |
| 17:Dr:222:ILE:HA | 17:Dr:238:THR:HG22 | 1.98 | 0.43 |
| 19:Dt:200:GLU:OE1 | 19:Dt:200:GLU:N | 2.49 | 0.43 |
| 26:Ea:141:GLY:N | 26:Ea:146:THR:O | 2.51 | 0.43 |
| 3:DC:524:ARG:NH2 | 37:EL:140:ASP:O | 2.52 | 0.43 |
| 4:DD:451:THR:HG22 | 4:DD:452:SER:N | 2.33 | 0.43 |
| 12:DM:158:TYR:O | 44:ES:50:ASN:ND2 | 2.52 | 0.43 |
| 13:DN:332:TYR:O | 13:DN:337:LYS:N | 2.52 | 0.43 |
| 57:DO:501:CDL:H181 | 57:DO:501:CDL:H871 | 2.00 | 0.43 |
| 20:DU:184:VAL:O | 20:DU:184:VAL:HG12 | 2.19 | 0.43 |
| 28:EC:43:THR:HG22 | 28:EC:60:LEU:HD13 | 2.01 | 0.43 |
| 1:Da:191:TYR:O | 1:Da:191:TYR:CG | 2.72 | 0.43 |
| 13:Dn:24:ILE:HD12 | 29:Ed:5:ILE:HD12 | 2.01 | 0.43 |
| 20:Du:51:GLN:HB3 | 20:Du:316:MET:HE1 | 2.01 | 0.43 |
| 22:Dw:136:ILE:N | 22:Dw:136:ILE:HD12 | 2.33 | 0.43 |
| 24:Dy:122:THR:HG23 | 24:Dy:123:ARG:HG3 | 2.00 | 0.43 |
| 40:Eo:54:THR:HG22 | 40:Eo:55:THR:N | 2.34 | 0.43 |
| 2:DB:172:ASN:OD1 | 30:EE:82:ASN:ND2 | 2.41 | 0.43 |
| 3:DC:479:TYR:O | 3:DC:483:VAL:HG23 | 2.18 | 0.43 |
| 4:DD:175:LEU:HD21 | 4:DD:177:PHE:CE2 | 2.54 | 0.43 |
| 8:DH:14:TYR:OH | 12:DM:393:GLU:OE1 | 2.32 | 0.43 |
| 8:DH:81:LEU:HB2 | 13:DN:325:ILE:HD13 | 2.01 | 0.43 |
| 16:DQ:133:VAL:HG22 | 57:DQ:1501:CDL:H873 | 2.00 | 0.43 |
| 20:DU:88:VAL:HA | 20:DU:91:VAL:HG12 | 2.01 | 0.43 |
| 28:EC:71:LEU:HD13 | 28:EC:79:LEU:HD12 | 1.99 | 0.43 |
| 1:Da:216:ILE:HG23 | 27:Eb:192:ASP:OD2 | 2.18 | 0.43 |
| 3:Dc:126:ILE:O | 3:Dc:126:ILE:HG22 | 2.19 | 0.43 |
| 9:Di:140:PRO:O | 9:Di:143:GLN:NE2 | 2.48 | 0.43 |
| 13:Dn:189:ILE:HB | 36:Ek:46:VAL:HG13 | 2.01 | 0.43 |
| 16:Dq:333:THR:HG23 | 19:Dt:74:VAL:HG21 | 2.00 | 0.43 |
| 33:Eh:1:AME:HG2 | 33:Eh:1:AME:O | 2.18 | 0.43 |
| 36:Ek:61:ARG:O | 36:Ek:64:ILE:HG22 | 2.17 | 0.43 |
| 58:DC:608:PC1:H2I1 | 57:EL:902:CDL:H361 | 2.01 | 0.43 |
| 4:DD:283:TYR:O | 4:DD:287:THR:HG23 | 2.19 | 0.43 |
| 4:DD:403:ASP:OD1 | 4:DD:403:ASP:C | 2.62 | 0.43 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 4:DD:575:PHE:CZ | 4:DD:579:ILE:HD11 | 2.53 | 0.43 |
| 12:DM:188:LEU:O | 12:DM:191:ARG:NE | 2.52 | 0.43 |
| 14:DO:305:LEU:O | 14:DO:305:LEU:HD23 | 2.18 | 0.43 |
| 21:DV:59:ILE:HD13 | 21:DV:280:VAL:HG13 | 2.00 | 0.43 |
| 2:Db:175:VAL:HG22 | 2:Db:179:TRP:CE2 | 2.54 | 0.43 |
| 4:Dd:469:ARG:NH2 | 4:Dd:509:GLU:OE2 | 2.48 | 0.43 |
| 12:Dm:142:VAL:HG21 | 16:Dq:25:GLY:HA2 | 2.01 | 0.43 |
| 13:Dn:30:LEU:H | 13:Dn:30:LEU:HD12 | 1.83 | 0.43 |
| 18:Ds:47:SER:C | 18:Ds:100:ALA:HB1 | 2.43 | 0.43 |
| 20:Du:254:ARG:HH22 | 20:Du:277:THR:HG23 | 1.83 | 0.43 |
| 28:Ec:9:LEU:C | 28:Ec:9:LEU:HD12 | 2.43 | 0.43 |
| 3:DC:438:ARG:O | 3:DC:439:THR:HG23 | 2.18 | 0.43 |
| 4:DD:482:LEU:HD12 | 4:DD:499:GLU:HG2 | 2.00 | 0.43 |
| 12:DM:338:ILE:HB | 12:DM:339:PRO:HD3 | 2.01 | 0.43 |
| 47:EJ:31:LEU:O | 47:EJ:175:HIS:NE2 | 2.49 | 0.43 |
| 1:Da:57:TYR:OH | 1:Da:145:GLN:NE2 | 2.48 | 0.43 |
| 4:Dd:465:ARG:NH2 | 4:Dd:519:GLU:OE1 | 2.51 | 0.43 |
| 4:Dd:575:PHE:CZ | 4:Dd:579:ILE:HD11 | 2.52 | 0.43 |
| 10:Dj:107:TRP:NE1 | 58:Eo:201:PC1:O12 | 2.44 | 0.43 |
| 18:Ds:219:LEU:HB3 | 18:Ds:241:ILE:HD12 | 2.00 | 0.43 |
| 21:Dv:249:ASN:O | 21:Dv:255:ASN:ND2 | 2.43 | 0.43 |
| 25:Dz:171:LEU:HD23 | 25:Dz:171:LEU:C | 2.44 | 0.43 |
| 33:Eh:29:CYS:O | 33:Eh:30:LEU:HD12 | 2.19 | 0.43 |
| 2:DB:175:VAL:HG22 | 2:DB:179:TRP:CE2 | 2.54 | 0.43 |
| 21:DV:269:LEU:HD23 | 21:DV:269:LEU:C | 2.44 | 0.43 |
| 37:EL:63:PHE:CE2 | 37:EL:67:LEU:HD11 | 2.54 | 0.43 |
| 1:Da:335:VAL:CG2 | 1:Da:407:MET:HE2 | 2.49 | 0.43 |
| 1:Da:353:LEU:HD22 | 1:Da:389:PHE:CZ | 2.54 | 0.43 |
| 1:Da:380:ILE:HD11 | 2:Db:528:VAL:HG11 | 2.01 | 0.43 |
| 2:Db:287:ASN:O | 2:Db:290:LEU:N | 2.51 | 0.43 |
| 4:Dd:403:ASP:OD1 | 4:Dd:403:ASP:C | 2.61 | 0.43 |
| 15:Dp:160:ASP:OD2 | 15:Dp:186:ARG:NE | 2.52 | 0.43 |
| 15:Dp:164:ALA:HB1 | 15:Dp:214:THR:HG22 | 2.01 | 0.43 |
| 15:Dp:323:VAL:HG23 | 15:Dp:323:VAL:O | 2.17 | 0.43 |
| 18:Ds:152:VAL:N | 18:Ds:153:PRO:HD2 | 2.34 | 0.43 |
| 1:DA:450:ARG:NH1 | 10:DJ:154:GLU:OE2 | 2.52 | 0.43 |
| 2:DB:337:LEU:HD22 | 2:DB:337:LEU:N | 2.33 | 0.43 |
| 59:DG:204:3PE:H3I3 | 17:DR:201:LEU:HB3 | 1.99 | 0.43 |
| 18:DS:152:VAL:N | 18:DS:153:PRO:HD2 | 2.33 | 0.43 |
| 25:DZ:70:TYR:HB3 | 25:DZ:126:ILE:HD11 | 2.01 | 0.43 |
| 26:EA:158:VAL:HG23 | 26:EA:159:LEU:N | 2.34 | 0.43 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 39:EN:105:TRP:O | 39:EN:109:SER:OG | 2.21 | 0.43 |
| 2:Db:201:LEU:HD13 | 20:Du:55:ASN:HB2 | 2.00 | 0.43 |
| 2:Db:360:LEU:HD13 | 2:Db:393:PHE:CZ | 2.54 | 0.43 |
| 3:Dc:111:ILE:N | 3:Dc:111:ILE:HD12 | 2.34 | 0.43 |
| 3:Dc:356:ARG:NH1 | 58:Dc:607:PC1:O14 | 2.52 | 0.43 |
| 58:Dv:408:PC1:O12 | 27:Eb:169:ARG:NH2 | 2.47 | 0.43 |
| 1:DA:270:THR:OG1 | 1:DA:271:THR:N | 2.51 | 0.42 |
| 3:DC:80:LEU:HD12 | 14:DO:276:GLN:CD | 2.44 | 0.42 |
| 3:DC:116:GLU:OE1 | 20:DU:276:LYS:NZ | 2.31 | 0.42 |
| 3:DC:126:ILE:O | 3:DC:126:ILE:HG22 | 2.17 | 0.42 |
| 3:DC:164:ASN:OD1 | 3:DC:172:ARG:NH2 | 2.49 | 0.42 |
| 3:DC:457:PHE:O | 3:DC:460:ILE:HG13 | 2.18 | 0.42 |
| 4:DD:162:THR:O | 4:DD:173:HIS:N | 2.43 | 0.42 |
| 4:DD:377:GLU:OE1 | 4:DD:377:GLU:N | 2.50 | 0.42 |
| 4:DD:466:GLN:OE1 | 4:DD:547:ASN:ND2 | 2.45 | 0.42 |
| 59:DR:401:3PE:H3I3 | 59:DR:401:3PE:H3C2 | 2.01 | 0.42 |
| 18:DS:209:THR:HG23 | 18:DS:210:PHE:N | 2.34 | 0.42 |
| 30:EE:154:LEU:HD22 | 30:EE:174:PHE:CD2 | 2.54 | 0.42 |
| 1:Da:525:ALA:HB2 | 1:Da:578:LEU:CB | 2.48 | 0.42 |
| 58:Dc:607:PC1:H2I1 | 57:Eh:1601:CDL:H361 | 2.01 | 0.42 |
| 4:Dd:410:SER:OG | 4:Dd:412:ARG:NH1 | 2.52 | 0.42 |
| 26:Ea:109:TYR:HB3 | 26:Ea:164:THR:HG23 | 2.01 | 0.42 |
| 66:Ed:201:HEM:HBC2 | 66:Ed:201:HEM:CMC | 2.48 | 0.42 |
| 30:Ee:124:HIS:CE1 | 30:Ee:128:THR:HG21 | 2.54 | 0.42 |
| 45:Et:6:ILE:N | 45:Et:6:ILE:HD12 | 2.34 | 0.42 |
| 1:DA:644:LYS:NZ | 19:DT:230:TRP:O | 2.49 | 0.42 |
| 2:DB:157:GLN:NE2 | 2:DB:370:GLU:OE2 | 2.52 | 0.42 |
| 5:DE:34:ASP:OD1 | 5:DE:38:LYS:NZ | 2.43 | 0.42 |
| 57:DM:501:CDL:OA9 | 42:EQ:71:LEU:HD21 | 2.19 | 0.42 |
| 13:DN:380:PHE:CE1 | 57:DY:301:CDL:H473 | 2.53 | 0.42 |
| 57:DN:504:CDL:H273 | 57:EB:304:CDL:H572 | 2.00 | 0.42 |
| 14:DO:32:LEU:HD21 | 14:DO:181:THR:OG1 | 2.18 | 0.42 |
| 15:DP:272:ASP:OD1 | 15:DP:273:THR:N | 2.52 | 0.42 |
| 19:DT:259:THR:HG21 | 31:EF:149:ASN:HD22 | 1.85 | 0.42 |
| 28:EC:23:ALA:O | 28:EC:24:GLU:C | 2.62 | 0.42 |
| 29:ED:106:ILE:HD13 | 36:EK:60:ILE:CD1 | 2.48 | 0.42 |
| 40:EO:39:TYR:OH | 58:EO:206:PC1:O14 | 2.36 | 0.42 |
| 49:EX:21:LEU:HD23 | 49:EX:21:LEU:C | 2.45 | 0.42 |
| 1:Da:234:TRP:NE1 | 27:Eb:46:THR:O | 2.52 | 0.42 |
| 4:Dd:506:LEU:HD22 | 4:Dd:544:PHE:CZ | 2.54 | 0.42 |
| 57:Dd:702:CDL:OA4 | 42:Eq:74:ILE:HG21 | 2.18 | 0.42 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 5:De:13:ASN:OD1 | 37:El:83:ARG:NH2 | 2.45 | 0.42 |
| 16:Dq:374:GLN:OE1 | 16:Dq:374:GLN:N | 2.52 | 0.42 |
| 19:Dt:87:TYR:OH | 19:Dt:142:ASP:OD1 | 2.20 | 0.42 |
| 26:Ea:176:MET:HE3 | 26:Ea:179:LEU:HD12 | 2.01 | 0.42 |
| 65:El:906:UQ8:C8 | 65:El:906:UQ8:C1M | 2.97 | 0.42 |
| 45:Et:70:TYR:OH | 50:Ey:11:THR:OG1 | 2.30 | 0.42 |
| 53:Dl:248:PHE:HB2 | 53:Dl:269:LEU:HD21 | 2.01 | 0.42 |
| 54:DA:701:HEA:HBC1 | 54:DA:701:HEA:HMC3 | 2.01 | 0.42 |
| 2:DB:244:THR:N | 45:ET:10:GLU:OE2 | 2.51 | 0.42 |
| 3:DC:111:ILE:HD12 | 3:DC:111:ILE:N | 2.35 | 0.42 |
| 12:DM:30:THR:HG22 | 12:DM:31:ALA:N | 2.34 | 0.42 |
| 57:DQ:1501:CDL:H432 | 57:DQ:1501:CDL:H472 | 2.02 | 0.42 |
| 22:DW:136:ILE:HD12 | 22:DW:136:ILE:N | 2.34 | 0.42 |
| 37:EL:131:TRP:HH2 | 65:EL:906:UQ8:H3MB | 1.83 | 0.42 |
| 3:Dc:55:THR:HG23 | 3:Dc:58:ASN:H | 1.84 | 0.42 |
| 3:Dc:106:VAL:HG21 | 20:Du:248:LEU:CD2 | 2.49 | 0.42 |
| 3:Dc:131:TYR:OH | 14:Do:245:GLN:O | 2.23 | 0.42 |
| 3:Dc:457:PHE:O | 3:Dc:460:ILE:HG13 | 2.19 | 0.42 |
| 9:Di:186:THR:HG22 | 9:Di:188:ASP:CG | 2.44 | 0.42 |
| 16:Dq:72:PRO:HB3 | 16:Dq:274:VAL:HG23 | 2.00 | 0.42 |
| 17:Dr:209:ILE:N | 17:Dr:210:PRO:HD2 | 2.34 | 0.42 |
| 8:DH:84:TYR:CD2 | 13:DN:348:LEU:HD23 | 2.55 | 0.42 |
| 12:DM:431:LEU:HD12 | 12:DM:431:LEU:N | 2.34 | 0.42 |
| 20:DU:100:ILE:C | 20:DU:100:ILE:HD12 | 2.45 | 0.42 |
| 22:DW:305:LEU:HD23 | 22:DW:305:LEU:C | 2.45 | 0.42 |
| 42:EQ:26:ASP:O | 42:EQ:29:VAL:HG22 | 2.20 | 0.42 |
| 1:Da:391:HIS:HB3 | 1:Da:392:PRO:HD3 | 2.01 | 0.42 |
| 2:Db:337:LEU:HD22 | 2:Db:337:LEU:N | 2.34 | 0.42 |
| 2:Db:509:SER:OG | 2:Db:512:ILE:O | 2.33 | 0.42 |
| 9:Di:77:GLN:OE1 | 9:Di:79:TYR:OH | 2.17 | 0.42 |
| 14:Do:299:LEU:HD12 | 14:Do:299:LEU:N | 2.33 | 0.42 |
| 20:Du:135:LEU:HD21 | 20:Du:180:ILE:HD12 | 2.00 | 0.42 |
| 32:Eg:8:ASN:O | 32:Eg:12:VAL:HG23 | 2.18 | 0.42 |
| 3:DC:142:TYR:O | 3:DC:144:ASP:N | 2.52 | 0.42 |
| 4:DD:596:ASP:HA | 4:DD:599:ILE:HG22 | 2.00 | 0.42 |
| 57:DH:201:CDL:H673 | 57:EB:304:CDL:OB7 | 2.19 | 0.42 |
| 19:DT:258:ASN:O | 19:DT:258:ASN:ND2 | 2.53 | 0.42 |
| 20:DU:246:TYR:N | 20:DU:247:PRO:HD2 | 2.35 | 0.42 |
| 21:DV:23:VAL:O | 21:DV:26:ILE:HG13 | 2.19 | 0.42 |
| 22:DW:304:GLY:O | 22:DW:305:LEU:C | 2.62 | 0.42 |
| 28:EC:39:LEU:O | 28:EC:43:THR:HG23 | 2.20 | 0.42 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 42:EQ:1:AME:HT21 | 42:EQ:117:HIS:CD2 | 2.54 | 0.42 |
| 17:Dr:137:ILE:HD12 | 17:Dr:137:ILE:N | 2.34 | 0.42 |
| 20:Du:21:ILE:HG22 | 20:Du:22:ASP:N | 2.34 | 0.42 |
| 21:Dv:23:VAL:O | 21:Dv:26:ILE:HG13 | 2.18 | 0.42 |
| 24:Dy:81:LEU:N | 24:Dy:82:PRO:CD | 2.83 | 0.42 |
| 28:Ec:101:LEU:HD23 | 28:Ec:101:LEU:C | 2.44 | 0.42 |
| 31:Ef:50:ILE:HG22 | 31:Ef:51:THR:N | 2.34 | 0.42 |
| 1:DA:391:HIS:HB3 | 1:DA:392:PRO:HD3 | 2.01 | 0.42 |
| 2:DB:48:TYR:O | 2:DB:51:ILE:HG13 | 2.20 | 0.42 |
| 4:DD:260:ASP:OD2 | 19:DT:42:ARG:NH2 | 2.52 | 0.42 |
| 9:DI:133:GLN:NE2 | 19:DT:207:GLU:O | 2.47 | 0.42 |
| 10:DJ:99:ASN:OD1 | 10:DJ:99:ASN:N | 2.53 | 0.42 |
| 12:DM:299:PHE:O | 12:DM:303:ASN:ND2 | 2.47 | 0.42 |
| 18:DS:21:VAL:HG11 | 18:DS:330:VAL:HG23 | 2.01 | 0.42 |
| 22:DW:271:GLU:OE1 | 22:DW:271:GLU:N | 2.45 | 0.42 |
| 42:EQ:39:SER:HA | 42:EQ:42:VAL:HG12 | 2.02 | 0.42 |
| 43:ER:27:ASN:ND2 | 43:ER:84:MET:O | 2.42 | 0.42 |
| 1:Da:310:PHE:CZ | 1:Da:347:ALA:HA | 2.55 | 0.42 |
| 3:Dc:268:PHE:CE1 | 3:Dc:272:ILE:HG21 | 2.54 | 0.42 |
| 21:Dv:45:THR:O | 21:Dv:45:THR:HG22 | 2.19 | 0.42 |
| 27:Eb:19:THR:HG23 | 27:Eb:20:PHE:CD2 | 2.55 | 0.42 |
| 35:Ev:39:THR:O | 35:Ev:39:THR:HG22 | 2.19 | 0.42 |
| 45:Et:73:VAL:HG11 | 50:Ey:10:ALA:HA | 2.02 | 0.42 |
| 49:Ex:21:LEU:C | 49:Ex:21:LEU:HD23 | 2.45 | 0.42 |
| 53:Dl:237:ASP:OD1 | 53:Dl:237:ASP:N | 2.53 | 0.42 |
| 53:DL:271:ASN:ND2 | 53:DL:273:SER:OG | 2.52 | 0.42 |
| 1:DA:111:VAL:HB | 1:DA:112:PRO:HD3 | 2.02 | 0.42 |
| 11:DK:121:ASP:OD1 | 11:DK:122:THR:N | 2.52 | 0.42 |
| 14:DO:357:LEU:HD23 | 14:DO:358:PHE:N | 2.35 | 0.42 |
| 15:DP:236:PHE:HD2 | 15:DP:340:ILE:HG23 | 1.84 | 0.42 |
| 21:DV:26:ILE:HD11 | 21:DV:299:ILE:HD12 | 2.01 | 0.42 |
| 21:DV:244:ARG:NH2 | 21:DV:259:TYR:OH | 2.53 | 0.42 |
| 23:DX:134:LEU:HD23 | 23:DX:134:LEU:C | 2.45 | 0.42 |
| 65:ED:603:UQ8:H10A | 57:ED:604:CDL:H121 | 2.01 | 0.42 |
| 39:EN:49:LEU:HD23 | 39:EN:49:LEU:C | 2.45 | 0.42 |
| 44:ES:42:ALA:HB1 | 44:ES:53:LEU:HD11 | 2.00 | 0.42 |
| 3:Dc:366:VAL:O | 3:Dc:369:ILE:HG13 | 2.20 | 0.42 |
| 3:Dc:582:ARG:HD2 | 42:Eq:1:AME:HG2 | 2.00 | 0.42 |
| 23:Dx:109:ARG:NE | 58:Dx:1204:PC1:O14 | 2.51 | 0.42 |
| 3:DC:190:LEU:HD11 | 25:DZ:170:LEU:HD11 | 2.02 | 0.42 |
| 11:DK:40:GLN:NE2 | 11:DK:81:ARG:O | 2.48 | 0.42 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 18:DS:25:VAL:HG23 | 18:DS:25:VAL:O | 2.19 | 0.42 |
| 19:DT:249:ASN:ND2 | 31:EF:77:ILE:HD13 | 2.35 | 0.42 |
| 33:EH:1:AME:O | 33:EH:1:AME:HG2 | 2.20 | 0.42 |
| 50:EY:1:MET:HG3 | 50:EY:5:LEU:HD23 | 2.01 | 0.42 |
| 13:Dn:332:TYR:O | 13:Dn:337:LYS:N | 2.52 | 0.42 |
| 28:Ec:45:HIS:ND1 | 28:Ec:49:ASN:OD1 | 2.51 | 0.42 |
| 65:Ed:202:UQ8:H10B | 65:Ed:202:UQ8:H13 | 2.02 | 0.42 |
| 48:Ew:26:TYR:O | 48:Ew:30:VAL:HG12 | 2.19 | 0.42 |
| 16:DQ:34:THR:HG23 | 16:DQ:62:ARG:HH12 | 1.83 | 0.42 |
| 17:DR:124:TYR:CE2 | 17:DR:128:VAL:HG21 | 2.55 | 0.42 |
| 24:DY:81:LEU:HD12 | 24:DY:196:TYR:HD2 | 1.85 | 0.42 |
| 24:DY:81:LEU:N | 24:DY:82:PRO:CD | 2.83 | 0.42 |
| 24:DY:122:THR:HG23 | 24:DY:123:ARG:HG3 | 2.02 | 0.42 |
| 1:Da:217:LYS:C | 1:Da:218:LEU:HD12 | 2.45 | 0.42 |
| 3:Dc:479:TYR:O | 3:Dc:483:VAL:HG23 | 2.19 | 0.42 |
| 3:Dc:545:ARG:NH1 | 33:Eh:104:THR:OG1 | 2.47 | 0.42 |
| 4:Dd:286:TYR:CE2 | 4:Dd:290:LEU:HD11 | 2.55 | 0.42 |
| 20:Du:246:TYR:N | 20:Du:247:PRO:HD2 | 2.35 | 0.42 |
| 23:Dx:62:LEU:HD11 | 23:Dx:94:VAL:HG23 | 2.02 | 0.42 |
| 29:Ed:165:SER:OG | 29:Ed:166:ILE:N | 2.52 | 0.42 |
| 34:Ei:80:GLY:HA3 | 34:Ei:109:LEU:HD12 | 2.01 | 0.42 |
| 59:El:905:3PE:H2E2 | 59:El:905:3PE:H2I2 | 2.01 | 0.42 |
| 1:DA:342:THR:HG22 | 1:DA:396:VAL:HA | 2.01 | 0.42 |
| 4:DD:168:ASP:O | 40:EO:9:VAL:HG22 | 2.20 | 0.42 |
| 11:DK:38:VAL:HG21 | 11:DK:91:LEU:HD21 | 2.01 | 0.42 |
| 13:DN:218:ILE:HD12 | 13:DN:218:ILE:N | 2.35 | 0.42 |
| 15:DP:169:TRP:CD1 | 15:DP:170:VAL:HG23 | 2.55 | 0.42 |
| 21:DV:137:SER:N | 21:DV:138:PRO:HD2 | 2.35 | 0.42 |
| 3:Dc:239:ILE:HD11 | 27:Eb:122:PHE:HE1 | 1.85 | 0.42 |
| 4:Dd:97:TYR:OH | 4:Dd:225:GLU:OE1 | 2.27 | 0.42 |
| 4:Dd:370:PHE:CD1 | 4:Dd:557:VAL:HG22 | 2.54 | 0.42 |
| 11:Dk:74:ILE:O | 11:Dk:81:ARG:NH1 | 2.47 | 0.42 |
| 12:Dm:307:LYS:NZ | 57:Du:402:CDL:OB3 | 2.38 | 0.42 |
| 14:Do:471:PRO:O | 14:Do:472:SER:OG | 2.30 | 0.42 |
| 17:Dr:342:ARG:O | 19:Dt:249:ASN:ND2 | 2.53 | 0.42 |
| 29:Ed:156:ILE:HG22 | 29:Ed:157:TRP:N | 2.35 | 0.42 |
| 33:Eh:12:ASP:OD1 | 33:Eh:13:ARG:N | 2.44 | 0.42 |
| 65:El:906:UQ8:C8 | 65:El:906:UQ8:H1M | 2.49 | 0.42 |
| 41:Ep:101:ILE:C | 41:Ep:101:ILE:HD12 | 2.44 | 0.42 |
| 47:Ej:99:PHE:O | 47:Ej:100:PRO:C | 2.63 | 0.42 |
| 1:DA:310:PHE:CD1 | 1:DA:310:PHE:C | 2.97 | 0.41 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 57:DA:709:CDL:OB4 | 13:DN:359:SER:OG | 2.25 | 0.41 |
| 4:DD:120:THR:HG22 | 44:ES:25:TRP:CE3 | 2.54 | 0.41 |
| 12:DM:163:ARG:NH1 | 19:DT:71:ILE:O | 2.53 | 0.41 |
| 26:EA:102:LEU:HD23 | 26:EA:102:LEU:O | 2.19 | 0.41 |
| 2:Db:588:VAL:HG13 | 2:Db:589:SER:N | 2.35 | 0.41 |
| 3:Dc:578:LYS:NZ | 6:Df:200:ASN:OD1 | 2.28 | 0.41 |
| 25:Dz:193:HIS:NE2 | 42:Eq:70:ASN:O | 2.53 | 0.41 |
| 46:Eu:53:LEU:O | 46:Eu:53:LEU:HD23 | 2.19 | 0.41 |
| 1:DA:155:ILE:HG21 | 1:DA:295:LEU:HD11 | 2.01 | 0.41 |
| 3:DC:552:SER:N | 33:EH:142:GLN:OE1 | 2.53 | 0.41 |
| 57:DD:703:CDL:CA6 | 10:DJ:65:LEU:HD22 | 2.50 | 0.41 |
| 16:DQ:268:THR:HG21 | 16:DQ:273:ILE:HD11 | 2.02 | 0.41 |
| 21:DV:211:ILE:HG23 | 27:EB:174:TYR:O | 2.20 | 0.41 |
| 29:ED:165:SER:OG | 29:ED:166:ILE:N | 2.53 | 0.41 |
| 31:EF:35:ILE:HD12 | 31:EF:35:ILE:N | 2.35 | 0.41 |
| 44:ES:45:ILE:HD11 | 44:ES:52:GLU:OE2 | 2.20 | 0.41 |
| 9:Di:146:ILE:HD12 | 9:Di:146:ILE:N | 2.35 | 0.41 |
| 14:Do:447:VAL:HG22 | 14:Do:448:VAL:N | 2.35 | 0.41 |
| 20:Du:135:LEU:CD2 | 20:Du:180:ILE:HD12 | 2.50 | 0.41 |
| 23:Dx:143:ARG:NH2 | 23:Dx:149:GLU:OE2 | 2.52 | 0.41 |
| 45:Et:77:MET:HE2 | 45:Et:79:LEU:HD21 | 2.01 | 0.41 |
| 1:DA:242:GLU:OE2 | 27:EB:74:LYS:NZ | 2.41 | 0.41 |
| 1:DA:335:VAL:CG2 | 1:DA:407:MET:HE2 | 2.49 | 0.41 |
| 1:DA:415:ARG:NH1 | 1:DA:416:ARG:O | 2.53 | 0.41 |
| 2:DB:110:SER:HB3 | 6:DF:110:LEU:HD21 | 2.03 | 0.41 |
| 58:DC:608:PC1:H2I1 | 57:EL:902:CDL:C36 | 2.50 | 0.41 |
| 4:DD:273:MET:HE1 | 8:DH:28:TYR:HB3 | 2.02 | 0.41 |
| 6:DF:182:ASP:OD1 | 6:DF:183:ASP:N | 2.54 | 0.41 |
| 15:DP:365:THR:HG22 | 15:DP:366:LYS:N | 2.35 | 0.41 |
| 16:DQ:123:PHE:O | 16:DQ:124:LYS:C | 2.63 | 0.41 |
| 17:DR:140:PRO:HG2 | 17:DR:144:ILE:HD11 | 2.01 | 0.41 |
| 34:EI:47:GLU:O | 34:EI:54:ARG:NH2 | 2.53 | 0.41 |
| 1:Da:412:ASN:O | 1:Da:483:LYS:N | 2.52 | 0.41 |
| 3:Dc:106:VAL:HG21 | 20:Du:248:LEU:HD23 | 2.01 | 0.41 |
| 13:Dn:365:ARG:NH1 | 25:Dz:44:ASN:O | 2.53 | 0.41 |
| 20:Du:15:PHE:CE2 | 20:Du:19:LEU:HD11 | 2.55 | 0.41 |
| 1:DA:194:TYR:CE2 | 1:DA:198:LEU:HD11 | 2.55 | 0.41 |
| 1:DA:331:LEU:HD21 | 4:DD:171:GLU:CD | 2.45 | 0.41 |
| 1:DA:645:ARG:NE | 19:DT:146:ILE:HD11 | 2.35 | 0.41 |
| 3:DC:366:VAL:O | 3:DC:369:ILE:HG13 | 2.20 | 0.41 |
| 4:DD:435:LEU:HD23 | 4:DD:435:LEU:C | 2.46 | 0.41 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 4:DD:497:HIS:ND1 | 13:DN:191:TYR:OH | 2.31 | 0.41 |
| 10:DJ:115:TYR:O | 10:DJ:119:VAL:HG23 | 2.21 | 0.41 |
| 15:DP:190:LYS:O | 15:DP:193:ARG:NH1 | 2.45 | 0.41 |
| 29:ED:53:ASP:OD1 | 60:EI:402:LPP:O2 | 2.38 | 0.41 |
| 34:EI:145:ASP:N | 34:EI:145:ASP:OD1 | 2.53 | 0.41 |
| 2:Db:155:GLU:HB3 | 2:Db:158:THR:HG22 | 2.02 | 0.41 |
| 3:Dc:77:VAL:O | 3:Dc:77:VAL:HG22 | 2.20 | 0.41 |
| 8:Dh:88:TYR:OH | 13:Dn:341:ASN:O | 2.34 | 0.41 |
| 16:Dq:293:THR:O | 16:Dq:293:THR:HG22 | 2.19 | 0.41 |
| 57:Dv:404:CDL:H1O1 | 57:Dv:404:CDL:PA1 | 2.43 | 0.41 |
| 26:Ea:168:LEU:HD23 | 26:Ea:168:LEU:C | 2.46 | 0.41 |
| 1:DA:215:VAL:O | 1:DA:215:VAL:HG13 | 2.21 | 0.41 |
| 1:DA:247:ALA:O | 1:DA:251:VAL:HG11 | 2.20 | 0.41 |
| 4:DD:293:VAL:HG21 | 19:DT:54:VAL:HG12 | 2.02 | 0.41 |
| 9:DI:146:ILE:N | 9:DI:146:ILE:HD12 | 2.36 | 0.41 |
| 9:DI:236:ILE:HD12 | 9:DI:236:ILE:N | 2.36 | 0.41 |
| 10:DJ:140:THR:HG23 | 43:ER:85:TYR:OH | 2.20 | 0.41 |
| 16:DQ:277:VAL:HG12 | 16:DQ:278:ASN:N | 2.35 | 0.41 |
| 17:DR:209:ILE:HG22 | 17:DR:213:TRP:CD1 | 2.56 | 0.41 |
| 66:ED:602:HEM:HBC2 | 66:ED:602:HEM:CMC | 2.48 | 0.41 |
| 43:ER:93:TYR:CZ | 43:ER:97:LEU:HD11 | 2.55 | 0.41 |
| 5:De:125:ASP:OD1 | 5:De:126:GLU:N | 2.53 | 0.41 |
| 13:Dn:392:LYS:N | 13:Dn:393:PRO:HD2 | 2.35 | 0.41 |
| 20:Du:82:LEU:HD21 | 20:Du:140:PHE:CD2 | 2.55 | 0.41 |
| 24:Dy:120:LEU:HD23 | 24:Dy:120:LEU:C | 2.46 | 0.41 |
| 25:Dz:81:HIS:NE2 | 25:Dz:117:GLU:OE1 | 2.51 | 0.41 |
| 26:Ea:158:VAL:HG23 | 26:Ea:159:LEU:N | 2.35 | 0.41 |
| 43:Er:93:TYR:CZ | 43:Er:97:LEU:HD11 | 2.55 | 0.41 |
| 18:DS:156:LEU:HD12 | 18:DS:194:LEU:O | 2.20 | 0.41 |
| 31:EF:50:ILE:HG22 | 31:EF:51:THR:N | 2.36 | 0.41 |
| 37:EL:110:ASN:ND2 | 44:ES:62:ASN:O | 2.53 | 0.41 |
| 45:ET:6:ILE:HD12 | 45:ET:6:ILE:N | 2.35 | 0.41 |
| 45:ET:30:LEU:HD23 | 45:ET:30:LEU:C | 2.45 | 0.41 |
| 2:Db:195:ILE:HD12 | 2:Db:195:ILE:N | 2.35 | 0.41 |
| 25:Dz:25:ILE:HG22 | 25:Dz:26:TYR:CD2 | 2.56 | 0.41 |
| 29:Ed:128:LEU:O | 29:Ed:128:LEU:HD23 | 2.20 | 0.41 |
| 38:Em:138:ARG:NH1 | 38:Em:142:LEU:HD22 | 2.35 | 0.41 |
| 3:DC:143:ASN:N | 14:DO:251:GLN:O | 2.53 | 0.41 |
| 3:DC:413:LEU:C | 3:DC:413:LEU:HD12 | 2.46 | 0.41 |
| 14:DO:447:VAL:HG22 | 14:DO:448:VAL:N | 2.36 | 0.41 |
| 18:DS:57:VAL:HG22 | 59:DS:403:3PE:H352 | 2.02 | 0.41 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 26:EA:79:ASP:OD1 | 26:EA:106:ARG:NH2 | 2.53 | 0.41 |
| 34:EI:105:ILE:HG23 | 34:EI:106:CYS:N | 2.36 | 0.41 |
| 39:EN:146:ASN:OD1 | 39:EN:147:ARG:N | 2.54 | 0.41 |
| 2:Db:121:GLN:HA | 2:Db:122:TRP:HA | 1.85 | 0.41 |
| 57:Dn:501:CDL:H671 | 58:Dv:405:PC1:C3H | 2.50 | 0.41 |
| 18:Ds:301:PHE:N | 57:Ds:402:CDL:OA3 | 2.53 | 0.41 |
| 31:Ef:128:VAL:HG12 | 31:Ef:130:GLN:H | 1.85 | 0.41 |
| 42:Eq:68:VAL:HG12 | 42:Eq:76:ARG:HG3 | 2.03 | 0.41 |
| 53:DL:358:VAL:N | 53:DL:370:LEU:O | 2.49 | 0.41 |
| 3:DC:109:ALA:HB3 | 3:DC:110:PRO:HD3 | 2.03 | 0.41 |
| 13:DN:117:ILE:HD12 | 13:DN:136:PHE:HE1 | 1.86 | 0.41 |
| 20:DU:135:LEU:CD2 | 20:DU:180:ILE:HD12 | 2.50 | 0.41 |
| 1:Da:287:THR:O | 1:Da:364:ARG:NH2 | 2.48 | 0.41 |
| 1:Da:508:LEU:HD21 | 1:Da:522:TYR:HD2 | 1.86 | 0.41 |
| 3:Dc:378:THR:O | 3:Dc:378:THR:HG22 | 2.20 | 0.41 |
| 6:Df:155:PHE:O | 6:Df:158:VAL:HG13 | 2.21 | 0.41 |
| 10:Dj:111:VAL:HG21 | 58:Eo:201:PC1:H2A1 | 2.03 | 0.41 |
| 12:Dm:431:LEU:N | 12:Dm:431:LEU:HD12 | 2.36 | 0.41 |
| 14:Do:57:LEU:HD22 | 14:Do:106:VAL:HG13 | 2.02 | 0.41 |
| 16:Dq:247:TYR:CD1 | 19:Dt:316:ILE:HD11 | 2.56 | 0.41 |
| 18:Ds:99:TYR:CZ | 18:Ds:103:ILE:HG21 | 2.56 | 0.41 |
| 20:Du:64:ARG:NE | 20:Du:77:ASP:OD2 | 2.54 | 0.41 |
| 29:Ed:114:TYR:CD2 | 65:Ed:202:UQ8:H4M | 2.56 | 0.41 |
| 39:En:123:ASN:ND2 | 39:En:123:ASN:O | 2.54 | 0.41 |
| 58:Eo:204:PC1:H2I3 | 58:Eo:204:PC1:C2E | 2.51 | 0.41 |
| 41:Ep:48:ARG:NH1 | 41:Ep:127:LEU:OXT | 2.50 | 0.41 |
| 42:Eq:12:THR:HG22 | 42:Eq:13:HIS:N | 2.35 | 0.41 |
| 1:DA:125:TYR:CE1 | 19:DT:208:ILE:HD12 | 2.56 | 0.41 |
| 1:DA:258:LYS:HB2 | 1:DA:261:VAL:HG23 | 2.03 | 0.41 |
| 1:DA:566:TYR:OH | 65:DS:404:UQ8:O2 | 2.33 | 0.41 |
| 2:DB:203:LEU:C | 2:DB:203:LEU:HD13 | 2.46 | 0.41 |
| 4:DD:100:MET:SD | 4:DD:248:THR:HG23 | 2.61 | 0.41 |
| 57:DI:701:CDL:H273 | 57:DI:701:CDL:H473 | 2.02 | 0.41 |
| 12:DM:362:ASP:O | 12:DM:380:ARG:NH2 | 2.54 | 0.41 |
| 13:DN:94:LEU:HD21 | 29:ED:11:LYS:O | 2.19 | 0.41 |
| 13:DN:113:PHE:CE2 | 13:DN:117:ILE:HD11 | 2.56 | 0.41 |
| 13:DN:249:ILE:HD12 | 13:DN:249:ILE:O | 2.21 | 0.41 |
| 15:DP:164:ALA:HB1 | 15:DP:214:THR:HG22 | 2.02 | 0.41 |
| 18:DS:302:THR:O | 18:DS:302:THR:HG22 | 2.21 | 0.41 |
| 19:DT:270:TRP:O | 31:EF:127:ASN:ND2 | 2.54 | 0.41 |
| 19:DT:318:ILE:HD12 | 19:DT:318:ILE:C | 2.46 | 0.41 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 21:DV:256:ARG:NH2 | 39:EN:14:ALA:O | 2.54 | 0.41 |
| 29:ED:106:ILE:O | 29:ED:110:SER:OG | 2.33 | 0.41 |
| 30:EE:163:ASN:OD1 | 30:EE:166:ASP:N | 2.42 | 0.41 |
| 30:EE:164:VAL:HG22 | 49:EX:34:ASP:OD1 | 2.21 | 0.41 |
| 31:EF:58:LEU:C | 31:EF:58:LEU:HD23 | 2.46 | 0.41 |
| 41:EP:101:ILE:C | 41:EP:101:ILE:HD12 | 2.46 | 0.41 |
| 12:Dm:83:TYR:O | 12:Dm:87:VAL:HG23 | 2.20 | 0.41 |
| 12:Dm:309:HIS:ND1 | 42:Eq:43:GLU:OE2 | 2.47 | 0.41 |
| 14:Do:305:LEU:HD23 | 14:Do:305:LEU:O | 2.21 | 0.41 |
| 16:Dq:34:THR:OG1 | 16:Dq:34:THR:O | 2.39 | 0.41 |
| 23:Dx:156:ASN:ND2 | 32:Eg:99:TYR:OH | 2.51 | 0.41 |
| 24:Dy:140:TRP:CD1 | 24:Dy:144:LEU:HD13 | 2.56 | 0.41 |
| 46:Eu:35:ASN:O | 46:Eu:41:GLN:NE2 | 2.50 | 0.41 |
| 53:Dl:348:VAL:HG12 | 53:Dl:350:ARG:H | 1.85 | 0.41 |
| 4:DD:362:ARG:NH1 | 4:DD:383:ASP:OD2 | 2.48 | 0.41 |
| 9:DI:45:GLU:OE2 | 18:DS:277:ASN:ND2 | 2.54 | 0.41 |
| 18:DS:82:GLU:HA | 18:DS:85:LYS:HG2 | 2.03 | 0.41 |
| 2:Db:122:TRP:HD1 | 2:Db:553:CYS:HG | 1.65 | 0.41 |
| 2:Db:139:THR:HG21 | 2:Db:569:PHE:CZ | 2.55 | 0.41 |
| 2:Db:154:GLY:O | 6:Df:114:GLN:NE2 | 2.54 | 0.41 |
| 2:Db:169:ARG:NH2 | 30:Ee:72:ILE:HG23 | 2.36 | 0.41 |
| 13:Dn:386:ILE:HG21 | 27:Eb:131:VAL:CG2 | 2.51 | 0.41 |
| 20:Du:274:ASN:O | 20:Du:277:THR:HG22 | 2.21 | 0.41 |
| 35:Ev:1:AME:HT23 | 39:En:134:LEU:O | 2.21 | 0.41 |
| 3:DC:268:PHE:CE1 | 3:DC:272:ILE:HG21 | 2.56 | 0.40 |
| 18:DS:1:AME:HT23 | 18:DS:6:GLU:HB2 | 2.02 | 0.40 |
| 18:DS:258:VAL:O | 18:DS:258:VAL:HG12 | 2.21 | 0.40 |
| 24:DY:81:LEU:N | 24:DY:82:PRO:HD2 | 2.37 | 0.40 |
| 42:EQ:30:ASN:CG | 42:EQ:33:THR:HG1 | 2.17 | 0.40 |
| 45:ET:37:LEU:C | 45:ET:37:LEU:HD12 | 2.47 | 0.40 |
| 2:Db:203:LEU:C | 2:Db:203:LEU:HD13 | 2.46 | 0.40 |
| 12:Dm:261:ASN:OD1 | 12:Dm:262:ALA:N | 2.54 | 0.40 |
| 47:Ej:96:ILE:HG21 | 47:Ej:99:PHE:CD2 | 2.56 | 0.40 |
| 1:DA:616:ILE:HD11 | 59:DS:401:3PE:H3H1 | 2.03 | 0.40 |
| 13:DN:271:ILE:HD11 | 19:DT:55:GLN:OE1 | 2.22 | 0.40 |
| 15:DP:184:LYS:HG2 | 15:DP:296:THR:HG22 | 2.03 | 0.40 |
| 15:DP:225:GLN:OE1 | 15:DP:225:GLN:N | 2.54 | 0.40 |
| 16:DQ:188:LEU:HD23 | 16:DQ:188:LEU:C | 2.45 | 0.40 |
| 37:EL:75:ILE:HD11 | 37:EL:124:LEU:HD12 | 2.03 | 0.40 |
| 37:EL:140:ASP:OD2 | 37:EL:144:GLU:N | 2.54 | 0.40 |
| 38:EM:44:ASP:HB3 | 38:EM:47:LEU:HD13 | 2.02 | 0.40 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 3:Dc:50:GLU:OE1 | 3:Dc:51:ASN:N | 2.54 | 0.40 |
| 3:Dc:317:TRP:NE1 | 3:Dc:488:ASN:OD1 | 2.53 | 0.40 |
| 10:Dj:107:TRP:O | 10:Dj:111:VAL:HG23 | 2.21 | 0.40 |
| 13:Dn:127:ILE:HD12 | 13:Dn:135:ILE:HG23 | 2.03 | 0.40 |
| 18:Ds:91:LYS:O | 18:Ds:95:ASN:ND2 | 2.47 | 0.40 |
| 24:Dy:71:TYR:CD2 | 24:Dy:195:LEU:HD23 | 2.56 | 0.40 |
| 38:Em:52:VAL:HG13 | 38:Em:53:GLU:N | 2.37 | 0.40 |
| 40:Eo:109:THR:HG22 | 40:Eo:110:LEU:H | 1.84 | 0.40 |
| 45:Et:37:LEU:HD12 | 45:Et:37:LEU:C | 2.46 | 0.40 |
| 53:DL:87:THR:HG21 | 53:DL:95:THR:HA | 2.03 | 0.40 |
| 4:DD:119:VAL:HG23 | 4:DD:120:THR:N | 2.36 | 0.40 |
| 21:DV:26:ILE:HD11 | 21:DV:299:ILE:CD1 | 2.52 | 0.40 |
| 23:DX:84:PHE:CE2 | 23:DX:88:LEU:HD11 | 2.56 | 0.40 |
| 42:EQ:12:THR:HG22 | 42:EQ:13:HIS:N | 2.36 | 0.40 |
| 2:Db:1:MET:SD | 6:Df:81:VAL:HG11 | 2.61 | 0.40 |
| 3:Dc:176:ILE:N | 3:Dc:176:ILE:HD12 | 2.37 | 0.40 |
| 10:Dj:211:GLY:O | 40:Eo:69:TRP:N | 2.52 | 0.40 |
| 57:Dj:403:CDL:HB32 | 44:Es:63:THR:HG21 | 2.03 | 0.40 |
| 12:Dm:447:ASP:OD1 | 12:Dm:448:PHE:N | 2.54 | 0.40 |
| 14:Do:245:GLN:O | 14:Do:248:VAL:HG22 | 2.21 | 0.40 |
| 15:Dp:219:VAL:HG22 | 15:Dp:219:VAL:O | 2.22 | 0.40 |
| 15:Dp:365:THR:HG22 | 15:Dp:366:LYS:N | 2.36 | 0.40 |
| 21:Dv:137:SER:N | 21:Dv:138:PRO:HD2 | 2.35 | 0.40 |
| 35:Ev:35:VAL:HG12 | 35:Ev:36:ALA:N | 2.36 | 0.40 |
| 65:En:1203:UQ8:H46 | 65:En:1203:UQ8:H42A | 1.84 | 0.40 |
| 45:Et:48:THR:HG22 | 45:Et:49:GLN:N | 2.36 | 0.40 |
| 53:Dl:359:ASP:OD1 | 53:Dl:359:ASP:N | 2.54 | 0.40 |
| 1:DA:191:TYR:O | 1:DA:191:TYR:CG | 2.73 | 0.40 |
| 2:DB:118:ARG:NH1 | 5:DE:126:GLU:OE2 | 2.54 | 0.40 |
| 2:DB:588:VAL:HG13 | 2:DB:589:SER:N | 2.36 | 0.40 |
| 3:DC:106:VAL:HG13 | 20:DU:247:PRO:HG2 | 2.04 | 0.40 |
| 3:DC:142:TYR:O | 3:DC:143:ASN:C | 2.64 | 0.40 |
| 59:DC:606:3PE:H3I2 | 10:DJ:117:ILE:HD11 | 2.02 | 0.40 |
| 12:DM:37:LEU:HA | 12:DM:40:VAL:HG12 | 2.03 | 0.40 |
| 24:DY:160:LEU:O | 24:DY:164:LEU:HD13 | 2.21 | 0.40 |
| 38:EM:52:VAL:HG13 | 38:EM:53:GLU:N | 2.36 | 0.40 |
| 50:EY:62:LEU:O | 50:EY:64:LYS:NZ | 2.54 | 0.40 |
| 1:Da:127:VAL:O | 1:Da:322:MET:N | 2.52 | 0.40 |
| 3:Dc:53:LEU:N | 3:Dc:53:LEU:HD22 | 2.36 | 0.40 |
| 4:Dd:374:LEU:HD23 | 4:Dd:375:THR:H | 1.87 | 0.40 |
| 4:Dd:503:LEU:HB2 | 36:Ek:40:ILE:HD11 | 2.02 | 0.40 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 4:Dd:572:TRP:N | 57:Dd:705:CDL:OB4 | 2.45 | 0.40 |
| 8:Dh:67:HIS:O | 8:Dh:71:VAL:HG23 | 2.21 | 0.40 |
| 14:Do:357:LEU:HD23 | 14:Do:358:PHE:N | 2.36 | 0.40 |
| 29:Ed:89:TYR:CE2 | 29:Ed:93:LEU:HD11 | 2.57 | 0.40 |
| 42:Eq:39:SER:HA | 42:Eq:42:VAL:HG12 | 2.03 | 0.40 |
| 45:Et:30:LEU:HD23 | 45:Et:30:LEU:C | 2.46 | 0.40 |
| 47:Ej:79:VAL:O | 47:Ej:83:VAL:HG22 | 2.21 | 0.40 |
| 2:DB:25:ASP:OD1 | 2:DB:29:HIS:NE2 | 2.54 | 0.40 |
| 2:DB:176:LYS:NZ | 30:EE:78:GLU:OE2 | 2.40 | 0.40 |
| 2:DB:376:ILE:N | 2:DB:376:ILE:HD12 | 2.37 | 0.40 |
| 3:DC:578:LYS:NZ | 6:DF:198:ALA:O | 2.52 | 0.40 |
| 4:DD:77:SER:OG | 57:DM:501:CDL:OA4 | 2.27 | 0.40 |
| 12:DM:449:ILE:O | 12:DM:453:SER:OG | 2.36 | 0.40 |
| 16:DQ:293:THR:O | 16:DQ:293:THR:HG22 | 2.21 | 0.40 |
| 43:ER:79:ARG:O | 43:ER:94:ARG:NH2 | 2.44 | 0.40 |
| 47:EJ:41:VAL:HG11 | 47:EJ:52:ILE:CD1 | 2.52 | 0.40 |
| 3:Dc:60:ILE:O | 3:Dc:62:LEU:HD12 | 2.20 | 0.40 |
| 19:Dt:123:THR:HG22 | 19:Dt:124:ARG:N | 2.37 | 0.40 |
| 19:Dt:279:GLU:O | 19:Dt:283:VAL:HG23 | 2.22 | 0.40 |
| 21:Dv:224:LEU:HD11 | 21:Dv:293:ALA:HB1 | 2.04 | 0.40 |
| 21:Dv:269:LEU:C | 21:Dv:269:LEU:HD23 | 2.45 | 0.40 |
| 26:Ea:222:GLN:OE1 | 26:Ea:222:GLN:N | 2.47 | 0.40 |
| 31:Ef:58:LEU:C | 31:Ef:58:LEU:HD23 | 2.47 | 0.40 |
| 34:Ei:101:LEU:O | 34:Ei:105:ILE:HG22 | 2.21 | 0.40 |
| 49:Ex:3:ASP:O | 49:Ex:7:ILE:HD13 | 2.21 | 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 | DA | 669/688 (97%) | 654 (98%) | 15 (2%) | 0 | 100 | 100 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|---|---|---|---|---|---|---|---|
| 1 | Da | 669/688 (97%) | 657 (98%) | 12 (2%) | 0 | 100 | 100 |
| 2 | DB | 602/604 (100%) | 586 (97%) | 16 (3%) | 0 | 100 | 100 |
| 2 | Db | 602/604 (100%) | 592 (98%) | 10 (2%) | 0 | 100 | 100 |
| 3 | DC | 580/594 (98%) | 569 (98%) | 9 (2%) | 2 (0%) | 36 | 58 |
| 3 | Dc | 580/594 (98%) | 569 (98%) | 11 (2%) | 0 | 100 | 100 |
| 4 | DD | 554/637 (87%) | 551 (100%) | 3 (0%) | 0 | 100 | 100 |
| 4 | Dd | 554/637 (87%) | 551 (100%) | 3 (0%) | 0 | 100 | 100 |
| 5 | DE | 124/130 (95%) | 121 (98%) | 3 (2%) | 0 | 100 | 100 |
| 5 | De | 124/130 (95%) | 121 (98%) | 3 (2%) | 0 | 100 | 100 |
| 6 | DF | 220/230 (96%) | 216 (98%) | 4 (2%) | 0 | 100 | 100 |
| 6 | Df | 220/230 (96%) | 215 (98%) | 5 (2%) | 0 | 100 | 100 |
| 7 | DG | 96/103 (93%) | 94 (98%) | 2 (2%) | 0 | 100 | 100 |
| 7 | Dg | 96/103 (93%) | 95 (99%) | 1 (1%) | 0 | 100 | 100 |
| 8 | DH | 131/133 (98%) | 124 (95%) | 7 (5%) | 0 | 100 | 100 |
| 8 | Dh | 131/133 (98%) | 125 (95%) | 6 (5%) | 0 | 100 | 100 |
| 9 | DI | 203/236 (86%) | 198 (98%) | 4 (2%) | 1 (0%) | 24 | 46 |
| 9 | Di | 203/236 (86%) | 196 (97%) | 6 (3%) | 1 (0%) | 24 | 46 |
| 10 | DJ | 218/220 (99%) | 218 (100%) | 0 | 0 | 100 | 100 |
| 10 | Dj | 218/220 (99%) | 216 (99%) | 2 (1%) | 0 | 100 | 100 |
| 11 | DK | 128/990 (13%) | 120 (94%) | 8 (6%) | 0 | 100 | 100 |
| 11 | Dk | 128/990 (13%) | 121 (94%) | 7 (6%) | 0 | 100 | 100 |
| 12 | DM | 453/490 (92%) | 446 (98%) | 7 (2%) | 0 | 100 | 100 |
| 12 | Dm | 453/490 (92%) | 446 (98%) | 7 (2%) | 0 | 100 | 100 |
| 13 | DN | 451/453 (100%) | 444 (98%) | 7 (2%) | 0 | 100 | 100 |
| 13 | Dn | 451/453 (100%) | 444 (98%) | 7 (2%) | 0 | 100 | 100 |
| 14 | DO | 431/473 (91%) | 429 (100%) | 2 (0%) | 0 | 100 | 100 |
| 14 | Do | 431/473 (91%) | 427 (99%) | 4 (1%) | 0 | 100 | 100 |
| 15 | DP | 288/402 (72%) | 283 (98%) | 5 (2%) | 0 | 100 | 100 |
| 15 | Dp | 288/402 (72%) | 283 (98%) | 5 (2%) | 0 | 100 | 100 |
| 16 | DQ | 381/385 (99%) | 368 (97%) | 13 (3%) | 0 | 100 | 100 |
| 16 | Dq | 381/385 (99%) | 370 (97%) | 11 (3%) | 0 | 100 | 100 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|---|---|---|---|---|---|---|---|
| 17 | DR | 241/348 (69%) | 237 (98%) | 4 (2%) | 0 | 100 | 100 |
| 17 | Dr | 241/348 (69%) | 238 (99%) | 3 (1%) | 0 | 100 | 100 |
| 18 | DS | 344/346 (99%) | 343 (100%) | 1 (0%) | 0 | 100 | 100 |
| 18 | Ds | 344/346 (99%) | 343 (100%) | 1 (0%) | 0 | 100 | 100 |
| 19 | DT | 291/318 (92%) | 290 (100%) | 1 (0%) | 0 | 100 | 100 |
| 19 | Dt | 291/318 (92%) | 290 (100%) | 1 (0%) | 0 | 100 | 100 |
| 20 | DU | 327/330 (99%) | 321 (98%) | 6 (2%) | 0 | 100 | 100 |
| 20 | Du | 327/330 (99%) | 321 (98%) | 6 (2%) | 0 | 100 | 100 |
| 21 | DV | 316/318 (99%) | 312 (99%) | 4 (1%) | 0 | 100 | 100 |
| 21 | Dv | 316/318 (99%) | 311 (98%) | 5 (2%) | 0 | 100 | 100 |
| 22 | DW | 299/318 (94%) | 298 (100%) | 1 (0%) | 0 | 100 | 100 |
| 22 | Dw | 299/318 (94%) | 297 (99%) | 2 (1%) | 0 | 100 | 100 |
| 23 | DX | 249/252 (99%) | 246 (99%) | 3 (1%) | 0 | 100 | 100 |
| 23 | Dx | 249/252 (99%) | 248 (100%) | 1 (0%) | 0 | 100 | 100 |
| 24 | DY | 185/234 (79%) | 184 (100%) | 1 (0%) | 0 | 100 | 100 |
| 24 | Dy | 185/234 (79%) | 184 (100%) | 1 (0%) | 0 | 100 | 100 |
| 25 | DZ | 206/231 (89%) | 205 (100%) | 1 (0%) | 0 | 100 | 100 |
| 25 | Dz | 206/231 (89%) | 205 (100%) | 1 (0%) | 0 | 100 | 100 |
| 26 | EA | 191/215 (89%) | 187 (98%) | 4 (2%) | 0 | 100 | 100 |
| 26 | Ea | 191/215 (89%) | 189 (99%) | 2 (1%) | 0 | 100 | 100 |
| 27 | EB | 207/210 (99%) | 205 (99%) | 2 (1%) | 0 | 100 | 100 |
| 27 | Eb | 207/210 (99%) | 207 (100%) | 0 | 0 | 100 | 100 |
| 28 | EC | 210/212 (99%) | 202 (96%) | 8 (4%) | 0 | 100 | 100 |
| 28 | Ec | 210/212 (99%) | 203 (97%) | 7 (3%) | 0 | 100 | 100 |
| 29 | ED | 188/190 (99%) | 183 (97%) | 5 (3%) | 0 | 100 | 100 |
| 29 | Ed | 188/190 (99%) | 184 (98%) | 4 (2%) | 0 | 100 | 100 |
| 30 | EE | 123/193 (64%) | 121 (98%) | 2 (2%) | 0 | 100 | 100 |
| 30 | Ee | 123/193 (64%) | 121 (98%) | 2 (2%) | 0 | 100 | 100 |
| 31 | EF | 186/188 (99%) | 185 (100%) | 1 (0%) | 0 | 100 | 100 |
| 31 | Ef | 186/188 (99%) | 185 (100%) | 1 (0%) | 0 | 100 | 100 |
| 32 | EG | 96/100 (96%) | 94 (98%) | 2 (2%) | 0 | 100 | 100 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|---|---|---|---|---|---|---|---|
| 32 | Eg | 96/100 (96%) | 96 (100%) | 0 | 0 | 100 | 100 |
| 33 | EH | 171/173 (99%) | 169 (99%) | 2 (1%) | 0 | 100 | 100 |
| 33 | Eh | 171/173 (99%) | 168 (98%) | 3 (2%) | 0 | 100 | 100 |
| 34 | EI | 170/173 (98%) | 166 (98%) | 4 (2%) | 0 | 100 | 100 |
| 34 | Ei | 170/173 (98%) | 167 (98%) | 3 (2%) | 0 | 100 | 100 |
| 35 | EV | 76/88 (86%) | 75 (99%) | 1 (1%) | 0 | 100 | 100 |
| 35 | Ev | 76/88 (86%) | 75 (99%) | 1 (1%) | 0 | 100 | 100 |
| 36 | EK | 167/170 (98%) | 166 (99%) | 1 (1%) | 0 | 100 | 100 |
| 36 | Ek | 167/170 (98%) | 166 (99%) | 1 (1%) | 0 | 100 | 100 |
| 37 | EL | 151/158 (96%) | 149 (99%) | 2 (1%) | 0 | 100 | 100 |
| 37 | El | 151/158 (96%) | 150 (99%) | 1 (1%) | 0 | 100 | 100 |
| 38 | EM | 151/154 (98%) | 150 (99%) | 1 (1%) | 0 | 100 | 100 |
| 38 | Em | 151/154 (98%) | 149 (99%) | 2 (1%) | 0 | 100 | 100 |
| 39 | EN | 143/149 (96%) | 140 (98%) | 3 (2%) | 0 | 100 | 100 |
| 39 | En | 143/149 (96%) | 139 (97%) | 4 (3%) | 0 | 100 | 100 |
| 40 | EO | 121/124 (98%) | 118 (98%) | 3 (2%) | 0 | 100 | 100 |
| 40 | Eo | 121/124 (98%) | 119 (98%) | 2 (2%) | 0 | 100 | 100 |
| 41 | EP | 98/127 (77%) | 97 (99%) | 1 (1%) | 0 | 100 | 100 |
| 41 | Ep | 98/127 (77%) | 98 (100%) | 0 | 0 | 100 | 100 |
| 42 | EQ | 120/122 (98%) | 119 (99%) | 1 (1%) | 0 | 100 | 100 |
| 42 | Eq | 120/122 (98%) | 119 (99%) | 1 (1%) | 0 | 100 | 100 |
| 43 | ER | 102/105 (97%) | 101 (99%) | 1 (1%) | 0 | 100 | 100 |
| 43 | Er | 102/105 (97%) | 101 (99%) | 1 (1%) | 0 | 100 | 100 |
| 44 | ES | 87/89 (98%) | 87 (100%) | 0 | 0 | 100 | 100 |
| 44 | Es | 87/89 (98%) | 87 (100%) | 0 | 0 | 100 | 100 |
| 45 | ET | 80/93 (86%) | 80 (100%) | 0 | 0 | 100 | 100 |
| 45 | Et | 80/93 (86%) | 80 (100%) | 0 | 0 | 100 | 100 |
| 46 | EU | 86/90 (96%) | 85 (99%) | 1 (1%) | 0 | 100 | 100 |
| 46 | Eu | 86/90 (96%) | 85 (99%) | 1 (1%) | 0 | 100 | 100 |
| 47 | EJ | 173/175 (99%) | 171 (99%) | 2 (1%) | 0 | 100 | 100 |
| 47 | Ej | 173/175 (99%) | 170 (98%) | 3 (2%) | 0 | 100 | 100 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|---|---|---|---|---|---|---|---|
| 48 | EW | 61/81 (75%) | 61 (100%) | 0 | 0 | 100 | 100 |
| 48 | Ew | 61/81 (75%) | 60 (98%) | 1 (2%) | 0 | 100 | 100 |
| 49 | EX | 67/72 (93%) | 67 (100%) | 0 | 0 | 100 | 100 |
| 49 | Ex | 67/72 (93%) | 67 (100%) | 0 | 0 | 100 | 100 |
| 50 | EY | 68/72 (94%) | 68 (100%) | 0 | 0 | 100 | 100 |
| 50 | Ey | 68/72 (94%) | 68 (100%) | 0 | 0 | 100 | 100 |
| 51 | EZ | 56/68 (82%) | 55 (98%) | 1 (2%) | 0 | 100 | 100 |
| 51 | Ez | 56/68 (82%) | 56 (100%) | 0 | 0 | 100 | 100 |
| 52 | FA | 69/72 (96%) | 69 (100%) | 0 | 0 | 100 | 100 |
| 52 | Fa | 69/72 (96%) | 69 (100%) | 0 | 0 | 100 | 100 |
| 53 | DL | 378/536 (70%) | 364 (96%) | 14 (4%) | 0 | 100 | 100 |
| 53 | Dl | 378/536 (70%) | 364 (96%) | 14 (4%) | 0 | 100 | 100 |
| All | All | 23566/27324 (86%) | 23198 (98%) | 364 (2%) | 4 (0%) | 100 | 100 |

All (4) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 3 | DC | 143 | ASN |
| 9 | Di | 119 | GLU |
| 9 | DI | 119 | GLU |
| 3 | DC | 49 | ASN |

### 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 | DA | 596/613 (97%) | 590 (99%) | 6 (1%) | 68 | 86 |
| 1 | Da | 596/613 (97%) | 588 (99%) | 8 (1%) | 61 | 82 |
| 2 | DB | 569/569 (100%) | 561 (99%) | 8 (1%) | 59 | 81 |
| 2 | Db | 569/569 (100%) | 563 (99%) | 6 (1%) | 65 | 84 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|---|---|---|---|---|---|---|
| 3 | DC | 553/565 (98%) | 553 (100%) | 0 | 100 | 100 |
| 3 | Dc | 553/565 (98%) | 552 (100%) | 1 (0%) | 87 | 95 |
| 4 | DD | 506/579 (87%) | 503 (99%) | 3 (1%) | 78 | 91 |
| 4 | Dd | 506/579 (87%) | 503 (99%) | 3 (1%) | 78 | 91 |
| 5 | DE | 114/116 (98%) | 114 (100%) | 0 | 100 | 100 |
| 5 | De | 114/116 (98%) | 113 (99%) | 1 (1%) | 70 | 87 |
| 6 | DF | 200/207 (97%) | 198 (99%) | 2 (1%) | 68 | 86 |
| 6 | Df | 200/207 (97%) | 199 (100%) | 1 (0%) | 81 | 92 |
| 7 | DG | 84/88 (96%) | 83 (99%) | 1 (1%) | 63 | 83 |
| 7 | Dg | 84/88 (96%) | 84 (100%) | 0 | 100 | 100 |
| 8 | DH | 119/119 (100%) | 118 (99%) | 1 (1%) | 73 | 88 |
| 8 | Dh | 119/119 (100%) | 117 (98%) | 2 (2%) | 53 | 78 |
| 9 | DI | 193/218 (88%) | 191 (99%) | 2 (1%) | 68 | 86 |
| 9 | Di | 193/218 (88%) | 191 (99%) | 2 (1%) | 68 | 86 |
| 10 | DJ | 199/199 (100%) | 195 (98%) | 4 (2%) | 48 | 74 |
| 10 | Dj | 199/199 (100%) | 196 (98%) | 3 (2%) | 57 | 80 |
| 11 | DK | 121/943 (13%) | 120 (99%) | 1 (1%) | 73 | 88 |
| 11 | Dk | 121/943 (13%) | 121 (100%) | 0 | 100 | 100 |
| 12 | DM | 413/447 (92%) | 411 (100%) | 2 (0%) | 81 | 92 |
| 12 | Dm | 413/447 (92%) | 410 (99%) | 3 (1%) | 76 | 89 |
| 13 | DN | 442/442 (100%) | 439 (99%) | 3 (1%) | 76 | 89 |
| 13 | Dn | 442/442 (100%) | 438 (99%) | 4 (1%) | 70 | 87 |
| 14 | DO | 380/413 (92%) | 379 (100%) | 1 (0%) | 86 | 94 |
| 14 | Do | 380/413 (92%) | 379 (100%) | 1 (0%) | 86 | 94 |
| 15 | DP | 253/358 (71%) | 252 (100%) | 1 (0%) | 84 | 93 |
| 15 | Dp | 253/358 (71%) | 252 (100%) | 1 (0%) | 84 | 93 |
| 16 | DQ | 340/342 (99%) | 339 (100%) | 1 (0%) | 86 | 94 |
| 16 | Dq | 340/342 (99%) | 340 (100%) | 0 | 100 | 100 |
| 17 | DR | 219/318 (69%) | 218 (100%) | 1 (0%) | 81 | 92 |
| 17 | Dr | 219/318 (69%) | 219 (100%) | 0 | 100 | 100 |
| 18 | DS | 293/293 (100%) | 289 (99%) | 4 (1%) | 59 | 81 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles |
|---|---|---|---|---|---|
| 18 | Ds | 293/293 (100%) | 288 (98%) | 5 (2%) | 53 78 |
| 19 | DT | 267/289 (92%) | 267 (100%) | 0 | 100 100 |
| 19 | Dt | 267/289 (92%) | 267 (100%) | 0 | 100 100 |
| 20 | DU | 275/276 (100%) | 273 (99%) | 2 (1%) | 76 89 |
| 20 | Du | 275/276 (100%) | 271 (98%) | 4 (2%) | 57 80 |
| 21 | DV | 259/259 (100%) | 258 (100%) | 1 (0%) | 84 93 |
| 21 | Dv | 259/259 (100%) | 256 (99%) | 3 (1%) | 63 83 |
| 22 | DW | 258/272 (95%) | 257 (100%) | 1 (0%) | 84 93 |
| 22 | Dw | 258/272 (95%) | 257 (100%) | 1 (0%) | 84 93 |
| 23 | DX | 218/219 (100%) | 217 (100%) | 1 (0%) | 81 92 |
| 23 | Dx | 218/219 (100%) | 215 (99%) | 3 (1%) | 59 81 |
| 24 | DY | 169/216 (78%) | 169 (100%) | 0 | 100 100 |
| 24 | Dy | 169/216 (78%) | 168 (99%) | 1 (1%) | 78 91 |
| 25 | DZ | 189/213 (89%) | 188 (100%) | 1 (0%) | 81 92 |
| 25 | Dz | 189/213 (89%) | 188 (100%) | 1 (0%) | 81 92 |
| 26 | EA | 180/201 (90%) | 179 (99%) | 1 (1%) | 78 91 |
| 26 | Ea | 180/201 (90%) | 180 (100%) | 0 | 100 100 |
| 27 | EB | 180/181 (99%) | 180 (100%) | 0 | 100 100 |
| 27 | Eb | 180/181 (99%) | 179 (99%) | 1 (1%) | 78 91 |
| 28 | EC | 178/178 (100%) | 177 (99%) | 1 (1%) | 78 91 |
| 28 | Ec | 178/178 (100%) | 177 (99%) | 1 (1%) | 78 91 |
| 29 | ED | 185/185 (100%) | 183 (99%) | 2 (1%) | 65 84 |
| 29 | Ed | 185/185 (100%) | 183 (99%) | 2 (1%) | 65 84 |
| 30 | EE | 116/180 (64%) | 116 (100%) | 0 | 100 100 |
| 30 | Ee | 116/180 (64%) | 116 (100%) | 0 | 100 100 |
| 31 | EF | 164/164 (100%) | 161 (98%) | 3 (2%) | 51 76 |
| 31 | Ef | 164/164 (100%) | 163 (99%) | 1 (1%) | 78 91 |
| 32 | EG | 77/78 (99%) | 77 (100%) | 0 | 100 100 |
| 32 | Eg | 77/78 (99%) | 77 (100%) | 0 | 100 100 |
| 33 | EH | 156/156 (100%) | 155 (99%) | 1 (1%) | 78 91 |
| 33 | Eh | 156/156 (100%) | 156 (100%) | 0 | 100 100 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|---|---|---|---|---|---|---|
| 34 | EI | 156/157 (99%) | 154 (99%) | 2 (1%) | 61 | 82 |
| 34 | Ei | 156/157 (99%) | 153 (98%) | 3 (2%) | 50 | 75 |
| 35 | EV | 71/80 (89%) | 71 (100%) | 0 | 100 | 100 |
| 35 | Ev | 71/80 (89%) | 71 (100%) | 0 | 100 | 100 |
| 36 | EK | 153/154 (99%) | 151 (99%) | 2 (1%) | 61 | 82 |
| 36 | Ek | 153/154 (99%) | 150 (98%) | 3 (2%) | 48 | 74 |
| 37 | EL | 134/139 (96%) | 134 (100%) | 0 | 100 | 100 |
| 37 | El | 134/139 (96%) | 134 (100%) | 0 | 100 | 100 |
| 38 | EM | 137/138 (99%) | 136 (99%) | 1 (1%) | 76 | 89 |
| 38 | Em | 137/138 (99%) | 136 (99%) | 1 (1%) | 76 | 89 |
| 39 | EN | 132/135 (98%) | 131 (99%) | 1 (1%) | 73 | 88 |
| 39 | En | 132/135 (98%) | 131 (99%) | 1 (1%) | 73 | 88 |
| 40 | EO | 112/113 (99%) | 111 (99%) | 1 (1%) | 70 | 87 |
| 40 | Eo | 112/113 (99%) | 111 (99%) | 1 (1%) | 70 | 87 |
| 41 | EP | 87/113 (77%) | 87 (100%) | 0 | 100 | 100 |
| 41 | Ep | 87/113 (77%) | 87 (100%) | 0 | 100 | 100 |
| 42 | EQ | 104/104 (100%) | 101 (97%) | 3 (3%) | 37 | 65 |
| 42 | Eq | 104/104 (100%) | 101 (97%) | 3 (3%) | 37 | 65 |
| 43 | ER | 87/88 (99%) | 87 (100%) | 0 | 100 | 100 |
| 43 | Er | 87/88 (99%) | 87 (100%) | 0 | 100 | 100 |
| 44 | ES | 84/84 (100%) | 84 (100%) | 0 | 100 | 100 |
| 44 | Es | 84/84 (100%) | 84 (100%) | 0 | 100 | 100 |
| 45 | ET | 75/83 (90%) | 72 (96%) | 3 (4%) | 28 | 55 |
| 45 | Et | 75/83 (90%) | 72 (96%) | 3 (4%) | 28 | 55 |
| 46 | EU | 78/80 (98%) | 78 (100%) | 0 | 100 | 100 |
| 46 | Eu | 78/80 (98%) | 78 (100%) | 0 | 100 | 100 |
| 47 | EJ | 157/157 (100%) | 156 (99%) | 1 (1%) | 78 | 91 |
| 47 | Ej | 157/157 (100%) | 155 (99%) | 2 (1%) | 61 | 82 |
| 48 | EW | 57/66 (86%) | 56 (98%) | 1 (2%) | 51 | 76 |
| 48 | Ew | 57/66 (86%) | 56 (98%) | 1 (2%) | 51 | 76 |
| 49 | EX | 64/67 (96%) | 63 (98%) | 1 (2%) | 55 | 79 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles |
|---|---|---|---|---|---|
| 49 | Ex | 64/67 (96%) | 63 (98%) | 1 (2%) | 55 79 |
| 50 | EY | 62/63 (98%) | 62 (100%) | 0 | 100 100 |
| 50 | Ey | 62/63 (98%) | 62 (100%) | 0 | 100 100 |
| 51 | EZ | 55/63 (87%) | 54 (98%) | 1 (2%) | 51 76 |
| 51 | Ez | 55/63 (87%) | 54 (98%) | 1 (2%) | 51 76 |
| 52 | FA | 62/63 (98%) | 60 (97%) | 2 (3%) | 34 62 |
| 52 | Fa | 62/63 (98%) | 60 (97%) | 2 (3%) | 34 62 |
| 53 | DL | 308/441 (70%) | 307 (100%) | 1 (0%) | 86 94 |
| 53 | Dl | 308/441 (70%) | 307 (100%) | 1 (0%) | 86 94 |
| All | All | 21280/24568 (87%) | 21123 (99%) | 157 (1%) | 73 89 |

All (157) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | DA | 57 | TYR |
| 1 | DA | 232 | MET |
| 1 | DA | 389 | PHE |
| 1 | DA | 429 | VAL |
| 1 | DA | 447 | LEU |
| 1 | DA | 630 | ARG |
| 2 | DB | 45 | TRP |
| 2 | DB | 104 | ILE |
| 2 | DB | 133 | PHE |
| 2 | DB | 143 | ILE |
| 2 | DB | 175 | VAL |
| 2 | DB | 183 | LEU |
| 2 | DB | 224 | PHE |
| 2 | DB | 524 | LYS |
| 4 | DD | 214 | ASN |
| 4 | DD | 236 | LYS |
| 4 | DD | 247 | GLU |
| 6 | DF | 35 | LYS |
| 6 | DF | 90 | ASP |
| 7 | DG | 1 | MET |
| 8 | DH | 120 | ARG |
| 9 | DI | 115 | GLU |
| 9 | DI | 141 | ILE |
| 10 | DJ | 26 | LYS |
| 10 | DJ | 98 | LEU |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 10 | DJ | 99 | ASN |
| 10 | DJ | 204 | GLU |
| 11 | DK | 96 | GLU |
| 12 | DM | 386 | THR |
| 12 | DM | 414 | GLN |
| 13 | DN | 249 | ILE |
| 13 | DN | 262 | LEU |
| 13 | DN | 420 | ASN |
| 14 | DO | 272 | GLU |
| 15 | DP | 228 | LEU |
| 16 | DQ | 34 | THR |
| 17 | DR | 211 | ARG |
| 18 | DS | 58 | GLU |
| 18 | DS | 65 | THR |
| 18 | DS | 145 | LEU |
| 18 | DS | 232 | GLN |
| 20 | DU | 10 | LYS |
| 20 | DU | 213 | GLN |
| 21 | DV | 108 | LYS |
| 22 | DW | 156 | GLU |
| 23 | DX | 157 | GLU |
| 25 | DZ | 125 | GLN |
| 26 | EA | 110 | LEU |
| 28 | EC | 56 | LEU |
| 29 | ED | 174 | ARG |
| 29 | ED | 175 | LEU |
| 31 | EF | 51 | THR |
| 31 | EF | 105 | GLN |
| 31 | EF | 157 | ARG |
| 33 | EH | 70 | HIS |
| 34 | EI | 8 | TYR |
| 34 | EI | 132 | VAL |
| 36 | EK | 12 | ASN |
| 36 | EK | 121 | VAL |
| 38 | EM | 137 | GLU |
| 39 | EN | 144 | LEU |
| 40 | EO | 124 | LYS |
| 42 | EQ | 2 | GLU |
| 42 | EQ | 65 | PHE |
| 42 | EQ | 73 | ILE |
| 45 | ET | 38 | LEU |
| 45 | ET | 58 | CYS |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 45 | ET | 83 | GLU |
| 47 | EJ | 158 | LEU |
| 48 | EW | 62 | LYS |
| 49 | EX | 4 | LYS |
| 51 | EZ | 23 | CYS |
| 52 | FA | 50 | GLU |
| 52 | FA | 72 | LEU |
| 1 | Da | 57 | TYR |
| 1 | Da | 76 | ARG |
| 1 | Da | 429 | VAL |
| 1 | Da | 447 | LEU |
| 1 | Da | 503 | PHE |
| 1 | Da | 521 | PHE |
| 1 | Da | 526 | HIS |
| 1 | Da | 630 | ARG |
| 2 | Db | 45 | TRP |
| 2 | Db | 224 | PHE |
| 2 | Db | 230 | TYR |
| 2 | Db | 412 | THR |
| 2 | Db | 511 | ASP |
| 2 | Db | 524 | LYS |
| 3 | Dc | 50 | GLU |
| 4 | Dd | 214 | ASN |
| 4 | Dd | 236 | LYS |
| 4 | Dd | 247 | GLU |
| 5 | De | 126 | GLU |
| 6 | Df | 35 | LYS |
| 8 | Dh | 120 | ARG |
| 8 | Dh | 122 | GLU |
| 9 | Di | 141 | ILE |
| 9 | Di | 208 | ILE |
| 10 | Dj | 26 | LYS |
| 10 | Dj | 98 | LEU |
| 10 | Dj | 204 | GLU |
| 12 | Dm | 103 | LEU |
| 12 | Dm | 372 | ASP |
| 12 | Dm | 386 | THR |
| 13 | Dn | 30 | LEU |
| 13 | Dn | 210 | LEU |
| 13 | Dn | 262 | LEU |
| 13 | Dn | 420 | ASN |
| 14 | Do | 272 | GLU |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 15 | Dp | 228 | LEU |
| 18 | Ds | 58 | GLU |
| 18 | Ds | 65 | THR |
| 18 | Ds | 145 | LEU |
| 18 | Ds | 156 | LEU |
| 18 | Ds | 232 | GLN |
| 20 | Du | 10 | LYS |
| 20 | Du | 91 | VAL |
| 20 | Du | 250 | VAL |
| 20 | Du | 276 | LYS |
| 21 | Dv | 3 | TYR |
| 21 | Dv | 108 | LYS |
| 21 | Dv | 275 | ILE |
| 22 | Dw | 268 | ASP |
| 23 | Dx | 134 | LEU |
| 23 | Dx | 157 | GLU |
| 23 | Dx | 228 | ASN |
| 24 | Dy | 190 | ARG |
| 25 | Dz | 125 | GLN |
| 27 | Eb | 63 | ARG |
| 28 | Ec | 9 | LEU |
| 29 | Ed | 82 | TYR |
| 29 | Ed | 174 | ARG |
| 31 | Ef | 105 | GLN |
| 34 | Ei | 8 | TYR |
| 34 | Ei | 111 | TYR |
| 34 | Ei | 132 | VAL |
| 36 | Ek | 12 | ASN |
| 36 | Ek | 17 | LEU |
| 36 | Ek | 21 | ARG |
| 38 | Em | 137 | GLU |
| 39 | En | 144 | LEU |
| 40 | Eo | 124 | LYS |
| 42 | Eq | 2 | GLU |
| 42 | Eq | 65 | PHE |
| 42 | Eq | 73 | ILE |
| 45 | Et | 38 | LEU |
| 45 | Et | 58 | CYS |
| 45 | Et | 83 | GLU |
| 47 | Ej | 99 | PHE |
| 47 | Ej | 158 | LEU |
| 48 | Ew | 62 | LYS |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 49 | Ex | 4 | LYS |
| 51 | Ez | 23 | CYS |
| 52 | Fa | 50 | GLU |
| 52 | Fa | 72 | LEU |
| 53 | Dl | 326 | GLN |
| 53 | DL | 326 | GLN |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (156) such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | DA | 50 | HIS |
| 1 | DA | 101 | HIS |
| 1 | DA | 182 | ASN |
| 1 | DA | 367 | GLN |
| 1 | DA | 411 | HIS |
| 1 | DA | 526 | HIS |
| 1 | DA | 528 | HIS |
| 2 | DB | 32 | GLN |
| 2 | DB | 198 | GLN |
| 2 | DB | 207 | ASN |
| 2 | DB | 379 | ASN |
| 3 | DC | 129 | ASN |
| 3 | DC | 205 | ASN |
| 3 | DC | 224 | ASN |
| 4 | DD | 130 | ASN |
| 4 | DD | 134 | ASN |
| 4 | DD | 348 | HIS |
| 4 | DD | 471 | GLN |
| 4 | DD | 477 | HIS |
| 5 | DE | 73 | GLN |
| 7 | DG | 39 | HIS |
| 12 | DM | 67 | HIS |
| 12 | DM | 106 | GLN |
| 12 | DM | 333 | ASN |
| 13 | DN | 57 | ASN |
| 13 | DN | 88 | HIS |
| 13 | DN | 146 | ASN |
| 13 | DN | 298 | ASN |
| 14 | DO | 76 | GLN |
| 14 | DO | 251 | GLN |
| 14 | DO | 438 | GLN |
| 15 | DP | 315 | ASN |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 16 | DQ | 15 | ASN |
| 16 | DQ | 54 | ASN |
| 16 | DQ | 61 | ASN |
| 16 | DQ | 96 | GLN |
| 17 | DR | 256 | HIS |
| 17 | DR | 262 | GLN |
| 17 | DR | 268 | GLN |
| 18 | DS | 20 | ASN |
| 18 | DS | 339 | ASN |
| 19 | DT | 72 | ASN |
| 19 | DT | 249 | ASN |
| 20 | DU | 62 | HIS |
| 20 | DU | 66 | HIS |
| 20 | DU | 318 | GLN |
| 21 | DV | 42 | GLN |
| 21 | DV | 97 | ASN |
| 21 | DV | 143 | ASN |
| 22 | DW | 203 | HIS |
| 22 | DW | 232 | HIS |
| 22 | DW | 238 | GLN |
| 23 | DX | 156 | ASN |
| 24 | DY | 200 | ASN |
| 25 | DZ | 110 | ASN |
| 26 | EA | 170 | GLN |
| 26 | EA | 205 | ASN |
| 27 | EB | 167 | GLN |
| 27 | EB | 208 | HIS |
| 28 | EC | 153 | ASN |
| 28 | EC | 194 | GLN |
| 28 | EC | 202 | GLN |
| 30 | EE | 111 | GLN |
| 31 | EF | 150 | ASN |
| 33 | EH | 4 | ASN |
| 33 | EH | 70 | HIS |
| 35 | EV | 34 | ASN |
| 36 | EK | 28 | GLN |
| 36 | EK | 101 | GLN |
| 36 | EK | 105 | ASN |
| 36 | EK | 163 | HIS |
| 41 | EP | 123 | HIS |
| 43 | ER | 45 | ASN |
| 47 | EJ | 91 | GLN |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 47 | EJ | 105 | GLN |
| 48 | EW | 40 | GLN |
| 50 | EY | 20 | HIS |
| 1 | Da | 514 | ASN |
| 1 | Da | 526 | HIS |
| 2 | Db | 198 | GLN |
| 2 | Db | 266 | ASN |
| 2 | Db | 316 | GLN |
| 2 | Db | 385 | ASN |
| 2 | Db | 548 | GLN |
| 2 | Db | 558 | HIS |
| 3 | Dc | 52 | ASN |
| 3 | Dc | 129 | ASN |
| 3 | Dc | 224 | ASN |
| 4 | Dd | 348 | HIS |
| 5 | De | 26 | ASN |
| 5 | De | 56 | ASN |
| 5 | De | 73 | GLN |
| 5 | De | 112 | HIS |
| 7 | Dg | 39 | HIS |
| 10 | Dj | 62 | HIS |
| 12 | Dm | 147 | GLN |
| 12 | Dm | 333 | ASN |
| 12 | Dm | 451 | GLN |
| 12 | Dm | 454 | ASN |
| 13 | Dn | 215 | ASN |
| 13 | Dn | 268 | ASN |
| 14 | Do | 107 | ASN |
| 14 | Do | 245 | GLN |
| 14 | Do | 251 | GLN |
| 14 | Do | 438 | GLN |
| 16 | Dq | 255 | GLN |
| 17 | Dr | 262 | GLN |
| 17 | Dr | 268 | GLN |
| 18 | Ds | 34 | ASN |
| 19 | Dt | 220 | ASN |
| 19 | Dt | 249 | ASN |
| 20 | Du | 62 | HIS |
| 20 | Du | 66 | HIS |
| 20 | Du | 224 | HIS |
| 20 | Du | 268 | ASN |
| 21 | Dv | 24 | ASN |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 21 | Dv | 143 | ASN |
| 22 | Dw | 25 | ASN |
| 22 | Dw | 81 | ASN |
| 22 | Dw | 203 | HIS |
| 22 | Dw | 232 | HIS |
| 23 | Dx | 47 | GLN |
| 25 | Dz | 110 | ASN |
| 27 | Eb | 208 | HIS |
| 28 | Ec | 44 | HIS |
| 28 | Ec | 184 | GLN |
| 32 | Eg | 9 | ASN |
| 32 | Eg | 13 | ASN |
| 33 | Eh | 47 | HIS |
| 33 | Eh | 131 | GLN |
| 34 | Ei | 166 | ASN |
| 36 | Ek | 28 | GLN |
| 36 | Ek | 101 | GLN |
| 36 | Ek | 105 | ASN |
| 36 | Ek | 143 | HIS |
| 36 | Ek | 163 | HIS |
| 37 | El | 38 | ASN |
| 41 | Ep | 123 | HIS |
| 42 | Eq | 64 | ASN |
| 43 | Er | 45 | ASN |
| 45 | Et | 33 | GLN |
| 45 | Et | 60 | ASN |
| 47 | Ej | 29 | HIS |
| 47 | Ej | 105 | GLN |
| 47 | Ej | 164 | GLN |
| 48 | Ew | 40 | GLN |
| 51 | Ez | 37 | HIS |
| 53 | Dl | 84 | ASN |
| 53 | Dl | 90 | GLN |
| 53 | Dl | 260 | ASN |
| 53 | Dl | 271 | ASN |
| 53 | Dl | 386 | GLN |
| 53 | DL | 90 | GLN |
| 53 | DL | 141 | ASN |
| 53 | DL | 260 | ASN |
| 53 | DL | 271 | 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)

20 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\| > 2$ | Counts | RMSZ | $\#\|Z\| > 2$ |
| 4 | TPO | Dd | 387 | 4 | 8,10,11 | 1.58 | 1 (12%) | 10,14,16 | 1.87 | 1 (10%) |
| 33 | AME | EH | 1 | 33 | 9,10,11 | 0.21 | 0 | 9,11,13 | 0.47 | 0 |
| 9 | SEP | DI | 120 | 9 | 8,9,10 | 1.54 | 1 (12%) | 8,12,14 | 1.55 | 2 (25%) |
| 4 | SEP | Dd | 520 | 4 | 8,9,10 | 1.55 | 1 (12%) | 8,12,14 | 1.73 | 2 (25%) |
| 33 | AME | Eh | 1 | 33 | 9,10,11 | 0.23 | 0 | 9,11,13 | 0.46 | 0 |
| 42 | AME | Eq | 1 | 42 | 9,10,11 | 0.24 | 0 | 9,11,13 | 0.50 | 0 |
| 4 | TPO | DD | 387 | 4 | 8,10,11 | 1.57 | 1 (12%) | 10,14,16 | 1.88 | 1 (10%) |
| 9 | SEP | Di | 120 | 9 | 8,9,10 | 1.54 | 1 (12%) | 8,12,14 | 1.56 | 2 (25%) |
| 4 | SEP | DD | 520 | 4 | 8,9,10 | 1.54 | 1 (12%) | 8,12,14 | 1.70 | 2 (25%) |
| 35 | AME | Ev | 1 | 35 | 9,10,11 | 0.23 | 0 | 9,11,13 | 0.49 | 0 |
| 16 | AME | DQ | 1 | 16 | 9,10,11 | 0.23 | 0 | 9,11,13 | 0.47 | 0 |
| 8 | AME | Dh | 1 | 8 | 9,10,11 | 0.23 | 0 | 9,11,13 | 0.50 | 0 |
| 21 | AME | DV | 1 | 21 | 9,10,11 | 0.23 | 0 | 9,11,13 | 0.57 | 0 |
| 21 | AME | Dv | 1 | 21 | 9,10,11 | 0.22 | 0 | 9,11,13 | 0.58 | 0 |
| 18 | AME | Ds | 1 | 18 | 9,10,11 | 0.23 | 0 | 9,11,13 | 0.52 | 0 |
| 8 | AME | DH | 1 | 8 | 9,10,11 | 0.24 | 0 | 9,11,13 | 0.49 | 0 |
| 18 | AME | DS | 1 | 18 | 9,10,11 | 0.24 | 0 | 9,11,13 | 0.52 | 0 |
| 35 | AME | EV | 1 | 35 | 9,10,11 | 0.23 | 0 | 9,11,13 | 0.47 | 0 |
| 42 | AME | EQ | 1 | 42 | 9,10,11 | 0.22 | 0 | 9,11,13 | 0.51 | 0 |
| 16 | AME | Dq | 1 | 16 | 9,10,11 | 0.24 | 0 | 9,11,13 | 0.47 | 0 |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 4 | TPO | Dd | 387 | 4 | - | 2/9/11/13 | - |
| 33 | AME | EH | 1 | 33 | - | 0/9/10/12 | - |
| 9 | SEP | DI | 120 | 9 | - | 1/5/8/10 | - |
| 4 | SEP | Dd | 520 | 4 | - | 0/5/8/10 | - |
| 33 | AME | Eh | 1 | 33 | - | 2/9/10/12 | - |
| 42 | AME | Eq | 1 | 42 | - | 2/9/10/12 | - |
| 4 | TPO | DD | 387 | 4 | - | 2/9/11/13 | - |
| 9 | SEP | Di | 120 | 9 | - | 0/5/8/10 | - |
| 4 | SEP | DD | 520 | 4 | - | 0/5/8/10 | - |
| 35 | AME | Ev | 1 | 35 | - | 1/9/10/12 | - |
| 16 | AME | DQ | 1 | 16 | - | 1/9/10/12 | - |
| 8 | AME | Dh | 1 | 8 | - | 0/9/10/12 | - |
| 21 | AME | DV | 1 | 21 | - | 0/9/10/12 | - |
| 21 | AME | Dv | 1 | 21 | - | 0/9/10/12 | - |
| 18 | AME | Ds | 1 | 18 | - | 1/9/10/12 | - |
| 8 | AME | DH | 1 | 8 | - | 0/9/10/12 | - |
| 18 | AME | DS | 1 | 18 | - | 1/9/10/12 | - |
| 35 | AME | EV | 1 | 35 | - | 1/9/10/12 | - |
| 42 | AME | EQ | 1 | 42 | - | 2/9/10/12 | - |
| 16 | AME | Dq | 1 | 16 | - | 2/9/10/12 | - |

All (6) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 4 | Dd | 520 | SEP | P-O1P | 3.38 | 1.61 | 1.50 |
| 9 | Di | 120 | SEP | P-O1P | 3.37 | 1.61 | 1.50 |
| 4 | Dd | 387 | TPO | P-O1P | 3.37 | 1.61 | 1.50 |
| 4 | DD | 520 | SEP | P-O1P | 3.35 | 1.61 | 1.50 |
| 9 | DI | 120 | SEP | P-O1P | 3.35 | 1.61 | 1.50 |
| 4 | DD | 387 | TPO | P-O1P | 3.35 | 1.61 | 1.50 |

All (10) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 4 | Dd | 387 | TPO | P-OG1-CB | -5.38 | 106.95 | 123.21 |
| 4 | DD | 387 | TPO | P-OG1-CB | -5.36 | 107.02 | 123.21 |
| 4 | Dd | 520 | SEP | OG-CB-CA | 3.22 | 111.28 | 108.14 |
| 4 | DD | 520 | SEP | OG-CB-CA | 3.15 | 111.21 | 108.14 |
| 4 | Dd | 520 | SEP | P-OG-CB | -3.14 | 109.66 | 118.30 |
| 4 | DD | 520 | SEP | P-OG-CB | -3.08 | 109.81 | 118.30 |
| 9 | Di | 120 | SEP | P-OG-CB | -2.89 | 110.32 | 118.30 |
| 9 | DI | 120 | SEP | P-OG-CB | -2.79 | 110.60 | 118.30 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 9 | DI | 120 | SEP | OG-CB-CA | 2.76 | 110.83 | 108.14 |
| 9 | Di | 120 | SEP | OG-CB-CA | 2.73 | 110.80 | 108.14 |

There are no chirality outliers.

All (18) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 42 | EQ | 1 | AME | O-C-CA-CB |
| 33 | Eh | 1 | AME | O-C-CA-CB |
| 42 | Eq | 1 | AME | O-C-CA-CB |
| 42 | EQ | 1 | AME | CB-CG-SD-CE |
| 42 | Eq | 1 | AME | CB-CG-SD-CE |
| 18 | Ds | 1 | AME | CB-CG-SD-CE |
| 33 | Eh | 1 | AME | CB-CG-SD-CE |
| 35 | EV | 1 | AME | CB-CG-SD-CE |
| 16 | DQ | 1 | AME | CB-CG-SD-CE |
| 35 | Ev | 1 | AME | CB-CG-SD-CE |
| 16 | Dq | 1 | AME | C-CA-N-CT1 |
| 16 | Dq | 1 | AME | CB-CA-N-CT1 |
| 4 | DD | 387 | TPO | C-CA-CB-CG2 |
| 4 | Dd | 387 | TPO | C-CA-CB-CG2 |
| 9 | DI | 120 | SEP | CB-OG-P-O3P |
| 4 | DD | 387 | TPO | O-C-CA-CB |
| 4 | Dd | 387 | TPO | O-C-CA-CB |
| 18 | DS | 1 | AME | CB-CG-SD-CE |

There are no ring outliers.

14 monomers are involved in 27 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 33 | EH | 1 | AME | 2 | 0 |
| 9 | DI | 120 | SEP | 1 | 0 |
| 4 | Dd | 520 | SEP | 1 | 0 |
| 33 | Eh | 1 | AME | 3 | 0 |
| 42 | Eq | 1 | AME | 4 | 0 |
| 9 | Di | 120 | SEP | 1 | 0 |
| 35 | Ev | 1 | AME | 1 | 0 |
| 16 | DQ | 1 | AME | 2 | 0 |
| 21 | DV | 1 | AME | 2 | 0 |
| 21 | Dv | 1 | AME | 2 | 0 |
| 18 | Ds | 1 | AME | 2 | 0 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 18 | DS | 1 | AME | 1 | 0 |
| 42 | EQ | 1 | AME | 4 | 0 |
| 16 | Dq | 1 | AME | 1 | 0 |

## 5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry (i)

Of 245 ligands modelled in this entry, 9 are monoatomic - leaving 236 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 | $\#\|Z\| > 2$ |
| 57 | CDL | DC | 601 | - | 99,99,99 | 0.30 | 0 | 105,111,111 | 0.24 | 0 |
| 57 | CDL | DA | 710 | - | 99,99,99 | 0.29 | 0 | 105,111,111 | 0.25 | 0 |
| 68 | ATP | ER | 201 | - | 29,33,33 | 0.28 | 0 | 44,52,52 | 0.78 | 1 (2%) |
| 57 | CDL | En | 1202 | - | 99,99,99 | 0.29 | 0 | 105,111,111 | 0.25 | 0 |
| 57 | CDL | El | 901 | - | 99,99,99 | 0.30 | 0 | 105,111,111 | 0.25 | 0 |
| 54 | HEA | DA | 701 | 1 | 66,67,67 | 2.50 | 26 (39%) | 78,103,103 | 2.34 | 31 (39%) |
| 58 | PC1 | Dv | 408 | - | 53,53,53 | 0.29 | 0 | 59,61,61 | 0.26 | 0 |
| 66 | HEM | Ed | 201 | - | 50,50,50 | 1.54 | 5 (10%) | 66,82,82 | 1.61 | 11 (16%) |
| 57 | CDL | Dm | 502 | - | 99,99,99 | 0.30 | 0 | 105,111,111 | 0.25 | 0 |
| 57 | CDL | Du | 403 | - | 99,99,99 | 0.30 | 0 | 105,111,111 | 0.24 | 0 |
| 59 | 3PE | DA | 708 | - | 50,50,50 | 0.26 | 0 | 53,55,55 | 0.20 | 0 |
| 57 | CDL | DZ | 501 | - | 99,99,99 | 0.30 | 0 | 105,111,111 | 0.24 | 0 |
| 59 | 3PE | Dr | 404 | - | 50,50,50 | 0.26 | 0 | 53,55,55 | 0.20 | 0 |
| 58 | PC1 | DC | 608 | - | 53,53,53 | 0.28 | 0 | 59,61,61 | 0.26 | 0 |
| 58 | PC1 | Dj | 406 | - | 53,53,53 | 0.29 | 0 | 59,61,61 | 0.26 | 0 |
| 58 | PC1 | DC | 604 | - | 53,53,53 | 0.28 | 0 | 59,61,61 | 0.27 | 0 |
| 57 | CDL | Dd | 704 | - | 99,99,99 | 0.30 | 0 | 105,111,111 | 0.25 | 0 |
| 54 | HEA | Da | 702 | - | 66,67,67 | 2.49 | 26 (39%) | 78,103,103 | 2.37 | 32 (41%) |
| 60 | LPP | DN | 503 | - | 43,43,43 | 0.22 | 0 | 47,48,48 | 0.28 | 0 |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\|>2$ | Counts | RMSZ | $\#\|Z\|>2$ |
| 62 | CUA | DB | 701 | 2 | 0,1,1 | - | - | - | | |
| 57 | CDL | Dn | 505 | - | 99,99,99 | 0.30 | 0 | 105,111,111 | 0.27 | 0 |
| 58 | PC1 | DA | 706 | - | 53,53,53 | 0.28 | 0 | 59,61,61 | 0.27 | 0 |
| 57 | CDL | Ds | 405 | - | 99,99,99 | 0.30 | 0 | 105,111,111 | 0.24 | 0 |
| 57 | CDL | Dm | 501 | - | 99,99,99 | 0.30 | 0 | 105,111,111 | 0.25 | 0 |
| 57 | CDL | DN | 504 | - | 99,99,99 | 0.29 | 0 | 105,111,111 | 0.25 | 0 |
| 59 | 3PE | Dx | 1206 | - | 50,50,50 | 0.27 | 0 | 53,55,55 | 0.21 | 0 |
| 58 | PC1 | Eo | 204 | - | 53,53,53 | 0.29 | 0 | 59,61,61 | 0.26 | 0 |
| 58 | PC1 | DV | 406 | - | 53,53,53 | 0.29 | 0 | 59,61,61 | 0.27 | 0 |
| 57 | CDL | DV | 404 | - | 99,99,99 | 0.30 | 0 | 105,111,111 | 0.25 | 0 |
| 57 | CDL | DA | 705 | - | 99,99,99 | 0.30 | 0 | 105,111,111 | 0.25 | 0 |
| 57 | CDL | DD | 702 | - | 99,99,99 | 0.29 | 0 | 105,111,111 | 0.25 | 0 |
| 57 | CDL | EU | 101 | - | 99,99,99 | 0.30 | 0 | 105,111,111 | 0.25 | 0 |
| 57 | CDL | Dg | 202 | - | 99,99,99 | 0.30 | 0 | 105,111,111 | 0.24 | 0 |
| 58 | PC1 | Dx | 1208 | - | 53,53,53 | 0.29 | 0 | 59,61,61 | 0.27 | 0 |
| 60 | LPP | Dl | 1101 | - | 43,43,43 | 0.23 | 0 | 47,48,48 | 0.27 | 0 |
| 57 | CDL | Dj | 403 | - | 99,99,99 | 0.30 | 0 | 105,111,111 | 0.25 | 0 |
| 57 | CDL | Eh | 1601 | - | 99,99,99 | 0.31 | 0 | 105,111,111 | 0.23 | 0 |
| 57 | CDL | ED | 604 | - | 99,99,99 | 0.30 | 0 | 105,111,111 | 0.24 | 0 |
| 58 | PC1 | DX | 306 | - | 53,53,53 | 0.29 | 0 | 59,61,61 | 0.26 | 0 |
| 57 | CDL | El | 902 | - | 99,99,99 | 0.30 | 0 | 105,111,111 | 0.24 | 0 |
| 57 | CDL | Dd | 702 | - | 99,99,99 | 0.30 | 0 | 105,111,111 | 0.25 | 0 |
| 57 | CDL | Do | 501 | - | 99,99,99 | 0.30 | 0 | 105,111,111 | 0.25 | 0 |
| 57 | CDL | Dj | 401 | - | 99,99,99 | 0.30 | 0 | 105,111,111 | 0.25 | 0 |
| 57 | CDL | DH | 201 | - | 99,99,99 | 0.29 | 0 | 105,111,111 | 0.25 | 0 |
| 57 | CDL | DD | 704 | - | 99,99,99 | 0.30 | 0 | 105,111,111 | 0.24 | 0 |
| 58 | PC1 | Dy | 302 | - | 53,53,53 | 0.28 | 0 | 59,61,61 | 0.26 | 0 |
| 57 | CDL | DI | 701 | - | 99,99,99 | 0.30 | 0 | 105,111,111 | 0.24 | 0 |
| 58 | PC1 | DG | 203 | - | 53,53,53 | 0.28 | 0 | 59,61,61 | 0.27 | 0 |
| 57 | CDL | EA | 301 | - | 99,99,99 | 0.29 | 0 | 105,111,111 | 0.24 | 0 |
| 57 | CDL | Dq | 402 | - | 99,99,99 | 0.30 | 0 | 105,111,111 | 0.25 | 0 |
| 58 | PC1 | DS | 406 | - | 53,53,53 | 0.29 | 0 | 59,61,61 | 0.25 | 0 |
| 57 | CDL | EL | 901 | - | 99,99,99 | 0.30 | 0 | 105,111,111 | 0.25 | 0 |
| 57 | CDL | Eu | 101 | - | 99,99,99 | 0.30 | 0 | 105,111,111 | 0.25 | 0 |
| 59 | 3PE | Ds | 401 | - | 50,50,50 | 0.26 | 0 | 53,55,55 | 0.23 | 0 |
| 59 | 3PE | Da | 708 | - | 50,50,50 | 0.26 | 0 | 53,55,55 | 0.21 | 0 |
| 65 | UQ8 | ED | 603 | - | 53,53,53 | 0.51 | 0 | 64,67,67 | 0.72 | 3 (4%) |
| 58 | PC1 | DC | 602 | - | 53,53,53 | 0.28 | 0 | 59,61,61 | 0.27 | 0 |
| 57 | CDL | DR | 403 | - | 99,99,99 | 0.30 | 0 | 105,111,111 | 0.24 | 0 |
| 58 | PC1 | Dg | 203 | - | 53,53,53 | 0.29 | 0 | 59,61,61 | 0.27 | 0 |
| 58 | PC1 | EB | 301 | - | 53,53,53 | 0.28 | 0 | 59,61,61 | 0.25 | 0 |
| 59 | 3PE | DR | 401 | - | 50,50,50 | 0.27 | 0 | 53,55,55 | 0.21 | 0 |
| 60 | LPP | DA | 711 | - | 43,43,43 | 0.22 | 0 | 47,48,48 | 0.28 | 0 |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\|>2$ | Counts | RMSZ | $\#\|Z\|>2$ |
| 58 | PC1 | Eb | 301 | - | 53,53,53 | 0.28 | 0 | 59,61,61 | 0.25 | 0 |
| 57 | CDL | DS | 402 | - | 99,99,99 | 0.30 | 0 | 105,111,111 | 0.25 | 0 |
| 59 | 3PE | DC | 607 | - | 50,50,50 | 0.27 | 0 | 53,55,55 | 0.21 | 0 |
| 58 | PC1 | DV | 405 | - | 53,53,53 | 0.29 | 0 | 59,61,61 | 0.26 | 0 |
| 68 | ATP | Er | 201 | - | 29,33,33 | 0.28 | 0 | 44,52,52 | 0.78 | 1 (2%) |
| 57 | CDL | EL | 902 | - | 99,99,99 | 0.30 | 0 | 105,111,111 | 0.25 | 0 |
| 57 | CDL | Dn | 501 | - | 99,99,99 | 0.30 | 0 | 105,111,111 | 0.26 | 0 |
| 59 | 3PE | Ds | 407 | - | 50,50,50 | 0.27 | 0 | 53,55,55 | 0.20 | 0 |
| 58 | PC1 | Di | 702 | - | 53,53,53 | 0.29 | 0 | 59,61,61 | 0.26 | 0 |
| 60 | LPP | Dn | 504 | - | 43,43,43 | 0.22 | 0 | 47,48,48 | 0.33 | 0 |
| 58 | PC1 | Eo | 205 | - | 53,53,53 | 0.29 | 0 | 59,61,61 | 0.27 | 0 |
| 57 | CDL | Dx | 1203 | - | 99,99,99 | 0.31 | 0 | 105,111,111 | 0.24 | 0 |
| 57 | CDL | DO | 501 | - | 99,99,99 | 0.30 | 0 | 105,111,111 | 0.24 | 0 |
| 58 | PC1 | Dx | 1204 | - | 53,53,53 | 0.29 | 0 | 59,61,61 | 0.27 | 0 |
| 65 | UQ8 | EN | 1204 | - | 53,53,53 | 0.50 | 0 | 64,67,67 | 0.67 | 2 (3%) |
| 57 | CDL | DQ | 1502 | - | 99,99,99 | 0.30 | 0 | 105,111,111 | 0.24 | 0 |
| 58 | PC1 | DX | 302 | - | 53,53,53 | 0.28 | 0 | 59,61,61 | 0.27 | 0 |
| 57 | CDL | DM | 502 | - | 99,99,99 | 0.29 | 0 | 105,111,111 | 0.25 | 0 |
| 57 | CDL | DR | 402 | - | 99,99,99 | 0.29 | 0 | 105,111,111 | 0.25 | 0 |
| 58 | PC1 | DV | 407 | - | 53,53,53 | 0.28 | 0 | 59,61,61 | 0.26 | 0 |
| 57 | CDL | Dy | 301 | - | 99,99,99 | 0.30 | 0 | 105,111,111 | 0.24 | 0 |
| 57 | CDL | Dd | 706 | - | 99,99,99 | 0.29 | 0 | 105,111,111 | 0.24 | 0 |
| 65 | UQ8 | El | 906 | - | 53,53,53 | 0.52 | 0 | 64,67,67 | 0.83 | 3 (4%) |
| 59 | 3PE | Ds | 403 | - | 50,50,50 | 0.27 | 0 | 53,55,55 | 0.20 | 0 |
| 59 | 3PE | Eo | 202 | - | 50,50,50 | 0.27 | 0 | 53,55,55 | 0.20 | 0 |
| 65 | UQ8 | Ed | 202 | - | 53,53,53 | 0.52 | 0 | 64,67,67 | 0.72 | 3 (4%) |
| 57 | CDL | Du | 401 | - | 99,99,99 | 0.29 | 0 | 105,111,111 | 0.25 | 0 |
| 58 | PC1 | Dv | 405 | - | 53,53,53 | 0.29 | 0 | 59,61,61 | 0.27 | 0 |
| 59 | 3PE | DS | 403 | - | 50,50,50 | 0.27 | 0 | 53,55,55 | 0.20 | 0 |
| 58 | PC1 | Dc | 604 | - | 53,53,53 | 0.28 | 0 | 59,61,61 | 0.27 | 0 |
| 59 | 3PE | EN | 1203 | - | 50,50,50 | 0.27 | 0 | 53,55,55 | 0.20 | 0 |
| 57 | CDL | Dj | 404 | - | 99,99,99 | 0.30 | 0 | 105,111,111 | 0.24 | 0 |
| 58 | PC1 | EB | 303 | - | 53,53,53 | 0.29 | 0 | 59,61,61 | 0.26 | 0 |
| 57 | CDL | ED | 601 | - | 99,99,99 | 0.30 | 0 | 105,111,111 | 0.24 | 0 |
| 57 | CDL | Dr | 402 | - | 99,99,99 | 0.30 | 0 | 105,111,111 | 0.24 | 0 |
| 58 | PC1 | EO | 207 | - | 53,53,53 | 0.29 | 0 | 59,61,61 | 0.26 | 0 |
| 57 | CDL | DU | 401 | - | 99,99,99 | 0.30 | 0 | 105,111,111 | 0.25 | 0 |
| 57 | CDL | Dh | 201 | - | 99,99,99 | 0.29 | 0 | 105,111,111 | 0.24 | 0 |
| 57 | CDL | DG | 201 | - | 99,99,99 | 0.30 | 0 | 105,111,111 | 0.25 | 0 |
| 65 | UQ8 | EL | 906 | - | 53,53,53 | 0.51 | 0 | 64,67,67 | 0.78 | 3 (4%) |
| 57 | CDL | Dn | 507 | - | 99,99,99 | 0.29 | 0 | 105,111,111 | 0.25 | 0 |
| 57 | CDL | Dj | 405 | - | 99,99,99 | 0.30 | 0 | 105,111,111 | 0.25 | 0 |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\|>2$ | Counts | RMSZ | $\#\|Z\|>2$ |
| 58 | PC1 | DS | 407 | - | 53,53,53 | 0.29 | 0 | 59,61,61 | 0.25 | 0 |
| 57 | CDL | DJ | 305 | - | 99,99,99 | 0.30 | 0 | 105,111,111 | 0.24 | 0 |
| 58 | PC1 | Dc | 603 | - | 53,53,53 | 0.28 | 0 | 59,61,61 | 0.26 | 0 |
| 58 | PC1 | Eo | 201 | - | 53,53,53 | 0.29 | 0 | 59,61,61 | 0.27 | 0 |
| 58 | PC1 | DC | 603 | - | 53,53,53 | 0.28 | 0 | 59,61,61 | 0.26 | 0 |
| 57 | CDL | DX | 307 | - | 99,99,99 | 0.30 | 0 | 105,111,111 | 0.24 | 0 |
| 57 | CDL | EL | 903 | - | 99,99,99 | 0.30 | 0 | 105,111,111 | 0.24 | 0 |
| 57 | CDL | EN | 1202 | - | 99,99,99 | 0.30 | 0 | 105,111,111 | 0.25 | 0 |
| 59 | 3PE | Dx | 1207 | - | 50,50,50 | 0.27 | 0 | 53,55,55 | 0.20 | 0 |
| 59 | 3PE | EO | 203 | - | 50,50,50 | 0.27 | 0 | 53,55,55 | 0.21 | 0 |
| 59 | 3PE | DX | 305 | - | 50,50,50 | 0.27 | 0 | 53,55,55 | 0.21 | 0 |
| 57 | CDL | DV | 402 | - | 99,99,99 | 0.30 | 0 | 105,111,111 | 0.25 | 0 |
| 57 | CDL | Ek | 201 | - | 99,99,99 | 0.30 | 0 | 105,111,111 | 0.25 | 0 |
| 67 | FES | EF | 202 | 31 | 0,4,4 | - | - | - | | |
| 59 | 3PE | DX | 303 | - | 50,50,50 | 0.26 | 0 | 53,55,55 | 0.19 | 0 |
| 59 | 3PE | Dx | 1205 | - | 50,50,50 | 0.27 | 0 | 53,55,55 | 0.21 | 0 |
| 60 | LPP | DN | 502 | - | 43,43,43 | 0.23 | 0 | 47,48,48 | 0.36 | 0 |
| 57 | CDL | Du | 402 | - | 99,99,99 | 0.29 | 0 | 105,111,111 | 0.25 | 0 |
| 57 | CDL | Dn | 502 | - | 99,99,99 | 0.30 | 0 | 105,111,111 | 0.24 | 0 |
| 59 | 3PE | DC | 606 | - | 50,50,50 | 0.27 | 0 | 53,55,55 | 0.22 | 0 |
| 59 | 3PE | EO | 204 | - | 50,50,50 | 0.27 | 0 | 53,55,55 | 0.22 | 0 |
| 58 | PC1 | Dq | 405 | - | 53,53,53 | 0.29 | 0 | 59,61,61 | 0.26 | 0 |
| 57 | CDL | Da | 705 | - | 99,99,99 | 0.29 | 0 | 105,111,111 | 0.25 | 0 |
| 58 | PC1 | DI | 702 | - | 53,53,53 | 0.29 | 0 | 59,61,61 | 0.26 | 0 |
| 58 | PC1 | Dc | 607 | - | 53,53,53 | 0.28 | 0 | 59,61,61 | 0.27 | 0 |
| 59 | 3PE | Eo | 203 | - | 50,50,50 | 0.27 | 0 | 53,55,55 | 0.21 | 0 |
| 57 | CDL | Dr | 403 | - | 99,99,99 | 0.30 | 0 | 105,111,111 | 0.24 | 0 |
| 57 | CDL | EB | 304 | - | 99,99,99 | 0.30 | 0 | 105,111,111 | 0.25 | 0 |
| 57 | CDL | El | 903 | - | 99,99,99 | 0.30 | 0 | 105,111,111 | 0.25 | 0 |
| 59 | 3PE | Dr | 401 | - | 50,50,50 | 0.27 | 0 | 53,55,55 | 0.22 | 0 |
| 57 | CDL | Dj | 408 | - | 99,99,99 | 0.30 | 0 | 105,111,111 | 0.25 | 0 |
| 59 | 3PE | Dg | 204 | - | 50,50,50 | 0.26 | 0 | 53,55,55 | 0.23 | 0 |
| 58 | PC1 | Da | 706 | - | 53,53,53 | 0.29 | 0 | 59,61,61 | 0.27 | 0 |
| 57 | CDL | Dj | 402 | - | 99,99,99 | 0.30 | 0 | 105,111,111 | 0.24 | 0 |
| 58 | PC1 | Db | 702 | - | 53,53,53 | 0.29 | 0 | 59,61,61 | 0.25 | 0 |
| 58 | PC1 | El | 904 | - | 53,53,53 | 0.28 | 0 | 59,61,61 | 0.28 | 0 |
| 57 | CDL | DG | 202 | - | 99,99,99 | 0.30 | 0 | 105,111,111 | 0.25 | 0 |
| 57 | CDL | Ea | 301 | - | 99,99,99 | 0.29 | 0 | 105,111,111 | 0.24 | 0 |
| 57 | CDL | En | 1201 | - | 99,99,99 | 0.29 | 0 | 105,111,111 | 0.25 | 0 |
| 58 | PC1 | DJ | 306 | - | 53,53,53 | 0.29 | 0 | 59,61,61 | 0.26 | 0 |
| 62 | CUA | Db | 701 | 2 | 0,1,1 | - | - | - | | |
| 65 | UQ8 | DS | 404 | - | 53,53,53 | 0.50 | 0 | 64,67,67 | 0.66 | 2 (3%) |
| 60 | LPP | Ed | 203 | - | 43,43,43 | 0.22 | 0 | 47,48,48 | 0.27 | 0 |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\|>2$ | Counts | RMSZ | $\#\|Z\|>2$ |
| 58 | PC1 | Ds | 406 | - | 53,53,53 | 0.29 | 0 | 59,61,61 | 0.26 | 0 |
| 57 | CDL | Dd | 705 | - | 99,99,99 | 0.30 | 0 | 105,111,111 | 0.25 | 0 |
| 57 | CDL | Dv | 401 | - | 99,99,99 | 0.30 | 0 | 105,111,111 | 0.24 | 0 |
| 57 | CDL | DQ | 1501 | - | 99,99,99 | 0.29 | 0 | 105,111,111 | 0.26 | 0 |
| 57 | CDL | Dq | 401 | - | 99,99,99 | 0.30 | 0 | 105,111,111 | 0.25 | 0 |
| 57 | CDL | DJ | 302 | - | 99,99,99 | 0.30 | 0 | 105,111,111 | 0.25 | 0 |
| 58 | PC1 | Dv | 406 | - | 53,53,53 | 0.29 | 0 | 59,61,61 | 0.25 | 0 |
| 59 | 3PE | DG | 204 | - | 50,50,50 | 0.27 | 0 | 53,55,55 | 0.20 | 0 |
| 67 | FES | Ef | 1002 | 31 | 0,4,4 | - | - | - | | |
| 58 | PC1 | DA | 707 | - | 53,53,53 | 0.29 | 0 | 59,61,61 | 0.27 | 0 |
| 67 | FES | Ef | 1003 | 31 | 0,4,4 | - | - | - | | |
| 57 | CDL | Dc | 601 | - | 99,99,99 | 0.30 | 0 | 105,111,111 | 0.24 | 0 |
| 65 | UQ8 | En | 1203 | - | 53,53,53 | 0.51 | 0 | 64,67,67 | 0.62 | 2 (3%) |
| 57 | CDL | Dx | 1201 | - | 99,99,99 | 0.30 | 0 | 105,111,111 | 0.25 | 0 |
| 57 | CDL | Du | 404 | - | 99,99,99 | 0.30 | 0 | 105,111,111 | 0.24 | 0 |
| 67 | FES | EF | 201 | 31 | 0,4,4 | - | - | - | | |
| 57 | CDL | DU | 402 | - | 99,99,99 | 0.29 | 0 | 105,111,111 | 0.25 | 0 |
| 57 | CDL | Ed | 204 | - | 99,99,99 | 0.29 | 0 | 105,111,111 | 0.25 | 0 |
| 58 | PC1 | EO | 206 | - | 53,53,53 | 0.29 | 0 | 59,61,61 | 0.26 | 0 |
| 57 | CDL | DU | 404 | - | 99,99,99 | 0.30 | 0 | 105,111,111 | 0.25 | 0 |
| 58 | PC1 | EO | 205 | - | 53,53,53 | 0.28 | 0 | 59,61,61 | 0.28 | 0 |
| 58 | PC1 | Dv | 407 | - | 53,53,53 | 0.29 | 0 | 59,61,61 | 0.26 | 0 |
| 59 | 3PE | DJ | 301 | - | 50,50,50 | 0.27 | 0 | 53,55,55 | 0.21 | 0 |
| 60 | LPP | Dn | 506 | - | 43,43,43 | 0.22 | 0 | 47,48,48 | 0.28 | 0 |
| 58 | PC1 | EO | 201 | - | 53,53,53 | 0.30 | 0 | 59,61,61 | 0.27 | 0 |
| 59 | 3PE | Em | 901 | - | 50,50,50 | 0.27 | 0 | 53,55,55 | 0.19 | 0 |
| 57 | CDL | Di | 701 | - | 99,99,99 | 0.30 | 0 | 105,111,111 | 0.24 | 0 |
| 58 | PC1 | DY | 302 | - | 53,53,53 | 0.28 | 0 | 59,61,61 | 0.26 | 0 |
| 57 | CDL | EI | 401 | - | 99,99,99 | 0.29 | 0 | 105,111,111 | 0.25 | 0 |
| 57 | CDL | DU | 403 | - | 99,99,99 | 0.30 | 0 | 105,111,111 | 0.24 | 0 |
| 57 | CDL | DN | 505 | - | 99,99,99 | 0.30 | 0 | 105,111,111 | 0.25 | 0 |
| 57 | CDL | EK | 201 | - | 99,99,99 | 0.30 | 0 | 105,111,111 | 0.25 | 0 |
| 57 | CDL | Eg | 101 | - | 99,99,99 | 0.29 | 0 | 105,111,111 | 0.25 | 0 |
| 66 | HEM | ED | 602 | - | 50,50,50 | 1.55 | 6 (12%) | 66,82,82 | 1.60 | 10 (15%) |
| 54 | HEA | Da | 701 | 1 | 66,67,67 | 2.50 | 26 (39%) | 78,103,103 | 2.36 | 31 (39%) |
| 57 | CDL | Ds | 402 | - | 99,99,99 | 0.30 | 0 | 105,111,111 | 0.24 | 0 |
| 57 | CDL | Ed | 205 | - | 99,99,99 | 0.29 | 0 | 105,111,111 | 0.24 | 0 |
| 57 | CDL | Dq | 404 | - | 99,99,99 | 0.30 | 0 | 105,111,111 | 0.24 | 0 |
| 57 | CDL | EL | 904 | - | 99,99,99 | 0.30 | 0 | 105,111,111 | 0.24 | 0 |
| 58 | PC1 | Eb | 302 | - | 53,53,53 | 0.29 | 0 | 59,61,61 | 0.27 | 0 |
| 59 | 3PE | DG | 205 | - | 50,50,50 | 0.27 | 0 | 53,55,55 | 0.21 | 0 |
| 57 | CDL | Dv | 403 | - | 99,99,99 | 0.30 | 0 | 105,111,111 | 0.24 | 0 |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\|>2$ | Counts | RMSZ | $\#\|Z\|>2$ |
| 58 | PC1 | Dx | 1202 | - | 53,53,53 | 0.28 | 0 | 59,61,61 | 0.26 | 0 |
| 57 | CDL | Dz | 501 | - | 99,99,99 | 0.30 | 0 | 105,111,111 | 0.24 | 0 |
| 57 | CDL | DX | 301 | - | 99,99,99 | 0.30 | 0 | 105,111,111 | 0.25 | 0 |
| 59 | 3PE | Dd | 703 | - | 50,50,50 | 0.27 | 0 | 53,55,55 | 0.20 | 0 |
| 57 | CDL | Dh | 202 | - | 99,99,99 | 0.30 | 0 | 105,111,111 | 0.24 | 0 |
| 59 | 3PE | EM | 901 | - | 50,50,50 | 0.27 | 0 | 53,55,55 | 0.20 | 0 |
| 57 | CDL | Da | 709 | - | 99,99,99 | 0.29 | 0 | 105,111,111 | 0.24 | 0 |
| 57 | CDL | EB | 302 | - | 99,99,99 | 0.30 | 0 | 105,111,111 | 0.27 | 0 |
| 59 | 3PE | Dj | 407 | - | 50,50,50 | 0.27 | 0 | 53,55,55 | 0.21 | 0 |
| 57 | CDL | Ei | 401 | - | 99,99,99 | 0.29 | 0 | 105,111,111 | 0.24 | 0 |
| 57 | CDL | DA | 709 | - | 99,99,99 | 0.30 | 0 | 105,111,111 | 0.25 | 0 |
| 58 | PC1 | Da | 707 | - | 53,53,53 | 0.29 | 0 | 59,61,61 | 0.27 | 0 |
| 59 | 3PE | EL | 905 | - | 50,50,50 | 0.27 | 0 | 53,55,55 | 0.22 | 0 |
| 57 | CDL | DS | 405 | - | 99,99,99 | 0.30 | 0 | 105,111,111 | 0.24 | 0 |
| 57 | CDL | DN | 501 | - | 99,99,99 | 0.30 | 0 | 105,111,111 | 0.25 | 0 |
| 59 | 3PE | DX | 304 | - | 50,50,50 | 0.26 | 0 | 53,55,55 | 0.21 | 0 |
| 57 | CDL | EH | 202 | - | 99,99,99 | 0.29 | 0 | 105,111,111 | 0.25 | 0 |
| 58 | PC1 | Dc | 602 | - | 53,53,53 | 0.28 | 0 | 59,61,61 | 0.27 | 0 |
| 59 | 3PE | El | 905 | - | 50,50,50 | 0.28 | 0 | 53,55,55 | 0.21 | 0 |
| 57 | CDL | EH | 201 | - | 99,99,99 | 0.29 | 0 | 105,111,111 | 0.25 | 0 |
| 57 | CDL | DD | 703 | - | 99,99,99 | 0.29 | 0 | 105,111,111 | 0.25 | 0 |
| 57 | CDL | Ep | 701 | - | 99,99,99 | 0.29 | 0 | 105,111,111 | 0.25 | 0 |
| 57 | CDL | DJ | 307 | - | 99,99,99 | 0.30 | 0 | 105,111,111 | 0.25 | 0 |
| 57 | CDL | Dq | 403 | - | 99,99,99 | 0.29 | 0 | 105,111,111 | 0.26 | 0 |
| 59 | 3PE | Dc | 606 | - | 50,50,50 | 0.27 | 0 | 53,55,55 | 0.20 | 0 |
| 58 | PC1 | Dc | 605 | - | 53,53,53 | 0.29 | 0 | 59,61,61 | 0.26 | 0 |
| 57 | CDL | DY | 301 | - | 99,99,99 | 0.30 | 0 | 105,111,111 | 0.24 | 0 |
| 57 | CDL | DQ | 1504 | - | 99,99,99 | 0.30 | 0 | 105,111,111 | 0.25 | 0 |
| 58 | PC1 | DQ | 1503 | - | 53,53,53 | 0.28 | 0 | 59,61,61 | 0.26 | 0 |
| 57 | CDL | Dv | 404 | - | 99,99,99 | 0.30 | 0 | 105,111,111 | 0.25 | 0 |
| 57 | CDL | DV | 403 | - | 99,99,99 | 0.30 | 0 | 105,111,111 | 0.24 | 0 |
| 57 | CDL | DM | 501 | - | 99,99,99 | 0.29 | 0 | 105,111,111 | 0.24 | 0 |
| 57 | CDL | EO | 202 | - | 99,99,99 | 0.30 | 0 | 105,111,111 | 0.25 | 0 |
| 57 | CDL | Dg | 201 | - | 99,99,99 | 0.30 | 0 | 105,111,111 | 0.25 | 0 |
| 58 | PC1 | DB | 702 | - | 53,53,53 | 0.29 | 0 | 59,61,61 | 0.26 | 0 |
| 57 | CDL | DV | 401 | - | 99,99,99 | 0.30 | 0 | 105,111,111 | 0.24 | 0 |
| 58 | PC1 | Ef | 1001 | - | 53,53,53 | 0.28 | 0 | 59,61,61 | 0.26 | 0 |
| 58 | PC1 | DC | 605 | - | 53,53,53 | 0.29 | 0 | 59,61,61 | 0.26 | 0 |
| 57 | CDL | Dv | 402 | - | 99,99,99 | 0.30 | 0 | 105,111,111 | 0.25 | 0 |
| 59 | 3PE | DS | 401 | - | 50,50,50 | 0.26 | 0 | 53,55,55 | 0.23 | 0 |
| 57 | CDL | DJ | 304 | - | 99,99,99 | 0.30 | 0 | 105,111,111 | 0.25 | 0 |
| 65 | UQ8 | Ds | 404 | - | 53,53,53 | 0.50 | 0 | 64,67,67 | 0.66 | 1 (1%) |
| 57 | CDL | DJ | 303 | - | 99,99,99 | 0.30 | 0 | 105,111,111 | 0.26 | 0 |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\|>2$ | Counts | RMSZ | $\#\|Z\|>2$ |
| 57 | CDL | Dn | 503 | - | 99,99,99 | 0.29 | 0 | 105,111,111 | 0.24 | 0 |
| 60 | LPP | EI | 402 | - | 43,43,43 | 0.22 | 0 | 47,48,48 | 0.27 | 0 |
| 57 | CDL | EN | 1201 | - | 99,99,99 | 0.30 | 0 | 105,111,111 | 0.25 | 0 |
| 54 | HEA | DA | 702 | - | 66,67,67 | 2.49 | 26 (39%) | 78,103,103 | 2.38 | 31 (39%) |

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 |
|---|---|---|---|---|---|---|---|
| 57 | CDL | DC | 601 | - | - | 27/110/110/110 | - |
| 57 | CDL | DA | 710 | - | - | 25/110/110/110 | - |
| 68 | ATP | ER | 201 | - | - | 6/22/38/38 | 0/3/3/3 |
| 57 | CDL | En | 1202 | - | - | 25/110/110/110 | - |
| 57 | CDL | El | 901 | - | - | 40/110/110/110 | - |
| 54 | HEA | DA | 701 | 1 | - | 3/36/76/76 | - |
| 58 | PC1 | Dv | 408 | - | - | 9/57/57/57 | - |
| 66 | HEM | Ed | 201 | - | - | 2/14/54/54 | - |
| 57 | CDL | Dm | 502 | - | - | 20/110/110/110 | - |
| 57 | CDL | Du | 403 | - | - | 30/110/110/110 | - |
| 59 | 3PE | DA | 708 | - | - | 13/54/54/54 | - |
| 57 | CDL | DZ | 501 | - | - | 28/110/110/110 | - |
| 59 | 3PE | Dr | 404 | - | - | 10/54/54/54 | - |
| 58 | PC1 | DC | 608 | - | - | 18/57/57/57 | - |
| 58 | PC1 | Dj | 406 | - | - | 10/57/57/57 | - |
| 58 | PC1 | DC | 604 | - | - | 16/57/57/57 | - |
| 57 | CDL | Dd | 704 | - | - | 34/110/110/110 | - |
| 54 | HEA | Da | 702 | - | - | 9/36/76/76 | - |
| 60 | LPP | DN | 503 | - | - | 1/45/45/45 | - |
| 57 | CDL | Dn | 505 | - | - | 27/110/110/110 | - |
| 58 | PC1 | DA | 706 | - | - | 14/57/57/57 | - |
| 57 | CDL | Ds | 405 | - | - | 28/110/110/110 | - |
| 57 | CDL | Dm | 501 | - | - | 39/110/110/110 | - |
| 57 | CDL | DN | 504 | - | - | 28/110/110/110 | - |
| 59 | 3PE | Dx | 1206 | - | - | 20/54/54/54 | - |
| 58 | PC1 | Eo | 204 | - | - | 20/57/57/57 | - |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 58 | PC1 | DV | 406 | - | - | 11/57/57/57 | - |
| 57 | CDL | DV | 404 | - | - | 38/110/110/110 | - |
| 57 | CDL | DA | 705 | - | - | 28/110/110/110 | - |
| 57 | CDL | DD | 702 | - | - | 25/110/110/110 | - |
| 57 | CDL | EU | 101 | - | - | 33/110/110/110 | - |
| 57 | CDL | Dg | 202 | - | - | 22/110/110/110 | - |
| 58 | PC1 | Dx | 1208 | - | - | 5/57/57/57 | - |
| 60 | LPP | Dl | 1101 | - | - | 8/45/45/45 | - |
| 57 | CDL | Dj | 403 | - | - | 36/110/110/110 | - |
| 57 | CDL | Eh | 1601 | - | - | 35/110/110/110 | - |
| 57 | CDL | ED | 604 | - | - | 27/110/110/110 | - |
| 58 | PC1 | DX | 306 | - | - | 10/57/57/57 | - |
| 57 | CDL | El | 902 | - | - | 37/110/110/110 | - |
| 57 | CDL | Dd | 702 | - | - | 28/110/110/110 | - |
| 57 | CDL | Do | 501 | - | - | 29/110/110/110 | - |
| 57 | CDL | Dj | 401 | - | - | 32/110/110/110 | - |
| 57 | CDL | DH | 201 | - | - | 22/110/110/110 | - |
| 57 | CDL | DD | 704 | - | - | 34/110/110/110 | - |
| 58 | PC1 | Dy | 302 | - | - | 11/57/57/57 | - |
| 57 | CDL | DI | 701 | - | - | 26/110/110/110 | - |
| 58 | PC1 | DG | 203 | - | - | 8/57/57/57 | - |
| 57 | CDL | EA | 301 | - | - | 26/110/110/110 | - |
| 57 | CDL | Dq | 402 | - | - | 26/110/110/110 | - |
| 58 | PC1 | DS | 406 | - | - | 19/57/57/57 | - |
| 57 | CDL | EL | 901 | - | - | 36/110/110/110 | - |
| 57 | CDL | Eu | 101 | - | - | 30/110/110/110 | - |
| 59 | 3PE | Ds | 401 | - | - | 17/54/54/54 | - |
| 59 | 3PE | Da | 708 | - | - | 17/54/54/54 | - |
| 65 | UQ8 | ED | 603 | - | - | 8/51/75/75 | 0/1/1/1 |
| 58 | PC1 | DC | 602 | - | - | 17/57/57/57 | - |
| 57 | CDL | DR | 403 | - | - | 27/110/110/110 | - |
| 58 | PC1 | Dg | 203 | - | - | 12/57/57/57 | - |
| 58 | PC1 | EB | 301 | - | - | 12/57/57/57 | - |
| 59 | 3PE | DR | 401 | - | - | 9/54/54/54 | - |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 60 | LPP | DA | 711 | - | - | 7/45/45/45 | - |
| 58 | PC1 | Eb | 301 | - | - | 11/57/57/57 | - |
| 57 | CDL | DS | 402 | - | - | 30/110/110/110 | - |
| 59 | 3PE | DC | 607 | - | - | 16/54/54/54 | - |
| 58 | PC1 | DV | 405 | - | - | 14/57/57/57 | - |
| 68 | ATP | Er | 201 | - | - | 5/22/38/38 | 0/3/3/3 |
| 57 | CDL | EL | 902 | - | - | 26/110/110/110 | - |
| 57 | CDL | Dn | 501 | - | - | 35/110/110/110 | - |
| 59 | 3PE | Ds | 407 | - | - | 12/54/54/54 | - |
| 58 | PC1 | Di | 702 | - | - | 19/57/57/57 | - |
| 60 | LPP | Dn | 504 | - | - | 9/45/45/45 | - |
| 58 | PC1 | Eo | 205 | - | - | 14/57/57/57 | - |
| 57 | CDL | Dx | 1203 | - | - | 31/110/110/110 | - |
| 57 | CDL | DO | 501 | - | - | 26/110/110/110 | - |
| 58 | PC1 | Dx | 1204 | - | - | 14/57/57/57 | - |
| 65 | UQ8 | EN | 1204 | - | - | 16/51/75/75 | 0/1/1/1 |
| 57 | CDL | DQ | 1502 | - | - | 23/110/110/110 | - |
| 58 | PC1 | DX | 302 | - | - | 14/57/57/57 | - |
| 57 | CDL | DM | 502 | - | - | 17/110/110/110 | - |
| 57 | CDL | DR | 402 | - | - | 35/110/110/110 | - |
| 58 | PC1 | DV | 407 | - | - | 10/57/57/57 | - |
| 57 | CDL | Dy | 301 | - | - | 29/110/110/110 | - |
| 57 | CDL | Dd | 706 | - | - | 26/110/110/110 | - |
| 65 | UQ8 | El | 906 | - | - | 12/51/75/75 | 0/1/1/1 |
| 59 | 3PE | Ds | 403 | - | - | 19/54/54/54 | - |
| 59 | 3PE | Eo | 202 | - | - | 16/54/54/54 | - |
| 65 | UQ8 | Ed | 202 | - | - | 9/51/75/75 | 0/1/1/1 |
| 57 | CDL | Du | 401 | - | - | 30/110/110/110 | - |
| 58 | PC1 | Dv | 405 | - | - | 12/57/57/57 | - |
| 59 | 3PE | DS | 403 | - | - | 19/54/54/54 | - |
| 58 | PC1 | Dc | 604 | - | - | 12/57/57/57 | - |
| 59 | 3PE | EN | 1203 | - | - | 14/54/54/54 | - |
| 57 | CDL | Dj | 404 | - | - | 33/110/110/110 | - |
| 58 | PC1 | EB | 303 | - | - | 4/57/57/57 | - |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 57 | CDL | ED | 601 | - | - | 27/110/110/110 | - |
| 57 | CDL | Dr | 402 | - | - | 32/110/110/110 | - |
| 58 | PC1 | EO | 207 | - | - | 17/57/57/57 | - |
| 57 | CDL | DU | 401 | - | - | 32/110/110/110 | - |
| 57 | CDL | Dh | 201 | - | - | 25/110/110/110 | - |
| 57 | CDL | DG | 201 | - | - | 38/110/110/110 | - |
| 65 | UQ8 | EL | 906 | - | - | 10/51/75/75 | 0/1/1/1 |
| 57 | CDL | Dn | 507 | - | - | 22/110/110/110 | - |
| 57 | CDL | Dj | 405 | - | - | 23/110/110/110 | - |
| 58 | PC1 | DS | 407 | - | - | 16/57/57/57 | - |
| 57 | CDL | DJ | 305 | - | - | 25/110/110/110 | - |
| 58 | PC1 | Dc | 603 | - | - | 14/57/57/57 | - |
| 58 | PC1 | Eo | 201 | - | - | 15/57/57/57 | - |
| 58 | PC1 | DC | 603 | - | - | 13/57/57/57 | - |
| 57 | CDL | DX | 307 | - | - | 25/110/110/110 | - |
| 57 | CDL | EL | 903 | - | - | 37/110/110/110 | - |
| 57 | CDL | EN | 1202 | - | - | 31/110/110/110 | - |
| 59 | 3PE | Dx | 1207 | - | - | 13/54/54/54 | - |
| 59 | 3PE | EO | 203 | - | - | 18/54/54/54 | - |
| 59 | 3PE | DX | 305 | - | - | 13/54/54/54 | - |
| 57 | CDL | DV | 402 | - | - | 42/110/110/110 | - |
| 57 | CDL | Ek | 201 | - | - | 26/110/110/110 | - |
| 67 | FES | EF | 202 | 31 | - | - | 0/1/1/1 |
| 59 | 3PE | DX | 303 | - | - | 14/54/54/54 | - |
| 59 | 3PE | Dx | 1205 | - | - | 16/54/54/54 | - |
| 60 | LPP | DN | 502 | - | - | 8/45/45/45 | - |
| 57 | CDL | Du | 402 | - | - | 19/110/110/110 | - |
| 57 | CDL | Dn | 502 | - | - | 27/110/110/110 | - |
| 59 | 3PE | DC | 606 | - | - | 9/54/54/54 | - |
| 59 | 3PE | EO | 204 | - | - | 8/54/54/54 | - |
| 58 | PC1 | Dq | 405 | - | - | 9/57/57/57 | - |
| 57 | CDL | Da | 705 | - | - | 32/110/110/110 | - |
| 58 | PC1 | DI | 702 | - | - | 19/57/57/57 | - |
| 58 | PC1 | Dc | 607 | - | - | 17/57/57/57 | - |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 59 | 3PE | Eo | 203 | - | - | 7/54/54/54 | - |
| 57 | CDL | Dr | 403 | - | - | 23/110/110/110 | - |
| 57 | CDL | EB | 304 | - | - | 34/110/110/110 | - |
| 57 | CDL | El | 903 | - | - | 31/110/110/110 | - |
| 59 | 3PE | Dr | 401 | - | - | 16/54/54/54 | - |
| 57 | CDL | Dj | 408 | - | - | 33/110/110/110 | - |
| 59 | 3PE | Dg | 204 | - | - | 12/54/54/54 | - |
| 58 | PC1 | Da | 706 | - | - | 16/57/57/57 | - |
| 57 | CDL | Dj | 402 | - | - | 29/110/110/110 | - |
| 58 | PC1 | Db | 702 | - | - | 21/57/57/57 | - |
| 58 | PC1 | El | 904 | - | - | 10/57/57/57 | - |
| 57 | CDL | DG | 202 | - | - | 19/110/110/110 | - |
| 57 | CDL | Ea | 301 | - | - | 24/110/110/110 | - |
| 57 | CDL | En | 1201 | - | - | 24/110/110/110 | - |
| 58 | PC1 | DJ | 306 | - | - | 11/57/57/57 | - |
| 65 | UQ8 | DS | 404 | - | - | 9/51/75/75 | 0/1/1/1 |
| 60 | LPP | Ed | 203 | - | - | 2/45/45/45 | - |
| 58 | PC1 | Ds | 406 | - | - | 9/57/57/57 | - |
| 57 | CDL | Dd | 705 | - | - | 31/110/110/110 | - |
| 57 | CDL | Dv | 401 | - | - | 28/110/110/110 | - |
| 57 | CDL | DQ | 1501 | - | - | 31/110/110/110 | - |
| 57 | CDL | Dq | 401 | - | - | 25/110/110/110 | - |
| 57 | CDL | DJ | 302 | - | - | 19/110/110/110 | - |
| 58 | PC1 | Dv | 406 | - | - | 19/57/57/57 | - |
| 59 | 3PE | DG | 204 | - | - | 16/54/54/54 | - |
| 67 | FES | Ef | 1002 | 31 | - | - | 0/1/1/1 |
| 58 | PC1 | DA | 707 | - | - | 11/57/57/57 | - |
| 67 | FES | Ef | 1003 | 31 | - | - | 0/1/1/1 |
| 57 | CDL | Dc | 601 | - | - | 31/110/110/110 | - |
| 65 | UQ8 | En | 1203 | - | - | 9/51/75/75 | 0/1/1/1 |
| 57 | CDL | Dx | 1201 | - | - | 29/110/110/110 | - |
| 57 | CDL | Du | 404 | - | - | 26/110/110/110 | - |
| 67 | FES | EF | 201 | 31 | - | - | 0/1/1/1 |
| 57 | CDL | DU | 402 | - | - | 19/110/110/110 | - |
| 57 | CDL | Ed | 204 | - | - | 25/110/110/110 | - |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 58 | PC1 | EO | 206 | - | - | 26/57/57/57 | - |
| 57 | CDL | DU | 404 | - | - | 23/110/110/110 | - |
| 58 | PC1 | EO | 205 | - | - | 10/57/57/57 | - |
| 58 | PC1 | Dv | 407 | - | - | 13/57/57/57 | - |
| 59 | 3PE | DJ | 301 | - | - | 15/54/54/54 | - |
| 60 | LPP | Dn | 506 | - | - | 7/45/45/45 | - |
| 58 | PC1 | EO | 201 | - | - | 12/57/57/57 | - |
| 59 | 3PE | Em | 901 | - | - | 14/54/54/54 | - |
| 57 | CDL | Di | 701 | - | - | 32/110/110/110 | - |
| 58 | PC1 | DY | 302 | - | - | 10/57/57/57 | - |
| 57 | CDL | EI | 401 | - | - | 24/110/110/110 | - |
| 57 | CDL | DU | 403 | - | - | 19/110/110/110 | - |
| 57 | CDL | DN | 505 | - | - | 30/110/110/110 | - |
| 57 | CDL | EK | 201 | - | - | 26/110/110/110 | - |
| 57 | CDL | Eg | 101 | - | - | 34/110/110/110 | - |
| 66 | HEM | ED | 602 | - | - | 2/14/54/54 | - |
| 54 | HEA | Da | 701 | 1 | - | 5/36/76/76 | - |
| 57 | CDL | Ds | 402 | - | - | 32/110/110/110 | - |
| 57 | CDL | Ed | 205 | - | - | 25/110/110/110 | - |
| 57 | CDL | Dq | 404 | - | - | 21/110/110/110 | - |
| 57 | CDL | EL | 904 | - | - | 33/110/110/110 | - |
| 58 | PC1 | Eb | 302 | - | - | 5/57/57/57 | - |
| 59 | 3PE | DG | 205 | - | - | 14/54/54/54 | - |
| 57 | CDL | Dv | 403 | - | - | 24/110/110/110 | - |
| 58 | PC1 | Dx | 1202 | - | - | 14/57/57/57 | - |
| 57 | CDL | Dz | 501 | - | - | 28/110/110/110 | - |
| 57 | CDL | DX | 301 | - | - | 33/110/110/110 | - |
| 59 | 3PE | Dd | 703 | - | - | 17/54/54/54 | - |
| 57 | CDL | Dh | 202 | - | - | 32/110/110/110 | - |
| 59 | 3PE | EM | 901 | - | - | 13/54/54/54 | - |
| 57 | CDL | Da | 709 | - | - | 33/110/110/110 | - |
| 57 | CDL | EB | 302 | - | - | 27/110/110/110 | - |
| 59 | 3PE | Dj | 407 | - | - | 5/54/54/54 | - |
| 57 | CDL | Ei | 401 | - | - | 23/110/110/110 | - |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 57 | CDL | DA | 709 | - | - | 35/110/110/110 | - |
| 58 | PC1 | Da | 707 | - | - | 13/57/57/57 | - |
| 59 | 3PE | EL | 905 | - | - | 16/54/54/54 | - |
| 57 | CDL | DS | 405 | - | - | 32/110/110/110 | - |
| 57 | CDL | DN | 501 | - | - | 20/110/110/110 | - |
| 59 | 3PE | DX | 304 | - | - | 17/54/54/54 | - |
| 57 | CDL | EH | 202 | - | - | 24/110/110/110 | - |
| 58 | PC1 | Dc | 602 | - | - | 18/57/57/57 | - |
| 59 | 3PE | El | 905 | - | - | 17/54/54/54 | - |
| 57 | CDL | EH | 201 | - | - | 26/110/110/110 | - |
| 57 | CDL | DD | 703 | - | - | 25/110/110/110 | - |
| 57 | CDL | Ep | 701 | - | - | 30/110/110/110 | - |
| 57 | CDL | DJ | 307 | - | - | 32/110/110/110 | - |
| 57 | CDL | Dq | 403 | - | - | 24/110/110/110 | - |
| 59 | 3PE | Dc | 606 | - | - | 18/54/54/54 | - |
| 58 | PC1 | Dc | 605 | - | - | 16/57/57/57 | - |
| 57 | CDL | DY | 301 | - | - | 29/110/110/110 | - |
| 57 | CDL | DQ | 1504 | - | - | 33/110/110/110 | - |
| 58 | PC1 | DQ | 1503 | - | - | 11/57/57/57 | - |
| 57 | CDL | Dv | 404 | - | - | 41/110/110/110 | - |
| 57 | CDL | DV | 403 | - | - | 24/110/110/110 | - |
| 57 | CDL | DM | 501 | - | - | 31/110/110/110 | - |
| 57 | CDL | EO | 202 | - | - | 31/110/110/110 | - |
| 57 | CDL | Dg | 201 | - | - | 40/110/110/110 | - |
| 58 | PC1 | DB | 702 | - | - | 21/57/57/57 | - |
| 57 | CDL | DV | 401 | - | - | 28/110/110/110 | - |
| 58 | PC1 | Ef | 1001 | - | - | 18/57/57/57 | - |
| 58 | PC1 | DC | 605 | - | - | 11/57/57/57 | - |
| 57 | CDL | Dv | 402 | - | - | 40/110/110/110 | - |
| 59 | 3PE | DS | 401 | - | - | 17/54/54/54 | - |
| 57 | CDL | DJ | 304 | - | - | 37/110/110/110 | - |
| 65 | UQ8 | Ds | 404 | - | - | 12/51/75/75 | 0/1/1/1 |
| 57 | CDL | DJ | 303 | - | - | 36/110/110/110 | - |
| 57 | CDL | Dn | 503 | - | - | 24/110/110/110 | - |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 60 | LPP | EI | 402 | - | - | 8/45/45/45 | - |
| 57 | CDL | EN | 1201 | - | - | 27/110/110/110 | - |
| 54 | HEA | DA | 702 | - | - | 8/36/76/76 | - |

All (115) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 54 | Da | 701 | HEA | C3A-C2A | 5.89 | 1.49 | 1.36 |
| 54 | DA | 701 | HEA | C3A-C2A | 5.83 | 1.49 | 1.36 |
| 54 | Da | 702 | HEA | C3A-C2A | 5.82 | 1.49 | 1.36 |
| 54 | DA | 702 | HEA | C3A-C2A | 5.80 | 1.49 | 1.36 |
| 54 | DA | 702 | HEA | FE-NB | 5.55 | 2.12 | 1.94 |
| 54 | Da | 702 | HEA | FE-NB | 5.53 | 2.12 | 1.94 |
| 54 | Da | 701 | HEA | C3B-C2B | 5.52 | 1.47 | 1.34 |
| 54 | DA | 701 | HEA | C3B-C2B | 5.51 | 1.47 | 1.34 |
| 54 | Da | 701 | HEA | FE-NB | 5.48 | 2.11 | 1.94 |
| 54 | DA | 701 | HEA | FE-NB | 5.47 | 2.11 | 1.94 |
| 54 | DA | 702 | HEA | FE-ND | 5.46 | 2.11 | 1.94 |
| 66 | ED | 602 | HEM | FE-NB | 5.45 | 2.11 | 1.94 |
| 54 | Da | 702 | HEA | C3B-C2B | 5.43 | 1.46 | 1.34 |
| 54 | DA | 702 | HEA | C3B-C2B | 5.43 | 1.46 | 1.34 |
| 54 | Da | 702 | HEA | FE-ND | 5.42 | 2.11 | 1.94 |
| 66 | Ed | 201 | HEM | FE-NB | 5.42 | 2.11 | 1.94 |
| 54 | Da | 701 | HEA | FE-ND | 5.35 | 2.11 | 1.94 |
| 54 | DA | 701 | HEA | FE-ND | 5.32 | 2.11 | 1.94 |
| 54 | Da | 701 | HEA | C3D-C2D | 4.93 | 1.47 | 1.36 |
| 54 | DA | 702 | HEA | C3D-C2D | 4.90 | 1.47 | 1.36 |
| 54 | Da | 702 | HEA | C3D-C2D | 4.89 | 1.47 | 1.36 |
| 54 | DA | 701 | HEA | C3D-C2D | 4.89 | 1.47 | 1.36 |
| 54 | DA | 701 | HEA | FE-NC | 4.75 | 2.11 | 1.95 |
| 54 | Da | 701 | HEA | FE-NC | 4.75 | 2.11 | 1.95 |
| 54 | Da | 702 | HEA | FE-NC | 4.67 | 2.11 | 1.95 |
| 54 | DA | 702 | HEA | FE-NC | 4.64 | 2.10 | 1.95 |
| 54 | Da | 701 | HEA | CHA-C1A | 4.56 | 1.47 | 1.38 |
| 54 | DA | 702 | HEA | CHB-C4A | 4.55 | 1.47 | 1.38 |
| 54 | Da | 701 | HEA | CHC-C4B | 4.53 | 1.47 | 1.38 |
| 54 | DA | 701 | HEA | CHB-C4A | 4.53 | 1.47 | 1.38 |
| 54 | DA | 701 | HEA | CHC-C4B | 4.53 | 1.47 | 1.38 |
| 54 | DA | 701 | HEA | CHA-C1A | 4.52 | 1.47 | 1.38 |
| 54 | Da | 702 | HEA | CHC-C4B | 4.52 | 1.47 | 1.38 |
| 54 | Da | 702 | HEA | CHB-C4A | 4.51 | 1.47 | 1.38 |
| 54 | DA | 702 | HEA | CHA-C1A | 4.50 | 1.47 | 1.38 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 54 | DA | 702 | HEA | CHC-C4B | 4.48 | 1.47 | 1.38 |
| 54 | Da | 702 | HEA | CHA-C1A | 4.47 | 1.47 | 1.38 |
| 54 | Da | 701 | HEA | CHD-C1D | 4.42 | 1.47 | 1.38 |
| 54 | DA | 701 | HEA | CHD-C1D | 4.40 | 1.47 | 1.38 |
| 54 | DA | 702 | HEA | CHD-C1D | 4.40 | 1.47 | 1.38 |
| 54 | Da | 702 | HEA | CHD-C1D | 4.39 | 1.47 | 1.38 |
| 54 | Da | 701 | HEA | CHB-C4A | 4.36 | 1.46 | 1.38 |
| 66 | Ed | 201 | HEM | FE-NC | 4.27 | 2.09 | 1.95 |
| 66 | ED | 602 | HEM | FE-NC | 4.24 | 2.09 | 1.95 |
| 54 | Da | 701 | HEA | CHC-C1C | 3.82 | 1.48 | 1.39 |
| 54 | DA | 701 | HEA | CHC-C1C | 3.81 | 1.48 | 1.39 |
| 54 | Da | 701 | HEA | CHD-C4C | 3.74 | 1.47 | 1.39 |
| 54 | DA | 701 | HEA | CHD-C4C | 3.73 | 1.47 | 1.39 |
| 54 | Da | 702 | HEA | CHC-C1C | 3.72 | 1.47 | 1.39 |
| 54 | DA | 702 | HEA | CHC-C1C | 3.70 | 1.47 | 1.39 |
| 54 | Da | 702 | HEA | CHD-C4C | 3.70 | 1.47 | 1.39 |
| 54 | DA | 702 | HEA | CHD-C4C | 3.68 | 1.47 | 1.39 |
| 54 | Da | 702 | HEA | CHA-C4D | 3.62 | 1.47 | 1.39 |
| 54 | DA | 702 | HEA | CHA-C4D | 3.60 | 1.47 | 1.39 |
| 54 | Da | 701 | HEA | CHA-C4D | 3.59 | 1.47 | 1.39 |
| 54 | DA | 702 | HEA | CHB-C1B | 3.57 | 1.47 | 1.39 |
| 54 | Da | 702 | HEA | CHB-C1B | 3.57 | 1.47 | 1.39 |
| 54 | DA | 701 | HEA | CHB-C1B | 3.57 | 1.47 | 1.39 |
| 54 | Da | 701 | HEA | CHB-C1B | 3.53 | 1.47 | 1.39 |
| 54 | DA | 701 | HEA | CHA-C4D | 3.48 | 1.47 | 1.39 |
| 54 | Da | 701 | HEA | C1A-NA | 3.34 | 1.46 | 1.39 |
| 54 | DA | 701 | HEA | C1A-NA | 3.33 | 1.46 | 1.39 |
| 54 | DA | 702 | HEA | C1A-NA | 3.20 | 1.46 | 1.39 |
| 54 | Da | 702 | HEA | C1A-NA | 3.18 | 1.45 | 1.39 |
| 66 | Ed | 201 | HEM | C4D-ND | -3.14 | 1.34 | 1.40 |
| 66 | ED | 602 | HEM | C4D-ND | -3.09 | 1.35 | 1.40 |
| 66 | ED | 602 | HEM | C1B-NB | -3.05 | 1.35 | 1.40 |
| 66 | Ed | 201 | HEM | C1B-NB | -3.00 | 1.35 | 1.40 |
| 54 | Da | 702 | HEA | C4B-C3B | 2.93 | 1.49 | 1.44 |
| 54 | DA | 702 | HEA | C4B-C3B | 2.91 | 1.49 | 1.44 |
| 54 | Da | 701 | HEA | C4B-C3B | 2.81 | 1.49 | 1.44 |
| 54 | Da | 701 | HEA | C1A-C2A | 2.80 | 1.50 | 1.45 |
| 54 | Da | 702 | HEA | C1D-ND | -2.76 | 1.35 | 1.40 |
| 54 | DA | 701 | HEA | C4B-C3B | 2.75 | 1.49 | 1.44 |
| 54 | Da | 701 | HEA | C1D-ND | -2.75 | 1.35 | 1.40 |
| 54 | DA | 701 | HEA | C1A-C2A | 2.73 | 1.50 | 1.45 |
| 54 | DA | 702 | HEA | C1D-ND | -2.72 | 1.35 | 1.40 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 54 | DA | 701 | HEA | C4A-NA | 2.71 | 1.45 | 1.39 |
| 54 | Da | 701 | HEA | C1C-C2C | 2.70 | 1.49 | 1.43 |
| 54 | DA | 701 | HEA | C1D-ND | -2.69 | 1.35 | 1.40 |
| 54 | DA | 701 | HEA | C1C-C2C | 2.68 | 1.49 | 1.43 |
| 54 | DA | 702 | HEA | C4A-NA | 2.67 | 1.44 | 1.39 |
| 54 | Da | 701 | HEA | C4B-NB | -2.65 | 1.35 | 1.40 |
| 54 | DA | 701 | HEA | C4B-NB | -2.63 | 1.35 | 1.40 |
| 54 | Da | 702 | HEA | C4A-NA | 2.63 | 1.44 | 1.39 |
| 54 | Da | 702 | HEA | C1C-C2C | 2.62 | 1.49 | 1.43 |
| 54 | DA | 701 | HEA | C3C-C4C | 2.60 | 1.48 | 1.42 |
| 54 | Da | 701 | HEA | C3C-C4C | 2.60 | 1.48 | 1.42 |
| 54 | DA | 702 | HEA | C1A-C2A | 2.59 | 1.49 | 1.45 |
| 54 | Da | 701 | HEA | C4A-NA | 2.58 | 1.44 | 1.39 |
| 54 | Da | 702 | HEA | C1A-C2A | 2.58 | 1.49 | 1.45 |
| 54 | Da | 702 | HEA | C3C-C4C | 2.55 | 1.48 | 1.42 |
| 54 | DA | 702 | HEA | C1C-C2C | 2.52 | 1.49 | 1.43 |
| 54 | DA | 702 | HEA | C3C-C4C | 2.50 | 1.48 | 1.42 |
| 54 | DA | 702 | HEA | C4B-NB | -2.48 | 1.36 | 1.40 |
| 54 | Da | 702 | HEA | C4B-NB | -2.47 | 1.36 | 1.40 |
| 54 | DA | 702 | HEA | C4D-C3D | 2.47 | 1.49 | 1.45 |
| 54 | Da | 702 | HEA | C4D-C3D | 2.41 | 1.49 | 1.45 |
| 54 | DA | 701 | HEA | C1D-C2D | 2.29 | 1.49 | 1.44 |
| 54 | Da | 701 | HEA | C1D-C2D | 2.27 | 1.49 | 1.44 |
| 66 | ED | 602 | HEM | FE-ND | -2.25 | 1.87 | 1.94 |
| 54 | Da | 701 | HEA | C4D-C3D | 2.23 | 1.48 | 1.45 |
| 66 | Ed | 201 | HEM | FE-ND | -2.22 | 1.87 | 1.94 |
| 54 | DA | 701 | HEA | C4D-C3D | 2.21 | 1.48 | 1.45 |
| 54 | DA | 702 | HEA | C1B-C2B | 2.21 | 1.48 | 1.44 |
| 54 | Da | 702 | HEA | C1D-C2D | 2.20 | 1.48 | 1.44 |
| 54 | DA | 702 | HEA | C1D-C2D | 2.19 | 1.48 | 1.44 |
| 54 | DA | 702 | HEA | C4C-NC | -2.15 | 1.35 | 1.39 |
| 54 | Da | 702 | HEA | C1B-C2B | 2.15 | 1.48 | 1.44 |
| 54 | Da | 701 | HEA | C1B-C2B | 2.14 | 1.48 | 1.44 |
| 54 | DA | 701 | HEA | C1B-C2B | 2.13 | 1.48 | 1.44 |
| 54 | Da | 702 | HEA | C4C-NC | -2.13 | 1.35 | 1.39 |
| 54 | DA | 701 | HEA | C4C-NC | -2.11 | 1.35 | 1.39 |
| 54 | Da | 701 | HEA | C4C-NC | -2.07 | 1.35 | 1.39 |
| 66 | ED | 602 | HEM | C1C-C2C | -2.01 | 1.41 | 1.45 |

All (167) bond angle outliers are listed below:

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 54 | DA | 701 | HEA | C3C-C4C-NC | 6.87 | 114.47 | 110.25 |
| 54 | Da | 702 | HEA | C3C-C4C-NC | 6.84 | 114.46 | 110.25 |
| 54 | Da | 701 | HEA | C3C-C4C-NC | 6.79 | 114.43 | 110.25 |
| 54 | DA | 702 | HEA | C3C-C4C-NC | 6.71 | 114.37 | 110.25 |
| 54 | DA | 701 | HEA | C3D-C4D-ND | 5.99 | 116.16 | 110.36 |
| 54 | DA | 702 | HEA | C3D-C4D-ND | 5.93 | 116.10 | 110.36 |
| 54 | Da | 702 | HEA | C3D-C4D-ND | 5.92 | 116.09 | 110.36 |
| 54 | Da | 701 | HEA | C3D-C4D-ND | 5.89 | 116.06 | 110.36 |
| 54 | DA | 702 | HEA | C2D-C1D-ND | 5.36 | 116.19 | 109.84 |
| 54 | Da | 702 | HEA | C2D-C1D-ND | 5.31 | 116.13 | 109.84 |
| 54 | Da | 701 | HEA | C2B-C1B-NB | 5.27 | 116.19 | 109.88 |
| 54 | DA | 701 | HEA | C2D-C1D-ND | 5.25 | 116.06 | 109.84 |
| 54 | DA | 702 | HEA | C3B-C4B-NB | 5.24 | 116.05 | 109.84 |
| 54 | DA | 701 | HEA | C2B-C1B-NB | 5.22 | 116.13 | 109.88 |
| 54 | Da | 701 | HEA | C3C-C2C-C1C | -5.19 | 100.90 | 107.16 |
| 54 | DA | 702 | HEA | C2B-C1B-NB | 5.18 | 116.09 | 109.88 |
| 54 | Da | 702 | HEA | C2B-C1B-NB | 5.17 | 116.08 | 109.88 |
| 54 | Da | 701 | HEA | C2D-C1D-ND | 5.16 | 115.96 | 109.84 |
| 54 | DA | 701 | HEA | C3C-C2C-C1C | -5.14 | 100.95 | 107.16 |
| 54 | Da | 701 | HEA | C3B-C4B-NB | 5.14 | 115.93 | 109.84 |
| 54 | DA | 701 | HEA | C3B-C4B-NB | 5.13 | 115.92 | 109.84 |
| 54 | Da | 702 | HEA | C3B-C4B-NB | 5.13 | 115.92 | 109.84 |
| 54 | DA | 702 | HEA | C3C-C2C-C1C | -5.13 | 100.97 | 107.16 |
| 54 | Da | 702 | HEA | C3C-C2C-C1C | -5.11 | 101.00 | 107.16 |
| 66 | ED | 602 | HEM | CHC-C4B-NB | 5.09 | 129.95 | 124.42 |
| 66 | Ed | 201 | HEM | CHC-C4B-NB | 5.07 | 129.93 | 124.42 |
| 54 | Da | 701 | HEA | C2C-C1C-NC | 4.20 | 116.47 | 110.08 |
| 54 | DA | 701 | HEA | C2C-C1C-NC | 4.17 | 116.43 | 110.08 |
| 54 | DA | 702 | HEA | C2C-C1C-NC | 4.16 | 116.42 | 110.08 |
| 54 | DA | 701 | HEA | C1D-C2D-C3D | -4.15 | 102.59 | 106.96 |
| 54 | Da | 702 | HEA | C2C-C1C-NC | 4.14 | 116.38 | 110.08 |
| 66 | ED | 602 | HEM | CHD-C1D-ND | 4.11 | 128.88 | 124.42 |
| 54 | Da | 701 | HEA | C1D-C2D-C3D | -4.08 | 102.66 | 106.96 |
| 66 | Ed | 201 | HEM | CHD-C1D-ND | 4.03 | 128.80 | 124.42 |
| 54 | DA | 702 | HEA | C1D-C2D-C3D | -3.97 | 102.78 | 106.96 |
| 54 | Da | 702 | HEA | C1D-C2D-C3D | -3.94 | 102.81 | 106.96 |
| 65 | El | 906 | UQ8 | C7-C8-C9 | 3.83 | 133.16 | 126.79 |
| 66 | Ed | 201 | HEM | CHA-C4D-ND | 3.68 | 128.92 | 124.37 |
| 66 | Ed | 201 | HEM | C1B-NB-C4B | 3.67 | 108.87 | 105.07 |
| 65 | EL | 906 | UQ8 | C7-C8-C9 | 3.65 | 132.87 | 126.79 |
| 66 | ED | 602 | HEM | C1B-NB-C4B | 3.63 | 108.82 | 105.07 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 54 | Da | 701 | HEA | C1B-C2B-C3B | -3.54 | 102.57 | 106.80 |
| 66 | ED | 602 | HEM | CHA-C4D-ND | 3.52 | 128.72 | 124.37 |
| 54 | DA | 701 | HEA | C1B-C2B-C3B | -3.50 | 102.61 | 106.80 |
| 65 | El | 906 | UQ8 | C8-C7-C6 | 3.50 | 121.48 | 112.05 |
| 54 | DA | 702 | HEA | C13-C12-C11 | -3.45 | 109.16 | 114.35 |
| 54 | DA | 702 | HEA | C1B-C2B-C3B | -3.30 | 102.86 | 106.80 |
| 54 | DA | 702 | HEA | C26-C15-C16 | 3.29 | 120.81 | 115.27 |
| 54 | Da | 702 | HEA | C1B-C2B-C3B | -3.29 | 102.86 | 106.80 |
| 54 | Da | 702 | HEA | C27-C19-C20 | 3.24 | 120.73 | 115.27 |
| 54 | DA | 702 | HEA | C4D-C3D-C2D | -3.14 | 102.33 | 106.90 |
| 54 | Da | 702 | HEA | C4D-C3D-C2D | -3.13 | 102.33 | 106.90 |
| 54 | Da | 701 | HEA | CHB-C4A-NA | 3.12 | 127.81 | 124.44 |
| 66 | ED | 602 | HEM | C4C-NC-C1C | 3.09 | 108.37 | 105.35 |
| 54 | DA | 701 | HEA | CHA-C4D-C3D | -3.08 | 120.32 | 124.84 |
| 65 | Ed | 202 | UQ8 | C7-C8-C9 | 3.07 | 131.90 | 126.79 |
| 54 | Da | 701 | HEA | OMA-CMA-C3A | -3.03 | 118.83 | 125.69 |
| 54 | Da | 701 | HEA | C4D-C3D-C2D | -3.03 | 102.48 | 106.90 |
| 54 | DA | 701 | HEA | C4D-C3D-C2D | -3.01 | 102.51 | 106.90 |
| 65 | ED | 603 | UQ8 | C7-C8-C9 | 2.99 | 131.77 | 126.79 |
| 54 | Da | 701 | HEA | CHA-C4D-C3D | -2.98 | 120.45 | 124.84 |
| 54 | Da | 702 | HEA | C13-C12-C11 | -2.95 | 109.92 | 114.35 |
| 54 | DA | 701 | HEA | CHB-C1B-C2B | -2.94 | 120.38 | 124.98 |
| 66 | Ed | 201 | HEM | C4C-NC-C1C | 2.93 | 108.22 | 105.35 |
| 54 | DA | 702 | HEA | C4B-C3B-C2B | -2.91 | 102.43 | 107.41 |
| 54 | Da | 702 | HEA | CHB-C1B-C2B | -2.89 | 120.47 | 124.98 |
| 54 | Da | 701 | HEA | CHB-C1B-C2B | -2.88 | 120.47 | 124.98 |
| 54 | Da | 702 | HEA | C4B-C3B-C2B | -2.88 | 102.49 | 107.41 |
| 54 | DA | 702 | HEA | CHB-C1B-C2B | -2.85 | 120.53 | 124.98 |
| 54 | Da | 702 | HEA | CAD-C3D-C4D | 2.85 | 129.63 | 124.66 |
| 54 | Da | 701 | HEA | CHB-C4A-C3A | -2.85 | 120.39 | 125.26 |
| 65 | EL | 906 | UQ8 | C8-C7-C6 | 2.84 | 119.69 | 112.05 |
| 54 | DA | 701 | HEA | C4B-C3B-C2B | -2.80 | 102.63 | 107.41 |
| 54 | Da | 701 | HEA | C4B-C3B-C2B | -2.79 | 102.64 | 107.41 |
| 54 | Da | 701 | HEA | C3A-C2A-C1A | -2.79 | 104.41 | 107.08 |
| 54 | DA | 702 | HEA | CAD-C3D-C4D | 2.78 | 129.51 | 124.66 |
| 65 | Ds | 404 | UQ8 | C7-C8-C9 | 2.75 | 131.36 | 126.79 |
| 54 | Da | 702 | HEA | C26-C15-C16 | 2.72 | 119.84 | 115.27 |
| 54 | DA | 702 | HEA | C27-C19-C20 | 2.70 | 119.81 | 115.27 |
| 54 | DA | 702 | HEA | CMB-C2B-C1B | 2.67 | 129.10 | 125.04 |
| 65 | DS | 404 | UQ8 | C7-C8-C9 | 2.62 | 131.15 | 126.79 |
| 66 | Ed | 201 | HEM | CHB-C1B-NB | 2.60 | 127.58 | 124.37 |
| 54 | DA | 702 | HEA | CHB-C4A-NA | 2.59 | 127.25 | 124.44 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 54 | Da | 702 | HEA | CHB-C4A-NA | 2.59 | 127.24 | 124.44 |
| 54 | DA | 702 | HEA | CHC-C1C-C2C | -2.59 | 119.92 | 127.24 |
| 54 | Da | 701 | HEA | C13-C14-C15 | -2.58 | 121.46 | 127.66 |
| 54 | Da | 701 | HEA | CAA-CBA-CGA | -2.57 | 108.06 | 113.60 |
| 54 | Da | 702 | HEA | CHC-C1C-C2C | -2.57 | 119.99 | 127.24 |
| 54 | DA | 701 | HEA | C13-C14-C15 | -2.56 | 121.49 | 127.66 |
| 54 | Da | 702 | HEA | CHA-C4D-C3D | -2.56 | 121.08 | 124.84 |
| 54 | DA | 701 | HEA | C3A-C2A-C1A | -2.55 | 104.64 | 107.08 |
| 54 | DA | 701 | HEA | CHB-C4A-NA | 2.55 | 127.20 | 124.44 |
| 54 | DA | 702 | HEA | CHA-C4D-C3D | -2.54 | 121.10 | 124.84 |
| 54 | Da | 702 | HEA | CMB-C2B-C1B | 2.53 | 128.90 | 125.04 |
| 66 | ED | 602 | HEM | CHB-C1B-NB | 2.52 | 127.48 | 124.37 |
| 66 | ED | 602 | HEM | CHD-C1D-C2D | -2.51 | 121.06 | 124.98 |
| 54 | Da | 702 | HEA | CHD-C1D-C2D | -2.50 | 119.78 | 126.73 |
| 54 | DA | 702 | HEA | CHD-C1D-C2D | -2.49 | 119.83 | 126.73 |
| 54 | Da | 701 | HEA | CHC-C1C-C2C | -2.48 | 120.24 | 127.24 |
| 54 | Da | 701 | HEA | C27-C19-C20 | 2.47 | 119.43 | 115.27 |
| 65 | EL | 906 | UQ8 | C17-C18-C19 | -2.46 | 121.73 | 127.66 |
| 54 | DA | 701 | HEA | CHC-C1C-C2C | -2.46 | 120.29 | 127.24 |
| 66 | Ed | 201 | HEM | CHD-C1D-C2D | -2.46 | 121.14 | 124.98 |
| 54 | Da | 702 | HEA | C25-C23-C24 | 2.46 | 120.03 | 114.60 |
| 54 | DA | 701 | HEA | C27-C19-C20 | 2.45 | 119.39 | 115.27 |
| 54 | DA | 701 | HEA | CAA-CBA-CGA | -2.45 | 108.33 | 113.60 |
| 54 | DA | 701 | HEA | C25-C23-C24 | 2.44 | 120.00 | 114.60 |
| 54 | Da | 701 | HEA | C25-C23-C24 | 2.44 | 119.99 | 114.60 |
| 54 | DA | 702 | HEA | C4B-NB-C1B | -2.42 | 102.57 | 105.07 |
| 54 | Da | 701 | HEA | CHD-C1D-C2D | -2.42 | 120.00 | 126.73 |
| 66 | Ed | 201 | HEM | CHA-C4D-C3D | -2.41 | 120.80 | 125.33 |
| 65 | EN | 1204 | UQ8 | C17-C18-C19 | -2.40 | 121.88 | 127.66 |
| 54 | DA | 702 | HEA | C1D-ND-C4D | -2.40 | 102.60 | 105.07 |
| 54 | DA | 701 | HEA | CHB-C4A-C3A | -2.39 | 121.17 | 125.26 |
| 54 | DA | 701 | HEA | CHD-C1D-C2D | -2.38 | 120.11 | 126.73 |
| 54 | DA | 702 | HEA | C3A-C2A-C1A | -2.38 | 104.81 | 107.08 |
| 54 | DA | 702 | HEA | OMA-CMA-C3A | -2.37 | 120.33 | 125.69 |
| 54 | Da | 702 | HEA | C3A-C2A-C1A | -2.36 | 104.83 | 107.08 |
| 54 | DA | 702 | HEA | C25-C23-C24 | 2.36 | 119.81 | 114.60 |
| 54 | Da | 702 | HEA | C1D-ND-C4D | -2.35 | 102.64 | 105.07 |
| 54 | Da | 702 | HEA | C4B-NB-C1B | -2.35 | 102.65 | 105.07 |
| 54 | DA | 701 | HEA | CMD-C2D-C1D | 2.34 | 128.60 | 125.04 |
| 65 | Ed | 202 | UQ8 | C8-C7-C6 | 2.33 | 118.34 | 112.05 |
| 54 | DA | 701 | HEA | OMA-CMA-C3A | -2.33 | 120.42 | 125.69 |
| 65 | ED | 603 | UQ8 | C8-C7-C6 | 2.33 | 118.33 | 112.05 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 66 | ED | 602 | HEM | CHA-C4D-C3D | -2.33 | 120.95 | 125.33 |
| 54 | Da | 701 | HEA | C4B-NB-C1B | -2.33 | 102.67 | 105.07 |
| 54 | DA | 701 | HEA | C1D-ND-C4D | -2.33 | 102.67 | 105.07 |
| 54 | Da | 702 | HEA | CHB-C4A-C3A | -2.32 | 121.29 | 125.26 |
| 54 | Da | 702 | HEA | OMA-CMA-C3A | -2.31 | 120.45 | 125.69 |
| 54 | DA | 701 | HEA | C4B-NB-C1B | -2.29 | 102.71 | 105.07 |
| 65 | El | 906 | UQ8 | C17-C18-C19 | -2.29 | 122.15 | 127.66 |
| 54 | DA | 702 | HEA | CHB-C4A-C3A | -2.29 | 121.35 | 125.26 |
| 54 | Da | 701 | HEA | CMD-C2D-C1D | 2.26 | 128.49 | 125.04 |
| 65 | Ed | 202 | UQ8 | C21-C19-C18 | 2.23 | 125.63 | 121.12 |
| 65 | En | 1203 | UQ8 | C7-C8-C9 | 2.23 | 130.50 | 126.79 |
| 54 | DA | 702 | HEA | CMD-C2D-C1D | 2.22 | 128.42 | 125.04 |
| 54 | Da | 701 | HEA | C17-C18-C19 | -2.22 | 122.33 | 127.66 |
| 65 | ED | 603 | UQ8 | C21-C19-C18 | 2.21 | 125.59 | 121.12 |
| 54 | Da | 702 | HEA | CAD-CBD-CGD | -2.21 | 108.84 | 113.60 |
| 54 | DA | 702 | HEA | CAD-CBD-CGD | -2.21 | 108.84 | 113.60 |
| 54 | Da | 702 | HEA | CMD-C2D-C1D | 2.20 | 128.39 | 125.04 |
| 65 | EN | 1204 | UQ8 | C7-C8-C9 | 2.20 | 130.45 | 126.79 |
| 54 | DA | 701 | HEA | CMB-C2B-C1B | 2.20 | 128.38 | 125.04 |
| 54 | Da | 701 | HEA | CAD-C3D-C4D | 2.18 | 128.47 | 124.66 |
| 54 | Da | 701 | HEA | C1D-ND-C4D | -2.17 | 102.83 | 105.07 |
| 54 | Da | 701 | HEA | CHC-C4B-C3B | -2.17 | 120.22 | 125.80 |
| 66 | ED | 602 | HEM | C1A-CHA-C4D | -2.16 | 121.21 | 126.34 |
| 66 | Ed | 201 | HEM | C1A-CHA-C4D | -2.14 | 121.25 | 126.34 |
| 54 | DA | 701 | HEA | C17-C18-C19 | -2.13 | 122.52 | 127.66 |
| 54 | Da | 701 | HEA | C26-C15-C16 | 2.13 | 118.86 | 115.27 |
| 54 | DA | 701 | HEA | CHC-C4B-C3B | -2.13 | 120.31 | 125.80 |
| 54 | Da | 701 | HEA | CMB-C2B-C1B | 2.13 | 128.28 | 125.04 |
| 66 | Ed | 201 | HEM | CMD-C2D-C1D | 2.11 | 128.25 | 125.04 |
| 54 | DA | 701 | HEA | C26-C15-C16 | 2.10 | 118.81 | 115.27 |
| 54 | DA | 701 | HEA | CAD-C3D-C4D | 2.10 | 128.33 | 124.66 |
| 54 | DA | 702 | HEA | CAA-CBA-CGA | -2.10 | 109.09 | 113.60 |
| 66 | ED | 602 | HEM | CMD-C2D-C1D | 2.07 | 128.19 | 125.04 |
| 68 | Er | 201 | ATP | PB-O3B-PG | 2.07 | 139.93 | 132.83 |
| 54 | DA | 702 | HEA | CHC-C4B-C3B | -2.06 | 120.49 | 125.80 |
| 54 | Da | 702 | HEA | CHC-C4B-C3B | -2.05 | 120.51 | 125.80 |
| 54 | Da | 702 | HEA | CMC-C2C-C3C | 2.04 | 131.54 | 126.59 |
| 68 | ER | 201 | ATP | PB-O3B-PG | 2.04 | 139.82 | 132.83 |
| 54 | Da | 702 | HEA | CAA-CBA-CGA | -2.04 | 109.22 | 113.60 |
| 66 | Ed | 201 | HEM | CHD-C4C-NC | 2.03 | 126.64 | 124.44 |
| 65 | En | 1203 | UQ8 | C17-C18-C19 | -2.03 | 122.78 | 127.66 |
| 65 | DS | 404 | UQ8 | C8-C7-C6 | 2.02 | 117.49 | 112.05 |

There are no chirality outliers.

