# Full wwPDB EM Validation Report (i)

Aug 13, 2026 – 12:55 AM JST

| | | |
|---|---|---|
| PDB ID | : | 8ZO8 / pdb_00008zo8 |
| EMDB ID | : | EMD-60284 |
| Title | : | Respirasome open state 3 in presence of metformin (SC-MetO3) |
| Authors | : | Teng, F.; He, Z.X.; Hu, Y.Q.; Xu, C.Y.; Guo, R.Y.; Zhou, L. |
| Deposited on | : | 2024-05-28 |
| Resolution | : | 3.24 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 (i) symbol.

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

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

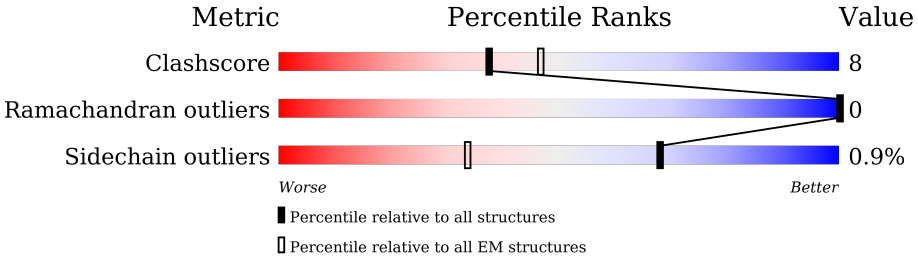
| | | |
|---|---|---|
| EMDB validation analysis | : | 0.0.1.dev133 |
| Mogul | : | 1.8.5 (274361), CSD as541be (2020) |
| MolProbity | : | 4-5-2 with Phenix2.0 |
| Buster-report | : | wwPDB partial adaption of 1.1.7 (2018) |
| Percentile statistics | : | 20250101.v01 (using entries in the PDB archive 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 |

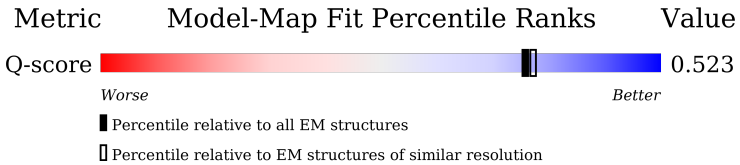
# 1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.24 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 | 14594 ( 2.74 - 3.74 ) |

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 | 4L | 98 | 82% 18% |
| 2 | 5A | 102 | 71% 29% |
| 3 | 5B | 95 | 71% 29% |
| 4 | 6A | 75 | 75% 25% |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 5 | 6B | 82 | 73% 27% |
| 6 | 6C | 70 | 79% 21% |
| 7 | 7A | 57 | 74% 25% |
| 8 | 7B | 50 | 86% 14% |
| 9 | 7C | 47 | 89% 11% |
| 10 | 8B | 43 | 72% 28% |
| 11 | A1 | 70 | 91% 9% |
| 12 | A2 | 85 | 88% 12% |
| 13 | A3 | 83 | 96% |
| 14 | A5 | 112 | 91% 9% |
| 15 | A6 | 114 | 85% 15% |
| 16 | A7 | 112 | 79% 7% 13% |
| 17 | A8 | 171 | 85% 15% |
| 18 | A9 | 341 | 82% 17% |
| 19 | AB | 156 | 40% 9% 51% |
| 19 | AC | 156 | 44% 11% 44% |
| 20 | AK | 320 | 79% 20% |
| 21 | AL | 140 | 88% 12% |
| 22 | AM | 143 | 88% 12% |
| 23 | AN | 142 | 82% 18% |
| 24 | B1 | 56 | 91% 9% |
| 25 | B2 | 67 | 90% 10% |
| 26 | B3 | 79 | 85% 15% |
| 27 | B4 | 128 | 88% 12% |
| 28 | B5 | 138 | 86% 14% |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 29 | B6 | 126 | 63% 17% 20% |
| 30 | B7 | 125 | 84% 16% |
| 31 | B8 | 156 | 89% 11% |
| 32 | B9 | 178 | 79% 21% |
| 33 | BK | 176 | 89% 10% |
| 34 | BL | 102 | 83% 14% |
| 35 | C1 | 514 | 71% 29% |
| 36 | C2 | 228 | 76% 23% |
| 37 | C3 | 260 | 81% 18% |
| 38 | C4 | 138 | 79% 21% |
| 39 | CA | 49 | 82% 16% |
| 40 | CB | 121 | 84% 16% |
| 41 | N1 | 318 | 77% 21% |
| 42 | N2 | 347 | 76% 24% |
| 43 | N3 | 115 | 71% 14% 15% |
| 44 | N4 | 459 | 80% 20% |
| 45 | N5 | 603 | 79% 20% |
| 46 | N6 | 173 | 74% 20% 6% |
| 47 | QA | 419 | 82% 18% |
| 47 | Qa | 419 | 77% 22% |
| 48 | QB | 446 | 83% 17% |
| 48 | Qb | 446 | 79% 18% |
| 49 | QC | 379 | 82% 17% |
| 49 | Qc | 379 | 86% 13% |
| 50 | QD | 241 | 88% 12% |

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| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 50 | Qd | 241 | 82% 17% |
| 51 | QE | 196 | 13% 72% 28% |
| 51 | Qe | 196 | 18% 74% 26% |
| 52 | QF | 67 | 88% 12% |
| 52 | Qf | 67 | 70% 25% |
| 53 | QG | 101 | 84% 15% |
| 53 | Qg | 101 | 86% 14% |
| 54 | QH | 79 | 80% 19% |
| 54 | Qh | 79 | 81% 19% |
| 55 | QI | 64 | 84% 12% |
| 55 | Qi | 64 | 83% 11% 6% |
| 56 | QJ | 49 | 94% 6% |
| 57 | QK | 78 | 8% 79% 14% 6% |
| 58 | Qj | 51 | 86% 14% |
| 59 | S1 | 689 | 76% 24% |
| 60 | S2 | 430 | 77% 21% |
| 61 | S3 | 207 | 85% 15% |
| 62 | S4 | 124 | 84% 16% |
| 63 | S5 | 100 | 89% 11% |
| 64 | S6 | 96 | 81% 19% |
| 65 | S7 | 156 | 84% 15% |
| 66 | S8 | 176 | 83% 17% |
| 67 | V1 | 431 | 77% 22% |
| 68 | V2 | 217 | 88% 12% |
| 69 | V3 | 42 | 76% 24% |

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

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|---|---|---|---|---|---|---|---|
| 84 | HEC | QD | 401 | X | - | - | - |
| 84 | HEC | Qd | 402 | X | - | - | - |
| 85 | FES | QE | 304 | - | - | X | - |
| 86 | SF4 | S8 | 302 | - | - | X | - |

# 2 Entry composition (i)

There are 87 unique types of molecules in this entry. The entry contains 116743 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called NADH-ubiquinone oxidoreductase chain 4L.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 1 | 4L | 98 | 748 | 493 | 113 | 128 | 14 | 0 | 0 |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 2 | 5A | 102 | 825 | 528 | 139 | 156 | 2 | 0 | 0 |

- Molecule 3 is a protein called Cytochrome c oxidase subunit 5B, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 3 | 5B | 95 | 724 | 449 | 128 | 141 | 6 | 0 | 0 |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 4 | 6A | 75 | 620 | 401 | 118 | 100 | 1 | 0 | 0 |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 5 | 6B | 82 | 684 | 431 | 125 | 123 | 5 | 0 | 0 |

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

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 6 | 6C | 70 | 574 | 375 | 101 | 95 | 3 | 0 | 0 |

- Molecule 7 is a protein called Cytochrome c oxidase subunit 7A1, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 7 | 7A | 57 | 447 | 287 | 76 | 81 | 3 | 0 | 0 |

- Molecule 8 is a protein called Cytochrome c oxidase subunit 7B, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 8 | 7B | 50 | 392 | 254 | 66 | 71 | 1 | 0 | 0 |

- Molecule 9 is a protein called Cytochrome c oxidase subunit 7C, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 9 | 7C | 47 | 387 | 257 | 65 | 63 | 2 | 0 | 0 |

- Molecule 10 is a protein called Cytochrome c oxidase subunit 8.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | | |
| 10 | 8B | 43 | 338 | 222 | 57 | 59 | 0 | 0 |

- Molecule 11 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 11 | A1 | 70 | 562 | 361 | 101 | 94 | 6 | 0 | 0 |

- Molecule 12 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 12 | A2 | 85 | 686 | 431 | 128 | 125 | 2 | 0 | 0 |

- Molecule 13 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 13 | A3 | 83 | 643 | 417 | 110 | 115 | 1 | 0 | 0 |

- Molecule 14 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 14 | A5 | 112 | 910 | 588 | 154 | 165 | 3 | 0 | 0 |

- Molecule 15 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 15 | A6 | 114 | 967 | 617 | 178 | 167 | 5 | 0 | 0 |

- Molecule 16 is a protein called Complex I-B14.5a.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 16 | A7 | 97 | 780 | 491 | 147 | 139 | 3 | 0 | 0 |

- Molecule 17 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 17 | A8 | 171 | 1398 | 887 | 250 | 251 | 10 | 0 | 0 |

- Molecule 18 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 18 | A9 | 337 | 2703 | 1750 | 472 | 472 | 9 | 0 | 0 |

- Molecule 19 is a protein called Acyl carrier protein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 19 | AB | 77 | 624 | 402 | 93 | 124 | 5 | 0 | 0 |
| 19 | AC | 87 | 702 | 452 | 103 | 142 | 5 | 0 | 0 |

- Molecule 20 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 20 | AK | 320 | 2590 | 1649 | 440 | 491 | 10 | 0 | 0 |

- Molecule 21 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 21 | AL | 140 | 1021 | 651 | 174 | 190 | 6 | 0 | 0 |

- Molecule 22 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 22 | AM | 143 | 1195 | 764 | 216 | 211 | 4 | 0 | 0 |

- Molecule 23 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 23 | AN | 142 | 1173 | 755 | 203 | 206 | 9 | 0 | 0 |

- Molecule 24 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 24 | B1 | 56 | 479 | 311 | 88 | 79 | 1 | 0 | 0 |

- Molecule 25 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 25 | B2 | 67 | 584 | 385 | 95 | 103 | 1 | 0 | 0 |

- Molecule 26 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 26 | B3 | 79 | 632 | 413 | 106 | 112 | 1 | 0 | 0 |

- Molecule 27 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | | |
| 27 | B4 | 128 | 1062 | 691 | 182 | 189 | 0 | 0 |

- Molecule 28 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 28 | B5 | 138 | 1151 | 754 | 195 | 199 | 3 | 0 | 0 |

- Molecule 29 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 29 | B6 | 101 | 861 | 562 | 153 | 145 | 1 | 0 | 0 |

- Molecule 30 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 30 | B7 | 125 | 1068 | 663 | 204 | 190 | 11 | 0 | 0 |

- Molecule 31 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 31 | B8 | 156 | 1315 | 853 | 213 | 241 | 8 | 0 | 0 |

- Molecule 32 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 32 | B9 | 178 | 1534 | 982 | 279 | 265 | 8 | 0 | 0 |

- Molecule 33 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 33 | BK | 174 | 1456 | 913 | 264 | 271 | 8 | 0 | 0 |

- Molecule 34 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 34 | BL | 99 | 828 | 531 | 137 | 156 | 4 | 0 | 0 |

- Molecule 35 is a protein called Cytochrome c oxidase subunit 1.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 35 | C1 | 514 | 4024 | 2692 | 625 | 675 | 32 | 0 | 0 |

- Molecule 36 is a protein called Cytochrome c oxidase subunit 2.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 36 | C2 | 228 | 1833 | 1193 | 282 | 340 | 18 | 0 | 0 |

- Molecule 37 is a protein called Cytochrome c oxidase subunit 3.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 37 | C3 | 260 | 2103 | 1403 | 337 | 353 | 10 | 0 | 0 |

- Molecule 38 is a protein called Cytochrome c oxidase subunit 4.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 38 | C4 | 138 | 1153 | 751 | 188 | 210 | 4 | 0 | 0 |

- Molecule 39 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | | |
| 39 | CA | 49 | 417 | 276 | 71 | 70 | 0 | 0 |

- Molecule 40 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C2.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 40 | CB | 121 | 1000 | 650 | 173 | 171 | 6 | 0 | 0 |

- Molecule 41 is a protein called NADH-ubiquinone oxidoreductase chain 1.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 41 | N1 | 311 | 2457 | 1644 | 377 | 415 | 21 | 0 | 0 |

- Molecule 42 is a protein called NADH-ubiquinone oxidoreductase chain 2.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 42 | N2 | 347 | 2710 | 1782 | 420 | 462 | 46 | 0 | 0 |

- Molecule 43 is a protein called NADH-ubiquinone oxidoreductase chain 3.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 43 | N3 | 98 | 786 | 535 | 114 | 132 | 5 | 0 | 0 |

- Molecule 44 is a protein called NADH-ubiquinone oxidoreductase chain 4.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 44 | N4 | 459 | 3631 | 2412 | 572 | 609 | 38 | 0 | 0 |

- Molecule 45 is a protein called NADH-ubiquinone oxidoreductase chain 5.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 45 | N5 | 603 | 4785 | 3173 | 741 | 820 | 51 | 0 | 0 |

- Molecule 46 is a protein called NADH-ubiquinone oxidoreductase chain 6.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 46 | N6 | 163 | 1236 | 831 | 177 | 217 | 11 | 0 | 0 |

- Molecule 47 is a protein called Cytochrome b-c1 complex subunit 2, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 47 | QA | 419 | 3147 | 1971 | 557 | 611 | 8 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 47 | Qa | 419 | 3147 | 1971 | 557 | 611 | 8 | 0 | 0 |

- Molecule 48 is a protein called Cytochrome b-c1 complex subunit 1, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 48 | QB | 446 | 3459 | 2161 | 605 | 674 | 19 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 48 | Qb | 433 | 3367 | 2103 | 592 | 653 | 19 | 0 | 0 |

- Molecule 49 is a protein called Cytochrome b.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 49 | QC | 379 | 3025 | 2031 | 471 | 502 | 21 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 49 | Qc | 379 | 3025 | 2031 | 471 | 502 | 21 | 0 | 0 |

- Molecule 50 is a protein called Cytochrome c domain-containing protein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 50 | QD | 241 | 1921 | 1225 | 330 | 350 | 16 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 50 | Qd | 239 | 1904 | 1215 | 327 | 346 | 16 | 0 | 0 |

- Molecule 51 is a protein called Rieske domain-containing protein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 51 | QE | 196 | 1517 | 955 | 265 | 290 | 7 | 0 | 0 |
| | | | Total | C | N | O | S | | |
| 51 | Qe | 196 | 1517 | 955 | 265 | 290 | 7 | 0 | 0 |

- Molecule 52 is a protein called Cytochrome b-c1 complex subunit 6.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 52 | QF | 67 | 552 | 336 | 100 | 111 | 5 | 0 | 0 |
| 52 | Qf | 64 | 528 | 320 | 97 | 106 | 5 | 0 | 0 |

- Molecule 53 is a protein called Cytochrome b-c1 complex subunit 7.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 53 | QG | 101 | 893 | 572 | 157 | 162 | 2 | 0 | 0 |
| 53 | Qg | 101 | 893 | 572 | 157 | 162 | 2 | 0 | 0 |

- Molecule 54 is a protein called Cytochrome b-c1 complex subunit 8.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 54 | QH | 78 | 662 | 432 | 121 | 107 | 2 | 0 | 0 |
| 54 | Qh | 79 | 666 | 434 | 122 | 108 | 2 | 0 | 0 |

- Molecule 55 is a protein called Ubiquinol-cytochrome c reductase complex.

| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | | |
| 55 | QI | 62 | 507 | 331 | 90 | 86 | 0 | 0 |
| 55 | Qi | 60 | 493 | 322 | 87 | 84 | 0 | 0 |

- Molecule 56 is a protein called Cytochrome b-c1 complex subunit 10.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 56 | QJ | 49 | 405 | 269 | 71 | 63 | 2 | 0 | 0 |

- Molecule 57 is a protein called Cytochrome b-c1 complex subunit Rieske, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 57 | QK | 73 | 520 | 328 | 98 | 92 | 2 | 0 | 0 |

- Molecule 58 is a protein called Cytochrome b-c1 complex subunit 10.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 58 | Qj | 51 | 421 | 281 | 74 | 65 | 1 | 0 | 0 |

- Molecule 59 is a protein called NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 59 | S1 | 689 | 5290 | 3317 | 922 | 1012 | 39 | 0 | 0 |

- Molecule 60 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 60 | S2 | 421 | 3391 | 2169 | 580 | 618 | 24 | 0 | 0 |

- Molecule 61 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 61 | S3 | 207 | 1729 | 1119 | 297 | 311 | 2 | 0 | 0 |

- Molecule 62 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 62 | S4 | 124 | 1007 | 637 | 179 | 188 | 3 | 0 | 0 |

- Molecule 63 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 5.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 63 | S5 | 100 | 825 | 525 | 153 | 141 | 6 | 0 | 0 |

- Molecule 64 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 64 | S6 | 96 | 741 | 452 | 140 | 146 | 3 | 0 | 0 |

- Molecule 65 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 65 | S7 | 156 | 1248 | 794 | 227 | 213 | 14 | 0 | 0 |

- Molecule 66 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 66 | S8 | 176 | 1412 | 887 | 243 | 269 | 13 | 0 | 0 |

- Molecule 67 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 67 | V1 | 431 | 3316 | 2092 | 592 | 612 | 20 | 0 | 0 |

- Molecule 68 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 68 | V2 | 217 | 1671 | 1065 | 281 | 315 | 10 | 0 | 0 |

- Molecule 69 is a protein called NADH:ubiquinone oxidoreductase subunit V3.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | |
| 69 | V3 | 42 | 355 | 219 | 67 | 68 | 1 | 0 | 0 |

- Molecule 70 is ZINC ION (CCD ID: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms | | AltConf |
|---|---|---|---|---|---|
| | | | Total | Zn | |
| 70 | 5B | 1 | 1 | 1 | 0 |

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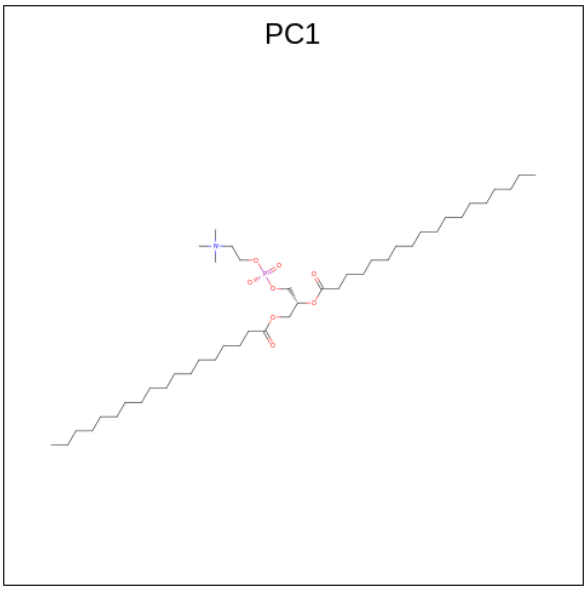
| Mol | Chain | Residues | Atoms | | AltConf |
|---|---|---|---|---|---|
| | | | Total | Zn | |
| 70 | S6 | 1 | 1 | 1 | 0 |

- Molecule 71 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: $C_{44}H_{88}NO_8P$).




| Mol | Chain | Residues | Atoms | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | |
| 71 | 6A | 1 | 45 | 35 | 1 | 8 | 1 | 0 |
| 71 | 7B | 1 | 54 | 44 | 1 | 8 | 1 | 0 |
| 71 | AL | 1 | 54 | 44 | 1 | 8 | 1 | 0 |
| 71 | C1 | 1 | 54 | 44 | 1 | 8 | 1 | 0 |
| 71 | C1 | 1 | 46 | 36 | 1 | 8 | 1 | 0 |
| 71 | C3 | 1 | 49 | 39 | 1 | 8 | 1 | 0 |
| 71 | C3 | 1 | 43 | 33 | 1 | 8 | 1 | 0 |
| 71 | N5 | 1 | 54 | 44 | 1 | 8 | 1 | 0 |
| 71 | N6 | 1 | 54 | 44 | 1 | 8 | 1 | 0 |
| 71 | QC | 1 | 54 | 44 | 1 | 8 | 1 | 0 |

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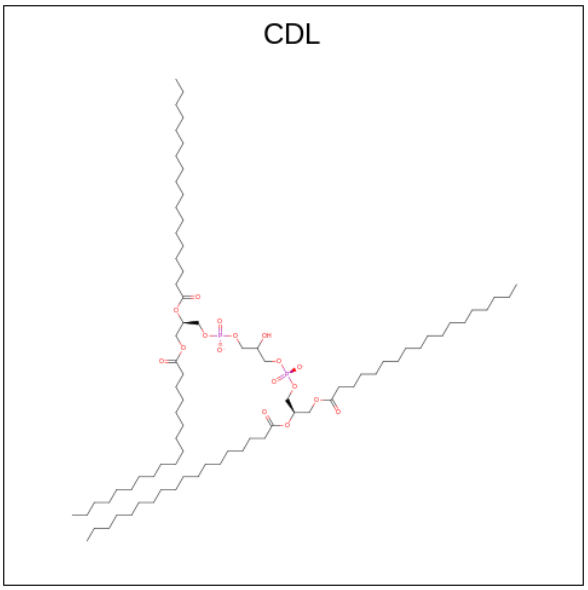
| Mol | Chain | Residues | Atoms | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | |
| 71 | QC | 1 | 54 | 44 | 1 | 8 | 1 | 0 |
| 71 | QH | 1 | 54 | 44 | 1 | 8 | 1 | 0 |
| 71 | Qb | 1 | 29 | 19 | 1 | 8 | 1 | 0 |
| 71 | Qj | 1 | 54 | 44 | 1 | 8 | 1 | 0 |

- Molecule 72 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).




| Mol | Chain | Residues | Atoms | | | | AltConf |
|---|---|---|---|---|---|---|---|
| | | | Total | C | O | P | |
| 72 | 6A | 1 | 69 | 50 | 17 | 2 | 0 |
| 72 | A8 | 1 | 83 | 64 | 17 | 2 | 0 |
| 72 | AL | 1 | 84 | 65 | 17 | 2 | 0 |
| 72 | AL | 1 | 93 | 74 | 17 | 2 | 0 |
| 72 | AL | 1 | 80 | 61 | 17 | 2 | 0 |
| 72 | AM | 1 | 51 | 32 | 17 | 2 | 0 |
| 72 | B5 | 1 | 100 | 81 | 17 | 2 | 0 |

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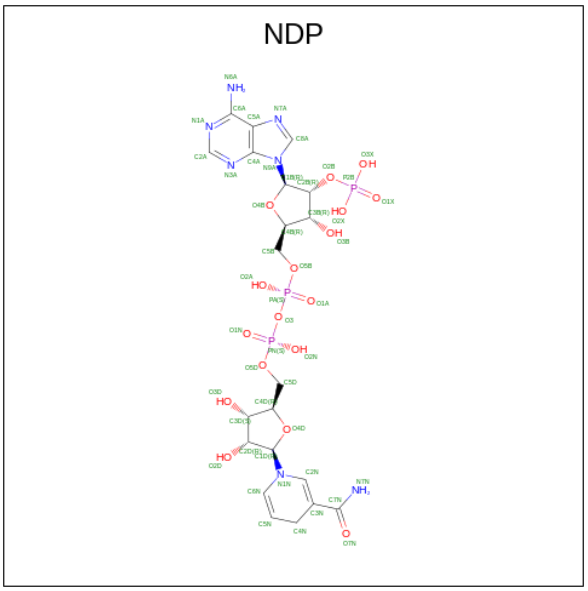
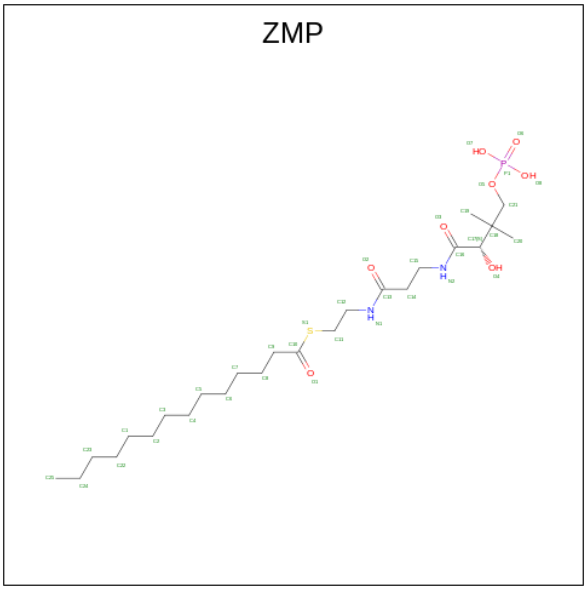
| Mol | Chain | Residues | Atoms | | | | AltConf |
|---|---|---|---|---|---|---|---|
| | | | Total | C | O | P | |
| 72 | CB | 1 | 100 | 81 | 17 | 2 | 0 |
| | | | Total | C | O | P | |
| 72 | N2 | 1 | 68 | 49 | 17 | 2 | 0 |
| | | | Total | C | O | P | |
| 72 | N5 | 1 | 89 | 70 | 17 | 2 | 0 |
| | | | Total | C | O | P | |
| 72 | N5 | 1 | 100 | 81 | 17 | 2 | 0 |
| | | | Total | C | O | P | |
| 72 | QB | 1 | 64 | 45 | 17 | 2 | 0 |
| | | | Total | C | O | P | |
| 72 | QC | 1 | 94 | 75 | 17 | 2 | 0 |
| | | | Total | C | O | P | |
| 72 | QC | 1 | 55 | 36 | 17 | 2 | 0 |
| | | | Total | C | O | P | |
| 72 | QH | 1 | 61 | 42 | 17 | 2 | 0 |
| | | | Total | C | O | P | |
| 72 | Qb | 1 | 64 | 45 | 17 | 2 | 0 |
| | | | Total | C | O | P | |
| 72 | Qd | 1 | 64 | 45 | 17 | 2 | 0 |
| | | | Total | C | O | P | |
| 72 | Qh | 1 | 64 | 45 | 17 | 2 | 0 |

- Molecule 73 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).



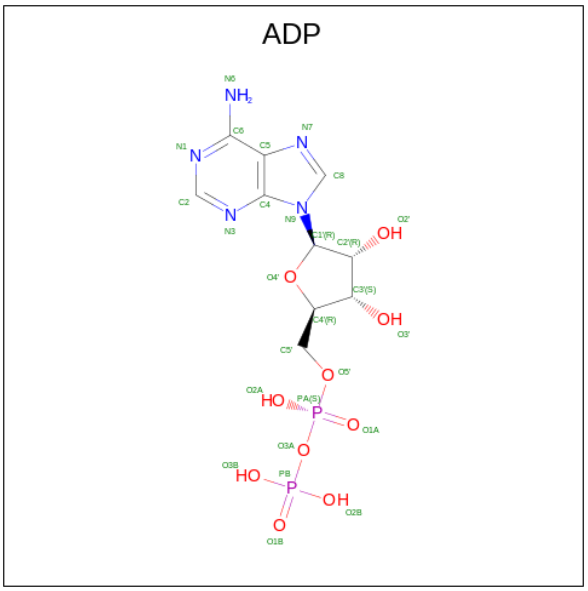
| Mol | Chain | Residues | Atoms | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | |
| 73 | A9 | 1 | 48 | 21 | 7 | 17 | 3 | 0 |

- Molecule 74 is S-[2-({N-[(2S)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-beta-alanyl}amino)ethyl] tetradecanethioate (CCD ID: ZMP) (formula: $C_{25}H_{49}N_2O_8PS$).



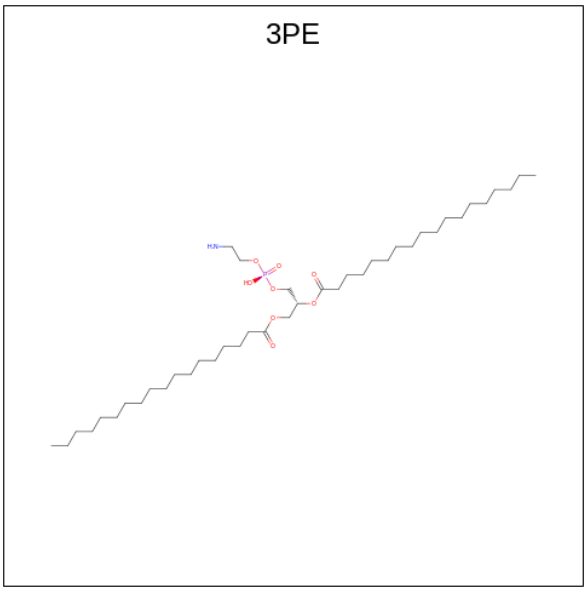

| Mol | Chain | Residues | Atoms | | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | S | |
| 74 | AB | 1 | 36 | 25 | 2 | 7 | 1 | 1 | 0 |
| 74 | AC | 1 | 36 | 25 | 2 | 7 | 1 | 1 | 0 |

- Molecule 75 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).




| Mol | Chain | Residues | Atoms | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | |
| 75 | AK | 1 | 27 | 10 | 5 | 10 | 2 | 0 |

- Molecule 76 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: $C_{41}H_{82}NO_8P$).




| Mol | Chain | Residues | Atoms | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | |
| 76 | AL | 1 | 51 | 41 | 1 | 8 | 1 | 0 |
| | | | Total | C | N | O | P | |
| 76 | C1 | 1 | 51 | 41 | 1 | 8 | 1 | 0 |

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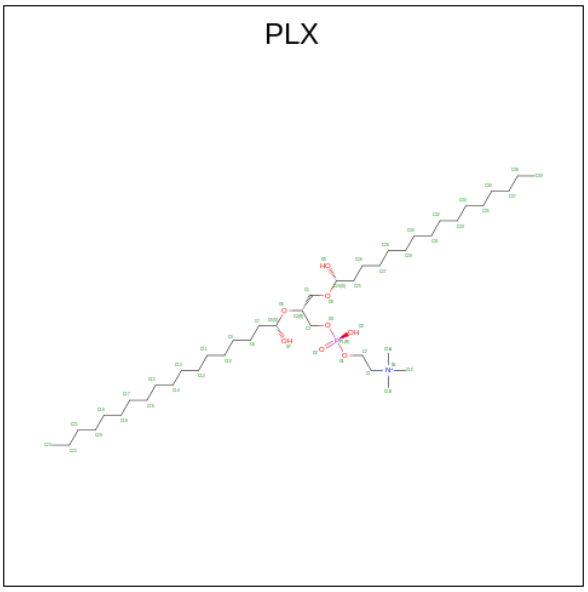
| Mol | Chain | Residues | Atoms | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | |
| 76 | C1 | 1 | 44 | 34 | 1 | 8 | 1 | 0 |
| 76 | CA | 1 | 51 | 41 | 1 | 8 | 1 | 0 |
| 76 | CB | 1 | 46 | 36 | 1 | 8 | 1 | 0 |
| 76 | N4 | 1 | 51 | 41 | 1 | 8 | 1 | 0 |
| 76 | QE | 1 | 44 | 34 | 1 | 8 | 1 | 0 |
| 76 | S7 | 1 | 51 | 41 | 1 | 8 | 1 | 0 |

- Molecule 77 is (9R,11S)-9-({[(1S)-1-HYDROXYHEXADECYL]OXY}METHYL)-2,2-DIMETHYL-5,7,10-TRIOXA-2LAMBDA 5 -AZA-6LAMBDA 5 -PHOSPHAOCTACOSANE-6,6,11-TRIOL (CCD ID: PLX) (formula: $C_{42}H_{89}NO_8P$).




| Mol | Chain | Residues | Atoms | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | |
| 77 | AL | 1 | 47 | 37 | 1 | 8 | 1 | 0 |
| 77 | AM | 1 | 52 | 42 | 1 | 8 | 1 | 0 |
| 77 | AM | 1 | 52 | 42 | 1 | 8 | 1 | 0 |
| 77 | B5 | 1 | 52 | 42 | 1 | 8 | 1 | 0 |

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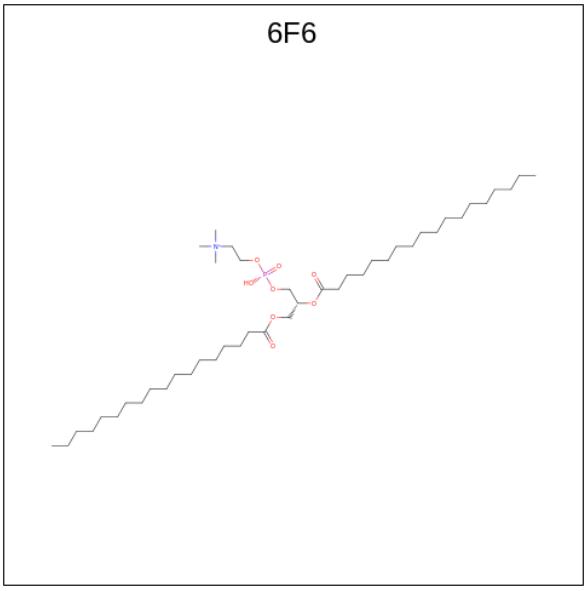
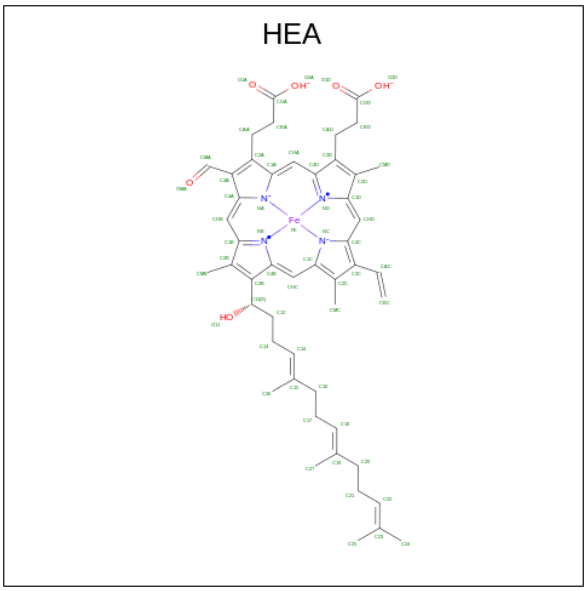
| Mol | Chain | Residues | Atoms | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | |
| 77 | C2 | 1 | 43 | 33 | 1 | 8 | 1 | 0 |
| | | | Total | C | N | O | P | |
| 77 | CB | 1 | 52 | 42 | 1 | 8 | 1 | 0 |
| | | | Total | C | N | O | P | |
| 77 | N4 | 1 | 52 | 42 | 1 | 8 | 1 | 0 |
| | | | Total | C | N | O | P | |
| 77 | QE | 1 | 46 | 36 | 1 | 8 | 1 | 0 |
| | | | Total | C | N | O | P | |
| 77 | QI | 1 | 52 | 42 | 1 | 8 | 1 | 0 |

- Molecule 78 is (4S,7R)-4-hydroxy-N,N,N-trimethyl-7-(octadecanoyloxy)-4,10-dioxo-3,5,9-trioxa-4lambda 5 -phosphaheptacosan-1-aminium (CCD ID: 6F6) (formula: $C_{44}H_{89}NO_8P$).




| Mol | Chain | Residues | Atoms | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | |
| 78 | B5 | 1 | 54 | 44 | 1 | 8 | 1 | 0 |
| | | | Total | C | N | O | P | |
| 78 | QJ | 1 | 54 | 44 | 1 | 8 | 1 | 0 |
| | | | Total | C | N | O | P | |
| 78 | Qc | 1 | 54 | 44 | 1 | 8 | 1 | 0 |

- Molecule 79 is HEME-A (CCD ID: HEA) (formula: $C_{49}H_{56}FeN_4O_6$).




| Mol | Chain | Residues | Atoms | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | Fe | N | O | |
| 79 | C1 | 1 | 60 | 49 | 1 | 4 | 6 | 0 |
| | | | Total | C | Fe | N | O | |
| 79 | C1 | 1 | 60 | 49 | 1 | 4 | 6 | 0 |

- Molecule 80 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

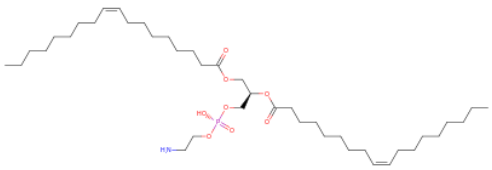
| Mol | Chain | Residues | Atoms | | AltConf |
|---|---|---|---|---|---|
| | | | Total | Cu | |
| 80 | C1 | 1 | 1 | 1 | 0 |
| | | | Total | Cu | |
| 80 | C2 | 2 | 2 | 2 | 0 |

- Molecule 81 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms | | AltConf |
|---|---|---|---|---|---|
| | | | Total | Mg | |
| 81 | C1 | 1 | 1 | 1 | 0 |
| | | | Total | Mg | |
| 81 | S1 | 1 | 1 | 1 | 0 |

- Molecule 82 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (CCD ID: PEE) (formula: $C_{41}H_{78}NO_8P$).

PEE



| Mol | Chain | Residues | Atoms | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | |
| 82 | C1 | 1 | 51 | 41 | 1 | 8 | 1 | 0 |
| 82 | N1 | 1 | 38 | 28 | 1 | 8 | 1 | 0 |
| 82 | N3 | 1 | 51 | 41 | 1 | 8 | 1 | 0 |
| 82 | N5 | 1 | 46 | 36 | 1 | 8 | 1 | 0 |
| 82 | QB | 1 | 27 | 17 | 1 | 8 | 1 | 0 |
| 82 | QB | 1 | 51 | 41 | 1 | 8 | 1 | 0 |
| 82 | QC | 1 | 51 | 41 | 1 | 8 | 1 | 0 |
| 82 | QC | 1 | 38 | 28 | 1 | 8 | 1 | 0 |
| 82 | QE | 1 | 47 | 37 | 1 | 8 | 1 | 0 |
| 82 | Qc | 1 | 42 | 32 | 1 | 8 | 1 | 0 |
| 82 | Qd | 1 | 51 | 41 | 1 | 8 | 1 | 0 |
| 82 | Qh | 1 | 41 | 31 | 1 | 8 | 1 | 0 |
| 82 | Qh | 1 | 51 | 41 | 1 | 8 | 1 | 0 |
| 82 | S2 | 1 | 48 | 38 | 1 | 8 | 1 | 0 |

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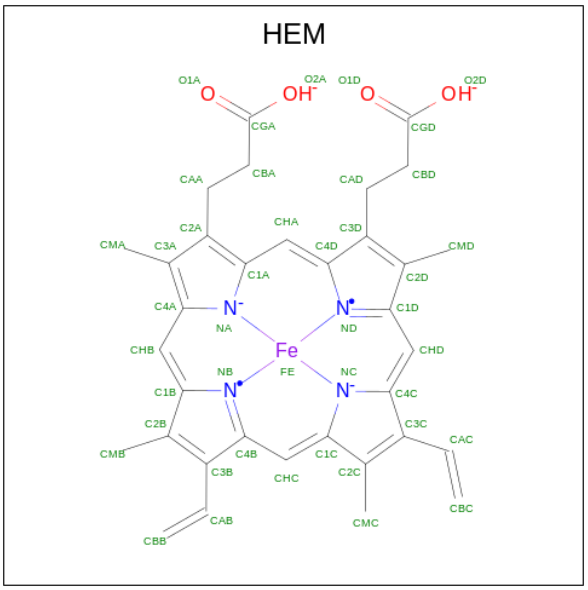
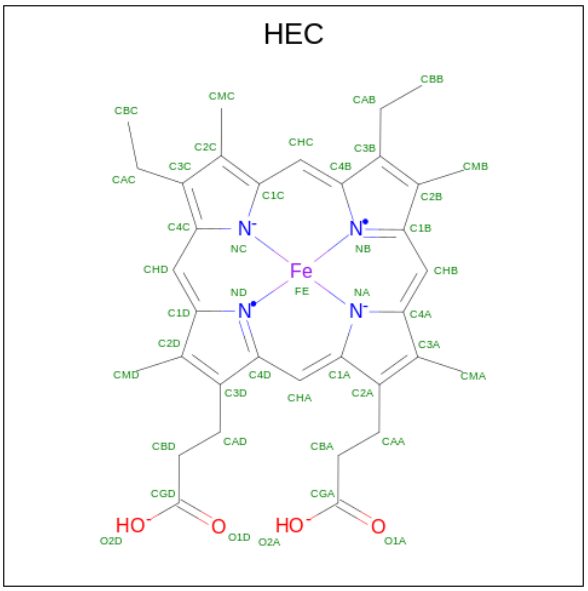
| Mol | Chain | Residues | Atoms | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | |
| 82 | S8 | 1 | 51 | 41 | 1 | 8 | 1 | 0 |

- Molecule 83 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



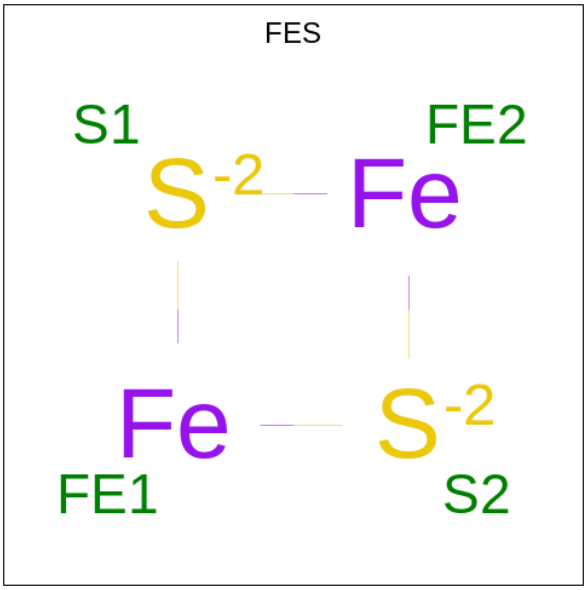

| Mol | Chain | Residues | Atoms | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | Fe | N | O | |
| 83 | QC | 1 | 43 | 34 | 1 | 4 | 4 | 0 |
| | | | Total | C | Fe | N | O | |
| 83 | QC | 1 | 43 | 34 | 1 | 4 | 4 | 0 |
| | | | Total | C | Fe | N | O | |
| 83 | Qc | 1 | 43 | 34 | 1 | 4 | 4 | 0 |
| | | | Total | C | Fe | N | O | |
| 83 | Qc | 1 | 43 | 34 | 1 | 4 | 4 | 0 |

- Molecule 84 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{36}FeN_4O_4$).




| Mol | Chain | Residues | Atoms | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | Fe | N | O | |
| 84 | QD | 1 | 43 | 34 | 1 | 4 | 4 | 0 |
| 84 | Qd | 1 | 43 | 34 | 1 | 4 | 4 | 0 |

- Molecule 85 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: $Fe_2S_2$).




| Mol | Chain | Residues | Atoms | | | AltConf |
|---|---|---|---|---|---|---|
| | | | Total | Fe | S | |
| 85 | QE | 1 | 4 | 2 | 2 | 0 |
| 85 | Qe | 1 | 4 | 2 | 2 | 0 |

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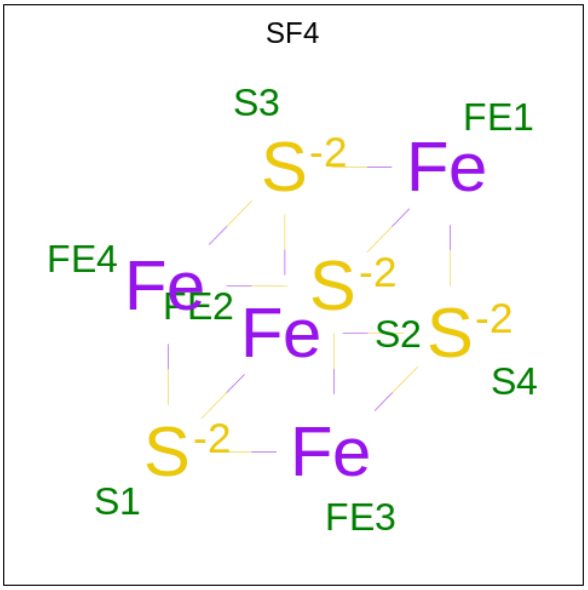
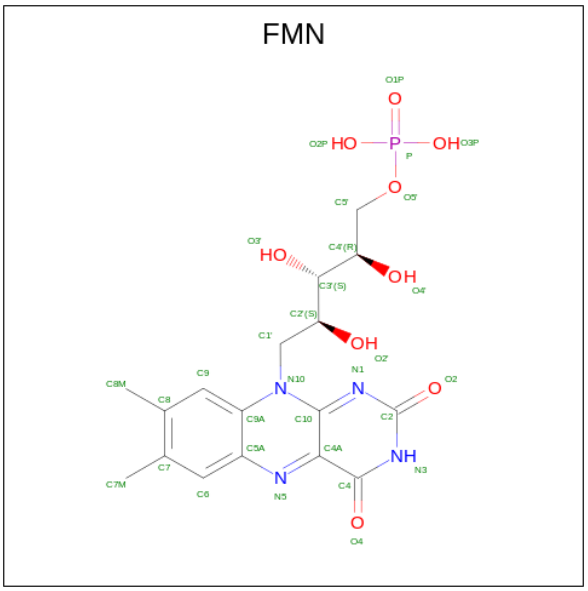
| Mol | Chain | Residues | Atoms | | | AltConf |
|---|---|---|---|---|---|---|
| | | | Total | Fe | S | |
| 85 | S1 | 1 | 4 | 2 | 2 | 0 |
| 85 | V2 | 1 | 4 | 2 | 2 | 0 |

- Molecule 86 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: $Fe_4S_4$).




| Mol | Chain | Residues | Atoms | | | AltConf |
|---|---|---|---|---|---|---|
| | | | Total | Fe | S | |
| 86 | S1 | 1 | 8 | 4 | 4 | 0 |
| 86 | S1 | 1 | 8 | 4 | 4 | 0 |
| 86 | S7 | 1 | 8 | 4 | 4 | 0 |
| 86 | S8 | 1 | 8 | 4 | 4 | 0 |
| 86 | S8 | 1 | 8 | 4 | 4 | 0 |
| 86 | V1 | 1 | 8 | 4 | 4 | 0 |

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




| Mol | Chain | Residues | Atoms | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | |
| 87 | V1 | 1 | 31 | 17 | 4 | 9 | 1 | 0 |

# 3 Residue-property plots (i)

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

• Molecule 1: NADH-ubiquinone oxidoreductase chain 4L

Chain 4L: 82% 18%

M1 P2 L3 M6 I9 L20 M21 Y22 R23 G35 M36 M37 L38 L55 A56 I62 L63 A67 A68 L73 C98

• Molecule 2: Cytochrome c oxidase subunit 5A, mitochondrial

Chain 5A: 71% 29%

T50 D55 D66 I67 D68 E71 L72 R73 L79 L84 V85 P86 I90 C98 L101 F104 A105 S106 A107 V108 R109 V113 V114 P126 Y127 V128 I129 Q130 P134 T135 L136 N137 E138 I141 S142 T143 P144 E145 E146 L147 K151

• Molecule 3: Cytochrome c oxidase subunit 5B, mitochondrial

Chain 5B: 71% 29%

S33 G34 P38 E41 T45 G46 A54 A55 R56 K57 G58 P61 Y62 A70 N78 S82 I83 T84 N85 K86 R87 N97 S98 V105 E109 T110 Q111 R112 T118 L122 L127