All (4794) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 57 | DA | 709 | CDL | CA2-OA2-PA1-OA3 |
| 57 | DA | 709 | CDL | CA2-OA2-PA1-OA4 |
| 57 | DA | 709 | CDL | CB2-OB2-PB2-OB3 |
| 57 | DA | 710 | CDL | CA3-OA5-PA1-OA2 |
| 57 | DA | 710 | CDL | CA3-OA5-PA1-OA3 |
| 57 | DA | 710 | CDL | CA3-OA5-PA1-OA4 |
| 57 | DA | 710 | CDL | C11-CA5-OA6-CA4 |
| 57 | DC | 601 | CDL | CA2-OA2-PA1-OA4 |
| 57 | DC | 601 | CDL | CB3-OB5-PB2-OB2 |
| 57 | DC | 601 | CDL | CB3-OB5-PB2-OB3 |
| 57 | DC | 601 | CDL | CB3-OB5-PB2-OB4 |
| 57 | DD | 702 | CDL | O1-C1-CA2-OA2 |
| 57 | DD | 702 | CDL | CA3-OA5-PA1-OA3 |
| 57 | DD | 702 | CDL | CA3-OA5-PA1-OA4 |
| 57 | DD | 702 | CDL | C11-CA5-OA6-CA4 |
| 57 | DD | 702 | CDL | OB6-CB4-CB6-OB8 |
| 57 | DD | 704 | CDL | CA2-OA2-PA1-OA3 |
| 57 | DD | 704 | CDL | CB3-OB5-PB2-OB2 |
| 57 | DD | 704 | CDL | C51-CB5-OB6-CB4 |
| 57 | DG | 201 | CDL | CB2-C1-CA2-OA2 |
| 57 | DG | 201 | CDL | CB2-OB2-PB2-OB3 |
| 57 | DG | 201 | CDL | CB3-OB5-PB2-OB2 |
| 57 | DH | 201 | CDL | CB2-C1-CA2-OA2 |
| 57 | DH | 201 | CDL | CA3-OA5-PA1-OA2 |
| 57 | DH | 201 | CDL | CA3-OA5-PA1-OA3 |
| 57 | DH | 201 | CDL | OA6-CA4-CA6-OA8 |
| 57 | DI | 701 | CDL | C11-CA5-OA6-CA4 |
| 57 | DI | 701 | CDL | C51-CB5-OB6-CB4 |
| 57 | DJ | 302 | CDL | CB2-C1-CA2-OA2 |
| 57 | DJ | 302 | CDL | C1-CA2-OA2-PA1 |
| 57 | DJ | 303 | CDL | CA2-OA2-PA1-OA4 |
| 57 | DJ | 303 | CDL | CA3-OA5-PA1-OA4 |
| 57 | DJ | 303 | CDL | C11-CA5-OA6-CA4 |
| 57 | DJ | 303 | CDL | CB3-OB5-PB2-OB4 |
| 57 | DJ | 305 | CDL | O1-C1-CA2-OA2 |
| 57 | DJ | 305 | CDL | CB2-C1-CA2-OA2 |
| 57 | DJ | 305 | CDL | CA3-OA5-PA1-OA3 |
| 57 | DJ | 305 | CDL | CA3-OA5-PA1-OA4 |
| 57 | DJ | 305 | CDL | CB2-OB2-PB2-OB3 |
| 57 | DJ | 307 | CDL | O1-C1-CB2-OB2 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 57 | DJ | 307 | CDL | CB2-OB2-PB2-OB3 |
| 57 | DJ | 307 | CDL | OB5-CB3-CB4-OB6 |
| 57 | DJ | 307 | CDL | C51-CB5-OB6-CB4 |
| 57 | DM | 501 | CDL | C1-CA2-OA2-PA1 |
| 57 | DM | 501 | CDL | CA3-OA5-PA1-OA3 |
| 57 | DM | 501 | CDL | CB2-OB2-PB2-OB4 |
| 57 | DM | 501 | CDL | C51-CB5-OB6-CB4 |
| 57 | DM | 502 | CDL | O1-C1-CB2-OB2 |
| 57 | DM | 502 | CDL | C51-CB5-OB6-CB4 |
| 57 | DN | 501 | CDL | CA3-OA5-PA1-OA4 |
| 57 | DN | 504 | CDL | CB3-OB5-PB2-OB3 |
| 57 | DN | 504 | CDL | C51-CB5-OB6-CB4 |
| 57 | DN | 505 | CDL | CB2-C1-CA2-OA2 |
| 57 | DN | 505 | CDL | C1-CA2-OA2-PA1 |
| 57 | DN | 505 | CDL | C11-CA5-OA6-CA4 |
| 57 | DO | 501 | CDL | C11-CA5-OA6-CA4 |
| 57 | DO | 501 | CDL | C51-CB5-OB6-CB4 |
| 57 | DQ | 1501 | CDL | CA3-OA5-PA1-OA2 |
| 57 | DQ | 1501 | CDL | CA3-OA5-PA1-OA3 |
| 57 | DQ | 1501 | CDL | CA3-OA5-PA1-OA4 |
| 57 | DQ | 1501 | CDL | C11-CA5-OA6-CA4 |
| 57 | DQ | 1501 | CDL | CB3-OB5-PB2-OB3 |
| 57 | DQ | 1502 | CDL | CA3-OA5-PA1-OA2 |
| 57 | DQ | 1502 | CDL | CA3-OA5-PA1-OA3 |
| 57 | DQ | 1502 | CDL | CA3-OA5-PA1-OA4 |
| 57 | DQ | 1502 | CDL | CB3-OB5-PB2-OB2 |
| 57 | DQ | 1502 | CDL | CB3-OB5-PB2-OB3 |
| 57 | DQ | 1504 | CDL | CA2-OA2-PA1-OA3 |
| 57 | DQ | 1504 | CDL | CA2-OA2-PA1-OA5 |
| 57 | DQ | 1504 | CDL | OA5-CA3-CA4-OA6 |
| 57 | DQ | 1504 | CDL | OA7-CA5-OA6-CA4 |
| 57 | DQ | 1504 | CDL | C11-CA5-OA6-CA4 |
| 57 | DQ | 1504 | CDL | CB3-OB5-PB2-OB2 |
| 57 | DR | 402 | CDL | CA3-OA5-PA1-OA3 |
| 57 | DR | 402 | CDL | CA3-OA5-PA1-OA4 |
| 57 | DR | 402 | CDL | CB2-OB2-PB2-OB5 |
| 57 | DR | 402 | CDL | CB3-OB5-PB2-OB3 |
| 57 | DR | 402 | CDL | CB3-OB5-PB2-OB4 |
| 57 | DR | 403 | CDL | O1-C1-CA2-OA2 |
| 57 | DR | 403 | CDL | CA2-OA2-PA1-OA3 |
| 57 | DS | 402 | CDL | CA2-OA2-PA1-OA3 |
| 57 | DS | 402 | CDL | CB3-OB5-PB2-OB2 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 57 | DS | 402 | CDL | CB4-CB3-OB5-PB2 |
| 57 | DS | 405 | CDL | CA2-OA2-PA1-OA3 |
| 57 | DS | 405 | CDL | CB3-OB5-PB2-OB3 |
| 57 | DU | 401 | CDL | CA2-OA2-PA1-OA3 |
| 57 | DU | 402 | CDL | C11-CA5-OA6-CA4 |
| 57 | DU | 402 | CDL | CB2-OB2-PB2-OB3 |
| 57 | DU | 403 | CDL | CA2-OA2-PA1-OA5 |
| 57 | DU | 403 | CDL | CB3-OB5-PB2-OB3 |
| 57 | DU | 404 | CDL | CA3-OA5-PA1-OA3 |
| 57 | DU | 404 | CDL | CA3-CA4-OA6-CA5 |
| 57 | DU | 404 | CDL | CB2-OB2-PB2-OB3 |
| 57 | DU | 404 | CDL | OB5-CB3-CB4-OB6 |
| 57 | DV | 401 | CDL | CA3-OA5-PA1-OA2 |
| 57 | DV | 401 | CDL | CA3-OA5-PA1-OA3 |
| 57 | DV | 401 | CDL | CA3-OA5-PA1-OA4 |
| 57 | DV | 401 | CDL | OA7-CA5-OA6-CA4 |
| 57 | DV | 402 | CDL | CA3-OA5-PA1-OA4 |
| 57 | DV | 402 | CDL | C11-CA5-OA6-CA4 |
| 57 | DV | 402 | CDL | CB3-OB5-PB2-OB2 |
| 57 | DV | 402 | CDL | CB3-OB5-PB2-OB3 |
| 57 | DV | 402 | CDL | CB3-OB5-PB2-OB4 |
| 57 | DV | 402 | CDL | C51-CB5-OB6-CB4 |
| 57 | DV | 403 | CDL | CA3-OA5-PA1-OA3 |
| 57 | DV | 403 | CDL | CA3-OA5-PA1-OA4 |
| 57 | DV | 404 | CDL | O1-C1-CA2-OA2 |
| 57 | DV | 404 | CDL | CA3-OA5-PA1-OA3 |
| 57 | DV | 404 | CDL | CB2-OB2-PB2-OB3 |
| 57 | DV | 404 | CDL | CB3-OB5-PB2-OB3 |
| 57 | DV | 404 | CDL | C51-CB5-OB6-CB4 |
| 57 | DX | 301 | CDL | CB3-OB5-PB2-OB4 |
| 57 | DY | 301 | CDL | CA3-OA5-PA1-OA2 |
| 57 | DY | 301 | CDL | CA3-OA5-PA1-OA3 |
| 57 | DY | 301 | CDL | CA3-OA5-PA1-OA4 |
| 57 | DY | 301 | CDL | C11-CA5-OA6-CA4 |
| 57 | DY | 301 | CDL | OB6-CB4-CB6-OB8 |
| 57 | DY | 301 | CDL | C51-CB5-OB6-CB4 |
| 57 | EA | 301 | CDL | CA2-OA2-PA1-OA3 |
| 57 | EA | 301 | CDL | CA2-OA2-PA1-OA4 |
| 57 | EA | 301 | CDL | CB2-OB2-PB2-OB3 |
| 57 | EA | 301 | CDL | CB3-OB5-PB2-OB3 |
| 57 | EB | 302 | CDL | C11-CA5-OA6-CA4 |
| 57 | EB | 302 | CDL | OB5-CB3-CB4-OB6 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 57 | EB | 302 | CDL | OB7-CB5-OB6-CB4 |
| 57 | EB | 304 | CDL | CA3-OA5-PA1-OA2 |
| 57 | EB | 304 | CDL | CA3-OA5-PA1-OA3 |
| 57 | EB | 304 | CDL | CA3-OA5-PA1-OA4 |
| 57 | EB | 304 | CDL | CB2-OB2-PB2-OB3 |
| 57 | EB | 304 | CDL | CB2-OB2-PB2-OB5 |
| 57 | ED | 601 | CDL | CA3-OA5-PA1-OA2 |
| 57 | ED | 601 | CDL | CA3-OA5-PA1-OA3 |
| 57 | ED | 601 | CDL | C11-CA5-OA6-CA4 |
| 57 | ED | 604 | CDL | CA3-OA5-PA1-OA2 |
| 57 | ED | 604 | CDL | CA3-OA5-PA1-OA3 |
| 57 | ED | 604 | CDL | CA3-OA5-PA1-OA4 |
| 57 | ED | 604 | CDL | OB5-CB3-CB4-OB6 |
| 57 | EH | 201 | CDL | CA3-OA5-PA1-OA3 |
| 57 | EH | 201 | CDL | CB3-OB5-PB2-OB3 |
| 57 | EH | 201 | CDL | CB3-OB5-PB2-OB4 |
| 57 | EH | 202 | CDL | CB2-OB2-PB2-OB3 |
| 57 | EI | 401 | CDL | CB3-OB5-PB2-OB3 |
| 57 | EL | 901 | CDL | CA3-OA5-PA1-OA3 |
| 57 | EL | 901 | CDL | OA6-CA4-CA6-OA8 |
| 57 | EL | 902 | CDL | CA2-C1-CB2-OB2 |
| 57 | EL | 902 | CDL | CA2-OA2-PA1-OA3 |
| 57 | EL | 902 | CDL | C11-CA5-OA6-CA4 |
| 57 | EL | 902 | CDL | CB3-OB5-PB2-OB3 |
| 57 | EL | 902 | CDL | C51-CB5-OB6-CB4 |
| 57 | EL | 903 | CDL | C11-CA5-OA6-CA4 |
| 57 | EL | 903 | CDL | CB3-OB5-PB2-OB4 |
| 57 | EL | 904 | CDL | CB2-OB2-PB2-OB3 |
| 57 | EL | 904 | CDL | CB3-OB5-PB2-OB3 |
| 57 | EL | 904 | CDL | CB3-OB5-PB2-OB4 |
| 57 | EL | 904 | CDL | C51-CB5-OB6-CB4 |
| 57 | EN | 1201 | CDL | O1-C1-CA2-OA2 |
| 57 | EN | 1201 | CDL | CA2-OA2-PA1-OA5 |
| 57 | EN | 1202 | CDL | C51-CB5-OB6-CB4 |
| 57 | EO | 202 | CDL | C11-CA5-OA6-CA4 |
| 57 | EO | 202 | CDL | C51-CB5-OB6-CB4 |
| 57 | EU | 101 | CDL | CA3-OA5-PA1-OA3 |
| 57 | EU | 101 | CDL | CB2-OB2-PB2-OB3 |
| 57 | EU | 101 | CDL | CB3-OB5-PB2-OB2 |
| 57 | Da | 705 | CDL | OA6-CA4-CA6-OA8 |
| 57 | Da | 705 | CDL | CB3-OB5-PB2-OB4 |
| 57 | Da | 709 | CDL | CA3-OA5-PA1-OA4 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 57 | Da | 709 | CDL | C11-CA5-OA6-CA4 |
| 57 | Da | 709 | CDL | CB3-OB5-PB2-OB3 |
| 57 | Dc | 601 | CDL | CB3-OB5-PB2-OB2 |
| 57 | Dc | 601 | CDL | CB3-OB5-PB2-OB3 |
| 57 | Dc | 601 | CDL | CB3-OB5-PB2-OB4 |
| 57 | Dd | 702 | CDL | CB2-C1-CA2-OA2 |
| 57 | Dd | 702 | CDL | CA3-OA5-PA1-OA2 |
| 57 | Dd | 702 | CDL | CA3-OA5-PA1-OA3 |
| 57 | Dd | 702 | CDL | CA3-OA5-PA1-OA4 |
| 57 | Dd | 702 | CDL | C11-CA5-OA6-CA4 |
| 57 | Dd | 704 | CDL | CB2-C1-CA2-OA2 |
| 57 | Dd | 704 | CDL | C1-CB2-OB2-PB2 |
| 57 | Dd | 705 | CDL | CA3-OA5-PA1-OA3 |
| 57 | Dd | 705 | CDL | CA3-OA5-PA1-OA4 |
| 57 | Dd | 706 | CDL | CB3-OB5-PB2-OB3 |
| 57 | Dg | 201 | CDL | CB2-C1-CA2-OA2 |
| 57 | Dg | 201 | CDL | C11-CA5-OA6-CA4 |
| 57 | Dg | 201 | CDL | CB3-OB5-PB2-OB2 |
| 57 | Dh | 201 | CDL | CB2-C1-CA2-OA2 |
| 57 | Dh | 201 | CDL | CA3-OA5-PA1-OA3 |
| 57 | Dh | 201 | CDL | OA6-CA4-CA6-OA8 |
| 57 | Dh | 201 | CDL | CB2-OB2-PB2-OB3 |
| 57 | Dh | 202 | CDL | CA3-OA5-PA1-OA2 |
| 57 | Dh | 202 | CDL | CA3-OA5-PA1-OA3 |
| 57 | Dh | 202 | CDL | CA3-OA5-PA1-OA4 |
| 57 | Di | 701 | CDL | C11-CA5-OA6-CA4 |
| 57 | Di | 701 | CDL | CB3-OB5-PB2-OB2 |
| 57 | Di | 701 | CDL | OB7-CB5-OB6-CB4 |
| 57 | Di | 701 | CDL | C51-CB5-OB6-CB4 |
| 57 | Dj | 401 | CDL | CB2-OB2-PB2-OB3 |
| 57 | Dj | 401 | CDL | CB3-OB5-PB2-OB4 |
| 57 | Dj | 401 | CDL | C51-CB5-OB6-CB4 |
| 57 | Dj | 402 | CDL | O1-C1-CA2-OA2 |
| 57 | Dj | 402 | CDL | CA2-OA2-PA1-OA5 |
| 57 | Dj | 402 | CDL | CA3-OA5-PA1-OA2 |
| 57 | Dj | 402 | CDL | C11-CA5-OA6-CA4 |
| 57 | Dj | 403 | CDL | CA2-OA2-PA1-OA3 |
| 57 | Dj | 403 | CDL | CA3-OA5-PA1-OA4 |
| 57 | Dj | 404 | CDL | CA3-OA5-PA1-OA3 |
| 57 | Dj | 404 | CDL | CA3-OA5-PA1-OA4 |
| 57 | Dj | 404 | CDL | OA7-CA5-OA6-CA4 |
| 57 | Dj | 404 | CDL | CB3-OB5-PB2-OB2 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 57 | Dj | 404 | CDL | C51-CB5-OB6-CB4 |
| 57 | Dj | 405 | CDL | CA3-OA5-PA1-OA3 |
| 57 | Dj | 405 | CDL | CA3-OA5-PA1-OA4 |
| 57 | Dj | 405 | CDL | CB2-OB2-PB2-OB3 |
| 57 | Dj | 408 | CDL | O1-C1-CB2-OB2 |
| 57 | Dj | 408 | CDL | CA2-OA2-PA1-OA5 |
| 57 | Dj | 408 | CDL | OA6-CA4-CA6-OA8 |
| 57 | Dj | 408 | CDL | C51-CB5-OB6-CB4 |
| 57 | Dm | 501 | CDL | CB2-OB2-PB2-OB5 |
| 57 | Dm | 502 | CDL | CA2-OA2-PA1-OA3 |
| 57 | Dm | 502 | CDL | CA3-OA5-PA1-OA3 |
| 57 | Dm | 502 | CDL | CA3-OA5-PA1-OA4 |
| 57 | Dm | 502 | CDL | C51-CB5-OB6-CB4 |
| 57 | Dn | 501 | CDL | CA2-OA2-PA1-OA3 |
| 57 | Dn | 501 | CDL | CA2-OA2-PA1-OA4 |
| 57 | Dn | 501 | CDL | CA2-OA2-PA1-OA5 |
| 57 | Dn | 501 | CDL | CA3-OA5-PA1-OA3 |
| 57 | Dn | 501 | CDL | CA3-OA5-PA1-OA4 |
| 57 | Dn | 502 | CDL | CA3-OA5-PA1-OA2 |
| 57 | Dn | 502 | CDL | CA3-OA5-PA1-OA3 |
| 57 | Dn | 502 | CDL | CA3-OA5-PA1-OA4 |
| 57 | Dn | 502 | CDL | CA4-CA3-OA5-PA1 |
| 57 | Dn | 503 | CDL | CA3-OA5-PA1-OA2 |
| 57 | Dn | 503 | CDL | CA3-OA5-PA1-OA3 |
| 57 | Dn | 503 | CDL | OA7-CA5-OA6-CA4 |
| 57 | Dn | 503 | CDL | C11-CA5-OA6-CA4 |
| 57 | Dn | 505 | CDL | O1-C1-CA2-OA2 |
| 57 | Dn | 505 | CDL | OA7-CA5-OA6-CA4 |
| 57 | Dn | 505 | CDL | CB3-OB5-PB2-OB3 |
| 57 | Dn | 505 | CDL | CB3-OB5-PB2-OB4 |
| 57 | Dn | 505 | CDL | OB7-CB5-OB6-CB4 |
| 57 | Dn | 505 | CDL | C51-CB5-OB6-CB4 |
| 57 | Dn | 507 | CDL | OB7-CB5-OB6-CB4 |
| 57 | Dn | 507 | CDL | C51-CB5-OB6-CB4 |
| 57 | Do | 501 | CDL | CA3-OA5-PA1-OA2 |
| 57 | Do | 501 | CDL | CA3-OA5-PA1-OA3 |
| 57 | Do | 501 | CDL | CA3-OA5-PA1-OA4 |
| 57 | Do | 501 | CDL | C51-CB5-OB6-CB4 |
| 57 | Dq | 401 | CDL | C1-CB2-OB2-PB2 |
| 57 | Dq | 401 | CDL | CB2-OB2-PB2-OB3 |
| 57 | Dq | 401 | CDL | C51-CB5-OB6-CB4 |
| 57 | Dq | 402 | CDL | OA7-CA5-OA6-CA4 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 57 | Dq | 402 | CDL | C51-CB5-OB6-CB4 |
| 57 | Dq | 403 | CDL | CA3-OA5-PA1-OA3 |
| 57 | Dq | 403 | CDL | CA3-OA5-PA1-OA4 |
| 57 | Dq | 403 | CDL | OA7-CA5-OA6-CA4 |
| 57 | Dq | 403 | CDL | C11-CA5-OA6-CA4 |
| 57 | Dq | 403 | CDL | CB3-OB5-PB2-OB3 |
| 57 | Dq | 404 | CDL | CA2-OA2-PA1-OA3 |
| 57 | Dq | 404 | CDL | CA3-OA5-PA1-OA4 |
| 57 | Dq | 404 | CDL | CB3-OB5-PB2-OB2 |
| 57 | Dr | 402 | CDL | CA3-OA5-PA1-OA3 |
| 57 | Dr | 402 | CDL | CA3-OA5-PA1-OA4 |
| 57 | Dr | 402 | CDL | CB2-OB2-PB2-OB4 |
| 57 | Dr | 402 | CDL | OB6-CB4-CB6-OB8 |
| 57 | Dr | 403 | CDL | O1-C1-CA2-OA2 |
| 57 | Dr | 403 | CDL | CA2-OA2-PA1-OA3 |
| 57 | Dr | 403 | CDL | CA2-OA2-PA1-OA5 |
| 57 | Dr | 403 | CDL | OB6-CB4-CB6-OB8 |
| 57 | Ds | 402 | CDL | CA2-OA2-PA1-OA3 |
| 57 | Ds | 402 | CDL | CB3-OB5-PB2-OB2 |
| 57 | Ds | 402 | CDL | CB4-CB3-OB5-PB2 |
| 57 | Ds | 405 | CDL | CA2-OA2-PA1-OA3 |
| 57 | Ds | 405 | CDL | CB3-OB5-PB2-OB3 |
| 57 | Du | 401 | CDL | CA2-OA2-PA1-OA3 |
| 57 | Du | 401 | CDL | CA3-OA5-PA1-OA3 |
| 57 | Du | 401 | CDL | OB7-CB5-OB6-CB4 |
| 57 | Du | 401 | CDL | C51-CB5-OB6-CB4 |
| 57 | Du | 402 | CDL | C11-CA5-OA6-CA4 |
| 57 | Du | 402 | CDL | CB3-OB5-PB2-OB2 |
| 57 | Du | 402 | CDL | CB3-OB5-PB2-OB3 |
| 57 | Du | 402 | CDL | CB3-OB5-PB2-OB4 |
| 57 | Du | 403 | CDL | CA2-OA2-PA1-OA5 |
| 57 | Du | 403 | CDL | CB3-OB5-PB2-OB2 |
| 57 | Du | 403 | CDL | CB3-OB5-PB2-OB3 |
| 57 | Du | 403 | CDL | CB3-OB5-PB2-OB4 |
| 57 | Du | 404 | CDL | CA3-OA5-PA1-OA3 |
| 57 | Du | 404 | CDL | CB3-OB5-PB2-OB3 |
| 57 | Dv | 401 | CDL | CA3-OA5-PA1-OA2 |
| 57 | Dv | 401 | CDL | CA3-OA5-PA1-OA3 |
| 57 | Dv | 401 | CDL | CA3-OA5-PA1-OA4 |
| 57 | Dv | 401 | CDL | OA7-CA5-OA6-CA4 |
| 57 | Dv | 401 | CDL | CB2-OB2-PB2-OB3 |
| 57 | Dv | 402 | CDL | CA3-OA5-PA1-OA3 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 57 | Dv | 402 | CDL | CA3-OA5-PA1-OA4 |
| 57 | Dv | 402 | CDL | OA7-CA5-OA6-CA4 |
| 57 | Dv | 402 | CDL | C11-CA5-OA6-CA4 |
| 57 | Dv | 402 | CDL | CB3-OB5-PB2-OB2 |
| 57 | Dv | 402 | CDL | CB3-OB5-PB2-OB3 |
| 57 | Dv | 402 | CDL | CB3-OB5-PB2-OB4 |
| 57 | Dv | 402 | CDL | C51-CB5-OB6-CB4 |
| 57 | Dv | 404 | CDL | CA2-OA2-PA1-OA3 |
| 57 | Dv | 404 | CDL | CA2-OA2-PA1-OA5 |
| 57 | Dv | 404 | CDL | CA3-OA5-PA1-OA2 |
| 57 | Dv | 404 | CDL | CA3-OA5-PA1-OA3 |
| 57 | Dv | 404 | CDL | CA3-OA5-PA1-OA4 |
| 57 | Dv | 404 | CDL | CB2-OB2-PB2-OB3 |
| 57 | Dv | 404 | CDL | CB3-OB5-PB2-OB3 |
| 57 | Dv | 404 | CDL | C51-CB5-OB6-CB4 |
| 57 | Dx | 1201 | CDL | CA2-OA2-PA1-OA4 |
| 57 | Dx | 1201 | CDL | CB2-OB2-PB2-OB4 |
| 57 | Dx | 1201 | CDL | CB3-OB5-PB2-OB4 |
| 57 | Dx | 1203 | CDL | CA2-OA2-PA1-OA3 |
| 57 | Dx | 1203 | CDL | CA2-OA2-PA1-OA5 |
| 57 | Dx | 1203 | CDL | OB5-CB3-CB4-OB6 |
| 57 | Dy | 301 | CDL | CA3-OA5-PA1-OA2 |
| 57 | Dy | 301 | CDL | CA3-OA5-PA1-OA3 |
| 57 | Dy | 301 | CDL | CA3-OA5-PA1-OA4 |
| 57 | Dy | 301 | CDL | C11-CA5-OA6-CA4 |
| 57 | Dy | 301 | CDL | C51-CB5-OB6-CB4 |
| 57 | Ea | 301 | CDL | C11-CA5-OA6-CA4 |
| 57 | Ea | 301 | CDL | CB2-OB2-PB2-OB3 |
| 57 | Ed | 204 | CDL | CA3-OA5-PA1-OA3 |
| 57 | Ed | 204 | CDL | CA3-OA5-PA1-OA4 |
| 57 | Ed | 204 | CDL | CB2-OB2-PB2-OB3 |
| 57 | Ed | 204 | CDL | CB2-OB2-PB2-OB4 |
| 57 | Ed | 204 | CDL | CB2-OB2-PB2-OB5 |
| 57 | Ed | 205 | CDL | CA3-OA5-PA1-OA3 |
| 57 | Ed | 205 | CDL | CB3-OB5-PB2-OB2 |
| 57 | Ed | 205 | CDL | CB3-OB5-PB2-OB3 |
| 57 | Eg | 101 | CDL | CA2-OA2-PA1-OA3 |
| 57 | Eg | 101 | CDL | CA2-OA2-PA1-OA5 |
| 57 | Eg | 101 | CDL | C11-CA5-OA6-CA4 |
| 57 | Eg | 101 | CDL | CB3-OB5-PB2-OB3 |
| 57 | Eh | 1601 | CDL | C11-CA5-OA6-CA4 |
| 57 | Eh | 1601 | CDL | CB3-OB5-PB2-OB3 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 57 | Ei | 401 | CDL | CA2-OA2-PA1-OA5 |
| 57 | Ei | 401 | CDL | C11-CA5-OA6-CA4 |
| 57 | Ei | 401 | CDL | CB3-OB5-PB2-OB4 |
| 57 | Ek | 201 | CDL | CA2-OA2-PA1-OA4 |
| 57 | Ek | 201 | CDL | CA3-OA5-PA1-OA3 |
| 57 | Ek | 201 | CDL | CA3-OA5-PA1-OA4 |
| 57 | El | 901 | CDL | CB2-C1-CA2-OA2 |
| 57 | El | 901 | CDL | CA3-OA5-PA1-OA2 |
| 57 | El | 901 | CDL | CA3-OA5-PA1-OA3 |
| 57 | El | 901 | CDL | CA3-OA5-PA1-OA4 |
| 57 | El | 901 | CDL | OB6-CB4-CB6-OB8 |
| 57 | El | 901 | CDL | C51-CB5-OB6-CB4 |
| 57 | El | 902 | CDL | CA2-C1-CB2-OB2 |
| 57 | El | 902 | CDL | C1-CB2-OB2-PB2 |
| 57 | El | 902 | CDL | CB3-OB5-PB2-OB4 |
| 57 | El | 902 | CDL | OB7-CB5-OB6-CB4 |
| 57 | El | 902 | CDL | C51-CB5-OB6-CB4 |
| 57 | El | 903 | CDL | CA3-OA5-PA1-OA4 |
| 57 | El | 903 | CDL | CB2-OB2-PB2-OB3 |
| 57 | El | 903 | CDL | CB3-OB5-PB2-OB3 |
| 57 | El | 903 | CDL | CB3-OB5-PB2-OB4 |
| 57 | El | 903 | CDL | C51-CB5-OB6-CB4 |
| 57 | En | 1201 | CDL | CA2-OA2-PA1-OA5 |
| 57 | En | 1202 | CDL | CA3-OA5-PA1-OA2 |
| 57 | En | 1202 | CDL | CA3-OA5-PA1-OA3 |
| 57 | En | 1202 | CDL | CA3-OA5-PA1-OA4 |
| 57 | En | 1202 | CDL | C51-CB5-OB6-CB4 |
| 57 | Ep | 701 | CDL | CB2-C1-CA2-OA2 |
| 57 | Ep | 701 | CDL | CA3-OA5-PA1-OA2 |
| 57 | Ep | 701 | CDL | CA3-OA5-PA1-OA3 |
| 57 | Ep | 701 | CDL | CA3-OA5-PA1-OA4 |
| 57 | Eu | 101 | CDL | O1-C1-CA2-OA2 |
| 58 | DA | 706 | PC1 | C11-O13-P-O14 |
| 58 | DA | 706 | PC1 | O21-C2-C3-O31 |
| 58 | DA | 707 | PC1 | C1-O11-P-O12 |
| 58 | DA | 707 | PC1 | C1-O11-P-O14 |
| 58 | DB | 702 | PC1 | C11-O13-P-O12 |
| 58 | DB | 702 | PC1 | C11-O13-P-O14 |
| 58 | DB | 702 | PC1 | C11-O13-P-O11 |
| 58 | DB | 702 | PC1 | O22-C21-O21-C2 |
| 58 | DC | 602 | PC1 | C1-O11-P-O12 |
| 58 | DC | 602 | PC1 | C1-O11-P-O14 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 58 | DC | 603 | PC1 | O13-C11-C12-N |
| 58 | DC | 604 | PC1 | C11-O13-P-O12 |
| 58 | DC | 604 | PC1 | C11-O13-P-O14 |
| 58 | DC | 604 | PC1 | C11-O13-P-O11 |
| 58 | DC | 604 | PC1 | C1-O11-P-O12 |
| 58 | DC | 604 | PC1 | C1-O11-P-O14 |
| 58 | DC | 605 | PC1 | C1-O11-P-O13 |
| 58 | DC | 605 | PC1 | C22-C21-O21-C2 |
| 58 | DC | 608 | PC1 | C11-O13-P-O12 |
| 58 | DC | 608 | PC1 | O22-C21-O21-C2 |
| 58 | DC | 608 | PC1 | C22-C21-O21-C2 |
| 58 | DI | 702 | PC1 | C1-O11-P-O12 |
| 58 | DI | 702 | PC1 | C1-O11-P-O14 |
| 58 | DI | 702 | PC1 | C1-O11-P-O13 |
| 58 | DJ | 306 | PC1 | C11-O13-P-O12 |
| 58 | DS | 406 | PC1 | C11-O13-P-O14 |
| 58 | DS | 406 | PC1 | C11-O13-P-O11 |
| 58 | DS | 406 | PC1 | C1-O11-P-O12 |
| 58 | DS | 406 | PC1 | C1-O11-P-O14 |
| 58 | DS | 406 | PC1 | C12-C11-O13-P |
| 58 | DS | 407 | PC1 | C11-O13-P-O14 |
| 58 | DV | 405 | PC1 | C11-O13-P-O12 |
| 58 | DV | 407 | PC1 | C11-O13-P-O12 |
| 58 | DV | 407 | PC1 | C11-O13-P-O14 |
| 58 | DV | 407 | PC1 | C1-O11-P-O12 |
| 58 | DV | 407 | PC1 | C1-O11-P-O14 |
| 58 | DV | 407 | PC1 | C1-O11-P-O13 |
| 58 | DX | 302 | PC1 | C11-O13-P-O14 |
| 58 | DX | 302 | PC1 | C1-O11-P-O12 |
| 58 | DX | 306 | PC1 | C11-O13-P-O12 |
| 58 | DX | 306 | PC1 | C22-C21-O21-C2 |
| 58 | DY | 302 | PC1 | O13-C11-C12-N |
| 58 | DY | 302 | PC1 | O22-C21-O21-C2 |
| 58 | EB | 303 | PC1 | O13-C11-C12-N |
| 58 | EO | 201 | PC1 | C12-C11-O13-P |
| 58 | EO | 201 | PC1 | O13-C11-C12-N |
| 58 | EO | 205 | PC1 | C11-O13-P-O12 |
| 58 | EO | 205 | PC1 | C1-O11-P-O12 |
| 58 | EO | 206 | PC1 | C11-O13-P-O12 |
| 58 | EO | 206 | PC1 | C11-O13-P-O14 |
| 58 | EO | 206 | PC1 | C11-O13-P-O11 |
| 58 | EO | 206 | PC1 | C1-O11-P-O12 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 58 | EO | 206 | PC1 | C22-C21-O21-C2 |
| 58 | EO | 207 | PC1 | C11-O13-P-O12 |
| 58 | EO | 207 | PC1 | C11-O13-P-O14 |
| 58 | EO | 207 | PC1 | C11-O13-P-O11 |
| 58 | EO | 207 | PC1 | C22-C21-O21-C2 |
| 58 | Da | 706 | PC1 | C11-O13-P-O14 |
| 58 | Da | 706 | PC1 | O21-C2-C3-O31 |
| 58 | Da | 707 | PC1 | C1-O11-P-O12 |
| 58 | Da | 707 | PC1 | C1-O11-P-O14 |
| 58 | Da | 707 | PC1 | C1-O11-P-O13 |
| 58 | Da | 707 | PC1 | O13-C11-C12-N |
| 58 | Db | 702 | PC1 | C22-C21-O21-C2 |
| 58 | Dc | 602 | PC1 | C1-O11-P-O12 |
| 58 | Dc | 602 | PC1 | C1-O11-P-O14 |
| 58 | Dc | 605 | PC1 | C11-O13-P-O14 |
| 58 | Dc | 605 | PC1 | C1-O11-P-O14 |
| 58 | Dc | 605 | PC1 | C22-C21-O21-C2 |
| 58 | Dc | 607 | PC1 | C11-O13-P-O12 |
| 58 | Dc | 607 | PC1 | O22-C21-O21-C2 |
| 58 | Dg | 203 | PC1 | C22-C21-O21-C2 |
| 58 | Di | 702 | PC1 | C11-O13-P-O12 |
| 58 | Di | 702 | PC1 | C1-O11-P-O14 |
| 58 | Dj | 406 | PC1 | C11-O13-P-O12 |
| 58 | Dj | 406 | PC1 | C1-O11-P-O13 |
| 58 | Ds | 406 | PC1 | O21-C2-C3-O31 |
| 58 | Dv | 406 | PC1 | C11-O13-P-O14 |
| 58 | Dv | 406 | PC1 | C11-O13-P-O11 |
| 58 | Dv | 406 | PC1 | C1-O11-P-O12 |
| 58 | Dv | 406 | PC1 | C1-O11-P-O14 |
| 58 | Dv | 406 | PC1 | C1-O11-P-O13 |
| 58 | Dv | 407 | PC1 | C1-O11-P-O14 |
| 58 | Dv | 408 | PC1 | C11-O13-P-O12 |
| 58 | Dv | 408 | PC1 | C11-O13-P-O14 |
| 58 | Dv | 408 | PC1 | C1-O11-P-O12 |
| 58 | Dx | 1202 | PC1 | C1-O11-P-O12 |
| 58 | Dx | 1202 | PC1 | C1-O11-P-O14 |
| 58 | Dx | 1202 | PC1 | O13-C11-C12-N |
| 58 | Dx | 1202 | PC1 | O11-C1-C2-O21 |
| 58 | Dx | 1204 | PC1 | C11-O13-P-O14 |
| 58 | Dy | 302 | PC1 | O13-C11-C12-N |
| 58 | Dy | 302 | PC1 | O22-C21-O21-C2 |
| 58 | Eb | 301 | PC1 | C1-O11-P-O14 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 58 | Eb | 302 | PC1 | O13-C11-C12-N |
| 58 | Ef | 1001 | PC1 | C1-O11-P-O13 |
| 58 | Ef | 1001 | PC1 | O13-C11-C12-N |
| 58 | El | 904 | PC1 | C11-O13-P-O12 |
| 58 | El | 904 | PC1 | C1-O11-P-O12 |
| 58 | Eo | 201 | PC1 | C11-O13-P-O11 |
| 58 | Eo | 201 | PC1 | C12-C11-O13-P |
| 58 | Eo | 201 | PC1 | O13-C11-C12-N |
| 58 | Eo | 204 | PC1 | C11-O13-P-O12 |
| 58 | Eo | 204 | PC1 | C11-O13-P-O14 |
| 58 | Eo | 204 | PC1 | C22-C21-O21-C2 |
| 58 | Eo | 205 | PC1 | C11-O13-P-O12 |
| 58 | Eo | 205 | PC1 | C11-O13-P-O14 |
| 58 | Eo | 205 | PC1 | C22-C21-O21-C2 |
| 59 | DC | 606 | 3PE | C1-O11-P-O12 |
| 59 | DC | 606 | 3PE | C1-O11-P-O14 |
| 59 | DC | 607 | 3PE | C11-O13-P-O14 |
| 59 | DC | 607 | 3PE | O13-C11-C12-N |
| 59 | DG | 204 | 3PE | C11-O13-P-O12 |
| 59 | DG | 204 | 3PE | C11-O13-P-O14 |
| 59 | DG | 205 | 3PE | C1-O11-P-O13 |
| 59 | DG | 205 | 3PE | C2-C1-O11-P |
| 59 | DJ | 301 | 3PE | C1-O11-P-O12 |
| 59 | DJ | 301 | 3PE | C11-O13-P-O11 |
| 59 | DR | 401 | 3PE | C11-O13-P-O14 |
| 59 | DR | 401 | 3PE | O21-C2-C3-O31 |
| 59 | DS | 401 | 3PE | C1-O11-P-O14 |
| 59 | DS | 401 | 3PE | C12-C11-O13-P |
| 59 | DS | 401 | 3PE | O21-C2-C3-O31 |
| 59 | DS | 403 | 3PE | C1-O11-P-O14 |
| 59 | DS | 403 | 3PE | C11-O13-P-O11 |
| 59 | DX | 303 | 3PE | C11-O13-P-O11 |
| 59 | DX | 303 | 3PE | C11-O13-P-O12 |
| 59 | DX | 303 | 3PE | C11-O13-P-O14 |
| 59 | DX | 303 | 3PE | O13-C11-C12-N |
| 59 | DX | 304 | 3PE | C1-O11-P-O12 |
| 59 | DX | 304 | 3PE | C1-O11-P-O13 |
| 59 | DX | 304 | 3PE | C1-O11-P-O14 |
| 59 | DX | 304 | 3PE | C11-O13-P-O14 |
| 59 | DX | 305 | 3PE | C1-O11-P-O12 |
| 59 | DX | 305 | 3PE | C1-O11-P-O13 |
| 59 | DX | 305 | 3PE | C1-O11-P-O14 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 59 | DX | 305 | 3PE | C11-O13-P-O12 |
| 59 | DX | 305 | 3PE | C11-O13-P-O14 |
| 59 | EL | 905 | 3PE | C1-O11-P-O12 |
| 59 | EL | 905 | 3PE | C1-O11-P-O14 |
| 59 | EL | 905 | 3PE | C11-O13-P-O14 |
| 59 | EM | 901 | 3PE | C1-O11-P-O12 |
| 59 | EM | 901 | 3PE | C1-O11-P-O13 |
| 59 | EM | 901 | 3PE | C1-O11-P-O14 |
| 59 | EN | 1203 | 3PE | C11-O13-P-O11 |
| 59 | EO | 203 | 3PE | C1-O11-P-O12 |
| 59 | EO | 203 | 3PE | C1-O11-P-O14 |
| 59 | EO | 203 | 3PE | C11-O13-P-O14 |
| 59 | EO | 203 | 3PE | O21-C2-C3-O31 |
| 59 | EO | 203 | 3PE | C22-C21-O21-C2 |
| 59 | EO | 204 | 3PE | C1-O11-P-O12 |
| 59 | Da | 708 | 3PE | C1-O11-P-O12 |
| 59 | Da | 708 | 3PE | C1-O11-P-O14 |
| 59 | Dc | 606 | 3PE | C1-O11-P-O14 |
| 59 | Dc | 606 | 3PE | C11-O13-P-O12 |
| 59 | Dc | 606 | 3PE | C11-O13-P-O14 |
| 59 | Dd | 703 | 3PE | C1-O11-P-O12 |
| 59 | Dr | 401 | 3PE | C1-O11-P-O12 |
| 59 | Dr | 404 | 3PE | C1-O11-P-O13 |
| 59 | Ds | 401 | 3PE | C1-O11-P-O13 |
| 59 | Ds | 401 | 3PE | C1-O11-P-O14 |
| 59 | Ds | 401 | 3PE | C12-C11-O13-P |
| 59 | Ds | 401 | 3PE | O21-C2-C3-O31 |
| 59 | Ds | 403 | 3PE | C1-O11-P-O14 |
| 59 | Ds | 403 | 3PE | C11-O13-P-O11 |
| 59 | Ds | 407 | 3PE | C11-O13-P-O11 |
| 59 | Ds | 407 | 3PE | C11-O13-P-O14 |
| 59 | Dx | 1205 | 3PE | C1-O11-P-O12 |
| 59 | Dx | 1205 | 3PE | C1-O11-P-O14 |
| 59 | Dx | 1205 | 3PE | C11-O13-P-O11 |
| 59 | Dx | 1205 | 3PE | C11-O13-P-O12 |
| 59 | Dx | 1205 | 3PE | C11-O13-P-O14 |
| 59 | Dx | 1205 | 3PE | O13-C11-C12-N |
| 59 | Dx | 1206 | 3PE | C1-O11-P-O14 |
| 59 | Dx | 1206 | 3PE | C11-O13-P-O11 |
| 59 | Dx | 1206 | 3PE | C11-O13-P-O12 |
| 59 | Dx | 1206 | 3PE | C11-O13-P-O14 |
| 59 | Dx | 1207 | 3PE | C1-O11-P-O12 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 59 | Dx | 1207 | 3PE | C1-O11-P-O13 |
| 59 | Dx | 1207 | 3PE | C1-O11-P-O14 |
| 59 | Dx | 1207 | 3PE | C11-O13-P-O12 |
| 59 | El | 905 | 3PE | C1-O11-P-O13 |
| 59 | El | 905 | 3PE | C11-O13-P-O14 |
| 59 | Em | 901 | 3PE | C1-O11-P-O12 |
| 59 | Em | 901 | 3PE | C1-O11-P-O13 |
| 59 | Em | 901 | 3PE | C1-O11-P-O14 |
| 59 | Eo | 202 | 3PE | C22-C21-O21-C2 |
| 59 | Eo | 203 | 3PE | C1-O11-P-O12 |
| 59 | Eo | 203 | 3PE | C1-O11-P-O14 |
| 60 | DA | 711 | LPP | C6-O5-P1-O2 |
| 60 | DA | 711 | LPP | C6-O5-P1-O3 |
| 60 | DA | 711 | LPP | C6-O5-P1-O4 |
| 60 | DN | 502 | LPP | C6-O5-P1-O2 |
| 60 | DN | 502 | LPP | C6-O5-P1-O3 |
| 60 | DN | 502 | LPP | C6-O5-P1-O4 |
| 60 | Dn | 504 | LPP | C6-O5-P1-O2 |
| 60 | Dn | 504 | LPP | C6-O5-P1-O3 |
| 60 | Dn | 504 | LPP | C6-O5-P1-O4 |
| 60 | Dl | 1101 | LPP | C6-O5-P1-O2 |
| 60 | Dl | 1101 | LPP | C6-O5-P1-O4 |
| 65 | EL | 906 | UQ8 | C30-C29-C31-C32 |
| 65 | EL | 906 | UQ8 | C28-C29-C31-C32 |
| 65 | EL | 906 | UQ8 | C5-C6-C7-C8 |
| 65 | Ds | 404 | UQ8 | C35-C34-C36-C37 |
| 65 | Ds | 404 | UQ8 | C33-C34-C36-C37 |
| 65 | El | 906 | UQ8 | C30-C29-C31-C32 |
| 65 | El | 906 | UQ8 | C28-C29-C31-C32 |
| 65 | El | 906 | UQ8 | C1-C6-C7-C8 |
| 65 | El | 906 | UQ8 | C5-C6-C7-C8 |
| 65 | En | 1203 | UQ8 | C25-C24-C26-C27 |
| 65 | En | 1203 | UQ8 | C23-C24-C26-C27 |
| 68 | ER | 201 | ATP | C5'-O5'-PA-O1A |
| 68 | ER | 201 | ATP | C5'-O5'-PA-O2A |
| 57 | DD | 703 | CDL | OA9-CA7-OA8-CA6 |
| 57 | DG | 201 | CDL | OB9-CB7-OB8-CB6 |
| 57 | DN | 504 | CDL | OA9-CA7-OA8-CA6 |
| 57 | DV | 403 | CDL | OA9-CA7-OA8-CA6 |
| 57 | EB | 304 | CDL | OB9-CB7-OB8-CB6 |
| 57 | EH | 202 | CDL | OA9-CA7-OA8-CA6 |
| 57 | EH | 202 | CDL | OB9-CB7-OB8-CB6 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 57 | Dh | 202 | CDL | OB9-CB7-OB8-CB6 |
| 57 | Dj | 402 | CDL | OA9-CA7-OA8-CA6 |
| 57 | Dv | 404 | CDL | OA9-CA7-OA8-CA6 |
| 57 | Ed | 204 | CDL | OA9-CA7-OA8-CA6 |
| 57 | Ei | 401 | CDL | OA9-CA7-OA8-CA6 |
| 57 | Ep | 701 | CDL | OB9-CB7-OB8-CB6 |
| 58 | Dj | 406 | PC1 | O32-C31-O31-C3 |
| 57 | DD | 703 | CDL | C31-CA7-OA8-CA6 |
| 57 | DS | 405 | CDL | C71-CB7-OB8-CB6 |
| 57 | EI | 401 | CDL | C31-CA7-OA8-CA6 |
| 57 | Dd | 704 | CDL | C31-CA7-OA8-CA6 |
| 57 | Dj | 402 | CDL | C31-CA7-OA8-CA6 |
| 57 | Ei | 401 | CDL | C31-CA7-OA8-CA6 |
| 58 | EB | 301 | PC1 | C32-C31-O31-C3 |
| 57 | DA | 709 | CDL | OB9-CB7-OB8-CB6 |
| 57 | DD | 703 | CDL | OB9-CB7-OB8-CB6 |
| 57 | DJ | 304 | CDL | OA9-CA7-OA8-CA6 |
| 57 | DJ | 305 | CDL | OB9-CB7-OB8-CB6 |
| 57 | DQ | 1504 | CDL | OB9-CB7-OB8-CB6 |
| 57 | DS | 402 | CDL | OB9-CB7-OB8-CB6 |
| 57 | DS | 405 | CDL | OB9-CB7-OB8-CB6 |
| 57 | DU | 402 | CDL | OB9-CB7-OB8-CB6 |
| 57 | DV | 402 | CDL | OA9-CA7-OA8-CA6 |
| 57 | DV | 404 | CDL | OA9-CA7-OA8-CA6 |
| 57 | DX | 301 | CDL | OA9-CA7-OA8-CA6 |
| 57 | EA | 301 | CDL | OA9-CA7-OA8-CA6 |
| 57 | EI | 401 | CDL | OA9-CA7-OA8-CA6 |
| 57 | EK | 201 | CDL | OB9-CB7-OB8-CB6 |
| 57 | EL | 901 | CDL | OB9-CB7-OB8-CB6 |
| 57 | EL | 902 | CDL | OB9-CB7-OB8-CB6 |
| 57 | EO | 202 | CDL | OB9-CB7-OB8-CB6 |
| 57 | EU | 101 | CDL | OA9-CA7-OA8-CA6 |
| 57 | Dd | 704 | CDL | OA9-CA7-OA8-CA6 |
| 57 | Dd | 704 | CDL | OB9-CB7-OB8-CB6 |
| 57 | Dg | 201 | CDL | OA9-CA7-OA8-CA6 |
| 57 | Dg | 201 | CDL | OB9-CB7-OB8-CB6 |
| 57 | Dj | 401 | CDL | OB9-CB7-OB8-CB6 |
| 57 | Dj | 403 | CDL | OA9-CA7-OA8-CA6 |
| 57 | Dj | 404 | CDL | OB9-CB7-OB8-CB6 |
| 57 | Dj | 405 | CDL | OB9-CB7-OB8-CB6 |
| 57 | Dn | 501 | CDL | OB9-CB7-OB8-CB6 |
| 57 | Dn | 507 | CDL | OA9-CA7-OA8-CA6 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 57 | Dq | 401 | CDL | OB9-CB7-OB8-CB6 |
| 57 | Dq | 402 | CDL | OA9-CA7-OA8-CA6 |
| 57 | Ds | 405 | CDL | OB9-CB7-OB8-CB6 |
| 57 | Du | 403 | CDL | OB9-CB7-OB8-CB6 |
| 57 | Dv | 402 | CDL | OA9-CA7-OA8-CA6 |
| 57 | Dv | 403 | CDL | OA9-CA7-OA8-CA6 |
| 57 | Ea | 301 | CDL | OA9-CA7-OA8-CA6 |
| 57 | El | 902 | CDL | OB9-CB7-OB8-CB6 |
| 57 | Eu | 101 | CDL | OA9-CA7-OA8-CA6 |
| 58 | DJ | 306 | PC1 | O32-C31-O31-C3 |
| 58 | DX | 302 | PC1 | O32-C31-O31-C3 |
| 58 | EB | 301 | PC1 | O32-C31-O31-C3 |
| 58 | Eb | 301 | PC1 | O32-C31-O31-C3 |
| 59 | Da | 708 | 3PE | O32-C31-O31-C3 |
| 59 | Dr | 401 | 3PE | O32-C31-O31-C3 |
| 57 | DD | 704 | CDL | OB7-CB5-OB6-CB4 |
| 57 | DG | 201 | CDL | OB7-CB5-OB6-CB4 |
| 57 | DI | 701 | CDL | OA7-CA5-OA6-CA4 |
| 57 | DI | 701 | CDL | OB7-CB5-OB6-CB4 |
| 57 | DJ | 303 | CDL | OA7-CA5-OA6-CA4 |
| 57 | DJ | 307 | CDL | OB7-CB5-OB6-CB4 |
| 57 | DM | 501 | CDL | OB7-CB5-OB6-CB4 |
| 57 | DM | 502 | CDL | OB7-CB5-OB6-CB4 |
| 57 | DN | 504 | CDL | OB7-CB5-OB6-CB4 |
| 57 | DN | 505 | CDL | OA7-CA5-OA6-CA4 |
| 57 | DO | 501 | CDL | OA7-CA5-OA6-CA4 |
| 57 | DO | 501 | CDL | OB7-CB5-OB6-CB4 |
| 57 | DQ | 1501 | CDL | OA7-CA5-OA6-CA4 |
| 57 | DU | 401 | CDL | OB7-CB5-OB6-CB4 |
| 57 | DV | 402 | CDL | OA7-CA5-OA6-CA4 |
| 57 | DV | 402 | CDL | OB7-CB5-OB6-CB4 |
| 57 | DV | 404 | CDL | OB7-CB5-OB6-CB4 |
| 57 | DY | 301 | CDL | OA7-CA5-OA6-CA4 |
| 57 | DY | 301 | CDL | OB7-CB5-OB6-CB4 |
| 57 | EB | 302 | CDL | OA7-CA5-OA6-CA4 |
| 57 | ED | 601 | CDL | OA7-CA5-OA6-CA4 |
| 57 | EL | 902 | CDL | OA7-CA5-OA6-CA4 |
| 57 | EL | 902 | CDL | OB7-CB5-OB6-CB4 |
| 57 | EL | 904 | CDL | OB7-CB5-OB6-CB4 |
| 57 | EN | 1202 | CDL | OB7-CB5-OB6-CB4 |
| 57 | EO | 202 | CDL | OB7-CB5-OB6-CB4 |
| 57 | EU | 101 | CDL | OA7-CA5-OA6-CA4 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 57 | Da | 709 | CDL | OA7-CA5-OA6-CA4 |
| 57 | Dd | 702 | CDL | OA7-CA5-OA6-CA4 |
| 57 | Dg | 201 | CDL | OA7-CA5-OA6-CA4 |
| 57 | Dj | 401 | CDL | OB7-CB5-OB6-CB4 |
| 57 | Dj | 402 | CDL | OA7-CA5-OA6-CA4 |
| 57 | Dj | 404 | CDL | OB7-CB5-OB6-CB4 |
| 57 | Dj | 408 | CDL | OB7-CB5-OB6-CB4 |
| 57 | Dm | 501 | CDL | OB7-CB5-OB6-CB4 |
| 57 | Dm | 502 | CDL | OB7-CB5-OB6-CB4 |
| 57 | Do | 501 | CDL | OB7-CB5-OB6-CB4 |
| 57 | Dq | 401 | CDL | OB7-CB5-OB6-CB4 |
| 57 | Dq | 402 | CDL | OB7-CB5-OB6-CB4 |
| 57 | Dq | 403 | CDL | OB7-CB5-OB6-CB4 |
| 57 | Du | 402 | CDL | OA7-CA5-OA6-CA4 |
| 57 | Dv | 402 | CDL | OB7-CB5-OB6-CB4 |
| 57 | Dv | 404 | CDL | OB7-CB5-OB6-CB4 |
| 57 | Dx | 1203 | CDL | OB7-CB5-OB6-CB4 |
| 57 | Ea | 301 | CDL | OA7-CA5-OA6-CA4 |
| 57 | Ed | 204 | CDL | OA7-CA5-OA6-CA4 |
| 57 | Eg | 101 | CDL | OA7-CA5-OA6-CA4 |
| 57 | Eh | 1601 | CDL | OA7-CA5-OA6-CA4 |
| 57 | Ei | 401 | CDL | OA7-CA5-OA6-CA4 |
| 57 | El | 901 | CDL | OB7-CB5-OB6-CB4 |
| 57 | El | 902 | CDL | OA7-CA5-OA6-CA4 |
| 57 | El | 903 | CDL | OB7-CB5-OB6-CB4 |
| 57 | En | 1202 | CDL | OB7-CB5-OB6-CB4 |
| 58 | DC | 605 | PC1 | O22-C21-O21-C2 |
| 58 | DG | 203 | PC1 | O22-C21-O21-C2 |
| 58 | DX | 306 | PC1 | O22-C21-O21-C2 |
| 58 | EO | 206 | PC1 | O22-C21-O21-C2 |
| 58 | EO | 207 | PC1 | O22-C21-O21-C2 |
| 58 | Db | 702 | PC1 | O22-C21-O21-C2 |
| 58 | Dc | 605 | PC1 | O22-C21-O21-C2 |
| 58 | Dg | 203 | PC1 | O22-C21-O21-C2 |
| 58 | Eo | 204 | PC1 | O22-C21-O21-C2 |
| 58 | Eo | 205 | PC1 | O22-C21-O21-C2 |
| 59 | DG | 204 | 3PE | O22-C21-O21-C2 |
| 59 | EO | 203 | 3PE | O22-C21-O21-C2 |
| 59 | Eo | 202 | 3PE | O22-C21-O21-C2 |
| 57 | DD | 703 | CDL | C71-CB7-OB8-CB6 |
| 57 | DG | 201 | CDL | C71-CB7-OB8-CB6 |
| 57 | DJ | 304 | CDL | C31-CA7-OA8-CA6 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 57 | DN | 504 | CDL | C31-CA7-OA8-CA6 |
| 57 | DV | 403 | CDL | C31-CA7-OA8-CA6 |
| 57 | DX | 301 | CDL | C31-CA7-OA8-CA6 |
| 57 | EA | 301 | CDL | C31-CA7-OA8-CA6 |
| 57 | EB | 304 | CDL | C71-CB7-OB8-CB6 |
| 57 | EH | 202 | CDL | C31-CA7-OA8-CA6 |
| 57 | EH | 202 | CDL | C71-CB7-OB8-CB6 |
| 57 | EL | 904 | CDL | C71-CB7-OB8-CB6 |
| 57 | EN | 1201 | CDL | C71-CB7-OB8-CB6 |
| 57 | EN | 1202 | CDL | C31-CA7-OA8-CA6 |
| 57 | Dd | 704 | CDL | C71-CB7-OB8-CB6 |
| 57 | Dg | 201 | CDL | C71-CB7-OB8-CB6 |
| 57 | Dh | 202 | CDL | C71-CB7-OB8-CB6 |
| 57 | Dj | 403 | CDL | C31-CA7-OA8-CA6 |
| 57 | Ds | 405 | CDL | C71-CB7-OB8-CB6 |
| 57 | Du | 401 | CDL | C31-CA7-OA8-CA6 |
| 57 | Dv | 401 | CDL | C31-CA7-OA8-CA6 |
| 57 | Dv | 404 | CDL | C31-CA7-OA8-CA6 |
| 57 | Ea | 301 | CDL | C31-CA7-OA8-CA6 |
| 57 | Ed | 204 | CDL | C31-CA7-OA8-CA6 |
| 57 | Ep | 701 | CDL | C71-CB7-OB8-CB6 |
| 58 | DJ | 306 | PC1 | C32-C31-O31-C3 |
| 58 | Dc | 604 | PC1 | C32-C31-O31-C3 |
| 58 | Dj | 406 | PC1 | C32-C31-O31-C3 |
| 59 | EN | 1203 | 3PE | C32-C31-O31-C3 |
| 59 | Da | 708 | 3PE | C32-C31-O31-C3 |
| 57 | DG | 201 | CDL | C51-CB5-OB6-CB4 |
| 57 | DU | 401 | CDL | C51-CB5-OB6-CB4 |
| 57 | DV | 401 | CDL | C11-CA5-OA6-CA4 |
| 57 | EB | 302 | CDL | C51-CB5-OB6-CB4 |
| 57 | EU | 101 | CDL | C11-CA5-OA6-CA4 |
| 57 | Dj | 404 | CDL | C11-CA5-OA6-CA4 |
| 57 | Dm | 501 | CDL | C51-CB5-OB6-CB4 |
| 57 | Dn | 505 | CDL | C11-CA5-OA6-CA4 |
| 57 | Dq | 402 | CDL | C11-CA5-OA6-CA4 |
| 57 | Dq | 403 | CDL | C51-CB5-OB6-CB4 |
| 57 | Dv | 401 | CDL | C11-CA5-OA6-CA4 |
| 57 | Dx | 1203 | CDL | C51-CB5-OB6-CB4 |
| 57 | Ed | 204 | CDL | C11-CA5-OA6-CA4 |
| 57 | El | 902 | CDL | C11-CA5-OA6-CA4 |
| 58 | DB | 702 | PC1 | C22-C21-O21-C2 |
| 58 | DG | 203 | PC1 | C22-C21-O21-C2 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 58 | DY | 302 | PC1 | C22-C21-O21-C2 |
| 58 | Dc | 607 | PC1 | C22-C21-O21-C2 |
| 58 | Dy | 302 | PC1 | C22-C21-O21-C2 |
| 59 | DG | 204 | 3PE | C22-C21-O21-C2 |
| 65 | DS | 404 | UQ8 | C35-C34-C36-C37 |
| 65 | DS | 404 | UQ8 | C33-C34-C36-C37 |
| 57 | DA | 705 | CDL | C71-CB7-OB8-CB6 |
| 57 | DA | 709 | CDL | C71-CB7-OB8-CB6 |
| 57 | DJ | 305 | CDL | C71-CB7-OB8-CB6 |
| 57 | DQ | 1504 | CDL | C71-CB7-OB8-CB6 |
| 57 | DS | 402 | CDL | C71-CB7-OB8-CB6 |
| 57 | DU | 402 | CDL | C71-CB7-OB8-CB6 |
| 57 | DV | 401 | CDL | C31-CA7-OA8-CA6 |
| 57 | DV | 402 | CDL | C31-CA7-OA8-CA6 |
| 57 | DV | 404 | CDL | C31-CA7-OA8-CA6 |
| 57 | EA | 301 | CDL | C71-CB7-OB8-CB6 |
| 57 | EK | 201 | CDL | C71-CB7-OB8-CB6 |
| 57 | EL | 901 | CDL | C71-CB7-OB8-CB6 |
| 57 | EL | 902 | CDL | C71-CB7-OB8-CB6 |
| 57 | EL | 903 | CDL | C71-CB7-OB8-CB6 |
| 57 | EO | 202 | CDL | C71-CB7-OB8-CB6 |
| 57 | EU | 101 | CDL | C31-CA7-OA8-CA6 |
| 57 | Da | 709 | CDL | C71-CB7-OB8-CB6 |
| 57 | Dc | 601 | CDL | C71-CB7-OB8-CB6 |
| 57 | Dg | 201 | CDL | C31-CA7-OA8-CA6 |
| 57 | Dh | 201 | CDL | C71-CB7-OB8-CB6 |
| 57 | Dh | 202 | CDL | C31-CA7-OA8-CA6 |
| 57 | Dj | 401 | CDL | C71-CB7-OB8-CB6 |
| 57 | Dj | 404 | CDL | C71-CB7-OB8-CB6 |
| 57 | Dj | 405 | CDL | C71-CB7-OB8-CB6 |
| 57 | Dn | 501 | CDL | C71-CB7-OB8-CB6 |
| 57 | Dn | 507 | CDL | C31-CA7-OA8-CA6 |
| 57 | Dq | 401 | CDL | C71-CB7-OB8-CB6 |
| 57 | Dq | 402 | CDL | C31-CA7-OA8-CA6 |
| 57 | Dq | 402 | CDL | C71-CB7-OB8-CB6 |
| 57 | Du | 402 | CDL | C71-CB7-OB8-CB6 |
| 57 | Du | 403 | CDL | C71-CB7-OB8-CB6 |
| 57 | Dv | 402 | CDL | C31-CA7-OA8-CA6 |
| 57 | Dv | 403 | CDL | C31-CA7-OA8-CA6 |
| 57 | Eh | 1601 | CDL | C71-CB7-OB8-CB6 |
| 57 | Ek | 201 | CDL | C71-CB7-OB8-CB6 |
| 57 | El | 902 | CDL | C71-CB7-OB8-CB6 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 57 | En | 1202 | CDL | C31-CA7-OA8-CA6 |
| 57 | Eu | 101 | CDL | C31-CA7-OA8-CA6 |
| 58 | DC | 602 | PC1 | C32-C31-O31-C3 |
| 58 | DC | 604 | PC1 | C32-C31-O31-C3 |
| 58 | DX | 302 | PC1 | C32-C31-O31-C3 |
| 58 | Eb | 301 | PC1 | C32-C31-O31-C3 |
| 58 | Ef | 1001 | PC1 | C32-C31-O31-C3 |
| 59 | Dr | 401 | 3PE | C32-C31-O31-C3 |
| 59 | Ds | 407 | 3PE | C32-C31-O31-C3 |
| 57 | DA | 710 | CDL | OA7-CA5-OA6-CA4 |
| 57 | DD | 702 | CDL | OA7-CA5-OA6-CA4 |
| 57 | DU | 402 | CDL | OA7-CA5-OA6-CA4 |
| 57 | EL | 903 | CDL | OA7-CA5-OA6-CA4 |
| 57 | EO | 202 | CDL | OA7-CA5-OA6-CA4 |
| 57 | Di | 701 | CDL | OA7-CA5-OA6-CA4 |
| 57 | Dy | 301 | CDL | OA7-CA5-OA6-CA4 |
| 57 | Dy | 301 | CDL | OB7-CB5-OB6-CB4 |
| 57 | Ek | 201 | CDL | OA7-CA5-OA6-CA4 |
| 57 | DA | 705 | CDL | OB9-CB7-OB8-CB6 |
| 57 | DJ | 307 | CDL | OA9-CA7-OA8-CA6 |
| 57 | DQ | 1504 | CDL | OA9-CA7-OA8-CA6 |
| 57 | DV | 401 | CDL | OA9-CA7-OA8-CA6 |
| 57 | EB | 304 | CDL | OA9-CA7-OA8-CA6 |
| 57 | EL | 903 | CDL | OB9-CB7-OB8-CB6 |
| 57 | EN | 1202 | CDL | OA9-CA7-OA8-CA6 |
| 57 | Da | 705 | CDL | OB9-CB7-OB8-CB6 |
| 57 | Dc | 601 | CDL | OB9-CB7-OB8-CB6 |
| 57 | Dh | 202 | CDL | OA9-CA7-OA8-CA6 |
| 57 | Dj | 408 | CDL | OA9-CA7-OA8-CA6 |
| 57 | Du | 402 | CDL | OB9-CB7-OB8-CB6 |
| 57 | Dv | 401 | CDL | OA9-CA7-OA8-CA6 |
| 57 | Dx | 1201 | CDL | OB9-CB7-OB8-CB6 |
| 57 | Eh | 1601 | CDL | OB9-CB7-OB8-CB6 |
| 57 | El | 901 | CDL | OB9-CB7-OB8-CB6 |
| 58 | DC | 602 | PC1 | O32-C31-O31-C3 |
| 58 | DC | 604 | PC1 | O32-C31-O31-C3 |
| 58 | DS | 407 | PC1 | O32-C31-O31-C3 |
| 58 | Dc | 602 | PC1 | O32-C31-O31-C3 |
| 58 | Ds | 406 | PC1 | O32-C31-O31-C3 |
| 59 | EO | 204 | 3PE | O32-C31-O31-C3 |
| 57 | DA | 710 | CDL | O1-C1-CB2-OB2 |
| 57 | DG | 201 | CDL | O1-C1-CA2-OA2 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 57 | DH | 201 | CDL | O1-C1-CA2-OA2 |
| 57 | DJ | 302 | CDL | O1-C1-CA2-OA2 |
| 57 | DN | 505 | CDL | O1-C1-CA2-OA2 |
| 57 | EB | 304 | CDL | O1-C1-CA2-OA2 |
| 57 | EL | 902 | CDL | O1-C1-CB2-OB2 |
| 57 | EU | 101 | CDL | O1-C1-CA2-OA2 |
| 57 | Dd | 704 | CDL | O1-C1-CA2-OA2 |
| 57 | Dd | 706 | CDL | O1-C1-CA2-OA2 |
| 57 | Dg | 202 | CDL | O1-C1-CA2-OA2 |
| 57 | Dh | 201 | CDL | O1-C1-CA2-OA2 |
| 57 | Dj | 405 | CDL | O1-C1-CA2-OA2 |
| 57 | Dm | 501 | CDL | O1-C1-CB2-OB2 |
| 57 | Du | 402 | CDL | O1-C1-CB2-OB2 |
| 57 | Ei | 401 | CDL | O1-C1-CA2-OA2 |
| 57 | El | 902 | CDL | O1-C1-CB2-OB2 |
| 57 | En | 1201 | CDL | O1-C1-CA2-OA2 |
| 57 | DC | 601 | CDL | C71-CB7-OB8-CB6 |
| 57 | DH | 201 | CDL | C71-CB7-OB8-CB6 |
| 57 | DO | 501 | CDL | C31-CA7-OA8-CA6 |
| 57 | Dn | 503 | CDL | C71-CB7-OB8-CB6 |
| 57 | Dx | 1201 | CDL | C71-CB7-OB8-CB6 |
| 58 | DS | 407 | PC1 | C32-C31-O31-C3 |
| 58 | DV | 406 | PC1 | C32-C31-O31-C3 |
| 58 | Ds | 406 | PC1 | C32-C31-O31-C3 |
| 57 | EA | 301 | CDL | OB9-CB7-OB8-CB6 |
| 57 | EL | 904 | CDL | OB9-CB7-OB8-CB6 |
| 57 | EN | 1201 | CDL | OB9-CB7-OB8-CB6 |
| 57 | Da | 709 | CDL | OB9-CB7-OB8-CB6 |
| 57 | Dn | 503 | CDL | OB9-CB7-OB8-CB6 |
| 57 | Du | 401 | CDL | OA9-CA7-OA8-CA6 |
| 57 | Ek | 201 | CDL | OB9-CB7-OB8-CB6 |
| 58 | Dc | 604 | PC1 | O32-C31-O31-C3 |
| 58 | Ef | 1001 | PC1 | O32-C31-O31-C3 |
| 59 | EN | 1203 | 3PE | O32-C31-O31-C3 |
| 57 | DJ | 304 | CDL | C11-CA5-OA6-CA4 |
| 57 | DJ | 305 | CDL | C11-CA5-OA6-CA4 |
| 57 | DJ | 305 | CDL | C51-CB5-OB6-CB4 |
| 57 | DM | 501 | CDL | C11-CA5-OA6-CA4 |
| 57 | DR | 403 | CDL | C11-CA5-OA6-CA4 |
| 57 | DU | 404 | CDL | C11-CA5-OA6-CA4 |
| 57 | DV | 401 | CDL | C51-CB5-OB6-CB4 |
| 57 | EK | 201 | CDL | C51-CB5-OB6-CB4 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 57 | EL | 903 | CDL | C51-CB5-OB6-CB4 |
| 57 | Dj | 403 | CDL | C11-CA5-OA6-CA4 |
| 57 | Dj | 405 | CDL | C11-CA5-OA6-CA4 |
| 57 | Dj | 408 | CDL | C11-CA5-OA6-CA4 |
| 57 | Dr | 403 | CDL | C11-CA5-OA6-CA4 |
| 57 | Ds | 402 | CDL | C11-CA5-OA6-CA4 |
| 57 | Ek | 201 | CDL | C11-CA5-OA6-CA4 |
| 57 | En | 1202 | CDL | C11-CA5-OA6-CA4 |
| 58 | Da | 707 | PC1 | C22-C21-O21-C2 |
| 58 | Dv | 406 | PC1 | C22-C21-O21-C2 |
| 58 | Dx | 1208 | PC1 | C22-C21-O21-C2 |
| 57 | Dd | 705 | CDL | CA5-C11-C12-C13 |
| 59 | Dc | 606 | 3PE | C2-C3-O31-C31 |
| 59 | Ds | 407 | 3PE | O32-C31-O31-C3 |
| 57 | DJ | 307 | CDL | C31-CA7-OA8-CA6 |
| 57 | DQ | 1504 | CDL | C31-CA7-OA8-CA6 |
| 57 | EB | 304 | CDL | C31-CA7-OA8-CA6 |
| 57 | Da | 705 | CDL | C71-CB7-OB8-CB6 |
| 57 | Dj | 408 | CDL | C31-CA7-OA8-CA6 |
| 57 | El | 901 | CDL | C71-CB7-OB8-CB6 |
| 58 | Dc | 602 | PC1 | C32-C31-O31-C3 |
| 59 | DJ | 301 | 3PE | C32-C31-O31-C3 |
| 59 | EO | 204 | 3PE | C32-C31-O31-C3 |
| 57 | DJ | 305 | CDL | OB7-CB5-OB6-CB4 |
| 58 | Dv | 406 | PC1 | O22-C21-O21-C2 |
| 58 | Dx | 1208 | PC1 | O22-C21-O21-C2 |
| 57 | DJ | 304 | CDL | CA4-CA3-OA5-PA1 |
| 57 | EL | 903 | CDL | C1-CB2-OB2-PB2 |
| 57 | EU | 101 | CDL | CA4-CA3-OA5-PA1 |
| 57 | Dg | 201 | CDL | CB4-CB3-OB5-PB2 |
| 57 | El | 903 | CDL | C1-CB2-OB2-PB2 |
| 58 | Da | 706 | PC1 | C2-C1-O11-P |
| 57 | DO | 501 | CDL | OA9-CA7-OA8-CA6 |
| 57 | Dh | 201 | CDL | OB9-CB7-OB8-CB6 |
| 57 | Dq | 402 | CDL | OB9-CB7-OB8-CB6 |
| 57 | En | 1202 | CDL | OA9-CA7-OA8-CA6 |
| 58 | DV | 406 | PC1 | O32-C31-O31-C3 |
| 65 | EN | 1204 | UQ8 | C25-C24-C26-C27 |
| 65 | EN | 1204 | UQ8 | C23-C24-C26-C27 |
| 57 | DC | 601 | CDL | OB9-CB7-OB8-CB6 |
| 57 | DH | 201 | CDL | OB9-CB7-OB8-CB6 |
| 59 | DJ | 301 | 3PE | O32-C31-O31-C3 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 54 | DA | 702 | HEA | C15-C16-C17-C18 |
| 54 | Da | 702 | HEA | C19-C20-C21-C22 |
| 65 | ED | 603 | UQ8 | C39-C41-C42-C43 |
| 65 | EN | 1204 | UQ8 | C34-C36-C37-C38 |
| 65 | En | 1203 | UQ8 | C19-C21-C22-C23 |
| 57 | DA | 710 | CDL | C31-CA7-OA8-CA6 |
| 57 | ED | 601 | CDL | C31-CA7-OA8-CA6 |
| 57 | Dr | 402 | CDL | C31-CA7-OA8-CA6 |
| 57 | Eg | 101 | CDL | C31-CA7-OA8-CA6 |
| 58 | Dq | 405 | PC1 | C32-C31-O31-C3 |
| 57 | DM | 502 | CDL | CA5-C11-C12-C13 |
| 58 | DA | 707 | PC1 | C3C-C3D-C3E-C3F |
| 57 | DA | 705 | CDL | C51-CB5-OB6-CB4 |
| 57 | Dv | 401 | CDL | C51-CB5-OB6-CB4 |
| 59 | El | 905 | 3PE | C22-C21-O21-C2 |
| 59 | Ds | 403 | 3PE | C2-C3-O31-C31 |
| 57 | DD | 702 | CDL | CB2-C1-CA2-OA2 |
| 57 | DJ | 304 | CDL | CB2-C1-CA2-OA2 |
| 57 | DR | 403 | CDL | CB2-C1-CA2-OA2 |
| 57 | DY | 301 | CDL | CB2-C1-CA2-OA2 |
| 57 | EN | 1201 | CDL | CB2-C1-CA2-OA2 |
| 57 | Dj | 402 | CDL | CB2-C1-CA2-OA2 |
| 57 | Dj | 405 | CDL | CB2-C1-CA2-OA2 |
| 57 | Dj | 408 | CDL | CA2-C1-CB2-OB2 |
| 57 | Dm | 501 | CDL | CA2-C1-CB2-OB2 |
| 57 | Dn | 505 | CDL | CB2-C1-CA2-OA2 |
| 57 | Dq | 401 | CDL | CB2-C1-CA2-OA2 |
| 57 | Dr | 403 | CDL | CB2-C1-CA2-OA2 |
| 57 | Ds | 402 | CDL | CA2-C1-CB2-OB2 |
| 57 | Dy | 301 | CDL | CB2-C1-CA2-OA2 |
| 57 | Ei | 401 | CDL | CB2-C1-CA2-OA2 |
| 57 | En | 1201 | CDL | CB2-C1-CA2-OA2 |
| 57 | DJ | 304 | CDL | OA7-CA5-OA6-CA4 |
| 57 | DR | 403 | CDL | OA7-CA5-OA6-CA4 |
| 57 | DU | 404 | CDL | OA7-CA5-OA6-CA4 |
| 57 | DV | 401 | CDL | OB7-CB5-OB6-CB4 |
| 57 | EK | 201 | CDL | OB7-CB5-OB6-CB4 |
| 57 | EL | 903 | CDL | OB7-CB5-OB6-CB4 |
| 57 | Dr | 403 | CDL | OA7-CA5-OA6-CA4 |
| 57 | Ds | 402 | CDL | OA7-CA5-OA6-CA4 |
| 57 | En | 1202 | CDL | OA7-CA5-OA6-CA4 |
| 57 | DA | 710 | CDL | OA9-CA7-OA8-CA6 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 57 | ED | 601 | CDL | OA9-CA7-OA8-CA6 |
| 57 | Dr | 402 | CDL | OA9-CA7-OA8-CA6 |
| 57 | DA | 709 | CDL | C31-CA7-OA8-CA6 |
| 57 | DD | 702 | CDL | C71-CB7-OB8-CB6 |
| 57 | DR | 402 | CDL | C31-CA7-OA8-CA6 |
| 57 | ED | 601 | CDL | C71-CB7-OB8-CB6 |
| 57 | EH | 201 | CDL | C71-CB7-OB8-CB6 |
| 57 | Da | 709 | CDL | C31-CA7-OA8-CA6 |
| 57 | Dd | 706 | CDL | C71-CB7-OB8-CB6 |
| 57 | Dg | 202 | CDL | C31-CA7-OA8-CA6 |
| 57 | Dm | 502 | CDL | C71-CB7-OB8-CB6 |
| 57 | Dn | 501 | CDL | C31-CA7-OA8-CA6 |
| 57 | Dn | 502 | CDL | C31-CA7-OA8-CA6 |
| 57 | Dn | 503 | CDL | C31-CA7-OA8-CA6 |
| 57 | Do | 501 | CDL | C31-CA7-OA8-CA6 |
| 57 | Dx | 1203 | CDL | C31-CA7-OA8-CA6 |
| 57 | Dx | 1203 | CDL | C71-CB7-OB8-CB6 |
| 57 | El | 903 | CDL | C71-CB7-OB8-CB6 |
| 58 | DA | 706 | PC1 | C32-C31-O31-C3 |
| 58 | DC | 608 | PC1 | C32-C31-O31-C3 |
| 58 | DQ | 1503 | PC1 | C32-C31-O31-C3 |
| 58 | Da | 706 | PC1 | C32-C31-O31-C3 |
| 58 | Dc | 607 | PC1 | C32-C31-O31-C3 |
| 58 | Dv | 407 | PC1 | C32-C31-O31-C3 |
| 59 | DC | 607 | 3PE | C32-C31-O31-C3 |
| 59 | DS | 403 | 3PE | C32-C31-O31-C3 |
| 59 | Dr | 404 | 3PE | C32-C31-O31-C3 |
| 59 | Ds | 403 | 3PE | C32-C31-O31-C3 |
| 57 | DJ | 304 | CDL | OB5-CB3-CB4-OB6 |
| 57 | DV | 404 | CDL | OB5-CB3-CB4-OB6 |
| 57 | Dv | 404 | CDL | OB5-CB3-CB4-OB6 |
| 58 | DQ | 1503 | PC1 | O11-C1-C2-O21 |
| 57 | DG | 201 | CDL | O1-C1-CB2-OB2 |
| 57 | DJ | 304 | CDL | O1-C1-CA2-OA2 |
| 57 | DJ | 307 | CDL | O1-C1-CA2-OA2 |
| 57 | EB | 302 | CDL | O1-C1-CA2-OA2 |
| 57 | ED | 601 | CDL | O1-C1-CA2-OA2 |
| 57 | Dd | 702 | CDL | O1-C1-CA2-OA2 |
| 57 | Dd | 702 | CDL | O1-C1-CB2-OB2 |
| 57 | Dg | 201 | CDL | O1-C1-CA2-OA2 |
| 57 | Dj | 408 | CDL | O1-C1-CA2-OA2 |
| 57 | Du | 404 | CDL | O1-C1-CA2-OA2 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 57 | Dv | 404 | CDL | O1-C1-CA2-OA2 |
| 57 | Ep | 701 | CDL | O1-C1-CA2-OA2 |
| 57 | El | 901 | CDL | CA5-C11-C12-C13 |
| 57 | DA | 705 | CDL | OA6-CA4-CA6-OA8 |
| 57 | DJ | 303 | CDL | OB6-CB4-CB6-OB8 |
| 57 | DR | 402 | CDL | OB6-CB4-CB6-OB8 |
| 57 | DR | 403 | CDL | OB6-CB4-CB6-OB8 |
| 57 | Dg | 201 | CDL | OA6-CA4-CA6-OA8 |
| 58 | DS | 407 | PC1 | O21-C2-C3-O31 |
| 57 | DA | 709 | CDL | OA9-CA7-OA8-CA6 |
| 57 | EH | 201 | CDL | OB9-CB7-OB8-CB6 |
| 57 | Dn | 503 | CDL | OA9-CA7-OA8-CA6 |
| 59 | DC | 607 | 3PE | O32-C31-O31-C3 |
| 57 | DJ | 305 | CDL | OA7-CA5-OA6-CA4 |
| 57 | DM | 501 | CDL | OA7-CA5-OA6-CA4 |
| 57 | Dj | 403 | CDL | OA7-CA5-OA6-CA4 |
| 57 | Dj | 408 | CDL | OA7-CA5-OA6-CA4 |
| 57 | DD | 704 | CDL | C11-CA5-OA6-CA4 |
| 57 | DJ | 302 | CDL | C11-CA5-OA6-CA4 |
| 57 | DM | 502 | CDL | C11-CA5-OA6-CA4 |
| 57 | Dg | 201 | CDL | C51-CB5-OB6-CB4 |
| 57 | Dm | 502 | CDL | C11-CA5-OA6-CA4 |
| 57 | Do | 501 | CDL | C11-CA5-OA6-CA4 |
| 58 | Da | 707 | PC1 | C3C-C3D-C3E-C3F |
| 57 | DU | 404 | CDL | CA5-C11-C12-C13 |
| 57 | EL | 901 | CDL | CA5-C11-C12-C13 |
| 57 | Dz | 501 | CDL | CA7-C31-C32-C33 |
| 57 | El | 902 | CDL | CA5-C11-C12-C13 |
| 59 | EM | 901 | 3PE | C21-C22-C23-C24 |
| 57 | DD | 702 | CDL | OB9-CB7-OB8-CB6 |
| 57 | ED | 601 | CDL | OB9-CB7-OB8-CB6 |
| 57 | Dd | 706 | CDL | OB9-CB7-OB8-CB6 |
| 57 | Dn | 501 | CDL | OA9-CA7-OA8-CA6 |
| 57 | Dn | 502 | CDL | OA9-CA7-OA8-CA6 |
| 57 | Do | 501 | CDL | OA9-CA7-OA8-CA6 |
| 57 | Dx | 1203 | CDL | OA9-CA7-OA8-CA6 |
| 57 | Dx | 1203 | CDL | OB9-CB7-OB8-CB6 |
| 57 | El | 903 | CDL | OB9-CB7-OB8-CB6 |
| 58 | DA | 706 | PC1 | O32-C31-O31-C3 |
| 58 | Da | 706 | PC1 | O32-C31-O31-C3 |
| 59 | DS | 403 | 3PE | O32-C31-O31-C3 |
| 59 | Ds | 403 | 3PE | O32-C31-O31-C3 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 57 | DJ | 303 | CDL | C71-CB7-OB8-CB6 |
| 57 | DN | 505 | CDL | C31-CA7-OA8-CA6 |
| 57 | DN | 505 | CDL | C71-CB7-OB8-CB6 |
| 57 | Ed | 204 | CDL | C71-CB7-OB8-CB6 |
| 57 | Eh | 1601 | CDL | C31-CA7-OA8-CA6 |
| 57 | En | 1201 | CDL | C71-CB7-OB8-CB6 |
| 59 | Em | 901 | 3PE | C32-C31-O31-C3 |
| 57 | DG | 202 | CDL | CA5-C11-C12-C13 |
| 57 | DV | 402 | CDL | CA5-C11-C12-C13 |
| 57 | Dc | 601 | CDL | CA5-C11-C12-C13 |
| 57 | Dj | 408 | CDL | CA5-C11-C12-C13 |
| 57 | Dv | 402 | CDL | CA5-C11-C12-C13 |
| 58 | EO | 201 | PC1 | C31-C32-C33-C34 |
| 57 | DR | 402 | CDL | OA9-CA7-OA8-CA6 |
| 57 | DJ | 304 | CDL | CA5-C11-C12-C13 |
| 57 | DN | 501 | CDL | CA5-C11-C12-C13 |
| 57 | EB | 304 | CDL | CA5-C11-C12-C13 |
| 57 | ED | 601 | CDL | CA5-C11-C12-C13 |
| 57 | EL | 902 | CDL | CA5-C11-C12-C13 |
| 57 | Dh | 202 | CDL | CA5-C11-C12-C13 |
| 57 | Dm | 501 | CDL | CA5-C11-C12-C13 |
| 57 | Du | 402 | CDL | CA5-C11-C12-C13 |
| 57 | Dx | 1201 | CDL | CA5-C11-C12-C13 |
| 57 | Dy | 301 | CDL | CA5-C11-C12-C13 |
| 57 | Ei | 401 | CDL | CA5-C11-C12-C13 |
| 57 | Dq | 403 | CDL | C19-C20-C21-C22 |
| 59 | DG | 205 | 3PE | C32-C31-O31-C3 |
| 59 | Dc | 606 | 3PE | C32-C31-O31-C3 |
| 57 | Dj | 405 | CDL | OA7-CA5-OA6-CA4 |
| 57 | Dv | 401 | CDL | OB7-CB5-OB6-CB4 |
| 58 | Da | 707 | PC1 | O22-C21-O21-C2 |
| 57 | Ep | 701 | CDL | C1-CA2-OA2-PA1 |
| 57 | DU | 401 | CDL | CA5-C11-C12-C13 |
| 57 | DZ | 501 | CDL | CA5-C11-C12-C13 |
| 57 | DU | 402 | CDL | C14-C15-C16-C17 |
| 57 | Eu | 101 | CDL | C11-CA5-OA6-CA4 |
| 59 | Eo | 203 | 3PE | C22-C21-O21-C2 |
| 57 | Dm | 502 | CDL | OB9-CB7-OB8-CB6 |
| 58 | DQ | 1503 | PC1 | O32-C31-O31-C3 |
| 58 | Dc | 607 | PC1 | O32-C31-O31-C3 |
| 57 | Dg | 202 | CDL | OA9-CA7-OA8-CA6 |
| 65 | Ed | 202 | UQ8 | C39-C41-C42-C43 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 65 | El | 906 | UQ8 | C14-C16-C17-C18 |
| 65 | En | 1203 | UQ8 | C34-C36-C37-C38 |
| 57 | DH | 201 | CDL | CA5-C11-C12-C13 |
| 57 | DD | 704 | CDL | O1-C1-CA2-OA2 |
| 57 | DS | 402 | CDL | O1-C1-CB2-OB2 |
| 57 | DX | 301 | CDL | O1-C1-CB2-OB2 |
| 57 | DY | 301 | CDL | O1-C1-CA2-OA2 |
| 57 | EL | 903 | CDL | O1-C1-CB2-OB2 |
| 57 | EN | 1202 | CDL | O1-C1-CA2-OA2 |
| 57 | Dd | 704 | CDL | O1-C1-CB2-OB2 |
| 57 | Dq | 401 | CDL | O1-C1-CA2-OA2 |
| 57 | Ds | 402 | CDL | O1-C1-CB2-OB2 |
| 57 | Dy | 301 | CDL | O1-C1-CA2-OA2 |
| 57 | El | 901 | CDL | O1-C1-CA2-OA2 |
| 57 | En | 1202 | CDL | O1-C1-CA2-OA2 |
| 57 | DA | 705 | CDL | OB7-CB5-OB6-CB4 |
| 57 | DD | 704 | CDL | OA7-CA5-OA6-CA4 |
| 57 | DJ | 302 | CDL | OA7-CA5-OA6-CA4 |
| 57 | Dg | 201 | CDL | OB7-CB5-OB6-CB4 |
| 57 | Dm | 502 | CDL | OA7-CA5-OA6-CA4 |
| 59 | El | 905 | 3PE | O22-C21-O21-C2 |
| 58 | DI | 702 | PC1 | C32-C31-O31-C3 |
| 57 | Da | 709 | CDL | OA9-CA7-OA8-CA6 |
| 57 | Eg | 101 | CDL | OA9-CA7-OA8-CA6 |
| 58 | Dq | 405 | PC1 | O32-C31-O31-C3 |
| 58 | Dv | 407 | PC1 | O32-C31-O31-C3 |
| 59 | Dr | 404 | 3PE | O32-C31-O31-C3 |
| 59 | Em | 901 | 3PE | O32-C31-O31-C3 |
| 57 | DQ | 1504 | CDL | CB5-C51-C52-C53 |
| 57 | Dm | 502 | CDL | CA5-C11-C12-C13 |
| 57 | DQ | 1501 | CDL | C19-C20-C21-C22 |
| 57 | Ed | 204 | CDL | OB9-CB7-OB8-CB6 |
| 57 | Eh | 1601 | CDL | OA9-CA7-OA8-CA6 |
| 58 | DC | 608 | PC1 | O32-C31-O31-C3 |
| 59 | Dc | 606 | 3PE | O32-C31-O31-C3 |
| 57 | DQ | 1502 | CDL | C11-CA5-OA6-CA4 |
| 57 | DQ | 1504 | CDL | C51-CB5-OB6-CB4 |
| 57 | DU | 401 | CDL | C11-CA5-OA6-CA4 |
| 57 | EB | 304 | CDL | C11-CA5-OA6-CA4 |
| 57 | EI | 401 | CDL | C11-CA5-OA6-CA4 |
| 57 | EN | 1202 | CDL | C11-CA5-OA6-CA4 |
| 57 | Dh | 201 | CDL | C11-CA5-OA6-CA4 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 57 | Dh | 202 | CDL | C11-CA5-OA6-CA4 |
| 57 | Dr | 402 | CDL | C51-CB5-OB6-CB4 |
| 59 | Ds | 407 | 3PE | C22-C21-O21-C2 |
| 57 | Dg | 201 | CDL | C23-C24-C25-C26 |
| 57 | DA | 709 | CDL | CA2-OA2-PA1-OA5 |
| 57 | DA | 709 | CDL | CB3-OB5-PB2-OB2 |
| 57 | DC | 601 | CDL | CB2-OB2-PB2-OB5 |
| 57 | DD | 702 | CDL | CA3-OA5-PA1-OA2 |
| 57 | DD | 703 | CDL | CB2-OB2-PB2-OB5 |
| 57 | DD | 704 | CDL | CA2-OA2-PA1-OA5 |
| 57 | DJ | 303 | CDL | CA2-OA2-PA1-OA5 |
| 57 | DJ | 304 | CDL | CA3-OA5-PA1-OA2 |
| 57 | DJ | 305 | CDL | CA3-OA5-PA1-OA2 |
| 57 | DM | 501 | CDL | CB2-OB2-PB2-OB5 |
| 57 | DN | 505 | CDL | CA2-OA2-PA1-OA5 |
| 57 | DN | 505 | CDL | CA3-OA5-PA1-OA2 |
| 57 | DO | 501 | CDL | CA3-OA5-PA1-OA2 |
| 57 | DO | 501 | CDL | CB3-OB5-PB2-OB2 |
| 57 | DQ | 1501 | CDL | CB3-OB5-PB2-OB2 |
| 57 | DR | 402 | CDL | CA3-OA5-PA1-OA2 |
| 57 | DR | 402 | CDL | CB3-OB5-PB2-OB2 |
| 57 | DS | 405 | CDL | CA2-OA2-PA1-OA5 |
| 57 | DS | 405 | CDL | CB3-OB5-PB2-OB2 |
| 57 | DU | 401 | CDL | CA2-OA2-PA1-OA5 |
| 57 | DU | 403 | CDL | CB3-OB5-PB2-OB2 |
| 57 | DV | 403 | CDL | CA3-OA5-PA1-OA2 |
| 57 | DX | 301 | CDL | CB2-OB2-PB2-OB5 |
| 57 | DZ | 501 | CDL | CA2-OA2-PA1-OA5 |
| 57 | EA | 301 | CDL | CA2-OA2-PA1-OA5 |
| 57 | EA | 301 | CDL | CB2-OB2-PB2-OB5 |
| 57 | EB | 302 | CDL | CB3-OB5-PB2-OB2 |
| 57 | EB | 304 | CDL | CB3-OB5-PB2-OB2 |
| 57 | EH | 201 | CDL | CB3-OB5-PB2-OB2 |
| 57 | EH | 202 | CDL | CA3-OA5-PA1-OA2 |
| 57 | EH | 202 | CDL | CB3-OB5-PB2-OB2 |
| 57 | EI | 401 | CDL | CB3-OB5-PB2-OB2 |
| 57 | EK | 201 | CDL | CA2-OA2-PA1-OA5 |
| 57 | EK | 201 | CDL | CA3-OA5-PA1-OA2 |
| 57 | EL | 903 | CDL | CB2-OB2-PB2-OB5 |
| 57 | EL | 903 | CDL | CB3-OB5-PB2-OB2 |
| 57 | EL | 904 | CDL | CB3-OB5-PB2-OB2 |
| 57 | EU | 101 | CDL | CA3-OA5-PA1-OA2 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 57 | Da | 709 | CDL | CA3-OA5-PA1-OA2 |
| 57 | Da | 709 | CDL | CB3-OB5-PB2-OB2 |
| 57 | Dc | 601 | CDL | CB2-OB2-PB2-OB5 |
| 57 | Dd | 704 | CDL | CB2-OB2-PB2-OB5 |
| 57 | Dd | 705 | CDL | CA3-OA5-PA1-OA2 |
| 57 | Dh | 202 | CDL | CB2-OB2-PB2-OB5 |
| 57 | Dh | 202 | CDL | CB3-OB5-PB2-OB2 |
| 57 | Dj | 401 | CDL | CB3-OB5-PB2-OB2 |
| 57 | Dj | 404 | CDL | CA3-OA5-PA1-OA2 |
| 57 | Dj | 405 | CDL | CA3-OA5-PA1-OA2 |
| 57 | Dj | 408 | CDL | CB2-OB2-PB2-OB5 |
| 57 | Dm | 501 | CDL | CA3-OA5-PA1-OA2 |
| 57 | Dm | 502 | CDL | CA3-OA5-PA1-OA2 |
| 57 | Dn | 501 | CDL | CA3-OA5-PA1-OA2 |
| 57 | Dn | 502 | CDL | CB3-OB5-PB2-OB2 |
| 57 | Dn | 505 | CDL | CB3-OB5-PB2-OB2 |
| 57 | Do | 501 | CDL | CB3-OB5-PB2-OB2 |
| 57 | Dq | 401 | CDL | CB3-OB5-PB2-OB2 |
| 57 | Dq | 402 | CDL | CA2-OA2-PA1-OA5 |
| 57 | Dq | 403 | CDL | CA3-OA5-PA1-OA2 |
| 57 | Dq | 404 | CDL | CA3-OA5-PA1-OA2 |
| 57 | Dr | 402 | CDL | CA3-OA5-PA1-OA2 |
| 57 | Dr | 402 | CDL | CB2-OB2-PB2-OB5 |
| 57 | Ds | 405 | CDL | CA2-OA2-PA1-OA5 |
| 57 | Du | 401 | CDL | CA2-OA2-PA1-OA5 |
| 57 | Du | 403 | CDL | CA3-OA5-PA1-OA2 |
| 57 | Du | 404 | CDL | CB3-OB5-PB2-OB2 |
| 57 | Dv | 402 | CDL | CA3-OA5-PA1-OA2 |
| 57 | Dv | 403 | CDL | CA3-OA5-PA1-OA2 |
| 57 | Dx | 1201 | CDL | CA2-OA2-PA1-OA5 |
| 57 | Dx | 1201 | CDL | CB2-OB2-PB2-OB5 |
| 57 | Dx | 1201 | CDL | CB3-OB5-PB2-OB2 |
| 57 | Dx | 1203 | CDL | CA3-OA5-PA1-OA2 |
| 57 | Dx | 1203 | CDL | CB3-OB5-PB2-OB2 |
| 57 | Ea | 301 | CDL | CA2-OA2-PA1-OA5 |
| 57 | Ea | 301 | CDL | CB2-OB2-PB2-OB5 |
| 57 | Ed | 204 | CDL | CA3-OA5-PA1-OA2 |
| 57 | Ed | 204 | CDL | CB3-OB5-PB2-OB2 |
| 57 | Ed | 205 | CDL | CA3-OA5-PA1-OA2 |
| 57 | Ei | 401 | CDL | CB3-OB5-PB2-OB2 |
| 57 | Ek | 201 | CDL | CA2-OA2-PA1-OA5 |
| 57 | Ek | 201 | CDL | CA3-OA5-PA1-OA2 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 57 | El | 902 | CDL | CB2-OB2-PB2-OB5 |
| 57 | El | 902 | CDL | CB3-OB5-PB2-OB2 |
| 57 | El | 903 | CDL | CB2-OB2-PB2-OB5 |
| 57 | El | 903 | CDL | CB3-OB5-PB2-OB2 |
| 58 | DA | 707 | PC1 | C1-O11-P-O13 |
| 58 | DC | 602 | PC1 | C11-O13-P-O11 |
| 58 | DC | 602 | PC1 | C1-O11-P-O13 |
| 58 | DC | 603 | PC1 | C11-O13-P-O11 |
| 58 | DC | 604 | PC1 | C1-O11-P-O13 |
| 58 | DC | 608 | PC1 | C11-O13-P-O11 |
| 58 | DI | 702 | PC1 | C11-O13-P-O11 |
| 58 | DJ | 306 | PC1 | C11-O13-P-O11 |
| 58 | DJ | 306 | PC1 | C1-O11-P-O13 |
| 58 | DQ | 1503 | PC1 | C11-O13-P-O11 |
| 58 | DS | 406 | PC1 | C1-O11-P-O13 |
| 58 | DV | 405 | PC1 | C11-O13-P-O11 |
| 58 | DV | 406 | PC1 | C11-O13-P-O11 |
| 58 | DV | 407 | PC1 | C11-O13-P-O11 |
| 58 | DX | 302 | PC1 | C1-O11-P-O13 |
| 58 | DX | 306 | PC1 | C11-O13-P-O11 |
| 58 | EB | 301 | PC1 | C11-O13-P-O11 |
| 58 | EB | 301 | PC1 | C1-O11-P-O13 |
| 58 | EO | 201 | PC1 | C11-O13-P-O11 |
| 58 | EO | 205 | PC1 | C11-O13-P-O11 |
| 58 | EO | 205 | PC1 | C1-O11-P-O13 |
| 58 | Db | 702 | PC1 | C11-O13-P-O11 |
| 58 | Dc | 602 | PC1 | C11-O13-P-O11 |
| 58 | Dc | 602 | PC1 | C1-O11-P-O13 |
| 58 | Dc | 603 | PC1 | C11-O13-P-O11 |
| 58 | Dc | 604 | PC1 | C11-O13-P-O11 |
| 58 | Dc | 604 | PC1 | C1-O11-P-O13 |
| 58 | Dc | 605 | PC1 | C1-O11-P-O13 |
| 58 | Dc | 607 | PC1 | C11-O13-P-O11 |
| 58 | Di | 702 | PC1 | C11-O13-P-O11 |
| 58 | Di | 702 | PC1 | C1-O11-P-O13 |
| 58 | Dj | 406 | PC1 | C11-O13-P-O11 |
| 58 | Dq | 405 | PC1 | C11-O13-P-O11 |
| 58 | Dv | 407 | PC1 | C11-O13-P-O11 |
| 58 | Dv | 408 | PC1 | C11-O13-P-O11 |
| 58 | Dv | 408 | PC1 | C1-O11-P-O13 |
| 58 | Dx | 1202 | PC1 | C1-O11-P-O13 |
| 58 | El | 904 | PC1 | C11-O13-P-O11 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 58 | El | 904 | PC1 | C1-O11-P-O13 |
| 58 | Eo | 204 | PC1 | C11-O13-P-O11 |
| 58 | Eo | 205 | PC1 | C11-O13-P-O11 |
| 59 | DC | 606 | 3PE | C1-O11-P-O13 |
| 59 | DC | 607 | 3PE | C11-O13-P-O11 |
| 59 | DG | 204 | 3PE | C1-O11-P-O13 |
| 59 | DG | 204 | 3PE | C11-O13-P-O11 |
| 59 | DJ | 301 | 3PE | C1-O11-P-O13 |
| 59 | DS | 401 | 3PE | C1-O11-P-O13 |
| 59 | DS | 403 | 3PE | C1-O11-P-O13 |
| 59 | DX | 304 | 3PE | C11-O13-P-O11 |
| 59 | DX | 305 | 3PE | C11-O13-P-O11 |
| 59 | EL | 905 | 3PE | C1-O11-P-O13 |
| 59 | EO | 203 | 3PE | C1-O11-P-O13 |
| 59 | EO | 203 | 3PE | C11-O13-P-O11 |
| 59 | EO | 204 | 3PE | C1-O11-P-O13 |
| 59 | Da | 708 | 3PE | C1-O11-P-O13 |
| 59 | Dc | 606 | 3PE | C11-O13-P-O11 |
| 59 | Dd | 703 | 3PE | C1-O11-P-O13 |
| 59 | Dr | 401 | 3PE | C1-O11-P-O13 |
| 59 | Ds | 403 | 3PE | C1-O11-P-O13 |
| 59 | Dx | 1205 | 3PE | C1-O11-P-O13 |
| 59 | Dx | 1206 | 3PE | C1-O11-P-O13 |
| 59 | Eo | 203 | 3PE | C1-O11-P-O13 |
| 57 | EN | 1201 | CDL | CA5-C11-C12-C13 |
| 57 | Eh | 1601 | CDL | CA5-C11-C12-C13 |
| 57 | Ek | 201 | CDL | CA5-C11-C12-C13 |
| 57 | DG | 202 | CDL | C31-CA7-OA8-CA6 |
| 57 | Eu | 101 | CDL | C71-CB7-OB8-CB6 |
| 58 | Di | 702 | PC1 | C32-C31-O31-C3 |
| 57 | DH | 201 | CDL | C38-C39-C40-C41 |
| 57 | Du | 404 | CDL | CA5-C11-C12-C13 |
| 57 | DD | 704 | CDL | CB2-C1-CA2-OA2 |
| 57 | DJ | 307 | CDL | CA2-C1-CB2-OB2 |
| 57 | DM | 502 | CDL | CA2-C1-CB2-OB2 |
| 57 | DV | 404 | CDL | CB2-C1-CA2-OA2 |
| 57 | DX | 301 | CDL | CA2-C1-CB2-OB2 |
| 57 | EL | 903 | CDL | CA2-C1-CB2-OB2 |
| 57 | EN | 1202 | CDL | CB2-C1-CA2-OA2 |
| 57 | Dd | 704 | CDL | CA2-C1-CB2-OB2 |
| 57 | En | 1202 | CDL | CB2-C1-CA2-OA2 |
| 57 | Eu | 101 | CDL | CB2-C1-CA2-OA2 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 57 | DM | 502 | CDL | OA7-CA5-OA6-CA4 |
| 57 | DQ | 1502 | CDL | OA7-CA5-OA6-CA4 |
| 57 | DQ | 1504 | CDL | OB7-CB5-OB6-CB4 |
| 57 | DU | 401 | CDL | OA7-CA5-OA6-CA4 |
| 57 | EB | 304 | CDL | OA7-CA5-OA6-CA4 |
| 57 | EI | 401 | CDL | OA7-CA5-OA6-CA4 |
| 57 | EN | 1202 | CDL | OA7-CA5-OA6-CA4 |
| 57 | Dh | 201 | CDL | OA7-CA5-OA6-CA4 |
| 57 | Dh | 202 | CDL | OA7-CA5-OA6-CA4 |
| 57 | Do | 501 | CDL | OA7-CA5-OA6-CA4 |
| 57 | Dr | 402 | CDL | OB7-CB5-OB6-CB4 |
| 57 | Eu | 101 | CDL | OA7-CA5-OA6-CA4 |
| 59 | Ds | 407 | 3PE | O22-C21-O21-C2 |
| 59 | Eo | 203 | 3PE | O22-C21-O21-C2 |
| 57 | DR | 402 | CDL | C71-CB7-OB8-CB6 |
| 57 | DZ | 501 | CDL | C71-CB7-OB8-CB6 |
| 57 | EL | 904 | CDL | C31-CA7-OA8-CA6 |
| 57 | Dd | 702 | CDL | C71-CB7-OB8-CB6 |
| 57 | Dj | 401 | CDL | C31-CA7-OA8-CA6 |
| 57 | Dr | 402 | CDL | C71-CB7-OB8-CB6 |
| 57 | Du | 401 | CDL | C71-CB7-OB8-CB6 |
| 57 | Du | 403 | CDL | C31-CA7-OA8-CA6 |
| 57 | Dv | 404 | CDL | C71-CB7-OB8-CB6 |
| 58 | Dx | 1204 | PC1 | C32-C31-O31-C3 |
| 57 | DV | 402 | CDL | C14-C15-C16-C17 |
| 57 | Dr | 403 | CDL | C13-C14-C15-C16 |
| 57 | Ds | 405 | CDL | C14-C15-C16-C17 |
| 57 | DH | 201 | CDL | C11-CA5-OA6-CA4 |
| 57 | DS | 402 | CDL | C11-CA5-OA6-CA4 |
| 57 | DX | 301 | CDL | C51-CB5-OB6-CB4 |
| 57 | DZ | 501 | CDL | C51-CB5-OB6-CB4 |
| 57 | EK | 201 | CDL | C11-CA5-OA6-CA4 |
| 57 | Dc | 601 | CDL | C11-CA5-OA6-CA4 |
| 57 | Dc | 601 | CDL | C51-CB5-OB6-CB4 |
| 57 | Dd | 705 | CDL | C11-CA5-OA6-CA4 |
| 57 | Dq | 404 | CDL | C11-CA5-OA6-CA4 |
| 58 | DA | 707 | PC1 | C22-C21-O21-C2 |
| 59 | Dg | 204 | 3PE | C22-C21-O21-C2 |
| 57 | DA | 710 | CDL | C17-C18-C19-C20 |
| 57 | EA | 301 | CDL | C11-C12-C13-C14 |
| 57 | Da | 705 | CDL | C75-C76-C77-C78 |
| 57 | Dd | 704 | CDL | C75-C76-C77-C78 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 57 | Dj | 403 | CDL | C55-C56-C57-C58 |
| 57 | Dv | 402 | CDL | C14-C15-C16-C17 |
| 57 | Dz | 501 | CDL | C39-C40-C41-C42 |
| 57 | El | 903 | CDL | C74-C75-C76-C77 |
| 58 | Dc | 607 | PC1 | C3D-C3E-C3F-C3G |
| 59 | DG | 205 | 3PE | O32-C31-O31-C3 |
| 57 | DV | 404 | CDL | C71-CB7-OB8-CB6 |
| 57 | Dm | 501 | CDL | C71-CB7-OB8-CB6 |
| 57 | Ds | 402 | CDL | C71-CB7-OB8-CB6 |
| 57 | DG | 202 | CDL | C80-C81-C82-C83 |
| 57 | DJ | 303 | CDL | C62-C63-C64-C65 |
| 57 | Dm | 501 | CDL | C55-C56-C57-C58 |
| 57 | Du | 404 | CDL | C11-C12-C13-C14 |
| 57 | Dx | 1201 | CDL | C14-C15-C16-C17 |
| 57 | Dx | 1203 | CDL | C19-C20-C21-C22 |
| 57 | Dz | 501 | CDL | C42-C43-C44-C45 |
| 58 | EB | 301 | PC1 | C27-C28-C29-C2A |
| 57 | DV | 402 | CDL | CB3-CB4-OB6-CB5 |
| 57 | Dv | 402 | CDL | CB3-CB4-OB6-CB5 |
| 58 | EO | 206 | PC1 | C1-C2-O21-C21 |
| 57 | DH | 201 | CDL | OA7-CA5-OA6-CA4 |
| 57 | DS | 402 | CDL | OA7-CA5-OA6-CA4 |
| 57 | DZ | 501 | CDL | OB7-CB5-OB6-CB4 |
| 57 | EK | 201 | CDL | OA7-CA5-OA6-CA4 |
| 57 | Dc | 601 | CDL | OA7-CA5-OA6-CA4 |
| 57 | Dc | 601 | CDL | OB7-CB5-OB6-CB4 |
| 57 | Dd | 705 | CDL | OA7-CA5-OA6-CA4 |
| 57 | Dq | 404 | CDL | OA7-CA5-OA6-CA4 |
| 58 | DA | 707 | PC1 | O22-C21-O21-C2 |
| 59 | Dg | 204 | 3PE | O22-C21-O21-C2 |
| 57 | DU | 404 | CDL | C11-C12-C13-C14 |
| 57 | Dj | 403 | CDL | C39-C40-C41-C42 |
| 57 | El | 901 | CDL | C80-C81-C82-C83 |
| 57 | En | 1202 | CDL | C57-C58-C59-C60 |
| 58 | EO | 207 | PC1 | C3E-C3F-C3G-C3H |
| 58 | Eb | 301 | PC1 | C27-C28-C29-C2A |
| 57 | Dj | 401 | CDL | C1-CB2-OB2-PB2 |
| 57 | Dm | 501 | CDL | C1-CB2-OB2-PB2 |
| 57 | Du | 401 | CDL | C1-CA2-OA2-PA1 |
| 57 | Eg | 101 | CDL | C1-CA2-OA2-PA1 |
| 57 | Ei | 401 | CDL | CB4-CB3-OB5-PB2 |
| 57 | DI | 701 | CDL | C13-C14-C15-C16 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 57 | DU | 404 | CDL | C80-C81-C82-C83 |
| 57 | EL | 904 | CDL | C63-C64-C65-C66 |
| 57 | Eu | 101 | CDL | C11-C12-C13-C14 |
| 57 | DJ | 303 | CDL | O1-C1-CB2-OB2 |
| 57 | EB | 302 | CDL | O1-C1-CB2-OB2 |
| 57 | DJ | 305 | CDL | C12-C13-C14-C15 |
| 57 | DQ | 1504 | CDL | C11-C12-C13-C14 |
| 57 | DR | 403 | CDL | C11-C12-C13-C14 |
| 57 | DU | 402 | CDL | C21-C22-C23-C24 |
| 57 | Dc | 601 | CDL | C13-C14-C15-C16 |
| 57 | Dd | 705 | CDL | C36-C37-C38-C39 |
| 57 | El | 901 | CDL | C55-C56-C57-C58 |
| 59 | Dd | 703 | 3PE | C25-C26-C27-C28 |
| 57 | EK | 201 | CDL | CA5-C11-C12-C13 |
| 57 | Dg | 202 | CDL | CA5-C11-C12-C13 |
| 57 | Dh | 201 | CDL | CA5-C11-C12-C13 |
| 57 | Ed | 204 | CDL | CA5-C11-C12-C13 |
| 57 | DJ | 307 | CDL | OA6-CA4-CA6-OA8 |
| 59 | Da | 708 | 3PE | O21-C2-C3-O31 |
| 59 | Ds | 401 | 3PE | C32-C31-O31-C3 |
| 57 | DM | 501 | CDL | C81-C82-C83-C84 |
| 57 | DX | 301 | CDL | C11-C12-C13-C14 |
| 57 | EL | 901 | CDL | C37-C38-C39-C40 |
| 57 | Dd | 704 | CDL | C22-C23-C24-C25 |
| 57 | Di | 701 | CDL | C13-C14-C15-C16 |
| 58 | DJ | 306 | PC1 | C3D-C3E-C3F-C3G |
| 58 | Dc | 605 | PC1 | C29-C2A-C2B-C2C |
| 57 | DG | 202 | CDL | OA9-CA7-OA8-CA6 |
| 57 | DJ | 303 | CDL | OB9-CB7-OB8-CB6 |
| 57 | DN | 505 | CDL | OA9-CA7-OA8-CA6 |
| 57 | DN | 505 | CDL | OB9-CB7-OB8-CB6 |
| 57 | En | 1201 | CDL | OB9-CB7-OB8-CB6 |
| 65 | El | 906 | UQ8 | C15-C14-C16-C17 |
| 57 | DQ | 1504 | CDL | C34-C35-C36-C37 |
| 57 | DR | 403 | CDL | C13-C14-C15-C16 |
| 57 | DX | 301 | CDL | C19-C20-C21-C22 |
| 57 | Ea | 301 | CDL | C13-C14-C15-C16 |
| 58 | DC | 604 | PC1 | C3B-C3C-C3D-C3E |
| 58 | Eo | 204 | PC1 | C2C-C2D-C2E-C2F |
| 65 | El | 906 | UQ8 | C13-C14-C16-C17 |
| 57 | Dq | 403 | CDL | CA5-C11-C12-C13 |
| 57 | DA | 705 | CDL | C75-C76-C77-C78 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 57 | EK | 201 | CDL | C40-C41-C42-C43 |
| 57 | Dq | 402 | CDL | C13-C14-C15-C16 |
| 57 | Dq | 403 | CDL | C12-C13-C14-C15 |
| 58 | DB | 702 | PC1 | C3C-C3D-C3E-C3F |
| 58 | Dj | 406 | PC1 | C3D-C3E-C3F-C3G |
| 60 | EI | 402 | LPP | C34-C35-C36-C37 |
| 58 | DI | 702 | PC1 | O32-C31-O31-C3 |
| 58 | Di | 702 | PC1 | O32-C31-O31-C3 |
| 57 | DX | 301 | CDL | C14-C15-C16-C17 |
| 57 | EL | 901 | CDL | C39-C40-C41-C42 |
| 57 | Dq | 401 | CDL | C35-C36-C37-C38 |
| 57 | Du | 403 | CDL | C14-C15-C16-C17 |
| 57 | Ek | 201 | CDL | C40-C41-C42-C43 |
| 58 | Dy | 302 | PC1 | C2E-C2F-C2G-C2H |
| 57 | DD | 703 | CDL | OA7-CA5-OA6-CA4 |
| 57 | DX | 301 | CDL | OB7-CB5-OB6-CB4 |
| 57 | Dm | 501 | CDL | OA7-CA5-OA6-CA4 |
| 57 | DA | 709 | CDL | C11-CA5-OA6-CA4 |
| 57 | DC | 601 | CDL | C11-CA5-OA6-CA4 |
| 57 | DD | 703 | CDL | C11-CA5-OA6-CA4 |
| 57 | EH | 202 | CDL | C11-CA5-OA6-CA4 |
| 57 | EL | 904 | CDL | C11-CA5-OA6-CA4 |
| 57 | Dm | 501 | CDL | C11-CA5-OA6-CA4 |
| 57 | Dn | 501 | CDL | C11-CA5-OA6-CA4 |
| 57 | El | 903 | CDL | C11-CA5-OA6-CA4 |
| 57 | DJ | 302 | CDL | C40-C41-C42-C43 |
| 57 | EL | 904 | CDL | C81-C82-C83-C84 |
| 57 | EU | 101 | CDL | C11-C12-C13-C14 |
| 57 | Dv | 403 | CDL | C13-C14-C15-C16 |
| 57 | El | 902 | CDL | C37-C38-C39-C40 |
| 58 | DI | 702 | PC1 | C27-C28-C29-C2A |
| 58 | Dc | 602 | PC1 | C3C-C3D-C3E-C3F |
| 58 | Eo | 201 | PC1 | C31-C32-C33-C34 |
| 57 | DA | 705 | CDL | C41-C42-C43-C44 |
| 57 | EH | 201 | CDL | C75-C76-C77-C78 |
| 57 | Da | 705 | CDL | C41-C42-C43-C44 |
| 57 | Ds | 402 | CDL | C74-C75-C76-C77 |
| 57 | Ds | 405 | CDL | C11-C12-C13-C14 |
| 57 | Du | 401 | CDL | C11-C12-C13-C14 |
| 57 | Dx | 1203 | CDL | C76-C77-C78-C79 |
| 57 | El | 902 | CDL | C39-C40-C41-C42 |
| 57 | En | 1202 | CDL | C11-C12-C13-C14 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 58 | DB | 702 | PC1 | C27-C28-C29-C2A |
| 58 | DC | 602 | PC1 | C3C-C3D-C3E-C3F |
| 58 | DY | 302 | PC1 | C2E-C2F-C2G-C2H |
| 58 | EO | 207 | PC1 | C3B-C3C-C3D-C3E |
| 58 | Dx | 1204 | PC1 | C24-C25-C26-C27 |
| 58 | Eo | 205 | PC1 | C3E-C3F-C3G-C3H |
| 65 | ED | 603 | UQ8 | C24-C26-C27-C28 |
| 57 | Dd | 705 | CDL | C13-C14-C15-C16 |
| 57 | Dg | 201 | CDL | C58-C59-C60-C61 |
| 57 | Dz | 501 | CDL | C77-C78-C79-C80 |
| 57 | Ed | 205 | CDL | C51-C52-C53-C54 |
| 57 | Eh | 1601 | CDL | C61-C62-C63-C64 |
| 59 | DJ | 301 | 3PE | C32-C33-C34-C35 |
| 59 | DX | 303 | 3PE | C39-C3A-C3B-C3C |
| 59 | DA | 708 | 3PE | O13-C11-C12-N |
| 59 | Dg | 204 | 3PE | O13-C11-C12-N |
| 57 | DA | 710 | CDL | C16-C17-C18-C19 |
| 57 | DI | 701 | CDL | C42-C43-C44-C45 |
| 57 | DM | 501 | CDL | C79-C80-C81-C82 |
| 57 | Dj | 408 | CDL | C13-C14-C15-C16 |
| 57 | Dn | 503 | CDL | C17-C18-C19-C20 |
| 57 | Du | 404 | CDL | C57-C58-C59-C60 |
| 57 | El | 901 | CDL | C12-C13-C14-C15 |
| 58 | DS | 406 | PC1 | C3B-C3C-C3D-C3E |
| 58 | Dc | 603 | PC1 | C2A-C2B-C2C-C2D |
| 59 | Eo | 202 | 3PE | C36-C37-C38-C39 |
| 57 | Dj | 403 | CDL | CA5-C11-C12-C13 |
| 57 | Dr | 402 | CDL | CA7-C31-C32-C33 |
| 59 | EN | 1203 | 3PE | C21-C22-C23-C24 |
| 57 | DR | 402 | CDL | OB9-CB7-OB8-CB6 |
| 57 | DZ | 501 | CDL | OB9-CB7-OB8-CB6 |
| 57 | EL | 904 | CDL | OA9-CA7-OA8-CA6 |
| 57 | DD | 702 | CDL | C74-C75-C76-C77 |
| 57 | DG | 201 | CDL | C14-C15-C16-C17 |
| 57 | DJ | 303 | CDL | C51-C52-C53-C54 |
| 57 | Da | 709 | CDL | C14-C15-C16-C17 |
| 57 | Dj | 402 | CDL | C52-C53-C54-C55 |
| 57 | Dv | 402 | CDL | C75-C76-C77-C78 |
| 57 | DU | 401 | CDL | C71-CB7-OB8-CB6 |
| 57 | DJ | 302 | CDL | C14-C15-C16-C17 |
| 57 | DN | 504 | CDL | C35-C36-C37-C38 |
| 57 | Dj | 402 | CDL | C62-C63-C64-C65 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 57 | Dv | 401 | CDL | C54-C55-C56-C57 |
| 57 | Dv | 404 | CDL | C13-C14-C15-C16 |
| 57 | Dv | 404 | CDL | C79-C80-C81-C82 |
| 57 | En | 1201 | CDL | C21-C22-C23-C24 |
| 57 | Ep | 701 | CDL | C11-C12-C13-C14 |
| 58 | Di | 702 | PC1 | C27-C28-C29-C2A |
| 57 | DJ | 307 | CDL | C54-C55-C56-C57 |
| 57 | DU | 404 | CDL | C33-C34-C35-C36 |
| 57 | EL | 901 | CDL | C80-C81-C82-C83 |
| 57 | Dn | 507 | CDL | C35-C36-C37-C38 |
| 57 | DA | 710 | CDL | CA5-C11-C12-C13 |
| 60 | EI | 402 | LPP | C11-C12-C13-C14 |
| 57 | DD | 704 | CDL | C41-C42-C43-C44 |
| 57 | DJ | 304 | CDL | C35-C36-C37-C38 |
| 57 | DN | 505 | CDL | C16-C17-C18-C19 |
| 57 | DV | 401 | CDL | C54-C55-C56-C57 |
| 57 | DV | 403 | CDL | C54-C55-C56-C57 |
| 57 | DV | 404 | CDL | C79-C80-C81-C82 |
| 57 | EN | 1201 | CDL | C77-C78-C79-C80 |
| 57 | Dj | 408 | CDL | C55-C56-C57-C58 |
| 57 | Dv | 401 | CDL | C80-C81-C82-C83 |
| 57 | El | 901 | CDL | C23-C24-C25-C26 |
| 57 | El | 903 | CDL | C81-C82-C83-C84 |
| 59 | EL | 905 | 3PE | C26-C27-C28-C29 |
| 59 | Ds | 407 | 3PE | C27-C28-C29-C2A |
| 57 | Dm | 502 | CDL | CA3-CA4-CA6-OA8 |
| 57 | Ed | 205 | CDL | CA3-CA4-CA6-OA8 |
| 58 | EO | 206 | PC1 | C1-C2-C3-O31 |
| 57 | DA | 709 | CDL | OA7-CA5-OA6-CA4 |
| 57 | DC | 601 | CDL | OA7-CA5-OA6-CA4 |
| 57 | EH | 202 | CDL | OA7-CA5-OA6-CA4 |
| 57 | El | 903 | CDL | OA7-CA5-OA6-CA4 |
| 57 | DU | 402 | CDL | C61-C62-C63-C64 |
| 57 | DV | 404 | CDL | C72-C73-C74-C75 |
| 57 | DX | 307 | CDL | C32-C33-C34-C35 |
| 57 | Dn | 501 | CDL | C73-C74-C75-C76 |
| 57 | Eg | 101 | CDL | C63-C64-C65-C66 |
| 58 | DC | 603 | PC1 | C2A-C2B-C2C-C2D |
| 59 | EN | 1203 | 3PE | C38-C39-C3A-C3B |
| 57 | DI | 701 | CDL | C62-C63-C64-C65 |
| 57 | DS | 402 | CDL | C16-C17-C18-C19 |
| 57 | DX | 307 | CDL | C11-C12-C13-C14 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 57 | DD | 704 | CDL | C71-CB7-OB8-CB6 |
| 57 | DJ | 307 | CDL | C71-CB7-OB8-CB6 |
| 57 | DN | 501 | CDL | C11-CA5-OA6-CA4 |
| 57 | DN | 504 | CDL | C11-CA5-OA6-CA4 |
| 57 | DU | 403 | CDL | C11-CA5-OA6-CA4 |
| 57 | DV | 403 | CDL | C11-CA5-OA6-CA4 |
| 57 | DX | 307 | CDL | C51-CB5-OB6-CB4 |
| 57 | ED | 604 | CDL | C11-CA5-OA6-CA4 |
| 57 | Dn | 503 | CDL | C51-CB5-OB6-CB4 |
| 57 | Dn | 507 | CDL | C11-CA5-OA6-CA4 |
| 57 | Du | 404 | CDL | C11-CA5-OA6-CA4 |
| 57 | Dv | 403 | CDL | C11-CA5-OA6-CA4 |
| 57 | Dx | 1201 | CDL | C11-CA5-OA6-CA4 |
| 57 | Dz | 501 | CDL | C51-CB5-OB6-CB4 |
| 57 | Ed | 205 | CDL | C11-CA5-OA6-CA4 |
| 59 | DA | 708 | 3PE | C22-C21-O21-C2 |
| 59 | DG | 205 | 3PE | C22-C21-O21-C2 |
| 59 | Dd | 703 | 3PE | C22-C21-O21-C2 |
| 59 | DS | 403 | 3PE | C2-C3-O31-C31 |
| 57 | DJ | 302 | CDL | C60-C61-C62-C63 |
| 57 | DD | 703 | CDL | C75-C76-C77-C78 |
| 57 | DG | 201 | CDL | C12-C13-C14-C15 |
| 57 | DN | 501 | CDL | C13-C14-C15-C16 |
| 57 | Dj | 403 | CDL | C13-C14-C15-C16 |
| 57 | Dj | 403 | CDL | C17-C18-C19-C20 |
| 57 | Dj | 404 | CDL | C16-C17-C18-C19 |
| 57 | Dr | 403 | CDL | C11-C12-C13-C14 |
| 57 | Dx | 1203 | CDL | C60-C61-C62-C63 |
| 57 | Eg | 101 | CDL | C16-C17-C18-C19 |
| 57 | El | 903 | CDL | C76-C77-C78-C79 |
| 58 | DX | 306 | PC1 | C3D-C3E-C3F-C3G |
| 59 | Dx | 1206 | 3PE | C3D-C3E-C3F-C3G |
| 57 | DU | 402 | CDL | CA5-C11-C12-C13 |
| 57 | DA | 709 | CDL | C73-C74-C75-C76 |
| 57 | DV | 403 | CDL | C13-C14-C15-C16 |
| 57 | EN | 1202 | CDL | C57-C58-C59-C60 |
| 57 | Dh | 201 | CDL | C38-C39-C40-C41 |
| 57 | Dh | 202 | CDL | C21-C22-C23-C24 |
| 57 | Ds | 402 | CDL | C57-C58-C59-C60 |
| 57 | Dx | 1203 | CDL | C56-C57-C58-C59 |
| 57 | DA | 710 | CDL | O1-C1-CA2-OA2 |
| 57 | DJ | 304 | CDL | C13-C14-C15-C16 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 57 | DY | 301 | CDL | C12-C13-C14-C15 |
| 57 | Dh | 202 | CDL | C37-C38-C39-C40 |
| 57 | Du | 401 | CDL | C36-C37-C38-C39 |
| 57 | Du | 404 | CDL | C80-C81-C82-C83 |
| 57 | DJ | 304 | CDL | C55-C56-C57-C58 |
| 57 | DM | 501 | CDL | C55-C56-C57-C58 |
| 57 | DR | 402 | CDL | C61-C62-C63-C64 |
| 57 | DY | 301 | CDL | C35-C36-C37-C38 |
| 57 | Dg | 201 | CDL | C11-C12-C13-C14 |
| 57 | Dv | 403 | CDL | C54-C55-C56-C57 |
| 57 | Dv | 404 | CDL | C72-C73-C74-C75 |
| 57 | Dj | 401 | CDL | OA9-CA7-OA8-CA6 |
| 57 | Dr | 402 | CDL | OB9-CB7-OB8-CB6 |
| 57 | Du | 401 | CDL | OB9-CB7-OB8-CB6 |
| 57 | Du | 403 | CDL | OA9-CA7-OA8-CA6 |
| 57 | Dv | 404 | CDL | OB9-CB7-OB8-CB6 |
| 57 | Eu | 101 | CDL | OB9-CB7-OB8-CB6 |
| 58 | Dx | 1204 | PC1 | O32-C31-O31-C3 |
| 57 | Dv | 401 | CDL | CA5-C11-C12-C13 |
| 57 | EB | 302 | CDL | CA2-C1-CB2-OB2 |
| 57 | EU | 101 | CDL | CB2-C1-CA2-OA2 |
| 57 | DD | 704 | CDL | C36-C37-C38-C39 |
| 57 | DM | 501 | CDL | C58-C59-C60-C61 |
| 57 | EN | 1201 | CDL | C21-C22-C23-C24 |
| 57 | Di | 701 | CDL | C37-C38-C39-C40 |
| 59 | DX | 304 | 3PE | C3D-C3E-C3F-C3G |
| 59 | Ds | 407 | 3PE | C38-C39-C3A-C3B |
| 57 | DN | 501 | CDL | OA7-CA5-OA6-CA4 |
| 57 | DN | 504 | CDL | OA7-CA5-OA6-CA4 |
| 57 | ED | 604 | CDL | OA7-CA5-OA6-CA4 |
| 57 | EL | 904 | CDL | OA7-CA5-OA6-CA4 |
| 57 | Dd | 705 | CDL | OB7-CB5-OB6-CB4 |
| 57 | Dn | 501 | CDL | OA7-CA5-OA6-CA4 |
| 57 | Dn | 503 | CDL | OB7-CB5-OB6-CB4 |
| 57 | Dn | 507 | CDL | OA7-CA5-OA6-CA4 |
| 57 | Du | 404 | CDL | OA7-CA5-OA6-CA4 |
| 57 | Dv | 403 | CDL | OA7-CA5-OA6-CA4 |
| 57 | Dx | 1201 | CDL | OA7-CA5-OA6-CA4 |
| 57 | Dz | 501 | CDL | OB7-CB5-OB6-CB4 |
| 57 | Ed | 205 | CDL | OA7-CA5-OA6-CA4 |
| 59 | DG | 205 | 3PE | O22-C21-O21-C2 |
| 59 | Dd | 703 | 3PE | O22-C21-O21-C2 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 57 | DI | 701 | CDL | C37-C38-C39-C40 |
| 57 | ED | 601 | CDL | C17-C18-C19-C20 |
| 57 | EL | 901 | CDL | C61-C62-C63-C64 |
| 57 | Di | 701 | CDL | C42-C43-C44-C45 |
| 57 | Dr | 402 | CDL | C57-C58-C59-C60 |
| 57 | Eh | 1601 | CDL | C20-C21-C22-C23 |
| 57 | Ei | 401 | CDL | C12-C13-C14-C15 |
| 57 | El | 901 | CDL | C33-C34-C35-C36 |
| 57 | DG | 201 | CDL | CA4-CA3-OA5-PA1 |
| 57 | EH | 202 | CDL | CA4-CA3-OA5-PA1 |
| 57 | DV | 404 | CDL | OB9-CB7-OB8-CB6 |
| 57 | Dd | 702 | CDL | OB9-CB7-OB8-CB6 |
| 57 | Dm | 501 | CDL | OB9-CB7-OB8-CB6 |
| 57 | Ds | 402 | CDL | OB9-CB7-OB8-CB6 |
| 57 | DH | 201 | CDL | C56-C57-C58-C59 |
| 57 | DJ | 304 | CDL | C17-C18-C19-C20 |
| 57 | DN | 501 | CDL | C36-C37-C38-C39 |
| 57 | DX | 307 | CDL | C14-C15-C16-C17 |
| 57 | EN | 1201 | CDL | C34-C35-C36-C37 |
| 57 | EO | 202 | CDL | C11-C12-C13-C14 |
| 57 | EO | 202 | CDL | C16-C17-C18-C19 |
| 57 | Di | 701 | CDL | C77-C78-C79-C80 |
| 57 | Eg | 101 | CDL | C81-C82-C83-C84 |
| 58 | DC | 605 | PC1 | C29-C2A-C2B-C2C |
| 58 | Dx | 1208 | PC1 | C3D-C3E-C3F-C3G |
| 58 | DI | 702 | PC1 | C11-C12-N-C14 |
| 57 | DZ | 501 | CDL | CB7-C71-C72-C73 |
| 57 | Dz | 501 | CDL | CA5-C11-C12-C13 |
| 57 | DG | 201 | CDL | C56-C57-C58-C59 |
| 57 | DO | 501 | CDL | C32-C33-C34-C35 |
| 57 | DV | 404 | CDL | C12-C13-C14-C15 |
| 57 | EB | 302 | CDL | C34-C35-C36-C37 |
| 57 | EI | 401 | CDL | C61-C62-C63-C64 |
| 57 | EL | 902 | CDL | C20-C21-C22-C23 |
| 57 | Dq | 401 | CDL | C11-C12-C13-C14 |
| 57 | Dx | 1201 | CDL | C77-C78-C79-C80 |
| 57 | Eh | 1601 | CDL | C23-C24-C25-C26 |
| 57 | Ei | 401 | CDL | C61-C62-C63-C64 |
| 59 | EN | 1203 | 3PE | C27-C28-C29-C2A |
| 57 | DM | 501 | CDL | C71-CB7-OB8-CB6 |
| 57 | DU | 401 | CDL | C31-CA7-OA8-CA6 |
| 57 | DU | 403 | CDL | C31-CA7-OA8-CA6 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 57 | EU | 101 | CDL | C71-CB7-OB8-CB6 |
| 57 | Dd | 702 | CDL | C31-CA7-OA8-CA6 |
| 58 | Eo | 204 | PC1 | C32-C31-O31-C3 |
| 59 | DR | 401 | 3PE | C32-C31-O31-C3 |
| 57 | DS | 405 | CDL | C51-CB5-OB6-CB4 |
| 57 | EN | 1201 | CDL | C11-CA5-OA6-CA4 |
| 57 | Dd | 705 | CDL | C51-CB5-OB6-CB4 |
| 57 | Ds | 405 | CDL | C11-CA5-OA6-CA4 |
| 57 | Dx | 1201 | CDL | C51-CB5-OB6-CB4 |
| 58 | DS | 406 | PC1 | C22-C21-O21-C2 |
| 58 | DX | 302 | PC1 | C22-C21-O21-C2 |
| 57 | DC | 601 | CDL | C14-C15-C16-C17 |
| 57 | DS | 402 | CDL | C57-C58-C59-C60 |
| 57 | DV | 401 | CDL | C80-C81-C82-C83 |
| 57 | EB | 304 | CDL | C21-C22-C23-C24 |
| 57 | EK | 201 | CDL | C74-C75-C76-C77 |
| 57 | Dh | 201 | CDL | C56-C57-C58-C59 |
| 57 | Dh | 202 | CDL | C74-C75-C76-C77 |
| 57 | Di | 701 | CDL | C71-C72-C73-C74 |
| 57 | Dv | 403 | CDL | C36-C37-C38-C39 |
| 57 | Dy | 301 | CDL | C35-C36-C37-C38 |
| 58 | DV | 406 | PC1 | C3C-C3D-C3E-C3F |
| 58 | Dv | 407 | PC1 | C3C-C3D-C3E-C3F |
| 59 | DA | 708 | 3PE | C28-C29-C2A-C2B |
| 59 | DS | 403 | 3PE | C37-C38-C39-C3A |
| 60 | Ed | 203 | LPP | C19-C20-C21-C22 |
| 59 | Ds | 401 | 3PE | O32-C31-O31-C3 |
| 57 | DR | 402 | CDL | CA7-C31-C32-C33 |
| 57 | Du | 402 | CDL | C57-C58-C59-C60 |
| 57 | Dv | 404 | CDL | C17-C18-C19-C20 |
| 57 | Eh | 1601 | CDL | C53-C54-C55-C56 |
| 58 | DA | 706 | PC1 | C24-C25-C26-C27 |
| 57 | El | 902 | CDL | C78-C79-C80-C81 |
| 58 | Eo | 204 | PC1 | C3A-C3B-C3C-C3D |
| 59 | Ds | 403 | 3PE | C37-C38-C39-C3A |
| 65 | Ed | 202 | UQ8 | C35-C34-C36-C37 |
| 57 | DD | 704 | CDL | OB9-CB7-OB8-CB6 |
| 57 | DJ | 307 | CDL | OB9-CB7-OB8-CB6 |
| 57 | DU | 401 | CDL | OB9-CB7-OB8-CB6 |
| 58 | Ds | 406 | PC1 | C2B-C2C-C2D-C2E |
| 59 | EO | 203 | 3PE | C36-C37-C38-C39 |
| 57 | DJ | 303 | CDL | OB7-CB5-OB6-CB4 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 57 | DS | 405 | CDL | OA7-CA5-OA6-CA4 |
| 57 | DU | 403 | CDL | OA7-CA5-OA6-CA4 |
| 57 | DV | 403 | CDL | OA7-CA5-OA6-CA4 |
| 57 | DV | 404 | CDL | OA7-CA5-OA6-CA4 |
| 57 | EL | 901 | CDL | OA7-CA5-OA6-CA4 |
| 57 | Da | 705 | CDL | OB7-CB5-OB6-CB4 |
| 58 | Dq | 405 | PC1 | O22-C21-O21-C2 |
| 58 | Dx | 1202 | PC1 | O22-C21-O21-C2 |
| 59 | DC | 606 | 3PE | O22-C21-O21-C2 |
| 59 | EO | 204 | 3PE | O22-C21-O21-C2 |
| 57 | DJ | 303 | CDL | CA5-C11-C12-C13 |
| 57 | DM | 502 | CDL | CB7-C71-C72-C73 |
| 57 | DY | 301 | CDL | CA5-C11-C12-C13 |
| 57 | Dn | 503 | CDL | CA5-C11-C12-C13 |
| 57 | DD | 702 | CDL | C31-CA7-OA8-CA6 |
| 57 | DY | 301 | CDL | C31-CA7-OA8-CA6 |
| 57 | Dq | 404 | CDL | C71-CB7-OB8-CB6 |
| 57 | Dz | 501 | CDL | C71-CB7-OB8-CB6 |
| 58 | Da | 707 | PC1 | C32-C31-O31-C3 |
| 59 | DS | 401 | 3PE | C32-C31-O31-C3 |
| 59 | EO | 203 | 3PE | C32-C31-O31-C3 |
| 57 | DI | 701 | CDL | C71-C72-C73-C74 |
| 57 | DO | 501 | CDL | C76-C77-C78-C79 |
| 57 | DU | 401 | CDL | C36-C37-C38-C39 |
| 57 | EB | 304 | CDL | C37-C38-C39-C40 |
| 57 | EN | 1201 | CDL | C53-C54-C55-C56 |
| 57 | Dn | 507 | CDL | C14-C15-C16-C17 |
| 57 | Dz | 501 | CDL | C11-C12-C13-C14 |
| 57 | Ea | 301 | CDL | C74-C75-C76-C77 |
| 57 | El | 901 | CDL | C61-C62-C63-C64 |
| 58 | DB | 702 | PC1 | C32-C33-C34-C35 |
| 57 | DG | 201 | CDL | C53-C54-C55-C56 |
| 57 | EL | 903 | CDL | C83-C84-C85-C86 |
| 57 | EN | 1201 | CDL | C39-C40-C41-C42 |
| 57 | EU | 101 | CDL | C36-C37-C38-C39 |
| 57 | Dd | 704 | CDL | C17-C18-C19-C20 |
| 57 | Dn | 505 | CDL | C34-C35-C36-C37 |
| 57 | Dz | 501 | CDL | C16-C17-C18-C19 |
| 57 | Ek | 201 | CDL | C77-C78-C79-C80 |
| 59 | EL | 905 | 3PE | C37-C38-C39-C3A |
| 57 | DU | 401 | CDL | OA9-CA7-OA8-CA6 |
| 57 | EL | 902 | CDL | C81-C82-C83-C84 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 57 | Dn | 501 | CDL | C57-C58-C59-C60 |
| 57 | Eh | 1601 | CDL | C81-C82-C83-C84 |
| 57 | En | 1201 | CDL | C82-C83-C84-C85 |
| 58 | DC | 602 | PC1 | C3D-C3E-C3F-C3G |
| 59 | DC | 606 | 3PE | C3E-C3F-C3G-C3H |
| 57 | DC | 601 | CDL | CA5-C11-C12-C13 |
| 57 | DG | 201 | CDL | CA5-C11-C12-C13 |
| 57 | DD | 703 | CDL | C17-C18-C19-C20 |
| 57 | DJ | 302 | CDL | C13-C14-C15-C16 |
| 57 | DO | 501 | CDL | C40-C41-C42-C43 |
| 57 | DR | 403 | CDL | C41-C42-C43-C44 |
| 57 | Dj | 401 | CDL | C53-C54-C55-C56 |
| 57 | Dj | 405 | CDL | C11-C12-C13-C14 |
| 57 | Dn | 507 | CDL | C36-C37-C38-C39 |
| 57 | Do | 501 | CDL | C40-C41-C42-C43 |
| 57 | Dq | 401 | CDL | C39-C40-C41-C42 |
| 57 | Dr | 402 | CDL | C75-C76-C77-C78 |
| 57 | Dx | 1201 | CDL | C20-C21-C22-C23 |
| 57 | Eg | 101 | CDL | C11-C12-C13-C14 |
| 57 | Eh | 1601 | CDL | C55-C56-C57-C58 |
| 57 | El | 901 | CDL | C39-C40-C41-C42 |
| 57 | En | 1201 | CDL | C39-C40-C41-C42 |
| 58 | Di | 702 | PC1 | C3A-C3B-C3C-C3D |
| 59 | Dr | 404 | 3PE | C3E-C3F-C3G-C3H |
| 59 | Ds | 407 | 3PE | C35-C36-C37-C38 |
| 57 | DG | 202 | CDL | CA4-CA6-OA8-CA7 |
| 57 | DA | 710 | CDL | C12-C13-C14-C15 |
| 57 | DV | 404 | CDL | C13-C14-C15-C16 |
| 57 | Dj | 402 | CDL | C58-C59-C60-C61 |
| 57 | Dn | 503 | CDL | C56-C57-C58-C59 |
| 57 | Do | 501 | CDL | C32-C33-C34-C35 |
| 57 | Do | 501 | CDL | C77-C78-C79-C80 |
| 59 | EO | 203 | 3PE | C3C-C3D-C3E-C3F |
| 59 | Eo | 202 | 3PE | C3C-C3D-C3E-C3F |
| 57 | Dv | 401 | CDL | C71-CB7-OB8-CB6 |
| 65 | EN | 1204 | UQ8 | C19-C21-C22-C23 |
| 57 | DA | 709 | CDL | C57-C58-C59-C60 |
| 57 | DD | 703 | CDL | C63-C64-C65-C66 |
| 57 | DN | 504 | CDL | C36-C37-C38-C39 |
| 57 | DR | 403 | CDL | C12-C13-C14-C15 |
| 57 | EL | 901 | CDL | C42-C43-C44-C45 |
| 57 | Dd | 702 | CDL | C35-C36-C37-C38 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 57 | Dr | 403 | CDL | C41-C42-C43-C44 |
| 57 | Ds | 405 | CDL | C38-C39-C40-C41 |
| 57 | Dv | 402 | CDL | C20-C21-C22-C23 |
| 57 | Dv | 404 | CDL | C82-C83-C84-C85 |
| 57 | Ea | 301 | CDL | C81-C82-C83-C84 |
| 57 | El | 902 | CDL | C75-C76-C77-C78 |
| 58 | DS | 407 | PC1 | C2B-C2C-C2D-C2E |
| 58 | EO | 206 | PC1 | C3A-C3B-C3C-C3D |
| 58 | Dj | 406 | PC1 | C22-C23-C24-C25 |
| 59 | DS | 403 | 3PE | C39-C3A-C3B-C3C |
| 59 | DX | 304 | 3PE | C26-C27-C28-C29 |
| 57 | Dz | 501 | CDL | CB7-C71-C72-C73 |
| 57 | DC | 601 | CDL | C51-CB5-OB6-CB4 |
| 57 | DJ | 303 | CDL | C51-CB5-OB6-CB4 |
| 57 | DJ | 307 | CDL | C11-CA5-OA6-CA4 |
| 57 | DQ | 1501 | CDL | C51-CB5-OB6-CB4 |
| 57 | DQ | 1502 | CDL | C51-CB5-OB6-CB4 |
| 57 | DS | 405 | CDL | C11-CA5-OA6-CA4 |
| 57 | DU | 402 | CDL | C51-CB5-OB6-CB4 |
| 57 | DV | 404 | CDL | C11-CA5-OA6-CA4 |
| 57 | DX | 307 | CDL | C11-CA5-OA6-CA4 |
| 57 | ED | 604 | CDL | C51-CB5-OB6-CB4 |
| 57 | EL | 901 | CDL | C11-CA5-OA6-CA4 |
| 57 | Da | 705 | CDL | C51-CB5-OB6-CB4 |
| 57 | Dg | 202 | CDL | C11-CA5-OA6-CA4 |
| 57 | Dj | 405 | CDL | C51-CB5-OB6-CB4 |
| 57 | Ds | 405 | CDL | C51-CB5-OB6-CB4 |
| 57 | Du | 401 | CDL | C11-CA5-OA6-CA4 |
| 57 | Du | 403 | CDL | C11-CA5-OA6-CA4 |
| 57 | Dv | 404 | CDL | C11-CA5-OA6-CA4 |
| 57 | Dz | 501 | CDL | C11-CA5-OA6-CA4 |
| 57 | Eh | 1601 | CDL | C51-CB5-OB6-CB4 |
| 57 | El | 901 | CDL | C11-CA5-OA6-CA4 |
| 57 | Ep | 701 | CDL | C11-CA5-OA6-CA4 |
| 58 | Dq | 405 | PC1 | C22-C21-O21-C2 |
| 58 | Dx | 1202 | PC1 | C22-C21-O21-C2 |
| 58 | Ef | 1001 | PC1 | C22-C21-O21-C2 |
| 59 | DC | 606 | 3PE | C22-C21-O21-C2 |
| 59 | DX | 304 | 3PE | C22-C21-O21-C2 |
| 59 | EO | 204 | 3PE | C22-C21-O21-C2 |
| 59 | Dx | 1205 | 3PE | C22-C21-O21-C2 |
| 59 | Dx | 1206 | 3PE | C22-C21-O21-C2 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 57 | DX | 301 | CDL | OB5-CB3-CB4-OB6 |
| 57 | Dj | 403 | CDL | OB5-CB3-CB4-OB6 |
| 58 | DS | 407 | PC1 | O11-C1-C2-O21 |
| 58 | Dq | 405 | PC1 | O11-C1-C2-O21 |
| 57 | DV | 402 | CDL | C75-C76-C77-C78 |
| 57 | DV | 404 | CDL | C82-C83-C84-C85 |
| 57 | DZ | 501 | CDL | C16-C17-C18-C19 |
| 57 | ED | 604 | CDL | C51-C52-C53-C54 |
| 57 | EL | 903 | CDL | C38-C39-C40-C41 |
| 57 | Da | 709 | CDL | C76-C77-C78-C79 |
| 57 | Dn | 502 | CDL | C12-C13-C14-C15 |
| 57 | Dq | 404 | CDL | C51-C52-C53-C54 |
| 57 | Ek | 201 | CDL | C53-C54-C55-C56 |
| 57 | El | 901 | CDL | C37-C38-C39-C40 |
| 57 | Eu | 101 | CDL | C36-C37-C38-C39 |
| 59 | DA | 708 | 3PE | C25-C26-C27-C28 |
| 59 | EO | 203 | 3PE | C27-C28-C29-C2A |
| 59 | Dx | 1207 | 3PE | C27-C28-C29-C2A |
| 57 | DM | 501 | CDL | OB9-CB7-OB8-CB6 |
| 57 | Dg | 201 | CDL | C19-C20-C21-C22 |
| 57 | Dj | 404 | CDL | C11-C12-C13-C14 |
| 57 | Ds | 402 | CDL | C61-C62-C63-C64 |
| 57 | Dv | 403 | CDL | C81-C82-C83-C84 |
| 59 | El | 905 | 3PE | C26-C27-C28-C29 |
| 57 | Dh | 202 | CDL | O1-C1-CA2-OA2 |
| 57 | DJ | 307 | CDL | OA7-CA5-OA6-CA4 |
| 57 | DS | 405 | CDL | OB7-CB5-OB6-CB4 |
| 57 | DX | 307 | CDL | OB7-CB5-OB6-CB4 |
| 57 | ED | 604 | CDL | OB7-CB5-OB6-CB4 |
| 57 | EN | 1201 | CDL | OA7-CA5-OA6-CA4 |
| 57 | Dg | 202 | CDL | OA7-CA5-OA6-CA4 |
| 57 | Dj | 405 | CDL | OB7-CB5-OB6-CB4 |
| 57 | Du | 401 | CDL | OA7-CA5-OA6-CA4 |
| 57 | Du | 403 | CDL | OA7-CA5-OA6-CA4 |
| 57 | Dx | 1201 | CDL | OB7-CB5-OB6-CB4 |
| 57 | Dz | 501 | CDL | OA7-CA5-OA6-CA4 |
| 57 | El | 901 | CDL | OA7-CA5-OA6-CA4 |
| 58 | DS | 406 | PC1 | O22-C21-O21-C2 |
| 58 | DX | 302 | PC1 | O22-C21-O21-C2 |
| 58 | Ef | 1001 | PC1 | O22-C21-O21-C2 |
| 59 | DA | 708 | 3PE | O22-C21-O21-C2 |
| 59 | DX | 304 | 3PE | O22-C21-O21-C2 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 57 | Dg | 202 | CDL | CB7-C71-C72-C73 |
| 59 | Em | 901 | 3PE | C21-C22-C23-C24 |
| 57 | Ds | 405 | CDL | C62-C63-C64-C65 |
| 57 | Dx | 1203 | CDL | C17-C18-C19-C20 |
| 57 | Eg | 101 | CDL | C60-C61-C62-C63 |
| 57 | En | 1202 | CDL | C34-C35-C36-C37 |
| 59 | EO | 203 | 3PE | C2C-C2D-C2E-C2F |
| 57 | DA | 710 | CDL | OA6-CA4-CA6-OA8 |
| 57 | DM | 501 | CDL | OA6-CA4-CA6-OA8 |
| 57 | DX | 307 | CDL | OA6-CA4-CA6-OA8 |
| 57 | EL | 901 | CDL | OB6-CB4-CB6-OB8 |
| 57 | Da | 709 | CDL | OA6-CA4-CA6-OA8 |
| 57 | Dj | 401 | CDL | OA6-CA4-CA6-OA8 |
| 57 | Dy | 301 | CDL | OB6-CB4-CB6-OB8 |
| 57 | En | 1201 | CDL | OA6-CA4-CA6-OA8 |
| 58 | DV | 407 | PC1 | O21-C2-C3-O31 |
| 58 | EO | 206 | PC1 | O21-C2-C3-O31 |
| 58 | Ef | 1001 | PC1 | O21-C2-C3-O31 |
| 59 | DA | 708 | 3PE | O21-C2-C3-O31 |
| 57 | DO | 501 | CDL | C15-C16-C17-C18 |
| 57 | DQ | 1502 | CDL | C51-C52-C53-C54 |
| 57 | DS | 402 | CDL | C61-C62-C63-C64 |
| 57 | DV | 402 | CDL | C20-C21-C22-C23 |
| 57 | DY | 301 | CDL | C82-C83-C84-C85 |
| 57 | ED | 604 | CDL | C61-C62-C63-C64 |
| 57 | Dv | 401 | CDL | C39-C40-C41-C42 |
| 57 | Dv | 404 | CDL | C12-C13-C14-C15 |
| 57 | En | 1201 | CDL | C54-C55-C56-C57 |
| 58 | EO | 207 | PC1 | C3C-C3D-C3E-C3F |
| 58 | Db | 702 | PC1 | C32-C33-C34-C35 |
| 59 | DG | 205 | 3PE | C3E-C3F-C3G-C3H |
| 59 | Dx | 1206 | 3PE | C26-C27-C28-C29 |
| 59 | Eo | 202 | 3PE | C2C-C2D-C2E-C2F |
| 59 | DR | 401 | 3PE | O32-C31-O31-C3 |
| 58 | Di | 702 | PC1 | C11-C12-N-C14 |
| 57 | DD | 704 | CDL | C62-C63-C64-C65 |
| 57 | DJ | 304 | CDL | C60-C61-C62-C63 |
| 57 | DV | 401 | CDL | C57-C58-C59-C60 |
| 57 | DV | 402 | CDL | C37-C38-C39-C40 |
| 57 | DV | 404 | CDL | C17-C18-C19-C20 |
| 57 | DY | 301 | CDL | C56-C57-C58-C59 |
| 57 | EK | 201 | CDL | C33-C34-C35-C36 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 57 | Dj | 405 | CDL | C37-C38-C39-C40 |
| 57 | Dq | 401 | CDL | C53-C54-C55-C56 |
| 57 | Dq | 403 | CDL | C53-C54-C55-C56 |
| 57 | Ds | 402 | CDL | C16-C17-C18-C19 |
| 57 | Dx | 1201 | CDL | C43-C44-C45-C46 |
| 57 | Dy | 301 | CDL | C56-C57-C58-C59 |
| 57 | Eh | 1601 | CDL | C57-C58-C59-C60 |
| 57 | El | 902 | CDL | C12-C13-C14-C15 |
| 59 | EM | 901 | 3PE | C26-C27-C28-C29 |
| 59 | EM | 901 | 3PE | C2A-C2B-C2C-C2D |
| 59 | Dr | 404 | 3PE | C22-C23-C24-C25 |
| 59 | Eo | 202 | 3PE | C27-C28-C29-C2A |
| 60 | Dn | 504 | LPP | C31-C32-C33-C34 |
| 57 | DD | 702 | CDL | CA5-C11-C12-C13 |
| 57 | DR | 403 | CDL | CA7-C31-C32-C33 |
| 57 | DA | 710 | CDL | C40-C41-C42-C43 |
| 57 | DG | 201 | CDL | C63-C64-C65-C66 |
| 57 | DJ | 307 | CDL | C51-C52-C53-C54 |
| 57 | DM | 502 | CDL | C14-C15-C16-C17 |
| 57 | EB | 304 | CDL | C63-C64-C65-C66 |
| 57 | EL | 901 | CDL | C33-C34-C35-C36 |
| 57 | EO | 202 | CDL | C31-C32-C33-C34 |
| 57 | Dd | 704 | CDL | C11-C12-C13-C14 |
| 57 | Dy | 301 | CDL | C82-C83-C84-C85 |
| 60 | DN | 502 | LPP | C35-C36-C37-C38 |
| 60 | EI | 402 | LPP | C15-C16-C17-C18 |
| 60 | EI | 402 | LPP | C20-C21-C22-C23 |
| 57 | DU | 403 | CDL | C36-C37-C38-C39 |
| 57 | Dd | 706 | CDL | C75-C76-C77-C78 |
| 57 | Ek | 201 | CDL | C33-C34-C35-C36 |
| 58 | DC | 608 | PC1 | C2C-C2D-C2E-C2F |
| 58 | Dx | 1202 | PC1 | C2B-C2C-C2D-C2E |
| 57 | DJ | 304 | CDL | C23-C24-C25-C26 |
| 57 | DS | 405 | CDL | C62-C63-C64-C65 |
| 57 | DV | 403 | CDL | C36-C37-C38-C39 |
| 57 | DX | 307 | CDL | C43-C44-C45-C46 |
| 57 | EA | 301 | CDL | C81-C82-C83-C84 |
| 57 | EN | 1201 | CDL | C17-C18-C19-C20 |
| 57 | Dd | 705 | CDL | C62-C63-C64-C65 |
| 57 | Di | 701 | CDL | C74-C75-C76-C77 |
| 57 | Ed | 205 | CDL | C16-C17-C18-C19 |
| 57 | Ed | 205 | CDL | C61-C62-C63-C64 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 57 | Ek | 201 | CDL | C74-C75-C76-C77 |
| 58 | DC | 603 | PC1 | C35-C36-C37-C38 |
| 58 | DI | 702 | PC1 | C2C-C2D-C2E-C2F |
| 58 | EO | 206 | PC1 | C33-C34-C35-C36 |
| 58 | Da | 707 | PC1 | C3E-C3F-C3G-C3H |
| 57 | DJ | 304 | CDL | C72-C73-C74-C75 |
| 57 | DJ | 307 | CDL | C77-C78-C79-C80 |
| 57 | DN | 505 | CDL | C12-C13-C14-C15 |
| 57 | Dr | 402 | CDL | C60-C61-C62-C63 |
| 57 | Dx | 1203 | CDL | C32-C33-C34-C35 |
| 57 | El | 903 | CDL | C20-C21-C22-C23 |
| 58 | Db | 702 | PC1 | C27-C28-C29-C2A |
| 58 | Eo | 201 | PC1 | C3B-C3C-C3D-C3E |
| 59 | EN | 1203 | 3PE | C35-C36-C37-C38 |
| 60 | DN | 502 | LPP | C31-C32-C33-C34 |
| 57 | DU | 403 | CDL | OA9-CA7-OA8-CA6 |
| 57 | Dd | 702 | CDL | OA9-CA7-OA8-CA6 |
| 57 | Dq | 404 | CDL | OB9-CB7-OB8-CB6 |
| 58 | Eo | 204 | PC1 | O32-C31-O31-C3 |
| 57 | DC | 601 | CDL | OB7-CB5-OB6-CB4 |
| 57 | DU | 402 | CDL | OB7-CB5-OB6-CB4 |
| 57 | Ds | 405 | CDL | OA7-CA5-OA6-CA4 |
| 57 | Ds | 405 | CDL | OB7-CB5-OB6-CB4 |
| 57 | Dv | 404 | CDL | OA7-CA5-OA6-CA4 |
| 57 | Ep | 701 | CDL | OA7-CA5-OA6-CA4 |
| 59 | Dx | 1206 | 3PE | O22-C21-O21-C2 |
| 57 | Dd | 702 | CDL | C51-CB5-OB6-CB4 |
| 57 | Dd | 706 | CDL | C51-CB5-OB6-CB4 |
| 59 | Dj | 407 | 3PE | C22-C21-O21-C2 |
| 57 | DC | 601 | CDL | C33-C34-C35-C36 |
| 57 | DN | 501 | CDL | C41-C42-C43-C44 |
| 57 | DQ | 1504 | CDL | C53-C54-C55-C56 |
| 57 | EH | 202 | CDL | C80-C81-C82-C83 |
| 57 | Dj | 405 | CDL | C41-C42-C43-C44 |
| 57 | Dj | 408 | CDL | C82-C83-C84-C85 |
| 57 | Dv | 402 | CDL | C37-C38-C39-C40 |
| 57 | Dv | 403 | CDL | C62-C63-C64-C65 |
| 57 | Dx | 1201 | CDL | C11-C12-C13-C14 |
| 57 | El | 903 | CDL | C56-C57-C58-C59 |
| 58 | EO | 205 | PC1 | C3C-C3D-C3E-C3F |
| 58 | Da | 706 | PC1 | C24-C25-C26-C27 |
| 58 | Di | 702 | PC1 | C2C-C2D-C2E-C2F |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 59 | Ds | 403 | 3PE | C39-C3A-C3B-C3C |
| 57 | DA | 709 | CDL | CA3-OA5-PA1-OA2 |
| 57 | DJ | 303 | CDL | CA3-OA5-PA1-OA2 |
| 57 | DJ | 303 | CDL | CB3-OB5-PB2-OB2 |
| 57 | DU | 404 | CDL | CB2-OB2-PB2-OB5 |
| 57 | DV | 402 | CDL | CA3-OA5-PA1-OA2 |
| 57 | DV | 404 | CDL | CB2-OB2-PB2-OB5 |
| 57 | DX | 301 | CDL | CA3-OA5-PA1-OA2 |
| 57 | DX | 301 | CDL | CB3-OB5-PB2-OB2 |
| 57 | DX | 307 | CDL | CA2-OA2-PA1-OA5 |
| 57 | EA | 301 | CDL | CB3-OB5-PB2-OB2 |
| 57 | EH | 202 | CDL | CB2-OB2-PB2-OB5 |
| 57 | Da | 705 | CDL | CB3-OB5-PB2-OB2 |
| 57 | Dq | 402 | CDL | CB3-OB5-PB2-OB2 |
| 57 | Dq | 403 | CDL | CB3-OB5-PB2-OB2 |
| 57 | Ds | 405 | CDL | CB3-OB5-PB2-OB2 |
| 57 | Eg | 101 | CDL | CA3-OA5-PA1-OA2 |
| 58 | DA | 706 | PC1 | C11-O13-P-O11 |
| 58 | DS | 407 | PC1 | C11-O13-P-O11 |
| 58 | EO | 206 | PC1 | C1-O11-P-O13 |
| 58 | Da | 706 | PC1 | C11-O13-P-O11 |
| 58 | Dx | 1202 | PC1 | C11-O13-P-O11 |
| 58 | Eb | 301 | PC1 | C1-O11-P-O13 |
| 59 | EL | 905 | 3PE | C11-O13-P-O11 |
| 59 | Dr | 401 | 3PE | C11-O13-P-O11 |
| 59 | Dx | 1207 | 3PE | C11-O13-P-O11 |
| 59 | El | 905 | 3PE | C11-O13-P-O11 |
| 57 | DJ | 307 | CDL | C82-C83-C84-C85 |
| 57 | DU | 402 | CDL | C11-C12-C13-C14 |
| 57 | DV | 401 | CDL | C39-C40-C41-C42 |
| 57 | ED | 601 | CDL | C56-C57-C58-C59 |
| 57 | ED | 604 | CDL | C16-C17-C18-C19 |
| 57 | Dc | 601 | CDL | C12-C13-C14-C15 |
| 57 | Dj | 405 | CDL | C20-C21-C22-C23 |
| 57 | Ed | 204 | CDL | C76-C77-C78-C79 |
| 58 | EO | 206 | PC1 | C2D-C2E-C2F-C2G |
| 57 | DG | 201 | CDL | CB4-CB3-OB5-PB2 |
| 57 | DN | 501 | CDL | CA4-CA3-OA5-PA1 |
| 57 | DU | 401 | CDL | C1-CA2-OA2-PA1 |
| 57 | EI | 401 | CDL | CB4-CB3-OB5-PB2 |
| 57 | Da | 705 | CDL | CB4-CB3-OB5-PB2 |
| 57 | Dv | 404 | CDL | CB4-CB3-OB5-PB2 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 58 | DA | 706 | PC1 | C2-C1-O11-P |
| 57 | DJ | 304 | CDL | C79-C80-C81-C82 |
| 57 | DJ | 305 | CDL | C41-C42-C43-C44 |
| 57 | DN | 505 | CDL | C80-C81-C82-C83 |
| 57 | DV | 403 | CDL | C81-C82-C83-C84 |
| 57 | Dx | 1201 | CDL | C74-C75-C76-C77 |
| 58 | DJ | 306 | PC1 | C22-C23-C24-C25 |
| 60 | DN | 502 | LPP | C37-C38-C39-C40 |
| 57 | Dj | 402 | CDL | C71-CB7-OB8-CB6 |
| 57 | DA | 705 | CDL | OB5-CB3-CB4-CB6 |
| 57 | DJ | 307 | CDL | OB5-CB3-CB4-CB6 |
| 57 | DQ | 1504 | CDL | OA5-CA3-CA4-CA6 |
| 57 | DS | 402 | CDL | OB5-CB3-CB4-CB6 |
| 57 | DU | 401 | CDL | OB5-CB3-CB4-CB6 |
| 57 | EB | 302 | CDL | OB5-CB3-CB4-CB6 |
| 57 | ED | 604 | CDL | OB5-CB3-CB4-CB6 |
| 57 | EH | 202 | CDL | OB5-CB3-CB4-CB6 |
| 57 | EN | 1202 | CDL | OA5-CA3-CA4-CA6 |
| 57 | Dc | 601 | CDL | OB5-CB3-CB4-CB6 |
| 57 | Di | 701 | CDL | OB5-CB3-CB4-CB6 |
| 57 | Dj | 405 | CDL | OB5-CB3-CB4-CB6 |
| 57 | Dm | 501 | CDL | OA5-CA3-CA4-CA6 |
| 57 | Do | 501 | CDL | OA5-CA3-CA4-CA6 |
| 57 | Dq | 402 | CDL | OB5-CB3-CB4-CB6 |
| 57 | Ds | 402 | CDL | OB5-CB3-CB4-CB6 |
| 57 | Dx | 1203 | CDL | OB5-CB3-CB4-CB6 |
| 57 | Ep | 701 | CDL | OA5-CA3-CA4-CA6 |
| 58 | Dc | 603 | PC1 | O11-C1-C2-C3 |
| 58 | Di | 702 | PC1 | O11-C1-C2-C3 |
| 59 | Dj | 407 | 3PE | O11-C1-C2-C3 |
| 59 | Dr | 404 | 3PE | O11-C1-C2-C3 |
| 57 | DJ | 303 | CDL | C33-C34-C35-C36 |
| 57 | Dc | 601 | CDL | C33-C34-C35-C36 |
| 57 | Dg | 201 | CDL | C44-C45-C46-C47 |
| 57 | Do | 501 | CDL | C15-C16-C17-C18 |
| 57 | Dv | 402 | CDL | C76-C77-C78-C79 |
| 57 | Eu | 101 | CDL | C17-C18-C19-C20 |
| 59 | El | 905 | 3PE | C3E-C3F-C3G-C3H |
| 57 | Dj | 404 | CDL | C31-C32-C33-C34 |
| 57 | Du | 402 | CDL | C21-C22-C23-C24 |
| 57 | Du | 403 | CDL | C37-C38-C39-C40 |
| 57 | Dv | 401 | CDL | C21-C22-C23-C24 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 58 | DV | 405 | PC1 | C3B-C3C-C3D-C3E |
| 57 | EU | 101 | CDL | OB9-CB7-OB8-CB6 |
| 57 | DN | 505 | CDL | C55-C56-C57-C58 |
| 57 | DS | 405 | CDL | C53-C54-C55-C56 |
| 57 | DX | 301 | CDL | C74-C75-C76-C77 |
| 57 | EU | 101 | CDL | C17-C18-C19-C20 |
| 57 | Da | 709 | CDL | C16-C17-C18-C19 |
| 57 | Dd | 704 | CDL | C63-C64-C65-C66 |
| 57 | Dh | 202 | CDL | C63-C64-C65-C66 |
| 57 | Dq | 401 | CDL | C17-C18-C19-C20 |
| 57 | Dq | 404 | CDL | C38-C39-C40-C41 |
| 57 | Dr | 402 | CDL | C20-C21-C22-C23 |
| 57 | Eg | 101 | CDL | C79-C80-C81-C82 |
| 58 | DX | 302 | PC1 | C33-C34-C35-C36 |
| 57 | DQ | 1501 | CDL | C53-C54-C55-C56 |
| 57 | DQ | 1504 | CDL | C40-C41-C42-C43 |
| 57 | DX | 301 | CDL | C35-C36-C37-C38 |
| 57 | Dg | 202 | CDL | C35-C36-C37-C38 |
| 57 | Dq | 402 | CDL | C17-C18-C19-C20 |
| 57 | Du | 403 | CDL | C12-C13-C14-C15 |
| 57 | El | 903 | CDL | C61-C62-C63-C64 |
| 58 | Dx | 1204 | PC1 | C25-C26-C27-C28 |
| 59 | DX | 305 | 3PE | C27-C28-C29-C2A |
| 59 | Dc | 606 | 3PE | C34-C35-C36-C37 |
| 57 | EU | 101 | CDL | CA5-C11-C12-C13 |
| 57 | DA | 709 | CDL | C35-C36-C37-C38 |
| 57 | DC | 601 | CDL | C40-C41-C42-C43 |
| 57 | DV | 402 | CDL | C57-C58-C59-C60 |
| 57 | Dg | 201 | CDL | C63-C64-C65-C66 |
| 57 | Ds | 405 | CDL | C53-C54-C55-C56 |
| 57 | El | 902 | CDL | C63-C64-C65-C66 |
| 57 | En | 1201 | CDL | C17-C18-C19-C20 |
| 58 | Dc | 607 | PC1 | C2C-C2D-C2E-C2F |
| 57 | DV | 401 | CDL | C71-CB7-OB8-CB6 |
| 58 | EO | 207 | PC1 | C32-C31-O31-C3 |
| 57 | DR | 403 | CDL | CA2-C1-CB2-OB2 |
| 57 | DS | 402 | CDL | CA2-C1-CB2-OB2 |
| 57 | EB | 304 | CDL | CB2-C1-CA2-OA2 |
| 57 | Dd | 706 | CDL | CB2-C1-CA2-OA2 |
| 57 | Du | 402 | CDL | CA2-C1-CB2-OB2 |
| 57 | Dv | 403 | CDL | CA2-C1-CB2-OB2 |
| 57 | Eg | 101 | CDL | CB2-C1-CA2-OA2 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 59 | Dx | 1205 | 3PE | O22-C21-O21-C2 |
| 57 | DD | 703 | CDL | C11-C12-C13-C14 |
| 57 | DD | 703 | CDL | C82-C83-C84-C85 |
| 57 | Dn | 505 | CDL | C20-C21-C22-C23 |
| 57 | Dv | 402 | CDL | C79-C80-C81-C82 |
| 59 | Em | 901 | 3PE | C2A-C2B-C2C-C2D |
| 60 | DA | 711 | LPP | C40-C41-C42-C43 |
| 57 | DG | 201 | CDL | C31-C32-C33-C34 |
| 57 | DN | 504 | CDL | C43-C44-C45-C46 |
| 57 | DZ | 501 | CDL | C38-C39-C40-C41 |
| 57 | EK | 201 | CDL | C77-C78-C79-C80 |
| 57 | EL | 904 | CDL | C56-C57-C58-C59 |
| 57 | Dd | 704 | CDL | C82-C83-C84-C85 |
| 57 | Dv | 401 | CDL | C57-C58-C59-C60 |
| 57 | Dx | 1203 | CDL | C35-C36-C37-C38 |
| 57 | En | 1202 | CDL | C37-C38-C39-C40 |
| 58 | DG | 203 | PC1 | C28-C29-C2A-C2B |
| 58 | DQ | 1503 | PC1 | C34-C35-C36-C37 |
| 58 | Dq | 405 | PC1 | C34-C35-C36-C37 |
| 58 | Eo | 201 | PC1 | C25-C26-C27-C28 |
| 57 | Dd | 702 | CDL | CA5-C11-C12-C13 |
| 57 | Du | 401 | CDL | CA5-C11-C12-C13 |
| 57 | DD | 702 | CDL | OA9-CA7-OA8-CA6 |
| 57 | Dz | 501 | CDL | OB9-CB7-OB8-CB6 |
| 58 | Da | 707 | PC1 | O32-C31-O31-C3 |
| 57 | DN | 501 | CDL | C14-C15-C16-C17 |
| 57 | DV | 401 | CDL | C21-C22-C23-C24 |
| 57 | Dn | 501 | CDL | C35-C36-C37-C38 |
| 57 | Dn | 507 | CDL | C82-C83-C84-C85 |
| 57 | Ed | 204 | CDL | C80-C81-C82-C83 |
| 57 | Eg | 101 | CDL | C42-C43-C44-C45 |
| 58 | Dx | 1208 | PC1 | C24-C25-C26-C27 |
| 58 | Eo | 204 | PC1 | C33-C34-C35-C36 |
| 59 | EL | 905 | 3PE | C3E-C3F-C3G-C3H |
| 59 | Dx | 1207 | 3PE | C39-C3A-C3B-C3C |
| 60 | Dn | 504 | LPP | C37-C38-C39-C40 |
| 57 | DA | 709 | CDL | CA3-CA4-CA6-OA8 |
| 57 | DA | 710 | CDL | CA3-CA4-CA6-OA8 |
| 57 | DC | 601 | CDL | CA3-CA4-CA6-OA8 |
| 57 | DD | 702 | CDL | CB3-CB4-CB6-OB8 |
| 57 | DH | 201 | CDL | CA3-CA4-CA6-OA8 |
| 57 | DJ | 303 | CDL | CB3-CB4-CB6-OB8 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 57 | DM | 501 | CDL | CA3-CA4-CA6-OA8 |
| 57 | DR | 402 | CDL | CB3-CB4-CB6-OB8 |
| 57 | DS | 402 | CDL | CA3-CA4-CA6-OA8 |
| 57 | DU | 401 | CDL | C11-C12-C13-C14 |
| 57 | DU | 401 | CDL | CB3-CB4-CB6-OB8 |
| 57 | DV | 403 | CDL | C23-C24-C25-C26 |
| 57 | DX | 301 | CDL | C38-C39-C40-C41 |
| 57 | EB | 304 | CDL | CB3-CB4-CB6-OB8 |
| 57 | ED | 601 | CDL | CB3-CB4-CB6-OB8 |
| 57 | EH | 201 | CDL | CB3-CB4-CB6-OB8 |
| 57 | EK | 201 | CDL | CA3-CA4-CA6-OA8 |
| 57 | EK | 201 | CDL | C53-C54-C55-C56 |
| 57 | EL | 901 | CDL | C82-C83-C84-C85 |
| 57 | EL | 903 | CDL | C63-C64-C65-C66 |
| 57 | Da | 705 | CDL | CB3-CB4-CB6-OB8 |
| 57 | Da | 709 | CDL | CA3-CA4-CA6-OA8 |
| 57 | Dc | 601 | CDL | CA3-CA4-CA6-OA8 |
| 57 | Dc | 601 | CDL | C40-C41-C42-C43 |
| 57 | Dd | 702 | CDL | CA3-CA4-CA6-OA8 |
| 57 | Dd | 704 | CDL | CB3-CB4-CB6-OB8 |
| 57 | Dd | 706 | CDL | CB3-CB4-CB6-OB8 |
| 57 | Dg | 201 | CDL | CB3-CB4-CB6-OB8 |
| 57 | Dh | 202 | CDL | CB3-CB4-CB6-OB8 |
| 57 | Dj | 401 | CDL | CA3-CA4-CA6-OA8 |
| 57 | Dj | 408 | CDL | CA3-CA4-CA6-OA8 |
| 57 | Dr | 403 | CDL | CB3-CB4-CB6-OB8 |
| 57 | Ds | 405 | CDL | C55-C56-C57-C58 |
| 57 | Du | 402 | CDL | CA3-CA4-CA6-OA8 |
| 57 | Du | 403 | CDL | CB3-CB4-CB6-OB8 |
| 57 | Dv | 404 | CDL | CA3-CA4-CA6-OA8 |
| 57 | Dx | 1201 | CDL | CA3-CA4-CA6-OA8 |
| 57 | El | 902 | CDL | CA3-CA4-CA6-OA8 |
| 57 | El | 903 | CDL | CA3-CA4-CA6-OA8 |
| 57 | Ep | 701 | CDL | CA3-CA4-CA6-OA8 |
| 57 | Eu | 101 | CDL | CB3-CB4-CB6-OB8 |
| 58 | DC | 608 | PC1 | C1-C2-C3-O31 |
| 58 | DI | 702 | PC1 | C3A-C3B-C3C-C3D |
| 58 | DS | 406 | PC1 | C1-C2-C3-O31 |
| 58 | DV | 406 | PC1 | C2D-C2E-C2F-C2G |
| 58 | DV | 407 | PC1 | C1-C2-C3-O31 |
| 58 | DX | 302 | PC1 | C1-C2-C3-O31 |
| 58 | DY | 302 | PC1 | C1-C2-C3-O31 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 58 | EO | 207 | PC1 | C1-C2-C3-O31 |
| 58 | Dc | 605 | PC1 | C1-C2-C3-O31 |
| 58 | Ds | 406 | PC1 | C1-C2-C3-O31 |
| 58 | Dy | 302 | PC1 | C1-C2-C3-O31 |
| 58 | El | 904 | PC1 | C3C-C3D-C3E-C3F |
| 59 | DC | 607 | 3PE | C34-C35-C36-C37 |
| 59 | DR | 401 | 3PE | C1-C2-C3-O31 |
| 59 | DX | 305 | 3PE | C1-C2-C3-O31 |
| 59 | EM | 901 | 3PE | C1-C2-C3-O31 |
| 59 | EN | 1203 | 3PE | C1-C2-C3-O31 |
| 59 | EO | 203 | 3PE | C1-C2-C3-O31 |
| 59 | Da | 708 | 3PE | C1-C2-C3-O31 |
| 59 | Em | 901 | 3PE | C26-C27-C28-C29 |
| 57 | EB | 302 | CDL | C71-CB7-OB8-CB6 |
| 57 | DJ | 305 | CDL | C37-C38-C39-C40 |
| 57 | DX | 307 | CDL | C20-C21-C22-C23 |
| 57 | EL | 901 | CDL | C19-C20-C21-C22 |
| 57 | Dd | 702 | CDL | C14-C15-C16-C17 |
| 57 | Dv | 403 | CDL | C23-C24-C25-C26 |
| 58 | EO | 201 | PC1 | C3B-C3C-C3D-C3E |
| 59 | El | 905 | 3PE | C37-C38-C39-C3A |
| 59 | DS | 401 | 3PE | O32-C31-O31-C3 |
| 65 | EL | 906 | UQ8 | C1-C6-C7-C8 |
| 57 | Dv | 404 | CDL | C41-C42-C43-C44 |
| 57 | Dx | 1203 | CDL | C54-C55-C56-C57 |
| 57 | El | 901 | CDL | C51-C52-C53-C54 |
| 58 | DV | 405 | PC1 | C3F-C3G-C3H-C3I |
| 59 | DX | 305 | 3PE | C39-C3A-C3B-C3C |
| 57 | DQ | 1502 | CDL | C38-C39-C40-C41 |
| 57 | DR | 402 | CDL | C82-C83-C84-C85 |
| 57 | DS | 405 | CDL | C38-C39-C40-C41 |
| 57 | DS | 405 | CDL | C55-C56-C57-C58 |
| 57 | Da | 709 | CDL | C21-C22-C23-C24 |
| 57 | Dh | 201 | CDL | C12-C13-C14-C15 |
| 57 | Dj | 408 | CDL | C59-C60-C61-C62 |
| 57 | Dv | 402 | CDL | C60-C61-C62-C63 |
| 57 | Eh | 1601 | CDL | C14-C15-C16-C17 |
| 58 | Dv | 405 | PC1 | C3F-C3G-C3H-C3I |
| 58 | Dv | 407 | PC1 | C2D-C2E-C2F-C2G |
| 58 | Dv | 407 | PC1 | O31-C31-C32-C33 |
| 57 | DY | 301 | CDL | OA9-CA7-OA8-CA6 |
| 59 | EO | 203 | 3PE | O32-C31-O31-C3 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 57 | DV | 404 | CDL | C43-C44-C45-C46 |
| 57 | DY | 301 | CDL | C14-C15-C16-C17 |
| 57 | Dj | 403 | CDL | C35-C36-C37-C38 |
| 57 | Dm | 501 | CDL | C58-C59-C60-C61 |
| 57 | Dv | 401 | CDL | C14-C15-C16-C17 |
| 57 | DJ | 305 | CDL | C77-C78-C79-C80 |
| 57 | DN | 505 | CDL | C42-C43-C44-C45 |
| 57 | DQ | 1504 | CDL | C17-C18-C19-C20 |
| 57 | DX | 301 | CDL | C12-C13-C14-C15 |
| 57 | EA | 301 | CDL | C13-C14-C15-C16 |
| 57 | EA | 301 | CDL | C75-C76-C77-C78 |
| 57 | EB | 302 | CDL | C20-C21-C22-C23 |
| 57 | Dg | 201 | CDL | C17-C18-C19-C20 |
| 57 | Dj | 401 | CDL | C37-C38-C39-C40 |
| 57 | Dj | 403 | CDL | C60-C61-C62-C63 |
| 57 | Dn | 502 | CDL | C41-C42-C43-C44 |
| 57 | Dr | 403 | CDL | C34-C35-C36-C37 |
| 57 | Du | 402 | CDL | C42-C43-C44-C45 |
| 57 | Dz | 501 | CDL | C12-C13-C14-C15 |
| 57 | Ed | 205 | CDL | C23-C24-C25-C26 |
| 58 | DB | 702 | PC1 | C2D-C2E-C2F-C2G |
| 58 | DX | 306 | PC1 | C24-C25-C26-C27 |
| 59 | DS | 401 | 3PE | C35-C36-C37-C38 |
| 57 | Dj | 403 | CDL | C58-C59-C60-C61 |
| 57 | Dj | 404 | CDL | C19-C20-C21-C22 |
| 57 | Dn | 502 | CDL | C36-C37-C38-C39 |
| 57 | Dn | 507 | CDL | C43-C44-C45-C46 |
| 59 | DC | 607 | 3PE | C25-C26-C27-C28 |
| 59 | Da | 708 | 3PE | C28-C29-C2A-C2B |
| 57 | DV | 401 | CDL | CA5-C11-C12-C13 |
| 57 | DX | 307 | CDL | CA5-C11-C12-C13 |
| 57 | DM | 501 | CDL | C14-C15-C16-C17 |
| 57 | DS | 405 | CDL | C58-C59-C60-C61 |
| 57 | Dj | 403 | CDL | C11-C12-C13-C14 |
| 57 | Dj | 404 | CDL | C18-C19-C20-C21 |
| 57 | Ds | 405 | CDL | C58-C59-C60-C61 |
| 58 | Dv | 406 | PC1 | C3B-C3C-C3D-C3E |
| 59 | DJ | 301 | 3PE | C22-C21-O21-C2 |
| 57 | EB | 304 | CDL | C73-C74-C75-C76 |
| 57 | Dj | 401 | CDL | C39-C40-C41-C42 |
| 57 | Dj | 401 | CDL | C82-C83-C84-C85 |
| 58 | DB | 702 | PC1 | C2E-C2F-C2G-C2H |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 58 | Dc | 604 | PC1 | C3F-C3G-C3H-C3I |
| 65 | DS | 404 | UQ8 | C30-C29-C31-C32 |
| 65 | Ds | 404 | UQ8 | C30-C29-C31-C32 |
| 58 | Db | 702 | PC1 | C2C-C2D-C2E-C2F |
| 65 | Ds | 404 | UQ8 | C28-C29-C31-C32 |
| 57 | EL | 903 | CDL | CA5-C11-C12-C13 |
| 57 | Dd | 704 | CDL | CA5-C11-C12-C13 |
| 57 | DD | 704 | CDL | C31-CA7-OA8-CA6 |
| 57 | DQ | 1501 | CDL | C71-CB7-OB8-CB6 |
| 57 | DQ | 1502 | CDL | C71-CB7-OB8-CB6 |
| 57 | DD | 704 | CDL | C82-C83-C84-C85 |
| 57 | ED | 604 | CDL | C23-C24-C25-C26 |
| 57 | EL | 903 | CDL | C36-C37-C38-C39 |
| 57 | EL | 904 | CDL | C20-C21-C22-C23 |
| 57 | Dz | 501 | CDL | C34-C35-C36-C37 |
| 58 | DA | 706 | PC1 | C29-C2A-C2B-C2C |
| 58 | DJ | 306 | PC1 | C37-C38-C39-C3A |
| 58 | Dc | 603 | PC1 | C35-C36-C37-C38 |
| 57 | DI | 701 | CDL | C79-C80-C81-C82 |
| 57 | DY | 301 | CDL | C79-C80-C81-C82 |
| 57 | Da | 709 | CDL | C18-C19-C20-C21 |
| 57 | Dv | 404 | CDL | C43-C44-C45-C46 |
| 58 | Dg | 203 | PC1 | C28-C29-C2A-C2B |
| 58 | Eo | 204 | PC1 | C3F-C3G-C3H-C3I |
| 57 | Dq | 404 | CDL | CB6-CB4-OB6-CB5 |
| 57 | Dx | 1203 | CDL | CB6-CB4-OB6-CB5 |
| 58 | DS | 406 | PC1 | C1-C2-O21-C21 |
| 58 | Eo | 204 | PC1 | C1-C2-O21-C21 |
| 57 | Dv | 401 | CDL | OB9-CB7-OB8-CB6 |
| 57 | DG | 202 | CDL | C51-C52-C53-C54 |
| 57 | DV | 402 | CDL | C17-C18-C19-C20 |
| 57 | En | 1201 | CDL | C53-C54-C55-C56 |
| 57 | Eu | 101 | CDL | C63-C64-C65-C66 |
| 57 | DG | 201 | CDL | C13-C14-C15-C16 |
| 57 | DV | 402 | CDL | C60-C61-C62-C63 |
| 57 | EN | 1201 | CDL | C14-C15-C16-C17 |
| 57 | Di | 701 | CDL | C80-C81-C82-C83 |
| 57 | Dj | 403 | CDL | C23-C24-C25-C26 |
| 57 | Dj | 408 | CDL | C51-C52-C53-C54 |
| 57 | Dm | 501 | CDL | C81-C82-C83-C84 |
| 58 | DC | 608 | PC1 | C3D-C3E-C3F-C3G |
| 58 | Eo | 205 | PC1 | C3B-C3C-C3D-C3E |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 60 | EI | 402 | LPP | C18-C19-C20-C21 |
| 57 | Eu | 101 | CDL | CA4-CA3-OA5-PA1 |
| 59 | DG | 204 | 3PE | C2-C1-O11-P |
| 60 | Dl | 1101 | LPP | C6-O5-P1-O3 |
| 57 | DS | 402 | CDL | C80-C81-C82-C83 |
| 57 | DV | 404 | CDL | C53-C54-C55-C56 |
| 57 | EO | 202 | CDL | C53-C54-C55-C56 |
| 57 | EO | 202 | CDL | C62-C63-C64-C65 |
| 57 | Dj | 405 | CDL | C77-C78-C79-C80 |
| 57 | Dq | 402 | CDL | C40-C41-C42-C43 |
| 57 | Dq | 403 | CDL | C36-C37-C38-C39 |
| 57 | Dr | 403 | CDL | C12-C13-C14-C15 |
| 57 | Dv | 402 | CDL | C17-C18-C19-C20 |
| 57 | Dy | 301 | CDL | C43-C44-C45-C46 |
| 58 | EO | 201 | PC1 | C2B-C2C-C2D-C2E |
| 59 | Ds | 401 | 3PE | C35-C36-C37-C38 |
| 57 | DJ | 302 | CDL | C71-CB7-OB8-CB6 |
| 57 | Du | 404 | CDL | C71-CB7-OB8-CB6 |
| 57 | Dv | 403 | CDL | C71-CB7-OB8-CB6 |
| 57 | Ep | 701 | CDL | C31-CA7-OA8-CA6 |
| 58 | DS | 406 | PC1 | C32-C31-O31-C3 |
| 58 | Dc | 603 | PC1 | C32-C31-O31-C3 |
| 58 | Dv | 406 | PC1 | C32-C31-O31-C3 |
| 57 | EL | 902 | CDL | OA5-CA3-CA4-OA6 |
| 57 | Di | 701 | CDL | OB5-CB3-CB4-OB6 |
| 57 | Du | 401 | CDL | OA5-CA3-CA4-OA6 |
| 57 | Dy | 301 | CDL | OA5-CA3-CA4-OA6 |
| 57 | Dz | 501 | CDL | OB5-CB3-CB4-OB6 |
| 57 | Ed | 205 | CDL | OB5-CB3-CB4-OB6 |
| 58 | Ef | 1001 | PC1 | O11-C1-C2-O21 |
| 57 | DN | 504 | CDL | C14-C15-C16-C17 |
| 57 | DN | 505 | CDL | C60-C61-C62-C63 |
| 57 | DZ | 501 | CDL | C12-C13-C14-C15 |
| 57 | Dq | 401 | CDL | C82-C83-C84-C85 |
| 58 | Db | 702 | PC1 | C2A-C2B-C2C-C2D |
| 57 | EU | 101 | CDL | C63-C64-C65-C66 |
| 57 | Dd | 705 | CDL | C82-C83-C84-C85 |
| 57 | El | 903 | CDL | C79-C80-C81-C82 |
| 57 | DI | 701 | CDL | O1-C1-CA2-OA2 |
| 57 | Dj | 402 | CDL | OB9-CB7-OB8-CB6 |
| 57 | DA | 710 | CDL | C42-C43-C44-C45 |
| 57 | DU | 404 | CDL | C23-C24-C25-C26 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 57 | Du | 403 | CDL | C19-C20-C21-C22 |
| 58 | EB | 301 | PC1 | C36-C37-C38-C39 |
| 58 | Dv | 405 | PC1 | C2A-C2B-C2C-C2D |
| 58 | El | 904 | PC1 | C3B-C3C-C3D-C3E |
| 57 | DD | 703 | CDL | C14-C15-C16-C17 |
| 57 | DV | 402 | CDL | C12-C13-C14-C15 |
| 57 | ED | 604 | CDL | OA6-CA4-CA6-OA8 |
| 57 | Dd | 702 | CDL | OB6-CB4-CB6-OB8 |
| 57 | Dm | 502 | CDL | OA6-CA4-CA6-OA8 |
| 57 | Dn | 503 | CDL | OB6-CB4-CB6-OB8 |
| 57 | Dv | 404 | CDL | OA6-CA4-CA6-OA8 |
| 57 | Dx | 1201 | CDL | OA6-CA4-CA6-OA8 |
| 57 | Ed | 205 | CDL | OA6-CA4-CA6-OA8 |
| 58 | DA | 707 | PC1 | O21-C2-C3-O31 |
| 58 | Dy | 302 | PC1 | O21-C2-C3-O31 |
| 59 | EN | 1203 | 3PE | O21-C2-C3-O31 |
| 57 | DJ | 303 | CDL | C19-C20-C21-C22 |
| 57 | Dq | 402 | CDL | C35-C36-C37-C38 |
| 58 | Eb | 301 | PC1 | C36-C37-C38-C39 |
| 59 | Dc | 606 | 3PE | C25-C26-C27-C28 |
| 57 | DQ | 1501 | CDL | OB7-CB5-OB6-CB4 |
| 57 | DX | 307 | CDL | OA7-CA5-OA6-CA4 |
| 57 | DV | 401 | CDL | OB9-CB7-OB8-CB6 |
| 57 | EB | 302 | CDL | OB9-CB7-OB8-CB6 |
| 58 | EO | 207 | PC1 | O32-C31-O31-C3 |
| 57 | Dj | 404 | CDL | C53-C54-C55-C56 |
| 58 | Dg | 203 | PC1 | C3D-C3E-C3F-C3G |
| 60 | Dn | 504 | LPP | C35-C36-C37-C38 |
| 54 | DA | 701 | HEA | C26-C15-C16-C17 |
| 57 | DV | 403 | CDL | C62-C63-C64-C65 |
| 57 | Dn | 507 | CDL | C40-C41-C42-C43 |
| 57 | Dr | 402 | CDL | C82-C83-C84-C85 |
| 58 | Dj | 406 | PC1 | C37-C38-C39-C3A |
| 57 | DC | 601 | CDL | C80-C81-C82-C83 |
| 57 | DV | 404 | CDL | C41-C42-C43-C44 |
| 57 | DX | 301 | CDL | C61-C62-C63-C64 |
| 57 | EL | 904 | CDL | C61-C62-C63-C64 |
| 57 | Dc | 601 | CDL | C14-C15-C16-C17 |
| 57 | Dh | 202 | CDL | C42-C43-C44-C45 |
| 58 | DX | 302 | PC1 | C26-C27-C28-C29 |
| 58 | EO | 206 | PC1 | C2E-C2F-C2G-C2H |
| 57 | Eu | 101 | CDL | CA5-C11-C12-C13 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 57 | DS | 405 | CDL | C43-C44-C45-C46 |
| 57 | ED | 604 | CDL | C11-C12-C13-C14 |
| 57 | Dg | 201 | CDL | C52-C53-C54-C55 |
| 57 | Dr | 403 | CDL | C35-C36-C37-C38 |
| 57 | Dv | 404 | CDL | C53-C54-C55-C56 |
| 58 | Da | 706 | PC1 | C29-C2A-C2B-C2C |
| 58 | Dc | 602 | PC1 | C3D-C3E-C3F-C3G |
| 59 | Ds | 401 | 3PE | C39-C3A-C3B-C3C |
| 57 | Dm | 502 | CDL | C31-CA7-OA8-CA6 |
| 57 | Ed | 205 | CDL | C31-CA7-OA8-CA6 |
| 59 | Dd | 703 | 3PE | C32-C31-O31-C3 |
| 57 | DU | 404 | CDL | C13-C14-C15-C16 |
| 57 | Da | 709 | CDL | C74-C75-C76-C77 |
| 57 | Dy | 301 | CDL | C79-C80-C81-C82 |
| 57 | En | 1202 | CDL | C23-C24-C25-C26 |
| 58 | DV | 405 | PC1 | C2A-C2B-C2C-C2D |
| 57 | Dn | 507 | CDL | C56-C57-C58-C59 |
| 58 | DB | 702 | PC1 | C2B-C2C-C2D-C2E |
| 58 | DS | 406 | PC1 | C3F-C3G-C3H-C3I |
| 58 | Dc | 605 | PC1 | C3F-C3G-C3H-C3I |
| 59 | Ds | 407 | 3PE | C3E-C3F-C3G-C3H |
| 57 | DJ | 305 | CDL | C20-C21-C22-C23 |
| 57 | DR | 402 | CDL | C33-C34-C35-C36 |
| 57 | Di | 701 | CDL | C19-C20-C21-C22 |
| 57 | Dn | 502 | CDL | C11-C12-C13-C14 |
| 57 | Dv | 402 | CDL | C57-C58-C59-C60 |
| 58 | DG | 203 | PC1 | C26-C27-C28-C29 |
| 58 | Db | 702 | PC1 | C2E-C2F-C2G-C2H |
| 58 | Dx | 1204 | PC1 | C3D-C3E-C3F-C3G |
| 59 | EN | 1203 | 3PE | C3E-C3F-C3G-C3H |
| 57 | EB | 302 | CDL | CB2-C1-CA2-OA2 |
| 57 | ED | 601 | CDL | CB2-C1-CA2-OA2 |
| 57 | EH | 201 | CDL | CA2-C1-CB2-OB2 |
| 57 | Du | 404 | CDL | CB2-C1-CA2-OA2 |
| 57 | Du | 404 | CDL | CA2-C1-CB2-OB2 |
| 57 | DQ | 1502 | CDL | OB7-CB5-OB6-CB4 |
| 57 | DJ | 304 | CDL | C51-CB5-OB6-CB4 |
| 57 | EH | 201 | CDL | C51-CB5-OB6-CB4 |
| 57 | DJ | 303 | CDL | C13-C14-C15-C16 |
| 57 | DZ | 501 | CDL | C34-C35-C36-C37 |
| 57 | EL | 903 | CDL | C74-C75-C76-C77 |
| 57 | Dc | 601 | CDL | C79-C80-C81-C82 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 57 | Dg | 201 | CDL | C56-C57-C58-C59 |
| 57 | Dm | 501 | CDL | C76-C77-C78-C79 |
| 57 | Dn | 502 | CDL | C19-C20-C21-C22 |
| 57 | Dv | 403 | CDL | C75-C76-C77-C78 |
| 57 | Eh | 1601 | CDL | C83-C84-C85-C86 |
| 59 | DS | 403 | 3PE | C2B-C2C-C2D-C2E |
| 60 | Dl | 1101 | LPP | C41-C42-C43-C44 |
| 57 | DU | 404 | CDL | C31-CA7-OA8-CA6 |
| 57 | ED | 604 | CDL | C31-CA7-OA8-CA6 |
| 57 | Ed | 205 | CDL | C71-CB7-OB8-CB6 |
| 58 | Db | 702 | PC1 | C32-C31-O31-C3 |
| 57 | Ds | 405 | CDL | C43-C44-C45-C46 |
| 58 | Dv | 406 | PC1 | C3F-C3G-C3H-C3I |
| 58 | Eo | 204 | PC1 | C2A-C2B-C2C-C2D |
| 59 | DS | 401 | 3PE | C39-C3A-C3B-C3C |
| 57 | DI | 701 | CDL | C19-C20-C21-C22 |
| 57 | Dc | 601 | CDL | C80-C81-C82-C83 |
| 57 | Dh | 202 | CDL | C53-C54-C55-C56 |
| 57 | Dn | 503 | CDL | C83-C84-C85-C86 |
| 58 | DC | 604 | PC1 | C3F-C3G-C3H-C3I |
| 54 | DA | 702 | HEA | C4D-C3D-CAD-CBD |
| 57 | DV | 401 | CDL | C18-C19-C20-C21 |
| 57 | EB | 304 | CDL | C42-C43-C44-C45 |
| 57 | EO | 202 | CDL | C37-C38-C39-C40 |
| 57 | DG | 201 | CDL | OA5-CA3-CA4-CA6 |
| 57 | DJ | 304 | CDL | OB5-CB3-CB4-CB6 |
| 57 | DO | 501 | CDL | OA5-CA3-CA4-CA6 |
| 57 | DU | 404 | CDL | OB5-CB3-CB4-CB6 |
| 57 | DV | 404 | CDL | OB5-CB3-CB4-CB6 |
| 57 | DX | 301 | CDL | OB5-CB3-CB4-CB6 |
| 57 | EB | 302 | CDL | OA5-CA3-CA4-CA6 |
| 57 | EI | 401 | CDL | OB5-CB3-CB4-CB6 |
| 57 | EL | 901 | CDL | OB5-CB3-CB4-CB6 |
| 57 | Da | 705 | CDL | OB5-CB3-CB4-CB6 |
| 57 | Dd | 705 | CDL | OA5-CA3-CA4-CA6 |
| 57 | Dm | 501 | CDL | OB5-CB3-CB4-CB6 |
| 57 | Dn | 502 | CDL | OB5-CB3-CB4-CB6 |
| 57 | Dq | 404 | CDL | OB5-CB3-CB4-CB6 |
| 57 | Ds | 405 | CDL | OB5-CB3-CB4-CB6 |
| 57 | Du | 401 | CDL | OB5-CB3-CB4-CB6 |
| 57 | Dv | 404 | CDL | OB5-CB3-CB4-CB6 |
| 57 | Dz | 501 | CDL | OB5-CB3-CB4-CB6 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 57 | El | 901 | CDL | OA5-CA3-CA4-CA6 |
| 57 | Eu | 101 | CDL | OA5-CA3-CA4-CA6 |
| 58 | DG | 203 | PC1 | O11-C1-C2-C3 |
| 58 | DI | 702 | PC1 | O11-C1-C2-C3 |
| 58 | DQ | 1503 | PC1 | O11-C1-C2-C3 |
| 58 | DS | 407 | PC1 | O11-C1-C2-C3 |
| 58 | Dg | 203 | PC1 | O11-C1-C2-C3 |
| 58 | Dq | 405 | PC1 | O11-C1-C2-C3 |
| 59 | Da | 708 | 3PE | O11-C1-C2-C3 |
| 59 | Dx | 1206 | 3PE | O11-C1-C2-C3 |
| 57 | Dd | 702 | CDL | CB7-C71-C72-C73 |
| 57 | Dy | 301 | CDL | CB5-C51-C52-C53 |
| 57 | DN | 504 | CDL | C56-C57-C58-C59 |
| 57 | Dx | 1203 | CDL | C36-C37-C38-C39 |
| 59 | Ds | 403 | 3PE | C2B-C2C-C2D-C2E |
| 57 | DU | 403 | CDL | C71-CB7-OB8-CB6 |
| 57 | DG | 202 | CDL | C35-C36-C37-C38 |
| 57 | EL | 901 | CDL | C53-C54-C55-C56 |
| 57 | EN | 1202 | CDL | C23-C24-C25-C26 |
| 54 | Da | 701 | HEA | C26-C15-C16-C17 |
| 65 | ED | 603 | UQ8 | C40-C39-C41-C42 |
| 54 | DA | 701 | HEA | C14-C15-C16-C17 |
| 65 | DS | 404 | UQ8 | C28-C29-C31-C32 |
| 65 | ED | 603 | UQ8 | C38-C39-C41-C42 |
| 57 | DX | 301 | CDL | CA7-C31-C32-C33 |
| 57 | DA | 705 | CDL | C34-C35-C36-C37 |
| 57 | DJ | 307 | CDL | C59-C60-C61-C62 |
| 57 | Dd | 704 | CDL | C38-C39-C40-C41 |
| 57 | DV | 403 | CDL | O1-C1-CB2-OB2 |
| 57 | DX | 307 | CDL | O1-C1-CA2-OA2 |
| 57 | Dd | 705 | CDL | O1-C1-CB2-OB2 |
| 57 | El | 902 | CDL | O1-C1-CA2-OA2 |
| 57 | Eh | 1601 | CDL | OB7-CB5-OB6-CB4 |
| 57 | DQ | 1502 | CDL | OB9-CB7-OB8-CB6 |
| 57 | DD | 704 | CDL | C13-C14-C15-C16 |
| 57 | DN | 504 | CDL | C40-C41-C42-C43 |
| 58 | DB | 702 | PC1 | C38-C39-C3A-C3B |
| 57 | Dj | 401 | CDL | C35-C36-C37-C38 |
| 58 | EB | 301 | PC1 | C3C-C3D-C3E-C3F |
| 57 | Dn | 505 | CDL | C31-CA7-OA8-CA6 |
| 57 | Eg | 101 | CDL | C71-CB7-OB8-CB6 |
| 58 | DC | 603 | PC1 | C32-C31-O31-C3 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 58 | Dy | 302 | PC1 | C32-C31-O31-C3 |
| 58 | DC | 604 | PC1 | O21-C21-C22-C23 |
| 57 | EN | 1202 | CDL | C34-C35-C36-C37 |
| 58 | DC | 603 | PC1 | C2C-C2D-C2E-C2F |
| 59 | DA | 708 | 3PE | C3A-C3B-C3C-C3D |
| 59 | DS | 401 | 3PE | C38-C39-C3A-C3B |
| 57 | DD | 704 | CDL | CA4-CA3-OA5-PA1 |
| 57 | DJ | 305 | CDL | C1-CB2-OB2-PB2 |
| 57 | DS | 405 | CDL | C1-CA2-OA2-PA1 |
| 57 | EK | 201 | CDL | C1-CA2-OA2-PA1 |
| 57 | Da | 705 | CDL | CA4-CA3-OA5-PA1 |
| 57 | Dd | 702 | CDL | C1-CA2-OA2-PA1 |
| 57 | Dg | 201 | CDL | C1-CA2-OA2-PA1 |
| 57 | Dj | 405 | CDL | C1-CB2-OB2-PB2 |
| 57 | DN | 504 | CDL | C82-C83-C84-C85 |
| 57 | DS | 402 | CDL | C76-C77-C78-C79 |
| 57 | Dv | 401 | CDL | C18-C19-C20-C21 |
| 59 | DS | 403 | 3PE | C27-C28-C29-C2A |
| 57 | EI | 401 | CDL | C11-C12-C13-C14 |
| 57 | En | 1201 | CDL | C34-C35-C36-C37 |
| 58 | EO | 206 | PC1 | C2B-C2C-C2D-C2E |
| 57 | DG | 202 | CDL | CA7-C31-C32-C33 |
| 57 | DU | 403 | CDL | C14-C15-C16-C17 |
| 57 | EL | 902 | CDL | C83-C84-C85-C86 |
| 57 | EU | 101 | CDL | C72-C73-C74-C75 |
| 57 | DR | 402 | CDL | C23-C24-C25-C26 |
| 58 | EO | 205 | PC1 | C3B-C3C-C3D-C3E |
| 57 | DA | 705 | CDL | CA3-CA4-CA6-OA8 |
| 57 | DA | 705 | CDL | CB3-CB4-CB6-OB8 |
| 57 | DG | 201 | CDL | CB3-CB4-CB6-OB8 |
| 57 | DG | 202 | CDL | CB3-CB4-CB6-OB8 |
| 57 | DI | 701 | CDL | CA3-CA4-CA6-OA8 |
| 57 | DJ | 307 | CDL | CA3-CA4-CA6-OA8 |
| 57 | DN | 505 | CDL | CB3-CB4-CB6-OB8 |
| 57 | DR | 403 | CDL | CB3-CB4-CB6-OB8 |
| 57 | DU | 401 | CDL | CA3-CA4-CA6-OA8 |
| 57 | DX | 307 | CDL | CA3-CA4-CA6-OA8 |
| 57 | DY | 301 | CDL | CA3-CA4-CA6-OA8 |
| 57 | DY | 301 | CDL | CB3-CB4-CB6-OB8 |
| 57 | ED | 604 | CDL | CA3-CA4-CA6-OA8 |
| 57 | EL | 901 | CDL | CA3-CA4-CA6-OA8 |
| 57 | EL | 901 | CDL | CB3-CB4-CB6-OB8 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 57 | EL | 903 | CDL | CA3-CA4-CA6-OA8 |
| 57 | EO | 202 | CDL | CB3-CB4-CB6-OB8 |
| 57 | EU | 101 | CDL | CB3-CB4-CB6-OB8 |
| 57 | Dg | 201 | CDL | CA3-CA4-CA6-OA8 |
| 57 | Dg | 202 | CDL | CB3-CB4-CB6-OB8 |
| 57 | Dh | 201 | CDL | CA3-CA4-CA6-OA8 |
| 57 | Di | 701 | CDL | CA3-CA4-CA6-OA8 |
| 57 | Dn | 505 | CDL | CB3-CB4-CB6-OB8 |
| 57 | Dr | 402 | CDL | CA3-CA4-CA6-OA8 |
| 57 | Dr | 402 | CDL | CB3-CB4-CB6-OB8 |
| 57 | Ds | 402 | CDL | CA3-CA4-CA6-OA8 |
| 57 | Dy | 301 | CDL | CA3-CA4-CA6-OA8 |
| 57 | Dy | 301 | CDL | CB3-CB4-CB6-OB8 |
| 57 | Ei | 401 | CDL | CA3-CA4-CA6-OA8 |
| 57 | Ep | 701 | CDL | CB3-CB4-CB6-OB8 |
| 58 | DA | 707 | PC1 | C1-C2-C3-O31 |
| 58 | DC | 605 | PC1 | C1-C2-C3-O31 |
| 58 | DS | 407 | PC1 | C1-C2-C3-O31 |
| 58 | DV | 405 | PC1 | C1-C2-C3-O31 |
| 58 | Da | 706 | PC1 | C1-C2-C3-O31 |
| 58 | Dc | 607 | PC1 | C1-C2-C3-O31 |
| 58 | Dv | 405 | PC1 | C1-C2-C3-O31 |
| 58 | Dv | 406 | PC1 | C1-C2-C3-O31 |
| 58 | Ef | 1001 | PC1 | C1-C2-C3-O31 |
| 58 | Eo | 201 | PC1 | C1-C2-C3-O31 |
| 59 | DA | 708 | 3PE | C1-C2-C3-O31 |
| 59 | EL | 905 | 3PE | C1-C2-C3-O31 |
| 59 | Ds | 401 | 3PE | C1-C2-C3-O31 |
| 59 | Em | 901 | 3PE | C1-C2-C3-O31 |
| 57 | Dd | 702 | CDL | OB7-CB5-OB6-CB4 |
| 58 | Dc | 603 | PC1 | C3D-C3E-C3F-C3G |
| 60 | Dn | 506 | LPP | C35-C36-C37-C38 |
| 57 | DD | 704 | CDL | OA9-CA7-OA8-CA6 |
| 57 | Dv | 403 | CDL | OB9-CB7-OB8-CB6 |
| 57 | DC | 601 | CDL | C79-C80-C81-C82 |
| 57 | EB | 304 | CDL | C44-C45-C46-C47 |
| 57 | EI | 401 | CDL | C76-C77-C78-C79 |
| 57 | Dm | 501 | CDL | C82-C83-C84-C85 |
| 59 | Dd | 703 | 3PE | C35-C36-C37-C38 |
| 57 | DI | 701 | CDL | C73-C74-C75-C76 |
| 57 | DZ | 501 | CDL | C77-C78-C79-C80 |
| 58 | Ef | 1001 | PC1 | C2B-C2C-C2D-C2E |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 59 | Dc | 606 | 3PE | C2F-C2G-C2H-C2I |
| 57 | DG | 202 | CDL | C14-C15-C16-C17 |
| 57 | DJ | 303 | CDL | C40-C41-C42-C43 |
| 57 | DJ | 302 | CDL | OB9-CB7-OB8-CB6 |
| 57 | DQ | 1501 | CDL | OB9-CB7-OB8-CB6 |
| 57 | Du | 404 | CDL | OB9-CB7-OB8-CB6 |
| 57 | Ea | 301 | CDL | C71-CB7-OB8-CB6 |
| 58 | DI | 702 | PC1 | C11-C12-N-C13 |
| 65 | Ed | 202 | UQ8 | C33-C34-C36-C37 |
| 68 | Er | 201 | ATP | PG-O3B-PB-O3A |
| 57 | DV | 404 | CDL | C40-C41-C42-C43 |
| 57 | Dx | 1203 | CDL | C20-C21-C22-C23 |
| 58 | Dg | 203 | PC1 | C26-C27-C28-C29 |
| 57 | DQ | 1501 | CDL | C36-C37-C38-C39 |
| 57 | DV | 403 | CDL | C75-C76-C77-C78 |
| 57 | ED | 601 | CDL | CB2-OB2-PB2-OB5 |
| 57 | EL | 902 | CDL | CB3-OB5-PB2-OB2 |
| 57 | Dh | 201 | CDL | CA3-OA5-PA1-OA2 |
| 57 | Dj | 403 | CDL | CB2-OB2-PB2-OB5 |
| 57 | Dq | 403 | CDL | CA2-OA2-PA1-OA5 |
| 57 | Dv | 404 | CDL | CB2-OB2-PB2-OB5 |
| 57 | Eg | 101 | CDL | CB3-OB5-PB2-OB2 |
| 57 | El | 903 | CDL | CA3-OA5-PA1-OA2 |
| 58 | Dx | 1204 | PC1 | C11-O13-P-O11 |
| 57 | Dh | 202 | CDL | C44-C45-C46-C47 |
| 57 | Dq | 401 | CDL | C37-C38-C39-C40 |
| 57 | DU | 402 | CDL | C56-C57-C58-C59 |
| 58 | Eo | 205 | PC1 | C29-C2A-C2B-C2C |
| 57 | DQ | 1501 | CDL | OB5-CB3-CB4-OB6 |
| 57 | DS | 405 | CDL | OB5-CB3-CB4-OB6 |
| 57 | DX | 307 | CDL | OB5-CB3-CB4-OB6 |
| 57 | DZ | 501 | CDL | OB5-CB3-CB4-OB6 |
| 57 | EA | 301 | CDL | OA5-CA3-CA4-OA6 |
| 57 | EI | 401 | CDL | OB5-CB3-CB4-OB6 |
| 57 | EN | 1202 | CDL | OA5-CA3-CA4-OA6 |
| 57 | Dc | 601 | CDL | OB5-CB3-CB4-OB6 |
| 57 | Ds | 402 | CDL | OB5-CB3-CB4-OB6 |
| 57 | Ds | 405 | CDL | OB5-CB3-CB4-OB6 |
| 57 | Du | 401 | CDL | OB5-CB3-CB4-OB6 |
| 57 | Du | 404 | CDL | OB5-CB3-CB4-OB6 |
| 57 | Dv | 403 | CDL | OA5-CA3-CA4-OA6 |
| 57 | Ep | 701 | CDL | OA5-CA3-CA4-OA6 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 58 | DI | 702 | PC1 | O11-C1-C2-O21 |
| 58 | Dc | 607 | PC1 | O11-C1-C2-O21 |
| 58 | Eo | 201 | PC1 | O11-C1-C2-O21 |
| 59 | DS | 403 | 3PE | O11-C1-C2-O21 |
| 59 | DX | 303 | 3PE | O11-C1-C2-O21 |
| 59 | Dg | 204 | 3PE | O11-C1-C2-O21 |
| 59 | Dr | 404 | 3PE | O11-C1-C2-O21 |
| 59 | Ds | 403 | 3PE | O11-C1-C2-O21 |
| 57 | Dd | 706 | CDL | OB7-CB5-OB6-CB4 |
| 58 | DC | 605 | PC1 | C32-C31-O31-C3 |
| 57 | Dj | 401 | CDL | C13-C14-C15-C16 |
| 57 | Ep | 701 | CDL | C60-C61-C62-C63 |
| 58 | DS | 406 | PC1 | O32-C31-O31-C3 |
| 58 | Dc | 603 | PC1 | O32-C31-O31-C3 |
| 58 | Dv | 406 | PC1 | O32-C31-O31-C3 |
| 57 | Dv | 402 | CDL | C42-C43-C44-C45 |
| 59 | Dx | 1205 | 3PE | C2F-C2G-C2H-C2I |
| 57 | DR | 402 | CDL | C20-C21-C22-C23 |
| 58 | DC | 603 | PC1 | C3D-C3E-C3F-C3G |
| 58 | Dc | 607 | PC1 | C2B-C2C-C2D-C2E |
| 57 | Ep | 701 | CDL | OA9-CA7-OA8-CA6 |
| 59 | DJ | 301 | 3PE | C35-C36-C37-C38 |
| 65 | EL | 906 | UQ8 | C2-C3-O3-C3M |
| 57 | DM | 501 | CDL | C77-C78-C79-C80 |
| 57 | EL | 901 | CDL | C23-C24-C25-C26 |
| 57 | Dj | 404 | CDL | C77-C78-C79-C80 |
| 57 | Dn | 501 | CDL | C76-C77-C78-C79 |
| 57 | DA | 709 | CDL | OA6-CA4-CA6-OA8 |
| 57 | DJ | 302 | CDL | OA6-CA4-CA6-OA8 |
| 57 | DS | 402 | CDL | OA6-CA4-CA6-OA8 |
| 57 | DY | 301 | CDL | OA6-CA4-CA6-OA8 |
| 57 | ED | 601 | CDL | OB6-CB4-CB6-OB8 |
| 57 | EH | 202 | CDL | OA6-CA4-CA6-OA8 |
| 57 | EI | 401 | CDL | OA6-CA4-CA6-OA8 |
| 57 | EL | 903 | CDL | OB6-CB4-CB6-OB8 |
| 57 | EO | 202 | CDL | OB6-CB4-CB6-OB8 |
| 57 | Dg | 201 | CDL | OB6-CB4-CB6-OB8 |
| 57 | Dr | 402 | CDL | OA6-CA4-CA6-OA8 |
| 57 | Ds | 402 | CDL | OA6-CA4-CA6-OA8 |
| 57 | Eg | 101 | CDL | OA6-CA4-CA6-OA8 |
| 57 | Ei | 401 | CDL | OA6-CA4-CA6-OA8 |
| 57 | El | 902 | CDL | OA6-CA4-CA6-OA8 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 57 | El | 903 | CDL | OA6-CA4-CA6-OA8 |
| 57 | Ep | 701 | CDL | OA6-CA4-CA6-OA8 |
| 58 | DS | 406 | PC1 | O21-C2-C3-O31 |
| 58 | EO | 207 | PC1 | O21-C2-C3-O31 |
| 58 | Dc | 607 | PC1 | O21-C2-C3-O31 |
| 59 | DC | 607 | 3PE | O21-C2-C3-O31 |
| 59 | DX | 305 | 3PE | O21-C2-C3-O31 |
| 59 | Dr | 401 | 3PE | O21-C2-C3-O31 |
| 59 | Dx | 1207 | 3PE | O21-C2-C3-O31 |
| 59 | Em | 901 | 3PE | O21-C2-C3-O31 |
| 58 | DY | 302 | PC1 | C32-C31-O31-C3 |
| 58 | DV | 406 | PC1 | O31-C31-C32-C33 |
| 57 | DQ | 1504 | CDL | C36-C37-C38-C39 |
| 57 | Dv | 404 | CDL | C40-C41-C42-C43 |
| 60 | EI | 402 | LPP | C38-C39-C40-C41 |
| 57 | Dj | 401 | CDL | CA5-C11-C12-C13 |
| 57 | DU | 401 | CDL | C60-C61-C62-C63 |
| 57 | Dv | 402 | CDL | C16-C17-C18-C19 |
| 58 | Dc | 603 | PC1 | C2C-C2D-C2E-C2F |
| 57 | DA | 710 | CDL | CA2-C1-CB2-OB2 |
| 57 | DJ | 307 | CDL | CB2-C1-CA2-OA2 |
| 57 | DV | 403 | CDL | CA2-C1-CB2-OB2 |
| 57 | Dg | 202 | CDL | CB2-C1-CA2-OA2 |
| 57 | Dv | 404 | CDL | CB2-C1-CA2-OA2 |
| 57 | Ed | 204 | CDL | CA2-C1-CB2-OB2 |
| 65 | EN | 1204 | UQ8 | C14-C16-C17-C18 |
| 57 | EL | 904 | CDL | C77-C78-C79-C80 |
| 57 | El | 902 | CDL | C34-C35-C36-C37 |
| 59 | Dj | 407 | 3PE | O22-C21-O21-C2 |
| 54 | Da | 701 | HEA | C14-C15-C16-C17 |
| 57 | DV | 402 | CDL | C79-C80-C81-C82 |
| 57 | Do | 501 | CDL | C11-C12-C13-C14 |
| 58 | DA | 706 | PC1 | C37-C38-C39-C3A |
| 57 | EB | 304 | CDL | C53-C54-C55-C56 |
| 57 | EL | 903 | CDL | C34-C35-C36-C37 |
| 57 | Dg | 201 | CDL | C12-C13-C14-C15 |
| 57 | Dr | 402 | CDL | C84-C85-C86-C87 |
| 57 | Ds | 405 | CDL | C12-C13-C14-C15 |
| 60 | Dl | 1101 | LPP | C18-C19-C20-C21 |
| 60 | Dl | 1101 | LPP | C39-C40-C41-C42 |
| 57 | DA | 705 | CDL | CA4-CA3-OA5-PA1 |
| 57 | DD | 702 | CDL | C1-CA2-OA2-PA1 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 57 | DJ | 305 | CDL | CB4-CB3-OB5-PB2 |
| 57 | DQ | 1504 | CDL | C1-CA2-OA2-PA1 |
| 57 | ED | 604 | CDL | C1-CB2-OB2-PB2 |
| 57 | EI | 401 | CDL | C1-CA2-OA2-PA1 |
| 57 | EO | 202 | CDL | CB4-CB3-OB5-PB2 |
| 57 | Dg | 201 | CDL | CA4-CA3-OA5-PA1 |
| 57 | Dm | 501 | CDL | CA4-CA3-OA5-PA1 |
| 57 | Dn | 507 | CDL | C1-CB2-OB2-PB2 |
| 57 | Dq | 402 | CDL | C1-CA2-OA2-PA1 |
| 57 | Dr | 403 | CDL | CA4-CA3-OA5-PA1 |
| 57 | Ds | 405 | CDL | C1-CA2-OA2-PA1 |
| 57 | Du | 403 | CDL | C1-CA2-OA2-PA1 |
| 57 | Du | 404 | CDL | C1-CA2-OA2-PA1 |
| 57 | Dx | 1203 | CDL | CA4-CA3-OA5-PA1 |
| 57 | Ea | 301 | CDL | CA4-CA3-OA5-PA1 |
| 57 | En | 1202 | CDL | C1-CA2-OA2-PA1 |
| 59 | Dc | 606 | 3PE | C2-C1-O11-P |
| 57 | Dm | 502 | CDL | OA9-CA7-OA8-CA6 |
| 57 | Ed | 205 | CDL | OA9-CA7-OA8-CA6 |
| 58 | Db | 702 | PC1 | O32-C31-O31-C3 |
| 59 | Dd | 703 | 3PE | O32-C31-O31-C3 |
| 57 | DN | 504 | CDL | C11-C12-C13-C14 |
| 57 | EU | 101 | CDL | C40-C41-C42-C43 |
| 57 | Dj | 401 | CDL | C11-C12-C13-C14 |
| 57 | Dx | 1203 | CDL | C40-C41-C42-C43 |
| 58 | Da | 706 | PC1 | C37-C38-C39-C3A |
| 58 | Di | 702 | PC1 | C11-C12-N-C13 |
| 58 | Eo | 204 | PC1 | C11-C12-N-C13 |
| 57 | DQ | 1504 | CDL | C57-C58-C59-C60 |
| 57 | DR | 402 | CDL | C41-C42-C43-C44 |
| 57 | DX | 301 | CDL | C40-C41-C42-C43 |
| 59 | DC | 606 | 3PE | C2A-C2B-C2C-C2D |
| 57 | DD | 704 | CDL | C84-C85-C86-C87 |
| 57 | Dd | 705 | CDL | C84-C85-C86-C87 |
| 57 | DR | 402 | CDL | C84-C85-C86-C87 |
| 57 | EL | 901 | CDL | C11-C12-C13-C14 |
| 57 | Du | 403 | CDL | C34-C35-C36-C37 |
| 57 | DJ | 304 | CDL | OB7-CB5-OB6-CB4 |
| 59 | DJ | 301 | 3PE | O22-C21-O21-C2 |
| 57 | Ek | 201 | CDL | C51-CB5-OB6-CB4 |
| 59 | EL | 905 | 3PE | C22-C21-O21-C2 |
| 57 | DQ | 1501 | CDL | C43-C44-C45-C46 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 58 | Db | 702 | PC1 | C3E-C3F-C3G-C3H |
| 59 | Ds | 401 | 3PE | C38-C39-C3A-C3B |
| 57 | Dj | 402 | CDL | C56-C57-C58-C59 |
| 57 | Di | 701 | CDL | C79-C80-C81-C82 |
| 57 | Dm | 501 | CDL | C11-C12-C13-C14 |
| 57 | DI | 701 | CDL | OB5-CB3-CB4-CB6 |
| 57 | DQ | 1501 | CDL | OB5-CB3-CB4-CB6 |
| 57 | DQ | 1502 | CDL | OB5-CB3-CB4-CB6 |
| 57 | DS | 405 | CDL | OB5-CB3-CB4-CB6 |
| 57 | DV | 404 | CDL | OA5-CA3-CA4-CA6 |
| 57 | DX | 307 | CDL | OB5-CB3-CB4-CB6 |
| 57 | DZ | 501 | CDL | OB5-CB3-CB4-CB6 |
| 57 | EA | 301 | CDL | OA5-CA3-CA4-CA6 |
| 57 | EH | 202 | CDL | OA5-CA3-CA4-CA6 |
| 57 | EO | 202 | CDL | OA5-CA3-CA4-CA6 |
| 57 | EU | 101 | CDL | OA5-CA3-CA4-CA6 |
| 57 | Da | 709 | CDL | OB5-CB3-CB4-CB6 |
| 57 | Dj | 403 | CDL | OB5-CB3-CB4-CB6 |
| 57 | Dv | 404 | CDL | OA5-CA3-CA4-CA6 |
| 57 | Eg | 101 | CDL | OB5-CB3-CB4-CB6 |
| 58 | Dx | 1202 | PC1 | O11-C1-C2-C3 |
| 59 | DS | 403 | 3PE | O11-C1-C2-C3 |
| 59 | Dg | 204 | 3PE | O11-C1-C2-C3 |
| 57 | Eg | 101 | CDL | O1-C1-CA2-OA2 |
| 57 | DU | 401 | CDL | C13-C14-C15-C16 |
| 57 | DV | 402 | CDL | C16-C17-C18-C19 |
| 58 | DB | 702 | PC1 | C3B-C3C-C3D-C3E |
| 59 | Dc | 606 | 3PE | C3B-C3C-C3D-C3E |
| 57 | ED | 604 | CDL | OA9-CA7-OA8-CA6 |
| 57 | DV | 402 | CDL | C42-C43-C44-C45 |
| 57 | DZ | 501 | CDL | C11-C12-C13-C14 |
| 59 | Da | 708 | 3PE | C3A-C3B-C3C-C3D |
| 57 | Dh | 201 | CDL | C31-CA7-OA8-CA6 |
| 57 | Dq | 401 | CDL | C31-CA7-OA8-CA6 |
| 59 | DR | 401 | 3PE | C35-C36-C37-C38 |
| 57 | DU | 404 | CDL | OA9-CA7-OA8-CA6 |
| 59 | Dc | 606 | 3PE | C22-C21-O21-C2 |
| 57 | EL | 903 | CDL | C79-C80-C81-C82 |
| 57 | DV | 403 | CDL | C71-CB7-OB8-CB6 |
| 57 | Dm | 501 | CDL | C52-C51-CB5-OB6 |
| 57 | EL | 903 | CDL | C78-C79-C80-C81 |
| 57 | Da | 709 | CDL | C39-C40-C41-C42 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 57 | Dj | 402 | CDL | C54-C55-C56-C57 |
| 58 | DS | 406 | PC1 | C29-C2A-C2B-C2C |
| 58 | DS | 406 | PC1 | C32-C33-C34-C35 |
| 57 | DJ | 304 | CDL | C58-C59-C60-C61 |
| 57 | Dg | 201 | CDL | C83-C84-C85-C86 |
| 59 | Ds | 403 | 3PE | C27-C28-C29-C2A |
| 57 | Dj | 403 | CDL | C79-C80-C81-C82 |
| 58 | EO | 206 | PC1 | C2A-C2B-C2C-C2D |
| 57 | DG | 201 | CDL | CB3-CB4-OB6-CB5 |
| 57 | DI | 701 | CDL | CA6-CA4-OA6-CA5 |
| 57 | DJ | 305 | CDL | CB6-CB4-OB6-CB5 |
| 57 | DZ | 501 | CDL | CB6-CB4-OB6-CB5 |
| 57 | EB | 302 | CDL | CA6-CA4-OA6-CA5 |
| 57 | Dg | 201 | CDL | CA3-CA4-OA6-CA5 |
| 57 | Dn | 502 | CDL | CA6-CA4-OA6-CA5 |
| 57 | Dq | 403 | CDL | CA6-CA4-OA6-CA5 |
| 57 | Dy | 301 | CDL | CB3-CB4-OB6-CB5 |
| 57 | Dz | 501 | CDL | CB6-CB4-OB6-CB5 |
| 57 | Ea | 301 | CDL | CA6-CA4-OA6-CA5 |
| 57 | Eh | 1601 | CDL | CB3-CB4-OB6-CB5 |
| 59 | Eo | 203 | 3PE | C3-C2-O21-C21 |
| 57 | EH | 201 | CDL | OB7-CB5-OB6-CB4 |
| 57 | Dv | 402 | CDL | C77-C78-C79-C80 |
| 57 | El | 902 | CDL | C52-C53-C54-C55 |
| 58 | Db | 702 | PC1 | C38-C39-C3A-C3B |
| 57 | DN | 501 | CDL | C31-CA7-OA8-CA6 |
| 58 | EO | 206 | PC1 | C32-C31-O31-C3 |
| 57 | DH | 201 | CDL | C21-C22-C23-C24 |
| 57 | EO | 202 | CDL | C77-C78-C79-C80 |
| 59 | EL | 905 | 3PE | C2B-C2C-C2D-C2E |
| 65 | DS | 404 | UQ8 | C5-C4-O4-C4M |
| 65 | Ed | 202 | UQ8 | C2-C3-O3-C3M |
| 57 | Dx | 1203 | CDL | C64-C65-C66-C67 |
| 57 | DA | 709 | CDL | CB7-C71-C72-C73 |
| 57 | Dn | 501 | CDL | CB7-C71-C72-C73 |
| 57 | DG | 202 | CDL | CA3-CA4-CA6-OA8 |
| 57 | DJ | 302 | CDL | CA3-CA4-CA6-OA8 |
| 57 | DR | 402 | CDL | CA3-CA4-CA6-OA8 |
| 57 | DR | 403 | CDL | CA4-CA3-OA5-PA1 |
| 57 | DR | 403 | CDL | C1-CB2-OB2-PB2 |
| 57 | DS | 402 | CDL | CB3-CB4-CB6-OB8 |
| 57 | DV | 402 | CDL | C1-CA2-OA2-PA1 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 57 | DX | 301 | CDL | CA4-CA3-OA5-PA1 |
| 57 | DX | 307 | CDL | C1-CB2-OB2-PB2 |
| 57 | EI | 401 | CDL | CA3-CA4-CA6-OA8 |
| 57 | EL | 903 | CDL | CB3-CB4-CB6-OB8 |
| 57 | EN | 1202 | CDL | CB3-CB4-CB6-OB8 |
| 57 | EO | 202 | CDL | CA4-CA3-OA5-PA1 |
| 57 | Da | 705 | CDL | CA3-CA4-CA6-OA8 |
| 57 | Dh | 202 | CDL | C1-CB2-OB2-PB2 |
| 57 | Dm | 501 | CDL | CA3-CA4-CA6-OA8 |
| 57 | Dn | 501 | CDL | CA3-CA4-CA6-OA8 |
| 57 | Dn | 502 | CDL | C1-CB2-OB2-PB2 |
| 57 | Dr | 402 | CDL | CA4-CA3-OA5-PA1 |
| 57 | Ed | 204 | CDL | C1-CA2-OA2-PA1 |
| 57 | Eg | 101 | CDL | CA3-CA4-CA6-OA8 |
| 57 | Ek | 201 | CDL | C1-CA2-OA2-PA1 |
| 57 | El | 901 | CDL | CB3-CB4-CB6-OB8 |
| 58 | DA | 706 | PC1 | C1-C2-C3-O31 |
| 58 | DC | 602 | PC1 | C1-C2-C3-O31 |
| 58 | Db | 702 | PC1 | C2-C1-O11-P |
| 58 | Dc | 602 | PC1 | C1-C2-C3-O31 |
| 59 | DS | 401 | 3PE | C1-C2-C3-O31 |
| 59 | Da | 708 | 3PE | C2-C1-O11-P |
| 59 | Dc | 606 | 3PE | C1-C2-C3-O31 |
| 59 | Dr | 401 | 3PE | C1-C2-C3-O31 |
| 59 | Dx | 1207 | 3PE | C1-C2-C3-O31 |
| 60 | DN | 502 | LPP | C7-C6-O5-P1 |
| 58 | DY | 302 | PC1 | O32-C31-O31-C3 |
| 57 | Dn | 502 | CDL | C11-CA5-OA6-CA4 |
| 57 | EO | 202 | CDL | C63-C64-C65-C66 |
| 58 | EO | 201 | PC1 | C28-C29-C2A-C2B |
| 57 | DG | 201 | CDL | OA5-CA3-CA4-OA6 |
| 57 | DI | 701 | CDL | OB5-CB3-CB4-OB6 |
| 57 | DO | 501 | CDL | OA5-CA3-CA4-OA6 |
| 57 | DQ | 1504 | CDL | OB5-CB3-CB4-OB6 |
| 57 | DS | 405 | CDL | OA5-CA3-CA4-OA6 |
| 57 | DV | 404 | CDL | OA5-CA3-CA4-OA6 |
| 57 | EB | 302 | CDL | OA5-CA3-CA4-OA6 |
| 57 | ED | 601 | CDL | OB5-CB3-CB4-OB6 |
| 57 | EL | 901 | CDL | OB5-CB3-CB4-OB6 |
| 57 | EL | 904 | CDL | OA5-CA3-CA4-OA6 |
| 57 | EO | 202 | CDL | OA5-CA3-CA4-OA6 |
| 57 | Da | 705 | CDL | OB5-CB3-CB4-OB6 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 57 | Dj | 402 | CDL | OB5-CB3-CB4-OB6 |
| 57 | Dm | 501 | CDL | OA5-CA3-CA4-OA6 |
| 57 | Dm | 501 | CDL | OB5-CB3-CB4-OB6 |
| 57 | Do | 501 | CDL | OA5-CA3-CA4-OA6 |
| 57 | Dv | 404 | CDL | OA5-CA3-CA4-OA6 |
| 57 | Eg | 101 | CDL | OB5-CB3-CB4-OB6 |
| 57 | El | 901 | CDL | OA5-CA3-CA4-OA6 |
| 57 | Eu | 101 | CDL | OA5-CA3-CA4-OA6 |
| 58 | Dc | 603 | PC1 | O11-C1-C2-O21 |
| 58 | Dg | 203 | PC1 | O11-C1-C2-O21 |
| 58 | Di | 702 | PC1 | O11-C1-C2-O21 |
| 59 | Da | 708 | 3PE | O11-C1-C2-O21 |
| 59 | El | 905 | 3PE | O11-C1-C2-O21 |
| 57 | Dd | 705 | CDL | CA2-C1-CB2-OB2 |
| 57 | Dj | 408 | CDL | CB2-C1-CA2-OA2 |
| 57 | Dn | 502 | CDL | OA7-CA5-OA6-CA4 |
| 57 | Ek | 201 | CDL | OB7-CB5-OB6-CB4 |
| 59 | Dc | 606 | 3PE | O22-C21-O21-C2 |
| 57 | DS | 402 | CDL | C72-C73-C74-C75 |
| 57 | DU | 403 | CDL | OB9-CB7-OB8-CB6 |
| 57 | Ed | 205 | CDL | OB9-CB7-OB8-CB6 |
| 58 | DC | 603 | PC1 | O32-C31-O31-C3 |
| 58 | DC | 605 | PC1 | O32-C31-O31-C3 |
| 57 | DG | 201 | CDL | C58-C59-C60-C61 |
| 57 | DU | 402 | CDL | C42-C43-C44-C45 |
| 57 | Eu | 101 | CDL | C40-C41-C42-C43 |
| 59 | DC | 607 | 3PE | C3B-C3C-C3D-C3E |
| 54 | DA | 702 | HEA | C2D-C3D-CAD-CBD |
| 57 | EL | 903 | CDL | C52-C53-C54-C55 |
| 57 | Dd | 705 | CDL | C38-C39-C40-C41 |
| 58 | DS | 407 | PC1 | C3C-C3D-C3E-C3F |
| 57 | DA | 705 | CDL | OB6-CB4-CB6-OB8 |
| 57 | DA | 709 | CDL | OB6-CB4-CB6-OB8 |
| 57 | DD | 703 | CDL | OA6-CA4-CA6-OA8 |
| 57 | DG | 202 | CDL | OA6-CA4-CA6-OA8 |
| 57 | DH | 201 | CDL | OB6-CB4-CB6-OB8 |
| 57 | DR | 402 | CDL | OA6-CA4-CA6-OA8 |
| 57 | DU | 401 | CDL | OB6-CB4-CB6-OB8 |
| 57 | ED | 601 | CDL | OA6-CA4-CA6-OA8 |
| 57 | EH | 201 | CDL | OB6-CB4-CB6-OB8 |
| 57 | EK | 201 | CDL | OA6-CA4-CA6-OA8 |
| 57 | EN | 1201 | CDL | OA6-CA4-CA6-OA8 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 57 | EU | 101 | CDL | OB6-CB4-CB6-OB8 |
| 57 | Dd | 704 | CDL | OB6-CB4-CB6-OB8 |
| 57 | Dd | 706 | CDL | OB6-CB4-CB6-OB8 |
| 57 | Di | 701 | CDL | OA6-CA4-CA6-OA8 |
| 57 | Dm | 501 | CDL | OA6-CA4-CA6-OA8 |
| 57 | Dn | 501 | CDL | OA6-CA4-CA6-OA8 |
| 57 | Dn | 505 | CDL | OB6-CB4-CB6-OB8 |
| 57 | Du | 402 | CDL | OA6-CA4-CA6-OA8 |
| 57 | Dv | 402 | CDL | OB6-CB4-CB6-OB8 |
| 57 | Dy | 301 | CDL | OA6-CA4-CA6-OA8 |
| 57 | Eu | 101 | CDL | OB6-CB4-CB6-OB8 |
| 58 | DC | 602 | PC1 | O21-C2-C3-O31 |
| 58 | DV | 405 | PC1 | O21-C2-C3-O31 |
| 58 | DX | 302 | PC1 | O21-C2-C3-O31 |
| 58 | DY | 302 | PC1 | O21-C2-C3-O31 |
| 58 | Dc | 602 | PC1 | O21-C2-C3-O31 |
| 58 | Dc | 605 | PC1 | O21-C2-C3-O31 |
| 58 | Eo | 204 | PC1 | O21-C2-C3-O31 |
| 59 | Dc | 606 | 3PE | O21-C2-C3-O31 |
| 59 | Eo | 202 | 3PE | O21-C2-C3-O31 |
| 57 | DV | 404 | CDL | C31-C32-C33-C34 |
| 58 | DC | 608 | PC1 | C3C-C3D-C3E-C3F |
| 58 | Dy | 302 | PC1 | O32-C31-O31-C3 |
| 57 | DJ | 304 | CDL | C11-C12-C13-C14 |
| 58 | EO | 206 | PC1 | C11-C12-N-C13 |
| 68 | ER | 201 | ATP | C5'-O5'-PA-O3A |
| 57 | Do | 501 | CDL | C76-C77-C78-C79 |
| 57 | Dx | 1201 | CDL | C38-C39-C40-C41 |
| 57 | Dj | 403 | CDL | C51-CB5-OB6-CB4 |
| 65 | EN | 1204 | UQ8 | C40-C39-C41-C42 |
| 57 | Dv | 402 | CDL | C12-C13-C14-C15 |
| 57 | Dn | 505 | CDL | OA9-CA7-OA8-CA6 |
| 57 | Ea | 301 | CDL | OB9-CB7-OB8-CB6 |
| 57 | Eg | 101 | CDL | OB9-CB7-OB8-CB6 |
| 58 | Dx | 1204 | PC1 | C31-C32-C33-C34 |
| 57 | EO | 202 | CDL | C13-C14-C15-C16 |
| 57 | Eh | 1601 | CDL | C13-C14-C15-C16 |
| 58 | EB | 303 | PC1 | C2E-C2F-C2G-C2H |
| 59 | EL | 905 | 3PE | O22-C21-O21-C2 |
| 57 | Dg | 202 | CDL | CA4-CA6-OA8-CA7 |
| 57 | Dn | 507 | CDL | C11-C12-C13-C14 |
| 57 | Dr | 402 | CDL | C61-C62-C63-C64 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 57 | El | 901 | CDL | C18-C19-C20-C21 |
| 58 | Dv | 406 | PC1 | C29-C2A-C2B-C2C |
| 57 | Dh | 201 | CDL | OA9-CA7-OA8-CA6 |
| 57 | DQ | 1501 | CDL | C81-C82-C83-C84 |
| 57 | DZ | 501 | CDL | C73-C74-C75-C76 |
| 57 | EN | 1201 | CDL | C11-C12-C13-C14 |
| 57 | Dh | 201 | CDL | C21-C22-C23-C24 |
| 57 | El | 901 | CDL | C64-C65-C66-C67 |
| 60 | Dn | 506 | LPP | C38-C39-C40-C41 |
| 57 | Dr | 402 | CDL | C13-C14-C15-C16 |
| 57 | DJ | 307 | CDL | C72-C71-CB7-OB8 |
| 57 | DD | 702 | CDL | C23-C24-C25-C26 |
| 58 | Dc | 602 | PC1 | C3F-C3G-C3H-C3I |
| 57 | DV | 403 | CDL | OB9-CB7-OB8-CB6 |
| 57 | Dq | 401 | CDL | OA9-CA7-OA8-CA6 |
| 57 | El | 903 | CDL | C31-CA7-OA8-CA6 |
| 58 | DA | 707 | PC1 | C32-C31-O31-C3 |
| 58 | Dg | 203 | PC1 | C32-C31-O31-C3 |
| 54 | Da | 702 | HEA | C4D-C3D-CAD-CBD |
| 57 | Du | 402 | CDL | C14-C15-C16-C17 |
| 58 | EO | 201 | PC1 | C25-C26-C27-C28 |
| 58 | Dc | 605 | PC1 | C3E-C3F-C3G-C3H |
| 58 | Eb | 301 | PC1 | C3C-C3D-C3E-C3F |
| 59 | DS | 403 | 3PE | C34-C35-C36-C37 |
| 57 | DV | 403 | CDL | C82-C83-C84-C85 |
| 58 | DC | 603 | PC1 | C3B-C3C-C3D-C3E |
| 57 | Dq | 404 | CDL | OB7-CB5-OB6-CB4 |
| 57 | Dq | 403 | CDL | C17-C18-C19-C20 |
| 57 | EB | 302 | CDL | C31-CA7-OA8-CA6 |
| 57 | Dj | 403 | CDL | C71-CB7-OB8-CB6 |
| 57 | Dm | 501 | CDL | C31-CA7-OA8-CA6 |
| 58 | DX | 306 | PC1 | C32-C31-O31-C3 |
| 57 | DA | 709 | CDL | CB2-OB2-PB2-OB5 |
| 57 | DG | 201 | CDL | CB2-OB2-PB2-OB5 |
| 57 | DM | 501 | CDL | CA3-OA5-PA1-OA2 |
| 57 | DN | 501 | CDL | CA3-OA5-PA1-OA2 |
| 57 | DU | 402 | CDL | CB3-OB5-PB2-OB2 |
| 57 | DU | 404 | CDL | CA3-OA5-PA1-OA2 |
| 57 | DV | 404 | CDL | CA3-OA5-PA1-OA2 |
| 57 | EL | 901 | CDL | CA3-OA5-PA1-OA2 |
| 57 | EL | 901 | CDL | CB3-OB5-PB2-OB2 |
| 57 | EL | 902 | CDL | CA2-OA2-PA1-OA5 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 57 | Dj | 401 | CDL | CB2-OB2-PB2-OB5 |
| 57 | Dj | 403 | CDL | CA2-OA2-PA1-OA5 |
| 57 | Dj | 403 | CDL | CA3-OA5-PA1-OA2 |
| 57 | Dq | 401 | CDL | CB2-OB2-PB2-OB5 |
| 57 | Dq | 404 | CDL | CA2-OA2-PA1-OA5 |
| 57 | Ds | 402 | CDL | CA2-OA2-PA1-OA5 |
| 57 | Dv | 401 | CDL | CB2-OB2-PB2-OB5 |
| 57 | Dv | 404 | CDL | CB3-OB5-PB2-OB2 |
| 58 | Eb | 301 | PC1 | C11-O13-P-O11 |
| 59 | DC | 607 | 3PE | C1-O11-P-O13 |
| 59 | Da | 708 | 3PE | C11-O13-P-O11 |
| 59 | Dg | 204 | 3PE | C1-O11-P-O13 |
| 59 | Eo | 202 | 3PE | C11-O13-P-O11 |
| 57 | DG | 202 | CDL | C63-C64-C65-C66 |
| 58 | DC | 602 | PC1 | C3F-C3G-C3H-C3I |
| 57 | DQ | 1501 | CDL | O1-C1-CA2-OA2 |
| 57 | DR | 403 | CDL | O1-C1-CB2-OB2 |
| 57 | Dv | 403 | CDL | O1-C1-CB2-OB2 |
| 57 | DA | 705 | CDL | C15-C16-C17-C18 |
| 57 | DR | 403 | CDL | C17-C18-C19-C20 |
| 57 | EI | 401 | CDL | C52-C51-CB5-OB6 |
| 57 | DA | 705 | CDL | CB4-CB3-OB5-PB2 |
| 57 | DD | 703 | CDL | CB4-CB3-OB5-PB2 |
| 57 | DG | 201 | CDL | C1-CA2-OA2-PA1 |
| 57 | DG | 201 | CDL | C1-CB2-OB2-PB2 |
| 57 | DN | 504 | CDL | C1-CB2-OB2-PB2 |
| 57 | DU | 404 | CDL | C1-CB2-OB2-PB2 |
| 57 | DV | 404 | CDL | CB4-CB3-OB5-PB2 |
| 57 | EA | 301 | CDL | CA4-CA3-OA5-PA1 |
| 57 | EB | 304 | CDL | C1-CB2-OB2-PB2 |
| 57 | EN | 1202 | CDL | C1-CA2-OA2-PA1 |
| 57 | Da | 705 | CDL | C1-CB2-OB2-PB2 |
| 57 | Dd | 706 | CDL | CA4-CA3-OA5-PA1 |
| 57 | Dj | 403 | CDL | C1-CA2-OA2-PA1 |
| 57 | Dj | 404 | CDL | CB4-CB3-OB5-PB2 |
| 57 | Dn | 502 | CDL | C1-CA2-OA2-PA1 |
| 57 | Dr | 403 | CDL | C1-CB2-OB2-PB2 |
| 57 | Dv | 402 | CDL | C1-CA2-OA2-PA1 |
| 57 | Dv | 404 | CDL | C1-CA2-OA2-PA1 |
| 57 | Dz | 501 | CDL | C1-CB2-OB2-PB2 |
| 57 | Eh | 1601 | CDL | C1-CA2-OA2-PA1 |
| 57 | Ei | 401 | CDL | C1-CB2-OB2-PB2 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 60 | Dn | 504 | LPP | C7-C6-O5-P1 |
| 57 | Ea | 301 | CDL | C11-C12-C13-C14 |
| 59 | Dj | 407 | 3PE | C29-C2A-C2B-C2C |
| 59 | Ds | 401 | 3PE | C34-C35-C36-C37 |
| 58 | EO | 206 | PC1 | O32-C31-O31-C3 |
| 57 | DA | 709 | CDL | CA3-OA5-PA1-OA3 |
| 57 | DA | 709 | CDL | CA3-OA5-PA1-OA4 |
| 57 | DA | 709 | CDL | CB3-OB5-PB2-OB4 |
| 57 | DC | 601 | CDL | CB2-OB2-PB2-OB3 |
| 57 | DD | 703 | CDL | CB2-OB2-PB2-OB3 |
| 57 | DD | 704 | CDL | CA2-OA2-PA1-OA4 |
| 57 | DJ | 303 | CDL | CA3-OA5-PA1-OA3 |
| 57 | DJ | 303 | CDL | CB3-OB5-PB2-OB3 |
| 57 | DJ | 304 | CDL | CA3-OA5-PA1-OA3 |
| 57 | DN | 501 | CDL | CA3-OA5-PA1-OA3 |
| 57 | DN | 505 | CDL | CA2-OA2-PA1-OA3 |
| 57 | DN | 505 | CDL | CA3-OA5-PA1-OA3 |
| 57 | DN | 505 | CDL | CA3-OA5-PA1-OA4 |
| 57 | DO | 501 | CDL | CA3-OA5-PA1-OA3 |
| 57 | DO | 501 | CDL | CB3-OB5-PB2-OB3 |
| 57 | DQ | 1501 | CDL | CB3-OB5-PB2-OB4 |
| 57 | DQ | 1504 | CDL | CB3-OB5-PB2-OB4 |
| 57 | DR | 402 | CDL | CB2-OB2-PB2-OB4 |
| 57 | DS | 402 | CDL | CB3-OB5-PB2-OB4 |
| 57 | DS | 405 | CDL | CA2-OA2-PA1-OA4 |
| 57 | DS | 405 | CDL | CB3-OB5-PB2-OB4 |
| 57 | DU | 401 | CDL | CA2-OA2-PA1-OA4 |
| 57 | DU | 403 | CDL | CA2-OA2-PA1-OA4 |
| 57 | DU | 403 | CDL | CB3-OB5-PB2-OB4 |
| 57 | DU | 404 | CDL | CB2-OB2-PB2-OB4 |
| 57 | DV | 402 | CDL | CA3-OA5-PA1-OA3 |
| 57 | DX | 301 | CDL | CB2-OB2-PB2-OB3 |
| 57 | DX | 301 | CDL | CB3-OB5-PB2-OB3 |
| 57 | DZ | 501 | CDL | CA2-OA2-PA1-OA3 |
| 57 | EA | 301 | CDL | CB2-OB2-PB2-OB4 |
| 57 | EB | 302 | CDL | CB3-OB5-PB2-OB3 |
| 57 | EB | 304 | CDL | CB3-OB5-PB2-OB3 |
| 57 | EH | 202 | CDL | CA3-OA5-PA1-OA3 |
| 57 | EH | 202 | CDL | CB3-OB5-PB2-OB3 |
| 57 | EI | 401 | CDL | CB3-OB5-PB2-OB4 |
| 57 | EK | 201 | CDL | CA2-OA2-PA1-OA3 |
| 57 | EK | 201 | CDL | CA3-OA5-PA1-OA3 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 57 | EK | 201 | CDL | CA3-OA5-PA1-OA4 |
| 57 | EL | 903 | CDL | CB2-OB2-PB2-OB3 |
| 57 | EL | 903 | CDL | CB2-OB2-PB2-OB4 |
| 57 | EN | 1201 | CDL | CA2-OA2-PA1-OA4 |
| 57 | EU | 101 | CDL | CA3-OA5-PA1-OA4 |
| 57 | EU | 101 | CDL | CB3-OB5-PB2-OB4 |
| 57 | Da | 705 | CDL | CB3-OB5-PB2-OB3 |
| 57 | Da | 709 | CDL | CA3-OA5-PA1-OA3 |
| 57 | Da | 709 | CDL | CB3-OB5-PB2-OB4 |
| 57 | Dc | 601 | CDL | CB2-OB2-PB2-OB3 |
| 57 | Dd | 704 | CDL | CB2-OB2-PB2-OB3 |
| 57 | Dg | 201 | CDL | CB3-OB5-PB2-OB4 |
| 57 | Dh | 202 | CDL | CB2-OB2-PB2-OB3 |
| 57 | Dh | 202 | CDL | CB3-OB5-PB2-OB3 |
| 57 | Dj | 401 | CDL | CB3-OB5-PB2-OB3 |
| 57 | Dj | 402 | CDL | CA2-OA2-PA1-OA4 |
| 57 | Dj | 402 | CDL | CA3-OA5-PA1-OA4 |
| 57 | Dj | 403 | CDL | CA3-OA5-PA1-OA3 |
| 57 | Dj | 404 | CDL | CB3-OB5-PB2-OB4 |
| 57 | Dj | 408 | CDL | CA2-OA2-PA1-OA4 |
| 57 | Dj | 408 | CDL | CB2-OB2-PB2-OB3 |
| 57 | Dm | 501 | CDL | CA3-OA5-PA1-OA3 |
| 57 | Dm | 501 | CDL | CB2-OB2-PB2-OB4 |
| 57 | Dn | 502 | CDL | CB3-OB5-PB2-OB3 |
| 57 | Do | 501 | CDL | CB3-OB5-PB2-OB3 |
| 57 | Dq | 401 | CDL | CB3-OB5-PB2-OB3 |
| 57 | Dq | 402 | CDL | CA2-OA2-PA1-OA3 |
| 57 | Dq | 403 | CDL | CB3-OB5-PB2-OB4 |
| 57 | Dq | 404 | CDL | CA3-OA5-PA1-OA3 |
| 57 | Dq | 404 | CDL | CB3-OB5-PB2-OB3 |
| 57 | Ds | 402 | CDL | CB3-OB5-PB2-OB4 |
| 57 | Ds | 405 | CDL | CA2-OA2-PA1-OA4 |
| 57 | Ds | 405 | CDL | CB3-OB5-PB2-OB4 |
| 57 | Du | 401 | CDL | CA2-OA2-PA1-OA4 |
| 57 | Du | 403 | CDL | CA3-OA5-PA1-OA3 |
| 57 | Du | 403 | CDL | CA3-OA5-PA1-OA4 |
| 57 | Du | 404 | CDL | CB3-OB5-PB2-OB4 |
| 57 | Dv | 403 | CDL | CA3-OA5-PA1-OA3 |
| 57 | Dx | 1201 | CDL | CB3-OB5-PB2-OB3 |
| 57 | Dx | 1203 | CDL | CA3-OA5-PA1-OA3 |
| 57 | Dx | 1203 | CDL | CA3-OA5-PA1-OA4 |
| 57 | Dx | 1203 | CDL | CB3-OB5-PB2-OB3 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 57 | Ea | 301 | CDL | CA2-OA2-PA1-OA3 |
| 57 | Ea | 301 | CDL | CA2-OA2-PA1-OA4 |
| 57 | Ea | 301 | CDL | CB2-OB2-PB2-OB4 |
| 57 | Ed | 204 | CDL | CB3-OB5-PB2-OB3 |
| 57 | Ed | 205 | CDL | CA3-OA5-PA1-OA4 |
| 57 | Ei | 401 | CDL | CB3-OB5-PB2-OB3 |
| 57 | El | 902 | CDL | CB2-OB2-PB2-OB3 |
| 57 | El | 902 | CDL | CB2-OB2-PB2-OB4 |
| 57 | El | 902 | CDL | CB3-OB5-PB2-OB3 |
| 57 | El | 903 | CDL | CA3-OA5-PA1-OA3 |
| 57 | El | 903 | CDL | CB2-OB2-PB2-OB4 |
| 57 | Eu | 101 | CDL | CB2-OB2-PB2-OB3 |
| 58 | DC | 602 | PC1 | C11-O13-P-O12 |
| 58 | DC | 602 | PC1 | C11-O13-P-O14 |
| 58 | DC | 603 | PC1 | C11-O13-P-O14 |
| 58 | DC | 605 | PC1 | C1-O11-P-O12 |
| 58 | DI | 702 | PC1 | C11-O13-P-O12 |
| 58 | DI | 702 | PC1 | C11-O13-P-O14 |
| 58 | DJ | 306 | PC1 | C11-O13-P-O14 |
| 58 | DJ | 306 | PC1 | C1-O11-P-O14 |
| 58 | DQ | 1503 | PC1 | C11-O13-P-O14 |
| 58 | DS | 407 | PC1 | C11-O13-P-O12 |
| 58 | DV | 405 | PC1 | C11-O13-P-O14 |
| 58 | DV | 406 | PC1 | C11-O13-P-O14 |
| 58 | DX | 302 | PC1 | C1-O11-P-O14 |
| 58 | DX | 306 | PC1 | C11-O13-P-O14 |
| 58 | EB | 301 | PC1 | C11-O13-P-O12 |
| 58 | EB | 301 | PC1 | C1-O11-P-O12 |
| 58 | EB | 301 | PC1 | C1-O11-P-O14 |
| 58 | EO | 201 | PC1 | C11-O13-P-O14 |
| 58 | EO | 206 | PC1 | C1-O11-P-O14 |
| 58 | EO | 206 | PC1 | C11-C12-N-C15 |
| 58 | Da | 706 | PC1 | C11-O13-P-O12 |
| 58 | Db | 702 | PC1 | C11-O13-P-O14 |
| 58 | Dc | 602 | PC1 | C11-O13-P-O12 |
| 58 | Dc | 602 | PC1 | C11-O13-P-O14 |
| 58 | Dc | 603 | PC1 | C11-O13-P-O14 |
| 58 | Dc | 604 | PC1 | C11-O13-P-O14 |
| 58 | Dc | 604 | PC1 | C1-O11-P-O12 |
| 58 | Dc | 604 | PC1 | C1-O11-P-O14 |
| 58 | Dc | 605 | PC1 | C1-O11-P-O12 |
| 58 | Di | 702 | PC1 | C11-O13-P-O14 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 58 | Di | 702 | PC1 | C1-O11-P-O12 |
| 58 | Dj | 406 | PC1 | C11-O13-P-O14 |
| 58 | Dj | 406 | PC1 | C1-O11-P-O14 |
| 58 | Dq | 405 | PC1 | C11-O13-P-O14 |
| 58 | Dv | 405 | PC1 | C11-O13-P-O12 |
| 58 | Dv | 407 | PC1 | C11-O13-P-O14 |
| 58 | Dv | 408 | PC1 | C1-O11-P-O14 |
| 58 | Eb | 301 | PC1 | C1-O11-P-O12 |
| 58 | Ef | 1001 | PC1 | C1-O11-P-O14 |
| 58 | Eo | 201 | PC1 | C11-O13-P-O14 |
| 58 | Eo | 204 | PC1 | C11-C12-N-C15 |
| 59 | DC | 607 | 3PE | C1-O11-P-O12 |
| 59 | DC | 607 | 3PE | C1-O11-P-O14 |
| 59 | DC | 607 | 3PE | C11-O13-P-O12 |
| 59 | DG | 204 | 3PE | C1-O11-P-O12 |
| 59 | DG | 204 | 3PE | C1-O11-P-O14 |
| 59 | DG | 205 | 3PE | C1-O11-P-O12 |
| 59 | DJ | 301 | 3PE | C11-O13-P-O12 |
| 59 | DS | 403 | 3PE | C1-O11-P-O12 |
| 59 | DS | 403 | 3PE | C11-O13-P-O12 |
| 59 | DX | 304 | 3PE | C11-O13-P-O12 |
| 59 | EL | 905 | 3PE | C11-O13-P-O12 |
| 59 | EN | 1203 | 3PE | C11-O13-P-O12 |
| 59 | Da | 708 | 3PE | C11-O13-P-O14 |
| 59 | Dr | 401 | 3PE | C11-O13-P-O12 |
| 59 | Dr | 401 | 3PE | C11-O13-P-O14 |
| 59 | Dr | 404 | 3PE | C1-O11-P-O12 |
| 59 | Ds | 403 | 3PE | C1-O11-P-O12 |
| 59 | Ds | 403 | 3PE | C11-O13-P-O12 |
| 59 | Dx | 1206 | 3PE | C1-O11-P-O12 |
| 59 | Dx | 1207 | 3PE | C11-O13-P-O14 |
| 59 | El | 905 | 3PE | C1-O11-P-O12 |
| 59 | El | 905 | 3PE | C11-O13-P-O12 |
| 57 | Da | 705 | CDL | C62-C63-C64-C65 |
| 58 | DX | 302 | PC1 | C23-C24-C25-C26 |
| 57 | Dr | 403 | CDL | C71-CB7-OB8-CB6 |
| 57 | DQ | 1504 | CDL | OB5-CB3-CB4-CB6 |
| 57 | DS | 405 | CDL | OA5-CA3-CA4-CA6 |
| 57 | ED | 601 | CDL | OB5-CB3-CB4-CB6 |
| 57 | EL | 902 | CDL | OA5-CA3-CA4-CA6 |
| 57 | EL | 902 | CDL | OB5-CB3-CB4-CB6 |
| 57 | EL | 904 | CDL | OA5-CA3-CA4-CA6 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 57 | Dd | 704 | CDL | OA5-CA3-CA4-CA6 |
| 57 | Dn | 503 | CDL | OB5-CB3-CB4-CB6 |
| 57 | Du | 404 | CDL | OB5-CB3-CB4-CB6 |
| 57 | Dv | 403 | CDL | OA5-CA3-CA4-CA6 |
| 57 | Eh | 1601 | CDL | OA5-CA3-CA4-CA6 |
| 59 | DX | 303 | 3PE | O11-C1-C2-C3 |
| 59 | Dx | 1205 | 3PE | O11-C1-C2-C3 |
| 59 | El | 905 | 3PE | O11-C1-C2-C3 |
| 57 | Du | 404 | CDL | C13-C14-C15-C16 |
| 57 | DN | 501 | CDL | OA9-CA7-OA8-CA6 |
| 57 | Ei | 401 | CDL | C52-C51-CB5-OB6 |
| 57 | DX | 307 | CDL | C78-C79-C80-C81 |
| 58 | EO | 201 | PC1 | C32-C33-C34-C35 |
| 57 | Dd | 704 | CDL | C74-C75-C76-C77 |
| 57 | Di | 701 | CDL | C33-C34-C35-C36 |
| 65 | EL | 906 | UQ8 | C5-C4-O4-C4M |
| 57 | Dj | 408 | CDL | C52-C53-C54-C55 |
| 58 | DB | 702 | PC1 | C12-C11-O13-P |
| 58 | DS | 407 | PC1 | C12-C11-O13-P |
| 58 | Db | 702 | PC1 | C12-C11-O13-P |
| 58 | Dv | 406 | PC1 | C12-C11-O13-P |
| 58 | Dx | 1202 | PC1 | C12-C11-O13-P |
| 59 | DX | 303 | 3PE | C12-C11-O13-P |
| 59 | Dg | 204 | 3PE | C12-C11-O13-P |
| 59 | Dx | 1205 | 3PE | C12-C11-O13-P |
| 57 | EL | 902 | CDL | C73-C74-C75-C76 |
| 57 | Dg | 202 | CDL | C13-C14-C15-C16 |
| 58 | Dv | 405 | PC1 | C3B-C3C-C3D-C3E |
| 57 | Dr | 403 | CDL | C17-C18-C19-C20 |
| 58 | Eb | 302 | PC1 | C2E-C2F-C2G-C2H |
| 59 | Dg | 204 | 3PE | C2A-C2B-C2C-C2D |
| 59 | El | 905 | 3PE | C33-C34-C35-C36 |
| 57 | Dn | 502 | CDL | CA5-C11-C12-C13 |
| 57 | Da | 705 | CDL | C34-C35-C36-C37 |
| 57 | Dn | 507 | CDL | C37-C38-C39-C40 |
| 57 | El | 901 | CDL | C31-CA7-OA8-CA6 |
| 57 | DX | 307 | CDL | CB2-C1-CA2-OA2 |
| 57 | EK | 201 | CDL | CB2-C1-CA2-OA2 |
| 57 | Dj | 403 | CDL | OB7-CB5-OB6-CB4 |
| 57 | EH | 201 | CDL | C23-C24-C25-C26 |
| 57 | EL | 901 | CDL | C55-C56-C57-C58 |
| 57 | EN | 1202 | CDL | C37-C38-C39-C40 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 58 | Dg | 203 | PC1 | C23-C24-C25-C26 |
| 57 | DC | 601 | CDL | OB5-CB3-CB4-OB6 |
| 57 | DD | 703 | CDL | OB5-CB3-CB4-OB6 |
| 57 | DJ | 304 | CDL | OA5-CA3-CA4-OA6 |
| 57 | DQ | 1502 | CDL | OB5-CB3-CB4-OB6 |
| 57 | EH | 202 | CDL | OA5-CA3-CA4-OA6 |
| 57 | EH | 202 | CDL | OB5-CB3-CB4-OB6 |
| 57 | EL | 902 | CDL | OB5-CB3-CB4-OB6 |
| 57 | EU | 101 | CDL | OA5-CA3-CA4-OA6 |
| 57 | Da | 709 | CDL | OB5-CB3-CB4-OB6 |
| 57 | Dd | 704 | CDL | OA5-CA3-CA4-OA6 |
| 57 | Dd | 705 | CDL | OA5-CA3-CA4-OA6 |
| 57 | Dj | 405 | CDL | OB5-CB3-CB4-OB6 |
| 57 | Dn | 502 | CDL | OB5-CB3-CB4-OB6 |
| 57 | Dn | 503 | CDL | OB5-CB3-CB4-OB6 |
| 57 | Dq | 402 | CDL | OA5-CA3-CA4-OA6 |
| 57 | Dq | 402 | CDL | OB5-CB3-CB4-OB6 |
| 57 | Dq | 404 | CDL | OB5-CB3-CB4-OB6 |
| 57 | Eh | 1601 | CDL | OA5-CA3-CA4-OA6 |
| 58 | DG | 203 | PC1 | O11-C1-C2-O21 |
| 58 | Db | 702 | PC1 | O11-C1-C2-O21 |
| 59 | Dx | 1206 | 3PE | O11-C1-C2-O21 |
| 57 | EO | 202 | CDL | C58-C59-C60-C61 |
| 57 | El | 901 | CDL | C32-C33-C34-C35 |
| 58 | Dg | 203 | PC1 | O32-C31-O31-C3 |
| 57 | DR | 402 | CDL | C13-C14-C15-C16 |
| 57 | Dr | 402 | CDL | C59-C60-C61-C62 |
| 57 | Dv | 401 | CDL | C78-C79-C80-C81 |
| 58 | Eo | 205 | PC1 | C3D-C3E-C3F-C3G |
| 57 | Dx | 1203 | CDL | C14-C15-C16-C17 |
| 57 | Dq | 404 | CDL | C51-CB5-OB6-CB4 |
| 57 | Ed | 205 | CDL | C51-CB5-OB6-CB4 |
| 57 | EN | 1202 | CDL | C58-C59-C60-C61 |
| 57 | Du | 401 | CDL | C60-C61-C62-C63 |
| 57 | EB | 302 | CDL | OA9-CA7-OA8-CA6 |
| 57 | Dj | 403 | CDL | OB9-CB7-OB8-CB6 |
| 57 | Dm | 501 | CDL | OA9-CA7-OA8-CA6 |
| 57 | El | 903 | CDL | OA9-CA7-OA8-CA6 |
| 58 | DA | 707 | PC1 | O32-C31-O31-C3 |
| 58 | DX | 306 | PC1 | O32-C31-O31-C3 |
| 57 | EO | 202 | CDL | O1-C1-CA2-OA2 |
| 57 | Du | 404 | CDL | O1-C1-CB2-OB2 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 54 | Da | 702 | HEA | C2D-C3D-CAD-CBD |
| 58 | DS | 407 | PC1 | C11-C12-N-C13 |
| 57 | DA | 705 | CDL | C62-C63-C64-C65 |
| 57 | DA | 709 | CDL | C76-C77-C78-C79 |
| 57 | Dh | 202 | CDL | C71-C72-C73-C74 |
| 57 | Ep | 701 | CDL | C84-C85-C86-C87 |
| 58 | Dv | 406 | PC1 | C32-C33-C34-C35 |
| 57 | DH | 201 | CDL | CB3-CB4-CB6-OB8 |
| 57 | DN | 505 | CDL | CA3-CA4-CA6-OA8 |
| 57 | DS | 405 | CDL | C33-C34-C35-C36 |
| 57 | DV | 402 | CDL | C76-C77-C78-C79 |
| 57 | ED | 601 | CDL | CA3-CA4-CA6-OA8 |
| 57 | EL | 903 | CDL | C13-C14-C15-C16 |
| 57 | Dd | 702 | CDL | CB3-CB4-CB6-OB8 |
| 57 | Dh | 201 | CDL | CB3-CB4-CB6-OB8 |
| 57 | Ek | 201 | CDL | CA3-CA4-CA6-OA8 |
| 57 | En | 1201 | CDL | CA3-CA4-CA6-OA8 |
| 58 | DB | 702 | PC1 | O13-C11-C12-N |
| 58 | DC | 604 | PC1 | O13-C11-C12-N |
| 58 | DS | 406 | PC1 | O13-C11-C12-N |
| 58 | DV | 406 | PC1 | O13-C11-C12-N |
| 58 | EO | 205 | PC1 | O13-C11-C12-N |
| 58 | Db | 702 | PC1 | O13-C11-C12-N |
| 58 | Dc | 604 | PC1 | O13-C11-C12-N |
| 58 | Dc | 605 | PC1 | O13-C11-C12-N |
| 58 | Dv | 406 | PC1 | O13-C11-C12-N |
| 58 | Dv | 407 | PC1 | O13-C11-C12-N |
| 58 | El | 904 | PC1 | O13-C11-C12-N |
| 57 | DC | 601 | CDL | OA6-CA4-CA6-OA8 |
| 57 | DG | 202 | CDL | OB6-CB4-CB6-OB8 |
| 57 | DI | 701 | CDL | OA6-CA4-CA6-OA8 |
| 57 | DM | 502 | CDL | OB6-CB4-CB6-OB8 |
| 57 | DN | 505 | CDL | OA6-CA4-CA6-OA8 |
| 57 | DN | 505 | CDL | OB6-CB4-CB6-OB8 |
| 57 | DU | 401 | CDL | OA6-CA4-CA6-OA8 |
| 57 | EB | 304 | CDL | OB6-CB4-CB6-OB8 |
| 57 | EL | 903 | CDL | OA6-CA4-CA6-OA8 |
| 57 | Dc | 601 | CDL | OA6-CA4-CA6-OA8 |
| 57 | Dd | 702 | CDL | OA6-CA4-CA6-OA8 |
| 57 | Dg | 202 | CDL | OB6-CB4-CB6-OB8 |
| 57 | Dh | 201 | CDL | OB6-CB4-CB6-OB8 |
| 57 | Du | 403 | CDL | OB6-CB4-CB6-OB8 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 57 | Ep | 701 | CDL | OB6-CB4-CB6-OB8 |
| 58 | DC | 605 | PC1 | O21-C2-C3-O31 |
| 58 | DC | 608 | PC1 | O21-C2-C3-O31 |
| 58 | Dv | 405 | PC1 | O21-C2-C3-O31 |
| 58 | Dv | 406 | PC1 | O21-C2-C3-O31 |
| 58 | Eo | 201 | PC1 | O21-C2-C3-O31 |
| 59 | EL | 905 | 3PE | O21-C2-C3-O31 |
| 57 | DQ | 1504 | CDL | C51-C52-C53-C54 |
| 57 | Dd | 704 | CDL | C21-C22-C23-C24 |
| 58 | DG | 203 | PC1 | C23-C24-C25-C26 |
| 58 | DG | 203 | PC1 | C3B-C3C-C3D-C3E |
| 59 | Ds | 403 | 3PE | C28-C29-C2A-C2B |
| 57 | El | 901 | CDL | C13-C14-C15-C16 |
| 57 | DA | 709 | CDL | CB4-CB3-OB5-PB2 |
| 57 | DN | 505 | CDL | CA4-CA3-OA5-PA1 |
| 57 | Dx | 1201 | CDL | C1-CB2-OB2-PB2 |
| 57 | Dj | 402 | CDL | C16-C17-C18-C19 |
| 57 | Dj | 404 | CDL | C63-C64-C65-C66 |
| 57 | Dr | 403 | CDL | OB9-CB7-OB8-CB6 |
| 57 | El | 901 | CDL | OA9-CA7-OA8-CA6 |
| 65 | Ed | 202 | UQ8 | C40-C39-C41-C42 |
| 57 | DX | 307 | CDL | C71-CB7-OB8-CB6 |
| 57 | Dj | 404 | CDL | C31-CA7-OA8-CA6 |
| 57 | DQ | 1504 | CDL | C61-C62-C63-C64 |
| 57 | Da | 705 | CDL | C82-C83-C84-C85 |
| 57 | DR | 403 | CDL | C34-C35-C36-C37 |
| 57 | DX | 301 | CDL | C33-C34-C35-C36 |
| 57 | Dd | 704 | CDL | C20-C21-C22-C23 |
| 57 | Dn | 505 | CDL | C54-C55-C56-C57 |
| 58 | Db | 702 | PC1 | C3B-C3C-C3D-C3E |
| 65 | El | 906 | UQ8 | C39-C41-C42-C43 |
| 57 | DX | 307 | CDL | OB9-CB7-OB8-CB6 |
| 57 | En | 1201 | CDL | C12-C11-CA5-OA6 |
| 58 | DI | 702 | PC1 | C11-C12-N-C15 |
| 58 | Di | 702 | PC1 | C11-C12-N-C15 |
| 57 | DD | 704 | CDL | C40-C41-C42-C43 |
| 57 | Dr | 402 | CDL | C53-C54-C55-C56 |
| 57 | Dx | 1201 | CDL | C32-C33-C34-C35 |
| 58 | EO | 201 | PC1 | C29-C2A-C2B-C2C |
| 57 | Dv | 401 | CDL | C72-C71-CB7-OB8 |
| 60 | Dl | 1101 | LPP | O27-C29-C30-C31 |
| 57 | DM | 502 | CDL | C19-C20-C21-C22 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 59 | El | 905 | 3PE | C2F-C2G-C2H-C2I |
| 57 | EB | 304 | CDL | CB5-C51-C52-C53 |
| 58 | Eo | 201 | PC1 | C2B-C2C-C2D-C2E |
| 65 | EN | 1204 | UQ8 | C2-C3-O3-C3M |
| 65 | Ds | 404 | UQ8 | C2-C3-O3-C3M |
| 65 | Ds | 404 | UQ8 | C5-C4-O4-C4M |
| 65 | El | 906 | UQ8 | C2-C3-O3-C3M |
| 57 | DV | 401 | CDL | C72-C71-CB7-OB8 |
| 57 | Dj | 408 | CDL | C72-C71-CB7-OB8 |
| 57 | DG | 202 | CDL | C72-C73-C74-C75 |
| 57 | EL | 901 | CDL | C83-C84-C85-C86 |
| 65 | EN | 1204 | UQ8 | C38-C39-C41-C42 |
| 57 | En | 1201 | CDL | C14-C15-C16-C17 |
| 57 | Dn | 503 | CDL | C14-C15-C16-C17 |
| 57 | DH | 201 | CDL | C12-C13-C14-C15 |
| 57 | DI | 701 | CDL | C33-C34-C35-C36 |
| 57 | ED | 601 | CDL | C35-C36-C37-C38 |
| 58 | Dc | 607 | PC1 | O31-C31-C32-C33 |
| 57 | DA | 709 | CDL | CB6-CB4-OB6-CB5 |
| 57 | DC | 601 | CDL | CB6-CB4-OB6-CB5 |
| 57 | DD | 703 | CDL | CA6-CA4-OA6-CA5 |
| 57 | DD | 703 | CDL | CB3-CB4-OB6-CB5 |
| 57 | DJ | 303 | CDL | CB3-CB4-OB6-CB5 |
| 57 | DN | 501 | CDL | CA6-CA4-OA6-CA5 |
| 57 | DN | 504 | CDL | CA3-CA4-OA6-CA5 |
| 57 | DO | 501 | CDL | CB6-CB4-OB6-CB5 |
| 57 | DQ | 1502 | CDL | CB6-CB4-OB6-CB5 |
| 57 | DQ | 1504 | CDL | CA6-CA4-OA6-CA5 |
| 57 | DR | 403 | CDL | CA6-CA4-OA6-CA5 |
| 57 | DS | 402 | CDL | CB3-CB4-OB6-CB5 |
| 57 | EK | 201 | CDL | CB3-CB4-OB6-CB5 |
| 57 | EL | 901 | CDL | CA3-CA4-OA6-CA5 |
| 57 | EO | 202 | CDL | CB3-CB4-OB6-CB5 |
| 57 | Da | 709 | CDL | CA3-CA4-OA6-CA5 |
| 57 | Dc | 601 | CDL | CB6-CB4-OB6-CB5 |
| 57 | Di | 701 | CDL | CA6-CA4-OA6-CA5 |
| 57 | Dj | 405 | CDL | CB6-CB4-OB6-CB5 |
| 57 | Dn | 505 | CDL | CA6-CA4-OA6-CA5 |
| 57 | Dn | 507 | CDL | CA3-CA4-OA6-CA5 |
| 57 | Dq | 402 | CDL | CA6-CA4-OA6-CA5 |
| 57 | Dr | 403 | CDL | CA6-CA4-OA6-CA5 |
| 57 | Ds | 402 | CDL | CB3-CB4-OB6-CB5 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 57 | Du | 404 | CDL | CA3-CA4-OA6-CA5 |
| 57 | Dv | 404 | CDL | CA3-CA4-OA6-CA5 |
| 57 | Ek | 201 | CDL | CB3-CB4-OB6-CB5 |
| 57 | El | 903 | CDL | CA3-CA4-OA6-CA5 |
| 57 | En | 1202 | CDL | CB6-CB4-OB6-CB5 |
| 58 | Db | 702 | PC1 | C1-C2-O21-C21 |
| 58 | Dc | 605 | PC1 | C3-C2-O21-C21 |
| 58 | Dv | 406 | PC1 | C1-C2-O21-C21 |
| 58 | Eo | 205 | PC1 | C3-C2-O21-C21 |
| 59 | DC | 606 | 3PE | C1-C2-O21-C21 |
| 59 | EO | 203 | 3PE | C1-C2-O21-C21 |
| 59 | EO | 204 | 3PE | C1-C2-O21-C21 |
| 59 | Dr | 401 | 3PE | C1-C2-O21-C21 |
| 57 | DD | 703 | CDL | OB5-CB3-CB4-CB6 |
| 57 | DJ | 304 | CDL | OA5-CA3-CA4-CA6 |
| 59 | Ds | 403 | 3PE | O11-C1-C2-C3 |
| 57 | Dc | 601 | CDL | C31-CA7-OA8-CA6 |
| 57 | Da | 705 | CDL | C17-C18-C19-C20 |
| 58 | DI | 702 | PC1 | C35-C36-C37-C38 |
| 57 | El | 901 | CDL | CB5-C51-C52-C53 |
| 57 | Eh | 1601 | CDL | C21-C22-C23-C24 |
| 58 | Ds | 406 | PC1 | C3C-C3D-C3E-C3F |
| 58 | DC | 608 | PC1 | O31-C31-C32-C33 |
| 57 | Dj | 404 | CDL | OA9-CA7-OA8-CA6 |
| 57 | Dh | 202 | CDL | C79-C80-C81-C82 |
| 57 | Eu | 101 | CDL | C72-C73-C74-C75 |
| 57 | DV | 401 | CDL | C1-CA2-OA2-PA1 |
| 57 | DV | 403 | CDL | C1-CA2-OA2-PA1 |
| 57 | ED | 601 | CDL | C1-CB2-OB2-PB2 |
| 57 | Dj | 403 | CDL | CA4-CA3-OA5-PA1 |
| 57 | Dj | 404 | CDL | C1-CB2-OB2-PB2 |
| 57 | Dv | 401 | CDL | C1-CA2-OA2-PA1 |
| 59 | Dd | 703 | 3PE | C2-C1-O11-P |
| 57 | DG | 202 | CDL | C34-C35-C36-C37 |
| 57 | EL | 904 | CDL | C84-C85-C86-C87 |
| 57 | Dj | 404 | CDL | C61-C62-C63-C64 |
| 57 | Ds | 405 | CDL | C33-C34-C35-C36 |
| 59 | DS | 401 | 3PE | C34-C35-C36-C37 |
| 57 | Dj | 402 | CDL | CA4-CA6-OA8-CA7 |
| 57 | Dc | 601 | CDL | OA9-CA7-OA8-CA6 |
| 57 | DA | 705 | CDL | OB5-CB3-CB4-OB6 |
| 57 | DS | 402 | CDL | OB5-CB3-CB4-OB6 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 57 | DU | 401 | CDL | OB5-CB3-CB4-OB6 |
| 59 | Dj | 407 | 3PE | O11-C1-C2-O21 |
| 59 | Dx | 1205 | 3PE | O11-C1-C2-O21 |
| 57 | Dd | 702 | CDL | C23-C24-C25-C26 |
| 57 | Dd | 704 | CDL | C12-C13-C14-C15 |
| 58 | DS | 407 | PC1 | C11-C12-N-C15 |
| 58 | Eo | 204 | PC1 | C11-C12-N-C14 |
| 57 | El | 903 | CDL | CA5-C11-C12-C13 |
| 57 | Ed | 205 | CDL | OB7-CB5-OB6-CB4 |
| 57 | Eu | 101 | CDL | OB7-CB5-OB6-CB4 |
| 57 | DS | 405 | CDL | C14-C15-C16-C17 |
| 58 | DC | 604 | PC1 | C27-C28-C29-C2A |
| 57 | Dm | 502 | CDL | CB7-C71-C72-C73 |
| 57 | EH | 201 | CDL | C44-C45-C46-C47 |
| 57 | DV | 402 | CDL | O1-C1-CB2-OB2 |
| 57 | DO | 501 | CDL | C11-C12-C13-C14 |
| 57 | Dj | 401 | CDL | C17-C18-C19-C20 |
| 57 | Eu | 101 | CDL | C51-CB5-OB6-CB4 |
| 59 | EL | 905 | 3PE | C2F-C2G-C2H-C2I |
| 57 | Dj | 404 | CDL | C62-C63-C64-C65 |
| 58 | Dx | 1204 | PC1 | C2B-C2C-C2D-C2E |
| 57 | Ds | 402 | CDL | OA9-CA7-OA8-CA6 |
| 57 | EN | 1202 | CDL | OB6-CB4-CB6-OB8 |
| 57 | Da | 705 | CDL | OB6-CB4-CB6-OB8 |
| 57 | Dh | 202 | CDL | OB6-CB4-CB6-OB8 |
| 57 | Dn | 501 | CDL | OB6-CB4-CB6-OB8 |
| 57 | Eh | 1601 | CDL | OB6-CB4-CB6-OB8 |
| 59 | EM | 901 | 3PE | O21-C2-C3-O31 |
| 57 | Di | 701 | CDL | C62-C63-C64-C65 |
| 57 | El | 901 | CDL | C36-C37-C38-C39 |
| 57 | DZ | 501 | CDL | C31-CA7-OA8-CA6 |
| 57 | DA | 710 | CDL | CB2-OB2-PB2-OB5 |
| 57 | DH | 201 | CDL | CA2-OA2-PA1-OA5 |
| 57 | DH | 201 | CDL | CB2-OB2-PB2-OB5 |
| 57 | DI | 701 | CDL | CB2-OB2-PB2-OB5 |
| 57 | DJ | 302 | CDL | CB2-OB2-PB2-OB5 |
| 57 | DJ | 304 | CDL | CA2-OA2-PA1-OA5 |
| 57 | DJ | 304 | CDL | CB3-OB5-PB2-OB2 |
| 57 | DJ | 305 | CDL | CB2-OB2-PB2-OB5 |
| 57 | DJ | 307 | CDL | CA2-OA2-PA1-OA5 |
| 57 | DJ | 307 | CDL | CB2-OB2-PB2-OB5 |
| 57 | DM | 502 | CDL | CA2-OA2-PA1-OA5 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 57 | DM | 502 | CDL | CB2-OB2-PB2-OB5 |
| 57 | DN | 501 | CDL | CB2-OB2-PB2-OB5 |
| 57 | DN | 504 | CDL | CB3-OB5-PB2-OB2 |
| 57 | DN | 505 | CDL | CB3-OB5-PB2-OB2 |
| 57 | DQ | 1501 | CDL | CA2-OA2-PA1-OA5 |
| 57 | DQ | 1502 | CDL | CA2-OA2-PA1-OA5 |
| 57 | DR | 403 | CDL | CA2-OA2-PA1-OA5 |
| 57 | DS | 402 | CDL | CA2-OA2-PA1-OA5 |
| 57 | DV | 401 | CDL | CB2-OB2-PB2-OB5 |
| 57 | DV | 404 | CDL | CB3-OB5-PB2-OB2 |
| 57 | DX | 301 | CDL | CA2-OA2-PA1-OA5 |
| 57 | DY | 301 | CDL | CA2-OA2-PA1-OA5 |
| 57 | DY | 301 | CDL | CB3-OB5-PB2-OB2 |
| 57 | EB | 302 | CDL | CA2-OA2-PA1-OA5 |
| 57 | EB | 302 | CDL | CB2-OB2-PB2-OB5 |
| 57 | ED | 601 | CDL | CA2-OA2-PA1-OA5 |
| 57 | ED | 601 | CDL | CB3-OB5-PB2-OB2 |
| 57 | ED | 604 | CDL | CB3-OB5-PB2-OB2 |
| 57 | EI | 401 | CDL | CA2-OA2-PA1-OA5 |
| 57 | EL | 904 | CDL | CB2-OB2-PB2-OB5 |
| 57 | EN | 1201 | CDL | CB2-OB2-PB2-OB5 |
| 57 | EN | 1202 | CDL | CA2-OA2-PA1-OA5 |
| 57 | EN | 1202 | CDL | CB2-OB2-PB2-OB5 |
| 57 | EO | 202 | CDL | CB3-OB5-PB2-OB2 |
| 57 | EU | 101 | CDL | CA2-OA2-PA1-OA5 |
| 57 | EU | 101 | CDL | CB2-OB2-PB2-OB5 |
| 57 | Dd | 705 | CDL | CB3-OB5-PB2-OB2 |
| 57 | Dg | 201 | CDL | CB2-OB2-PB2-OB5 |
| 57 | Dh | 201 | CDL | CA2-OA2-PA1-OA5 |
| 57 | Dh | 201 | CDL | CB2-OB2-PB2-OB5 |
| 57 | Dj | 403 | CDL | CB3-OB5-PB2-OB2 |
| 57 | Dj | 404 | CDL | CA2-OA2-PA1-OA5 |
| 57 | Dj | 405 | CDL | CB2-OB2-PB2-OB5 |
| 57 | Dm | 501 | CDL | CA2-OA2-PA1-OA5 |
| 57 | Dm | 502 | CDL | CA2-OA2-PA1-OA5 |
| 57 | Dn | 501 | CDL | CB2-OB2-PB2-OB5 |
| 57 | Dn | 501 | CDL | CB3-OB5-PB2-OB2 |
| 57 | Dn | 503 | CDL | CA2-OA2-PA1-OA5 |
| 57 | Dn | 505 | CDL | CA2-OA2-PA1-OA5 |
| 57 | Dq | 401 | CDL | CA2-OA2-PA1-OA5 |
| 57 | Du | 402 | CDL | CB2-OB2-PB2-OB5 |
| 57 | Du | 404 | CDL | CA3-OA5-PA1-OA2 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 57 | Dy | 301 | CDL | CA2-OA2-PA1-OA5 |
| 57 | Dy | 301 | CDL | CB3-OB5-PB2-OB2 |
| 57 | Dz | 501 | CDL | CA2-OA2-PA1-OA5 |
| 57 | Ed | 204 | CDL | CA2-OA2-PA1-OA5 |
| 57 | Eh | 1601 | CDL | CA2-OA2-PA1-OA5 |
| 57 | Ei | 401 | CDL | CA3-OA5-PA1-OA2 |
| 57 | En | 1201 | CDL | CB2-OB2-PB2-OB5 |
| 57 | En | 1202 | CDL | CA2-OA2-PA1-OA5 |
| 57 | En | 1202 | CDL | CB2-OB2-PB2-OB5 |
| 57 | Ep | 701 | CDL | CB2-OB2-PB2-OB5 |
| 57 | Eu | 101 | CDL | CA2-OA2-PA1-OA5 |
| 57 | Eu | 101 | CDL | CB2-OB2-PB2-OB5 |
| 57 | Eu | 101 | CDL | CB3-OB5-PB2-OB2 |
| 58 | DV | 405 | PC1 | C1-O11-P-O13 |
| 58 | DX | 302 | PC1 | C11-O13-P-O11 |
| 58 | EB | 303 | PC1 | C1-O11-P-O13 |
| 58 | Dc | 605 | PC1 | C11-O13-P-O11 |
| 58 | Dv | 407 | PC1 | C1-O11-P-O13 |
| 58 | Eb | 302 | PC1 | C1-O11-P-O13 |
| 58 | Ef | 1001 | PC1 | C11-O13-P-O11 |
| 59 | DR | 401 | 3PE | C1-O11-P-O13 |
| 59 | DS | 401 | 3PE | C11-O13-P-O11 |
| 59 | DX | 303 | 3PE | C1-O11-P-O13 |
| 59 | Dd | 703 | 3PE | C11-O13-P-O11 |
| 59 | Ds | 401 | 3PE | C11-O13-P-O11 |
| 59 | Ds | 407 | 3PE | C1-O11-P-O13 |
| 57 | DA | 709 | CDL | C12-C13-C14-C15 |
| 57 | DO | 501 | CDL | C36-C37-C38-C39 |
| 57 | DV | 404 | CDL | C14-C15-C16-C17 |
| 57 | DG | 201 | CDL | OA7-CA5-OA6-CA4 |
| 57 | Dj | 408 | CDL | C77-C78-C79-C80 |
| 57 | DM | 502 | CDL | CB3-CB4-CB6-OB8 |
| 57 | Dj | 402 | CDL | CB3-CB4-CB6-OB8 |
| 57 | Dj | 404 | CDL | CA3-CA4-CA6-OA8 |
| 57 | Dn | 503 | CDL | CB3-CB4-CB6-OB8 |
| 57 | Dq | 402 | CDL | CB3-CB4-CB6-OB8 |
| 57 | Dn | 505 | CDL | C39-C40-C41-C42 |
| 58 | DA | 706 | PC1 | C35-C36-C37-C38 |
| 57 | DI | 701 | CDL | C74-C75-C76-C77 |
| 57 | DV | 402 | CDL | C78-C79-C80-C81 |
| 58 | Dc | 603 | PC1 | C34-C35-C36-C37 |
| 58 | Eb | 302 | PC1 | C34-C35-C36-C37 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 57 | Do | 501 | CDL | C12-C13-C14-C15 |
| 57 | Dq | 403 | CDL | C21-C22-C23-C24 |
| 57 | DO | 501 | CDL | C77-C78-C79-C80 |
| 57 | Dj | 401 | CDL | C18-C19-C20-C21 |
| 58 | Dg | 203 | PC1 | O31-C31-C32-C33 |
| 58 | Dv | 407 | PC1 | O21-C21-C22-C23 |
| 57 | Dj | 402 | CDL | C57-C58-C59-C60 |
| 57 | DR | 402 | CDL | C36-C37-C38-C39 |
| 57 | DV | 401 | CDL | C78-C79-C80-C81 |
| 57 | DD | 703 | CDL | C1-CB2-OB2-PB2 |
| 57 | DH | 201 | CDL | CA4-CA3-OA5-PA1 |
| 57 | DJ | 303 | CDL | C1-CB2-OB2-PB2 |
| 57 | DR | 402 | CDL | CA4-CA3-OA5-PA1 |
| 57 | EB | 304 | CDL | CB4-CB3-OB5-PB2 |
| 57 | EK | 201 | CDL | CB4-CB3-OB5-PB2 |
| 57 | EL | 902 | CDL | CB4-CB3-OB5-PB2 |
| 57 | EL | 903 | CDL | CB4-CB3-OB5-PB2 |
| 57 | EL | 904 | CDL | C1-CB2-OB2-PB2 |
| 57 | Dm | 501 | CDL | C1-CA2-OA2-PA1 |
| 57 | Dn | 501 | CDL | CB4-CB3-OB5-PB2 |
| 57 | Dv | 403 | CDL | C1-CB2-OB2-PB2 |
| 57 | Dz | 501 | CDL | CA4-CA3-OA5-PA1 |
| 58 | EO | 205 | PC1 | C2-C1-O11-P |
| 58 | Eb | 302 | PC1 | C2-C1-O11-P |
| 58 | El | 904 | PC1 | C2-C1-O11-P |
| 59 | DX | 304 | 3PE | C2-C1-O11-P |
| 57 | DR | 402 | CDL | C42-C43-C44-C45 |
| 57 | Dv | 403 | CDL | C82-C83-C84-C85 |
| 59 | Ds | 403 | 3PE | C34-C35-C36-C37 |
| 57 | DS | 402 | CDL | OA9-CA7-OA8-CA6 |
| 57 | DV | 402 | CDL | CA2-C1-CB2-OB2 |
| 57 | Dd | 702 | CDL | CA2-C1-CB2-OB2 |
| 57 | Dd | 706 | CDL | OA7-CA5-OA6-CA4 |
| 57 | Ep | 701 | CDL | C76-C77-C78-C79 |
| 59 | EN | 1203 | 3PE | C36-C37-C38-C39 |
| 65 | ED | 603 | UQ8 | C35-C34-C36-C37 |
| 65 | DS | 404 | UQ8 | C31-C32-C33-C34 |
| 57 | Do | 501 | CDL | C36-C37-C38-C39 |
| 57 | DA | 705 | CDL | C31-CA7-OA8-CA6 |
| 57 | DJ | 304 | CDL | C71-CB7-OB8-CB6 |
| 57 | DS | 402 | CDL | C31-CA7-OA8-CA6 |
| 57 | DV | 402 | CDL | C71-CB7-OB8-CB6 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 57 | ED | 604 | CDL | C71-CB7-OB8-CB6 |
| 57 | Do | 501 | CDL | C71-CB7-OB8-CB6 |
| 57 | Ds | 402 | CDL | C31-CA7-OA8-CA6 |
| 59 | EM | 901 | 3PE | C32-C31-O31-C3 |
| 58 | Dv | 407 | PC1 | O32-C31-C32-C33 |
| 60 | DA | 711 | LPP | C17-C18-C19-C20 |
| 57 | DA | 705 | CDL | OA9-CA7-OA8-CA6 |
| 57 | DZ | 501 | CDL | OA9-CA7-OA8-CA6 |
| 57 | Dd | 705 | CDL | OB9-CB7-OB8-CB6 |
| 57 | Do | 501 | CDL | OB9-CB7-OB8-CB6 |
| 57 | EL | 901 | CDL | C44-C45-C46-C47 |
| 57 | Di | 701 | CDL | C55-C56-C57-C58 |
| 57 | DQ | 1504 | CDL | C55-C56-C57-C58 |
| 57 | DX | 307 | CDL | C39-C40-C41-C42 |
| 57 | EL | 902 | CDL | C78-C79-C80-C81 |
| 59 | DG | 205 | 3PE | C29-C2A-C2B-C2C |
| 57 | DU | 401 | CDL | C20-C21-C22-C23 |
| 57 | ED | 604 | CDL | OB9-CB7-OB8-CB6 |
| 57 | DG | 201 | CDL | C31-CA7-OA8-CA6 |
| 57 | Dd | 705 | CDL | C71-CB7-OB8-CB6 |
| 57 | DJ | 304 | CDL | CA7-C31-C32-C33 |
| 57 | ED | 604 | CDL | CA5-C11-C12-C13 |
| 57 | DQ | 1504 | CDL | C72-C73-C74-C75 |
| 57 | Dd | 706 | CDL | C77-C78-C79-C80 |
| 58 | EO | 206 | PC1 | C11-C12-N-C14 |
| 57 | DM | 501 | CDL | C62-C63-C64-C65 |
| 57 | EO | 202 | CDL | C18-C19-C20-C21 |
| 57 | Dj | 401 | CDL | C36-C37-C38-C39 |
| 57 | Dj | 401 | CDL | C59-C60-C61-C62 |
| 57 | DD | 704 | CDL | OB5-CB3-CB4-CB6 |
| 57 | Dj | 402 | CDL | OA5-CA3-CA4-CA6 |
| 57 | EH | 202 | CDL | C74-C75-C76-C77 |
| 59 | DG | 204 | 3PE | O13-C11-C12-N |
| 59 | Da | 708 | 3PE | O13-C11-C12-N |
| 57 | DA | 705 | CDL | C55-C56-C57-C58 |
| 57 | DJ | 307 | CDL | OA5-CA3-CA4-OA6 |
| 57 | DO | 501 | CDL | OB5-CB3-CB4-OB6 |
| 57 | Dn | 505 | CDL | OB5-CB3-CB4-OB6 |
| 57 | El | 902 | CDL | OB5-CB3-CB4-OB6 |
| 58 | DB | 702 | PC1 | O11-C1-C2-O21 |
| 58 | DJ | 306 | PC1 | C23-C24-C25-C26 |
| 57 | EB | 304 | CDL | C74-C75-C76-C77 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 57 | Da | 705 | CDL | C55-C56-C57-C58 |
| 59 | Dd | 703 | 3PE | C39-C3A-C3B-C3C |
| 58 | Eo | 205 | PC1 | C3C-C3D-C3E-C3F |
| 57 | DV | 402 | CDL | OB9-CB7-OB8-CB6 |
| 57 | DA | 705 | CDL | C82-C83-C84-C85 |
| 57 | EH | 201 | CDL | O1-C1-CB2-OB2 |
| 57 | Dq | 403 | CDL | O1-C1-CA2-OA2 |
| 58 | DQ | 1503 | PC1 | O22-C21-O21-C2 |
| 59 | Dr | 401 | 3PE | O22-C21-O21-C2 |
| 57 | DJ | 302 | CDL | C84-C85-C86-C87 |
| 57 | DU | 402 | CDL | C58-C59-C60-C61 |
| 57 | DU | 402 | CDL | C60-C61-C62-C63 |
| 57 | Dg | 202 | CDL | C80-C81-C82-C83 |
| 57 | Dv | 402 | CDL | C72-C73-C74-C75 |
| 57 | Dx | 1201 | CDL | C81-C82-C83-C84 |
| 57 | El | 901 | CDL | C11-C12-C13-C14 |
| 66 | Ed | 201 | HEM | CAA-CBA-CGA-O1A |
| 57 | DU | 403 | CDL | C17-C18-C19-C20 |
| 58 | Dy | 302 | PC1 | C3B-C3C-C3D-C3E |
| 57 | DA | 705 | CDL | C17-C18-C19-C20 |
| 59 | DR | 401 | 3PE | C3D-C3E-C3F-C3G |
| 59 | EM | 901 | 3PE | O32-C31-O31-C3 |
| 66 | ED | 602 | HEM | CAA-CBA-CGA-O1A |
| 57 | DD | 704 | CDL | OA6-CA4-CA6-OA8 |
| 57 | DQ | 1501 | CDL | OB6-CB4-CB6-OB8 |
| 57 | DV | 402 | CDL | OB6-CB4-CB6-OB8 |
| 57 | EN | 1202 | CDL | OA6-CA4-CA6-OA8 |
| 57 | Dd | 705 | CDL | OA6-CA4-CA6-OA8 |
| 57 | Dn | 502 | CDL | OB6-CB4-CB6-OB8 |
| 57 | Dq | 401 | CDL | OB6-CB4-CB6-OB8 |
| 58 | Dv | 408 | PC1 | O21-C2-C3-O31 |
| 57 | EI | 401 | CDL | C14-C15-C16-C17 |
| 58 | Dv | 406 | PC1 | O31-C31-C32-C33 |
| 65 | Ds | 404 | UQ8 | C31-C32-C33-C34 |
| 57 | Ds | 405 | CDL | C31-C32-C33-C34 |
| 58 | DV | 406 | PC1 | C3B-C3C-C3D-C3E |
| 57 | DR | 402 | CDL | C1-CB2-OB2-PB2 |
| 57 | DZ | 501 | CDL | C1-CB2-OB2-PB2 |
| 57 | EO | 202 | CDL | C1-CB2-OB2-PB2 |
| 57 | Ek | 201 | CDL | CB4-CB3-OB5-PB2 |
| 57 | EB | 304 | CDL | C51-C52-C53-C54 |
| 57 | Ei | 401 | CDL | C76-C77-C78-C79 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 59 | Dx | 1205 | 3PE | C3A-C3B-C3C-C3D |
| 59 | Dx | 1206 | 3PE | C3F-C3G-C3H-C3I |
| 60 | DA | 711 | LPP | C18-C19-C20-C21 |
| 58 | Di | 702 | PC1 | O22-C21-O21-C2 |
| 60 | DA | 711 | LPP | O27-C29-C30-C31 |
| 57 | Ds | 402 | CDL | C78-C79-C80-C81 |
| 54 | DA | 702 | HEA | CAD-CBD-CGD-O1D |
| 65 | DS | 404 | UQ8 | C40-C39-C41-C42 |
| 65 | En | 1203 | UQ8 | C35-C34-C36-C37 |
| 57 | DQ | 1502 | CDL | C12-C13-C14-C15 |
| 58 | Dg | 203 | PC1 | C3F-C3G-C3H-C3I |
| 57 | Dn | 501 | CDL | C78-C79-C80-C81 |
| 57 | Ds | 402 | CDL | C80-C81-C82-C83 |
| 57 | EH | 201 | CDL | C76-C77-C78-C79 |
| 58 | Dc | 603 | PC1 | C3B-C3C-C3D-C3E |
| 57 | DU | 404 | CDL | C71-CB7-OB8-CB6 |
| 57 | EL | 903 | CDL | C31-CA7-OA8-CA6 |
| 57 | En | 1201 | CDL | C31-CA7-OA8-CA6 |
| 57 | Do | 501 | CDL | C33-C34-C35-C36 |
| 57 | EB | 302 | CDL | C12-C13-C14-C15 |
| 57 | DA | 709 | CDL | CB3-CB4-CB6-OB8 |
| 57 | DD | 702 | CDL | CA3-CA4-CA6-OA8 |
| 57 | DD | 704 | CDL | CA3-CA4-CA6-OA8 |
| 57 | DJ | 302 | CDL | CB3-CB4-CB6-OB8 |
| 57 | DX | 301 | CDL | CB3-CB4-CB6-OB8 |
| 57 | Dd | 705 | CDL | CA3-CA4-CA6-OA8 |
| 57 | Dm | 502 | CDL | CB3-CB4-CB6-OB8 |
| 57 | Dq | 402 | CDL | CA3-CA4-CA6-OA8 |
| 57 | Dv | 402 | CDL | CB3-CB4-CB6-OB8 |
| 57 | Eh | 1601 | CDL | CB3-CB4-CB6-OB8 |
| 57 | En | 1202 | CDL | CB3-CB4-CB6-OB8 |
| 58 | Dv | 408 | PC1 | C1-C2-C3-O31 |
| 58 | Dx | 1204 | PC1 | C1-C2-C3-O31 |
| 58 | Eo | 204 | PC1 | C1-C2-C3-O31 |
| 59 | DC | 606 | 3PE | C1-C2-C3-O31 |
| 59 | El | 905 | 3PE | C1-C2-C3-O31 |
| 57 | DS | 402 | CDL | C11-C12-C13-C14 |
| 57 | Di | 701 | CDL | C32-C33-C34-C35 |
| 57 | DM | 501 | CDL | C52-C51-CB5-OB6 |
| 57 | EB | 302 | CDL | C11-C12-C13-C14 |
| 58 | Eo | 201 | PC1 | C33-C34-C35-C36 |
| 57 | DJ | 304 | CDL | OB9-CB7-OB8-CB6 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 57 | EL | 903 | CDL | OA9-CA7-OA8-CA6 |
| 57 | Eh | 1601 | CDL | C18-C19-C20-C21 |
| 57 | El | 902 | CDL | C13-C14-C15-C16 |
| 57 | DZ | 501 | CDL | O1-C1-CA2-OA2 |
| 57 | EB | 304 | CDL | C79-C80-C81-C82 |
| 58 | DV | 407 | PC1 | C32-C33-C34-C35 |
| 59 | DJ | 301 | 3PE | C3C-C3D-C3E-C3F |
| 59 | DX | 305 | 3PE | C2E-C2F-C2G-C2H |
| 57 | El | 902 | CDL | C83-C84-C85-C86 |
| 57 | Ep | 701 | CDL | C80-C81-C82-C83 |
| 57 | DN | 504 | CDL | C37-C38-C39-C40 |
| 57 | DJ | 307 | CDL | CB6-CB4-OB6-CB5 |
| 57 | DQ | 1501 | CDL | CA6-CA4-OA6-CA5 |
| 57 | DV | 401 | CDL | CB3-CB4-OB6-CB5 |
| 57 | DV | 404 | CDL | CA3-CA4-OA6-CA5 |
| 57 | EA | 301 | CDL | CA6-CA4-OA6-CA5 |
| 57 | EN | 1202 | CDL | CB6-CB4-OB6-CB5 |
| 57 | Dd | 704 | CDL | CB3-CB4-OB6-CB5 |
| 57 | Dg | 201 | CDL | CB3-CB4-OB6-CB5 |
| 57 | Dj | 404 | CDL | CB3-CB4-OB6-CB5 |
| 57 | Dn | 501 | CDL | CB6-CB4-OB6-CB5 |
| 57 | Dv | 401 | CDL | CB3-CB4-OB6-CB5 |
| 58 | DC | 608 | PC1 | C1-C2-O21-C21 |
| 58 | DC | 608 | PC1 | C3-C2-O21-C21 |
| 58 | EO | 207 | PC1 | C1-C2-O21-C21 |
| 58 | Eo | 205 | PC1 | C1-C2-O21-C21 |
| 59 | Dg | 204 | 3PE | C1-C2-O21-C21 |
| 57 | EN | 1201 | CDL | C80-C81-C82-C83 |
| 58 | DS | 407 | PC1 | C11-C12-N-C14 |
| 59 | Dr | 401 | 3PE | C22-C21-O21-C2 |
| 57 | Dg | 201 | CDL | C21-C22-C23-C24 |
| 57 | Dj | 402 | CDL | C51-C52-C53-C54 |
| 57 | Dj | 403 | CDL | C34-C35-C36-C37 |
| 59 | Ds | 401 | 3PE | C32-C33-C34-C35 |
| 54 | Da | 702 | HEA | CAD-CBD-CGD-O1D |
| 57 | DN | 505 | CDL | C81-C82-C83-C84 |
| 58 | EO | 201 | PC1 | C23-C24-C25-C26 |
| 59 | DX | 304 | 3PE | C3F-C3G-C3H-C3I |
| 57 | Da | 709 | CDL | C22-C23-C24-C25 |
| 57 | Du | 403 | CDL | C79-C80-C81-C82 |
| 59 | Ds | 401 | 3PE | C3A-C3B-C3C-C3D |
| 57 | DJ | 305 | CDL | CB3-OB5-PB2-OB2 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 57 | EH | 201 | CDL | CA3-OA5-PA1-OA2 |
| 57 | Dc | 601 | CDL | CA3-OA5-PA1-OA2 |
| 57 | Du | 401 | CDL | CA3-OA5-PA1-OA2 |
| 58 | Dc | 604 | PC1 | O21-C21-C22-C23 |
| 57 | DR | 402 | CDL | CA5-C11-C12-C13 |
| 54 | DA | 702 | HEA | CAD-CBD-CGD-O2D |
| 66 | ED | 602 | HEM | CAA-CBA-CGA-O2A |
| 57 | DN | 504 | CDL | C13-C14-C15-C16 |
| 57 | Da | 705 | CDL | C77-C78-C79-C80 |
| 57 | EL | 904 | CDL | C43-C44-C45-C46 |
| 59 | Ds | 403 | 3PE | C3E-C3F-C3G-C3H |
| 59 | Dx | 1207 | 3PE | C2B-C2C-C2D-C2E |
| 57 | DU | 401 | CDL | OA5-CA3-CA4-OA6 |
| 57 | EL | 903 | CDL | OB5-CB3-CB4-OB6 |
| 58 | DC | 608 | PC1 | O11-C1-C2-O21 |
| 58 | Ds | 406 | PC1 | O11-C1-C2-O21 |
| 58 | DS | 406 | PC1 | O31-C31-C32-C33 |
| 57 | EL | 904 | CDL | C41-C42-C43-C44 |
| 57 | DG | 201 | CDL | C43-C44-C45-C46 |
| 57 | DM | 501 | CDL | C54-C55-C56-C57 |
| 57 | DU | 403 | CDL | C12-C13-C14-C15 |
| 57 | EN | 1201 | CDL | C79-C80-C81-C82 |
| 57 | Dr | 402 | CDL | C51-C52-C53-C54 |
| 57 | En | 1202 | CDL | C32-C33-C34-C35 |
| 58 | DC | 608 | PC1 | C2B-C2C-C2D-C2E |
| 57 | DJ | 305 | CDL | OB5-CB3-CB4-CB6 |
| 57 | DR | 402 | CDL | OB5-CB3-CB4-CB6 |
| 57 | EL | 901 | CDL | OA5-CA3-CA4-CA6 |
| 57 | Dd | 706 | CDL | OA5-CA3-CA4-CA6 |
| 57 | Dj | 401 | CDL | OA5-CA3-CA4-CA6 |
| 57 | Ed | 204 | CDL | OB5-CB3-CB4-CB6 |
| 57 | Ed | 205 | CDL | OB5-CB3-CB4-CB6 |
| 57 | El | 902 | CDL | OB5-CB3-CB4-CB6 |
| 58 | Db | 702 | PC1 | O11-C1-C2-C3 |
| 57 | DM | 501 | CDL | C82-C83-C84-C85 |
| 57 | EL | 901 | CDL | C78-C79-C80-C81 |
| 59 | DX | 303 | 3PE | C2C-C2D-C2E-C2F |
| 57 | Dd | 706 | CDL | C11-CA5-OA6-CA4 |
| 58 | DQ | 1503 | PC1 | C22-C21-O21-C2 |
| 65 | Ds | 404 | UQ8 | C40-C39-C41-C42 |
| 57 | Di | 701 | CDL | CA7-C31-C32-C33 |
| 65 | DS | 404 | UQ8 | C38-C39-C41-C42 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 65 | Ed | 202 | UQ8 | C38-C39-C41-C42 |
| 57 | DD | 704 | CDL | O1-C1-CB2-OB2 |
| 57 | EH | 201 | CDL | C39-C40-C41-C42 |
| 57 | DG | 201 | CDL | OA9-CA7-OA8-CA6 |
| 57 | DU | 404 | CDL | OB9-CB7-OB8-CB6 |
| 57 | En | 1201 | CDL | OA9-CA7-OA8-CA6 |
| 57 | Da | 705 | CDL | C15-C16-C17-C18 |
| 58 | Dx | 1204 | PC1 | O22-C21-O21-C2 |
| 57 | DS | 402 | CDL | C13-C14-C15-C16 |
| 57 | DG | 201 | CDL | OB6-CB4-CB6-OB8 |
| 57 | Dq | 402 | CDL | OB6-CB4-CB6-OB8 |
| 57 | Ek | 201 | CDL | OA6-CA4-CA6-OA8 |
| 58 | Da | 707 | PC1 | O21-C2-C3-O31 |
| 59 | Eo | 202 | 3PE | C32-C31-O31-C3 |
| 57 | EH | 202 | CDL | CA5-C11-C12-C13 |
| 57 | DJ | 307 | CDL | C52-C53-C54-C55 |
| 57 | Dd | 706 | CDL | C80-C81-C82-C83 |
| 60 | Dn | 506 | LPP | C37-C38-C39-C40 |
| 54 | Da | 701 | HEA | CAD-CBD-CGD-O1D |
| 66 | Ed | 201 | HEM | CAA-CBA-CGA-O2A |
| 57 | DS | 402 | CDL | C74-C75-C76-C77 |
| 57 | Dg | 202 | CDL | C42-C43-C44-C45 |
| 57 | Eh | 1601 | CDL | C73-C74-C75-C76 |
| 59 | Dr | 401 | 3PE | C3D-C3E-C3F-C3G |
| 57 | Dg | 202 | CDL | C14-C15-C16-C17 |
| 57 | En | 1202 | CDL | C36-C37-C38-C39 |
| 59 | EM | 901 | 3PE | C25-C26-C27-C28 |
| 57 | DJ | 307 | CDL | C32-C31-CA7-OA8 |
| 57 | DG | 201 | CDL | CA2-C1-CB2-OB2 |
| 57 | EA | 301 | CDL | CB2-C1-CA2-OA2 |
| 65 | EL | 906 | UQ8 | C14-C16-C17-C18 |
| 54 | Da | 702 | HEA | CAD-CBD-CGD-O2D |
| 65 | EN | 1204 | UQ8 | C12-C11-C9-C10 |
| 65 | En | 1203 | UQ8 | C30-C29-C31-C32 |
| 57 | EO | 202 | CDL | C59-C60-C61-C62 |
| 60 | Dl | 1101 | LPP | C17-C18-C19-C20 |
| 65 | En | 1203 | UQ8 | C33-C34-C36-C37 |
| 57 | Dq | 402 | CDL | C72-C73-C74-C75 |
| 57 | DH | 201 | CDL | C18-C19-C20-C21 |
| 59 | Ds | 407 | 3PE | C36-C37-C38-C39 |
| 57 | EN | 1202 | CDL | C36-C37-C38-C39 |
| 57 | Du | 402 | CDL | C24-C25-C26-C27 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 57 | En | 1202 | CDL | C59-C60-C61-C62 |
| 57 | Eu | 101 | CDL | C71-C72-C73-C74 |
| 59 | Dr | 404 | 3PE | C29-C2A-C2B-C2C |
| 57 | DI | 701 | CDL | C57-C58-C59-C60 |
| 57 | Dd | 705 | CDL | C1-CB2-OB2-PB2 |
| 58 | Di | 702 | PC1 | C22-C21-O21-C2 |
| 68 | ER | 201 | ATP | PA-O3A-PB-O1B |
| 65 | EN | 1204 | UQ8 | C11-C12-C13-C14 |
| 57 | En | 1201 | CDL | C52-C53-C54-C55 |
| 59 | DS | 401 | 3PE | C3A-C3B-C3C-C3D |
| 57 | EN | 1201 | CDL | C13-C14-C15-C16 |
| 57 | Dh | 201 | CDL | C18-C19-C20-C21 |
| 59 | EO | 203 | 3PE | C26-C27-C28-C29 |
| 57 | Ed | 205 | CDL | C11-C12-C13-C14 |
| 59 | Eo | 202 | 3PE | O32-C31-O31-C3 |
| 57 | Dd | 705 | CDL | C40-C41-C42-C43 |
| 57 | Eg | 101 | CDL | C54-C55-C56-C57 |
| 58 | DA | 707 | PC1 | C3E-C3F-C3G-C3H |
| 57 | Dz | 501 | CDL | C72-C71-CB7-OB8 |
| 57 | DI | 701 | CDL | C53-C54-C55-C56 |
| 57 | DQ | 1501 | CDL | C21-C22-C23-C24 |
| 57 | DV | 401 | CDL | C43-C44-C45-C46 |
| 57 | Dn | 501 | CDL | CB3-CB4-CB6-OB8 |
| 58 | EO | 207 | PC1 | C3D-C3E-C3F-C3G |
| 58 | Da | 707 | PC1 | C1-C2-C3-O31 |
| 57 | EN | 1202 | CDL | C14-C15-C16-C17 |
| 57 | Di | 701 | CDL | C57-C58-C59-C60 |
| 57 | DJ | 304 | CDL | C16-C17-C18-C19 |
| 57 | EL | 902 | CDL | C14-C15-C16-C17 |
| 59 | Ds | 401 | 3PE | C36-C37-C38-C39 |
| 59 | El | 905 | 3PE | C22-C23-C24-C25 |
| 54 | Da | 702 | HEA | C27-C19-C20-C21 |
| 65 | EN | 1204 | UQ8 | C35-C34-C36-C37 |
| 65 | Ed | 202 | UQ8 | C12-C11-C9-C10 |
| 57 | DJ | 302 | CDL | C52-C51-CB5-OB6 |
| 57 | El | 902 | CDL | OA9-CA7-OA8-CA6 |
| 57 | Dq | 403 | CDL | C76-C77-C78-C79 |
| 57 | DG | 201 | CDL | C11-CA5-OA6-CA4 |
| 58 | DC | 604 | PC1 | C26-C27-C28-C29 |
| 57 | DY | 301 | CDL | C57-C58-C59-C60 |
| 57 | Ds | 402 | CDL | C12-C13-C14-C15 |
| 57 | El | 902 | CDL | C44-C45-C46-C47 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 59 | EO | 204 | 3PE | C2F-C2G-C2H-C2I |
| 57 | DU | 402 | CDL | OA9-CA7-OA8-CA6 |
| 57 | EL | 904 | CDL | C71-C72-C73-C74 |
| 57 | EO | 202 | CDL | C12-C13-C14-C15 |
| 57 | Da | 709 | CDL | C38-C39-C40-C41 |
| 57 | Dj | 404 | CDL | C55-C56-C57-C58 |
| 57 | Dn | 505 | CDL | C12-C13-C14-C15 |
| 57 | DM | 502 | CDL | C12-C13-C14-C15 |
| 57 | Dd | 706 | CDL | C44-C45-C46-C47 |
| 59 | DX | 305 | 3PE | C35-C36-C37-C38 |
| 57 | DR | 402 | CDL | OB5-CB3-CB4-OB6 |
| 57 | EU | 101 | CDL | OB5-CB3-CB4-OB6 |
| 57 | Dj | 402 | CDL | OA5-CA3-CA4-OA6 |
| 57 | Dn | 505 | CDL | OA5-CA3-CA4-OA6 |
| 57 | Do | 501 | CDL | OB5-CB3-CB4-OB6 |
| 57 | Dz | 501 | CDL | OA5-CA3-CA4-OA6 |
| 59 | DG | 205 | 3PE | O11-C1-C2-O21 |
| 54 | Da | 701 | HEA | CAD-CBD-CGD-O2D |
| 65 | ED | 603 | UQ8 | C2-C3-O3-C3M |
| 57 | DJ | 303 | CDL | C75-C76-C77-C78 |
| 57 | DN | 501 | CDL | C12-C13-C14-C15 |
| 57 | EN | 1202 | CDL | C11-C12-C13-C14 |
| 57 | Da | 709 | CDL | C40-C41-C42-C43 |
| 57 | DV | 401 | CDL | C14-C15-C16-C17 |
| 57 | EB | 304 | CDL | C35-C36-C37-C38 |
| 58 | Dv | 407 | PC1 | C3B-C3C-C3D-C3E |
| 57 | EN | 1201 | CDL | C40-C41-C42-C43 |
| 57 | DC | 601 | CDL | OB5-CB3-CB4-CB6 |
| 57 | EH | 201 | CDL | OA5-CA3-CA4-CA6 |
| 57 | Du | 401 | CDL | OA5-CA3-CA4-CA6 |
| 57 | Dy | 301 | CDL | OA5-CA3-CA4-CA6 |
| 57 | Dz | 501 | CDL | OA5-CA3-CA4-CA6 |
| 58 | DC | 603 | PC1 | O11-C1-C2-C3 |
| 58 | Dc | 607 | PC1 | O11-C1-C2-C3 |
| 58 | Ef | 1001 | PC1 | O11-C1-C2-C3 |
| 59 | DG | 204 | 3PE | O11-C1-C2-C3 |
| 58 | Eb | 301 | PC1 | O31-C31-C32-C33 |
| 57 | Da | 705 | CDL | OA9-CA7-OA8-CA6 |
| 65 | EN | 1204 | UQ8 | C15-C14-C16-C17 |
| 65 | El | 906 | UQ8 | C12-C11-C9-C10 |
| 65 | EL | 906 | UQ8 | C39-C41-C42-C43 |
| 58 | DC | 604 | PC1 | O22-C21-C22-C23 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 57 | Dg | 202 | CDL | C40-C41-C42-C43 |
| 57 | Ds | 402 | CDL | C56-C57-C58-C59 |
| 58 | Dv | 405 | PC1 | C29-C2A-C2B-C2C |
| 59 | DG | 204 | 3PE | C2A-C2B-C2C-C2D |
| 59 | DS | 401 | 3PE | C36-C37-C38-C39 |
| 54 | Da | 702 | HEA | C18-C19-C20-C21 |
| 57 | DU | 402 | CDL | C31-CA7-OA8-CA6 |
| 57 | DA | 709 | CDL | C36-C37-C38-C39 |
| 58 | DY | 302 | PC1 | C3E-C3F-C3G-C3H |
| 58 | Eo | 201 | PC1 | C3F-C3G-C3H-C3I |
| 59 | DX | 305 | 3PE | C26-C27-C28-C29 |
| 59 | Dd | 703 | 3PE | C3C-C3D-C3E-C3F |
| 59 | Em | 901 | 3PE | C25-C26-C27-C28 |
| 57 | DM | 501 | CDL | C41-C42-C43-C44 |
| 57 | Dd | 706 | CDL | C39-C40-C41-C42 |
| 57 | DJ | 304 | CDL | C1-CB2-OB2-PB2 |
| 57 | Da | 705 | CDL | CB2-C1-CA2-OA2 |
| 57 | Ds | 402 | CDL | C11-C12-C13-C14 |
| 57 | DV | 404 | CDL | OA6-CA4-CA6-OA8 |
| 57 | Dj | 404 | CDL | OA6-CA4-CA6-OA8 |
| 58 | DB | 702 | PC1 | O32-C31-O31-C3 |
| 57 | Dh | 202 | CDL | CB5-C51-C52-C53 |
| 57 | ED | 601 | CDL | C80-C81-C82-C83 |
| 57 | Dd | 705 | CDL | C12-C11-CA5-OA6 |
| 57 | Dj | 408 | CDL | C52-C51-CB5-OB6 |
| 58 | EO | 207 | PC1 | O21-C21-C22-C23 |
| 58 | Da | 706 | PC1 | O31-C31-C32-C33 |
| 59 | DG | 204 | 3PE | O21-C21-C22-C23 |
| 59 | DX | 303 | 3PE | O21-C21-C22-C23 |
| 59 | Dx | 1206 | 3PE | O21-C21-C22-C23 |
| 60 | Dn | 504 | LPP | O27-C29-C30-C31 |
| 57 | DU | 404 | CDL | C22-C23-C24-C25 |
| 57 | Du | 401 | CDL | C71-C72-C73-C74 |
| 68 | ER | 201 | ATP | PG-O3B-PB-O3A |
| 57 | DM | 502 | CDL | C52-C53-C54-C55 |
| 65 | El | 906 | UQ8 | C11-C12-C13-C14 |
| 57 | Da | 705 | CDL | C31-CA7-OA8-CA6 |
| 57 | El | 902 | CDL | C31-CA7-OA8-CA6 |
| 57 | DN | 505 | CDL | CA5-C11-C12-C13 |
| 57 | DQ | 1501 | CDL | C72-C71-CB7-OB8 |
| 57 | Da | 709 | CDL | C52-C51-CB5-OB6 |
| 57 | Ed | 205 | CDL | C12-C11-CA5-OA6 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 59 | Dd | 703 | 3PE | O21-C21-C22-C23 |
| 65 | En | 1203 | UQ8 | C12-C11-C9-C10 |
| 57 | Di | 701 | CDL | C61-C62-C63-C64 |
| 57 | El | 903 | CDL | C43-C44-C45-C46 |
| 57 | DC | 601 | CDL | CA2-OA2-PA1-OA5 |
| 57 | DD | 704 | CDL | CA3-OA5-PA1-OA2 |
| 57 | DG | 202 | CDL | CA3-OA5-PA1-OA2 |
| 57 | Di | 701 | CDL | CB2-OB2-PB2-OB5 |
| 58 | Ds | 406 | PC1 | C11-O13-P-O11 |
| 58 | Dv | 405 | PC1 | C1-O11-P-O13 |
| 65 | Ds | 404 | UQ8 | C38-C39-C41-C42 |
| 57 | EL | 903 | CDL | C16-C17-C18-C19 |
| 57 | DJ | 303 | CDL | C12-C11-CA5-OA6 |
| 58 | DC | 603 | PC1 | O21-C21-C22-C23 |
| 58 | Dx | 1202 | PC1 | O31-C31-C32-C33 |
| 59 | DG | 205 | 3PE | O31-C31-C32-C33 |
| 59 | DS | 401 | 3PE | O21-C21-C22-C23 |
| 59 | DS | 403 | 3PE | O21-C21-C22-C23 |
| 59 | DR | 401 | 3PE | C3F-C3G-C3H-C3I |
| 57 | EL | 902 | CDL | C35-C36-C37-C38 |
| 57 | Dn | 505 | CDL | C14-C15-C16-C17 |
| 57 | Du | 403 | CDL | C57-C58-C59-C60 |
| 54 | Da | 702 | HEA | CAA-CBA-CGA-O1A |
| 57 | Ed | 204 | CDL | O1-C1-CA2-OA2 |
| 57 | DD | 703 | CDL | C52-C51-CB5-OB6 |
| 57 | DU | 401 | CDL | C72-C71-CB7-OB8 |
| 57 | DZ | 501 | CDL | C72-C71-CB7-OB8 |
| 57 | ED | 604 | CDL | C12-C11-CA5-OA6 |
| 57 | Dr | 403 | CDL | C52-C51-CB5-OB6 |
| 57 | Dx | 1201 | CDL | C52-C51-CB5-OB6 |
| 59 | Dx | 1206 | 3PE | O31-C31-C32-C33 |
| 57 | DR | 402 | CDL | C76-C77-C78-C79 |
| 57 | DS | 405 | CDL | C31-C32-C33-C34 |
| 58 | DC | 602 | PC1 | C2E-C2F-C2G-C2H |
| 59 | DC | 607 | 3PE | C2F-C2G-C2H-C2I |
| 59 | DX | 303 | 3PE | C2B-C2C-C2D-C2E |
| 57 | DQ | 1501 | CDL | CA3-CA4-OA6-CA5 |
| 57 | DR | 403 | CDL | CA3-CA4-OA6-CA5 |
| 57 | Dd | 705 | CDL | CB6-CB4-OB6-CB5 |
| 57 | Do | 501 | CDL | CB3-CB4-OB6-CB5 |
| 57 | Do | 501 | CDL | CB6-CB4-OB6-CB5 |
| 57 | Dr | 403 | CDL | CA3-CA4-OA6-CA5 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 58 | Db | 702 | PC1 | C3-C2-O21-C21 |
| 59 | Dg | 204 | 3PE | C3-C2-O21-C21 |
| 57 | Dd | 706 | CDL | C56-C57-C58-C59 |
| 57 | Dh | 201 | CDL | C59-C60-C61-C62 |
| 57 | DD | 702 | CDL | OB7-CB5-OB6-CB4 |
| 57 | EH | 201 | CDL | C34-C35-C36-C37 |
| 59 | DX | 304 | 3PE | C32-C33-C34-C35 |
| 54 | DA | 702 | HEA | CAA-CBA-CGA-O1A |
| 57 | DV | 402 | CDL | C72-C73-C74-C75 |
| 58 | DB | 702 | PC1 | C3E-C3F-C3G-C3H |
| 57 | DN | 504 | CDL | C72-C71-CB7-OB8 |
| 57 | Dm | 501 | CDL | C72-C71-CB7-OB8 |
| 57 | Dn | 502 | CDL | C32-C31-CA7-OA8 |
| 57 | Du | 401 | CDL | C72-C71-CB7-OB8 |
| 57 | Dv | 401 | CDL | C52-C51-CB5-OB6 |
| 58 | Dv | 405 | PC1 | O31-C31-C32-C33 |
| 59 | DJ | 301 | 3PE | O21-C21-C22-C23 |
| 59 | DX | 304 | 3PE | O21-C21-C22-C23 |
| 59 | Dc | 606 | 3PE | O21-C21-C22-C23 |
| 59 | Eo | 202 | 3PE | O31-C31-C32-C33 |
| 57 | En | 1201 | CDL | C83-C84-C85-C86 |
| 58 | Ef | 1001 | PC1 | C2A-C2B-C2C-C2D |
| 57 | DQ | 1504 | CDL | C13-C14-C15-C16 |
| 57 | Ds | 405 | CDL | C41-C42-C43-C44 |
| 57 | DX | 301 | CDL | C24-C25-C26-C27 |
| 65 | EN | 1204 | UQ8 | C12-C11-C9-C8 |
| 57 | DM | 501 | CDL | C12-C11-CA5-OA6 |
| 57 | DQ | 1501 | CDL | C32-C31-CA7-OA8 |
| 57 | DR | 403 | CDL | C52-C51-CB5-OB6 |
| 57 | EA | 301 | CDL | C52-C51-CB5-OB6 |
| 57 | EH | 202 | CDL | C72-C71-CB7-OB8 |
| 57 | Da | 709 | CDL | C12-C11-CA5-OA6 |
| 57 | Ea | 301 | CDL | C72-C71-CB7-OB8 |
| 57 | Ek | 201 | CDL | C32-C31-CA7-OA8 |
| 58 | DA | 706 | PC1 | O31-C31-C32-C33 |
| 58 | DV | 405 | PC1 | O31-C31-C32-C33 |
| 58 | EO | 205 | PC1 | O21-C21-C22-C23 |
| 58 | Dx | 1204 | PC1 | O31-C31-C32-C33 |
| 58 | El | 904 | PC1 | O21-C21-C22-C23 |
| 59 | DJ | 301 | 3PE | O31-C31-C32-C33 |
| 59 | Ds | 403 | 3PE | O21-C21-C22-C23 |
| 57 | Dj | 401 | CDL | C60-C61-C62-C63 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 58 | DQ | 1503 | PC1 | C3D-C3E-C3F-C3G |
| 58 | DV | 407 | PC1 | C3D-C3E-C3F-C3G |
| 59 | DS | 403 | 3PE | C28-C29-C2A-C2B |
| 59 | Dx | 1207 | 3PE | C35-C36-C37-C38 |
| 65 | Ds | 404 | UQ8 | C39-C41-C42-C43 |
| 57 | DU | 403 | CDL | C15-C16-C17-C18 |
| 57 | EB | 304 | CDL | C20-C21-C22-C23 |
| 57 | DM | 501 | CDL | C1-CB2-OB2-PB2 |
| 57 | EA | 301 | CDL | CA3-CA4-CA6-OA8 |
| 57 | EL | 901 | CDL | CB4-CB3-OB5-PB2 |
| 57 | EN | 1202 | CDL | CA3-CA4-CA6-OA8 |
| 57 | Dn | 503 | CDL | CB4-CB3-OB5-PB2 |
| 57 | Eg | 101 | CDL | CB4-CB3-OB5-PB2 |
| 59 | DC | 607 | 3PE | C1-C2-C3-O31 |
| 59 | Eo | 202 | 3PE | C1-C2-C3-O31 |
| 57 | Dj | 408 | CDL | OB9-CB7-OB8-CB6 |
| 57 | DY | 301 | CDL | OA5-CA3-CA4-OA6 |
| 57 | EH | 201 | CDL | OA5-CA3-CA4-OA6 |
| 57 | Dd | 706 | CDL | OA5-CA3-CA4-OA6 |
| 57 | Dd | 706 | CDL | OB5-CB3-CB4-OB6 |
| 57 | Dj | 408 | CDL | OB5-CB3-CB4-OB6 |
| 57 | Dn | 502 | CDL | OA5-CA3-CA4-OA6 |
| 58 | DY | 302 | PC1 | O11-C1-C2-O21 |
| 59 | DG | 204 | 3PE | O11-C1-C2-O21 |
| 57 | DO | 501 | CDL | C72-C71-CB7-OB8 |
| 57 | DV | 401 | CDL | C52-C51-CB5-OB6 |
| 57 | Dj | 408 | CDL | C32-C31-CA7-OA8 |
| 57 | Do | 501 | CDL | C72-C71-CB7-OB8 |
| 57 | Dq | 402 | CDL | C32-C31-CA7-OA8 |
| 57 | Dv | 402 | CDL | C12-C11-CA5-OA6 |
| 57 | Dv | 404 | CDL | C52-C51-CB5-OB6 |
| 57 | Dz | 501 | CDL | C32-C31-CA7-OA8 |
| 57 | El | 901 | CDL | C32-C31-CA7-OA8 |
| 57 | Eu | 101 | CDL | C72-C71-CB7-OB8 |
| 58 | DC | 602 | PC1 | O21-C21-C22-C23 |
| 58 | Dc | 603 | PC1 | O21-C21-C22-C23 |
| 60 | Dn | 506 | LPP | O27-C29-C30-C31 |
| 57 | Dm | 501 | CDL | C78-C79-C80-C81 |
| 60 | DN | 503 | LPP | C35-C36-C37-C38 |
| 57 | DN | 501 | CDL | C57-C58-C59-C60 |
| 57 | DV | 402 | CDL | C77-C78-C79-C80 |
| 57 | DV | 404 | CDL | C83-C84-C85-C86 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 57 | En | 1201 | CDL | C43-C44-C45-C46 |
| 57 | Dq | 401 | CDL | CA4-CA6-OA8-CA7 |
| 59 | Dr | 401 | 3PE | C3F-C3G-C3H-C3I |
| 57 | DA | 709 | CDL | C72-C71-CB7-OB8 |
| 57 | DQ | 1502 | CDL | C32-C31-CA7-OA8 |
| 57 | DQ | 1502 | CDL | C72-C71-CB7-OB8 |
| 57 | DU | 403 | CDL | C32-C31-CA7-OA8 |
| 57 | DV | 403 | CDL | C72-C71-CB7-OB8 |
| 57 | Ea | 301 | CDL | C52-C51-CB5-OB6 |
| 57 | DN | 504 | CDL | C81-C82-C83-C84 |
| 57 | DV | 402 | CDL | C81-C82-C83-C84 |
| 57 | Dg | 202 | CDL | C78-C79-C80-C81 |
| 57 | EL | 904 | CDL | C83-C84-C85-C86 |
| 58 | Di | 702 | PC1 | C34-C35-C36-C37 |
| 59 | Em | 901 | 3PE | C3B-C3C-C3D-C3E |
| 57 | Du | 403 | CDL | O1-C1-CB2-OB2 |
| 57 | Ed | 204 | CDL | O1-C1-CB2-OB2 |
| 58 | Dc | 604 | PC1 | O22-C21-O21-C2 |
| 57 | Dd | 702 | CDL | C78-C79-C80-C81 |
| 54 | Da | 702 | HEA | CAA-CBA-CGA-O2A |
| 65 | ED | 603 | UQ8 | C12-C11-C9-C10 |
| 57 | DV | 402 | CDL | C12-C11-CA5-OA6 |
| 57 | DV | 404 | CDL | C52-C51-CB5-OB6 |
| 57 | Da | 705 | CDL | C72-C71-CB7-OB8 |
| 57 | Dm | 501 | CDL | C12-C11-CA5-OA6 |
| 57 | Dq | 404 | CDL | C72-C71-CB7-OB8 |
| 57 | Dv | 403 | CDL | C72-C71-CB7-OB8 |
| 57 | Ea | 301 | CDL | C12-C11-CA5-OA6 |
| 59 | DG | 205 | 3PE | O21-C21-C22-C23 |
| 59 | DX | 304 | 3PE | O31-C31-C32-C33 |
| 65 | EN | 1204 | UQ8 | C33-C34-C36-C37 |
| 65 | En | 1203 | UQ8 | C12-C11-C9-C8 |
| 57 | DV | 403 | CDL | C77-C78-C79-C80 |
| 57 | Ds | 402 | CDL | C82-C83-C84-C85 |
| 58 | DV | 405 | PC1 | C29-C2A-C2B-C2C |
| 57 | Da | 705 | CDL | OA5-CA3-CA4-CA6 |
| 57 | Dd | 704 | CDL | OB5-CB3-CB4-CB6 |
| 57 | Dn | 505 | CDL | OA5-CA3-CA4-CA6 |
| 57 | Ed | 204 | CDL | OA5-CA3-CA4-CA6 |
| 58 | Eo | 201 | PC1 | O11-C1-C2-C3 |
| 57 | Dd | 704 | CDL | C35-C36-C37-C38 |
| 57 | Dn | 507 | CDL | C81-C82-C83-C84 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 58 | Da | 706 | PC1 | C2C-C2D-C2E-C2F |
| 57 | Dd | 705 | CDL | C72-C71-CB7-OB8 |
| 57 | Di | 701 | CDL | C72-C71-CB7-OB8 |
| 57 | Du | 403 | CDL | C32-C31-CA7-OA8 |
| 57 | Du | 404 | CDL | C72-C71-CB7-OB8 |
| 57 | El | 902 | CDL | C52-C51-CB5-OB6 |
| 57 | Ep | 701 | CDL | C12-C11-CA5-OA6 |
| 58 | DC | 608 | PC1 | O21-C21-C22-C23 |
| 59 | EN | 1203 | 3PE | O21-C21-C22-C23 |
| 57 | DD | 702 | CDL | C35-C36-C37-C38 |
| 57 | DJ | 303 | CDL | C24-C25-C26-C27 |
| 57 | DJ | 304 | CDL | C19-C20-C21-C22 |
| 57 | DS | 402 | CDL | C56-C57-C58-C59 |
| 57 | EK | 201 | CDL | C13-C14-C15-C16 |
| 57 | Dg | 202 | CDL | C63-C64-C65-C66 |
| 57 | Ep | 701 | CDL | C78-C79-C80-C81 |
| 58 | DB | 702 | PC1 | C26-C27-C28-C29 |
| 57 | DQ | 1504 | CDL | OB6-CB4-CB6-OB8 |
| 57 | Ed | 205 | CDL | OB6-CB4-CB6-OB8 |
| 57 | El | 901 | CDL | OA6-CA4-CA6-OA8 |
| 58 | DB | 702 | PC1 | C32-C31-O31-C3 |
| 57 | DQ | 1504 | CDL | C76-C77-C78-C79 |
| 57 | DG | 202 | CDL | C31-C32-C33-C34 |
| 57 | EL | 901 | CDL | C77-C78-C79-C80 |
| 57 | Dn | 501 | CDL | C12-C13-C14-C15 |
| 59 | EL | 905 | 3PE | C34-C35-C36-C37 |
| 57 | DU | 401 | CDL | C32-C31-CA7-OA8 |
| 57 | DZ | 501 | CDL | C32-C31-CA7-OA8 |
| 57 | EI | 401 | CDL | C12-C11-CA5-OA6 |
| 57 | EI | 401 | CDL | C72-C71-CB7-OB8 |
| 57 | EL | 904 | CDL | C12-C11-CA5-OA6 |
| 57 | Dg | 201 | CDL | C12-C11-CA5-OA6 |
| 57 | Dn | 501 | CDL | C72-C71-CB7-OB8 |
| 57 | Dq | 401 | CDL | C72-C71-CB7-OB8 |
| 57 | Ei | 401 | CDL | C72-C71-CB7-OB8 |
| 58 | EO | 206 | PC1 | O21-C21-C22-C23 |
| 58 | Dc | 602 | PC1 | O21-C21-C22-C23 |
| 58 | Eo | 205 | PC1 | O21-C21-C22-C23 |
| 59 | EM | 901 | 3PE | O21-C21-C22-C23 |
| 59 | Ds | 401 | 3PE | O21-C21-C22-C23 |
| 59 | Dx | 1205 | 3PE | O21-C21-C22-C23 |
| 57 | DA | 705 | CDL | C77-C78-C79-C80 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 57 | DN | 504 | CDL | C59-C60-C61-C62 |
| 57 | DX | 301 | CDL | C78-C79-C80-C81 |
| 57 | Dg | 202 | CDL | C31-C32-C33-C34 |
| 54 | DA | 702 | HEA | CAA-CBA-CGA-O2A |
| 68 | Er | 201 | ATP | C5'-O5'-PA-O3A |
| 57 | Du | 401 | CDL | C37-C38-C39-C40 |
| 57 | DU | 401 | CDL | CA7-C31-C32-C33 |
| 59 | Eo | 202 | 3PE | C38-C39-C3A-C3B |
| 57 | DD | 702 | CDL | C51-CB5-OB6-CB4 |
| 58 | Dx | 1204 | PC1 | C22-C21-O21-C2 |
| 57 | Dj | 401 | CDL | CA4-CA6-OA8-CA7 |
| 57 | Dq | 404 | CDL | C14-C15-C16-C17 |
| 57 | Du | 403 | CDL | C58-C59-C60-C61 |
| 65 | EN | 1204 | UQ8 | C13-C14-C16-C17 |
| 58 | DB | 702 | PC1 | C2-C1-O11-P |
| 57 | DA | 709 | CDL | C77-C78-C79-C80 |
| 57 | DX | 307 | CDL | C63-C64-C65-C66 |
| 57 | EK | 201 | CDL | C32-C31-CA7-OA8 |
| 57 | Dh | 202 | CDL | C72-C71-CB7-OB8 |
| 57 | Eh | 1601 | CDL | C52-C51-CB5-OB6 |
| 58 | EO | 206 | PC1 | O31-C31-C32-C33 |
| 59 | Dg | 204 | 3PE | O21-C21-C22-C23 |
| 57 | DS | 405 | CDL | C18-C19-C20-C21 |
| 57 | DX | 301 | CDL | C32-C33-C34-C35 |
| 57 | Dr | 402 | CDL | C41-C42-C43-C44 |
| 57 | Dj | 408 | CDL | C52-C51-CB5-OB7 |
| 65 | Ed | 202 | UQ8 | C24-C26-C27-C28 |
| 57 | Dv | 404 | CDL | C83-C84-C85-C86 |
| 57 | DM | 501 | CDL | C17-C18-C19-C20 |
| 58 | Da | 706 | PC1 | C35-C36-C37-C38 |
| 58 | Dc | 602 | PC1 | C2E-C2F-C2G-C2H |
| 65 | EL | 906 | UQ8 | C3-C4-O4-C4M |
| 65 | Ds | 404 | UQ8 | C4-C3-O3-C3M |
| 65 | Ed | 202 | UQ8 | C4-C3-O3-C3M |
| 57 | DZ | 501 | CDL | C39-C40-C41-C42 |
| 57 | Dv | 402 | CDL | C81-C82-C83-C84 |
| 57 | El | 901 | CDL | C62-C63-C64-C65 |
| 60 | EI | 402 | LPP | C40-C41-C42-C43 |
| 57 | Dj | 408 | CDL | C71-CB7-OB8-CB6 |
| 57 | DD | 704 | CDL | C72-C71-CB7-OB8 |
| 57 | DJ | 303 | CDL | C72-C71-CB7-OB8 |
| 57 | Dq | 403 | CDL | C72-C71-CB7-OB8 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 57 | DJ | 303 | CDL | C12-C11-CA5-OA7 |
| 58 | Dc | 603 | PC1 | O22-C21-C22-C23 |
| 68 | ER | 201 | ATP | PA-O3A-PB-O2B |
| 68 | Er | 201 | ATP | PG-O3B-PB-O1B |
| 57 | DR | 403 | CDL | C52-C53-C54-C55 |
| 57 | EN | 1201 | CDL | C54-C55-C56-C57 |
| 57 | Da | 705 | CDL | C16-C17-C18-C19 |
| 65 | El | 906 | UQ8 | C36-C37-C38-C39 |
| 58 | Dv | 405 | PC1 | O32-C31-C32-C33 |
| 57 | Du | 401 | CDL | C13-C14-C15-C16 |
| 59 | DA | 708 | 3PE | C2C-C2D-C2E-C2F |
| 57 | Dj | 401 | CDL | C72-C71-CB7-OB8 |
| 57 | Dr | 402 | CDL | C52-C51-CB5-OB6 |
| 57 | EA | 301 | CDL | C78-C79-C80-C81 |
| 57 | Eg | 101 | CDL | C73-C74-C75-C76 |
| 57 | El | 903 | CDL | C83-C84-C85-C86 |
| 57 | DV | 403 | CDL | C11-C12-C13-C14 |
| 57 | Du | 403 | CDL | C33-C34-C35-C36 |
| 58 | DV | 405 | PC1 | C2D-C2E-C2F-C2G |
| 59 | DS | 403 | 3PE | C3E-C3F-C3G-C3H |
| 57 | DQ | 1501 | CDL | C72-C71-CB7-OB9 |
| 57 | EA | 301 | CDL | C52-C51-CB5-OB7 |
| 57 | Ea | 301 | CDL | C72-C71-CB7-OB9 |
| 58 | DC | 603 | PC1 | O22-C21-C22-C23 |
| 59 | DS | 403 | 3PE | O22-C21-C22-C23 |
| 59 | DX | 303 | 3PE | O22-C21-C22-C23 |
| 59 | Dx | 1206 | 3PE | O22-C21-C22-C23 |
| 59 | DA | 708 | 3PE | C2D-C2E-C2F-C2G |
| 60 | EI | 402 | LPP | C21-C22-C23-C24 |
| 57 | DS | 405 | CDL | C78-C79-C80-C81 |
| 65 | ED | 603 | UQ8 | C33-C34-C36-C37 |
| 57 | Di | 701 | CDL | C53-C54-C55-C56 |
| 57 | Dn | 502 | CDL | C61-C62-C63-C64 |
| 59 | Dr | 404 | 3PE | C28-C29-C2A-C2B |
| 57 | EH | 202 | CDL | C72-C71-CB7-OB9 |
| 57 | Da | 705 | CDL | C72-C71-CB7-OB9 |
| 57 | Dn | 502 | CDL | C32-C31-CA7-OA9 |
| 58 | DV | 406 | PC1 | O32-C31-C32-C33 |
| 58 | El | 904 | PC1 | O22-C21-C22-C23 |
| 59 | Ds | 403 | 3PE | O22-C21-C22-C23 |
| 57 | DD | 704 | CDL | OB5-CB3-CB4-OB6 |
| 57 | Dv | 402 | CDL | C71-CB7-OB8-CB6 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 57 | Ds | 402 | CDL | C54-C55-C56-C57 |
| 57 | DS | 405 | CDL | CA7-C31-C32-C33 |
| 57 | DO | 501 | CDL | C33-C34-C35-C36 |
| 57 | Dd | 704 | CDL | C37-C38-C39-C40 |
| 57 | DO | 501 | CDL | C72-C71-CB7-OB9 |
| 57 | DV | 403 | CDL | C72-C71-CB7-OB9 |
| 57 | Da | 709 | CDL | C52-C51-CB5-OB7 |
| 57 | Dd | 705 | CDL | C12-C11-CA5-OA7 |
| 57 | Dj | 408 | CDL | C32-C31-CA7-OA9 |
| 57 | Ed | 205 | CDL | C12-C11-CA5-OA7 |
| 58 | EO | 205 | PC1 | O22-C21-C22-C23 |
| 58 | Da | 706 | PC1 | O32-C31-C32-C33 |
| 58 | Dx | 1204 | PC1 | O32-C31-C32-C33 |
| 59 | DG | 204 | 3PE | O22-C21-C22-C23 |
| 59 | Dd | 703 | 3PE | O22-C21-C22-C23 |
| 60 | Dn | 504 | LPP | O28-C29-C30-C31 |
| 60 | Dn | 506 | LPP | O28-C29-C30-C31 |
| 57 | DA | 709 | CDL | C11-C12-C13-C14 |
| 58 | Dc | 607 | PC1 | C3C-C3D-C3E-C3F |
| 59 | DS | 401 | 3PE | C32-C33-C34-C35 |
| 57 | EN | 1202 | CDL | C71-CB7-OB8-CB6 |
| 57 | DD | 703 | CDL | C52-C51-CB5-OB7 |
| 57 | DR | 403 | CDL | C52-C51-CB5-OB7 |
| 57 | DU | 401 | CDL | C72-C71-CB7-OB9 |
| 57 | Dq | 404 | CDL | C72-C71-CB7-OB9 |
| 57 | Dv | 401 | CDL | C52-C51-CB5-OB7 |
| 57 | Dv | 403 | CDL | C72-C71-CB7-OB9 |
| 57 | Ea | 301 | CDL | C12-C11-CA5-OA7 |
| 58 | EO | 207 | PC1 | O22-C21-C22-C23 |
| 59 | DJ | 301 | 3PE | O22-C21-C22-C23 |
| 59 | DS | 401 | 3PE | O22-C21-C22-C23 |
| 59 | DX | 304 | 3PE | O32-C31-C32-C33 |
| 59 | Dc | 606 | 3PE | O22-C21-C22-C23 |
| 59 | Dg | 204 | 3PE | O22-C21-C22-C23 |
| 57 | DU | 401 | CDL | C37-C38-C39-C40 |
| 57 | Dh | 202 | CDL | C51-C52-C53-C54 |
| 57 | Dj | 403 | CDL | C19-C20-C21-C22 |
| 57 | DD | 703 | CDL | CA3-CA4-CA6-OA8 |
| 57 | EB | 302 | CDL | CB3-CB4-CB6-OB8 |
| 57 | EH | 202 | CDL | CA3-CA4-CA6-OA8 |
| 57 | EN | 1201 | CDL | CA3-CA4-CA6-OA8 |
| 57 | Eg | 101 | CDL | CB3-CB4-CB6-OB8 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 57 | DA | 710 | CDL | C12-C11-CA5-OA6 |
| 57 | Dn | 503 | CDL | C32-C31-CA7-OA8 |
| 58 | Ef | 1001 | PC1 | O31-C31-C32-C33 |
| 57 | Dh | 202 | CDL | C55-C56-C57-C58 |
| 59 | DA | 708 | 3PE | C36-C37-C38-C39 |
| 59 | Dx | 1207 | 3PE | C2E-C2F-C2G-C2H |
| 57 | Eh | 1601 | CDL | CB3-OB5-PB2-OB2 |
| 57 | DQ | 1501 | CDL | C14-C15-C16-C17 |
| 57 | DU | 401 | CDL | C71-C72-C73-C74 |
| 57 | Dg | 201 | CDL | C75-C76-C77-C78 |
| 57 | Dg | 202 | CDL | C36-C37-C38-C39 |
| 58 | Da | 706 | PC1 | C3A-C3B-C3C-C3D |
| 57 | ED | 604 | CDL | C12-C11-CA5-OA7 |
| 57 | Dm | 501 | CDL | C72-C71-CB7-OB9 |
| 57 | Du | 401 | CDL | C72-C71-CB7-OB9 |
| 57 | Ek | 201 | CDL | C32-C31-CA7-OA9 |
| 59 | DJ | 301 | 3PE | O32-C31-C32-C33 |
| 57 | EN | 1202 | CDL | C32-C33-C34-C35 |
| 57 | El | 902 | CDL | C79-C80-C81-C82 |
| 57 | EN | 1202 | CDL | OB9-CB7-OB8-CB6 |
| 57 | Dv | 402 | CDL | OB9-CB7-OB8-CB6 |
| 59 | Eo | 202 | 3PE | C26-C27-C28-C29 |
| 60 | DN | 502 | LPP | O27-C29-C30-C31 |
| 57 | DA | 705 | CDL | C1-CB2-OB2-PB2 |
| 57 | Dg | 201 | CDL | C1-CB2-OB2-PB2 |
| 57 | Eg | 101 | CDL | CA4-CA3-OA5-PA1 |
| 58 | EB | 301 | PC1 | C2-C1-O11-P |
| 58 | EB | 303 | PC1 | C2-C1-O11-P |
| 57 | DQ | 1501 | CDL | C32-C31-CA7-OA9 |
| 57 | Dm | 501 | CDL | C12-C11-CA5-OA7 |
| 57 | Dq | 402 | CDL | C32-C31-CA7-OA9 |
| 57 | Du | 404 | CDL | C72-C71-CB7-OB9 |
| 57 | Dv | 402 | CDL | C12-C11-CA5-OA7 |
| 57 | Ea | 301 | CDL | C52-C51-CB5-OB7 |
| 57 | El | 901 | CDL | C32-C31-CA7-OA9 |
| 57 | Ep | 701 | CDL | C12-C11-CA5-OA7 |
| 58 | DV | 405 | PC1 | O32-C31-C32-C33 |
| 58 | Dx | 1202 | PC1 | O32-C31-C32-C33 |
| 59 | DG | 205 | 3PE | O32-C31-C32-C33 |
| 58 | Dv | 408 | PC1 | C3C-C3D-C3E-C3F |
| 60 | Dn | 506 | LPP | C30-C31-C32-C33 |
| 57 | EL | 901 | CDL | C73-C74-C75-C76 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 57 | Ds | 402 | CDL | C22-C23-C24-C25 |
| 58 | DA | 706 | PC1 | C2C-C2D-C2E-C2F |
| 57 | DA | 705 | CDL | CB3-OB5-PB2-OB3 |
| 57 | DA | 710 | CDL | CB2-OB2-PB2-OB3 |
| 57 | DC | 601 | CDL | CA2-OA2-PA1-OA3 |
| 57 | DD | 704 | CDL | CA3-OA5-PA1-OA3 |
| 57 | DD | 704 | CDL | CB3-OB5-PB2-OB4 |
| 57 | DG | 201 | CDL | CB3-OB5-PB2-OB4 |
| 57 | DG | 202 | CDL | CA3-OA5-PA1-OA3 |
| 57 | DJ | 302 | CDL | CA2-OA2-PA1-OA3 |
| 57 | DJ | 305 | CDL | CB3-OB5-PB2-OB3 |
| 57 | DJ | 307 | CDL | CB3-OB5-PB2-OB3 |
| 57 | DM | 502 | CDL | CB2-OB2-PB2-OB3 |
| 57 | DN | 501 | CDL | CA2-OA2-PA1-OA3 |
| 57 | DN | 504 | CDL | CB3-OB5-PB2-OB4 |
| 57 | DN | 505 | CDL | CB3-OB5-PB2-OB3 |
| 57 | DQ | 1502 | CDL | CA2-OA2-PA1-OA3 |
| 57 | DX | 301 | CDL | CA3-OA5-PA1-OA3 |
| 57 | DX | 301 | CDL | CB2-OB2-PB2-OB4 |
| 57 | DY | 301 | CDL | CA2-OA2-PA1-OA3 |
| 57 | DY | 301 | CDL | CB3-OB5-PB2-OB3 |
| 57 | ED | 601 | CDL | CA2-OA2-PA1-OA3 |
| 57 | ED | 601 | CDL | CB2-OB2-PB2-OB3 |
| 57 | EL | 904 | CDL | CA2-OA2-PA1-OA3 |
| 57 | EL | 904 | CDL | CA2-OA2-PA1-OA4 |
| 57 | EL | 904 | CDL | CB2-OB2-PB2-OB4 |
| 57 | EN | 1202 | CDL | CB2-OB2-PB2-OB3 |
| 57 | EU | 101 | CDL | CA2-OA2-PA1-OA3 |
| 57 | Dc | 601 | CDL | CA2-OA2-PA1-OA3 |
| 57 | Dc | 601 | CDL | CA2-OA2-PA1-OA4 |
| 57 | Dd | 706 | CDL | CB3-OB5-PB2-OB4 |
| 57 | Dg | 202 | CDL | CA3-OA5-PA1-OA3 |
| 57 | Di | 701 | CDL | CB3-OB5-PB2-OB4 |
| 57 | Dj | 402 | CDL | CB3-OB5-PB2-OB3 |
| 57 | Dj | 403 | CDL | CB2-OB2-PB2-OB3 |
| 57 | Dj | 403 | CDL | CB3-OB5-PB2-OB3 |
| 57 | Dj | 404 | CDL | CA2-OA2-PA1-OA3 |
| 57 | Dn | 501 | CDL | CB2-OB2-PB2-OB3 |
| 57 | Dn | 501 | CDL | CB3-OB5-PB2-OB3 |
| 57 | Dn | 503 | CDL | CA2-OA2-PA1-OA3 |
| 57 | Du | 401 | CDL | CA3-OA5-PA1-OA4 |
| 57 | Du | 403 | CDL | CA2-OA2-PA1-OA4 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 57 | Dy | 301 | CDL | CA2-OA2-PA1-OA3 |
| 57 | Dz | 501 | CDL | CA2-OA2-PA1-OA3 |
| 57 | Ed | 204 | CDL | CA2-OA2-PA1-OA3 |
| 57 | Eg | 101 | CDL | CA3-OA5-PA1-OA3 |
| 57 | Eh | 1601 | CDL | CA2-OA2-PA1-OA3 |
| 57 | Eh | 1601 | CDL | CB3-OB5-PB2-OB4 |
| 57 | Ei | 401 | CDL | CA2-OA2-PA1-OA4 |
| 57 | En | 1201 | CDL | CA2-OA2-PA1-OA4 |
| 57 | En | 1201 | CDL | CB2-OB2-PB2-OB3 |
| 57 | En | 1202 | CDL | CB2-OB2-PB2-OB3 |
| 57 | Eu | 101 | CDL | CA3-OA5-PA1-OA3 |
| 58 | DS | 407 | PC1 | C1-O11-P-O14 |
| 58 | DV | 405 | PC1 | C1-O11-P-O14 |
| 58 | DV | 406 | PC1 | C1-O11-P-O14 |
| 58 | DX | 306 | PC1 | C1-O11-P-O14 |
| 58 | Dv | 405 | PC1 | C11-O13-P-O14 |
| 58 | Dv | 405 | PC1 | C1-O11-P-O14 |
| 58 | Dx | 1202 | PC1 | C11-O13-P-O14 |
| 58 | Dx | 1208 | PC1 | C11-O13-P-O14 |
| 58 | Dy | 302 | PC1 | C11-O13-P-O14 |
| 58 | Dy | 302 | PC1 | C1-O11-P-O14 |
| 58 | Ef | 1001 | PC1 | C11-O13-P-O14 |
| 58 | Eo | 204 | PC1 | C1-O11-P-O14 |
| 59 | Dd | 703 | 3PE | C11-O13-P-O14 |
| 59 | Eo | 202 | 3PE | C11-O13-P-O14 |
| 59 | Eo | 203 | 3PE | C11-O13-P-O14 |
| 68 | Er | 201 | ATP | C5'-O5'-PA-O1A |
| 68 | Er | 201 | ATP | C5'-O5'-PA-O2A |
| 58 | Dc | 604 | PC1 | C22-C21-O21-C2 |
| 57 | Ds | 405 | CDL | CA7-C31-C32-C33 |
| 57 | DD | 702 | CDL | C14-C15-C16-C17 |
| 57 | DM | 501 | CDL | C40-C41-C42-C43 |
| 57 | DS | 405 | CDL | C41-C42-C43-C44 |
| 57 | Dh | 202 | CDL | C20-C21-C22-C23 |
| 57 | Dj | 401 | CDL | C79-C80-C81-C82 |
| 57 | DQ | 1502 | CDL | C32-C31-CA7-OA9 |
| 57 | DQ | 1502 | CDL | C72-C71-CB7-OB9 |
| 57 | DU | 403 | CDL | C32-C31-CA7-OA9 |
| 57 | DV | 402 | CDL | C12-C11-CA5-OA7 |
| 57 | DV | 404 | CDL | C52-C51-CB5-OB7 |
| 57 | EI | 401 | CDL | C12-C11-CA5-OA7 |
| 57 | EI | 401 | CDL | C72-C71-CB7-OB9 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 57 | Dg | 201 | CDL | C12-C11-CA5-OA7 |
| 57 | Dn | 501 | CDL | C72-C71-CB7-OB9 |
| 57 | El | 902 | CDL | C52-C51-CB5-OB7 |
| 59 | DG | 205 | 3PE | O22-C21-C22-C23 |
| 59 | EN | 1203 | 3PE | O22-C21-C22-C23 |
| 59 | Ds | 401 | 3PE | O22-C21-C22-C23 |
| 58 | DQ | 1503 | PC1 | O31-C31-C32-C33 |
| 57 | DO | 501 | CDL | OB5-CB3-CB4-CB6 |
| 57 | Dj | 402 | CDL | OB5-CB3-CB4-CB6 |
| 57 | DJ | 304 | CDL | C83-C84-C85-C86 |
| 59 | Dx | 1206 | 3PE | C32-C33-C34-C35 |
| 57 | EL | 903 | CDL | C84-C85-C86-C87 |
| 59 | Dr | 401 | 3PE | O13-C11-C12-N |
| 57 | DD | 704 | CDL | C72-C71-CB7-OB9 |
| 57 | Eu | 101 | CDL | C72-C71-CB7-OB9 |
| 58 | Dc | 602 | PC1 | O22-C21-C22-C23 |
| 59 | DX | 304 | 3PE | O22-C21-C22-C23 |
| 59 | Eo | 202 | 3PE | O32-C31-C32-C33 |
| 57 | DG | 201 | CDL | C17-C18-C19-C20 |
| 57 | DG | 201 | CDL | C41-C42-C43-C44 |
| 57 | DI | 701 | CDL | C36-C37-C38-C39 |
| 57 | DS | 402 | CDL | C54-C55-C56-C57 |
| 57 | DR | 403 | CDL | C72-C71-CB7-OB8 |
| 57 | Da | 709 | CDL | C32-C31-CA7-OA8 |
| 59 | Dd | 703 | 3PE | O31-C31-C32-C33 |
| 57 | ED | 604 | CDL | C75-C76-C77-C78 |
| 57 | DN | 504 | CDL | C20-C21-C22-C23 |
| 57 | DN | 504 | CDL | C72-C71-CB7-OB9 |
| 57 | EK | 201 | CDL | C32-C31-CA7-OA9 |
| 57 | Dj | 401 | CDL | C72-C71-CB7-OB9 |
| 57 | Dr | 403 | CDL | C52-C51-CB5-OB7 |
| 57 | Dx | 1201 | CDL | C52-C51-CB5-OB7 |
| 59 | Dx | 1206 | 3PE | O32-C31-C32-C33 |
| 57 | Dj | 404 | CDL | C58-C59-C60-C61 |
| 57 | DR | 403 | CDL | C37-C38-C39-C40 |
| 57 | DJ | 305 | CDL | C72-C71-CB7-OB8 |
| 57 | Dj | 402 | CDL | C12-C11-CA5-OA6 |
| 57 | Dq | 403 | CDL | C52-C51-CB5-OB6 |
| 57 | DA | 709 | CDL | C83-C84-C85-C86 |
| 57 | DD | 702 | CDL | C73-C74-C75-C76 |
| 60 | Ed | 203 | LPP | C18-C19-C20-C21 |
| 57 | DZ | 501 | CDL | C32-C31-CA7-OA9 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 57 | Do | 501 | CDL | C72-C71-CB7-OB9 |
| 58 | DC | 602 | PC1 | O22-C21-C22-C23 |
| 58 | Eo | 205 | PC1 | O22-C21-C22-C23 |
| 57 | EL | 901 | CDL | C32-C33-C34-C35 |
| 57 | DH | 201 | CDL | C60-C61-C62-C63 |
| 57 | DM | 501 | CDL | C83-C84-C85-C86 |
| 57 | DN | 505 | CDL | C53-C54-C55-C56 |
| 57 | EU | 101 | CDL | C71-C72-C73-C74 |
| 57 | Dj | 403 | CDL | C63-C64-C65-C66 |
| 57 | Du | 402 | CDL | C20-C21-C22-C23 |
| 54 | DA | 701 | HEA | CAD-CBD-CGD-O2D |
| 54 | DA | 702 | HEA | C3B-C11-C12-C13 |
| 57 | DA | 710 | CDL | CA3-CA4-OA6-CA5 |
| 57 | DJ | 307 | CDL | CB3-CB4-OB6-CB5 |
| 57 | DO | 501 | CDL | CB3-CB4-OB6-CB5 |
| 57 | DV | 401 | CDL | CA3-CA4-OA6-CA5 |
| 57 | EA | 301 | CDL | CA3-CA4-OA6-CA5 |
| 57 | EN | 1202 | CDL | CB3-CB4-OB6-CB5 |
| 57 | EO | 202 | CDL | CB6-CB4-OB6-CB5 |
| 57 | Dd | 705 | CDL | CB3-CB4-OB6-CB5 |
| 57 | Dd | 706 | CDL | CB6-CB4-OB6-CB5 |
| 57 | Dj | 402 | CDL | CB3-CB4-OB6-CB5 |
| 57 | Dj | 404 | CDL | CA3-CA4-OA6-CA5 |
| 58 | EB | 301 | PC1 | C12-C11-O13-P |
| 58 | EO | 207 | PC1 | C3-C2-O21-C21 |
| 58 | Da | 707 | PC1 | C12-C11-O13-P |
| 58 | Dc | 607 | PC1 | C1-C2-O21-C21 |
| 58 | Eb | 301 | PC1 | C12-C11-O13-P |
| 58 | Ef | 1001 | PC1 | C12-C11-O13-P |
| 59 | DA | 708 | 3PE | C12-C11-O13-P |
| 59 | DG | 204 | 3PE | C12-C11-O13-P |
| 59 | EO | 203 | 3PE | C12-C11-O13-P |
| 57 | DM | 501 | CDL | C12-C11-CA5-OA7 |
| 57 | DV | 401 | CDL | C52-C51-CB5-OB7 |
| 57 | Da | 709 | CDL | C12-C11-CA5-OA7 |
| 57 | Dm | 501 | CDL | C52-C51-CB5-OB7 |
| 57 | Dq | 403 | CDL | C72-C71-CB7-OB9 |
| 57 | Dv | 404 | CDL | C52-C51-CB5-OB7 |
| 57 | Dz | 501 | CDL | C32-C31-CA7-OA9 |
| 57 | Eh | 1601 | CDL | C52-C51-CB5-OB7 |
| 58 | DA | 706 | PC1 | O32-C31-C32-C33 |
| 58 | EO | 206 | PC1 | O32-C31-C32-C33 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 59 | Dx | 1205 | 3PE | O22-C21-C22-C23 |
| 57 | DR | 403 | CDL | C20-C21-C22-C23 |
| 57 | Da | 709 | CDL | C36-C37-C38-C39 |
| 57 | Dn | 501 | CDL | C83-C84-C85-C86 |
| 59 | DA | 708 | 3PE | C3C-C3D-C3E-C3F |
| 59 | Da | 708 | 3PE | C3C-C3D-C3E-C3F |
| 59 | Da | 708 | 3PE | C2D-C2E-C2F-C2G |
| 57 | EN | 1201 | CDL | C42-C43-C44-C45 |
| 57 | Dd | 704 | CDL | C40-C41-C42-C43 |
| 57 | Dn | 501 | CDL | C77-C78-C79-C80 |
| 57 | DA | 709 | CDL | C55-C56-C57-C58 |
| 57 | Dd | 704 | CDL | C83-C84-C85-C86 |
| 57 | Dd | 705 | CDL | C72-C71-CB7-OB9 |
| 57 | DU | 404 | CDL | C14-C15-C16-C17 |
| 57 | EL | 903 | CDL | C33-C34-C35-C36 |
| 57 | DC | 601 | CDL | C72-C71-CB7-OB8 |
| 57 | DD | 702 | CDL | C32-C31-CA7-OA8 |
| 57 | DS | 405 | CDL | C12-C11-CA5-OA6 |
| 57 | EH | 201 | CDL | C32-C31-CA7-OA8 |
| 57 | EH | 201 | CDL | C52-C51-CB5-OB6 |
| 57 | EL | 901 | CDL | C72-C71-CB7-OB8 |
| 57 | EU | 101 | CDL | C72-C71-CB7-OB8 |
| 57 | Dd | 702 | CDL | C32-C31-CA7-OA8 |
| 57 | Dd | 702 | CDL | C72-C71-CB7-OB8 |
| 57 | Dg | 201 | CDL | C32-C31-CA7-OA8 |
| 57 | Dj | 405 | CDL | C72-C71-CB7-OB8 |
| 57 | Dm | 502 | CDL | C12-C11-CA5-OA6 |
| 57 | Dn | 505 | CDL | C12-C11-CA5-OA6 |
| 57 | Dy | 301 | CDL | C72-C71-CB7-OB8 |
| 57 | Eg | 101 | CDL | C12-C11-CA5-OA6 |
| 57 | El | 901 | CDL | C72-C71-CB7-OB8 |
| 58 | DC | 605 | PC1 | O21-C21-C22-C23 |
| 59 | Em | 901 | 3PE | O21-C21-C22-C23 |
| 57 | Dn | 501 | CDL | C64-C65-C66-C67 |
| 57 | Du | 404 | CDL | C76-C77-C78-C79 |
| 59 | DX | 303 | 3PE | C26-C27-C28-C29 |
| 57 | DZ | 501 | CDL | C35-C36-C37-C38 |
| 57 | Ek | 201 | CDL | C11-C12-C13-C14 |
| 60 | Dn | 506 | LPP | C41-C42-C43-C44 |
| 57 | Ds | 402 | CDL | C76-C77-C78-C79 |
| 57 | Dv | 402 | CDL | C82-C83-C84-C85 |
| 57 | DG | 201 | CDL | C21-C22-C23-C24 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 57 | DZ | 501 | CDL | C33-C34-C35-C36 |
| 57 | Du | 404 | CDL | C61-C62-C63-C64 |
| 57 | DA | 710 | CDL | C32-C31-CA7-OA8 |
| 57 | DD | 704 | CDL | C52-C51-CB5-OB6 |
| 57 | DI | 701 | CDL | C72-C71-CB7-OB8 |
| 57 | DJ | 302 | CDL | C32-C31-CA7-OA8 |
| 57 | DJ | 304 | CDL | C72-C71-CB7-OB8 |
| 57 | DV | 402 | CDL | C52-C51-CB5-OB6 |
| 57 | EL | 903 | CDL | C32-C31-CA7-OA8 |
| 57 | Dc | 601 | CDL | C72-C71-CB7-OB8 |
| 57 | Dd | 706 | CDL | C32-C31-CA7-OA8 |
| 57 | Dn | 502 | CDL | C52-C51-CB5-OB6 |
| 57 | Ds | 402 | CDL | C12-C11-CA5-OA6 |
| 57 | Dv | 402 | CDL | C32-C31-CA7-OA8 |
| 57 | Dx | 1201 | CDL | C72-C71-CB7-OB8 |
| 57 | Ep | 701 | CDL | C32-C31-CA7-OA8 |
| 58 | DI | 702 | PC1 | O21-C21-C22-C23 |
| 58 | Dc | 602 | PC1 | O31-C31-C32-C33 |
| 58 | Dc | 605 | PC1 | O21-C21-C22-C23 |
| 58 | Eo | 204 | PC1 | O21-C21-C22-C23 |
| 59 | El | 905 | 3PE | O21-C21-C22-C23 |
| 65 | DS | 404 | UQ8 | C11-C12-C13-C14 |
| 57 | DA | 710 | CDL | CB2-C1-CA2-OA2 |
| 57 | Dj | 403 | CDL | CB2-C1-CA2-OA2 |
| 57 | EO | 202 | CDL | C72-C73-C74-C75 |
| 57 | Ep | 701 | CDL | C55-C56-C57-C58 |
| 57 | EI | 401 | CDL | CA5-C11-C12-C13 |
| 57 | DC | 601 | CDL | C72-C71-CB7-OB9 |
| 57 | DU | 401 | CDL | C32-C31-CA7-OA9 |
| 57 | Dc | 601 | CDL | C72-C71-CB7-OB9 |
| 57 | Di | 701 | CDL | C72-C71-CB7-OB9 |
| 57 | Dq | 401 | CDL | C72-C71-CB7-OB9 |
| 57 | Ei | 401 | CDL | C72-C71-CB7-OB9 |
| 59 | EM | 901 | 3PE | O22-C21-C22-C23 |
| 57 | Dv | 403 | CDL | C77-C78-C79-C80 |
| 57 | Dj | 408 | CDL | C1-CA2-OA2-PA1 |
| 57 | Dd | 706 | CDL | C34-C35-C36-C37 |
| 57 | Dd | 704 | CDL | OB5-CB3-CB4-OB6 |
| 59 | Dr | 401 | 3PE | O11-C1-C2-O21 |
| 57 | DA | 709 | CDL | C72-C71-CB7-OB9 |
| 57 | DA | 710 | CDL | C12-C11-CA5-OA7 |
| 57 | Du | 403 | CDL | C32-C31-CA7-OA9 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 58 | DC | 608 | PC1 | O22-C21-C22-C23 |
| 58 | Dc | 605 | PC1 | O22-C21-C22-C23 |
| 58 | Ef | 1001 | PC1 | O32-C31-C32-C33 |
| 59 | Em | 901 | 3PE | O22-C21-C22-C23 |
| 57 | Dm | 501 | CDL | C41-C42-C43-C44 |
| 57 | Dr | 402 | CDL | C74-C75-C76-C77 |
| 57 | DA | 705 | CDL | C72-C71-CB7-OB8 |
| 57 | DJ | 303 | CDL | C32-C31-CA7-OA8 |
| 57 | DV | 402 | CDL | C32-C31-CA7-OA8 |
| 57 | DX | 307 | CDL | C52-C51-CB5-OB6 |
| 57 | EB | 302 | CDL | C12-C11-CA5-OA6 |
| 57 | ED | 604 | CDL | C32-C31-CA7-OA8 |
| 57 | EN | 1201 | CDL | C12-C11-CA5-OA6 |
| 57 | Dn | 505 | CDL | C72-C71-CB7-OB8 |
| 57 | Dn | 507 | CDL | C72-C71-CB7-OB8 |
| 57 | Du | 401 | CDL | C32-C31-CA7-OA8 |
| 57 | Dv | 402 | CDL | C52-C51-CB5-OB6 |
| 58 | Dc | 607 | PC1 | O21-C21-C22-C23 |
| 59 | DC | 607 | 3PE | O21-C21-C22-C23 |
| 57 | DD | 704 | CDL | C37-C38-C39-C40 |
| 57 | DJ | 303 | CDL | C59-C60-C61-C62 |
| 57 | DR | 402 | CDL | C75-C76-C77-C78 |
| 57 | EL | 902 | CDL | C64-C65-C66-C67 |
| 57 | Dn | 501 | CDL | C43-C44-C45-C46 |
| 57 | DA | 705 | CDL | C16-C17-C18-C19 |
| 57 | DX | 307 | CDL | C42-C43-C44-C45 |
| 57 | EL | 904 | CDL | C14-C15-C16-C17 |
| 58 | DC | 604 | PC1 | C3C-C3D-C3E-C3F |
| 57 | DA | 705 | CDL | C72-C71-CB7-OB9 |
| 57 | DI | 701 | CDL | C72-C71-CB7-OB9 |
| 57 | EH | 201 | CDL | C32-C31-CA7-OA9 |
| 57 | EU | 101 | CDL | C72-C71-CB7-OB9 |
| 57 | Dn | 503 | CDL | C32-C31-CA7-OA9 |
| 58 | EO | 206 | PC1 | O22-C21-C22-C23 |
| 57 | DJ | 303 | CDL | C16-C17-C18-C19 |
| 57 | DQ | 1501 | CDL | C12-C13-C14-C15 |
| 57 | DR | 402 | CDL | C31-C32-C33-C34 |
| 59 | Dx | 1206 | 3PE | C35-C36-C37-C38 |
| 57 | DM | 501 | CDL | C72-C71-CB7-OB8 |
| 57 | DN | 501 | CDL | C52-C51-CB5-OB6 |
| 57 | DN | 504 | CDL | C32-C31-CA7-OA8 |
| 57 | DS | 405 | CDL | C32-C31-CA7-OA8 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 57 | Di | 701 | CDL | C52-C51-CB5-OB6 |
| 57 | Dn | 507 | CDL | C12-C11-CA5-OA6 |
| 57 | Dy | 301 | CDL | C52-C51-CB5-OB6 |
| 58 | DC | 602 | PC1 | O31-C31-C32-C33 |
| 65 | EN | 1204 | UQ8 | C4-C3-O3-C3M |
| 65 | Ds | 404 | UQ8 | C3-C4-O4-C4M |
| 58 | DC | 605 | PC1 | C3B-C3C-C3D-C3E |
| 57 | DD | 702 | CDL | C32-C31-CA7-OA9 |
| 57 | DJ | 303 | CDL | C72-C71-CB7-OB9 |
| 57 | DV | 402 | CDL | C52-C51-CB5-OB7 |
| 57 | EL | 904 | CDL | C12-C11-CA5-OA7 |
| 57 | Dn | 505 | CDL | C12-C11-CA5-OA7 |
| 57 | Du | 401 | CDL | C32-C31-CA7-OA9 |
| 57 | Dv | 402 | CDL | C52-C51-CB5-OB7 |
| 58 | DI | 702 | PC1 | O22-C21-C22-C23 |
| 65 | EL | 906 | UQ8 | C9-C11-C12-C13 |
| 57 | DN | 504 | CDL | C74-C75-C76-C77 |
| 57 | Dh | 201 | CDL | C60-C61-C62-C63 |
| 59 | Dx | 1206 | 3PE | C38-C39-C3A-C3B |
| 57 | DN | 501 | CDL | C12-C11-CA5-OA6 |
| 57 | DY | 301 | CDL | C72-C71-CB7-OB8 |
| 57 | EB | 304 | CDL | C72-C71-CB7-OB8 |
| 57 | Dn | 507 | CDL | C32-C31-CA7-OA8 |
| 57 | Dv | 401 | CDL | C32-C31-CA7-OA8 |
| 58 | Eo | 201 | PC1 | O31-C31-C32-C33 |
| 57 | DD | 703 | CDL | C74-C75-C76-C77 |
| 57 | DU | 403 | CDL | C33-C34-C35-C36 |
| 57 | DV | 402 | CDL | C71-C72-C73-C74 |
| 57 | Eg | 101 | CDL | C12-C13-C14-C15 |
| 57 | DJ | 303 | CDL | C32-C31-CA7-OA9 |
| 57 | EH | 201 | CDL | C52-C51-CB5-OB7 |
| 57 | Dg | 201 | CDL | C32-C31-CA7-OA9 |
| 57 | Dn | 507 | CDL | C72-C71-CB7-OB9 |
| 57 | Dr | 402 | CDL | C52-C51-CB5-OB7 |
| 57 | Eg | 101 | CDL | C12-C11-CA5-OA7 |
| 57 | Ep | 701 | CDL | C32-C31-CA7-OA9 |
| 59 | Dd | 703 | 3PE | O32-C31-C32-C33 |
| 54 | Da | 701 | HEA | CAA-CBA-CGA-O1A |
| 57 | Ek | 201 | CDL | C13-C14-C15-C16 |
| 57 | DJ | 304 | CDL | C72-C71-CB7-OB9 |
| 57 | Dm | 502 | CDL | C12-C11-CA5-OA7 |
| 57 | Dy | 301 | CDL | C72-C71-CB7-OB9 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 57 | El | 901 | CDL | C72-C71-CB7-OB9 |
| 58 | Dc | 602 | PC1 | O32-C31-C32-C33 |
| 57 | DJ | 307 | CDL | C61-C62-C63-C64 |
| 57 | EH | 201 | CDL | C80-C81-C82-C83 |
| 57 | Dx | 1203 | CDL | C57-C58-C59-C60 |
| 57 | Dd | 706 | CDL | C52-C51-CB5-OB6 |
| 57 | Du | 403 | CDL | C12-C11-CA5-OA6 |
| 58 | Ds | 406 | PC1 | O31-C31-C32-C33 |