• Molecule 4: Cytochrome c oxidase subunit

Chain 6A: 75% 25%

T23 W28 R29 T32 H50 H53 H54 I60 P61 Y62 H63 H64 L65 R66 I67 R68 T69 H79 T80 L81 F82 H83 N88 P97

• Molecule 5: Cytochrome c oxidase subunit

Chain 6B: 73% 27%

I5 Q6 T7 R8 I9 K10 N11 Y12 C30 W31 Q32 N33 Y34 L35 D36 F37 H38 R39 W56 Y57 R58 R59 V60 Y61 K62 C65 R76 K85 I86

• Molecule 6: Cytochrome c oxidase subunit 6C

Chain 6C: 79% 21%

L6 T7 I23 K38 K47 A48 Y49 A50 D51 F52 Y53 K60 E63 E64 K65 R66 G69 I70 F71 Q72 S73 A74 K75

• Molecule 7: Cytochrome c oxidase subunit 7A1, mitochondrial

Chain 7A: 74% 25%

L22 E23 N24 R25 Q30 F33 P40 V41 H42 L43 N50 I51 L52 Y53 C60 G72 S75 F76 P77 H78

• Molecule 8: Cytochrome c oxidase subunit 7B, mitochondrial

Chain 7B: 86% 14%

A30 H34 W53 I60 V69 G70 R71 V72 E79

• Molecule 9: Cytochrome c oxidase subunit 7C, mitochondrial

Chain 7C: 89% 11%

S17 H18 Y19 T42 L43 Y44 Q59 K62 K63

• Molecule 10: Cytochrome c oxidase subunit 8

Chain 8B: 72% 28%

I25 K28 R31 L43 T46 F47 L48 S49 F50 L51 I52 P53 A54 G55 S59 S67

• Molecule 11: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1

Chain A1: 91% 9%

M1 E4 N46 R50 L66 I69 D70

• Molecule 12: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2

Chain A2: 88% 12%

L14 E18 C24 C58 S59 D60 R68 Y69 K75 R89 E92 K98

• Molecule 13: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3

Chain A3: 96%

A87 S121 A127 V151 L169

• Molecule 14: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5

Chain A5: 91% 9%

L5 P20 D33 Y44 T48 I51 Q76 I77 V80 K93 R96 I116

• Molecule 15: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6

Chain A6: 85% 15%

T41 S42 P45 S48 E53 R63 Y66 L78 R86 D87 K88 M92 L107 T127 M130 R131 R140 L145 P154

• Molecule 16: Complex I-B14.5a

Chain A7: 79% 7% 13%

A2 S3 R27 I31 S32 K33 R34 T35 Q36 V43 Y54 K74 VAL LEU ALA SER GLY LYS PRO ALA GLU SER SER ALA VAL ALA GLU T90 I101 L113

• Molecule 17: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

Chain A8: 85% 15%

P79 L84 V95 K96 V97 N117 M121 R124 I151 K152 E157 P158 F159 T160 W163 F174 R178 R196 P197 D198 E201 L202 K207 Y219 N228 L235 K239 R243 L244 F245 F246 M249

• Molecule 18: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial

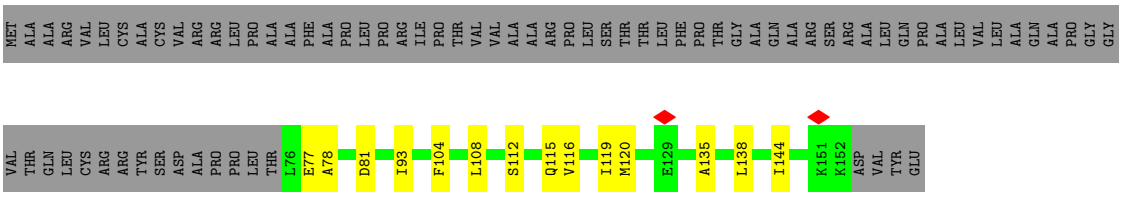
Chain A9: 82% 17%

L36 S50 I54 A61 F64 R67 M76 V82 N109 D112 K118 V126 L129 V161 E162 K163 I167 S168 H169 L170 N171 A172 D173 S176 K184 E188 A198 T199 I200 P203 S204 D205 I206 D211 N215 Y216 R221

Q238 S246 I250 I253 G260 K261 T262 V266 G267 P268 N269 R270 Y279 R286 L293 P294 R303 T314 T315 R316 M327 P333 P344 L345 E346 L347 R357 T358 Y359 ARG TRP LEU THR S364 E365 V369 K370 P371 A372 N376

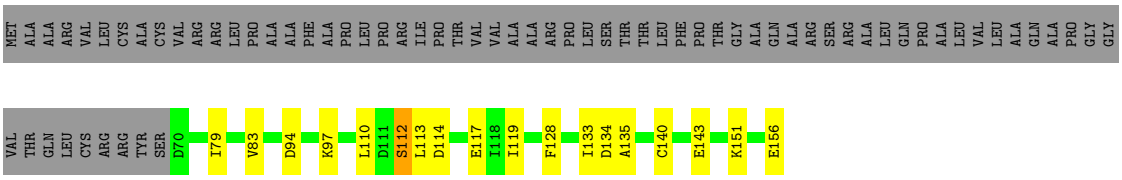
• Molecule 19: Acyl carrier protein

Chain AB: 40% 9% 51%



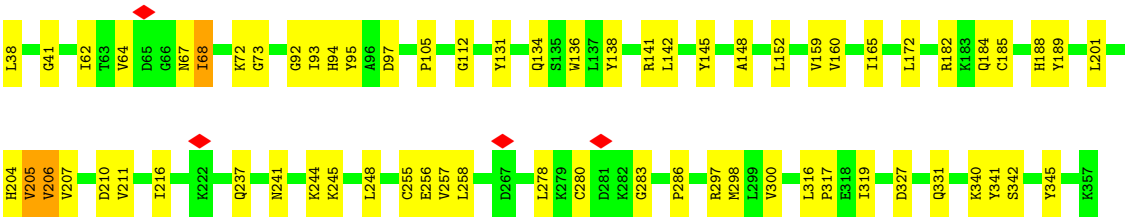

• Molecule 19: Acyl carrier protein

Chain AC: 44% 11% 44%



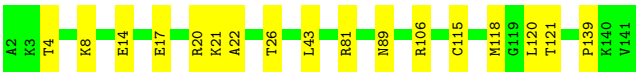

• Molecule 20: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

Chain AK: 79% 20%



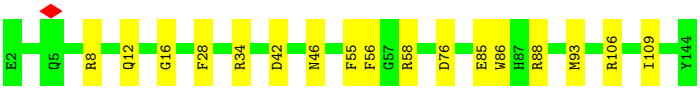

• Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11

Chain AL: 88% 12%



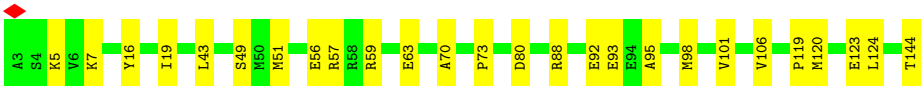

• Molecule 22: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

Chain AM: 88% 12%




• Molecule 23: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13

Chain AN: 82% 18%

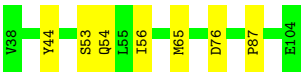


• Molecule 24: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1

Chain B1:

• Molecule 25: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial

Chain B2:

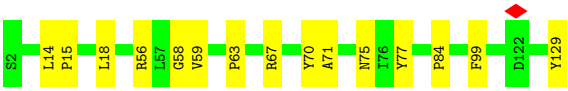



• Molecule 26: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3

Chain B3:

• Molecule 27: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4

Chain B4:

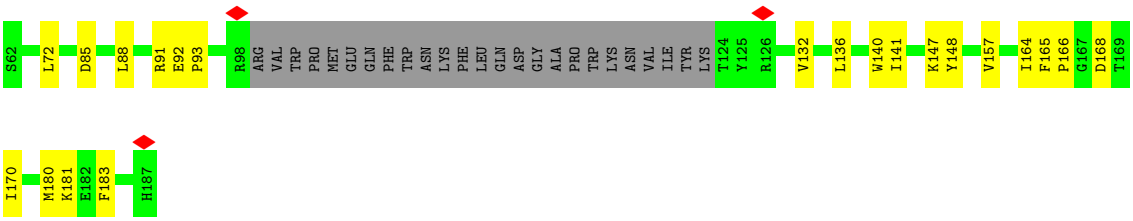



• Molecule 28: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial

Chain B5:

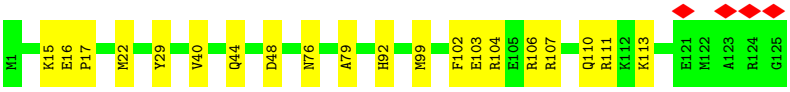
• Molecule 29: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6

Chain B6:



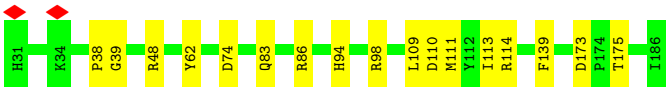
• Molecule 30: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7

Chain B7:



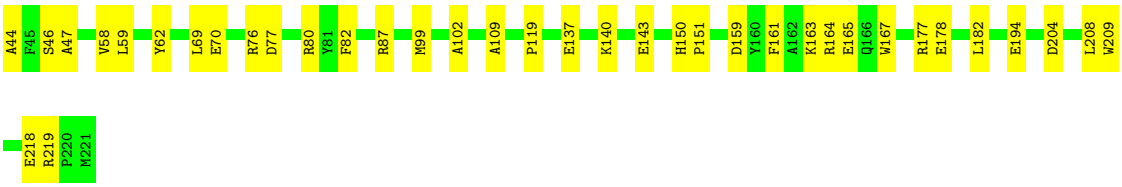

• Molecule 31: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

Chain B8:



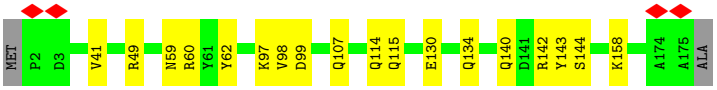

• Molecule 32: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9

Chain B9:



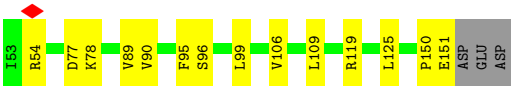

• Molecule 33: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10

Chain BK:



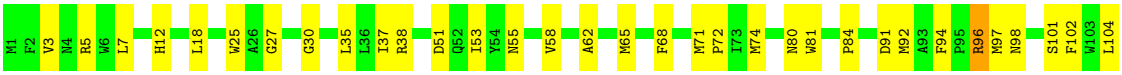

• Molecule 34: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial

Chain BL:




• Molecule 35: Cytochrome c oxidase subunit 1

Chain C1:



P107 S108 F109 S115 S116 M117 V118 T124 T127 V128 L132 A133 G134 N135 S142 V143 D144 F148 S156 T166 I169 K172 P173 M176 S177 Q178 Y179 Q180 L183 F184 L195 L202 R213 N214 L215 N216 T217 T218 I229 L230 H233

W236 F237 F238 G239 H240 V243 Y244 I245 L246 I247 F251 I254 S255 H256 K265 E266 M273 M292 D300 T301 Y304 S307 A308 I311 I312 A313 T316 K319 V320 F321 H328 N331 W334 F344 L347 F348 T349 G352 V357 N360

D364 H368 D369 T370 Y371 Y372 V373 V374 F377 H378 Y379 V380 L381 S382 M383 I389 M390 N406 W409 I412 H413 M417 V421 N422 M423 T424 F425 F426 P427 G432 M436 P437 R438 D442 Y443 P444 D445 A446 Y447 T448 A449 W450 N451 S454 S458

L462 M466 L467 M468 I469 F470 I471 E481 V482 S483 T490 N491 L492 L495 P501 T504 P508 K514

- Molecule 36: Cytochrome c oxidase subunit 2

Chain C2: 76% 23%

M1 D11 T27 L28 M29 I30 V31 V38 T48 M56 W65 L73 N91 N92 P93 K98 H102 Q103 W104 Y110 T111 L116 K129 P130 G131 E132 M133 R134 E137 V138 D139 V143 L144 P145 R151 M152 L153 V154 E157 D158 V159 L160 H161

S162 W163 A164 V165 K171 T172 D173 A174 I175 N180 S186 T187 R188 G194 Q195 C196 S197 C200 N203 M207 E212 L213 F219 W222 T228

- Molecule 37: Cytochrome c oxidase subunit 3

Chain C3: 81% 18%

T2 H3 P15 T19 L25 T32 T49 T53 M54 W57 W58 R63 T66 F67 L79 F86 A100 L112 P118 N125 P126 L127 E128 L137 G141 I144 T145 W146 A147 H148 L151 R156 M159 L163 A178 Y181

A184 T187 D190 G202 F203 H204 G205 V208 V217 R221 Q222 L223 F233 G234 F235 V245 W249 Y253 Y257 S261

- Molecule 38: Cytochrome c oxidase subunit 4

Chain C4: 79% 21%

E31 D32 Y33 V39 D40 R41 R42 L46 L62 K65 E66 S74 M75 D76 E77 K78 L81 F90 M93 W100 T106 F109 F110 I111 A115 K122 P130 F133 W137 L146 D147 I153 Q154 G155 A158 W167 K168

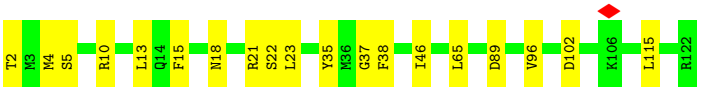
- Molecule 39: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial

Chain CA: 82% 16%

K28 K43 T47 W55 I59 K60 E64 E68 R72 E76

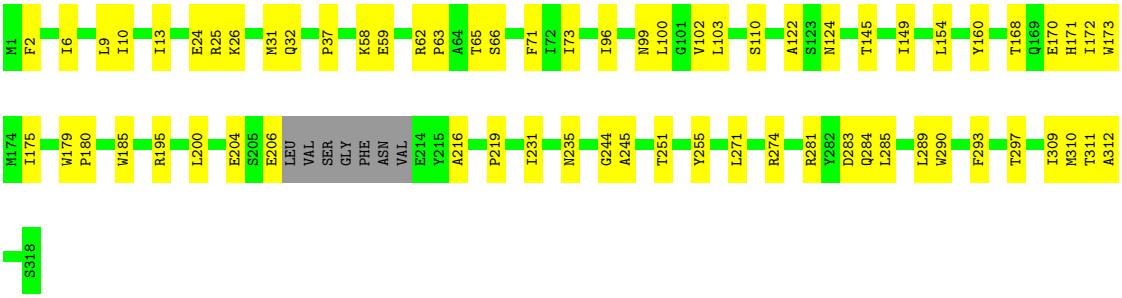
- Molecule 40: NADH dehydrogenase [ubiquinone] 1 subunit C2

Chain CB: 84% 16%



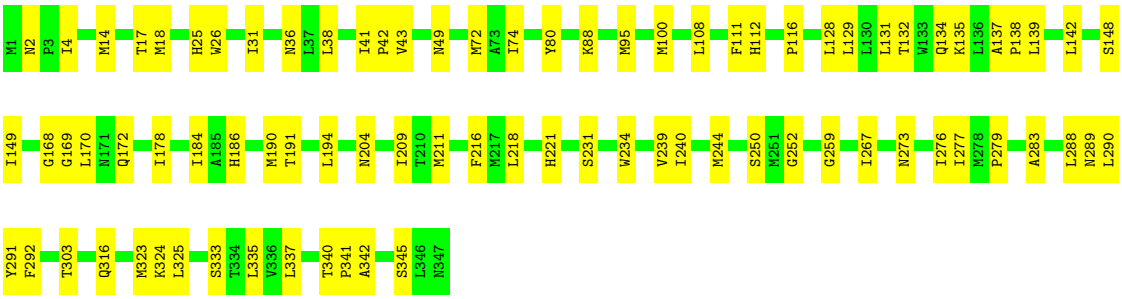

- Molecule 41: NADH-ubiquinone oxidoreductase chain 1

Chain N1:




- Molecule 42: NADH-ubiquinone oxidoreductase chain 2

Chain N2:

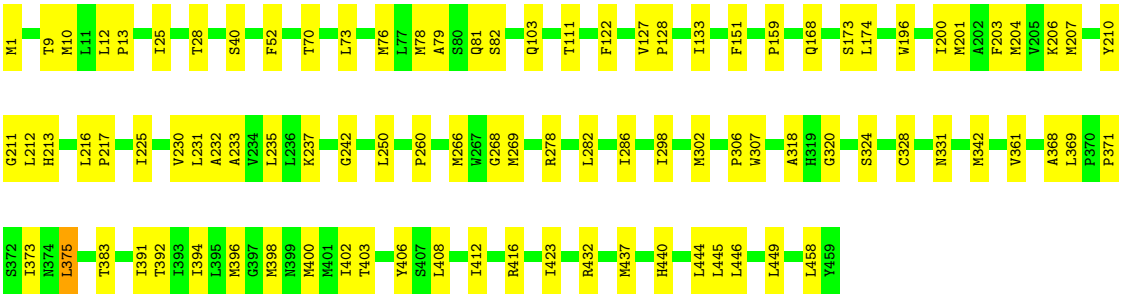



- Molecule 43: NADH-ubiquinone oxidoreductase chain 3

Chain N3:

- Molecule 44: NADH-ubiquinone oxidoreductase chain 4

Chain N4:



• Molecule 45: NADH-ubiquinone oxidoreductase chain 5

Chain N5: 79% 20%

M1 N2 P3 F4 A5 S6 L7 T8 L9 T10 T11 I14 L15 N23 A43 L46 V49 P50 M53 M61 I62 H67 Q72 E75 L76 L94 T97 I100 M101 E102 F103 L125 F141 I149 T162 T166 I172 R176 I180

V183 L190 N194 A195 W196 Q200 M203 L204 C208 P209 L213 H230 L233 P234 T241 L246 L247 H248 S249 V253 L260 V273 Q274 L286 A289 L290 C291 A292 I293 T294 Q295 N296 D297 I301 F304 S305 T306 L310 N320

L327 M331 F340 M341 G344 S345 I346 L362 A365 M366 P367 I375 M383 P384 Y385 L386 T387 G388 F389 D393 V399 L409 I410 M411 L418 T419 A420 A421 Y422 S423 T424 R425 F431 P435 L450 R456 L457 L458 G465 T481 F498

L504 T507 M525 L526 P530 H534 R535 L536 P537 S545 L558 E559 L562 P563 K564 T565 T566 S567 Q570 M571 K572 S578 N579 Q580 I584 F588 L589 S590 F591 I595 N603

• Molecule 46: NADH-ubiquinone oxidoreductase chain 6

Chain N6: 74% 20% 6%

M3 F17 V18 G19 F20 S21 S22 L33 I34 G37 M55 V56 F57 L61 G62 G63 M64 L65 V66 A75 THR GLU MET TYR PRO GLU VAL TRP VAL SER N86 M103 Y106 E112 I116 F117 K118 F119 N120 G121 L122 G123 D124 W125 V126 I127 T130 G131 D132

G150 V165 V166 V167 I168 M169 E170 R173 G174 N175

• Molecule 47: Cytochrome b-c1 complex subunit 2, mitochondrial

Chain QA: 82% 18%

P35 S51 R60 I65 K66 A67 G68 S69 R70 L77 L82 T90 T91 K92 S95 R116 V123 E124 C125 L133 L138 A142 A143 R148 V151 A152 A153 L154 Q155 S156 L177 H178 A179 A180 R183 N184 A185 N188 S189 R196 L205

H206 Y207 Y208 N211 T214 R217 M218 L230 F237 L238 N239 M240 R241 A249 R254 E257 I258 R259 L271 V272 Q290 L293 H298 R301 N304 A305 T306 S307 V313 Q319 F326 Y330 S331 D332 F336 G337 G348 D349 V350

I361 Q399 V402 M438 P448 F449 V450 L453

• Molecule 47: Cytochrome b-c1 complex subunit 2, mitochondrial

Chain Qa: 77% 22%

P35 I49 A50 S51 S59 R60 L63 F64 I65 K66 A67 G68 S69 R70 Y71 E72 H81 R84 L85 L89 T90 T91 K92 S95 K109 S114 T115 R116 E117 S118 V123 E124 C125 I130 L133 V140 T141 A142 A143 R148 W149 E150 V151 L154 Q155

S156 Q157 K162 A163 V164 L177 A180 R183 N188 C192 P193 D194 Y195 R196 I197 G198 K199 V200 H212 F213 T214 R217 M218 A219 L220 I221 H227 L230 K231 A234 F237 L238 N239 M240 R241 L244 K252 Y253 R254 I258 N262 A270 L271

V272 P297 R301 N304 V313 Q319 P320 V323 G337 T369 D370 V371 K375 L378 K379 G391 F392 L393 D394 E395 V396 Q408 P409 L413 I416 D421 R435 M438 G442 L453

- Molecule 48: Cytochrome b-c1 complex subunit 1, mitochondrial

Chain QB: 83% 17%

T35 D54 N55 G56 L57 V71 R80 N87 F92 G100 G106 E110 V113 E114 L120 N121 A122 T125 R126 Y132 I133 L146 L156 R165 D176 D181 T190 A191 F192 T195 P196 L197 A198 Q199 P204 N207 V208 R209 K210

L211 S212 R213 H223 Y224 K225 A226 P227 R228 M229 Y257 V258 C268 R269 F270 T271 E274 I275 R276 D279 D280 I289 E292 N301 L304 I310 F341 C347 E350 L354 F358 M363 D366 V388 V400 I413 R423 L426

A438 C445 F449 G460 P461 I462 E463 Q464 D467 F480

- Molecule 48: Cytochrome b-c1 complex subunit 1, mitochondrial

Chain Qb: 79% 18%

THR A36 T37 Y38 L42 T70 W74 I75 D76 N87 F92 V93 E94 T101 K102 N103 R104 L109 V113 M116 N121 R126 Y132 E145 L146 D149 Q152 N153 L156 E157 I161 R165 L172 D181 T190 G194 T195

Q199 S200 V201 E202 G203 P204 V208 R213 R228 F250 S251 S252 LEU SER GLY THR TYR VAL GLU ASP ALA VAL PRO ALA F265 R269 E274 I275 R276 H277 R278 D279 I289 V302 P303 L304 I310 Y314 D315 S316 T317 M324 S330 F341 Q342 L354

G355 A356 H357 F358 V359 C360 M363 M368 M369 F370 F371 L372 V388 K392 N393 R396 N397 T407 P408 E411 L418 L426 E430 A438 D451 E463 Q464 L465 P466 F480

- Molecule 49: Cytochrome b

Chain QC: 82% 17%

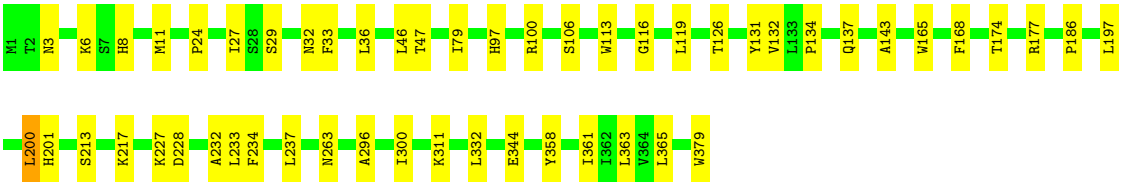
M1 T2 S25 N26 I27 S28 S29 L43 T47 L51 R71 I79 R80 Y81 I92 I96 H97 V98 G99 R100 G101 L102 Y103 T112 G116 L119 T126 G130 Y131 V132 L133 P134 Q137 M138 S139 F140 W141 T158 D159 L160 W165 D171

T174 P186 H196 L197 L200 H201 N207 I211 D216 Y223 Y224 I229 L233 M236 L237 S246 L249 N255 N263 T264 P265 I268 A277 L281 L294 I300 M304 S310 M316 F317 R318 S321 M327 T336

V343 E344 L363 S370 W379

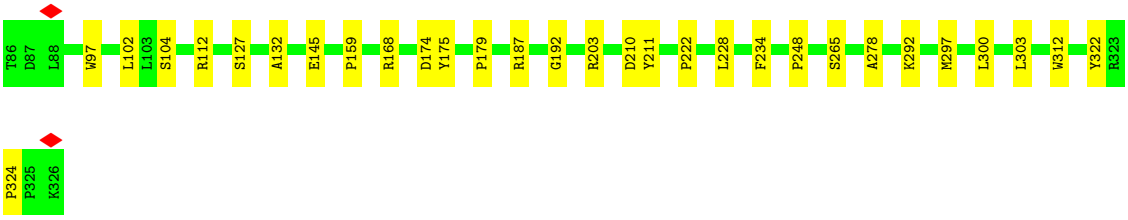
- Molecule 49: Cytochrome b

Chain Qc: 86% 13%




• Molecule 50: Cytochrome c domain-containing protein

Chain QD:

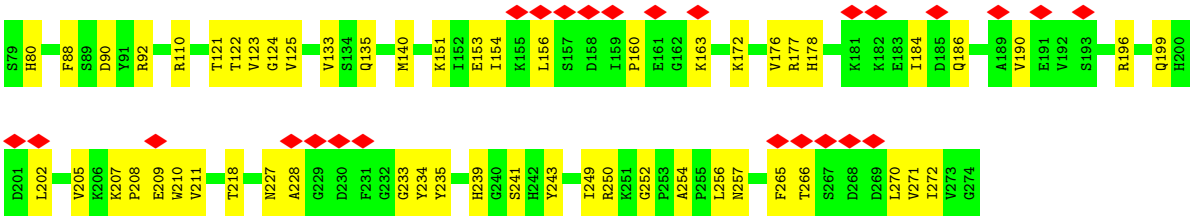



• Molecule 50: Cytochrome c domain-containing protein

Chain Qd:

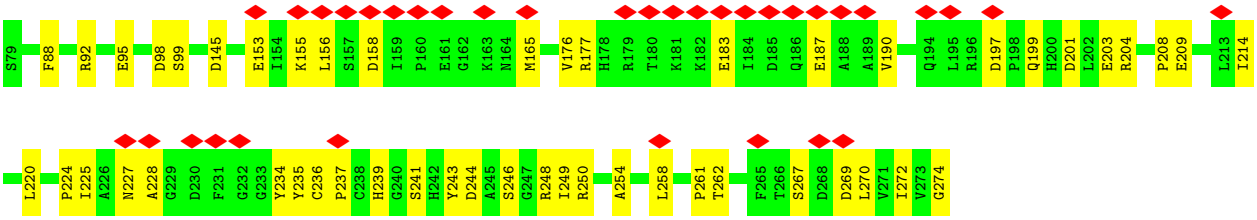
• Molecule 51: Rieske domain-containing protein

Chain QE:




• Molecule 51: Rieske domain-containing protein

Chain Qe:



• Molecule 52: Cytochrome b-c1 complex subunit 6

Chain QF: 88% 12%

E25 R34 E38 R47 R56 R60 T63 E64 E65 L71 K91

• Molecule 52: Cytochrome b-c1 complex subunit 6

Chain Qf: 70% 25%

GLU LEU VAL D28 P29 L30 T31 T32 V33 R34 E35 E38 Q39 I40 C43 R47 E51 L52 C53 R56 R60 R78 C81 V82 K91

• Molecule 53: Cytochrome b-c1 complex subunit 7

Chain QG: 84% 15%

S11 K19 R34 D35 D36 T37 D41 V44 I48 R49 R50 R62 M71 R72 Q73 Q74 E85 I99 K103 K110 K111

• Molecule 53: Cytochrome b-c1 complex subunit 7

Chain Qg: 86% 14%

S11 K12 D36 V44 K45 E46 A47 I48 R49 R50 L51 P52 E53 N54 L55 R62 K88 F89 Y90 K110 K111

• Molecule 54: Cytochrome b-c1 complex subunit 8

Chain QH: 80% 19%

GLY R3 G6 R12 S20 Q24 R25 A26 F27 P28 H29 K33 G34 I35 P36 N37 R40 F67 R72 Y78 E79 N80

• Molecule 54: Cytochrome b-c1 complex subunit 8

Chain Qh: 81% 19%

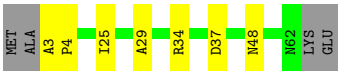
G2 H7 R12 Y17 S18 L19 S20 P21 F22 E23 Q24 N37 V38 L39 R40 R41 P52 Y57 F67 Y78 E79 N80

• Molecule 55: Ubiquinol-cytochrome c reductase complex

Chain QI: 84% 12%

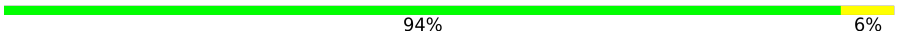
• Molecule 55: Ubiquinol-cytochrome c reductase complex

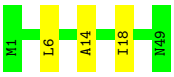
Chain Qi:




• Molecule 56: Cytochrome b-c1 complex subunit 10

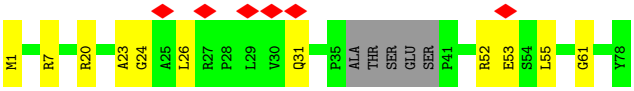
Chain QJ:



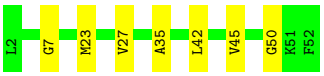

• Molecule 57: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain QK:



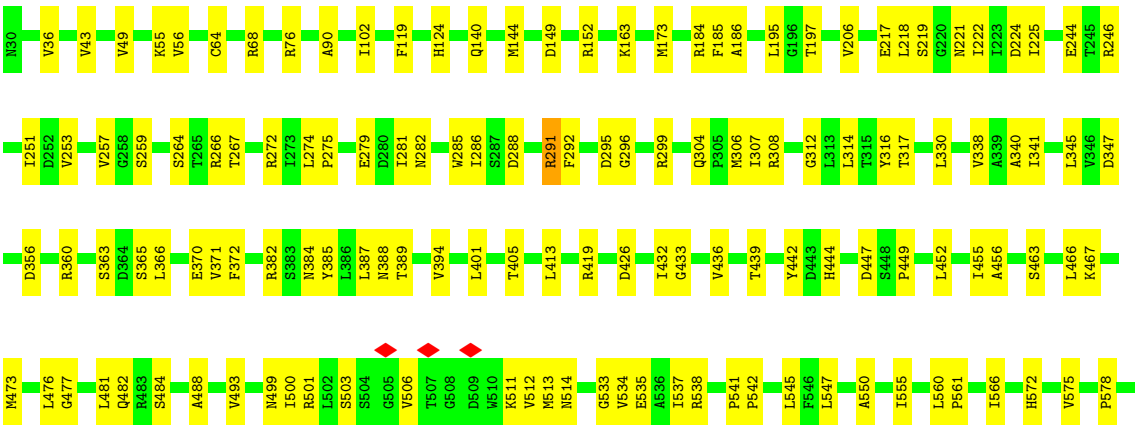

• Molecule 58: Cytochrome b-c1 complex subunit 10

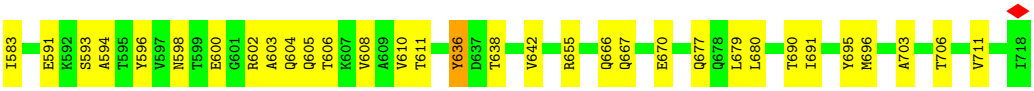
Chain Qj:




• Molecule 59: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

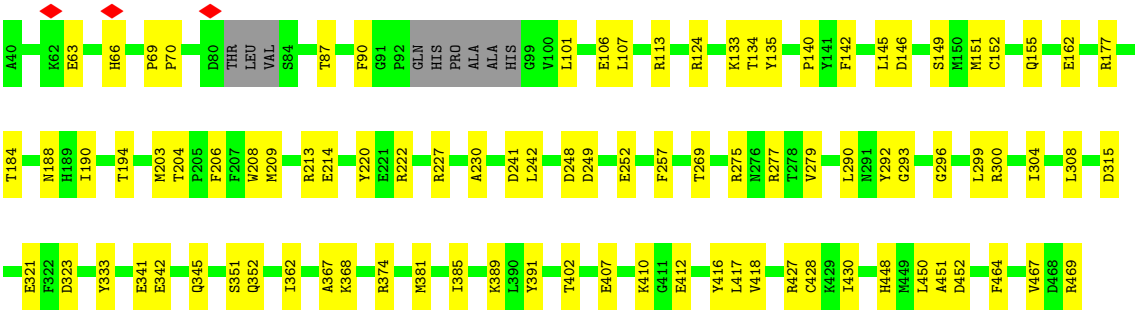
Chain S1:





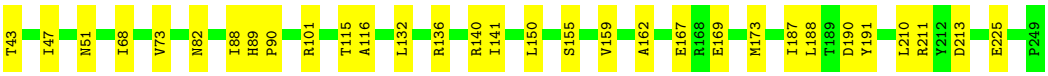

• Molecule 60: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial

Chain S2:



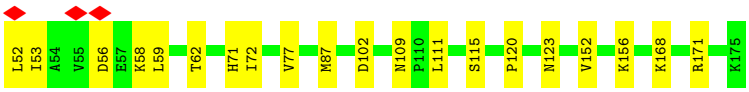

• Molecule 61: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial

Chain S3:




• Molecule 62: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

Chain S4:

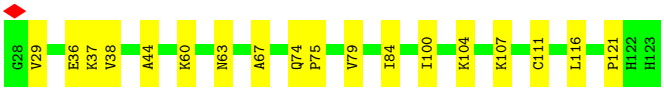



• Molecule 63: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5

Chain S5:

• Molecule 64: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial

Chain S6:




• Molecule 65: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial

Chain S7:

S41 D51 N55 L62 M65 T66 F67 C71 E75 D87 R88 V91 V92 M103 G107 T108 L117 P125 V130 C136 G140 G141 Y142 Y143 H144 D154 V159 K185 L190 R196

• Molecule 66: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial

Chain S8: 83% 17%

T37 D49 W63 L66 L74 S75 Y76 L77 F78 R79 E89 L93 R98 R105 S108 G109 E110 I114 V122 C123 P124 R144 Y145 D146 T150 I153 Y154 C155 D165 P171 H180 E200 I205 Y209 R212

• Molecule 67: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

Chain V1: 77% 22%

T30 D39 R40 T43 N44 L45 Y46 H49 G55 S58 R59 W62 Y63 K64 T65 L69 L70 K71 E79 R88 P94 L97 K98 W99 P110 K111 Y112 L113 V114 V115 D118 E119 R128 K137 L138 V139 E140 G141 C142 R147 A148 M149 G150 A151

R152 A153 A154 F162 E165 N168 Y177 L181 Y191 A203 Y204 I205 C206 G207 E208 E209 T210 A211 E217 K222 P223 R224 V235 T240 N244 V245 P252 R256 R257 G258 F265 N270 G280 H281 V282 N283 V288 E289 V294 K302

H303 A304 G305 G306 V307 W311 E333 T334 D338 F339 T347 G348 D358 V364 E377 S378 C379 G380 P384 C385 R386 E387 M396 V400 L412 W413 E414 I415 H422 R460

• Molecule 68: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

Chain V2: 88% 12%

G33 A34 G35 L38 N59 I66 V67 K68 P81 V82 L83 D84 L85 Q89 W92 P108 R111 A116 R124 K125 P126 T137 T138 R143 E150 N182 Q187 D190 E194 P237 P238 Q246 L249

• Molecule 69: NADH:ubiquinone oxidoreductase subunit V3

Chain V3: 76% 24%

D382 Y386 R387 N388 F399 L400 S407 K408 F409 R410 M411 R418 Q419 S420 H423

# 4 Experimental information (i)

| Property | Value | Source |
|---|---|---|
| EM reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, Not provided | |
| Number of particles used | 181922 | 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 ($e^-/Å^2$) | 51.9 | Depositor |
| Minimum defocus (nm) | 600 | Depositor |
| Maximum defocus (nm) | 1800 | Depositor |
| Magnification | 105000 | Depositor |
| Image detector | FEI FALCON IV (4k x 4k) | Depositor |
| Maximum map value | 47.701 | Depositor |
| Minimum map value | -16.089 | Depositor |
| Average map value | -0.009 | Depositor |
| Map value standard deviation | 1.062 | Depositor |
| Recommended contour level | 4 | Depositor |
| Map size (Å) | 576.0, 576.0, 576.0 | wwPDB |
| Map dimensions | 480, 480, 480 | wwPDB |
| Map angles (°) | 90.0, 90.0, 90.0 | wwPDB |
| Pixel spacing (Å) | 1.2, 1.2, 1.2 | Depositor |

# 5 Model quality (i)

## 5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: SF4, FES, PEE, HEC, 6F6, HEA, FMN, NDP, 2MR, PC1, PLX, 3PE, CU, ZN, CDL, HEM, ZMP, ADP, MG

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 | 4L | 0.20 | 0/759 | 0.28 | 0/1029 |
| 2 | 5A | 0.16 | 0/843 | 0.28 | 0/1145 |
| 3 | 5B | 0.18 | 0/739 | 0.33 | 0/1002 |
| 4 | 6A | 0.13 | 0/648 | 0.25 | 0/888 |
| 5 | 6B | 0.19 | 0/704 | 0.39 | 0/951 |
| 6 | 6C | 0.16 | 0/587 | 0.25 | 0/781 |
| 7 | 7A | 0.15 | 0/457 | 0.28 | 0/620 |
| 8 | 7B | 0.12 | 0/405 | 0.22 | 0/555 |
| 9 | 7C | 0.17 | 0/400 | 0.24 | 0/536 |
| 10 | 8B | 0.15 | 0/349 | 0.32 | 0/477 |
| 11 | A1 | 0.17 | 0/577 | 0.27 | 0/777 |
| 12 | A2 | 0.15 | 0/697 | 0.27 | 0/938 |
| 13 | A3 | 0.15 | 0/664 | 0.24 | 0/912 |
| 14 | A5 | 0.16 | 0/929 | 0.24 | 0/1258 |
| 15 | A6 | 0.17 | 0/991 | 0.28 | 0/1335 |
| 16 | A7 | 0.16 | 0/798 | 0.25 | 0/1079 |
| 17 | A8 | 0.17 | 0/1436 | 0.26 | 0/1938 |
| 18 | A9 | 0.17 | 0/2777 | 0.31 | 2/3762 (0.1%) |
| 19 | AB | 0.10 | 0/633 | 0.22 | 0/851 |
| 19 | AC | 0.18 | 0/714 | 0.25 | 0/965 |
| 20 | AK | 0.16 | 0/2650 | 0.34 | 2/3588 (0.1%) |
| 21 | AL | 0.14 | 0/1042 | 0.23 | 0/1411 |
| 22 | AM | 0.15 | 0/1236 | 0.24 | 0/1683 |
| 23 | AN | 0.18 | 0/1204 | 0.27 | 0/1624 |
| 24 | B1 | 0.16 | 0/491 | 0.26 | 0/663 |
| 25 | B2 | 0.18 | 0/610 | 0.28 | 0/836 |
| 26 | B3 | 0.16 | 0/651 | 0.27 | 0/880 |
| 27 | B4 | 0.18 | 0/1092 | 0.26 | 0/1481 |
| 28 | B5 | 0.19 | 0/1184 | 0.27 | 0/1603 |
| 29 | B6 | 0.19 | 0/888 | 0.32 | 0/1208 |
| 30 | B7 | 0.17 | 0/1092 | 0.26 | 0/1459 |

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | #\|Z\| >5 | RMSZ | #\|Z\| >5 |
| 31 | B8 | 0.17 | 0/1371 | 0.25 | 0/1875 |
| 32 | B9 | 0.19 | 0/1590 | 0.30 | 0/2155 |
| 33 | BK | 0.18 | 0/1489 | 0.26 | 0/2008 |
| 34 | BL | 0.19 | 0/851 | 0.30 | 0/1155 |
| 35 | C1 | 0.21 | 0/4164 | 0.34 | 0/5689 |
| 36 | C2 | 0.18 | 0/1880 | 0.32 | 0/2564 |
| 37 | C3 | 0.19 | 0/2186 | 0.30 | 0/2991 |
| 38 | C4 | 0.16 | 0/1187 | 0.26 | 0/1606 |
| 39 | CA | 0.15 | 0/430 | 0.24 | 0/581 |
| 40 | CB | 0.19 | 0/1031 | 0.28 | 0/1394 |
| 41 | N1 | 0.20 | 0/2528 | 0.33 | 0/3455 |
| 42 | N2 | 0.22 | 0/2773 | 0.34 | 0/3768 |
| 43 | N3 | 0.18 | 0/804 | 0.27 | 0/1097 |
| 44 | N4 | 0.23 | 0/3723 | 0.34 | 0/5078 |
| 45 | N5 | 0.21 | 0/4914 | 0.35 | 0/6683 |
| 46 | N6 | 0.18 | 0/1266 | 0.32 | 0/1712 |
| 47 | QA | 0.18 | 0/3200 | 0.29 | 0/4333 |
| 47 | Qa | 0.17 | 0/3200 | 0.28 | 0/4333 |
| 48 | QB | 0.19 | 0/3531 | 0.30 | 0/4793 |
| 48 | Qb | 0.18 | 0/3436 | 0.28 | 0/4659 |
| 49 | QC | 0.20 | 0/3123 | 0.32 | 0/4269 |
| 49 | Qc | 0.21 | 0/3123 | 0.31 | 0/4269 |
| 50 | QD | 0.18 | 0/1979 | 0.27 | 0/2684 |
| 50 | Qd | 0.18 | 0/1962 | 0.28 | 0/2663 |
| 51 | QE | 0.13 | 0/1550 | 0.25 | 0/2098 |
| 51 | Qe | 0.13 | 0/1550 | 0.27 | 0/2098 |
| 52 | QF | 0.14 | 0/558 | 0.22 | 0/747 |
| 52 | Qf | 0.16 | 0/534 | 0.25 | 0/714 |
| 53 | QG | 0.17 | 0/913 | 0.27 | 0/1223 |
| 53 | Qg | 0.18 | 0/913 | 0.26 | 0/1223 |
| 54 | QH | 0.17 | 0/684 | 0.30 | 0/926 |
| 54 | Qh | 0.17 | 0/688 | 0.29 | 0/931 |
| 55 | QI | 0.15 | 0/520 | 0.19 | 0/701 |
| 55 | Qi | 0.18 | 0/506 | 0.24 | 0/683 |
| 56 | QJ | 0.13 | 0/420 | 0.21 | 0/576 |
| 57 | QK | 0.12 | 0/528 | 0.26 | 0/716 |
| 58 | Qj | 0.16 | 0/437 | 0.29 | 0/598 |
| 59 | S1 | 0.21 | 0/5378 | 0.32 | 0/7287 |
| 60 | S2 | 0.23 | 0/3465 | 0.31 | 0/4691 |
| 61 | S3 | 0.22 | 0/1780 | 0.29 | 0/2424 |
| 62 | S4 | 0.20 | 0/1030 | 0.29 | 0/1391 |
| 63 | S5 | 0.18 | 0/845 | 0.25 | 0/1129 |
| 64 | S6 | 0.17 | 0/755 | 0.27 | 0/1018 |

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | #\|Z\| >5 | RMSZ | #\|Z\| >5 |
| 65 | S7 | 0.22 | 0/1279 | 0.29 | 0/1730 |
| 66 | S8 | 0.22 | 0/1443 | 0.28 | 0/1952 |
| 67 | V1 | 0.20 | 0/3391 | 0.31 | 0/4583 |
| 68 | V2 | 0.17 | 0/1711 | 0.30 | 0/2328 |
| 69 | V3 | 0.15 | 0/365 | 0.29 | 0/493 |
| All | All | 0.19 | 0/115231 | 0.30 | 4/156309 (0.0%) |

There are no bond length outliers.