There are no ring outliers.

132 monomers are involved in 215 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 57 | DC | 601 | CDL | 1 | 0 |
| 68 | ER | 201 | ATP | 2 | 0 |
| 57 | En | 1202 | CDL | 2 | 0 |
| 57 | El | 901 | CDL | 1 | 0 |
| 54 | DA | 701 | HEA | 1 | 0 |
| 58 | Dv | 408 | PC1 | 1 | 0 |
| 66 | Ed | 201 | HEM | 4 | 0 |
| 57 | Dm | 502 | CDL | 1 | 0 |
| 57 | DZ | 501 | CDL | 1 | 0 |
| 58 | DC | 608 | PC1 | 2 | 0 |
| 57 | Dd | 704 | CDL | 1 | 0 |
| 57 | Ds | 405 | CDL | 1 | 0 |
| 57 | DN | 504 | CDL | 2 | 0 |
| 59 | Dx | 1206 | 3PE | 1 | 0 |
| 58 | Eo | 204 | PC1 | 3 | 0 |
| 57 | DD | 702 | CDL | 2 | 0 |
| 57 | Dg | 202 | CDL | 2 | 0 |
| 57 | Dj | 403 | CDL | 2 | 0 |
| 57 | Eh | 1601 | CDL | 2 | 0 |
| 57 | ED | 604 | CDL | 1 | 0 |
| 58 | DX | 306 | PC1 | 1 | 0 |
| 57 | El | 902 | CDL | 2 | 0 |
| 57 | Dd | 702 | CDL | 2 | 0 |
| 57 | Do | 501 | CDL | 1 | 0 |
| 57 | Dj | 401 | CDL | 1 | 0 |
| 57 | DH | 201 | CDL | 4 | 0 |
| 57 | DI | 701 | CDL | 1 | 0 |
| 58 | DG | 203 | PC1 | 2 | 0 |
| 57 | EA | 301 | CDL | 1 | 0 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 57 | EL | 901 | CDL | 3 | 0 |
| 65 | ED | 603 | UQ8 | 5 | 0 |
| 59 | DR | 401 | 3PE | 2 | 0 |
| 57 | DS | 402 | CDL | 2 | 0 |
| 59 | DC | 607 | 3PE | 1 | 0 |
| 68 | Er | 201 | ATP | 2 | 0 |
| 57 | EL | 902 | CDL | 5 | 0 |
| 57 | Dn | 501 | CDL | 1 | 0 |
| 58 | Di | 702 | PC1 | 1 | 0 |
| 57 | Dx | 1203 | CDL | 2 | 0 |
| 57 | DO | 501 | CDL | 1 | 0 |
| 58 | Dx | 1204 | PC1 | 1 | 0 |
| 65 | EN | 1204 | UQ8 | 2 | 0 |
| 57 | DQ | 1502 | CDL | 2 | 0 |
| 58 | DX | 302 | PC1 | 1 | 0 |
| 57 | Dd | 706 | CDL | 1 | 0 |
| 65 | El | 906 | UQ8 | 2 | 0 |
| 59 | Ds | 403 | 3PE | 1 | 0 |
| 65 | Ed | 202 | UQ8 | 5 | 0 |
| 57 | Du | 401 | CDL | 1 | 0 |
| 58 | Dv | 405 | PC1 | 1 | 0 |
| 59 | DS | 403 | 3PE | 2 | 0 |
| 57 | Dj | 404 | CDL | 1 | 0 |
| 58 | EB | 303 | PC1 | 1 | 0 |
| 57 | Dr | 402 | CDL | 3 | 0 |
| 57 | Dh | 201 | CDL | 3 | 0 |
| 57 | DG | 201 | CDL | 1 | 0 |
| 65 | EL | 906 | UQ8 | 2 | 0 |
| 57 | Dn | 507 | CDL | 2 | 0 |
| 58 | Eo | 201 | PC1 | 3 | 0 |
| 57 | DX | 307 | CDL | 2 | 0 |
| 57 | EL | 903 | CDL | 1 | 0 |
| 57 | EN | 1202 | CDL | 3 | 0 |
| 57 | DV | 402 | CDL | 2 | 0 |
| 57 | Ek | 201 | CDL | 1 | 0 |
| 59 | Dx | 1205 | 3PE | 2 | 0 |
| 57 | Du | 402 | CDL | 2 | 0 |
| 57 | Dn | 502 | CDL | 3 | 0 |
| 59 | DC | 606 | 3PE | 2 | 0 |
| 59 | EO | 204 | 3PE | 1 | 0 |
| 58 | DI | 702 | PC1 | 1 | 0 |
| 58 | Dc | 607 | PC1 | 2 | 0 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 57 | EB | 304 | CDL | 3 | 0 |
| 57 | El | 903 | CDL | 1 | 0 |
| 59 | Dr | 401 | 3PE | 1 | 0 |
| 59 | Dg | 204 | 3PE | 1 | 0 |
| 57 | En | 1201 | CDL | 2 | 0 |
| 65 | DS | 404 | UQ8 | 2 | 0 |
| 60 | Ed | 203 | LPP | 1 | 0 |
| 57 | Dd | 705 | CDL | 3 | 0 |
| 57 | Dv | 401 | CDL | 2 | 0 |
| 57 | DQ | 1501 | CDL | 3 | 0 |
| 57 | Dq | 401 | CDL | 1 | 0 |
| 57 | DJ | 302 | CDL | 2 | 0 |
| 59 | DG | 204 | 3PE | 1 | 0 |
| 58 | DA | 707 | PC1 | 1 | 0 |
| 57 | Dc | 601 | CDL | 1 | 0 |
| 65 | En | 1203 | UQ8 | 4 | 0 |
| 57 | Dx | 1201 | CDL | 3 | 0 |
| 58 | EO | 206 | PC1 | 1 | 0 |
| 58 | EO | 205 | PC1 | 2 | 0 |
| 58 | EO | 201 | PC1 | 2 | 0 |
| 57 | Di | 701 | CDL | 1 | 0 |
| 57 | DN | 505 | CDL | 1 | 0 |
| 57 | Eg | 101 | CDL | 2 | 0 |
| 66 | ED | 602 | HEM | 5 | 0 |
| 54 | Da | 701 | HEA | 3 | 0 |
| 57 | Ds | 402 | CDL | 1 | 0 |
| 58 | Eb | 302 | PC1 | 1 | 0 |
| 57 | Dv | 403 | CDL | 2 | 0 |
| 58 | Dx | 1202 | PC1 | 2 | 0 |
| 57 | DX | 301 | CDL | 1 | 0 |
| 57 | Dh | 202 | CDL | 2 | 0 |
| 59 | EM | 901 | 3PE | 2 | 0 |
| 57 | Da | 709 | CDL | 3 | 0 |
| 57 | EB | 302 | CDL | 1 | 0 |
| 59 | Dj | 407 | 3PE | 2 | 0 |
| 57 | DA | 709 | CDL | 1 | 0 |
| 58 | Da | 707 | PC1 | 1 | 0 |
| 59 | EL | 905 | 3PE | 2 | 0 |
| 57 | DS | 405 | CDL | 1 | 0 |
| 59 | DX | 304 | 3PE | 1 | 0 |
| 59 | El | 905 | 3PE | 1 | 0 |
| 57 | DD | 703 | CDL | 1 | 0 |

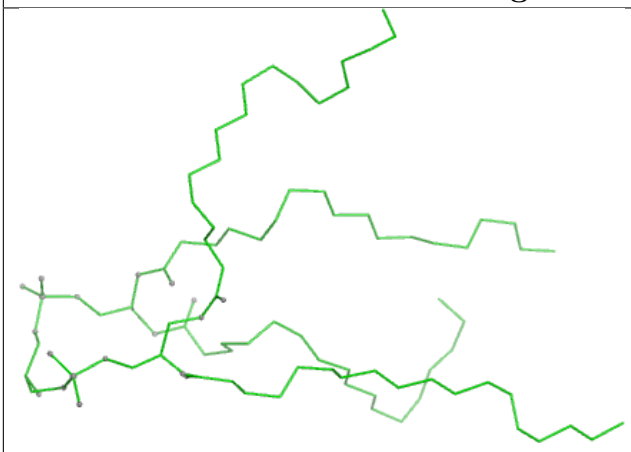
*Continued on next page...*

*Continued from previous page...*

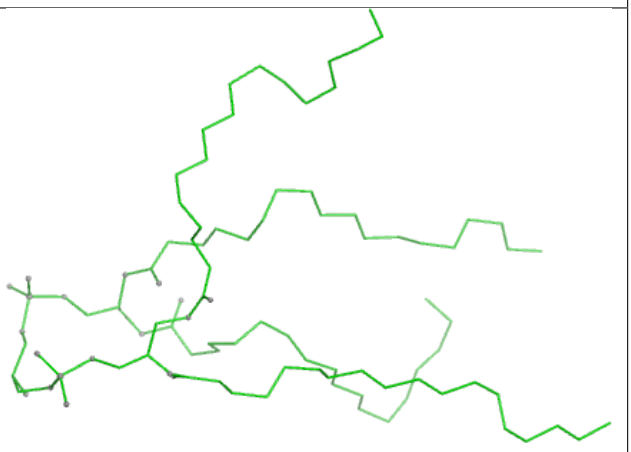
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 57 | Ep | 701 | CDL | 1 | 0 |
| 57 | DY | 301 | CDL | 1 | 0 |
| 57 | DQ | 1504 | CDL | 1 | 0 |
| 58 | DQ | 1503 | PC1 | 1 | 0 |
| 57 | Dv | 404 | CDL | 1 | 0 |
| 57 | DV | 403 | CDL | 1 | 0 |
| 57 | DM | 501 | CDL | 2 | 0 |
| 57 | Dg | 201 | CDL | 5 | 0 |
| 57 | DV | 401 | CDL | 2 | 0 |
| 58 | Ef | 1001 | PC1 | 1 | 0 |
| 58 | DC | 605 | PC1 | 1 | 0 |
| 57 | Dv | 402 | CDL | 3 | 0 |
| 59 | DS | 401 | 3PE | 1 | 0 |
| 57 | DJ | 304 | CDL | 1 | 0 |
| 65 | Ds | 404 | UQ8 | 3 | 0 |
| 57 | DJ | 303 | CDL | 2 | 0 |
| 57 | Dn | 503 | CDL | 2 | 0 |
| 60 | EI | 402 | LPP | 1 | 0 |
| 54 | DA | 702 | HEA | 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.