All (4) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 18 | A9 | 369 | VAL | CA-C-N | 7.40 | 135.01 | 120.94 |
| 18 | A9 | 369 | VAL | C-N-CA | 7.40 | 135.01 | 120.94 |
| 20 | AK | 204 | HIS | CA-C-N | -5.49 | 116.29 | 122.93 |
| 20 | AK | 204 | HIS | C-N-CA | -5.49 | 116.29 | 122.93 |

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts (i)

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 1 | 4L | 748 | 0 | 799 | 19 | 0 |
| 2 | 5A | 825 | 0 | 823 | 19 | 0 |
| 3 | 5B | 724 | 0 | 705 | 17 | 0 |
| 4 | 6A | 620 | 0 | 589 | 19 | 0 |
| 5 | 6B | 684 | 0 | 649 | 20 | 0 |
| 6 | 6C | 574 | 0 | 590 | 14 | 0 |
| 7 | 7A | 447 | 0 | 443 | 10 | 0 |
| 8 | 7B | 392 | 0 | 372 | 7 | 0 |
| 9 | 7C | 387 | 0 | 385 | 6 | 0 |
| 10 | 8B | 338 | 0 | 342 | 9 | 0 |
| 11 | A1 | 562 | 0 | 557 | 6 | 0 |
| 12 | A2 | 686 | 0 | 699 | 6 | 0 |
| 13 | A3 | 643 | 0 | 642 | 3 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 14 | A5 | 910 | 0 | 950 | 5 | 0 |
| 15 | A6 | 967 | 0 | 972 | 13 | 0 |
| 16 | A7 | 780 | 0 | 808 | 6 | 0 |
| 17 | A8 | 1398 | 0 | 1372 | 22 | 0 |
| 18 | A9 | 2703 | 0 | 2720 | 33 | 0 |
| 19 | AB | 624 | 0 | 625 | 10 | 0 |
| 19 | AC | 702 | 0 | 694 | 14 | 0 |
| 20 | AK | 2590 | 0 | 2551 | 43 | 0 |
| 21 | AL | 1021 | 0 | 1025 | 9 | 0 |
| 22 | AM | 1195 | 0 | 1149 | 12 | 0 |
| 23 | AN | 1173 | 0 | 1166 | 21 | 0 |
| 24 | B1 | 479 | 0 | 486 | 4 | 0 |
| 25 | B2 | 584 | 0 | 529 | 7 | 0 |
| 26 | B3 | 632 | 0 | 612 | 8 | 0 |
| 27 | B4 | 1062 | 0 | 1072 | 13 | 0 |
| 28 | B5 | 1151 | 0 | 1164 | 17 | 0 |
| 29 | B6 | 861 | 0 | 877 | 20 | 0 |
| 30 | B7 | 1068 | 0 | 1041 | 15 | 0 |
| 31 | B8 | 1315 | 0 | 1208 | 14 | 0 |
| 32 | B9 | 1534 | 0 | 1470 | 29 | 0 |
| 33 | BK | 1456 | 0 | 1424 | 15 | 0 |
| 34 | BL | 828 | 0 | 788 | 11 | 0 |
| 35 | C1 | 4024 | 0 | 4005 | 114 | 0 |
| 36 | C2 | 1833 | 0 | 1843 | 44 | 0 |
| 37 | C3 | 2103 | 0 | 2034 | 48 | 0 |
| 38 | C4 | 1153 | 0 | 1130 | 25 | 0 |
| 39 | CA | 417 | 0 | 422 | 6 | 0 |
| 40 | CB | 1000 | 0 | 994 | 19 | 0 |
| 41 | N1 | 2457 | 0 | 2554 | 52 | 0 |
| 42 | N2 | 2710 | 0 | 2874 | 59 | 0 |
| 43 | N3 | 786 | 0 | 836 | 14 | 0 |
| 44 | N4 | 3631 | 0 | 3839 | 74 | 0 |
| 45 | N5 | 4785 | 0 | 4933 | 96 | 0 |
| 46 | N6 | 1236 | 0 | 1241 | 30 | 0 |
| 47 | QA | 3147 | 0 | 3129 | 48 | 0 |
| 47 | Qa | 3147 | 0 | 3129 | 62 | 0 |
| 48 | QB | 3459 | 0 | 3350 | 46 | 0 |
| 48 | Qb | 3367 | 0 | 3262 | 52 | 0 |
| 49 | QC | 3025 | 0 | 3090 | 50 | 0 |
| 49 | Qc | 3025 | 0 | 3090 | 37 | 0 |
| 50 | QD | 1921 | 0 | 1867 | 24 | 0 |
| 50 | Qd | 1904 | 0 | 1849 | 28 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 51 | QE | 1517 | 0 | 1500 | 45 | 0 |
| 51 | Qe | 1517 | 0 | 1500 | 33 | 0 |
| 52 | QF | 552 | 0 | 536 | 7 | 0 |
| 52 | Qf | 528 | 0 | 510 | 11 | 0 |
| 53 | QG | 893 | 0 | 888 | 10 | 0 |
| 53 | Qg | 893 | 0 | 888 | 10 | 0 |
| 54 | QH | 662 | 0 | 660 | 13 | 0 |
| 54 | Qh | 666 | 0 | 663 | 14 | 0 |
| 55 | QI | 507 | 0 | 509 | 6 | 0 |
| 55 | Qi | 493 | 0 | 491 | 6 | 0 |
| 56 | QJ | 405 | 0 | 405 | 2 | 0 |
| 57 | QK | 520 | 0 | 554 | 10 | 0 |
| 58 | Qj | 421 | 0 | 418 | 5 | 0 |
| 59 | S1 | 5290 | 0 | 5321 | 105 | 0 |
| 60 | S2 | 3391 | 0 | 3328 | 67 | 0 |
| 61 | S3 | 1729 | 0 | 1687 | 18 | 0 |
| 62 | S4 | 1007 | 0 | 1008 | 15 | 0 |
| 63 | S5 | 825 | 0 | 834 | 13 | 0 |
| 64 | S6 | 741 | 0 | 701 | 13 | 0 |
| 65 | S7 | 1248 | 0 | 1254 | 17 | 0 |
| 66 | S8 | 1412 | 0 | 1363 | 25 | 0 |
| 67 | V1 | 3316 | 0 | 3272 | 68 | 0 |
| 68 | V2 | 1671 | 0 | 1673 | 17 | 0 |
| 69 | V3 | 355 | 0 | 329 | 10 | 0 |
| 70 | 5B | 1 | 0 | 0 | 0 | 0 |
| 70 | S6 | 1 | 0 | 0 | 0 | 0 |
| 71 | 6A | 45 | 0 | 64 | 16 | 0 |
| 71 | 7B | 54 | 0 | 88 | 4 | 0 |
| 71 | AL | 54 | 0 | 88 | 2 | 0 |
| 71 | C1 | 100 | 0 | 157 | 4 | 0 |
| 71 | C3 | 92 | 0 | 138 | 8 | 0 |
| 71 | N5 | 54 | 0 | 88 | 1 | 0 |
| 71 | N6 | 54 | 0 | 88 | 0 | 0 |
| 71 | QC | 108 | 0 | 176 | 6 | 0 |
| 71 | QH | 54 | 0 | 88 | 5 | 0 |
| 71 | Qb | 29 | 0 | 32 | 1 | 0 |
| 71 | Qj | 54 | 0 | 88 | 0 | 0 |
| 72 | 6A | 69 | 0 | 85 | 4 | 0 |
| 72 | A8 | 83 | 0 | 113 | 4 | 0 |
| 72 | AL | 257 | 0 | 361 | 7 | 0 |
| 72 | AM | 51 | 0 | 46 | 1 | 0 |
| 72 | B5 | 100 | 0 | 156 | 3 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 72 | CB | 100 | 0 | 156 | 11 | 0 |
| 72 | N2 | 68 | 0 | 80 | 2 | 0 |
| 72 | N5 | 189 | 0 | 284 | 15 | 0 |
| 72 | QB | 64 | 0 | 72 | 0 | 0 |
| 72 | QC | 149 | 0 | 192 | 10 | 0 |
| 72 | QH | 61 | 0 | 66 | 3 | 0 |
| 72 | Qb | 64 | 0 | 72 | 2 | 0 |
| 72 | Qd | 64 | 0 | 72 | 6 | 0 |
| 72 | Qh | 64 | 0 | 72 | 3 | 0 |
| 73 | A9 | 48 | 0 | 26 | 2 | 0 |
| 74 | AB | 36 | 0 | 47 | 1 | 0 |
| 74 | AC | 36 | 0 | 47 | 4 | 0 |
| 75 | AK | 27 | 0 | 12 | 4 | 0 |
| 76 | AL | 51 | 0 | 82 | 2 | 0 |
| 76 | C1 | 95 | 0 | 147 | 2 | 0 |
| 76 | CA | 51 | 0 | 82 | 2 | 0 |
| 76 | CB | 46 | 0 | 69 | 2 | 0 |
| 76 | N4 | 51 | 0 | 82 | 4 | 0 |
| 76 | QE | 44 | 0 | 65 | 3 | 0 |
| 76 | S7 | 51 | 0 | 82 | 4 | 0 |
| 77 | AL | 47 | 0 | 75 | 5 | 0 |
| 77 | AM | 104 | 0 | 176 | 9 | 0 |
| 77 | B5 | 52 | 0 | 88 | 5 | 0 |
| 77 | C2 | 43 | 0 | 67 | 1 | 0 |
| 77 | CB | 52 | 0 | 88 | 4 | 0 |
| 77 | N4 | 52 | 0 | 88 | 1 | 0 |
| 77 | QE | 46 | 0 | 73 | 6 | 0 |
| 77 | QI | 52 | 0 | 88 | 5 | 0 |
| 78 | B5 | 54 | 0 | 0 | 0 | 0 |
| 78 | QJ | 54 | 0 | 0 | 0 | 0 |
| 78 | Qc | 54 | 0 | 0 | 1 | 0 |
| 79 | C1 | 120 | 0 | 108 | 23 | 0 |
| 80 | C1 | 1 | 0 | 0 | 0 | 0 |
| 80 | C2 | 2 | 0 | 0 | 0 | 0 |
| 81 | C1 | 1 | 0 | 0 | 0 | 0 |
| 81 | S1 | 1 | 0 | 0 | 0 | 0 |
| 82 | C1 | 51 | 0 | 82 | 3 | 0 |
| 82 | N1 | 38 | 0 | 50 | 1 | 0 |
| 82 | N3 | 51 | 0 | 82 | 2 | 0 |
| 82 | N5 | 46 | 0 | 69 | 5 | 0 |
| 82 | QB | 78 | 0 | 110 | 2 | 0 |
| 82 | QC | 89 | 0 | 132 | 3 | 0 |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 82 | QE | 47 | 0 | 71 | 5 | 0 |
| 82 | Qc | 42 | 0 | 61 | 0 | 0 |
| 82 | Qd | 51 | 0 | 82 | 4 | 0 |
| 82 | Qh | 92 | 0 | 138 | 8 | 0 |
| 82 | S2 | 48 | 0 | 73 | 3 | 0 |
| 82 | S8 | 51 | 0 | 82 | 1 | 0 |
| 83 | QC | 86 | 0 | 60 | 10 | 0 |
| 83 | Qc | 86 | 0 | 60 | 7 | 0 |
| 84 | QD | 43 | 0 | 30 | 2 | 0 |
| 84 | Qd | 43 | 0 | 32 | 3 | 0 |
| 85 | QE | 4 | 0 | 0 | 2 | 0 |
| 85 | Qe | 4 | 0 | 0 | 1 | 0 |
| 85 | S1 | 4 | 0 | 0 | 0 | 0 |
| 85 | V2 | 4 | 0 | 0 | 0 | 0 |
| 86 | S1 | 16 | 0 | 0 | 0 | 0 |
| 86 | S7 | 8 | 0 | 0 | 1 | 0 |
| 86 | S8 | 16 | 0 | 0 | 2 | 0 |
| 86 | V1 | 8 | 0 | 0 | 1 | 0 |
| 87 | V1 | 31 | 0 | 19 | 1 | 0 |
| All | All | 116743 | 0 | 117808 | 1761 | 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 8.