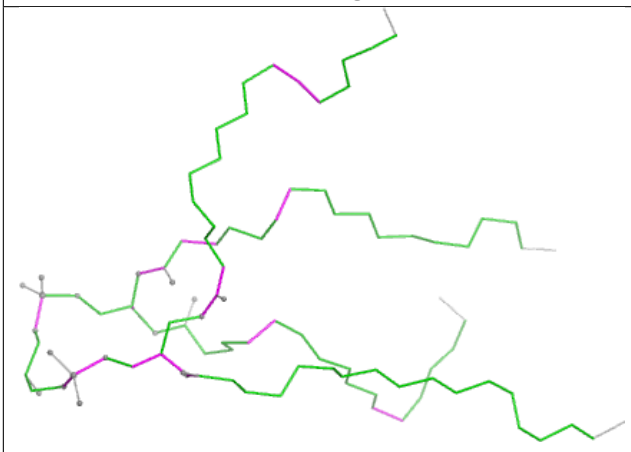
**Ligand CDL DC 601**



**Bond lengths**



**Bond angles**

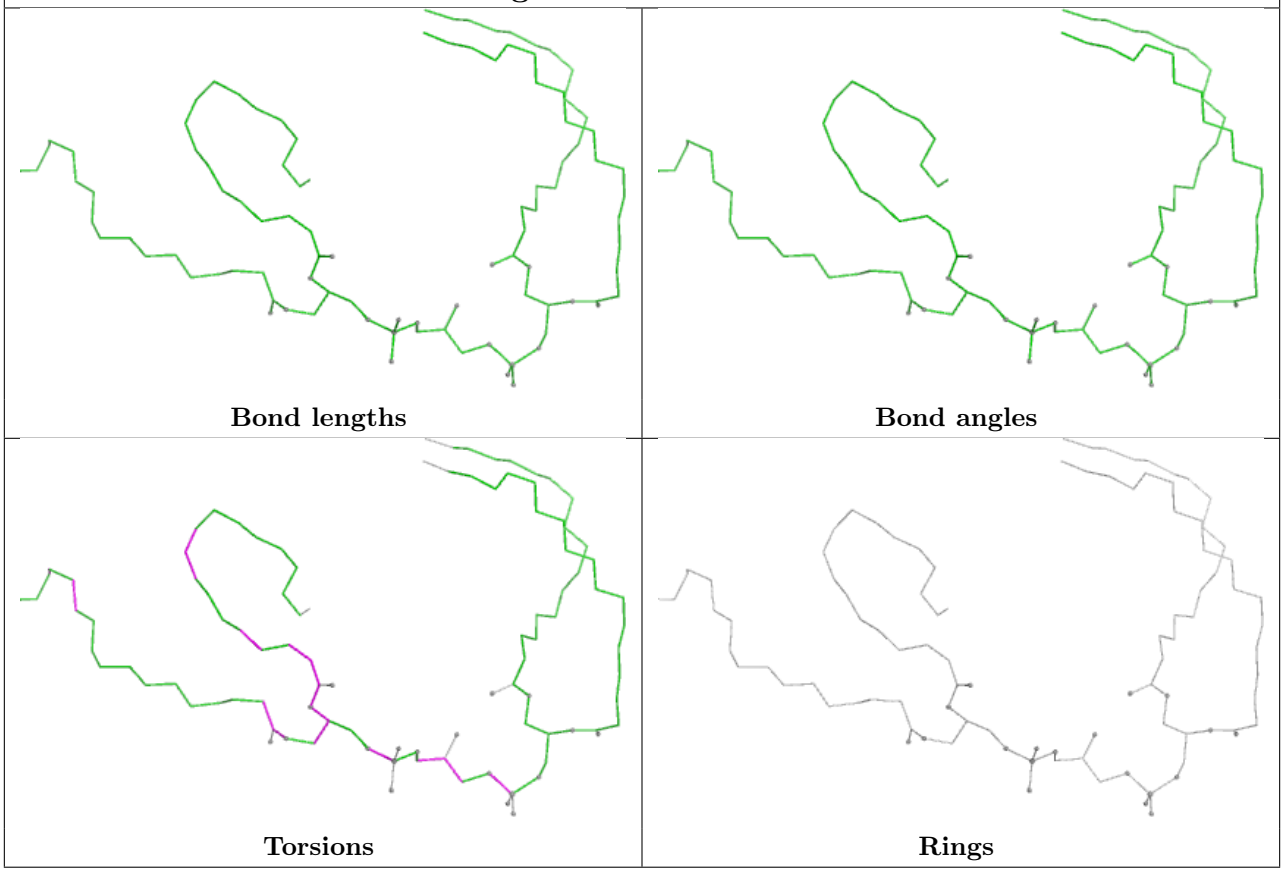


**Torsions**

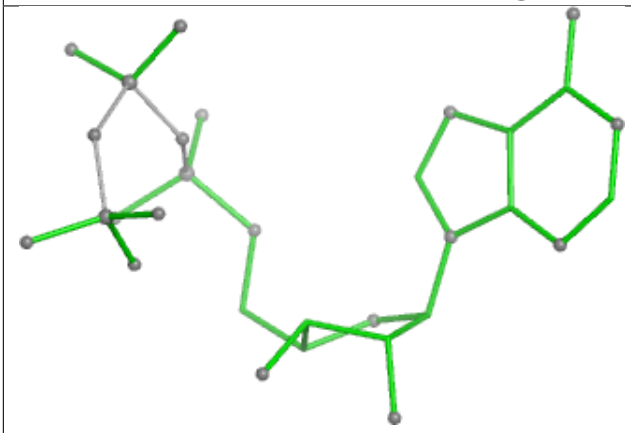


**Rings**

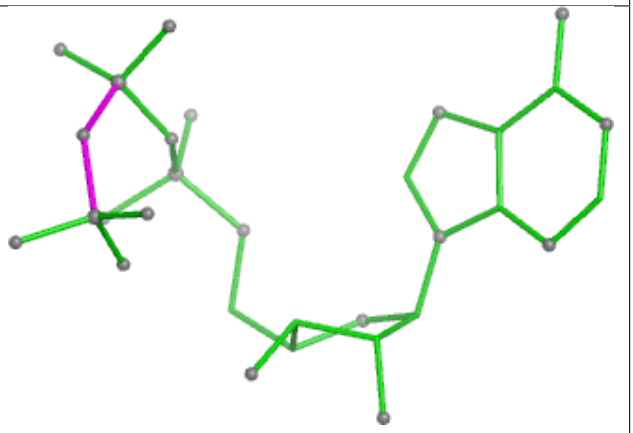
**Ligand CDL DA 710**



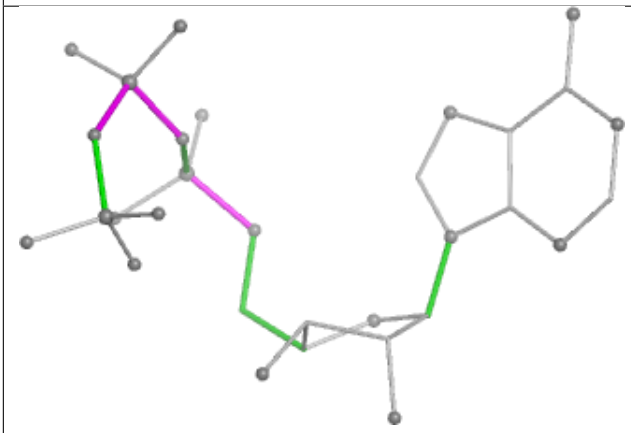
**Ligand ATP ER 201**



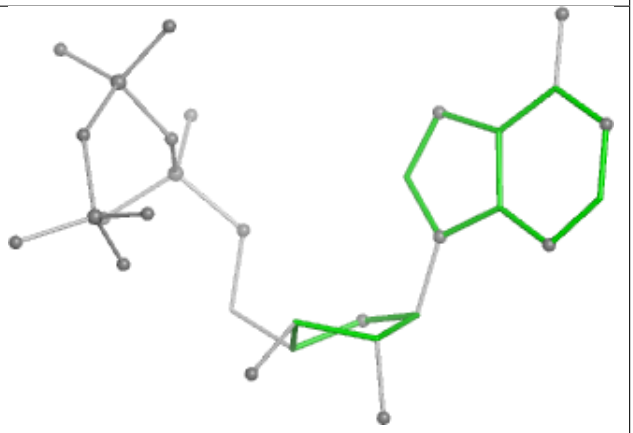
**Bond lengths**



**Bond angles**

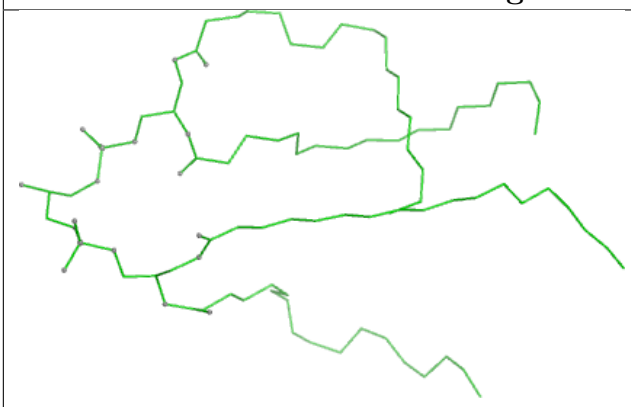


**Torsions**

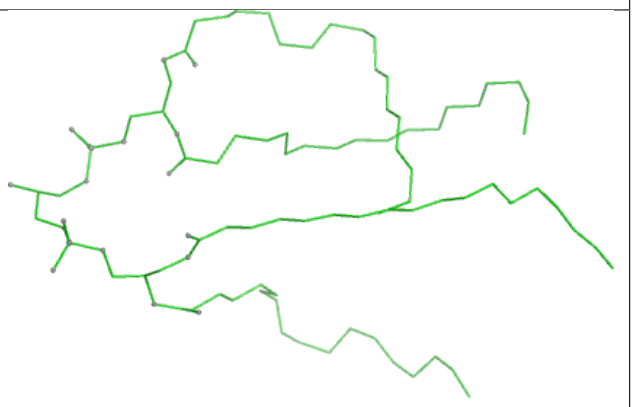


**Rings**

**Ligand CDL En 1202**



**Bond lengths**



**Bond angles**

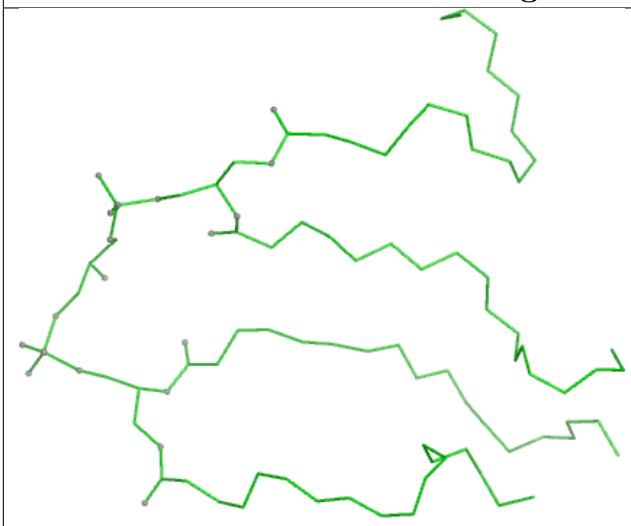


**Torsions**

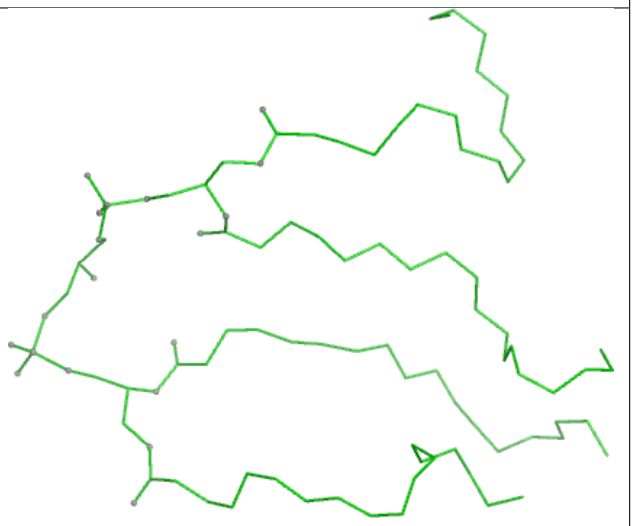


**Rings**

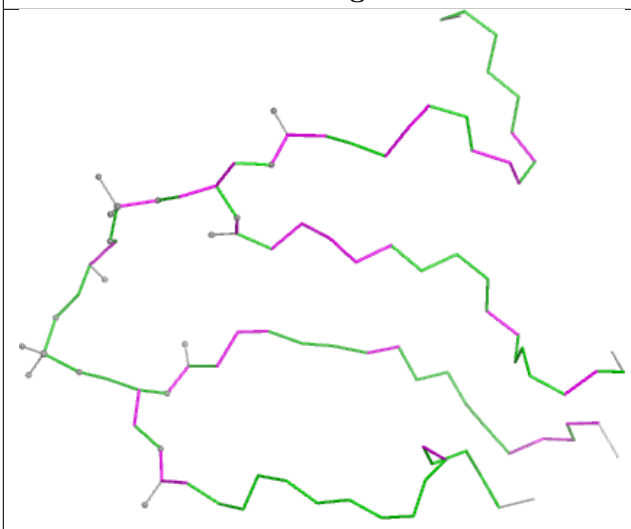
**Ligand CDL El 901**



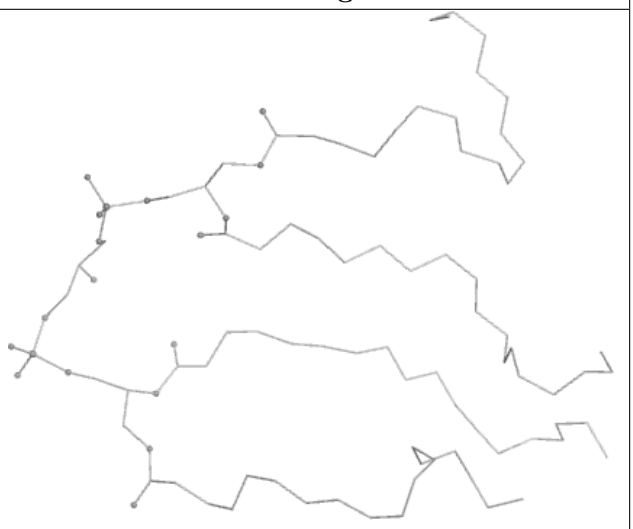
**Bond lengths**



**Bond angles**

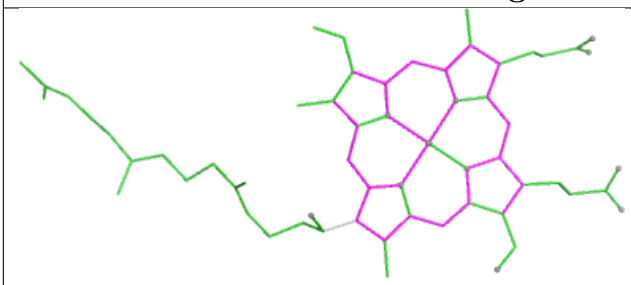


**Torsions**

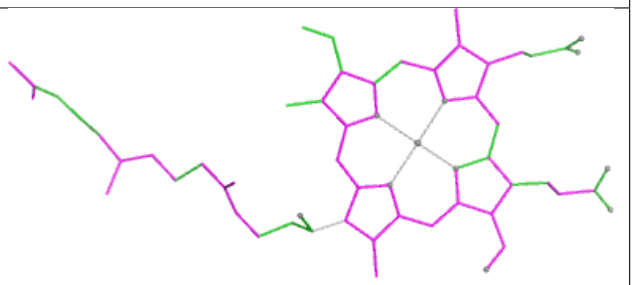


**Rings**

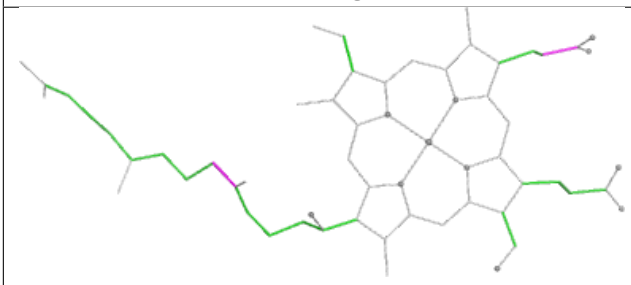
## Ligand HEA DA 701



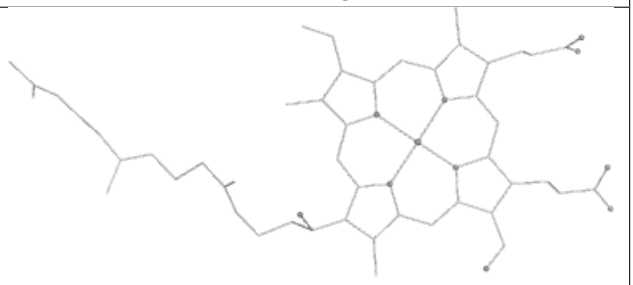
Bond lengths



Bond angles

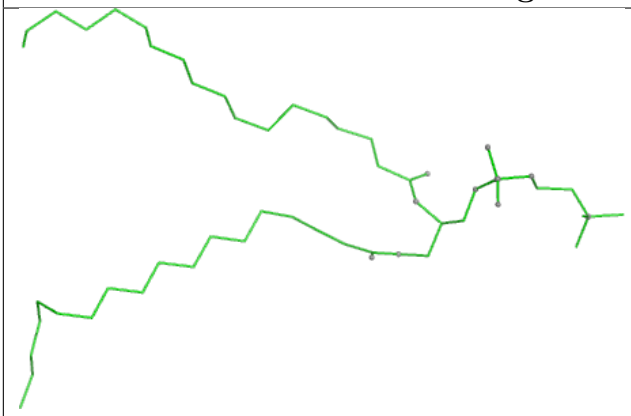


Torsions

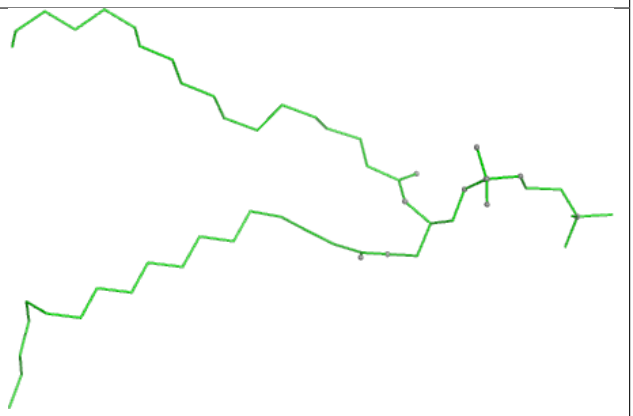


Rings

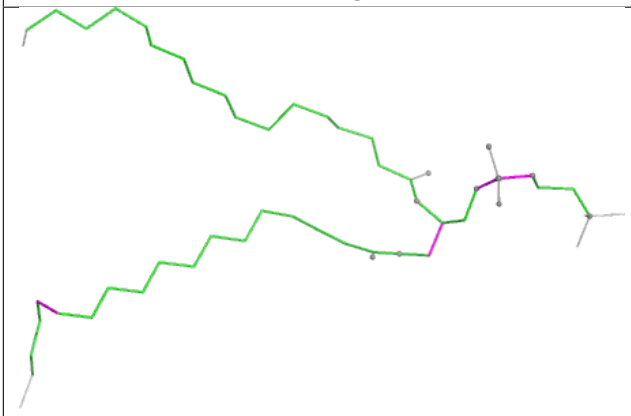
## Ligand PC1 Dv 408



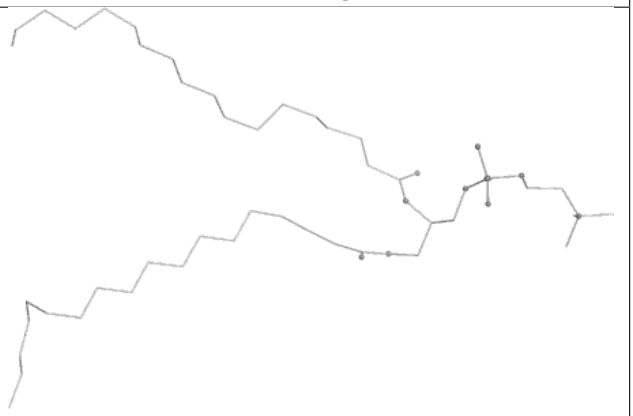
Bond lengths



Bond angles

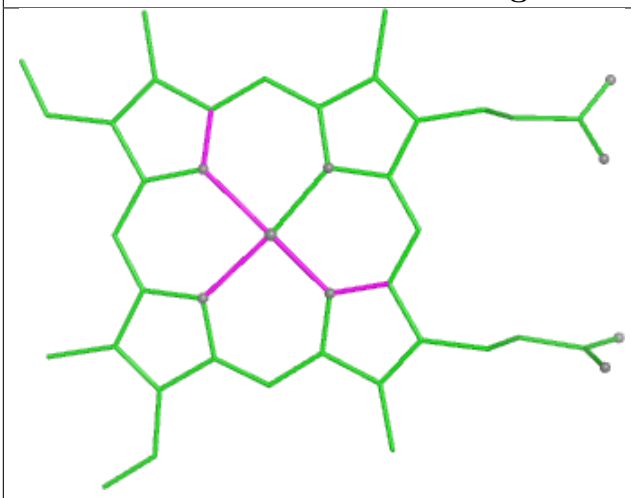


Torsions

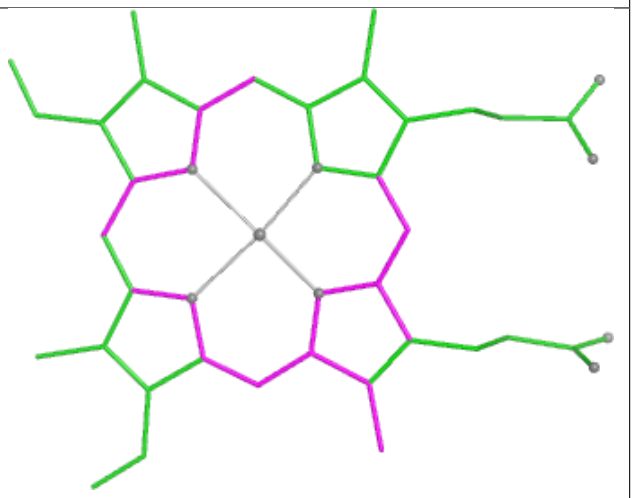


Rings

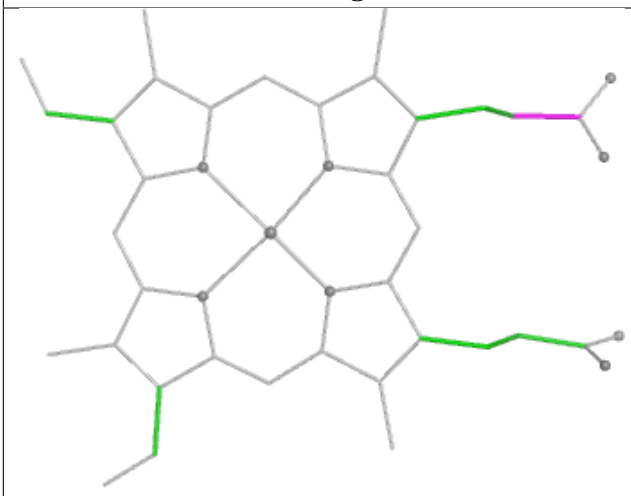
**Ligand HEM Ed 201**



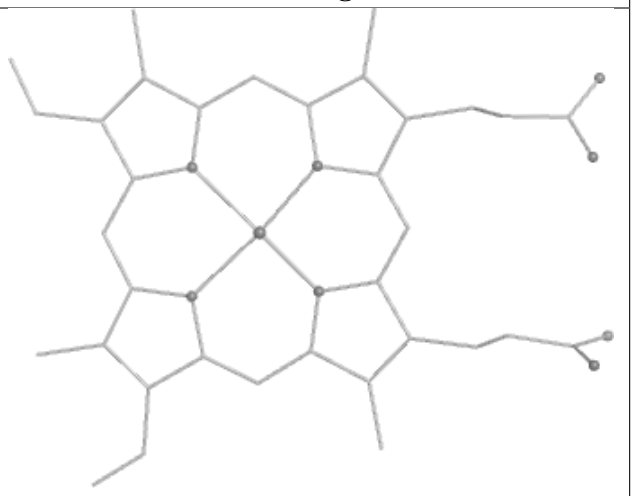
**Bond lengths**



**Bond angles**

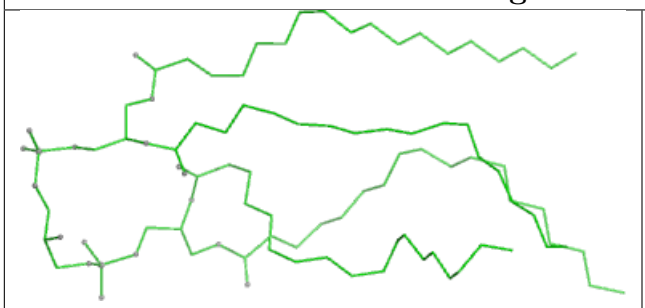


**Torsions**

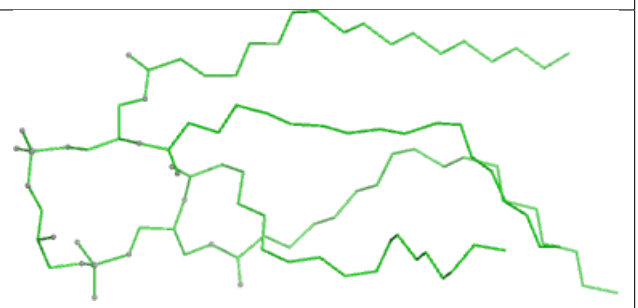


**Rings**

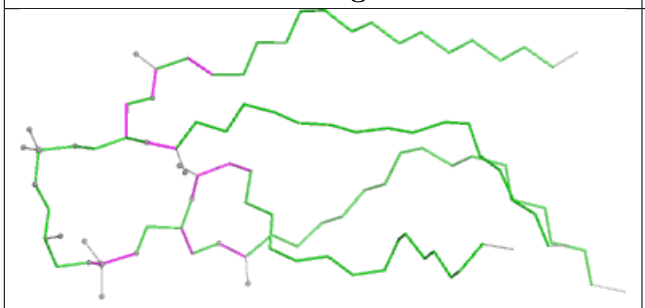
**Ligand CDL Dm 502**



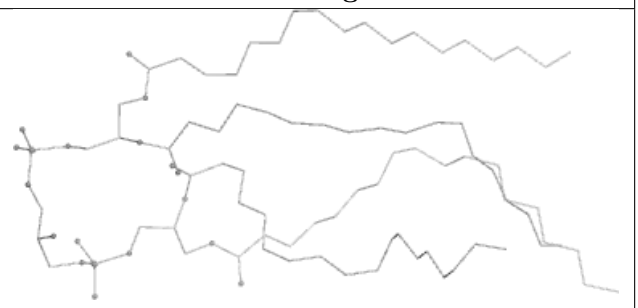
Bond lengths



Bond angles

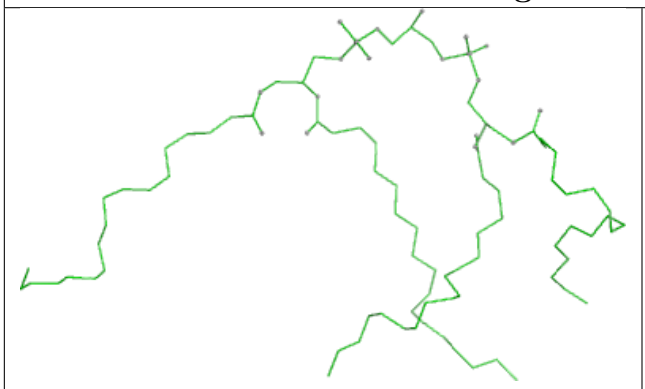


Torsions

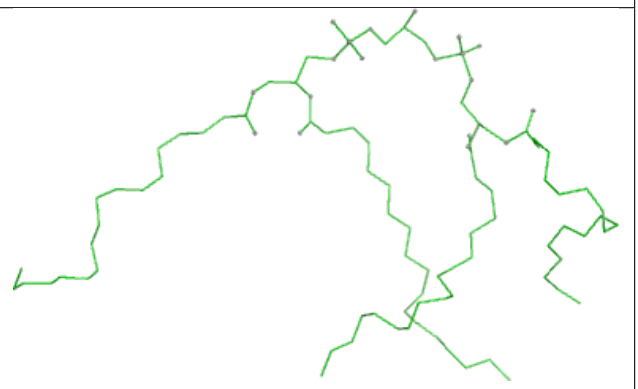


Rings

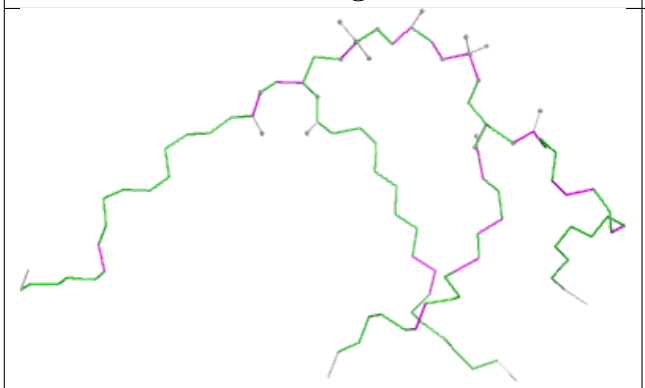
**Ligand CDL Du 403**



Bond lengths



Bond angles

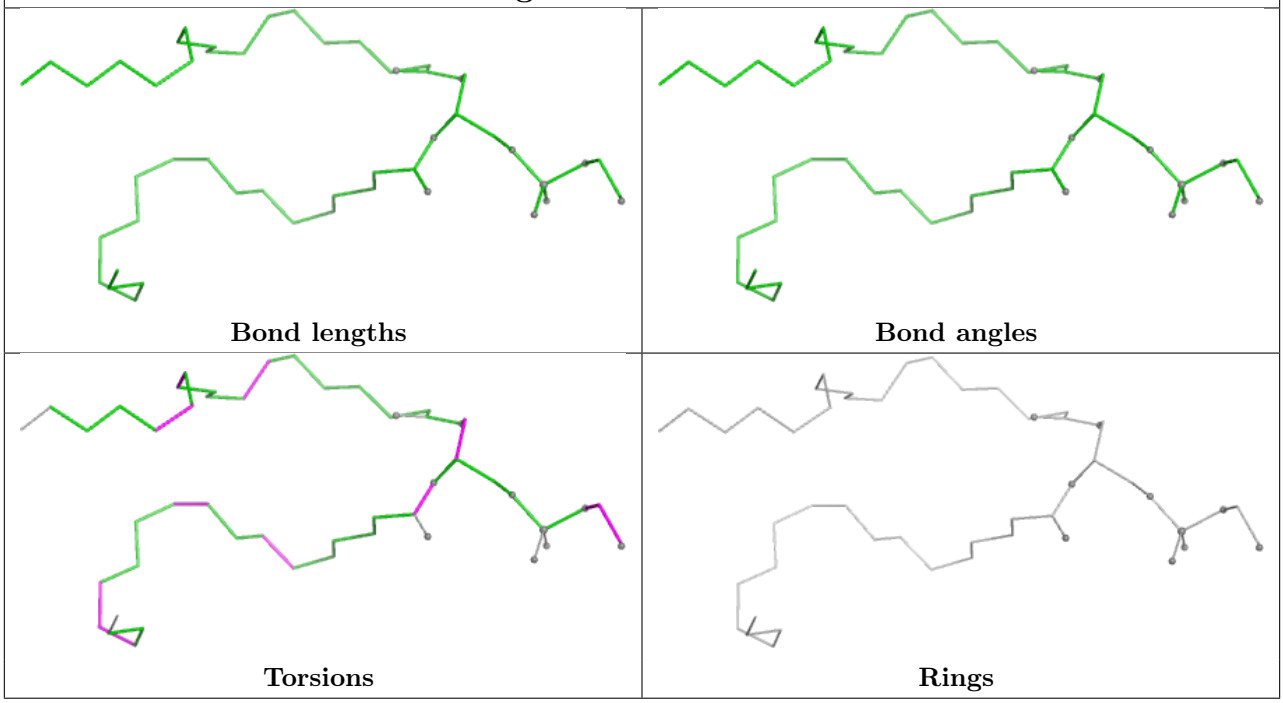


Torsions

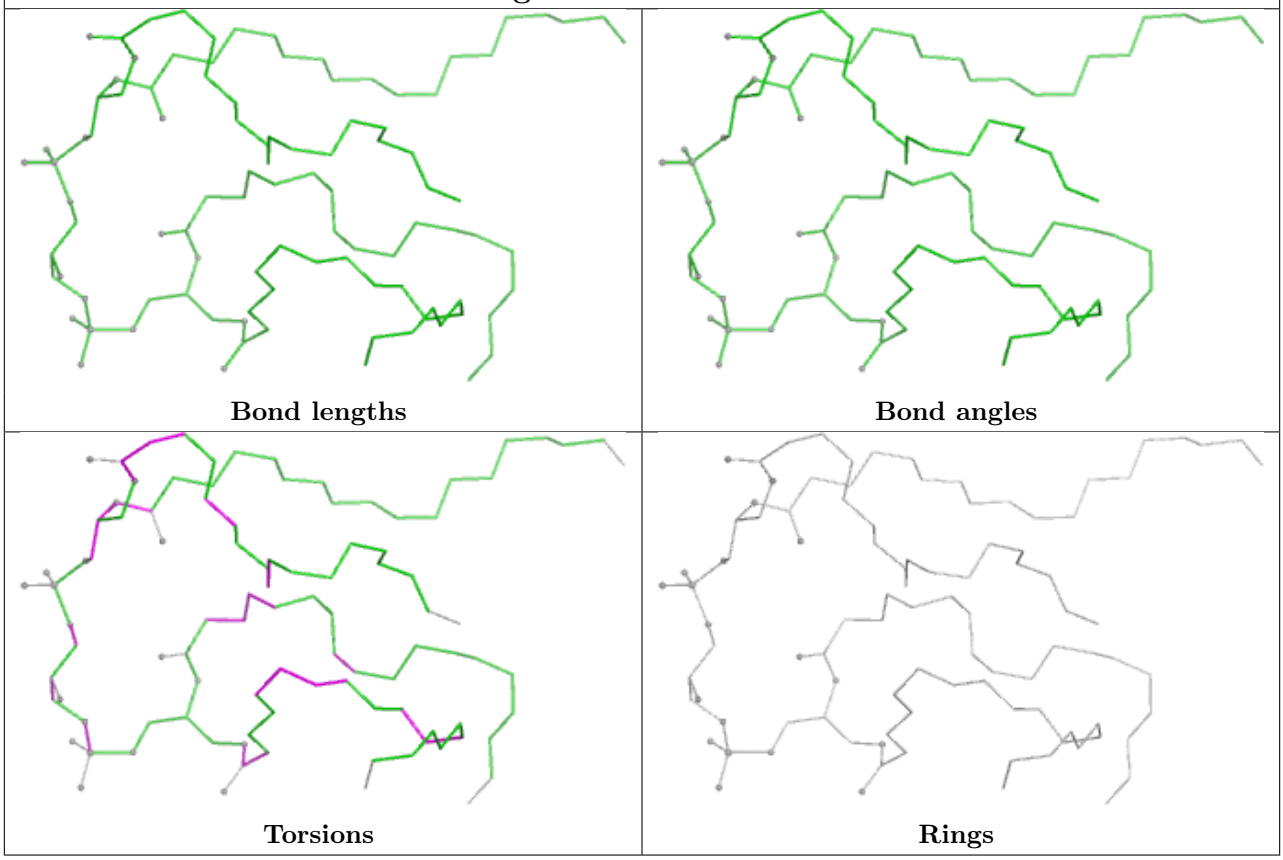


Rings

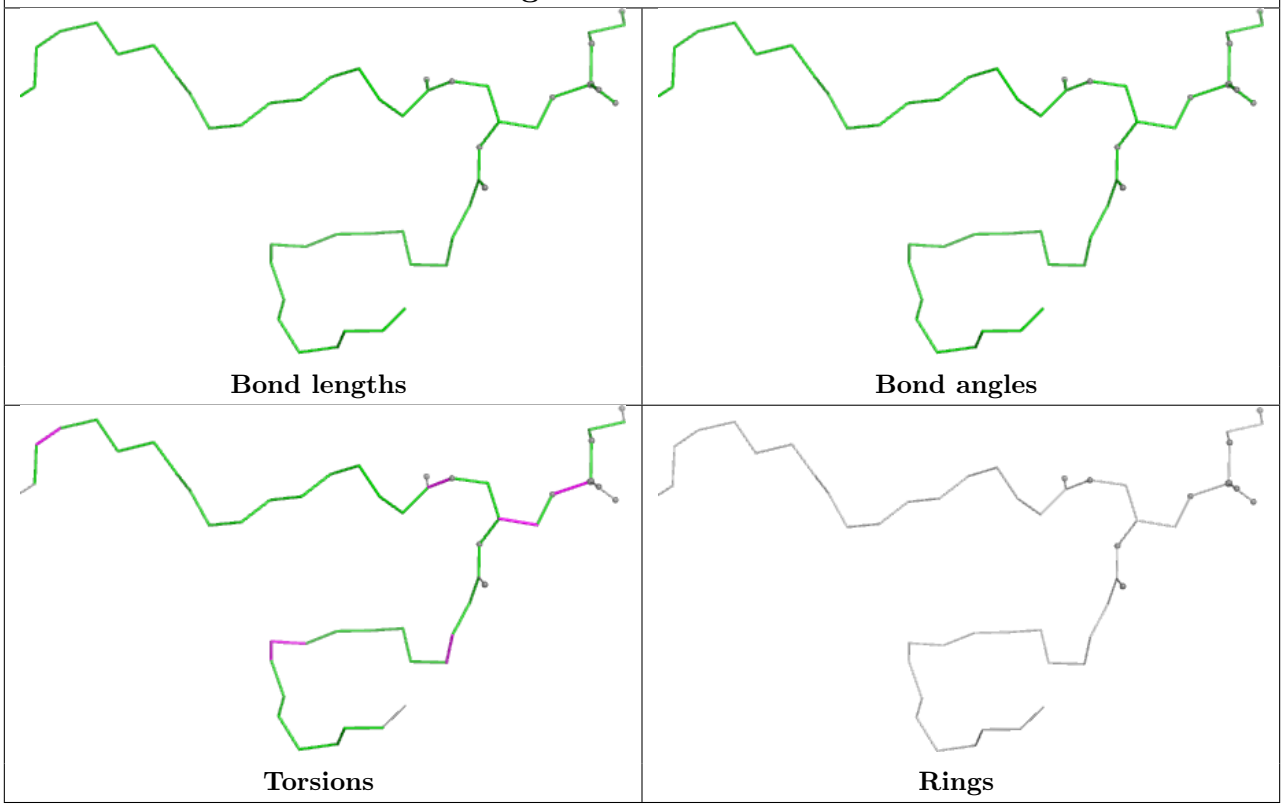
## Ligand 3PE DA 708



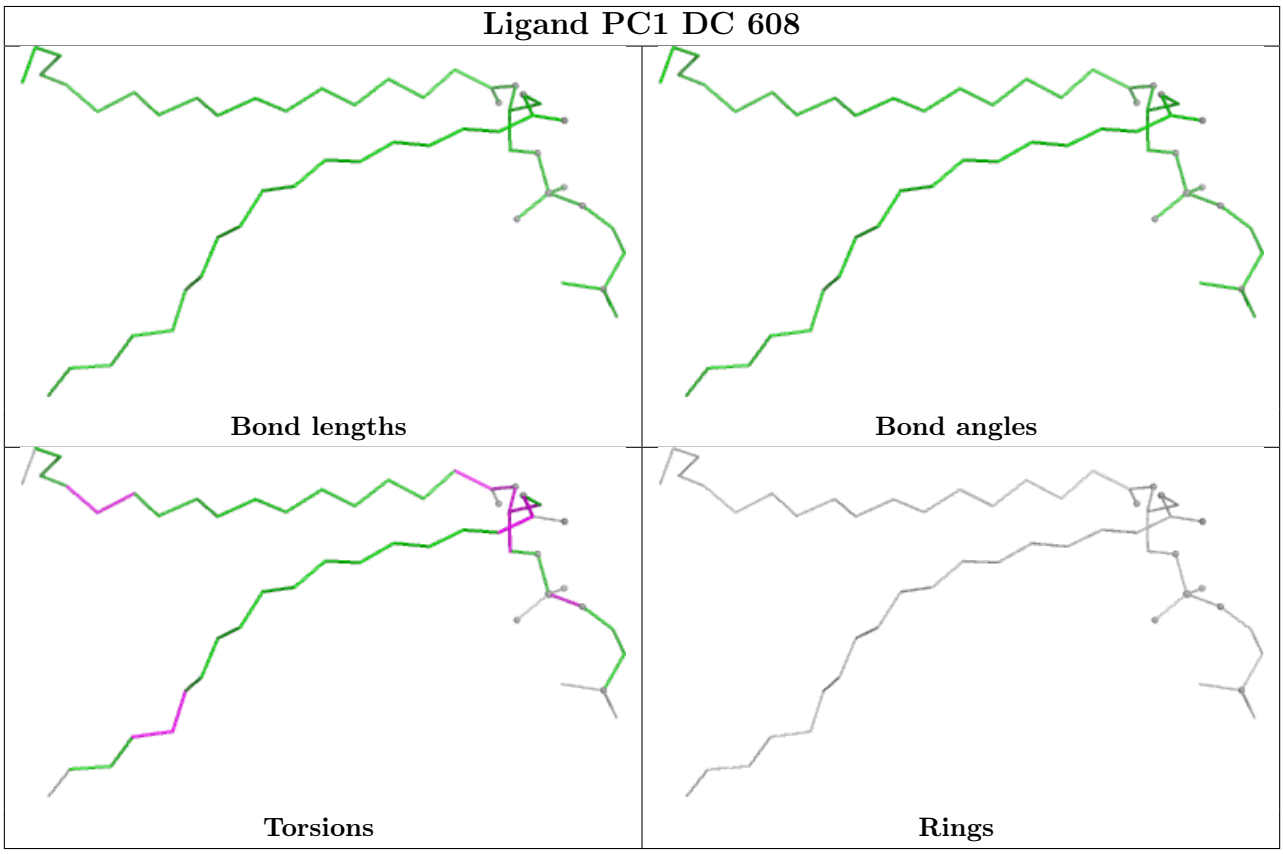

## Ligand CDL DZ 501



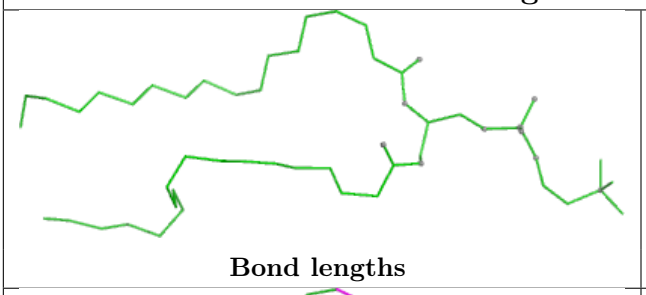
## Ligand 3PE Dr 404



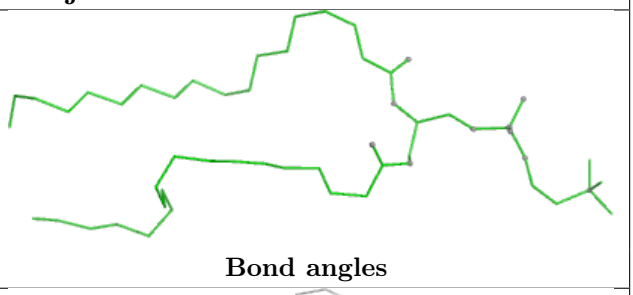

## Ligand PC1 DC 608



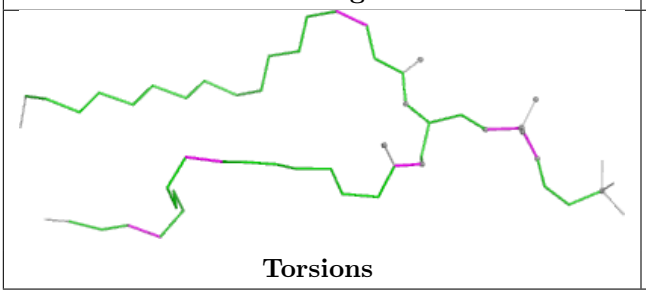
**Ligand PC1 Dj 406**



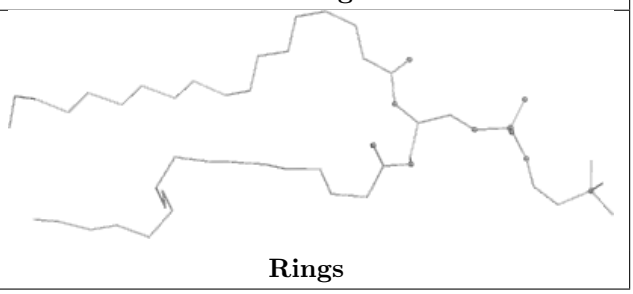
Bond lengths



Bond angles

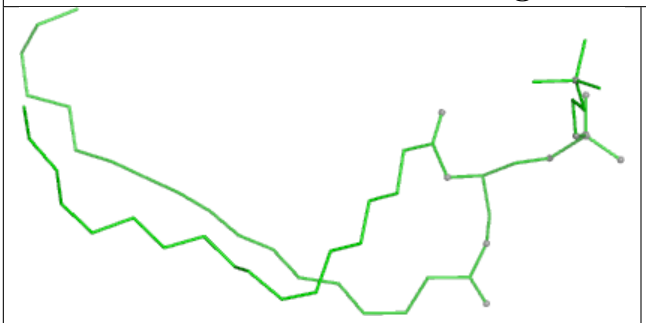


Torsions

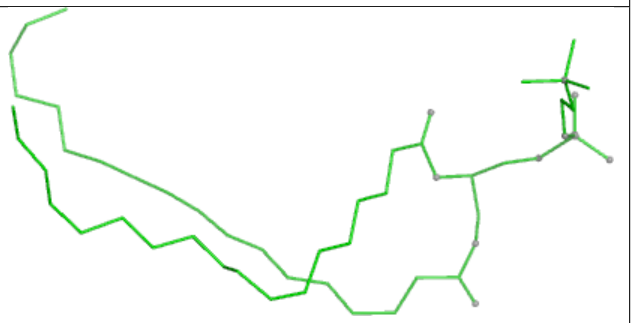


Rings

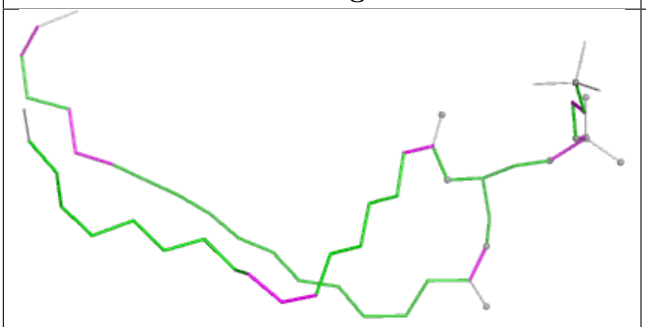
**Ligand PC1 DC 604**



Bond lengths



Bond angles

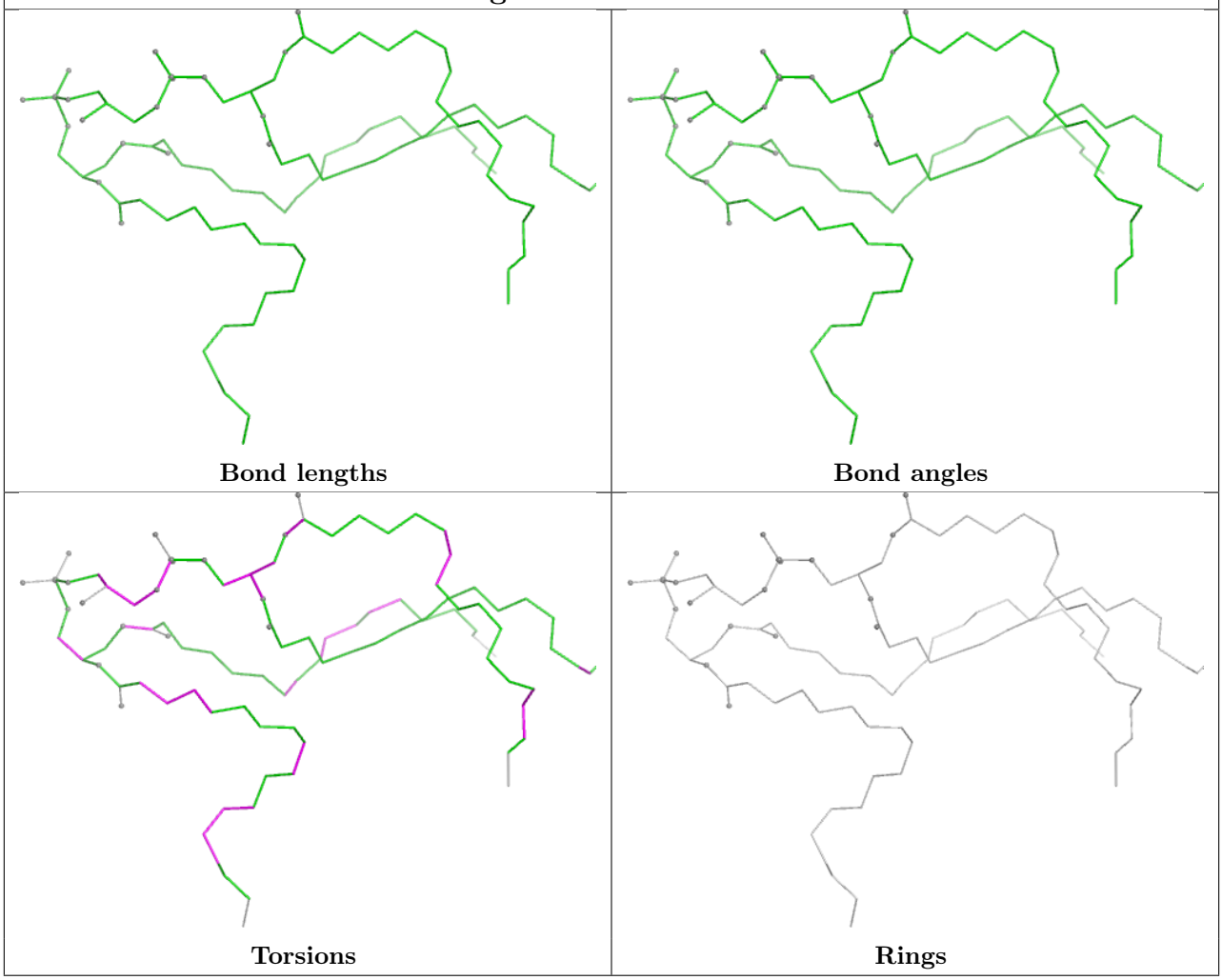


Torsions

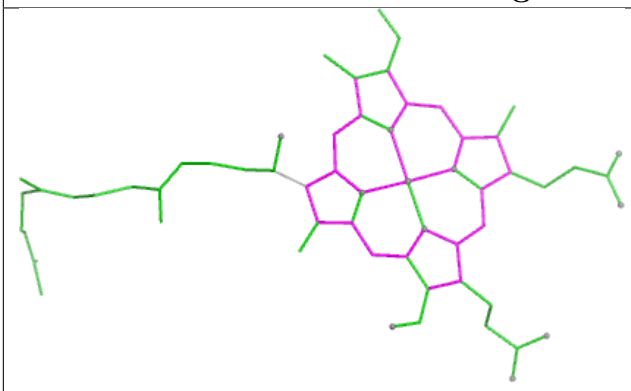


Rings

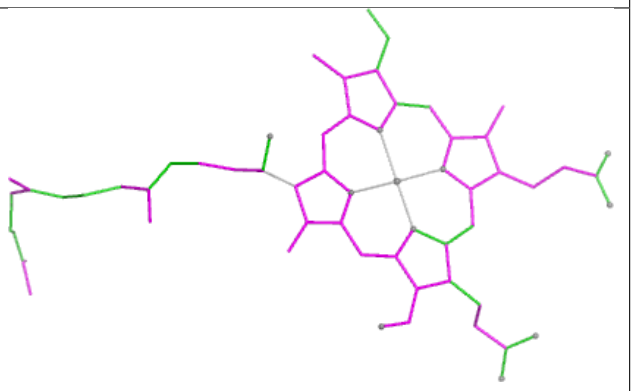
**Ligand CDL Dd 704**



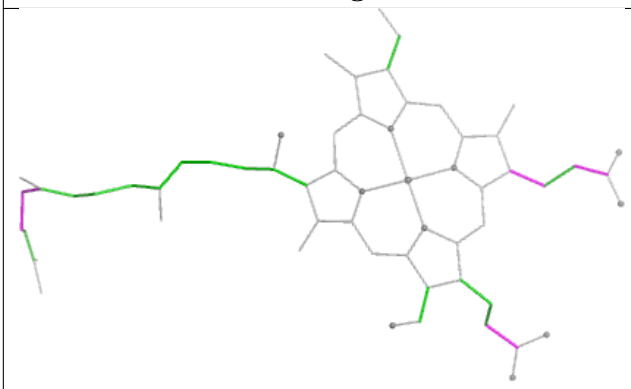
**Ligand HEA Da 702**



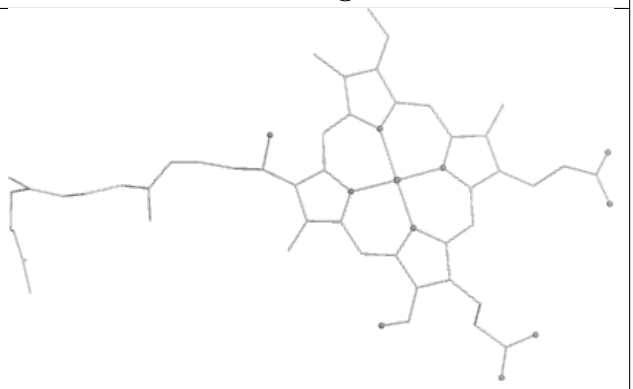
**Bond lengths**



**Bond angles**

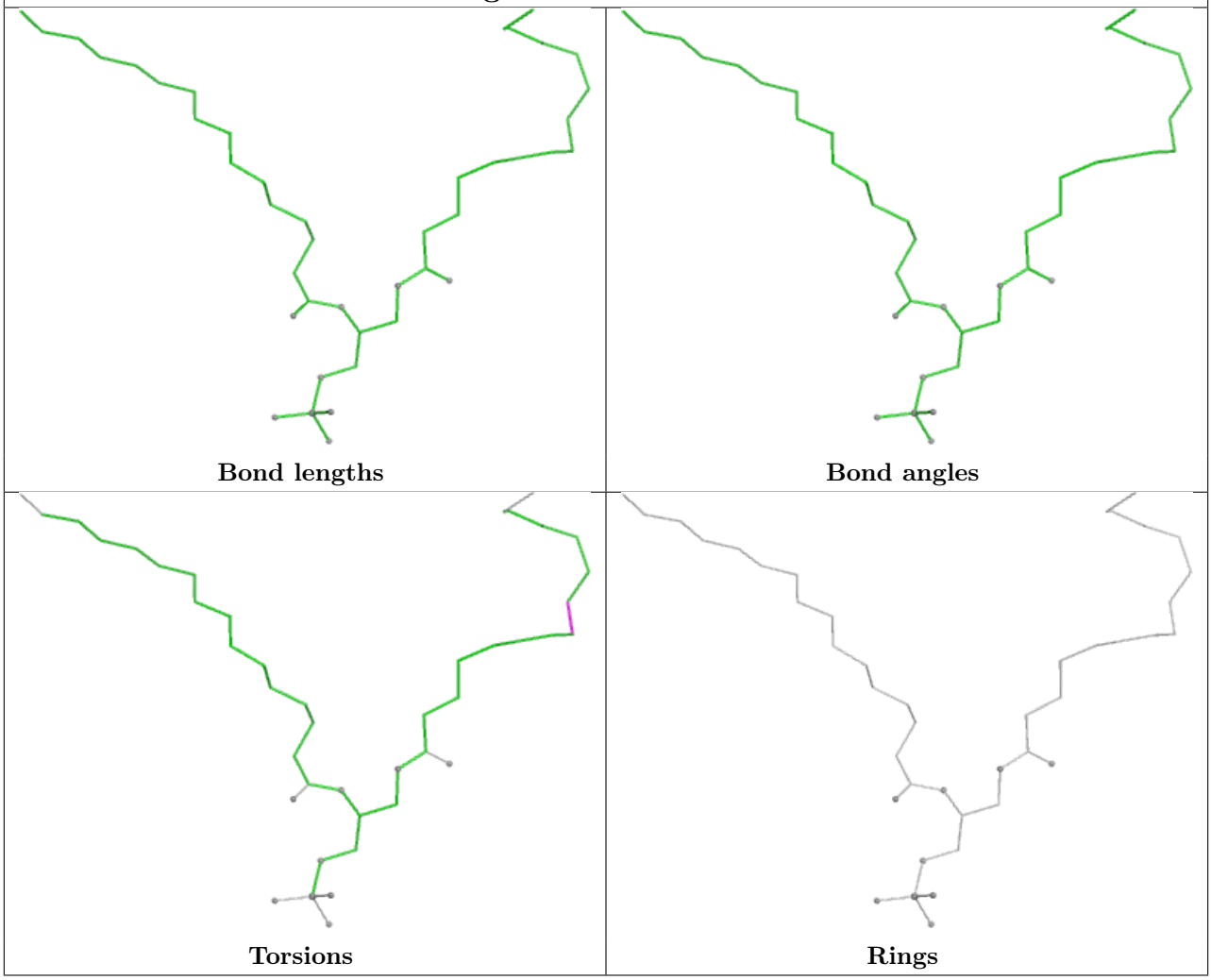


**Torsions**

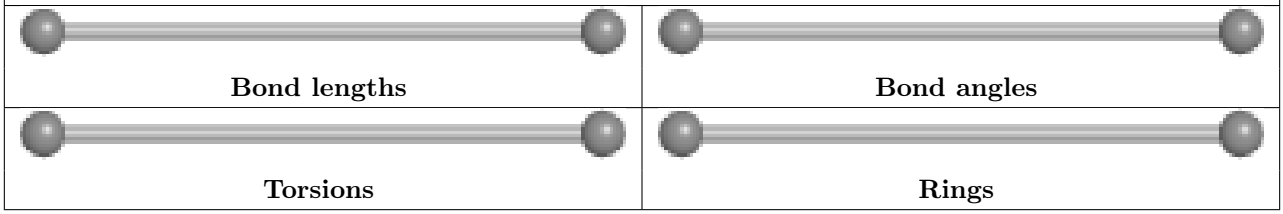


**Rings**

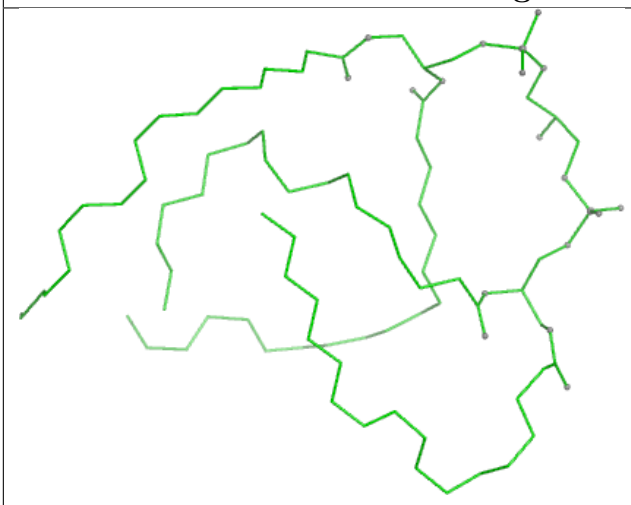
**Ligand LPP DN 503**



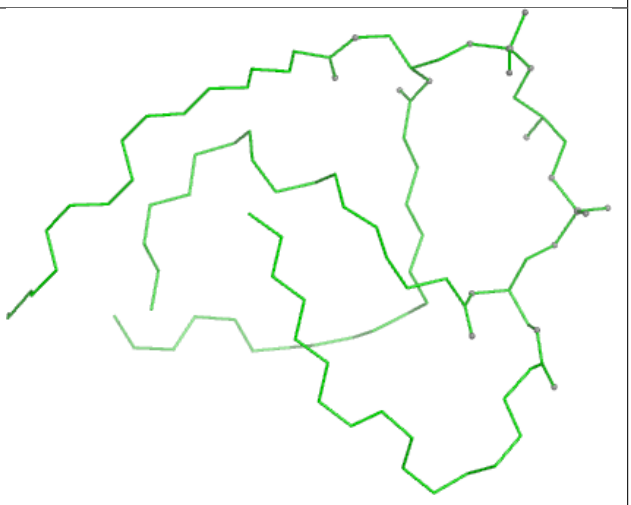

**Ligand CUA DB 701**



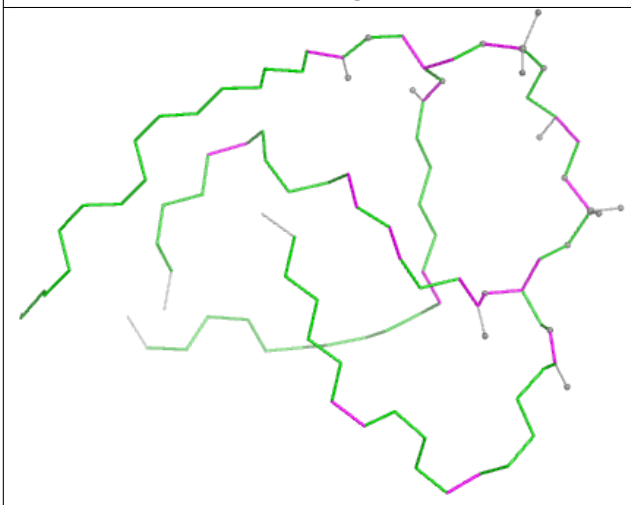
## Ligand CDL Dn 505



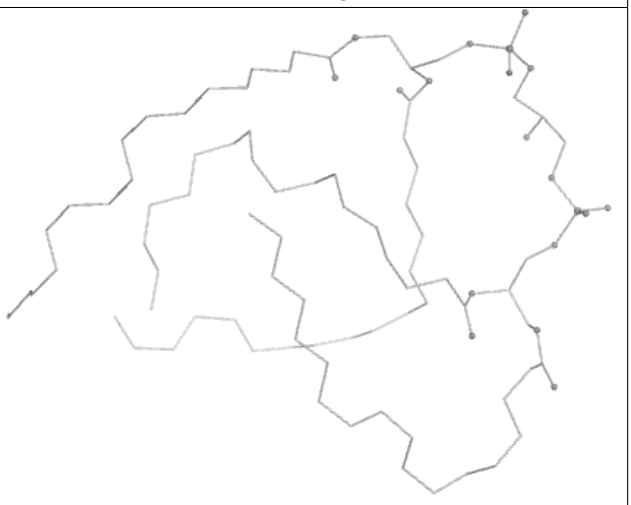
Bond lengths



Bond angles

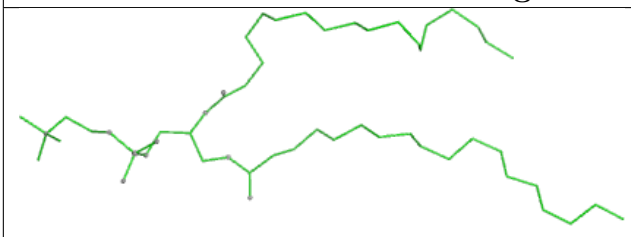


Torsions

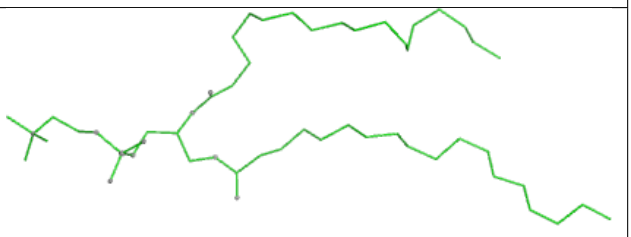


Rings

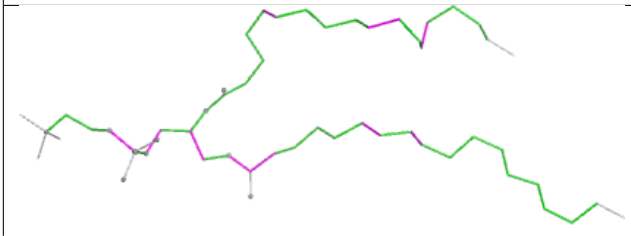
## Ligand PC1 DA 706



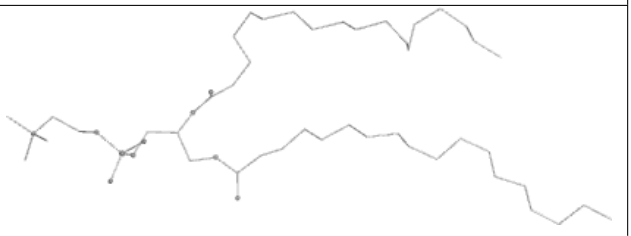
Bond lengths



Bond angles

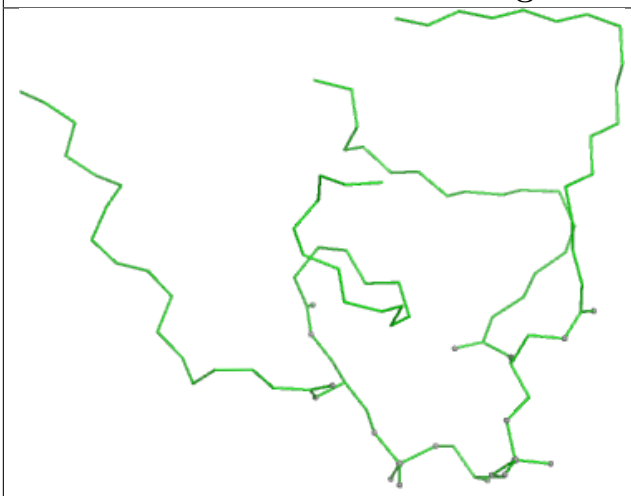


Torsions

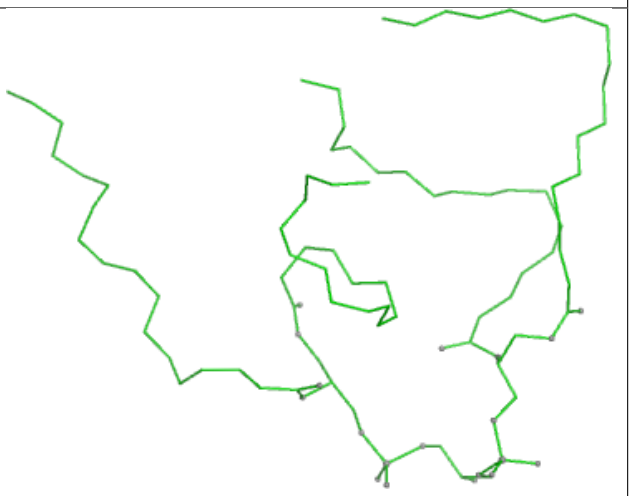


Rings

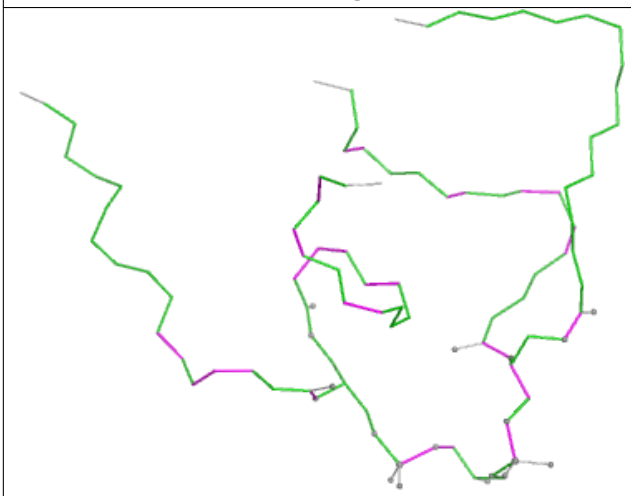
**Ligand CDL Ds 405**



**Bond lengths**



**Bond angles**

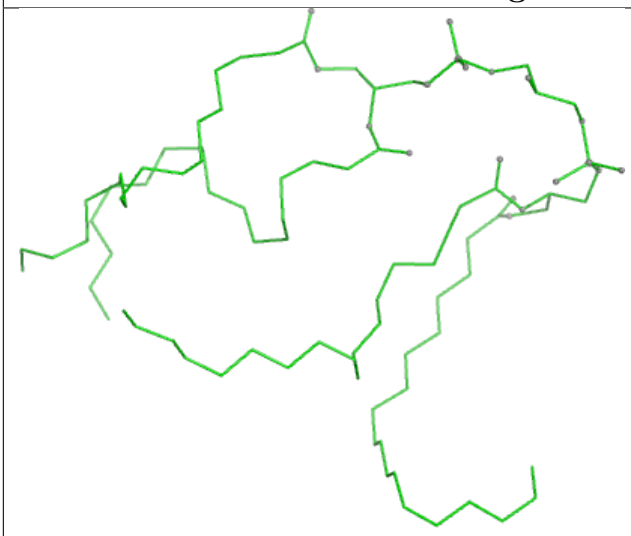


**Torsions**

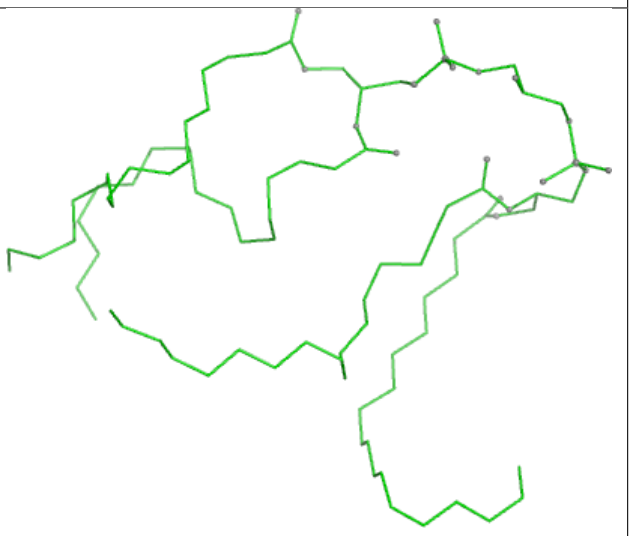


**Rings**

**Ligand CDL Dm 501**



**Bond lengths**



**Bond angles**

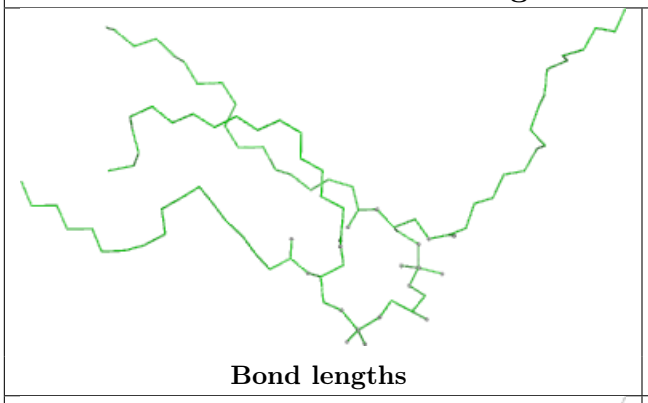


**Torsions**

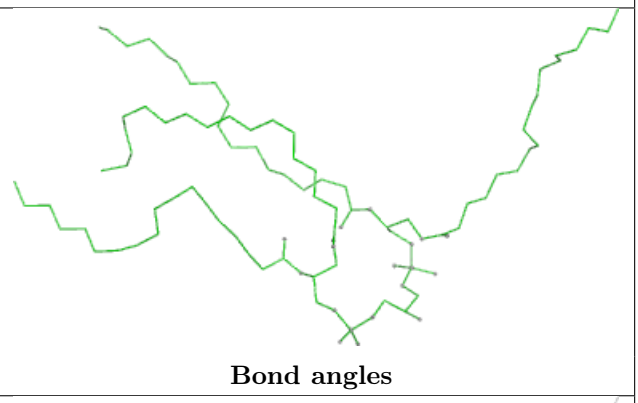


**Rings**

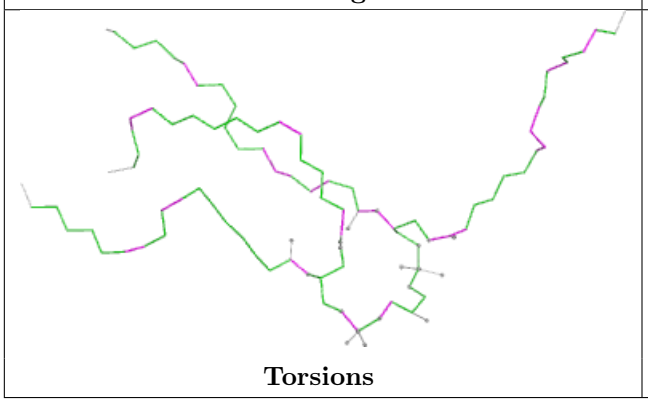
## Ligand CDL DN 504



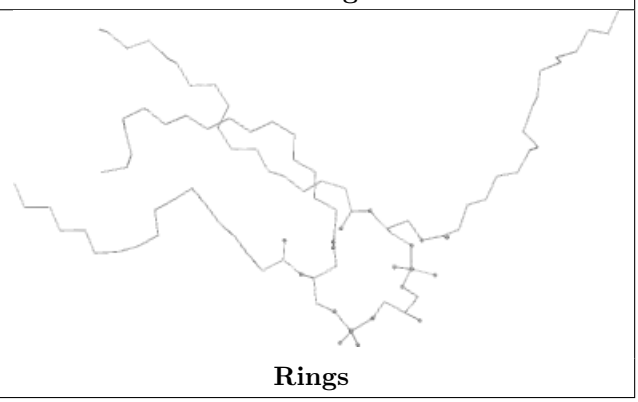
Bond lengths



Bond angles

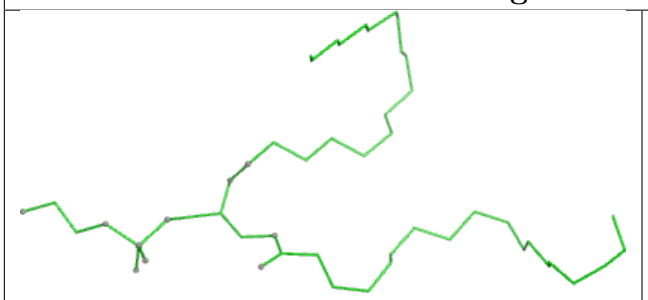


Torsions

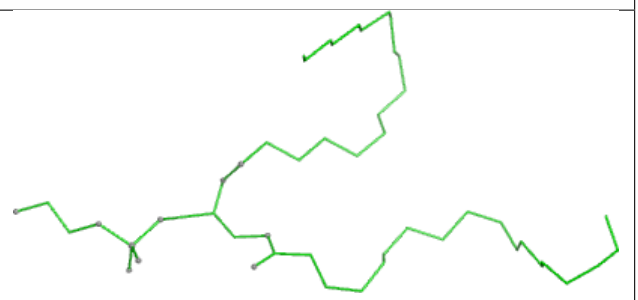


Rings

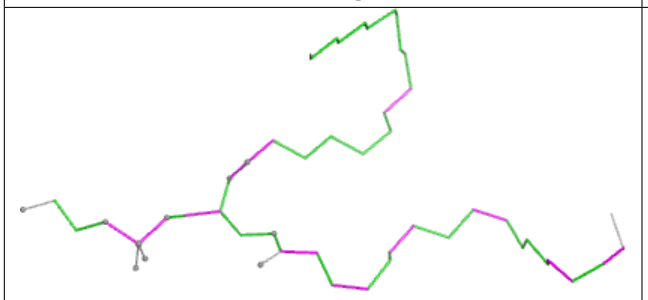
## Ligand 3PE Dx 1206



Bond lengths



Bond angles

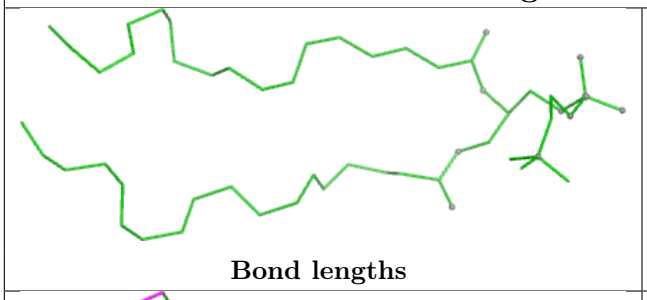


Torsions

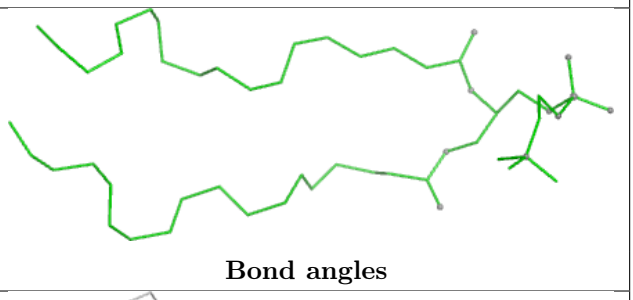


Rings

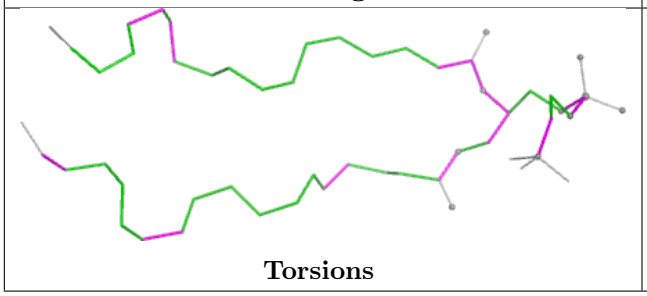
## Ligand PC1 Eo 204



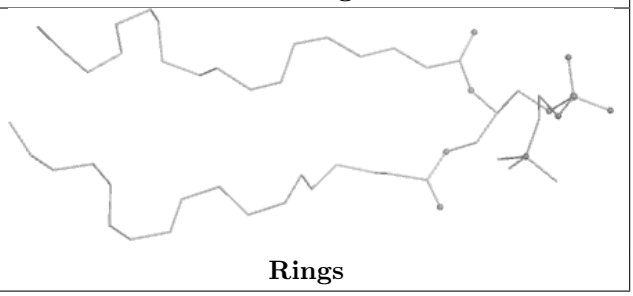
Bond lengths



Bond angles

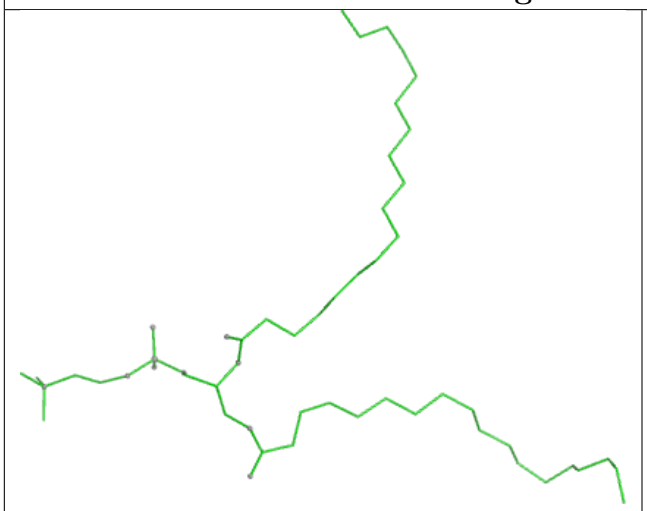


Torsions

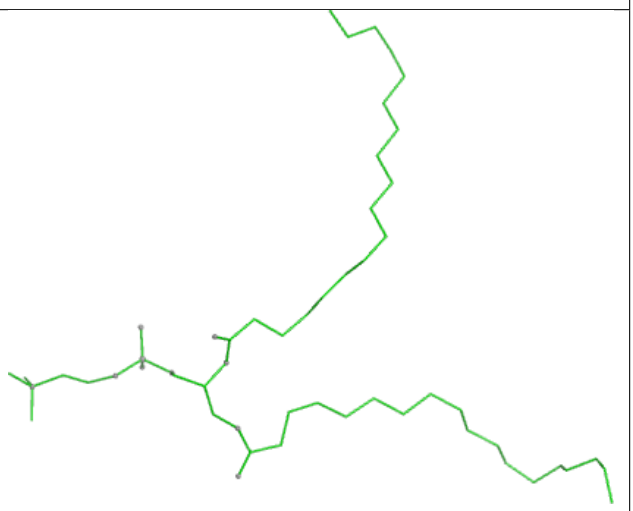


Rings

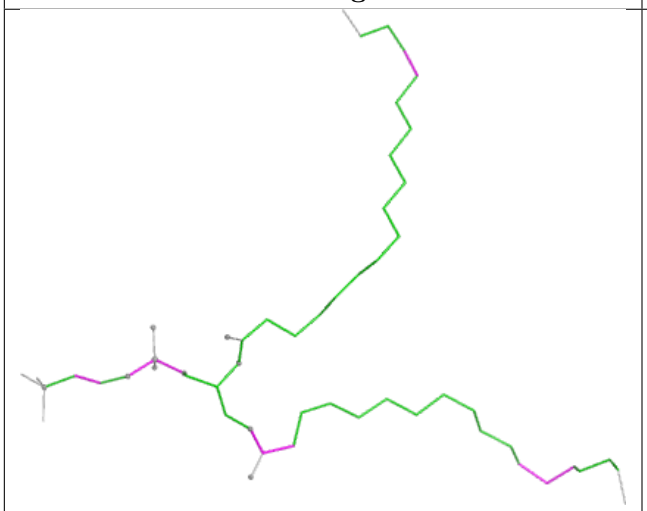
## Ligand PC1 DV 406



Bond lengths



Bond angles

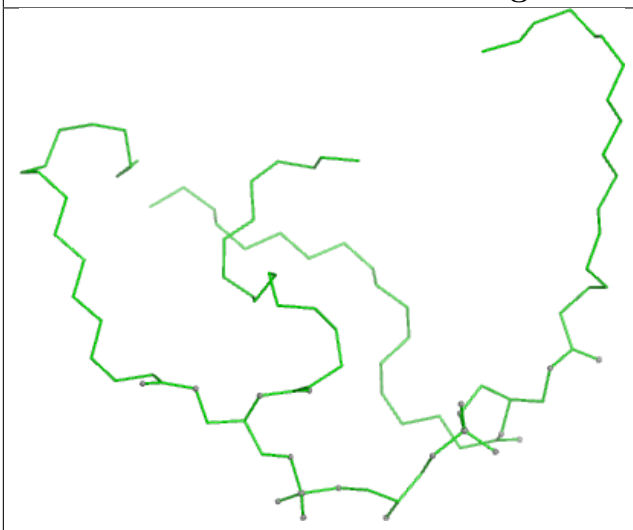


Torsions

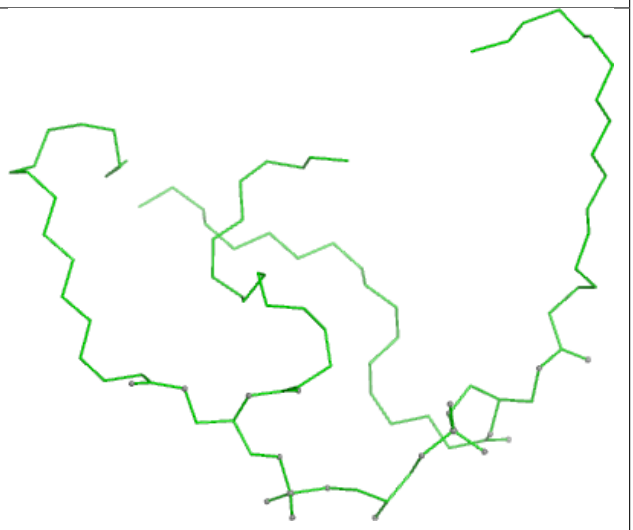


Rings

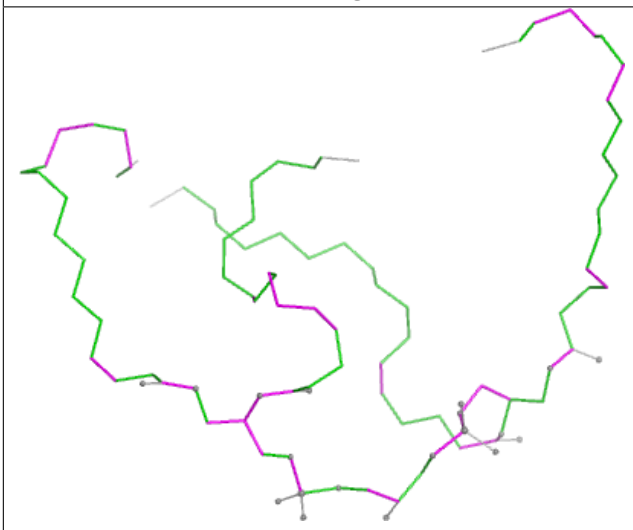
**Ligand CDL DV 404**



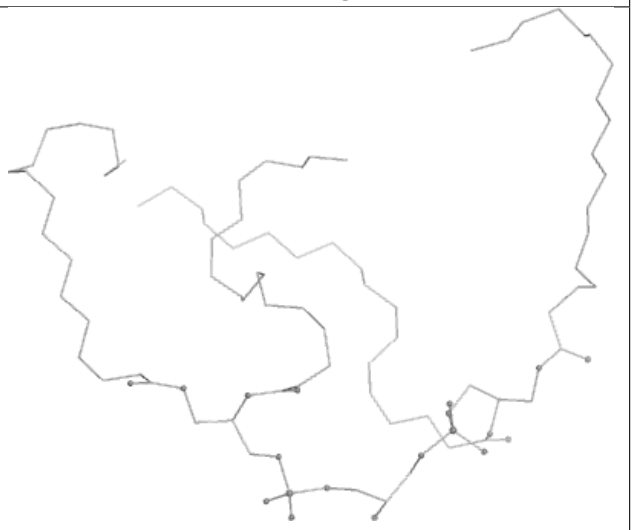
**Bond lengths**



**Bond angles**

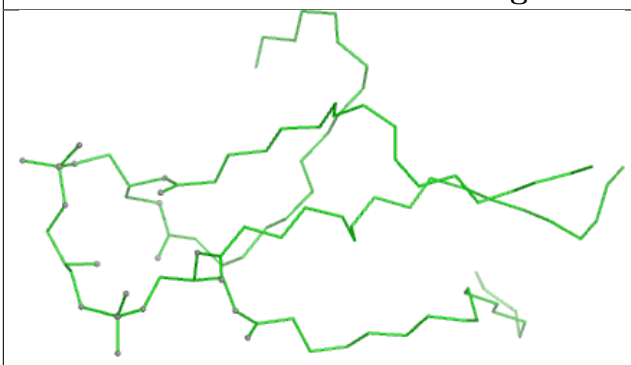


**Torsions**

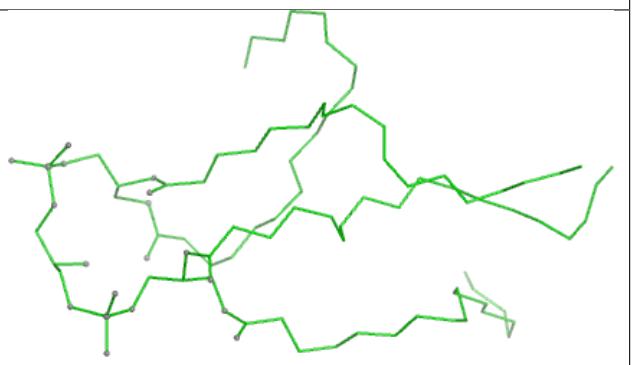


**Rings**

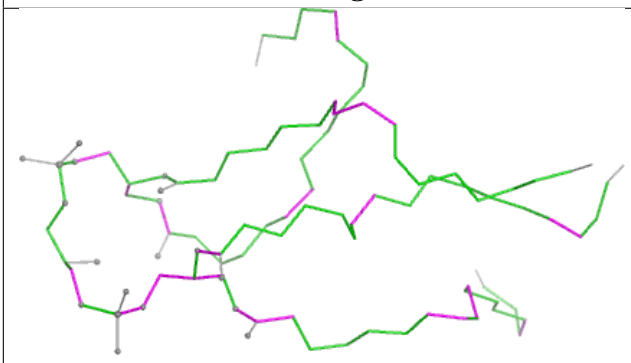
**Ligand CDL DA 705**



**Bond lengths**



**Bond angles**

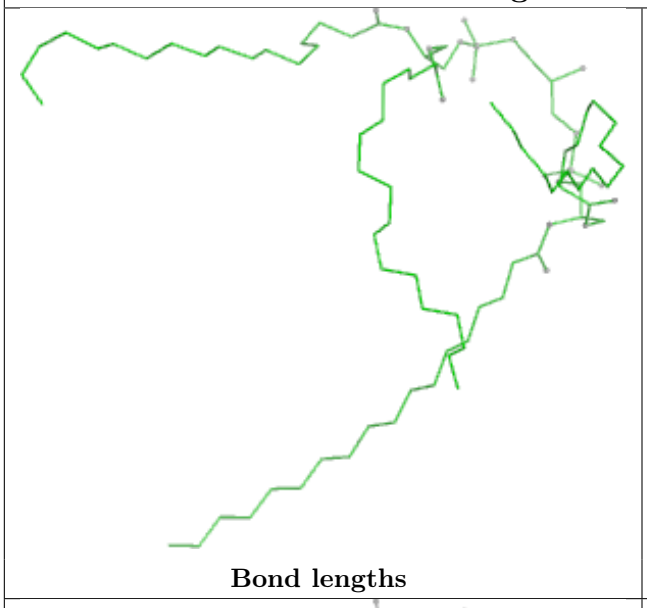


**Torsions**

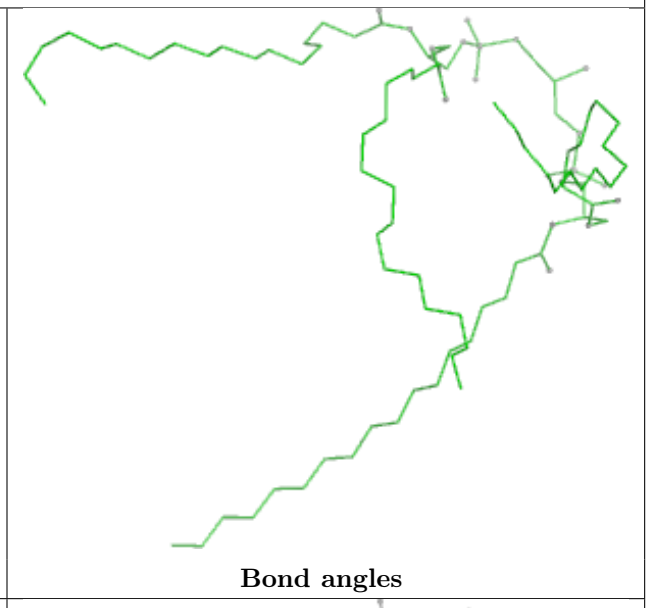


**Rings**

**Ligand CDL DD 702**



**Bond lengths**



**Bond angles**

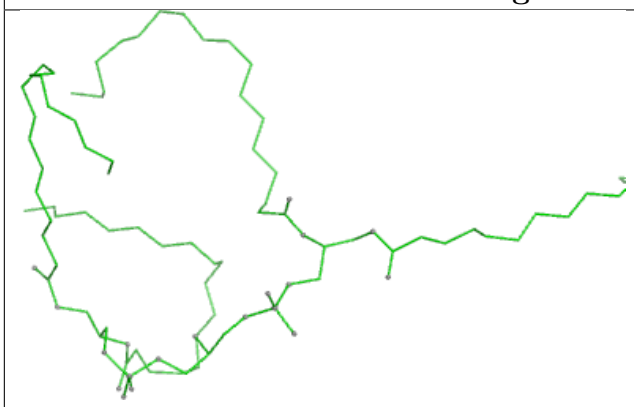


**Torsions**

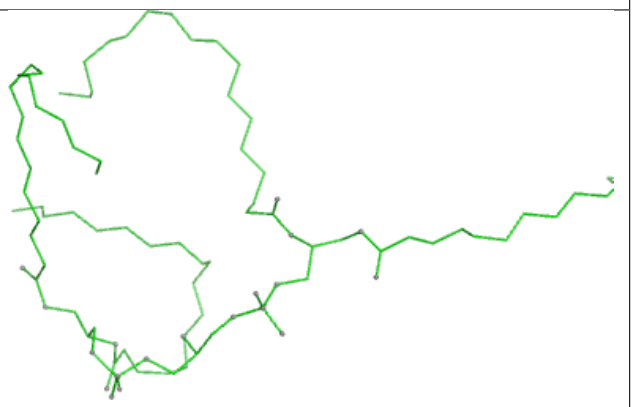


**Rings**

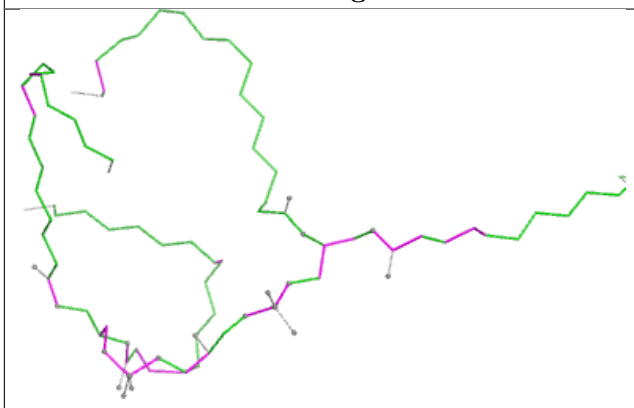
**Ligand CDL EU 101**



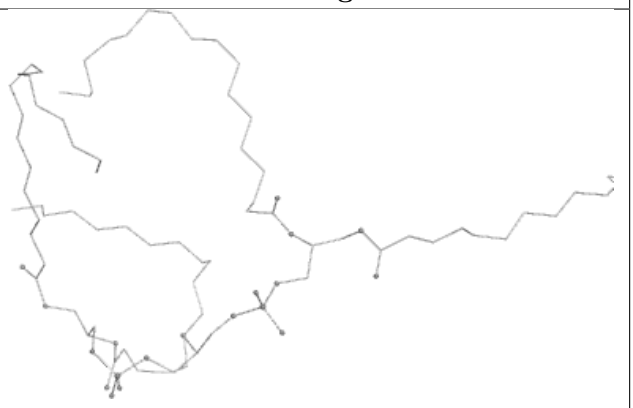
**Bond lengths**



**Bond angles**

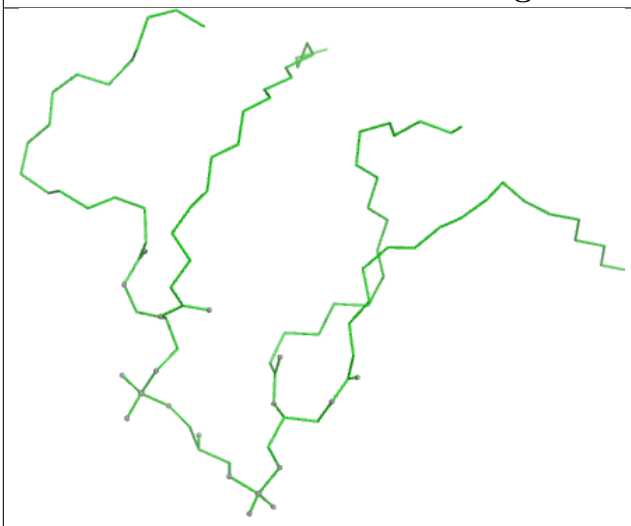


**Torsions**

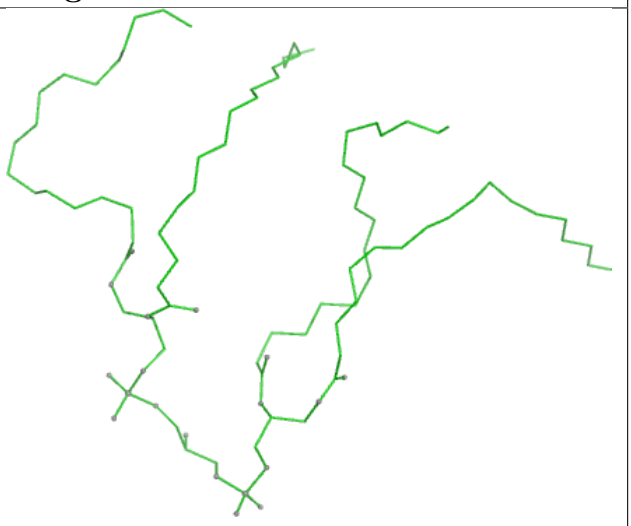


**Rings**

**Ligand CDL Dg 202**



**Bond lengths**



**Bond angles**

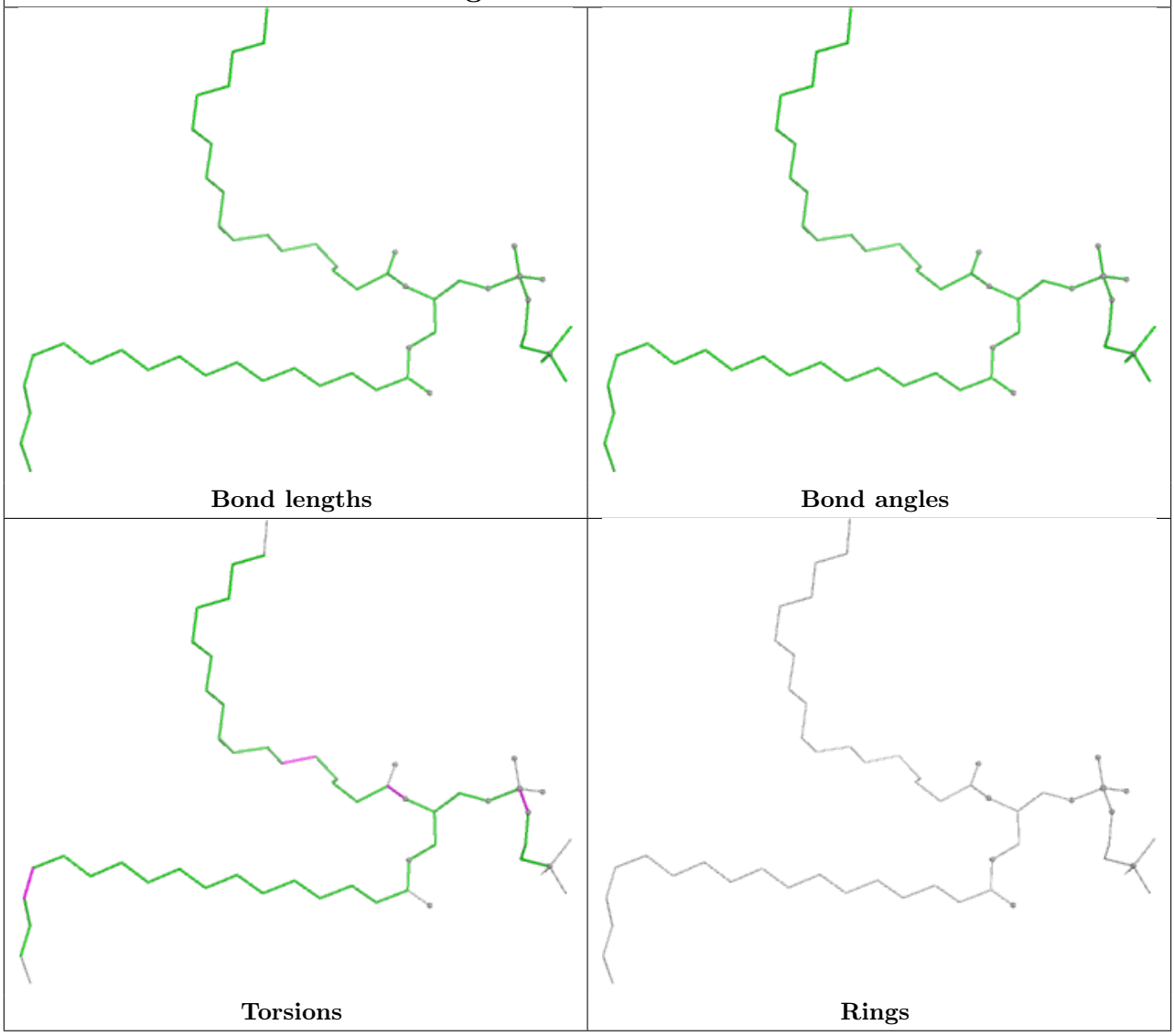


**Torsions**

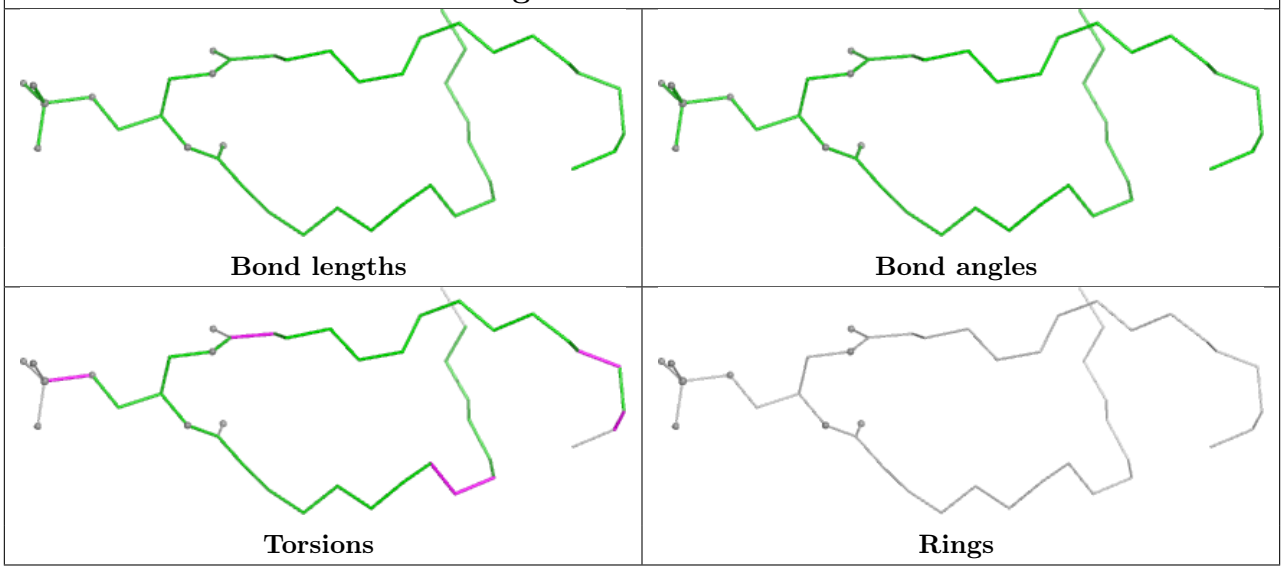


**Rings**

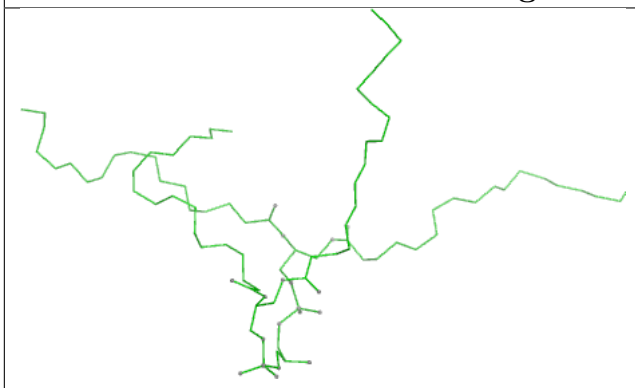
## Ligand PC1 Dx 1208



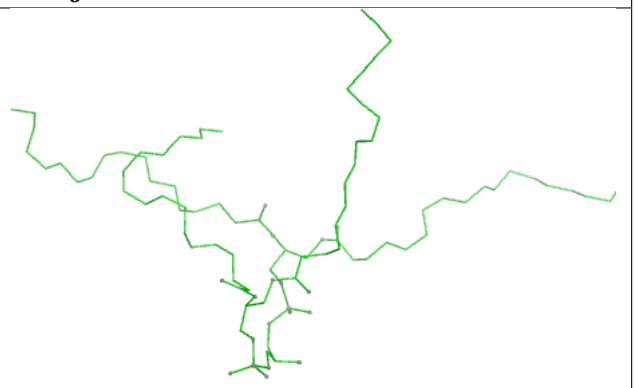

## Ligand LPP Dl 1101



**Ligand CDL Dj 403**



**Bond lengths**



**Bond angles**

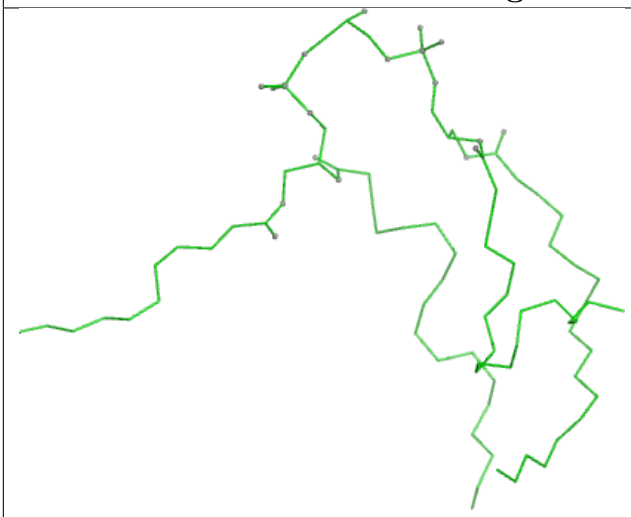


**Torsions**

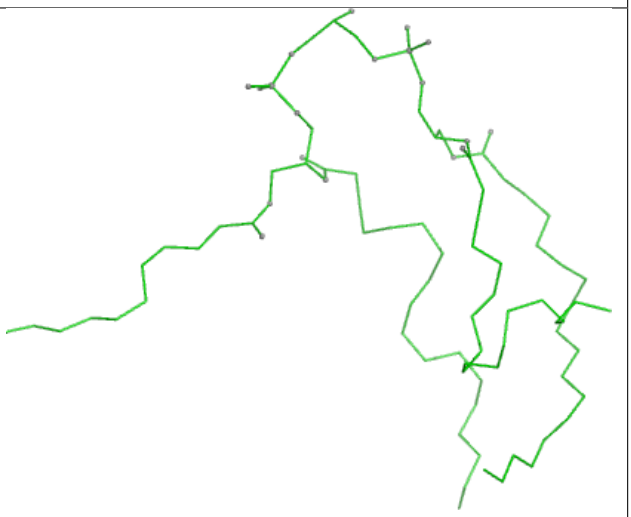


**Rings**

**Ligand CDL Eh 1601**



**Bond lengths**



**Bond angles**

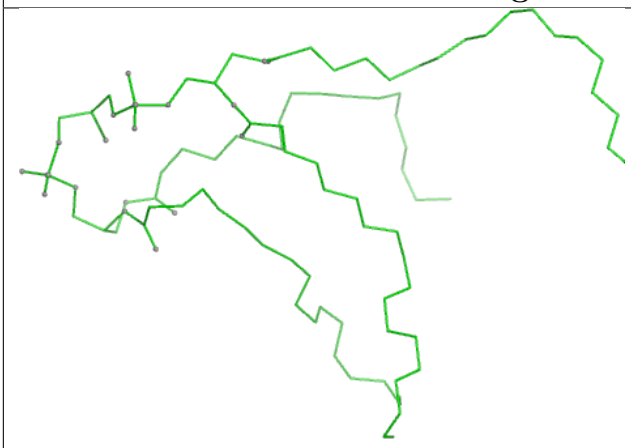


**Torsions**

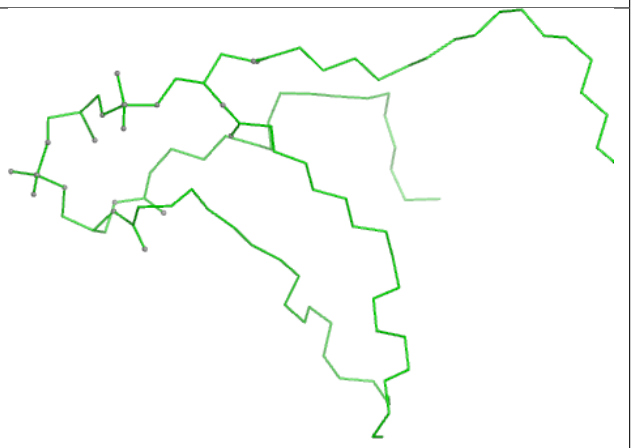


**Rings**

**Ligand CDL ED 604**



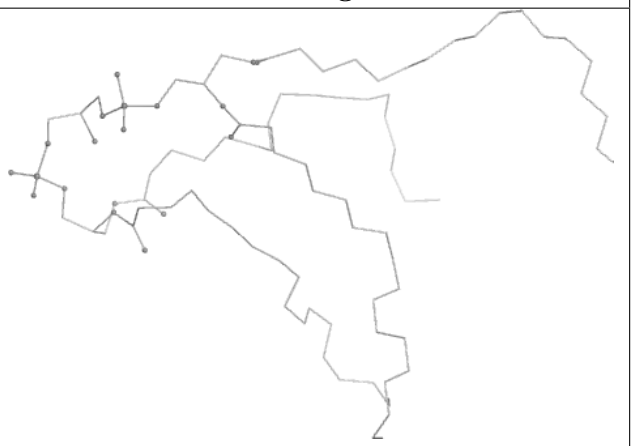
**Bond lengths**



**Bond angles**

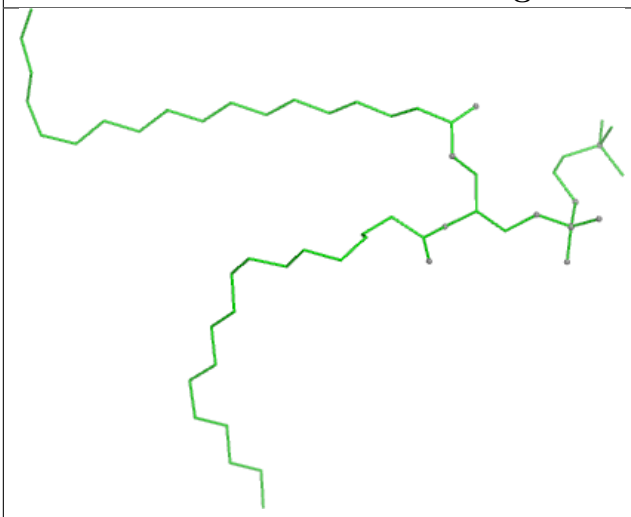


**Torsions**

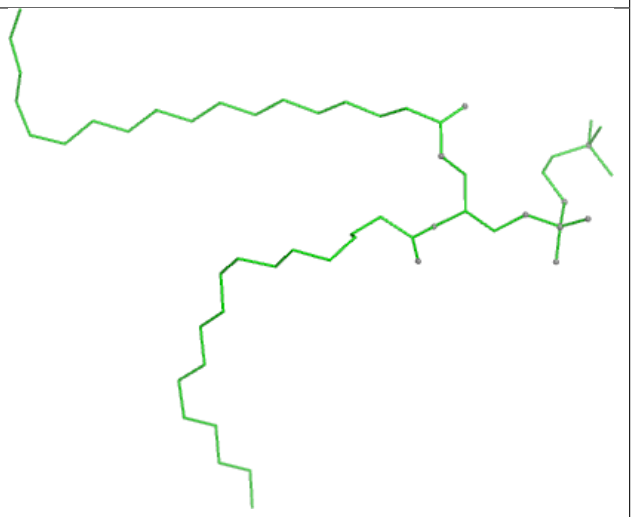


**Rings**

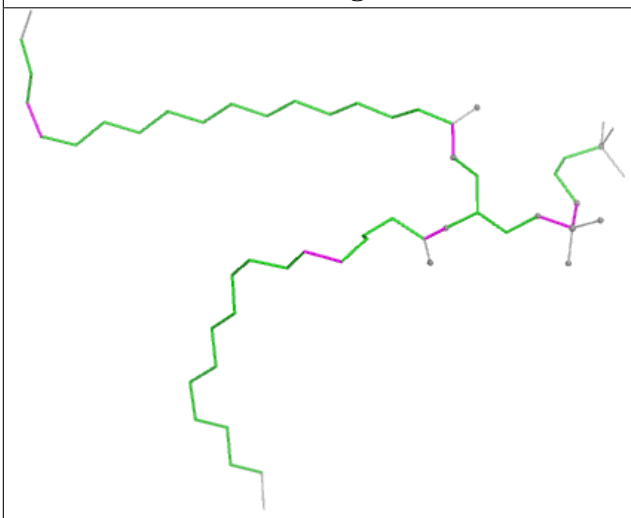
**Ligand PC1 DX 306**



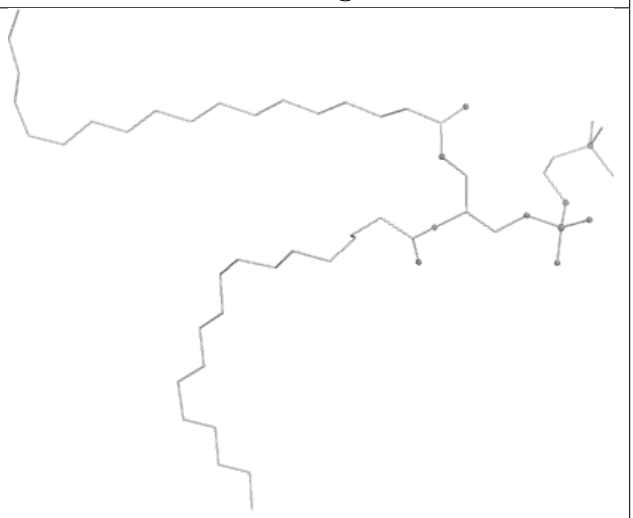
**Bond lengths**



**Bond angles**

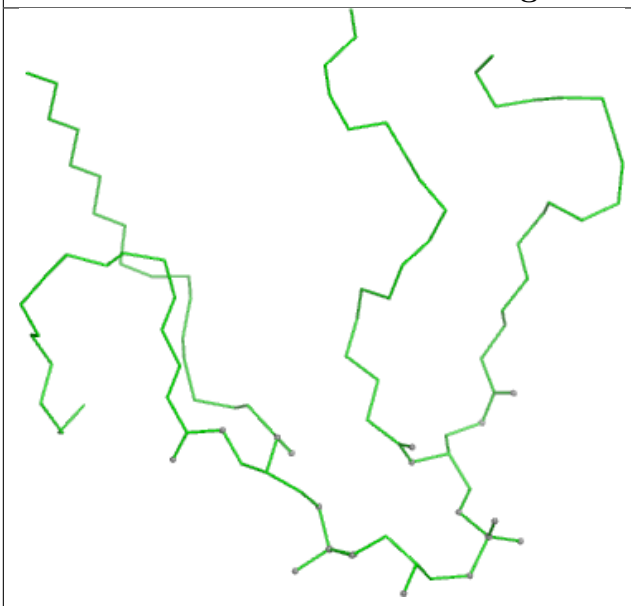


**Torsions**

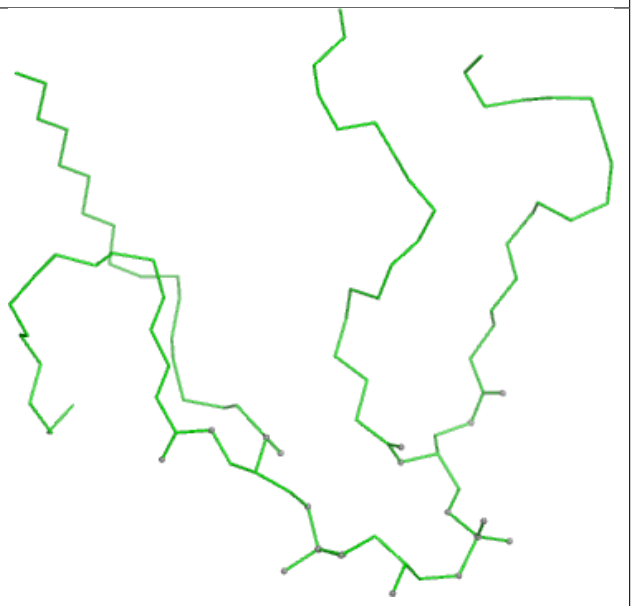


**Rings**

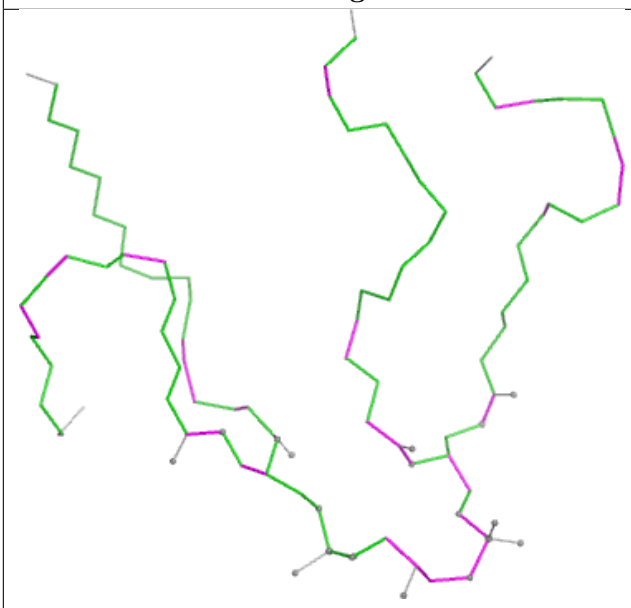
**Ligand CDL El 902**



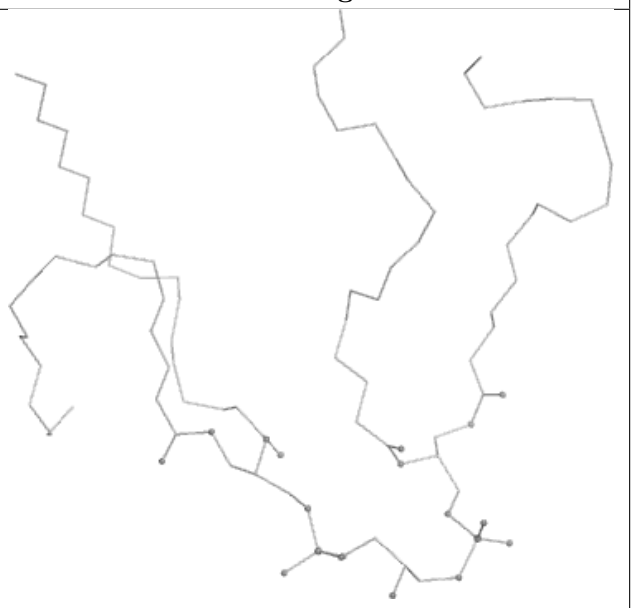
**Bond lengths**



**Bond angles**

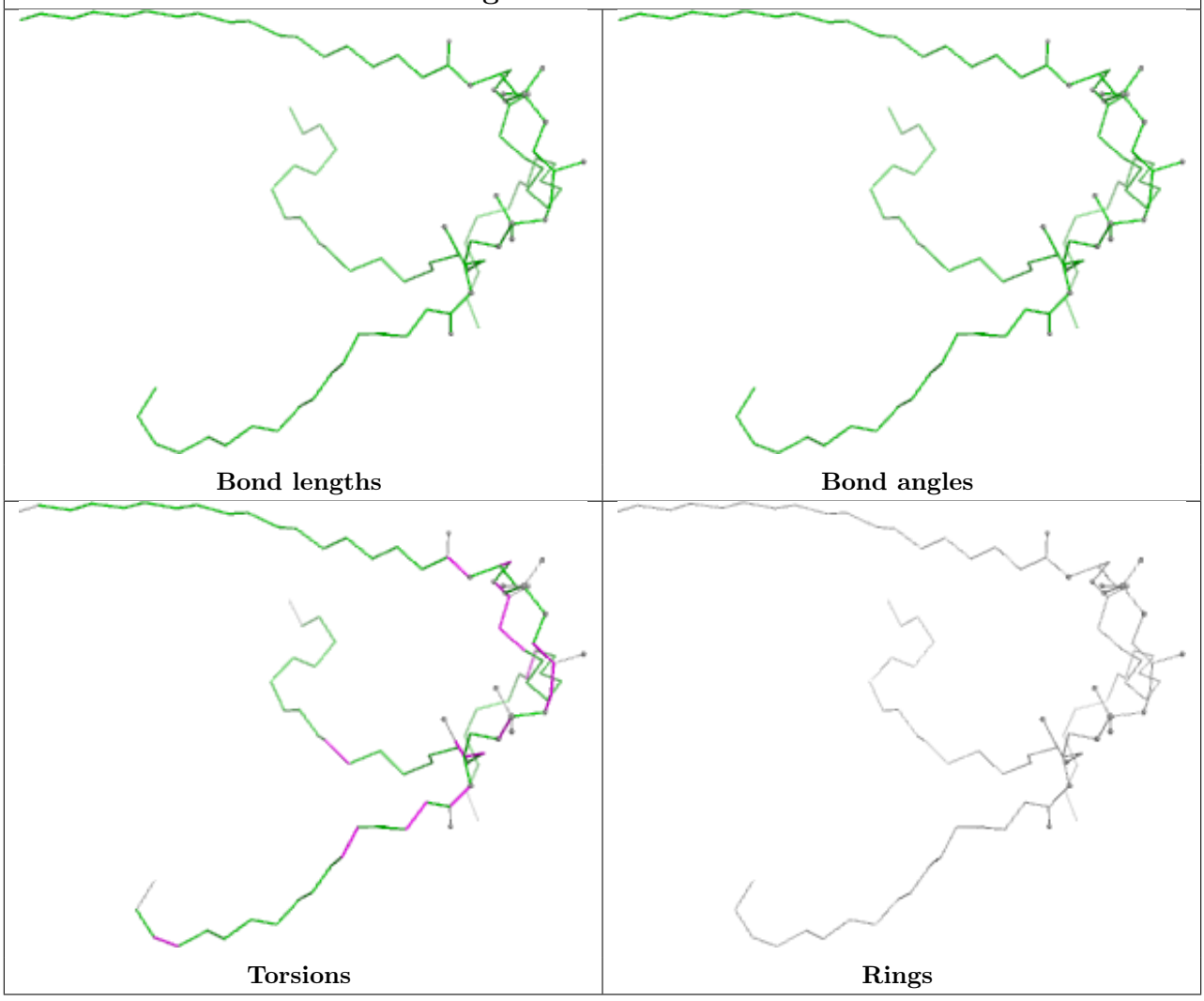


**Torsions**

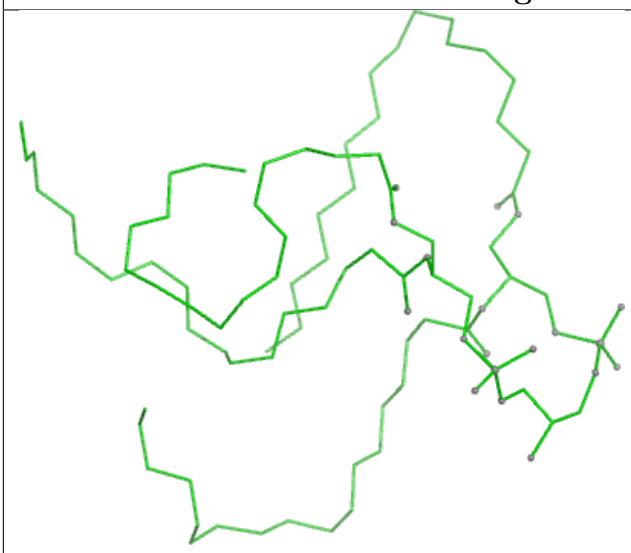


**Rings**

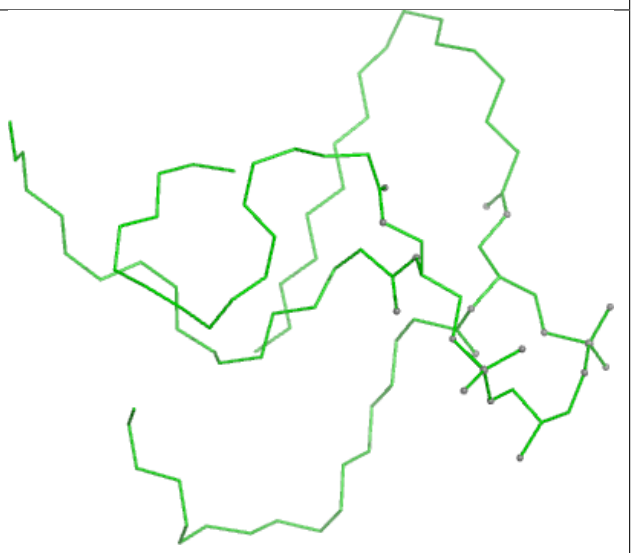
**Ligand CDL Dd 702**



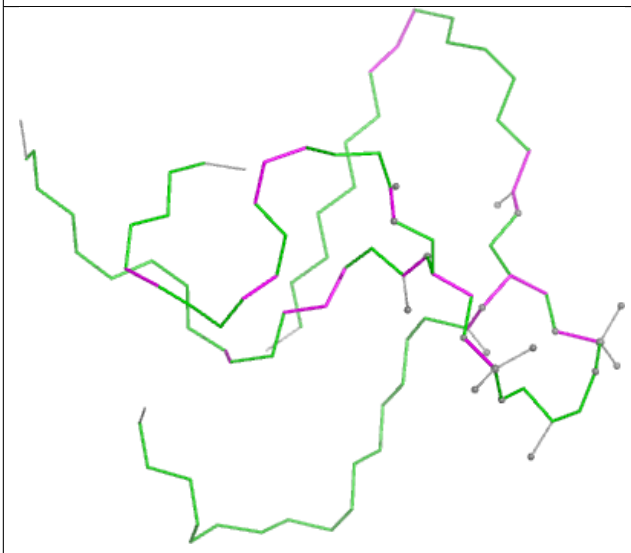
**Ligand CDL Do 501**



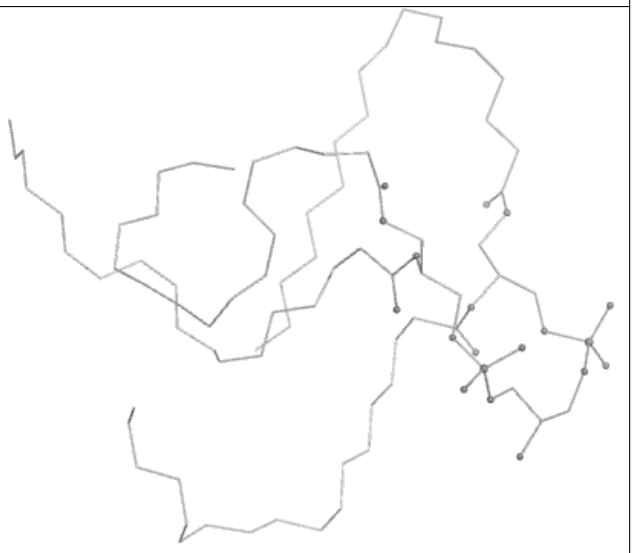
**Bond lengths**



**Bond angles**

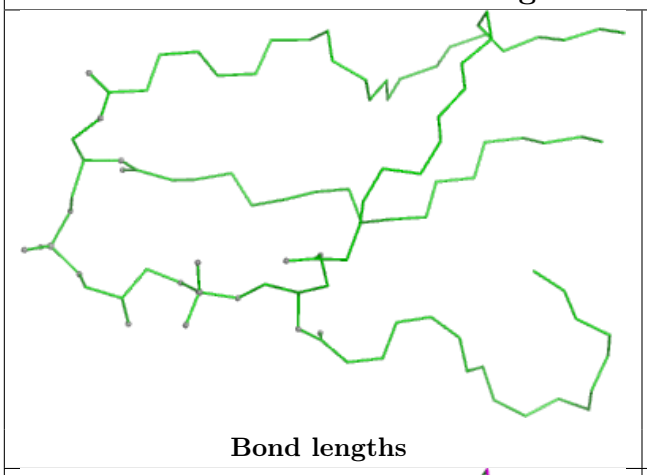


**Torsions**

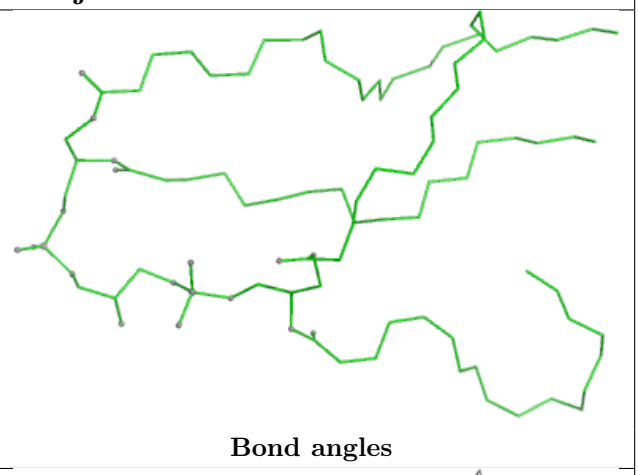


**Rings**

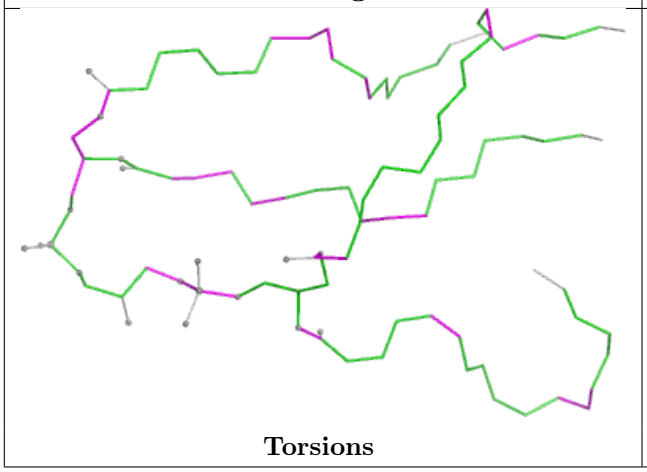
**Ligand CDL Dj 401**



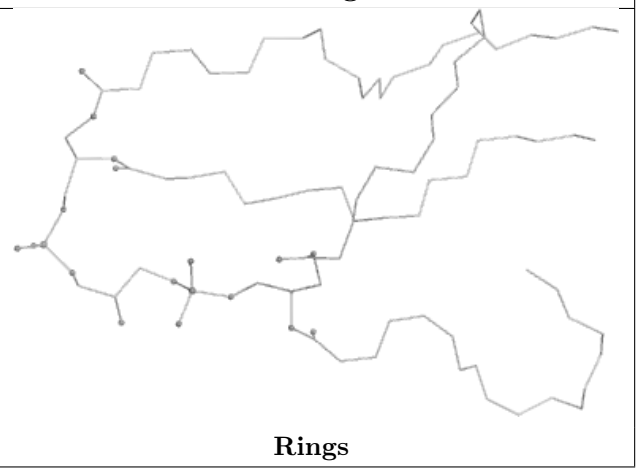
**Bond lengths**



**Bond angles**

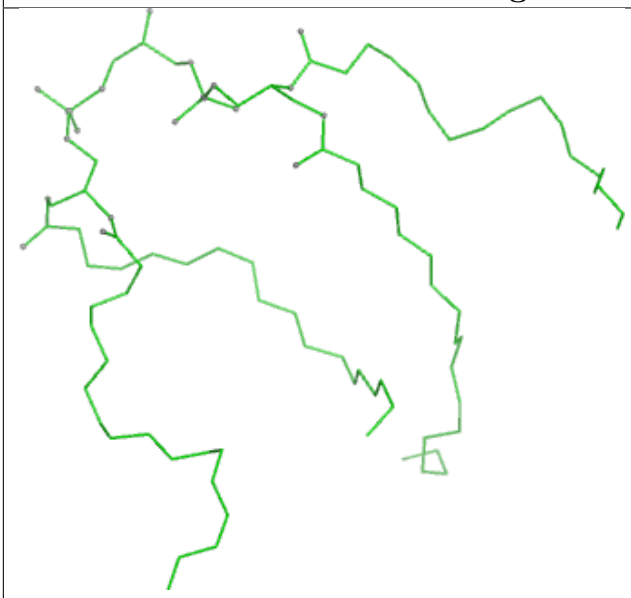


**Torsions**



**Rings**

**Ligand CDL DH 201**



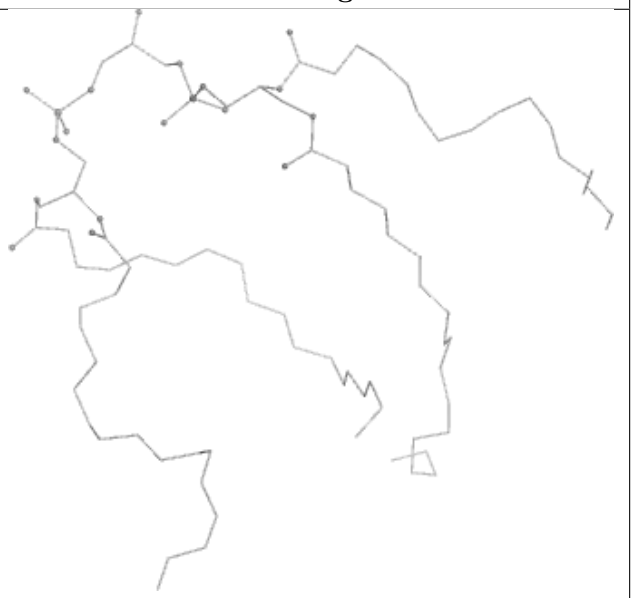
**Bond lengths**



**Bond angles**

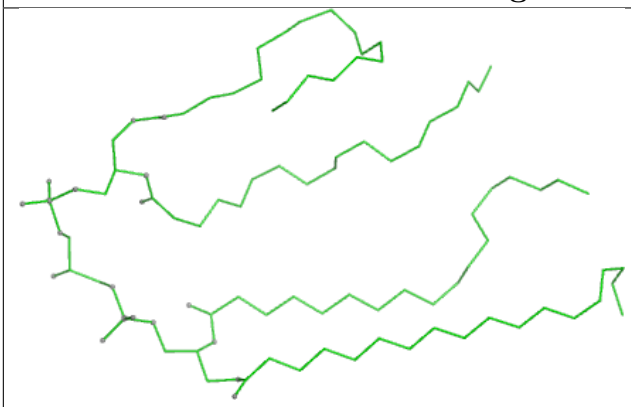


**Torsions**

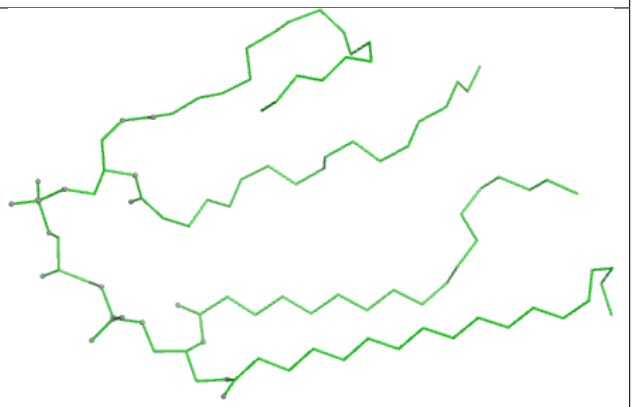


**Rings**

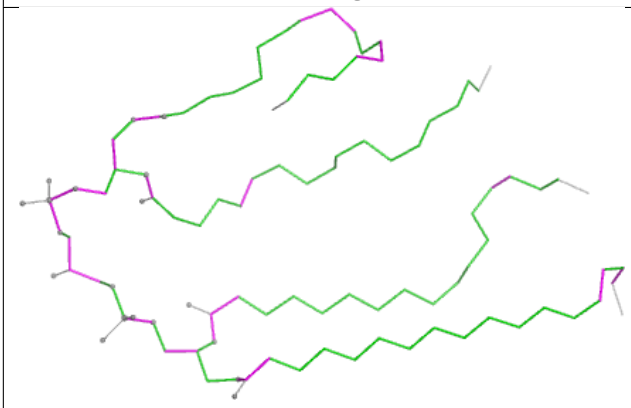
**Ligand CDL DD 704**



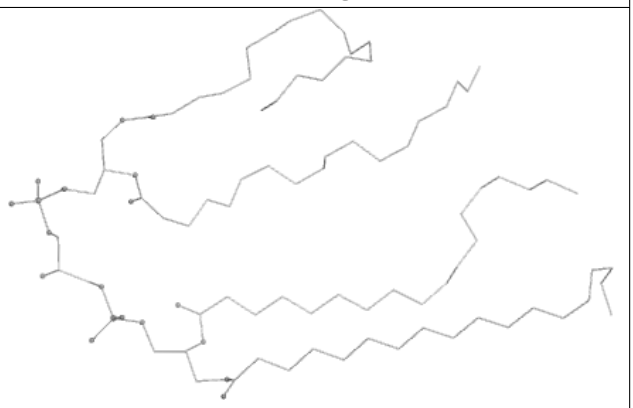
**Bond lengths**



**Bond angles**

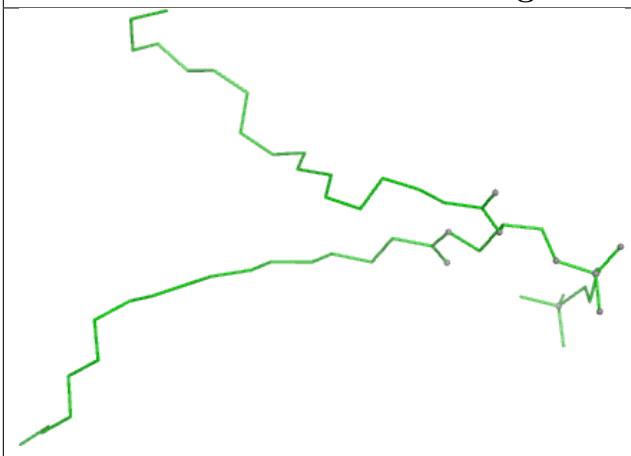


**Torsions**

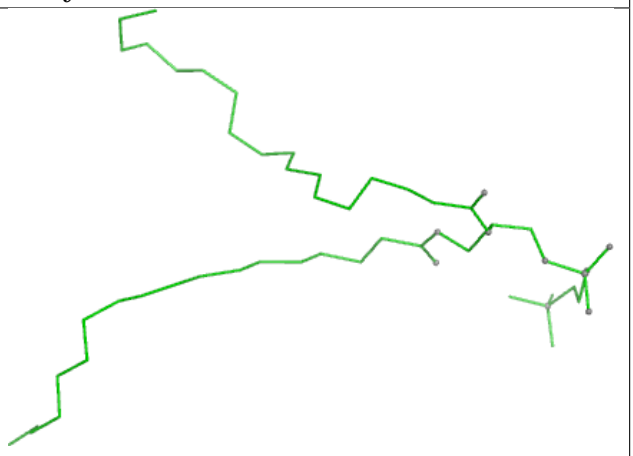


**Rings**

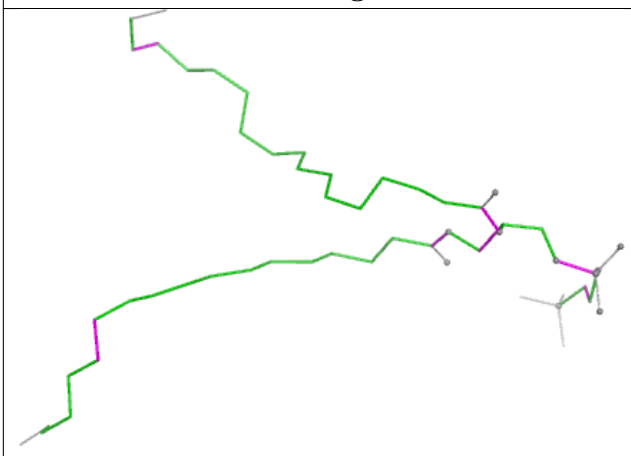
**Ligand PC1 Dy 302**



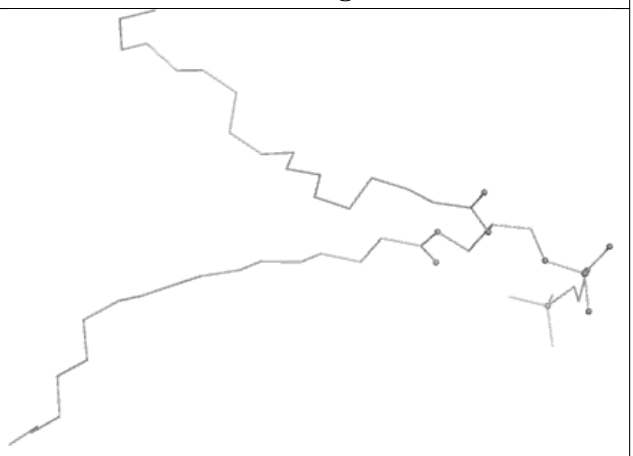
**Bond lengths**



**Bond angles**



**Torsions**



**Rings**

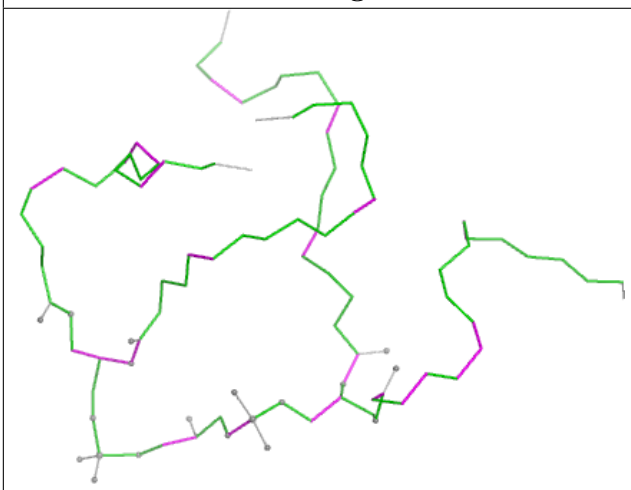
## Ligand CDL DI 701



Bond lengths



Bond angles

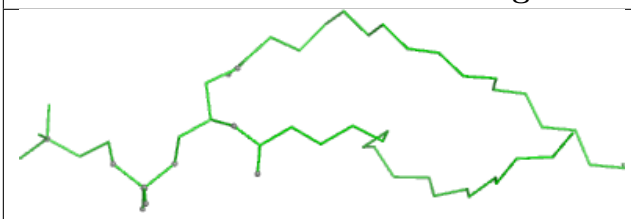


Torsions

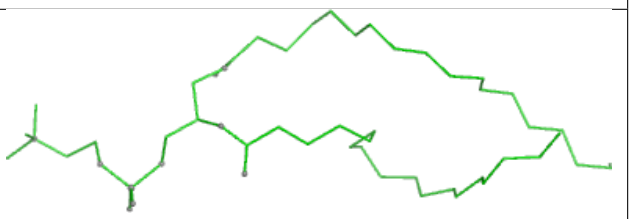


Rings

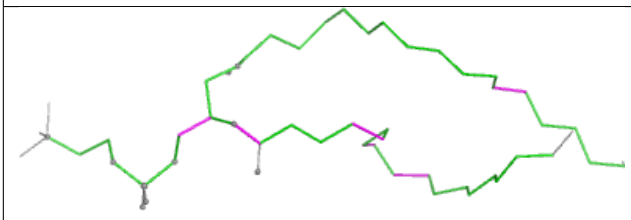
## Ligand PC1 DG 203



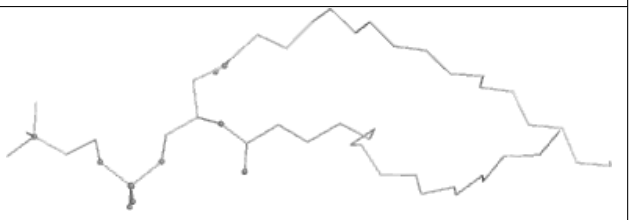
Bond lengths



Bond angles

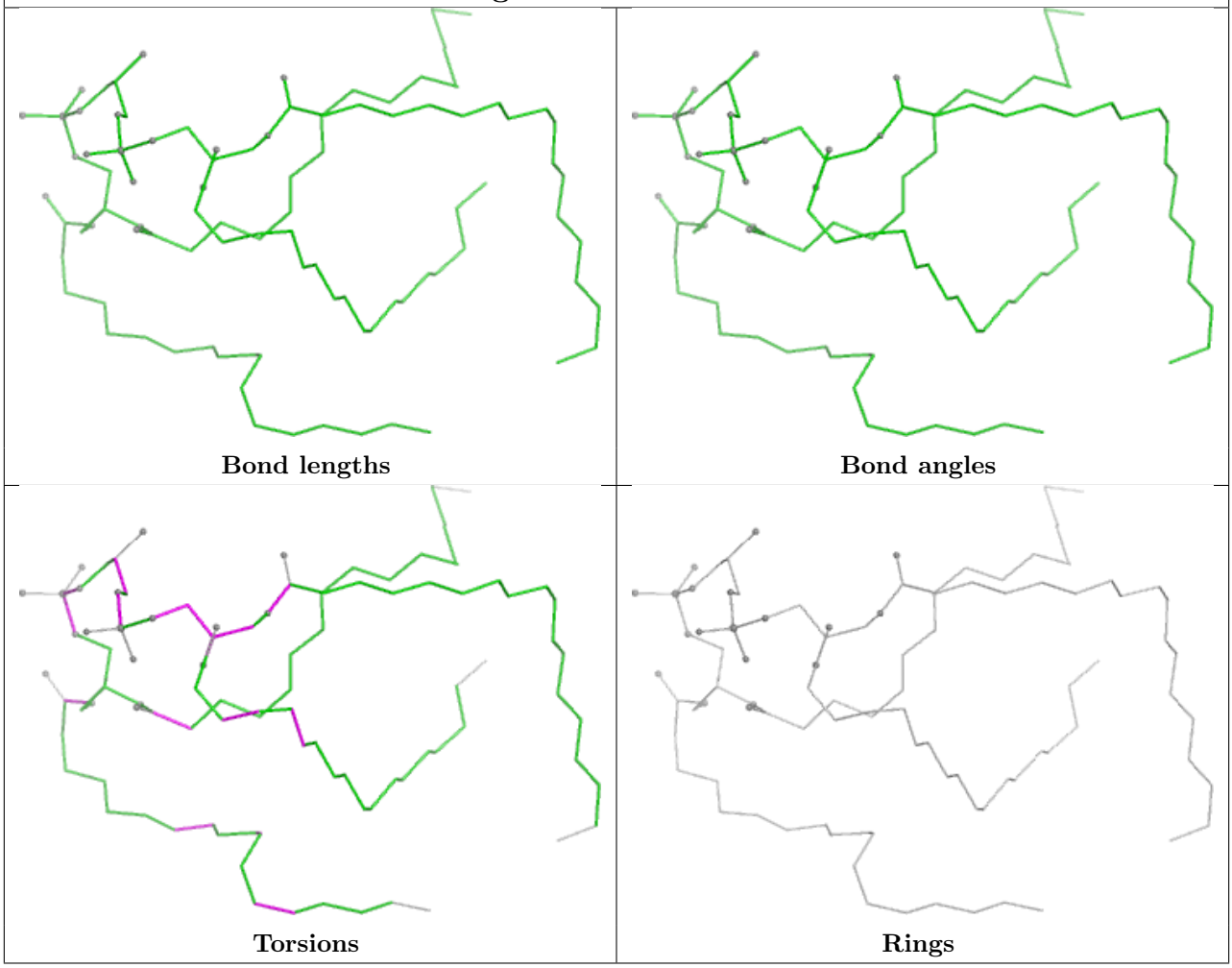


Torsions

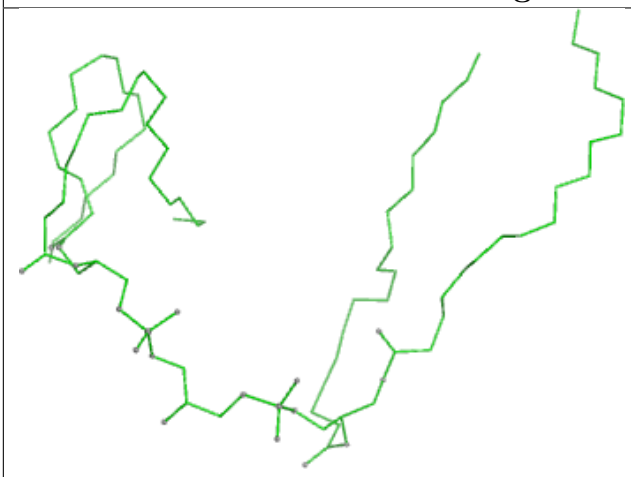


Rings

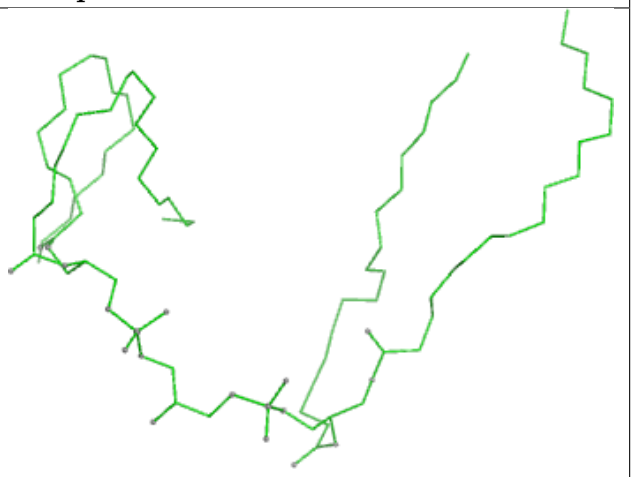
**Ligand CDL EA 301**



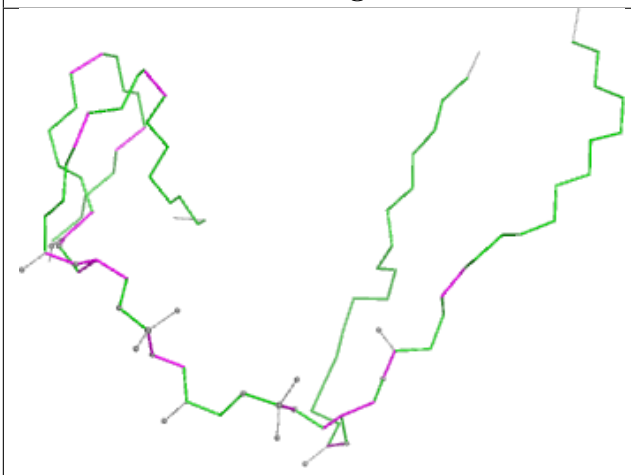
**Ligand CDL Dq 402**



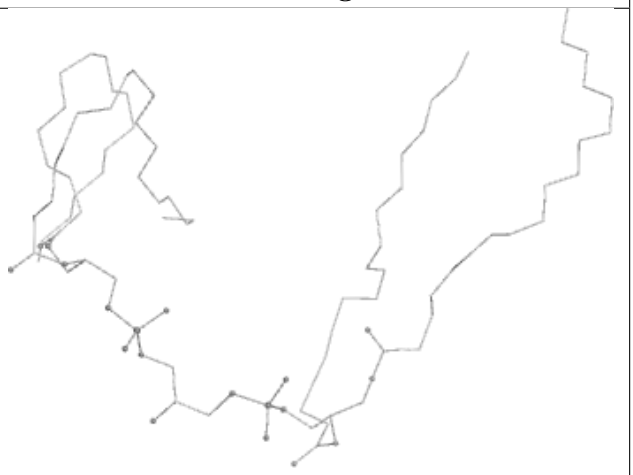
**Bond lengths**



**Bond angles**

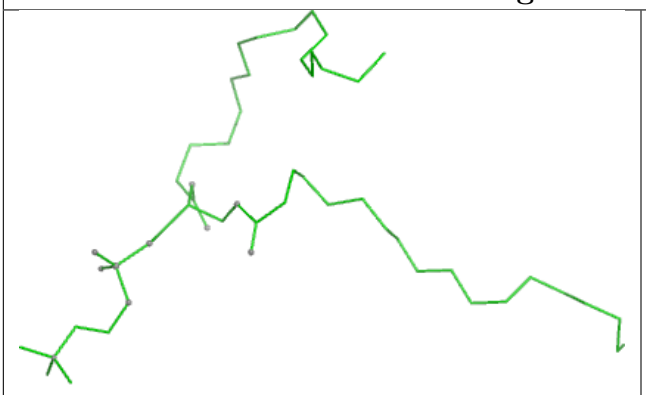


**Torsions**

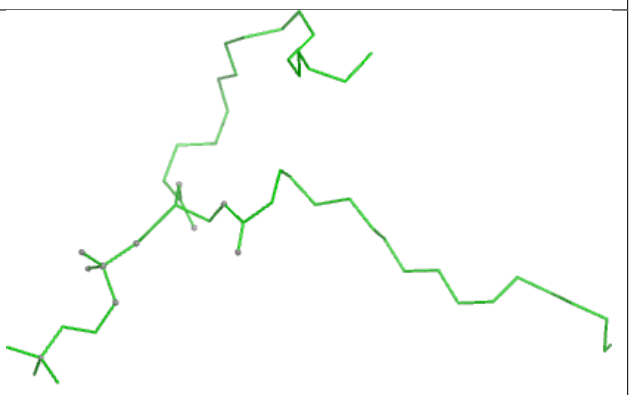


**Rings**

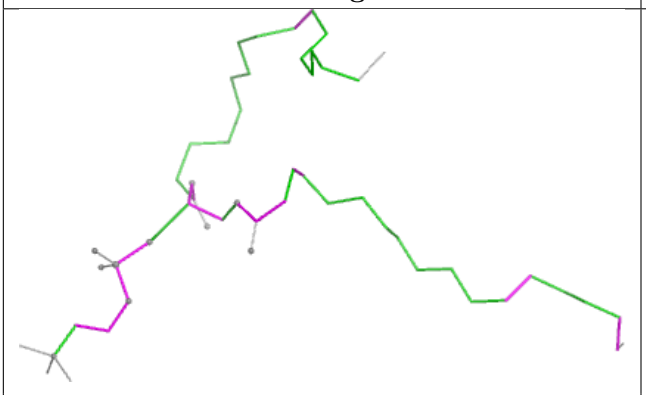
**Ligand PC1 DS 406**



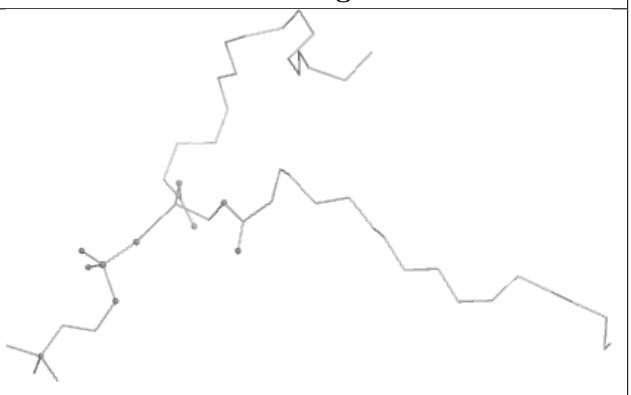
**Bond lengths**



**Bond angles**

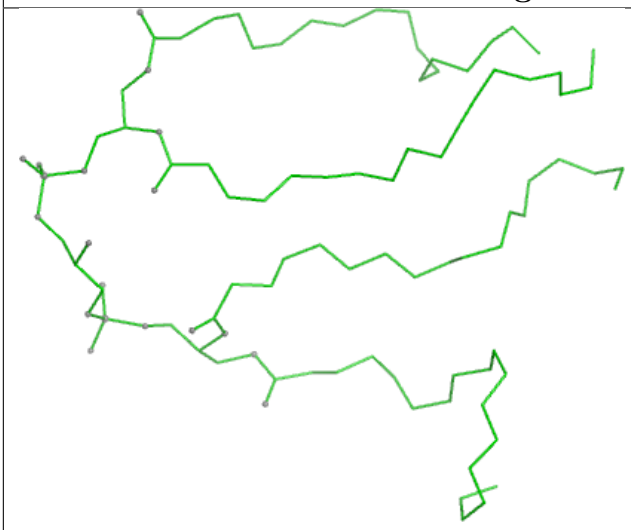


**Torsions**

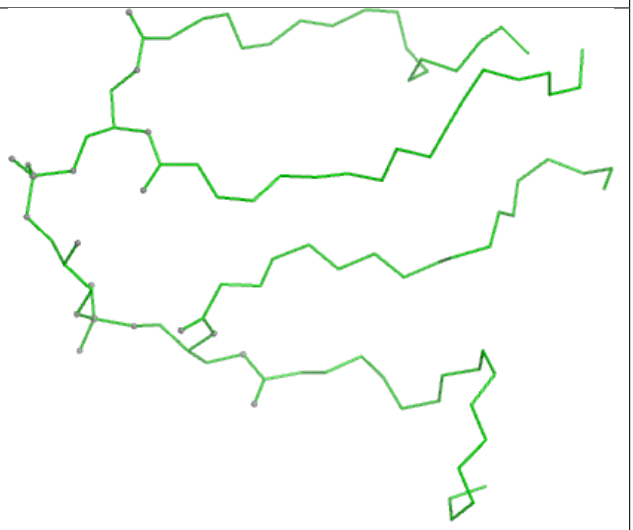


**Rings**

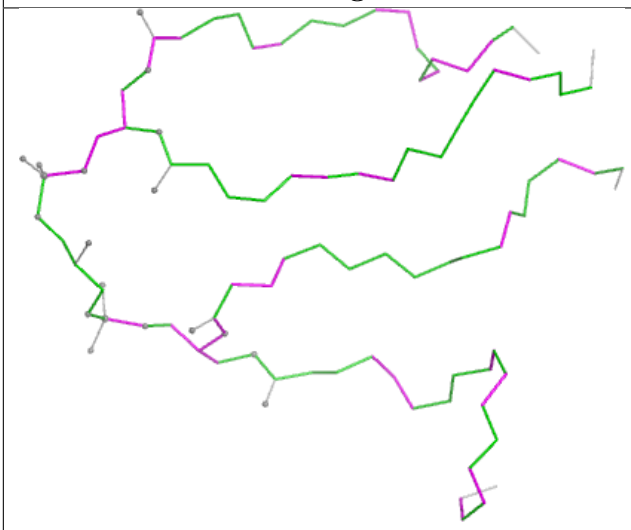
**Ligand CDL EL 901**



**Bond lengths**



**Bond angles**

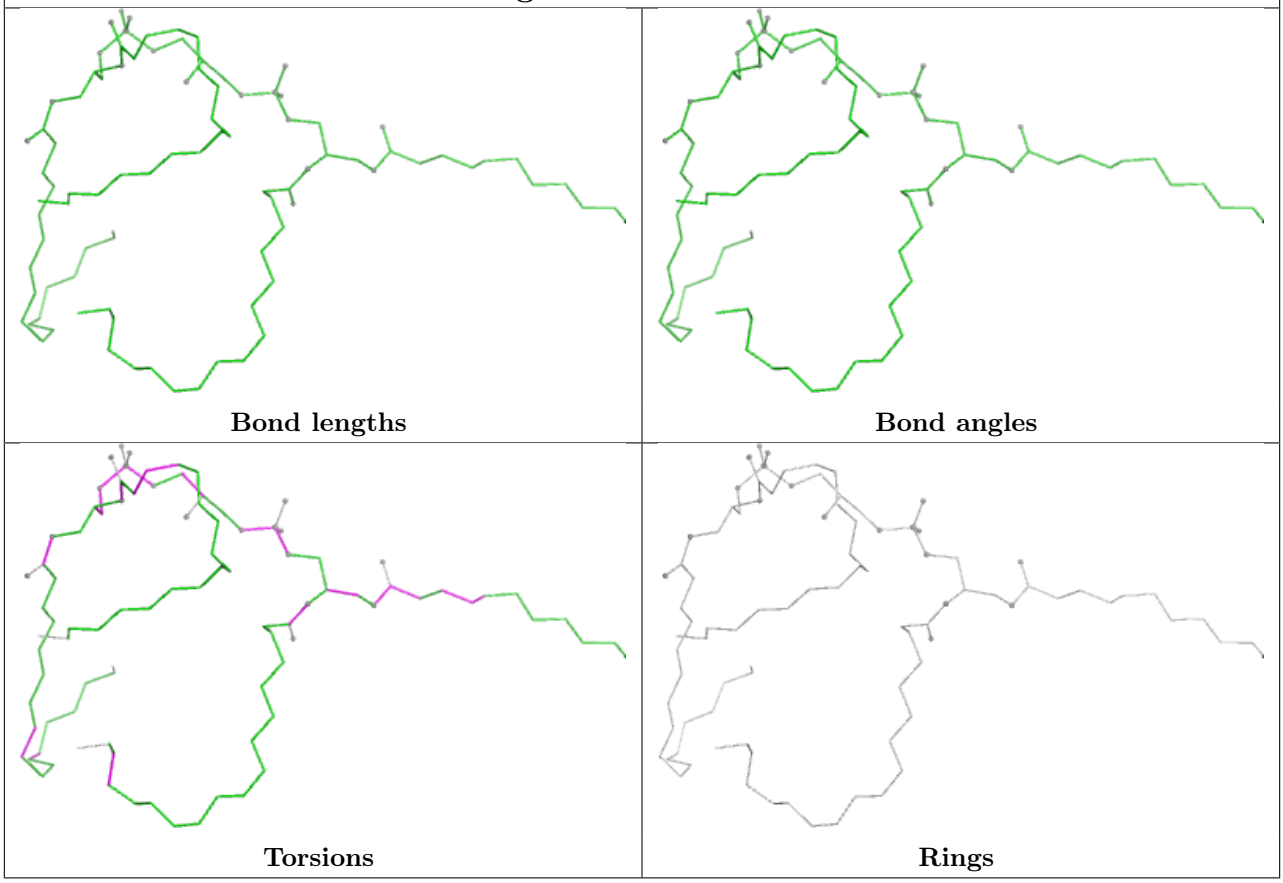


**Torsions**

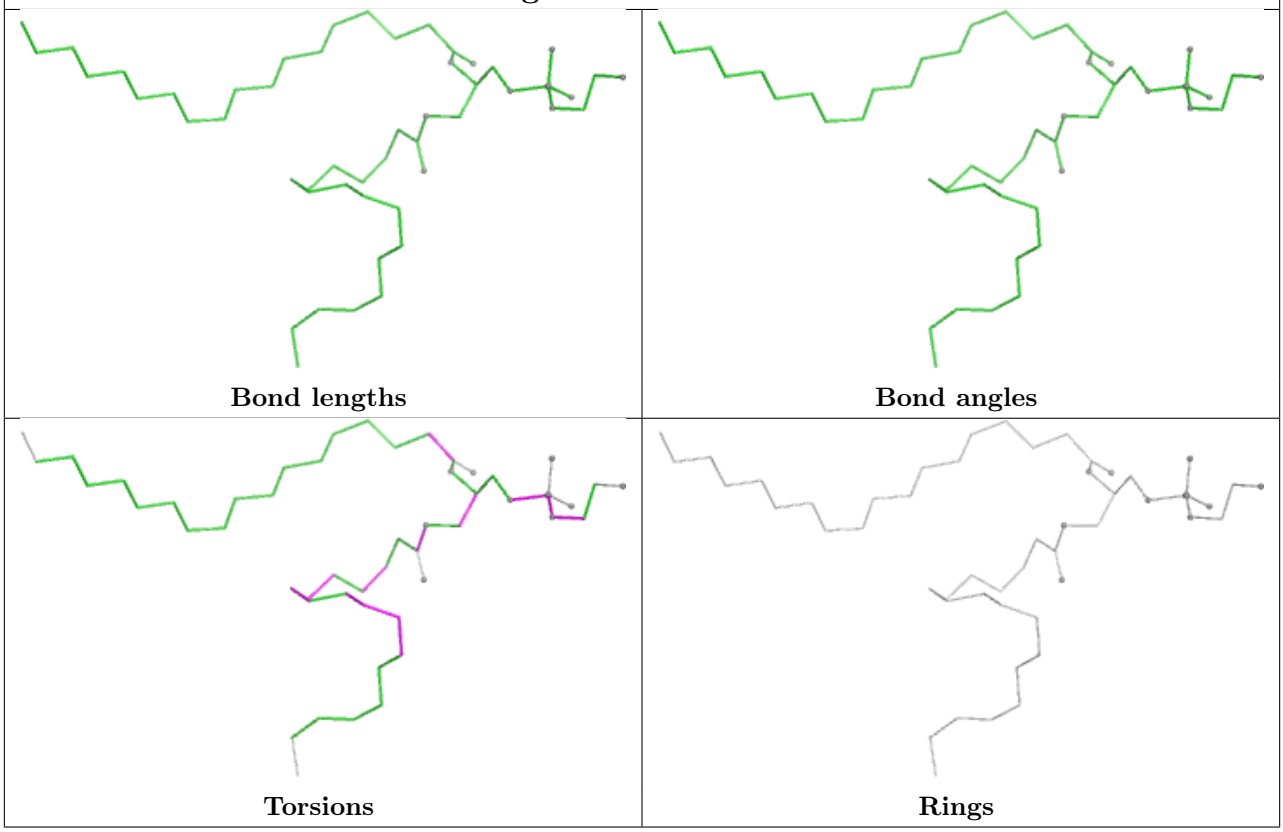


**Rings**

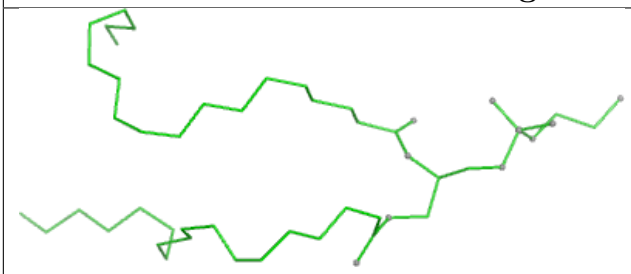
## Ligand CDL Eu 101



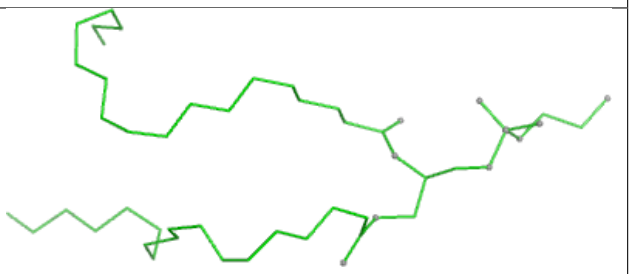

## Ligand 3PE Ds 401



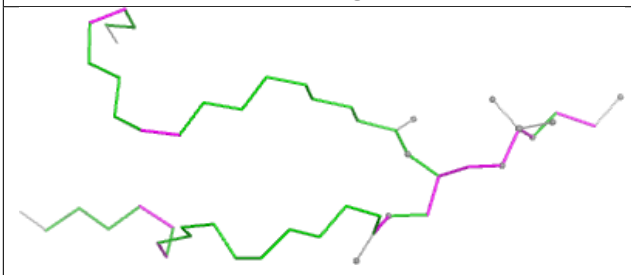
## Ligand 3PE Da 708



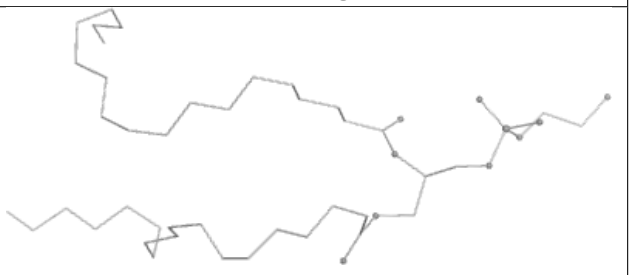
Bond lengths



Bond angles

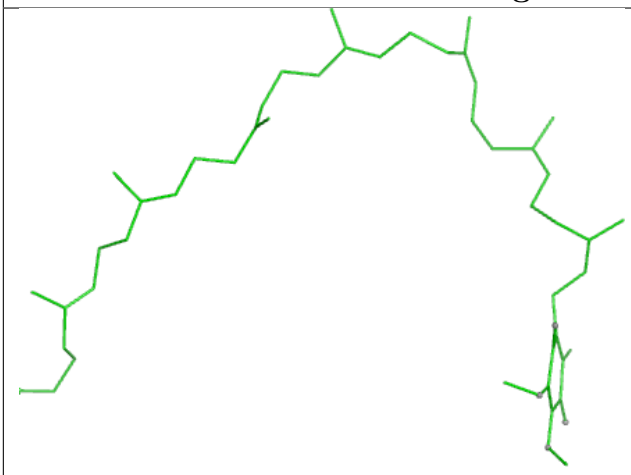


Torsions

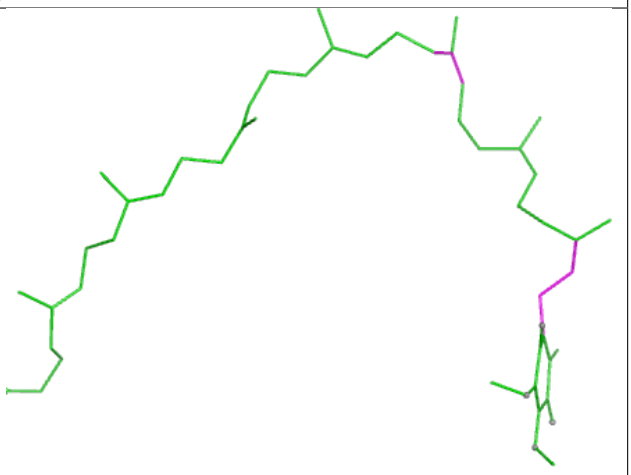


Rings

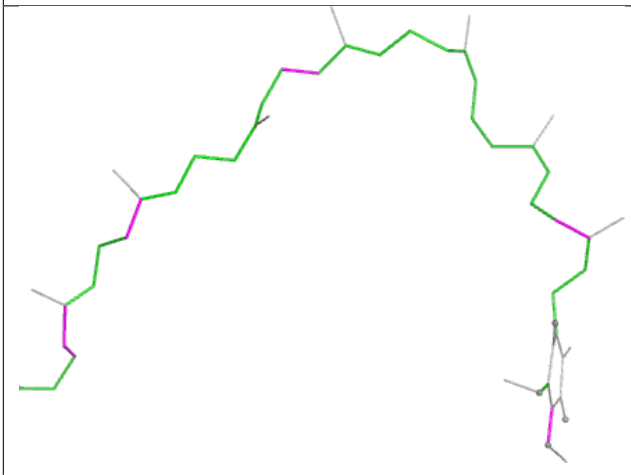
## Ligand UQ8 ED 603



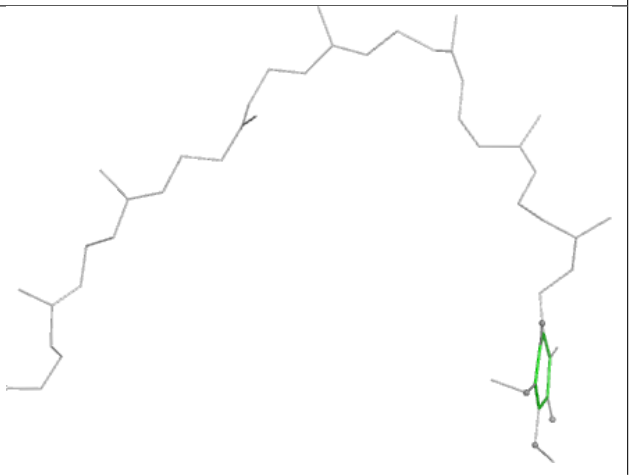
Bond lengths



Bond angles

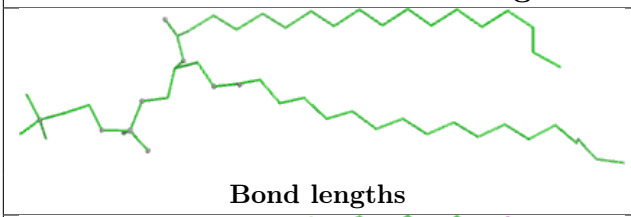


Torsions

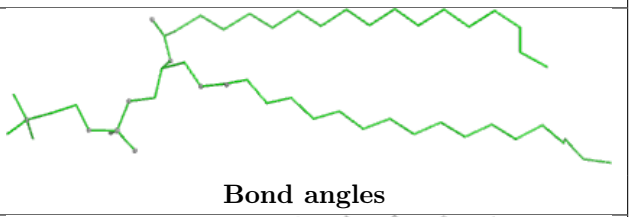


Rings

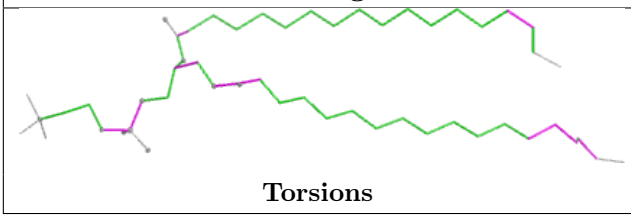
**Ligand PC1 DC 602**



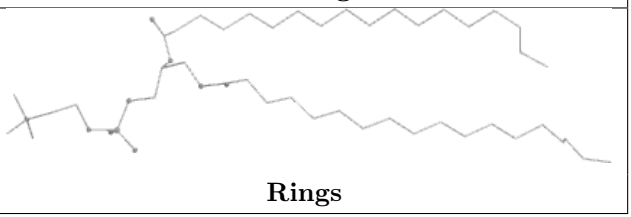
**Bond lengths**



**Bond angles**

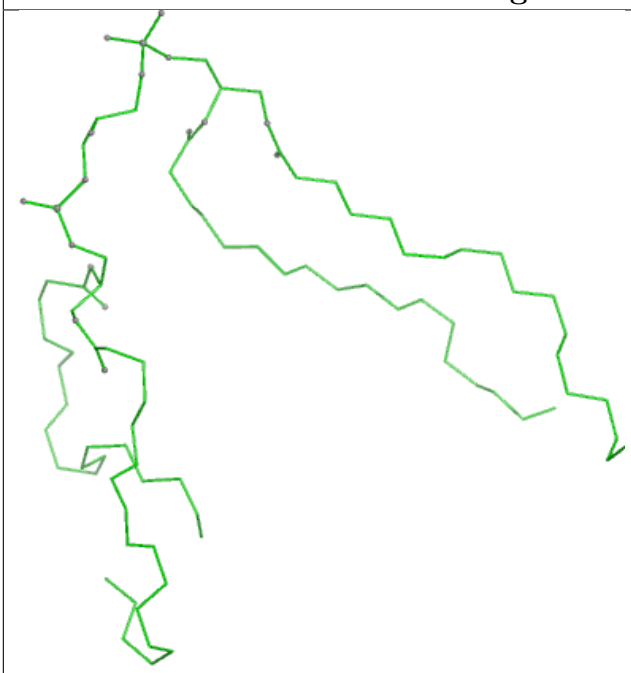


**Torsions**

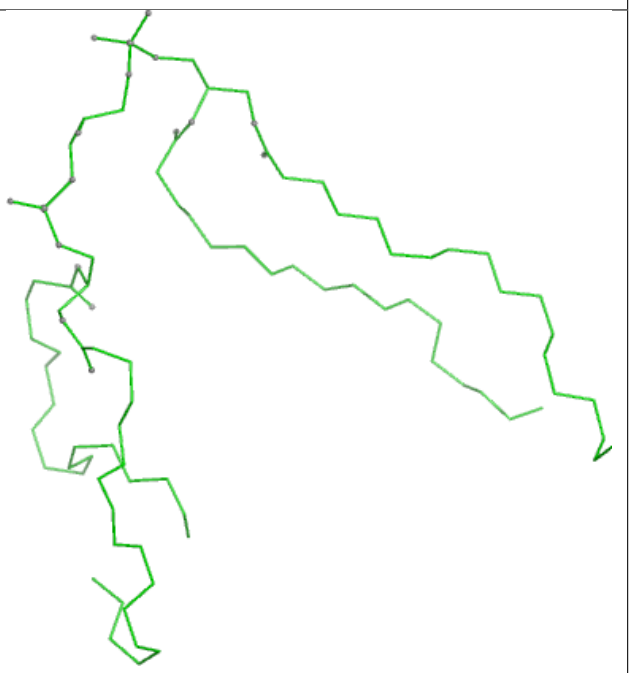


**Rings**

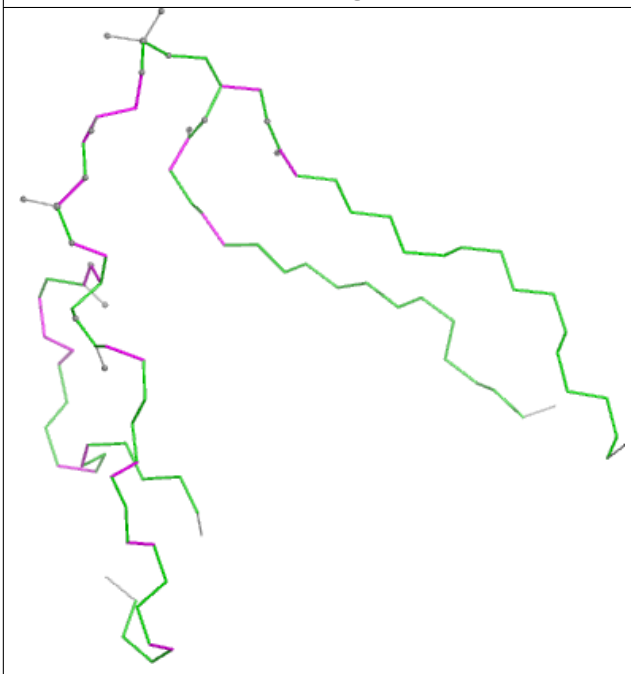
**Ligand CDL DR 403**



**Bond lengths**



**Bond angles**

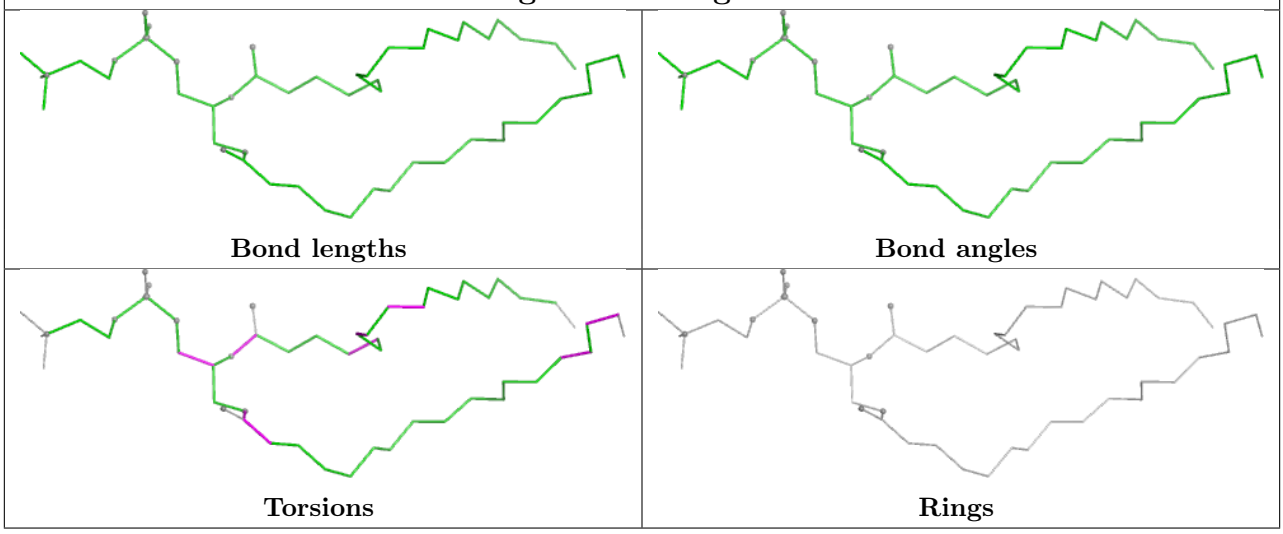


**Torsions**

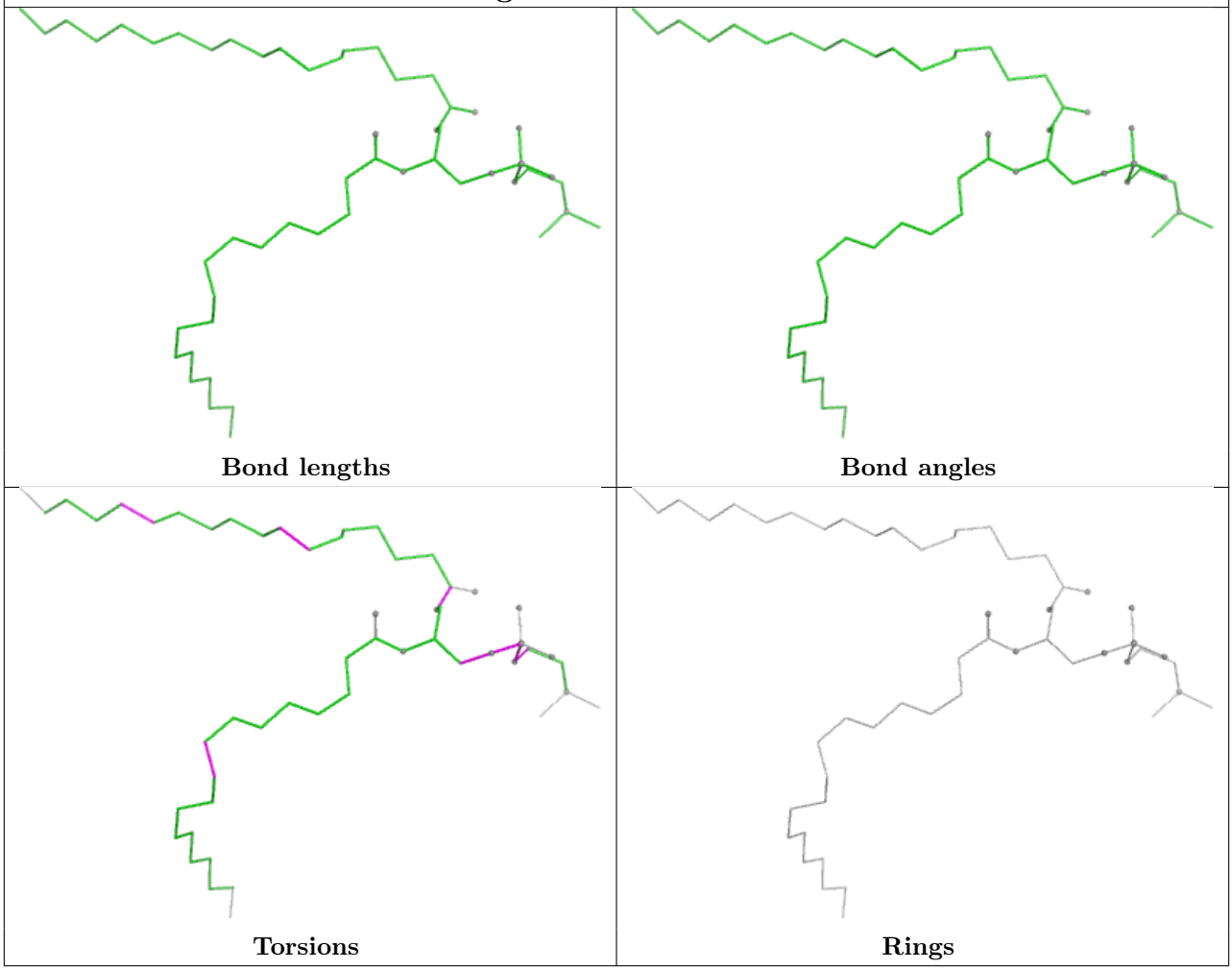


**Rings**

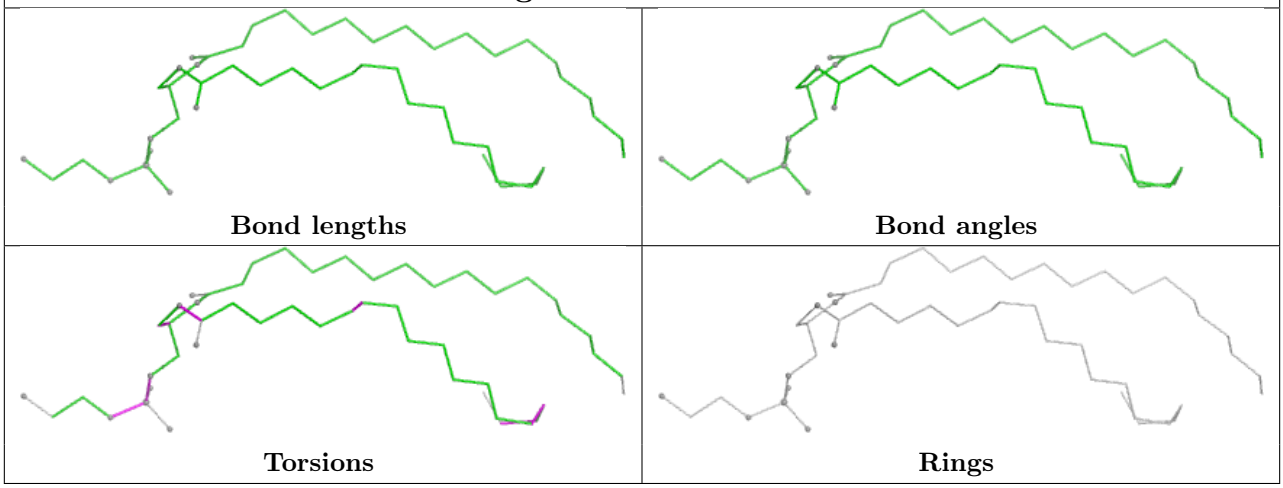
## Ligand PC1 Dg 203



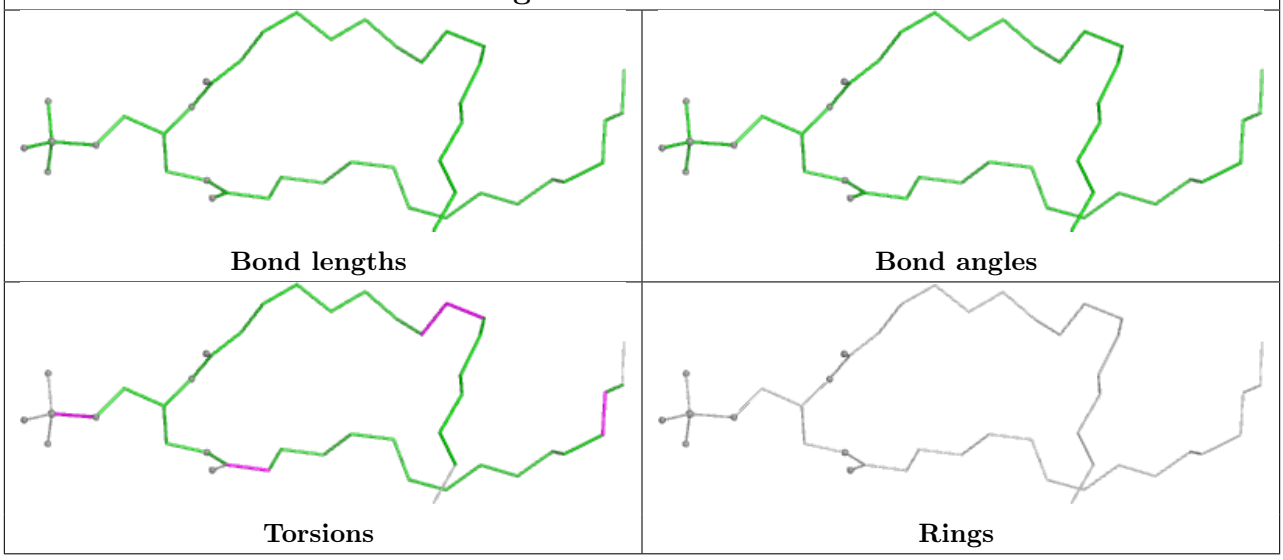

## Ligand PC1 EB 301



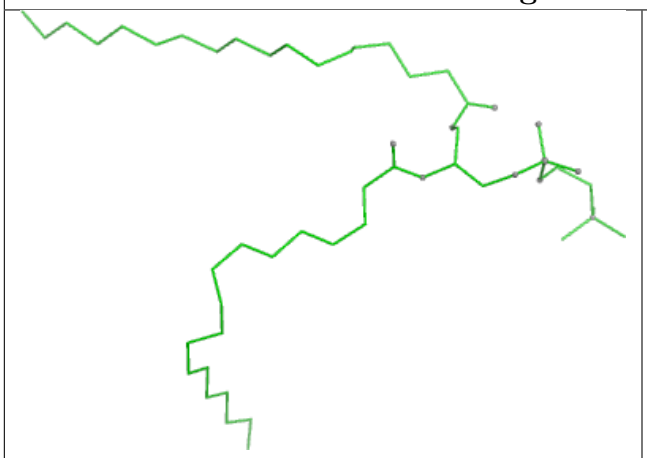
**Ligand 3PE DR 401**



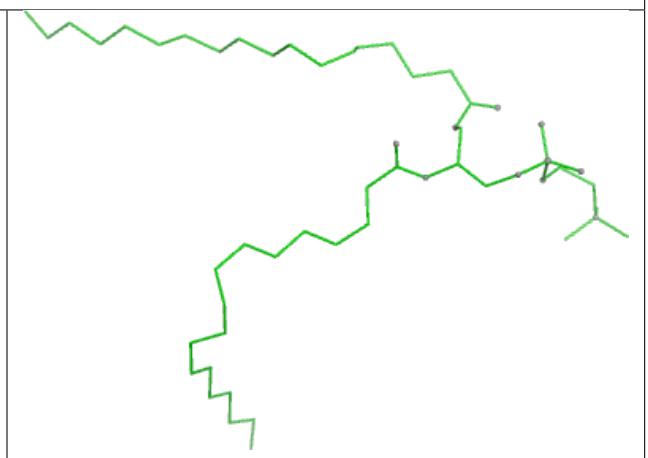

**Ligand LPP DA 711**



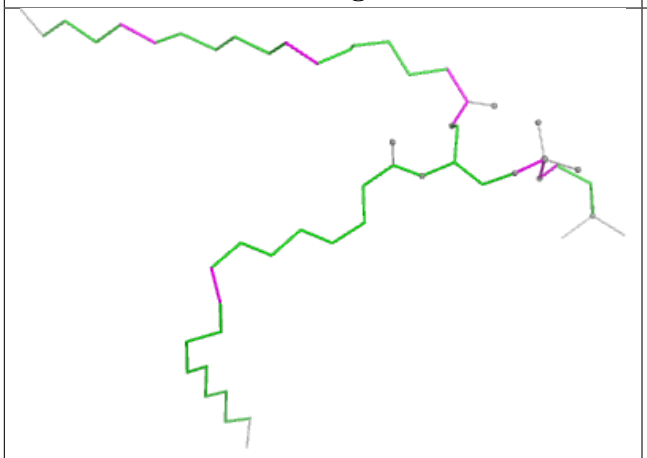
**Ligand PC1 Eb 301**



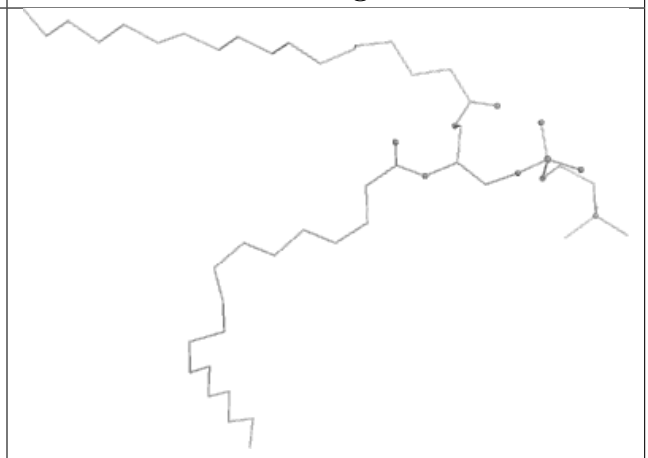
**Bond lengths**



**Bond angles**

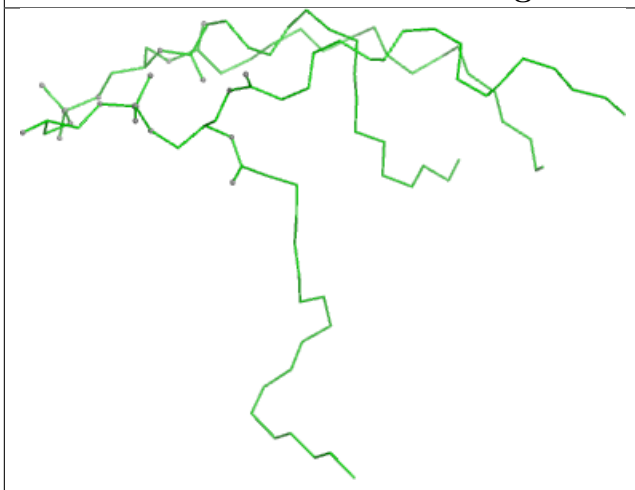


**Torsions**

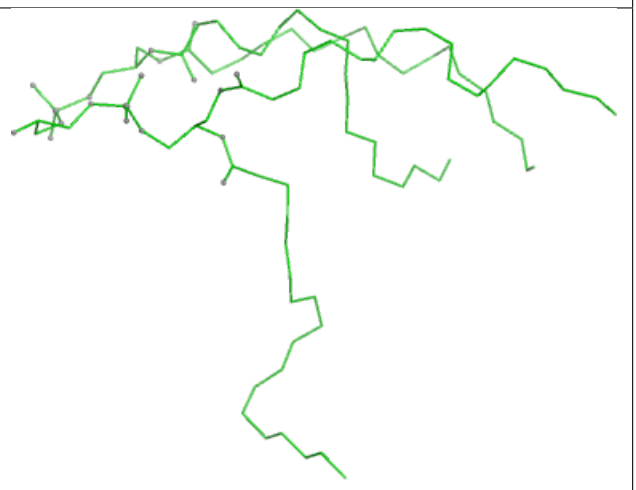


**Rings**

**Ligand CDL DS 402**



**Bond lengths**



**Bond angles**

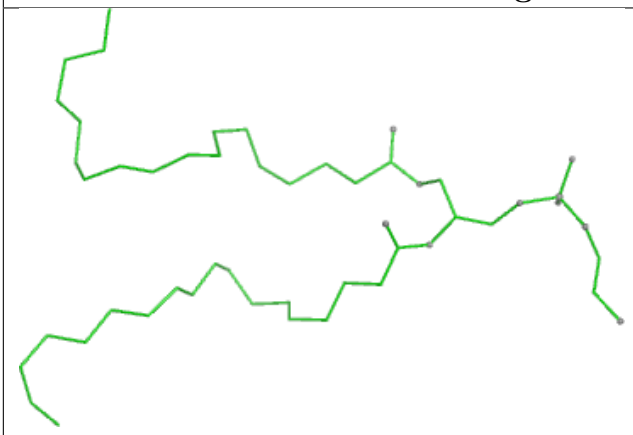


**Torsions**

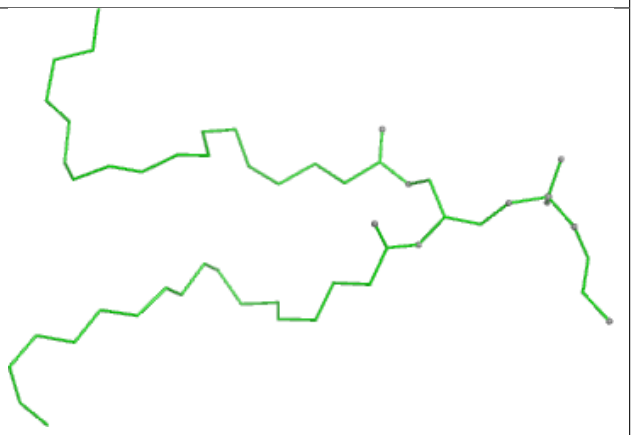


**Rings**

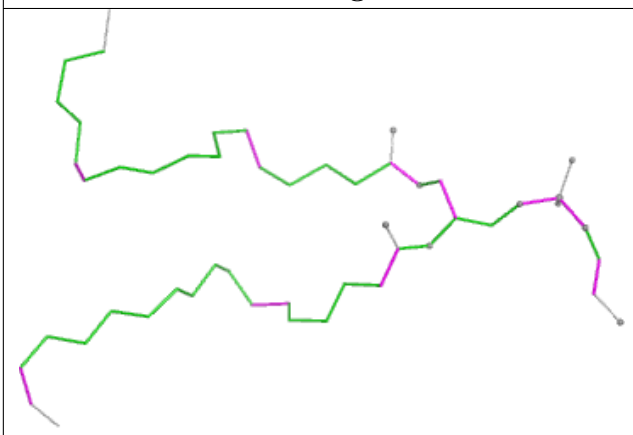
## Ligand 3PE DC 607



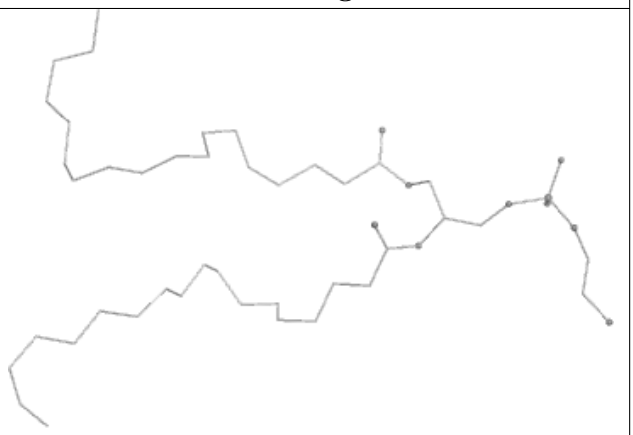
Bond lengths



Bond angles

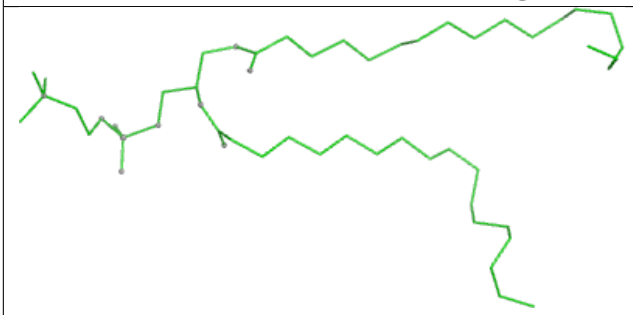


Torsions

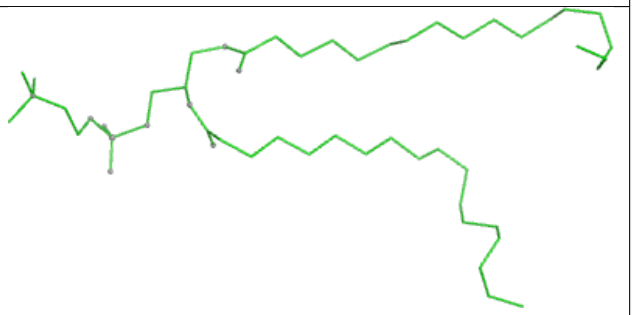


Rings

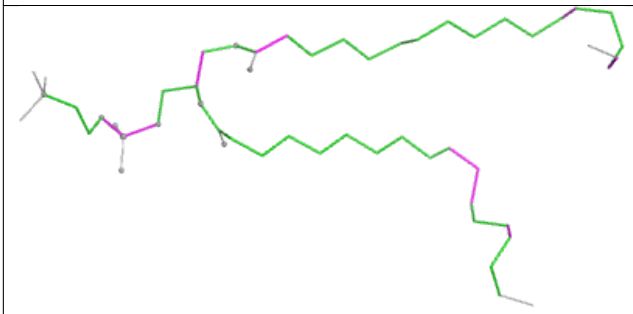
## Ligand PC1 DV 405



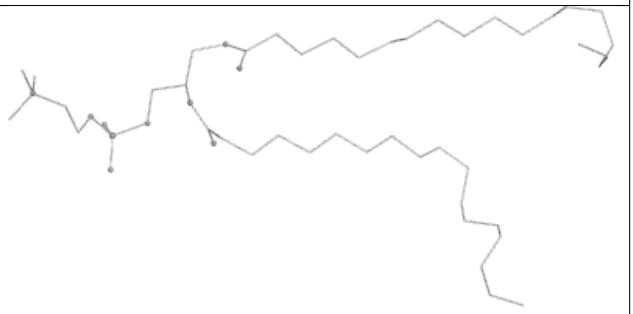
Bond lengths



Bond angles

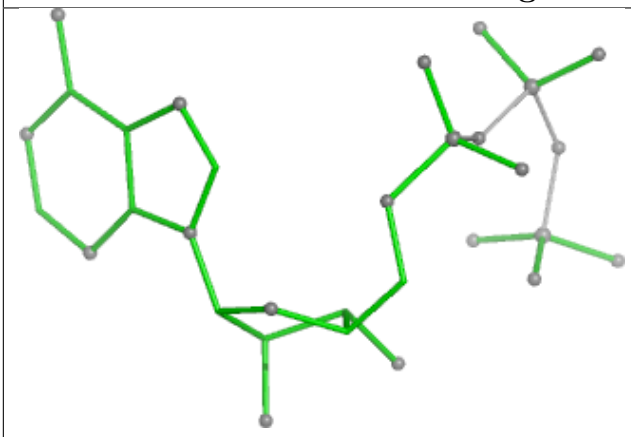


Torsions

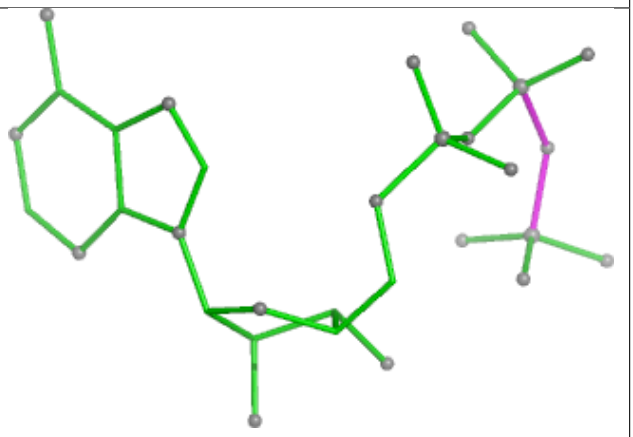


Rings

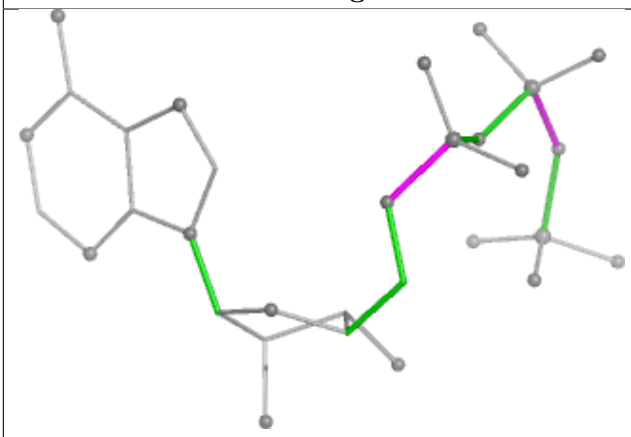
**Ligand ATP Er 201**



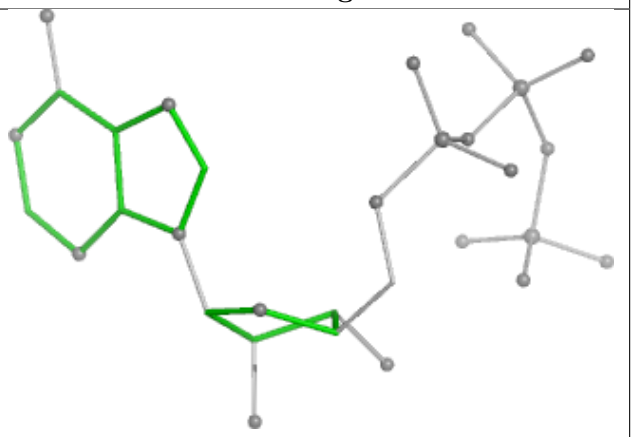
**Bond lengths**



**Bond angles**

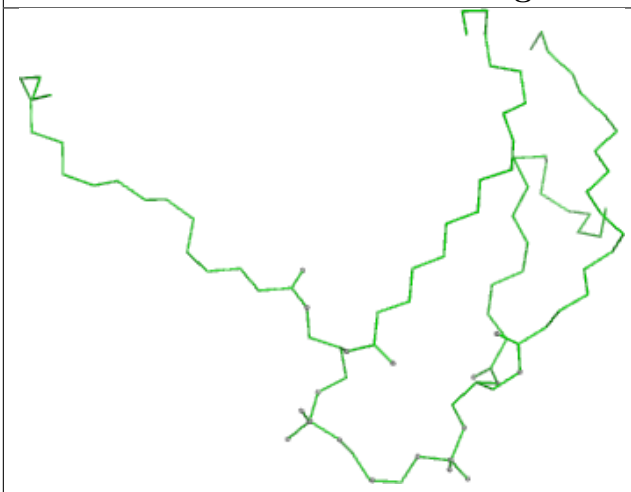


**Torsions**

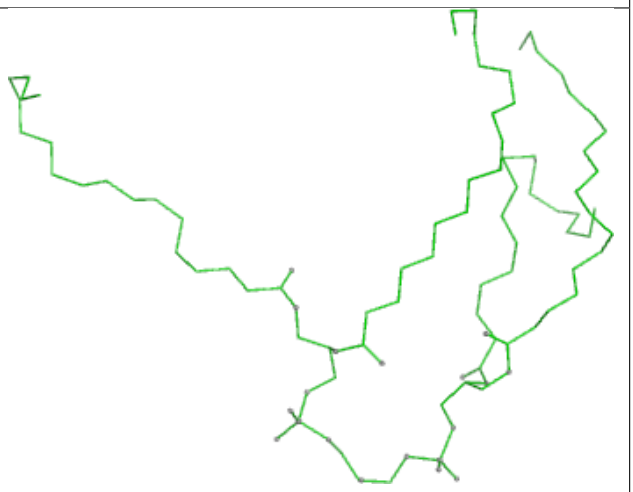


**Rings**

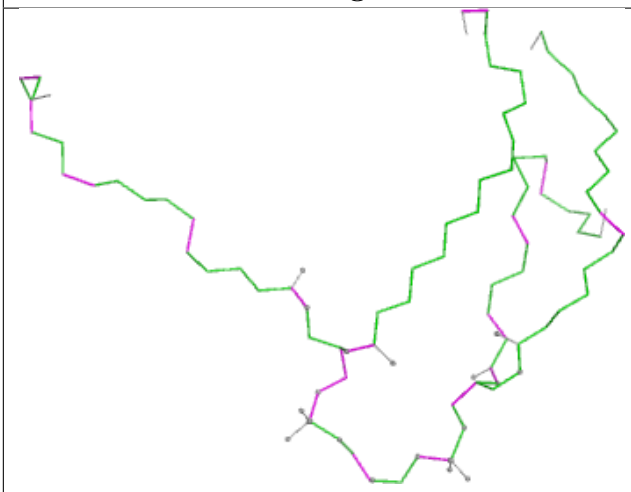
**Ligand CDL EL 902**



**Bond lengths**



**Bond angles**

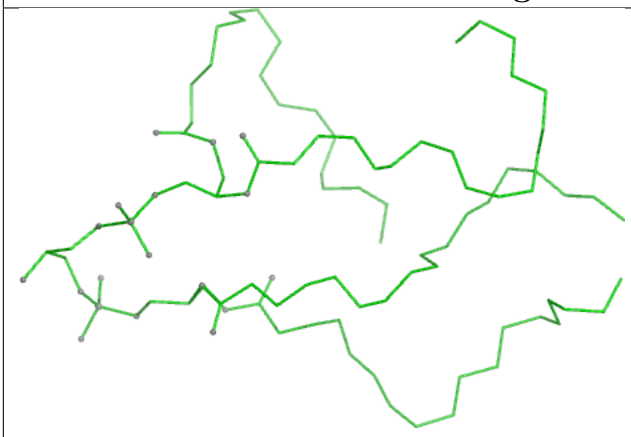


**Torsions**

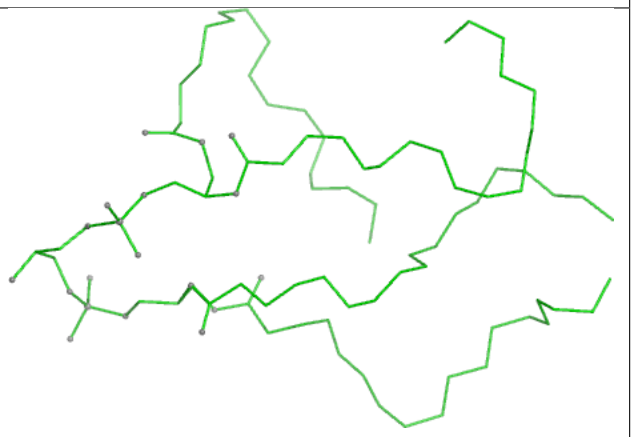


**Rings**

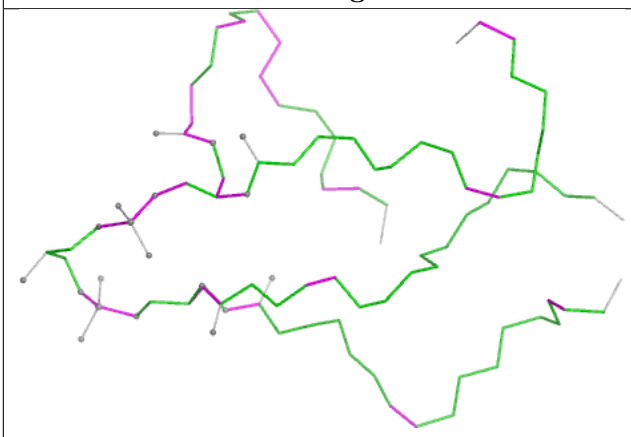
**Ligand CDL Dn 501**



**Bond lengths**



**Bond angles**

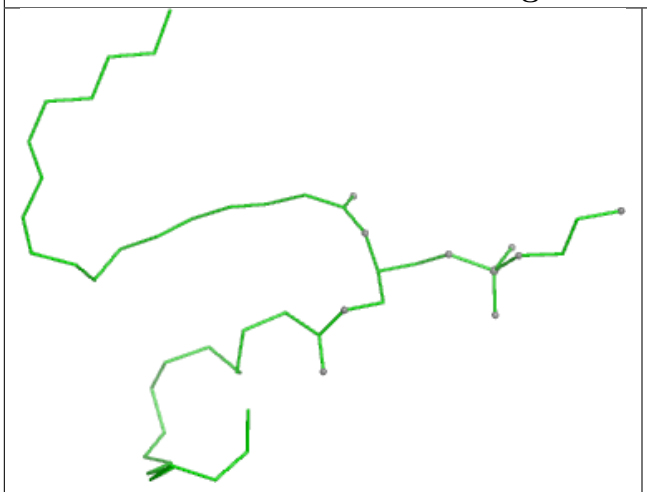


**Torsions**

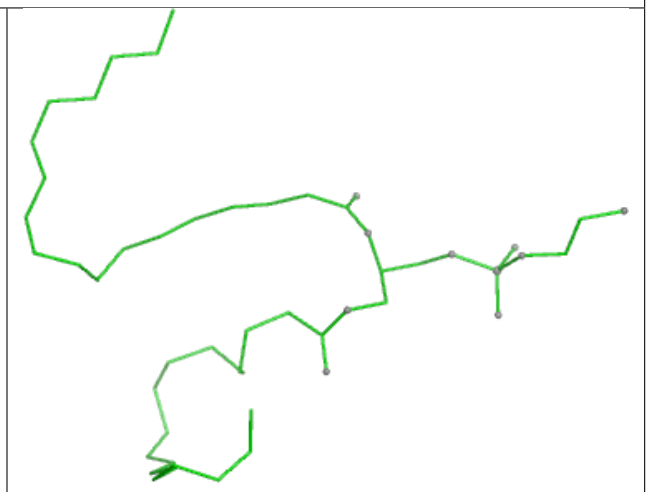


**Rings**

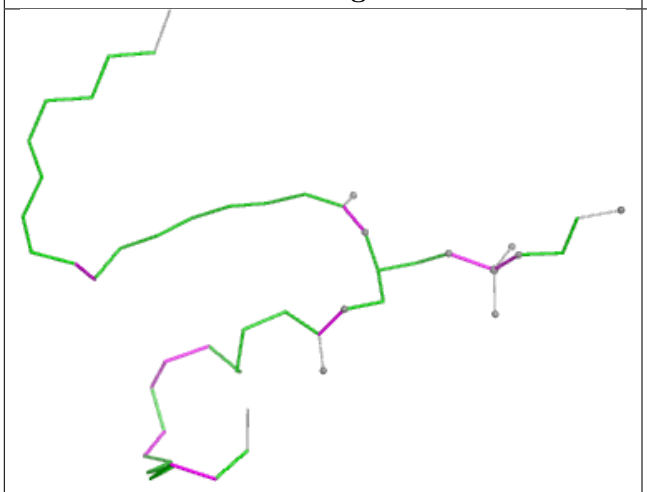
**Ligand 3PE Ds 407**



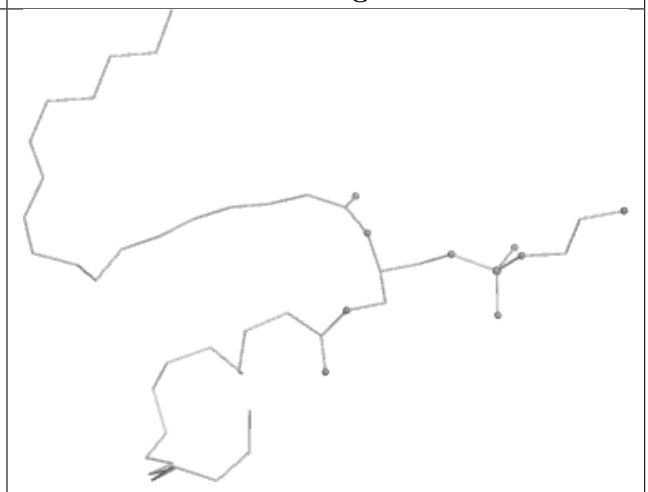
**Bond lengths**



**Bond angles**

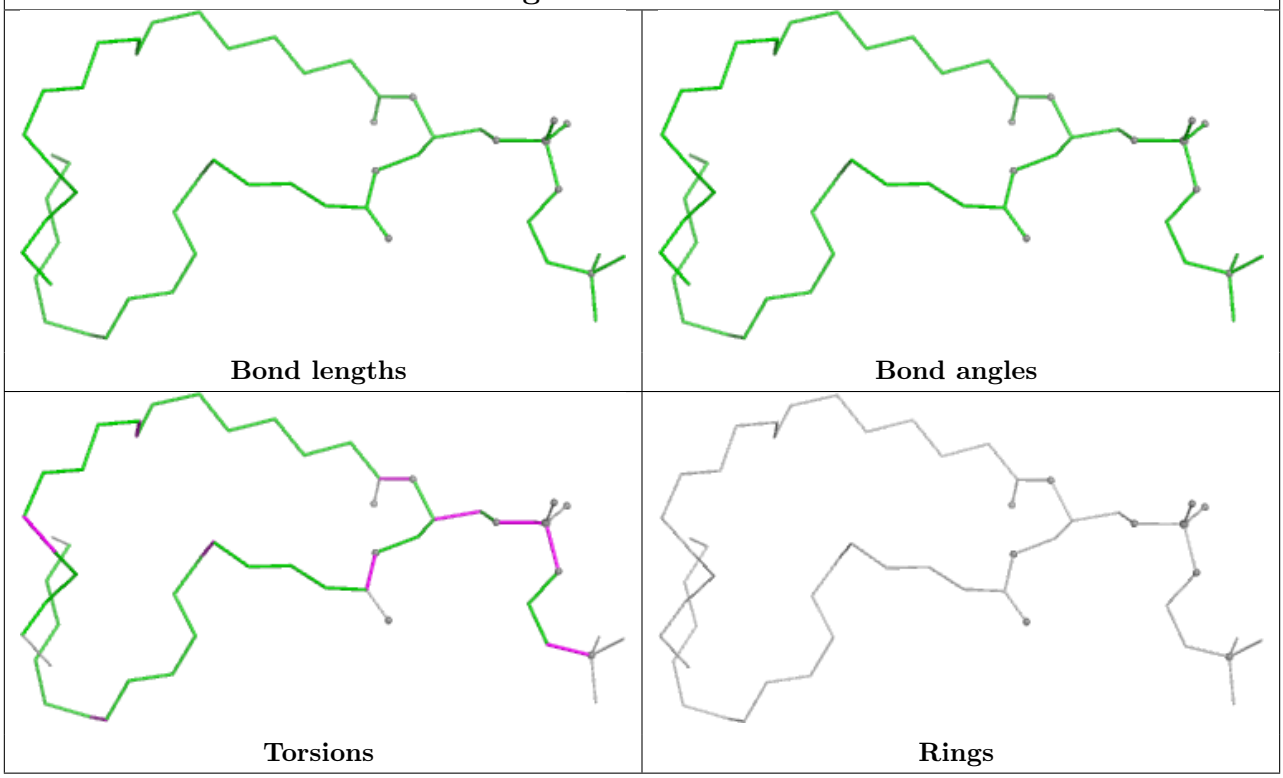


**Torsions**

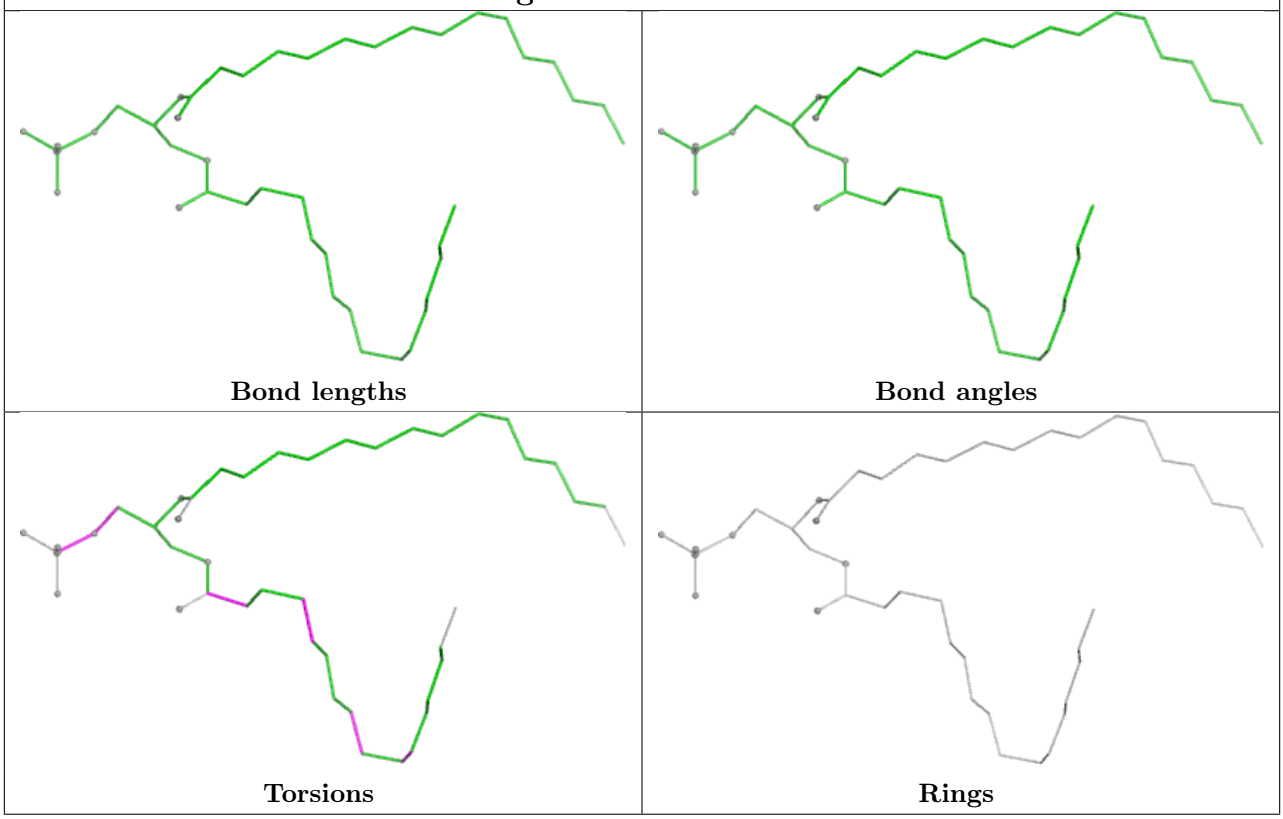


**Rings**

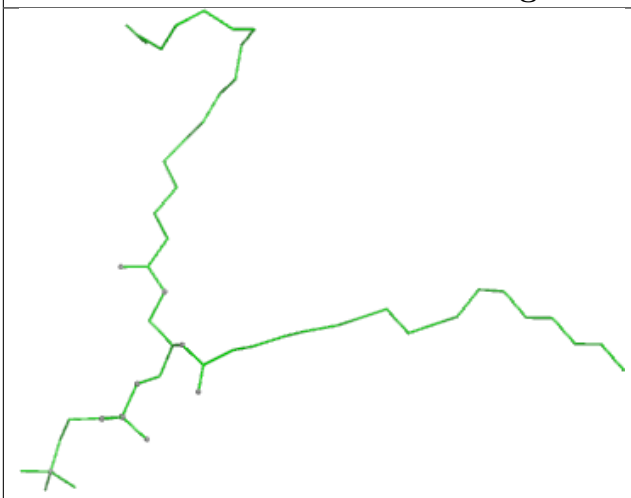
## Ligand PC1 Di 702



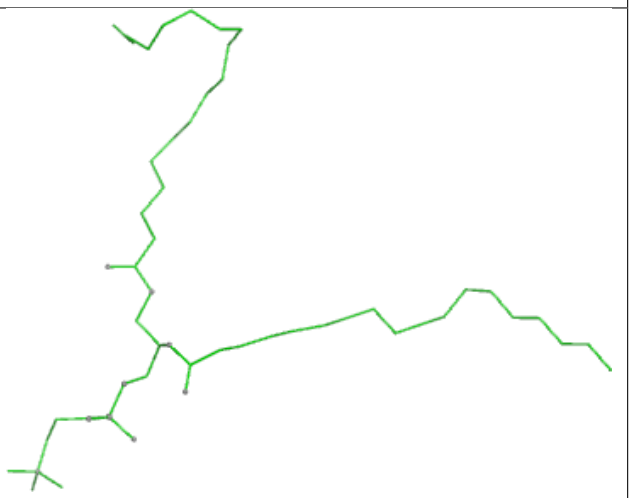

## Ligand LPP Dn 504



**Ligand PC1 Eo 205**



**Bond lengths**



**Bond angles**

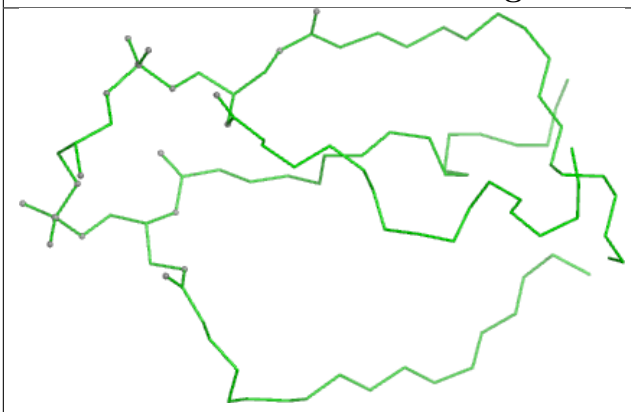


**Torsions**



**Rings**

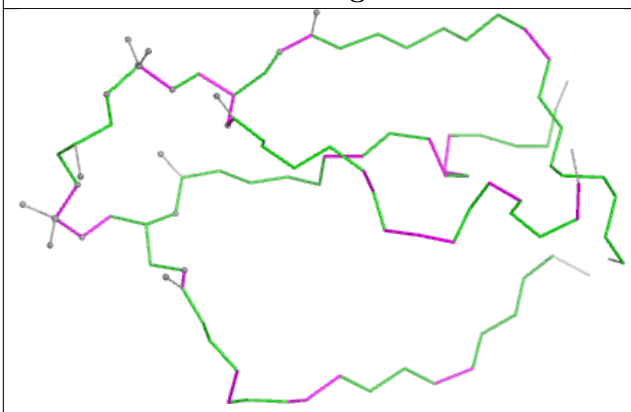
**Ligand CDL Dx 1203**



**Bond lengths**



**Bond angles**

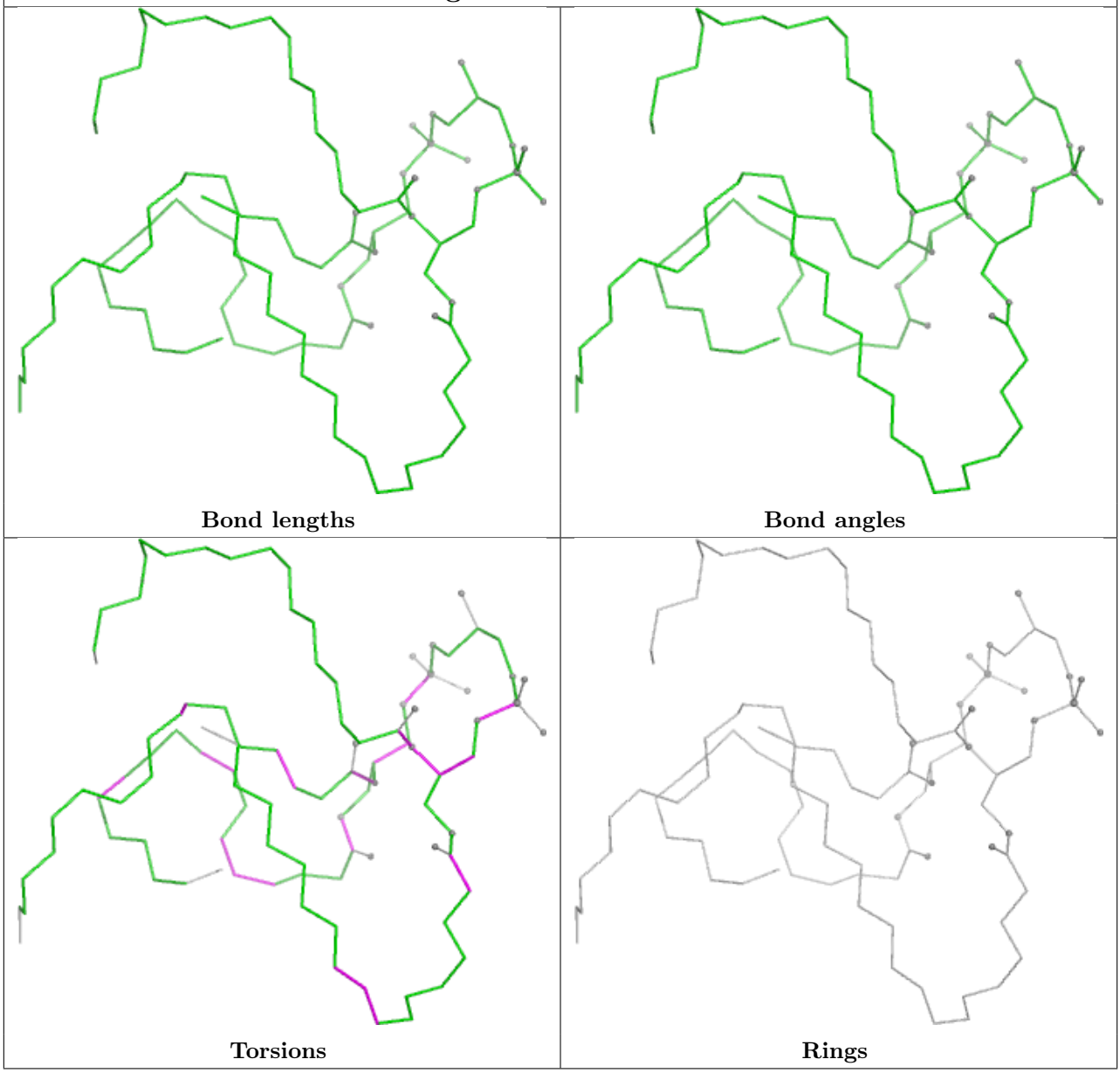


**Torsions**

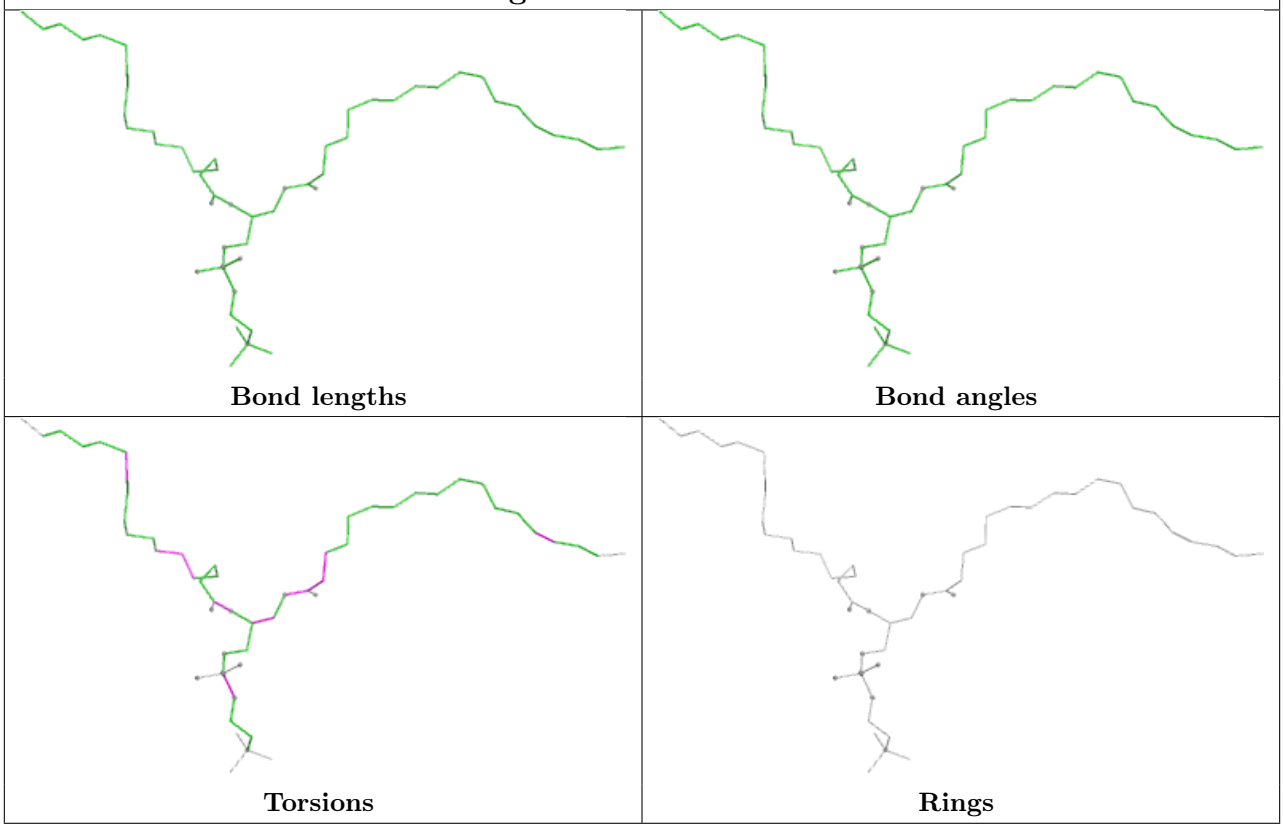


**Rings**

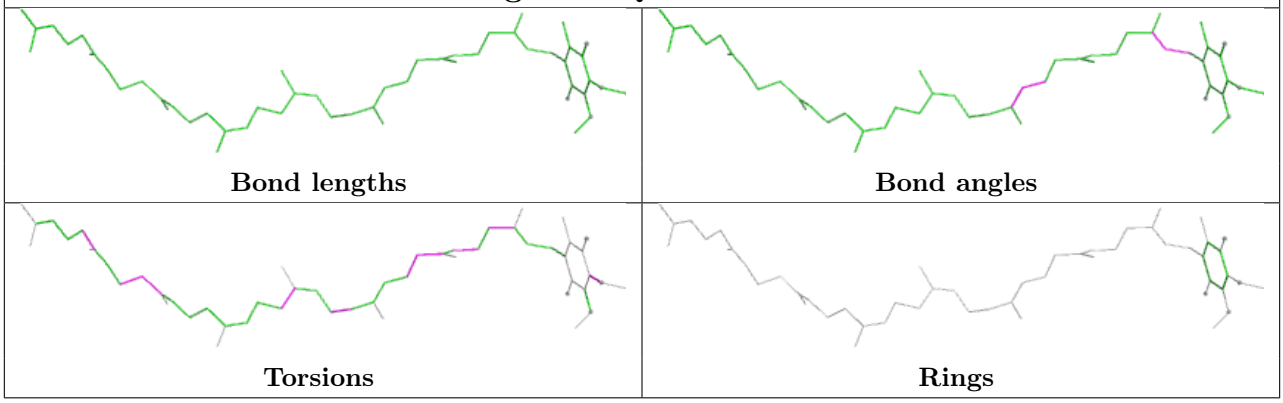
**Ligand CDL DO 501**



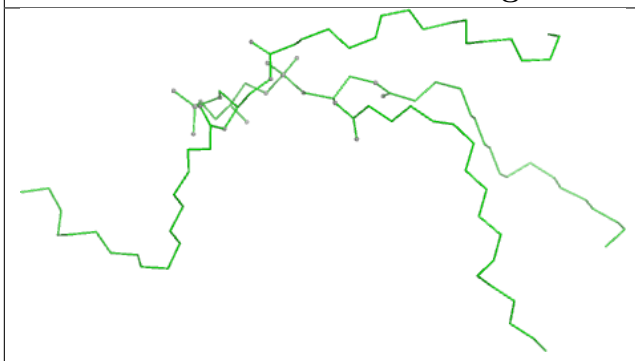
**Ligand PC1 Dx 1204**




**Ligand UQ8 EN 1204**



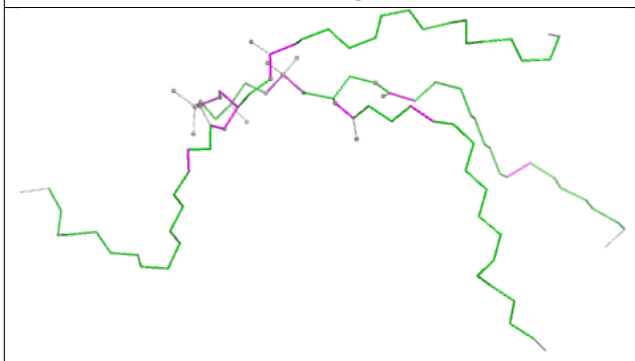
**Ligand CDL DQ 1502**



**Bond lengths**



**Bond angles**

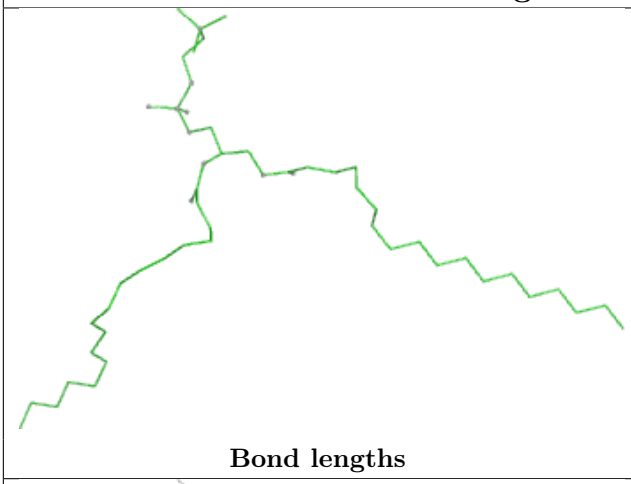


**Torsions**

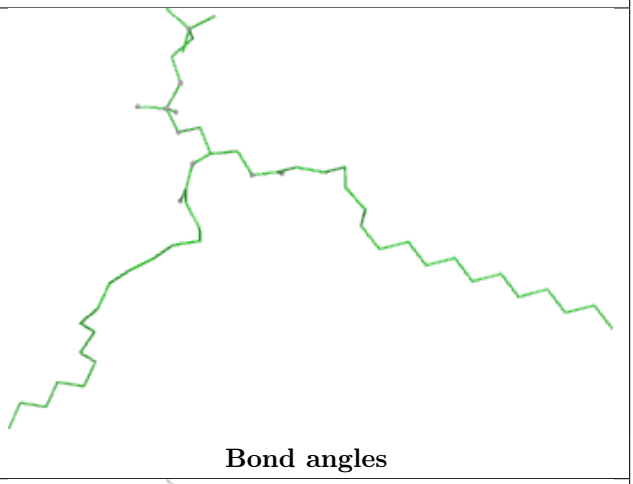


**Rings**

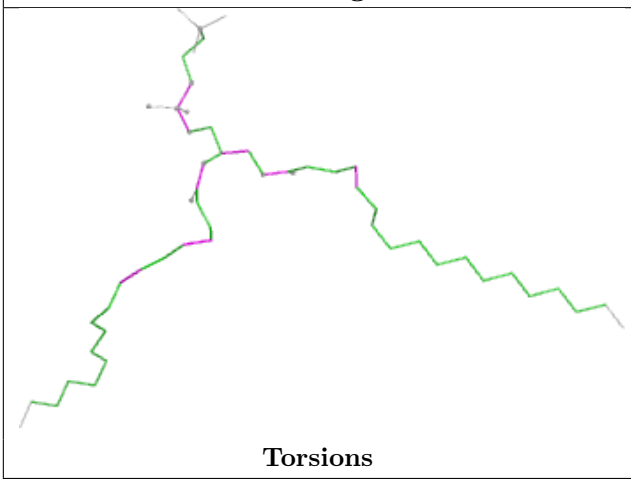
## Ligand PC1 DX 302



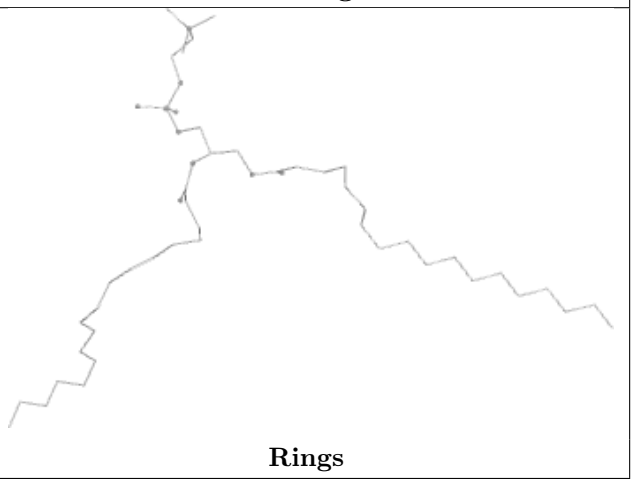
Bond lengths



Bond angles

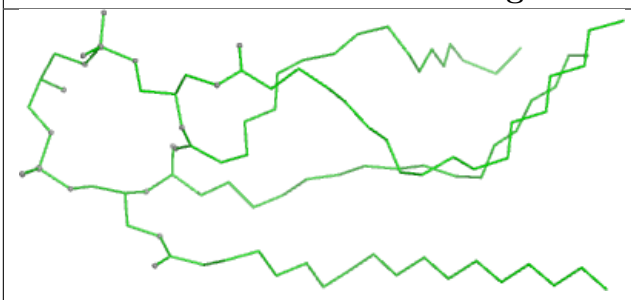


Torsions

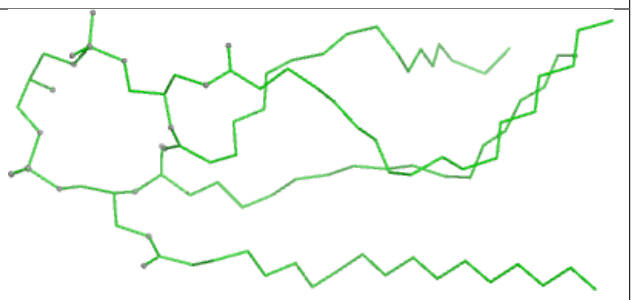


Rings

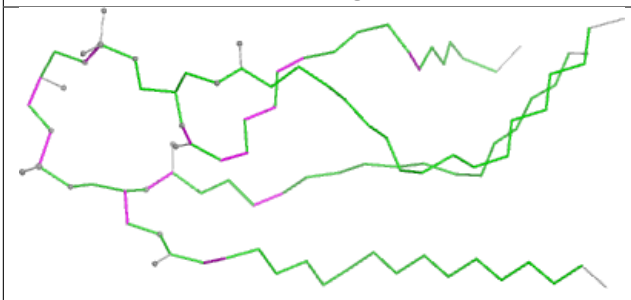
## Ligand CDL DM 502



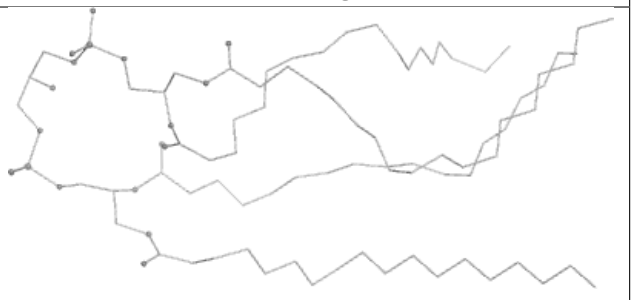
Bond lengths



Bond angles

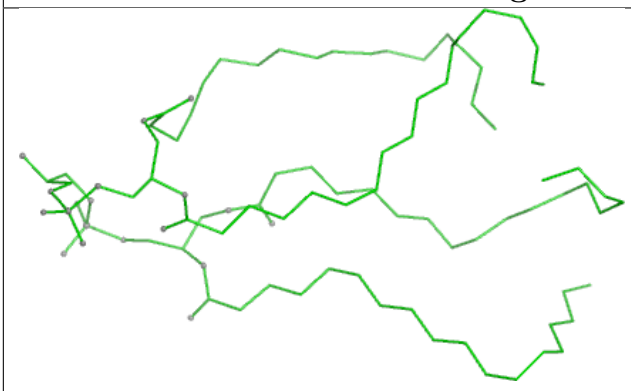


Torsions

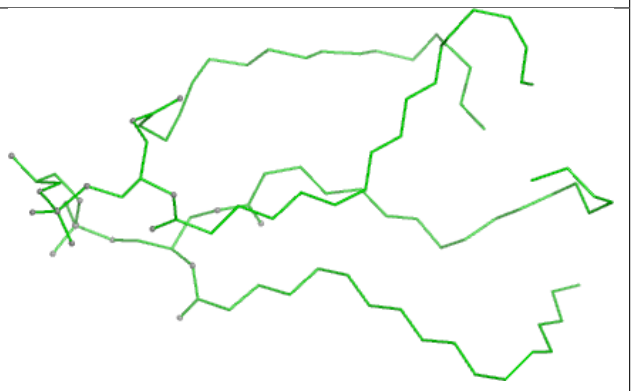


Rings

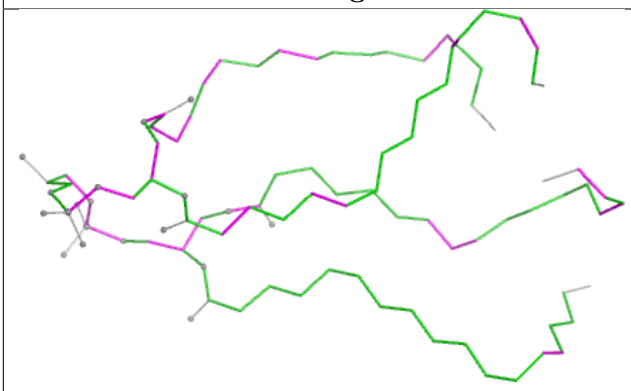
**Ligand CDL DR 402**



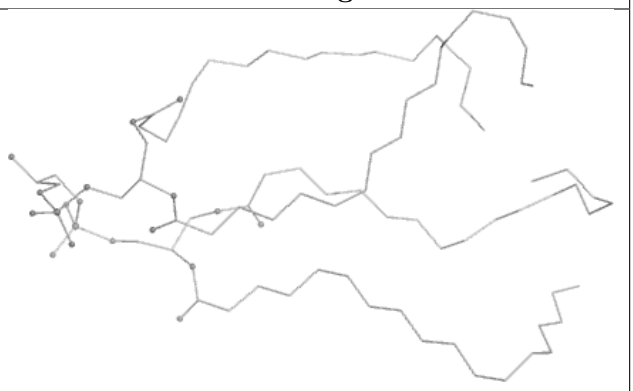
**Bond lengths**



**Bond angles**

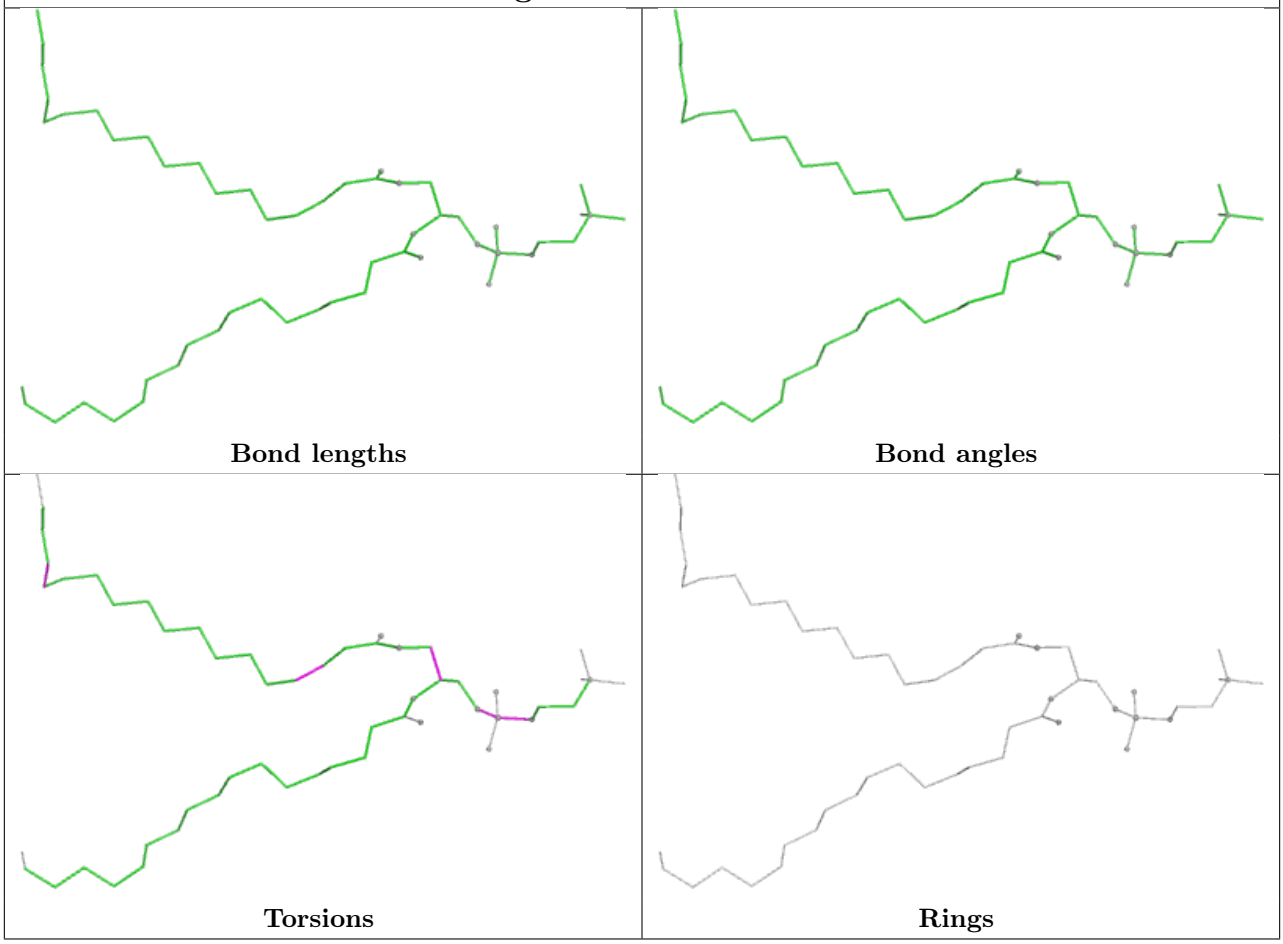


**Torsions**

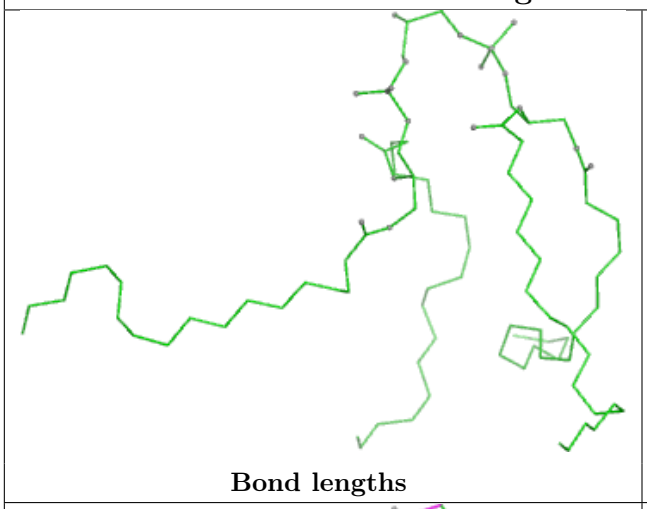


**Rings**

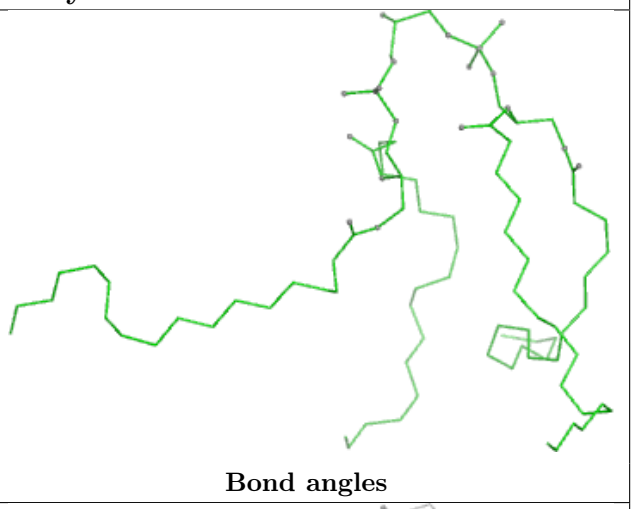
**Ligand PC1 DV 407**



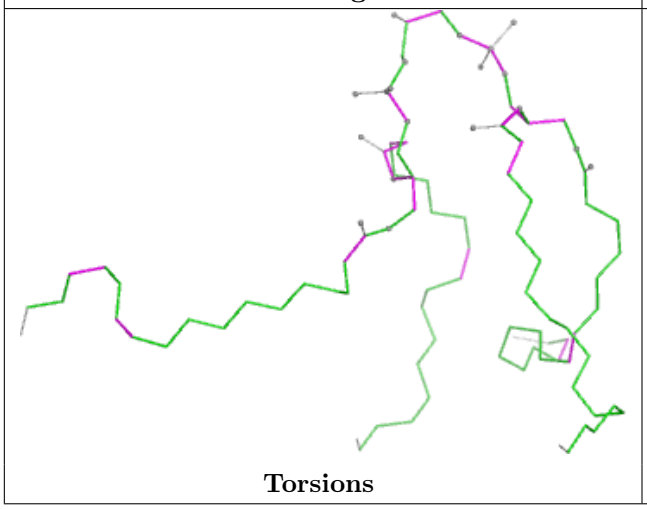
**Ligand CDL Dy 301**



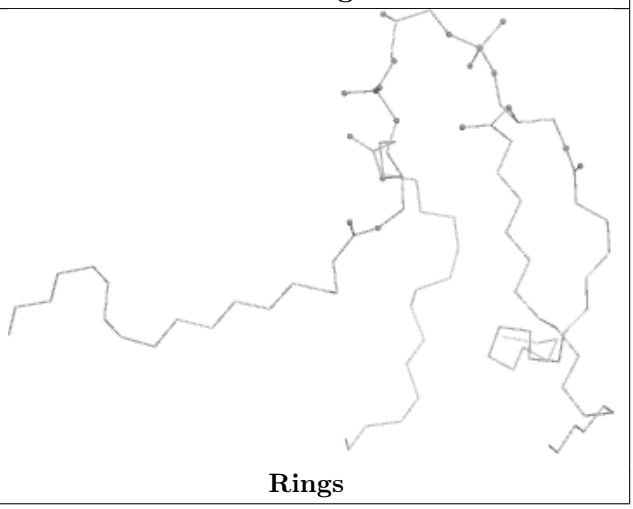
**Bond lengths**



**Bond angles**

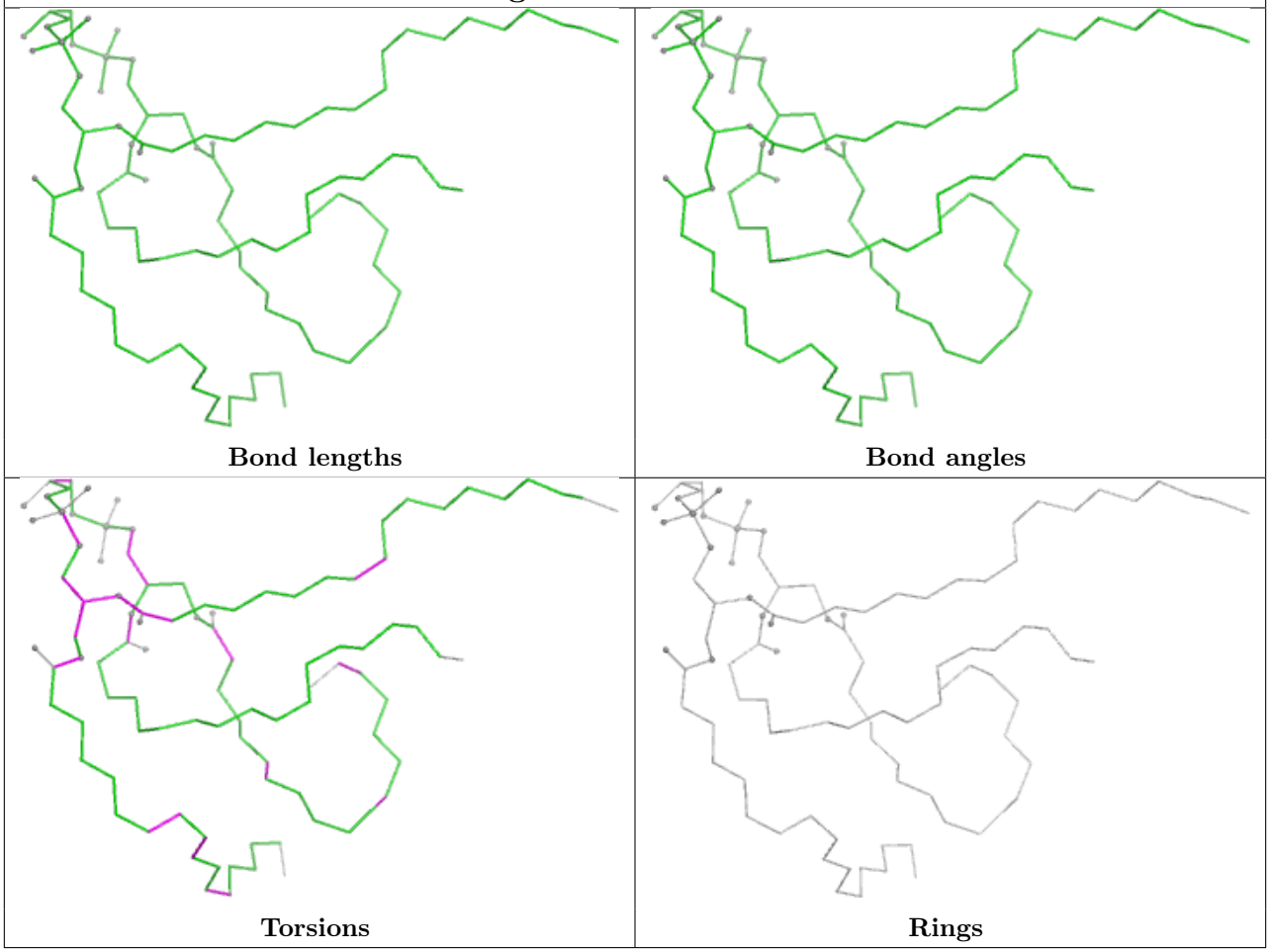


**Torsions**

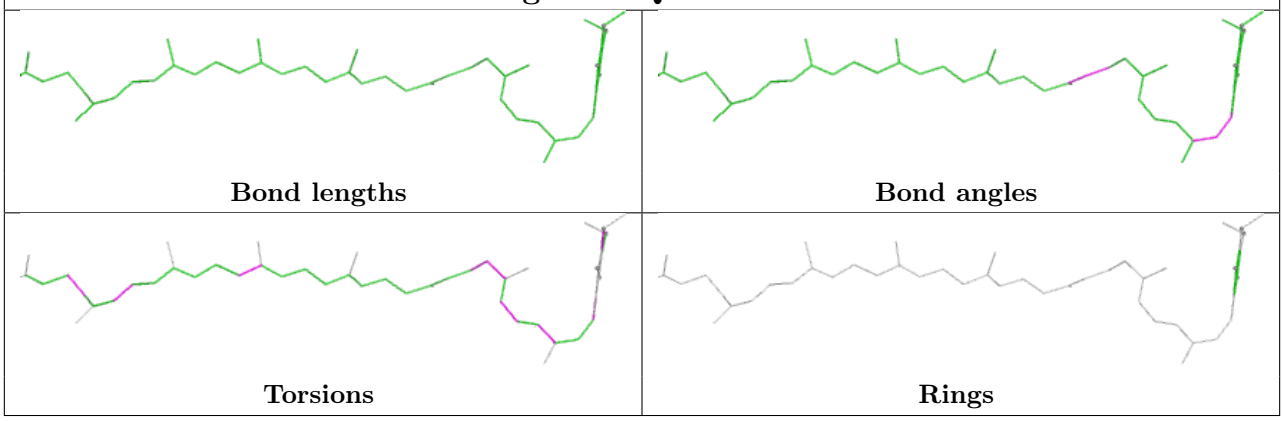


**Rings**

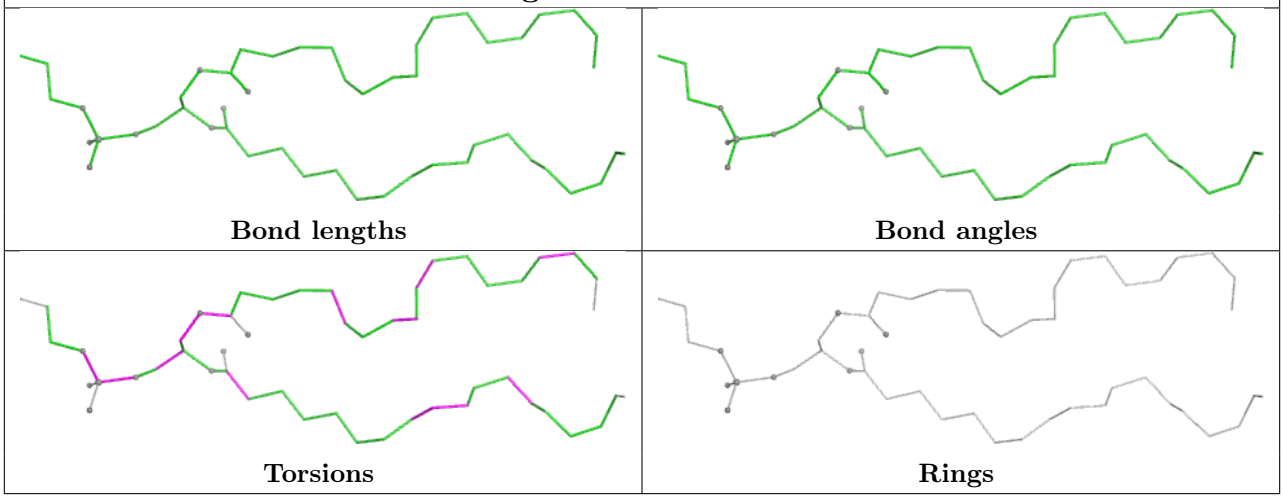
**Ligand CDL Dd 706**



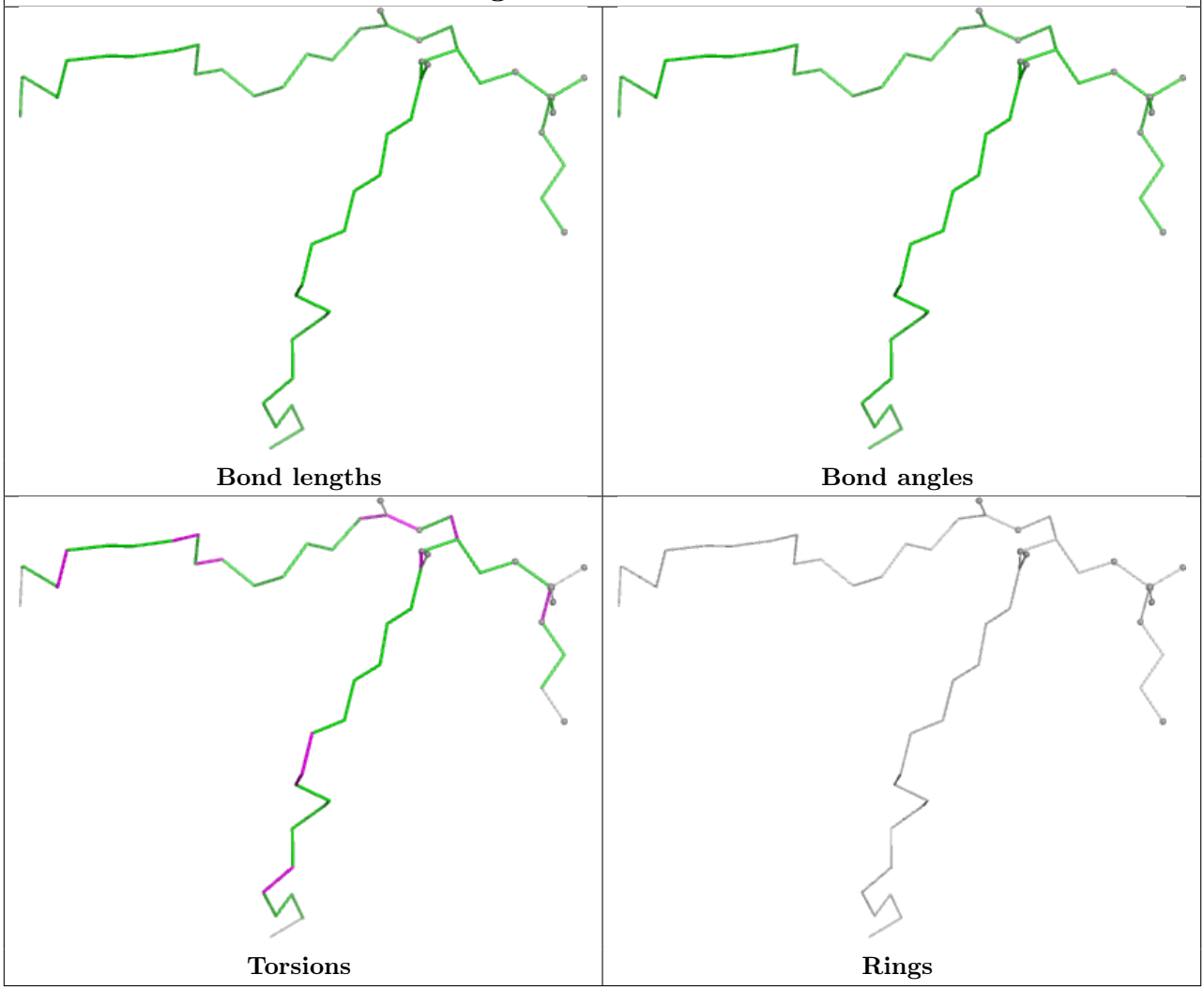

**Ligand UQ8 El 906**



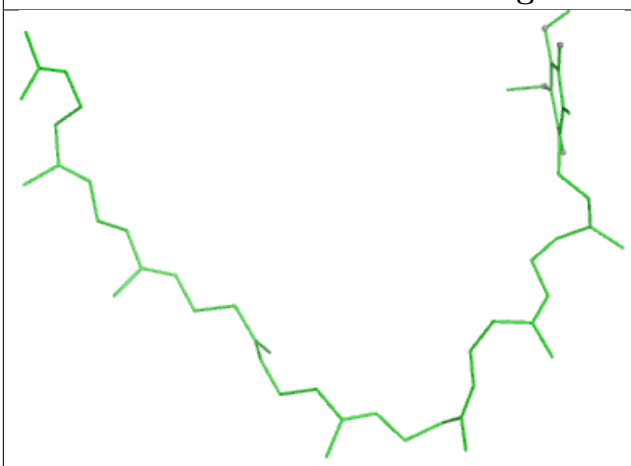
**Ligand 3PE Ds 403**



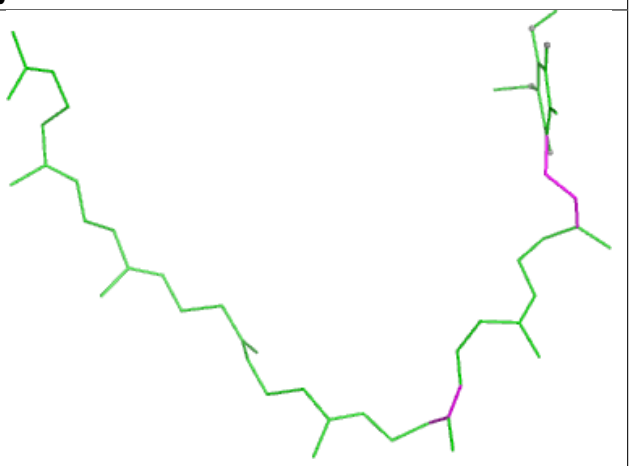

**Ligand 3PE Eo 202**



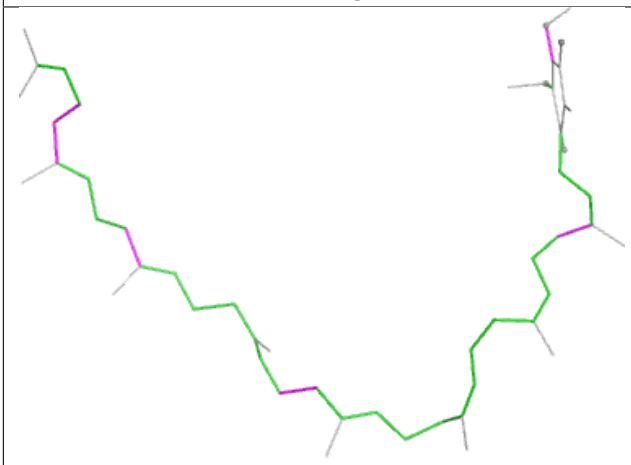
**Ligand UQ8 Ed 202**



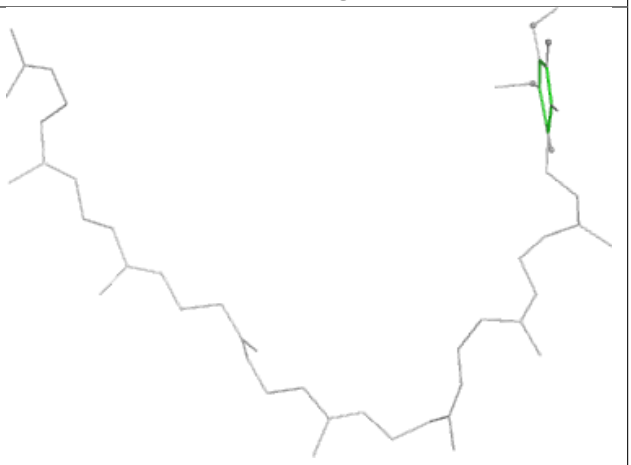
**Bond lengths**



**Bond angles**



**Torsions**



**Rings**

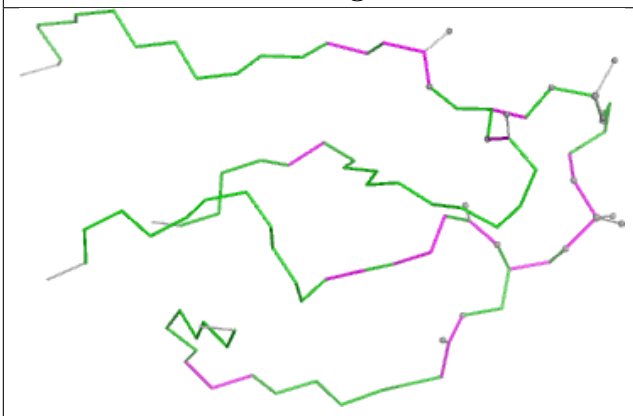
## Ligand CDL Du 401



Bond lengths



Bond angles

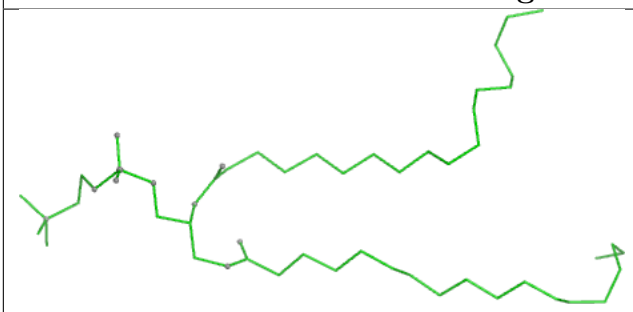


Torsions

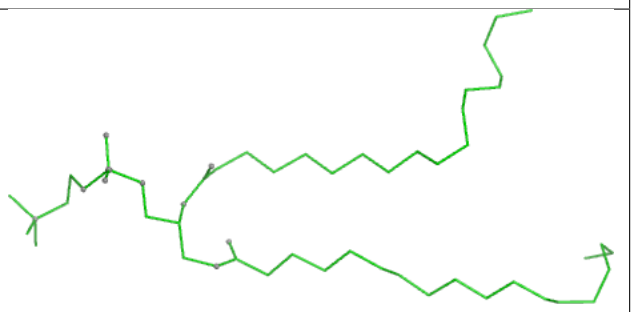


Rings

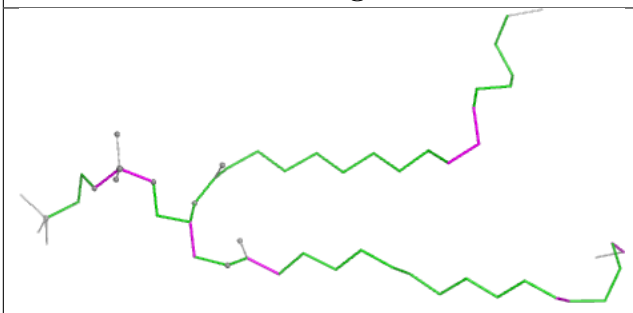
## Ligand PC1 Dv 405



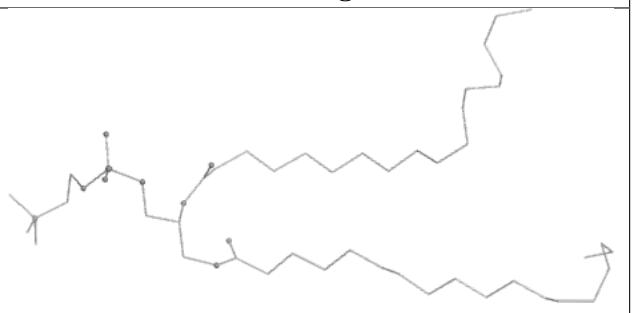
Bond lengths



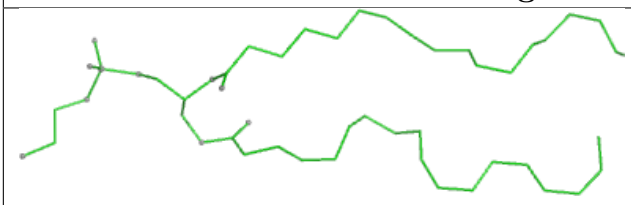
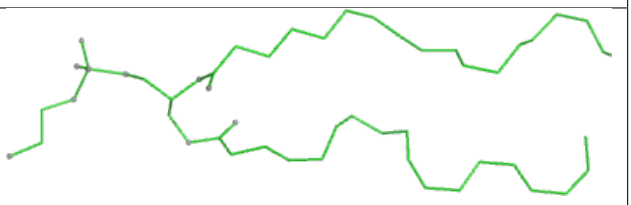
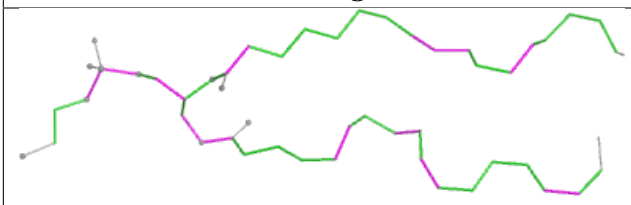
Bond angles