All (1761) 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) |
|---|---|---|---|
| 33:BK:140:GLN:O | 33:BK:144:SER:HB2 | 1.72 | 0.89 |
| 71:7B:101:PC1:H2D1 | 71:7B:101:PC1:H3E1 | 1.57 | 0.84 |
| 36:C2:196:CYS:HB3 | 36:C2:207:MET:SD | 2.18 | 0.82 |
| 66:S8:205:ILE:O | 66:S8:209:TYR:HB3 | 1.80 | 0.81 |
| 36:C2:196:CYS:CB | 36:C2:207:MET:SD | 2.69 | 0.80 |
| 18:A9:198:ALA:O | 18:A9:260:GLY:HA2 | 1.81 | 0.80 |
| 29:B6:88:LEU:HD22 | 29:B6:92:GLU:HG2 | 1.67 | 0.77 |
| 44:N4:306:PRO:HA | 44:N4:458:LEU:HD23 | 1.67 | 0.76 |
| 47:Qa:155:GLN:HE22 | 47:Qa:200:VAL:HB | 1.50 | 0.75 |
| 67:V1:110:PRO:HB3 | 67:V1:152:ARG:HD3 | 1.69 | 0.75 |
| 59:S1:124:HIS:HD2 | 60:S2:381:MET:HE2 | 1.52 | 0.75 |
| 44:N4:371:PRO:HD2 | 72:N5:702:CDL:H391 | 1.67 | 0.74 |
| 74:AC:201:ZMP:H5 | 32:B9:109:ALA:HB1 | 1.68 | 0.73 |
| 45:N5:3:PRO:HB2 | 45:N5:53:MET:HE1 | 1.70 | 0.73 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:N1:62:ARG:HH11 | 41:N1:63:PRO:HD2 | 1.53 | 0.73 |
| 51:QE:177:ARG:HH12 | 51:QE:233:GLY:HA2 | 1.54 | 0.73 |
| 42:N2:108:LEU:HD11 | 42:N2:191:THR:HG21 | 1.70 | 0.73 |
| 59:S1:251:ILE:HG12 | 59:S1:606:THR:HG22 | 1.69 | 0.73 |
| 41:N1:65:THR:HG21 | 41:N1:71:PHE:HB2 | 1.69 | 0.72 |
| 49:QC:237:LEU:HB2 | 50:QD:297:MET:HE2 | 1.70 | 0.72 |
| 41:N1:100:LEU:HD23 | 41:N1:103:LEU:HD12 | 1.72 | 0.72 |
| 47:Qa:81:HIS:HD2 | 47:Qa:192:CYS:H | 1.36 | 0.72 |
| 72:CB:203:CDL:HA21 | 72:CB:203:CDL:HB61 | 1.71 | 0.72 |
| 4:6A:83:HIS:HA | 71:6A:101:PC1:H132 | 1.73 | 0.70 |
| 47:Qa:90:THR:HG23 | 47:Qa:95:SER:HA | 1.73 | 0.70 |
| 77:AM:203:PLX:H111 | 77:AM:203:PLX:H271 | 1.72 | 0.70 |
| 7:7A:77:PRO:HG3 | 9:7C:62:LYS:HG3 | 1.72 | 0.70 |
| 51:Qe:153:GLU:HG2 | 51:Qe:272:ILE:HG12 | 1.72 | 0.70 |
| 12:A2:24:CYS:N | 12:A2:58:CYS:SG | 2.65 | 0.70 |
| 51:Qe:190:VAL:HG21 | 51:Qe:250:ARG:HH22 | 1.55 | 0.70 |
| 48:QB:100:GLY:HA2 | 48:QB:106:GLY:H | 1.57 | 0.69 |
| 5:6B:35:LEU:HA | 5:6B:86:ILE:HD11 | 1.74 | 0.69 |
| 5:6B:38:HIS:HB2 | 5:6B:86:ILE:HD13 | 1.74 | 0.69 |
| 76:C1:601:3PE:H2F1 | 38:C4:109:PHE:HB3 | 1.73 | 0.69 |
| 49:QC:98:VAL:HG22 | 83:QC:403:HEM:HBC2 | 1.75 | 0.69 |
| 67:V1:235:VAL:HG12 | 67:V1:240:THR:HG21 | 1.75 | 0.69 |
| 59:S1:456:ALA:O | 59:S1:499:ASN:ND2 | 2.26 | 0.69 |
| 47:QA:116:ARG:NH1 | 47:QA:188:ASN:O | 2.25 | 0.68 |
| 10:8B:28:LYS:HG3 | 35:C1:483:SER:HB3 | 1.76 | 0.68 |
| 68:V2:38:LEU:O | 68:V2:124:ARG:NH2 | 2.25 | 0.68 |
| 72:6A:102:CDL:H231 | 72:6A:102:CDL:H122 | 1.76 | 0.68 |
| 60:S2:290:LEU:O | 60:S2:293:GLY:N | 2.26 | 0.68 |
| 45:N5:5:ALA:HB2 | 45:N5:61:MET:HE1 | 1.76 | 0.68 |
| 60:S2:162:GLU:OE2 | 60:S2:177:ARG:NH2 | 2.24 | 0.67 |
| 77:B5:201:PLX:H91 | 44:N4:40:SER:HB3 | 1.76 | 0.67 |
| 42:N2:88:LYS:HG3 | 42:N2:148:SER:HB3 | 1.77 | 0.67 |
| 49:QC:2:THR:O | 82:QC:401:PEE:N | 2.28 | 0.67 |
| 51:Qe:177:ARG:HH12 | 51:Qe:227:ASN:HD21 | 1.42 | 0.67 |
| 26:B3:27:THR:HG22 | 26:B3:29:LEU:H | 1.57 | 0.67 |
| 3:5B:105:VAL:HA | 3:5B:111:GLN:HG3 | 1.77 | 0.67 |
| 51:Qe:204:ARG:NH2 | 51:Qe:258:LEU:O | 2.27 | 0.67 |
| 54:QH:27:PHE:H | 71:QH:102:PC1:H143 | 1.60 | 0.67 |
| 60:S2:300:ARG:NH2 | 60:S2:407:GLU:OE2 | 2.28 | 0.67 |
| 41:N1:200:LEU:HD11 | 41:N1:285:LEU:HD21 | 1.77 | 0.66 |
| 67:V1:111:LYS:HB2 | 67:V1:151:ALA:HA | 1.76 | 0.66 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:5A:143:THR:HB | 2:5A:146:GLU:HG3 | 1.78 | 0.66 |
| 71:6A:101:PC1:H322 | 37:C3:202:GLY:HA3 | 1.76 | 0.66 |
| 67:V1:40:ARG:NH1 | 67:V1:289:GLU:O | 2.29 | 0.66 |
| 36:C2:132:GLU:HB3 | 36:C2:137:GLU:HG3 | 1.76 | 0.66 |
| 72:Qd:401:CDL:H721 | 72:Qd:401:CDL:H312 | 1.78 | 0.66 |
| 45:N5:530:PRO:O | 45:N5:534:HIS:HB2 | 1.96 | 0.66 |
| 49:Qc:300:ILE:HD11 | 49:Qc:363:LEU:HD21 | 1.78 | 0.66 |
| 47:Qa:123:VAL:HB | 47:Qa:133:LEU:HD23 | 1.78 | 0.66 |
| 59:S1:356:ASP:OD2 | 59:S1:636:TYR:OH | 2.14 | 0.66 |
| 68:V2:182:ASN:HB3 | 68:V2:194:GLU:HB3 | 1.76 | 0.66 |
| 27:B4:71:ALA:HB2 | 31:B8:38:PRO:HG2 | 1.78 | 0.66 |
| 20:AK:64:VAL:HA | 20:AK:205:VAL:O | 1.96 | 0.65 |
| 50:Qd:125:CYS:SG | 84:Qd:402:HEC:HAC | 2.36 | 0.65 |
| 67:V1:112:TYR:HB2 | 67:V1:240:THR:HG22 | 1.77 | 0.65 |
| 37:C3:151:LEU:HD13 | 37:C3:159:MET:HG2 | 1.77 | 0.65 |
| 53:Qg:53:GLU:OE2 | 54:Qh:12:ARG:NH1 | 2.29 | 0.65 |
| 59:S1:149:ASP:HB2 | 60:S2:367:ALA:HB3 | 1.77 | 0.65 |
| 47:Qa:313:VAL:HG21 | 47:Qa:323:VAL:HG11 | 1.78 | 0.65 |
| 3:5B:86:LYS:NZ | 38:C4:33:TYR:OH | 2.29 | 0.65 |
| 72:AL:204:CDL:H852 | 45:N5:558:LEU:HD21 | 1.77 | 0.65 |
| 40:CB:2:THR:HB | 40:CB:5:SER:HB3 | 1.78 | 0.65 |
| 35:C1:304:TYR:HB2 | 82:C1:609:PEE:H61 | 1.79 | 0.65 |
| 41:N1:180:PRO:HB3 | 82:S8:303:PEE:H21 | 1.78 | 0.65 |
| 29:B6:132:VAL:O | 29:B6:136:LEU:HB3 | 1.97 | 0.65 |
| 47:Qa:51:SER:HB3 | 47:Qa:230:LEU:HD12 | 1.78 | 0.65 |
| 6:6C:53:TYR:OH | 36:C2:188:ARG:NH1 | 2.29 | 0.64 |
| 35:C1:424:THR:HA | 35:C1:454:SER:HA | 1.80 | 0.64 |
| 54:QH:37:ASN:ND2 | 72:Qd:401:CDL:OB4 | 2.30 | 0.64 |
| 59:S1:405:THR:HB | 59:S1:477:GLY:HA3 | 1.79 | 0.64 |
| 16:A7:32:SER:OG | 16:A7:36:GLN:NE2 | 2.31 | 0.64 |
| 20:AK:182:ARG:NH1 | 20:AK:184:GLN:OE1 | 2.30 | 0.64 |
| 50:Qd:289:MET:HG2 | 82:Qd:403:PEE:H2 | 1.77 | 0.64 |
| 51:Qe:244:ASP:OD2 | 51:Qe:250:ARG:NH2 | 2.29 | 0.64 |
| 37:C3:221:ARG:HH22 | 71:C3:301:PC1:H111 | 1.62 | 0.64 |
| 59:S1:338:VAL:O | 59:S1:365:SER:HB2 | 1.97 | 0.64 |
| 59:S1:387:LEU:HD12 | 59:S1:514:ASN:HB3 | 1.80 | 0.64 |
| 60:S2:412:GLU:OE2 | 61:S3:140:ARG:NH2 | 2.30 | 0.64 |
| 22:AM:34:ARG:NH2 | 66:S8:89:GLU:OE2 | 2.31 | 0.64 |
| 51:Qe:234:TYR:HB2 | 51:Qe:243:TYR:HB2 | 1.78 | 0.64 |
| 8:7B:53:TRP:HE1 | 38:C4:111:ILE:HG22 | 1.63 | 0.64 |
| 59:S1:266:ARG:HD2 | 59:S1:267:THR:HG23 | 1.80 | 0.64 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 71:6A:101:PC1:H392 | 71:6A:101:PC1:H281 | 1.80 | 0.64 |
| 20:AK:64:VAL:HG13 | 20:AK:207:VAL:HB | 1.79 | 0.64 |
| 52:Qf:60:ARG:NH1 | 54:Qh:78:TYR:O | 2.31 | 0.64 |
| 35:C1:124:THR:HG21 | 35:C1:133:ALA:HB2 | 1.79 | 0.63 |
| 67:V1:281:HIS:ND1 | 67:V1:358:ASP:OD1 | 2.31 | 0.63 |
| 77:QE:301:PLX:H291 | 76:QE:303:3PE:H2I3 | 1.80 | 0.63 |
| 51:Qe:187:GLU:OE1 | 51:Qe:248:ARG:NH2 | 2.32 | 0.63 |
| 72:CB:203:CDL:H231 | 72:CB:203:CDL:H401 | 1.81 | 0.63 |
| 59:S1:484:SER:HB2 | 59:S1:680:LEU:HD11 | 1.80 | 0.63 |
| 47:QA:77:LEU:O | 47:QA:196:ARG:NH1 | 2.25 | 0.63 |
| 47:Qa:51:SER:HG | 47:Qa:227:HIS:HD1 | 1.47 | 0.63 |
| 59:S1:246:ARG:HH22 | 62:S4:123:ASN:HD21 | 1.47 | 0.63 |
| 59:S1:299:ARG:NH1 | 59:S1:703:ALA:O | 2.31 | 0.63 |
| 60:S2:308:LEU:HB2 | 60:S2:407:GLU:HB2 | 1.81 | 0.63 |
| 67:V1:280:GLY:O | 68:V2:143:ARG:NH1 | 2.32 | 0.63 |
| 48:QB:301:ASN:ND2 | 48:QB:347:CYS:SG | 2.68 | 0.63 |
| 51:QE:140:MET:O | 49:Qc:177:ARG:NH2 | 2.32 | 0.63 |
| 51:Qe:262:THR:HB | 51:Qe:274:GLY:O | 1.99 | 0.63 |
| 65:S7:51:ASP:OD1 | 65:S7:55:ASN:ND2 | 2.31 | 0.63 |
| 11:A1:46:ASN:ND2 | 46:N6:132:ASP:OD2 | 2.32 | 0.62 |
| 20:AK:62:ILE:O | 20:AK:160:VAL:HA | 1.98 | 0.62 |
| 35:C1:96:ARG:HD2 | 37:C3:57:TRP:HE1 | 1.63 | 0.62 |
| 40:CB:13:LEU:HD21 | 63:S5:4:PHE:HB3 | 1.81 | 0.62 |
| 47:QA:90:THR:HG23 | 47:QA:95:SER:HA | 1.81 | 0.62 |
| 49:QC:165:TRP:O | 49:QC:174:THR:OG1 | 2.17 | 0.62 |
| 49:QC:233:LEU:HG | 50:QD:297:MET:HE1 | 1.80 | 0.62 |
| 35:C1:169:ILE:O | 35:C1:172:LYS:NZ | 2.33 | 0.62 |
| 60:S2:155:GLN:NE2 | 60:S2:315:ASP:OD2 | 2.32 | 0.62 |
| 47:QA:70:ARG:HD2 | 47:QA:185:ALA:HB1 | 1.82 | 0.62 |
| 53:QG:72:ARG:NH1 | 53:QG:74:GLN:OE1 | 2.32 | 0.62 |
| 72:AL:204:CDL:HA32 | 72:AL:204:CDL:H521 | 1.81 | 0.62 |
| 42:N2:289:ASN:HA | 42:N2:292:PHE:CE2 | 2.34 | 0.62 |
| 17:A8:219:TYR:OH | 28:B5:189:ASN:ND2 | 2.32 | 0.62 |
| 38:C4:155:GLY:H | 38:C4:158:ALA:HB3 | 1.64 | 0.62 |
| 31:B8:110:ASP:HB3 | 44:N4:278:ARG:HH11 | 1.65 | 0.62 |
| 33:BK:60:ARG:NH1 | 33:BK:62:TYR:OH | 2.32 | 0.62 |
| 42:N2:252:GLY:HA3 | 42:N2:290:LEU:HD13 | 1.81 | 0.62 |
| 45:N5:387:THR:HG22 | 45:N5:465:GLY:H | 1.65 | 0.62 |
| 60:S2:222:ARG:NH1 | 60:S2:249:ASP:OD2 | 2.28 | 0.62 |
| 18:A9:50:SER:OG | 61:S3:225:GLU:OE2 | 2.17 | 0.62 |
| 1:4L:23:ARG:HH21 | 46:N6:86:ASN:HD22 | 1.48 | 0.62 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 25:B2:87:PRO:HD2 | 30:B7:99:MET:HE1 | 1.82 | 0.62 |
| 72:CB:203:CDL:H421 | 72:CB:203:CDL:H822 | 1.82 | 0.62 |
| 41:N1:24:GLU:OE2 | 41:N1:274:ARG:NH1 | 2.33 | 0.62 |
| 48:Qb:87:ASN:HD22 | 48:Qb:204:PRO:HD3 | 1.64 | 0.62 |
| 59:S1:308:ARG:NH1 | 59:S1:312:GLY:O | 2.33 | 0.62 |
| 34:BL:89:VAL:HG21 | 44:N4:25:ILE:HG23 | 1.81 | 0.61 |
| 62:S4:62:THR:HG23 | 62:S4:72:ILE:HD13 | 1.80 | 0.61 |
| 15:A6:66:TYR:O | 15:A6:86:ARG:NH1 | 2.32 | 0.61 |
| 41:N1:231:ILE:O | 41:N1:235:ASN:ND2 | 2.34 | 0.61 |
| 43:N3:31:SER:O | 43:N3:33:LYS:NZ | 2.33 | 0.61 |
| 27:B4:15:PRO:HG2 | 27:B4:18:LEU:HB2 | 1.82 | 0.61 |
| 67:V1:128:ARG:NH2 | 68:V2:194:GLU:OE2 | 2.32 | 0.61 |
| 49:QC:81:TYR:OH | 50:QD:203:ARG:NH1 | 2.34 | 0.61 |
| 59:S1:433:GLY:O | 59:S1:444:HIS:NE2 | 2.31 | 0.61 |
| 48:QB:280:ASP:HA | 48:QB:461:PRO:HB3 | 1.83 | 0.61 |
| 64:S6:104:LYS:HE3 | 64:S6:107:LYS:HD3 | 1.81 | 0.61 |
| 68:V2:108:PRO:HB2 | 68:V2:111:ARG:HG2 | 1.82 | 0.61 |
| 20:AK:94:HIS:HA | 20:AK:97:ASP:HB2 | 1.81 | 0.61 |
| 59:S1:224:ASP:OD2 | 59:S1:291:ARG:NH2 | 2.33 | 0.61 |
| 48:Qb:388:VAL:HG21 | 48:Qb:438:ALA:HA | 1.83 | 0.61 |
| 59:S1:433:GLY:HA2 | 59:S1:447:ASP:HA | 1.82 | 0.61 |
| 60:S2:214:GLU:OE2 | 60:S2:227:ARG:NH2 | 2.33 | 0.61 |
| 2:5A:98:CYS:SG | 2:5A:106:SER:OG | 2.52 | 0.61 |
| 45:N5:100:ILE:HG21 | 45:N5:246:LEU:HB2 | 1.83 | 0.61 |
| 47:QA:92:LYS:HD2 | 47:QA:143:ALA:HB1 | 1.83 | 0.61 |
| 67:V1:140:GLU:OE2 | 67:V1:256:ARG:NH1 | 2.32 | 0.61 |
| 3:5B:41:GLU:HG2 | 3:5B:56:ARG:HH22 | 1.66 | 0.61 |
| 71:QC:407:PC1:H3E2 | 77:QI:301:PLX:H381 | 1.81 | 0.61 |
| 68:V2:68:LYS:NZ | 69:V3:407:SER:OG | 2.31 | 0.61 |
| 71:6A:101:PC1:H112 | 37:C3:187:THR:HA | 1.82 | 0.60 |
| 19:AB:116:VAL:HG12 | 19:AB:120:MET:HE2 | 1.83 | 0.60 |
| 59:S1:426:ASP:OD2 | 69:V3:418:ARG:NH2 | 2.34 | 0.60 |
| 66:S8:144:ARG:NH1 | 66:S8:146:ASP:OD2 | 2.31 | 0.60 |
| 18:A9:129:LEU:HD23 | 18:A9:167:ILE:HG13 | 1.82 | 0.60 |
| 40:CB:13:LEU:HD11 | 63:S5:6:VAL:HG12 | 1.83 | 0.60 |
| 51:QE:227:ASN:N | 51:QE:233:GLY:O | 2.32 | 0.60 |
| 67:V1:113:LEU:HD13 | 67:V1:149:MET:HE1 | 1.84 | 0.60 |
| 22:AM:106:ARG:HB2 | 22:AM:109:ILE:HG13 | 1.82 | 0.60 |
| 37:C3:156:ARG:NH1 | 37:C3:222:GLN:O | 2.33 | 0.60 |
| 53:QG:19:LYS:NZ | 53:QG:85:GLU:OE2 | 2.33 | 0.60 |
| 47:Qa:66:LYS:HB2 | 47:Qa:217:ARG:HB3 | 1.83 | 0.60 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 76:S7:302:3PE:H391 | 76:S7:302:3PE:H3E1 | 1.83 | 0.60 |
| 9:7C:62:LYS:NZ | 35:C1:117:MET:O | 2.35 | 0.60 |
| 72:CB:203:CDL:H401 | 72:CB:203:CDL:H262 | 1.83 | 0.60 |
| 51:QE:196:ARG:NH1 | 51:QE:254:ALA:O | 2.35 | 0.60 |
| 48:Qb:195:THR:HG21 | 48:Qb:269:ARG:H | 1.67 | 0.60 |
| 71:C1:606:PC1:H11 | 71:C1:606:PC1:H132 | 1.83 | 0.60 |
| 60:S2:145:LEU:HD13 | 60:S2:430:ILE:HG21 | 1.84 | 0.60 |
| 11:A1:66:LEU:HB3 | 17:A8:152:LYS:HE2 | 1.84 | 0.60 |
| 49:QC:47:THR:HG22 | 49:QC:79:ILE:HG23 | 1.83 | 0.60 |
| 62:S4:171:ARG:NH1 | 67:V1:217:GLU:OE1 | 2.27 | 0.60 |
| 21:AL:17:GLU:HG3 | 21:AL:20:ARG:HH21 | 1.66 | 0.60 |
| 59:S1:282:ASN:ND2 | 59:S1:285:TRP:O | 2.35 | 0.60 |
| 17:A8:174:PHE:HB3 | 17:A8:178:ARG:HH12 | 1.66 | 0.60 |
| 57:QK:1:MET:O | 57:QK:7:ARG:NH1 | 2.35 | 0.60 |
| 48:Qb:104:ARG:NH2 | 48:Qb:145:GLU:OE2 | 2.34 | 0.60 |
| 60:S2:63:GLU:HA | 60:S2:66:HIS:CD2 | 2.36 | 0.60 |
| 48:QB:156:LEU:O | 48:QB:213:ARG:NH1 | 2.34 | 0.59 |
| 51:QE:110:ARG:NH1 | 54:Qh:22:PHE:O | 2.34 | 0.59 |
| 36:C2:173:ASP:O | 36:C2:180:ASN:ND2 | 2.34 | 0.59 |
| 49:QC:229:ILE:HG23 | 77:QE:301:PLX:H151 | 1.83 | 0.59 |
| 35:C1:178:GLN:H | 71:C1:607:PC1:H142 | 1.68 | 0.59 |
| 48:QB:467:ASP:OD2 | 49:QC:223:TYR:OH | 2.20 | 0.59 |
| 52:Qf:38:GLU:OE1 | 52:Qf:47:ARG:NH2 | 2.34 | 0.59 |
| 52:Qf:53:CYS:SG | 52:Qf:56:ARG:NH2 | 2.74 | 0.59 |
| 60:S2:188:ASN:OD1 | 60:S2:410:LYS:NZ | 2.36 | 0.59 |
| 60:S2:374:ARG:NH2 | 66:S8:165:ASP:OD1 | 2.36 | 0.59 |
| 2:5A:130:GLN:HG3 | 6:6C:6:LEU:HD23 | 1.84 | 0.59 |
| 18:A9:279:TYR:HB2 | 18:A9:372:ALA:HB2 | 1.84 | 0.59 |
| 20:AK:241:ASN:HB3 | 20:AK:245:LYS:HE2 | 1.84 | 0.59 |
| 44:N4:122:PHE:HZ | 44:N4:206:LYS:HG3 | 1.67 | 0.59 |
| 33:BK:99:ASP:OD2 | 33:BK:142:ARG:NH1 | 2.34 | 0.59 |
| 35:C1:62:ALA:HB2 | 79:C1:602:HEA:HBD1 | 1.84 | 0.59 |
| 2:5A:68:ASP:HA | 2:5A:101:LEU:HD21 | 1.83 | 0.59 |
| 48:QB:181:ASP:OD1 | 48:QB:181:ASP:N | 2.36 | 0.59 |
| 59:S1:666:GLN:NE2 | 59:S1:670:GLU:OE2 | 2.35 | 0.59 |
| 77:AM:201:PLX:H72 | 77:AM:203:PLX:H91 | 1.85 | 0.58 |
| 31:B8:83:GLN:HA | 31:B8:86:ARG:HG3 | 1.84 | 0.58 |
| 35:C1:349:THR:HG21 | 36:C2:38:VAL:HG11 | 1.85 | 0.58 |
| 46:N6:103:MET:HA | 46:N6:106:TYR:CZ | 2.37 | 0.58 |
| 18:A9:204:SER:HB2 | 18:A9:266:VAL:HG12 | 1.84 | 0.58 |
| 20:AK:72:LYS:NZ | 75:AK:401:ADP:O1A | 2.36 | 0.58 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 23:AN:51:MET:HE2 | 41:N1:311:THR:HB | 1.84 | 0.58 |
| 35:C1:438:ARG:NH1 | 79:C1:603:HEA:O1D | 2.35 | 0.58 |
| 49:QC:100:ARG:NH2 | 83:QC:403:HEM:O1A | 2.36 | 0.58 |
| 67:V1:118:ASP:HB3 | 67:V1:207:GLY:HA2 | 1.85 | 0.58 |
| 2:5A:143:THR:HG22 | 2:5A:145:GLU:H | 1.69 | 0.58 |
| 13:A3:151:VAL:O | 17:A8:207:LYS:NZ | 2.30 | 0.58 |
| 47:QA:148:ARG:NH2 | 53:QG:50:ARG:O | 2.35 | 0.58 |
| 48:QB:204:PRO:HG2 | 48:QB:207:ASN:HB2 | 1.84 | 0.58 |
| 14:A5:20:PRO:HB3 | 14:A5:77:ILE:HG21 | 1.86 | 0.58 |
| 28:B5:92:PHE:O | 33:BK:59:ASN:ND2 | 2.36 | 0.58 |
| 35:C1:51:ASP:OD1 | 35:C1:55:ASN:ND2 | 2.37 | 0.58 |
| 36:C2:110:TYR:HB2 | 36:C2:116:LEU:HD12 | 1.86 | 0.58 |
| 36:C2:111:THR:O | 36:C2:111:THR:OG1 | 2.21 | 0.58 |
| 45:N5:295:GLN:O | 45:N5:425:ARG:NH1 | 2.36 | 0.58 |
| 55:QI:48:ASN:HD21 | 50:Qd:104:SER:HA | 1.69 | 0.58 |
| 44:N4:392:THR:O | 44:N4:396:MET:HG2 | 2.03 | 0.58 |
| 47:QA:116:ARG:HH12 | 47:QA:189:SER:HA | 1.67 | 0.58 |
| 20:AK:67:ASN:OD1 | 20:AK:68:ILE:N | 2.26 | 0.58 |
| 43:N3:68:GLU:HG3 | 43:N3:98:LEU:HD13 | 1.84 | 0.58 |
| 44:N4:369:LEU:HD21 | 45:N5:149:ILE:HD13 | 1.85 | 0.58 |
| 50:QD:292:LYS:NZ | 55:Qi:37:ASP:OD1 | 2.30 | 0.58 |
| 54:QH:26:ALA:H | 71:QH:102:PC1:H132 | 1.68 | 0.58 |
| 49:Qc:200:LEU:HD23 | 49:Qc:201:HIS:HD2 | 1.68 | 0.58 |
| 17:A8:196:ARG:NH2 | 23:AN:63:GLU:OE2 | 2.36 | 0.58 |
| 51:QE:125:VAL:HG21 | 77:QE:301:PLX:H111 | 1.85 | 0.58 |
| 48:Qb:42:LEU:HD22 | 48:Qb:426:LEU:HB3 | 1.85 | 0.58 |
| 8:7B:53:TRP:CE2 | 38:C4:115:ALA:HB2 | 2.39 | 0.58 |
| 35:C1:38:ARG:NH2 | 35:C1:451:ASN:O | 2.36 | 0.58 |
| 67:V1:113:LEU:O | 67:V1:154:ALA:HA | 2.02 | 0.58 |
| 2:5A:104:PHE:N | 38:C4:66:GLU:OE2 | 2.33 | 0.58 |
| 9:7C:59:GLN:NE2 | 35:C1:116:SER:O | 2.36 | 0.58 |
| 20:AK:255:CYS:SG | 20:AK:256:GLU:N | 2.71 | 0.58 |
| 49:Qc:237:LEU:HD13 | 50:Qd:297:MET:HG2 | 1.85 | 0.58 |
| 49:QC:138:MET:HE1 | 49:QC:268:ILE:HA | 1.86 | 0.58 |
| 49:Qc:213:SER:OG | 49:Qc:217:LYS:NZ | 2.37 | 0.58 |
| 53:Qg:36:ASP:OD2 | 53:Qg:62:ARG:NH1 | 2.37 | 0.58 |
| 59:S1:251:ILE:HG21 | 59:S1:604:GLN:HB3 | 1.85 | 0.58 |
| 59:S1:593:SER:HA | 59:S1:606:THR:O | 2.04 | 0.58 |
| 20:AK:134:GLN:HE22 | 75:AK:401:ADP:HN62 | 1.52 | 0.57 |
| 42:N2:26:TRP:HB3 | 42:N2:74:ILE:HD13 | 1.86 | 0.57 |
| 47:QA:70:ARG:NH2 | 47:QA:332:ASP:OD2 | 2.35 | 0.57 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 51:QE:205:VAL:HG11 | 51:QE:211:VAL:HG22 | 1.85 | 0.57 |
| 20:AK:92:GLY:H | 20:AK:95:TYR:HB3 | 1.68 | 0.57 |
| 35:C1:347:LEU:HD13 | 35:C1:383:MET:HB3 | 1.85 | 0.57 |
| 44:N4:445:LEU:HB3 | 72:N5:702:CDL:H452 | 1.85 | 0.57 |
| 5:6B:33:ASN:HB2 | 5:6B:61:TYR:CE2 | 2.40 | 0.57 |
| 35:C1:101:SER:O | 35:C1:156:SER:OG | 2.20 | 0.57 |
| 36:C2:161:HIS:CE1 | 36:C2:207:MET:HE1 | 2.39 | 0.57 |
| 51:QE:172:LYS:NZ | 49:Qc:168:PHE:O | 2.37 | 0.57 |
| 52:Qf:40:ILE:HG13 | 52:Qf:43:CYS:H | 1.69 | 0.57 |
| 59:S1:419:ARG:NH1 | 59:S1:439:THR:O | 2.37 | 0.57 |
| 2:5A:55:ASP:HA | 2:5A:90:ILE:HD11 | 1.87 | 0.57 |
| 20:AK:317:PRO:HB3 | 34:BL:54:ARG:HA | 1.85 | 0.57 |
| 25:B2:54:GLN:NE2 | 45:N5:367:PRO:HD2 | 2.19 | 0.57 |
| 47:QA:151:VAL:O | 47:QA:155:GLN:HG2 | 2.04 | 0.57 |
| 5:6B:7:THR:O | 5:6B:11:ASN:ND2 | 2.38 | 0.57 |
| 17:A8:84:LEU:O | 23:AN:88:ARG:NH1 | 2.38 | 0.57 |
| 41:N1:173:TRP:HB3 | 41:N1:175:ILE:HG22 | 1.86 | 0.57 |
| 60:S2:146:ASP:OD2 | 60:S2:149:SER:OG | 2.22 | 0.57 |
| 5:6B:39:ARG:NH2 | 5:6B:85:LYS:O | 2.36 | 0.57 |
| 72:CB:203:CDL:H722 | 72:CB:203:CDL:H321 | 1.85 | 0.57 |
| 42:N2:95:MET:HE2 | 42:N2:149:ILE:HA | 1.87 | 0.57 |
| 42:N2:170:LEU:HD11 | 42:N2:288:LEU:HD22 | 1.86 | 0.57 |
| 67:V1:288:VAL:HG21 | 67:V1:303:HIS:CD2 | 2.40 | 0.57 |
| 2:5A:114:VAL:HG11 | 2:5A:128:VAL:HG11 | 1.86 | 0.57 |
| 41:N1:24:GLU:HA | 41:N1:271:LEU:HD13 | 1.86 | 0.57 |
| 42:N2:42:PRO:HG2 | 46:N6:167:VAL:HG22 | 1.86 | 0.57 |
| 48:QB:126:ARG:NH1 | 48:QB:199:GLN:O | 2.38 | 0.57 |
| 36:C2:102:HIS:CD2 | 36:C2:157:GLU:HG3 | 2.40 | 0.57 |
| 72:CB:203:CDL:HA62 | 42:N2:239:VAL:HG22 | 1.87 | 0.57 |
| 50:QD:112:ARG:NH2 | 50:QD:145:GLU:OE1 | 2.37 | 0.57 |
| 48:Qb:274:GLU:OE2 | 48:Qb:276:ARG:NE | 2.29 | 0.57 |
| 49:Qc:126:THR:HG21 | 83:Qc:402:HEM:HBB2 | 1.85 | 0.57 |
| 22:AM:76:ASP:OD1 | 65:S7:185:LYS:NZ | 2.37 | 0.57 |
| 42:N2:131:LEU:O | 42:N2:135:LYS:HG2 | 2.05 | 0.57 |
| 50:QD:127:SER:HB3 | 50:QD:179:PRO:HD2 | 1.87 | 0.57 |
| 50:Qd:232:LEU:HD13 | 50:Qd:242:ALA:HB1 | 1.87 | 0.57 |
| 59:S1:219:SER:OG | 59:S1:288:ASP:OD2 | 2.22 | 0.57 |
| 60:S2:469:ARG:NH2 | 61:S3:169:GLU:OE2 | 2.38 | 0.57 |
| 47:Qa:301:ARG:NH2 | 48:Qb:94:GLU:OE2 | 2.38 | 0.57 |
| 51:QE:234:TYR:HB2 | 51:QE:243:TYR:HB2 | 1.87 | 0.56 |
| 52:Qf:33:VAL:HG12 | 52:Qf:82:VAL:HG22 | 1.87 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 18:A9:61:ALA:HB3 | 18:A9:82:VAL:HG13 | 1.87 | 0.56 |
| 18:A9:211:ASP:O | 18:A9:215:ASN:ND2 | 2.36 | 0.56 |
| 72:AL:201:CDL:H122 | 76:AL:202:3PE:H242 | 1.87 | 0.56 |
| 42:N2:323:MET:N | 42:N2:323:MET:SD | 2.77 | 0.56 |
| 6:6C:63:GLU:OE1 | 6:6C:66:ARG:NH2 | 2.37 | 0.56 |
| 29:B6:85:ASP:O | 32:B9:163:LYS:NZ | 2.37 | 0.56 |
| 35:C1:107:PRO:HB3 | 37:C3:25:LEU:HB2 | 1.87 | 0.56 |
| 47:QA:69:SER:HB3 | 47:QA:188:ASN:HB2 | 1.88 | 0.56 |
| 47:Qa:151:VAL:O | 47:Qa:155:GLN:HG2 | 2.05 | 0.56 |
| 60:S2:275:ARG:O | 60:S2:279:VAL:HB | 2.05 | 0.56 |
| 1:4L:6:MET:HE3 | 46:N6:103:MET:HE3 | 1.87 | 0.56 |
| 3:5B:84:THR:OG1 | 3:5B:85:ASN:N | 2.38 | 0.56 |
| 71:6A:101:PC1:H152 | 37:C3:187:THR:HA | 1.86 | 0.56 |
| 35:C1:352:GLY:C | 79:C1:603:HEA:H162 | 2.30 | 0.56 |
| 35:C1:406:ASN:HB3 | 35:C1:409:TRP:HB2 | 1.87 | 0.56 |
| 44:N4:403:THR:HA | 44:N4:406:TYR:CE2 | 2.41 | 0.56 |
| 49:QC:71:ARG:NH2 | 50:QD:278:ALA:O | 2.33 | 0.56 |
| 61:S3:132:LEU:HB2 | 61:S3:141:ILE:HG22 | 1.86 | 0.56 |
| 17:A8:198:ASP:N | 17:A8:201:GLU:OE1 | 2.38 | 0.56 |
| 17:A8:243:ARG:NH2 | 40:CB:89:ASP:OD1 | 2.31 | 0.56 |
| 33:BK:142:ARG:NH1 | 33:BK:143:TYR:OH | 2.39 | 0.56 |
| 5:6B:65:CYS:O | 36:C2:98:LYS:NZ | 2.37 | 0.56 |
| 35:C1:347:LEU:HD13 | 35:C1:383:MET:HE2 | 1.88 | 0.56 |
| 35:C1:443:TYR:O | 36:C2:134:ARG:NH2 | 2.38 | 0.56 |
| 52:QF:60:ARG:HD3 | 52:QF:63:THR:HG21 | 1.87 | 0.56 |
| 54:Qh:57:TYR:HD1 | 82:Qh:101:PEE:H11 | 1.71 | 0.56 |
| 59:S1:279:GLU:OE2 | 62:S4:156:LYS:NZ | 2.38 | 0.56 |
| 1:4L:73:LEU:HD21 | 42:N2:41:ILE:HG13 | 1.88 | 0.56 |
| 36:C2:200:CYS:SG | 36:C2:207:MET:CE | 2.93 | 0.56 |
| 76:CA:101:3PE:H3E1 | 42:N2:325:LEU:HD11 | 1.88 | 0.56 |
| 45:N5:97:THR:HG21 | 45:N5:125:LEU:HD22 | 1.87 | 0.56 |
| 48:QB:388:VAL:HG21 | 48:QB:438:ALA:HA | 1.88 | 0.56 |
| 20:AK:94:HIS:HB3 | 20:AK:105:PRO:HB3 | 1.86 | 0.56 |
| 47:Qa:379:LYS:HG2 | 47:Qa:413:LEU:HD22 | 1.87 | 0.56 |
| 3:5B:109:GLU:OE1 | 3:5B:110:THR:N | 2.38 | 0.56 |
| 6:6C:47:LYS:NZ | 6:6C:51:ASP:OD2 | 2.38 | 0.56 |
| 77:AM:201:PLX:H291 | 77:AM:201:PLX:H102 | 1.88 | 0.56 |
| 35:C1:374:VAL:HA | 35:C1:377:PHE:CE2 | 2.40 | 0.56 |
| 44:N4:70:THR:HA | 44:N4:103:GLN:HE21 | 1.70 | 0.56 |
| 51:Qe:153:GLU:HB3 | 51:Qe:270:LEU:HD11 | 1.88 | 0.56 |
| 72:Qh:102:CDL:H311 | 72:Qh:102:CDL:H721 | 1.88 | 0.56 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 24:B1:50:ARG:NH2 | 28:B5:106:VAL:O | 2.39 | 0.56 |
| 41:N1:149:ILE:HG21 | 41:N1:185:TRP:HB2 | 1.88 | 0.56 |
| 42:N2:36:ASN:OD1 | 42:N2:134:GLN:NE2 | 2.37 | 0.56 |
| 50:Qd:211:TYR:OH | 84:Qd:402:HEC:O1A | 2.20 | 0.56 |
| 59:S1:43:VAL:HG12 | 59:S1:55:LYS:HD2 | 1.88 | 0.56 |
| 59:S1:244:GLU:OE1 | 59:S1:266:ARG:NH1 | 2.37 | 0.56 |
| 5:6B:30:CYS:HA | 5:6B:61:TYR:CE1 | 2.41 | 0.55 |
| 35:C1:184:PHE:H | 35:C1:256:HIS:HE1 | 1.53 | 0.55 |
| 51:QE:209:GLU:HG3 | 51:QE:210:TRP:CD1 | 2.41 | 0.55 |
| 67:V1:88:ARG:O | 67:V1:244:ASN:ND2 | 2.39 | 0.55 |
| 1:4L:98:CYS:HB3 | 45:N5:580:GLN:HB2 | 1.87 | 0.55 |
| 35:C1:135:ASN:ND2 | 35:C1:213:ARG:O | 2.40 | 0.55 |
| 50:QD:159:PRO:HB2 | 50:Qd:184:GLU:HG3 | 1.88 | 0.55 |
| 19:AB:115:GLN:NE2 | 19:AB:135:ALA:O | 2.37 | 0.55 |
| 19:AC:156:GLU:OE1 | 28:B5:52:LYS:NZ | 2.39 | 0.55 |
| 45:N5:11:THR:HG22 | 45:N5:46:LEU:HB3 | 1.89 | 0.55 |
| 45:N5:23:ASN:HD22 | 72:N5:702:CDL:HB4 | 1.70 | 0.55 |
| 49:QC:43:LEU:O | 49:QC:47:THR:OG1 | 2.25 | 0.55 |
| 72:QH:101:CDL:H711 | 72:Qd:401:CDL:H152 | 1.88 | 0.55 |
| 14:A5:44:TYR:O | 14:A5:48:THR:HG22 | 2.06 | 0.55 |
| 22:AM:88:ARG:HD3 | 66:S8:200:GLU:HG3 | 1.88 | 0.55 |
| 35:C1:265:LYS:HD2 | 35:C1:490:THR:HG21 | 1.87 | 0.55 |
| 45:N5:375:ILE:HD12 | 45:N5:458:LEU:HD11 | 1.89 | 0.55 |
| 5:6B:62:LYS:O | 36:C2:111:THR:OG1 | 2.23 | 0.55 |
| 18:A9:173:ASP:HB3 | 18:A9:176:SER:HB2 | 1.88 | 0.55 |
| 77:CB:201:PLX:H1B3 | 63:S5:2:PRO:HD2 | 1.89 | 0.55 |
| 45:N5:249:SER:HA | 45:N5:306:THR:HG21 | 1.87 | 0.55 |
| 49:Qc:106:SER:OG | 83:Qc:403:HEM:O1D | 2.19 | 0.55 |
| 50:Qd:216:LEU:HB3 | 50:Qd:249:ILE:HD11 | 1.87 | 0.55 |
| 68:V2:187:GLN:HE21 | 68:V2:190:ASP:HA | 1.70 | 0.55 |
| 18:A9:188:GLU:HG3 | 18:A9:200:ILE:HD13 | 1.87 | 0.55 |
| 19:AC:119:ILE:HG21 | 19:AC:135:ALA:HB1 | 1.89 | 0.55 |
| 59:S1:144:MET:HG3 | 60:S2:389:LYS:HG3 | 1.89 | 0.55 |
| 46:N6:34:ILE:HD13 | 46:N6:61:LEU:HD22 | 1.89 | 0.55 |
| 47:QA:180:ALA:HB2 | 47:QA:258:ILE:HG13 | 1.87 | 0.55 |
| 34:BL:77:ASP:OD1 | 34:BL:78:LYS:N | 2.39 | 0.55 |
| 49:QC:126:THR:HG21 | 83:QC:402:HEM:HBB2 | 1.89 | 0.55 |
| 48:Qb:165:ARG:NH1 | 48:Qb:208:VAL:O | 2.39 | 0.55 |
| 72:Qh:102:CDL:H362 | 72:Qh:102:CDL:H762 | 1.88 | 0.55 |
| 59:S1:667:GLN:OE1 | 59:S1:667:GLN:N | 2.38 | 0.55 |
| 39:CA:72:ARG:NH2 | 40:CB:18:ASN:OD1 | 2.40 | 0.55 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 44:N4:1:MET:HE2 | 44:N4:111:THR:HG21 | 1.89 | 0.55 |
| 47:QA:313:VAL:HG11 | 47:QA:350:VAL:HG13 | 1.89 | 0.55 |
| 51:QE:199:GLN:NE2 | 51:QE:257:ASN:OD1 | 2.40 | 0.55 |
| 52:QF:38:GLU:OE1 | 52:QF:47:ARG:NH2 | 2.40 | 0.55 |
| 59:S1:476:LEU:HD21 | 59:S1:481:LEU:HD21 | 1.88 | 0.55 |
| 36:C2:98:LYS:HG2 | 36:C2:153:LEU:HB2 | 1.89 | 0.54 |
| 44:N4:282:LEU:HD13 | 44:N4:342:MET:HG3 | 1.88 | 0.54 |
| 2:5A:73:ARG:HA | 38:C4:46:LEU:HD12 | 1.90 | 0.54 |
| 45:N5:103:PHE:HB2 | 45:N5:341:MET:HE3 | 1.89 | 0.54 |
| 82:N5:701:PEE:H33 | 72:N5:702:CDL:H231 | 1.89 | 0.54 |
| 49:QC:25:SER:OG | 49:QC:216:ASP:OD2 | 2.24 | 0.54 |
| 49:QC:197:LEU:HD11 | 83:QC:403:HEM:HMA3 | 1.88 | 0.54 |
| 51:Qe:244:ASP:HB3 | 51:Qe:250:ARG:HE | 1.71 | 0.54 |
| 1:4L:37:MET:HE3 | 1:4L:67:ALA:HB2 | 1.87 | 0.54 |
| 6:6C:49:TYR:CE1 | 38:C4:153:ILE:HD13 | 2.43 | 0.54 |
| 18:A9:238:GLN:OE1 | 18:A9:270:ARG:NH1 | 2.41 | 0.54 |
| 35:C1:184:PHE:H | 35:C1:256:HIS:CE1 | 2.25 | 0.54 |
| 49:QC:100:ARG:NH1 | 83:QC:403:HEM:HBD1 | 2.21 | 0.54 |
| 47:Qa:84:ARG:NH1 | 47:Qa:114:SER:OG | 2.40 | 0.54 |
| 28:B5:152:LYS:HD3 | 40:CB:96:VAL:HG21 | 1.88 | 0.54 |
| 35:C1:74:MET:HE3 | 35:C1:389:ILE:HG13 | 1.88 | 0.54 |
| 35:C1:316:THR:HG22 | 79:C1:603:HEA:H18 | 1.89 | 0.54 |
| 45:N5:253:VAL:HG23 | 45:N5:310:LEU:HD21 | 1.89 | 0.54 |
| 72:QH:101:CDL:H722 | 72:Qd:401:CDL:H172 | 1.89 | 0.54 |
| 51:Qe:204:ARG:NE | 51:Qe:246:SER:O | 2.35 | 0.54 |
| 22:AM:55:PHE:CZ | 22:AM:58:ARG:HG3 | 2.42 | 0.54 |
| 35:C1:37:ILE:HD11 | 35:C1:58:VAL:HA | 1.89 | 0.54 |
| 44:N4:211:GLY:H | 44:N4:213:HIS:CD2 | 2.25 | 0.54 |
| 47:QA:178:HIS:NE2 | 47:QA:330:TYR:OH | 2.34 | 0.54 |
| 47:QA:207:TYR:O | 47:QA:211:ASN:ND2 | 2.30 | 0.54 |
| 48:Qb:276:ARG:NH2 | 48:Qb:466:PRO:O | 2.41 | 0.54 |
| 8:7B:71:ARG:HG3 | 8:7B:72:VAL:HG23 | 1.89 | 0.54 |
| 47:Qa:177:LEU:HD11 | 47:Qa:272:VAL:HG22 | 1.89 | 0.54 |
| 47:Qa:319:GLN:HE21 | 47:Qa:320:PRO:HD2 | 1.72 | 0.54 |
| 5:6B:33:ASN:HB2 | 5:6B:61:TYR:OH | 2.07 | 0.54 |
| 6:6C:60:LYS:NZ | 6:6C:64:GLU:OE2 | 2.34 | 0.54 |
| 27:B4:14:LEU:HD12 | 27:B4:15:PRO:HD2 | 1.90 | 0.54 |
| 44:N4:122:PHE:CZ | 44:N4:206:LYS:HG3 | 2.43 | 0.54 |
| 44:N4:391:ILE:HG23 | 44:N4:394:ILE:HD12 | 1.88 | 0.54 |
| 52:QF:71:LEU:HD22 | 50:Qd:223:PRO:HG3 | 1.89 | 0.54 |
| 47:Qa:214:THR:HG22 | 47:Qa:241:ARG:HB3 | 1.90 | 0.54 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 48:Qb:370:PHE:HE1 | 72:Qb:501:CDL:HA21 | 1.73 | 0.54 |
| 5:6B:9:ILE:HG12 | 5:6B:56:TRP:HB2 | 1.90 | 0.54 |
| 25:B2:44:TYR:HB2 | 26:B3:14:MET:HE1 | 1.90 | 0.54 |
| 44:N4:373:ILE:HD11 | 44:N4:444:LEU:HD23 | 1.90 | 0.54 |
| 47:Qa:81:HIS:CD2 | 47:Qa:192:CYS:H | 2.20 | 0.54 |
| 51:Qe:95:GLU:N | 51:Qe:95:GLU:OE1 | 2.39 | 0.54 |
| 53:Qg:36:ASP:OD1 | 53:Qg:90:TYR:OH | 2.16 | 0.54 |
| 59:S1:388:ASN:ND2 | 59:S1:513:MET:O | 2.32 | 0.54 |
| 6:6C:49:TYR:HE1 | 38:C4:153:ILE:HD13 | 1.71 | 0.54 |
| 47:Qa:65:ILE:HG12 | 47:Qa:218:MET:HG2 | 1.89 | 0.54 |
| 44:N4:361:VAL:HG22 | 72:N5:702:CDL:H311 | 1.90 | 0.54 |
| 61:S3:155:SER:OG | 61:S3:167:GLU:OE1 | 2.26 | 0.54 |
| 6:6C:38:LYS:HE2 | 36:C2:29:MET:HE1 | 1.88 | 0.53 |
| 35:C1:233:HIS:CD2 | 35:C1:292:MET:HE1 | 2.44 | 0.53 |
| 37:C3:112:LEU:HD13 | 37:C3:118:PRO:HG3 | 1.90 | 0.53 |
| 40:CB:37:GLY:HA3 | 76:CB:202:3PE:H271 | 1.90 | 0.53 |
| 41:N1:25:ARG:NH1 | 65:S7:87:ASP:OD1 | 2.41 | 0.53 |
| 45:N5:274:GLN:NE2 | 45:N5:320:ASN:OD1 | 2.41 | 0.53 |
| 49:QC:92:ILE:HD11 | 72:QC:406:CDL:H742 | 1.90 | 0.53 |
| 59:S1:394:VAL:HA | 59:S1:473:MET:HE1 | 1.90 | 0.53 |
| 64:S6:74:GLN:HG3 | 66:S8:108:SER:HB2 | 1.90 | 0.53 |
| 19:AC:94:ASP:HB3 | 19:AC:97:LYS:HG2 | 1.90 | 0.53 |
| 23:AN:98:MET:HE3 | 23:AN:101:VAL:HG21 | 1.89 | 0.53 |
| 35:C1:447:TYR:O | 35:C1:451:ASN:ND2 | 2.42 | 0.53 |
| 45:N5:362:LEU:HA | 45:N5:365:ALA:HB3 | 1.89 | 0.53 |
| 48:QB:195:THR:HG21 | 48:QB:268:CYS:HB3 | 1.89 | 0.53 |
| 77:QI:301:PLX:H192 | 49:Qc:232:ALA:HB1 | 1.89 | 0.53 |
| 37:C3:2:THR:OG1 | 37:C3:3:HIS:N | 2.37 | 0.53 |
| 48:QB:165:ARG:HD3 | 48:QB:209:ARG:HA | 1.90 | 0.53 |
| 63:S5:15:ASP:N | 63:S5:15:ASP:OD1 | 2.39 | 0.53 |
| 69:V3:399:PHE:HD2 | 69:V3:400:LEU:HD12 | 1.74 | 0.53 |
| 20:AK:141:ARG:NH2 | 75:AK:401:ADP:N7 | 2.55 | 0.53 |
| 35:C1:352:GLY:HA3 | 79:C1:603:HEA:H14 | 1.91 | 0.53 |
| 44:N4:446:LEU:HB3 | 77:N4:501:PLX:H272 | 1.90 | 0.53 |
| 50:QD:187:ARG:HB3 | 50:QD:192:GLY:HA2 | 1.90 | 0.53 |
| 59:S1:274:LEU:HD21 | 62:S4:87:MET:HE2 | 1.88 | 0.53 |
| 3:5B:45:THR:OG1 | 3:5B:46:GLY:N | 2.40 | 0.53 |
| 30:B7:29:TYR:OH | 30:B7:111:ARG:NH2 | 2.42 | 0.53 |
| 72:QC:406:CDL:H792 | 82:Qh:101:PEE:H23 | 1.91 | 0.53 |
| 49:Qc:137:GLN:NE2 | 49:Qc:263:ASN:O | 2.42 | 0.53 |
| 16:A7:34:ARG:NH2 | 66:S8:93:LEU:O | 2.42 | 0.53 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 24:B1:47:ARG:NH2 | 24:B1:53:GLU:OE2 | 2.42 | 0.53 |
| 28:B5:163:ARG:NH1 | 40:CB:102:ASP:OD2 | 2.26 | 0.53 |
| 42:N2:128:LEU:HD12 | 42:N2:216:PHE:HB3 | 1.91 | 0.53 |
| 51:QE:196:ARG:NH2 | 51:QE:252:GLY:O | 2.36 | 0.53 |
| 21:AL:43:LEU:HD12 | 72:AL:201:CDL:H522 | 1.90 | 0.53 |
| 30:B7:44:GLN:NE2 | 30:B7:48:ASP:OD1 | 2.42 | 0.53 |
| 43:N3:73:LEU:HD13 | 46:N6:55:MET:HE1 | 1.90 | 0.53 |
| 45:N5:76:LEU:HD21 | 45:N5:196:TRP:HE3 | 1.74 | 0.53 |
| 65:S7:62:LEU:O | 65:S7:91:VAL:HA | 2.09 | 0.53 |
| 22:AM:42:ASP:OD2 | 22:AM:46:ASN:ND2 | 2.40 | 0.53 |
| 35:C1:173:PRO:HD2 | 35:C1:176:MET:HE2 | 1.90 | 0.53 |
| 37:C3:187:THR:N | 37:C3:190:ASP:OD2 | 2.34 | 0.53 |
| 48:QB:460:GLY:HA2 | 48:QB:462:ILE:HG12 | 1.91 | 0.53 |
| 74:AC:201:ZMP:H19 | 32:B9:58:VAL:HG11 | 1.91 | 0.53 |
| 35:C1:65:MET:HB3 | 79:C1:602:HEA:CAC | 2.39 | 0.53 |
| 41:N1:99:ASN:N | 82:N1:401:PEE:O2P | 2.32 | 0.53 |
| 44:N4:408:LEU:HD12 | 45:N5:172:ILE:HG21 | 1.90 | 0.53 |
| 50:Qd:118:TYR:HA | 50:Qd:122:CYS:SG | 2.48 | 0.53 |
| 54:Qh:37:ASN:ND2 | 72:Qh:102:CDL:OB4 | 2.37 | 0.53 |
| 68:V2:59:ASN:ND2 | 68:V2:89:GLN:OE1 | 2.41 | 0.53 |
| 18:A9:171:ASN:ND2 | 18:A9:327:MET:H | 2.07 | 0.53 |
| 41:N1:37:PRO:HA | 65:S7:88:ARG:HA | 1.91 | 0.53 |
| 46:N6:112:GLU:HB3 | 46:N6:119:PHE:HD2 | 1.74 | 0.53 |
| 48:QB:195:THR:HG22 | 48:QB:197:LEU:H | 1.73 | 0.53 |
| 49:Qc:311:LYS:NZ | 49:Qc:379:TRP:OXT | 2.41 | 0.53 |
| 59:S1:512:VAL:O | 59:S1:514:ASN:ND2 | 2.41 | 0.53 |
| 61:S3:187:ILE:HG23 | 61:S3:188:LEU:HG | 1.90 | 0.53 |
| 4:6A:88:ASN:ND2 | 71:6A:101:PC1:H151 | 2.24 | 0.52 |
| 17:A8:202:LEU:HD13 | 23:AN:70:ALA:HB2 | 1.90 | 0.52 |
| 48:QB:121:ASN:ND2 | 48:QB:132:TYR:OH | 2.42 | 0.52 |
| 48:Qb:278:ARG:NH2 | 48:Qb:463:GLU:OE1 | 2.43 | 0.52 |
| 48:QB:54:ASP:OD1 | 48:QB:54:ASP:N | 2.41 | 0.52 |
| 72:QC:408:CDL:H512 | 72:QC:408:CDL:HA61 | 1.90 | 0.52 |
| 50:Qd:243:ILE:HG12 | 50:Qd:245:MET:H | 1.74 | 0.52 |
| 35:C1:229:ILE:HD11 | 36:C2:175:ILE:HG12 | 1.91 | 0.52 |
| 46:N6:33:LEU:HG | 46:N6:65:LEU:HD11 | 1.90 | 0.52 |
| 59:S1:591:GLU:HG2 | 59:S1:610:VAL:HG23 | 1.90 | 0.52 |
| 60:S2:101:LEU:HD13 | 60:S2:464:PHE:HZ | 1.74 | 0.52 |
| 29:B6:147:LYS:HE3 | 29:B6:148:TYR:CZ | 2.44 | 0.52 |
| 32:B9:218:GLU:HG2 | 32:B9:219:ARG:HG2 | 1.91 | 0.52 |
| 35:C1:352:GLY:HA3 | 79:C1:603:HEA:H162 | 1.90 | 0.52 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 45:N5:421:ALA:O | 45:N5:424:THR:OG1 | 2.26 | 0.52 |
| 48:QB:87:ASN:HD21 | 48:QB:199:GLN:HB3 | 1.74 | 0.52 |
| 72:QC:406:CDL:H141 | 72:QC:406:CDL:H182 | 1.91 | 0.52 |
| 47:Qa:92:LYS:HD3 | 47:Qa:143:ALA:HB1 | 1.92 | 0.52 |
| 53:Qg:46:GLU:OE2 | 53:Qg:49:ARG:NH1 | 2.43 | 0.52 |
| 59:S1:452:LEU:HD21 | 59:S1:493:VAL:HG13 | 1.92 | 0.52 |
| 60:S2:464:PHE:HA | 60:S2:467:VAL:HB | 1.91 | 0.52 |
| 1:4L:56:ALA:HA | 63:S5:18:MET:HE3 | 1.92 | 0.52 |
| 18:A9:357:ARG:NH1 | 18:A9:365:GLU:OE1 | 2.40 | 0.52 |
| 19:AC:112:SER:HB3 | 32:B9:59:LEU:HD11 | 1.92 | 0.52 |
| 35:C1:334:TRP:HZ3 | 71:C1:606:PC1:H332 | 1.74 | 0.52 |
| 44:N4:232:ALA:O | 44:N4:237:LYS:NZ | 2.43 | 0.52 |
| 45:N5:419:THR:HA | 45:N5:422:TYR:CE2 | 2.45 | 0.52 |
| 45:N5:536:LEU:HB3 | 45:N5:537:PRO:HD3 | 1.92 | 0.52 |
| 59:S1:488:ALA:HB2 | 59:S1:677:GLN:HG3 | 1.90 | 0.52 |
| 3:5B:87:ARG:NH2 | 35:C1:508:PRO:O | 2.43 | 0.52 |
| 6:6C:69:GLY:HA3 | 8:7B:79:GLU:HG3 | 1.92 | 0.52 |
| 35:C1:3:VAL:HG13 | 35:C1:7:LEU:HD12 | 1.91 | 0.52 |
| 37:C3:204:HIS:O | 37:C3:208:VAL:HG13 | 2.10 | 0.52 |
| 72:CB:203:CDL:H661 | 44:N4:13:PRO:HG3 | 1.90 | 0.52 |
| 42:N2:337:LEU:O | 42:N2:340:THR:OG1 | 2.27 | 0.52 |
| 49:QC:51:LEU:HD13 | 83:QC:402:HEM:HBD1 | 1.92 | 0.52 |
| 52:QF:34:ARG:O | 52:QF:38:GLU:HG2 | 2.09 | 0.52 |
| 49:Qc:8:HIS:HB3 | 49:Qc:11:MET:HB2 | 1.91 | 0.52 |
| 19:AC:134:ASP:OD2 | 32:B9:44:ALA:N | 2.42 | 0.52 |
| 36:C2:91:ASN:OD1 | 36:C2:92:ASN:N | 2.39 | 0.52 |
| 51:QE:154:ILE:HB | 51:QE:271:VAL:HG23 | 1.92 | 0.52 |
| 51:QE:184:ILE:HD11 | 51:QE:209:GLU:HA | 1.92 | 0.52 |
| 64:S6:36:GLU:OE2 | 64:S6:60:LYS:NZ | 2.34 | 0.52 |
| 67:V1:43:THR:HG21 | 67:V1:59:ARG:HG2 | 1.92 | 0.52 |
| 19:AC:128:PHE:HE2 | 19:AC:151:LYS:HD3 | 1.75 | 0.52 |
| 33:BK:107:GLN:HE22 | 45:N5:194:ASN:ND2 | 2.08 | 0.52 |
| 35:C1:316:THR:HB | 79:C1:603:HEA:H262 | 1.91 | 0.52 |
| 47:QA:298:HIS:HB2 | 48:QB:114:GLU:HG2 | 1.91 | 0.52 |
| 59:S1:356:ASP:O | 59:S1:360:ARG:HG2 | 2.10 | 0.52 |
| 61:S3:89:HIS:CG | 61:S3:90:PRO:HD2 | 2.44 | 0.52 |
| 37:C3:204:HIS:CE1 | 37:C3:249:TRP:HB2 | 2.45 | 0.51 |
| 47:QA:326:PHE:HA | 57:QK:61:GLY:HA2 | 1.91 | 0.51 |
| 50:Qd:122:CYS:SG | 84:Qd:402:HEC:HAB | 2.50 | 0.51 |
| 51:Qe:190:VAL:HG21 | 51:Qe:250:ARG:NH2 | 2.25 | 0.51 |
| 51:Qe:241:SER:OG | 85:Qe:301:FES:S2 | 2.63 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 60:S2:300:ARG:NH1 | 60:S2:342:GLU:OE2 | 2.43 | 0.51 |
| 4:6A:69:THR:N | 35:C1:216:ASN:OD1 | 2.42 | 0.51 |
| 4:6A:82:PHE:O | 71:6A:101:PC1:H143 | 2.11 | 0.51 |
| 20:AK:210:ASP:OD1 | 20:AK:244:LYS:NZ | 2.29 | 0.51 |
| 72:AM:202:CDL:H521 | 72:AM:202:CDL:HA61 | 1.93 | 0.51 |
| 36:C2:162:SER:HB3 | 36:C2:197:SER:H | 1.76 | 0.51 |
| 38:C4:39:VAL:HG22 | 38:C4:41:ARG:HG3 | 1.91 | 0.51 |
| 44:N4:211:GLY:H | 44:N4:213:HIS:HD2 | 1.58 | 0.51 |
| 72:QC:406:CDL:H522 | 82:Qh:101:PEE:H15 | 1.92 | 0.51 |
| 71:QC:407:PC1:H133 | 71:QC:407:PC1:H32 | 1.93 | 0.51 |
| 54:QH:25:ARG:HD2 | 71:QH:102:PC1:H141 | 1.91 | 0.51 |
| 33:BK:107:GLN:HE22 | 45:N5:194:ASN:HD22 | 1.57 | 0.51 |
| 49:QC:141:TRP:CD1 | 49:QC:265:PRO:HD3 | 2.46 | 0.51 |
| 67:V1:380:GLY:O | 67:V1:386:ARG:NH1 | 2.40 | 0.51 |
| 34:BL:95:PHE:O | 34:BL:99:LEU:HB2 | 2.10 | 0.51 |
| 44:N4:383:THR:HG21 | 45:N5:190:LEU:HD22 | 1.92 | 0.51 |
| 59:S1:197:THR:HG22 | 59:S1:206:VAL:HG22 | 1.93 | 0.51 |
| 6:6C:73:SER:HB2 | 36:C2:222:TRP:HB2 | 1.92 | 0.51 |
| 12:A2:18:GLU:HG2 | 12:A2:68:ARG:HB3 | 1.93 | 0.51 |
| 22:AM:12:GLN:O | 22:AM:16:GLY:N | 2.44 | 0.51 |
| 47:QA:60:ARG:NH1 | 47:QA:124:GLU:OE1 | 2.43 | 0.51 |
| 49:QC:112:THR:HG22 | 49:QC:196:HIS:CE1 | 2.46 | 0.51 |
| 52:Qf:38:GLU:OE2 | 52:Qf:78:ARG:NH1 | 2.43 | 0.51 |
| 59:S1:306:MET:HB2 | 59:S1:583:ILE:HB | 1.92 | 0.51 |
| 67:V1:162:PHE:HB3 | 67:V1:165:GLU:HB2 | 1.92 | 0.51 |
| 10:8B:55:GLY:O | 10:8B:59:SER:N | 2.44 | 0.51 |
| 32:B9:137:GLU:OE2 | 32:B9:140:LYS:NZ | 2.43 | 0.51 |
| 44:N4:216:LEU:HB3 | 44:N4:217:PRO:HD3 | 1.93 | 0.51 |
| 45:N5:248:HIS:O | 45:N5:253:VAL:HG22 | 2.10 | 0.51 |
| 46:N6:122:LEU:HD23 | 46:N6:126:VAL:HG11 | 1.91 | 0.51 |
| 17:A8:121:MET:HE2 | 23:AN:73:PRO:HA | 1.92 | 0.51 |
| 30:B7:107:ARG:HA | 30:B7:110:GLN:HG2 | 1.93 | 0.51 |
| 36:C2:129:LYS:N | 36:C2:132:GLU:OE1 | 2.43 | 0.51 |
| 51:QE:156:LEU:HD11 | 51:QE:271:VAL:HG13 | 1.92 | 0.51 |
| 59:S1:185:PHE:CZ | 59:S1:221:ASN:HB2 | 2.45 | 0.51 |
| 67:V1:112:TYR:O | 67:V1:240:THR:HA | 2.11 | 0.51 |
| 33:BK:115:GLN:HG2 | 45:N5:62:ILE:HG12 | 1.92 | 0.51 |
| 42:N2:342:ALA:O | 42:N2:345:SER:OG | 2.23 | 0.51 |
| 49:QC:344:GLU:HG3 | 54:Qh:67:PHE:HE1 | 1.76 | 0.51 |
| 47:Qa:162:LYS:NZ | 47:Qa:194:ASP:OD1 | 2.31 | 0.51 |
| 67:V1:217:GLU:OE2 | 67:V1:224:ARG:NH2 | 2.44 | 0.51 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 24:B1:29:ARG:NH2 | 77:B5:201:PLX:O3 | 2.44 | 0.51 |
| 37:C3:163:LEU:HD21 | 37:C3:235:PHE:HE1 | 1.76 | 0.51 |
| 44:N4:233:ALA:HA | 44:N4:320:GLY:HA2 | 1.92 | 0.51 |
| 48:QB:80:ARG:NH2 | 48:QB:350:GLU:OE1 | 2.44 | 0.51 |
| 67:V1:270:ASN:OD1 | 67:V1:270:ASN:N | 2.43 | 0.51 |
| 3:5B:98:SER:OG | 35:C1:266:GLU:OE1 | 2.23 | 0.51 |
| 4:6A:63:HIS:HB2 | 5:6B:76:ARG:HH21 | 1.76 | 0.51 |
| 28:B5:74:TYR:O | 34:BL:96:SER:OG | 2.26 | 0.51 |
| 72:B5:202:CDL:H822 | 72:N5:702:CDL:H473 | 1.91 | 0.51 |
| 39:CA:43:LYS:O | 39:CA:47:THR:OG1 | 2.29 | 0.51 |
| 47:QA:66:LYS:HB2 | 47:QA:217:ARG:HB3 | 1.92 | 0.51 |
| 47:QA:123:VAL:HB | 47:QA:133:LEU:HD23 | 1.93 | 0.51 |
| 48:Qb:396:ARG:NE | 48:Qb:430:GLU:OE2 | 2.44 | 0.51 |
| 67:V1:94:PRO:HB2 | 67:V1:97:LEU:HB2 | 1.93 | 0.51 |
| 47:QA:138:LEU:O | 47:QA:142:ALA:HB3 | 2.11 | 0.50 |
| 54:Qh:37:ASN:OD1 | 54:Qh:40:ARG:NH2 | 2.34 | 0.50 |
| 59:S1:389:THR:HG21 | 59:S1:473:MET:HE2 | 1.94 | 0.50 |
| 77:AM:203:PLX:H391 | 76:S7:302:3PE:H2E2 | 1.93 | 0.50 |
| 34:BL:151:GLU:OE1 | 34:BL:151:GLU:N | 2.44 | 0.50 |
| 35:C1:236:TRP:HH2 | 79:C1:603:HEA:HBD1 | 1.76 | 0.50 |
| 35:C1:406:ASN:HD22 | 35:C1:409:TRP:H | 1.60 | 0.50 |
| 47:QA:399:GLN:HA | 47:QA:402:VAL:HG22 | 1.93 | 0.50 |
| 67:V1:204:TYR:HB3 | 67:V1:377:GLU:HB3 | 1.93 | 0.50 |
| 23:AN:16:TYR:OH | 60:S2:248:ASP:OD1 | 2.25 | 0.50 |
| 23:AN:93:GLU:HG3 | 63:S5:98:HIS:CD2 | 2.46 | 0.50 |
| 42:N2:100:MET:HE1 | 45:N5:595:ILE:HG23 | 1.93 | 0.50 |
| 42:N2:112:HIS:O | 42:N2:116:PRO:HD2 | 2.11 | 0.50 |
| 47:Qa:63:LEU:HD23 | 47:Qa:141:THR:HG21 | 1.93 | 0.50 |
| 48:Qb:393:ASN:OD1 | 48:Qb:396:ARG:NH1 | 2.44 | 0.50 |
| 50:Qd:147:LYS:NZ | 50:Qd:151:GLU:OE2 | 2.30 | 0.50 |
| 59:S1:251:ILE:HD11 | 59:S1:596:TYR:HB2 | 1.92 | 0.50 |
| 59:S1:306:MET:HE2 | 59:S1:314:LEU:HB3 | 1.93 | 0.50 |
| 60:S2:194:THR:HB | 60:S2:206:PHE:HA | 1.92 | 0.50 |
| 5:6B:33:ASN:C | 5:6B:61:TYR:HE2 | 2.19 | 0.50 |
| 14:A5:93:LYS:HG2 | 14:A5:96:ARG:HH22 | 1.75 | 0.50 |
| 31:B8:48:ARG:NH2 | 31:B8:62:TYR:O | 2.44 | 0.50 |
| 79:C1:603:HEA:HBA2 | 79:C1:603:HEA:HMA | 1.92 | 0.50 |
| 44:N4:445:LEU:HD22 | 72:N5:702:CDL:H401 | 1.92 | 0.50 |
| 45:N5:327:LEU:O | 45:N5:331:MET:HG2 | 2.12 | 0.50 |
| 20:AK:206:VAL:HG13 | 20:AK:257:VAL:HG13 | 1.94 | 0.50 |
| 35:C1:27:GLY:HA3 | 79:C1:602:HEA:H273 | 1.94 | 0.50 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 35:C1:244:TYR:HA | 35:C1:247:ILE:HG22 | 1.94 | 0.50 |
| 49:QC:137:GLN:NE2 | 49:QC:263:ASN:O | 2.44 | 0.50 |
| 51:QE:151:LYS:HB3 | 51:QE:272:ILE:HD11 | 1.94 | 0.50 |
| 48:Qb:102:LYS:HG2 | 48:Qb:153:ASN:HB3 | 1.93 | 0.50 |
| 60:S2:107:LEU:HD21 | 60:S2:450:LEU:HD11 | 1.94 | 0.50 |
| 60:S2:133:LYS:HE2 | 66:S8:124:PRO:O | 2.12 | 0.50 |
| 60:S2:321:GLU:O | 60:S2:352:GLN:NE2 | 2.44 | 0.50 |
| 67:V1:311:TRP:NE1 | 67:V1:333:GLU:OE1 | 2.37 | 0.50 |
| 72:AL:204:CDL:H111 | 54:Qh:39:LEU:HD13 | 1.94 | 0.50 |
| 29:B6:165:PHE:O | 29:B6:168:ASP:HB2 | 2.12 | 0.50 |
| 36:C2:200:CYS:SG | 36:C2:207:MET:HE1 | 2.51 | 0.50 |
| 38:C4:90:PHE:HA | 38:C4:93:MET:HG2 | 1.93 | 0.50 |
| 44:N4:133:ILE:HD11 | 44:N4:231:LEU:HD11 | 1.94 | 0.50 |
| 44:N4:412:ILE:HG12 | 44:N4:416:ARG:HD2 | 1.93 | 0.50 |
| 45:N5:559:GLU:O | 45:N5:564:LYS:HB2 | 2.12 | 0.50 |
| 76:QE:303:3PE:H232 | 76:QE:303:3PE:H272 | 1.94 | 0.50 |
| 1:4L:68:ALA:HB2 | 46:N6:64:MET:HE2 | 1.93 | 0.50 |
| 21:AL:4:THR:HG22 | 21:AL:8:LYS:HE3 | 1.93 | 0.50 |
| 44:N4:82:SER:HB2 | 44:N4:432:ARG:CZ | 2.42 | 0.50 |
| 45:N5:15:LEU:HD11 | 45:N5:94:LEU:HD21 | 1.94 | 0.50 |
| 45:N5:566:THR:O | 45:N5:570:GLN:HG2 | 2.12 | 0.50 |
| 55:QI:51:LYS:NZ | 50:Qd:98:SER:O | 2.45 | 0.50 |
| 59:S1:307:ILE:HG23 | 59:S1:317:THR:HG21 | 1.94 | 0.50 |
| 59:S1:455:ILE:O | 59:S1:463:SER:OG | 2.27 | 0.50 |
| 1:4L:73:LEU:HD22 | 42:N2:38:LEU:HD12 | 1.93 | 0.50 |
| 5:6B:12:TYR:CE2 | 5:6B:59:ARG:HB3 | 2.46 | 0.50 |
| 71:AL:206:PC1:H262 | 71:AL:206:PC1:H321 | 1.93 | 0.50 |
| 35:C1:251:PHE:HB3 | 35:C1:319:LYS:HE2 | 1.94 | 0.50 |
| 36:C2:160:LEU:O | 36:C2:161:HIS:ND1 | 2.45 | 0.50 |
| 44:N4:76:MET:SD | 44:N4:230:VAL:HB | 2.52 | 0.50 |
| 71:QH:102:PC1:H2B1 | 71:QH:102:PC1:H382 | 1.94 | 0.50 |
| 47:Qa:164:VAL:HG21 | 48:Qb:317:THR:HG21 | 1.93 | 0.50 |
| 51:Qe:183:GLU:O | 51:Qe:187:GLU:HG2 | 2.12 | 0.50 |
| 59:S1:49:VAL:HG13 | 59:S1:102:ILE:HD13 | 1.93 | 0.50 |
| 35:C1:300:ASP:OD1 | 35:C1:301:THR:N | 2.45 | 0.50 |
| 36:C2:28:LEU:HA | 36:C2:31:VAL:HG22 | 1.94 | 0.50 |
| 46:N6:17:PHE:HA | 46:N6:20:PHE:CD2 | 2.47 | 0.50 |
| 47:Qa:91:THR:HG21 | 47:Qa:140:VAL:HA | 1.94 | 0.50 |
| 60:S2:135:TYR:HE1 | 60:S2:417:LEU:HD21 | 1.77 | 0.50 |
| 3:5B:97:ASN:O | 35:C1:180:GLN:NE2 | 2.35 | 0.49 |
| 37:C3:66:THR:HB | 71:C3:301:PC1:H142 | 1.94 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 39:CA:68:GLU:HG2 | 40:CB:21:ARG:HB3 | 1.93 | 0.49 |
| 41:N1:195:ARG:HH12 | 41:N1:274:ARG:HD2 | 1.77 | 0.49 |
| 18:A9:126:VAL:HG23 | 18:A9:161:VAL:HG11 | 1.94 | 0.49 |
| 35:C1:183:LEU:HD13 | 35:C1:273:MET:HG2 | 1.94 | 0.49 |
| 51:QE:123:VAL:HG13 | 55:Qi:29:ALA:HA | 1.94 | 0.49 |
| 57:QK:31:GLN:HE22 | 48:Qb:342:GLN:HB3 | 1.77 | 0.49 |
| 29:B6:141:ILE:HG23 | 82:N5:701:PEE:H60 | 1.94 | 0.49 |
| 37:C3:253:TYR:HA | 37:C3:257:TYR:HD1 | 1.76 | 0.49 |
| 41:N1:110:SER:HB3 | 46:N6:62:GLY:HA3 | 1.94 | 0.49 |
| 41:N1:145:THR:OG1 | 41:N1:289:LEU:HD11 | 2.12 | 0.49 |
| 42:N2:132:THR:HG21 | 72:N2:401:CDL:H372 | 1.94 | 0.49 |
| 60:S2:296:GLY:HA2 | 60:S2:300:ARG:HH21 | 1.78 | 0.49 |
| 17:A8:228:ASN:OD1 | 63:S5:51:ARG:NH1 | 2.44 | 0.49 |
| 72:AL:204:CDL:H522 | 27:B4:84:PRO:HG3 | 1.94 | 0.49 |
| 35:C1:466:MET:O | 35:C1:469:ILE:HG22 | 2.13 | 0.49 |
| 45:N5:383:MET:O | 45:N5:389:PHE:HB2 | 2.12 | 0.49 |
| 48:QB:192:PHE:O | 48:QB:198:ALA:HB2 | 2.12 | 0.49 |
| 48:QB:275:ILE:HG22 | 54:Qh:17:TYR:CD1 | 2.48 | 0.49 |
| 59:S1:347:ASP:OD1 | 59:S1:347:ASP:N | 2.43 | 0.49 |
| 65:S7:108:THR:HA | 65:S7:136:CYS:HB3 | 1.93 | 0.49 |
| 48:QB:120:LEU:HD13 | 48:QB:133:ILE:HG12 | 1.94 | 0.49 |
| 59:S1:603:ALA:O | 59:S1:604:GLN:HG3 | 2.12 | 0.49 |
| 45:N5:562:LEU:HB3 | 45:N5:563:PRO:HD3 | 1.95 | 0.49 |
| 47:QA:82:LEU:HD23 | 47:QA:205:LEU:HD11 | 1.94 | 0.49 |
| 48:Qb:194:GLY:O | 51:Qe:99:SER:OG | 2.30 | 0.49 |
| 60:S2:269:THR:O | 60:S2:333:TYR:OH | 2.28 | 0.49 |
| 66:S8:153:ILE:HG12 | 86:S8:302:SF4:S1 | 2.53 | 0.49 |
| 14:A5:48:THR:HA | 14:A5:51:ILE:HG12 | 1.95 | 0.49 |
| 71:QC:405:PC1:H3D1 | 71:QC:405:PC1:H392 | 1.94 | 0.49 |
| 51:Qe:224:PRO:HA | 51:Qe:236:CYS:HA | 1.94 | 0.49 |
| 55:Qi:34:ARG:HH21 | 58:Qj:50:GLY:HA3 | 1.78 | 0.49 |
| 71:6A:101:PC1:H321 | 71:C3:302:PC1:H271 | 1.93 | 0.49 |
| 18:A9:109:ASN:HB3 | 18:A9:112:ASP:HB2 | 1.94 | 0.49 |
| 18:A9:206:ILE:HG13 | 73:A9:401:NDP:H42N | 1.95 | 0.49 |
| 48:QB:366:ASP:HB2 | 48:QB:464:GLN:HG2 | 1.92 | 0.49 |
| 7:7A:75:SER:HA | 35:C1:118:VAL:HG12 | 1.94 | 0.49 |
| 42:N2:42:PRO:HG3 | 46:N6:167:VAL:HG13 | 1.95 | 0.49 |
| 42:N2:324:LYS:HB2 | 72:N2:401:CDL:H112 | 1.93 | 0.49 |
| 51:QE:160:PRO:HD2 | 51:QE:163:LYS:HG2 | 1.95 | 0.49 |
| 47:Qa:253:TYR:OH | 47:Qa:435:ARG:O | 2.19 | 0.49 |
| 53:Qg:52:PRO:HD2 | 53:Qg:55:LEU:HD12 | 1.95 | 0.49 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 59:S1:64:CYS:O | 59:S1:184:ARG:NH2 | 2.30 | 0.49 |
| 67:V1:112:TYR:CD1 | 67:V1:153:ALA:HB3 | 2.48 | 0.49 |
| 5:6B:30:CYS:SG | 5:6B:31:TRP:N | 2.86 | 0.49 |
| 23:AN:124:LEU:HD12 | 46:N6:130:THR:HG21 | 1.95 | 0.49 |
| 32:B9:143:GLU:O | 32:B9:164:ARG:NH2 | 2.46 | 0.49 |
| 44:N4:375:LEU:HD11 | 45:N5:141:PHE:HE2 | 1.77 | 0.49 |
| 47:QA:65:ILE:HG23 | 47:QA:218:MET:HG2 | 1.95 | 0.49 |
| 83:QC:402:HEM:HBC2 | 83:QC:402:HEM:HMC1 | 1.94 | 0.49 |
| 48:Qb:302:VAL:HB | 48:Qb:303:PRO:HD3 | 1.94 | 0.49 |
| 59:S1:466:LEU:HD13 | 59:S1:500:ILE:HD11 | 1.93 | 0.49 |
| 64:S6:100:ILE:HD11 | 64:S6:111:CYS:HB2 | 1.94 | 0.49 |
| 47:Qa:371:VAL:HG12 | 47:Qa:375:LYS:HE3 | 1.94 | 0.48 |
| 49:Qc:116:GLY:HA3 | 83:Qc:403:HEM:HBC2 | 1.94 | 0.48 |
| 49:Qc:227:LYS:HG2 | 50:Qd:308:LYS:HE2 | 1.94 | 0.48 |
| 60:S2:190:ILE:HD11 | 60:S2:257:PHE:HZ | 1.78 | 0.48 |
| 23:AN:57:ARG:NH1 | 41:N1:168:THR:OG1 | 2.46 | 0.48 |
| 29:B6:140:TRP:HD1 | 33:BK:41:VAL:HG13 | 1.78 | 0.48 |
| 35:C1:321:PHE:HB3 | 36:C2:65:TRP:CZ2 | 2.48 | 0.48 |
| 51:QE:178:HIS:CE1 | 51:QE:209:GLU:HB2 | 2.47 | 0.48 |
| 59:S1:163:LYS:HD3 | 59:S1:173:MET:HG3 | 1.94 | 0.48 |
| 59:S1:264:SER:HB2 | 59:S1:272:ARG:HB3 | 1.96 | 0.48 |
| 20:AK:142:LEU:HA | 20:AK:165:ILE:HD11 | 1.94 | 0.48 |
| 43:N3:79:SER:HA | 43:N3:87:MET:HE2 | 1.95 | 0.48 |
| 45:N5:7:LEU:O | 45:N5:11:THR:HG23 | 2.12 | 0.48 |
| 76:QE:303:3PE:H271 | 58:Qj:35:ALA:HB1 | 1.94 | 0.48 |
| 47:Qa:155:GLN:HB3 | 47:Qa:198:GLY:HA2 | 1.96 | 0.48 |
| 50:Qd:292:LYS:HD2 | 82:Qd:403:PEE:H3 | 1.95 | 0.48 |
| 77:AM:203:PLX:H191 | 77:AM:203:PLX:H393 | 1.94 | 0.48 |
| 77:AM:203:PLX:H201 | 76:S7:302:3PE:H2F2 | 1.96 | 0.48 |
| 40:CB:35:TYR:OH | 42:N2:335:LEU:O | 2.29 | 0.48 |
| 43:N3:28:ASN:ND2 | 76:S7:302:3PE:H251 | 2.28 | 0.48 |
| 47:QA:214:THR:HA | 47:QA:241:ARG:HB3 | 1.94 | 0.48 |
| 62:S4:109:ASN:ND2 | 62:S4:111:LEU:O | 2.47 | 0.48 |
| 28:B5:175:ASP:HA | 63:S5:45:HIS:HD2 | 1.78 | 0.48 |
| 37:C3:54:MET:HB3 | 37:C3:58:TRP:CZ3 | 2.49 | 0.48 |
| 37:C3:125:ASN:HD22 | 37:C3:128:GLU:HG3 | 1.78 | 0.48 |
| 45:N5:567:SER:OG | 82:S2:501:PEE:O3 | 2.31 | 0.48 |
| 48:QB:190:THR:HG22 | 48:QB:275:ILE:HG23 | 1.94 | 0.48 |
| 71:QC:405:PC1:H2G2 | 82:Qh:103:PEE:H76 | 1.94 | 0.48 |
| 71:QC:407:PC1:H2I1 | 77:QI:301:PLX:H362 | 1.96 | 0.48 |
| 50:QD:104:SER:HA | 55:Qi:48:ASN:HD21 | 1.79 | 0.48 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 47:Qa:63:LEU:HD21 | 47:Qa:218:MET:HE3 | 1.96 | 0.48 |
| 48:Qb:104:ARG:NH1 | 48:Qb:149:ASP:OD2 | 2.45 | 0.48 |
| 59:S1:224:ASP:CG | 59:S1:291:ARG:HH12 | 2.20 | 0.48 |
| 17:A8:95:VAL:HG12 | 17:A8:97:VAL:HG22 | 1.95 | 0.48 |
| 29:B6:181:LYS:HG3 | 30:B7:40:VAL:HG13 | 1.95 | 0.48 |
| 30:B7:29:TYR:O | 30:B7:104:ARG:NH2 | 2.47 | 0.48 |
| 41:N1:200:LEU:O | 41:N1:204:GLU:N | 2.46 | 0.48 |
| 48:QB:279:ASP:H | 48:QB:460:GLY:HA3 | 1.77 | 0.48 |
| 51:QE:190:VAL:HG21 | 51:QE:250:ARG:HH22 | 1.79 | 0.48 |
| 47:Qa:70:ARG:HD2 | 47:Qa:117:GLU:HG2 | 1.95 | 0.48 |
| 65:S7:130:VAL:HB | 65:S7:159:VAL:HA | 1.96 | 0.48 |
| 68:V2:92:TRP:CE2 | 68:V2:126:PRO:HG3 | 2.49 | 0.48 |
| 5:6B:5:ILE:HG13 | 5:6B:7:THR:H | 1.79 | 0.48 |
| 37:C3:66:THR:HB | 71:C3:301:PC1:H153 | 1.95 | 0.48 |
| 45:N5:49:VAL:HB | 45:N5:50:PRO:HD3 | 1.96 | 0.48 |
| 47:QA:153:ALA:O | 47:QA:156:SER:OG | 2.25 | 0.48 |
| 51:QE:207:LYS:HE3 | 51:QE:210:TRP:CD1 | 2.48 | 0.48 |
| 51:QE:234:TYR:N | 51:QE:243:TYR:O | 2.38 | 0.48 |
| 10:8B:52:ILE:HB | 10:8B:53:PRO:HD3 | 1.96 | 0.48 |
| 29:B6:157:VAL:HG13 | 45:N5:61:MET:HE3 | 1.95 | 0.48 |
| 35:C1:18:LEU:HB3 | 35:C1:102:PHE:CZ | 2.49 | 0.48 |
| 42:N2:49:ASN:OD1 | 42:N2:49:ASN:N | 2.47 | 0.48 |
| 82:N3:201:PEE:H22 | 82:N3:201:PEE:H27 | 1.65 | 0.48 |
| 45:N5:8:THR:O | 45:N5:11:THR:OG1 | 2.26 | 0.48 |
| 46:N6:150:GLY:HA2 | 63:S5:17:TRP:CZ2 | 2.49 | 0.48 |
| 59:S1:535:GLU:OE2 | 59:S1:538:ARG:NH1 | 2.46 | 0.48 |
| 60:S2:194:THR:HG21 | 60:S2:209:MET:HB2 | 1.94 | 0.48 |
| 60:S2:248:ASP:O | 60:S2:252:GLU:HG2 | 2.14 | 0.48 |
| 68:V2:85:LEU:HD13 | 69:V3:400:LEU:HD22 | 1.94 | 0.48 |
| 4:6A:65:LEU:HD22 | 37:C3:190:ASP:HB3 | 1.96 | 0.48 |
| 5:6B:62:LYS:HD3 | 5:6B:62:LYS:HA | 1.72 | 0.48 |
| 42:N2:139:LEU:HD13 | 42:N2:190:MET:HE1 | 1.96 | 0.48 |
| 49:Qc:200:LEU:HD23 | 49:Qc:201:HIS:CD2 | 2.48 | 0.48 |
| 66:S8:49:ASP:N | 66:S8:49:ASP:OD1 | 2.40 | 0.48 |
| 10:8B:46:THR:O | 10:8B:49:SER:OG | 2.31 | 0.48 |
| 66:S8:75:SER:O | 66:S8:79:ARG:HG3 | 2.14 | 0.48 |
| 35:C1:360:ASN:O | 35:C1:364:ASP:N | 2.41 | 0.47 |
| 35:C1:462:LEU:HG | 35:C1:466:MET:HE2 | 1.96 | 0.47 |
| 41:N1:65:THR:HG23 | 41:N1:122:ALA:HB1 | 1.96 | 0.47 |
| 57:QK:20:ARG:HH11 | 57:QK:23:ALA:HA | 1.79 | 0.47 |
| 51:Qe:267:SER:HB3 | 51:Qe:270:LEU:HB3 | 1.96 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 59:S1:338:VAL:HB | 59:S1:363:SER:HB2 | 1.96 | 0.47 |
| 18:A9:198:ALA:O | 18:A9:260:GLY:CA | 2.59 | 0.47 |
| 18:A9:268:PRO:HG2 | 18:A9:269:ASN:HD22 | 1.78 | 0.47 |
| 18:A9:293:LEU:HD12 | 18:A9:294:PRO:HD2 | 1.96 | 0.47 |
| 20:AK:93:ILE:HA | 20:AK:136:TRP:HE1 | 1.79 | 0.47 |
| 49:QC:300:ILE:HD11 | 49:QC:363:LEU:HD21 | 1.95 | 0.47 |
| 48:Qb:465:LEU:HD12 | 48:Qb:466:PRO:HD2 | 1.96 | 0.47 |
| 67:V1:138:LEU:HD13 | 67:V1:245:VAL:HG13 | 1.95 | 0.47 |
| 2:5A:126:PRO:O | 2:5A:130:GLN:HG2 | 2.13 | 0.47 |
| 5:6B:30:CYS:HA | 5:6B:61:TYR:CZ | 2.49 | 0.47 |
| 35:C1:12:HIS:HD2 | 35:C1:81:TRP:HA | 1.79 | 0.47 |
| 47:Qa:408:GLN:HE21 | 47:Qa:409:PRO:HD2 | 1.78 | 0.47 |
| 60:S2:241:ASP:OD1 | 60:S2:242:LEU:N | 2.46 | 0.47 |
| 2:5A:66:ASP:OD1 | 2:5A:66:ASP:N | 2.44 | 0.47 |
| 43:N3:64:LEU:HD13 | 46:N6:165:VAL:HG22 | 1.95 | 0.47 |
| 47:Qa:71:TYR:HB3 | 47:Qa:212:HIS:CE1 | 2.50 | 0.47 |
| 47:Qa:85:LEU:HD13 | 47:Qa:157:GLN:HG3 | 1.96 | 0.47 |
| 47:Qa:421:ASP:N | 47:Qa:421:ASP:OD1 | 2.47 | 0.47 |
| 59:S1:340:ALA:HB3 | 59:S1:366:LEU:HD23 | 1.95 | 0.47 |
| 59:S1:476:LEU:HD22 | 59:S1:493:VAL:HG21 | 1.96 | 0.47 |
| 67:V1:302:LYS:HE3 | 67:V1:303:HIS:CE1 | 2.49 | 0.47 |
| 7:7A:23:GLU:H | 7:7A:25:ARG:CZ | 2.27 | 0.47 |
| 17:A8:235:LEU:HB3 | 40:CB:23:LEU:HD21 | 1.95 | 0.47 |
| 20:AK:131:TYR:OH | 20:AK:188:HIS:ND1 | 2.40 | 0.47 |
| 35:C1:68:PHE:HA | 35:C1:72:PRO:HG2 | 1.96 | 0.47 |
| 41:N1:59:GLU:HB2 | 43:N3:30:TYR:CD2 | 2.49 | 0.47 |
| 45:N5:14:ILE:HD11 | 45:N5:43:ALA:HA | 1.96 | 0.47 |
| 45:N5:293:ILE:HD12 | 72:N5:703:CDL:H521 | 1.96 | 0.47 |
| 46:N6:124:ASP:N | 46:N6:124:ASP:OD1 | 2.47 | 0.47 |
| 65:S7:65:MET:HE2 | 65:S7:103:MET:HG3 | 1.97 | 0.47 |
| 65:S7:67:PHE:HE2 | 65:S7:117:LEU:HA | 1.80 | 0.47 |
| 67:V1:71:LYS:HE3 | 68:V2:249:LEU:HD23 | 1.95 | 0.47 |
| 2:5A:142:SER:HB2 | 2:5A:147:LEU:HD21 | 1.97 | 0.47 |
| 4:6A:81:LEU:HD11 | 72:6A:102:CDL:H321 | 1.96 | 0.47 |
| 24:B1:32:ASP:OD2 | 28:B5:131:LYS:NZ | 2.36 | 0.47 |
| 28:B5:126:TYR:OH | 44:N4:40:SER:O | 2.33 | 0.47 |
| 32:B9:177:ARG:HH12 | 32:B9:204:ASP:HA | 1.80 | 0.47 |
| 33:BK:144:SER:HB3 | 33:BK:158:LYS:NZ | 2.29 | 0.47 |
| 34:BL:106:VAL:HA | 34:BL:109:LEU:HG | 1.97 | 0.47 |
| 35:C1:80:ASN:ND2 | 35:C1:98:ASN:HD21 | 2.11 | 0.47 |
| 36:C2:161:HIS:CE1 | 36:C2:200:CYS:SG | 3.06 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 40:CB:46:ILE:HG12 | 72:CB:203:CDL:H741 | 1.97 | 0.47 |
| 41:N1:216:ALA:HB3 | 41:N1:219:PRO:HD2 | 1.96 | 0.47 |
| 42:N2:112:HIS:HB2 | 42:N2:184:ILE:HD13 | 1.97 | 0.47 |
| 47:QA:304:ASN:HB3 | 47:QA:307:SER:HB3 | 1.95 | 0.47 |
| 50:QD:265:SER:OG | 52:Qf:30:LEU:HB2 | 2.15 | 0.47 |
| 50:QD:300:LEU:HD21 | 51:QE:124:GLY:HA3 | 1.95 | 0.47 |
| 49:Qc:234:PHE:CZ | 72:Qd:401:CDL:H321 | 2.49 | 0.47 |
| 51:Qe:201:ASP:C | 51:Qe:203:GLU:H | 2.23 | 0.47 |
| 51:Qe:214:ILE:HG13 | 51:Qe:261:PRO:HD3 | 1.96 | 0.47 |
| 59:S1:222:ILE:HA | 59:S1:225:ILE:HG12 | 1.96 | 0.47 |
| 60:S2:140:PRO:HB2 | 65:S7:142:TYR:CE2 | 2.50 | 0.47 |
| 5:6B:33:ASN:HB2 | 5:6B:61:TYR:CZ | 2.50 | 0.47 |
| 35:C1:35:LEU:HD22 | 35:C1:462:LEU:HD22 | 1.95 | 0.47 |
| 35:C1:124:THR:HG23 | 35:C1:132:LEU:HG | 1.97 | 0.47 |
| 35:C1:357:VAL:HG22 | 36:C2:27:THR:HG22 | 1.97 | 0.47 |
| 37:C3:126:PRO:HB3 | 37:C3:257:TYR:HB3 | 1.96 | 0.47 |
| 41:N1:173:TRP:NE1 | 41:N1:244:GLY:O | 2.48 | 0.47 |
| 42:N2:231:SER:O | 42:N2:234:TRP:HD1 | 1.97 | 0.47 |
| 45:N5:241:THR:HG21 | 45:N5:344:GLY:HA3 | 1.97 | 0.47 |
| 48:QB:413:ILE:HG12 | 48:QB:423:ARG:HD2 | 1.97 | 0.47 |
| 49:QC:246:SER:HB2 | 49:QC:249:LEU:HB2 | 1.95 | 0.47 |
| 50:QD:132:ALA:HA | 50:QD:175:TYR:HA | 1.96 | 0.47 |
| 77:QE:301:PLX:H233 | 82:QE:302:PEE:H28 | 1.97 | 0.47 |
| 82:Qh:103:PEE:H25 | 82:Qh:103:PEE:H50 | 1.97 | 0.47 |
| 61:S3:101:ARG:NH1 | 61:S3:159:VAL:O | 2.47 | 0.47 |
| 67:V1:88:ARG:C | 67:V1:244:ASN:HD22 | 2.23 | 0.47 |
| 4:6A:28:TRP:HB3 | 37:C3:146:TRP:HB2 | 1.96 | 0.47 |
| 31:B8:114:ARG:HB2 | 45:N5:162:THR:HG21 | 1.96 | 0.47 |
| 35:C1:148:PHE:CE2 | 37:C3:32:THR:HG23 | 2.49 | 0.47 |
| 50:Qd:182:ASN:OD1 | 50:Qd:185:ALA:N | 2.43 | 0.47 |
| 59:S1:401:LEU:HD11 | 59:S1:432:ILE:HG13 | 1.96 | 0.47 |
| 59:S1:575:VAL:C | 59:S1:578:PRO:HD2 | 2.40 | 0.47 |
| 20:AK:256:GLU:HG3 | 20:AK:278:LEU:HG | 1.97 | 0.47 |
| 51:Qe:145:ASP:OD1 | 51:Qe:145:ASP:N | 2.48 | 0.47 |
| 60:S2:299:LEU:HD22 | 60:S2:304:ILE:HD12 | 1.97 | 0.47 |
| 1:4L:20:LEU:HD23 | 45:N5:588:PHE:HD2 | 1.80 | 0.47 |
| 18:A9:64:PHE:O | 18:A9:67:ARG:HG2 | 2.15 | 0.47 |
| 18:A9:168:SER:OG | 18:A9:169:HIS:N | 2.47 | 0.47 |
| 23:AN:56:GLU:OE1 | 23:AN:59:ARG:NH2 | 2.37 | 0.47 |
| 47:QA:293:LEU:HD21 | 47:QA:361:ILE:HD12 | 1.97 | 0.47 |
| 48:QB:113:VAL:HG12 | 48:QB:146:LEU:HD23 | 1.97 | 0.47 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 49:QC:159:ASP:OD1 | 49:QC:160:LEU:N | 2.48 | 0.47 |
| 48:Qb:126:ARG:NH1 | 48:Qb:199:GLN:O | 2.48 | 0.47 |
| 49:Qc:97:HIS:HD1 | 49:Qc:100:ARG:NH2 | 2.13 | 0.47 |
| 51:Qe:225:ILE:HG12 | 51:Qe:237:PRO:HD3 | 1.97 | 0.47 |
| 4:6A:81:LEU:HB3 | 71:6A:101:PC1:H12 | 1.97 | 0.46 |
| 17:A8:160:THR:HA | 17:A8:163:TRP:CD1 | 2.49 | 0.46 |
| 29:B6:132:VAL:O | 29:B6:136:LEU:CB | 2.62 | 0.46 |
| 34:BL:90:VAL:HG22 | 44:N4:28:THR:HG21 | 1.97 | 0.46 |
| 50:QD:248:PRO:HB2 | 84:QD:401:HEC:HBB2 | 1.97 | 0.46 |
| 48:Qb:74:TRP:CZ2 | 48:Qb:411:GLU:HA | 2.51 | 0.46 |
| 48:Qb:315:ASP:OD1 | 48:Qb:316:SER:N | 2.48 | 0.46 |
| 51:Qe:155:LYS:HB3 | 51:Qe:158:ASP:HB2 | 1.98 | 0.46 |
| 21:AL:118:MET:HA | 21:AL:121:THR:HG22 | 1.98 | 0.46 |
| 23:AN:49:SER:HB2 | 41:N1:172:ILE:HD13 | 1.97 | 0.46 |
| 30:B7:103:GLU:O | 30:B7:107:ARG:HG2 | 2.15 | 0.46 |
| 31:B8:62:TYR:OH | 31:B8:74:ASP:O | 2.29 | 0.46 |
| 32:B9:119:PRO:HB3 | 45:N5:525:MET:HE2 | 1.96 | 0.46 |
| 35:C1:436:MET:HE3 | 35:C1:443:TYR:HB3 | 1.96 | 0.46 |
| 71:C1:606:PC1:H222 | 38:C4:100:TRP:HB3 | 1.96 | 0.46 |
| 45:N5:293:ILE:HD13 | 45:N5:418:LEU:HD22 | 1.96 | 0.46 |
| 47:QA:138:LEU:HD13 | 47:QA:237:PHE:HB2 | 1.97 | 0.46 |
| 47:Qa:272:VAL:HA | 47:Qa:337:GLY:HA3 | 1.98 | 0.46 |
| 49:Qc:3:ASN:HD22 | 49:Qc:6:LYS:HE2 | 1.80 | 0.46 |
| 59:S1:382:ARG:C | 59:S1:384:ASN:H | 2.23 | 0.46 |
| 2:5A:67:ILE:HG13 | 2:5A:71:GLU:HB2 | 1.96 | 0.46 |
| 3:5B:61:PRO:HG2 | 3:5B:62:TYR:CD1 | 2.51 | 0.46 |
| 6:6C:49:TYR:CE1 | 38:C4:153:ILE:HG21 | 2.51 | 0.46 |
| 37:C3:112:LEU:HD22 | 37:C3:118:PRO:HB3 | 1.98 | 0.46 |
| 41:N1:10:ILE:HD11 | 43:N3:10:ASN:HD21 | 1.79 | 0.46 |
| 53:QG:110:LYS:HB2 | 58:Qj:7:GLY:HA3 | 1.97 | 0.46 |
| 48:Qb:310:ILE:HD11 | 48:Qb:388:VAL:HA | 1.97 | 0.46 |
| 59:S1:594:ALA:O | 59:S1:605:GLN:HA | 2.14 | 0.46 |
| 1:4L:1:MET:SD | 42:N2:80:TYR:OH | 2.72 | 0.46 |
| 71:6A:101:PC1:H31 | 71:6A:101:PC1:O12 | 2.15 | 0.46 |
| 16:A7:27:ARG:HD2 | 16:A7:31:ILE:HD11 | 1.98 | 0.46 |
| 20:AK:62:ILE:HG23 | 20:AK:205:VAL:CG2 | 2.46 | 0.46 |
| 21:AL:120:LEU:HD11 | 76:N4:502:3PE:H342 | 1.96 | 0.46 |
| 34:BL:119:ARG:NH2 | 45:N5:75:GLU:OE2 | 2.48 | 0.46 |
| 44:N4:278:ARG:HG3 | 45:N5:545:SER:HB2 | 1.98 | 0.46 |
| 44:N4:324:SER:OG | 44:N4:440:HIS:NE2 | 2.39 | 0.46 |
| 52:Qf:47:ARG:O | 52:Qf:51:GLU:HG2 | 2.15 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 59:S1:281:ILE:HD11 | 59:S1:602:ARG:HD2 | 1.97 | 0.46 |
| 59:S1:389:THR:OG1 | 59:S1:511:LYS:O | 2.34 | 0.46 |
| 60:S2:203:MET:O | 60:S2:206:PHE:HB3 | 2.16 | 0.46 |
| 60:S2:341:GLU:O | 60:S2:345:GLN:HG2 | 2.15 | 0.46 |
| 64:S6:29:VAL:HG21 | 64:S6:37:LYS:HD2 | 1.98 | 0.46 |
| 67:V1:203:ALA:HB3 | 67:V1:206:CYS:HB2 | 1.97 | 0.46 |
| 5:6B:56:TRP:O | 5:6B:60:VAL:HG23 | 2.16 | 0.46 |
| 11:A1:66:LEU:O | 11:A1:69:ILE:HG13 | 2.16 | 0.46 |
| 13:A3:121:SER:OG | 41:N1:310:MET:O | 2.28 | 0.46 |
| 72:A8:301:CDL:H542 | 72:A8:301:CDL:H162 | 1.95 | 0.46 |
| 19:AB:104:PHE:HD1 | 19:AB:108:LEU:HD12 | 1.81 | 0.46 |
| 23:AN:144:THR:HB | 41:N1:96:ILE:HG23 | 1.97 | 0.46 |
| 41:N1:66:SER:OG | 41:N1:124:ASN:ND2 | 2.35 | 0.46 |
| 76:N4:502:3PE:H2D2 | 45:N5:562:LEU:HD13 | 1.97 | 0.46 |
| 51:QE:186:GLN:O | 51:QE:190:VAL:HG23 | 2.15 | 0.46 |
| 52:QF:65:GLU:HB2 | 54:QH:78:TYR:CD1 | 2.51 | 0.46 |
| 52:Qf:28:ASP:HB3 | 52:Qf:29:PRO:HD3 | 1.97 | 0.46 |
| 67:V1:119:GLU:HA | 87:V1:502:FMN:HM71 | 1.96 | 0.46 |
| 2:5A:79:LEU:HD21 | 2:5A:86:PRO:HB3 | 1.97 | 0.46 |
| 32:B9:182:LEU:HD11 | 32:B9:208:LEU:HG | 1.96 | 0.46 |
| 37:C3:253:TYR:HA | 37:C3:257:TYR:CD1 | 2.50 | 0.46 |
| 53:QG:71:MET:HE2 | 50:Qd:316:LYS:HD3 | 1.98 | 0.46 |
| 50:Qd:119:LYS:O | 50:Qd:123:SER:OG | 2.27 | 0.46 |
| 60:S2:227:ARG:NH1 | 65:S7:75:GLU:OE1 | 2.48 | 0.46 |
| 35:C1:144:ASP:OD1 | 35:C1:213:ARG:NE | 2.36 | 0.46 |
| 35:C1:501:PRO:O | 35:C1:504:THR:HG23 | 2.16 | 0.46 |
| 39:CA:60:LYS:O | 39:CA:64:GLU:HG2 | 2.16 | 0.46 |
| 48:Qb:304:LEU:HD13 | 48:Qb:354:LEU:HD22 | 1.98 | 0.46 |
| 59:S1:291:ARG:HG2 | 59:S1:292:PHE:CE2 | 2.51 | 0.46 |
| 61:S3:115:THR:OG1 | 61:S3:116:ALA:N | 2.48 | 0.46 |
| 7:7A:33:PHE:HB2 | 37:C3:67:PHE:HB3 | 1.97 | 0.46 |
| 12:A2:59:SER:HB2 | 59:S1:655:ARG:HD3 | 1.97 | 0.46 |
| 15:A6:42:SER:HB2 | 62:S4:52:LEU:N | 2.31 | 0.46 |
| 19:AC:110:LEU:HB3 | 19:AC:114:ASP:HB2 | 1.97 | 0.46 |
| 74:AC:201:ZMP:H8 | 32:B9:109:ALA:HB2 | 1.98 | 0.46 |
| 22:AM:8:ARG:HD3 | 22:AM:8:ARG:HA | 1.76 | 0.46 |
| 27:B4:56:ARG:NH1 | 27:B4:58:GLY:O | 2.48 | 0.46 |
| 30:B7:103:GLU:OE2 | 30:B7:106:ARG:NH2 | 2.49 | 0.46 |
| 35:C1:230:LEU:HD21 | 37:C3:100:ALA:HA | 1.98 | 0.46 |
| 35:C1:412:ILE:HD13 | 38:C4:106:THR:HG21 | 1.97 | 0.46 |
| 76:CA:101:3PE:H231 | 40:CB:65:LEU:HD23 | 1.98 | 0.46 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 41:N1:31:MET:HG2 | 66:S8:77:LEU:HB2 | 1.98 | 0.46 |
| 46:N6:19:GLY:O | 46:N6:22:SER:OG | 2.28 | 0.46 |
| 53:QG:44:VAL:O | 53:QG:48:ILE:HG12 | 2.16 | 0.46 |
| 67:V1:283:ASN:ND2 | 67:V1:305:GLY:O | 2.33 | 0.46 |
| 7:7A:72:GLY:O | 7:7A:75:SER:OG | 2.32 | 0.46 |
| 35:C1:378:HIS:O | 35:C1:382:SER:OG | 2.25 | 0.46 |
| 48:QB:80:ARG:HH22 | 48:QB:350:GLU:CD | 2.24 | 0.46 |
| 51:QE:135:GLN:HE22 | 82:QE:302:PEE:H16 | 1.80 | 0.46 |
| 51:QE:207:LYS:HE3 | 51:QE:210:TRP:HD1 | 1.80 | 0.46 |
| 47:Qa:59:SER:HB2 | 47:Qa:130:ILE:HG21 | 1.97 | 0.46 |
| 66:S8:74:LEU:HD12 | 66:S8:77:LEU:HD23 | 1.98 | 0.46 |
| 12:A2:60:ASP:N | 12:A2:60:ASP:OD1 | 2.49 | 0.46 |
| 18:A9:168:SER:O | 18:A9:203:PRO:HD2 | 2.16 | 0.46 |
| 48:Qb:70:THR:HG21 | 48:Qb:407:THR:HA | 1.98 | 0.46 |
| 50:Qd:106:LEU:HD13 | 50:Qd:111:ILE:HD11 | 1.97 | 0.46 |
| 50:Qd:322:TYR:CZ | 50:Qd:324:PRO:HG3 | 2.51 | 0.46 |
| 59:S1:246:ARG:HH22 | 62:S4:123:ASN:ND2 | 2.14 | 0.46 |
| 9:7C:42:THR:HG23 | 10:8B:49:SER:HB3 | 1.98 | 0.45 |
| 9:7C:44:TYR:OH | 35:C1:25:TRP:HB2 | 2.16 | 0.45 |
| 28:B5:147:ALA:HB2 | 44:N4:173:SER:HB2 | 1.98 | 0.45 |
| 76:N4:502:3PE:H3A2 | 76:N4:502:3PE:H2D1 | 1.98 | 0.45 |
| 47:QA:271:LEU:HD22 | 47:QA:453:LEU:HD13 | 1.98 | 0.45 |
| 49:QC:29:SER:OG | 72:QC:408:CDL:HB61 | 2.15 | 0.45 |
| 77:QE:301:PLX:H152 | 77:QE:301:PLX:H182 | 1.77 | 0.45 |
| 61:S3:73:VAL:HA | 61:S3:88:ILE:HG22 | 1.97 | 0.45 |
| 20:AK:131:TYR:CD1 | 20:AK:185:CYS:HB3 | 2.51 | 0.45 |
| 22:AM:93:MET:HE1 | 66:S8:171:PRO:HB2 | 1.98 | 0.45 |
| 36:C2:139:ASP:OD1 | 36:C2:139:ASP:N | 2.49 | 0.45 |
| 44:N4:369:LEU:HD23 | 72:N5:702:CDL:H362 | 1.98 | 0.45 |
| 48:QB:110:GLU:HA | 48:QB:113:VAL:HG22 | 1.97 | 0.45 |
| 53:QG:36:ASP:OD2 | 53:QG:62:ARG:NH1 | 2.47 | 0.45 |
| 61:S3:211:ARG:NH2 | 61:S3:213:ASP:OD1 | 2.44 | 0.45 |
| 4:6A:53:HIS:O | 4:6A:54:HIS:ND1 | 2.48 | 0.45 |
| 4:6A:88:ASN:OD1 | 71:6A:101:PC1:H141 | 2.17 | 0.45 |
| 71:6A:101:PC1:H142 | 37:C3:181:TYR:O | 2.16 | 0.45 |
| 72:A8:301:CDL:H261 | 44:N4:10:MET:HE3 | 1.99 | 0.45 |
| 28:B5:146:LYS:O | 28:B5:150:ARG:HG3 | 2.16 | 0.45 |
| 77:B5:201:PLX:H371 | 77:B5:201:PLX:H342 | 1.81 | 0.45 |
| 41:N1:281:ARG:HB2 | 41:N1:284:GLN:HG3 | 1.99 | 0.45 |
| 42:N2:137:ALA:HB3 | 42:N2:138:PRO:HD3 | 1.97 | 0.45 |
| 50:QD:168:ARG:NH1 | 50:QD:174:ASP:OD2 | 2.42 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 50:Qd:256:PHE:HD2 | 50:Qd:260:THR:HB | 1.82 | 0.45 |
| 60:S2:190:ILE:HG23 | 60:S2:209:MET:HB3 | 1.98 | 0.45 |
| 67:V1:55:GLY:O | 67:V1:58:SER:OG | 2.27 | 0.45 |
| 7:7A:40:PRO:HG2 | 7:7A:43:LEU:HB2 | 1.98 | 0.45 |
| 26:B3:24:ILE:O | 26:B3:30:GLU:HB3 | 2.17 | 0.45 |
| 31:B8:111:MET:SD | 44:N4:278:ARG:NH2 | 2.89 | 0.45 |
| 37:C3:137:LEU:HD12 | 37:C3:249:TRP:CD1 | 2.51 | 0.45 |
| 82:N5:701:PEE:H36 | 82:N5:701:PEE:H29 | 1.57 | 0.45 |
| 82:QE:302:PEE:H23 | 82:QE:302:PEE:H30 | 1.59 | 0.45 |
| 35:C1:328:HIS:HD2 | 36:C2:56:MET:HE1 | 1.81 | 0.45 |
| 44:N4:127:VAL:HB | 44:N4:128:PRO:HD3 | 1.98 | 0.45 |
| 48:QB:445:CYS:O | 48:QB:449:PHE:HB2 | 2.15 | 0.45 |
| 49:QC:116:GLY:HA3 | 83:QC:403:HEM:C3C | 2.52 | 0.45 |
| 49:QC:236:MET:HG2 | 82:QE:302:PEE:H61 | 1.98 | 0.45 |
| 50:QD:322:TYR:CE2 | 50:QD:324:PRO:HG3 | 2.51 | 0.45 |
| 77:QI:301:PLX:H22 | 77:QI:301:PLX:H1C3 | 1.56 | 0.45 |
| 54:Qh:19:LEU:HD23 | 54:Qh:24:GLN:HB3 | 1.97 | 0.45 |
| 59:S1:36:VAL:HG11 | 59:S1:56:VAL:HG21 | 1.99 | 0.45 |
| 59:S1:541:PRO:HB3 | 59:S1:561:PRO:HD3 | 1.99 | 0.45 |
| 66:S8:98:ARG:NH1 | 66:S8:154:TYR:O | 2.49 | 0.45 |
| 67:V1:177:TYR:CD1 | 69:V3:409:PHE:HB3 | 2.52 | 0.45 |
| 36:C2:154:VAL:HG12 | 36:C2:174:ALA:HB2 | 1.99 | 0.45 |
| 41:N1:66:SER:HG | 41:N1:124:ASN:HD21 | 1.60 | 0.45 |
| 44:N4:79:ALA:O | 44:N4:82:SER:HB3 | 2.17 | 0.45 |
| 57:QK:24:GLY:HA3 | 47:Qa:109:LYS:HB3 | 1.98 | 0.45 |
| 47:Qa:183:ARG:CG | 47:Qa:254:ARG:HB2 | 2.46 | 0.45 |
| 48:Qb:121:ASN:ND2 | 48:Qb:132:TYR:OH | 2.50 | 0.45 |
| 49:Qc:186:PRO:HG2 | 83:Qc:402:HEM:HMC3 | 1.98 | 0.45 |
| 60:S2:134:THR:HG22 | 60:S2:135:TYR:H | 1.82 | 0.45 |
| 69:V3:386:TYR:CZ | 69:V3:388:ASN:HB3 | 2.52 | 0.45 |
| 3:5B:70:ALA:N | 3:5B:78:ASN:OD1 | 2.30 | 0.45 |
| 72:6A:102:CDL:H121 | 72:6A:102:CDL:H152 | 1.85 | 0.45 |
| 71:7B:101:PC1:H2B1 | 35:C1:423:MET:HE1 | 1.98 | 0.45 |
| 29:B6:91:ARG:NH2 | 32:B9:159:ASP:OD1 | 2.50 | 0.45 |
| 35:C1:445:ASP:OD1 | 36:C2:134:ARG:NE | 2.34 | 0.45 |
| 79:C1:603:HEA:HBA2 | 79:C1:603:HEA:CMA | 2.47 | 0.45 |
| 37:C3:49:THR:O | 37:C3:53:THR:OG1 | 2.33 | 0.45 |
| 37:C3:204:HIS:NE2 | 37:C3:249:TRP:HB2 | 2.32 | 0.45 |
| 45:N5:584:ILE:O | 45:N5:588:PHE:HB2 | 2.16 | 0.45 |
| 48:QB:176:ASP:OD1 | 51:QE:80:HIS:ND1 | 2.37 | 0.45 |
| 51:Qe:165:MET:HB3 | 51:Qe:176:VAL:HG23 | 1.99 | 0.45 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 67:V1:364:VAL:HG12 | 67:V1:400:VAL:HG12 | 1.98 | 0.45 |
| 17:A8:239:LYS:O | 17:A8:243:ARG:NH1 | 2.49 | 0.45 |
| 20:AK:316:LEU:HB2 | 20:AK:319:ILE:HG12 | 1.98 | 0.45 |
| 21:AL:14:GLU:HA | 21:AL:21:LYS:HE3 | 1.99 | 0.45 |
| 77:AL:205:PLX:H101 | 77:AL:205:PLX:H292 | 1.99 | 0.45 |
| 26:B3:49:GLU:HG3 | 32:B9:80:ARG:HD2 | 1.99 | 0.45 |
| 35:C1:409:TRP:HB3 | 35:C1:471:ILE:HG12 | 1.98 | 0.45 |
| 41:N1:58:LYS:NZ | 65:S7:125:PRO:O | 2.50 | 0.45 |
| 48:Qb:356:ALA:HB3 | 48:Qb:372:LEU:HD21 | 1.99 | 0.45 |
| 59:S1:259:SER:HB3 | 59:S1:282:ASN:HD22 | 1.81 | 0.45 |
| 60:S2:190:ILE:HD11 | 60:S2:257:PHE:CZ | 2.52 | 0.45 |
| 6:6C:72:GLN:N | 36:C2:212:GLU:OE2 | 2.50 | 0.45 |
| 17:A8:246:PHE:HE1 | 72:A8:301:CDL:H341 | 1.82 | 0.45 |
| 18:A9:54:ILE:HD12 | 18:A9:76:MET:HE1 | 1.99 | 0.45 |
| 31:B8:173:ASP:OD1 | 31:B8:175:THR:OG1 | 2.35 | 0.45 |
| 44:N4:201:MET:HE1 | 44:N4:212:LEU:HD11 | 1.99 | 0.45 |
| 49:QC:207:ASN:ND2 | 49:QC:211:ILE:O | 2.37 | 0.45 |
| 49:QC:336:THR:HG21 | 72:QC:406:CDL:H512 | 1.98 | 0.45 |
| 50:QD:211:TYR:OH | 84:QD:401:HEC:O2A | 2.32 | 0.45 |
| 55:QI:58:HIS:CE1 | 55:QI:59:LYS:HG3 | 2.52 | 0.45 |
| 47:Qa:115:THR:HG23 | 47:Qa:117:GLU:H | 1.82 | 0.45 |
| 47:Qa:180:ALA:HB2 | 47:Qa:258:ILE:HG13 | 1.98 | 0.45 |
| 50:Qd:99:HIS:HB2 | 50:Qd:283:HIS:HE1 | 1.82 | 0.45 |
| 64:S6:38:VAL:HG22 | 64:S6:44:ALA:HB2 | 1.98 | 0.45 |
| 4:6A:64:HIS:ND1 | 4:6A:65:LEU:HG | 2.32 | 0.45 |
| 20:AK:138:TYR:CE1 | 20:AK:165:ILE:HG23 | 2.52 | 0.45 |
| 71:AL:206:PC1:H271 | 44:N4:159:PRO:HB3 | 1.99 | 0.45 |
| 31:B8:39:GLY:N | 31:B8:74:ASP:OD1 | 2.38 | 0.45 |
| 35:C1:413:HIS:CE1 | 35:C1:468:MET:HB2 | 2.51 | 0.45 |
| 35:C1:442:ASP:OD1 | 35:C1:443:TYR:N | 2.49 | 0.45 |
| 41:N1:293:PHE:O | 41:N1:297:THR:OG1 | 2.32 | 0.45 |
| 44:N4:225:ILE:HD13 | 44:N4:331:ASN:HB2 | 1.99 | 0.45 |
| 66:S8:155:CYS:N | 86:S8:302:SF4:S4 | 2.88 | 0.45 |
| 23:AN:43:LEU:HG | 41:N1:179:TRP:HE1 | 1.81 | 0.44 |
| 27:B4:70:TYR:HD2 | 31:B8:38:PRO:HD2 | 1.80 | 0.44 |
| 32:B9:77:ASP:OD1 | 32:B9:77:ASP:N | 2.50 | 0.44 |
| 44:N4:82:SER:HB2 | 44:N4:432:ARG:NH1 | 2.32 | 0.44 |
| 45:N5:346:ILE:HD11 | 45:N5:431:PHE:CZ | 2.52 | 0.44 |
| 51:QE:266:THR:OG1 | 51:QE:270:LEU:O | 2.32 | 0.44 |
| 59:S1:296:GLY:O | 59:S1:572:HIS:NE2 | 2.45 | 0.44 |
| 60:S2:142:PHE:HZ | 60:S2:428:CYS:SG | 2.41 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 4:6A:28:TRP:O | 4:6A:32:THR:N | 2.46 | 0.44 |
| 21:AL:139:PRO:HA | 42:N2:273:ASN:HD22 | 1.82 | 0.44 |
| 72:AL:203:CDL:H432 | 72:AL:203:CDL:H671 | 1.99 | 0.44 |
| 35:C1:377:PHE:HA | 35:C1:380:VAL:HG22 | 1.99 | 0.44 |
| 35:C1:492:LEU:HD12 | 35:C1:495:LEU:HD12 | 1.99 | 0.44 |
| 41:N1:283:ASP:OD1 | 41:N1:283:ASP:N | 2.48 | 0.44 |
| 48:QB:270:PHE:CG | 48:QB:292:GLU:HB2 | 2.52 | 0.44 |
| 49:QC:131:TYR:O | 49:QC:134:PRO:HD2 | 2.16 | 0.44 |
| 49:QC:186:PRO:HG2 | 83:QC:402:HEM:HMC3 | 1.99 | 0.44 |
| 59:S1:119:PHE:HB3 | 67:V1:387:GLU:HB2 | 1.99 | 0.44 |
| 2:5A:109:ARG:O | 2:5A:113:VAL:HG23 | 2.18 | 0.44 |
| 4:6A:88:ASN:CG | 71:6A:101:PC1:H131 | 2.42 | 0.44 |
| 21:AL:22:ALA:O | 21:AL:26:THR:OG1 | 2.33 | 0.44 |
| 35:C1:313:ALA:HB3 | 36:C2:73:LEU:HD11 | 1.98 | 0.44 |
| 35:C1:316:THR:HG21 | 79:C1:603:HEA:C14 | 2.46 | 0.44 |
| 35:C1:352:GLY:CA | 79:C1:603:HEA:H162 | 2.48 | 0.44 |
| 37:C3:79:LEU:HB3 | 37:C3:233:PHE:CZ | 2.52 | 0.44 |
| 44:N4:196:TRP:CD1 | 44:N4:250:LEU:HB3 | 2.52 | 0.44 |
| 44:N4:266:MET:HA | 44:N4:269:MET:HE2 | 1.99 | 0.44 |
| 47:QA:125:CYS:HB3 | 47:QA:133:LEU:HD22 | 2.00 | 0.44 |
| 47:QA:306:THR:HG22 | 48:QB:114:GLU:OE1 | 2.18 | 0.44 |
| 48:Qb:324:MET:O | 48:Qb:330:SER:OG | 2.36 | 0.44 |
| 67:V1:205:ILE:HG12 | 67:V1:379:CYS:SG | 2.56 | 0.44 |
| 67:V1:412:LEU:HD12 | 67:V1:415:ILE:HD11 | 1.98 | 0.44 |
| 26:B3:52:ARG:HD3 | 45:N5:435:PRO:O | 2.17 | 0.44 |
| 41:N1:309:ILE:HD12 | 43:N3:88:LEU:HD13 | 2.00 | 0.44 |
| 44:N4:78:MET:O | 44:N4:81:GLN:HG2 | 2.18 | 0.44 |
| 44:N4:168:GLN:HB2 | 44:N4:174:LEU:HG | 1.99 | 0.44 |
| 44:N4:318:ALA:HB2 | 44:N4:373:ILE:HG13 | 1.99 | 0.44 |
| 45:N5:526:LEU:HD12 | 45:N5:530:PRO:HG3 | 2.00 | 0.44 |
| 67:V1:99:TRP:CD1 | 67:V1:149:MET:HE2 | 2.53 | 0.44 |
| 67:V1:151:ALA:O | 67:V1:191:TYR:OH | 2.23 | 0.44 |
| 15:A6:66:TYR:CE2 | 15:A6:86:ARG:HD3 | 2.52 | 0.44 |
| 20:AK:297:ARG:HA | 20:AK:300:VAL:HG22 | 1.99 | 0.44 |
| 77:AM:201:PLX:H22 | 77:AM:201:PLX:H1A2 | 1.78 | 0.44 |
| 29:B6:164:ILE:HD12 | 29:B6:170:ILE:HD11 | 1.99 | 0.44 |
| 76:CB:202:3PE:H2C2 | 72:CB:203:CDL:H642 | 2.00 | 0.44 |
| 47:QA:82:LEU:HD11 | 47:QA:154:LEU:HB3 | 1.98 | 0.44 |
| 54:QH:29:HIS:O | 54:QH:33:LYS:HG2 | 2.17 | 0.44 |
| 47:Qa:217:ARG:HD2 | 47:Qa:244:LEU:O | 2.18 | 0.44 |
| 50:Qd:139:VAL:HG21 | 50:Qd:277:TRP:CZ2 | 2.52 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 51:Qe:208:PRO:O | 51:Qe:209:GLU:HG2 | 2.17 | 0.44 |
| 53:Qg:54:ASN:OD1 | 53:Qg:55:LEU:N | 2.50 | 0.44 |
| 59:S1:152:ARG:NH1 | 67:V1:414:GLU:OE1 | 2.48 | 0.44 |
| 64:S6:63:ASN:OD1 | 66:S8:105:ARG:NH2 | 2.50 | 0.44 |
| 18:A9:163:LYS:NZ | 18:A9:253:ILE:O | 2.33 | 0.44 |
| 40:CB:38:PHE:HZ | 72:CB:203:CDL:H812 | 1.83 | 0.44 |
| 41:N1:25:ARG:NH2 | 65:S7:92:VAL:HG22 | 2.33 | 0.44 |
| 72:N5:702:CDL:H161 | 72:N5:702:CDL:H192 | 1.78 | 0.44 |
| 46:N6:169:MET:HE2 | 46:N6:169:MET:HB3 | 1.80 | 0.44 |
| 47:Qa:262:ASN:OD1 | 47:Qa:442:GLY:N | 2.51 | 0.44 |
| 48:Qb:76:ASP:O | 48:Qb:228:ARG:NH1 | 2.50 | 0.44 |
| 59:S1:140:GLN:HG2 | 60:S2:385:ILE:HG23 | 1.99 | 0.44 |
| 60:S2:391:TYR:HD1 | 66:S8:122:VAL:HG21 | 1.82 | 0.44 |
| 60:S2:402:THR:O | 60:S2:416:TYR:HA | 2.18 | 0.44 |
| 60:S2:430:ILE:HB | 60:S2:469:ARG:HD2 | 2.00 | 0.44 |
| 61:S3:51:ASN:HB3 | 61:S3:82:ASN:HD21 | 1.82 | 0.44 |
| 67:V1:270:ASN:HD22 | 67:V1:339:PHE:HB2 | 1.83 | 0.44 |
| 29:B6:85:ASP:OD2 | 32:B9:167:TRP:NE1 | 2.40 | 0.44 |
| 32:B9:70:GLU:OE2 | 32:B9:76:ARG:NH1 | 2.34 | 0.44 |
| 36:C2:164:ALA:HB2 | 36:C2:171:LYS:HG3 | 1.99 | 0.44 |
| 41:N1:32:GLN:HG2 | 60:S2:204:THR:HG22 | 2.00 | 0.44 |
| 49:QC:96:ILE:HD11 | 72:QC:408:CDL:H771 | 1.99 | 0.44 |
| 49:QC:200:LEU:HD23 | 49:QC:201:HIS:CD2 | 2.53 | 0.44 |
| 57:QK:26:LEU:HD23 | 57:QK:26:LEU:HA | 1.90 | 0.44 |
| 47:Qa:89:LEU:HD22 | 47:Qa:150:GLU:HB3 | 1.98 | 0.44 |
| 67:V1:385:CYS:CB | 86:V1:501:SF4:S2 | 3.05 | 0.44 |
| 19:AB:115:GLN:O | 19:AB:119:ILE:HG12 | 2.17 | 0.44 |
| 20:AK:283:GLY:O | 20:AK:286:PRO:HD2 | 2.18 | 0.44 |
| 77:AM:201:PLX:H341 | 77:AM:201:PLX:H372 | 1.73 | 0.44 |
| 29:B6:136:LEU:HD12 | 29:B6:136:LEU:HA | 1.85 | 0.44 |
| 79:C1:602:HEA:HBA2 | 79:C1:602:HEA:HMA | 2.00 | 0.44 |
| 37:C3:178:ALA:HB2 | 71:C3:302:PC1:H2B2 | 1.99 | 0.44 |
| 51:Qe:98:ASP:OD1 | 51:Qe:99:SER:N | 2.51 | 0.44 |
| 67:V1:168:ASN:ND2 | 69:V3:388:ASN:HD21 | 2.15 | 0.44 |
| 67:V1:211:ALA:HB2 | 67:V1:223:PRO:HG3 | 1.99 | 0.44 |
| 1:4L:21:MET:HG2 | 45:N5:589:LEU:HD13 | 2.00 | 0.44 |
| 3:5B:82:SER:HB2 | 3:5B:122:LEU:HD11 | 2.00 | 0.44 |
| 17:A8:244:LEU:HD23 | 42:N2:341:PRO:HG3 | 2.00 | 0.44 |
| 73:A9:401:NDP:N7N | 73:A9:401:NDP:O2N | 2.50 | 0.44 |
| 20:AK:93:ILE:HG23 | 20:AK:136:TRP:NE1 | 2.32 | 0.44 |
| 35:C1:308:ALA:O | 35:C1:311:ILE:HG12 | 2.18 | 0.44 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 35:C1:383:MET:HE3 | 35:C1:421:VAL:HG23 | 2.00 | 0.44 |
| 37:C3:86:PHE:HZ | 71:C3:301:PC1:H3A1 | 1.82 | 0.44 |
| 37:C3:217:VAL:O | 37:C3:221:ARG:HG3 | 2.18 | 0.44 |
| 45:N5:286:LEU:HD22 | 45:N5:411:MET:SD | 2.58 | 0.44 |
| 49:QC:102:LEU:HD22 | 49:QC:304:MET:HE2 | 1.99 | 0.44 |
| 51:QE:241:SER:OG | 85:QE:304:FES:S1 | 2.73 | 0.44 |
| 48:Qb:341:PHE:HB2 | 48:Qb:358:PHE:HB3 | 1.99 | 0.44 |
| 60:S2:418:VAL:HB | 60:S2:427:ARG:HB3 | 1.99 | 0.44 |
| 82:S2:501:PEE:H49 | 82:S2:501:PEE:H54 | 1.81 | 0.44 |
| 66:S8:150:THR:HG21 | 66:S8:180:HIS:NE2 | 2.33 | 0.44 |
| 17:A8:157:GLU:HB2 | 17:A8:158:PRO:HD3 | 2.00 | 0.43 |
| 19:AB:138:LEU:HD23 | 19:AB:144:ILE:HD13 | 2.00 | 0.43 |
| 77:AL:205:PLX:H141 | 27:B4:99:PHE:HZ | 1.82 | 0.43 |
| 26:B3:85:GLU:O | 26:B3:89:GLU:HG2 | 2.18 | 0.43 |
| 27:B4:71:ALA:HA | 27:B4:75:ASN:HB3 | 2.00 | 0.43 |
| 72:B5:202:CDL:H1 | 82:N5:701:PEE:H49 | 2.00 | 0.43 |
| 42:N2:211:MET:HG2 | 42:N2:333:SER:HB2 | 2.00 | 0.43 |
| 47:Qa:148:ARG:NH2 | 53:Qg:50:ARG:O | 2.50 | 0.43 |
| 48:Qb:38:TYR:CZ | 48:Qb:42:LEU:HD11 | 2.53 | 0.43 |
| 8:7B:69:VAL:HG12 | 38:C4:167:TRP:CZ3 | 2.53 | 0.43 |
| 77:CB:201:PLX:H1C3 | 77:CB:201:PLX:H22 | 1.78 | 0.43 |
| 42:N2:132:THR:HG23 | 42:N2:209:ILE:HG12 | 1.99 | 0.43 |
| 44:N4:328:CYS:HB3 | 44:N4:437:MET:HE1 | 2.00 | 0.43 |
| 44:N4:361:VAL:HG13 | 72:N5:702:CDL:H332 | 1.99 | 0.43 |
| 47:QA:70:ARG:NH1 | 47:QA:249:ALA:O | 2.51 | 0.43 |
| 51:QE:90:ASP:OD1 | 51:QE:90:ASP:N | 2.42 | 0.43 |
| 57:QK:24:GLY:HA3 | 47:Qa:109:LYS:HE3 | 2.00 | 0.43 |
| 49:Qc:132:VAL:HG22 | 49:Qc:143:ALA:HB2 | 2.00 | 0.43 |
| 49:Qc:233:LEU:HD23 | 49:Qc:233:LEU:HA | 1.80 | 0.43 |
| 49:Qc:361:ILE:HG12 | 49:Qc:365:LEU:HD12 | 1.99 | 0.43 |
| 82:Qh:101:PEE:H19 | 82:Qh:101:PEE:H25 | 1.61 | 0.43 |
| 59:S1:217:GLU:HG2 | 59:S1:218:LEU:HG | 2.00 | 0.43 |
| 67:V1:222:LYS:HG2 | 67:V1:379:CYS:HB3 | 2.00 | 0.43 |
| 2:5A:136:LEU:HD22 | 2:5A:141:ILE:HB | 1.99 | 0.43 |
| 4:6A:67:ILE:HD13 | 35:C1:218:THR:HG21 | 2.00 | 0.43 |
| 19:AC:114:ASP:OD1 | 32:B9:87:ARG:NH2 | 2.50 | 0.43 |
| 20:AK:148:ALA:HB1 | 20:AK:159:VAL:HG21 | 1.99 | 0.43 |
| 20:AK:237:GLN:HG3 | 20:AK:241:ASN:HD21 | 1.82 | 0.43 |
| 20:AK:244:LYS:HA | 20:AK:248:LEU:HD12 | 2.01 | 0.43 |
| 35:C1:427:PRO:HB3 | 35:C1:450:TRP:HB3 | 2.01 | 0.43 |
| 82:N3:201:PEE:H56 | 82:N3:201:PEE:H50 | 1.69 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 44:N4:260:PRO:HG3 | 76:N4:502:3PE:H221 | 2.00 | 0.43 |
| 47:QA:154:LEU:HD12 | 47:QA:154:LEU:HA | 1.85 | 0.43 |
| 82:QB:502:PEE:H49 | 77:QE:301:PLX:H6 | 2.00 | 0.43 |
| 53:QG:99:ILE:O | 53:QG:103:LYS:HG2 | 2.18 | 0.43 |
| 54:QH:72:ARG:HA | 54:QH:72:ARG:HD3 | 1.88 | 0.43 |
| 47:Qa:378:LEU:HG | 47:Qa:416:ILE:HD13 | 2.00 | 0.43 |
| 48:Qb:121:ASN:HB3 | 48:Qb:132:TYR:CE1 | 2.54 | 0.43 |
| 10:8B:47:PHE:O | 10:8B:51:LEU:HG | 2.19 | 0.43 |
| 20:AK:112:GLY:HA2 | 20:AK:136:TRP:CD2 | 2.53 | 0.43 |
| 20:AK:342:SER:HB3 | 20:AK:345:TYR:HD1 | 1.84 | 0.43 |
| 33:BK:114:GLN:HG3 | 45:N5:203:MET:HG2 | 1.99 | 0.43 |
| 35:C1:30:GLY:C | 35:C1:65:MET:HE2 | 2.42 | 0.43 |
| 35:C1:368:HIS:HD1 | 79:C1:603:HEA:CGA | 2.31 | 0.43 |
| 35:C1:409:TRP:CZ3 | 35:C1:467:LEU:HD11 | 2.53 | 0.43 |
| 82:C1:609:PEE:H60 | 82:C1:609:PEE:H66 | 1.58 | 0.43 |
| 37:C3:141:GLY:O | 37:C3:144:ILE:HG22 | 2.19 | 0.43 |
| 38:C4:65:LYS:HB3 | 38:C4:65:LYS:HE2 | 1.72 | 0.43 |
| 42:N2:250:SER:O | 42:N2:259:GLY:HA3 | 2.19 | 0.43 |
| 45:N5:289:ALA:O | 45:N5:293:ILE:HG23 | 2.19 | 0.43 |
| 47:QA:230:LEU:HD23 | 47:QA:230:LEU:HA | 1.87 | 0.43 |
| 48:QB:310:ILE:HD11 | 48:QB:388:VAL:HA | 1.99 | 0.43 |
| 48:Qb:109:LEU:HD12 | 48:Qb:146:LEU:HD22 | 2.00 | 0.43 |
| 54:Qh:20:SER:O | 54:Qh:24:GLN:HG2 | 2.19 | 0.43 |
| 82:Qh:101:PEE:H19 | 82:Qh:101:PEE:H13 | 1.49 | 0.43 |
| 59:S1:186:ALA:HB2 | 59:S1:195:LEU:HD12 | 1.99 | 0.43 |
| 17:A8:160:THR:HA | 17:A8:163:TRP:NE1 | 2.34 | 0.43 |
| 34:BL:150:PRO:HG3 | 40:CB:115:LEU:HD22 | 2.01 | 0.43 |
| 35:C1:254:ILE:HG13 | 35:C1:344:PHE:CD2 | 2.53 | 0.43 |
| 79:C1:602:HEA:HBD2 | 79:C1:602:HEA:HHA | 2.00 | 0.43 |
| 42:N2:2:ASN:HD22 | 42:N2:4:ILE:H | 1.66 | 0.43 |
| 44:N4:12:LEU:HB2 | 44:N4:13:PRO:HD3 | 1.99 | 0.43 |
| 44:N4:449:LEU:HG | 72:N5:702:CDL:H441 | 2.00 | 0.43 |
| 44:N4:458:LEU:O | 45:N5:72:GLN:NE2 | 2.51 | 0.43 |
| 46:N6:124:ASP:O | 46:N6:127:ILE:HG12 | 2.18 | 0.43 |
| 50:QD:228:LEU:HD11 | 50:QD:234:PHE:HB2 | 2.00 | 0.43 |
| 53:QG:34:ARG:O | 53:QG:37:THR:HG22 | 2.18 | 0.43 |
| 48:Qb:152:GLN:NE2 | 48:Qb:250:PHE:HA | 2.33 | 0.43 |
| 66:S8:153:ILE:HG13 | 66:S8:155:CYS:HB3 | 2.00 | 0.43 |
| 67:V1:39:ASP:HB3 | 67:V1:265:PHE:CE2 | 2.54 | 0.43 |
| 67:V1:65:THR:O | 67:V1:69:LEU:HG | 2.19 | 0.43 |
| 67:V1:396:MET:O | 67:V1:400:VAL:HG13 | 2.18 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 68:V2:83:LEU:HD21 | 68:V2:116:ALA:HB2 | 2.01 | 0.43 |
| 35:C1:94:PHE:CZ | 35:C1:166:THR:HG21 | 2.53 | 0.43 |
| 35:C1:236:TRP:CH2 | 79:C1:603:HEA:HBD1 | 2.54 | 0.43 |
| 40:CB:4:MET:O | 40:CB:10:ARG:NH1 | 2.52 | 0.43 |
| 54:QH:12:ARG:NH1 | 48:Qb:279:ASP:OD1 | 2.50 | 0.43 |
| 71:QH:102:PC1:H142 | 71:QH:102:PC1:H111 | 1.82 | 0.43 |
| 48:Qb:314:TYR:HB3 | 48:Qb:341:PHE:CD2 | 2.54 | 0.43 |
| 48:Qb:360:CYS:SG | 48:Qb:368:MET:HG3 | 2.59 | 0.43 |
| 49:Qc:47:THR:HG23 | 49:Qc:79:ILE:HG23 | 1.99 | 0.43 |
| 58:Qj:23:MET:O | 58:Qj:27:VAL:HG23 | 2.19 | 0.43 |
| 59:S1:338:VAL:HB | 59:S1:363:SER:CB | 2.48 | 0.43 |
| 60:S2:149:SER:HA | 60:S2:184:THR:HG22 | 2.01 | 0.43 |
| 61:S3:190:ASP:OD1 | 61:S3:191:TYR:N | 2.51 | 0.43 |
| 67:V1:69:LEU:HD22 | 67:V1:147:ARG:HG2 | 2.01 | 0.43 |
| 67:V1:79:GLU:OE2 | 68:V2:246:GLN:NE2 | 2.48 | 0.43 |
| 67:V1:141:GLY:HA2 | 67:V1:252:PRO:HD3 | 1.99 | 0.43 |
| 11:A1:50:ARG:NH1 | 17:A8:97:VAL:O | 2.40 | 0.43 |
| 21:AL:81:ARG:HH11 | 21:AL:89:ASN:HD21 | 1.64 | 0.43 |
| 35:C1:104:LEU:HD23 | 35:C1:104:LEU:HA | 1.85 | 0.43 |
| 71:C3:301:PC1:H132 | 71:C3:301:PC1:H112 | 1.89 | 0.43 |
| 42:N2:276:ILE:C | 42:N2:279:PRO:HD2 | 2.43 | 0.43 |
| 43:N3:64:LEU:O | 43:N3:68:GLU:HG2 | 2.18 | 0.43 |
| 47:Qa:409:PRO:O | 47:Qa:413:LEU:HG | 2.19 | 0.43 |
| 54:Qh:7:HIS:ND1 | 54:Qh:7:HIS:O | 2.51 | 0.43 |
| 3:5B:112:ARG:HA | 3:5B:118:THR:O | 2.18 | 0.43 |
| 8:7B:34:HIS:NE2 | 76:C1:601:3PE:O22 | 2.52 | 0.43 |
| 19:AB:78:ALA:HA | 19:AB:81:ASP:OD2 | 2.19 | 0.43 |
| 20:AK:72:LYS:HG3 | 20:AK:73:GLY:N | 2.34 | 0.43 |
| 41:N1:160:TYR:OH | 43:N3:73:LEU:O | 2.35 | 0.43 |
| 47:Qa:154:LEU:HD23 | 47:Qa:154:LEU:HA | 1.89 | 0.43 |
| 47:Qa:221:ILE:HG12 | 47:Qa:396:VAL:HG12 | 2.01 | 0.43 |
| 47:Qa:408:GLN:NE2 | 47:Qa:409:PRO:HD2 | 2.34 | 0.43 |
| 49:Qc:131:TYR:O | 49:Qc:134:PRO:HD2 | 2.19 | 0.43 |
| 67:V1:44:ASN:ND2 | 67:V1:49:HIS:H | 2.15 | 0.43 |
| 3:5B:38:PRO:HG3 | 7:7A:24:ASN:HD21 | 1.83 | 0.43 |
| 8:7B:60:ILE:HD12 | 38:C4:122:LYS:HG2 | 2.01 | 0.43 |
| 29:B6:92:GLU:HB3 | 29:B6:93:PRO:HD3 | 1.99 | 0.43 |
| 29:B6:148:TYR:CE1 | 33:BK:49:ARG:HG2 | 2.54 | 0.43 |
| 29:B6:164:ILE:HB | 30:B7:48:ASP:HB3 | 2.01 | 0.43 |
| 29:B6:166:PRO:HG2 | 29:B6:180:MET:HG3 | 2.00 | 0.43 |
| 41:N1:179:TRP:CG | 41:N1:180:PRO:HD3 | 2.54 | 0.43 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 44:N4:207:MET:HB3 | 44:N4:298:ILE:HD11 | 2.01 | 0.43 |
| 44:N4:210:TYR:CG | 44:N4:268:GLY:HA3 | 2.54 | 0.43 |
| 45:N5:172:ILE:O | 45:N5:176:ARG:HG2 | 2.19 | 0.43 |
| 45:N5:233:LEU:HB3 | 45:N5:234:PRO:HD3 | 2.00 | 0.43 |
| 45:N5:399:VAL:HG12 | 45:N5:409:LEU:HD13 | 2.00 | 0.43 |
| 47:QA:348:GLY:HA2 | 47:QA:448:PRO:HD3 | 2.00 | 0.43 |
| 49:QC:223:TYR:O | 50:QD:312:TRP:NE1 | 2.39 | 0.43 |
| 54:QH:35:ILE:HG12 | 72:Qd:401:CDL:H542 | 2.00 | 0.43 |
| 47:Qa:270:ALA:O | 47:Qa:438:MET:HA | 2.19 | 0.43 |
| 48:Qb:126:ARG:HH12 | 48:Qb:200:SER:HA | 1.84 | 0.43 |
| 51:Qe:228:ALA:HB3 | 51:Qe:235:TYR:HB3 | 2.01 | 0.43 |
| 53:Qg:44:VAL:O | 53:Qg:48:ILE:HG12 | 2.19 | 0.43 |
| 63:S5:95:PRO:HG2 | 63:S5:98:HIS:HB2 | 2.01 | 0.43 |
| 64:S6:79:VAL:O | 64:S6:121:PRO:HD3 | 2.18 | 0.43 |
| 19:AB:77:GLU:CD | 19:AB:77:GLU:H | 2.27 | 0.43 |
| 74:AC:201:ZMP:H14 | 32:B9:102:ALA:HB1 | 2.00 | 0.43 |
| 20:AK:327:ASP:O | 20:AK:331:GLN:HG2 | 2.19 | 0.43 |
| 22:AM:85:GLU:HG2 | 22:AM:86:TRP:H | 1.84 | 0.43 |
| 39:CA:55:TRP:O | 39:CA:59:ILE:HG12 | 2.19 | 0.43 |
| 41:N1:24:GLU:HG3 | 41:N1:271:LEU:HD22 | 2.00 | 0.43 |
| 42:N2:142:LEU:HB3 | 42:N2:194:LEU:HD21 | 2.00 | 0.43 |
| 42:N2:172:GLN:OE1 | 45:N5:578:SER:OG | 2.22 | 0.43 |
| 45:N5:292:ALA:HB2 | 45:N5:304:PHE:HB3 | 2.01 | 0.43 |
| 47:QA:51:SER:OG | 47:QA:230:LEU:HD12 | 2.19 | 0.43 |
| 47:QA:319:GLN:O | 57:QK:52:ARG:NH2 | 2.40 | 0.43 |
| 51:QE:249:ILE:HG12 | 51:QE:254:ALA:HB3 | 2.00 | 0.43 |
| 48:Qb:113:VAL:HA | 48:Qb:116:MET:HE2 | 2.01 | 0.43 |
| 48:Qb:393:ASN:O | 48:Qb:397:ASN:ND2 | 2.39 | 0.43 |
| 3:5B:54:ALA:O | 3:5B:58:GLY:N | 2.51 | 0.42 |
| 36:C2:186:SER:OG | 36:C2:213:LEU:HD13 | 2.19 | 0.42 |
| 72:CB:203:CDL:H792 | 72:CB:203:CDL:H432 | 2.01 | 0.42 |
| 45:N5:190:LEU:HB2 | 45:N5:196:TRP:NE1 | 2.34 | 0.42 |
| 48:QB:225:LYS:HD2 | 48:QB:257:TYR:CE2 | 2.54 | 0.42 |
| 56:QJ:6:LEU:O | 53:Qg:110:LYS:HD2 | 2.19 | 0.42 |
| 52:Qf:40:ILE:HD13 | 52:Qf:81:CYS:SG | 2.59 | 0.42 |
| 59:S1:253:VAL:HG12 | 59:S1:345:LEU:HD22 | 2.01 | 0.42 |
| 59:S1:467:LYS:HE3 | 59:S1:503:SER:HB3 | 2.00 | 0.42 |
| 60:S2:190:ILE:HG21 | 60:S2:213:ARG:HG3 | 2.00 | 0.42 |
| 64:S6:84:ILE:HD12 | 64:S6:84:ILE:HA | 1.87 | 0.42 |
| 17:A8:124:ARG:NE | 23:AN:80:ASP:OD2 | 2.43 | 0.42 |
| 18:A9:344:PRO:HG2 | 18:A9:347:LEU:HD13 | 2.01 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 23:AN:95:ALA:HA | 23:AN:106:VAL:HG11 | 2.01 | 0.42 |
| 37:C3:156:ARG:HH22 | 37:C3:223:LEU:HA | 1.84 | 0.42 |
| 42:N2:221:HIS:CD2 | 42:N2:240:ILE:HG13 | 2.54 | 0.42 |
| 43:N3:105:GLU:HG2 | 43:N3:110:GLY:HA3 | 2.00 | 0.42 |
| 45:N5:420:ALA:O | 45:N5:424:THR:HG23 | 2.19 | 0.42 |
| 48:QB:271:THR:OG1 | 51:QE:92:ARG:NH2 | 2.44 | 0.42 |
| 49:QC:130:GLY:O | 49:QC:134:PRO:HD3 | 2.19 | 0.42 |
| 49:Qc:296:ALA:HB1 | 78:Qc:404:6F6:O14 | 2.19 | 0.42 |
| 82:Qd:403:PEE:H21 | 82:Qd:403:PEE:H15 | 1.58 | 0.42 |
| 67:V1:62:TRP:CD2 | 67:V1:181:LEU:HD13 | 2.55 | 0.42 |
| 67:V1:115:VAL:HG21 | 67:V1:142:CYS:SG | 2.59 | 0.42 |
| 67:V1:209:GLU:HG3 | 67:V1:210:THR:H | 1.83 | 0.42 |
| 1:4L:35:GLY:HA3 | 46:N6:20:PHE:HZ | 1.84 | 0.42 |
| 7:7A:60:CYS:SG | 37:C3:19:THR:HG23 | 2.59 | 0.42 |
| 71:7B:101:PC1:H222 | 71:7B:101:PC1:H361 | 2.01 | 0.42 |
| 9:7C:19:TYR:CE2 | 35:C1:5:ARG:HG3 | 2.53 | 0.42 |
| 20:AK:97:ASP:OD1 | 42:N2:316:GLN:NE2 | 2.33 | 0.42 |
| 40:CB:15:PHE:HE1 | 77:CB:201:PLX:H261 | 1.85 | 0.42 |
| 44:N4:203:PHE:CE1 | 44:N4:242:GLY:HA3 | 2.54 | 0.42 |
| 47:QA:290:GLN:HB2 | 47:QA:336:PHE:HE1 | 1.84 | 0.42 |
| 48:QB:400:VAL:HG22 | 48:QB:426:LEU:HD21 | 2.00 | 0.42 |
| 51:QE:228:ALA:HB3 | 51:QE:235:TYR:HB3 | 2.01 | 0.42 |
| 55:QI:11:TYR:CZ | 55:QI:16:ARG:HG3 | 2.53 | 0.42 |
| 48:Qb:152:GLN:HE22 | 48:Qb:250:PHE:HA | 1.84 | 0.42 |
| 59:S1:124:HIS:CD2 | 60:S2:381:MET:HE2 | 2.42 | 0.42 |
| 66:S8:150:THR:HG21 | 66:S8:180:HIS:CD2 | 2.54 | 0.42 |
| 67:V1:63:TYR:CE2 | 67:V1:64:LYS:HE3 | 2.54 | 0.42 |
| 2:5A:107:ALA:HB1 | 2:5A:141:ILE:HD13 | 2.02 | 0.42 |
| 71:6A:101:PC1:H153 | 37:C3:184:ALA:HB3 | 2.00 | 0.42 |
| 18:A9:303:ARG:HB2 | 18:A9:316:ARG:HD3 | 2.00 | 0.42 |
| 19:AC:128:PHE:CE2 | 19:AC:151:LYS:HD3 | 2.54 | 0.42 |
| 20:AK:207:VAL:HA | 20:AK:258:LEU:O | 2.20 | 0.42 |
| 32:B9:150:HIS:CD2 | 32:B9:151:PRO:HD2 | 2.54 | 0.42 |
| 35:C1:352:GLY:HA3 | 79:C1:603:HEA:C14 | 2.48 | 0.42 |
| 41:N1:9:LEU:O | 41:N1:13:ILE:HG12 | 2.19 | 0.42 |
| 45:N5:162:THR:O | 45:N5:166:THR:HG23 | 2.20 | 0.42 |
| 45:N5:230:HIS:H | 45:N5:230:HIS:CD2 | 2.36 | 0.42 |
| 45:N5:504:LEU:HD12 | 72:N5:703:CDL:H511 | 2.01 | 0.42 |
| 45:N5:563:PRO:HA | 82:S2:501:PEE:H29 | 2.00 | 0.42 |
| 47:QA:177:LEU:HD11 | 47:QA:272:VAL:HG22 | 2.00 | 0.42 |
| 48:QB:92:PHE:HD2 | 48:QB:211:LEU:HD12 | 1.84 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 49:QC:139:SER:OG | 49:QC:255:ASN:ND2 | 2.48 | 0.42 |
| 72:QC:406:CDL:H151 | 72:QC:406:CDL:H382 | 2.02 | 0.42 |
| 52:QF:56:ARG:NH1 | 52:QF:65:GLU:OE2 | 2.53 | 0.42 |
| 47:Qa:391:GLY:HA2 | 47:Qa:394:ASP:OD2 | 2.19 | 0.42 |
| 49:Qc:119:LEU:HD22 | 83:Qc:403:HEM:HBB2 | 2.00 | 0.42 |
| 50:Qd:222:PRO:HA | 50:Qd:223:PRO:HD3 | 1.94 | 0.42 |
| 59:S1:76:ARG:NH2 | 59:S1:90:ALA:HB2 | 2.34 | 0.42 |
| 62:S4:102:ASP:OD1 | 62:S4:102:ASP:N | 2.53 | 0.42 |
| 67:V1:64:LYS:HE2 | 67:V1:64:LYS:HB3 | 1.83 | 0.42 |
| 68:V2:237:PRO:HA | 68:V2:238:PRO:HD3 | 1.91 | 0.42 |
| 6:6C:49:TYR:CD1 | 38:C4:153:ILE:HG21 | 2.55 | 0.42 |
| 18:A9:262:THR:O | 18:A9:333:PRO:HD2 | 2.20 | 0.42 |
| 77:AL:205:PLX:H341 | 77:AL:205:PLX:H311 | 1.92 | 0.42 |
| 22:AM:28:PHE:HE1 | 77:AM:201:PLX:H112 | 1.84 | 0.42 |
| 26:B3:32:VAL:HG21 | 32:B9:77:ASP:HB2 | 2.02 | 0.42 |
| 27:B4:59:VAL:HG22 | 44:N4:423:ILE:HG12 | 1.99 | 0.42 |
| 30:B7:92:HIS:ND1 | 45:N5:481:THR:OG1 | 2.37 | 0.42 |
| 32:B9:161:PHE:O | 32:B9:165:GLU:HG2 | 2.20 | 0.42 |
| 42:N2:2:ASN:ND2 | 42:N2:4:ILE:H | 2.18 | 0.42 |
| 42:N2:17:THR:HG23 | 42:N2:137:ALA:HB2 | 2.00 | 0.42 |
| 49:QC:316:MET:HE3 | 82:QC:404:PEE:H10 | 2.01 | 0.42 |
| 50:QD:187:ARG:NH1 | 50:QD:192:GLY:O | 2.53 | 0.42 |
| 50:QD:222:PRO:HG3 | 50:QD:234:PHE:HB2 | 2.02 | 0.42 |
| 47:Qa:49:ILE:HG22 | 47:Qa:227:HIS:CE1 | 2.55 | 0.42 |
| 50:Qd:105:SER:HB2 | 50:Qd:284:ASP:CG | 2.45 | 0.42 |
| 52:Qf:31:THR:O | 52:Qf:35:GLU:HG2 | 2.19 | 0.42 |
| 66:S8:63:TRP:HB3 | 66:S8:66:LEU:HD12 | 2.00 | 0.42 |
| 67:V1:44:ASN:C | 67:V1:46:TYR:H | 2.27 | 0.42 |
| 2:5A:143:THR:O | 2:5A:147:LEU:HG | 2.19 | 0.42 |
| 15:A6:48:SER:HB3 | 15:A6:53:GLU:HB2 | 2.00 | 0.42 |
| 20:AK:340:LYS:HE3 | 20:AK:341:TYR:CZ | 2.55 | 0.42 |
| 35:C1:304:TYR:HB2 | 82:C1:609:PEE:H57 | 2.00 | 0.42 |
| 36:C2:104:TRP:CG | 36:C2:203:ASN:HB2 | 2.55 | 0.42 |
| 38:C4:74:SER:O | 38:C4:78:LYS:HG3 | 2.20 | 0.42 |
| 39:CA:72:ARG:HH11 | 40:CB:22:SER:HB3 | 1.84 | 0.42 |
| 42:N2:186:HIS:O | 42:N2:190:MET:HG3 | 2.19 | 0.42 |
| 42:N2:267:ILE:HD11 | 42:N2:283:ALA:HB2 | 2.00 | 0.42 |
| 46:N6:117:PHE:HB2 | 46:N6:119:PHE:CZ | 2.54 | 0.42 |
| 55:QI:11:TYR:OH | 48:Qb:451:ASP:OD2 | 2.30 | 0.42 |
| 49:Qc:113:TRP:HE3 | 83:Qc:403:HEM:HMD1 | 1.83 | 0.42 |
| 59:S1:370:GLU:O | 59:S1:533:GLY:N | 2.50 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 59:S1:537:ILE:HG23 | 59:S1:542:PRO:HD3 | 2.01 | 0.42 |
| 60:S2:113:ARG:HD2 | 60:S2:113:ARG:HA | 1.82 | 0.42 |
| 62:S4:71:HIS:CE1 | 62:S4:120:PRO:HD2 | 2.54 | 0.42 |
| 65:S7:107:GLY:HA2 | 86:S7:301:SF4:S4 | 2.59 | 0.42 |
| 67:V1:137:LYS:HE2 | 67:V1:137:LYS:HB2 | 1.86 | 0.42 |
| 1:4L:55:LEU:HD23 | 1:4L:55:LEU:HA | 1.87 | 0.42 |
| 3:5B:83:ILE:HD11 | 37:C3:2:THR:N | 2.34 | 0.42 |
| 18:A9:303:ARG:HD3 | 18:A9:316:ARG:CZ | 2.50 | 0.42 |
| 18:A9:346:GLU:HG2 | 18:A9:371:PRO:HB3 | 2.01 | 0.42 |
| 19:AC:133:ILE:HG13 | 32:B9:46:SER:HB2 | 2.01 | 0.42 |
| 25:B2:76:ASP:OD1 | 25:B2:76:ASP:N | 2.53 | 0.42 |
| 31:B8:139:PHE:CD2 | 72:N5:703:CDL:H851 | 2.54 | 0.42 |
| 33:BK:98:VAL:HG11 | 34:BL:125:LEU:HD12 | 2.01 | 0.42 |
| 36:C2:161:HIS:HB2 | 36:C2:174:ALA:HB3 | 2.00 | 0.42 |
| 38:C4:146:LEU:HD23 | 38:C4:146:LEU:HA | 1.82 | 0.42 |
| 42:N2:25:HIS:HB2 | 63:S5:15:ASP:HB2 | 2.02 | 0.42 |
| 42:N2:168:GLY:O | 42:N2:172:GLN:HG2 | 2.19 | 0.42 |
| 48:QB:165:ARG:NH1 | 48:QB:208:VAL:O | 2.52 | 0.42 |
| 51:QE:88:PHE:O | 51:QE:92:ARG:HG3 | 2.19 | 0.42 |
| 51:QE:207:LYS:HG3 | 51:QE:208:PRO:HD2 | 2.02 | 0.42 |
| 47:Qa:220:LEU:HD12 | 47:Qa:234:ALA:HB2 | 2.01 | 0.42 |
| 47:Qa:230:LEU:HD23 | 47:Qa:230:LEU:HA | 1.84 | 0.42 |
| 59:S1:432:ILE:HD11 | 59:S1:455:ILE:HD12 | 2.02 | 0.42 |
| 69:V3:420:SER:HB3 | 69:V3:423:HIS:ND1 | 2.35 | 0.42 |
| 11:A1:1:MET:HE2 | 11:A1:1:MET:HB3 | 1.88 | 0.42 |
| 15:A6:78:LEU:HD22 | 15:A6:130:MET:HE3 | 2.01 | 0.42 |
| 20:AK:211:VAL:HB | 20:AK:216:ILE:HD11 | 2.01 | 0.42 |
| 31:B8:94:HIS:O | 31:B8:98:ARG:N | 2.48 | 0.42 |
| 33:BK:130:GLU:OE2 | 33:BK:134:GLN:NE2 | 2.52 | 0.42 |
| 36:C2:165:VAL:HG22 | 36:C2:194:GLY:HA3 | 2.01 | 0.42 |
| 44:N4:73:LEU:HA | 44:N4:76:MET:HE2 | 2.01 | 0.42 |
| 71:N5:704:PC1:H262 | 71:N5:704:PC1:H391 | 2.02 | 0.42 |
| 49:QC:27:ILE:HG12 | 49:QC:224:TYR:OH | 2.20 | 0.42 |
| 48:Qb:172:LEU:HD21 | 48:Qb:202:GLU:HB3 | 2.02 | 0.42 |
| 48:Qb:388:VAL:O | 48:Qb:392:LYS:HG3 | 2.19 | 0.42 |
| 60:S2:87:THR:OG1 | 60:S2:106:GLU:OE1 | 2.23 | 0.42 |
| 67:V1:43:THR:OG1 | 67:V1:44:ASN:N | 2.51 | 0.42 |
| 68:V2:137:THR:HG22 | 68:V2:138:THR:H | 1.84 | 0.42 |
| 11:A1:4:GLU:OE1 | 41:N1:26:LYS:NZ | 2.47 | 0.42 |
| 13:A3:127:ALA:HB2 | 41:N1:312:ALA:HA | 2.01 | 0.42 |
| 14:A5:76:GLN:O | 14:A5:80:VAL:HG23 | 2.20 | 0.42 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 77:AL:205:PLX:H362 | 77:AL:205:PLX:H392 | 1.84 | 0.42 |
| 27:B4:77:TYR:CZ | 45:N5:564:LYS:HG2 | 2.55 | 0.42 |
| 28:B5:110:TRP:O | 28:B5:119:ARG:HG2 | 2.20 | 0.42 |
| 42:N2:169:GLY:HA3 | 42:N2:292:PHE:CE2 | 2.55 | 0.42 |
| 44:N4:10:MET:HE2 | 44:N4:10:MET:HA | 2.02 | 0.42 |
| 45:N5:208:CYS:HA | 45:N5:209:PRO:HD3 | 1.78 | 0.42 |
| 48:QB:121:ASN:OD1 | 48:QB:122:ALA:N | 2.52 | 0.42 |
| 48:QB:223:HIS:HA | 48:QB:228:ARG:HH21 | 1.85 | 0.42 |
| 49:QC:130:GLY:O | 49:QC:133:LEU:HB2 | 2.20 | 0.42 |
| 72:QC:408:CDL:OB4 | 54:Qh:41:ARG:NH2 | 2.53 | 0.42 |
| 50:QD:303:LEU:HB3 | 51:QE:121:THR:OG1 | 2.20 | 0.42 |
| 49:Qc:332:LEU:HD21 | 49:Qc:358:TYR:CE2 | 2.55 | 0.42 |
| 59:S1:68:ARG:HH12 | 59:S1:279:GLU:HG2 | 1.85 | 0.42 |
| 59:S1:501:ARG:NE | 59:S1:506:VAL:HG23 | 2.35 | 0.42 |
| 64:S6:67:ALA:HB1 | 66:S8:110:GLU:HA | 2.02 | 0.42 |
| 69:V3:411:MET:HE2 | 69:V3:411:MET:HB3 | 1.92 | 0.42 |
| 69:V3:418:ARG:NH1 | 69:V3:423:HIS:O | 2.51 | 0.42 |
| 12:A2:89:ARG:HA | 12:A2:92:GLU:HG2 | 2.02 | 0.42 |
| 15:A6:45:PRO:HB3 | 62:S4:53:ILE:HD13 | 2.02 | 0.42 |
| 17:A8:117:ASN:HB3 | 23:AN:73:PRO:HG2 | 2.02 | 0.42 |
| 19:AB:112:SER:H | 74:AB:201:ZMP:P1 | 2.42 | 0.42 |
| 19:AC:113:LEU:HB2 | 32:B9:87:ARG:HH21 | 1.84 | 0.42 |
| 20:AK:172:LEU:HD22 | 20:AK:189:TYR:CD1 | 2.54 | 0.42 |
| 29:B6:183:PHE:CE1 | 30:B7:40:VAL:HG11 | 2.55 | 0.42 |
| 31:B8:48:ARG:HE | 31:B8:48:ARG:HB3 | 1.71 | 0.42 |
| 35:C1:91:ASP:OD1 | 35:C1:92:MET:N | 2.41 | 0.42 |
| 35:C1:143:VAL:HB | 35:C1:213:ARG:CZ | 2.50 | 0.42 |
| 79:C1:603:HEA:HHA | 79:C1:603:HEA:HAD2 | 1.92 | 0.42 |
| 42:N2:14:MET:O | 42:N2:18:MET:HG2 | 2.19 | 0.42 |
| 42:N2:88:LYS:HE3 | 42:N2:88:LYS:HB3 | 1.87 | 0.42 |
| 42:N2:111:PHE:HA | 45:N5:591:PHE:CE1 | 2.55 | 0.42 |
| 42:N2:178:ILE:HG23 | 42:N2:292:PHE:CE1 | 2.55 | 0.42 |
| 45:N5:149:ILE:HD11 | 72:N5:702:CDL:H171 | 2.01 | 0.42 |
| 47:QA:438:MET:HB3 | 47:QA:450:VAL:HG22 | 2.02 | 0.42 |
| 49:QC:327:MET:HA | 54:Qh:52:PRO:HB3 | 2.01 | 0.42 |
| 54:QH:37:ASN:OD1 | 54:QH:40:ARG:NH2 | 2.41 | 0.42 |
| 47:Qa:183:ARG:HG3 | 47:Qa:254:ARG:HB2 | 2.02 | 0.42 |
| 59:S1:330:LEU:HD23 | 59:S1:330:LEU:HA | 1.93 | 0.42 |
| 61:S3:173:MET:HE2 | 61:S3:188:LEU:HB2 | 2.01 | 0.42 |
| 67:V1:384:PRO:HG2 | 67:V1:422:HIS:O | 2.19 | 0.42 |
| 72:6A:102:CDL:H152 | 72:6A:102:CDL:H182 | 1.84 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 35:C1:71:MET:HB2 | 35:C1:72:PRO:HD3 | 2.02 | 0.41 |
| 44:N4:400:MET:HE1 | 45:N5:183:VAL:HG21 | 2.02 | 0.41 |
| 45:N5:297:ASP:O | 45:N5:301:ILE:HG13 | 2.21 | 0.41 |
| 47:QA:239:ASN:OD1 | 47:QA:239:ASN:N | 2.53 | 0.41 |
| 47:QA:272:VAL:HA | 47:QA:337:GLY:HA3 | 2.02 | 0.41 |
| 48:QB:304:LEU:HD13 | 48:QB:354:LEU:HD22 | 2.00 | 0.41 |
| 51:QE:133:VAL:HG22 | 82:QE:302:PEE:H38 | 2.02 | 0.41 |
| 51:QE:239:HIS:HB2 | 85:QE:304:FES:S1 | 2.60 | 0.41 |
| 53:QG:41:ASP:OD1 | 53:QG:41:ASP:N | 2.45 | 0.41 |
| 72:QH:101:CDL:HB62 | 49:Qc:29:SER:HB2 | 2.02 | 0.41 |
| 47:Qa:72:GLU:O | 47:Qa:188:ASN:ND2 | 2.53 | 0.41 |
| 49:Qc:165:TRP:O | 49:Qc:174:THR:OG1 | 2.29 | 0.41 |
| 65:S7:154:ASP:OD1 | 65:S7:154:ASP:N | 2.48 | 0.41 |
| 4:6A:81:LEU:HD22 | 71:6A:101:PC1:H221 | 2.01 | 0.41 |
| 7:7A:53:TYR:CE1 | 37:C3:15:PRO:HG3 | 2.55 | 0.41 |
| 15:A6:140:ARG:HA | 15:A6:140:ARG:HE | 1.85 | 0.41 |
| 16:A7:54:TYR:CZ | 60:S2:368:LYS:HD2 | 2.55 | 0.41 |
| 19:AC:117:GLU:OE2 | 32:B9:62:TYR:OH | 2.38 | 0.41 |
| 23:AN:120:MET:HE2 | 23:AN:120:MET:HB3 | 1.88 | 0.41 |
| 28:B5:139:ILE:O | 28:B5:143:GLU:HG2 | 2.20 | 0.41 |
| 41:N1:73:ILE:HD13 | 41:N1:73:ILE:HA | 1.91 | 0.41 |
| 46:N6:170:GLU:CD | 46:N6:173:ARG:HH21 | 2.28 | 0.41 |
| 82:QB:503:PEE:H39 | 82:QB:503:PEE:H72 | 2.02 | 0.41 |
| 47:Qa:125:CYS:SG | 47:Qa:133:LEU:HD22 | 2.60 | 0.41 |
| 47:Qa:297:PRO:HB3 | 47:Qa:304:ASN:HD21 | 1.85 | 0.41 |
| 51:Qe:156:LEU:HB2 | 51:Qe:269:ASP:HA | 2.02 | 0.41 |
| 59:S1:304:GLN:HB2 | 59:S1:316:TYR:HD1 | 1.85 | 0.41 |
| 67:V1:347:THR:HG22 | 67:V1:348:GLY:H | 1.85 | 0.41 |
| 4:6A:79:HIS:HD2 | 4:6A:83:HIS:CD2 | 2.38 | 0.41 |
| 15:A6:127:THR:O | 15:A6:131:ARG:HG3 | 2.20 | 0.41 |
| 18:A9:168:SER:HA | 18:A9:184:LYS:NZ | 2.35 | 0.41 |
| 20:AK:145:TYR:OH | 20:AK:201:LEU:O | 2.21 | 0.41 |
| 77:AL:205:PLX:H1C3 | 77:AL:205:PLX:H21 | 1.84 | 0.41 |
| 27:B4:63:PRO:O | 27:B4:67:ARG:HG3 | 2.20 | 0.41 |
| 35:C1:372:TYR:N | 35:C1:432:GLY:HA3 | 2.35 | 0.41 |
| 36:C2:93:PRO:HG2 | 36:C2:151:ARG:CZ | 2.50 | 0.41 |
| 37:C3:205:GLY:O | 37:C3:208:VAL:HG22 | 2.20 | 0.41 |
| 77:CB:201:PLX:H112 | 77:CB:201:PLX:H81 | 1.76 | 0.41 |
| 47:QA:301:ARG:HG2 | 57:QK:53:GLU:HB3 | 2.03 | 0.41 |
| 48:QB:363:MET:O | 48:QB:464:GLN:NE2 | 2.54 | 0.41 |
| 50:QD:97:TRP:NE1 | 50:QD:210:ASP:OD1 | 2.42 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 52:QF:34:ARG:NH2 | 50:Qd:217:THR:O | 2.51 | 0.41 |
| 47:Qa:68:GLY:H | 47:Qa:71:TYR:HD2 | 1.68 | 0.41 |
| 51:Qe:249:ILE:HG12 | 51:Qe:254:ALA:O | 2.20 | 0.41 |
| 6:6C:70:ILE:HD11 | 38:C4:147:ASP:HB3 | 2.02 | 0.41 |
| 16:A7:31:ILE:HD12 | 22:AM:56:PHE:CG | 2.55 | 0.41 |
| 35:C1:438:ARG:NH2 | 79:C1:603:HEA:O2D | 2.53 | 0.41 |
| 36:C2:158:ASP:OD1 | 36:C2:159:VAL:HG22 | 2.21 | 0.41 |
| 44:N4:368:ALA:HB1 | 44:N4:375:LEU:HA | 2.02 | 0.41 |
| 59:S1:449:PRO:HB2 | 59:S1:679:LEU:HD13 | 2.02 | 0.41 |
| 1:4L:3:LEU:HG | 46:N6:121:GLY:HA3 | 2.01 | 0.41 |
| 1:4L:23:ARG:NH2 | 46:N6:86:ASN:HD22 | 2.16 | 0.41 |
| 10:8B:43:LEU:HD23 | 10:8B:43:LEU:HA | 1.90 | 0.41 |
| 18:A9:221:ARG:HD2 | 18:A9:286:ARG:NH1 | 2.35 | 0.41 |
| 79:C1:602:HEA:HBA2 | 79:C1:602:HEA:CMA | 2.51 | 0.41 |
| 37:C3:208:VAL:HG12 | 37:C3:245:VAL:CG1 | 2.51 | 0.41 |
| 43:N3:65:PHE:CD2 | 43:N3:98:LEU:HD11 | 2.55 | 0.41 |
| 45:N5:176:ARG:HA | 45:N5:176:ARG:HD2 | 1.85 | 0.41 |
| 45:N5:213:LEU:HB3 | 45:N5:273:VAL:HG11 | 2.03 | 0.41 |
| 46:N6:65:LEU:HA | 46:N6:65:LEU:HD23 | 1.76 | 0.41 |
| 47:QA:68:GLY:N | 47:QA:208:TYR:OH | 2.50 | 0.41 |
| 48:QB:57:LEU:HD12 | 48:QB:229:MET:O | 2.21 | 0.41 |
| 47:Qa:66:LYS:O | 47:Qa:217:ARG:NH2 | 2.48 | 0.41 |
| 49:Qc:46:LEU:HD21 | 82:Qd:403:PEE:H35 | 2.03 | 0.41 |
| 82:Qh:103:PEE:H26 | 82:Qh:103:PEE:H32 | 1.84 | 0.41 |
| 59:S1:534:VAL:HG22 | 59:S1:537:ILE:HB | 2.02 | 0.41 |
| 60:S2:230:ALA:O | 66:S8:98:ARG:NH2 | 2.54 | 0.41 |
| 61:S3:150:LEU:HD12 | 62:S4:59:LEU:HD11 | 2.03 | 0.41 |
| 15:A6:145:LEU:HD12 | 15:A6:145:LEU:HA | 1.87 | 0.41 |
| 27:B4:77:TYR:OH | 45:N5:564:LYS:HG2 | 2.21 | 0.41 |
| 35:C1:96:ARG:H | 35:C1:96:ARG:HG3 | 1.51 | 0.41 |
| 35:C1:331:ASN:HD21 | 38:C4:42:ARG:HB2 | 1.85 | 0.41 |
| 35:C1:417:MET:O | 35:C1:421:VAL:HG22 | 2.21 | 0.41 |
| 41:N1:102:VAL:HG21 | 41:N1:154:LEU:HD11 | 2.02 | 0.41 |
| 45:N5:420:ALA:HB1 | 45:N5:498:PHE:CD1 | 2.56 | 0.41 |
| 49:QC:318:ARG:NH1 | 49:QC:321:SER:OG | 2.53 | 0.41 |
| 51:QE:153:GLU:HB3 | 51:QE:270:LEU:HD11 | 2.03 | 0.41 |
| 54:QH:20:SER:O | 54:QH:24:GLN:HG2 | 2.20 | 0.41 |
| 48:Qb:156:LEU:HB2 | 48:Qb:213:ARG:NH1 | 2.35 | 0.41 |
| 59:S1:295:ASP:OD2 | 59:S1:706:THR:OG1 | 2.29 | 0.41 |
| 59:S1:547:LEU:HB3 | 59:S1:550:ALA:HB3 | 2.02 | 0.41 |
| 68:V2:66:ILE:HG21 | 68:V2:81:PRO:HB2 | 2.03 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 18:A9:216:TYR:HE1 | 18:A9:314:THR:HB | 1.86 | 0.41 |
| 19:AC:79:ILE:O | 19:AC:83:VAL:HG13 | 2.21 | 0.41 |
| 20:AK:134:GLN:NE2 | 75:AK:401:ADP:HN62 | 2.16 | 0.41 |
| 72:B5:202:CDL:H191 | 72:B5:202:CDL:H731 | 2.01 | 0.41 |
| 29:B6:72:LEU:HD23 | 29:B6:72:LEU:HA | 1.88 | 0.41 |
| 32:B9:69:LEU:HD21 | 32:B9:82:PHE:HB3 | 2.02 | 0.41 |
| 35:C1:115:SER:OG | 35:C1:142:SER:O | 2.38 | 0.41 |
| 35:C1:307:SER:O | 35:C1:311:ILE:HG23 | 2.20 | 0.41 |
| 41:N1:289:LEU:HA | 41:N1:293:PHE:HB2 | 2.03 | 0.41 |
| 45:N5:10:THR:O | 45:N5:14:ILE:HG23 | 2.20 | 0.41 |
| 45:N5:67:HIS:O | 82:N5:701:PEE:H11 | 2.21 | 0.41 |
| 46:N6:116:ILE:H | 46:N6:116:ILE:HD12 | 1.86 | 0.41 |
| 46:N6:123:GLY:O | 46:N6:127:ILE:HG23 | 2.21 | 0.41 |
| 49:QC:200:LEU:HD23 | 49:QC:201:HIS:HD2 | 1.85 | 0.41 |
| 57:QK:55:LEU:HA | 57:QK:55:LEU:HD23 | 1.84 | 0.41 |
| 51:Qe:88:PHE:O | 51:Qe:92:ARG:HG3 | 2.21 | 0.41 |
| 60:S2:69:PRO:HA | 60:S2:70:PRO:HD3 | 1.96 | 0.41 |
| 60:S2:151:MET:HG3 | 60:S2:220:TYR:CZ | 2.56 | 0.41 |
| 60:S2:290:LEU:O | 60:S2:293:GLY:CA | 2.69 | 0.41 |
| 64:S6:116:LEU:HD23 | 64:S6:116:LEU:HA | 1.93 | 0.41 |
| 65:S7:140:GLY:HA3 | 65:S7:144:HIS:CD2 | 2.56 | 0.41 |
| 1:4L:38:LEU:HD21 | 46:N6:37:GLY:HA2 | 2.02 | 0.41 |
| 4:6A:60:ILE:O | 4:6A:62:TYR:N | 2.50 | 0.41 |
| 15:A6:107:LEU:HD23 | 15:A6:107:LEU:HA | 1.94 | 0.41 |
| 15:A6:131:ARG:NH2 | 61:S3:210:LEU:HD21 | 2.36 | 0.41 |
| 18:A9:118:LYS:HE2 | 18:A9:118:LYS:HB3 | 1.86 | 0.41 |
| 28:B5:181:HIS:HE1 | 63:S5:38:LYS:HE2 | 1.86 | 0.41 |
| 77:B5:201:PLX:H21 | 77:B5:201:PLX:H1B3 | 1.89 | 0.41 |
| 30:B7:16:GLU:HA | 30:B7:17:PRO:HD3 | 1.95 | 0.41 |
| 37:C3:63:ARG:HA | 37:C3:67:PHE:CD2 | 2.56 | 0.41 |
| 44:N4:200:ILE:O | 44:N4:204:MET:HG2 | 2.21 | 0.41 |
| 45:N5:102:GLU:OE1 | 45:N5:456:ARG:NH2 | 2.29 | 0.41 |
| 45:N5:260:LEU:HD23 | 45:N5:260:LEU:HA | 1.88 | 0.41 |
| 49:QC:133:LEU:HD23 | 49:QC:133:LEU:HA | 1.78 | 0.41 |
| 47:Qa:60:ARG:HD3 | 47:Qa:393:LEU:HD22 | 2.03 | 0.41 |
| 48:Qb:157:GLU:O | 48:Qb:161:ILE:HG12 | 2.20 | 0.41 |
| 48:Qb:418:LEU:HD23 | 48:Qb:418:LEU:HA | 1.92 | 0.41 |
| 49:Qc:237:LEU:HB2 | 50:Qd:297:MET:HG2 | 2.03 | 0.41 |
| 59:S1:555:ILE:HD13 | 59:S1:555:ILE:HA | 1.94 | 0.41 |
| 59:S1:638:THR:O | 59:S1:642:VAL:HG23 | 2.21 | 0.41 |
| 67:V1:235:VAL:H | 67:V1:240:THR:HG21 | 1.85 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:4L:9:ILE:HG12 | 42:N2:72:MET:HE1 | 2.03 | 0.41 |
| 10:8B:31:ARG:HD2 | 35:C1:481:GLU:CD | 2.46 | 0.41 |
| 12:A2:69:TYR:HE2 | 12:A2:75:LYS:HD3 | 1.85 | 0.41 |
| 19:AB:93:ILE:HD12 | 19:AB:108:LEU:HD13 | 2.03 | 0.41 |
| 19:AC:140:CYS:HB3 | 19:AC:143:GLU:HG3 | 2.03 | 0.41 |
| 20:AK:41:GLY:HA2 | 20:AK:298:MET:SD | 2.61 | 0.41 |
| 20:AK:256:GLU:HG2 | 20:AK:280:CYS:SG | 2.61 | 0.41 |
| 76:AL:202:3PE:H3B1 | 76:AL:202:3PE:H382 | 1.92 | 0.41 |
| 23:AN:88:ARG:O | 23:AN:92:GLU:HG2 | 2.21 | 0.41 |
| 23:AN:119:PRO:HB3 | 23:AN:123:GLU:HB2 | 2.02 | 0.41 |
| 27:B4:129:TYR:O | 44:N4:307:TRP:HB2 | 2.21 | 0.41 |
| 77:B5:201:PLX:H271 | 77:B5:201:PLX:H24 | 1.83 | 0.41 |
| 32:B9:47:ALA:HB1 | 32:B9:194:GLU:HB2 | 2.03 | 0.41 |
| 35:C1:12:HIS:CG | 35:C1:84:PRO:HG2 | 2.55 | 0.41 |
| 35:C1:202:LEU:HD22 | 35:C1:238:PHE:CE2 | 2.55 | 0.41 |
| 36:C2:143:VAL:HG12 | 36:C2:219:PHE:HD1 | 1.86 | 0.41 |
| 36:C2:145:PRO:HG3 | 36:C2:219:PHE:CD2 | 2.56 | 0.41 |
| 37:C3:86:PHE:CZ | 71:C3:301:PC1:H3A1 | 2.56 | 0.41 |
| 37:C3:144:ILE:HD12 | 37:C3:144:ILE:HA | 1.84 | 0.41 |
| 37:C3:148:HIS:HB2 | 37:C3:235:PHE:HE2 | 1.85 | 0.41 |
| 38:C4:130:PRO:HG2 | 38:C4:133:PHE:CE1 | 2.56 | 0.41 |
| 42:N2:218:LEU:HB3 | 42:N2:244:MET:HE2 | 2.03 | 0.41 |
| 42:N2:291:TYR:HA | 44:N4:151:PHE:HZ | 1.85 | 0.41 |
| 47:QA:183:ARG:HG3 | 47:QA:254:ARG:HB2 | 2.03 | 0.41 |
| 49:QC:277:ALA:HB1 | 49:QC:294:LEU:HG | 2.03 | 0.41 |
| 51:QE:122:THR:HG21 | 55:Qi:25:ILE:HD13 | 2.03 | 0.41 |
| 54:QH:6:GLY:HA3 | 48:Qb:363:MET:SD | 2.61 | 0.41 |
| 47:Qa:125:CYS:HB3 | 47:Qa:133:LEU:HD22 | 2.03 | 0.41 |
| 48:Qb:190:THR:HB | 48:Qb:275:ILE:HG13 | 2.03 | 0.41 |
| 48:Qb:407:THR:HB | 48:Qb:408:PRO:HD3 | 2.03 | 0.41 |
| 51:Qe:156:LEU:N | 51:Qe:269:ASP:O | 2.45 | 0.41 |
| 51:Qe:197:ASP:O | 51:Qe:199:GLN:N | 2.53 | 0.41 |
| 51:Qe:220:LEU:HD12 | 51:Qe:239:HIS:HE1 | 1.86 | 0.41 |
| 53:Qg:88:LYS:HD3 | 53:Qg:88:LYS:HA | 1.89 | 0.41 |
| 59:S1:371:VAL:O | 59:S1:482:GLN:NE2 | 2.54 | 0.41 |
| 10:8B:50:PHE:O | 10:8B:53:PRO:HD2 | 2.21 | 0.41 |
| 25:B2:76:ASP:O | 45:N5:385:TYR:OH | 2.27 | 0.41 |
| 36:C2:11:ASP:OD1 | 36:C2:11:ASP:N | 2.54 | 0.41 |
| 47:QA:214:THR:O | 47:QA:218:MET:HG3 | 2.21 | 0.41 |
| 49:QC:119:LEU:HD22 | 83:QC:403:HEM:HBB2 | 2.03 | 0.41 |
| 51:QE:218:THR:HG21 | 51:QE:256:LEU:HB2 | 2.02 | 0.41 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 72:Qb:501:CDL:HA32 | 71:Qb:502:PC1:H151 | 2.02 | 0.41 |
| 59:S1:436:VAL:O | 59:S1:442:TYR:OH | 2.26 | 0.41 |
| 60:S2:277:ARG:NH2 | 60:S2:451:ALA:HB1 | 2.36 | 0.41 |
| 62:S4:168:LYS:HA | 62:S4:168:LYS:HD3 | 1.92 | 0.41 |
| 3:5B:33:SER:OG | 3:5B:34:GLY:N | 2.54 | 0.40 |
| 7:7A:52:LEU:HD23 | 7:7A:52:LEU:HA | 1.93 | 0.40 |
| 15:A6:88:LYS:O | 15:A6:92:MET:HG2 | 2.21 | 0.40 |
| 72:A8:301:CDL:H221 | 72:A8:301:CDL:H252 | 1.90 | 0.40 |
| 28:B5:176:LYS:H | 63:S5:45:HIS:CD2 | 2.39 | 0.40 |
| 31:B8:109:LEU:O | 31:B8:113:ILE:HG23 | 2.22 | 0.40 |
| 35:C1:38:ARG:HG3 | 35:C1:458:SER:CB | 2.51 | 0.40 |
| 35:C1:195:LEU:HD23 | 35:C1:245:ILE:HD13 | 2.02 | 0.40 |
| 44:N4:9:THR:O | 44:N4:13:PRO:HD3 | 2.21 | 0.40 |
| 45:N5:200:GLN:HE21 | 45:N5:204:LEU:HD11 | 1.85 | 0.40 |
| 45:N5:504:LEU:HD23 | 45:N5:504:LEU:HA | 1.90 | 0.40 |
| 71:QC:405:PC1:H242 | 50:QD:102:LEU:HD21 | 2.03 | 0.40 |
| 51:QE:202:LEU:HD11 | 51:QE:208:PRO:HB3 | 2.03 | 0.40 |
| 54:QH:67:PHE:HE1 | 49:Qc:344:GLU:HG3 | 1.86 | 0.40 |
| 55:QI:63:LYS:HE2 | 55:QI:63:LYS:HB2 | 1.94 | 0.40 |
| 47:Qa:115:THR:HG23 | 47:Qa:118:SER:H | 1.86 | 0.40 |
| 49:Qc:32:ASN:ND2 | 49:Qc:228:ASP:HA | 2.36 | 0.40 |
| 59:S1:691:ILE:HG12 | 59:S1:695:TYR:CE2 | 2.56 | 0.40 |
| 60:S2:149:SER:HA | 60:S2:184:THR:CG2 | 2.51 | 0.40 |
| 60:S2:204:THR:HB | 60:S2:208:TRP:CZ2 | 2.55 | 0.40 |
| 62:S4:56:ASP:OD1 | 62:S4:56:ASP:N | 2.54 | 0.40 |
| 65:S7:190:LEU:HD23 | 65:S7:190:LEU:HA | 1.86 | 0.40 |
| 71:6A:101:PC1:H241 | 35:C1:215:LEU:HD21 | 2.03 | 0.40 |
| 71:7B:101:PC1:H152 | 71:7B:101:PC1:H111 | 1.85 | 0.40 |
| 16:A7:101:ILE:HG22 | 61:S3:136:ARG:O | 2.21 | 0.40 |
| 18:A9:246:SER:O | 18:A9:250:ILE:HG12 | 2.22 | 0.40 |
| 30:B7:15:LYS:HD2 | 30:B7:113:LYS:HG3 | 2.03 | 0.40 |
| 30:B7:76:ASN:ND2 | 30:B7:79:ALA:HB2 | 2.36 | 0.40 |
| 38:C4:62:LEU:HG | 38:C4:81:LEU:HD21 | 2.03 | 0.40 |
| 41:N1:170:GLU:HG2 | 41:N1:171:HIS:HD2 | 1.86 | 0.40 |
| 41:N1:290:TRP:HB3 | 43:N3:111:LEU:HD13 | 2.03 | 0.40 |
| 44:N4:231:LEU:HD23 | 44:N4:235:LEU:HD12 | 2.02 | 0.40 |
| 44:N4:398:MET:O | 44:N4:402:ILE:HG13 | 2.21 | 0.40 |
| 51:QE:190:VAL:HG21 | 51:QE:250:ARG:NH2 | 2.36 | 0.40 |
| 56:QJ:14:ALA:O | 56:QJ:18:ILE:HG12 | 2.22 | 0.40 |
| 49:Qc:24:PRO:HB2 | 49:Qc:27:ILE:HG23 | 2.01 | 0.40 |
| 49:Qc:197:LEU:HD11 | 83:Qc:403:HEM:HMA3 | 2.02 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 58:Qj:42:LEU:HA | 58:Qj:45:VAL:HG22 | 2.03 | 0.40 |
| 59:S1:696:MET:HG2 | 59:S1:711:VAL:HG21 | 2.03 | 0.40 |
| 60:S2:149:SER:HB2 | 60:S2:152:CYS:HB2 | 2.04 | 0.40 |
| 60:S2:323:ASP:OD1 | 66:S8:37:THR:OG1 | 2.30 | 0.40 |
| 64:S6:74:GLN:NE2 | 64:S6:75:PRO:HD2 | 2.36 | 0.40 |
| 1:4L:37:MET:HE1 | 1:4L:63:LEU:HD11 | 2.04 | 0.40 |
| 1:4L:62:ILE:HG21 | 42:N2:31:ILE:HD11 | 2.03 | 0.40 |
| 2:5A:134:PRO:O | 2:5A:138:GLU:HG2 | 2.21 | 0.40 |
| 30:B7:22:MET:HE1 | 30:B7:102:PHE:CD2 | 2.56 | 0.40 |
| 32:B9:99:MET:HA | 32:B9:99:MET:HE2 | 2.04 | 0.40 |
| 32:B9:178:GLU:OE2 | 32:B9:209:TRP:NE1 | 2.52 | 0.40 |
| 35:C1:390:MET:HE2 | 79:C1:602:HEA:H202 | 2.03 | 0.40 |
| 35:C1:469:ILE:HD12 | 35:C1:469:ILE:HA | 1.93 | 0.40 |
| 36:C2:130:PRO:HA | 38:C4:137:TRP:CH2 | 2.57 | 0.40 |
| 41:N1:206:GLU:HB2 | 60:S2:90:PHE:CE2 | 2.56 | 0.40 |
| 42:N2:277:ILE:H | 42:N2:277:ILE:HD12 | 1.86 | 0.40 |
| 44:N4:1:MET:HG2 | 44:N4:52:PHE:CD2 | 2.56 | 0.40 |
| 45:N5:176:ARG:O | 45:N5:180:ILE:HG13 | 2.21 | 0.40 |
| 45:N5:290:LEU:O | 45:N5:293:ILE:HG12 | 2.22 | 0.40 |
| 48:QB:341:PHE:HB2 | 48:QB:358:PHE:HB3 | 2.02 | 0.40 |
| 49:QC:310:SER:HB2 | 49:QC:370:SER:HB3 | 2.02 | 0.40 |
| 51:QE:154:ILE:HD13 | 51:QE:176:VAL:HG21 | 2.03 | 0.40 |
| 51:QE:207:LYS:HE2 | 51:QE:265:PHE:CE1 | 2.56 | 0.40 |
| 77:QI:301:PLX:H122 | 77:QI:301:PLX:H91 | 1.98 | 0.40 |
| 59:S1:257:VAL:HG11 | 59:S1:413:LEU:HB2 | 2.03 | 0.40 |
| 59:S1:341:ILE:HG13 | 59:S1:545:LEU:HD11 | 2.02 | 0.40 |
| 59:S1:372:PHE:CZ | 59:S1:385:TYR:HB3 | 2.57 | 0.40 |
| 59:S1:598:ASN:HD21 | 59:S1:600:GLU:HG2 | 1.86 | 0.40 |
| 60:S2:292:TYR:O | 61:S3:162:ALA:HB2 | 2.20 | 0.40 |
| 64:S6:104:LYS:HG2 | 64:S6:107:LYS:HG2 | 2.04 | 0.40 |
| 4:6A:29:ARG:HB2 | 37:C3:146:TRP:CE2 | 2.56 | 0.40 |
| 5:6B:37:PHE:CE1 | 5:6B:58:ARG:HB2 | 2.57 | 0.40 |
| 15:A6:63:ARG:HG2 | 19:AB:120:MET:SD | 2.62 | 0.40 |
| 26:B3:47:ARG:HA | 26:B3:50:ALA:HB3 | 2.03 | 0.40 |
| 28:B5:163:ARG:HH22 | 40:CB:102:ASP:CG | 2.28 | 0.40 |
| 35:C1:240:HIS:O | 35:C1:243:VAL:HG22 | 2.21 | 0.40 |
| 77:C2:301:PLX:H21 | 77:C2:301:PLX:H1C3 | 1.65 | 0.40 |
| 41:N1:245:ALA:HB3 | 41:N1:255:TYR:CE2 | 2.56 | 0.40 |
| 42:N2:190:MET:HG2 | 42:N2:204:ASN:HB3 | 2.03 | 0.40 |
| 45:N5:572:LYS:HD3 | 45:N5:572:LYS:HA | 1.93 | 0.40 |
| 47:QA:257:GLU:OE2 | 47:QA:259:ARG:HD3 | 2.21 | 0.40 |