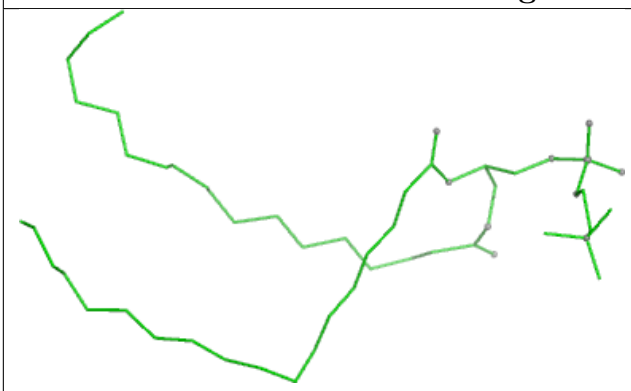
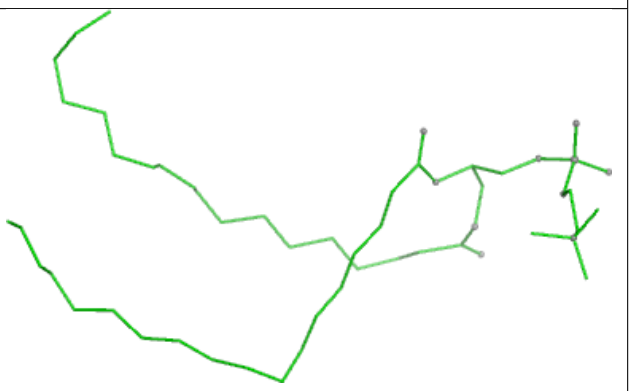
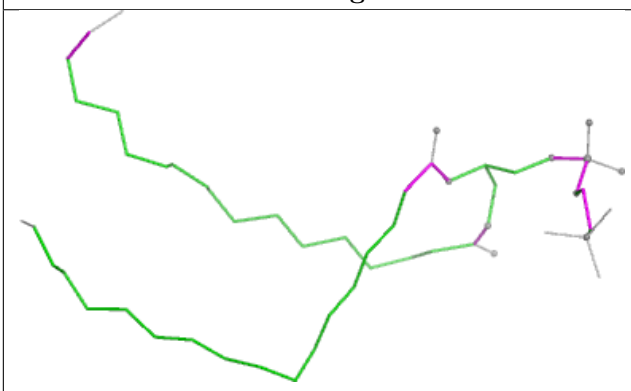
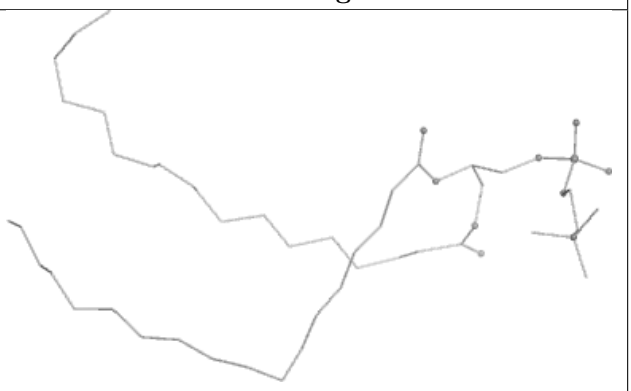


Torsions

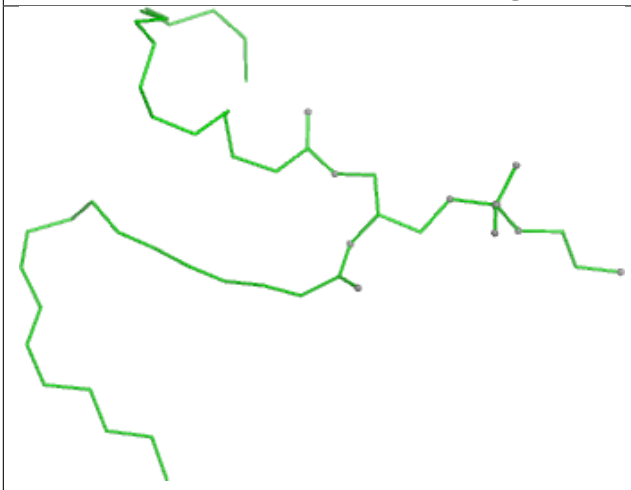


Rings

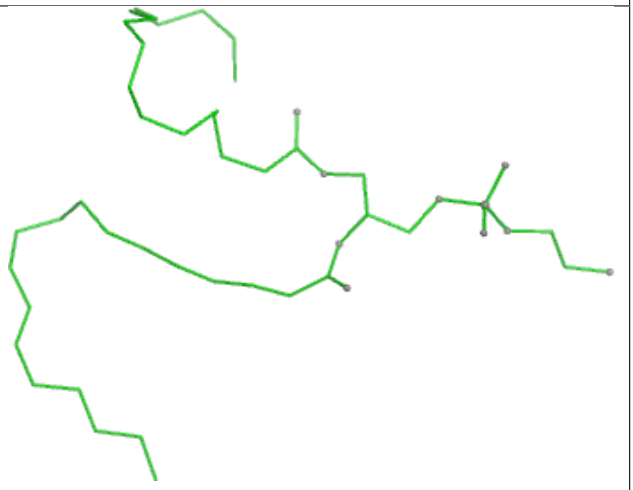
| Ligand 3PE DS 403 | |
|---|---|
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

| Ligand PC1 Dc 604 | |
|---|---|
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