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| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 48:QB:56:GLY:HA3 | 48:QB:227:PRO:HB3 | 2.03 | 0.40 |
| 47:Qa:195:TYR:CZ | 47:Qa:196:ARG:HG2 | 2.56 | 0.40 |
| 48:Qb:172:LEU:HD23 | 48:Qb:172:LEU:HA | 1.91 | 0.40 |
| 49:Qc:33:PHE:HA | 49:Qc:36:LEU:HB2 | 2.04 | 0.40 |
| 59:S1:560:LEU:HD12 | 59:S1:566:ILE:HD11 | 2.04 | 0.40 |
| 67:V1:244:ASN:OD1 | 67:V1:245:VAL:N | 2.53 | 0.40 |
| 23:AN:19:ILE:HD12 | 60:S2:351:SER:HB2 | 2.04 | 0.40 |
| 25:B2:53:SER:HA | 25:B2:56:ILE:HG12 | 2.04 | 0.40 |
| 25:B2:65:MET:SD | 45:N5:375:ILE:HG12 | 2.61 | 0.40 |
| 33:BK:97:LYS:HE3 | 33:BK:97:LYS:HB3 | 1.89 | 0.40 |
| 41:N1:2:PHE:CE2 | 41:N1:6:ILE:HD11 | 2.56 | 0.40 |
| 42:N2:43:VAL:HG11 | 42:N2:129:LEU:HD23 | 2.04 | 0.40 |
| 44:N4:282:LEU:O | 44:N4:286:ILE:HG13 | 2.21 | 0.40 |
| 44:N4:302:MET:HE2 | 44:N4:302:MET:HA | 2.03 | 0.40 |
| 45:N5:389:PHE:O | 45:N5:393:ASP:HB3 | 2.22 | 0.40 |
| 45:N5:504:LEU:O | 45:N5:507:THR:OG1 | 2.38 | 0.40 |
| 48:QB:274:GLU:CD | 48:QB:276:ARG:HH21 | 2.30 | 0.40 |
| 49:QC:103:TYR:CG | 82:QC:404:PEE:H16 | 2.56 | 0.40 |
| 55:Qi:3:ALA:HA | 55:Qi:4:PRO:HD3 | 1.98 | 0.40 |
| 59:S1:267:THR:HB | 62:S4:115:SER:HB2 | 2.03 | 0.40 |
| 59:S1:275:PRO:HG3 | 59:S1:286:ILE:HG12 | 2.04 | 0.40 |
| 60:S2:448:HIS:HB3 | 60:S2:452:ASP:HB2 | 2.04 | 0.40 |
| 67:V1:99:TRP:CD1 | 67:V1:99:TRP:N | 2.88 | 0.40 |
| 67:V1:258:GLY:HA2 | 68:V2:246:GLN:CD | 2.47 | 0.40 |
| 67:V1:270:ASN:ND2 | 67:V1:338:ASP:OD2 | 2.54 | 0.40 |

There are no symmetry-related clashes.

## 5.3 Torsion angles (i)

### 5.3.1 Protein backbone (i)

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

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles |
|---|---|---|---|---|---|---|
| 1 | 4L | 96/98 (98%) | 94 (98%) | 2 (2%) | 0 | 100 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|---|---|---|---|---|---|---|---|
| 2 | 5A | 100/102 (98%) | 99 (99%) | 1 (1%) | 0 | 100 | 100 |
| 3 | 5B | 93/95 (98%) | 88 (95%) | 5 (5%) | 0 | 100 | 100 |
| 4 | 6A | 73/75 (97%) | 70 (96%) | 3 (4%) | 0 | 100 | 100 |
| 5 | 6B | 80/82 (98%) | 76 (95%) | 4 (5%) | 0 | 100 | 100 |
| 6 | 6C | 68/70 (97%) | 66 (97%) | 2 (3%) | 0 | 100 | 100 |
| 7 | 7A | 55/57 (96%) | 55 (100%) | 0 | 0 | 100 | 100 |
| 8 | 7B | 48/50 (96%) | 46 (96%) | 2 (4%) | 0 | 100 | 100 |
| 9 | 7C | 45/47 (96%) | 44 (98%) | 1 (2%) | 0 | 100 | 100 |
| 10 | 8B | 41/43 (95%) | 41 (100%) | 0 | 0 | 100 | 100 |
| 11 | A1 | 68/70 (97%) | 68 (100%) | 0 | 0 | 100 | 100 |
| 12 | A2 | 83/85 (98%) | 79 (95%) | 4 (5%) | 0 | 100 | 100 |
| 13 | A3 | 81/83 (98%) | 78 (96%) | 3 (4%) | 0 | 100 | 100 |
| 14 | A5 | 110/112 (98%) | 105 (96%) | 5 (4%) | 0 | 100 | 100 |
| 15 | A6 | 112/114 (98%) | 107 (96%) | 5 (4%) | 0 | 100 | 100 |
| 16 | A7 | 93/112 (83%) | 89 (96%) | 4 (4%) | 0 | 100 | 100 |
| 17 | A8 | 169/171 (99%) | 166 (98%) | 3 (2%) | 0 | 100 | 100 |
| 18 | A9 | 333/341 (98%) | 322 (97%) | 11 (3%) | 0 | 100 | 100 |
| 19 | AB | 75/156 (48%) | 74 (99%) | 1 (1%) | 0 | 100 | 100 |
| 19 | AC | 85/156 (54%) | 85 (100%) | 0 | 0 | 100 | 100 |
| 20 | AK | 318/320 (99%) | 306 (96%) | 12 (4%) | 0 | 100 | 100 |
| 21 | AL | 138/140 (99%) | 136 (99%) | 2 (1%) | 0 | 100 | 100 |
| 22 | AM | 141/143 (99%) | 138 (98%) | 3 (2%) | 0 | 100 | 100 |
| 23 | AN | 140/142 (99%) | 132 (94%) | 8 (6%) | 0 | 100 | 100 |
| 24 | B1 | 54/56 (96%) | 54 (100%) | 0 | 0 | 100 | 100 |
| 25 | B2 | 65/67 (97%) | 65 (100%) | 0 | 0 | 100 | 100 |
| 26 | B3 | 77/79 (98%) | 75 (97%) | 2 (3%) | 0 | 100 | 100 |
| 27 | B4 | 126/128 (98%) | 124 (98%) | 2 (2%) | 0 | 100 | 100 |
| 28 | B5 | 136/138 (99%) | 131 (96%) | 5 (4%) | 0 | 100 | 100 |
| 29 | B6 | 97/126 (77%) | 93 (96%) | 4 (4%) | 0 | 100 | 100 |
| 30 | B7 | 123/125 (98%) | 118 (96%) | 5 (4%) | 0 | 100 | 100 |
| 31 | B8 | 154/156 (99%) | 149 (97%) | 5 (3%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|---|---|---|---|---|---|---|---|
| 32 | B9 | 176/178 (99%) | 172 (98%) | 4 (2%) | 0 | 100 | 100 |
| 33 | BK | 172/176 (98%) | 171 (99%) | 1 (1%) | 0 | 100 | 100 |
| 34 | BL | 97/102 (95%) | 90 (93%) | 7 (7%) | 0 | 100 | 100 |
| 35 | C1 | 512/514 (100%) | 495 (97%) | 17 (3%) | 0 | 100 | 100 |
| 36 | C2 | 226/228 (99%) | 221 (98%) | 5 (2%) | 0 | 100 | 100 |
| 37 | C3 | 258/260 (99%) | 246 (95%) | 12 (5%) | 0 | 100 | 100 |
| 38 | C4 | 136/138 (99%) | 127 (93%) | 9 (7%) | 0 | 100 | 100 |
| 39 | CA | 47/49 (96%) | 46 (98%) | 1 (2%) | 0 | 100 | 100 |
| 40 | CB | 119/121 (98%) | 118 (99%) | 1 (1%) | 0 | 100 | 100 |
| 41 | N1 | 307/318 (96%) | 295 (96%) | 12 (4%) | 0 | 100 | 100 |
| 42 | N2 | 345/347 (99%) | 337 (98%) | 8 (2%) | 0 | 100 | 100 |
| 43 | N3 | 94/115 (82%) | 91 (97%) | 3 (3%) | 0 | 100 | 100 |
| 44 | N4 | 457/459 (100%) | 451 (99%) | 6 (1%) | 0 | 100 | 100 |
| 45 | N5 | 601/603 (100%) | 568 (94%) | 33 (6%) | 0 | 100 | 100 |
| 46 | N6 | 159/173 (92%) | 146 (92%) | 13 (8%) | 0 | 100 | 100 |
| 47 | QA | 417/419 (100%) | 404 (97%) | 13 (3%) | 0 | 100 | 100 |
| 47 | Qa | 417/419 (100%) | 403 (97%) | 14 (3%) | 0 | 100 | 100 |
| 48 | QB | 444/446 (100%) | 430 (97%) | 14 (3%) | 0 | 100 | 100 |
| 48 | Qb | 429/446 (96%) | 421 (98%) | 8 (2%) | 0 | 100 | 100 |
| 49 | QC | 377/379 (100%) | 368 (98%) | 9 (2%) | 0 | 100 | 100 |
| 49 | Qc | 377/379 (100%) | 368 (98%) | 9 (2%) | 0 | 100 | 100 |
| 50 | QD | 239/241 (99%) | 231 (97%) | 8 (3%) | 0 | 100 | 100 |
| 50 | Qd | 237/241 (98%) | 234 (99%) | 3 (1%) | 0 | 100 | 100 |
| 51 | QE | 194/196 (99%) | 188 (97%) | 6 (3%) | 0 | 100 | 100 |
| 51 | Qe | 194/196 (99%) | 187 (96%) | 7 (4%) | 0 | 100 | 100 |
| 52 | QF | 65/67 (97%) | 65 (100%) | 0 | 0 | 100 | 100 |
| 52 | Qf | 62/67 (92%) | 61 (98%) | 1 (2%) | 0 | 100 | 100 |
| 53 | QG | 99/101 (98%) | 97 (98%) | 2 (2%) | 0 | 100 | 100 |
| 53 | Qg | 99/101 (98%) | 96 (97%) | 3 (3%) | 0 | 100 | 100 |
| 54 | QH | 76/79 (96%) | 74 (97%) | 2 (3%) | 0 | 100 | 100 |
| 54 | Qh | 77/79 (98%) | 76 (99%) | 1 (1%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|---|---|---|---|---|---|---|---|
| 55 | QI | 60/64 (94%) | 59 (98%) | 1 (2%) | 0 | 100 | 100 |
| 55 | Qi | 58/64 (91%) | 58 (100%) | 0 | 0 | 100 | 100 |
| 56 | QJ | 47/49 (96%) | 44 (94%) | 3 (6%) | 0 | 100 | 100 |
| 57 | QK | 69/78 (88%) | 68 (99%) | 1 (1%) | 0 | 100 | 100 |
| 58 | Qj | 49/51 (96%) | 47 (96%) | 2 (4%) | 0 | 100 | 100 |
| 59 | S1 | 687/689 (100%) | 653 (95%) | 34 (5%) | 0 | 100 | 100 |
| 60 | S2 | 414/430 (96%) | 392 (95%) | 22 (5%) | 0 | 100 | 100 |
| 61 | S3 | 205/207 (99%) | 192 (94%) | 13 (6%) | 0 | 100 | 100 |
| 62 | S4 | 122/124 (98%) | 118 (97%) | 4 (3%) | 0 | 100 | 100 |
| 63 | S5 | 98/100 (98%) | 95 (97%) | 3 (3%) | 0 | 100 | 100 |
| 64 | S6 | 94/96 (98%) | 93 (99%) | 1 (1%) | 0 | 100 | 100 |
| 65 | S7 | 154/156 (99%) | 148 (96%) | 6 (4%) | 0 | 100 | 100 |
| 66 | S8 | 174/176 (99%) | 169 (97%) | 5 (3%) | 0 | 100 | 100 |
| 67 | V1 | 429/431 (100%) | 404 (94%) | 25 (6%) | 0 | 100 | 100 |
| 68 | V2 | 215/217 (99%) | 208 (97%) | 7 (3%) | 0 | 100 | 100 |
| 69 | V3 | 40/42 (95%) | 36 (90%) | 4 (10%) | 0 | 100 | 100 |
| All | All | 13901/14350 (97%) | 13434 (97%) | 467 (3%) | 0 | 100 | 100 |

There are no Ramachandran outliers to report.

### 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 | 4L | 85/85 (100%) | 85 (100%) | 0 | 100 | 100 |
| 2 | 5A | 89/89 (100%) | 88 (99%) | 1 (1%) | 65 | 77 |
| 3 | 5B | 80/80 (100%) | 80 (100%) | 0 | 100 | 100 |
| 4 | 6A | 66/66 (100%) | 64 (97%) | 2 (3%) | 36 | 63 |
| 5 | 6B | 73/73 (100%) | 73 (100%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|---|---|---|---|---|---|---|
| 6 | 6C | 57/57 (100%) | 56 (98%) | 1 (2%) | 51 | 71 |
| 7 | 7A | 48/48 (100%) | 44 (92%) | 4 (8%) | 10 | 36 |
| 8 | 7B | 39/39 (100%) | 39 (100%) | 0 | 100 | 100 |
| 9 | 7C | 40/40 (100%) | 40 (100%) | 0 | 100 | 100 |
| 10 | 8B | 37/37 (100%) | 37 (100%) | 0 | 100 | 100 |
| 11 | A1 | 58/58 (100%) | 58 (100%) | 0 | 100 | 100 |
| 12 | A2 | 76/76 (100%) | 76 (100%) | 0 | 100 | 100 |
| 13 | A3 | 69/69 (100%) | 69 (100%) | 0 | 100 | 100 |
| 14 | A5 | 99/99 (100%) | 98 (99%) | 1 (1%) | 68 | 78 |
| 15 | A6 | 107/107 (100%) | 106 (99%) | 1 (1%) | 70 | 79 |
| 16 | A7 | 87/97 (90%) | 86 (99%) | 1 (1%) | 65 | 77 |
| 17 | A8 | 153/153 (100%) | 152 (99%) | 1 (1%) | 76 | 81 |
| 18 | A9 | 291/295 (99%) | 290 (100%) | 1 (0%) | 86 | 87 |
| 19 | AB | 71/132 (54%) | 71 (100%) | 0 | 100 | 100 |
| 19 | AC | 80/132 (61%) | 79 (99%) | 1 (1%) | 61 | 75 |
| 20 | AK | 283/283 (100%) | 278 (98%) | 5 (2%) | 51 | 71 |
| 21 | AL | 101/101 (100%) | 99 (98%) | 2 (2%) | 48 | 69 |
| 22 | AM | 129/129 (100%) | 129 (100%) | 0 | 100 | 100 |
| 23 | AN | 123/123 (100%) | 121 (98%) | 2 (2%) | 55 | 72 |
| 24 | B1 | 53/53 (100%) | 53 (100%) | 0 | 100 | 100 |
| 25 | B2 | 62/62 (100%) | 62 (100%) | 0 | 100 | 100 |
| 26 | B3 | 61/61 (100%) | 61 (100%) | 0 | 100 | 100 |
| 27 | B4 | 113/113 (100%) | 113 (100%) | 0 | 100 | 100 |
| 28 | B5 | 121/121 (100%) | 121 (100%) | 0 | 100 | 100 |
| 29 | B6 | 96/119 (81%) | 96 (100%) | 0 | 100 | 100 |
| 30 | B7 | 112/112 (100%) | 112 (100%) | 0 | 100 | 100 |
| 31 | B8 | 141/141 (100%) | 141 (100%) | 0 | 100 | 100 |
| 32 | B9 | 159/159 (100%) | 159 (100%) | 0 | 100 | 100 |
| 33 | BK | 155/156 (99%) | 155 (100%) | 0 | 100 | 100 |
| 34 | BL | 91/94 (97%) | 91 (100%) | 0 | 100 | 100 |
| 35 | C1 | 425/425 (100%) | 415 (98%) | 10 (2%) | 43 | 67 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|---|---|---|---|---|---|---|
| 36 | C2 | 212/212 (100%) | 209 (99%) | 3 (1%) | 59 | 74 |
| 37 | C3 | 224/224 (100%) | 222 (99%) | 2 (1%) | 70 | 79 |
| 38 | C4 | 123/123 (100%) | 122 (99%) | 1 (1%) | 73 | 80 |
| 39 | CA | 45/45 (100%) | 43 (96%) | 2 (4%) | 25 | 55 |
| 40 | CB | 108/108 (100%) | 108 (100%) | 0 | 100 | 100 |
| 41 | N1 | 269/275 (98%) | 268 (100%) | 1 (0%) | 84 | 85 |
| 42 | N2 | 311/311 (100%) | 310 (100%) | 1 (0%) | 86 | 87 |
| 43 | N3 | 86/100 (86%) | 86 (100%) | 0 | 100 | 100 |
| 44 | N4 | 410/410 (100%) | 409 (100%) | 1 (0%) | 87 | 88 |
| 45 | N5 | 537/537 (100%) | 533 (99%) | 4 (1%) | 76 | 81 |
| 46 | N6 | 129/139 (93%) | 127 (98%) | 2 (2%) | 55 | 72 |
| 47 | QA | 330/330 (100%) | 329 (100%) | 1 (0%) | 86 | 87 |
| 47 | Qa | 330/330 (100%) | 324 (98%) | 6 (2%) | 51 | 71 |
| 48 | QB | 372/372 (100%) | 367 (99%) | 5 (1%) | 61 | 75 |
| 48 | Qb | 362/372 (97%) | 357 (99%) | 5 (1%) | 59 | 74 |
| 49 | QC | 332/332 (100%) | 325 (98%) | 7 (2%) | 47 | 69 |
| 49 | Qc | 332/332 (100%) | 331 (100%) | 1 (0%) | 86 | 87 |
| 50 | QD | 206/206 (100%) | 206 (100%) | 0 | 100 | 100 |
| 50 | Qd | 204/206 (99%) | 202 (99%) | 2 (1%) | 68 | 78 |
| 51 | QE | 166/166 (100%) | 166 (100%) | 0 | 100 | 100 |
| 51 | Qe | 166/166 (100%) | 166 (100%) | 0 | 100 | 100 |
| 52 | QF | 64/64 (100%) | 64 (100%) | 0 | 100 | 100 |
| 52 | Qf | 61/64 (95%) | 61 (100%) | 0 | 100 | 100 |
| 53 | QG | 93/93 (100%) | 92 (99%) | 1 (1%) | 65 | 77 |
| 53 | Qg | 93/93 (100%) | 93 (100%) | 0 | 100 | 100 |
| 54 | QH | 70/70 (100%) | 70 (100%) | 0 | 100 | 100 |
| 54 | Qh | 70/70 (100%) | 70 (100%) | 0 | 100 | 100 |
| 55 | QI | 50/52 (96%) | 49 (98%) | 1 (2%) | 48 | 69 |
| 55 | Qi | 49/52 (94%) | 49 (100%) | 0 | 100 | 100 |
| 56 | QJ | 40/40 (100%) | 40 (100%) | 0 | 100 | 100 |
| 57 | QK | 55/59 (93%) | 55 (100%) | 0 | 100 | 100 |

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| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|---|---|---|---|---|---|---|
| 58 | Qj | 41/41 (100%) | 41 (100%) | 0 | 100 | 100 |
| 59 | S1 | 579/579 (100%) | 574 (99%) | 5 (1%) | 70 | 79 |
| 60 | S2 | 363/370 (98%) | 362 (100%) | 1 (0%) | 86 | 87 |
| 61 | S3 | 189/189 (100%) | 186 (98%) | 3 (2%) | 55 | 72 |
| 62 | S4 | 112/112 (100%) | 109 (97%) | 3 (3%) | 39 | 65 |
| 63 | S5 | 88/88 (100%) | 88 (100%) | 0 | 100 | 100 |
| 64 | S6 | 79/79 (100%) | 79 (100%) | 0 | 100 | 100 |
| 65 | S7 | 132/132 (100%) | 130 (98%) | 2 (2%) | 57 | 74 |
| 66 | S8 | 151/151 (100%) | 149 (99%) | 2 (1%) | 61 | 75 |
| 67 | V1 | 344/344 (100%) | 337 (98%) | 7 (2%) | 48 | 69 |
| 68 | V2 | 183/183 (100%) | 181 (99%) | 2 (1%) | 65 | 77 |
| 69 | V3 | 41/41 (100%) | 41 (100%) | 0 | 100 | 100 |
| All | All | 12131/12346 (98%) | 12027 (99%) | 104 (1%) | 68 | 79 |

All (104) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | 5A | 84 | LEU |
| 4 | 6A | 23 | THR |
| 4 | 6A | 50 | HIS |
| 6 | 6C | 23 | ILE |
| 7 | 7A | 25 | ARG |
| 7 | 7A | 30 | GLN |
| 7 | 7A | 41 | VAL |
| 7 | 7A | 50 | ASN |
| 14 | A5 | 33 | ASP |
| 15 | A6 | 41 | THR |
| 16 | A7 | 43 | VAL |
| 17 | A8 | 151 | ILE |
| 18 | A9 | 129 | LEU |
| 19 | AC | 112 | SER |
| 20 | AK | 38 | LEU |
| 20 | AK | 68 | ILE |
| 20 | AK | 152 | LEU |
| 20 | AK | 205 | VAL |
| 20 | AK | 206 | VAL |
| 21 | AL | 106 | ARG |
| 21 | AL | 115 | CYS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 23 | AN | 5 | LYS |
| 23 | AN | 7 | LYS |
| 35 | C1 | 53 | ILE |
| 35 | C1 | 96 | ARG |
| 35 | C1 | 97 | MET |
| 35 | C1 | 109 | PHE |
| 35 | C1 | 124 | THR |
| 35 | C1 | 127 | THR |
| 35 | C1 | 128 | VAL |
| 35 | C1 | 370 | THR |
| 35 | C1 | 426 | PHE |
| 35 | C1 | 448 | THR |
| 36 | C2 | 48 | THR |
| 36 | C2 | 111 | THR |
| 36 | C2 | 207 | MET |
| 37 | C3 | 32 | THR |
| 37 | C3 | 66 | THR |
| 38 | C4 | 76 | ASP |
| 39 | CA | 28 | LYS |
| 39 | CA | 47 | THR |
| 41 | N1 | 251 | THR |
| 42 | N2 | 303 | THR |
| 44 | N4 | 375 | LEU |
| 45 | N5 | 286 | LEU |
| 45 | N5 | 340 | PHE |
| 45 | N5 | 419 | THR |
| 45 | N5 | 450 | LEU |
| 46 | N6 | 57 | PHE |
| 46 | N6 | 66 | VAL |
| 47 | QA | 238 | LEU |
| 48 | QB | 71 | VAL |
| 48 | QB | 125 | THR |
| 48 | QB | 195 | THR |
| 48 | QB | 258 | VAL |
| 48 | QB | 289 | ILE |
| 49 | QC | 47 | THR |
| 49 | QC | 112 | THR |
| 49 | QC | 158 | THR |
| 49 | QC | 171 | ASP |
| 49 | QC | 200 | LEU |
| 49 | QC | 281 | LEU |
| 49 | QC | 343 | VAL |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 53 | QG | 37 | THR |
| 55 | QI | 5 | THR |
| 47 | Qa | 231 | LYS |
| 47 | Qa | 237 | PHE |
| 47 | Qa | 238 | LEU |
| 47 | Qa | 252 | LYS |
| 47 | Qa | 369 | THR |
| 47 | Qa | 421 | ASP |
| 48 | Qb | 92 | PHE |
| 48 | Qb | 101 | THR |
| 48 | Qb | 181 | ASP |
| 48 | Qb | 289 | ILE |
| 48 | Qb | 341 | PHE |
| 49 | Qc | 200 | LEU |
| 50 | Qd | 209 | GLU |
| 50 | Qd | 253 | VAL |
| 59 | S1 | 291 | ARG |
| 59 | S1 | 608 | VAL |
| 59 | S1 | 611 | THR |
| 59 | S1 | 636 | TYR |
| 59 | S1 | 690 | THR |
| 60 | S2 | 362 | ILE |
| 61 | S3 | 43 | THR |
| 61 | S3 | 47 | ILE |
| 61 | S3 | 68 | ILE |
| 62 | S4 | 58 | LYS |
| 62 | S4 | 77 | VAL |
| 62 | S4 | 152 | VAL |
| 65 | S7 | 67 | PHE |
| 65 | S7 | 71 | CYS |
| 66 | S8 | 76 | TYR |
| 66 | S8 | 114 | ILE |
| 67 | V1 | 270 | ASN |
| 67 | V1 | 294 | VAL |
| 67 | V1 | 307 | VAL |
| 67 | V1 | 334 | THR |
| 67 | V1 | 347 | THR |
| 67 | V1 | 379 | CYS |
| 67 | V1 | 385 | CYS |
| 68 | V2 | 137 | THR |
| 68 | V2 | 150 | GLU |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (268)

such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | 4L | 7 | ASN |
| 2 | 5A | 77 | ASN |
| 2 | 5A | 102 | ASN |
| 3 | 5B | 43 | GLN |
| 3 | 5B | 119 | HIS |
| 4 | 6A | 50 | HIS |
| 4 | 6A | 83 | HIS |
| 5 | 6B | 11 | ASN |
| 5 | 6B | 25 | ASN |
| 5 | 6B | 26 | GLN |
| 5 | 6B | 33 | ASN |
| 6 | 6C | 22 | HIS |
| 6 | 6C | 55 | ASN |
| 7 | 7A | 24 | ASN |
| 7 | 7A | 50 | ASN |
| 8 | 7B | 59 | GLN |
| 12 | A2 | 25 | GLN |
| 13 | A3 | 156 | GLN |
| 13 | A3 | 159 | GLN |
| 13 | A3 | 168 | ASN |
| 14 | A5 | 71 | GLN |
| 14 | A5 | 86 | ASN |
| 15 | A6 | 74 | HIS |
| 15 | A6 | 84 | GLN |
| 15 | A6 | 96 | ASN |
| 16 | A7 | 9 | GLN |
| 16 | A7 | 21 | GLN |
| 16 | A7 | 36 | GLN |
| 16 | A7 | 73 | GLN |
| 17 | A8 | 108 | HIS |
| 18 | A9 | 38 | HIS |
| 18 | A9 | 122 | HIS |
| 18 | A9 | 138 | ASN |
| 18 | A9 | 150 | HIS |
| 18 | A9 | 171 | ASN |
| 18 | A9 | 269 | ASN |
| 18 | A9 | 278 | GLN |
| 19 | AC | 101 | ASN |
| 19 | AC | 103 | HIS |
| 19 | AC | 142 | GLN |
| 20 | AK | 87 | HIS |
| 20 | AK | 134 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 20 | AK | 178 | GLN |
| 20 | AK | 221 | GLN |
| 20 | AK | 227 | HIS |
| 20 | AK | 259 | GLN |
| 21 | AL | 7 | HIS |
| 21 | AL | 89 | ASN |
| 22 | AM | 5 | GLN |
| 22 | AM | 31 | ASN |
| 22 | AM | 113 | HIS |
| 23 | AN | 61 | GLN |
| 24 | B1 | 3 | ASN |
| 24 | B1 | 6 | GLN |
| 24 | B1 | 14 | HIS |
| 25 | B2 | 49 | GLN |
| 25 | B2 | 54 | GLN |
| 25 | B2 | 57 | GLN |
| 26 | B3 | 21 | GLN |
| 26 | B3 | 33 | GLN |
| 27 | B4 | 50 | GLN |
| 27 | B4 | 123 | GLN |
| 28 | B5 | 181 | HIS |
| 28 | B5 | 189 | ASN |
| 29 | B6 | 143 | HIS |
| 30 | B7 | 110 | GLN |
| 31 | B8 | 94 | HIS |
| 31 | B8 | 115 | ASN |
| 31 | B8 | 154 | GLN |
| 32 | B9 | 104 | GLN |
| 32 | B9 | 108 | GLN |
| 32 | B9 | 117 | GLN |
| 32 | B9 | 211 | HIS |
| 33 | BK | 107 | GLN |
| 35 | C1 | 11 | ASN |
| 35 | C1 | 12 | HIS |
| 35 | C1 | 43 | GLN |
| 35 | C1 | 55 | ASN |
| 35 | C1 | 80 | ASN |
| 35 | C1 | 98 | ASN |
| 35 | C1 | 138 | HIS |
| 35 | C1 | 233 | HIS |
| 35 | C1 | 291 | HIS |
| 35 | C1 | 328 | HIS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 35 | C1 | 407 | GLN |
| 35 | C1 | 422 | ASN |
| 35 | C1 | 491 | ASN |
| 35 | C1 | 496 | HIS |
| 36 | C2 | 26 | HIS |
| 36 | C2 | 59 | GLN |
| 36 | C2 | 102 | HIS |
| 37 | C3 | 38 | ASN |
| 37 | C3 | 70 | HIS |
| 37 | C3 | 71 | HIS |
| 37 | C3 | 125 | ASN |
| 37 | C3 | 161 | GLN |
| 37 | C3 | 204 | HIS |
| 37 | C3 | 231 | HIS |
| 38 | C4 | 123 | HIS |
| 38 | C4 | 141 | GLN |
| 38 | C4 | 154 | GLN |
| 41 | N1 | 124 | ASN |
| 41 | N1 | 138 | GLN |
| 41 | N1 | 169 | GLN |
| 41 | N1 | 171 | HIS |
| 41 | N1 | 317 | GLN |
| 42 | N2 | 83 | GLN |
| 42 | N2 | 171 | ASN |
| 42 | N2 | 186 | HIS |
| 42 | N2 | 221 | HIS |
| 42 | N2 | 273 | ASN |
| 42 | N2 | 310 | ASN |
| 42 | N2 | 322 | GLN |
| 42 | N2 | 347 | ASN |
| 43 | N3 | 10 | ASN |
| 44 | N4 | 30 | HIS |
| 44 | N4 | 44 | GLN |
| 44 | N4 | 81 | GLN |
| 44 | N4 | 103 | GLN |
| 44 | N4 | 213 | HIS |
| 44 | N4 | 251 | ASN |
| 44 | N4 | 304 | GLN |
| 44 | N4 | 399 | ASN |
| 44 | N4 | 415 | GLN |
| 45 | N5 | 136 | ASN |
| 45 | N5 | 139 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 45 | N5 | 230 | HIS |
| 45 | N5 | 248 | HIS |
| 45 | N5 | 518 | GLN |
| 45 | N5 | 524 | ASN |
| 45 | N5 | 546 | GLN |
| 45 | N5 | 580 | GLN |
| 47 | QA | 168 | ASN |
| 47 | QA | 176 | ASN |
| 47 | QA | 184 | ASN |
| 47 | QA | 284 | ASN |
| 47 | QA | 291 | HIS |
| 47 | QA | 298 | HIS |
| 47 | QA | 365 | ASN |
| 47 | QA | 368 | ASN |
| 47 | QA | 399 | GLN |
| 47 | QA | 415 | GLN |
| 47 | QA | 426 | ASN |
| 48 | QB | 66 | GLN |
| 48 | QB | 173 | GLN |
| 48 | QB | 239 | HIS |
| 48 | QB | 301 | ASN |
| 48 | QB | 357 | HIS |
| 48 | QB | 464 | GLN |
| 49 | QC | 32 | ASN |
| 49 | QC | 68 | HIS |
| 49 | QC | 201 | HIS |
| 49 | QC | 267 | HIS |
| 49 | QC | 312 | GLN |
| 49 | QC | 322 | GLN |
| 49 | QC | 345 | HIS |
| 49 | QC | 374 | ASN |
| 50 | QD | 206 | HIS |
| 50 | QD | 266 | GLN |
| 50 | QD | 310 | HIS |
| 51 | QE | 135 | GLN |
| 51 | QE | 164 | ASN |
| 51 | QE | 186 | GLN |
| 51 | QE | 199 | GLN |
| 51 | QE | 257 | ASN |
| 52 | QF | 88 | ASN |
| 53 | QG | 80 | GLN |
| 54 | QH | 7 | HIS |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 55 | QI | 38 | GLN |
| 55 | QI | 46 | HIS |
| 55 | QI | 48 | ASN |
| 55 | QI | 55 | HIS |
| 57 | QK | 31 | GLN |
| 57 | QK | 58 | GLN |
| 47 | Qa | 36 | GLN |
| 47 | Qa | 81 | HIS |
| 47 | Qa | 139 | ASN |
| 47 | Qa | 155 | GLN |
| 47 | Qa | 167 | GLN |
| 47 | Qa | 172 | GLN |
| 47 | Qa | 212 | HIS |
| 47 | Qa | 290 | GLN |
| 47 | Qa | 304 | ASN |
| 47 | Qa | 319 | GLN |
| 47 | Qa | 376 | ASN |
| 47 | Qa | 408 | GLN |
| 48 | Qb | 43 | GLN |
| 48 | Qb | 87 | ASN |
| 48 | Qb | 95 | HIS |
| 48 | Qb | 152 | GLN |
| 48 | Qb | 153 | ASN |
| 48 | Qb | 160 | GLN |
| 48 | Qb | 170 | GLN |
| 48 | Qb | 188 | HIS |
| 48 | Qb | 223 | HIS |
| 48 | Qb | 239 | HIS |
| 48 | Qb | 249 | HIS |
| 48 | Qb | 357 | HIS |
| 49 | Qc | 3 | ASN |
| 49 | Qc | 201 | HIS |
| 49 | Qc | 260 | ASN |
| 49 | Qc | 341 | GLN |
| 50 | Qd | 116 | GLN |
| 50 | Qd | 190 | ASN |
| 50 | Qd | 206 | HIS |
| 50 | Qd | 251 | ASN |
| 50 | Qd | 283 | HIS |
| 51 | Qe | 135 | GLN |
| 51 | Qe | 186 | GLN |
| 51 | Qe | 199 | GLN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 51 | Qe | 227 | ASN |
| 52 | Qf | 36 | GLN |
| 52 | Qf | 55 | GLN |
| 53 | Qg | 23 | ASN |
| 55 | Qi | 38 | GLN |
| 55 | Qi | 48 | ASN |
| 58 | Qj | 16 | ASN |
| 59 | S1 | 39 | GLN |
| 59 | S1 | 51 | GLN |
| 59 | S1 | 123 | ASN |
| 59 | S1 | 202 | ASN |
| 59 | S1 | 282 | ASN |
| 59 | S1 | 331 | GLN |
| 59 | S1 | 336 | ASN |
| 59 | S1 | 424 | HIS |
| 59 | S1 | 425 | ASN |
| 59 | S1 | 453 | GLN |
| 59 | S1 | 498 | GLN |
| 59 | S1 | 652 | ASN |
| 59 | S1 | 677 | GLN |
| 59 | S1 | 688 | GLN |
| 60 | S2 | 66 | HIS |
| 60 | S2 | 239 | HIS |
| 60 | S2 | 240 | GLN |
| 61 | S3 | 51 | ASN |
| 61 | S3 | 75 | GLN |
| 61 | S3 | 82 | ASN |
| 61 | S3 | 107 | GLN |
| 61 | S3 | 123 | GLN |
| 61 | S3 | 131 | ASN |
| 61 | S3 | 247 | GLN |
| 62 | S4 | 92 | ASN |
| 62 | S4 | 93 | ASN |
| 62 | S4 | 123 | ASN |
| 62 | S4 | 163 | ASN |
| 63 | S5 | 25 | GLN |
| 63 | S5 | 34 | HIS |
| 63 | S5 | 45 | HIS |
| 64 | S6 | 43 | GLN |
| 64 | S6 | 74 | GLN |
| 64 | S6 | 120 | GLN |
| 67 | V1 | 44 | ASN |

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| Mol | Chain | Res | Type |
|---|---|---|---|
| 67 | V1 | 133 | HIS |
| 67 | V1 | 136 | HIS |
| 67 | V1 | 170 | GLN |
| 67 | V1 | 303 | HIS |
| 67 | V1 | 344 | GLN |
| 67 | V1 | 381 | GLN |
| 67 | V1 | 456 | GLN |
| 67 | V1 | 458 | GLN |
| 68 | V2 | 41 | HIS |
| 68 | V2 | 87 | GLN |
| 68 | V2 | 90 | ASN |
| 68 | V2 | 133 | GLN |
| 68 | V2 | 153 | GLN |
| 68 | V2 | 187 | GLN |
| 69 | V3 | 388 | ASN |
| 69 | V3 | 419 | GLN |

### 5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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 | $\#\|Z\| > 2$ |
| 60 | 2MR | S2 | 124 | 60 | 10,12,13 | 2.41 | 3 (30%) | 5,13,15 | 0.90 | 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 |
|---|---|---|---|---|---|---|---|
| 60 | 2MR | S2 | 124 | 60 | - | 3/10/13/15 | - |

All (3) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 60 | S2 | 124 | 2MR | CZ-NE | 5.08 | 1.45 | 1.34 |
| 60 | S2 | 124 | 2MR | CZ-NH2 | 4.94 | 1.44 | 1.33 |
| 60 | S2 | 124 | 2MR | CQ1-NH1 | -2.06 | 1.42 | 1.46 |

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 60 | S2 | 124 | 2MR | NE-CD-CG-CB |
| 60 | S2 | 124 | 2MR | CA-CB-CG-CD |
| 60 | S2 | 124 | 2MR | C-CA-CB-CG |

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry (i)