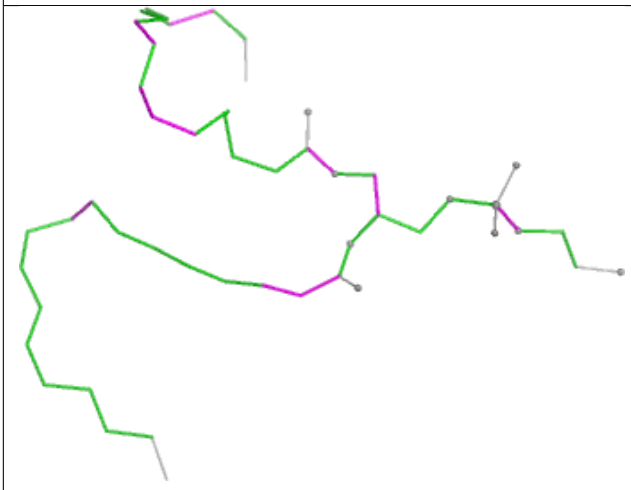
**Ligand 3PE EN 1203**



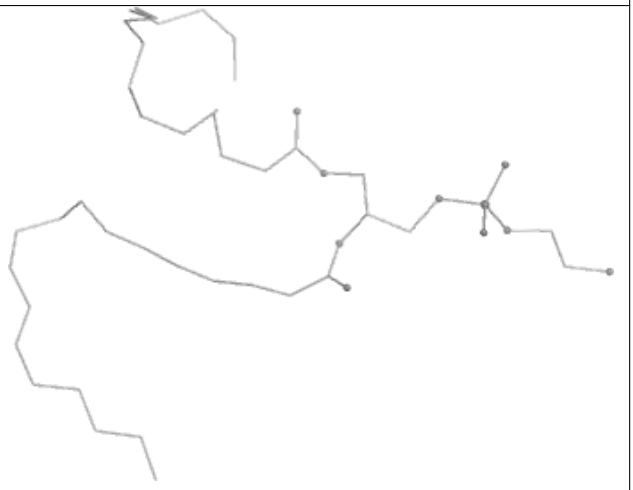
**Bond lengths**



**Bond angles**



**Torsions**



**Rings**

**Ligand CDL Dj 404**



**Bond lengths**



**Bond angles**

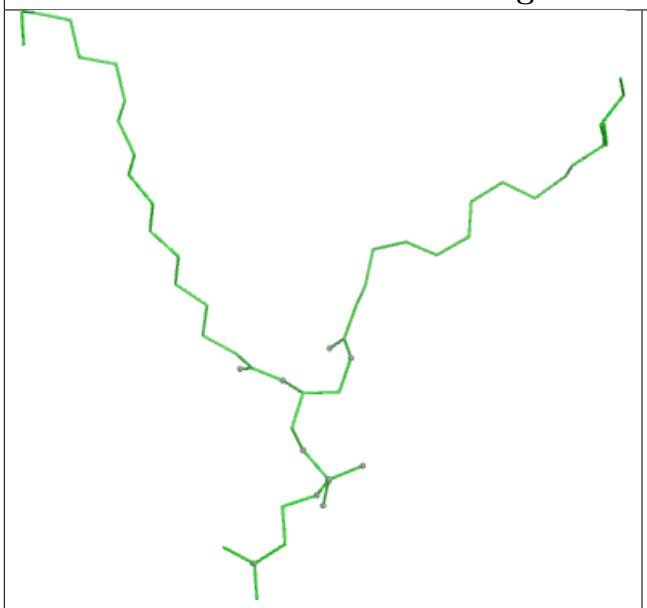


**Torsions**

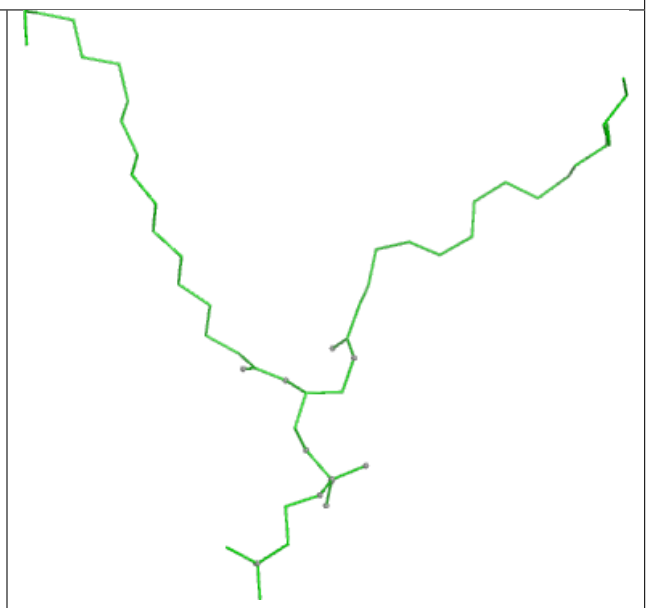


**Rings**

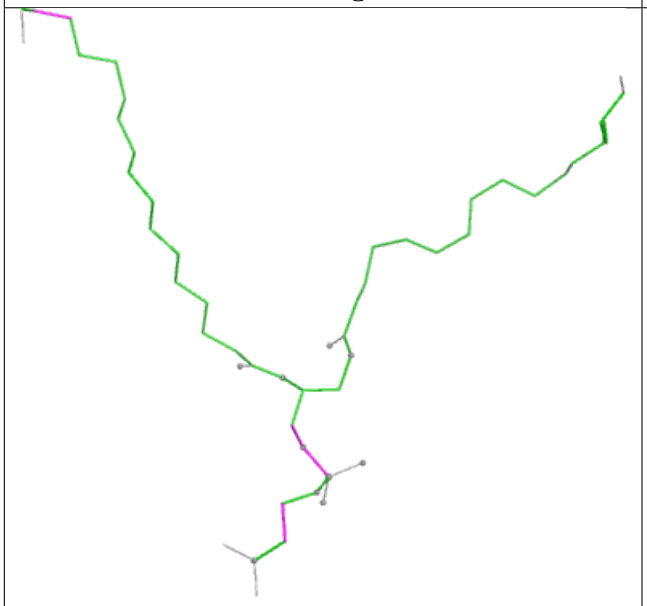
**Ligand PC1 EB 303**



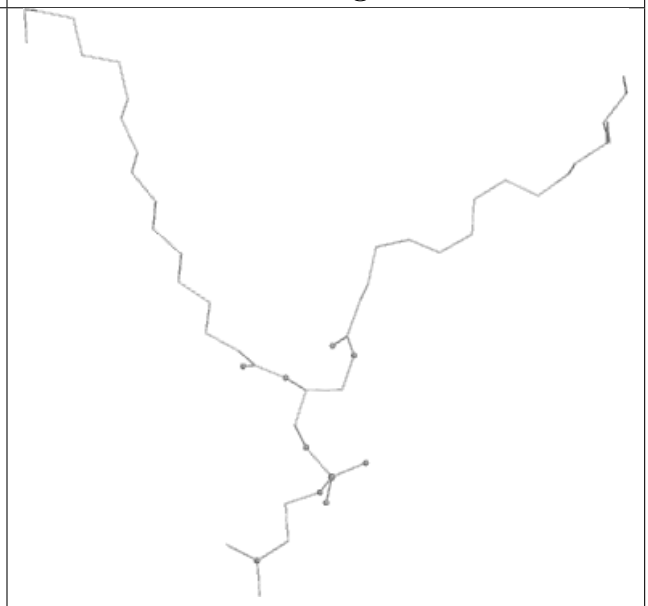
**Bond lengths**



**Bond angles**

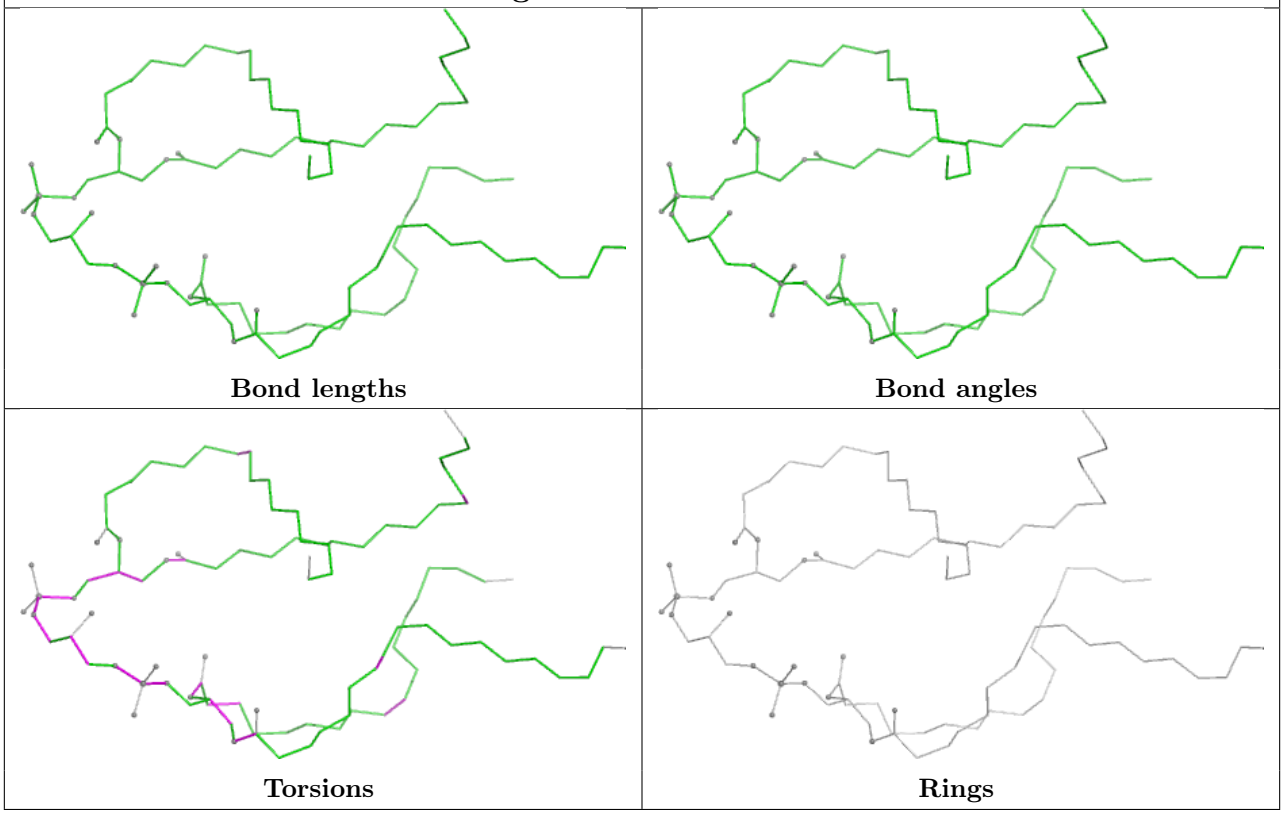


**Torsions**

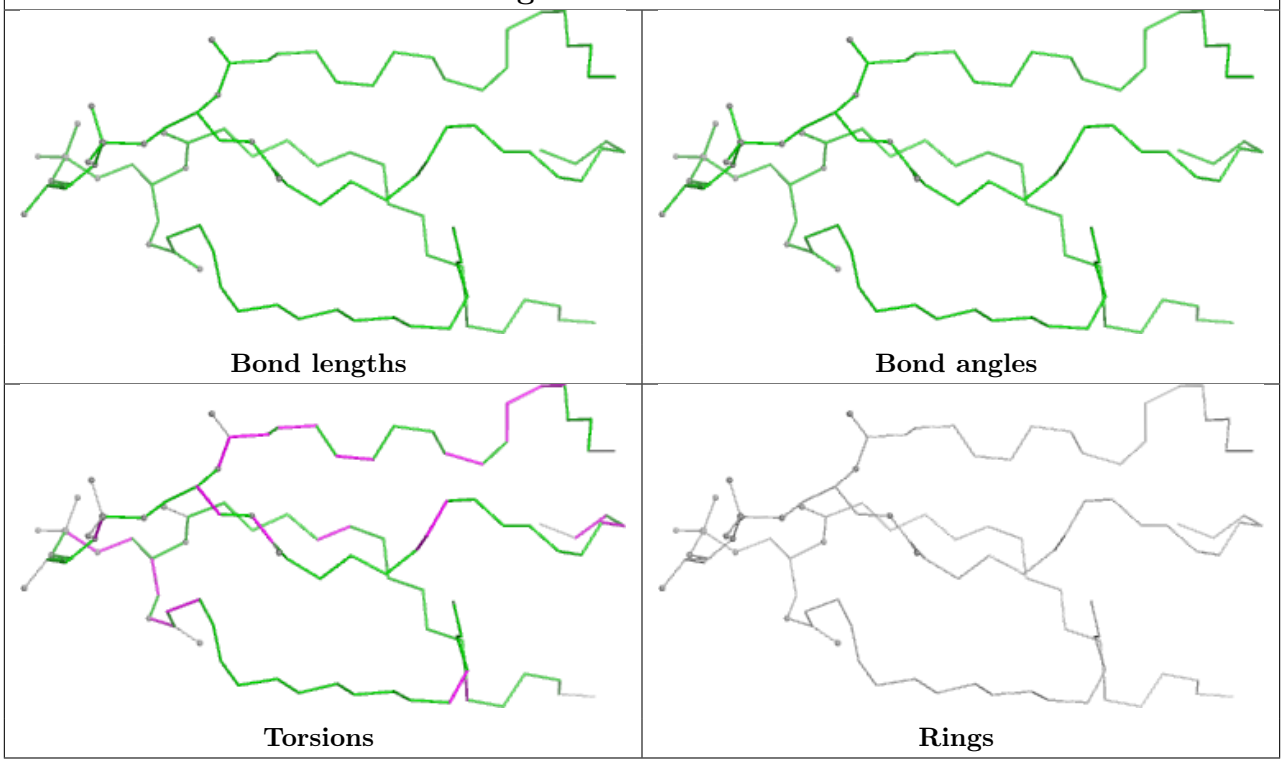


**Rings**

## Ligand CDL ED 601




## Ligand CDL Dr 402



**Ligand PC1 EO 207**



**Bond lengths**



**Bond angles**

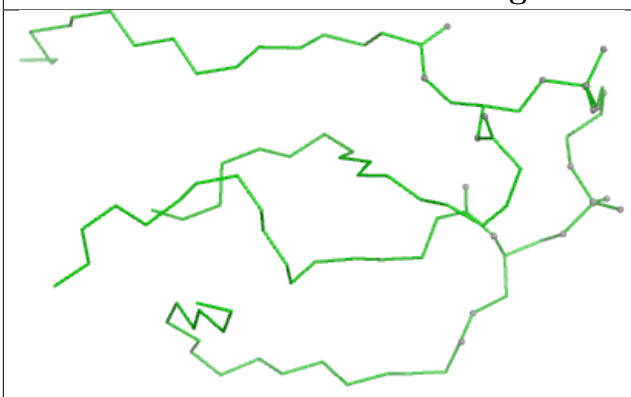


**Torsions**

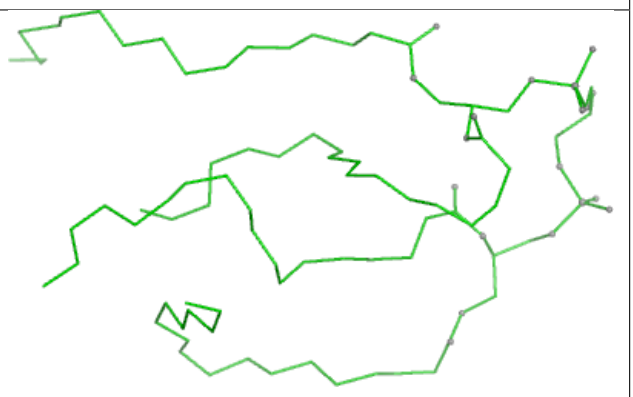


**Rings**

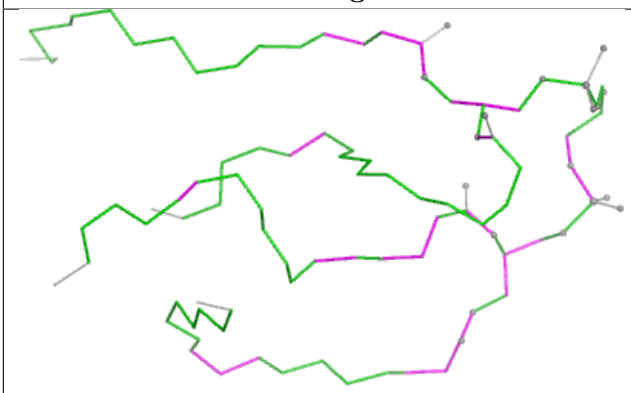
**Ligand CDL DU 401**



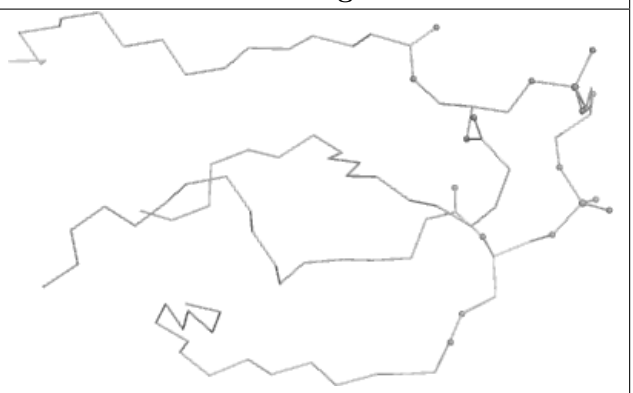
**Bond lengths**



**Bond angles**

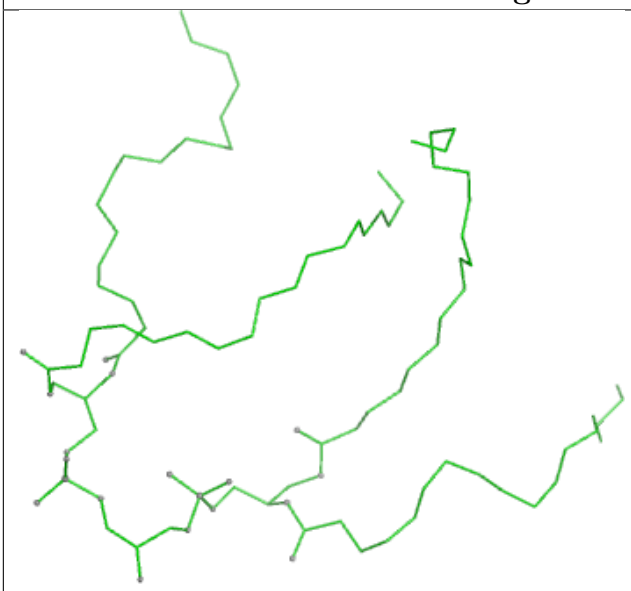


**Torsions**

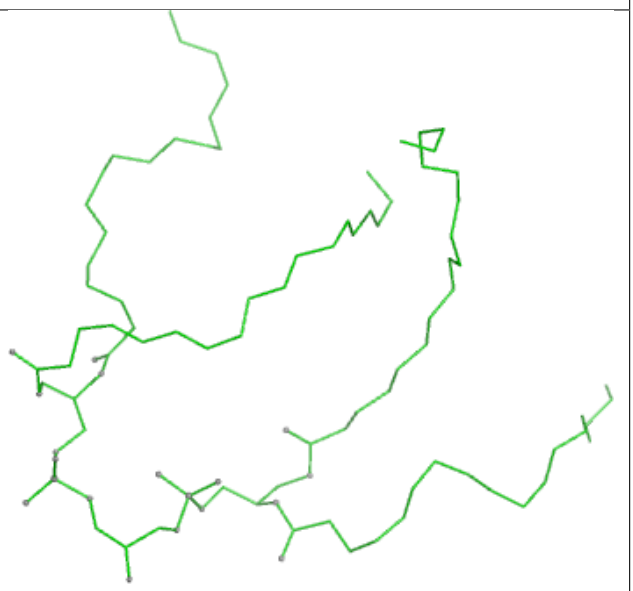


**Rings**

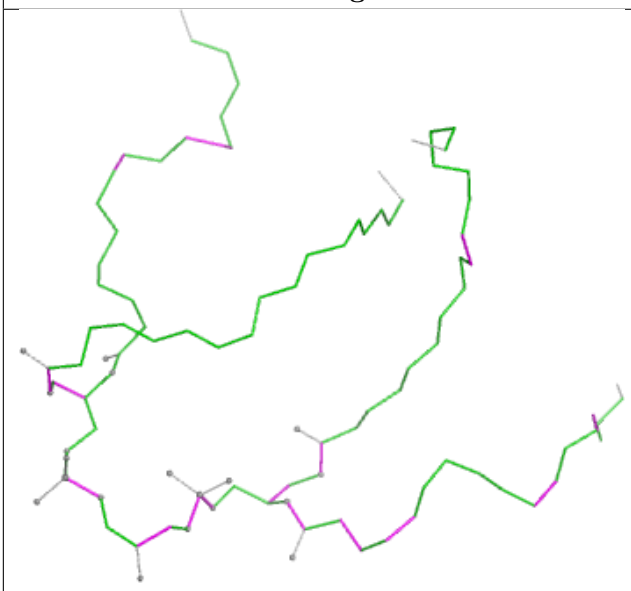
**Ligand CDL Dh 201**



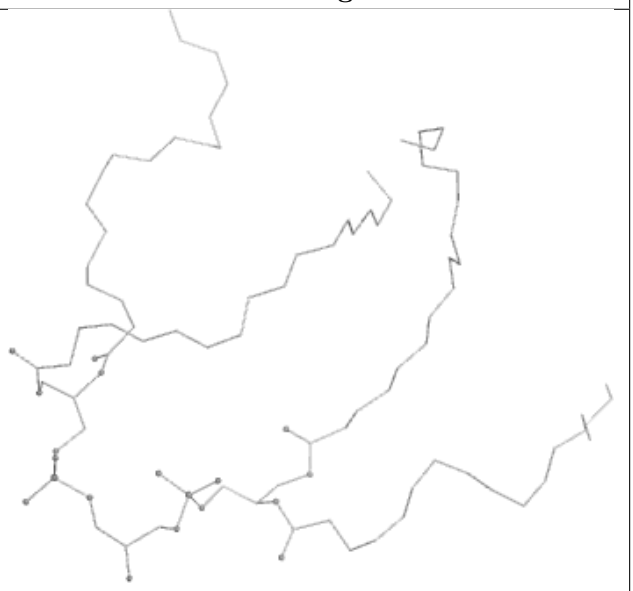
**Bond lengths**



**Bond angles**

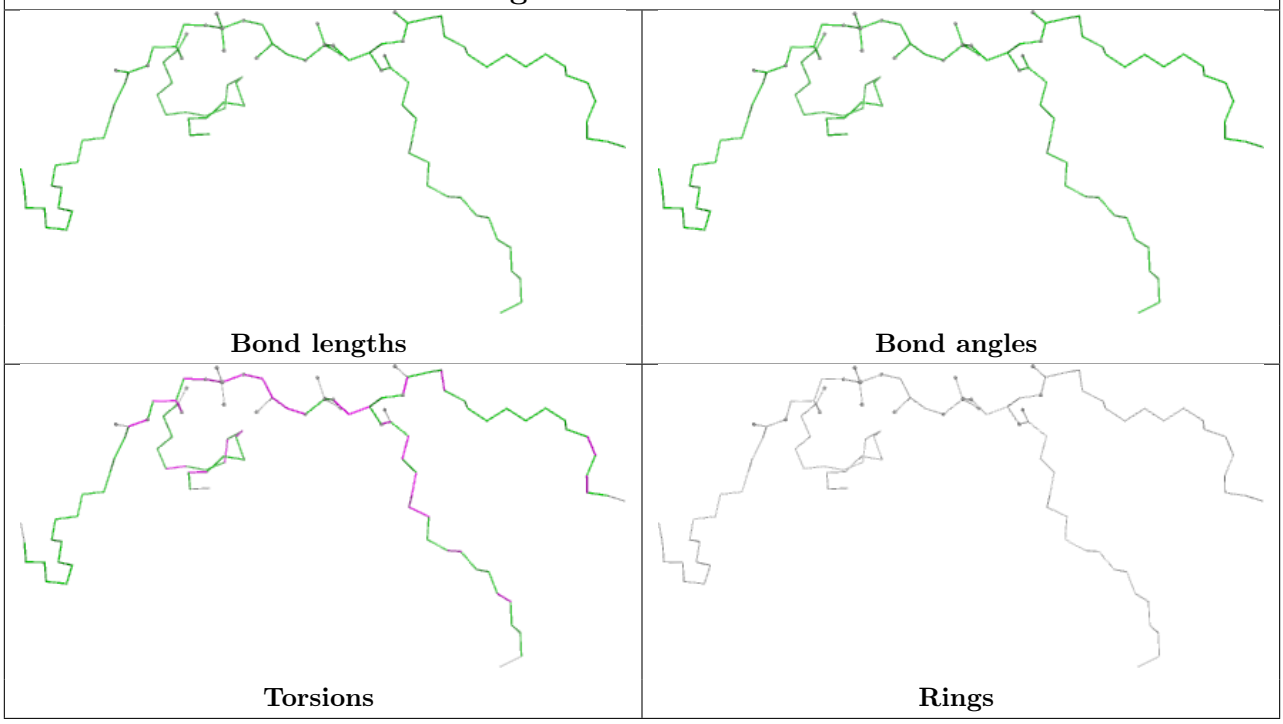


**Torsions**

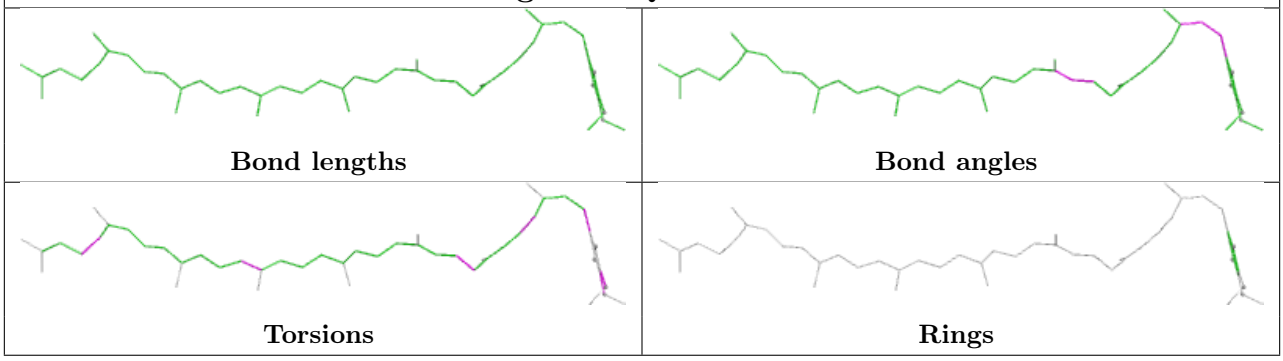


**Rings**

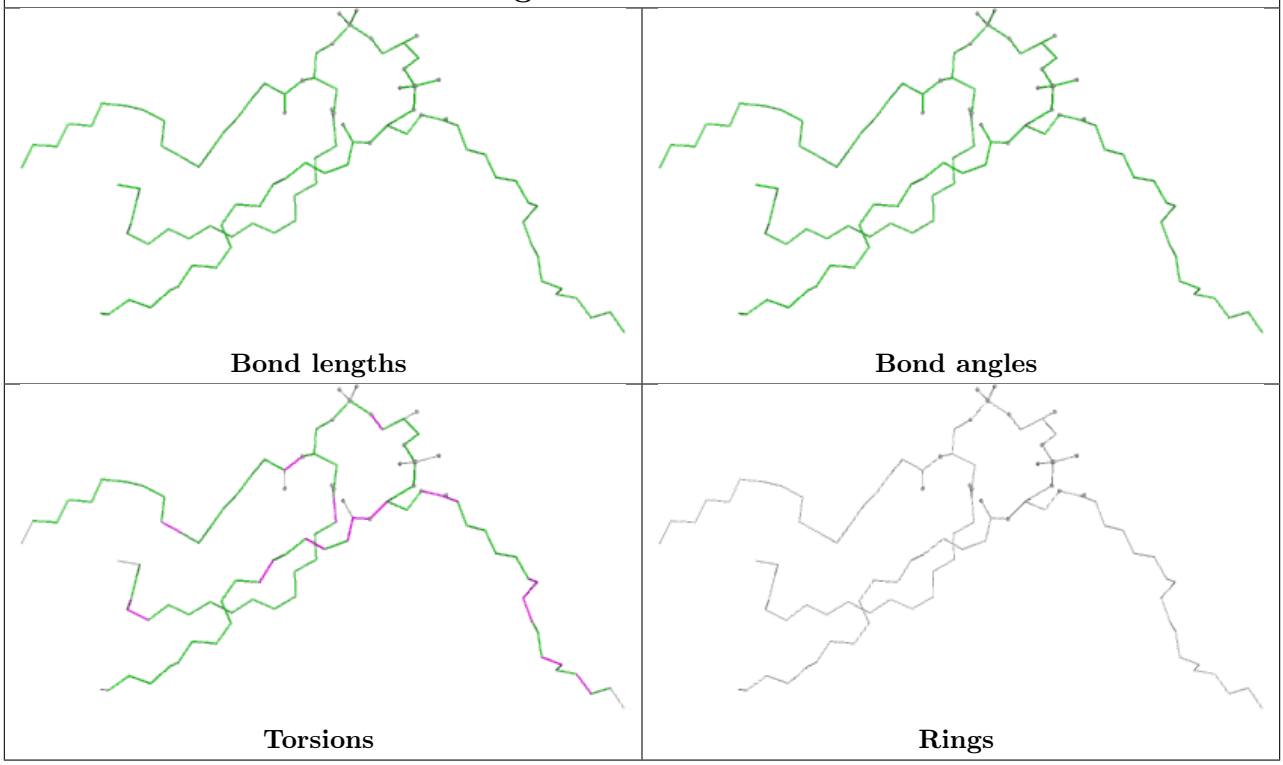
## Ligand CDL DG 201



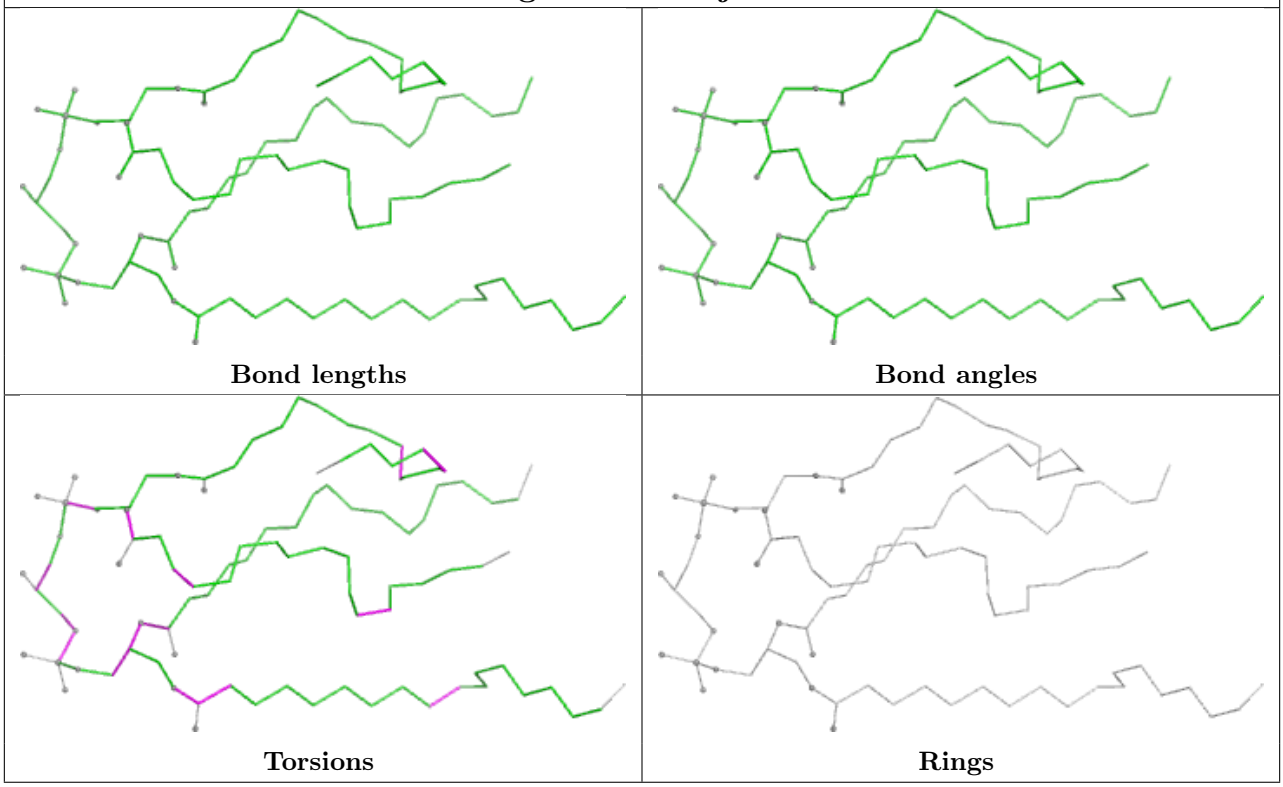

## Ligand UQ8 EL 906



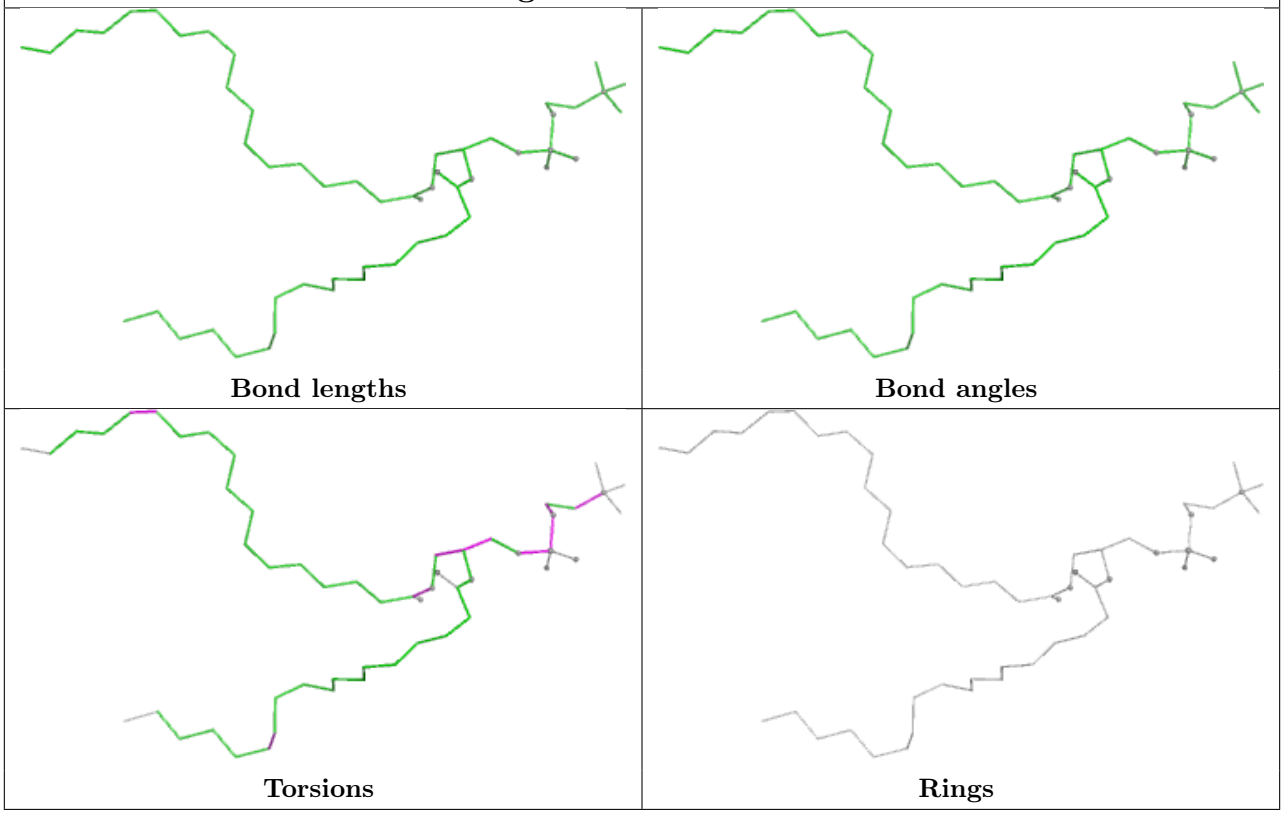
**Ligand CDL Dn 507**



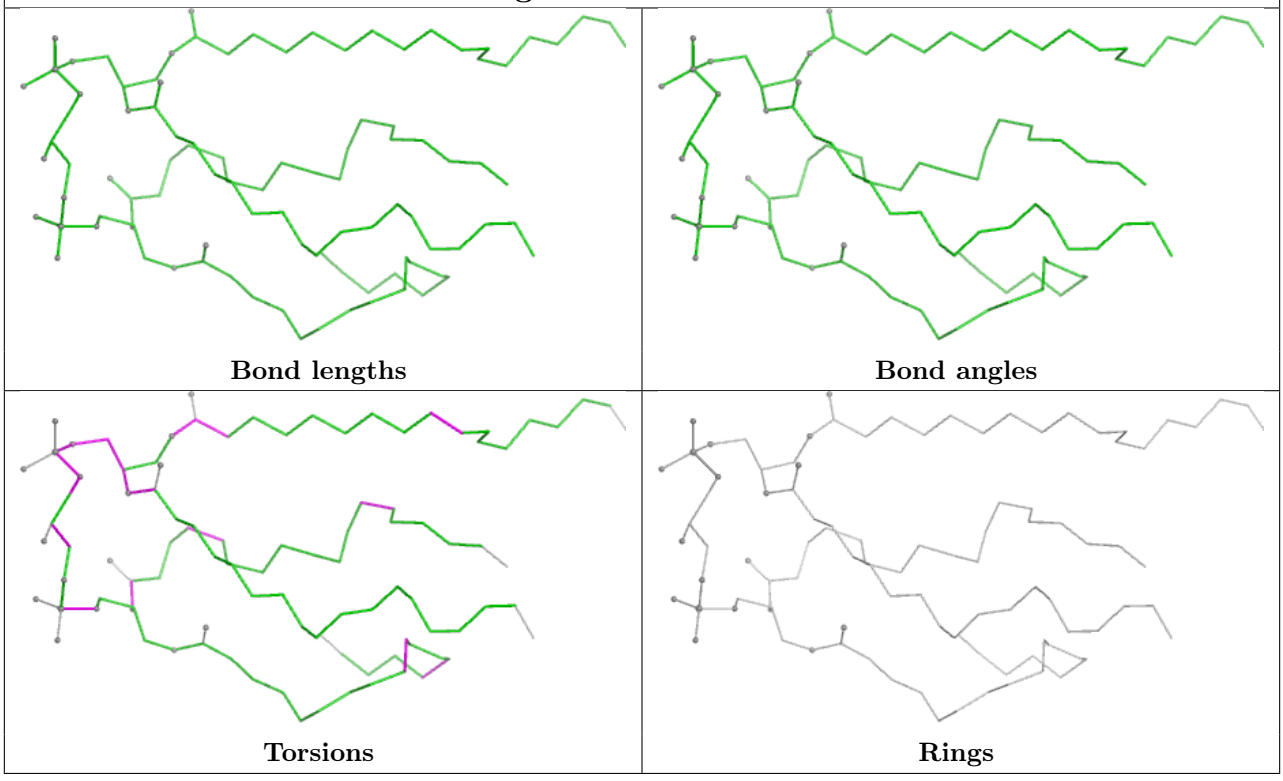

**Ligand CDL Dj 405**



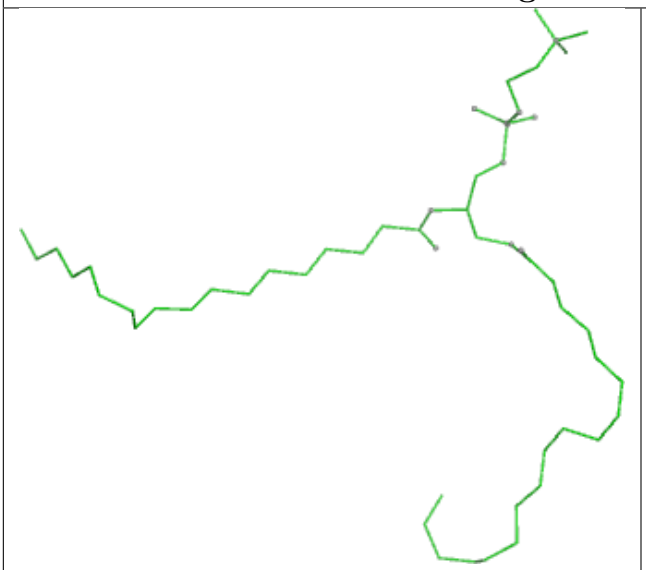
## Ligand PC1 DS 407



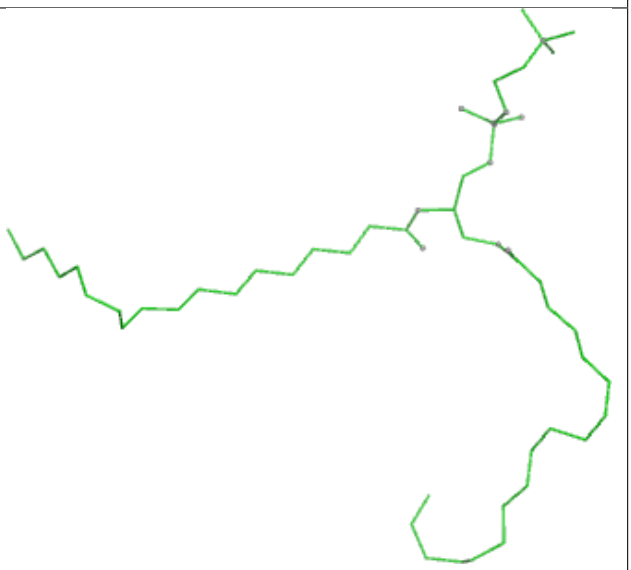

## Ligand CDL DJ 305



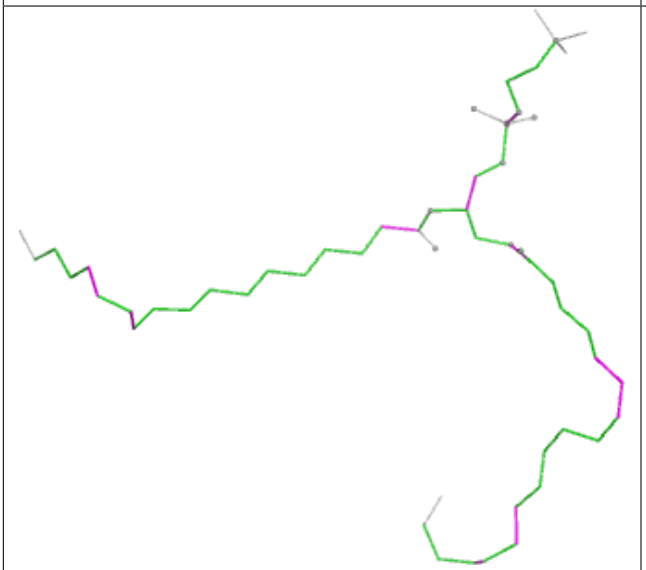
**Ligand PC1 Dc 603**



**Bond lengths**



**Bond angles**

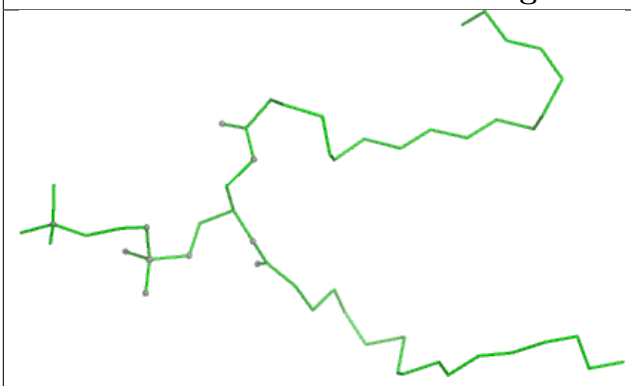


**Torsions**

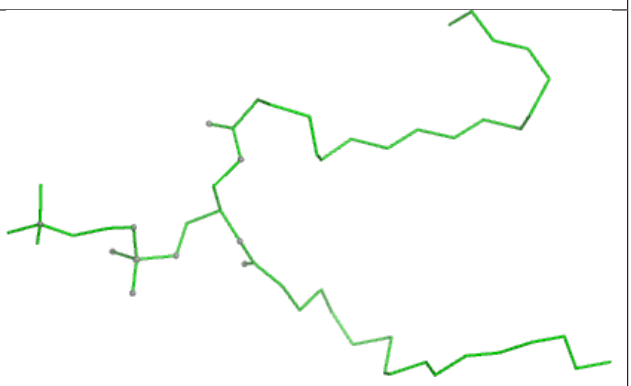


**Rings**

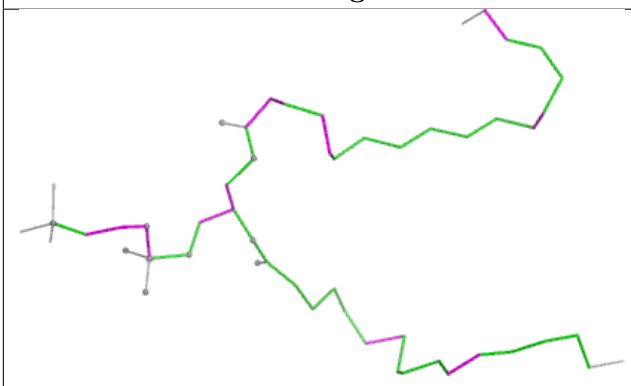
**Ligand PC1 Eo 201**



**Bond lengths**



**Bond angles**

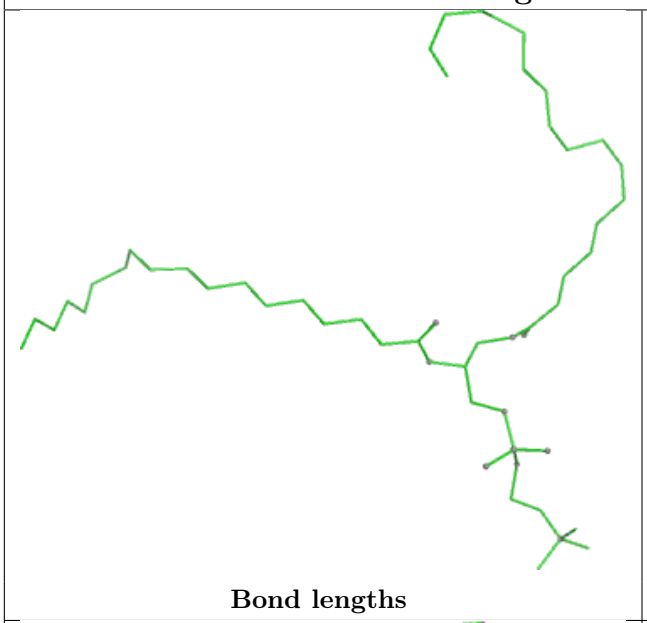


**Torsions**

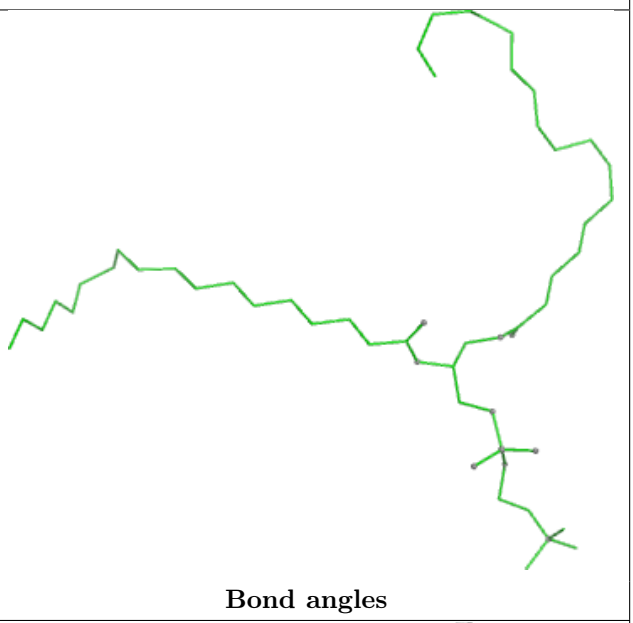


**Rings**

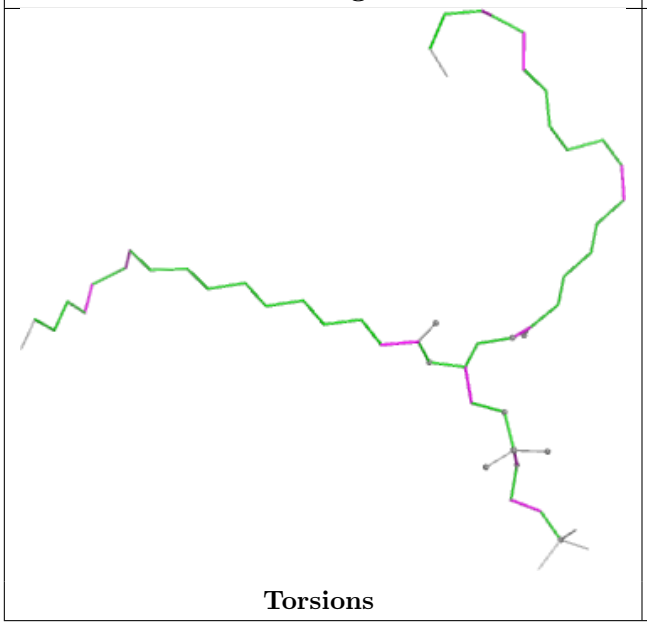
**Ligand PC1 DC 603**



**Bond lengths**



**Bond angles**

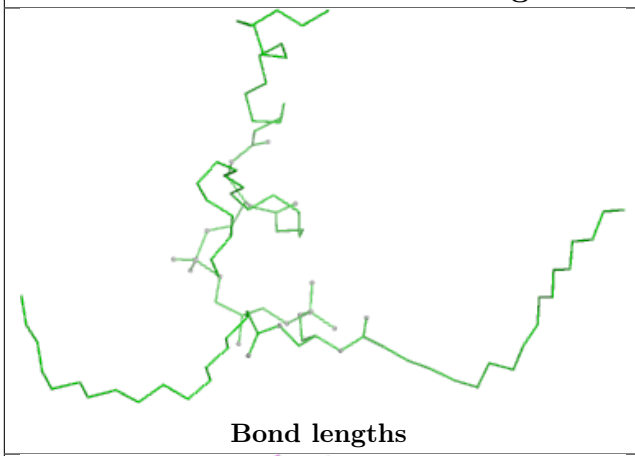


**Torsions**

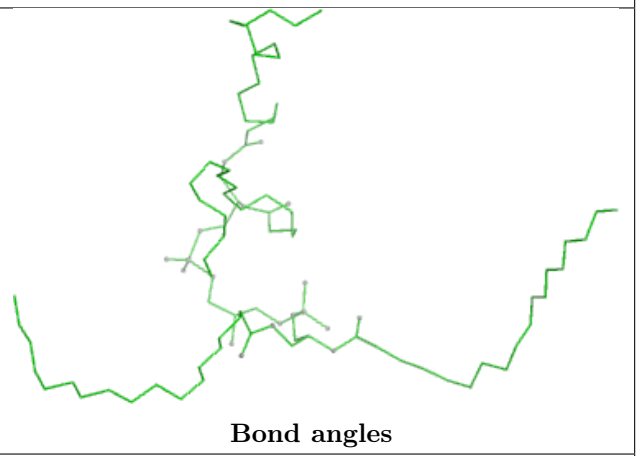


**Rings**

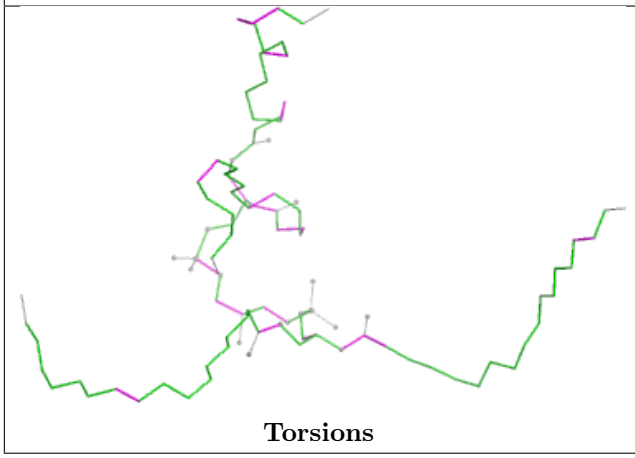
**Ligand CDL DX 307**



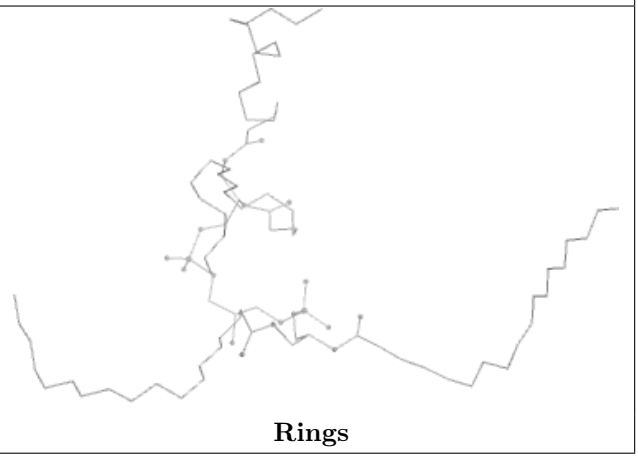
**Bond lengths**



**Bond angles**

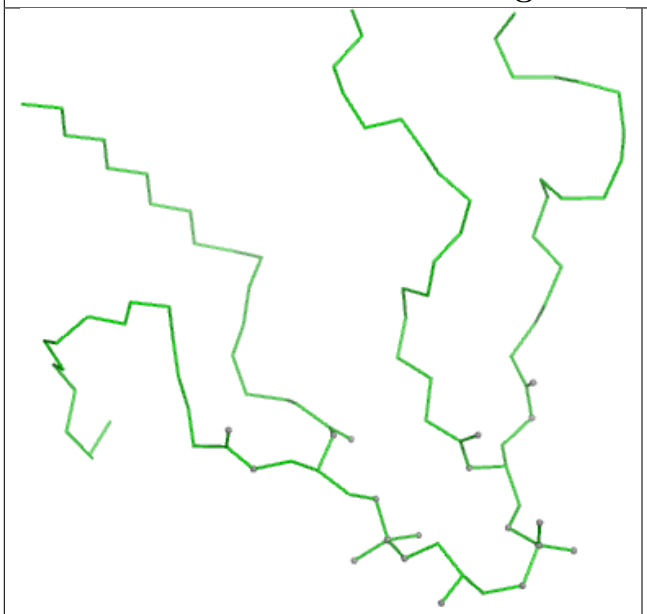


**Torsions**

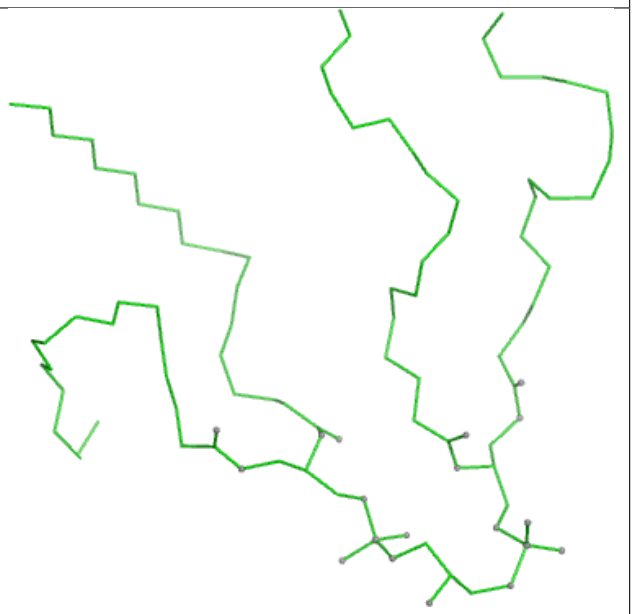


**Rings**

**Ligand CDL EL 903**



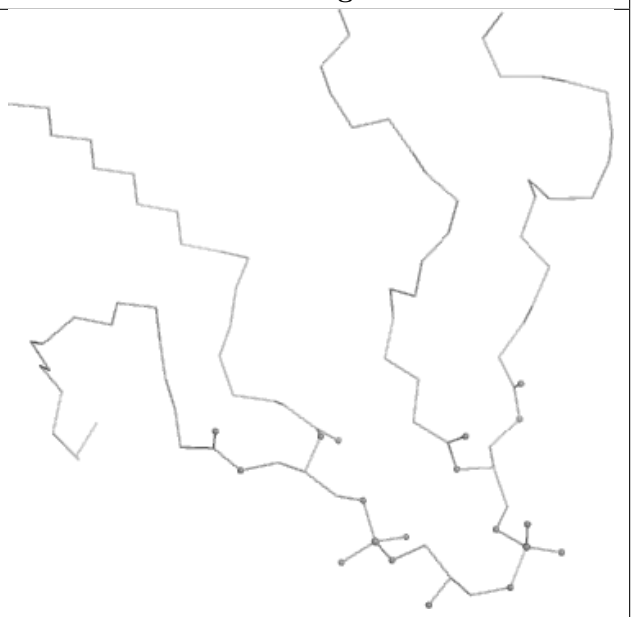
**Bond lengths**



**Bond angles**

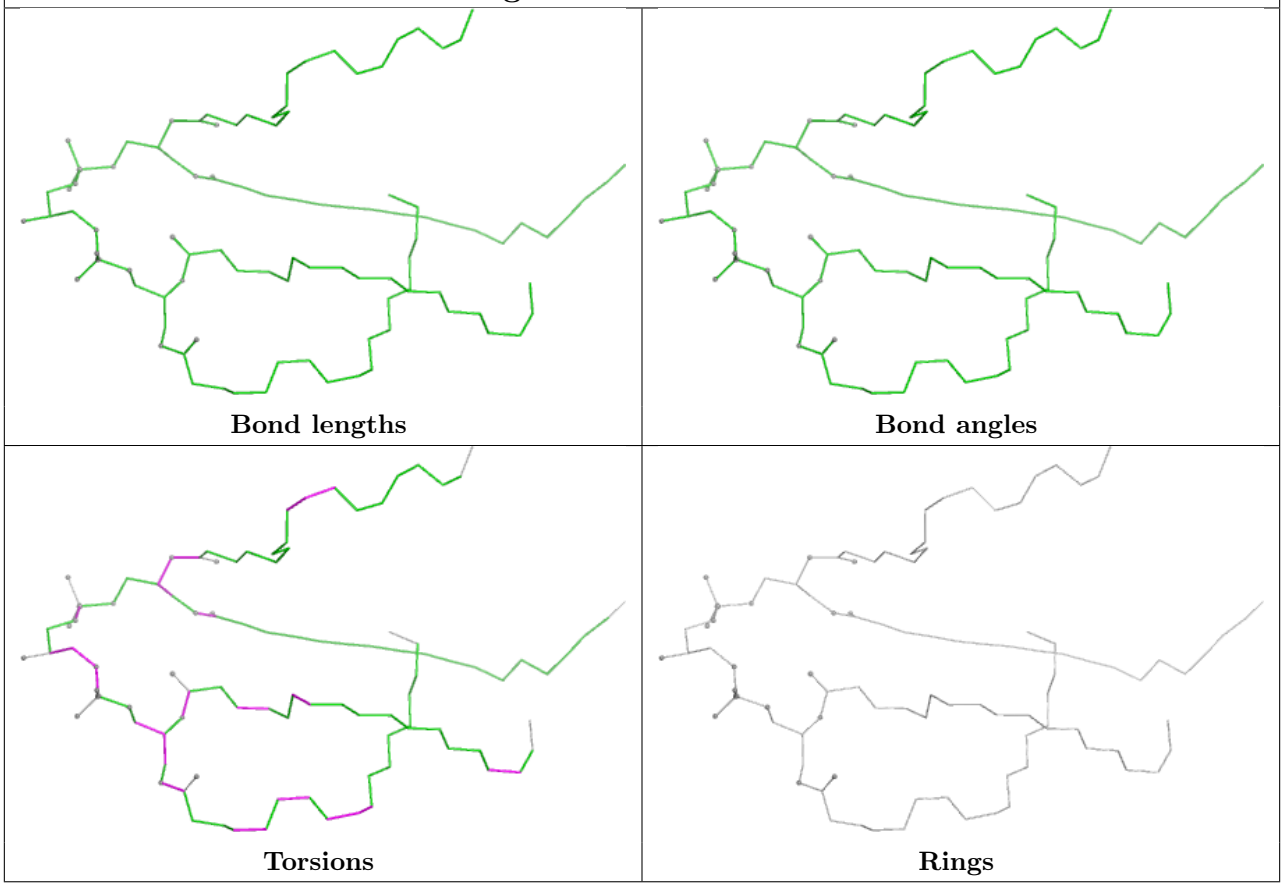


**Torsions**

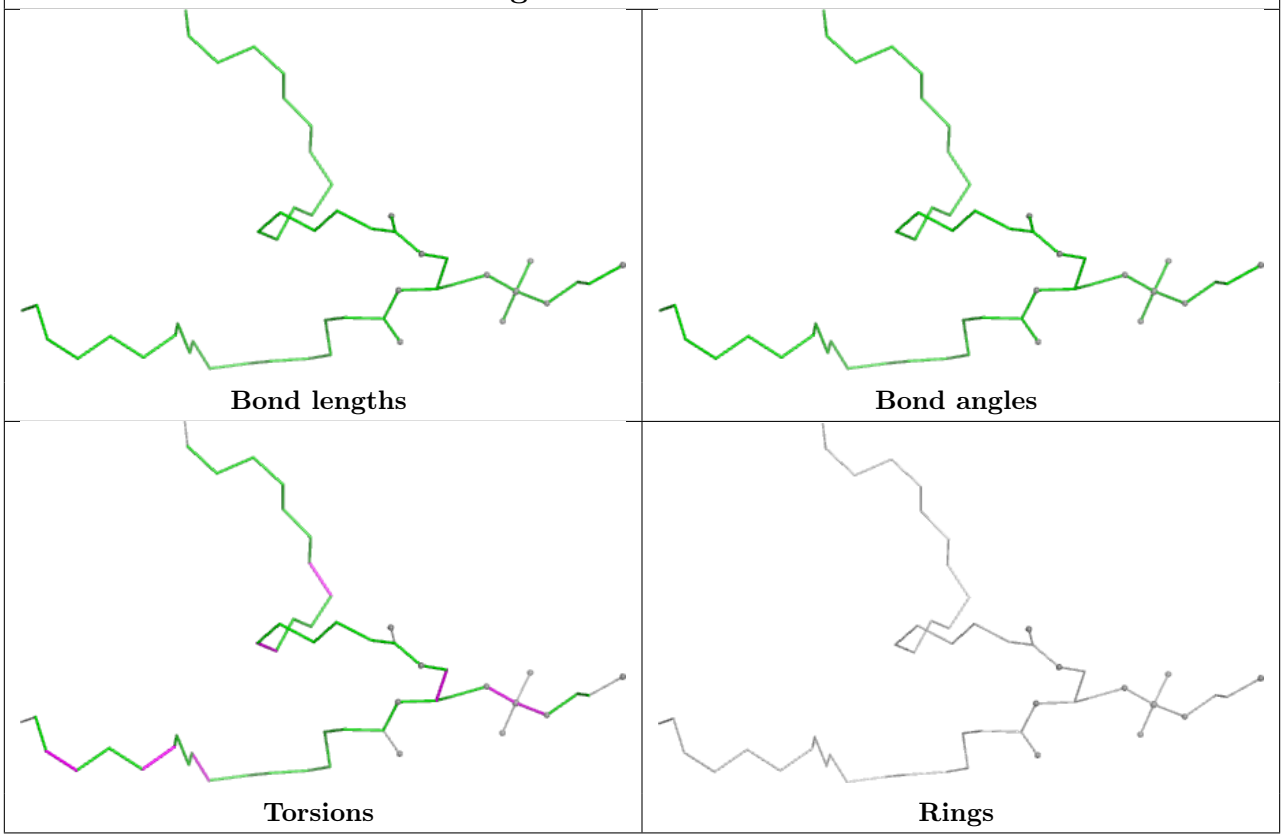


**Rings**

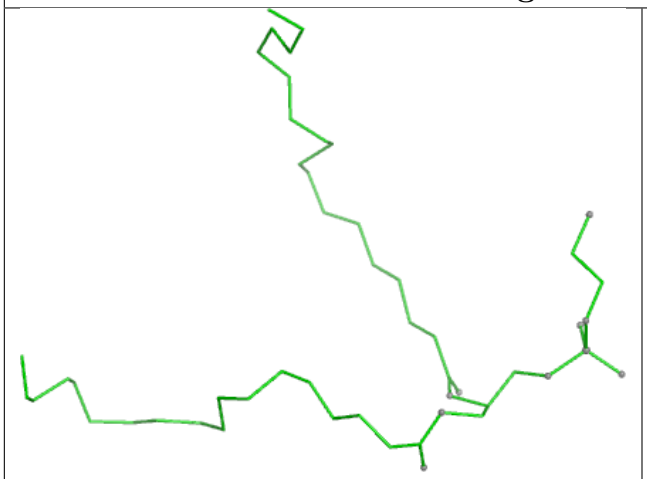
## Ligand CDL EN 1202



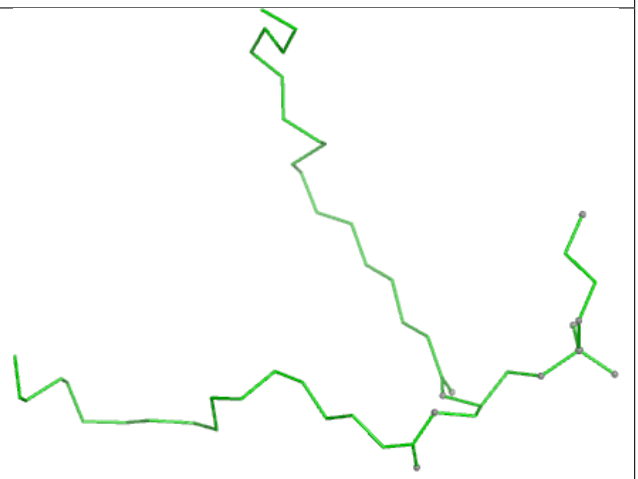

## Ligand 3PE Dx 1207



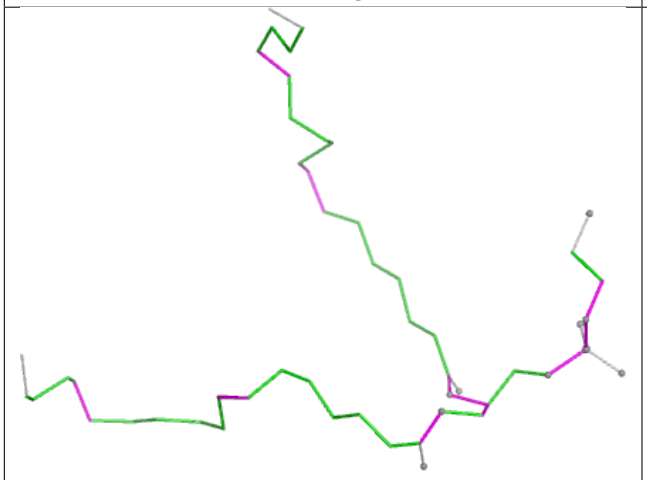
**Ligand 3PE EO 203**



**Bond lengths**



**Bond angles**

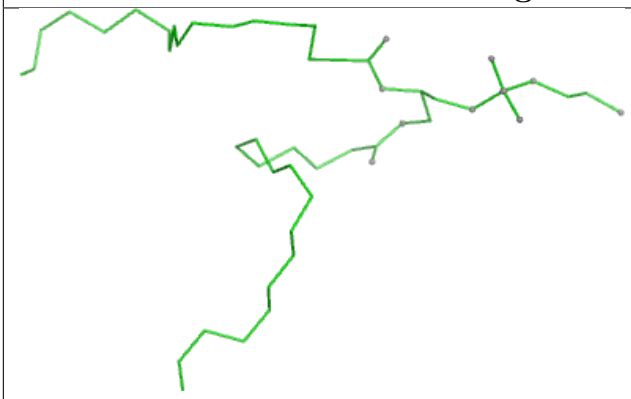


**Torsions**

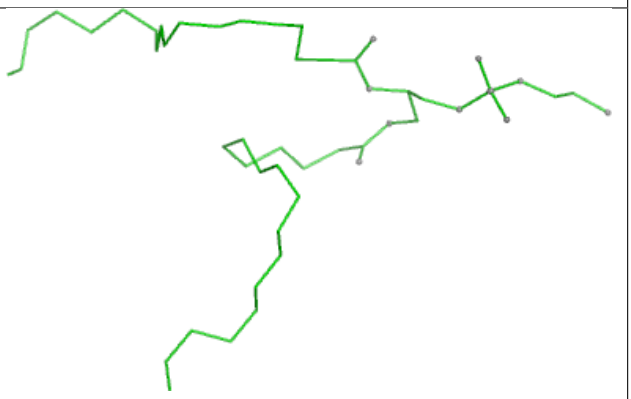


**Rings**

**Ligand 3PE DX 305**



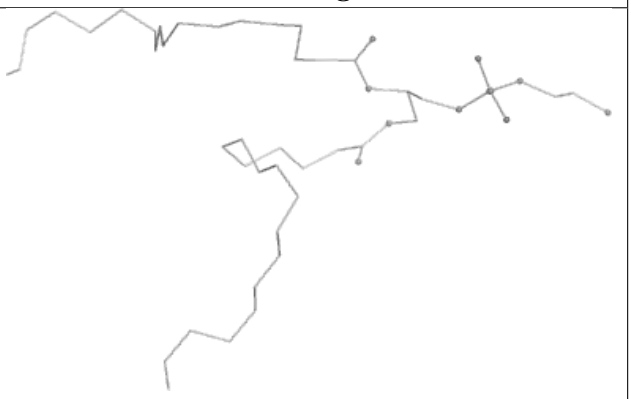
**Bond lengths**



**Bond angles**

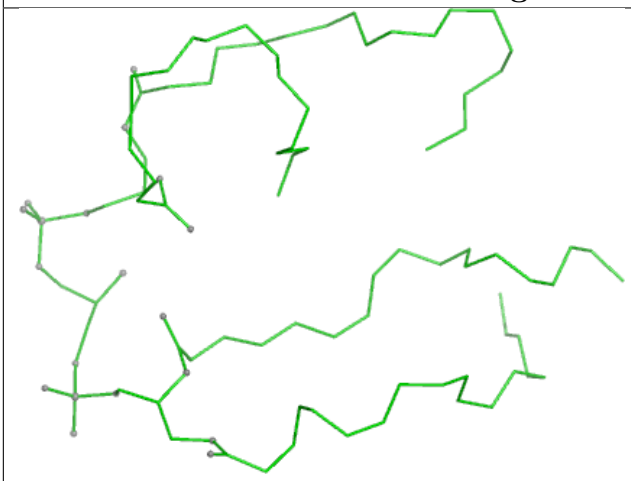


**Torsions**

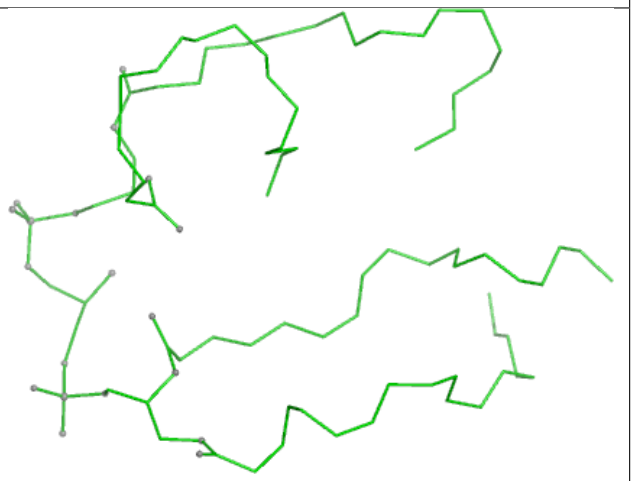


**Rings**

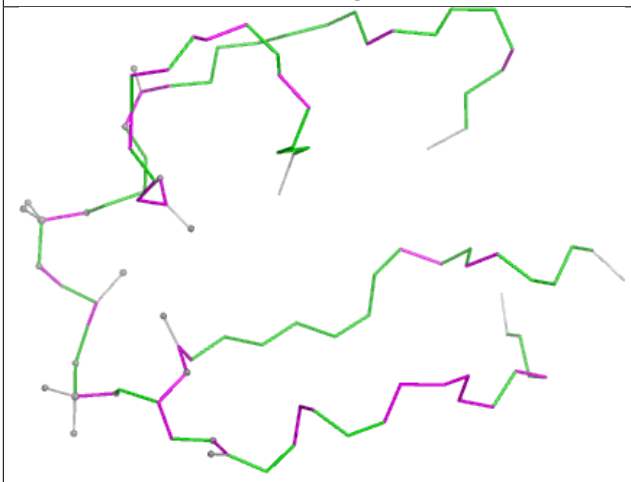
**Ligand CDL DV 402**



**Bond lengths**



**Bond angles**

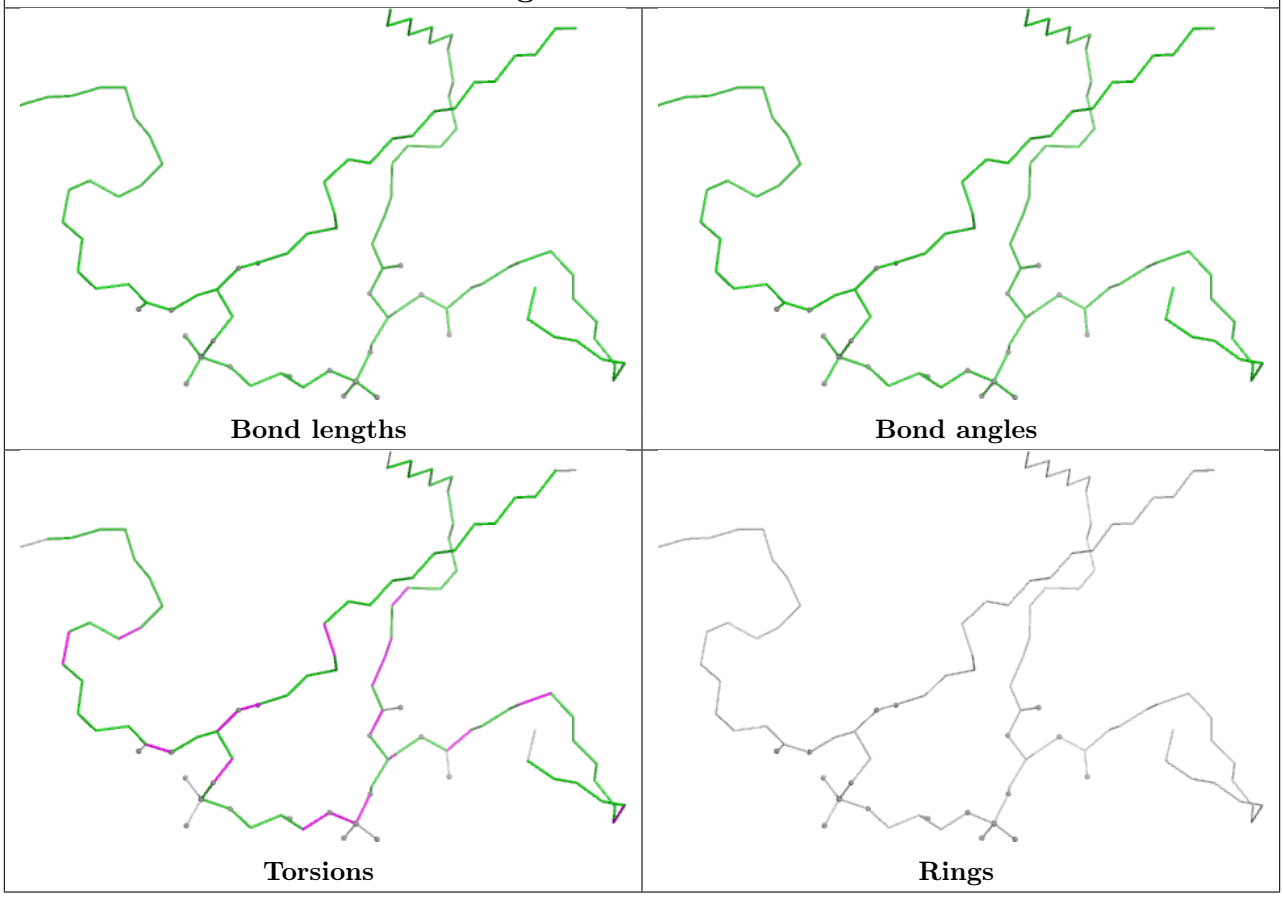


**Torsions**



**Rings**

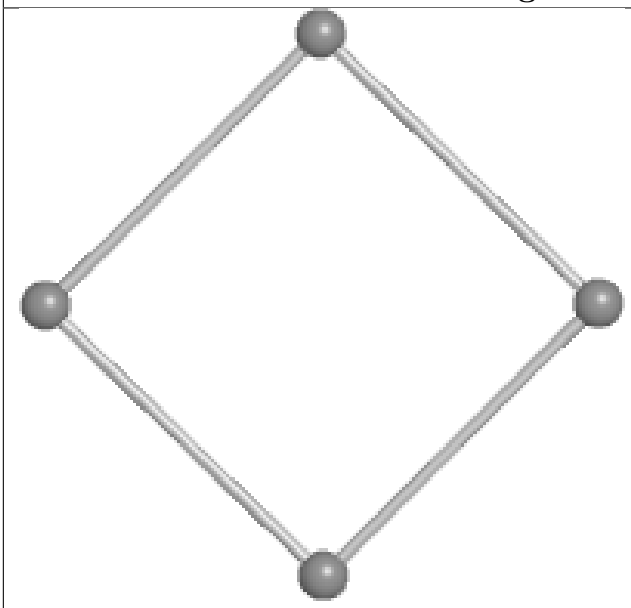
**Ligand CDL Ek 201**



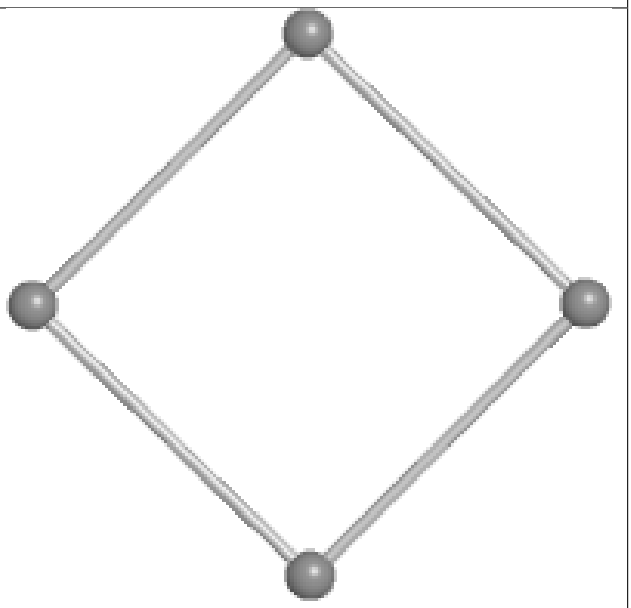
**Bond lengths** | **Bond angles**

**Torsions** | **Rings**

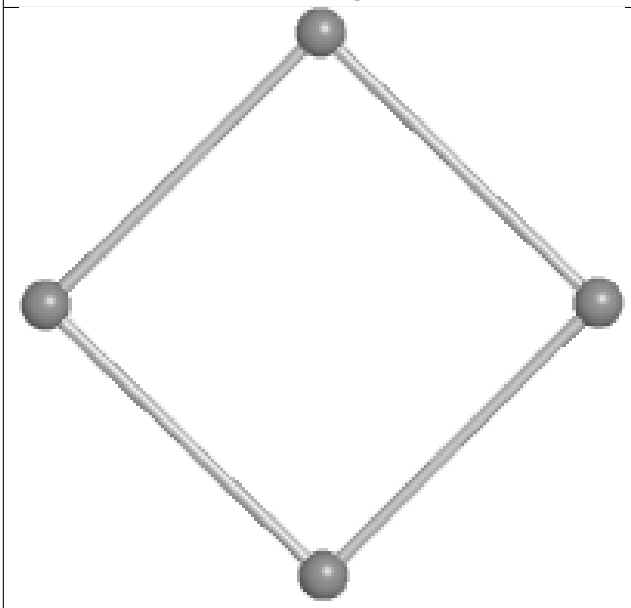
**Ligand FES EF 202**



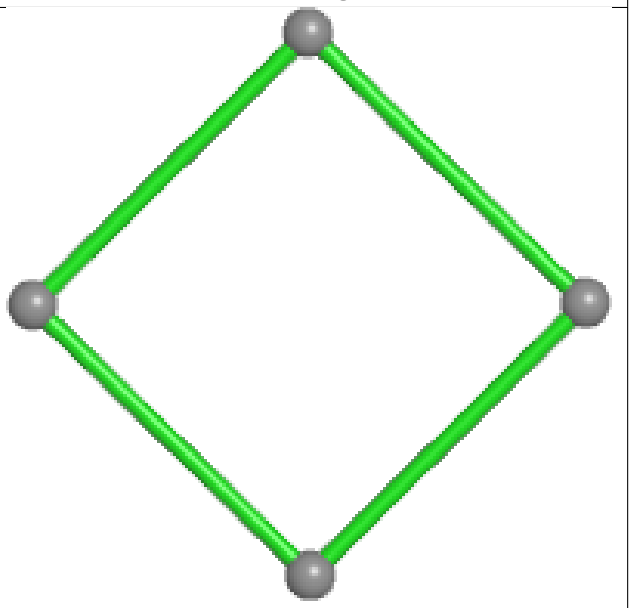
**Bond lengths**



**Bond angles**

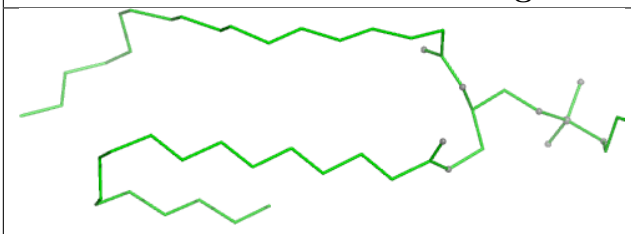


**Torsions**

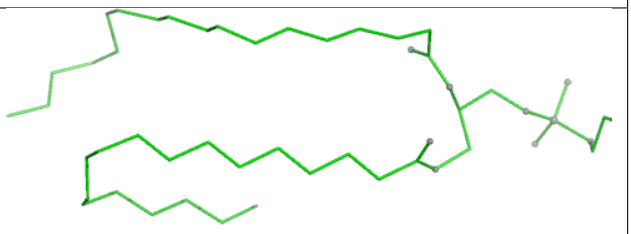


**Rings**

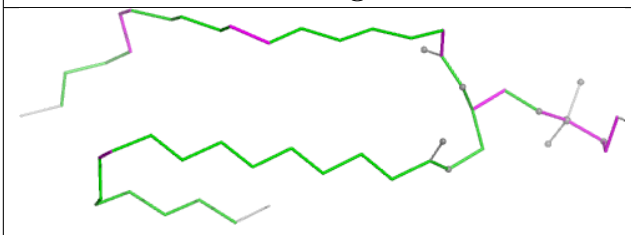
**Ligand 3PE DX 303**



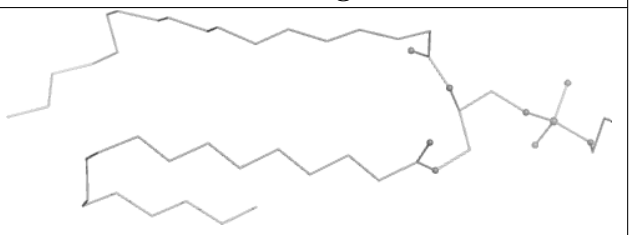
Bond lengths



Bond angles

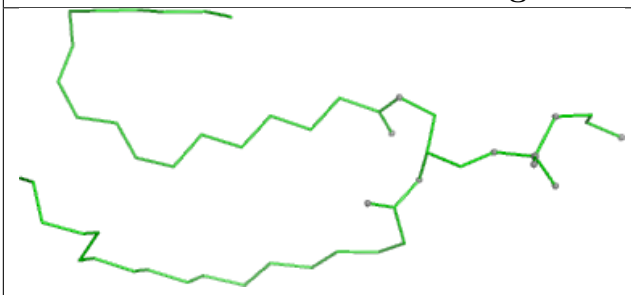


Torsions



Rings

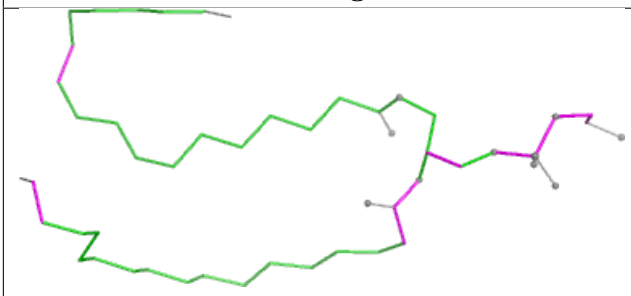
**Ligand 3PE Dx 1205**



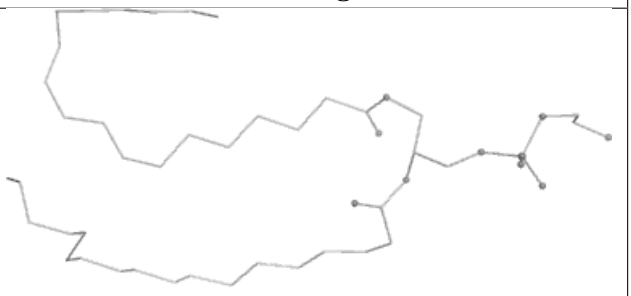
Bond lengths



Bond angles

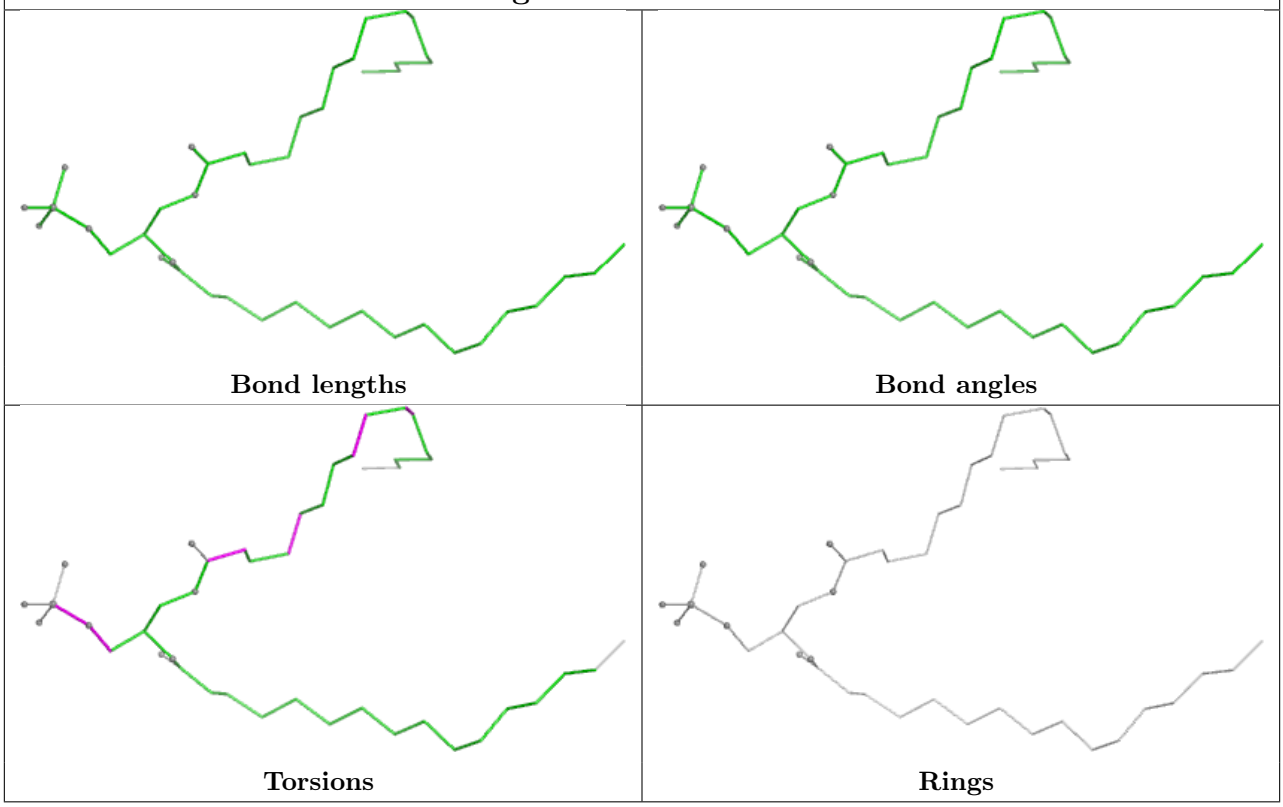


Torsions



Rings

**Ligand LPP DN 502**



**Ligand CDL Du 402**



**Bond lengths**



**Bond angles**

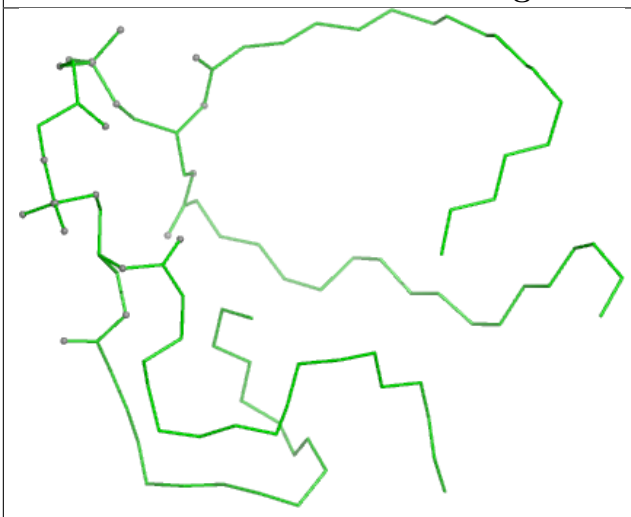


**Torsions**

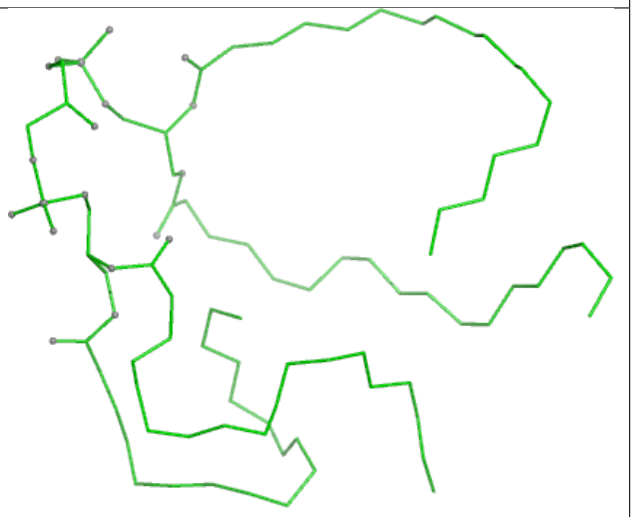


**Rings**

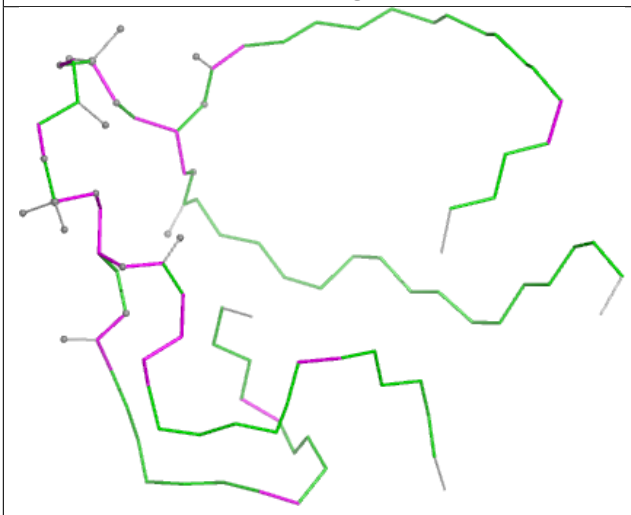
**Ligand CDL Dn 502**



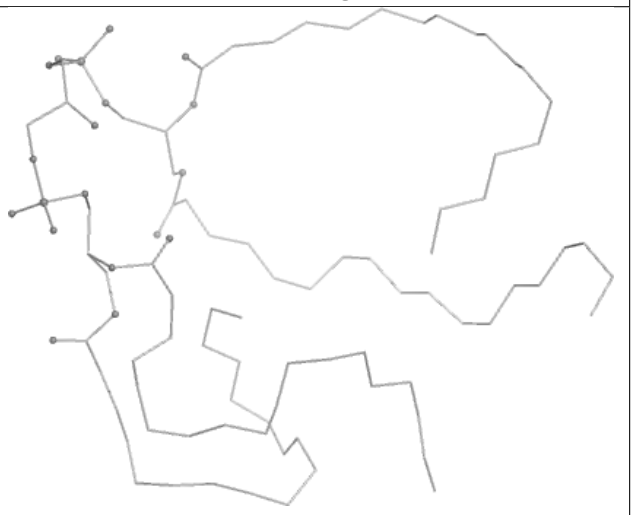
**Bond lengths**



**Bond angles**

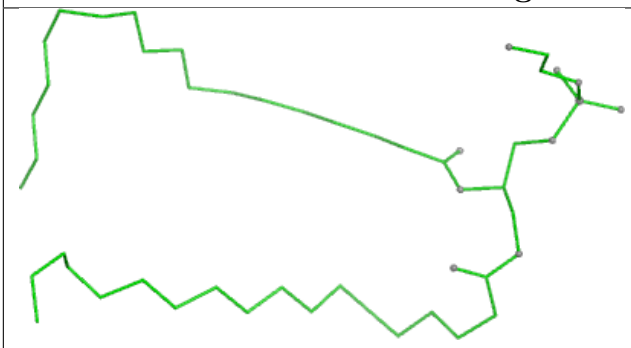


**Torsions**

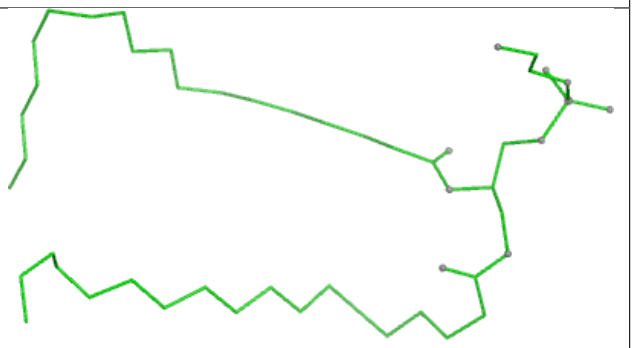


**Rings**

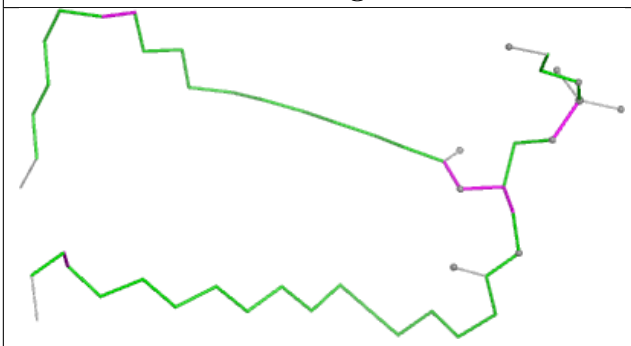
**Ligand 3PE DC 606**



Bond lengths



Bond angles

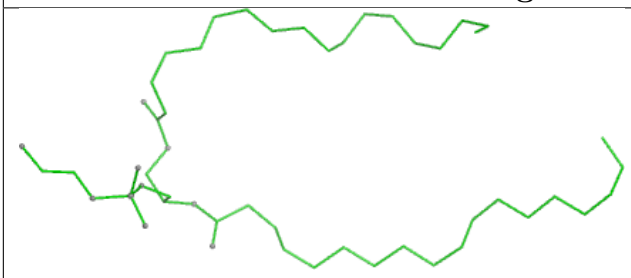


Torsions

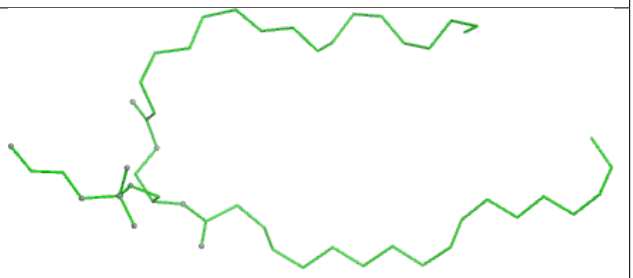


Rings

**Ligand 3PE EO 204**



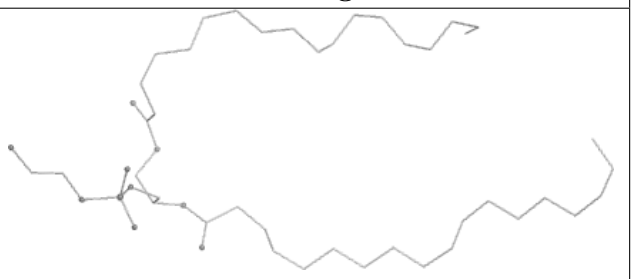
Bond lengths



Bond angles

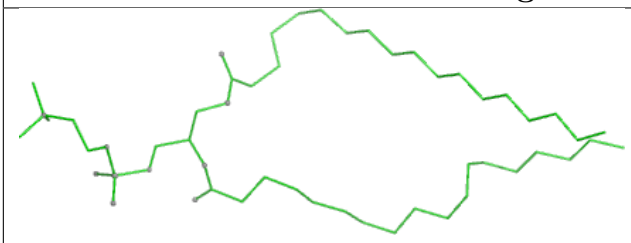


Torsions

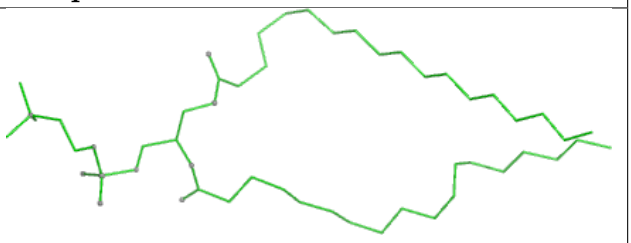


Rings

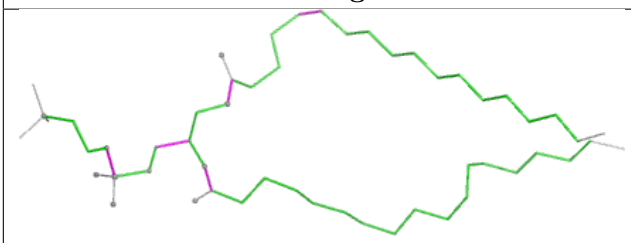
**Ligand PC1 Dq 405**



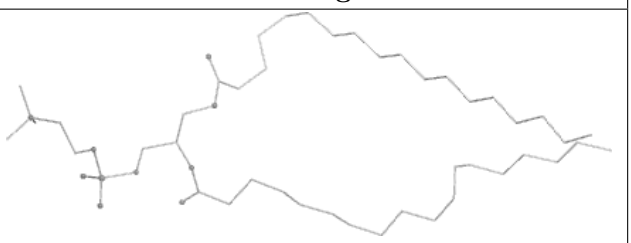
Bond lengths



Bond angles

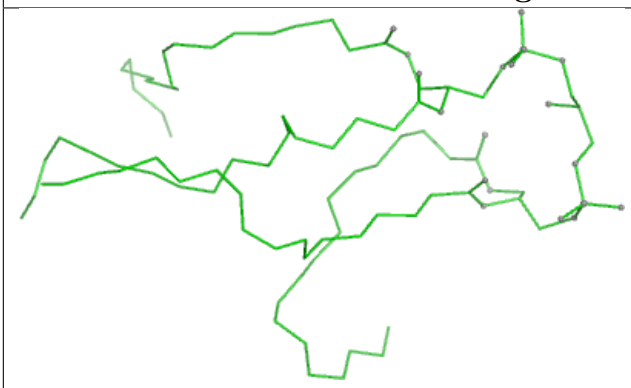


Torsions

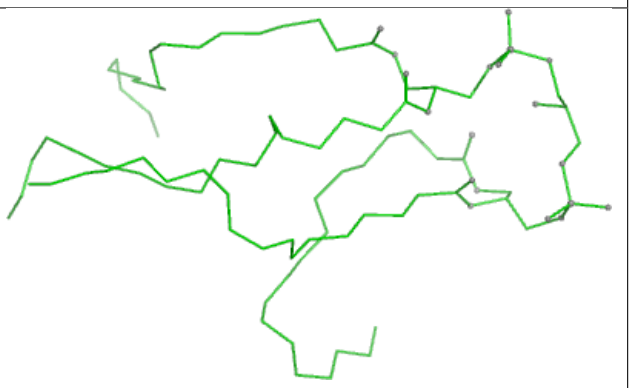


Rings

**Ligand CDL Da 705**



Bond lengths



Bond angles

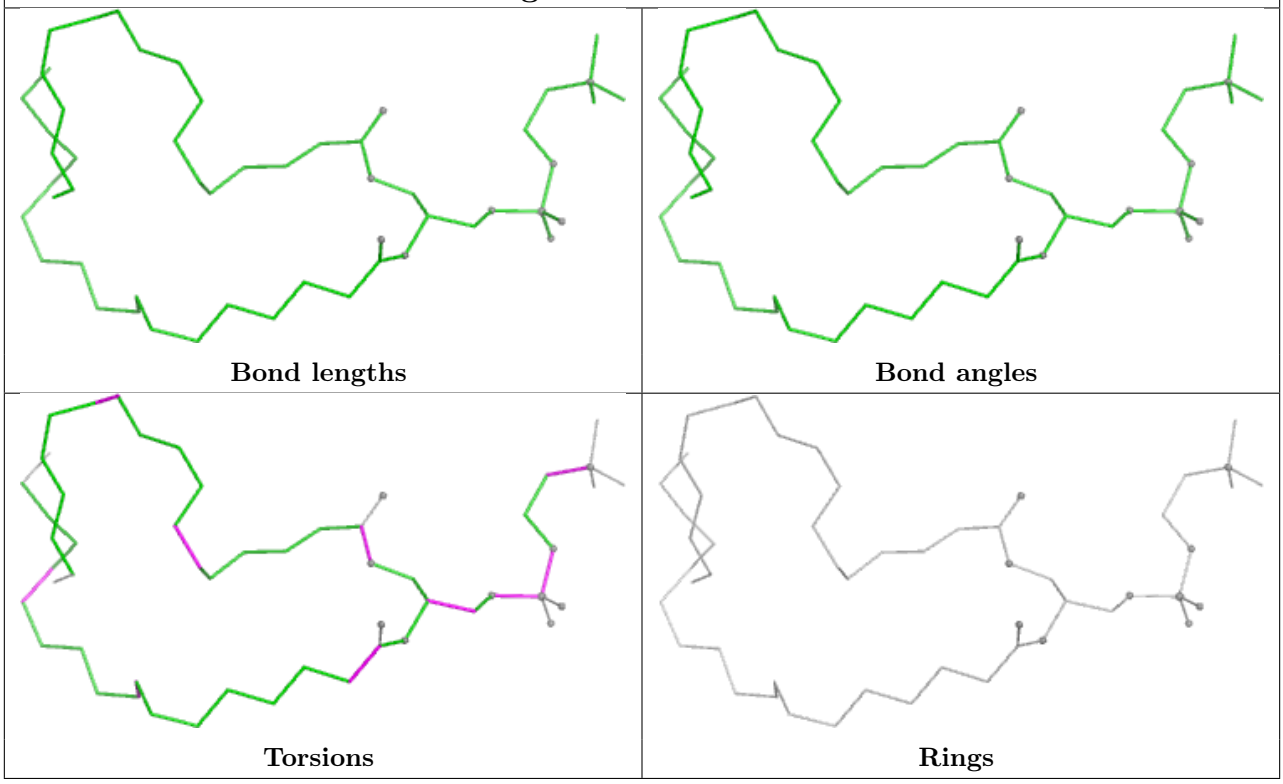


Torsions

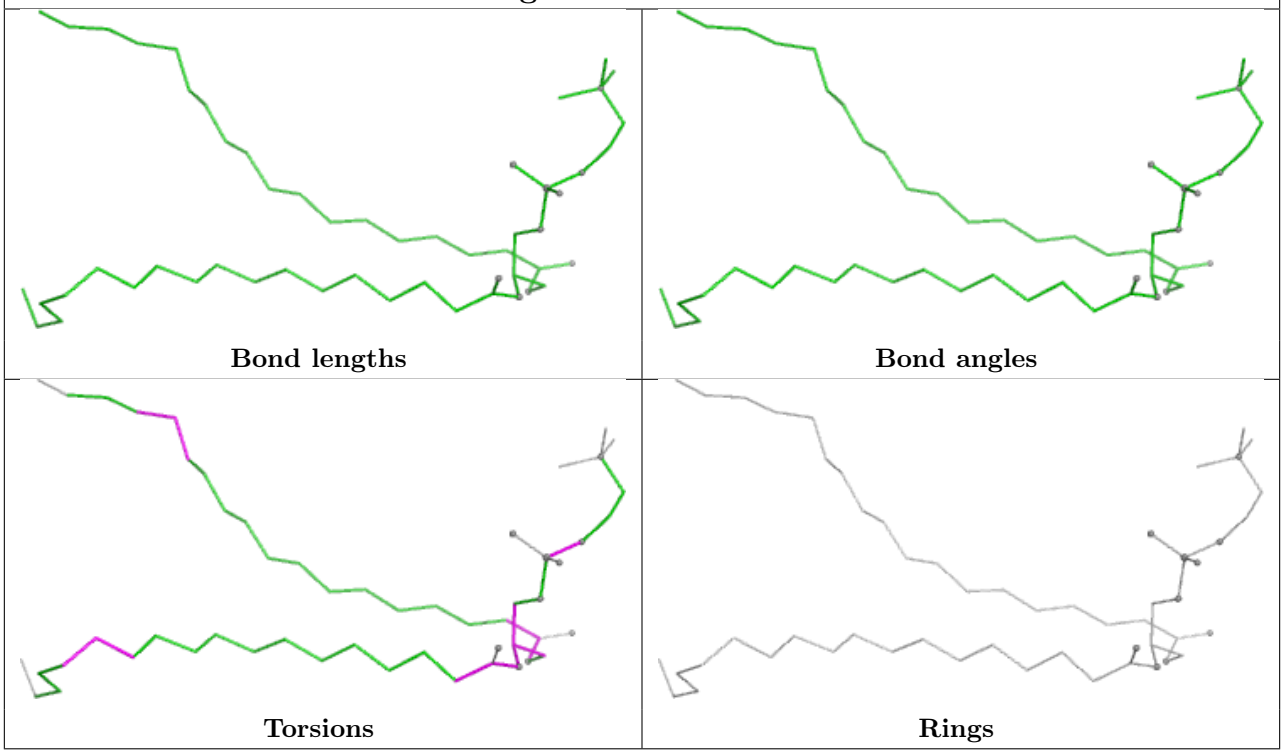


Rings

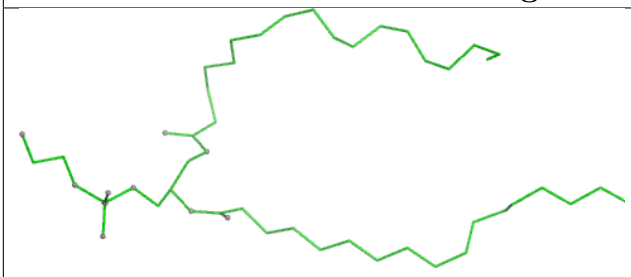
## Ligand PC1 DI 702



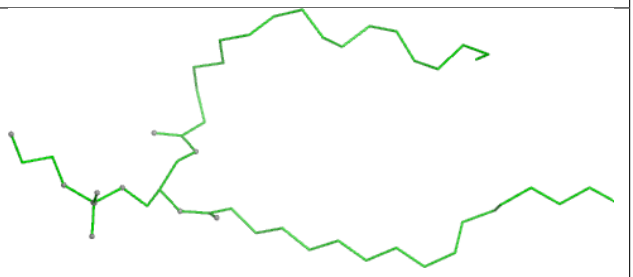

## Ligand PC1 Dc 607



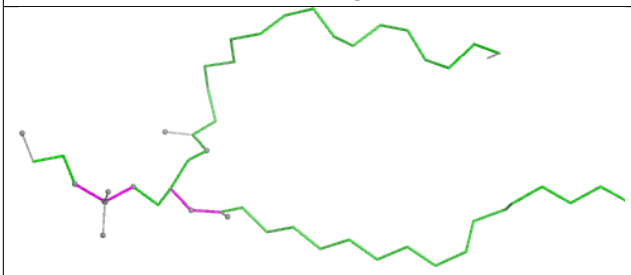
**Ligand 3PE Eo 203**



**Bond lengths**



**Bond angles**

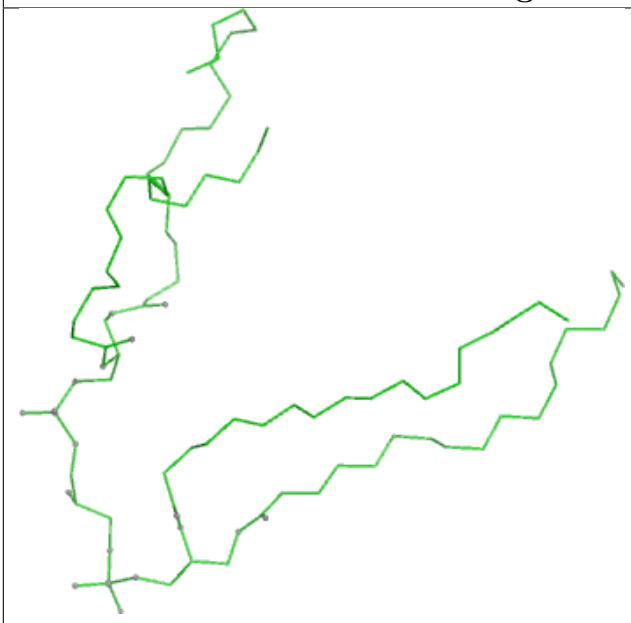


**Torsions**

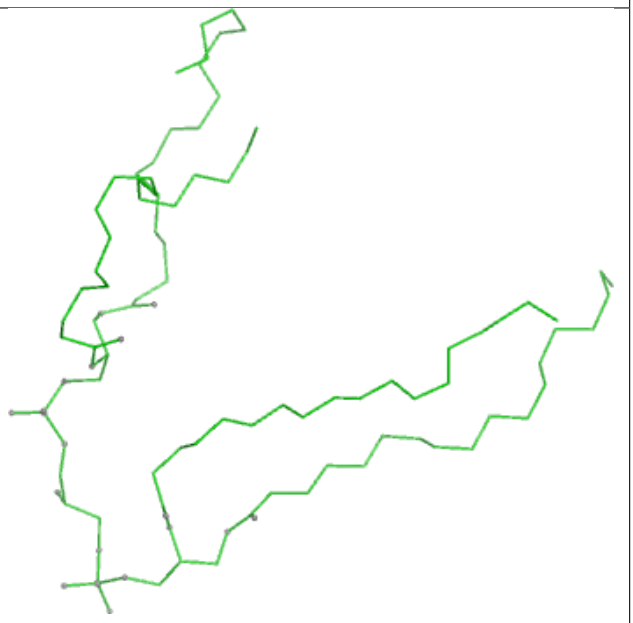


**Rings**

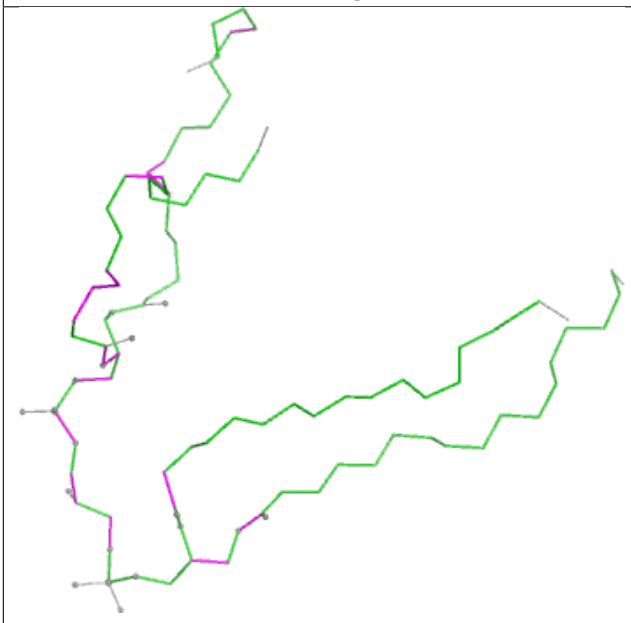
**Ligand CDL Dr 403**



**Bond lengths**



**Bond angles**

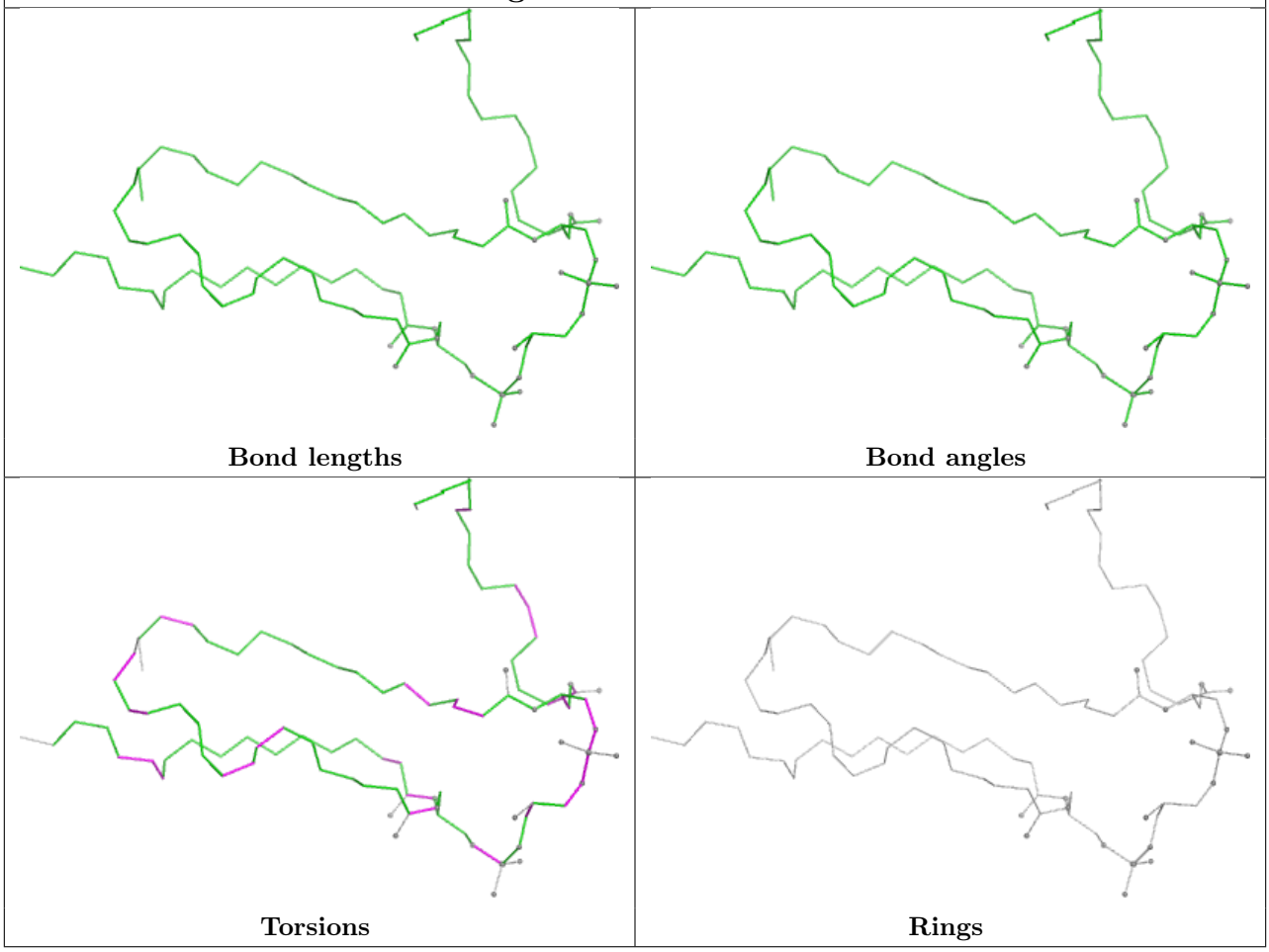


**Torsions**

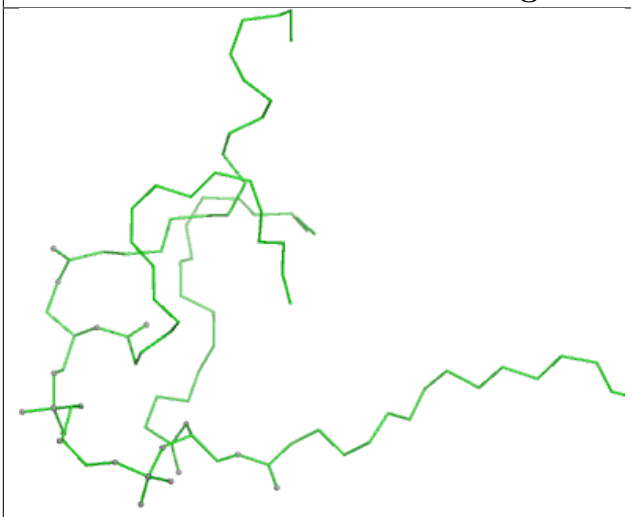


**Rings**

**Ligand CDL EB 304**



## Ligand CDL El 903



Bond lengths



Bond angles

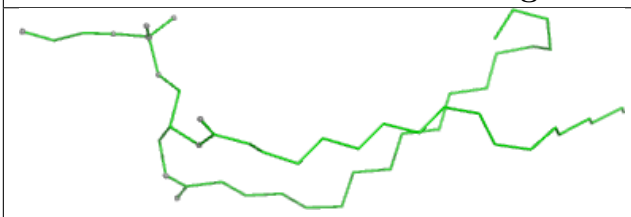


Torsions

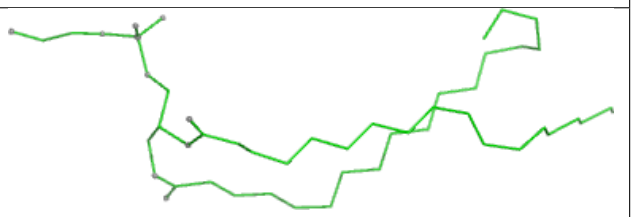


Rings

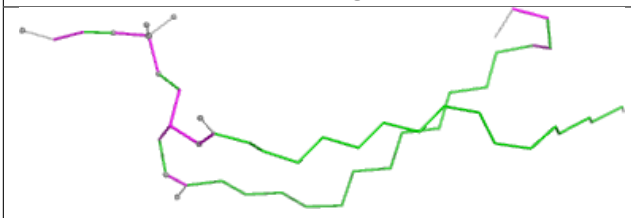
## Ligand 3PE Dr 401



Bond lengths



Bond angles

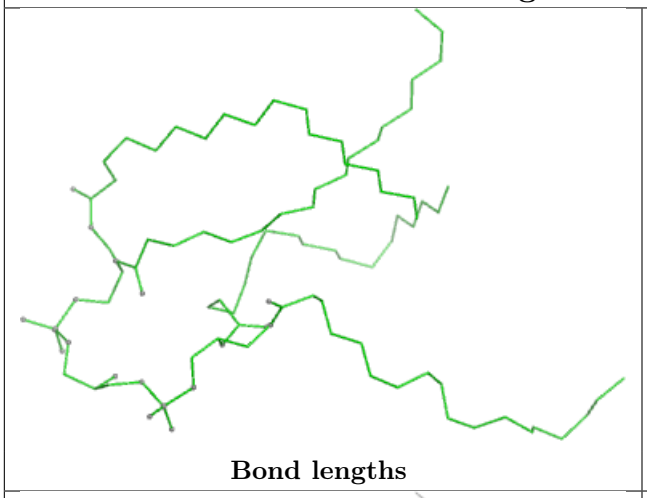


Torsions

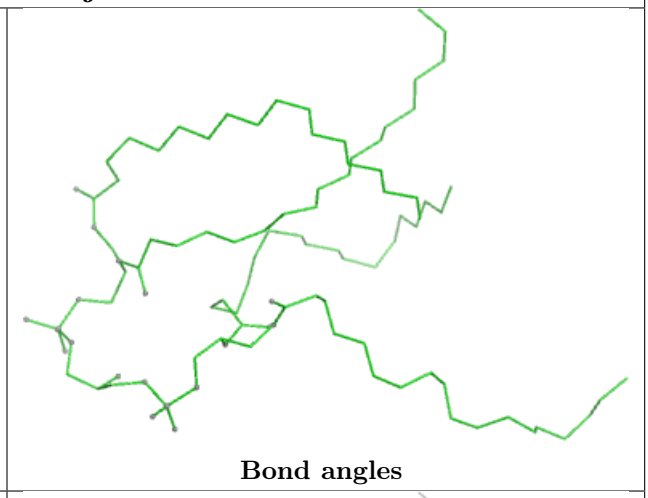


Rings

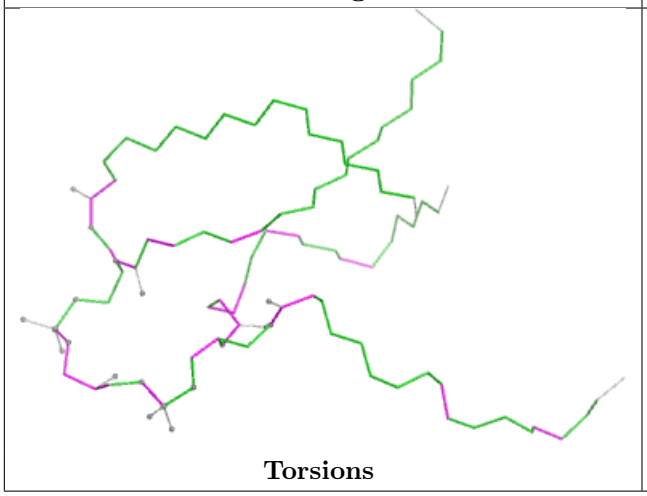
**Ligand CDL Dj 408**



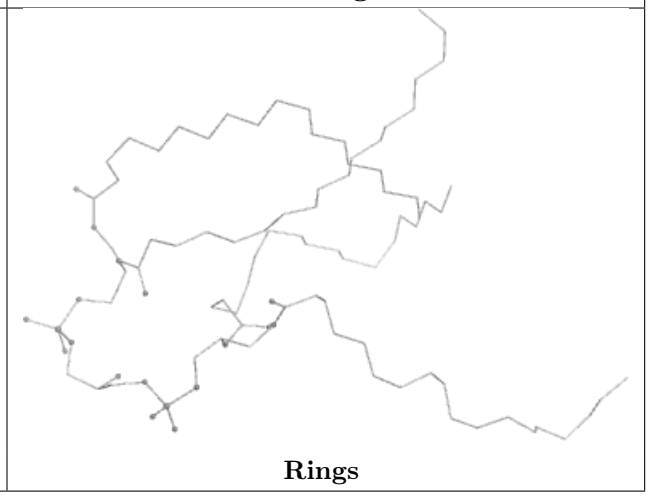
**Bond lengths**



**Bond angles**

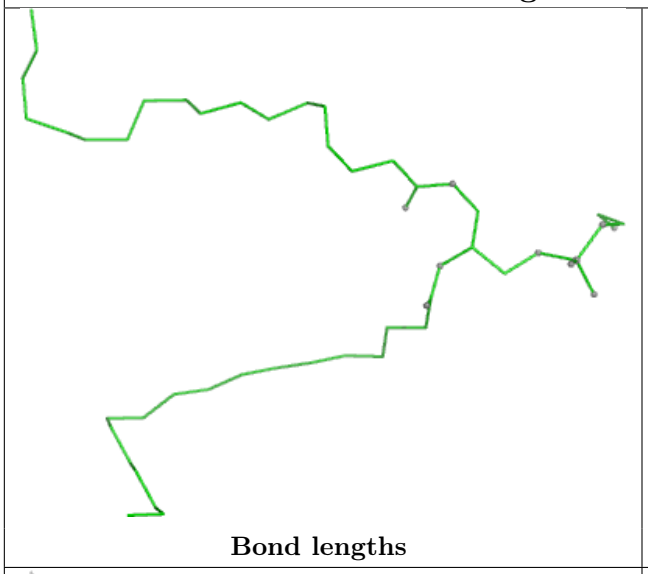


**Torsions**

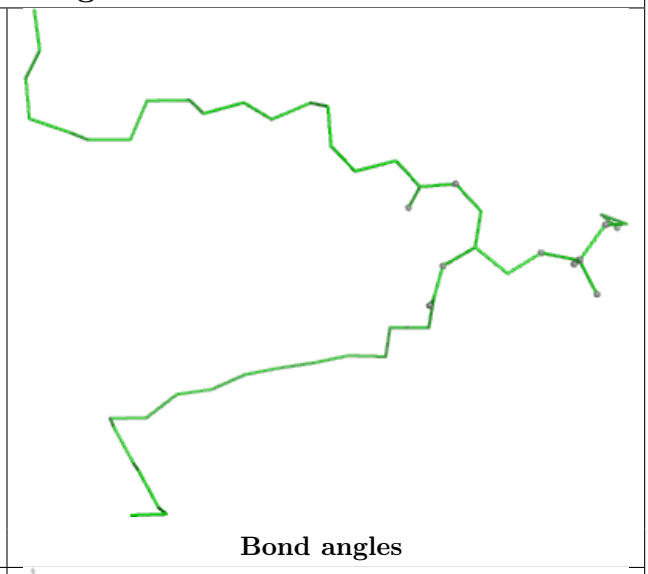


**Rings**

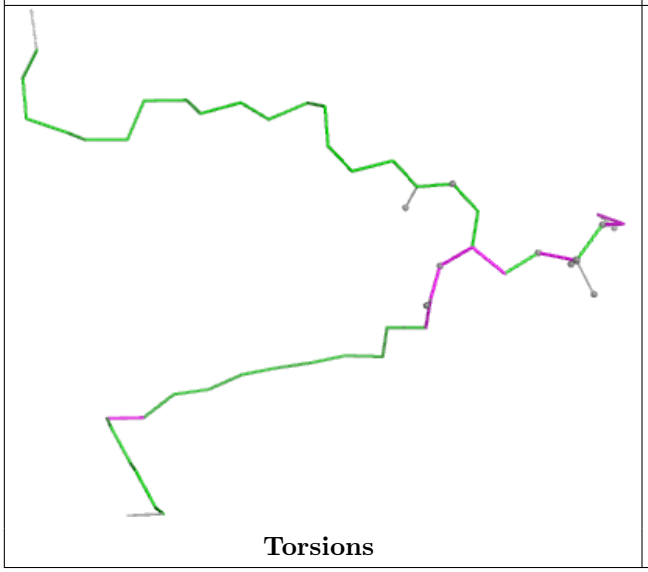
## Ligand 3PE Dg 204



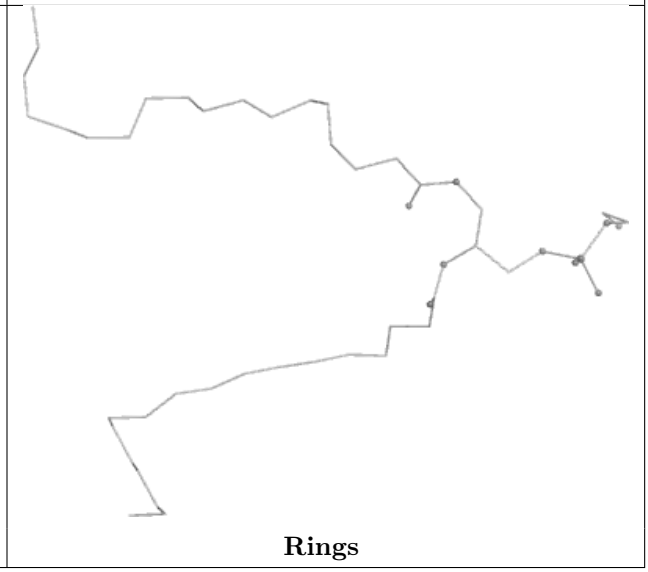
Bond lengths



Bond angles



Torsions

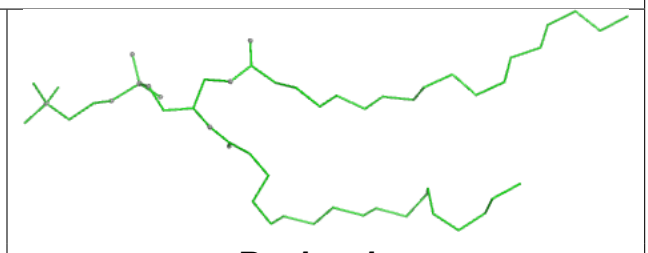


Rings

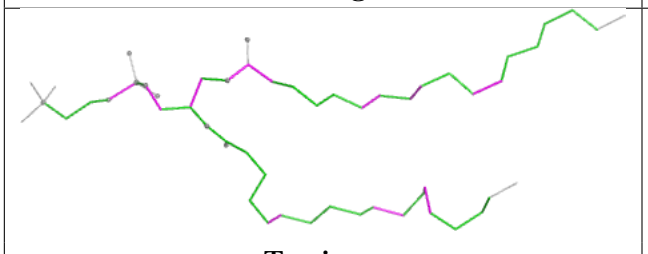
## Ligand PC1 Da 706



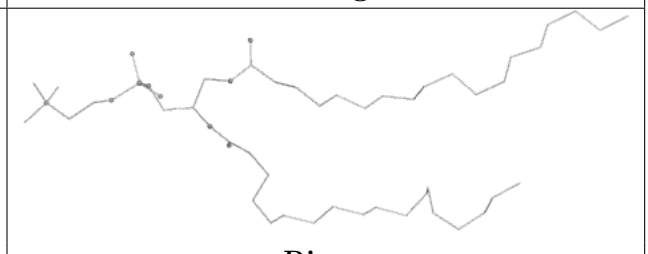
Bond lengths



Bond angles

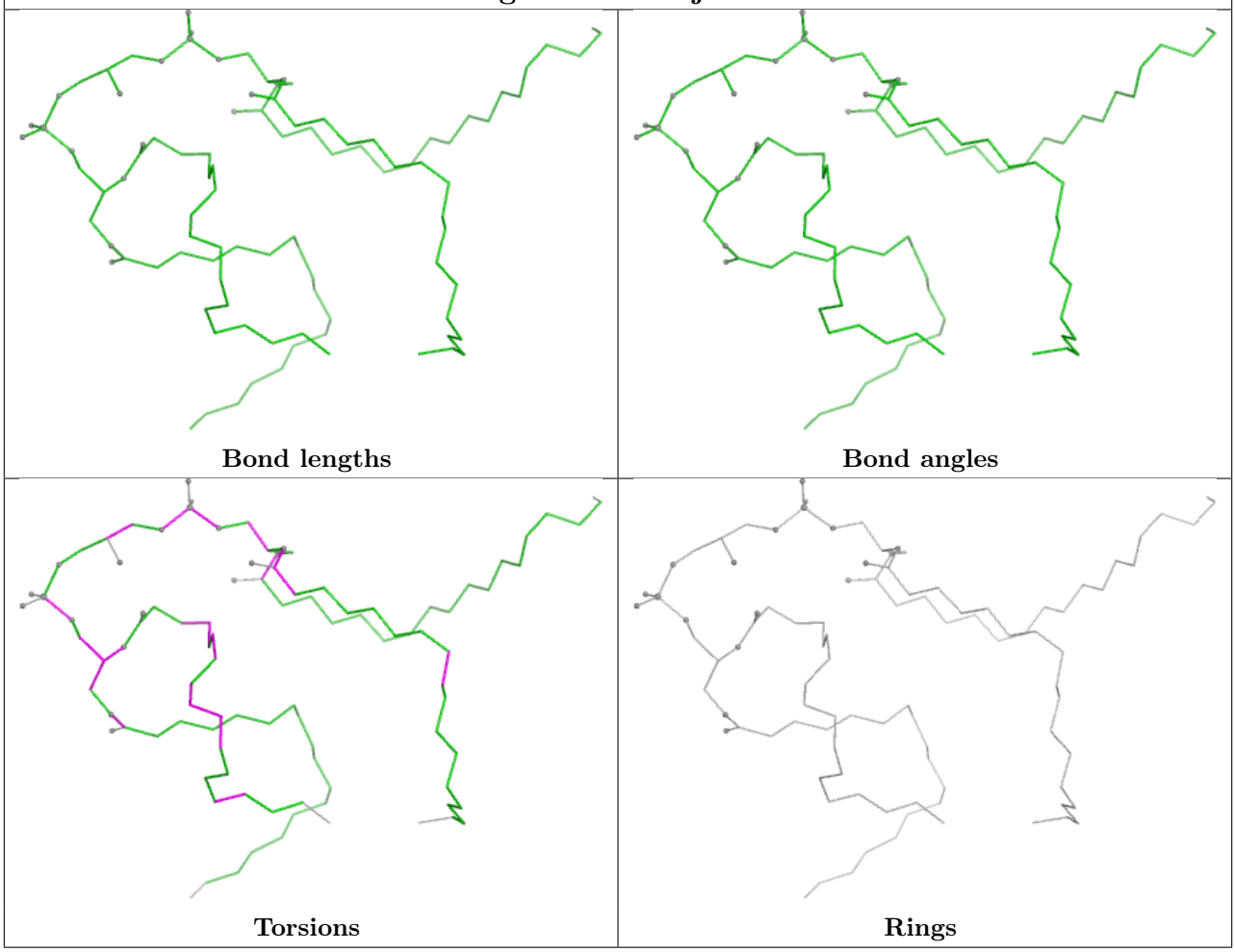


Torsions

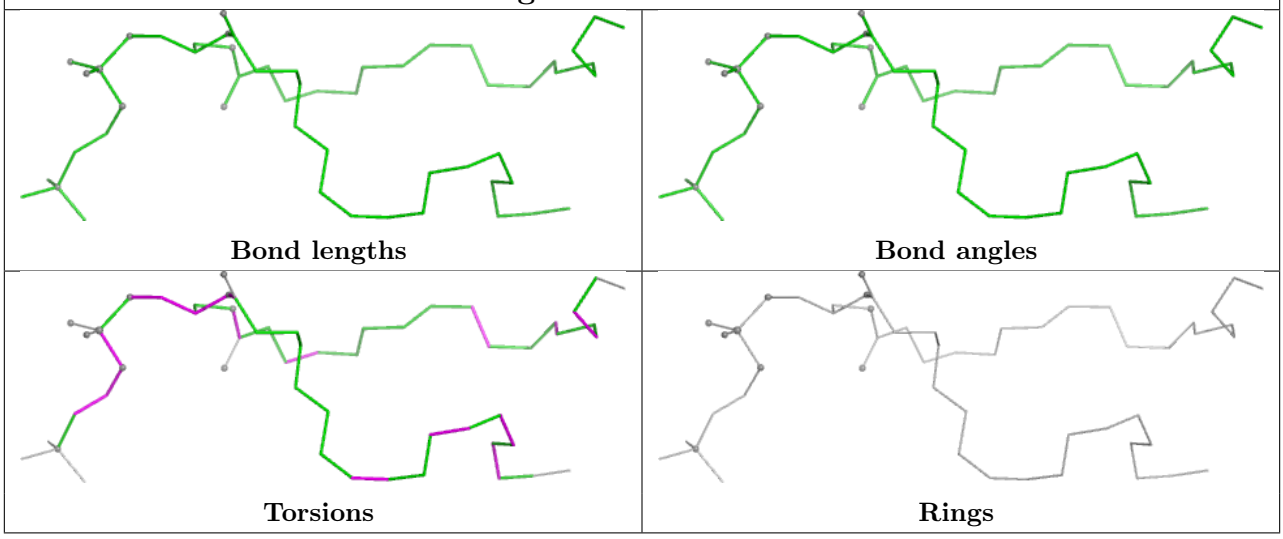


Rings

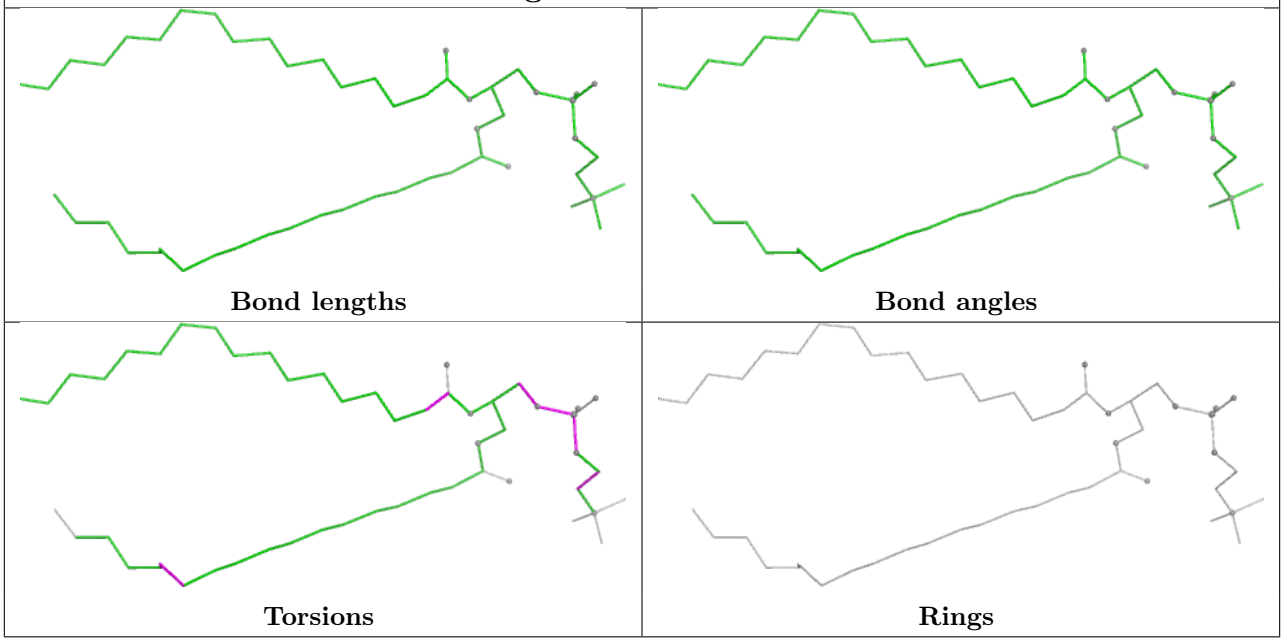
## Ligand CDL Dj 402



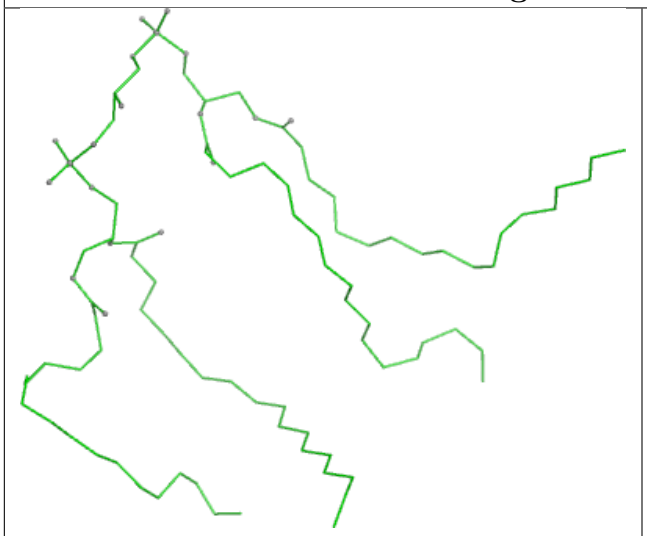

## Ligand PC1 Db 702



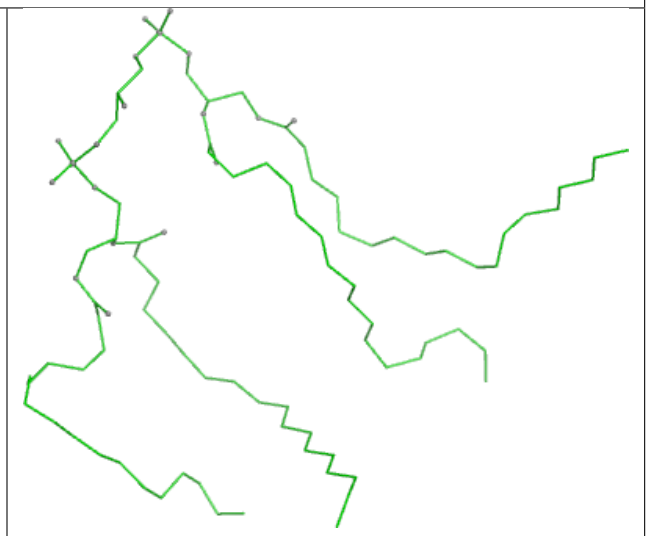
**Ligand PC1 El 904**



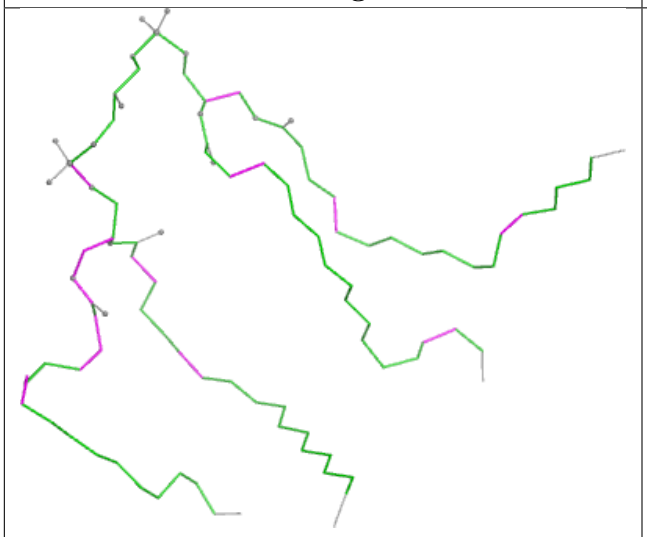
**Ligand CDL DG 202**



**Bond lengths**



**Bond angles**

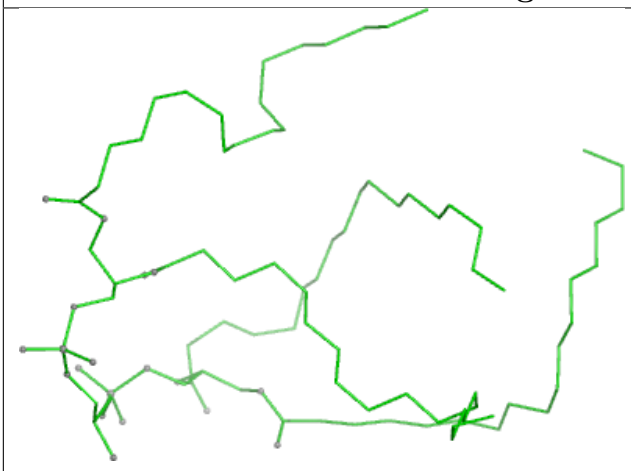


**Torsions**

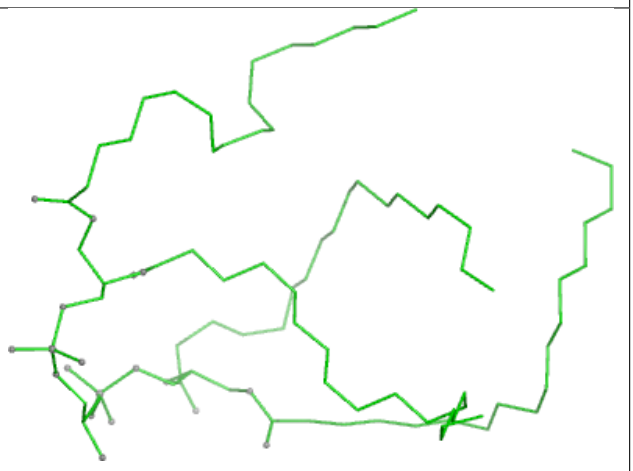


**Rings**

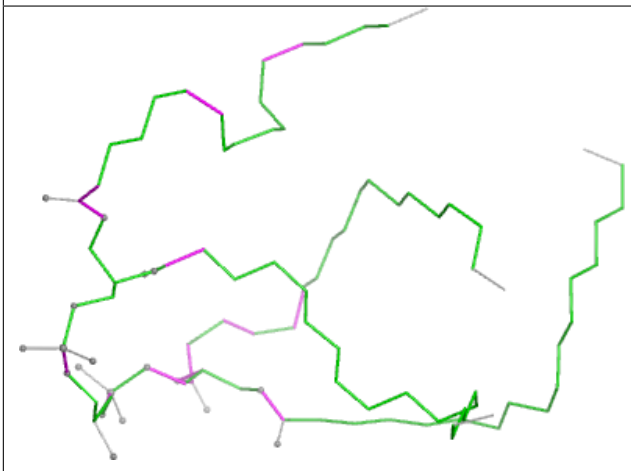
**Ligand CDL Ea 301**



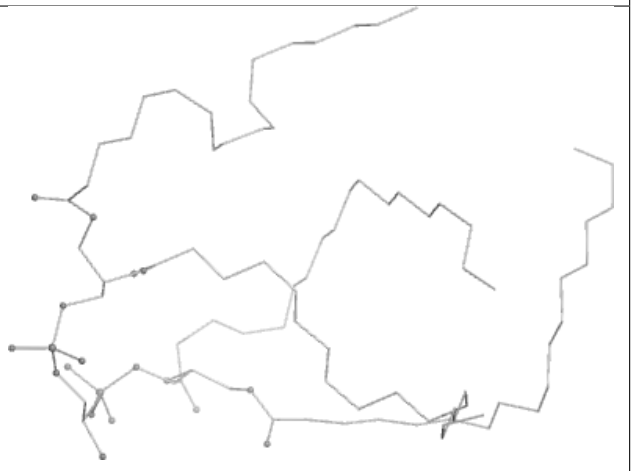
**Bond lengths**



**Bond angles**

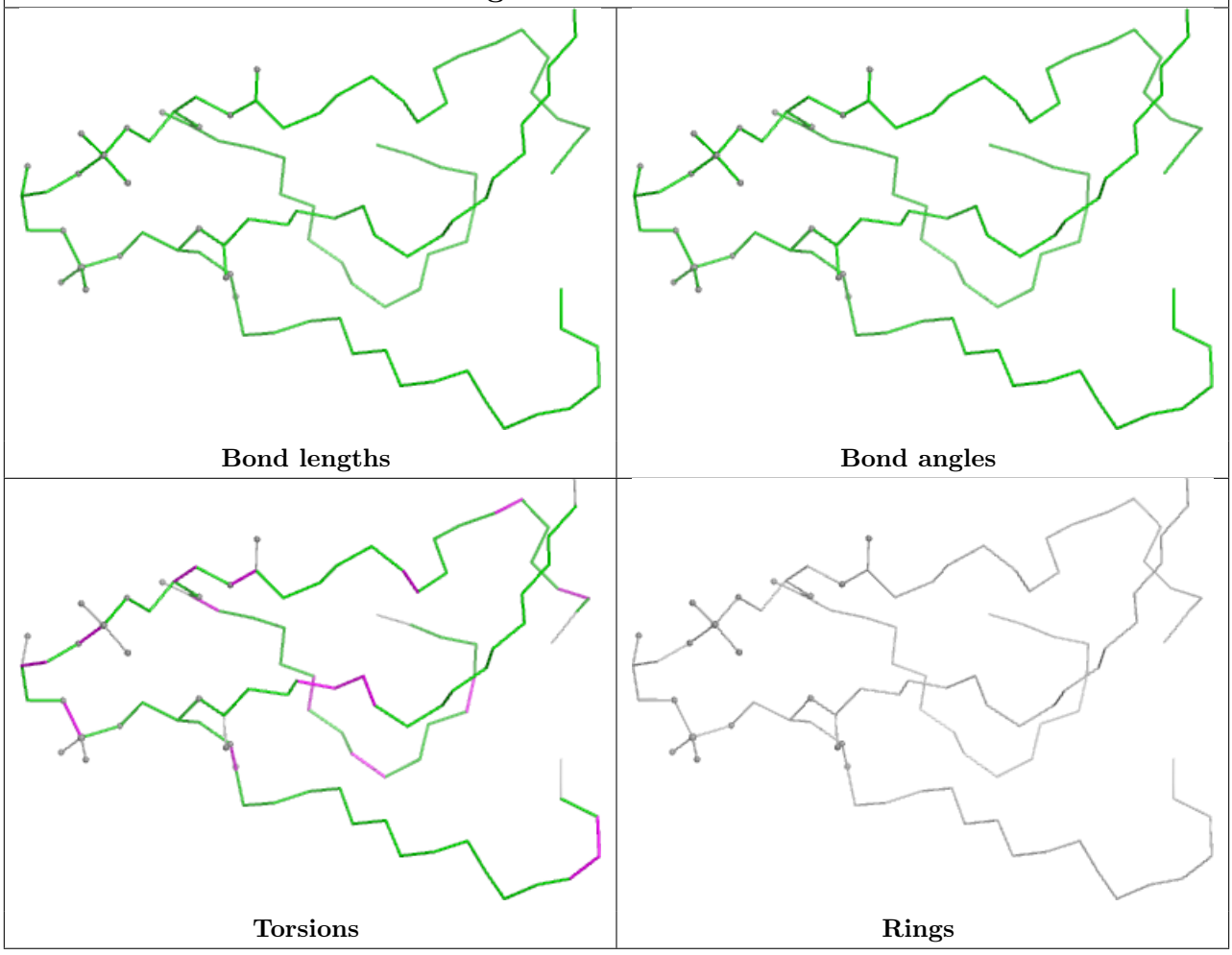


**Torsions**

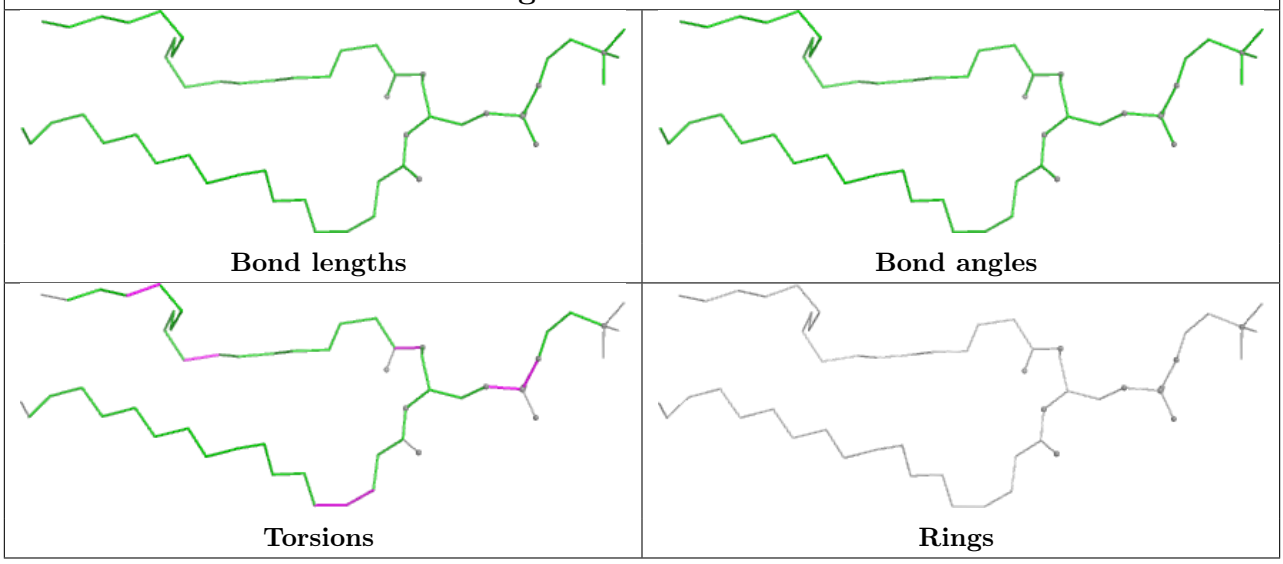


**Rings**

**Ligand CDL En 1201**



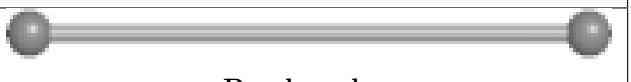

**Ligand PC1 DJ 306**



## Ligand CUA Db 701



Bond lengths



Bond angles

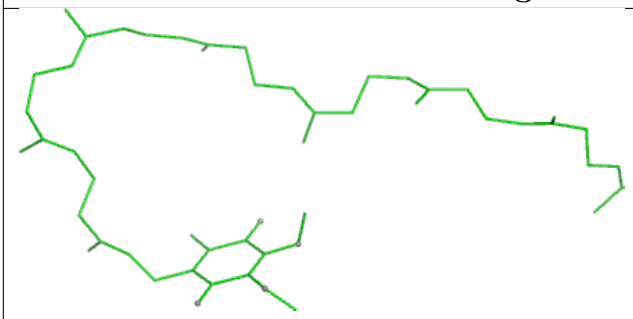


Torsions

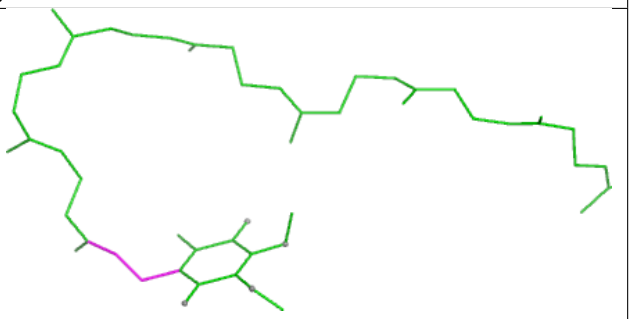


Rings

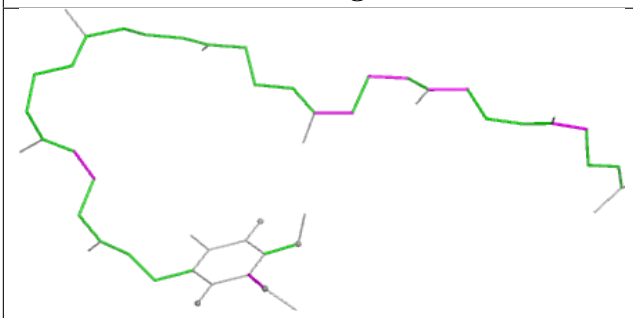
## Ligand UQ8 DS 404



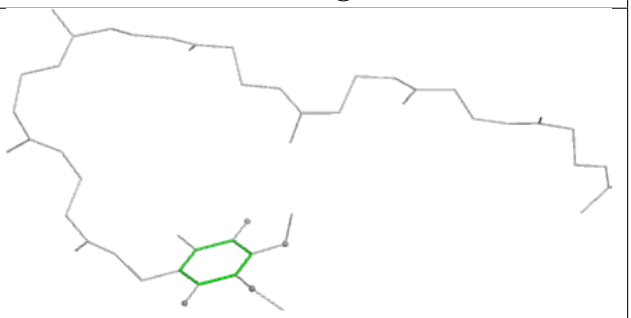
Bond lengths



Bond angles

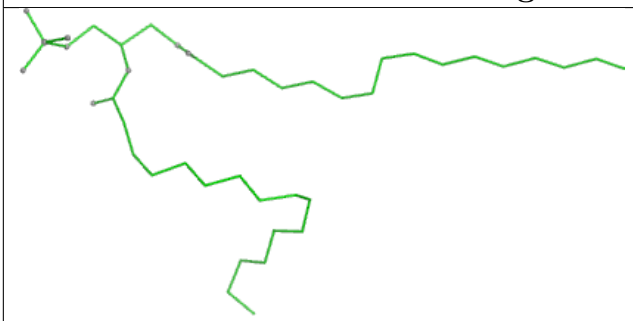


Torsions

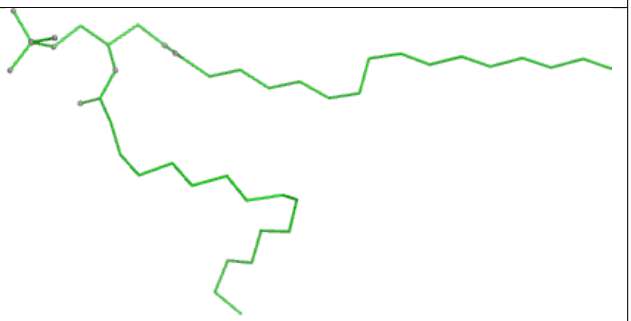


Rings

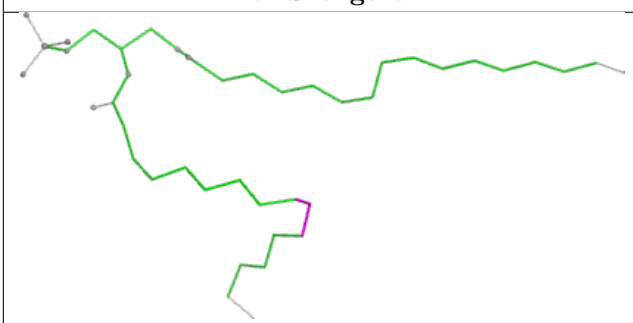
## Ligand LPP Ed 203



Bond lengths



Bond angles

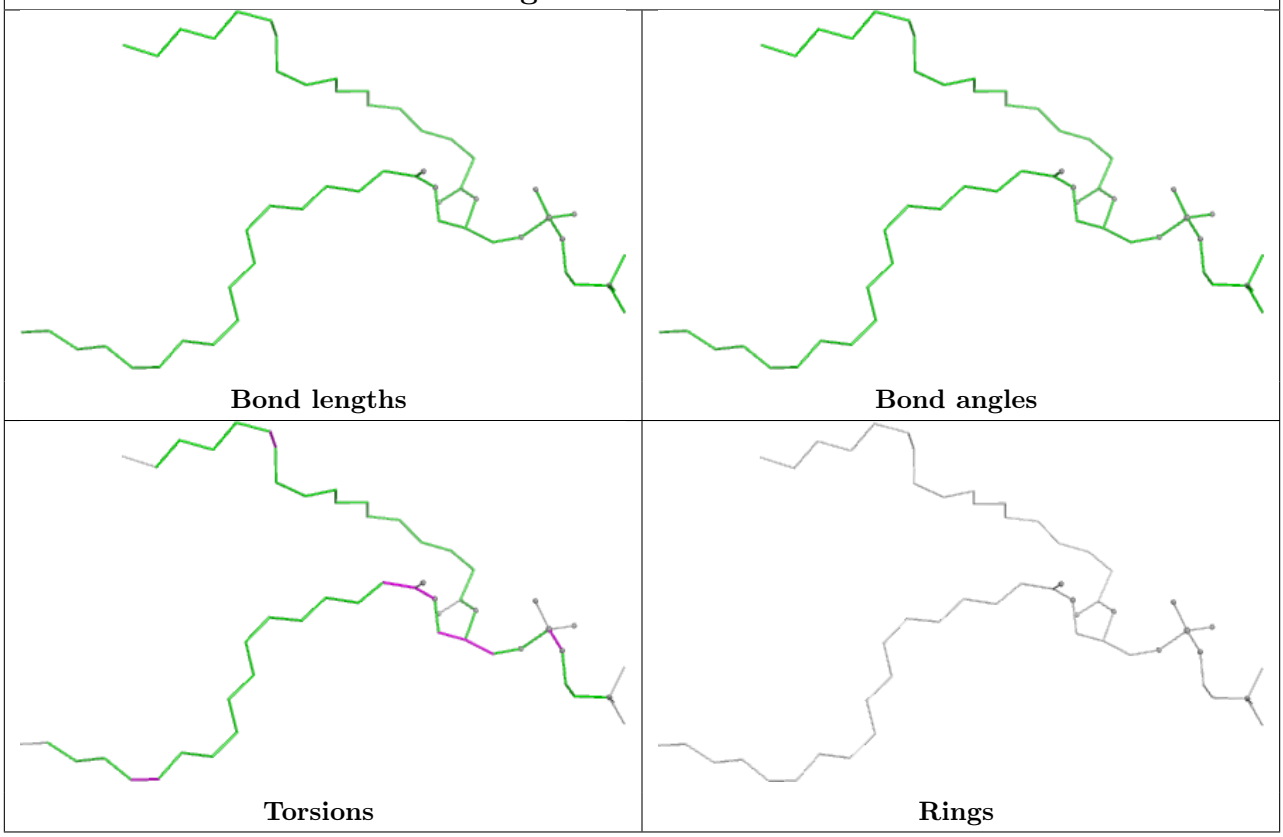


Torsions

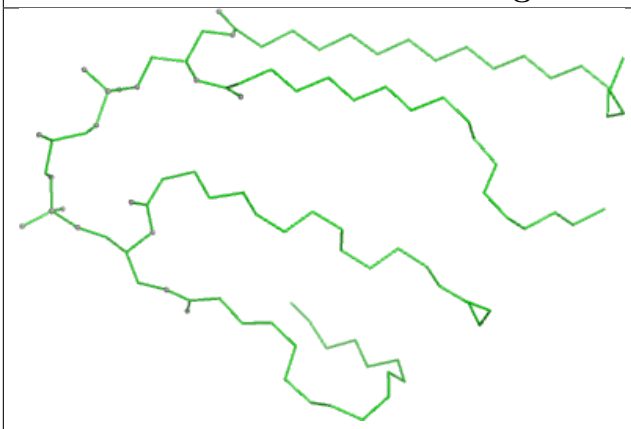


Rings

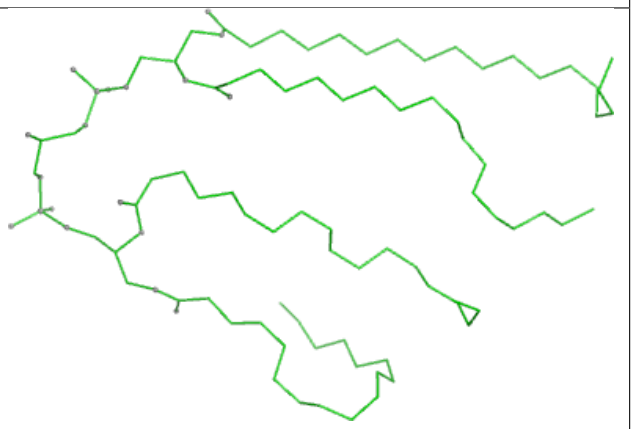
**Ligand PC1 Ds 406**



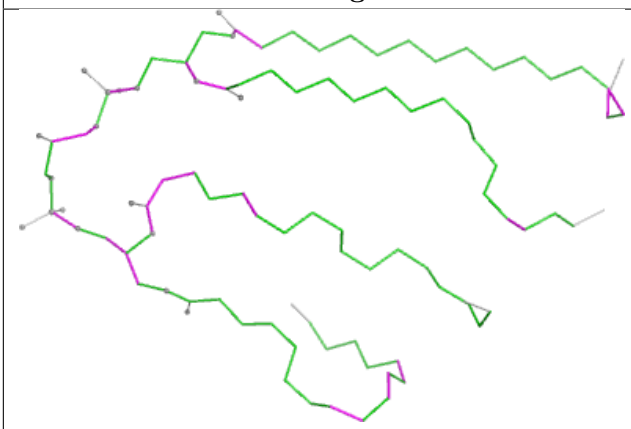
**Ligand CDL Dd 705**



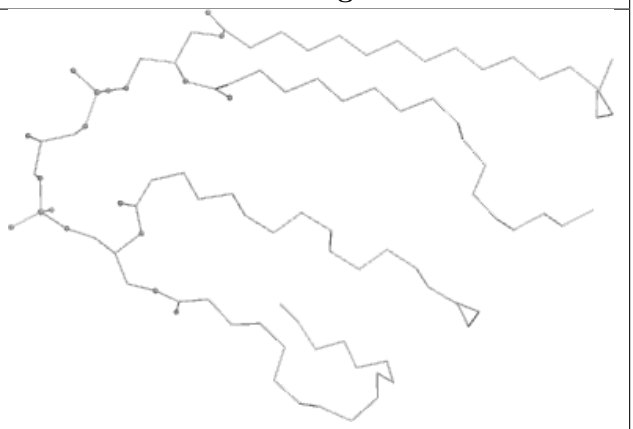
**Bond lengths**



**Bond angles**

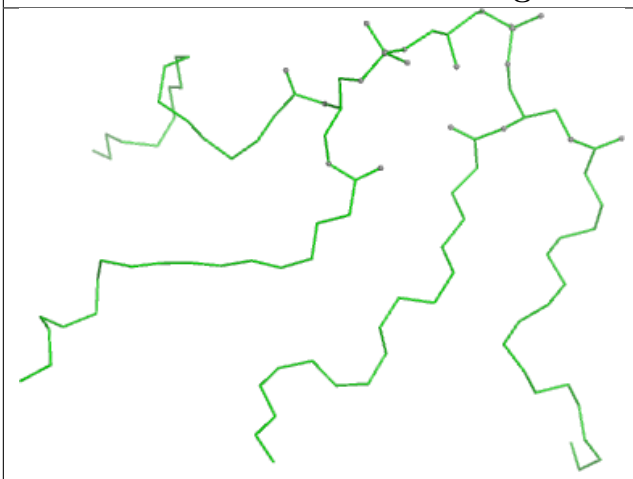


**Torsions**

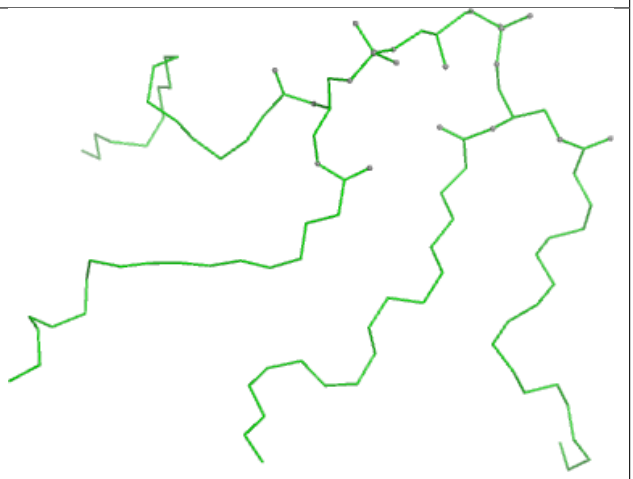


**Rings**

**Ligand CDL Dv 401**



**Bond lengths**



**Bond angles**

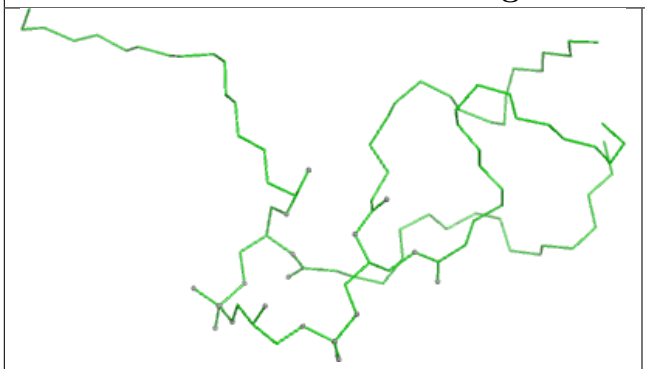


**Torsions**



**Rings**

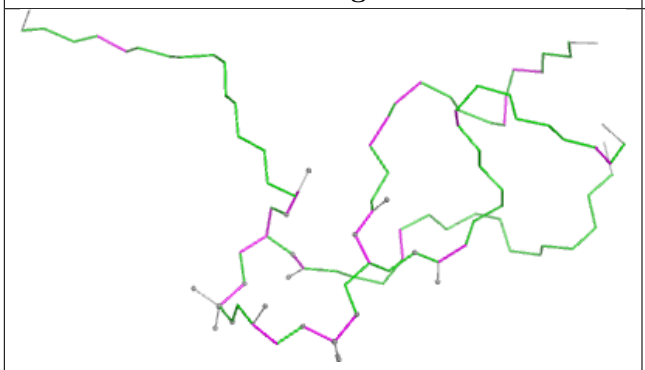
**Ligand CDL DQ 1501**



**Bond lengths**



**Bond angles**

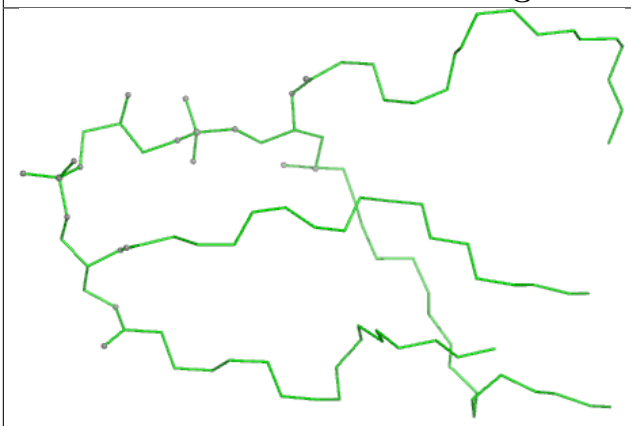


**Torsions**

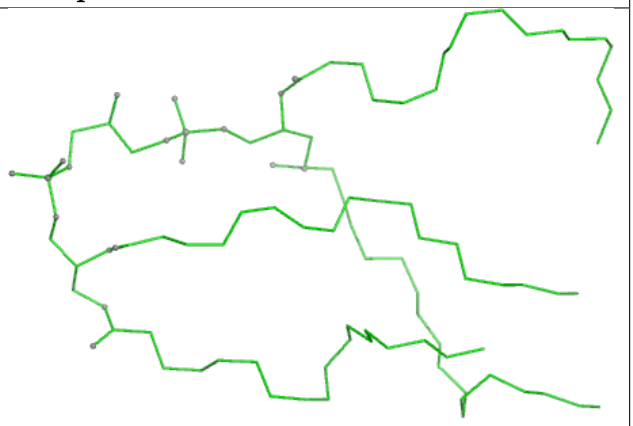


**Rings**

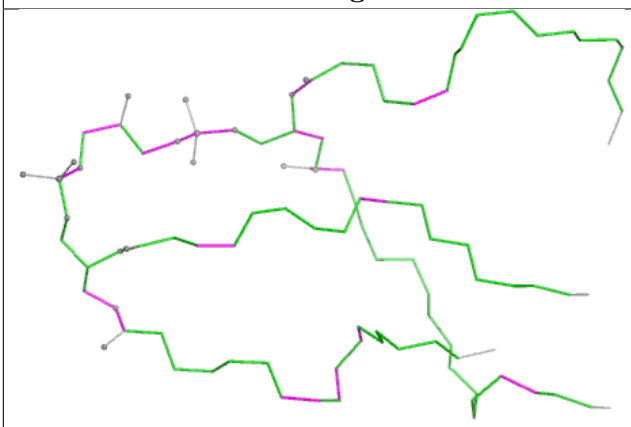
**Ligand CDL Dq 401**



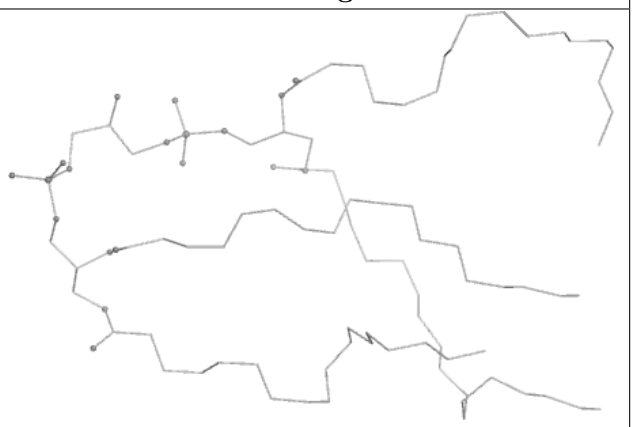
**Bond lengths**



**Bond angles**

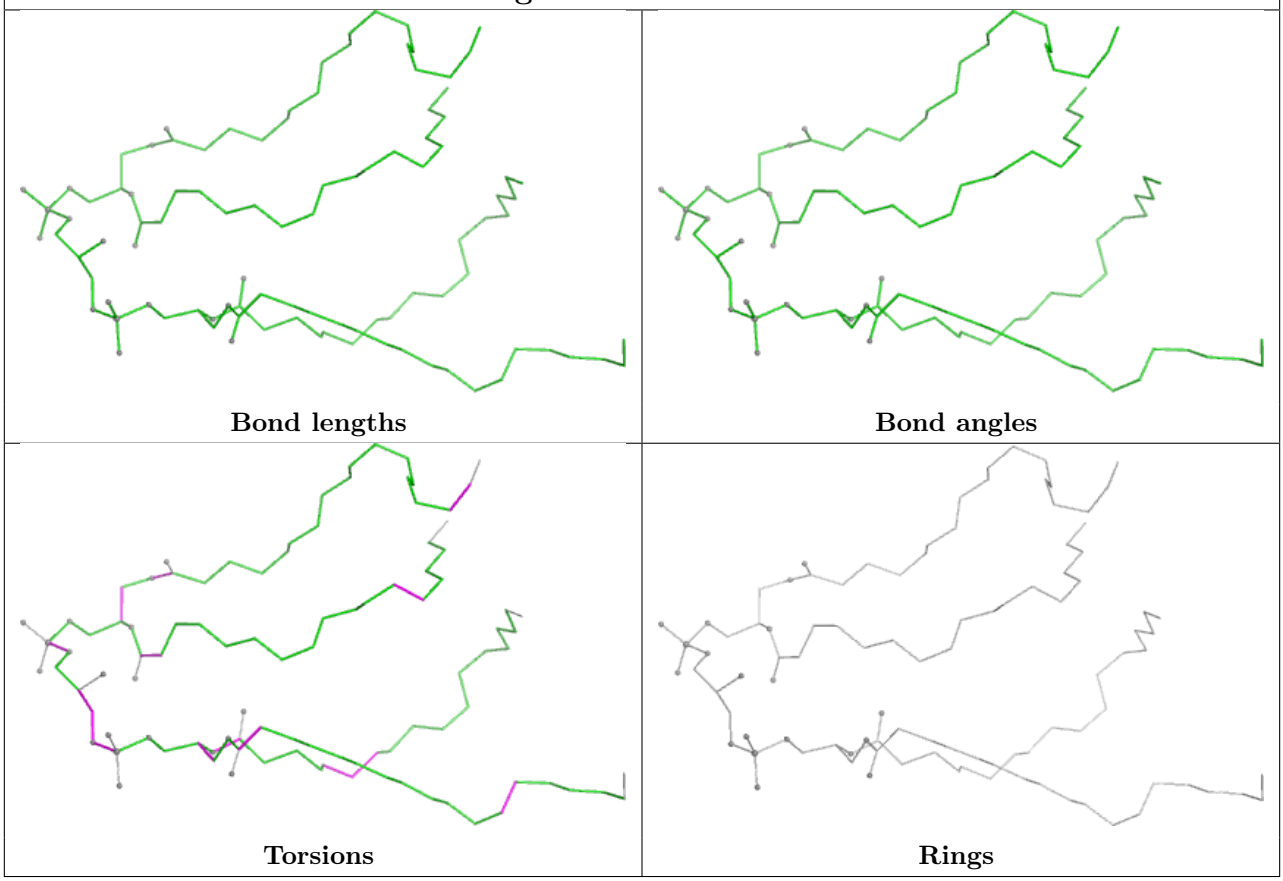


**Torsions**

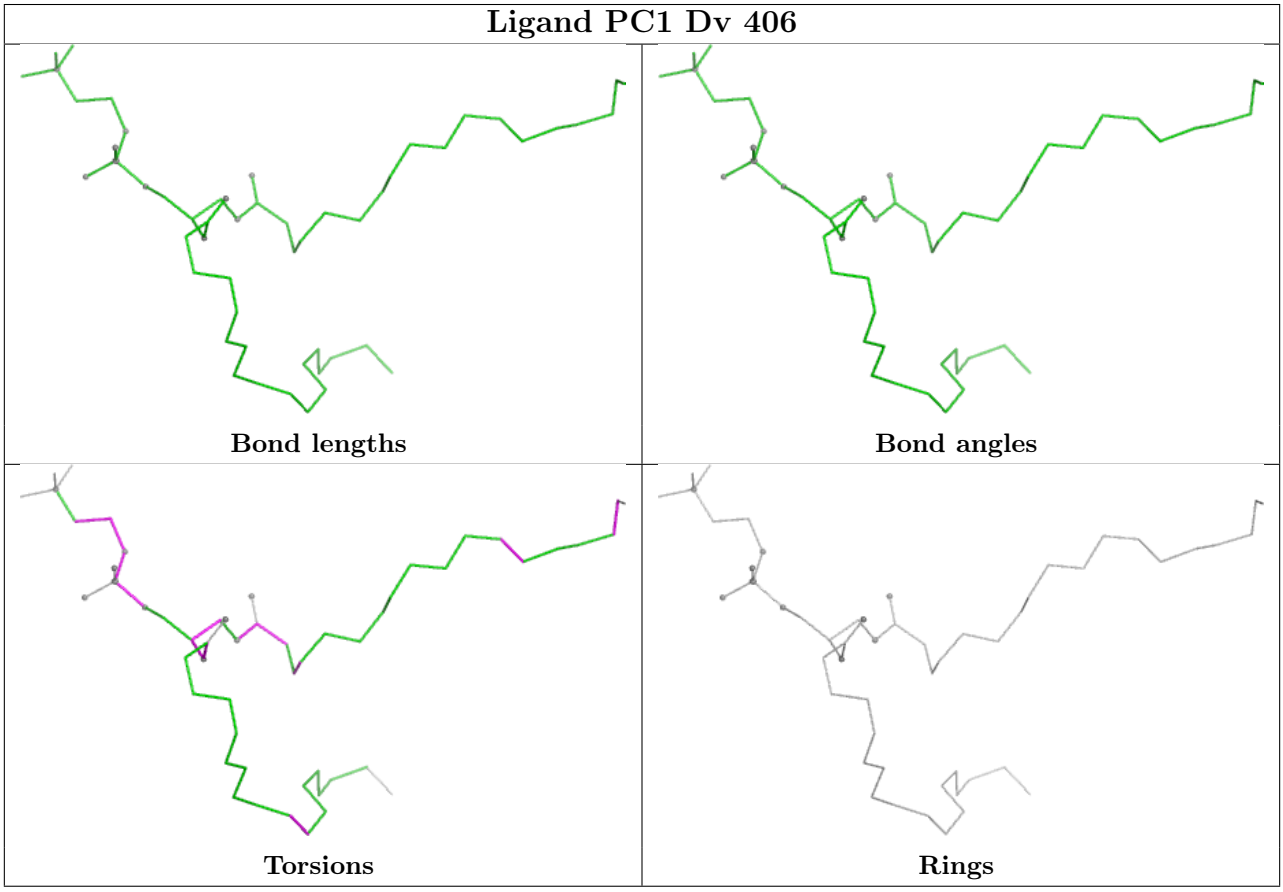


**Rings**

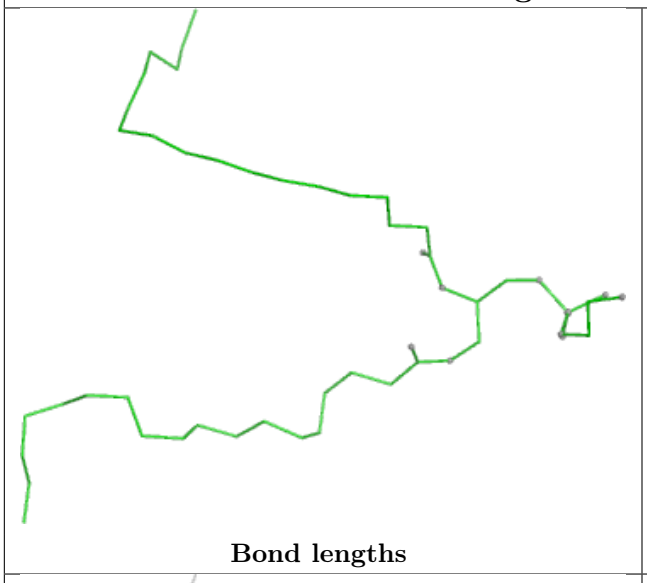
## Ligand CDL DJ 302



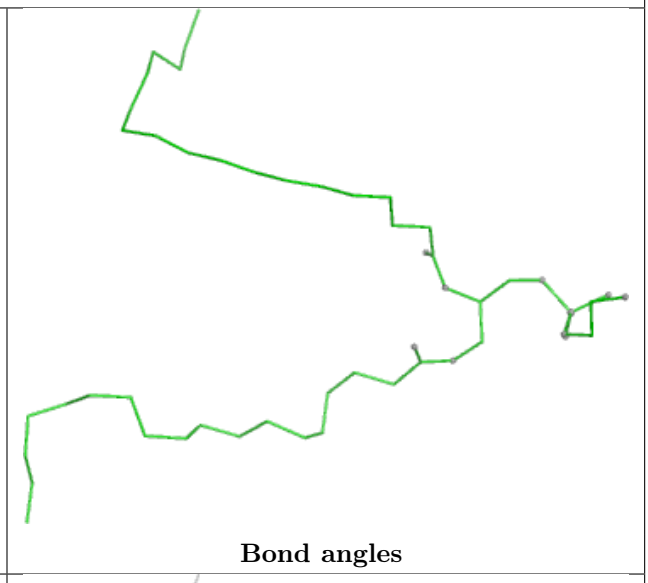

## Ligand PC1 Dv 406



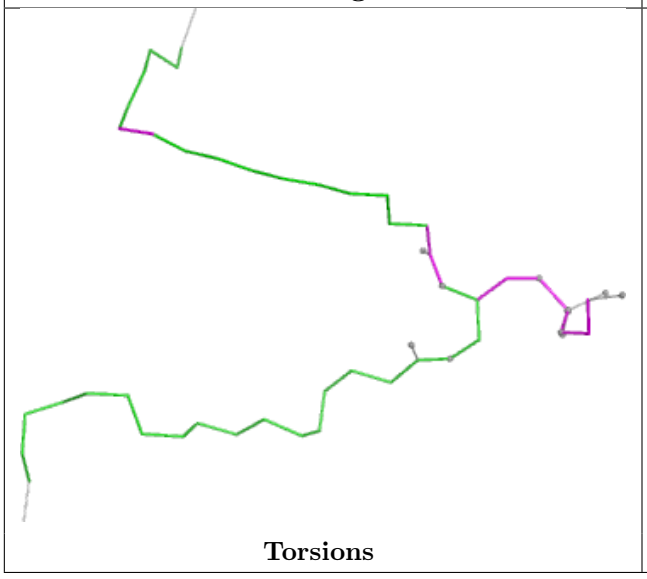
**Ligand 3PE DG 204**



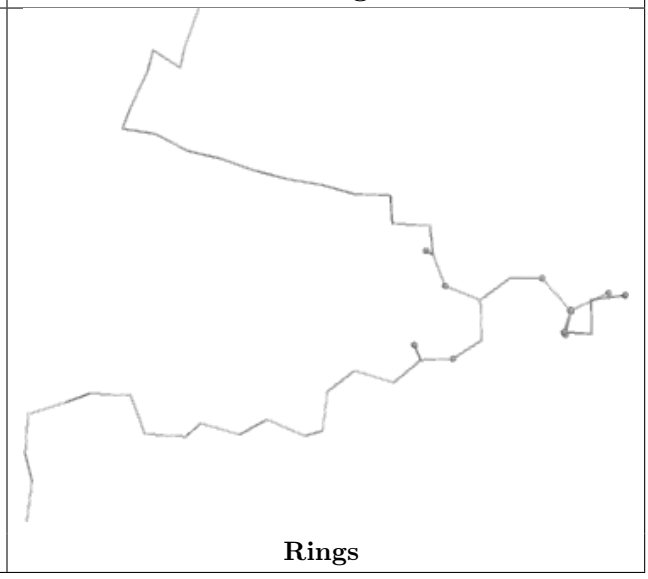
**Bond lengths**



**Bond angles**

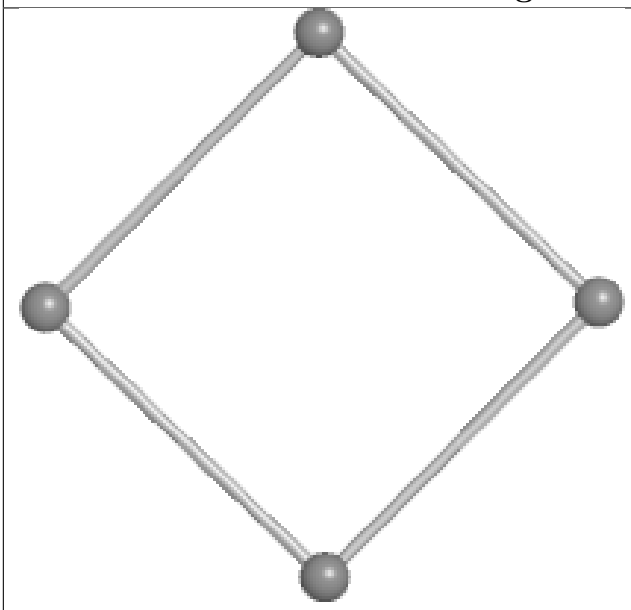


**Torsions**

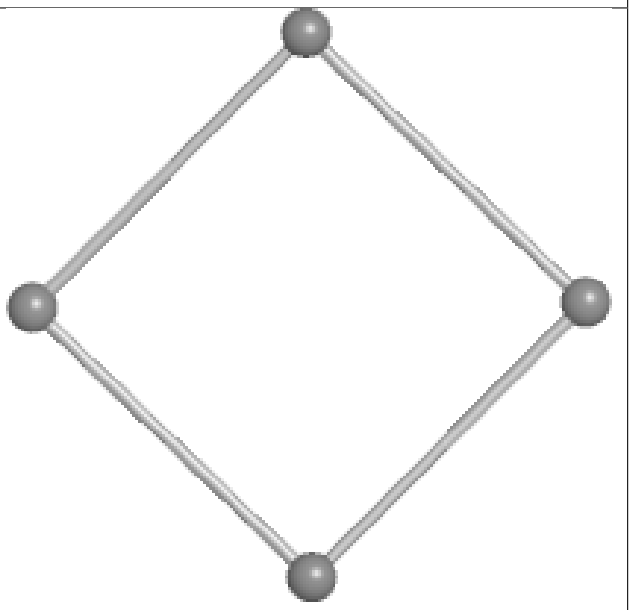


**Rings**

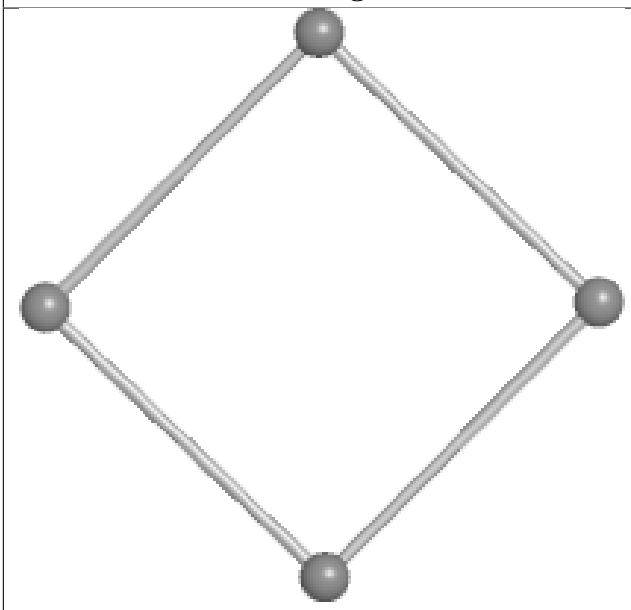
**Ligand FES Ef 1002**



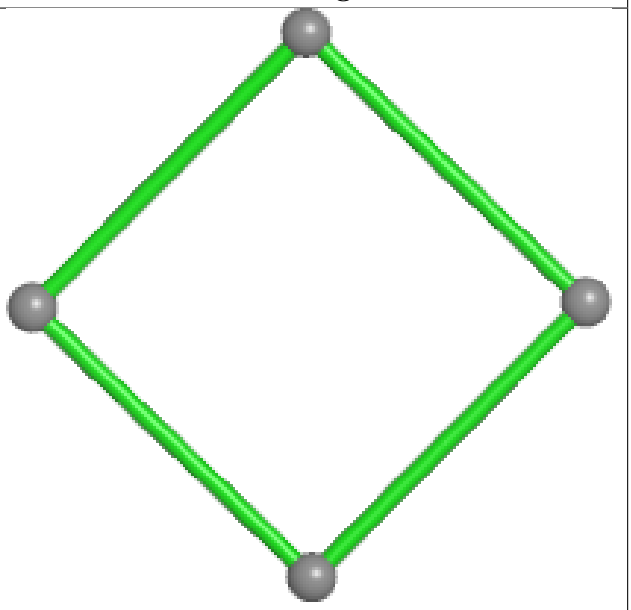
**Bond lengths**



**Bond angles**

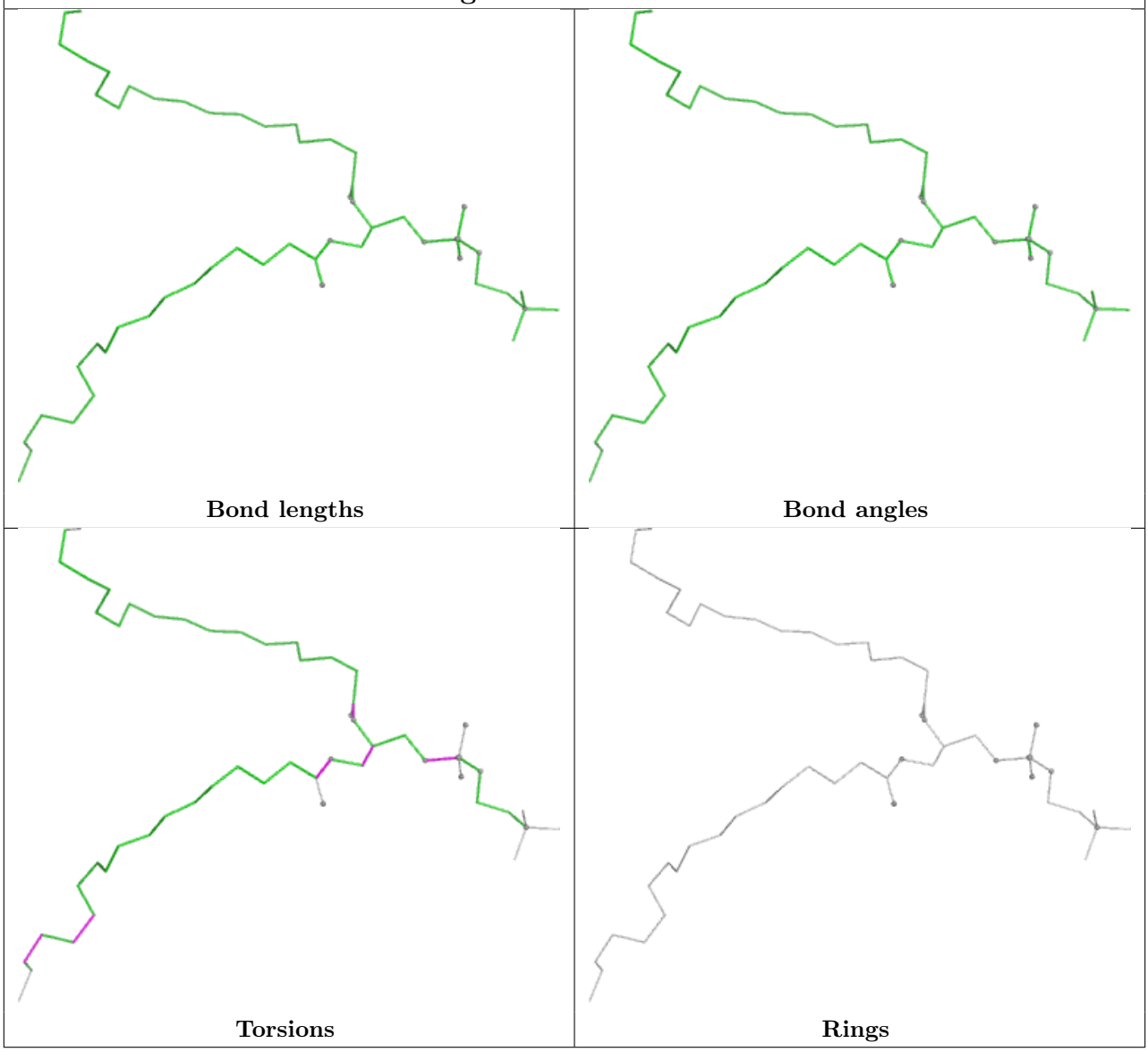


**Torsions**

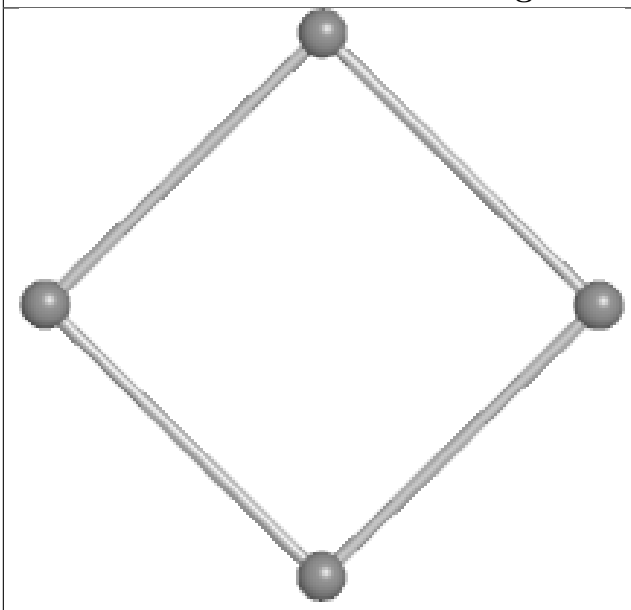


**Rings**

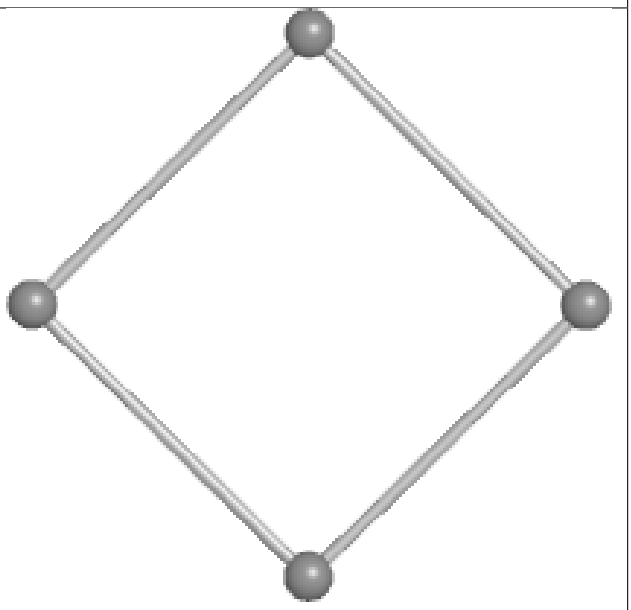
**Ligand PC1 DA 707**



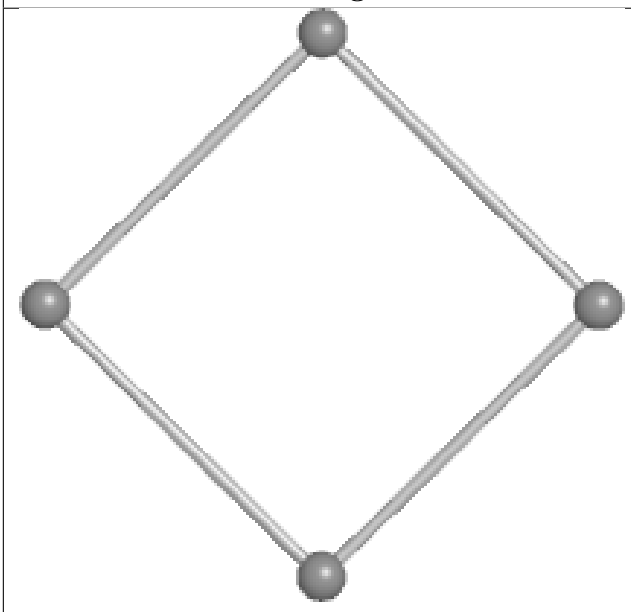
**Ligand FES Ef 1003**



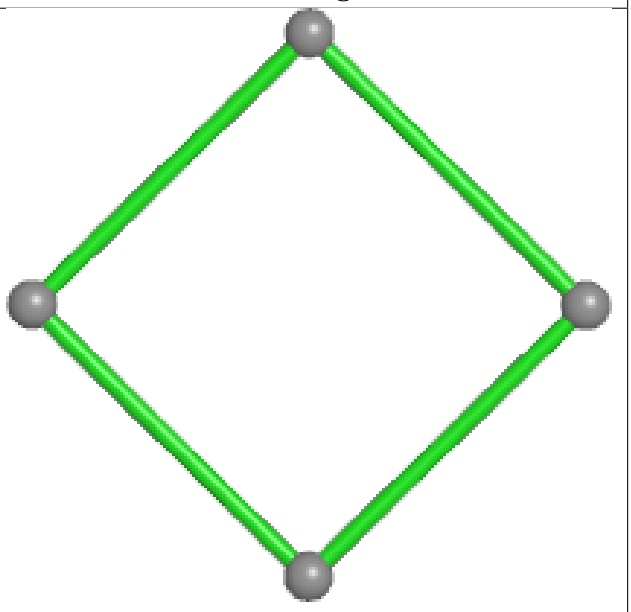
**Bond lengths**



**Bond angles**

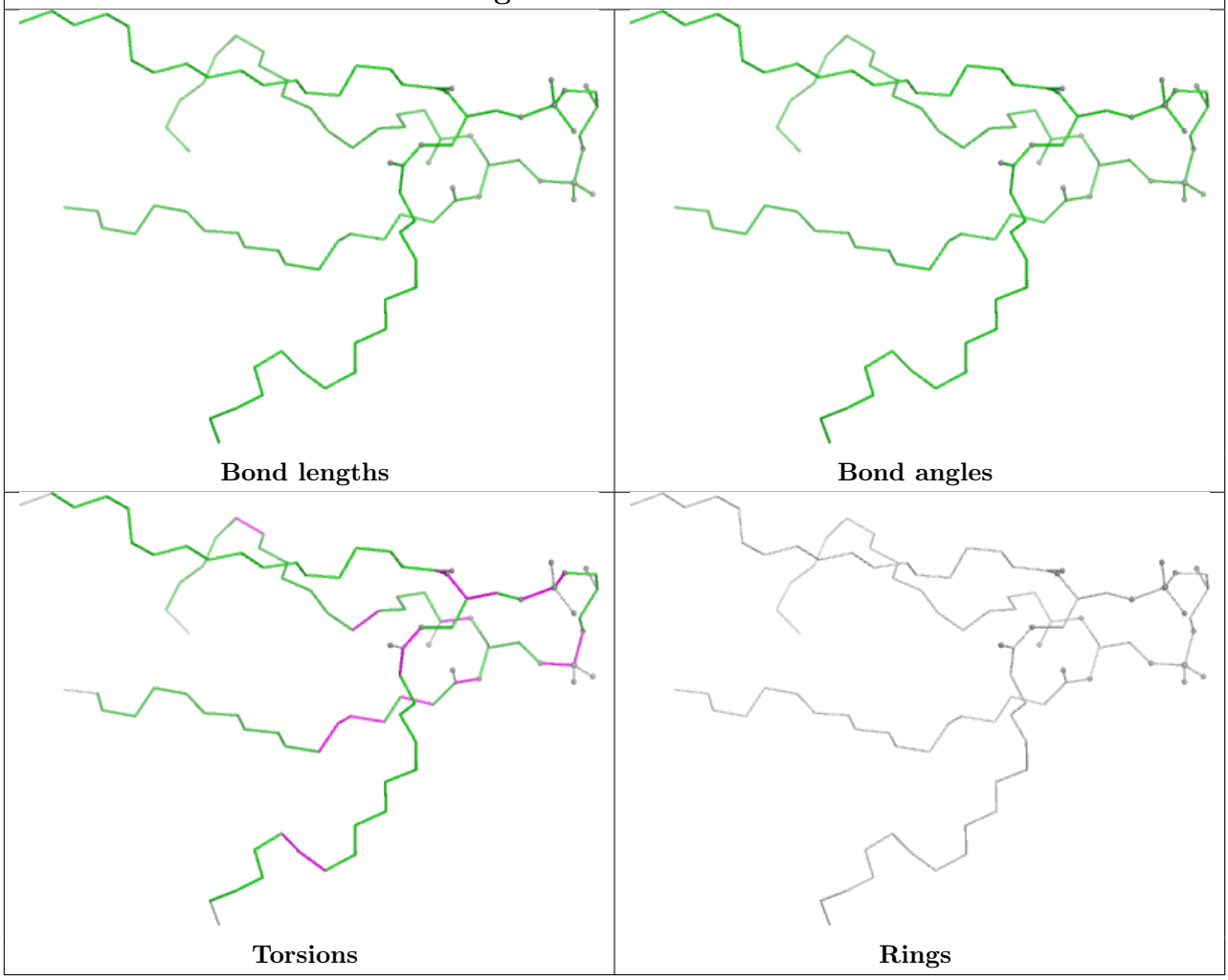


**Torsions**

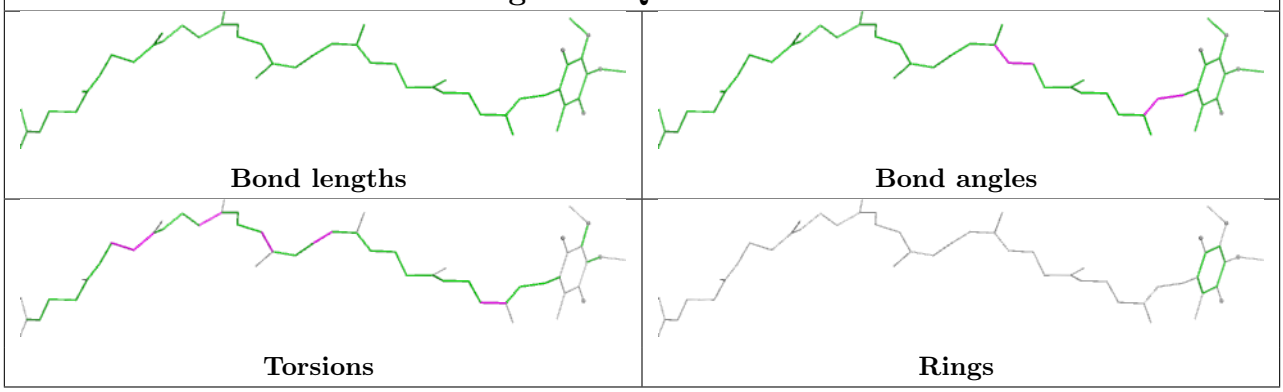


**Rings**

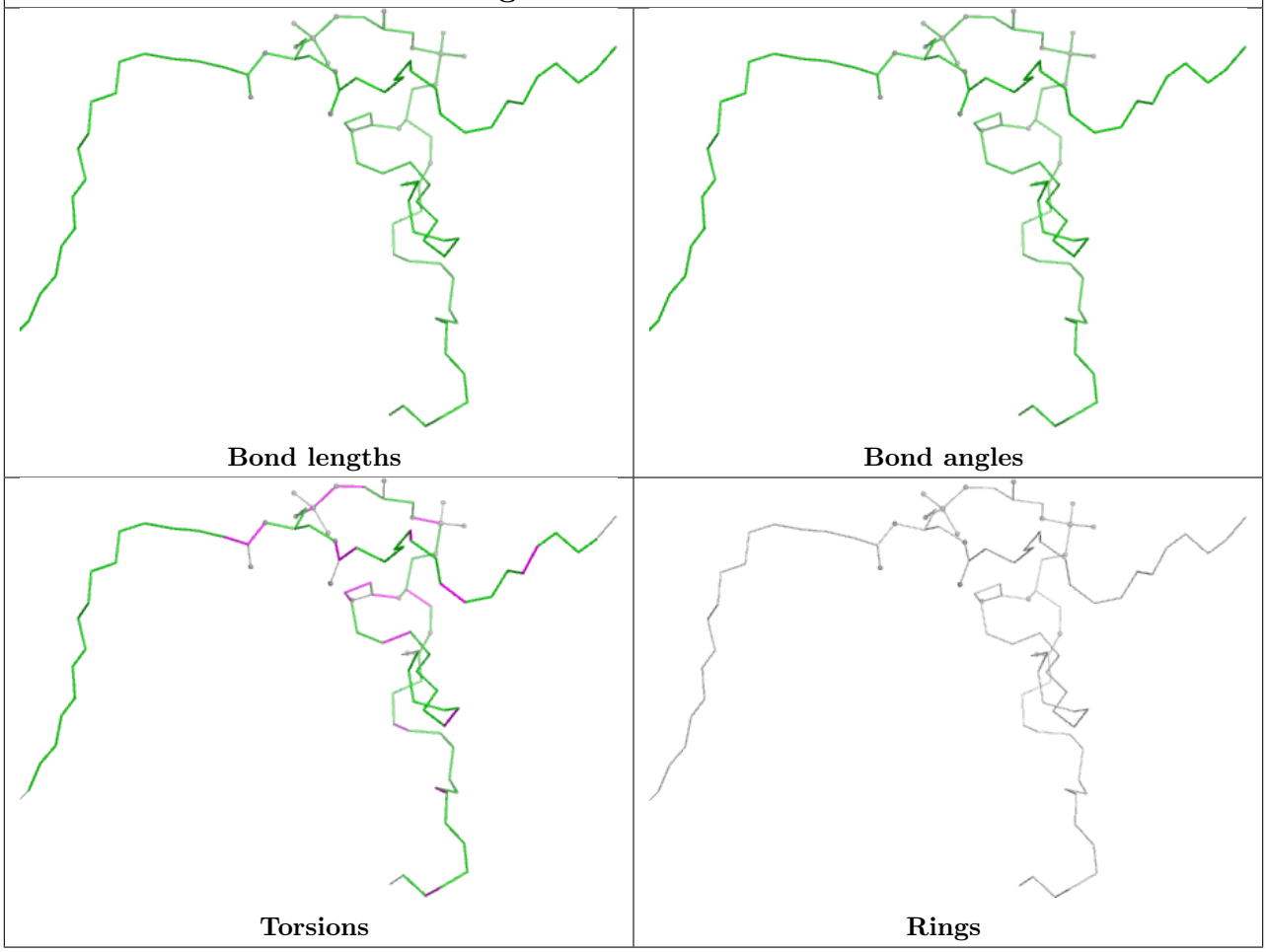
## Ligand CDL Dc 601



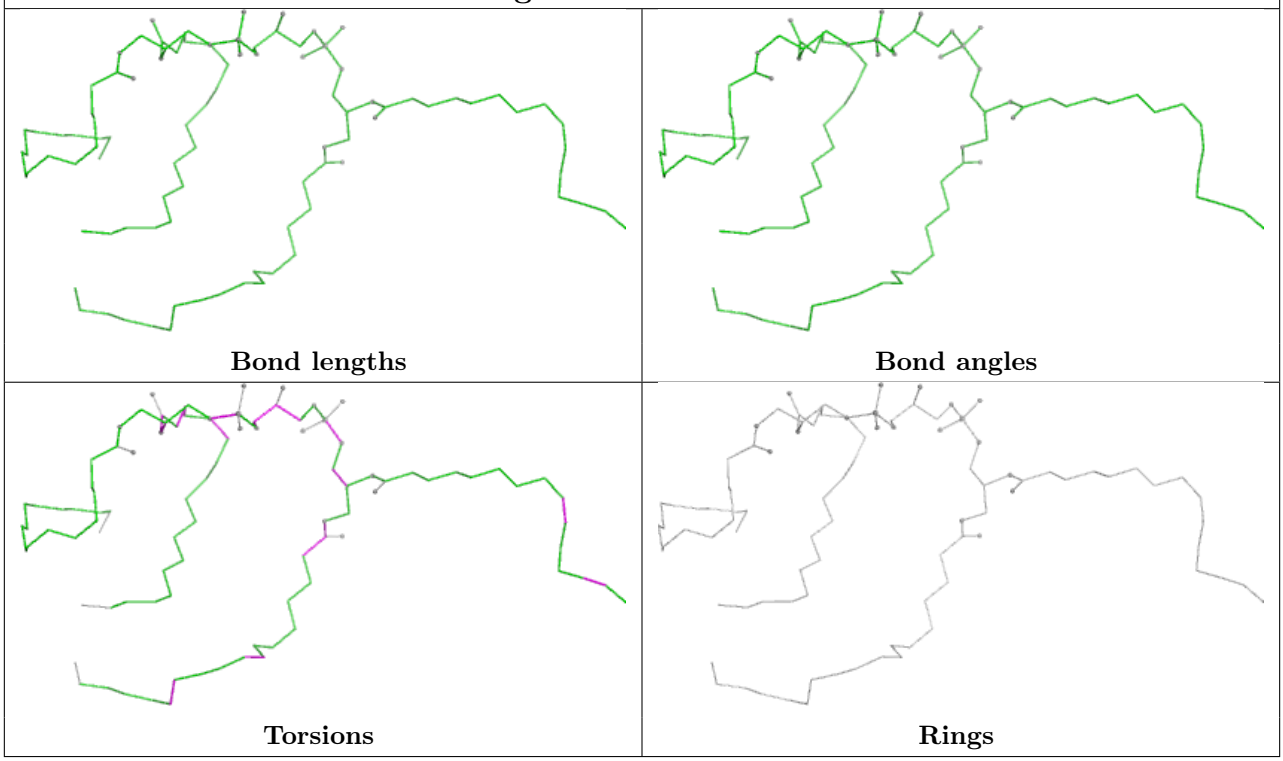

## Ligand UQ8 En 1203



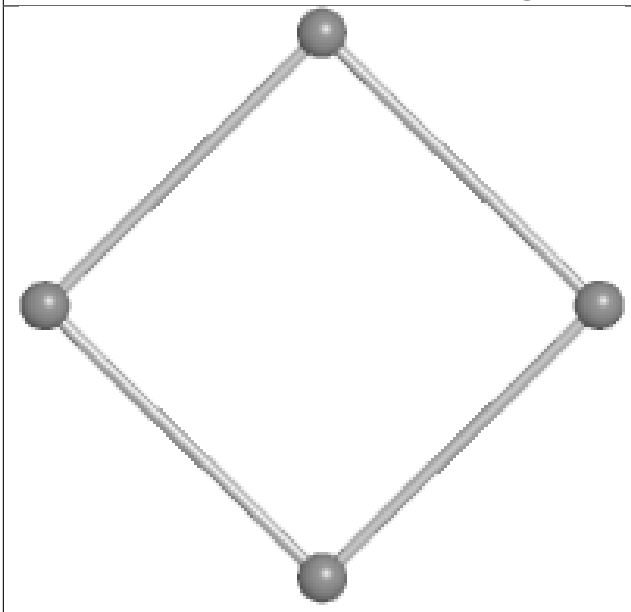
## Ligand CDL Dx 1201



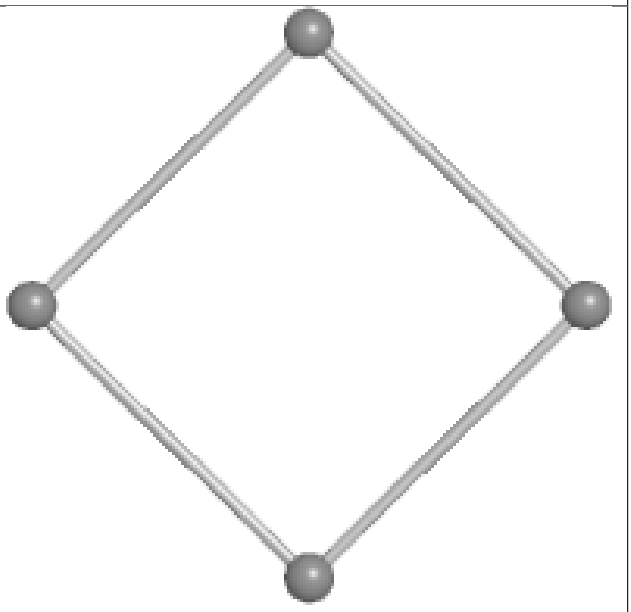

## Ligand CDL Du 404



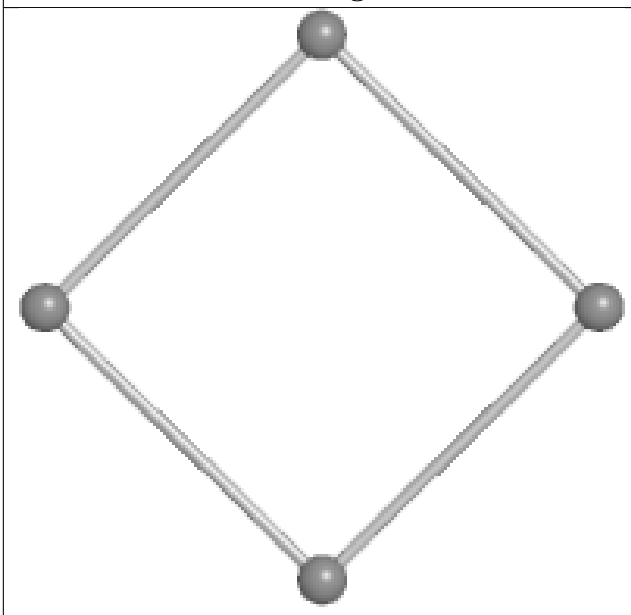
**Ligand FES EF 201**



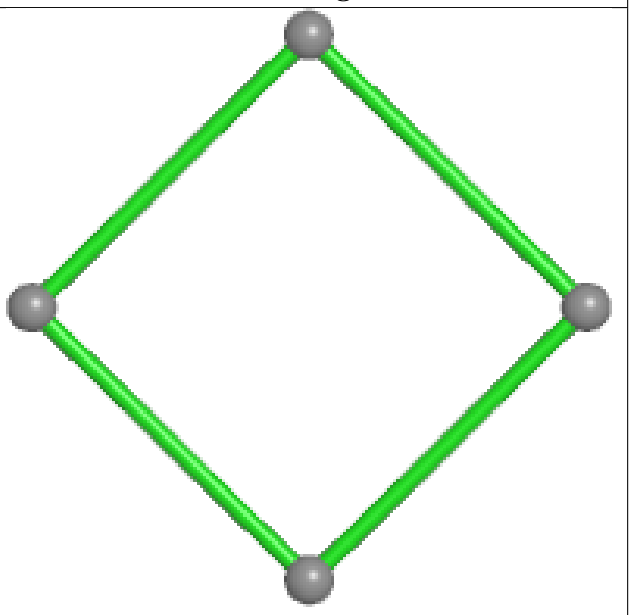
**Bond lengths**



**Bond angles**

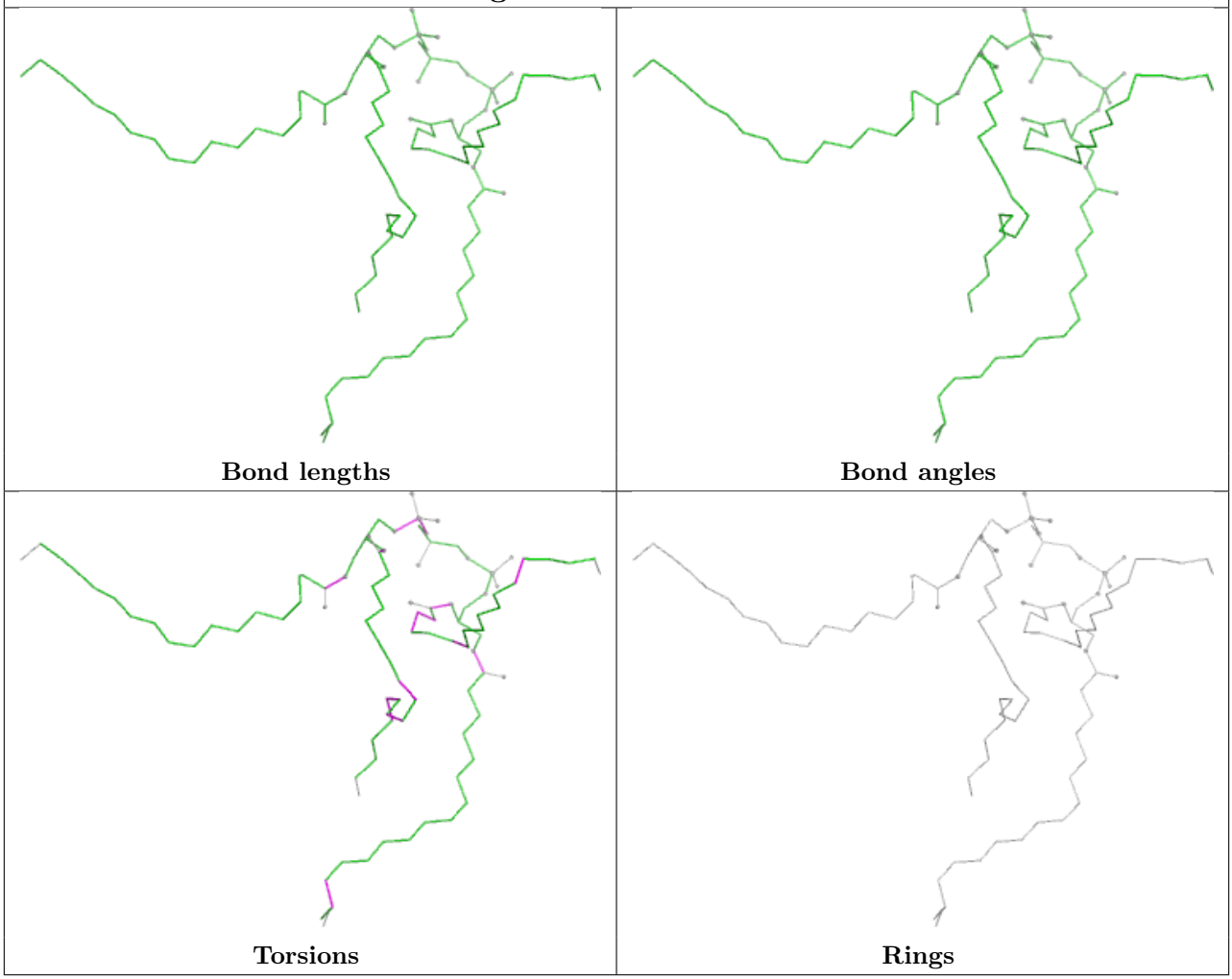


**Torsions**



**Rings**

**Ligand CDL DU 402**



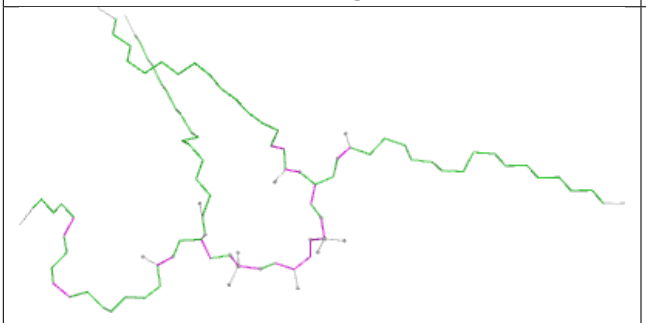
## Ligand CDL Ed 204



Bond lengths



Bond angles

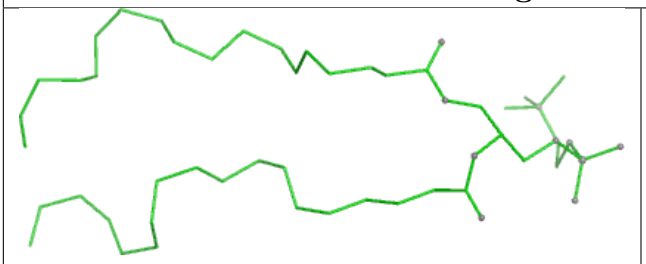


Torsions

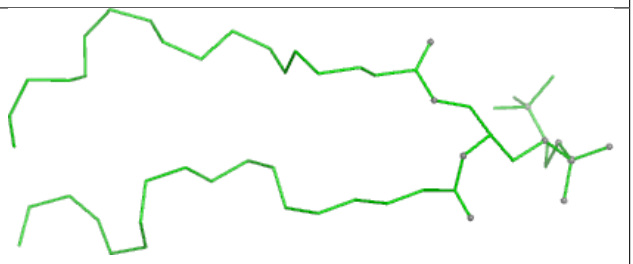


Rings

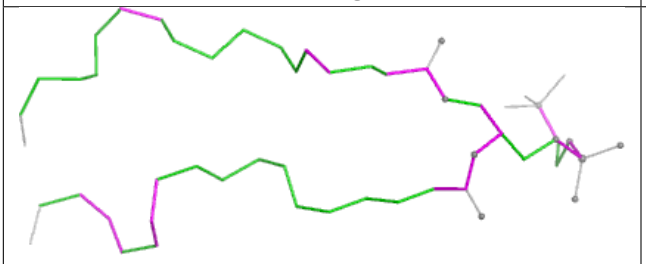
## Ligand PC1 EO 206



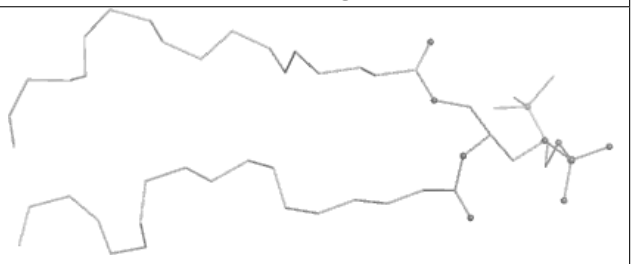
Bond lengths



Bond angles

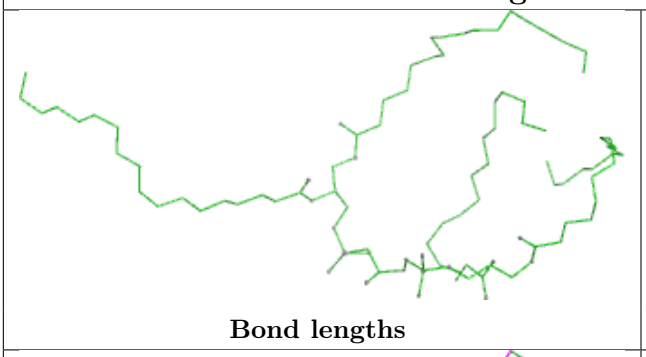


Torsions

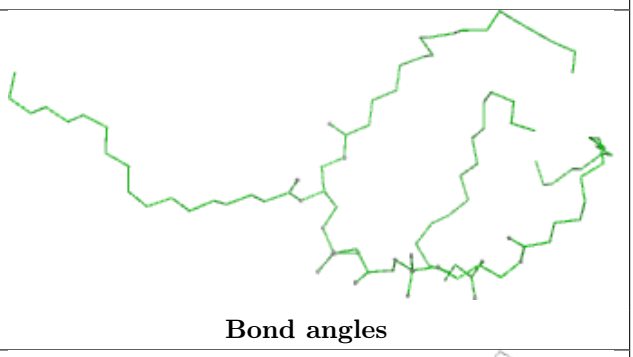


Rings

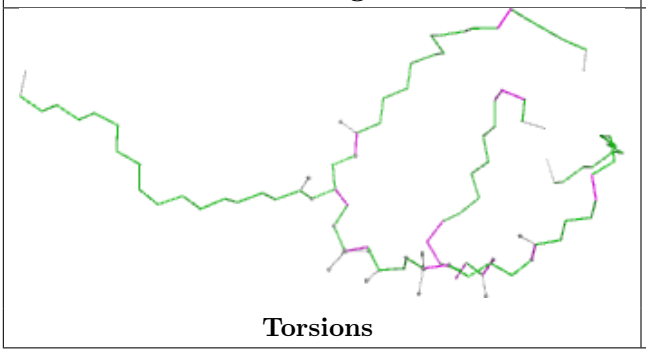
## Ligand CDL DU 404



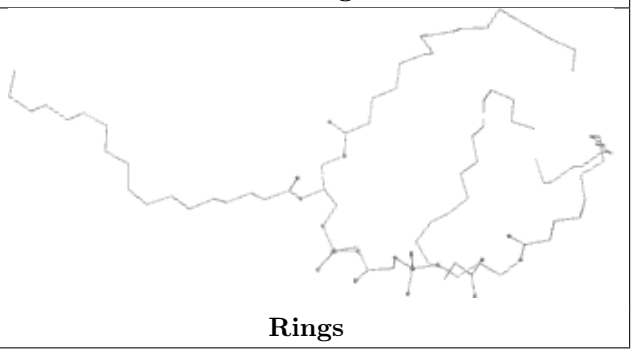
Bond lengths



Bond angles

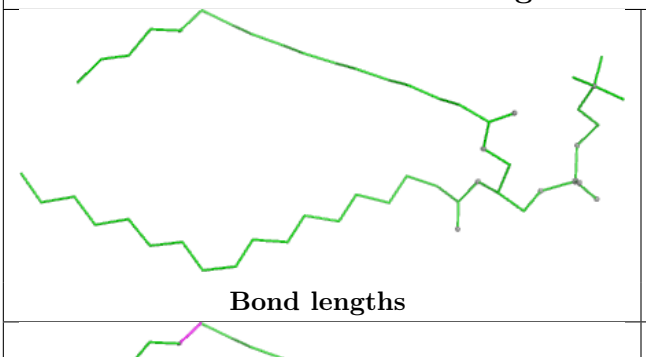


Torsions

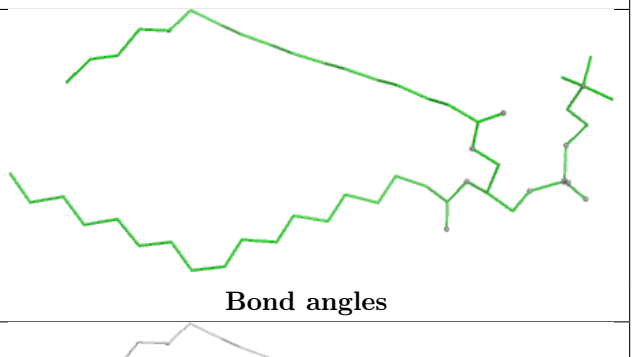


Rings

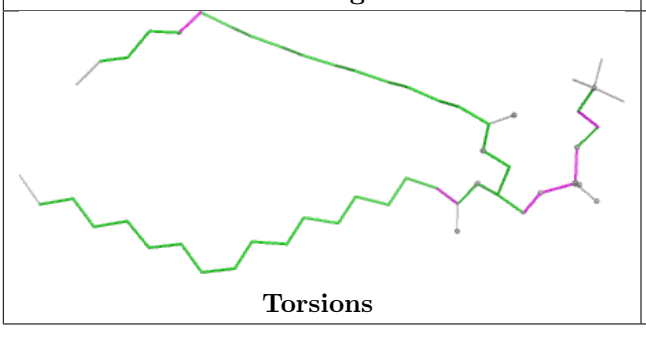
## Ligand PC1 EO 205



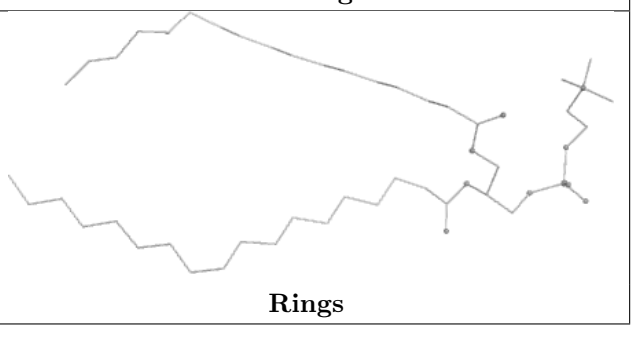
Bond lengths



Bond angles

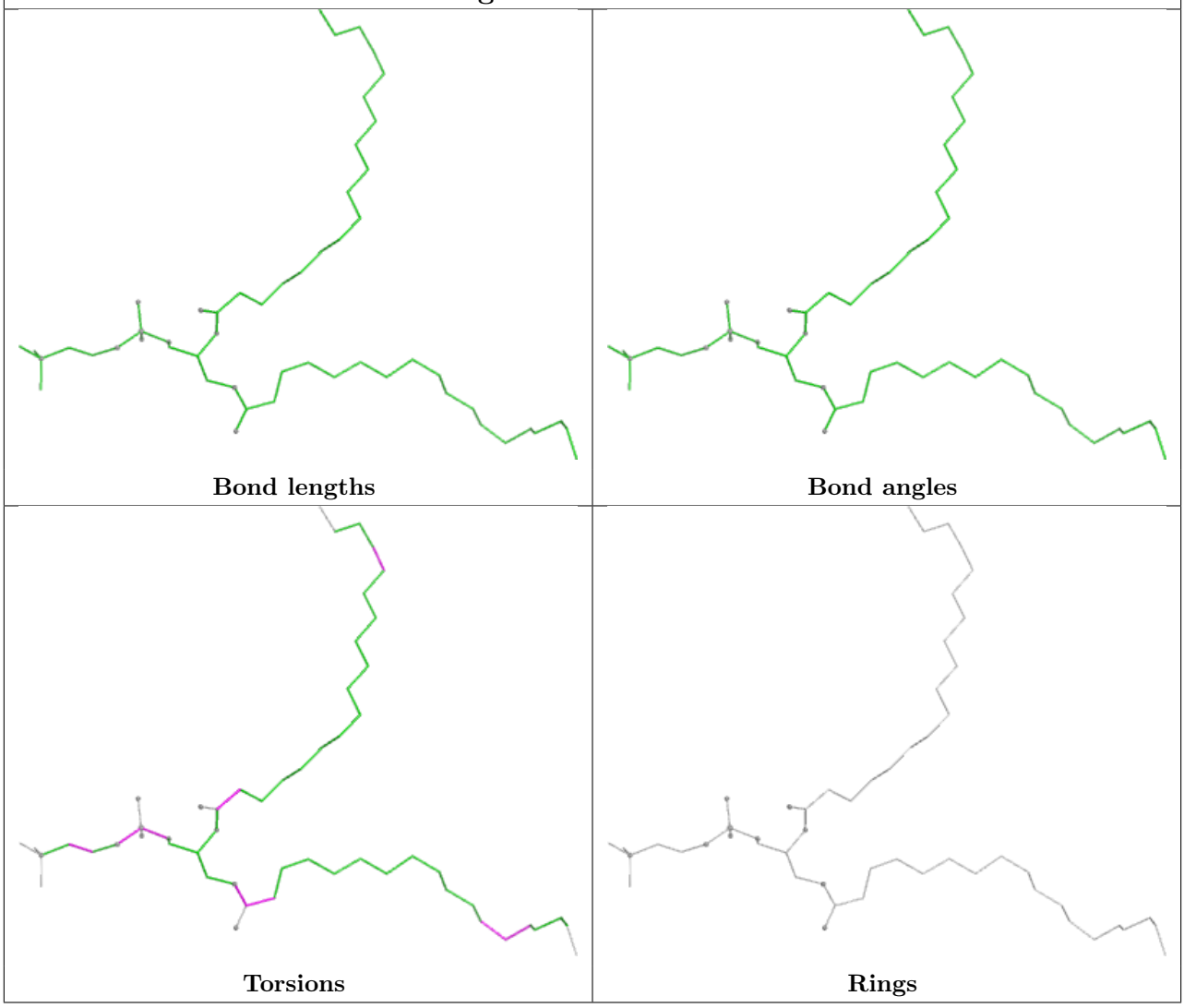


Torsions

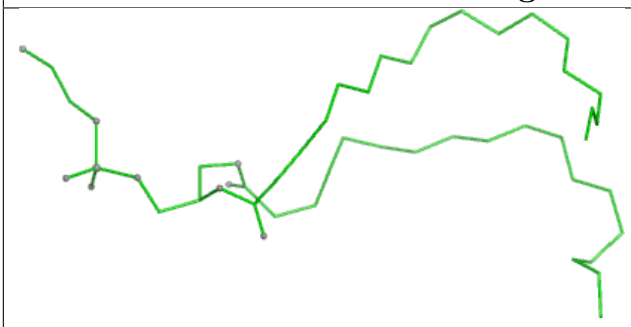


Rings

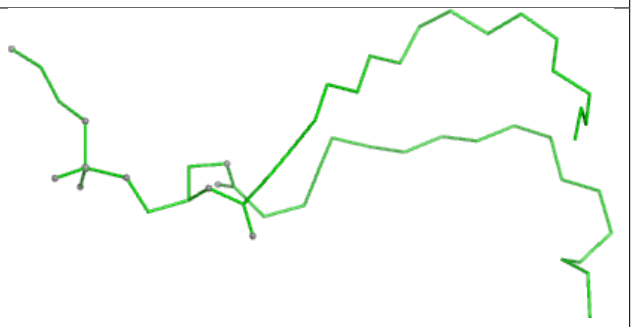
**Ligand PC1 Dv 407**



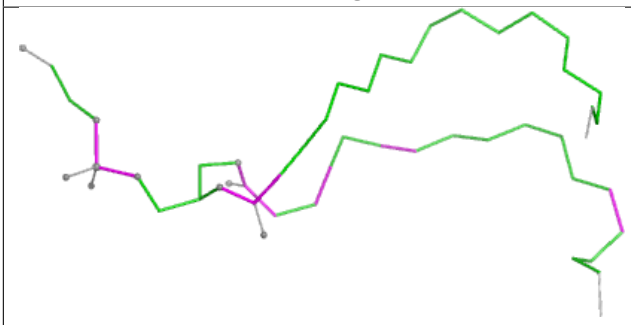
**Ligand 3PE DJ 301**



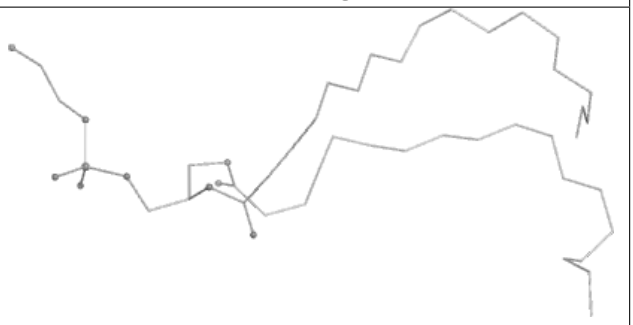
**Bond lengths**



**Bond angles**

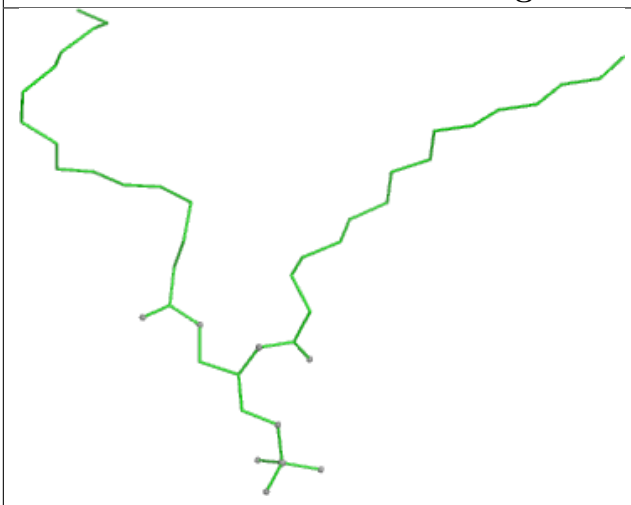


**Torsions**

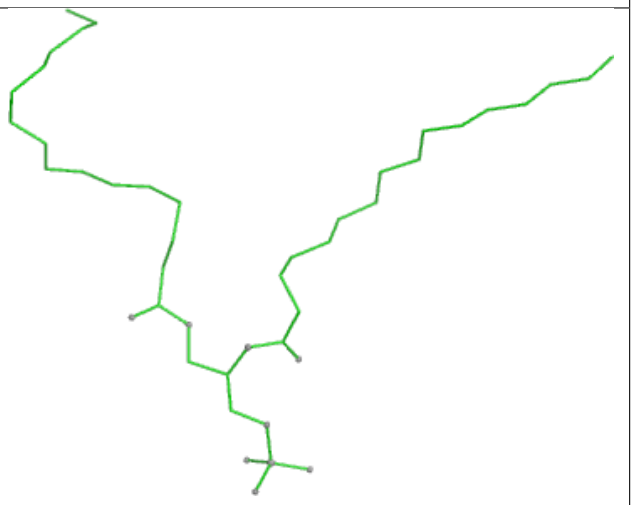


**Rings**

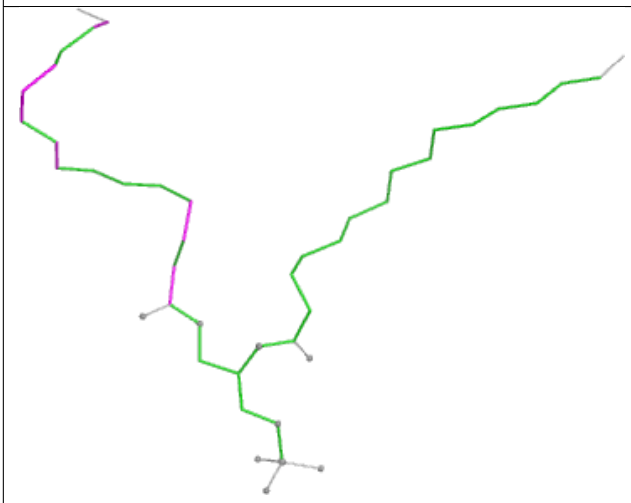
**Ligand LPP Dn 506**



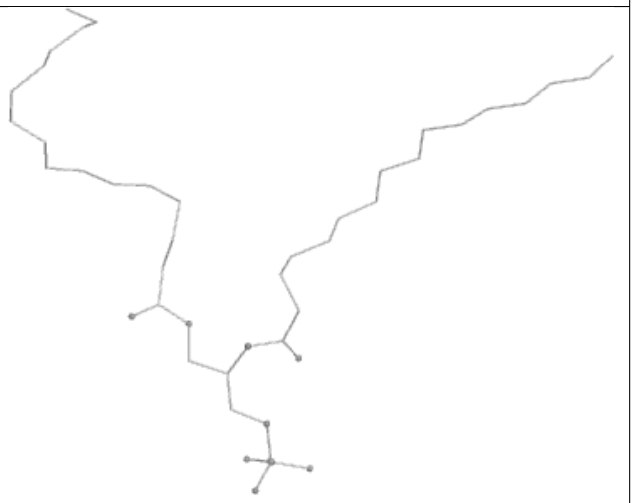
**Bond lengths**



**Bond angles**

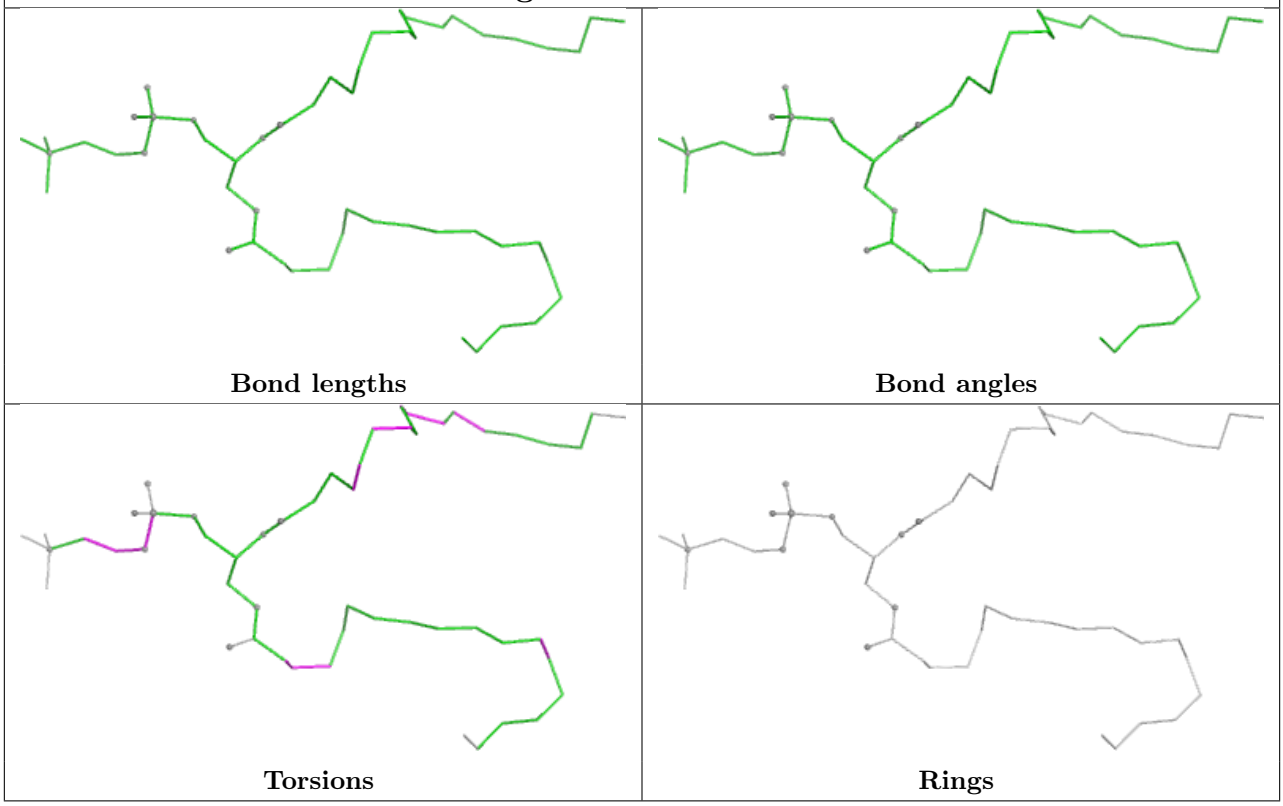


**Torsions**

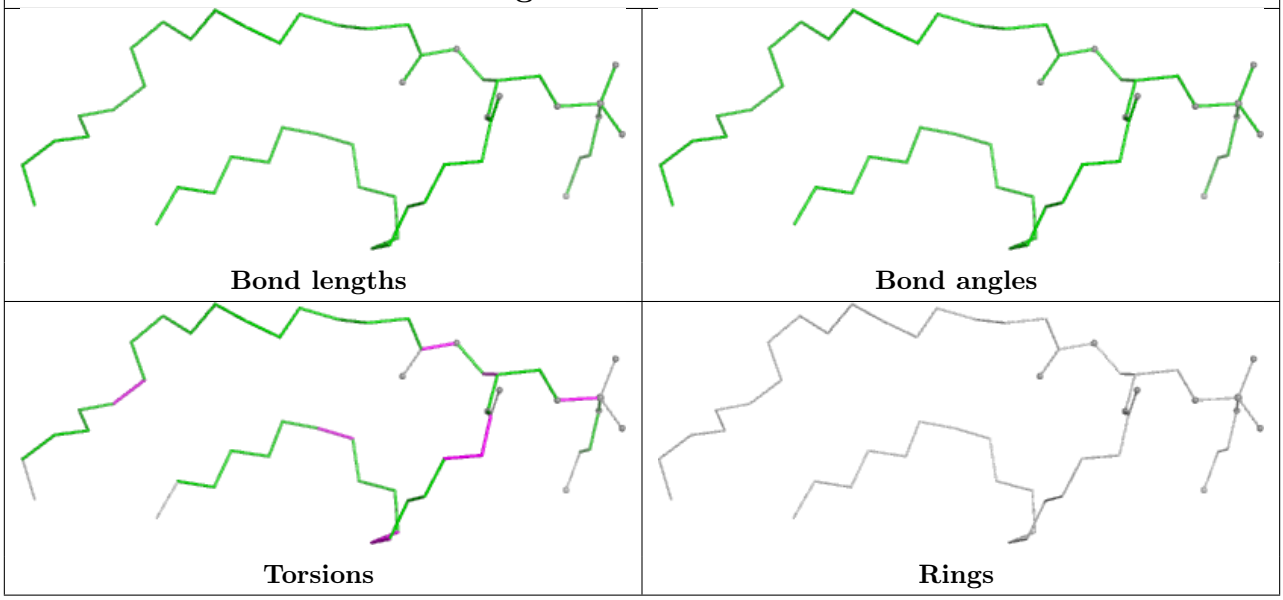


**Rings**

## Ligand PC1 EO 201




## Ligand 3PE Em 901



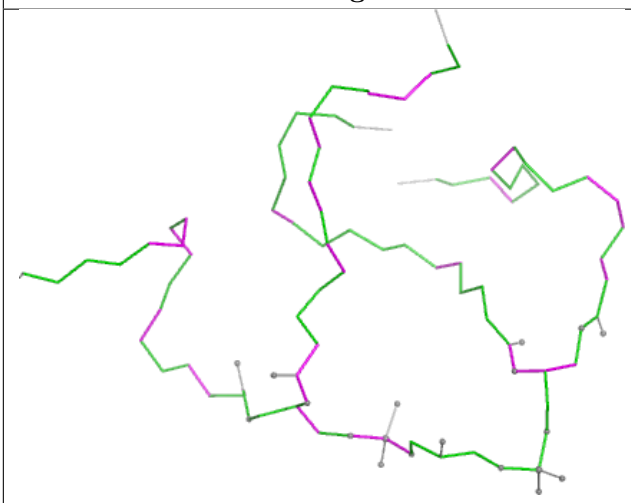
**Ligand CDL Di 701**



**Bond lengths**



**Bond angles**

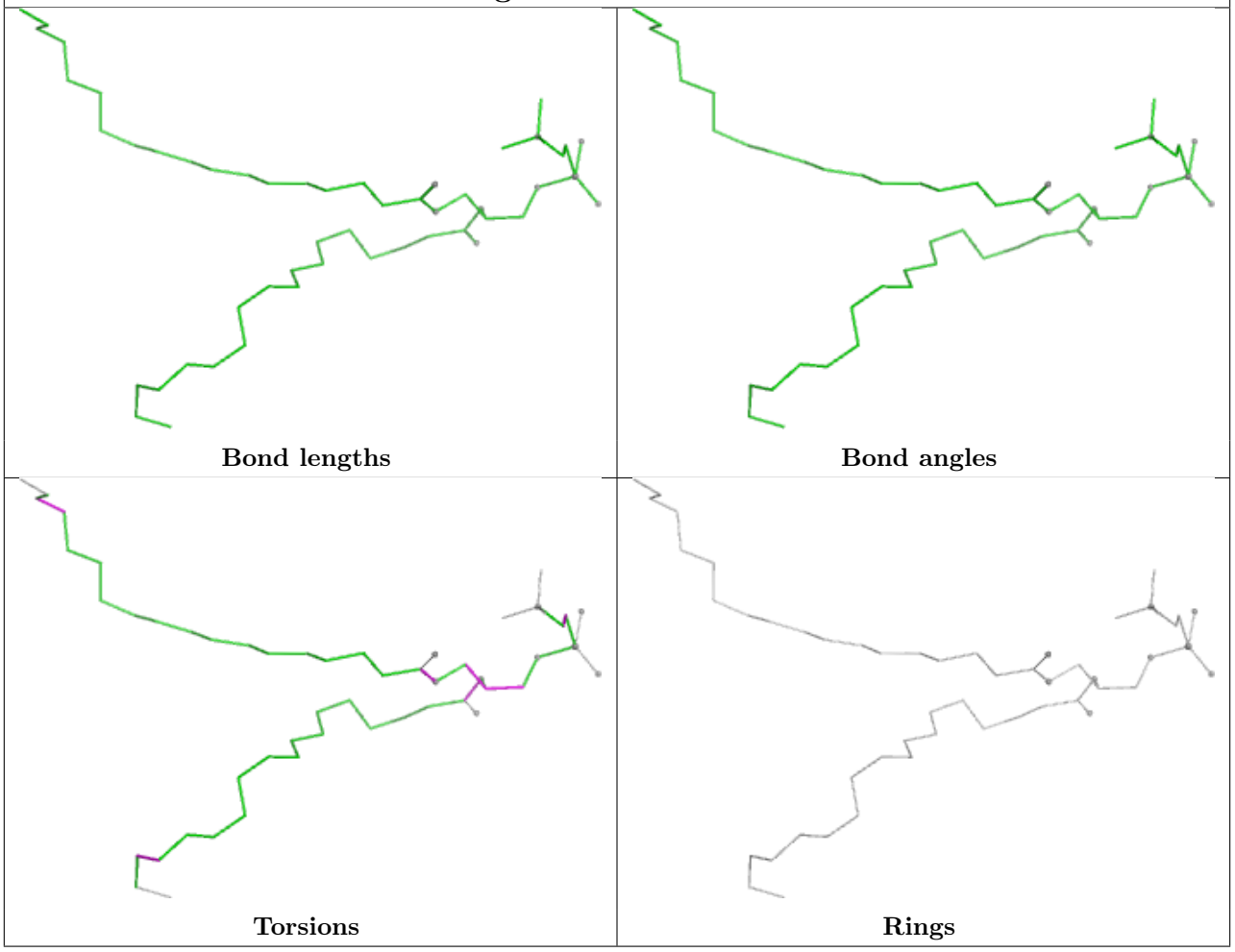


**Torsions**

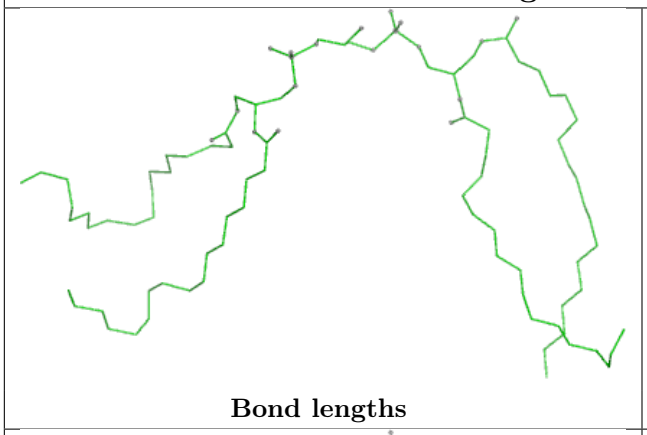


**Rings**

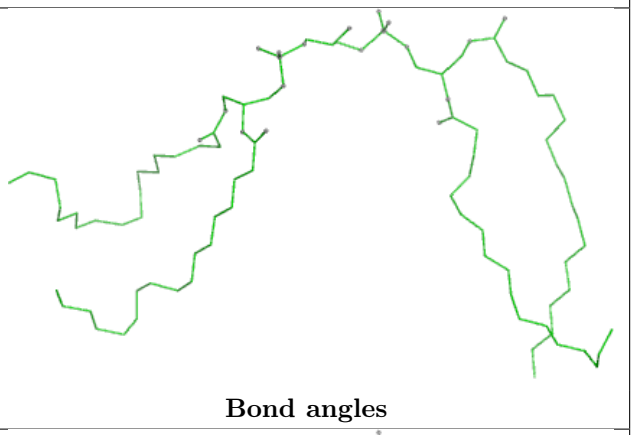
**Ligand PC1 DY 302**



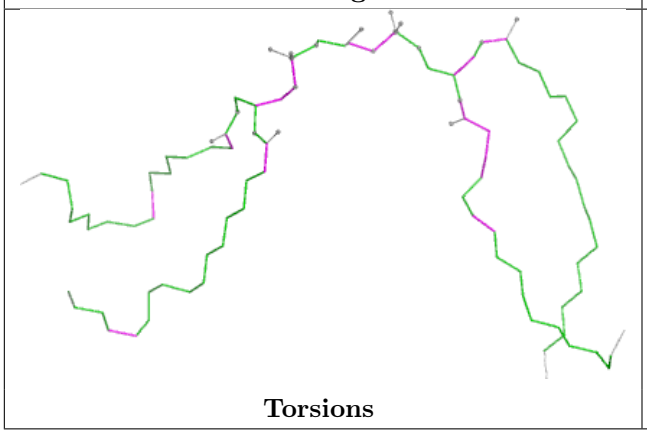
**Ligand CDL EI 401**



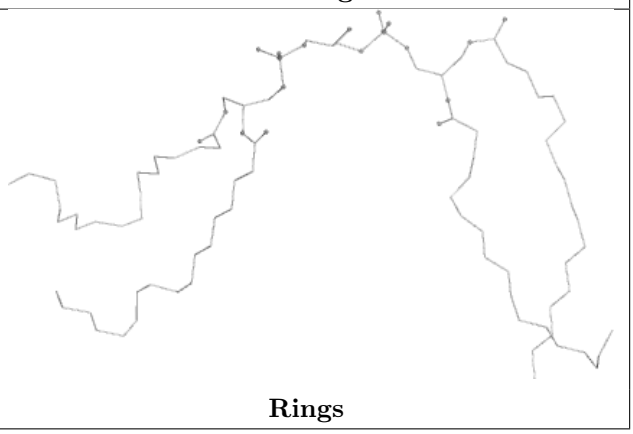
**Bond lengths**



**Bond angles**

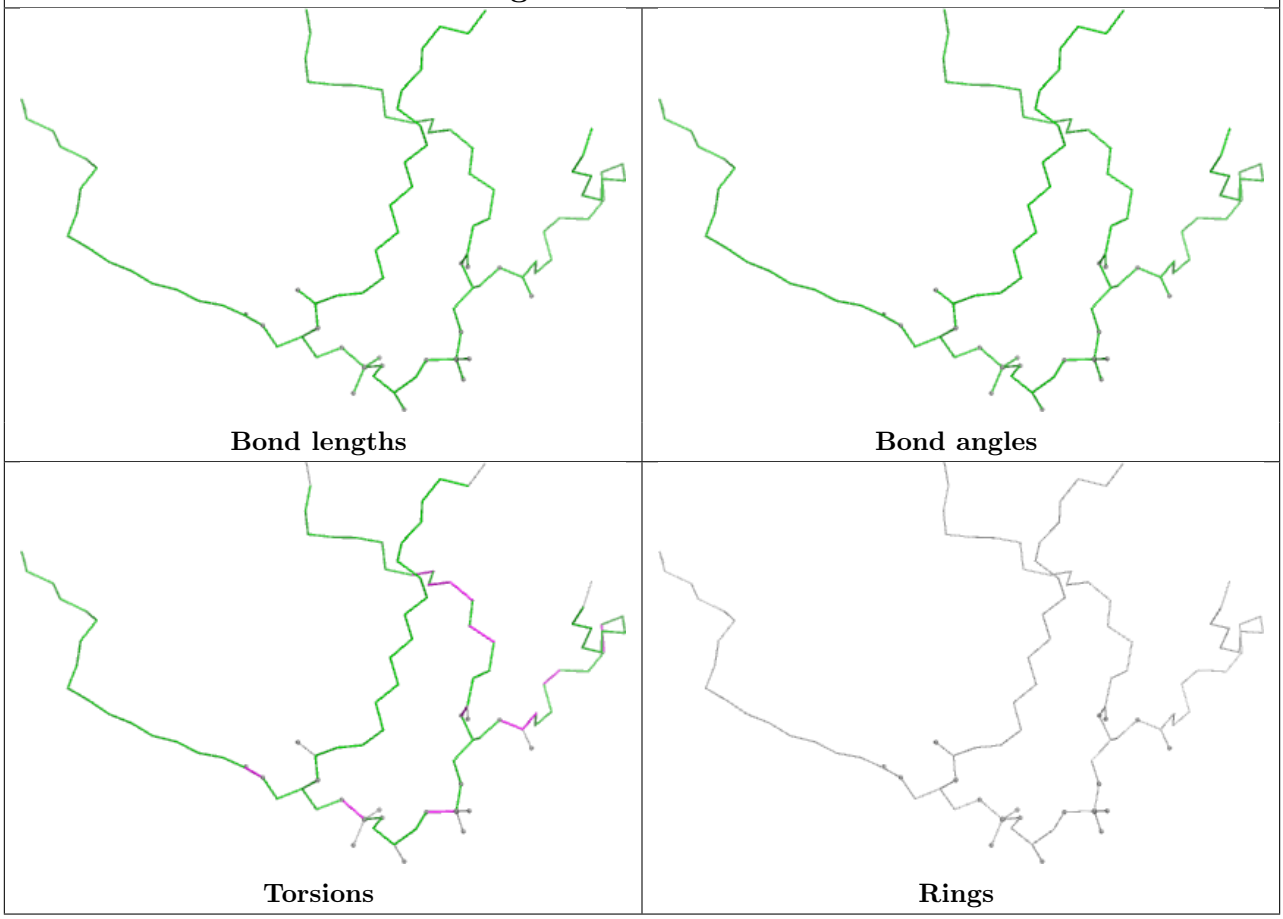


**Torsions**

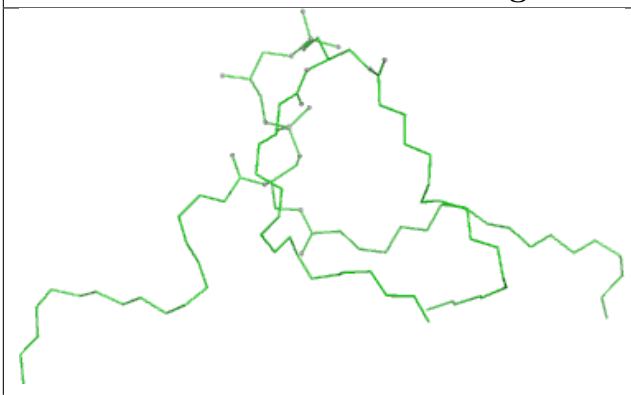


**Rings**

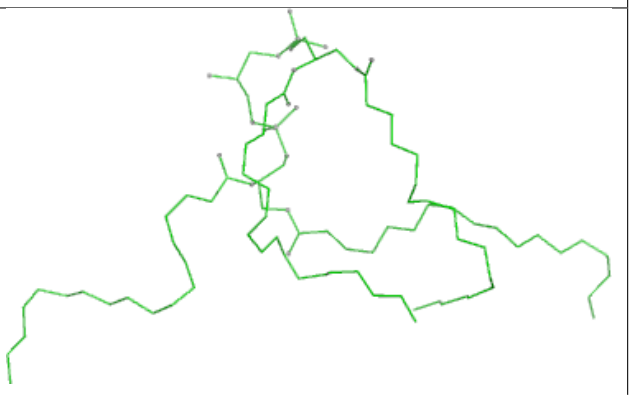
**Ligand CDL DU 403**



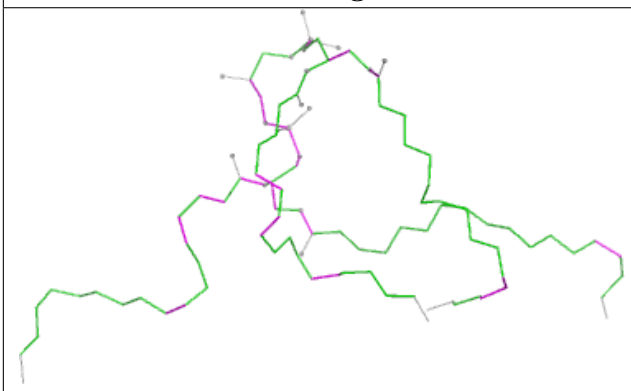
**Ligand CDL DN 505**



**Bond lengths**



**Bond angles**

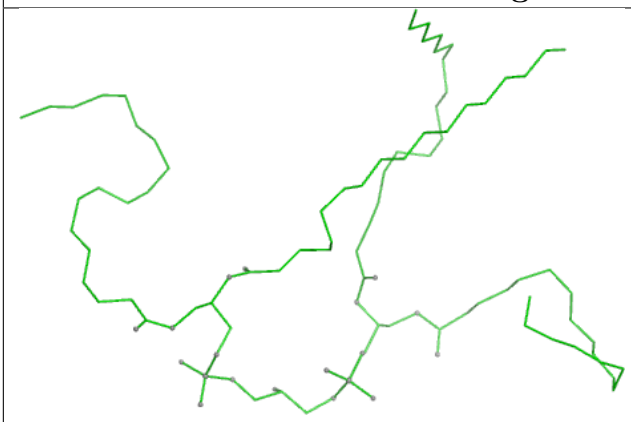


**Torsions**

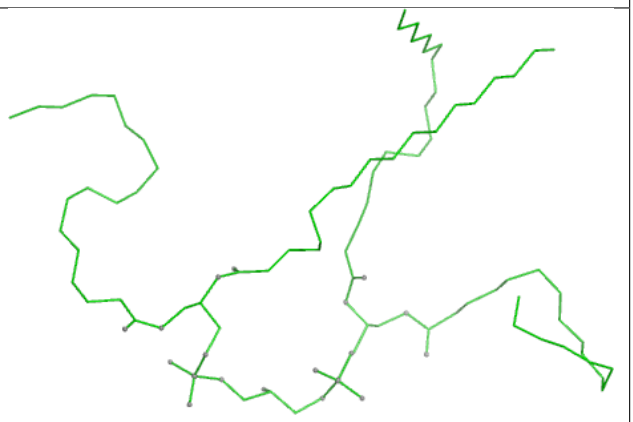


**Rings**

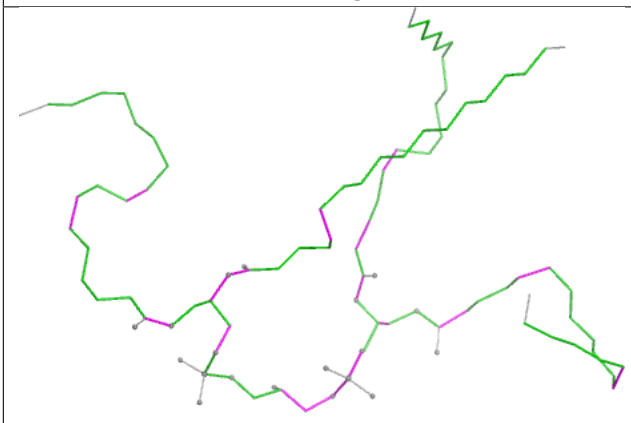
**Ligand CDL EK 201**



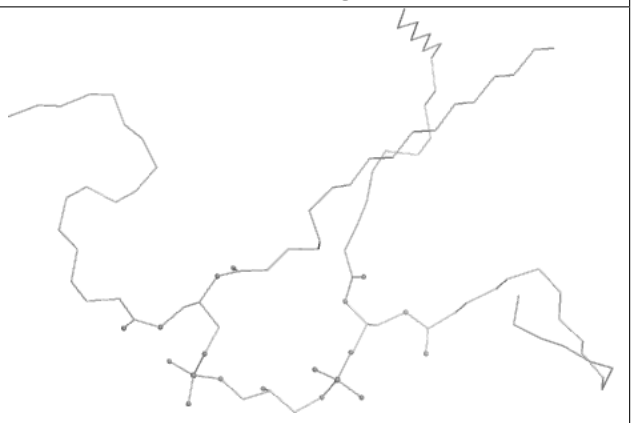
**Bond lengths**



**Bond angles**

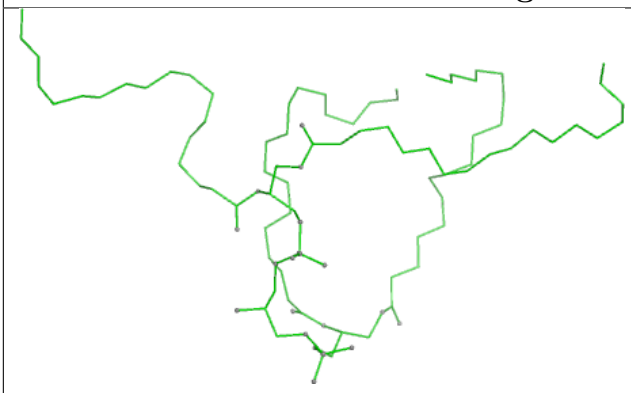


**Torsions**

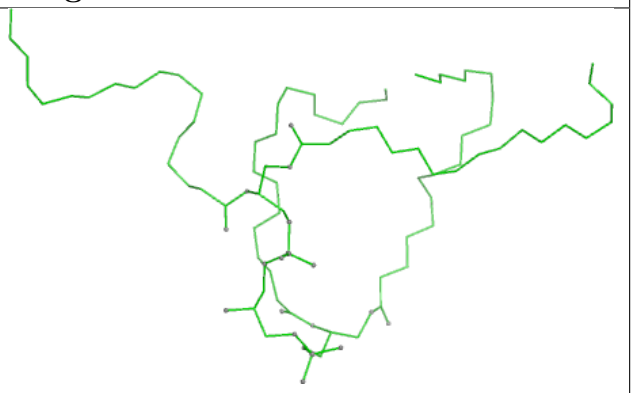


**Rings**

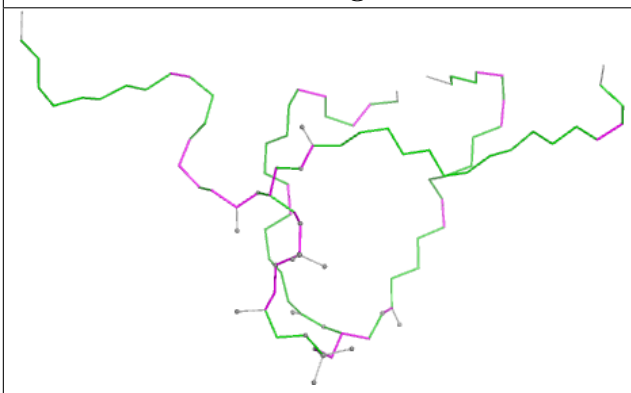
**Ligand CDL Eg 101**



**Bond lengths**



**Bond angles**

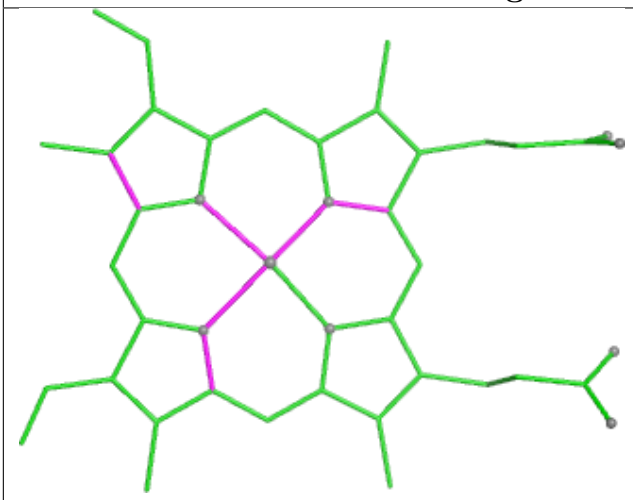


**Torsions**

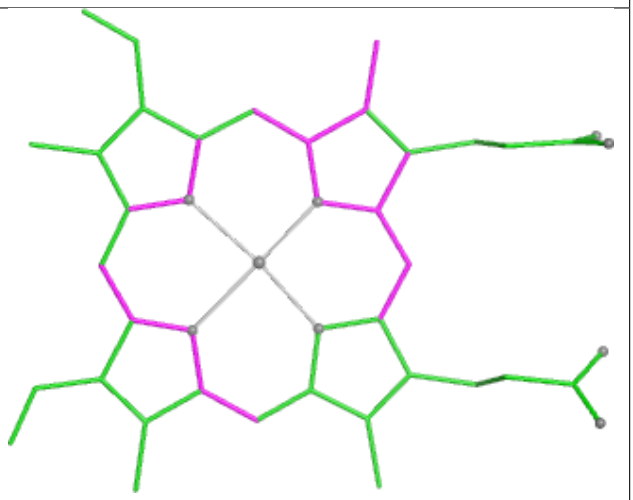


**Rings**

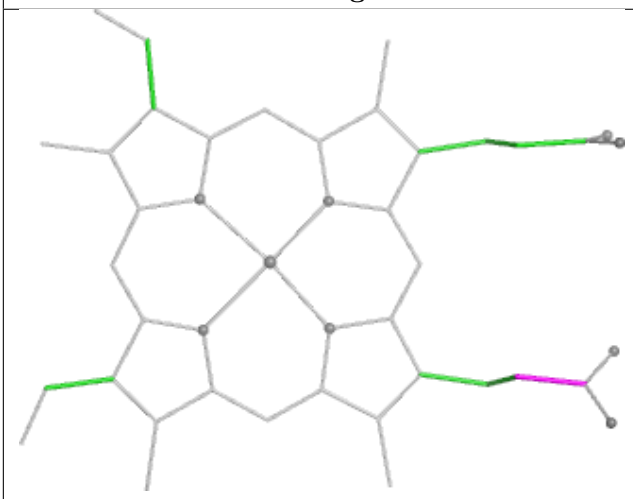
## Ligand HEM ED 602



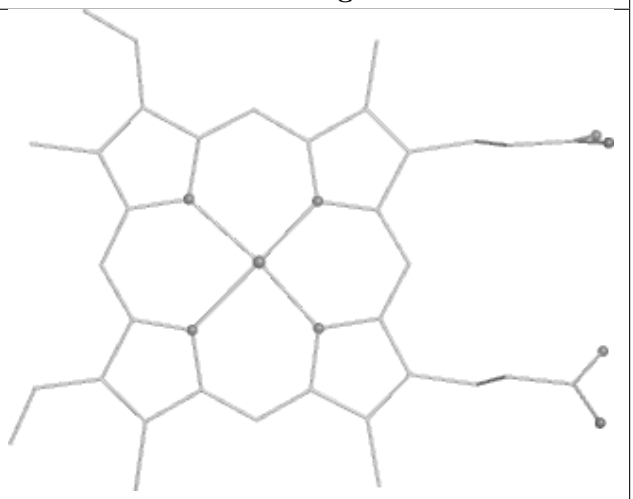
Bond lengths



Bond angles

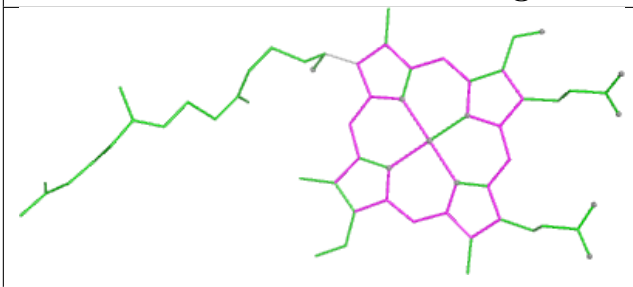


Torsions

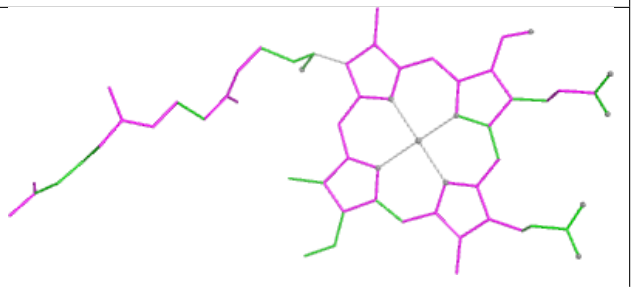


Rings

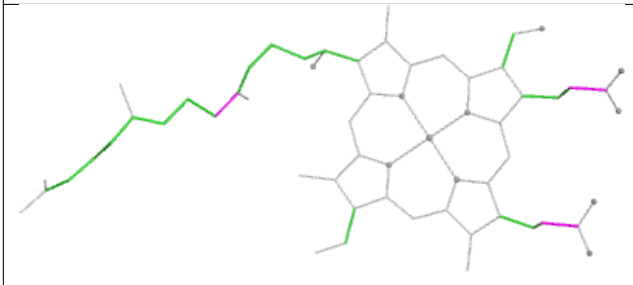
## Ligand HEA Da 701



Bond lengths



Bond angles

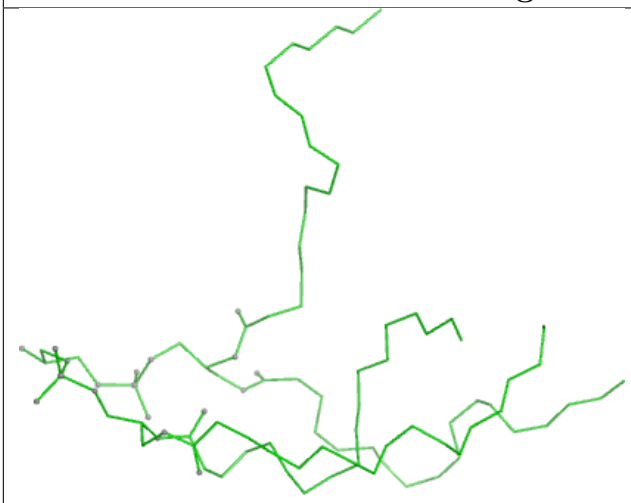


Torsions



Rings

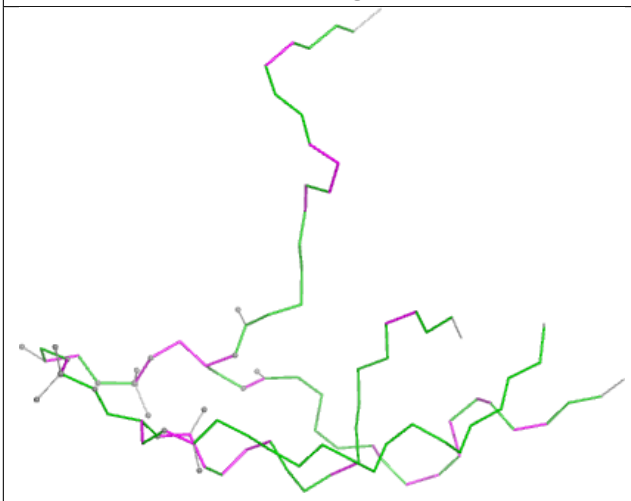
**Ligand CDL Ds 402**



**Bond lengths**



**Bond angles**

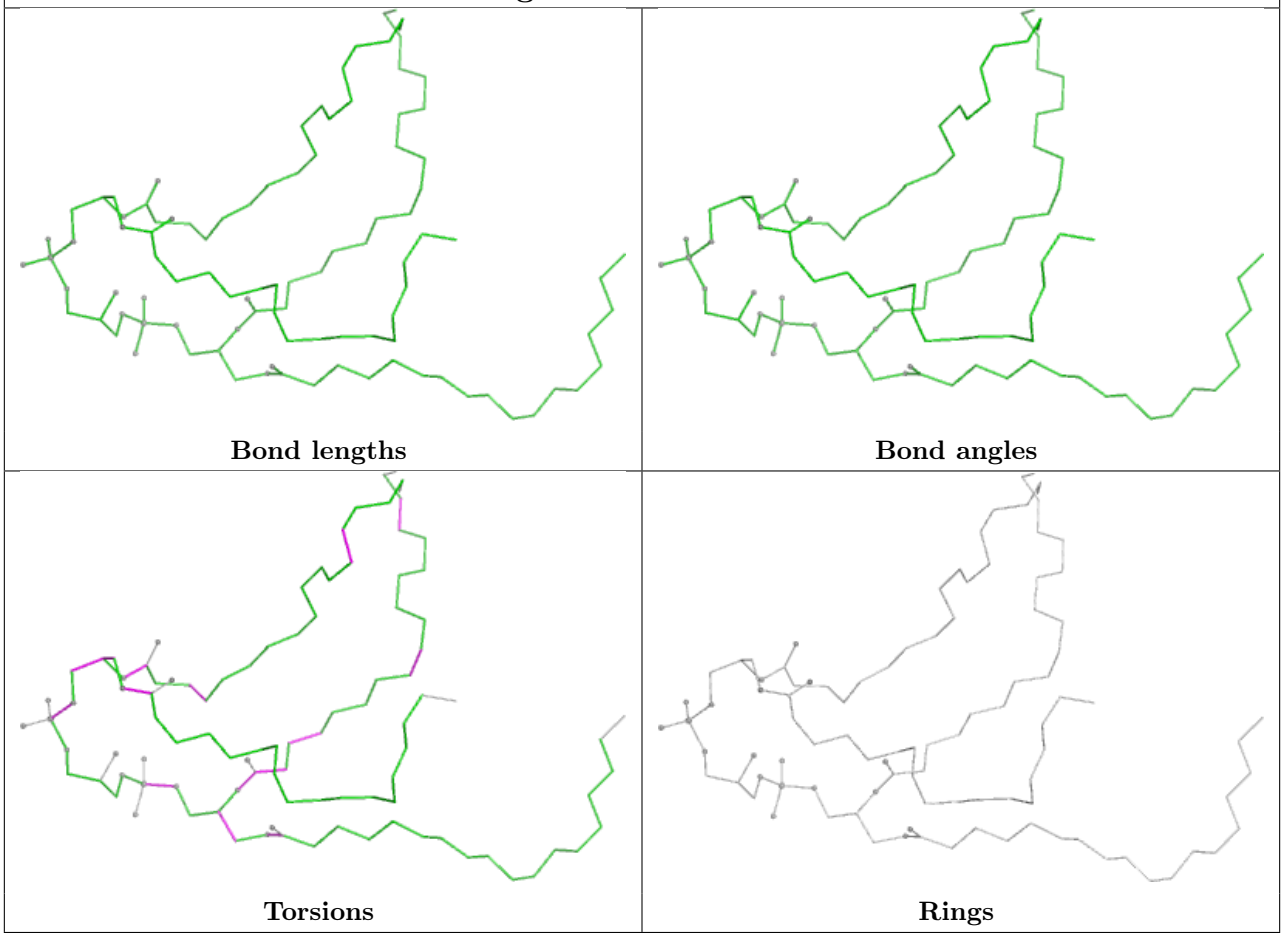


**Torsions**

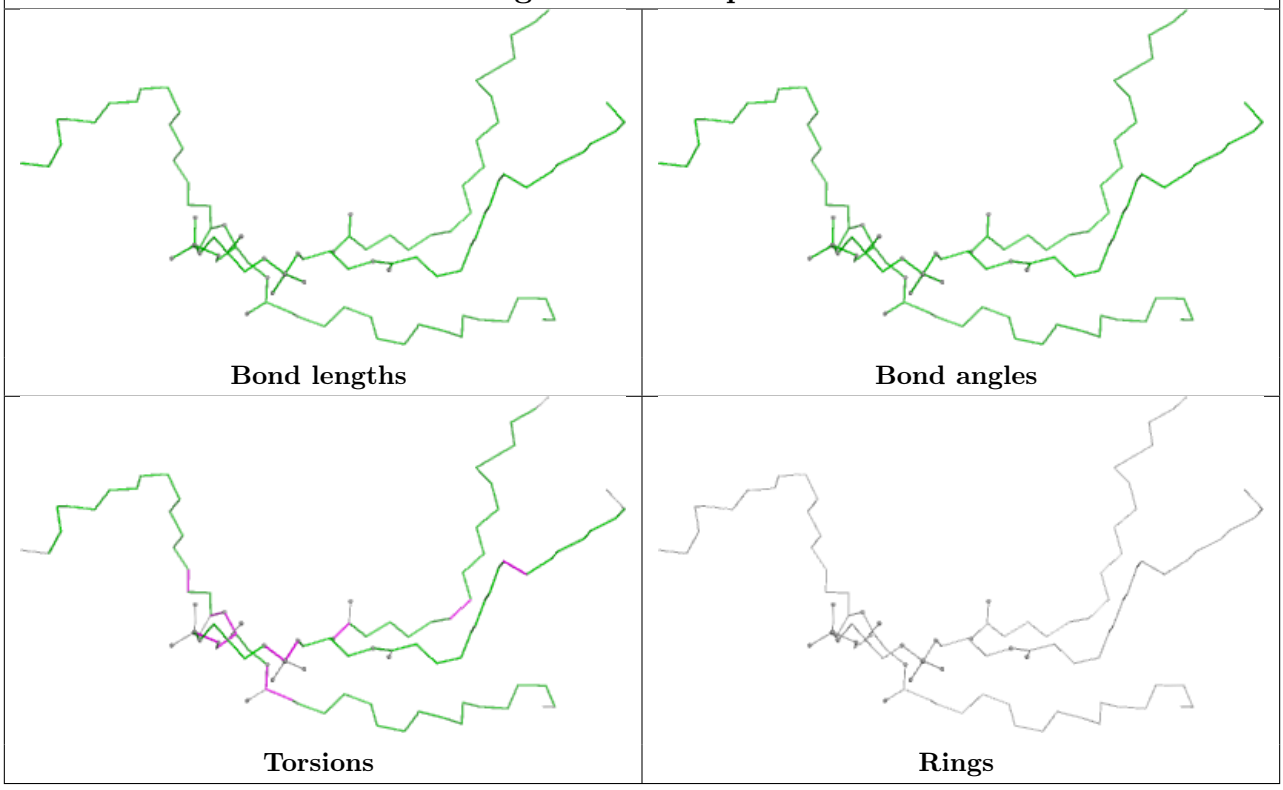


**Rings**

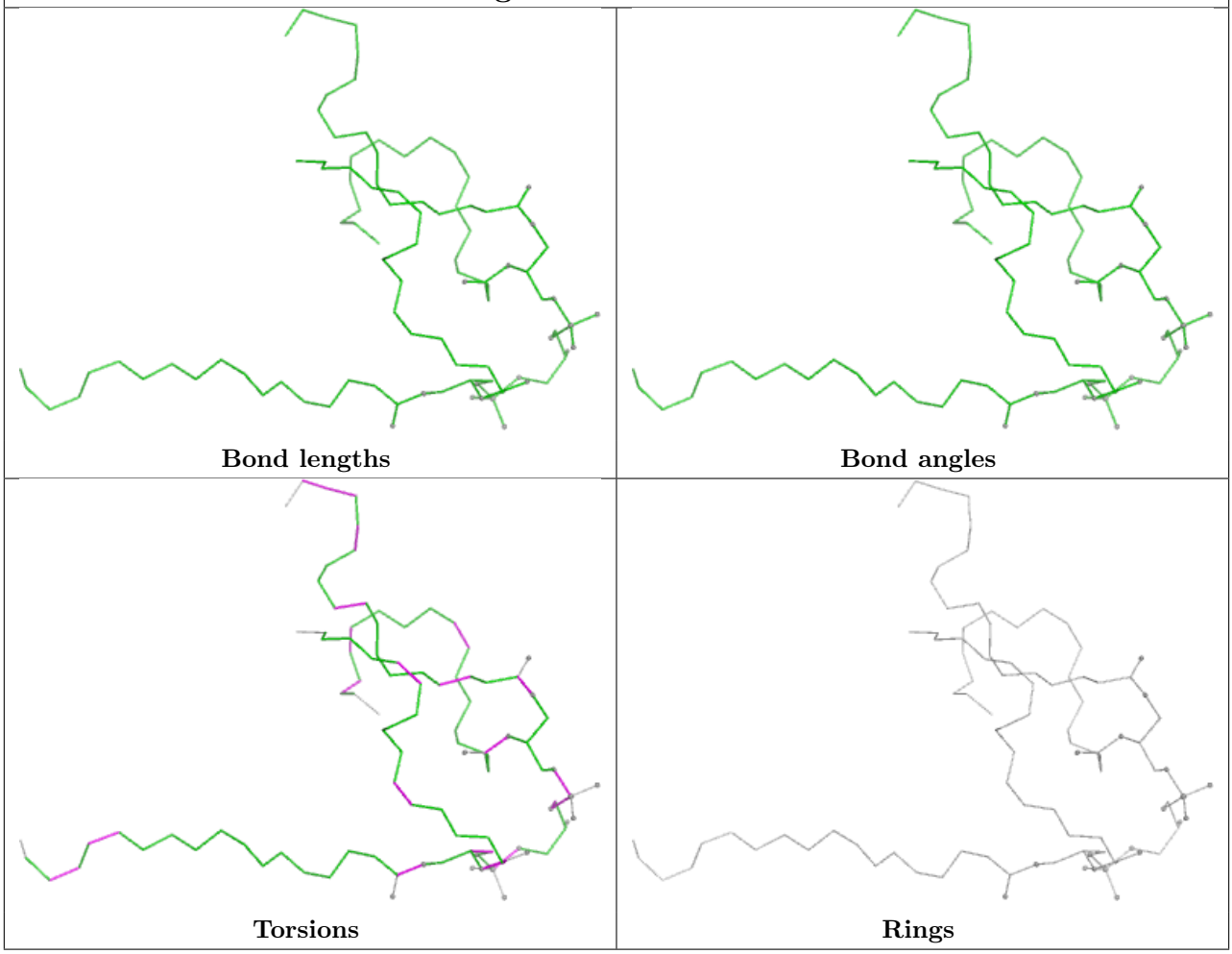
## Ligand CDL Ed 205



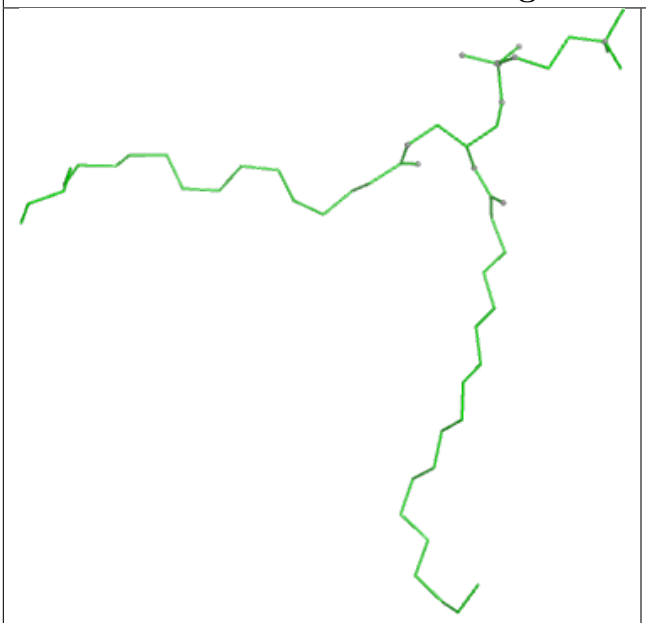

## Ligand CDL Dq 404



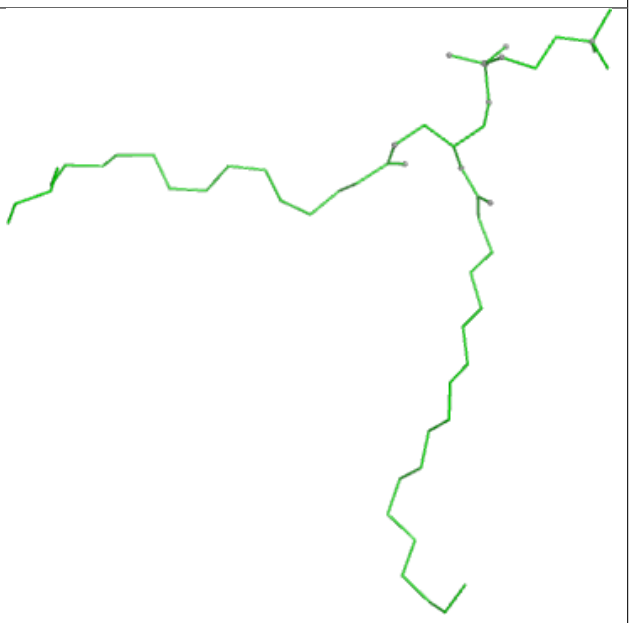
**Ligand CDL EL 904**



**Ligand PC1 Eb 302**



**Bond lengths**



**Bond angles**

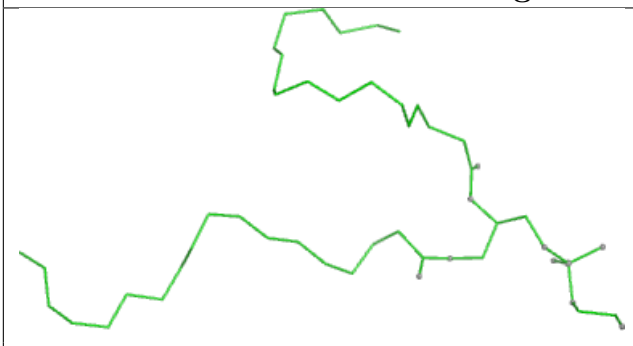


**Torsions**

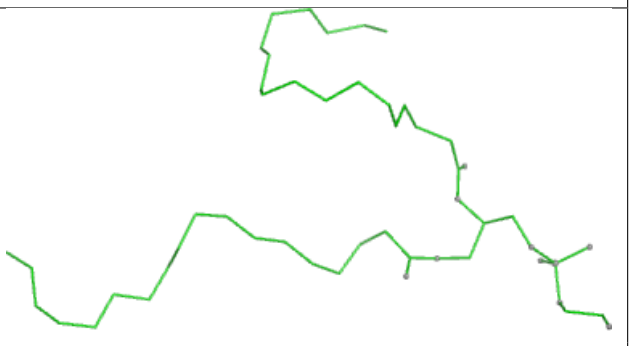


**Rings**

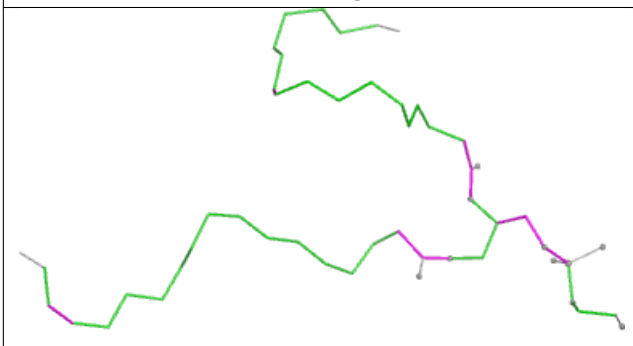
**Ligand 3PE DG 205**



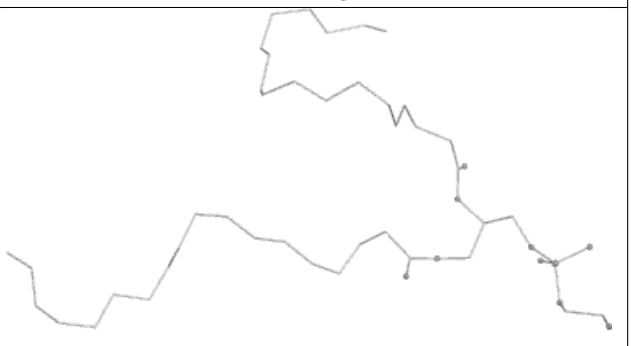
Bond lengths



Bond angles

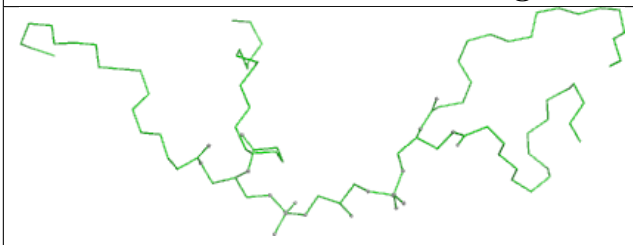


Torsions

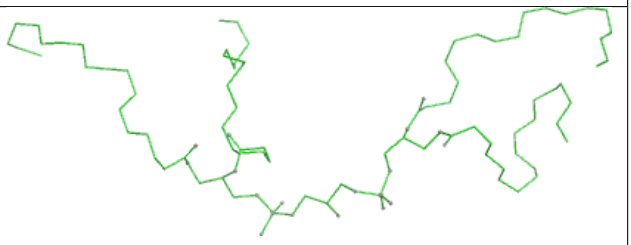


Rings

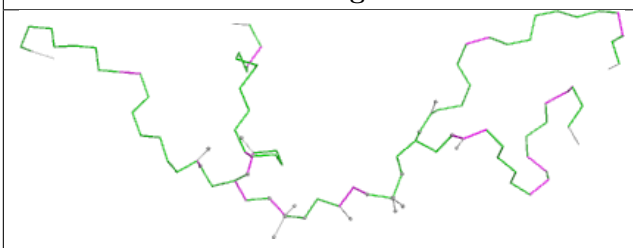
**Ligand CDL Dv 403**



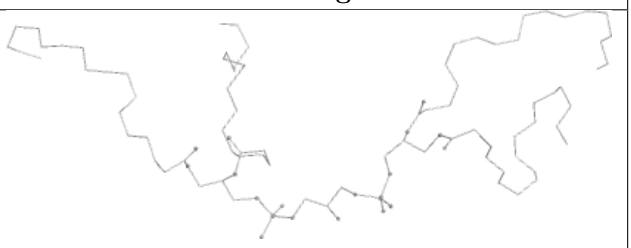
Bond lengths



Bond angles

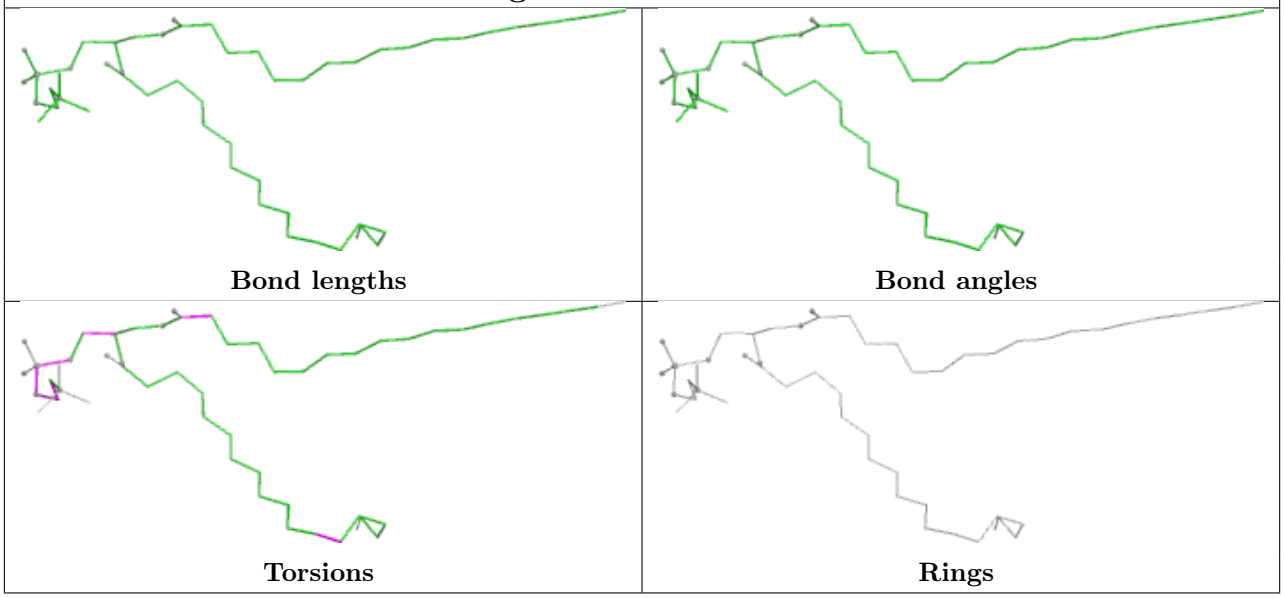


Torsions

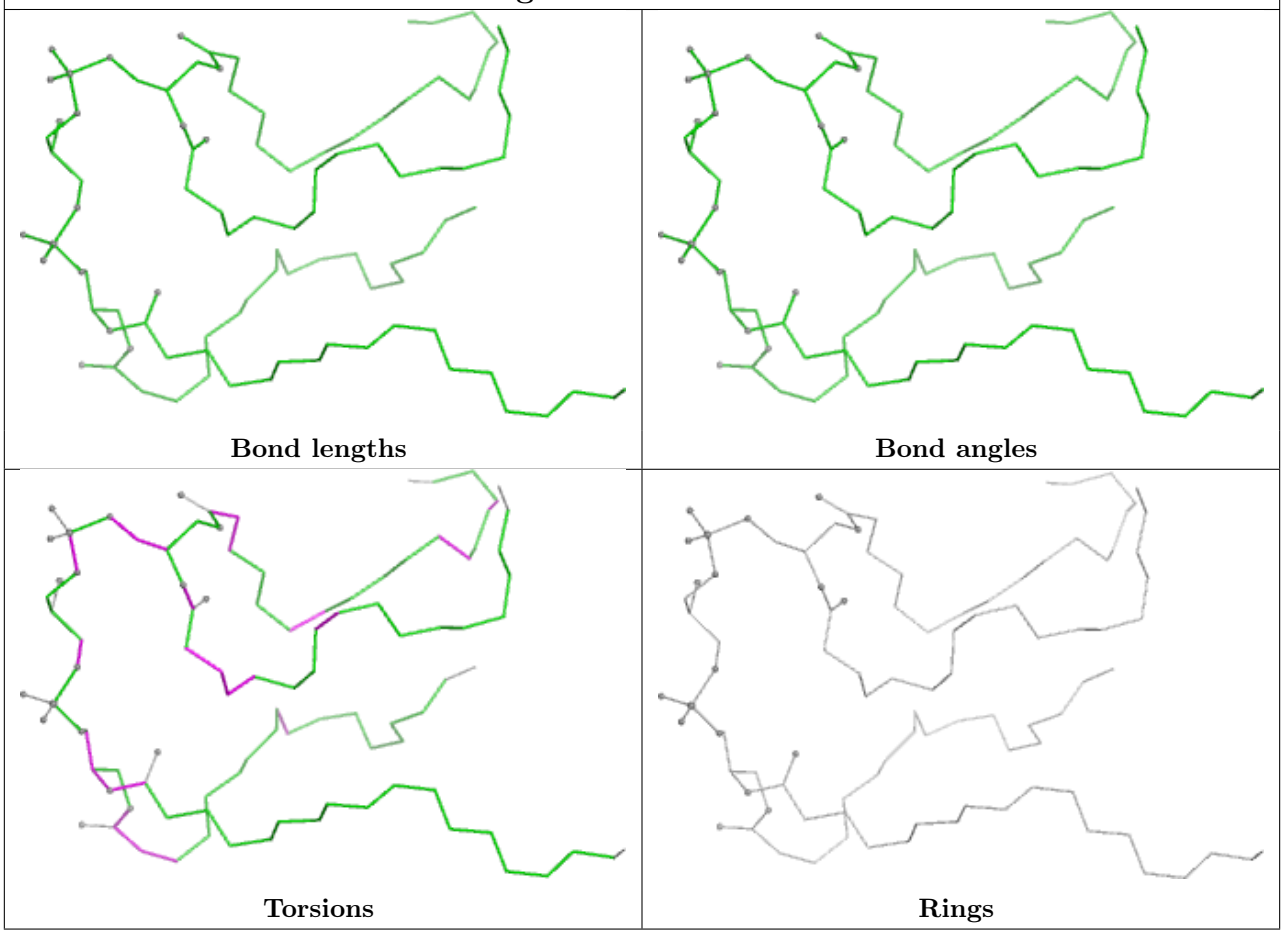


Rings

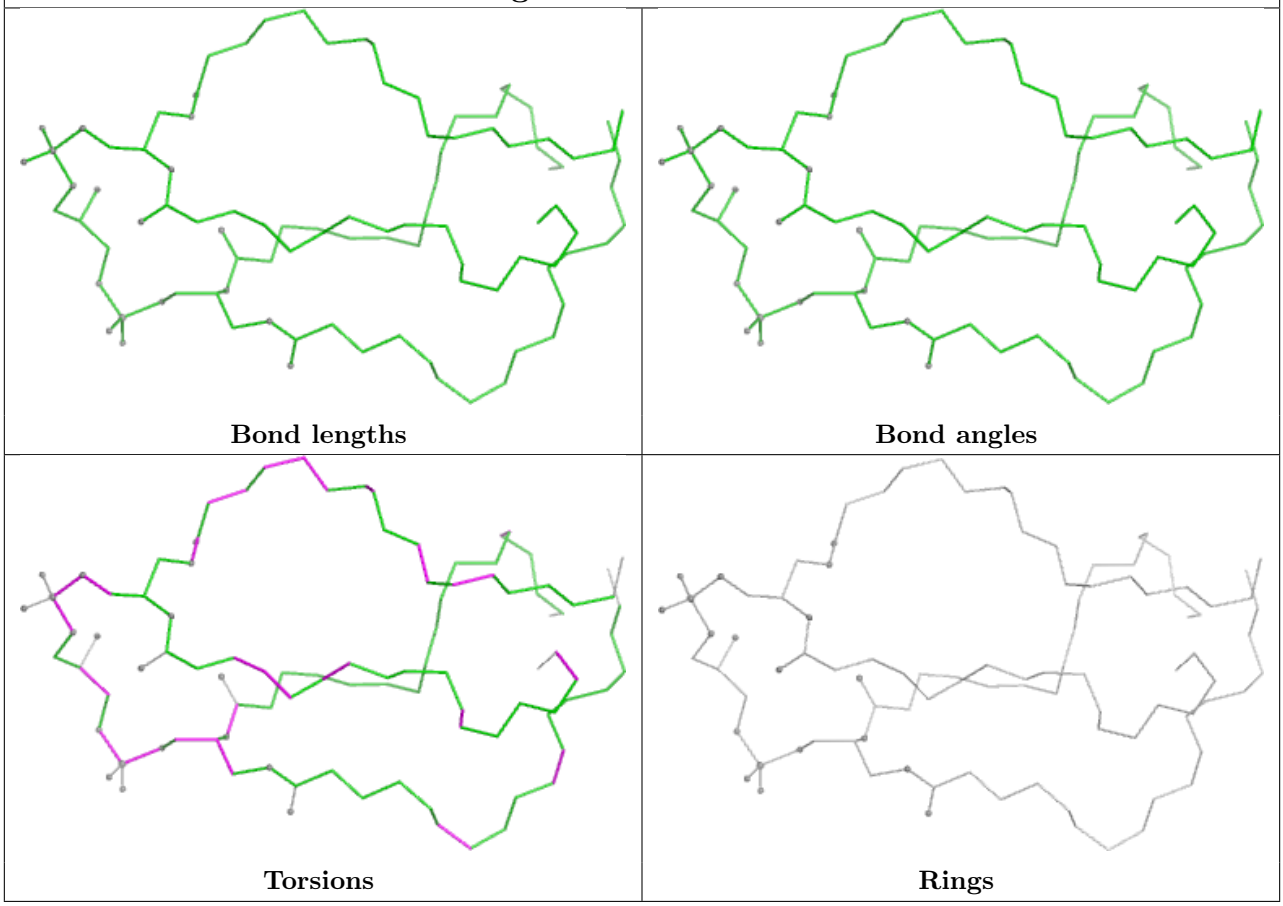
## Ligand PC1 Dx 1202



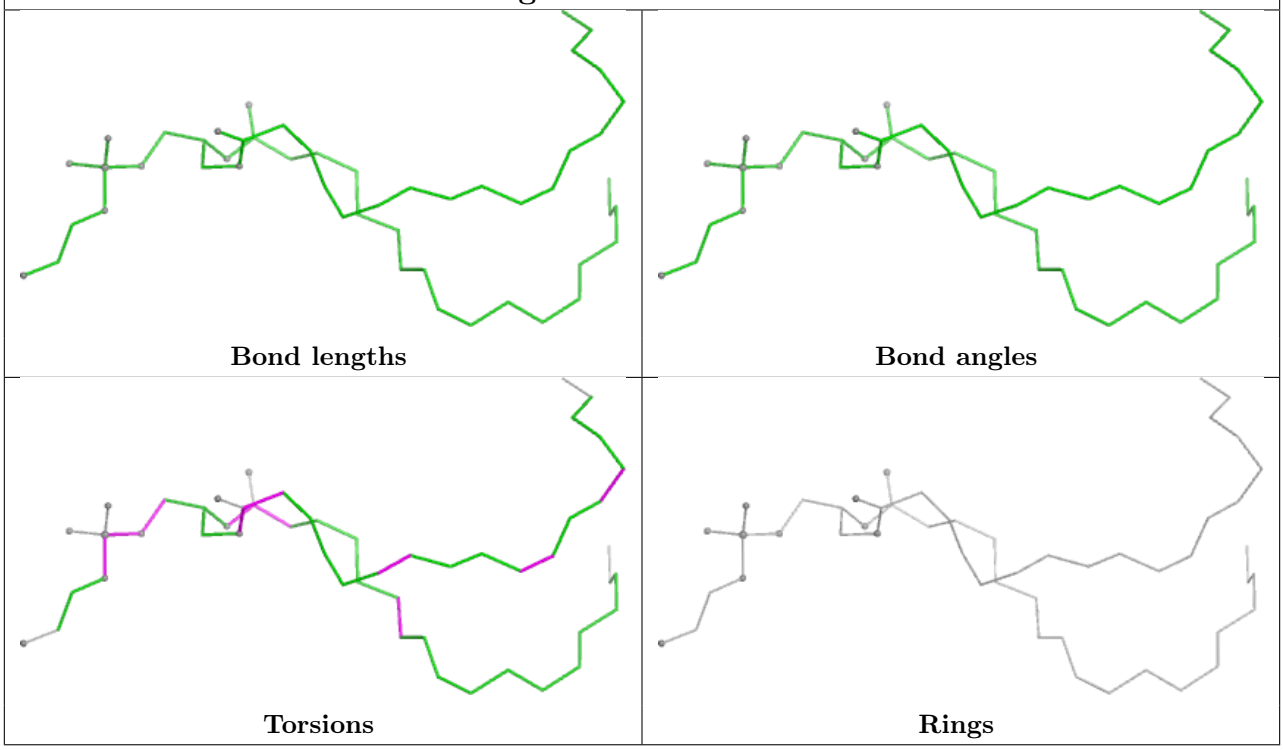

## Ligand CDL Dz 501



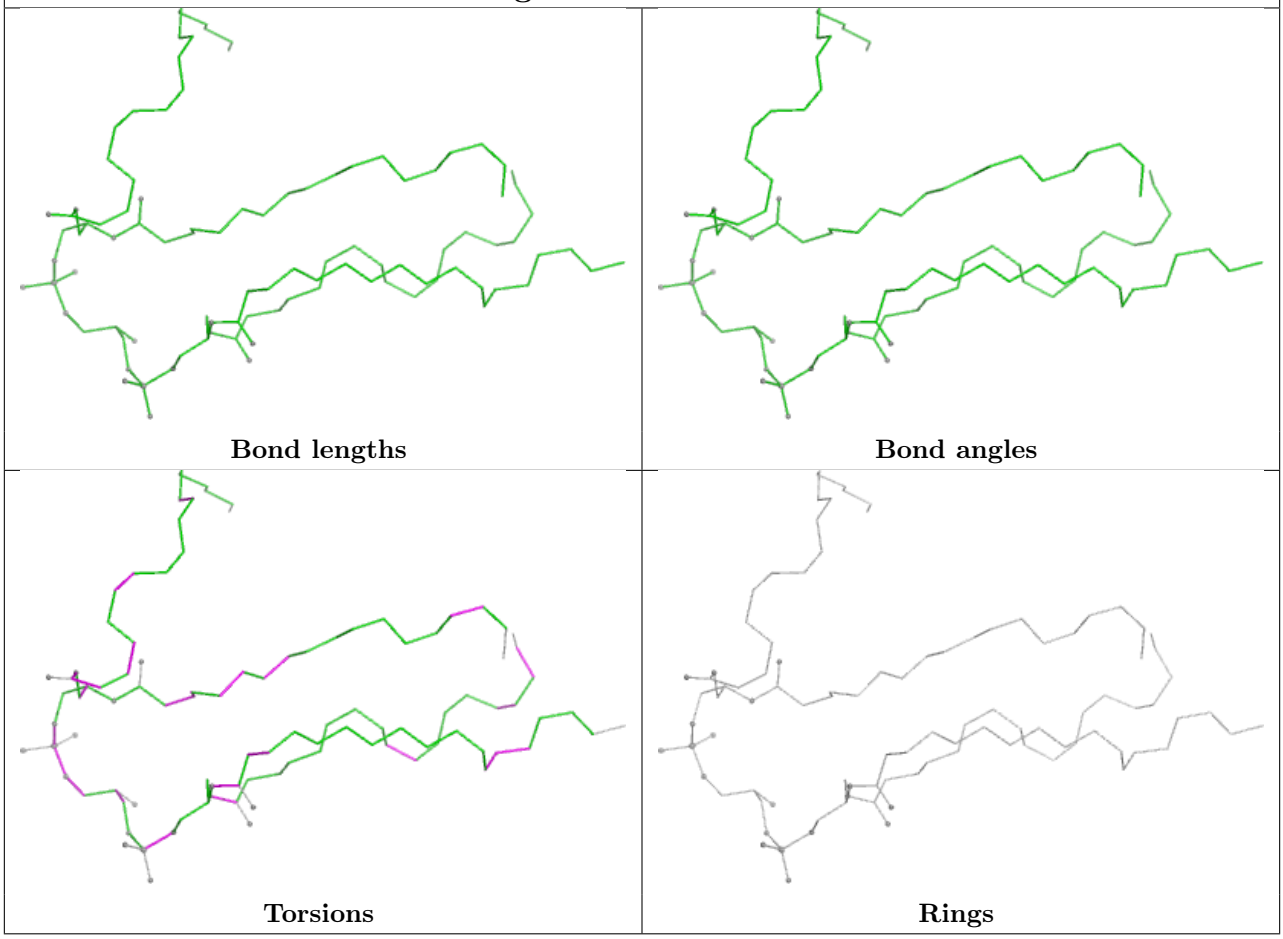
## Ligand CDL DX 301



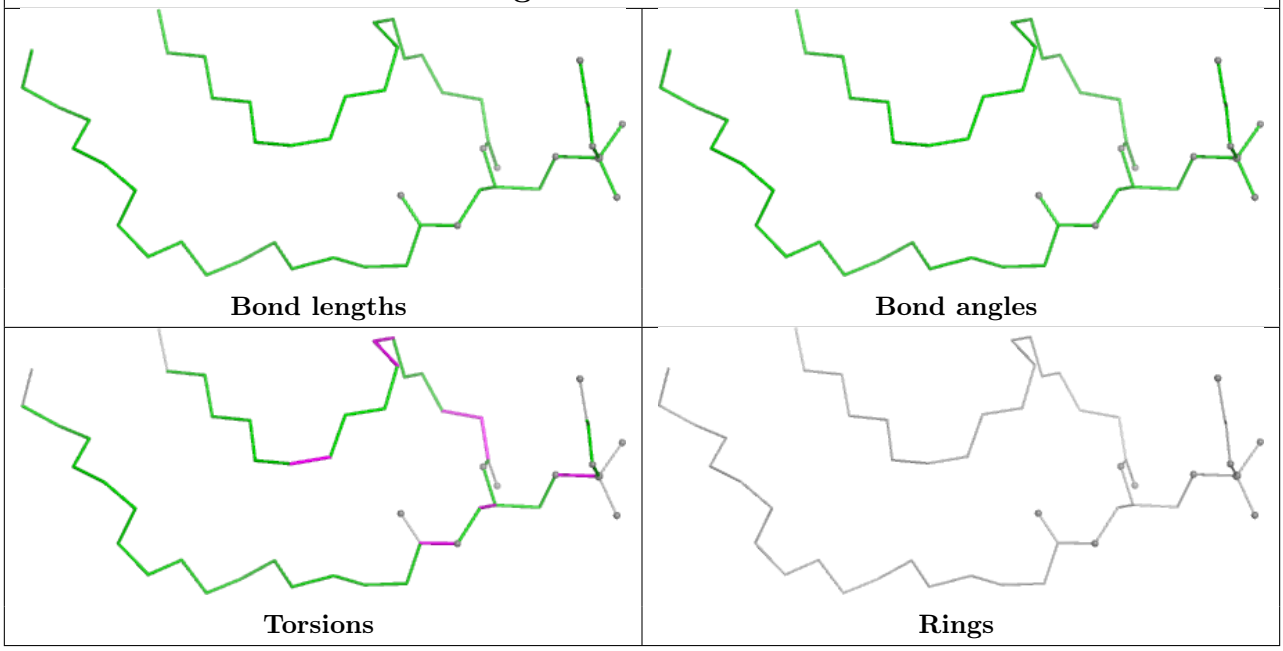

## Ligand 3PE Dd 703



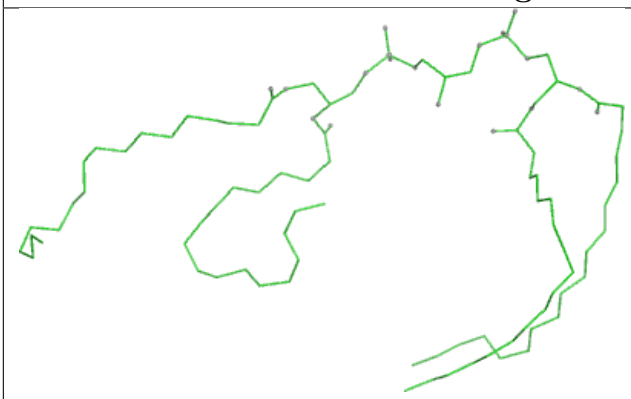
## Ligand CDL Dh 202



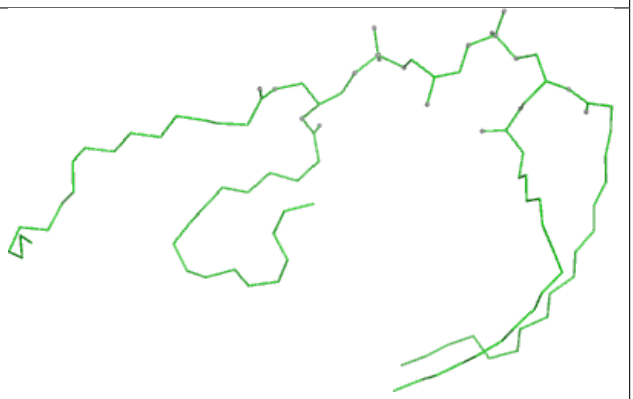

## Ligand 3PE EM 901



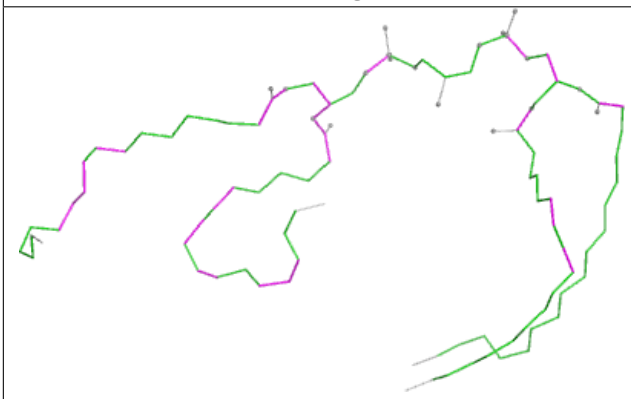
**Ligand CDL Da 709**



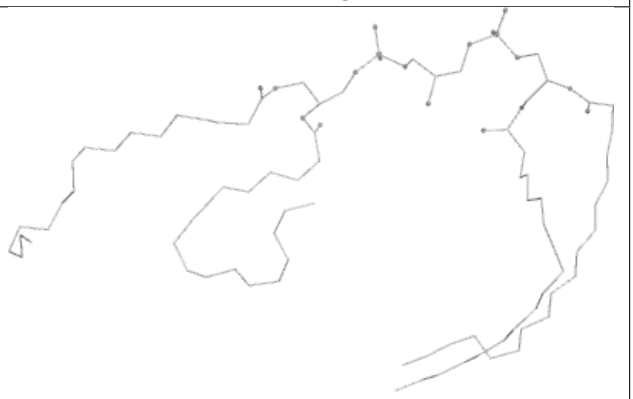
**Bond lengths**



**Bond angles**

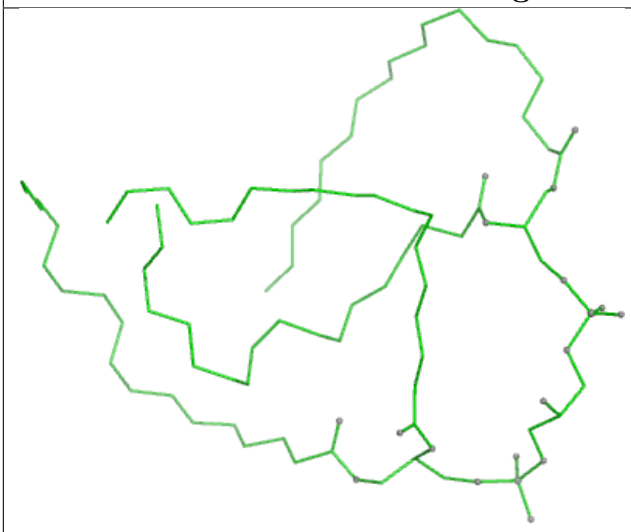


**Torsions**

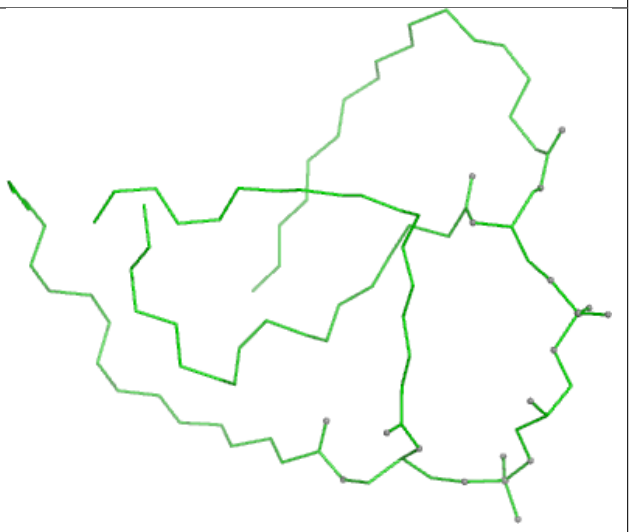


**Rings**

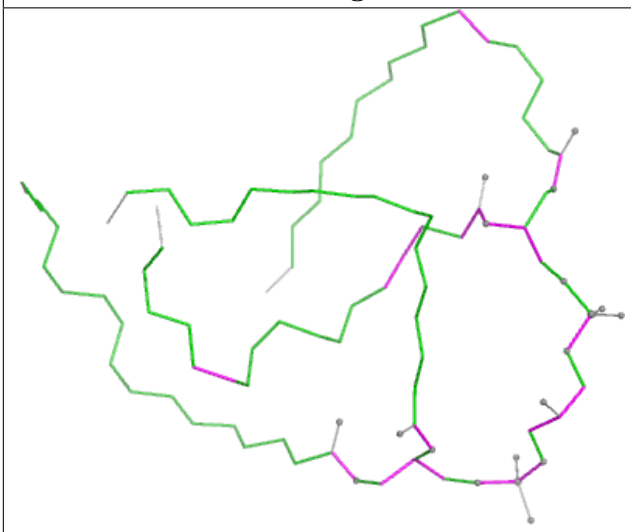
**Ligand CDL EB 302**



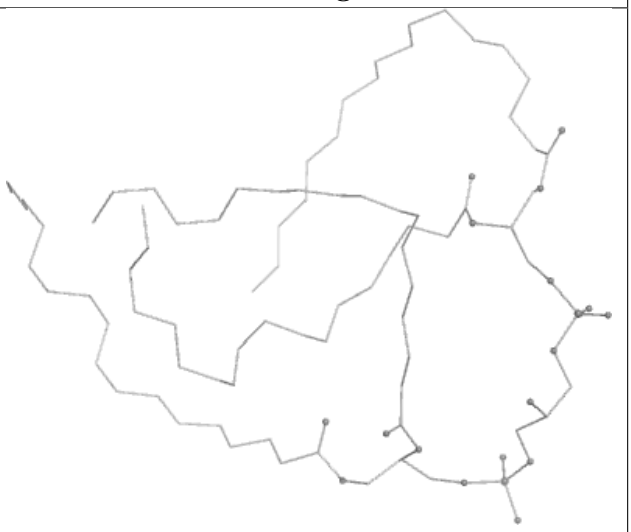
**Bond lengths**



**Bond angles**

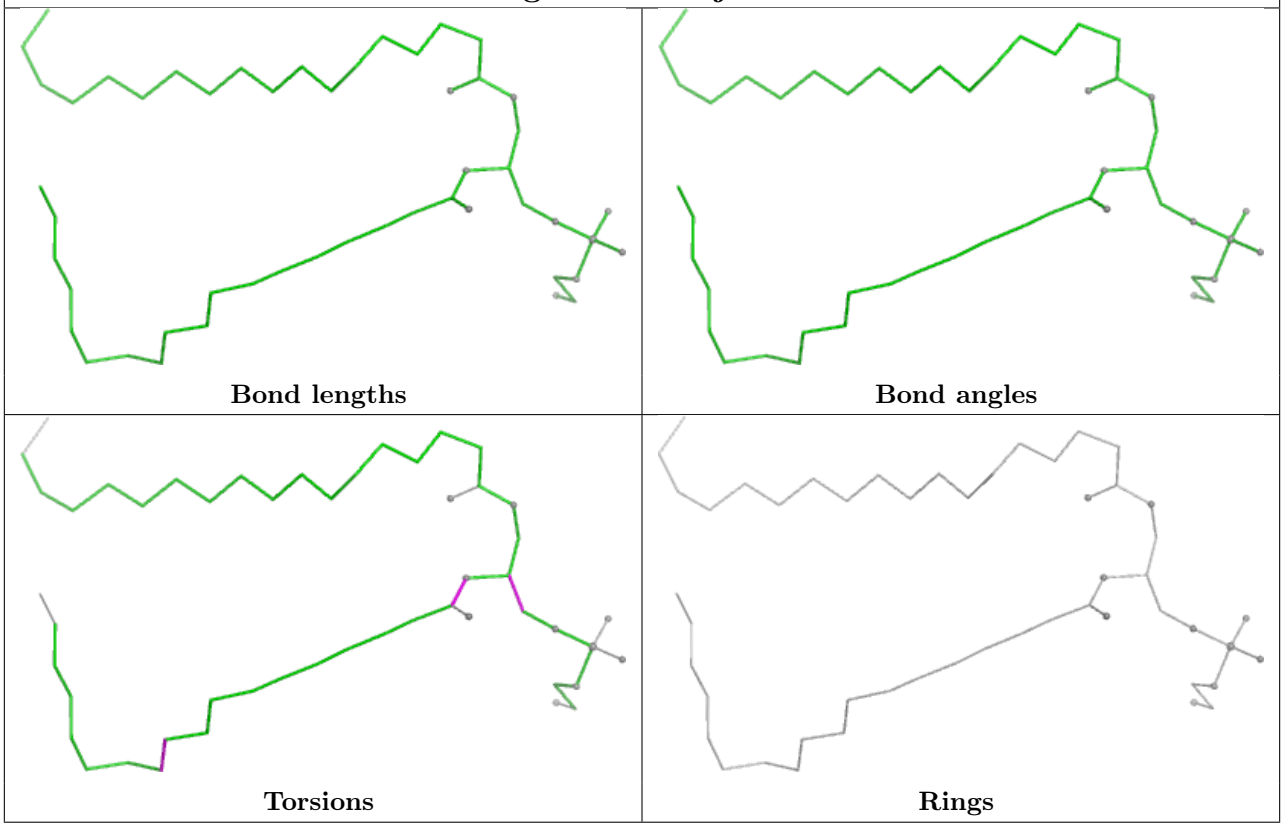


**Torsions**

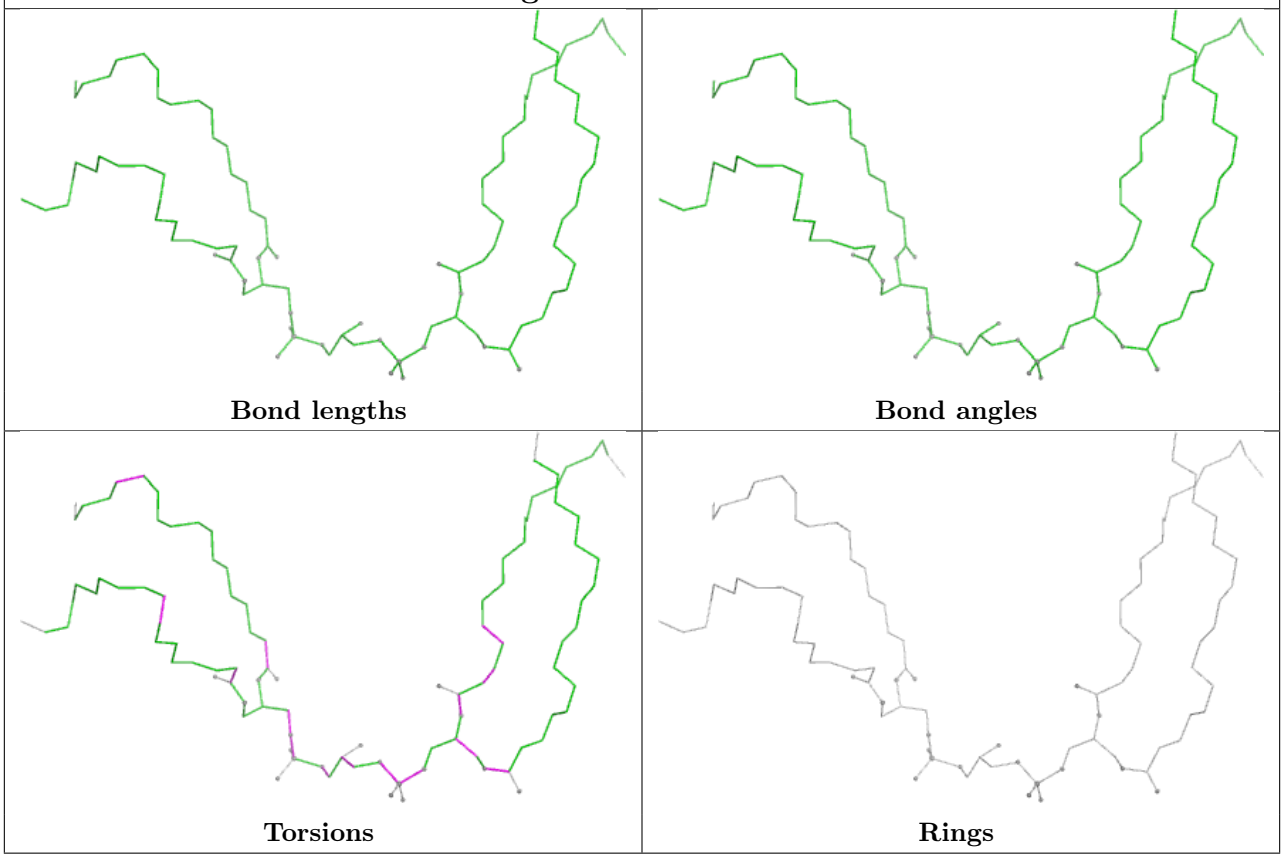


**Rings**

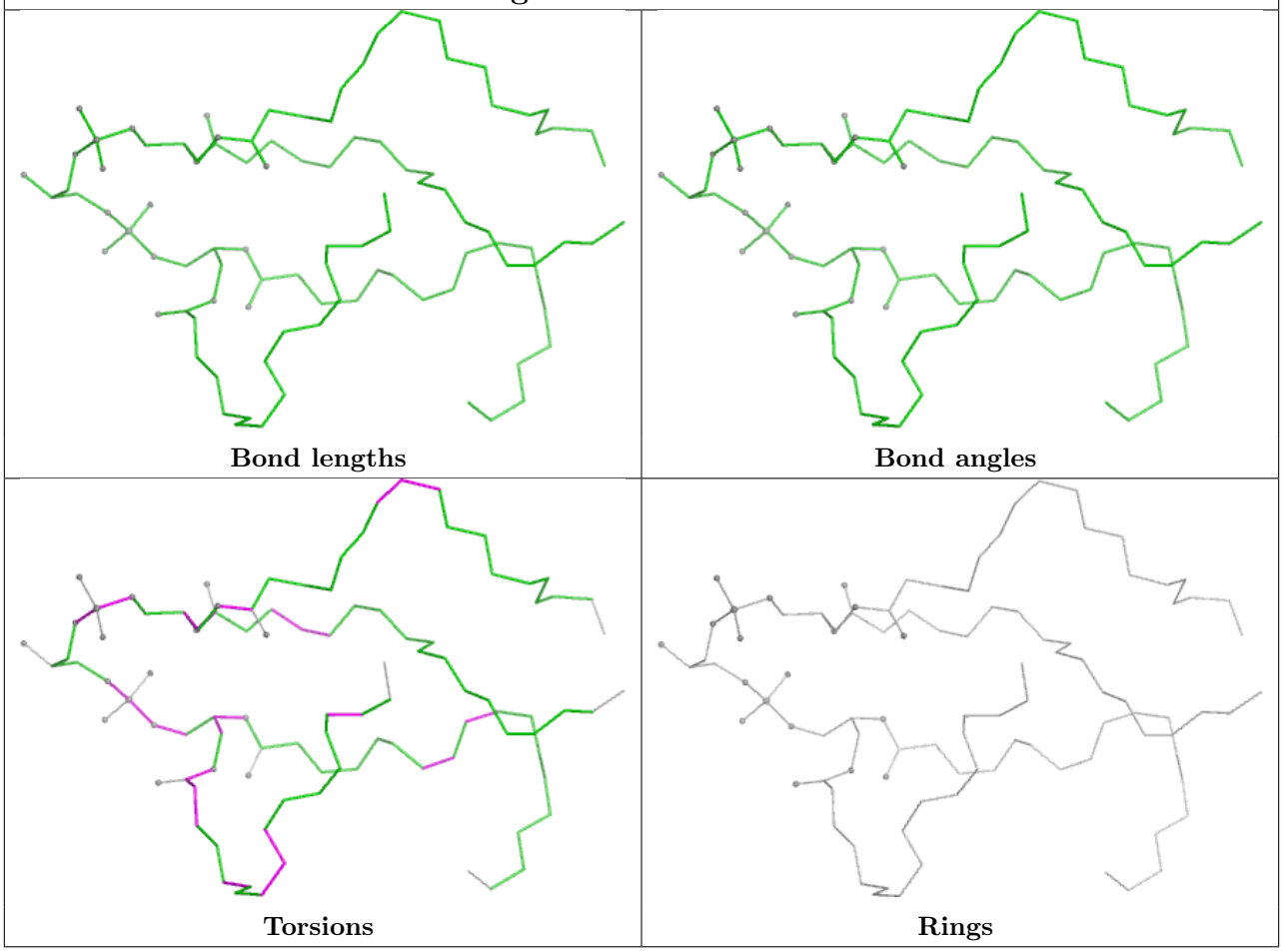
## Ligand 3PE Dj 407



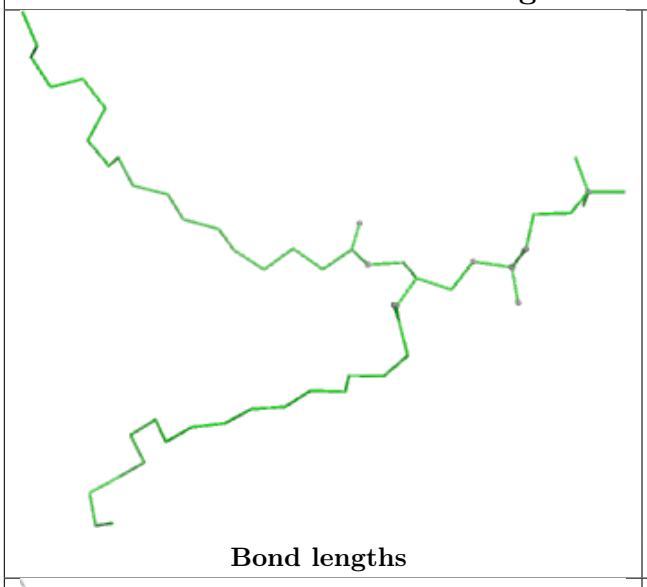

## Ligand CDL Ei 401



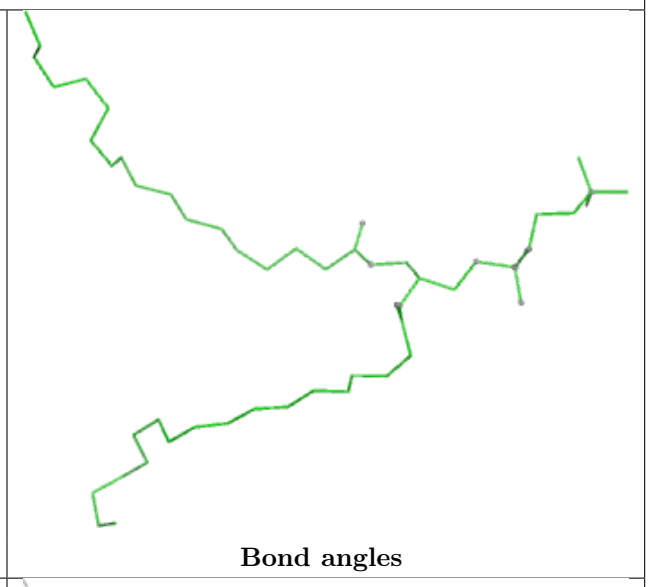
**Ligand CDL DA 709**



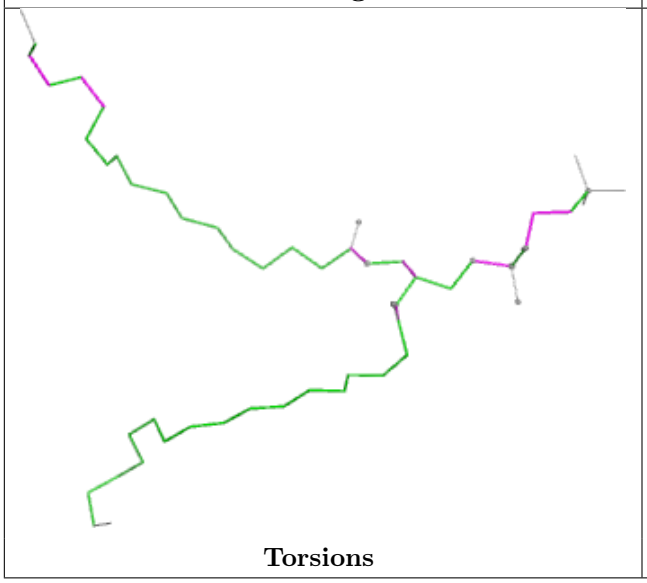
**Ligand PC1 Da 707**



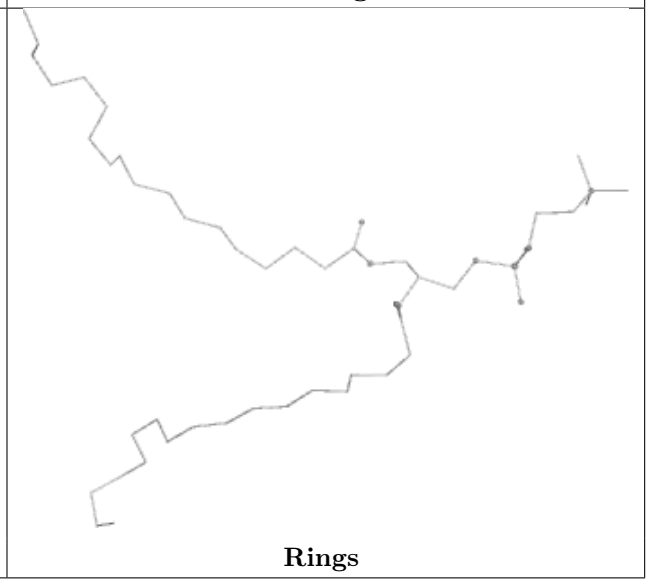
**Bond lengths**



**Bond angles**

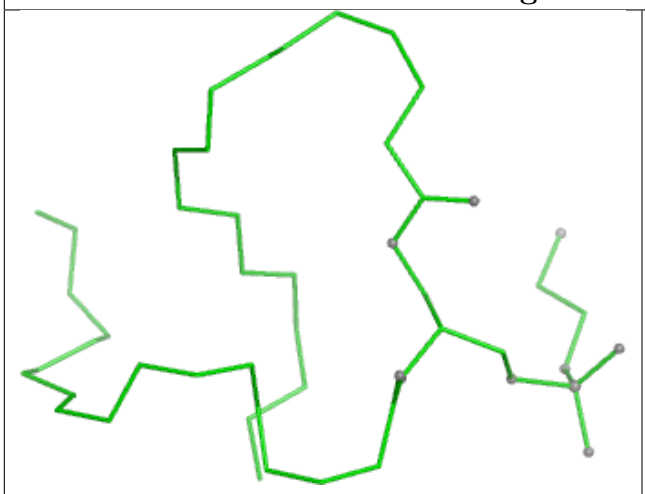


**Torsions**



**Rings**

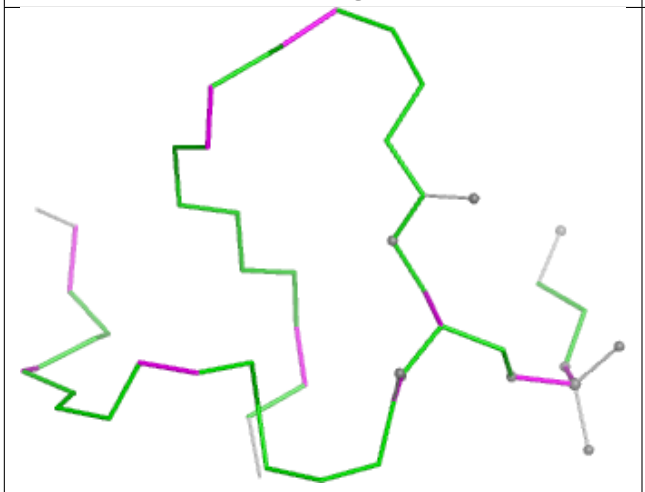
**Ligand 3PE EL 905**



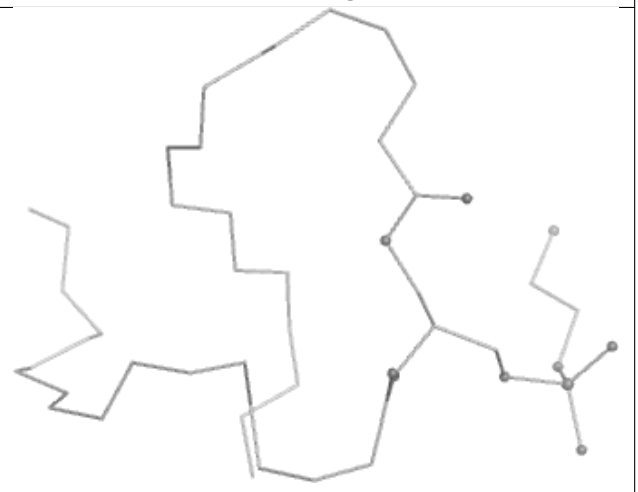
Bond lengths



Bond angles

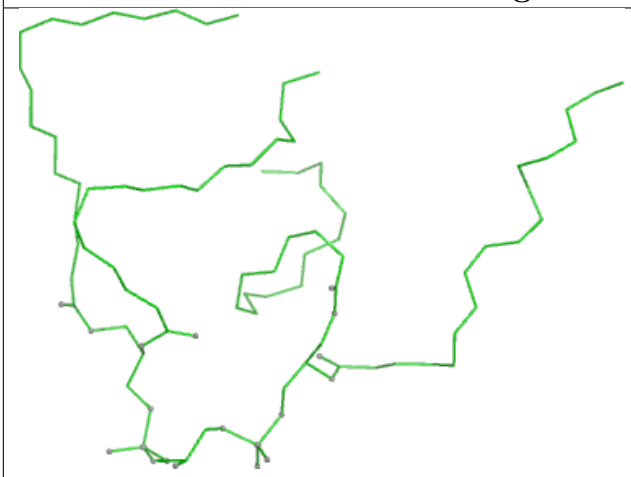


Torsions

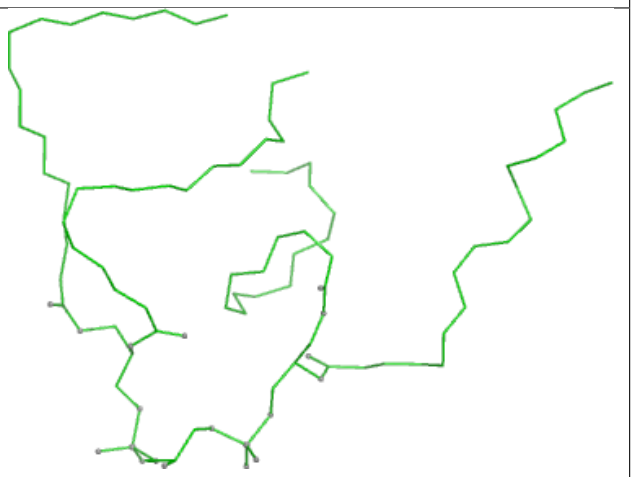


Rings

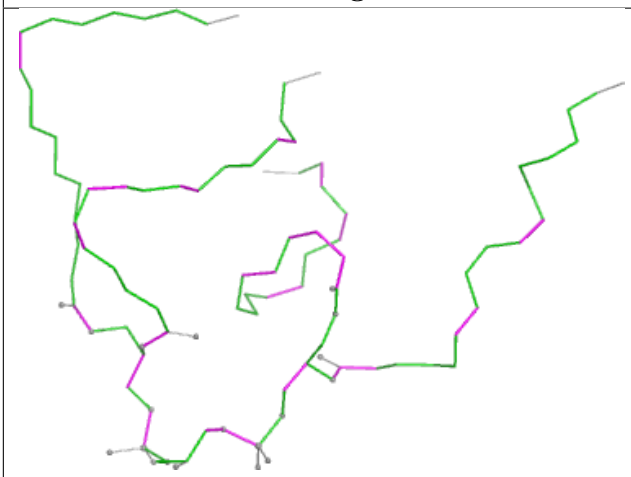
**Ligand CDL DS 405**



**Bond lengths**



**Bond angles**



**Torsions**



**Rings**

**Ligand CDL DN 501**



**Bond lengths**



**Bond angles**

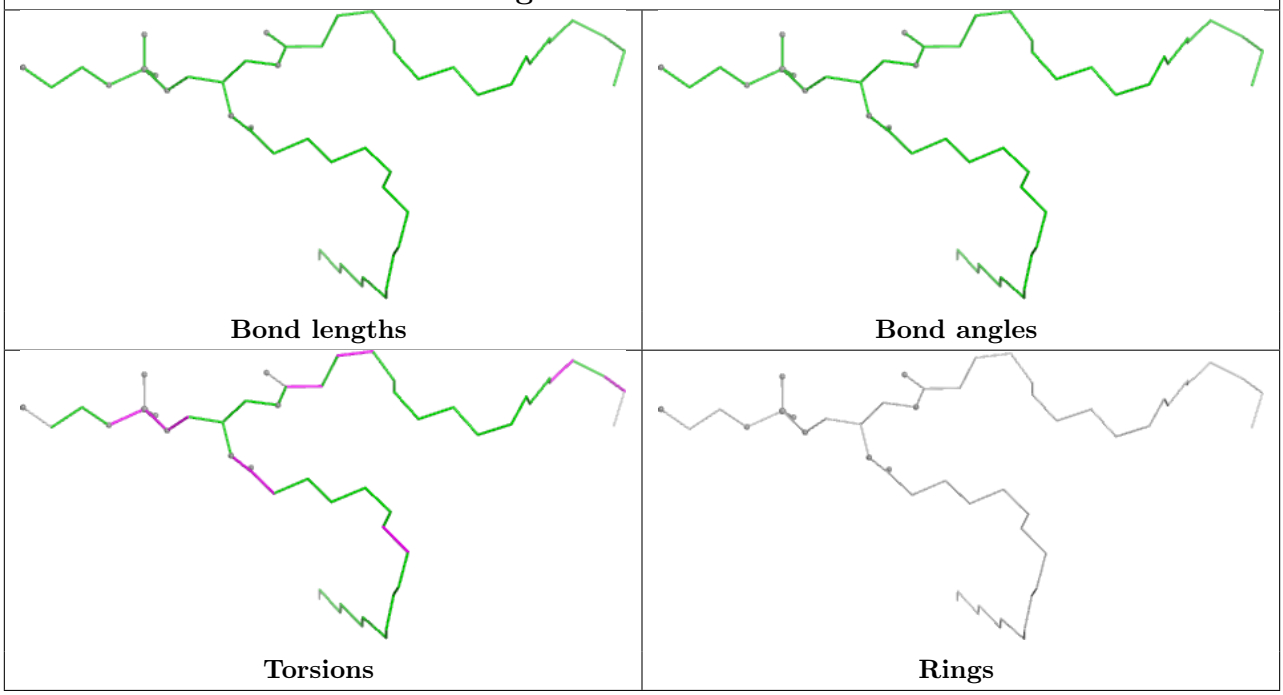


**Torsions**

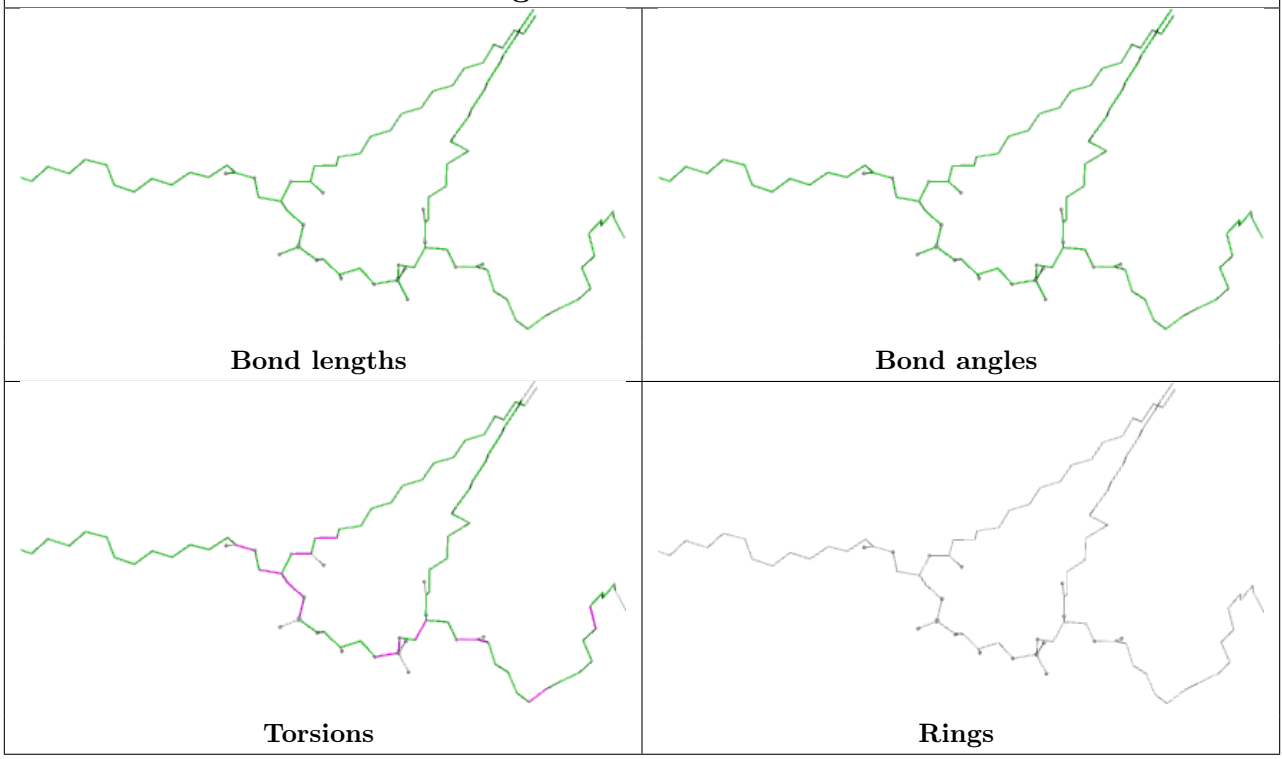


**Rings**

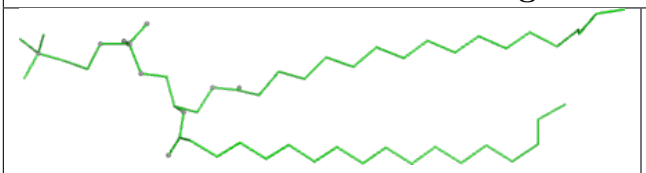
## Ligand 3PE DX 304



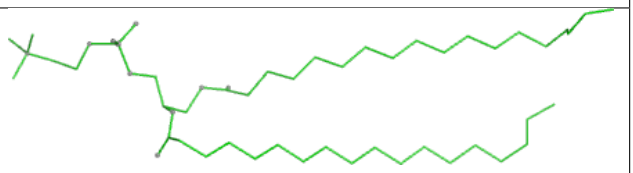

## Ligand CDL EH 202



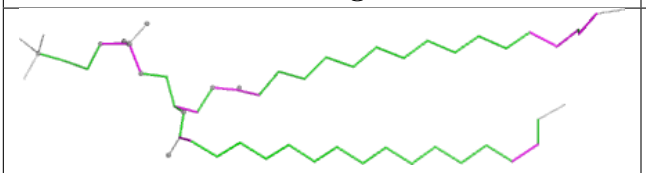
**Ligand PC1 Dc 602**



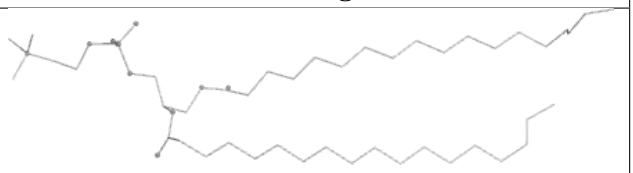
Bond lengths



Bond angles

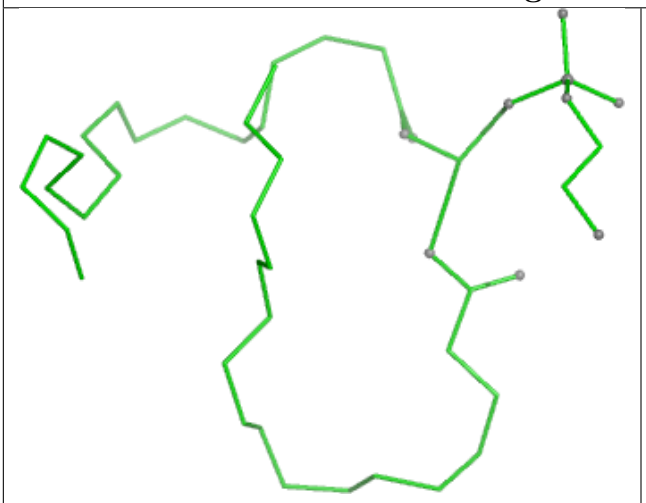


Torsions

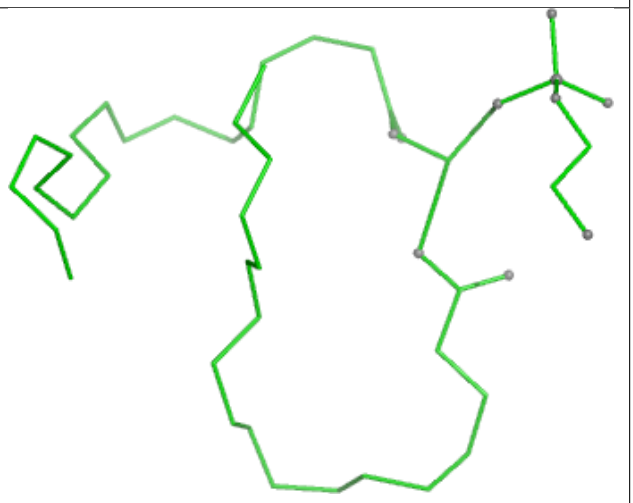


Rings

**Ligand 3PE El 905**



Bond lengths



Bond angles

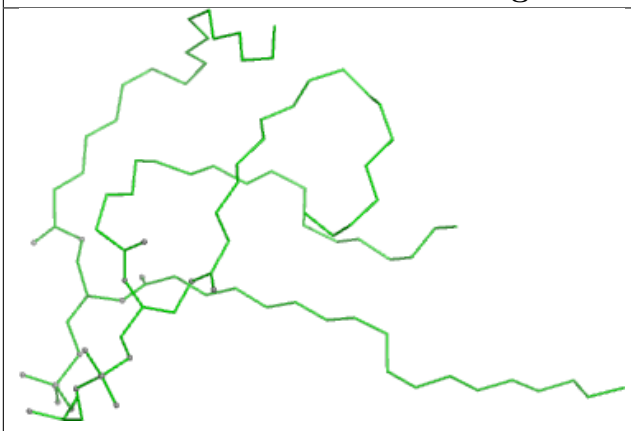


Torsions

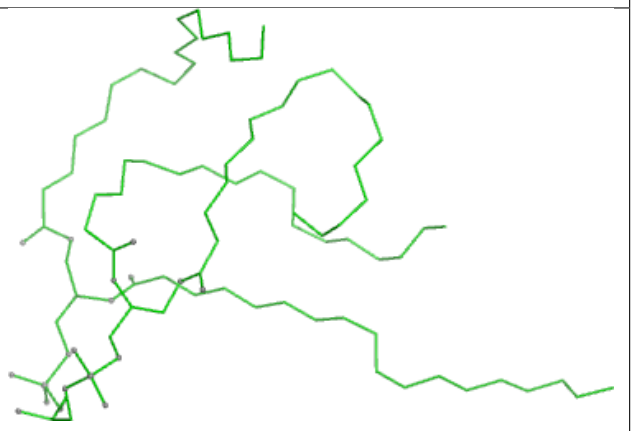


Rings

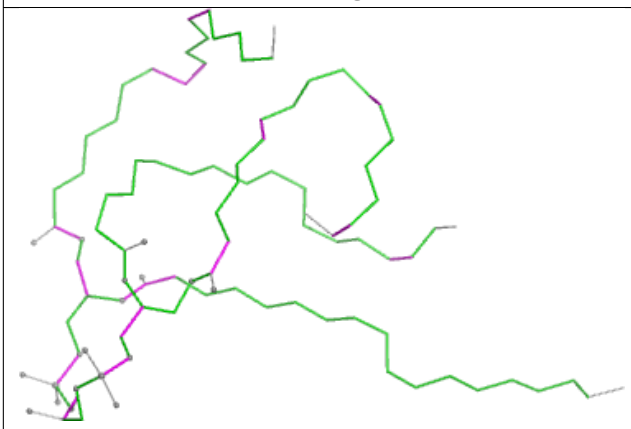
**Ligand CDL EH 201**



**Bond lengths**



**Bond angles**

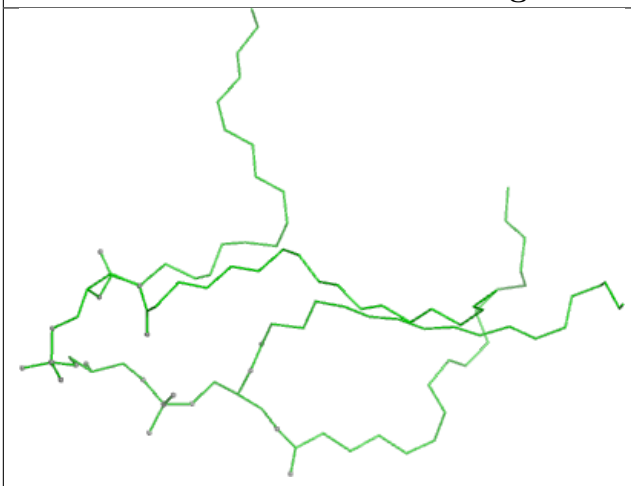


**Torsions**

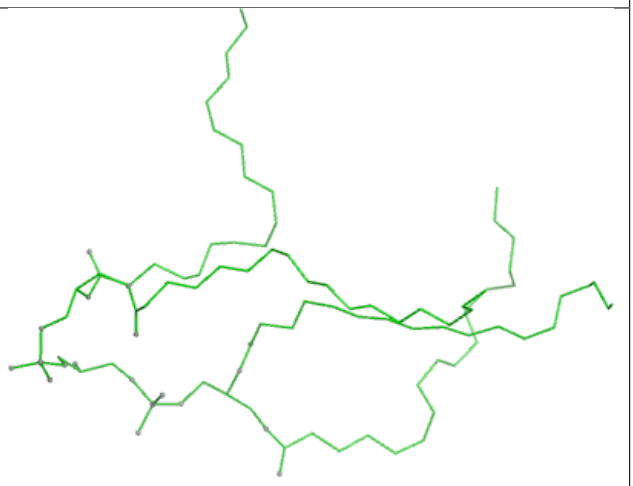


**Rings**

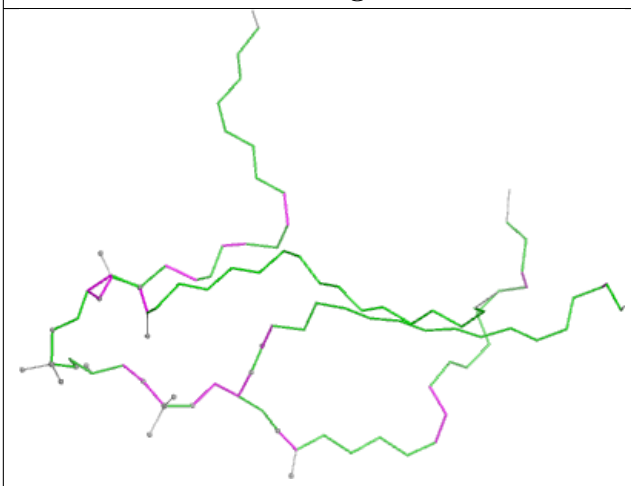
**Ligand CDL DD 703**



**Bond lengths**



**Bond angles**

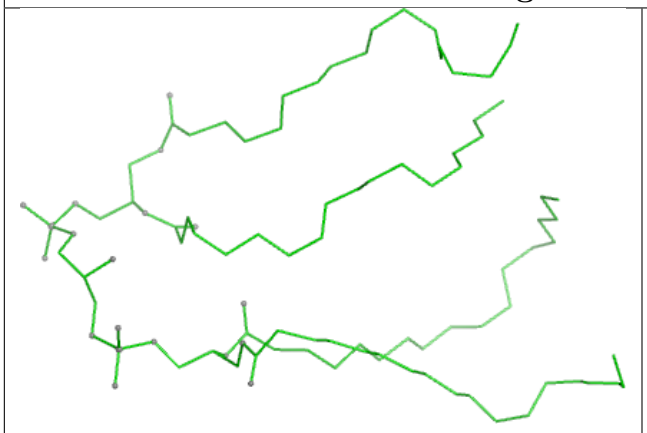


**Torsions**

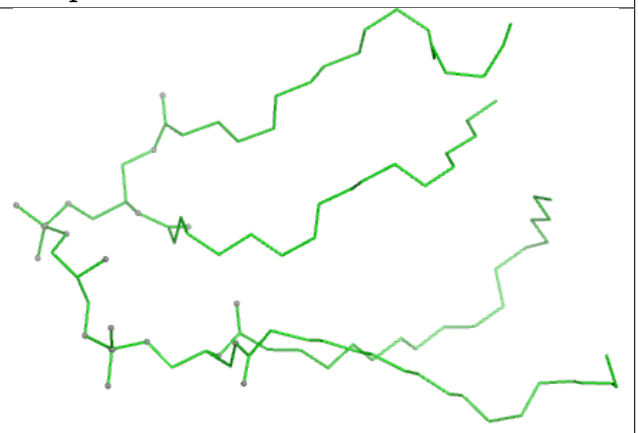


**Rings**

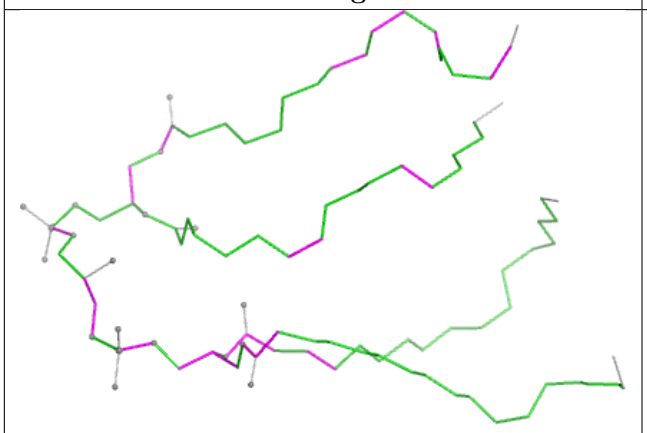
**Ligand CDL Ep 701**



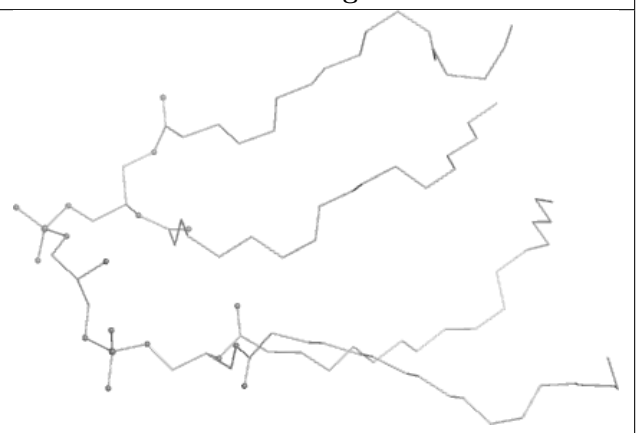
**Bond lengths**



**Bond angles**

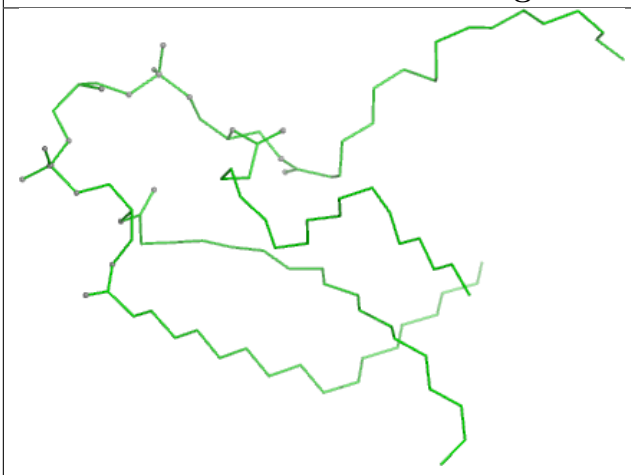


**Torsions**

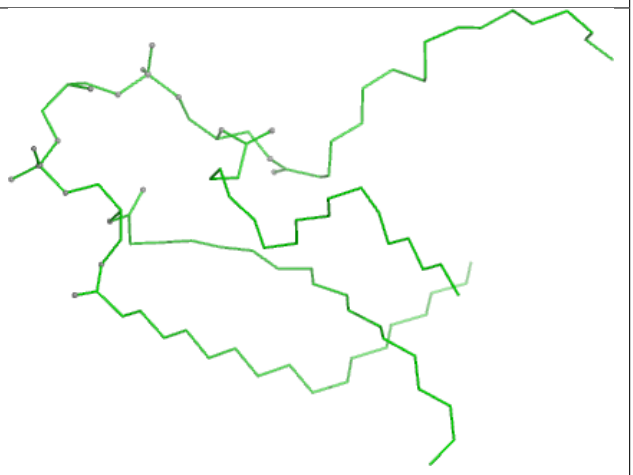


**Rings**

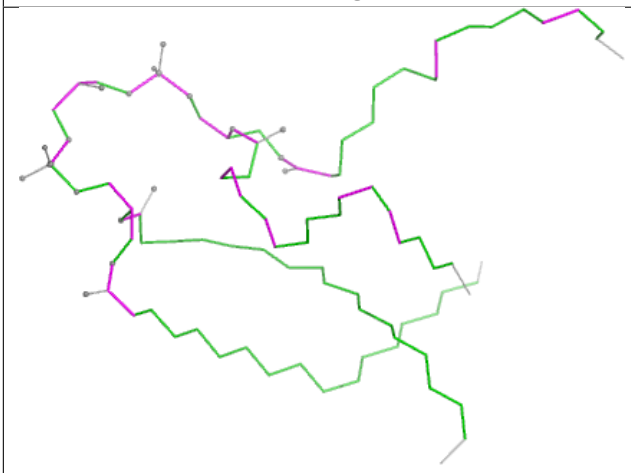
**Ligand CDL DJ 307**



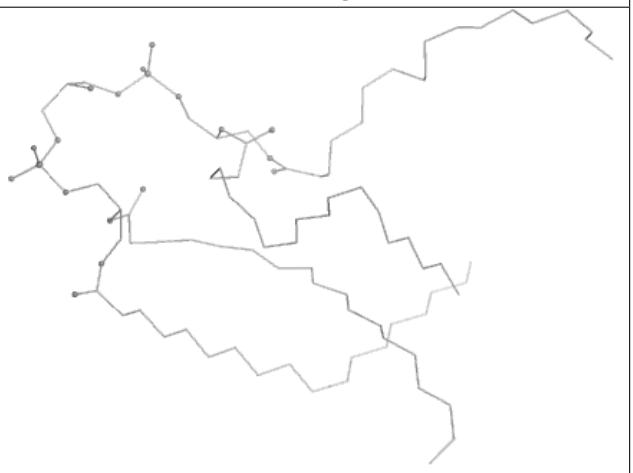
**Bond lengths**



**Bond angles**

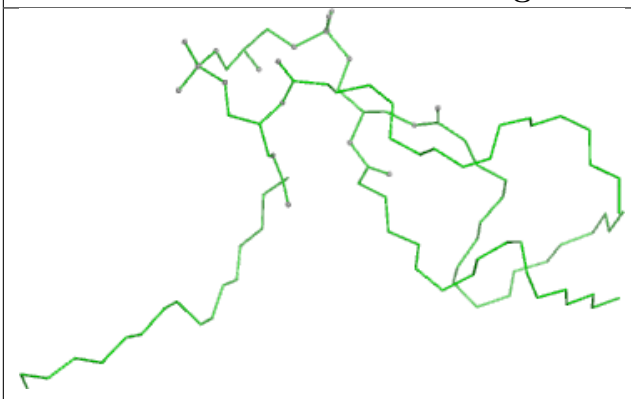


**Torsions**



**Rings**

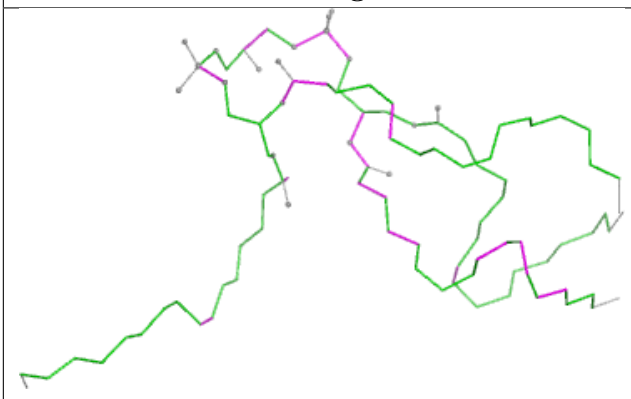
**Ligand CDL Dq 403**



**Bond lengths**



**Bond angles**

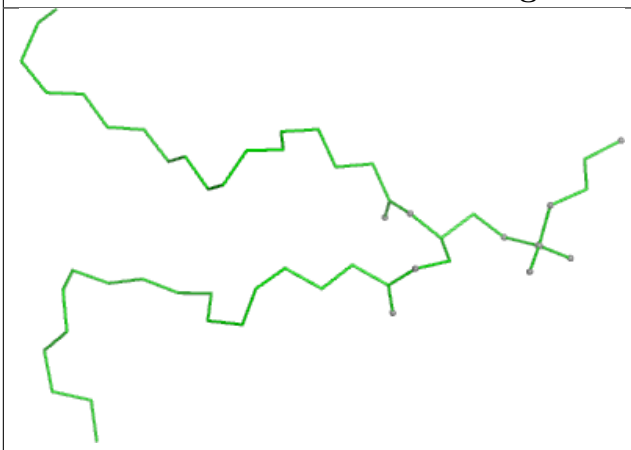


**Torsions**

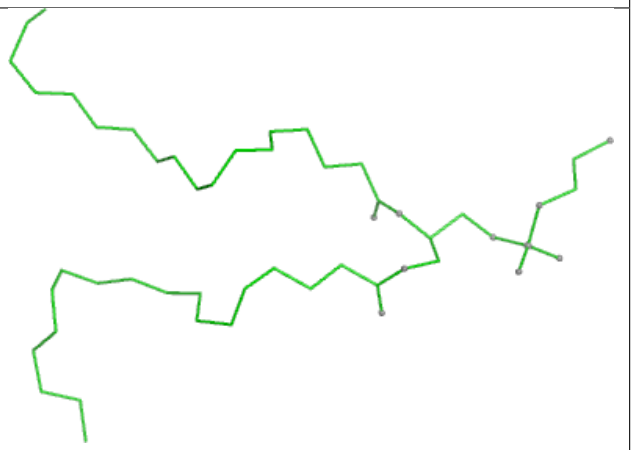


**Rings**

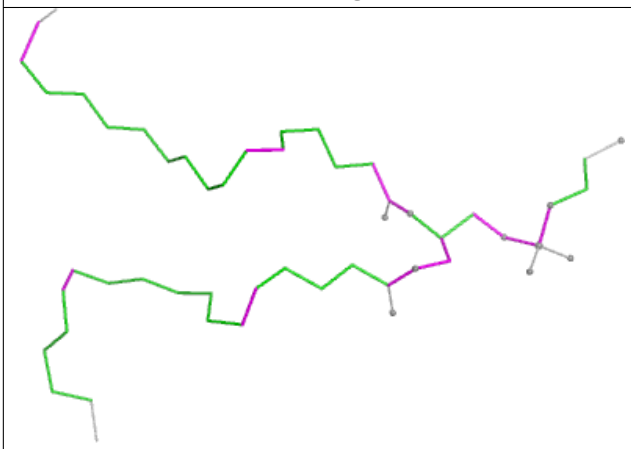
**Ligand 3PE Dc 606**



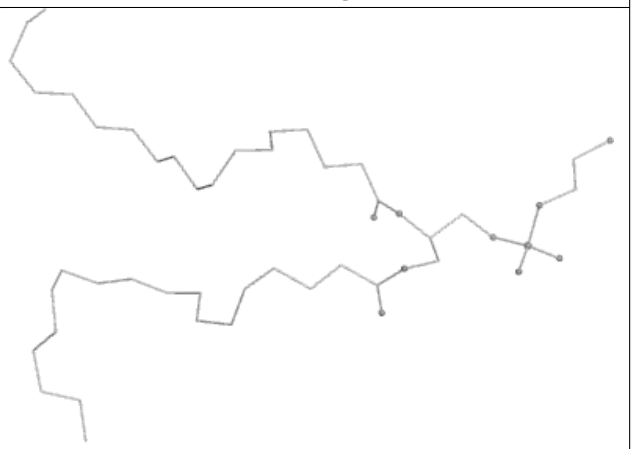
**Bond lengths**



**Bond angles**

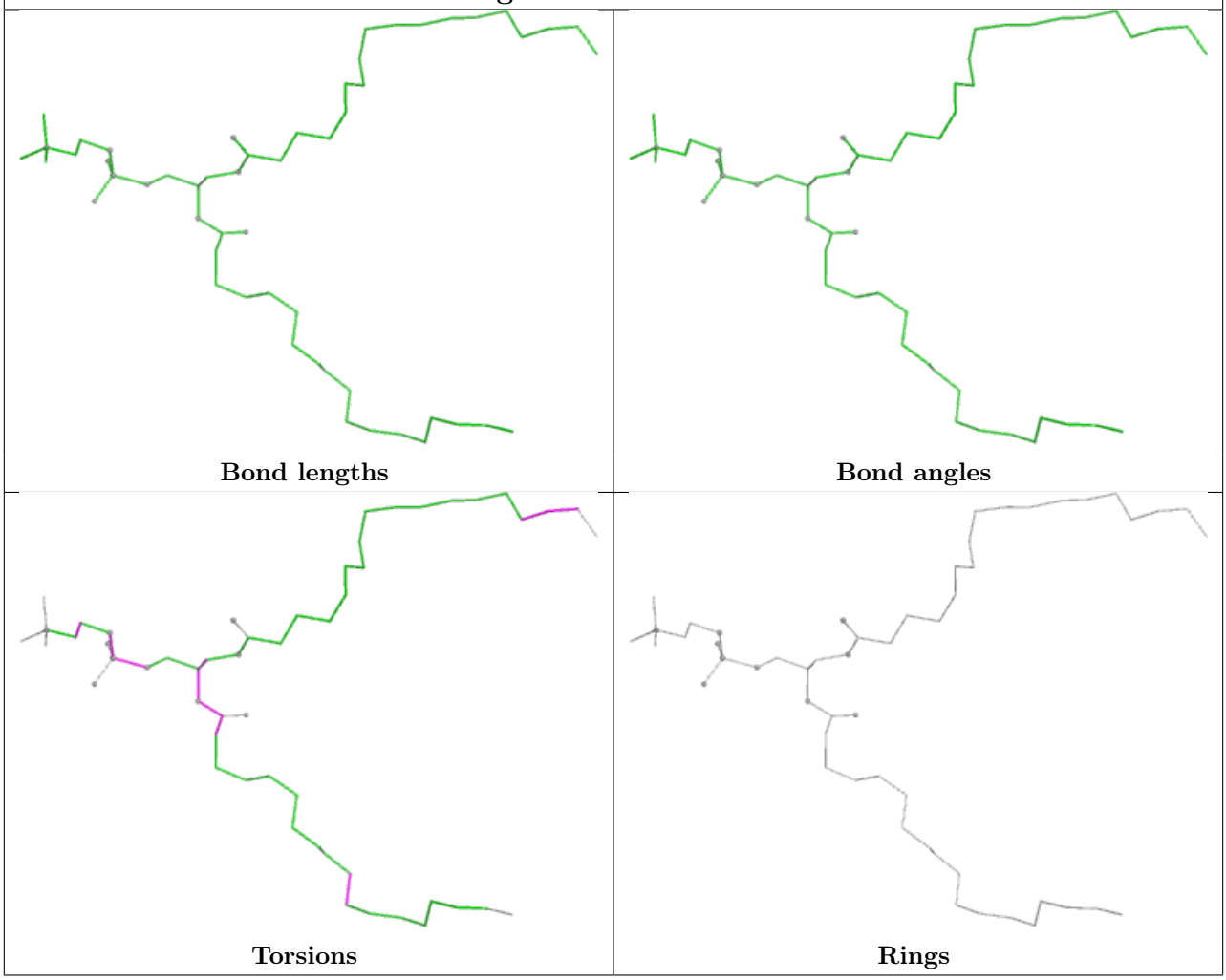


**Torsions**



**Rings**

**Ligand PC1 Dc 605**



**Ligand CDL DY 301**



**Bond lengths**



**Bond angles**

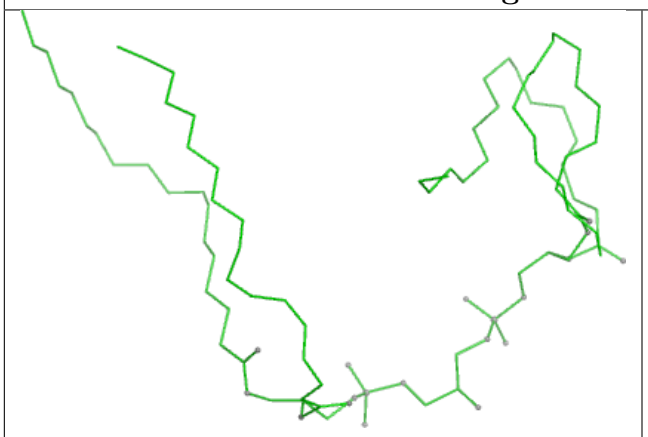


**Torsions**

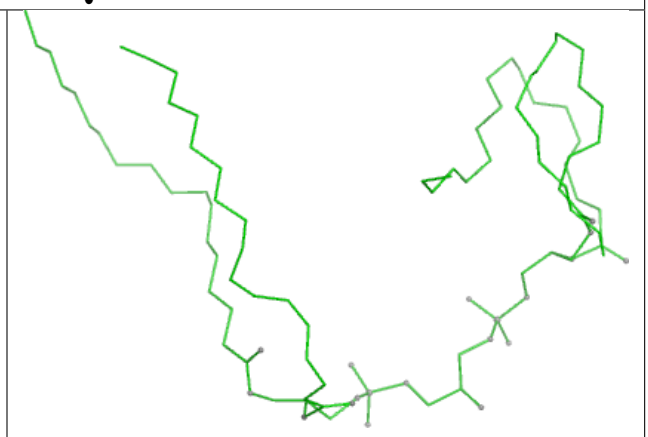


**Rings**

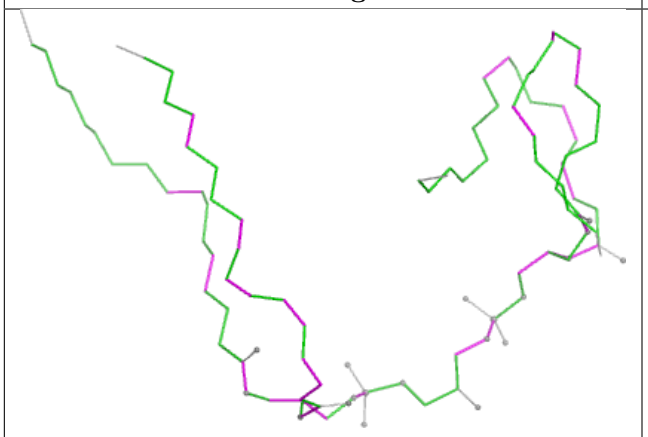
## Ligand CDL DQ 1504



Bond lengths



Bond angles

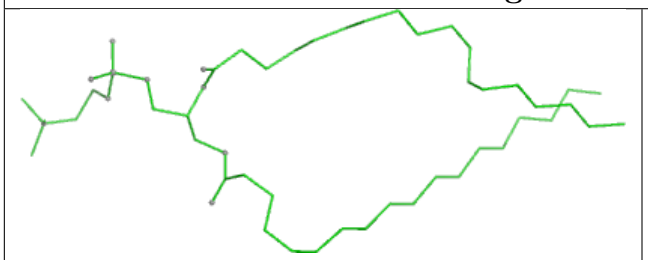


Torsions

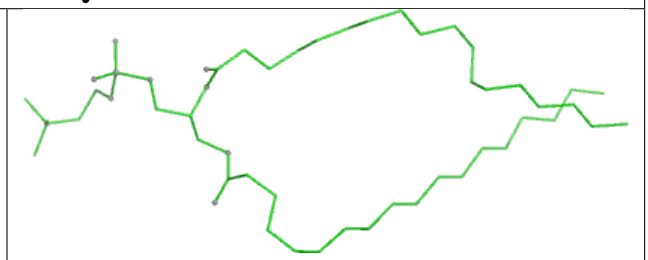


Rings

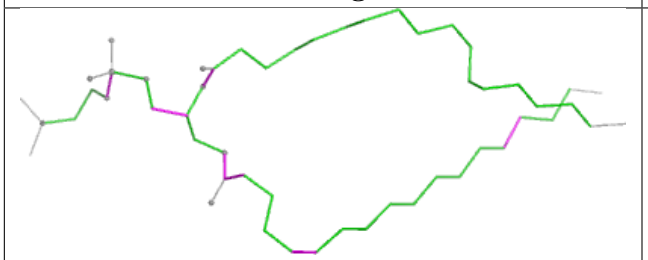
## Ligand PC1 DQ 1503



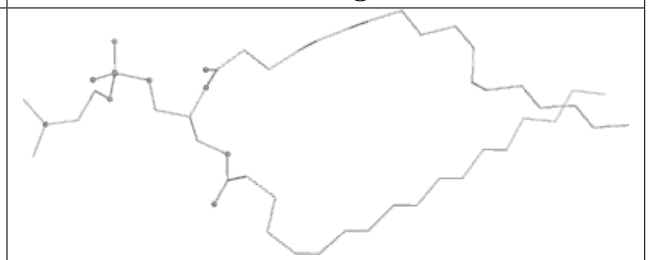
Bond lengths



Bond angles

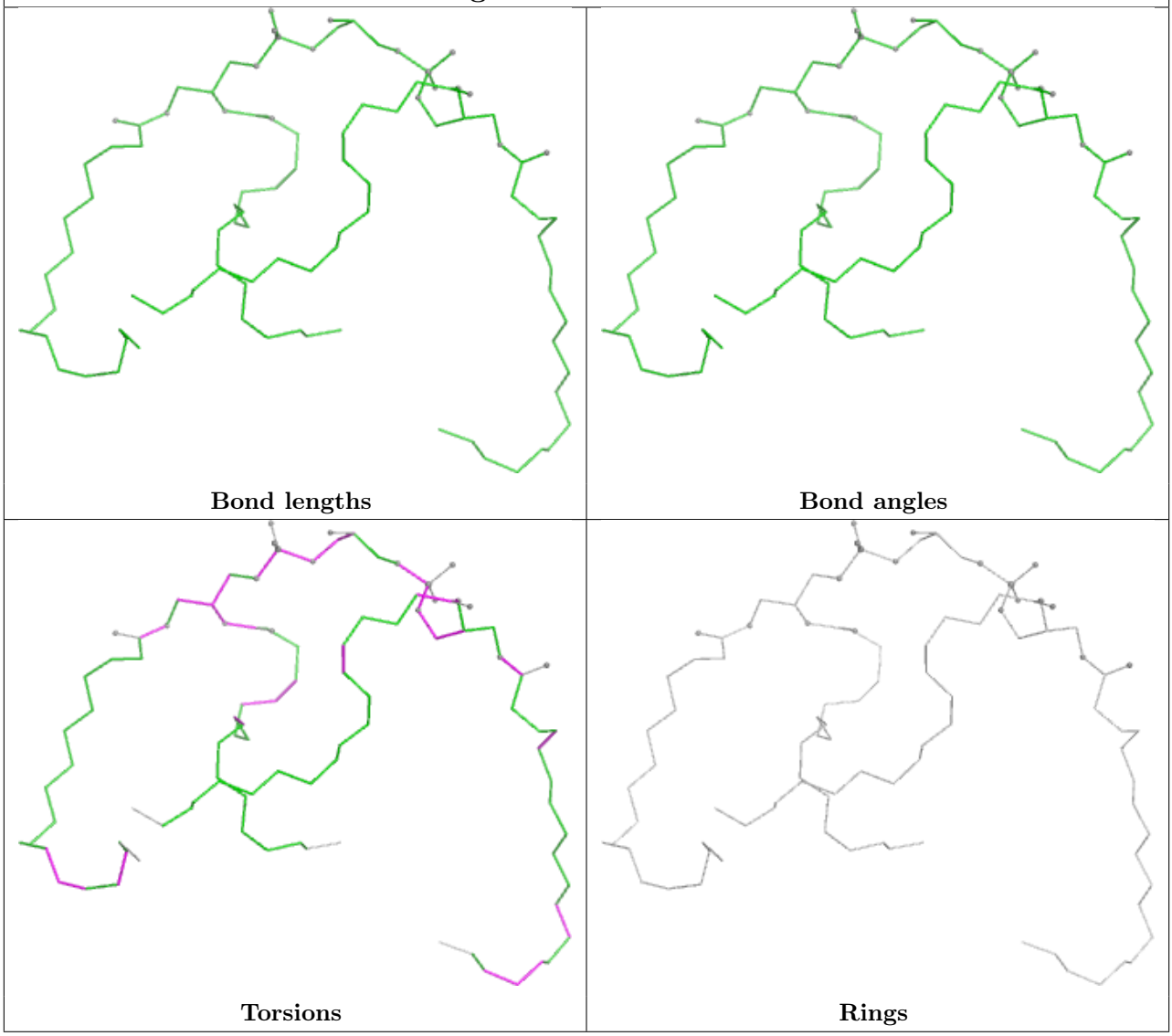


Torsions

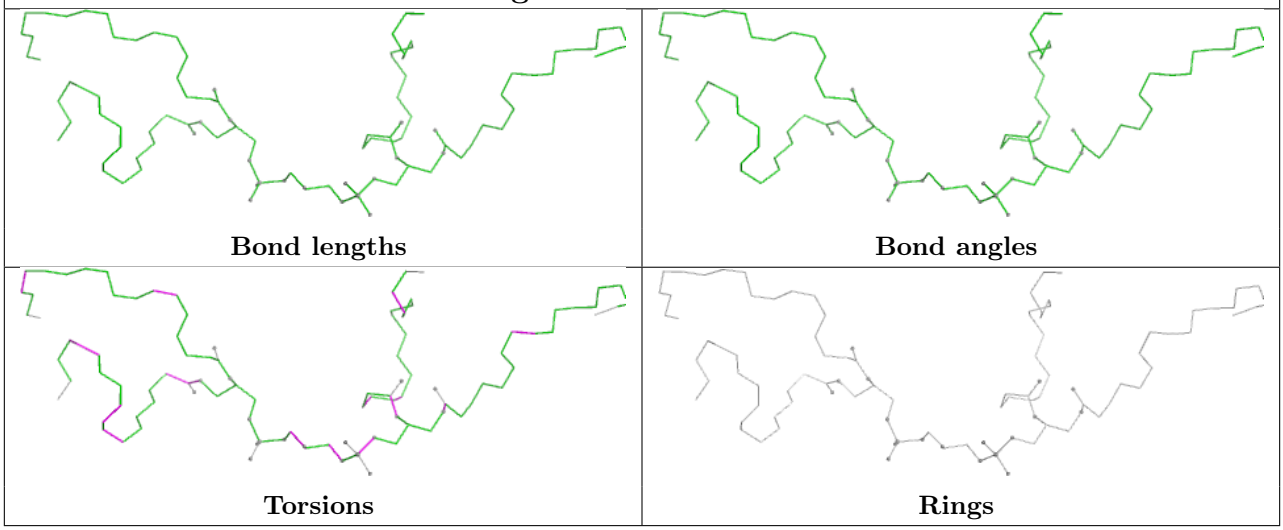


Rings

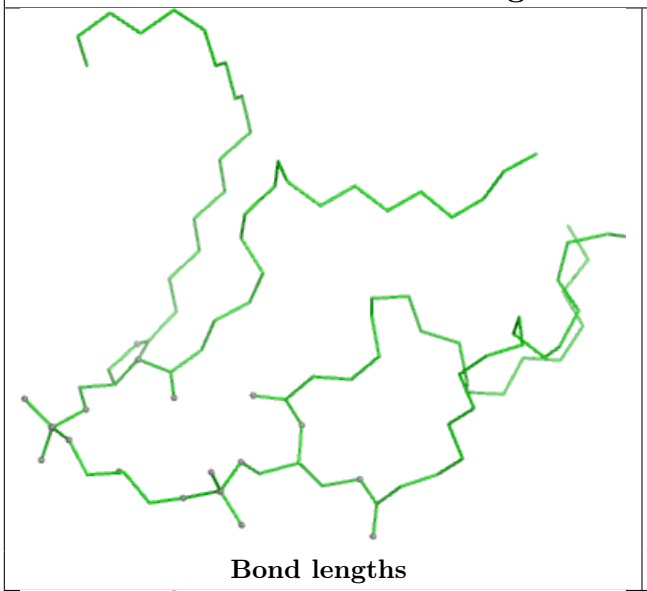
## Ligand CDL Dv 404



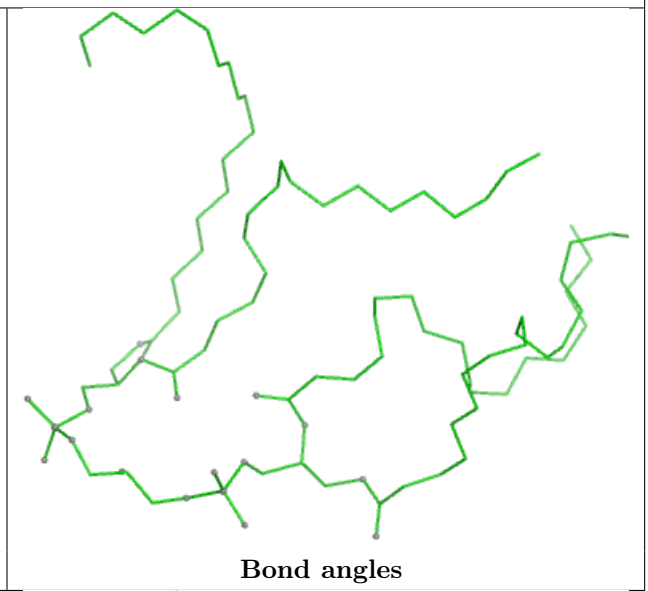

## Ligand CDL DV 403



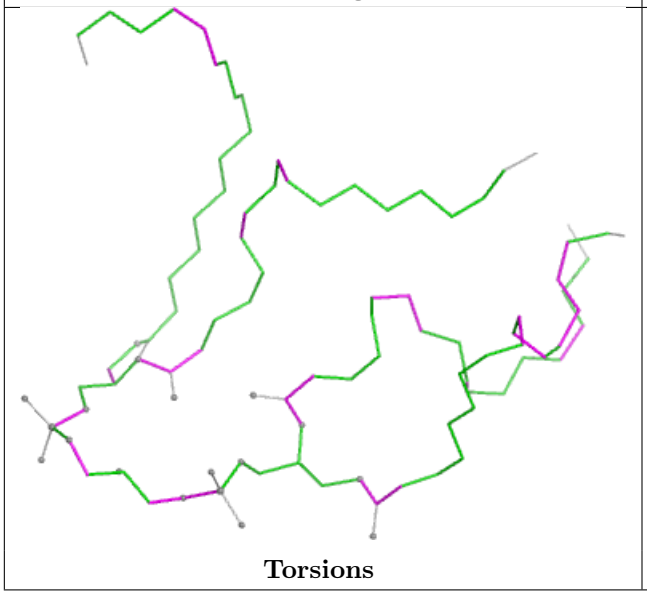
**Ligand CDL DM 501**



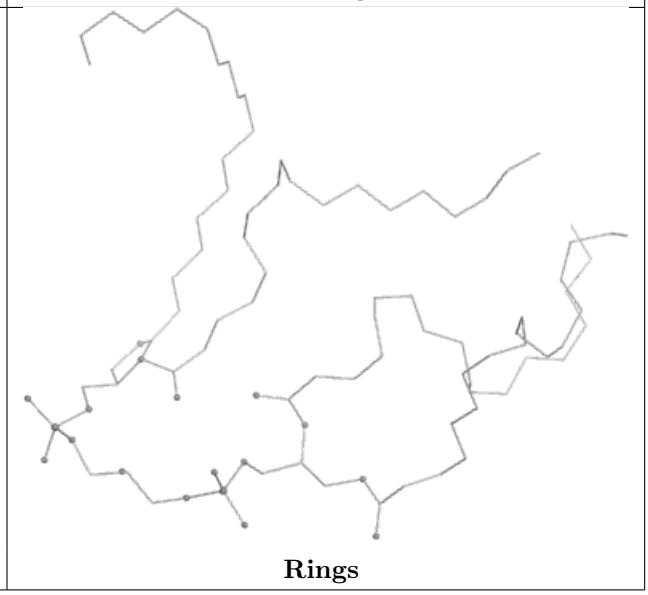
**Bond lengths**



**Bond angles**

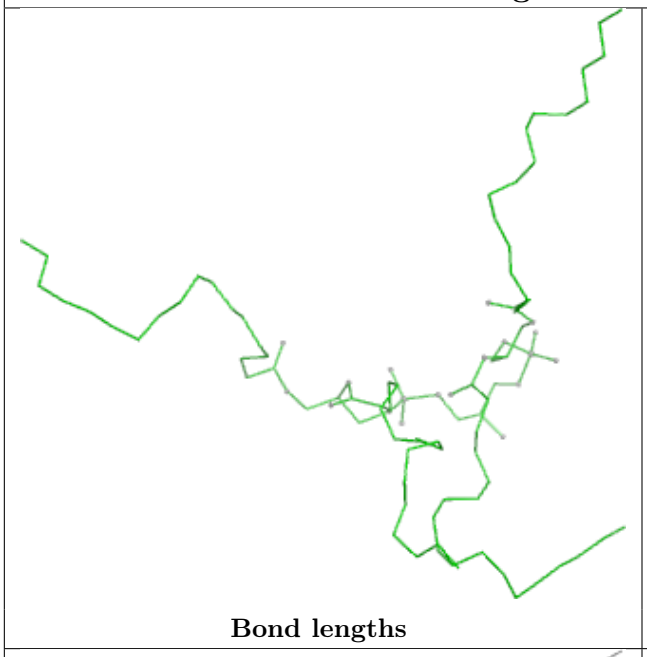


**Torsions**

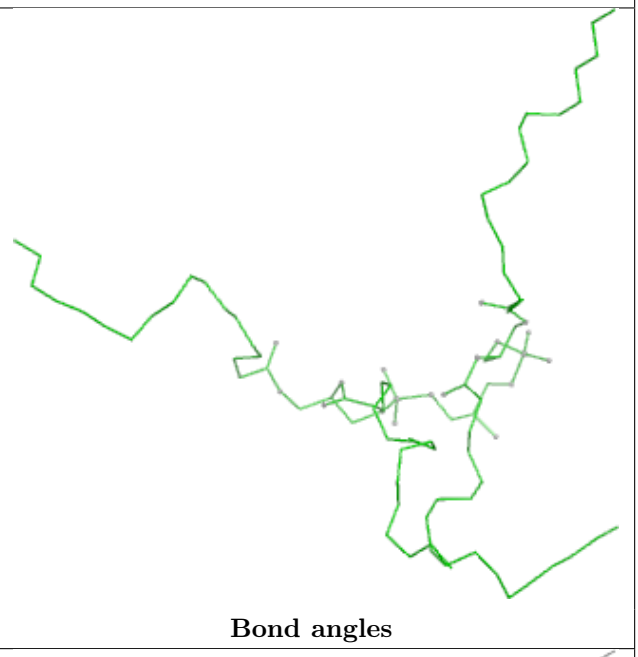


**Rings**

**Ligand CDL EO 202**



**Bond lengths**



**Bond angles**

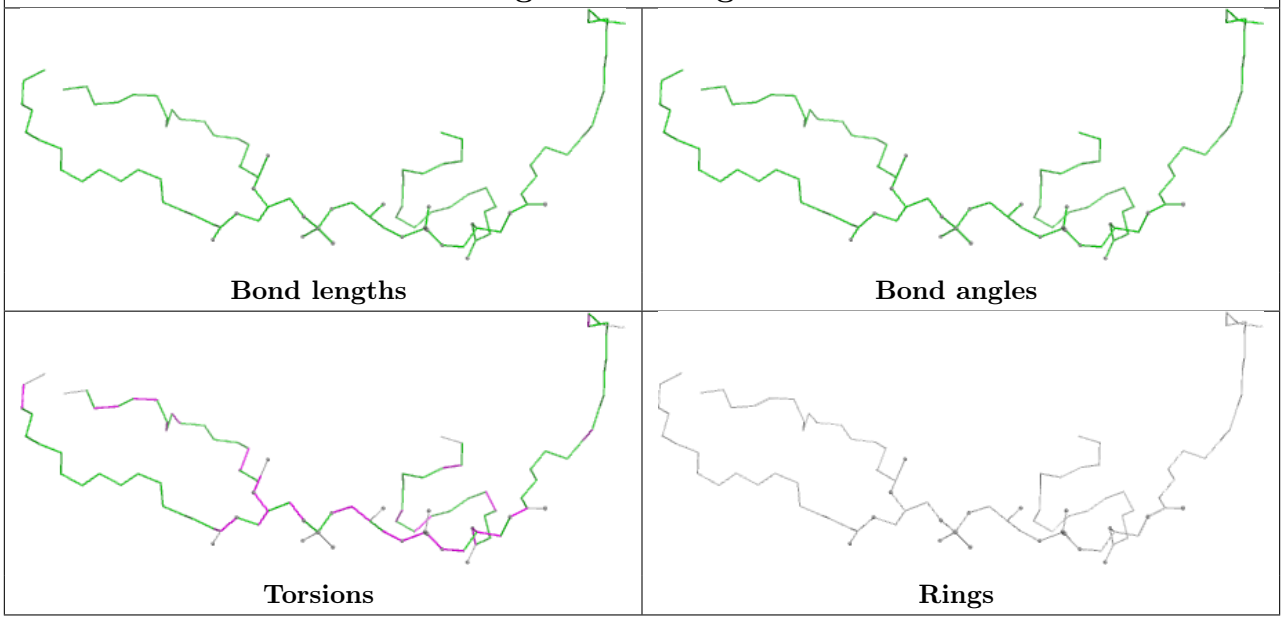


**Torsions**

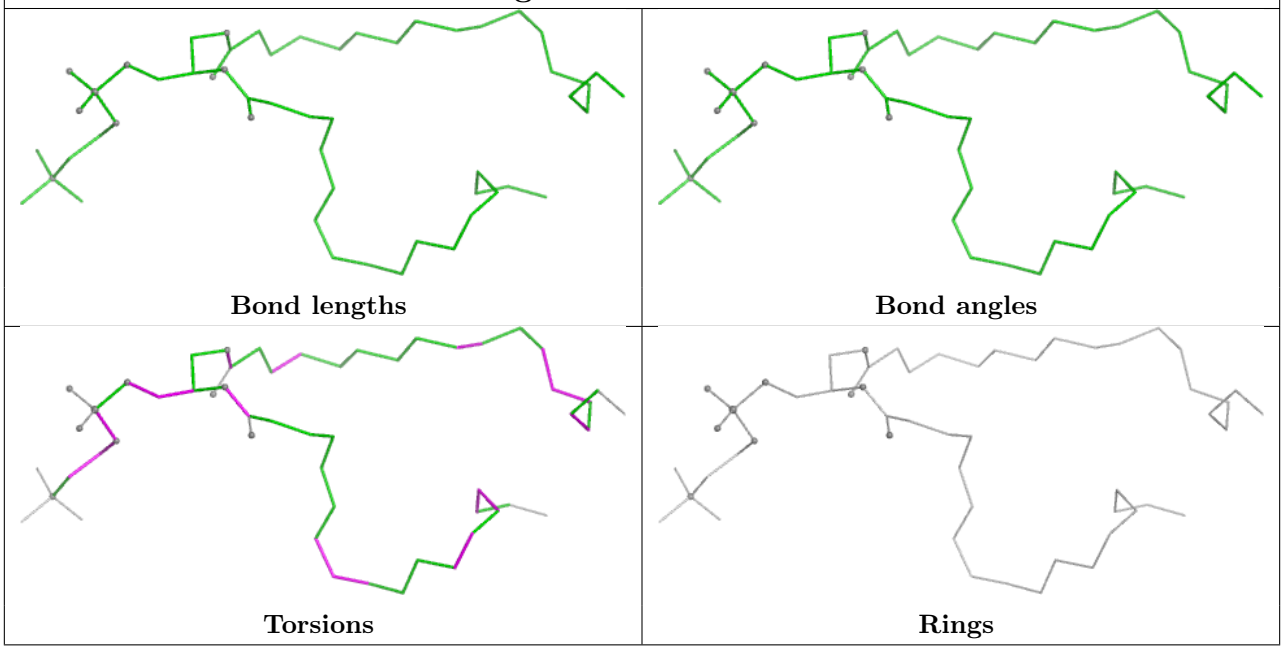


**Rings**

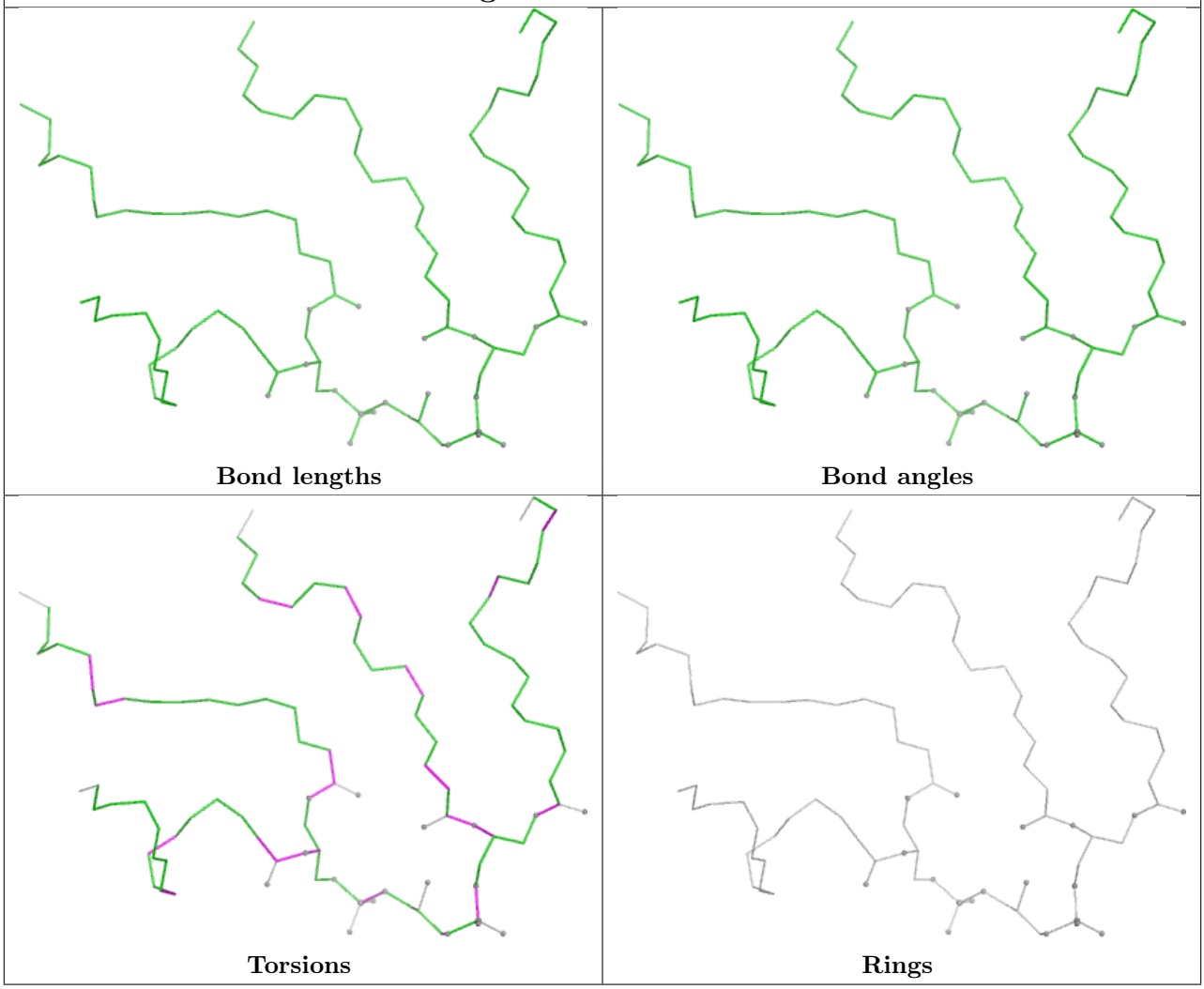
## Ligand CDL Dg 201



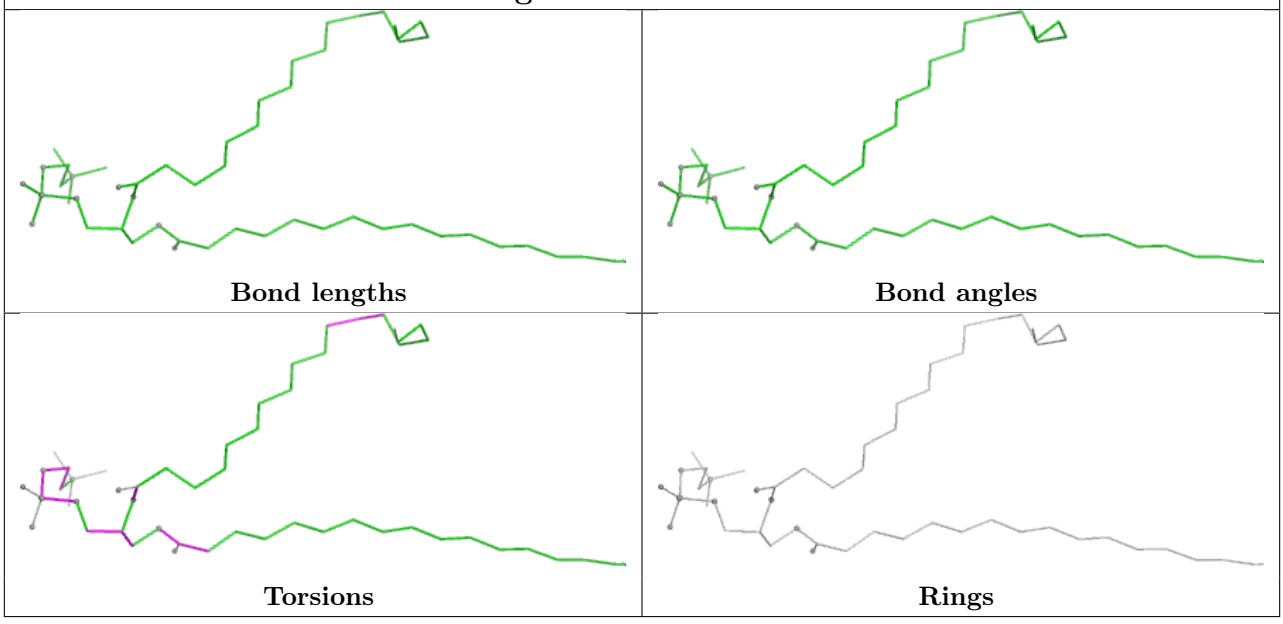

## Ligand PC1 DB 702



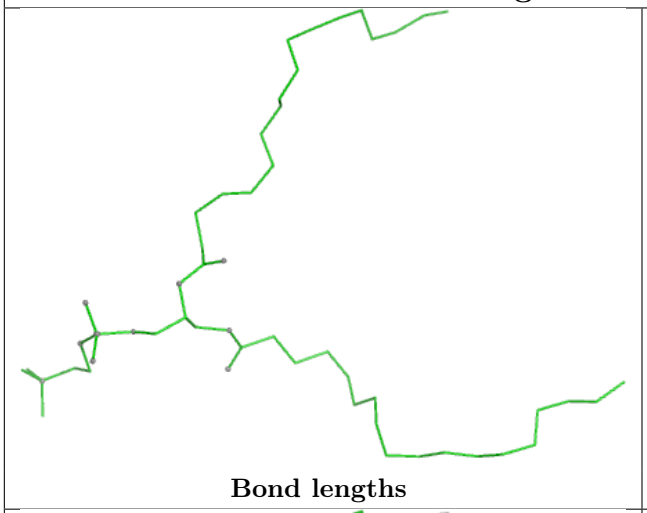
## Ligand CDL DV 401



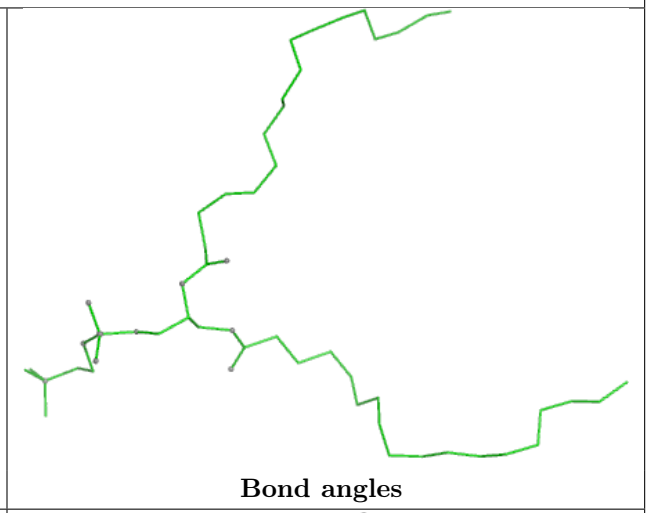

## Ligand PC1 Ef 1001



**Ligand PC1 DC 605**



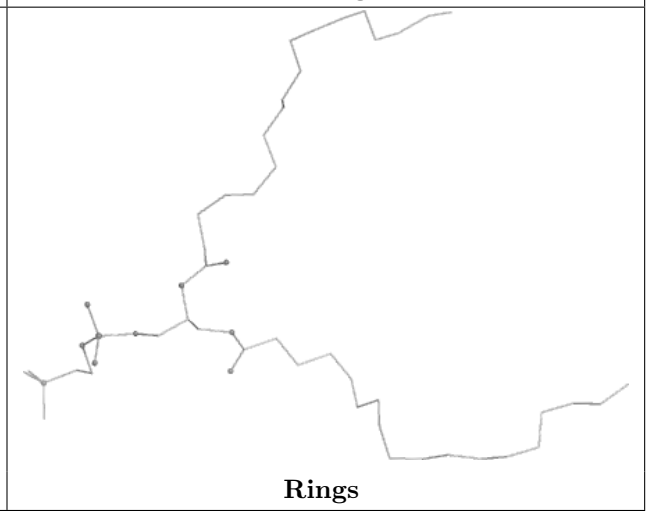
**Bond lengths**



**Bond angles**

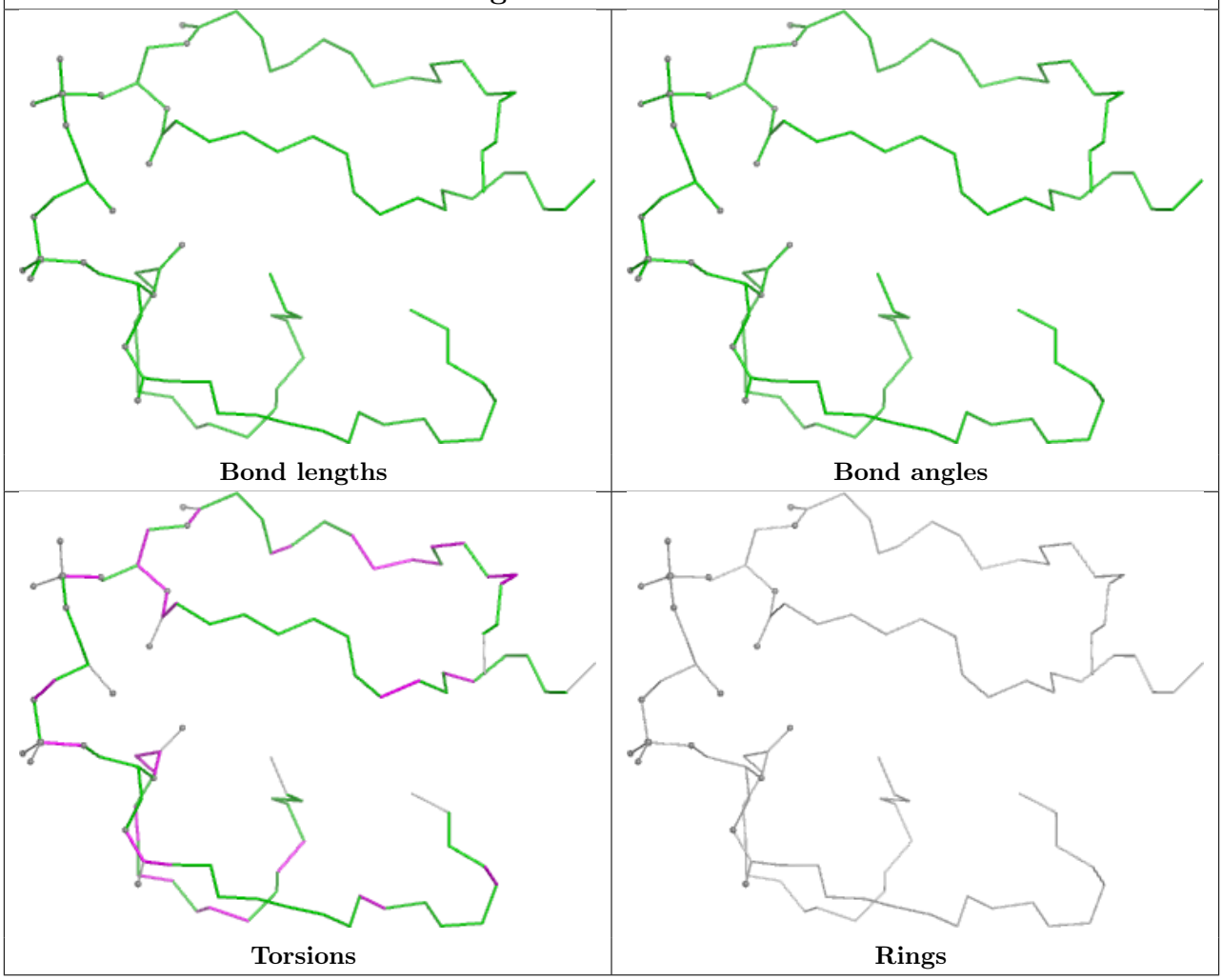


**Torsions**

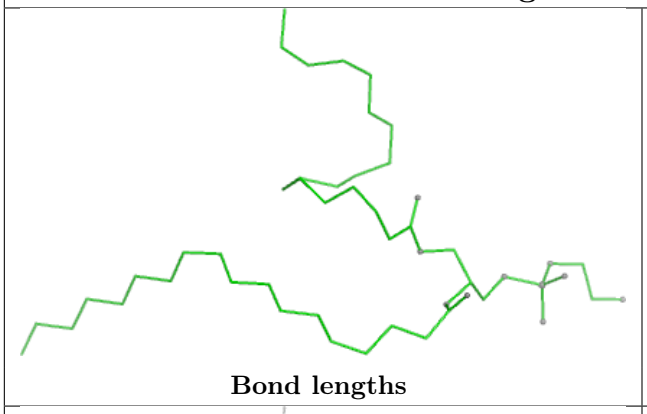


**Rings**

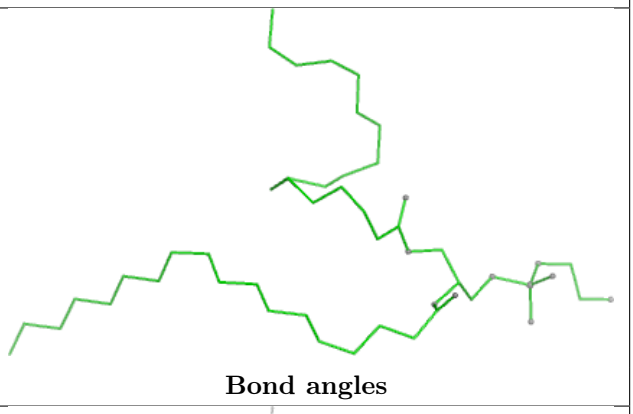
**Ligand CDL Dv 402**



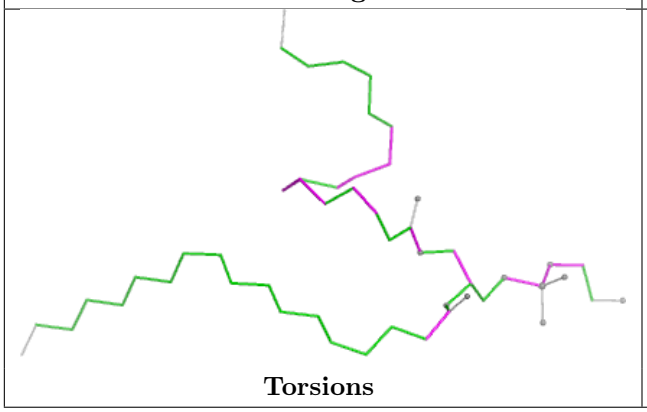
## Ligand 3PE DS 401



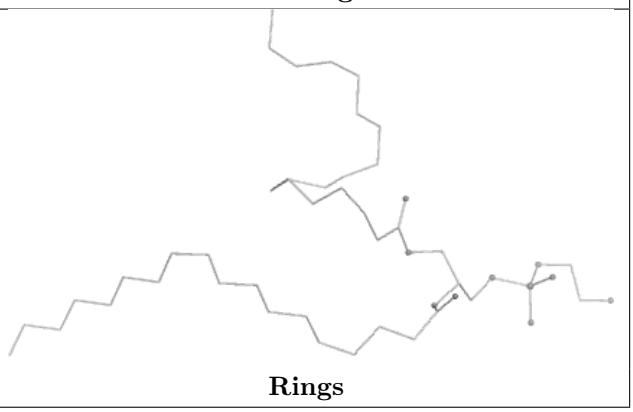
Bond lengths



Bond angles

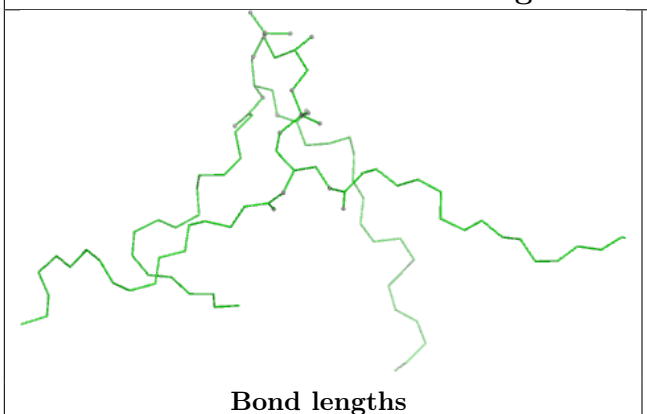


Torsions

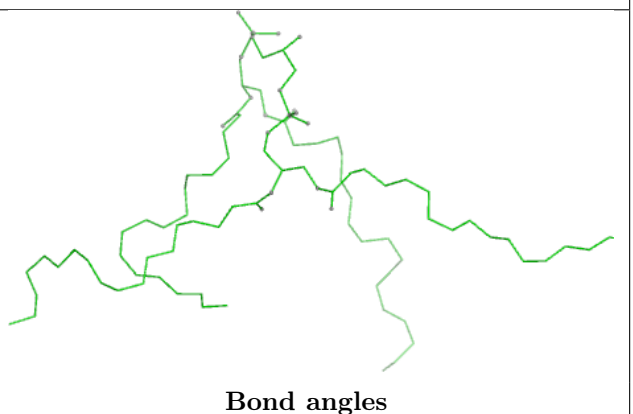


Rings

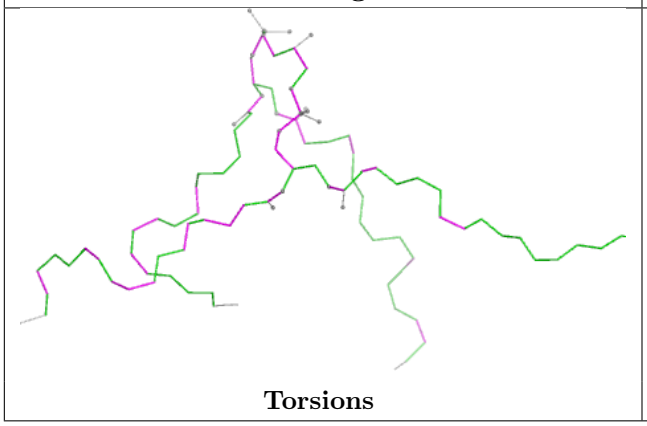
## Ligand CDL DJ 304



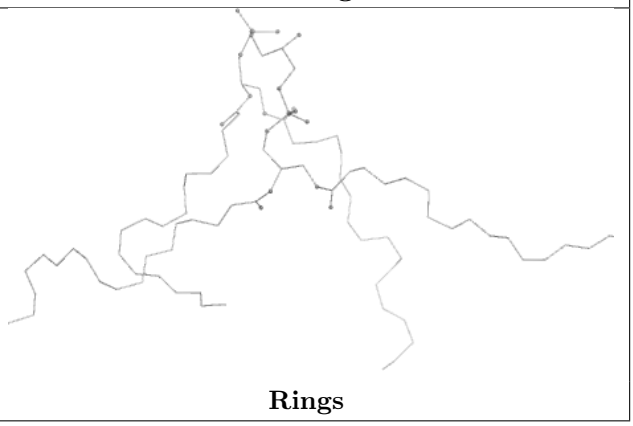
Bond lengths



Bond angles

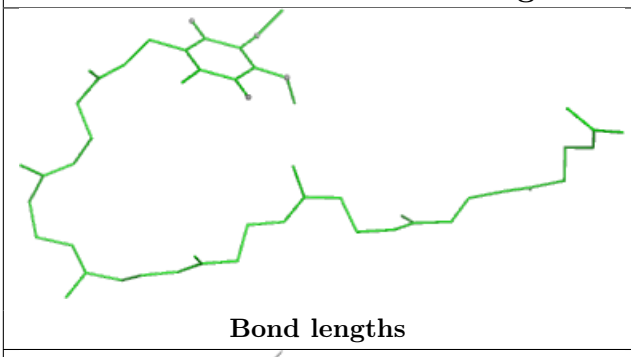


Torsions

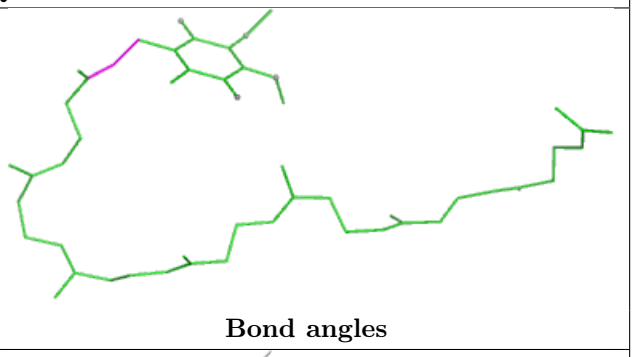


Rings

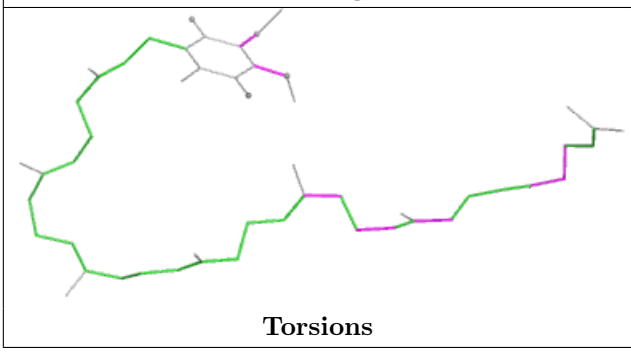
## Ligand UQ8 Ds 404



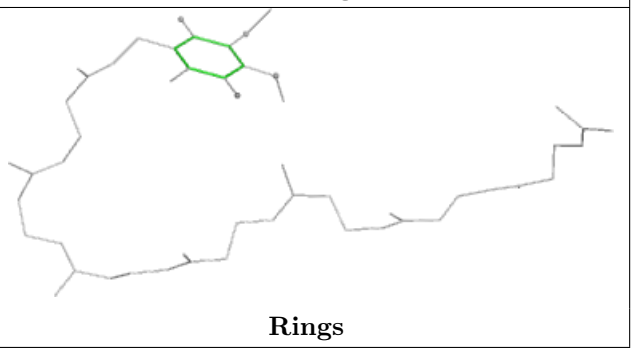
Bond lengths



Bond angles

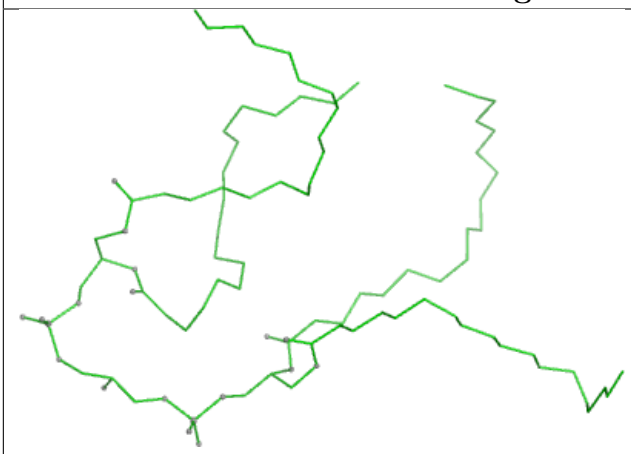


Torsions

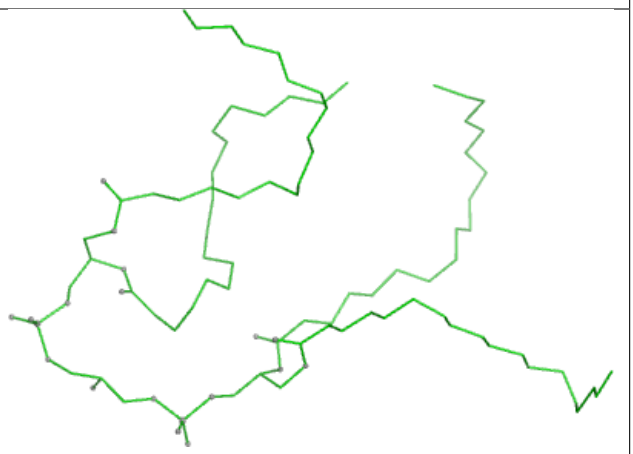


Rings

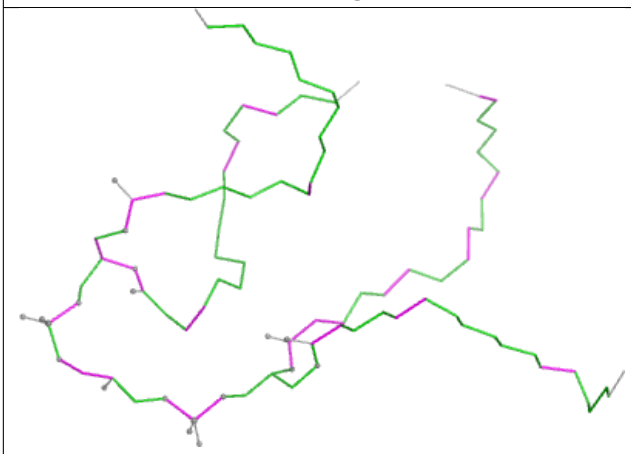
## Ligand CDL DJ 303



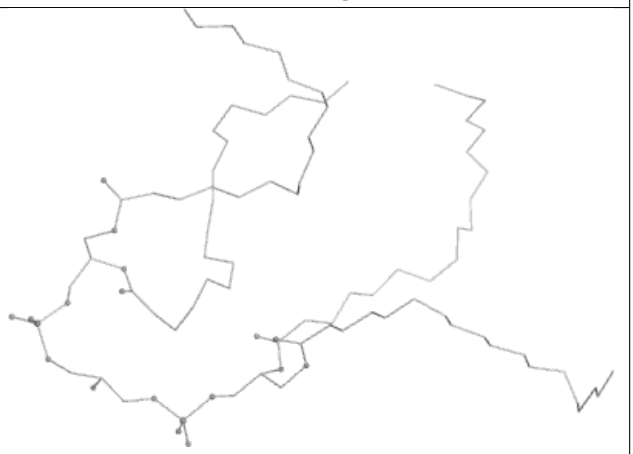
Bond lengths



Bond angles

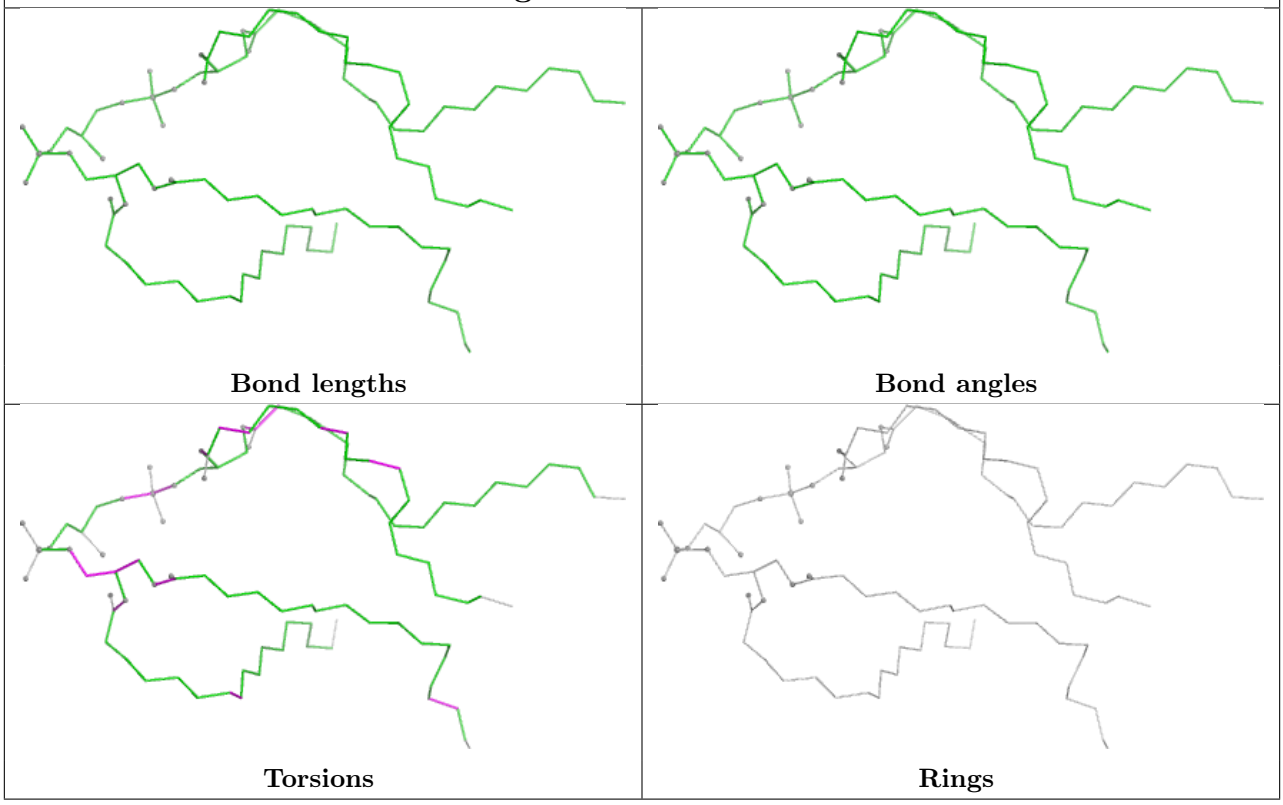


Torsions

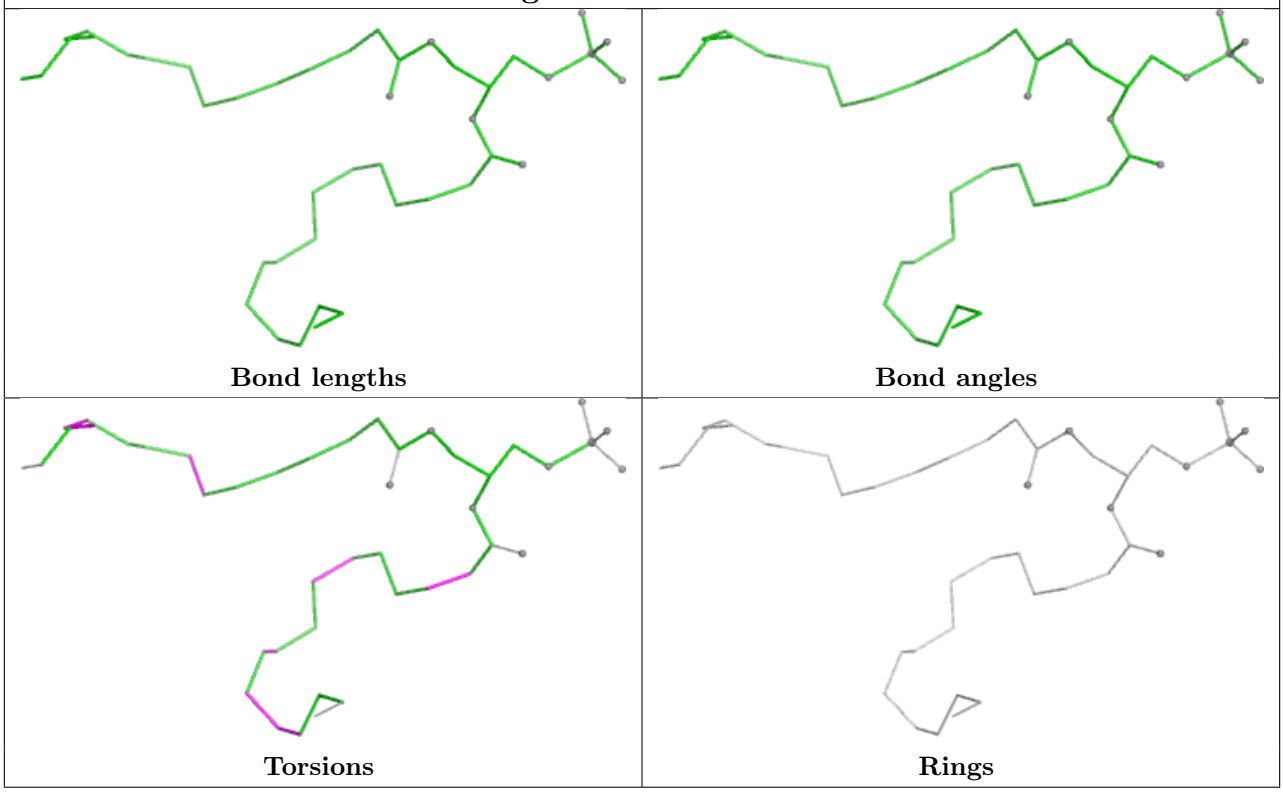


Rings

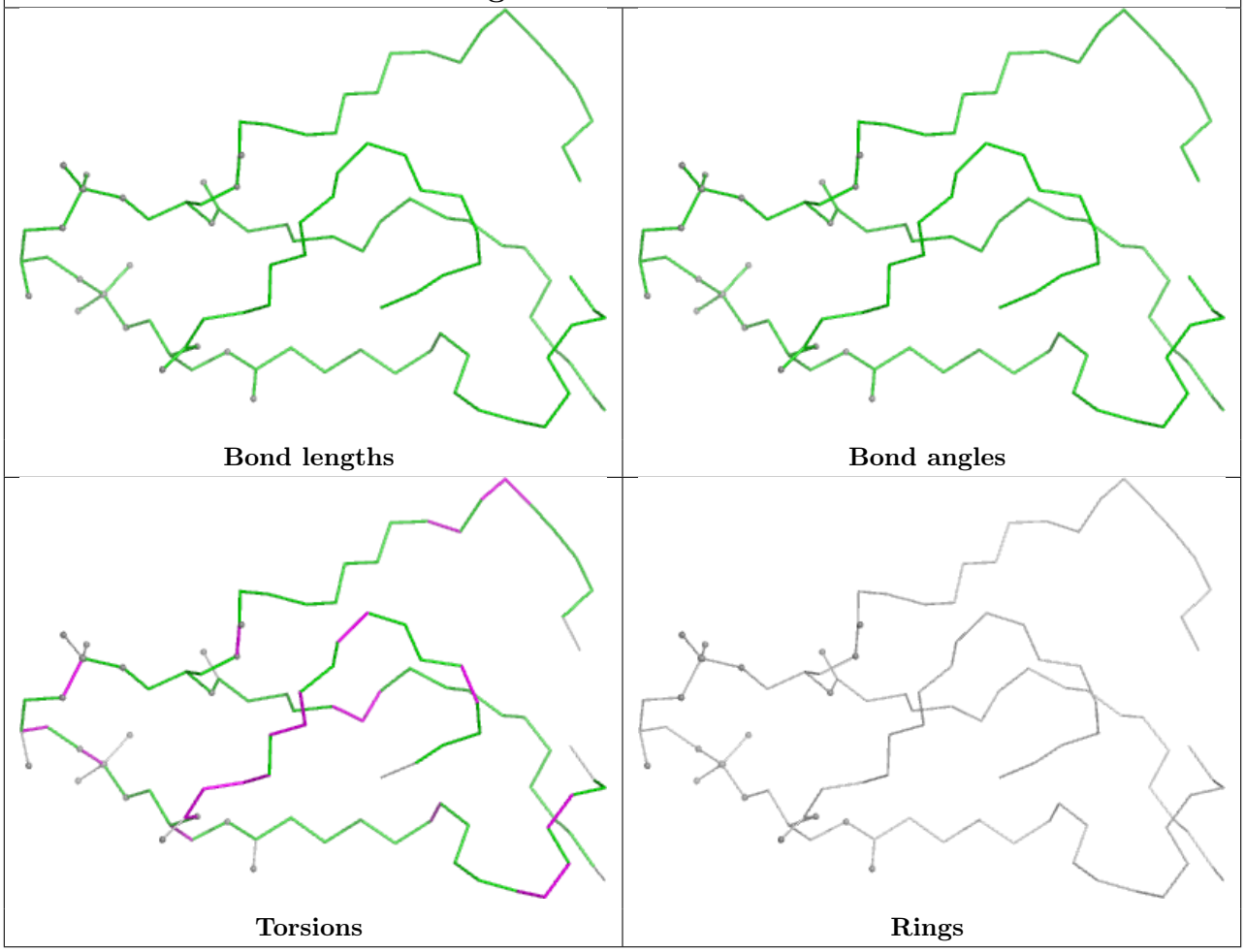
## Ligand CDL Dn 503



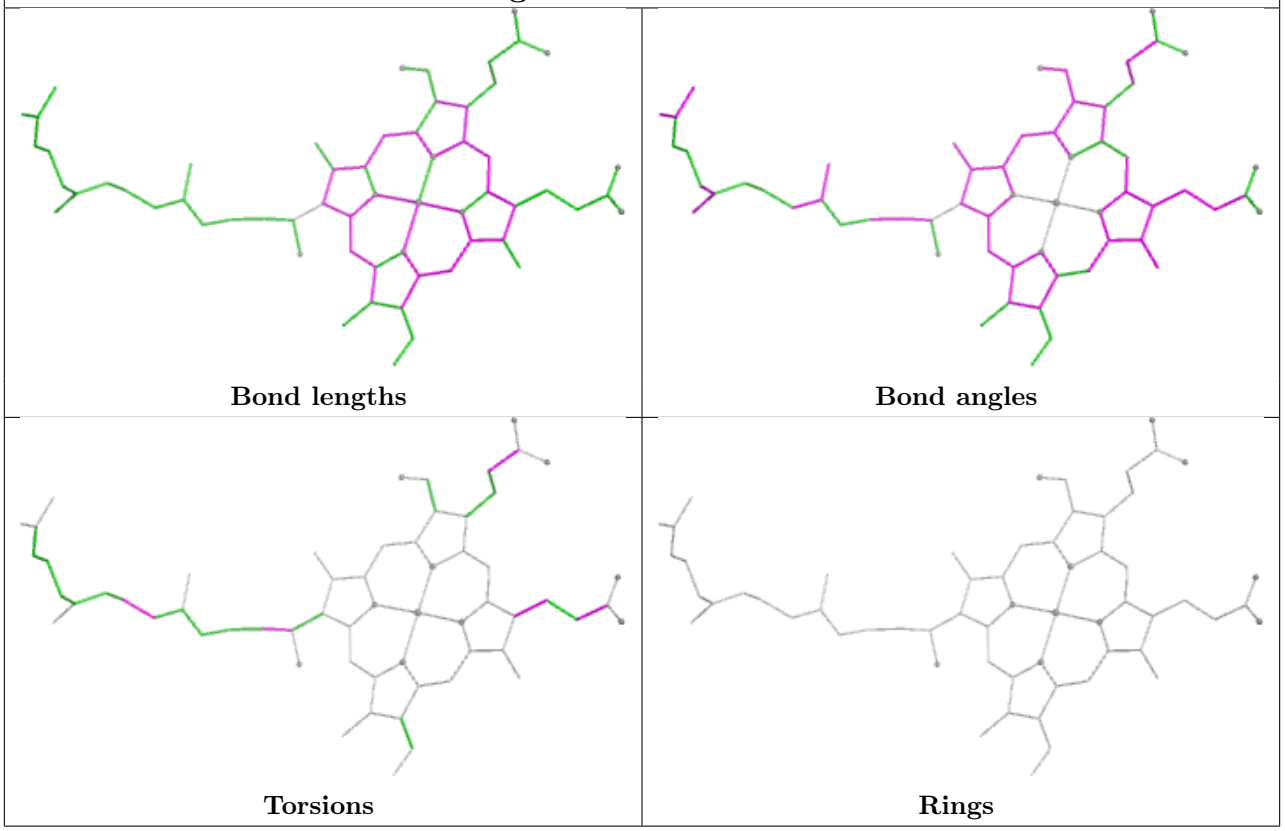

## Ligand LPP EI 402



**Ligand CDL EN 1201**



**Ligand HEA DA 702**




## 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.

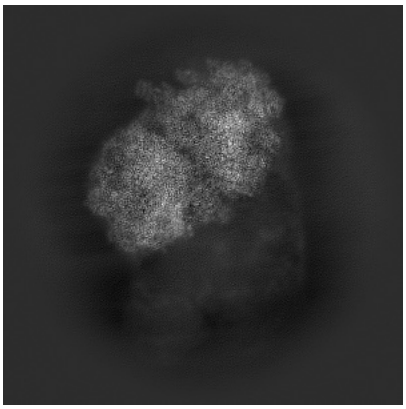
# 6 Map visualisation

This section contains visualisations of the EMDB entry EMD-15867. These allow visual inspection of the internal detail of the map and identification of artifacts.

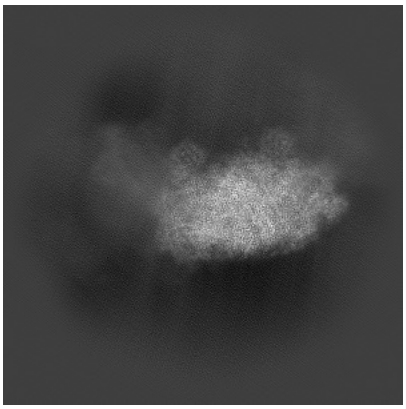
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

## 6.1 Orthogonal projections

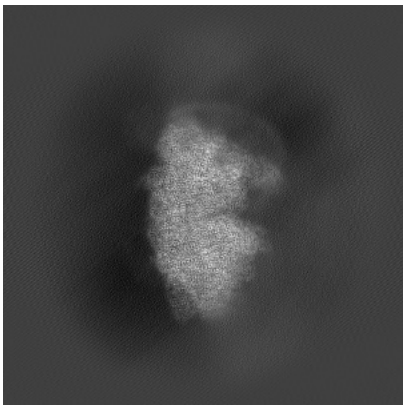
### 6.1.1 Primary map



X

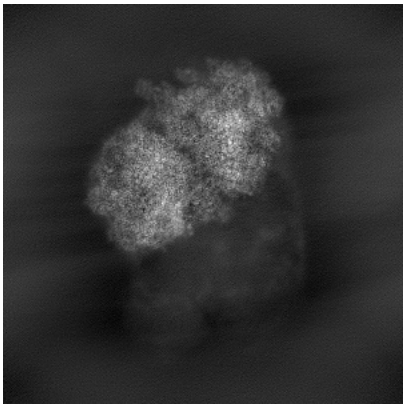


Y

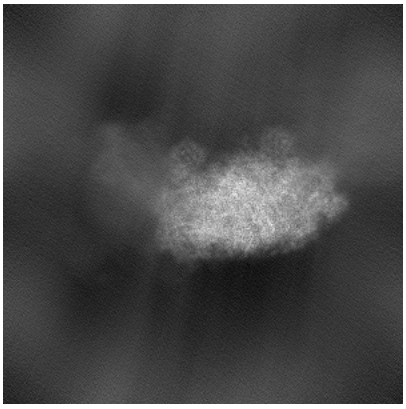


Z

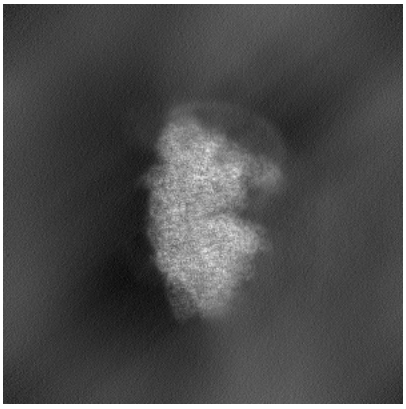
### 6.1.2 Raw map



X



Y

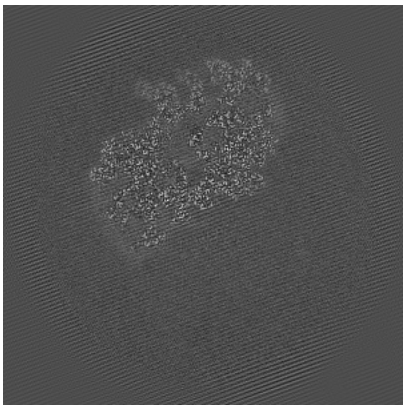


Z

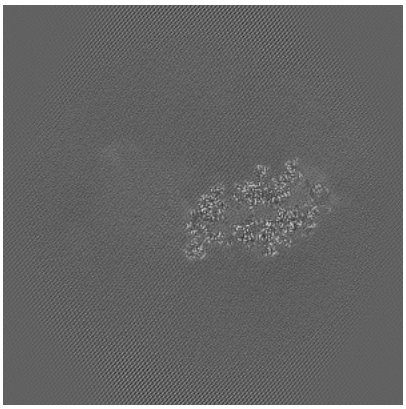
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices (i)

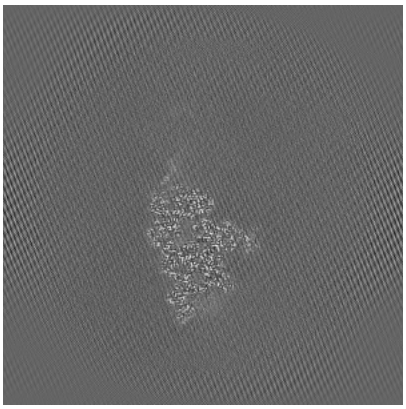
### 6.2.1 Primary map



X Index: 240

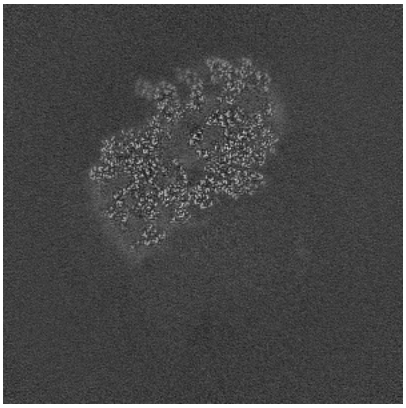


Y Index: 240

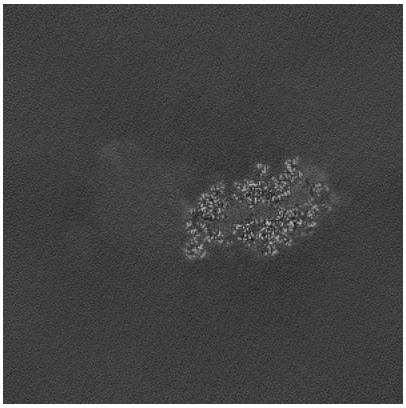


Z Index: 240

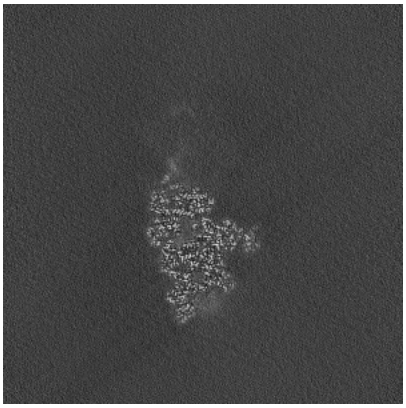
### 6.2.2 Raw map



X Index: 240



Y Index: 240

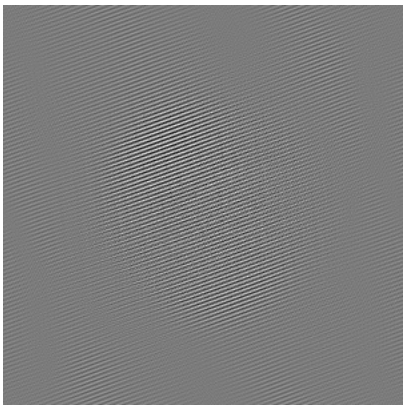


Z Index: 240

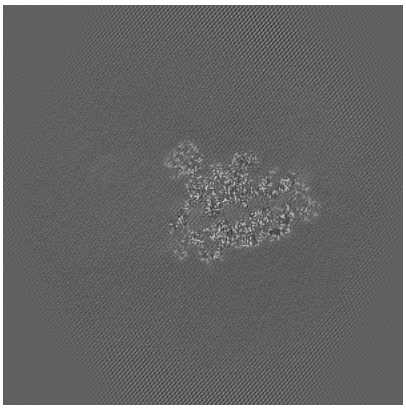
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices (i)

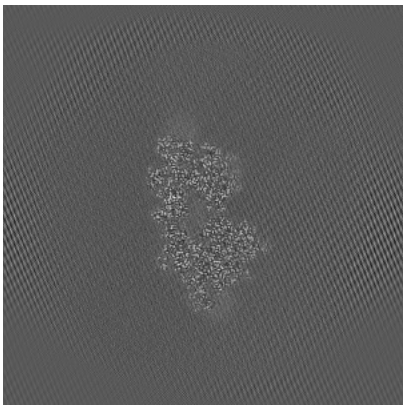
### 6.3.1 Primary map



X Index: 444

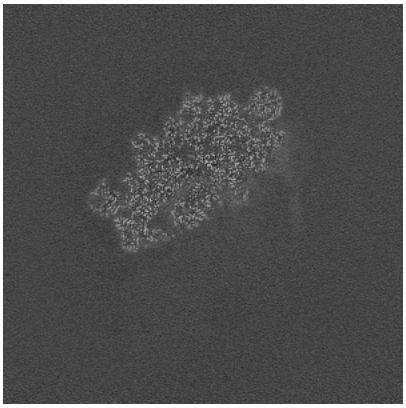


Y Index: 204

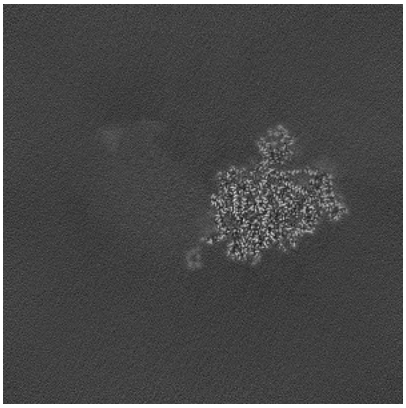


Z Index: 287

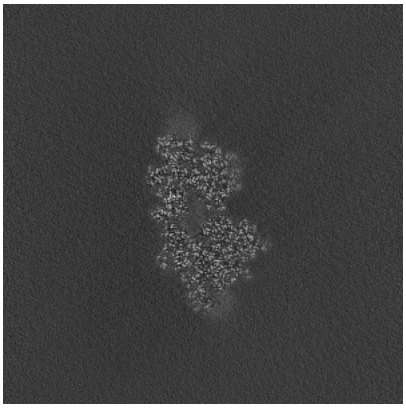
### 6.3.2 Raw map



X Index: 206



Y Index: 271

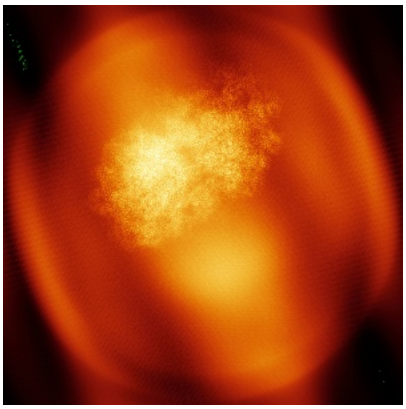


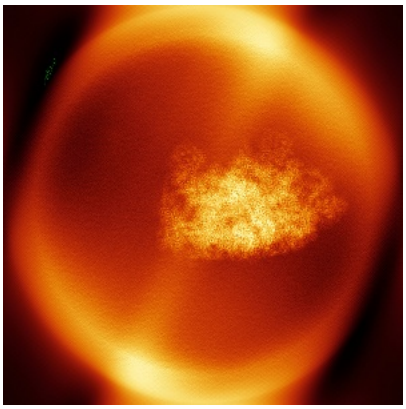
Z Index: 287

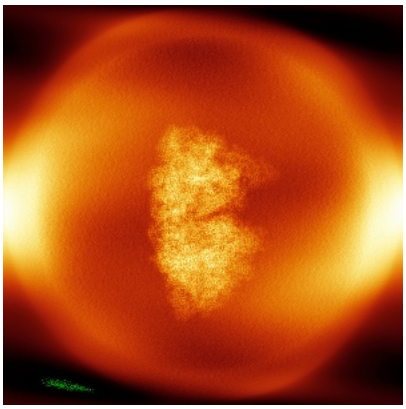
The images above show the largest variance slices of the map in three orthogonal directions.

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

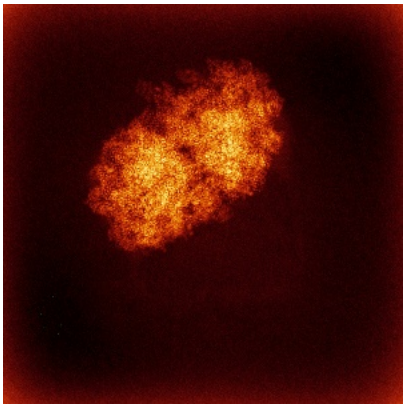
### 6.4.1 Primary map

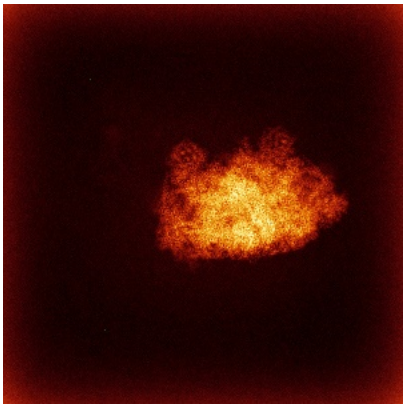

X

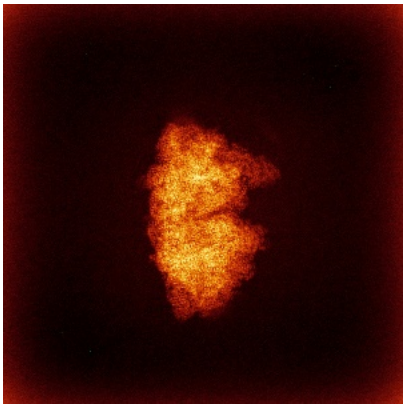

Y


Z

### 6.4.2 Raw map


X

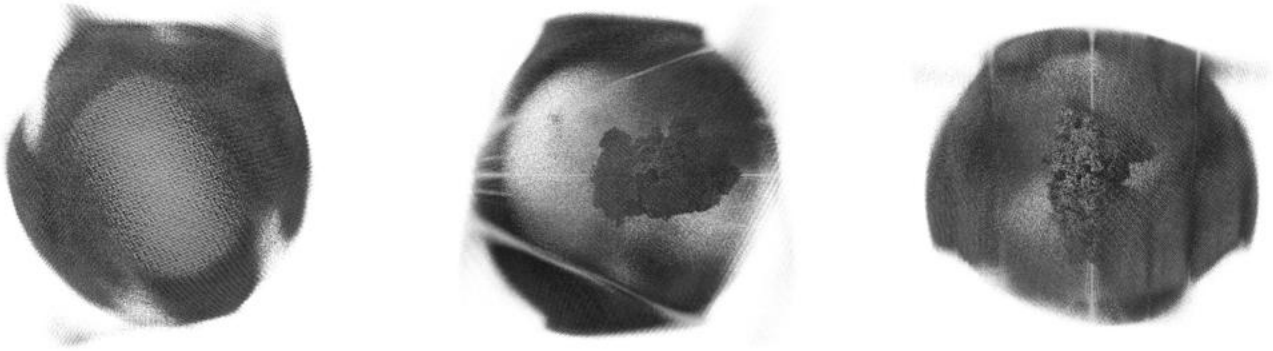

Y


Z

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

## 6.5 Orthogonal surface views (i)

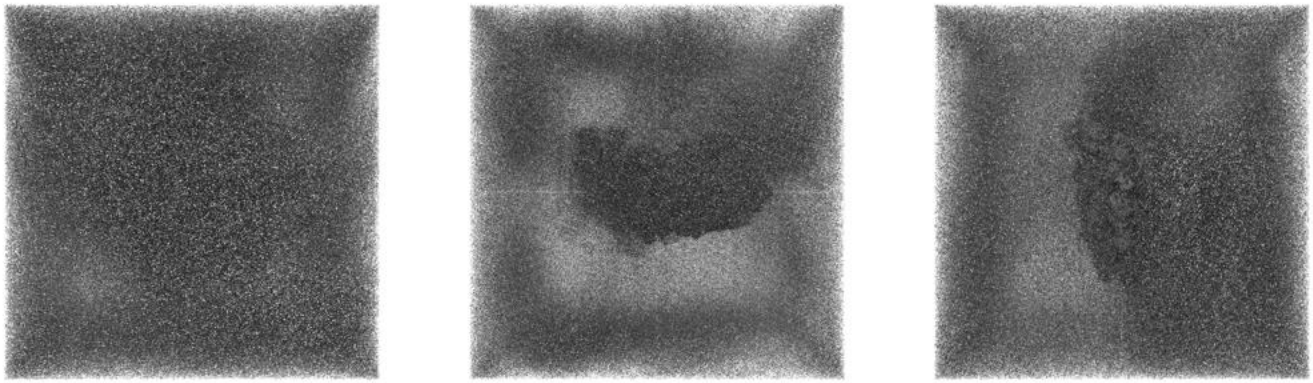
### 6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.85. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



X Y Z

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

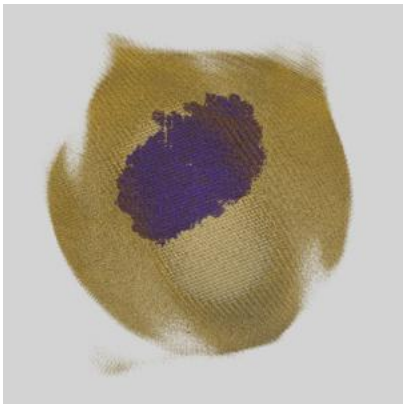
## 6.6 Mask visualisation

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

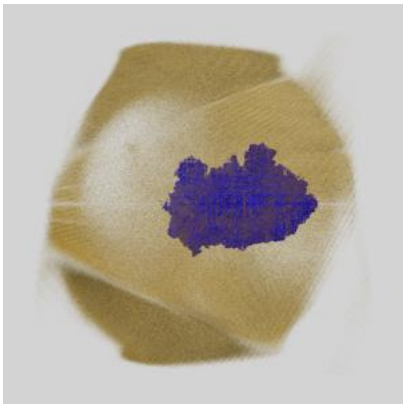
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

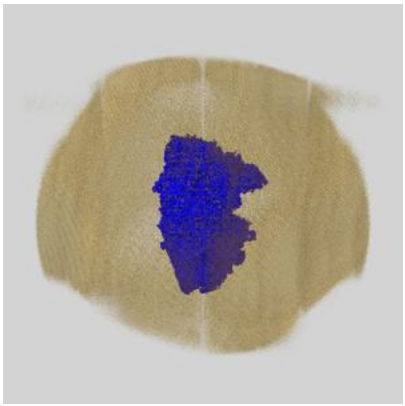
### 6.6.1 emd_15867_msk_1.map



X



Y

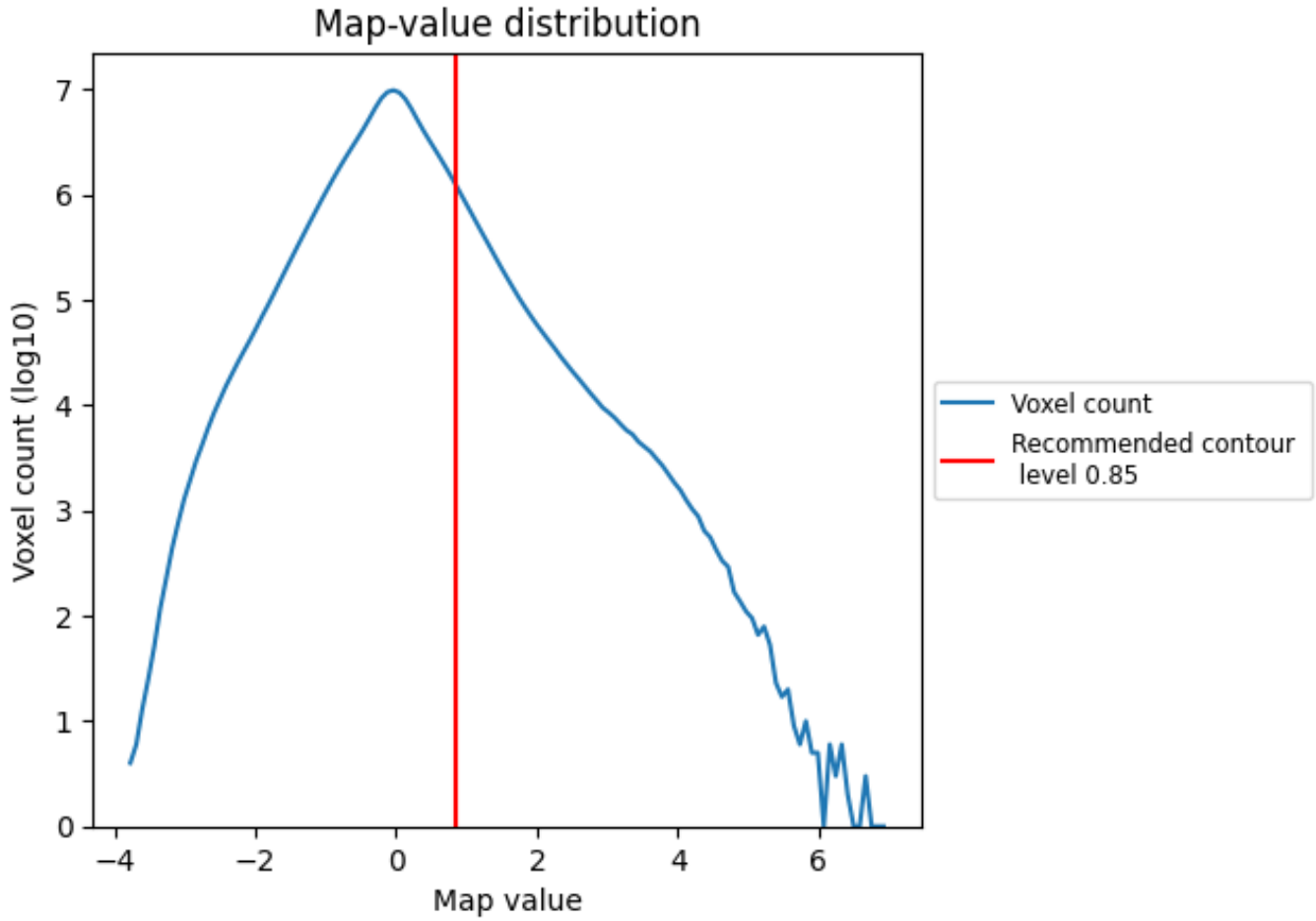


Z

# 7 Map analysis

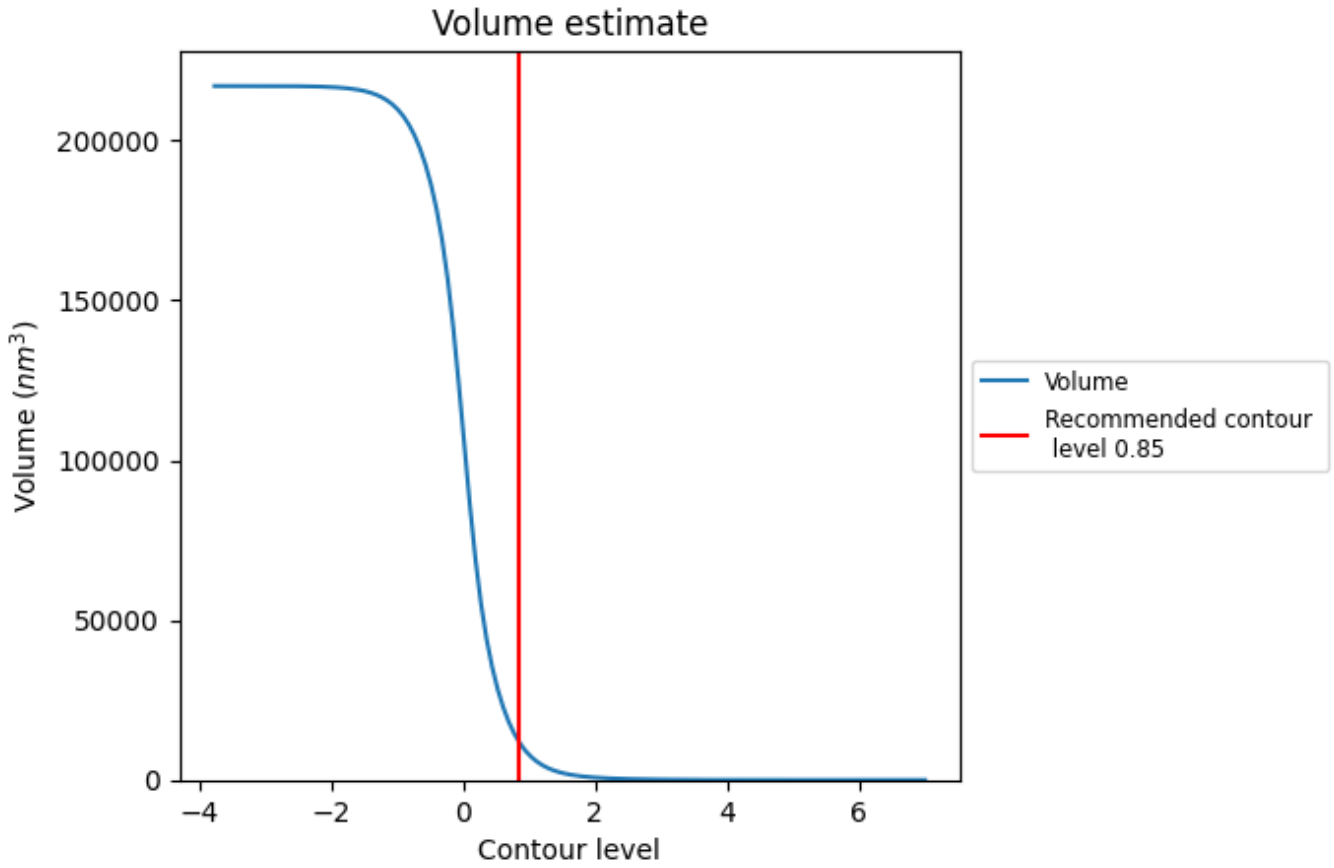
This section contains the results of statistical analysis of the map.

## 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.

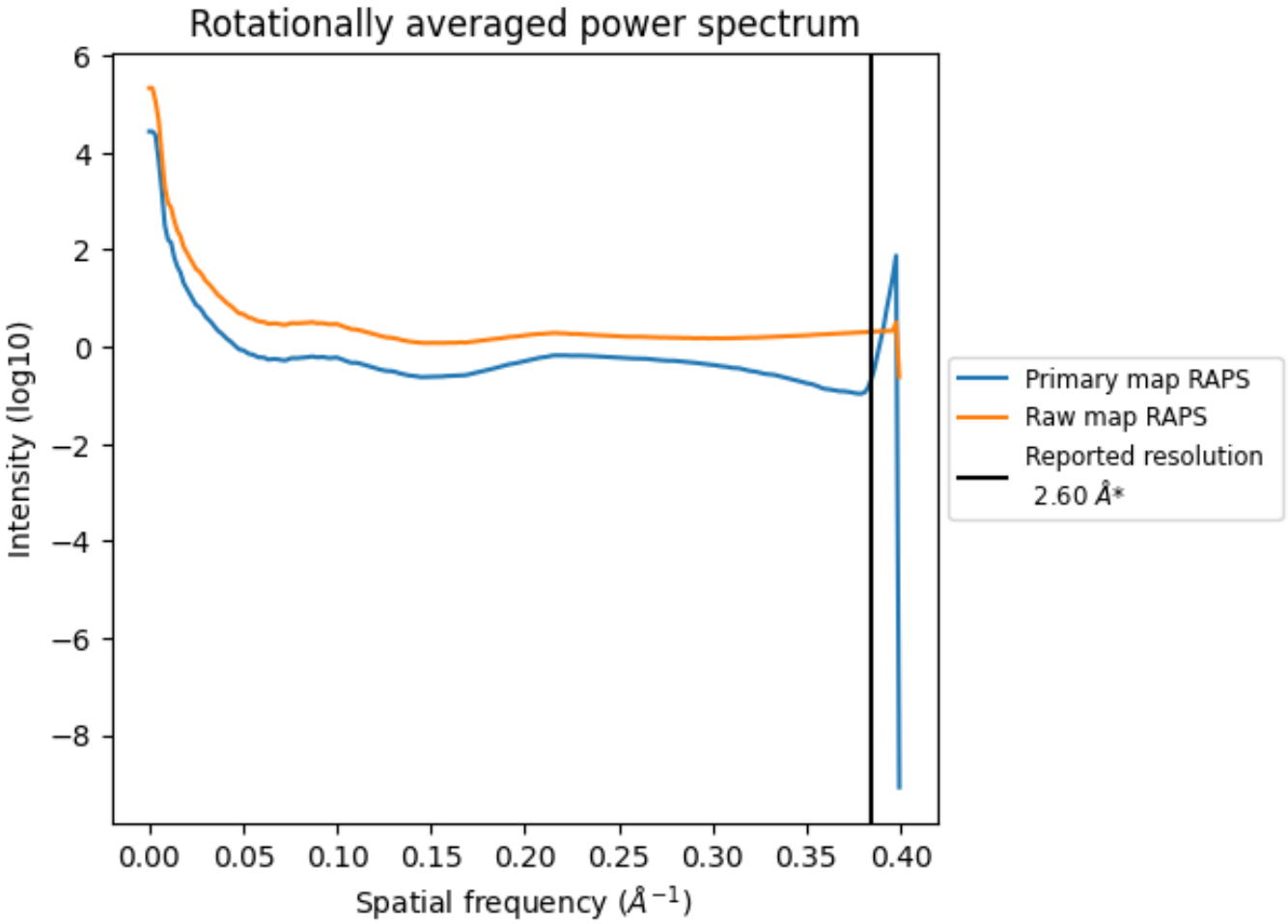
## 7.2 Volume estimate




The volume at the recommended contour level is 11769 $nm^3$; this corresponds to an approximate mass of 10631 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 (i)

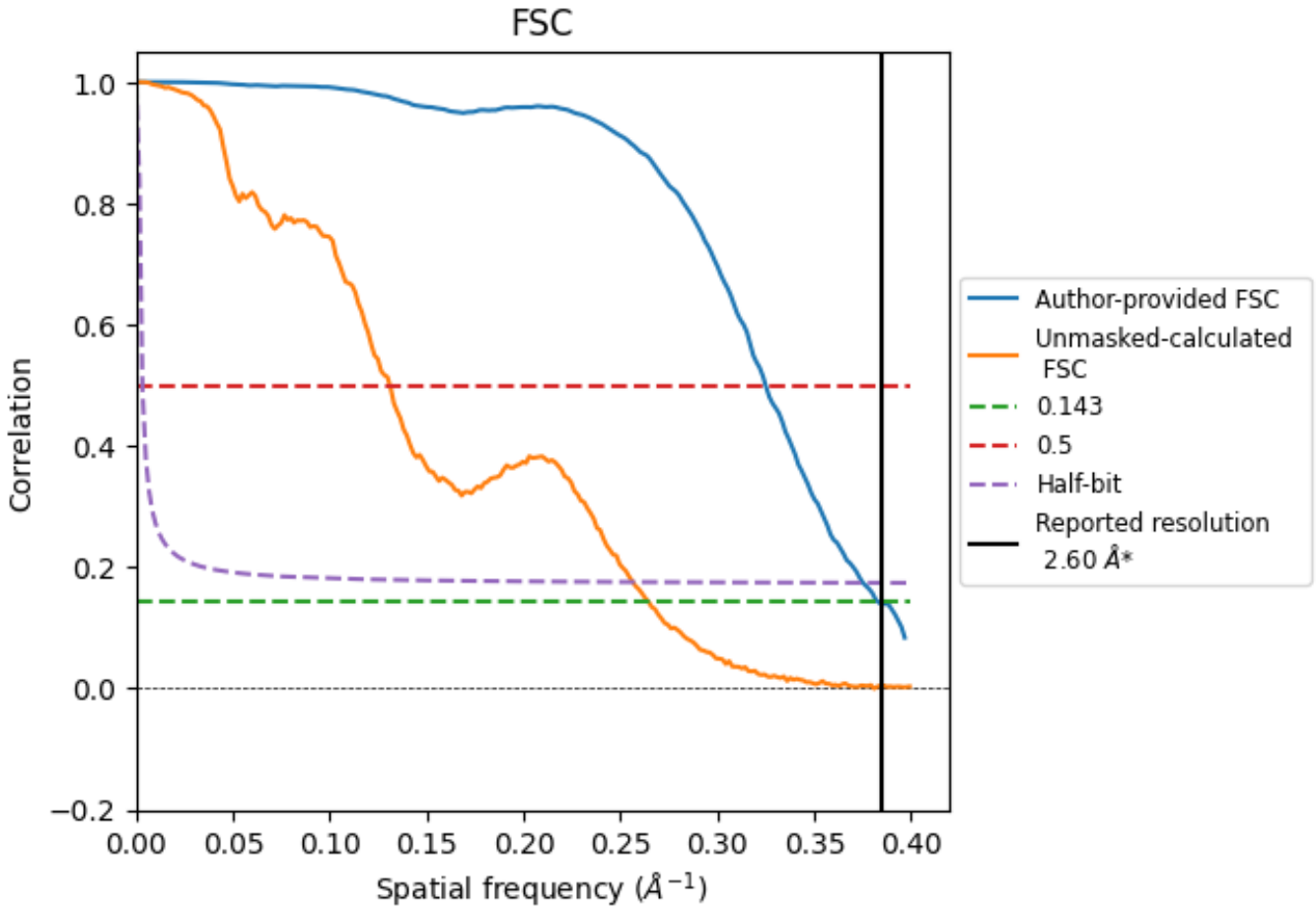



*Reported resolution corresponds to spatial frequency of 0.385 Å$^{-1}$

# 8 Fourier-Shell correlation

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

## 8.1 FSC




*Reported resolution corresponds to spatial frequency of 0.385 Å$^{-1}$

## 8.2 Resolution estimates (i)

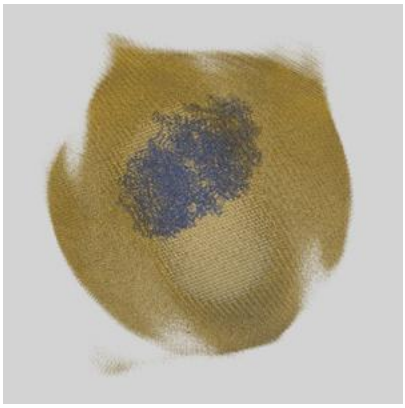
| Resolution estimate (Å) | Estimation criterion (FSC cut-off) | | |
|---|---|---|---|
| | 0.143 | 0.5 | Half-bit |
| Reported by author | 2.60 | - | - |
| Author-provided FSC curve | 2.61 | 3.08 | 2.66 |
| Unmasked-calculated* | 3.78 | 7.63 | 3.90 |

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.78 differs from the reported value 2.6 by more than 10 %

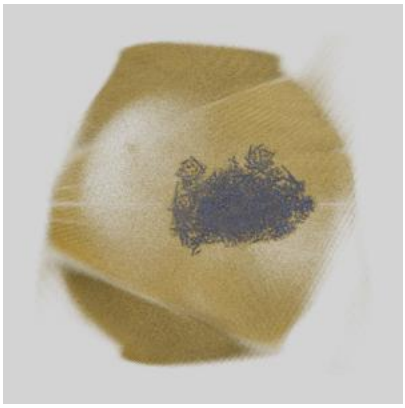
# 9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-15867 and PDB model 8B6H. Per-residue inclusion information can be found in section 3 on page 36.

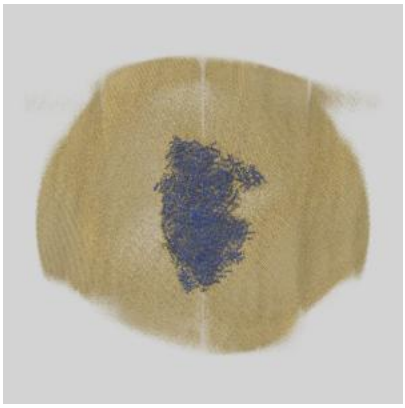
## 9.1 Map-model overlay



X



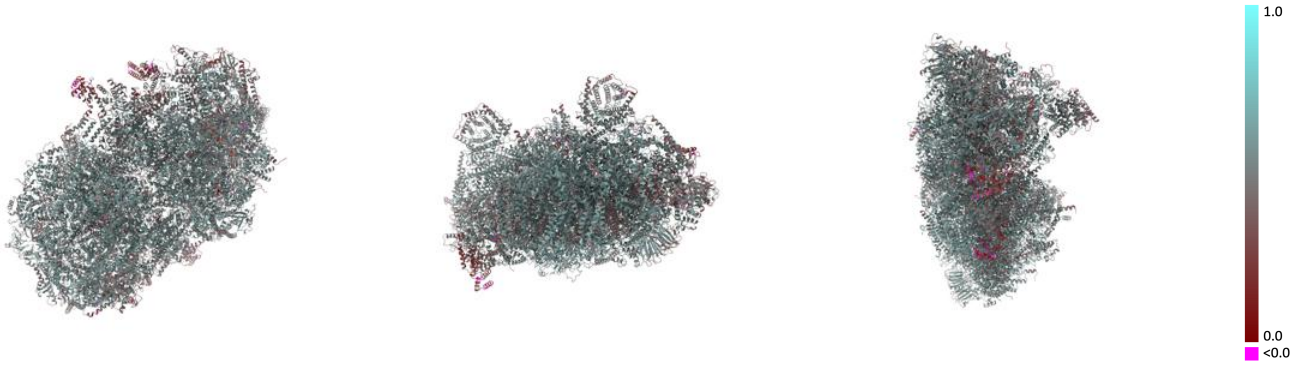
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.85 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

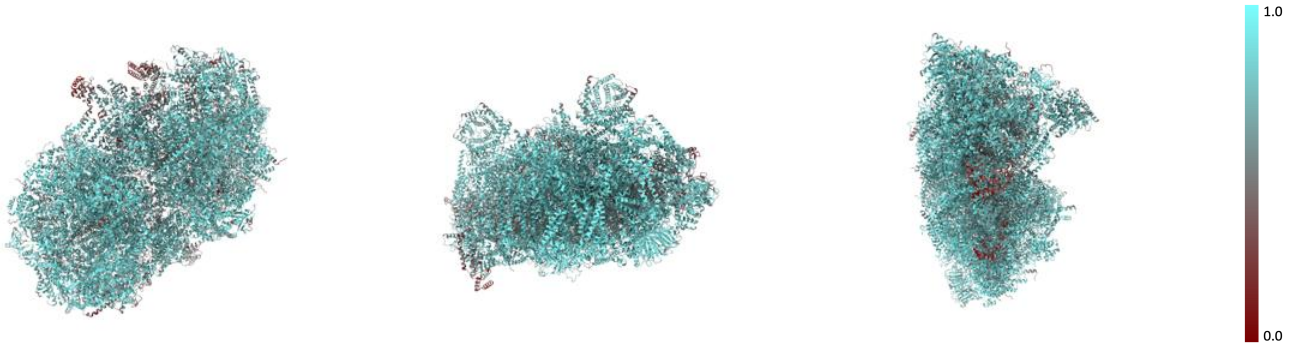
## 9.2 Q-score mapped to coordinate model




X Y Z

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

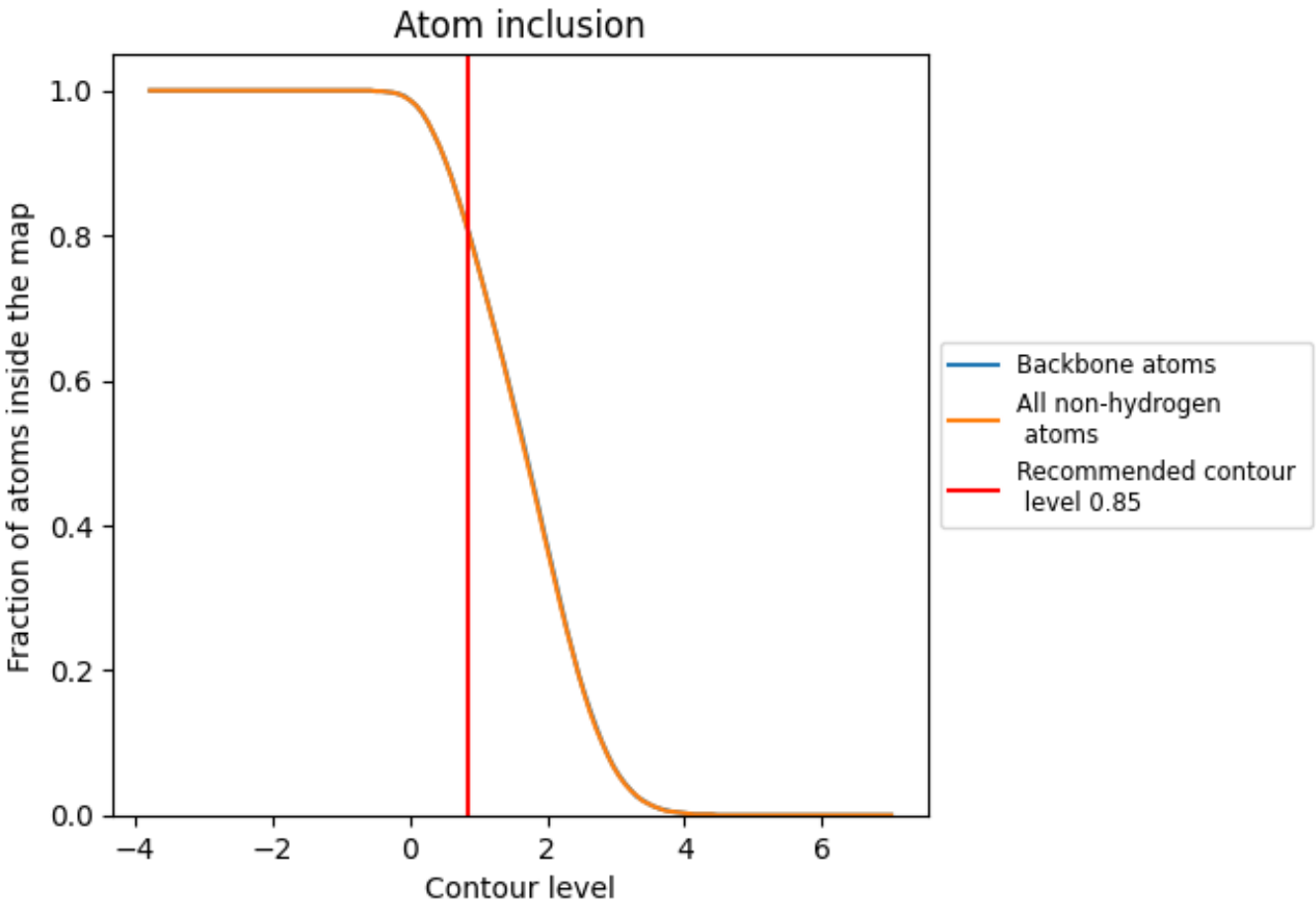
## 9.3 Atom inclusion mapped to coordinate model




X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.85).

## 9.4 Atom inclusion (i)




At the recommended contour level, 81% of all backbone atoms, 81% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.85) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion | Q-score |
|---|---|---|
| All | 0.8070 | 0.5310 |
| DA | 0.8810 | 0.5710 |
| DB | 0.8500 | 0.5430 |
| DC | 0.8300 | 0.5390 |
| DD | 0.8510 | 0.5550 |
| DE | 0.8880 | 0.5740 |
| DF | 0.8890 | 0.5670 |
| DG | 0.7980 | 0.5330 |
| DH | 0.8850 | 0.5740 |
| DI | 0.8520 | 0.5570 |
| DJ | 0.7770 | 0.5310 |
| DK | 0.8630 | 0.5500 |
| DL | 0.8360 | 0.5440 |
| DM | 0.8640 | 0.5680 |
| DN | 0.7760 | 0.5020 |
| DO | 0.6980 | 0.4450 |
| DP | 0.8050 | 0.5130 |
| DQ | 0.8430 | 0.5560 |
| DR | 0.8460 | 0.5530 |
| DS | 0.8390 | 0.5470 |
| DT | 0.9000 | 0.5850 |
| DU | 0.8200 | 0.5360 |
| DV | 0.8040 | 0.5240 |
| DW | 0.7730 | 0.4920 |
| DX | 0.7740 | 0.5200 |
| DY | 0.8330 | 0.5420 |
| DZ | 0.8440 | 0.5570 |
| Da | 0.8890 | 0.5800 |
| Db | 0.8280 | 0.5440 |
| Dc | 0.8030 | 0.5240 |
| Dd | 0.8080 | 0.5320 |
| De | 0.8870 | 0.5650 |
| Df | 0.8780 | 0.5640 |
| Dg | 0.8040 | 0.5350 |
| Dh | 0.8330 | 0.5540 |




*Continued on next page...*

*Continued from previous page...*

| Chain | Atom inclusion | Q-score |
|---|---|---|
| Di | 0.8280 | 0.5500 |
| Dj | 0.7660 | 0.5300 |
| Dk | 0.8440 | 0.5420 |
| Dl | 0.8090 | 0.5110 |
| Dm | 0.8380 | 0.5440 |
| Dn | 0.7040 | 0.4610 |
| Do | 0.5570 | 0.3840 |
| Dp | 0.7700 | 0.4890 |
| Dq | 0.8230 | 0.5440 |
| Dr | 0.8630 | 0.5640 |
| Ds | 0.8650 | 0.5640 |
| Dt | 0.8970 | 0.5890 |
| Du | 0.7640 | 0.5150 |
| Dv | 0.7940 | 0.5110 |
| Dw | 0.7680 | 0.5000 |
| Dx | 0.7520 | 0.5130 |
| Dy | 0.8110 | 0.5200 |
| Dz | 0.8030 | 0.5230 |
| EA | 0.8070 | 0.5260 |
| EB | 0.8090 | 0.5290 |
| EC | 0.6260 | 0.3840 |
| ED | 0.7530 | 0.5100 |
| EE | 0.8440 | 0.5340 |
| EF | 0.9090 | 0.5870 |
| EG | 0.8710 | 0.5720 |
| EH | 0.8430 | 0.5530 |
| EI | 0.8310 | 0.5470 |
| EJ | 0.8560 | 0.5500 |
| EK | 0.8080 | 0.5280 |
| EL | 0.7890 | 0.5330 |
| EM | 0.8530 | 0.5510 |
| EN | 0.8270 | 0.5410 |
| EO | 0.7610 | 0.5170 |
| EP | 0.8910 | 0.5920 |
| EQ | 0.9210 | 0.5850 |
| ER | 0.9190 | 0.5840 |
| ES | 0.9060 | 0.5920 |
| ET | 0.6820 | 0.4310 |
| EU | 0.7770 | 0.5170 |
| EV | 0.8080 | 0.5100 |
| EW | 0.7410 | 0.4740 |
| EX | 0.7180 | 0.4750 |

*Continued on next page...*

*Continued from previous page...*

| Chain | Atom inclusion | Q-score |
|---|---|---|
| EY | 0.7590 | 0.4680 |
| EZ | 0.8090 | 0.5170 |
| Ea | 0.7830 | 0.5220 |
| Eb | 0.8310 | 0.5440 |
| Ec | 0.4840 | 0.3370 |
| Ed | 0.6940 | 0.4880 |
| Ee | 0.8170 | 0.5240 |
| Ef | 0.8900 | 0.5800 |
| Eg | 0.7810 | 0.5430 |
| Eh | 0.8540 | 0.5680 |
| Ei | 0.7960 | 0.5310 |
| Ej | 0.7740 | 0.4980 |
| Ek | 0.7820 | 0.5210 |
| El | 0.7810 | 0.5470 |
| Em | 0.8570 | 0.5550 |
| En | 0.8240 | 0.5480 |
| Eo | 0.7860 | 0.5290 |
| Ep | 0.8270 | 0.5520 |
| Eq | 0.8960 | 0.5810 |
| Er | 0.9110 | 0.6000 |
| Es | 0.8860 | 0.5860 |
| Et | 0.6830 | 0.4060 |
| Eu | 0.7390 | 0.5030 |
| Ev | 0.8100 | 0.5100 |
| Ew | 0.7000 | 0.4350 |
| Ex | 0.6710 | 0.4530 |
| Ey | 0.7090 | 0.4490 |
| Ez | 0.7880 | 0.5110 |
| FA | 0.8150 | 0.5050 |
| Fa | 0.7740 | 0.4920 |