Of 97 ligands modelled in this entry, 7 are monoatomic - leaving 90 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 | $\#\|Z\| > 2$ |
| 82 | PEE | Qh | 101 | - | 40,40,50 | 1.47 | 5 (12%) | 42,45,55 | 1.14 | 3 (7%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\| > 2$ | Counts | RMSZ | $\#\|Z\| > 2$ |
| 83 | HEM | QC | 402 | 49 | 50,50,50 | 1.32 | 8 (16%) | 66,82,82 | 1.71 | 15 (22%) |
| 82 | PEE | Qd | 403 | - | 50,50,50 | 1.31 | 5 (10%) | 53,55,55 | 1.20 | 4 (7%) |
| 85 | FES | QE | 304 | 51 | 0,4,4 | - | - | - | | |
| 79 | HEA | C1 | 602 | 35 | 66,67,67 | 2.19 | 24 (36%) | 78,103,103 | 2.68 | 29 (37%) |
| 72 | CDL | QC | 406 | - | 93,93,99 | 0.31 | 0 | 99,105,111 | 0.33 | 0 |
| 86 | SF4 | S8 | 301 | 66 | 0,12,12 | - | - | - | | |
| 77 | PLX | AM | 201 | - | 51,51,51 | 1.11 | 4 (7%) | 55,59,59 | 0.88 | 1 (1%) |
| 72 | CDL | Qb | 501 | - | 63,63,99 | 0.37 | 0 | 69,75,111 | 0.38 | 0 |
| 79 | HEA | C1 | 603 | 35 | 66,67,67 | 2.21 | 25 (37%) | 78,103,103 | 2.66 | 28 (35%) |
| 77 | PLX | B5 | 201 | - | 51,51,51 | 1.11 | 3 (5%) | 55,59,59 | 0.91 | 1 (1%) |
| 86 | SF4 | S1 | 802 | 59 | 0,12,12 | - | - | - | | |
| 82 | PEE | QE | 302 | - | 46,46,50 | 1.35 | 5 (10%) | 49,51,55 | 1.28 | 4 (8%) |
| 76 | 3PE | N4 | 502 | - | 50,50,50 | 0.31 | 0 | 53,55,55 | 0.33 | 0 |
| 83 | HEM | Qc | 403 | 49 | 50,50,50 | 1.32 | 6 (12%) | 66,82,82 | 1.70 | 14 (21%) |
| 77 | PLX | QE | 301 | - | 45,45,51 | 1.18 | 3 (6%) | 49,53,59 | 0.92 | 1 (2%) |
| 72 | CDL | AL | 204 | - | 79,79,99 | 0.33 | 0 | 85,91,111 | 0.42 | 0 |
| 85 | FES | V2 | 301 | 68 | 0,4,4 | - | - | - | | |
| 72 | CDL | AM | 202 | - | 50,50,99 | 0.40 | 0 | 56,62,111 | 0.34 | 0 |
| 72 | CDL | N5 | 703 | - | 99,99,99 | 0.30 | 0 | 105,111,111 | 0.30 | 0 |
| 75 | ADP | AK | 401 | - | 27,29,29 | 1.34 | 4 (14%) | 42,45,45 | 1.99 | 10 (23%) |
| 86 | SF4 | S8 | 302 | 66 | 0,12,12 | - | - | - | | |
| 86 | SF4 | V1 | 501 | 67 | 0,12,12 | - | - | - | | |
| 82 | PEE | QB | 503 | - | 50,50,50 | 1.31 | 5 (10%) | 53,55,55 | 1.16 | 3 (5%) |
| 72 | CDL | QB | 501 | - | 63,63,99 | 0.37 | 0 | 69,75,111 | 0.41 | 0 |
| 72 | CDL | AL | 203 | - | 92,92,99 | 0.31 | 0 | 98,104,111 | 0.29 | 0 |
| 76 | 3PE | CB | 202 | - | 45,45,50 | 0.31 | 0 | 48,50,55 | 0.29 | 0 |
| 77 | PLX | QI | 301 | - | 51,51,51 | 1.12 | 3 (5%) | 55,59,59 | 0.89 | 1 (1%) |
| 86 | SF4 | S1 | 801 | 59 | 0,12,12 | - | - | - | | |
| 71 | PC1 | 7B | 101 | - | 53,53,53 | 0.29 | 0 | 59,61,61 | 0.27 | 0 |
| 82 | PEE | C1 | 609 | - | 50,50,50 | 1.32 | 5 (10%) | 53,55,55 | 1.16 | 3 (5%) |
| 72 | CDL | Qh | 102 | - | 63,63,99 | 0.37 | 0 | 69,75,111 | 0.37 | 0 |
| 71 | PC1 | QH | 102 | - | 53,53,53 | 0.29 | 0 | 59,61,61 | 0.32 | 0 |
| 72 | CDL | QH | 101 | - | 60,60,99 | 0.38 | 0 | 66,72,111 | 0.37 | 0 |
| 72 | CDL | AL | 201 | - | 83,83,99 | 0.32 | 0 | 89,95,111 | 0.34 | 0 |
| 71 | PC1 | C3 | 301 | - | 48,48,53 | 0.31 | 0 | 54,56,61 | 0.38 | 0 |
| 71 | PC1 | Qb | 502 | - | 28,28,53 | 0.39 | 0 | 34,36,61 | 0.40 | 0 |
| 72 | CDL | N5 | 702 | - | 88,88,99 | 0.31 | 0 | 94,100,111 | 0.32 | 0 |
| 83 | HEM | Qc | 402 | 49 | 50,50,50 | 1.32 | 7 (14%) | 66,82,82 | 1.73 | 15 (22%) |
| 71 | PC1 | QC | 405 | - | 53,53,53 | 0.30 | 0 | 59,61,61 | 0.30 | 0 |
| 78 | 6F6 | QJ | 101 | - | 53,53,53 | 0.29 | 0 | 59,61,61 | 0.30 | 0 |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | #\|Z\| > 2 | Counts | RMSZ | #\|Z\| > 2 |
| 76 | 3PE | C1 | 608 | - | 43,43,50 | 0.33 | 0 | 46,48,55 | 0.41 | 0 |
| 72 | CDL | CB | 203 | - | 99,99,99 | 0.30 | 0 | 105,111,111 | 0.29 | 0 |
| 77 | PLX | N4 | 501 | - | 51,51,51 | 1.11 | 3 (5%) | 55,59,59 | 0.92 | 2 (3%) |
| 74 | ZMP | AB | 201 | 19 | 29,35,36 | 0.70 | 1 (3%) | 34,42,45 | 0.90 | 2 (5%) |
| 76 | 3PE | QE | 303 | - | 43,43,50 | 0.32 | 0 | 46,48,55 | 0.30 | 0 |
| 82 | PEE | N5 | 701 | - | 45,45,50 | 1.38 | 5 (11%) | 48,50,55 | 1.18 | 2 (4%) |
| 76 | 3PE | C1 | 601 | - | 50,50,50 | 0.30 | 0 | 53,55,55 | 0.30 | 0 |
| 72 | CDL | A8 | 301 | - | 82,82,99 | 0.33 | 0 | 88,94,111 | 0.33 | 0 |
| 76 | 3PE | S7 | 302 | - | 50,50,50 | 0.31 | 0 | 53,55,55 | 0.34 | 0 |
| 82 | PEE | S2 | 501 | - | 47,47,50 | 1.35 | 5 (10%) | 50,52,55 | 1.18 | 3 (6%) |
| 74 | ZMP | AC | 201 | 19 | 29,35,36 | 0.73 | 1 (3%) | 34,42,45 | 0.76 | 0 |
| 82 | PEE | QC | 404 | - | 37,37,50 | 1.34 | 4 (10%) | 40,42,55 | 1.15 | 2 (5%) |
| 82 | PEE | QC | 401 | - | 50,50,50 | 1.32 | 5 (10%) | 53,55,55 | 1.22 | 3 (5%) |
| 76 | 3PE | CA | 101 | - | 50,50,50 | 0.30 | 0 | 53,55,55 | 0.33 | 0 |
| 71 | PC1 | C3 | 302 | - | 42,42,53 | 0.32 | 0 | 48,50,61 | 0.31 | 0 |
| 87 | FMN | V1 | 502 | - | 33,33,33 | 0.31 | 0 | 48,50,50 | 0.44 | 0 |
| 72 | CDL | QC | 408 | - | 54,54,99 | 0.39 | 0 | 60,66,111 | 0.38 | 0 |
| 83 | HEM | QC | 403 | 49 | 50,50,50 | 1.33 | 6 (12%) | 66,82,82 | 1.72 | 16 (24%) |
| 72 | CDL | Qd | 401 | - | 63,63,99 | 0.37 | 0 | 69,75,111 | 0.36 | 0 |
| 82 | PEE | N1 | 401 | - | 37,37,50 | 1.47 | 5 (13%) | 39,42,55 | 1.27 | 4 (10%) |
| 82 | PEE | Qc | 401 | - | 41,41,50 | 1.27 | 4 (9%) | 44,46,55 | 1.21 | 4 (9%) |
| 77 | PLX | AL | 205 | - | 46,46,51 | 1.13 | 4 (8%) | 50,54,59 | 0.93 | 2 (4%) |
| 71 | PC1 | C1 | 606 | - | 53,53,53 | 0.28 | 0 | 59,61,61 | 0.27 | 0 |
| 71 | PC1 | QC | 407 | - | 53,53,53 | 0.29 | 0 | 59,61,61 | 0.32 | 0 |
| 72 | CDL | B5 | 202 | - | 99,99,99 | 0.31 | 0 | 105,111,111 | 0.29 | 0 |
| 85 | FES | Qe | 301 | 51 | 0,4,4 | - | - | - | | |
| 85 | FES | S1 | 803 | 59 | 0,4,4 | - | - | - | | |
| 86 | SF4 | S7 | 301 | 65 | 0,12,12 | - | - | - | | |
| 71 | PC1 | N5 | 704 | - | 53,53,53 | 0.29 | 0 | 59,61,61 | 0.28 | 0 |
| 77 | PLX | CB | 201 | - | 51,51,51 | 1.11 | 3 (5%) | 55,59,59 | 0.92 | 1 (1%) |
| 71 | PC1 | Qj | 101 | - | 53,53,53 | 0.30 | 0 | 59,61,61 | 0.34 | 0 |
| 78 | 6F6 | Qc | 404 | - | 53,53,53 | 0.29 | 0 | 59,61,61 | 0.38 | 0 |
| 71 | PC1 | 6A | 101 | - | 44,44,53 | 0.32 | 0 | 50,52,61 | 0.33 | 0 |
| 71 | PC1 | AL | 206 | - | 53,53,53 | 0.29 | 0 | 59,61,61 | 0.31 | 0 |
| 84 | HEC | Qd | 402 | 50 | 50,50,50 | 1.32 | 5 (10%) | 68,82,82 | 1.20 | 3 (4%) |
| 78 | 6F6 | B5 | 203 | - | 53,53,53 | 0.29 | 0 | 59,61,61 | 0.33 | 0 |
| 82 | PEE | QB | 502 | - | 26,26,50 | 1.36 | 3 (11%) | 29,31,55 | 1.22 | 2 (6%) |
| 72 | CDL | 6A | 102 | - | 68,68,99 | 0.35 | 0 | 74,80,111 | 0.35 | 0 |
| 77 | PLX | C2 | 301 | - | 42,42,51 | 1.17 | 4 (9%) | 46,50,59 | 0.85 | 1 (2%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\| > 2$ | Counts | RMSZ | $\#\|Z\| > 2$ |
| 82 | PEE | Qh | 103 | - | 50,50,50 | 1.32 | 5 (10%) | 53,55,55 | 1.18 | 4 (7%) |
| 76 | 3PE | AL | 202 | - | 50,50,50 | 0.31 | 0 | 53,55,55 | 0.32 | 0 |
| 77 | PLX | AM | 203 | - | 51,51,51 | 1.10 | 3 (5%) | 55,59,59 | 0.89 | 1 (1%) |
| 82 | PEE | S8 | 303 | - | 50,50,50 | 1.30 | 5 (10%) | 53,55,55 | 1.19 | 4 (7%) |
| 82 | PEE | N3 | 201 | - | 50,50,50 | 1.30 | 5 (10%) | 53,55,55 | 1.19 | 5 (9%) |
| 71 | PC1 | C1 | 607 | - | 45,45,53 | 0.31 | 0 | 51,53,61 | 0.35 | 0 |
| 71 | PC1 | N6 | 201 | - | 53,53,53 | 0.30 | 0 | 59,61,61 | 0.26 | 0 |
| 84 | HEC | QD | 401 | 50 | 50,50,50 | 1.32 | 4 (8%) | 68,82,82 | 1.20 | 8 (11%) |
| 73 | NDP | A9 | 401 | - | 49,52,52 | 0.37 | 0 | 66,80,80 | 0.32 | 0 |
| 72 | CDL | N2 | 401 | - | 67,67,99 | 0.35 | 0 | 73,79,111 | 0.30 | 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 |
|---|---|---|---|---|---|---|---|
| 82 | PEE | Qh | 101 | - | - | 25/44/44/54 | - |
| 83 | HEM | QC | 402 | 49 | - | 7/14/54/54 | - |
| 82 | PEE | Qd | 403 | - | - | 24/54/54/54 | - |
| 85 | FES | QE | 304 | 51 | - | - | 0/1/1/1 |
| 79 | HEA | C1 | 602 | 35 | - | 13/36/76/76 | - |
| 72 | CDL | QC | 406 | - | - | 23/104/104/110 | - |
| 86 | SF4 | S8 | 301 | 66 | - | - | 0/6/5/5 |
| 77 | PLX | AM | 201 | - | - | 19/55/55/55 | - |
| 72 | CDL | Qb | 501 | - | - | 18/74/74/110 | - |
| 79 | HEA | C1 | 603 | 35 | - | 12/36/76/76 | - |
| 77 | PLX | B5 | 201 | - | - | 23/55/55/55 | - |
| 86 | SF4 | S1 | 802 | 59 | - | - | 0/6/5/5 |
| 82 | PEE | QE | 302 | - | - | 20/50/50/54 | - |
| 76 | 3PE | N4 | 502 | - | - | 12/54/54/54 | - |
| 83 | HEM | Qc | 403 | 49 | - | 9/14/54/54 | - |
| 77 | PLX | QE | 301 | - | - | 19/49/49/55 | - |
| 72 | CDL | AL | 204 | - | - | 25/90/90/110 | - |
| 85 | FES | V2 | 301 | 68 | - | - | 0/1/1/1 |
| 72 | CDL | AM | 202 | - | - | 9/61/61/110 | - |
| 72 | CDL | N5 | 703 | - | - | 21/110/110/110 | - |
| 75 | ADP | AK | 401 | - | - | 2/16/32/32 | 0/3/3/3 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 86 | SF4 | S8 | 302 | 66 | - | - | 0/6/5/5 |
| 86 | SF4 | V1 | 501 | 67 | - | - | 0/6/5/5 |
| 82 | PEE | QB | 503 | - | - | 23/54/54/54 | - |
| 72 | CDL | QB | 501 | - | - | 21/74/74/110 | - |
| 72 | CDL | AL | 203 | - | - | 22/103/103/110 | - |
| 76 | 3PE | CB | 202 | - | - | 8/49/49/54 | - |
| 77 | PLX | QI | 301 | - | - | 19/55/55/55 | - |
| 86 | SF4 | S1 | 801 | 59 | - | - | 0/6/5/5 |
| 71 | PC1 | 7B | 101 | - | - | 16/57/57/57 | - |
| 82 | PEE | C1 | 609 | - | - | 25/54/54/54 | - |
| 72 | CDL | Qh | 102 | - | - | 27/74/74/110 | - |
| 71 | PC1 | QH | 102 | - | - | 9/57/57/57 | - |
| 72 | CDL | QH | 101 | - | - | 12/71/71/110 | - |
| 72 | CDL | AL | 201 | - | - | 28/94/94/110 | - |
| 71 | PC1 | C3 | 301 | - | - | 17/52/52/57 | - |
| 71 | PC1 | Qb | 502 | - | - | 11/32/32/57 | - |
| 72 | CDL | N5 | 702 | - | - | 22/99/99/110 | - |
| 83 | HEM | Qc | 402 | 49 | - | 7/14/54/54 | - |
| 71 | PC1 | QC | 405 | - | - | 16/57/57/57 | - |
| 78 | 6F6 | QJ | 101 | - | - | 18/57/57/57 | - |
| 76 | 3PE | C1 | 608 | - | - | 12/47/47/54 | - |
| 72 | CDL | CB | 203 | - | - | 31/110/110/110 | - |
| 77 | PLX | N4 | 501 | - | - | 17/55/55/55 | - |
| 74 | ZMP | AB | 201 | 19 | - | 16/40/42/43 | - |
| 76 | 3PE | QE | 303 | - | - | 7/47/47/54 | - |
| 82 | PEE | N5 | 701 | - | - | 15/49/49/54 | - |
| 76 | 3PE | C1 | 601 | - | - | 11/54/54/54 | - |
| 72 | CDL | A8 | 301 | - | - | 24/93/93/110 | - |
| 76 | 3PE | S7 | 302 | - | - | 15/54/54/54 | - |
| 82 | PEE | S2 | 501 | - | - | 30/51/51/54 | - |
| 74 | ZMP | AC | 201 | 19 | - | 18/40/42/43 | - |
| 82 | PEE | QC | 404 | - | - | 12/41/41/54 | - |
| 82 | PEE | QC | 401 | - | - | 26/54/54/54 | - |
| 76 | 3PE | CA | 101 | - | - | 11/54/54/54 | - |
| 71 | PC1 | C3 | 302 | - | - | 9/46/46/57 | - |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 87 | FMN | V1 | 502 | - | - | 6/18/18/18 | 0/3/3/3 |
| 72 | CDL | QC | 408 | - | - | 18/65/65/110 | - |
| 83 | HEM | QC | 403 | 49 | - | 6/14/54/54 | - |
| 72 | CDL | Qd | 401 | - | - | 17/74/74/110 | - |
| 82 | PEE | N1 | 401 | - | - | 19/41/41/54 | - |
| 82 | PEE | Qc | 401 | - | - | 26/45/45/54 | - |
| 77 | PLX | AL | 205 | - | - | 21/50/50/55 | - |
| 71 | PC1 | C1 | 606 | - | - | 11/57/57/57 | - |
| 71 | PC1 | QC | 407 | - | - | 10/57/57/57 | - |
| 72 | CDL | B5 | 202 | - | - | 17/110/110/110 | - |
| 85 | FES | Qe | 301 | 51 | - | - | 0/1/1/1 |
| 85 | FES | S1 | 803 | 59 | - | - | 0/1/1/1 |
| 86 | SF4 | S7 | 301 | 65 | - | - | 0/6/5/5 |
| 71 | PC1 | N5 | 704 | - | - | 11/57/57/57 | - |
| 77 | PLX | CB | 201 | - | - | 27/55/55/55 | - |
| 71 | PC1 | Qj | 101 | - | - | 18/57/57/57 | - |
| 78 | 6F6 | Qc | 404 | - | - | 13/57/57/57 | - |
| 71 | PC1 | 6A | 101 | - | - | 15/48/48/57 | - |
| 71 | PC1 | AL | 206 | - | - | 15/57/57/57 | - |
| 84 | HEC | Qd | 402 | 50 | 1/1/3/7 | 1/14/54/54 | - |
| 78 | 6F6 | B5 | 203 | - | - | 11/57/57/57 | - |
| 82 | PEE | QB | 502 | - | - | 13/30/30/54 | - |
| 72 | CDL | 6A | 102 | - | - | 28/79/79/110 | - |
| 77 | PLX | C2 | 301 | - | - | 21/46/46/55 | - |
| 82 | PEE | Qh | 103 | - | - | 17/54/54/54 | - |
| 76 | 3PE | AL | 202 | - | - | 10/54/54/54 | - |
| 77 | PLX | AM | 203 | - | - | 24/55/55/55 | - |
| 82 | PEE | S8 | 303 | - | - | 22/54/54/54 | - |
| 82 | PEE | N3 | 201 | - | - | 24/54/54/54 | - |
| 71 | PC1 | C1 | 607 | - | - | 10/49/49/57 | - |
| 71 | PC1 | N6 | 201 | - | - | 6/57/57/57 | - |
| 84 | HEC | QD | 401 | 50 | 1/1/3/7 | 2/14/54/54 | - |
| 73 | NDP | A9 | 401 | - | - | 6/34/77/77 | 0/5/5/5 |
| 72 | CDL | N2 | 401 | - | - | 25/78/78/110 | - |

All (192) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 79 | C1 | 602 | HEA | C3B-C2B | 5.25 | 1.46 | 1.34 |
| 79 | C1 | 603 | HEA | C3B-C2B | 5.10 | 1.46 | 1.34 |
| 79 | C1 | 602 | HEA | FE-ND | 4.69 | 2.09 | 1.94 |
| 79 | C1 | 603 | HEA | FE-ND | 4.66 | 2.09 | 1.94 |
| 79 | C1 | 603 | HEA | FE-NB | 4.55 | 2.09 | 1.94 |
| 79 | C1 | 603 | HEA | C3A-C2A | 4.50 | 1.46 | 1.36 |
| 75 | AK | 401 | ADP | C5-C4 | 4.44 | 1.47 | 1.39 |
| 79 | C1 | 602 | HEA | FE-NB | 4.44 | 2.08 | 1.94 |
| 79 | C1 | 602 | HEA | C3A-C2A | 4.23 | 1.45 | 1.36 |
| 79 | C1 | 603 | HEA | C4B-NB | -4.17 | 1.33 | 1.40 |
| 79 | C1 | 603 | HEA | FE-NC | 4.14 | 2.09 | 1.95 |
| 79 | C1 | 602 | HEA | C1D-ND | -4.10 | 1.33 | 1.40 |
| 82 | Qh | 101 | PEE | C18-C19 | 4.08 | 1.55 | 1.31 |
| 82 | C1 | 609 | PEE | C18-C19 | 4.06 | 1.55 | 1.31 |
| 79 | C1 | 602 | HEA | CHC-C4B | 4.06 | 1.46 | 1.38 |
| 82 | QE | 302 | PEE | C18-C19 | 4.06 | 1.55 | 1.31 |
| 82 | QC | 404 | PEE | C18-C19 | 4.05 | 1.55 | 1.31 |
| 82 | N5 | 701 | PEE | C18-C19 | 4.04 | 1.55 | 1.31 |
| 82 | QC | 401 | PEE | C18-C19 | 4.04 | 1.55 | 1.31 |
| 82 | Qd | 403 | PEE | C18-C19 | 4.03 | 1.55 | 1.31 |
| 82 | S2 | 501 | PEE | C18-C19 | 4.03 | 1.55 | 1.31 |
| 82 | QB | 503 | PEE | C18-C19 | 4.02 | 1.55 | 1.31 |
| 79 | C1 | 603 | HEA | C1D-ND | -4.01 | 1.33 | 1.40 |
| 82 | Qh | 103 | PEE | C18-C19 | 4.01 | 1.55 | 1.31 |
| 79 | C1 | 602 | HEA | FE-NC | 3.99 | 2.08 | 1.95 |
| 82 | S8 | 303 | PEE | C18-C19 | 3.99 | 1.54 | 1.31 |
| 82 | Qc | 401 | PEE | C18-C19 | 3.99 | 1.54 | 1.31 |
| 82 | N3 | 201 | PEE | C18-C19 | 3.98 | 1.54 | 1.31 |
| 82 | C1 | 609 | PEE | C39-C38 | 3.96 | 1.54 | 1.31 |
| 82 | Qh | 101 | PEE | C39-C38 | 3.95 | 1.54 | 1.31 |
| 82 | Qh | 103 | PEE | C39-C38 | 3.95 | 1.54 | 1.31 |
| 82 | N5 | 701 | PEE | C39-C38 | 3.94 | 1.54 | 1.31 |
| 79 | C1 | 603 | HEA | CHC-C4B | 3.94 | 1.46 | 1.38 |
| 82 | QC | 401 | PEE | C39-C38 | 3.94 | 1.54 | 1.31 |
| 82 | QB | 503 | PEE | C39-C38 | 3.94 | 1.54 | 1.31 |
| 82 | S2 | 501 | PEE | C39-C38 | 3.93 | 1.54 | 1.31 |
| 82 | N1 | 401 | PEE | C39-C38 | 3.93 | 1.54 | 1.31 |
| 82 | S8 | 303 | PEE | C39-C38 | 3.92 | 1.54 | 1.31 |
| 82 | Qd | 403 | PEE | C39-C38 | 3.91 | 1.54 | 1.31 |
| 82 | QE | 302 | PEE | C39-C38 | 3.91 | 1.54 | 1.31 |
| 83 | QC | 403 | HEM | C4D-ND | -3.91 | 1.33 | 1.40 |
| 82 | N3 | 201 | PEE | C39-C38 | 3.90 | 1.54 | 1.31 |
| 83 | Qc | 403 | HEM | C4D-ND | -3.84 | 1.33 | 1.40 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 83 | QC | 402 | HEM | C4D-ND | -3.83 | 1.33 | 1.40 |
| 79 | C1 | 603 | HEA | C3D-C2D | 3.81 | 1.44 | 1.36 |
| 79 | C1 | 602 | HEA | C4B-NB | -3.79 | 1.33 | 1.40 |
| 79 | C1 | 602 | HEA | C3D-C2D | 3.74 | 1.44 | 1.36 |
| 83 | Qc | 402 | HEM | C4D-ND | -3.68 | 1.34 | 1.40 |
| 79 | C1 | 602 | HEA | CHA-C1A | 3.65 | 1.45 | 1.38 |
| 79 | C1 | 603 | HEA | C4C-NC | -3.63 | 1.32 | 1.39 |
| 79 | C1 | 602 | HEA | C4C-NC | -3.54 | 1.32 | 1.39 |
| 82 | N1 | 401 | PEE | C18-C19 | 3.41 | 1.55 | 1.29 |
| 79 | C1 | 603 | HEA | C1C-NC | -3.39 | 1.33 | 1.39 |
| 79 | C1 | 603 | HEA | CHA-C1A | 3.37 | 1.44 | 1.38 |
| 79 | C1 | 602 | HEA | CHD-C1D | 3.36 | 1.45 | 1.38 |
| 84 | Qd | 402 | HEC | CBC-CAC | -3.33 | 1.36 | 1.51 |
| 84 | QD | 401 | HEC | CBC-CAC | -3.33 | 1.36 | 1.51 |
| 77 | QE | 301 | PLX | O6-C4 | -3.32 | 1.40 | 1.44 |
| 82 | Qh | 101 | PEE | O3-C30 | 3.25 | 1.42 | 1.33 |
| 82 | QC | 401 | PEE | O3-C30 | 3.24 | 1.42 | 1.33 |
| 82 | Qh | 103 | PEE | O3-C30 | 3.24 | 1.42 | 1.33 |
| 83 | QC | 403 | HEM | C1B-NB | -3.24 | 1.34 | 1.40 |
| 82 | QB | 502 | PEE | O3-C30 | 3.23 | 1.42 | 1.33 |
| 82 | Qc | 401 | PEE | O3-C30 | 3.22 | 1.42 | 1.33 |
| 82 | C1 | 609 | PEE | O3-C30 | 3.21 | 1.42 | 1.33 |
| 82 | QB | 503 | PEE | O3-C30 | 3.21 | 1.42 | 1.33 |
| 79 | C1 | 603 | HEA | CHD-C1D | 3.20 | 1.45 | 1.38 |
| 83 | Qc | 403 | HEM | C1B-NB | -3.20 | 1.34 | 1.40 |
| 82 | QC | 404 | PEE | O3-C30 | 3.20 | 1.42 | 1.33 |
| 77 | CB | 201 | PLX | O6-C4 | -3.19 | 1.40 | 1.44 |
| 82 | S2 | 501 | PEE | O3-C30 | 3.18 | 1.42 | 1.33 |
| 79 | C1 | 602 | HEA | C1C-NC | -3.16 | 1.33 | 1.39 |
| 82 | S8 | 303 | PEE | O3-C30 | 3.14 | 1.42 | 1.33 |
| 82 | N3 | 201 | PEE | O3-C30 | 3.14 | 1.42 | 1.33 |
| 83 | Qc | 402 | HEM | C1B-NB | -3.13 | 1.34 | 1.40 |
| 82 | N5 | 701 | PEE | O3-C30 | 3.13 | 1.42 | 1.33 |
| 82 | Qd | 403 | PEE | O3-C30 | 3.12 | 1.42 | 1.33 |
| 77 | QI | 301 | PLX | O6-C4 | -3.11 | 1.40 | 1.44 |
| 82 | QE | 302 | PEE | O3-C30 | 3.11 | 1.42 | 1.33 |
| 83 | QC | 402 | HEM | C1B-NB | -3.10 | 1.35 | 1.40 |
| 77 | N4 | 501 | PLX | O6-C4 | -3.10 | 1.40 | 1.44 |
| 82 | N1 | 401 | PEE | O3-C30 | 3.09 | 1.42 | 1.33 |
| 77 | B5 | 201 | PLX | O6-C4 | -3.05 | 1.40 | 1.44 |
| 79 | C1 | 603 | HEA | C1B-NB | -3.03 | 1.32 | 1.38 |
| 79 | C1 | 602 | HEA | C1B-NB | -2.98 | 1.32 | 1.38 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 77 | AM | 203 | PLX | O6-C4 | -2.96 | 1.40 | 1.44 |
| 79 | C1 | 603 | HEA | CHC-C1C | 2.96 | 1.46 | 1.39 |
| 77 | AM | 201 | PLX | O6-C4 | -2.95 | 1.40 | 1.44 |
| 79 | C1 | 602 | HEA | C4D-ND | -2.94 | 1.32 | 1.38 |
| 83 | QC | 403 | HEM | C1C-C2C | -2.89 | 1.39 | 1.45 |
| 77 | C2 | 301 | PLX | O6-C4 | -2.87 | 1.40 | 1.44 |
| 79 | C1 | 602 | HEA | CHC-C1C | 2.85 | 1.45 | 1.39 |
| 74 | AC | 201 | ZMP | C9-C10 | -2.79 | 1.48 | 1.50 |
| 83 | QC | 403 | HEM | C1D-ND | -2.78 | 1.33 | 1.38 |
| 83 | Qc | 403 | HEM | C1C-C2C | -2.74 | 1.39 | 1.45 |
| 82 | N1 | 401 | PEE | O2-C10 | 2.73 | 1.42 | 1.34 |
| 82 | S8 | 303 | PEE | O2-C10 | 2.72 | 1.42 | 1.34 |
| 79 | C1 | 602 | HEA | CHD-C4C | 2.68 | 1.45 | 1.39 |
| 83 | Qc | 403 | HEM | C1D-ND | -2.66 | 1.33 | 1.38 |
| 82 | N5 | 701 | PEE | O2-C10 | 2.66 | 1.41 | 1.34 |
| 75 | AK | 401 | ADP | C5-C6 | 2.65 | 1.48 | 1.41 |
| 82 | Qd | 403 | PEE | O2-C10 | 2.65 | 1.41 | 1.34 |
| 82 | Qh | 101 | PEE | O2-C10 | 2.64 | 1.41 | 1.34 |
| 84 | Qd | 402 | HEC | CAC-C3C | 2.64 | 1.57 | 1.51 |
| 83 | Qc | 402 | HEM | C1D-ND | -2.64 | 1.33 | 1.38 |
| 82 | S2 | 501 | PEE | O2-C10 | 2.63 | 1.41 | 1.34 |
| 74 | AB | 201 | ZMP | C9-C10 | -2.63 | 1.48 | 1.50 |
| 82 | Qh | 103 | PEE | O2-C2 | -2.63 | 1.40 | 1.46 |
| 79 | C1 | 603 | HEA | CHB-C1B | 2.62 | 1.45 | 1.39 |
| 79 | C1 | 603 | HEA | C4D-ND | -2.62 | 1.33 | 1.38 |
| 82 | C1 | 609 | PEE | O2-C10 | 2.62 | 1.41 | 1.34 |
| 79 | C1 | 603 | HEA | C1A-NA | 2.62 | 1.44 | 1.39 |
| 84 | QD | 401 | HEC | CAC-C3C | 2.62 | 1.57 | 1.51 |
| 82 | QB | 503 | PEE | O2-C2 | -2.62 | 1.40 | 1.46 |
| 82 | Qc | 401 | PEE | O2-C2 | -2.61 | 1.40 | 1.46 |
| 82 | QB | 502 | PEE | O2-C10 | 2.61 | 1.41 | 1.34 |
| 83 | QC | 402 | HEM | C1D-ND | -2.61 | 1.33 | 1.38 |
| 79 | C1 | 603 | HEA | CHD-C4C | 2.60 | 1.45 | 1.39 |
| 82 | N3 | 201 | PEE | O2-C10 | 2.60 | 1.41 | 1.34 |
| 79 | C1 | 603 | HEA | CHB-C4A | 2.60 | 1.43 | 1.38 |
| 82 | QB | 502 | PEE | O2-C2 | -2.60 | 1.40 | 1.46 |
| 82 | QC | 401 | PEE | O2-C10 | 2.59 | 1.41 | 1.34 |
| 82 | QC | 401 | PEE | O2-C2 | -2.59 | 1.40 | 1.46 |
| 82 | QC | 404 | PEE | O2-C2 | -2.58 | 1.40 | 1.46 |
| 82 | QE | 302 | PEE | O2-C10 | 2.57 | 1.41 | 1.34 |
| 83 | Qc | 402 | HEM | C1C-C2C | -2.56 | 1.40 | 1.45 |
| 82 | QC | 404 | PEE | O2-C10 | 2.56 | 1.41 | 1.34 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 83 | QC | 402 | HEM | C1C-C2C | -2.55 | 1.40 | 1.45 |
| 79 | C1 | 602 | HEA | CHB-C1B | 2.53 | 1.45 | 1.39 |
| 79 | C1 | 602 | HEA | C1A-NA | 2.52 | 1.44 | 1.39 |
| 82 | Qh | 103 | PEE | O2-C10 | 2.52 | 1.41 | 1.34 |
| 82 | Qc | 401 | PEE | O2-C10 | 2.51 | 1.41 | 1.34 |
| 82 | QB | 503 | PEE | O2-C10 | 2.51 | 1.41 | 1.34 |
| 82 | N3 | 201 | PEE | O2-C2 | -2.51 | 1.40 | 1.46 |
| 82 | Qd | 403 | PEE | O2-C2 | -2.50 | 1.40 | 1.46 |
| 82 | QE | 302 | PEE | O2-C2 | -2.49 | 1.40 | 1.46 |
| 77 | AL | 205 | PLX | O6-C4 | -2.48 | 1.41 | 1.44 |
| 79 | C1 | 602 | HEA | CHB-C4A | 2.47 | 1.43 | 1.38 |
| 84 | Qd | 402 | HEC | CBB-CAB | -2.47 | 1.40 | 1.51 |
| 79 | C1 | 602 | HEA | O2D-CGD | -2.46 | 1.22 | 1.30 |
| 82 | C1 | 609 | PEE | O2-C2 | -2.46 | 1.40 | 1.46 |
| 82 | Qh | 101 | PEE | O2-C2 | -2.45 | 1.40 | 1.46 |
| 82 | N5 | 701 | PEE | O2-C2 | -2.45 | 1.40 | 1.46 |
| 79 | C1 | 602 | HEA | CHA-C4D | 2.44 | 1.44 | 1.39 |
| 82 | S2 | 501 | PEE | O2-C2 | -2.44 | 1.40 | 1.46 |
| 84 | QD | 401 | HEC | CBB-CAB | -2.43 | 1.40 | 1.51 |
| 79 | C1 | 602 | HEA | C4A-NA | 2.42 | 1.44 | 1.39 |
| 79 | C1 | 603 | HEA | O2D-CGD | -2.42 | 1.22 | 1.30 |
| 79 | C1 | 603 | HEA | O2A-CGA | -2.40 | 1.22 | 1.30 |
| 83 | Qc | 403 | HEM | FE-NB | 2.39 | 2.02 | 1.94 |
| 83 | Qc | 402 | HEM | FE-NB | 2.37 | 2.02 | 1.94 |
| 79 | C1 | 603 | HEA | C4A-NA | 2.34 | 1.44 | 1.39 |
| 79 | C1 | 602 | HEA | O2A-CGA | -2.34 | 1.22 | 1.30 |
| 77 | N4 | 501 | PLX | C1B-N1 | -2.34 | 1.43 | 1.50 |
| 75 | AK | 401 | ADP | C8-N7 | 2.34 | 1.36 | 1.31 |
| 83 | QC | 402 | HEM | FE-NB | 2.33 | 2.02 | 1.94 |
| 79 | C1 | 603 | HEA | CHA-C4D | 2.32 | 1.44 | 1.39 |
| 83 | QC | 403 | HEM | FE-NB | 2.31 | 2.02 | 1.94 |
| 77 | QE | 301 | PLX | C1B-N1 | -2.30 | 1.43 | 1.50 |
| 82 | N1 | 401 | PEE | O2-C2 | -2.30 | 1.40 | 1.46 |
| 79 | C1 | 603 | HEA | C4B-C3B | 2.28 | 1.48 | 1.44 |
| 82 | S8 | 303 | PEE | O2-C2 | -2.26 | 1.40 | 1.46 |
| 83 | Qc | 402 | HEM | C3C-C4C | -2.26 | 1.42 | 1.46 |
| 77 | B5 | 201 | PLX | C1B-N1 | -2.25 | 1.43 | 1.50 |
| 84 | Qd | 402 | HEC | CAB-C3B | 2.25 | 1.56 | 1.51 |
| 77 | CB | 201 | PLX | C1B-N1 | -2.23 | 1.43 | 1.50 |
| 77 | QI | 301 | PLX | C1B-N1 | -2.23 | 1.43 | 1.50 |
| 83 | QC | 402 | HEM | C3C-C4C | -2.21 | 1.42 | 1.46 |
| 77 | AL | 205 | PLX | C1B-N1 | -2.21 | 1.43 | 1.50 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 77 | AM | 203 | PLX | C1B-N1 | -2.20 | 1.43 | 1.50 |
| 75 | AK | 401 | ADP | C5-N7 | -2.20 | 1.34 | 1.39 |
| 77 | C2 | 301 | PLX | C1B-N1 | -2.17 | 1.43 | 1.50 |
| 77 | QE | 301 | PLX | C1C-N1 | -2.17 | 1.43 | 1.50 |
| 77 | AM | 201 | PLX | C1B-N1 | -2.14 | 1.43 | 1.50 |
| 77 | QI | 301 | PLX | C1C-N1 | -2.12 | 1.43 | 1.50 |
| 83 | Qc | 402 | HEM | FE-ND | 2.11 | 2.01 | 1.94 |
| 84 | QD | 401 | HEC | CAB-C3B | 2.10 | 1.56 | 1.51 |
| 77 | AM | 203 | PLX | C1C-N1 | -2.10 | 1.43 | 1.50 |
| 77 | AL | 205 | PLX | C1C-N1 | -2.10 | 1.43 | 1.50 |
| 77 | N4 | 501 | PLX | C1C-N1 | -2.10 | 1.43 | 1.50 |
| 77 | CB | 201 | PLX | C1C-N1 | -2.09 | 1.43 | 1.50 |
| 83 | QC | 402 | HEM | FE-ND | 2.08 | 2.01 | 1.94 |
| 83 | QC | 403 | HEM | C3C-C4C | -2.07 | 1.42 | 1.46 |
| 77 | B5 | 201 | PLX | C1C-N1 | -2.07 | 1.44 | 1.50 |
| 77 | AM | 201 | PLX | P1-O4 | 2.05 | 1.67 | 1.59 |
| 77 | C2 | 301 | PLX | C1C-N1 | -2.04 | 1.44 | 1.50 |
| 84 | Qd | 402 | HEC | CMD-C2D | 2.04 | 1.55 | 1.50 |
| 77 | C2 | 301 | PLX | P1-O4 | 2.04 | 1.67 | 1.59 |
| 83 | QC | 402 | HEM | C4B-NB | -2.03 | 1.34 | 1.38 |
| 77 | AM | 201 | PLX | C1C-N1 | -2.02 | 1.44 | 1.50 |
| 77 | AL | 205 | PLX | P1-O4 | 2.01 | 1.67 | 1.59 |
| 83 | Qc | 403 | HEM | C3C-C4C | -2.00 | 1.42 | 1.46 |

All (201) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 79 | C1 | 603 | HEA | CAD-CBD-CGD | -8.30 | 95.74 | 113.60 |
| 79 | C1 | 602 | HEA | C3C-C4C-NC | 7.81 | 115.05 | 110.25 |
| 79 | C1 | 602 | HEA | CAD-CBD-CGD | -7.80 | 96.81 | 113.60 |
| 79 | C1 | 603 | HEA | C3C-C4C-NC | 6.47 | 114.23 | 110.25 |
| 79 | C1 | 603 | HEA | CAA-CBA-CGA | -6.47 | 99.68 | 113.60 |
| 75 | AK | 401 | ADP | C5-C4-N3 | -6.31 | 118.52 | 126.75 |
| 79 | C1 | 602 | HEA | CAA-CBA-CGA | -6.20 | 100.27 | 113.60 |
| 79 | C1 | 603 | HEA | C3D-C4D-ND | 6.01 | 116.18 | 110.36 |
| 79 | C1 | 602 | HEA | C3D-C4D-ND | 5.65 | 115.83 | 110.36 |
| 79 | C1 | 602 | HEA | C13-C12-C11 | -5.51 | 106.07 | 114.35 |
| 79 | C1 | 603 | HEA | C3C-C2C-C1C | -5.44 | 100.59 | 107.16 |
| 79 | C1 | 602 | HEA | C3C-C2C-C1C | -5.41 | 100.64 | 107.16 |
| 79 | C1 | 603 | HEA | C13-C12-C11 | -5.08 | 106.72 | 114.35 |
| 79 | C1 | 603 | HEA | C2B-C1B-NB | 5.07 | 115.96 | 109.88 |
| 75 | AK | 401 | ADP | N3-C4-N9 | 4.99 | 135.30 | 127.08 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 79 | C1 | 602 | HEA | C1D-C2D-C3D | -4.95 | 101.75 | 106.96 |
| 79 | C1 | 602 | HEA | C2B-C1B-NB | 4.90 | 115.75 | 109.88 |
| 83 | Qc | 402 | HEM | CHD-C4C-NC | 4.90 | 129.74 | 124.44 |
| 83 | QC | 402 | HEM | CHC-C4B-NB | 4.79 | 129.62 | 124.42 |
| 83 | QC | 402 | HEM | CHD-C4C-NC | 4.78 | 129.61 | 124.44 |
| 83 | Qc | 403 | HEM | CHC-C4B-NB | 4.76 | 129.59 | 124.42 |
| 79 | C1 | 603 | HEA | CHB-C1B-C2B | -4.73 | 117.59 | 124.98 |
| 79 | C1 | 602 | HEA | CHB-C1B-C2B | -4.69 | 117.65 | 124.98 |
| 79 | C1 | 602 | HEA | C2D-C1D-ND | 4.68 | 115.38 | 109.84 |
| 83 | Qc | 402 | HEM | CHC-C4B-NB | 4.65 | 129.47 | 124.42 |
| 82 | QC | 401 | PEE | O2-C10-C11 | 4.61 | 121.44 | 111.50 |
| 79 | C1 | 603 | HEA | C2D-C1D-ND | 4.57 | 115.25 | 109.84 |
| 79 | C1 | 603 | HEA | C1D-C2D-C3D | -4.49 | 102.23 | 106.96 |
| 82 | QE | 302 | PEE | O2-C10-C11 | 4.41 | 121.00 | 111.50 |
| 83 | QC | 403 | HEM | CHC-C4B-NB | 4.37 | 129.17 | 124.42 |
| 83 | Qc | 403 | HEM | CHD-C4C-NC | 4.33 | 129.13 | 124.44 |
| 82 | Qd | 403 | PEE | O2-C10-C11 | 4.26 | 120.67 | 111.50 |
| 82 | QB | 502 | PEE | O2-C10-C11 | 4.25 | 120.66 | 111.50 |
| 79 | C1 | 602 | HEA | CHA-C4D-C3D | -4.15 | 118.73 | 124.84 |
| 83 | QC | 403 | HEM | C4D-ND-C1D | 4.12 | 109.32 | 105.07 |
| 83 | QC | 403 | HEM | CHD-C4C-NC | 4.05 | 128.82 | 124.44 |
| 79 | C1 | 603 | HEA | C3B-C4B-NB | 4.04 | 114.63 | 109.84 |
| 82 | S2 | 501 | PEE | O2-C10-C11 | 4.02 | 120.17 | 111.50 |
| 82 | C1 | 609 | PEE | O2-C10-C11 | 4.02 | 120.16 | 111.50 |
| 82 | N1 | 401 | PEE | O2-C10-C11 | 4.00 | 120.13 | 111.50 |
| 83 | QC | 402 | HEM | CHB-C1B-NB | 4.00 | 129.31 | 124.37 |
| 79 | C1 | 602 | HEA | C2C-C1C-NC | 3.99 | 116.16 | 110.08 |
| 79 | C1 | 602 | HEA | C3B-C4B-NB | 3.99 | 114.56 | 109.84 |
| 82 | N3 | 201 | PEE | O2-C10-C11 | 3.98 | 120.08 | 111.50 |
| 83 | Qc | 402 | HEM | CHB-C1B-NB | 3.95 | 129.25 | 124.37 |
| 82 | Qc | 401 | PEE | O2-C10-C11 | 3.93 | 119.98 | 111.50 |
| 82 | S8 | 303 | PEE | O2-C10-C11 | 3.92 | 119.96 | 111.50 |
| 82 | Qh | 101 | PEE | O2-C10-C11 | 3.92 | 119.94 | 111.50 |
| 83 | Qc | 403 | HEM | CHB-C1B-NB | 3.92 | 129.20 | 124.37 |
| 75 | AK | 401 | ADP | C2-N3-C4 | 3.91 | 120.99 | 111.75 |
| 82 | QB | 503 | PEE | O2-C10-C11 | 3.88 | 119.86 | 111.50 |
| 75 | AK | 401 | ADP | PA-O3A-PB | -3.86 | 119.57 | 132.83 |
| 82 | QC | 404 | PEE | O2-C10-C11 | 3.83 | 119.77 | 111.50 |
| 79 | C1 | 603 | HEA | CHA-C4D-C3D | -3.80 | 119.25 | 124.84 |
| 82 | N5 | 701 | PEE | O2-C10-C11 | 3.78 | 119.66 | 111.50 |
| 82 | Qh | 103 | PEE | O2-C10-C11 | 3.75 | 119.59 | 111.50 |
| 79 | C1 | 603 | HEA | C2C-C1C-NC | 3.71 | 115.73 | 110.08 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 83 | QC | 403 | HEM | CHB-C1B-NB | 3.69 | 128.93 | 124.37 |
| 79 | C1 | 603 | HEA | C4B-C3B-C2B | -3.63 | 101.21 | 107.41 |
| 79 | C1 | 602 | HEA | C4B-C3B-C2B | -3.55 | 101.34 | 107.41 |
| 83 | QC | 403 | HEM | C1B-NB-C4B | 3.50 | 108.68 | 105.07 |
| 83 | Qc | 403 | HEM | C4D-ND-C1D | 3.47 | 108.65 | 105.07 |
| 83 | Qc | 402 | HEM | C4D-ND-C1D | 3.25 | 108.43 | 105.07 |
| 83 | QC | 402 | HEM | C4D-ND-C1D | 3.24 | 108.42 | 105.07 |
| 79 | C1 | 603 | HEA | C17-C18-C19 | -3.17 | 120.03 | 127.66 |
| 75 | AK | 401 | ADP | C4-C5-N7 | -3.17 | 106.76 | 110.62 |
| 83 | QC | 402 | HEM | C1B-NB-C4B | 3.16 | 108.33 | 105.07 |
| 83 | QC | 403 | HEM | C4C-NC-C1C | 3.15 | 108.43 | 105.35 |
| 83 | Qc | 403 | HEM | C1B-NB-C4B | 3.12 | 108.29 | 105.07 |
| 75 | AK | 401 | ADP | N3-C2-N1 | -3.10 | 123.75 | 128.60 |
| 83 | Qc | 402 | HEM | C1B-NB-C4B | 3.04 | 108.22 | 105.07 |
| 83 | Qc | 403 | HEM | CHA-C4D-ND | 3.00 | 128.07 | 124.37 |
| 83 | Qc | 402 | HEM | CHA-C4D-ND | 2.97 | 128.04 | 124.37 |
| 83 | QC | 402 | HEM | CHA-C4D-ND | 2.97 | 128.03 | 124.37 |
| 83 | QC | 403 | HEM | C4A-NA-C1A | 2.96 | 108.24 | 105.35 |
| 84 | QD | 401 | HEC | O1D-CGD-CBD | -2.94 | 113.63 | 123.08 |
| 82 | QE | 302 | PEE | O3-C30-C31 | 2.88 | 120.95 | 111.91 |
| 79 | C1 | 603 | HEA | C27-C19-C20 | 2.86 | 120.08 | 115.27 |
| 82 | Qc | 401 | PEE | O3-C30-C31 | 2.85 | 120.85 | 111.91 |
| 83 | Qc | 402 | HEM | CHA-C1A-NA | 2.82 | 129.04 | 123.85 |
| 79 | C1 | 602 | HEA | C27-C19-C20 | 2.82 | 120.01 | 115.27 |
| 83 | Qc | 402 | HEM | CHD-C1D-ND | 2.81 | 127.47 | 124.42 |
| 79 | C1 | 602 | HEA | C17-C18-C19 | -2.80 | 120.92 | 127.66 |
| 83 | Qc | 403 | HEM | CAD-CBD-CGD | -2.79 | 107.60 | 113.60 |
| 79 | C1 | 603 | HEA | C13-C14-C15 | -2.79 | 120.94 | 127.66 |
| 82 | Qh | 103 | PEE | O3-C30-C31 | 2.79 | 120.65 | 111.91 |
| 82 | S8 | 303 | PEE | O3-C30-C31 | 2.78 | 120.63 | 111.91 |
| 84 | Qd | 402 | HEC | O1D-CGD-CBD | -2.77 | 114.17 | 123.08 |
| 83 | Qc | 403 | HEM | CHD-C1D-ND | 2.73 | 127.39 | 124.42 |
| 75 | AK | 401 | ADP | C5-N7-C8 | 2.71 | 107.36 | 103.51 |
| 79 | C1 | 602 | HEA | C13-C14-C15 | -2.71 | 121.14 | 127.66 |
| 83 | QC | 402 | HEM | CHA-C1A-NA | 2.70 | 128.82 | 123.85 |
| 83 | QC | 402 | HEM | CHD-C1D-ND | 2.68 | 127.33 | 124.42 |
| 83 | QC | 403 | HEM | CHA-C4D-ND | 2.68 | 127.67 | 124.37 |
| 82 | N1 | 401 | PEE | C17-C18-C19 | -2.66 | 109.90 | 131.07 |
| 82 | S2 | 501 | PEE | O3-C30-C31 | 2.66 | 120.25 | 111.91 |
| 82 | Qd | 403 | PEE | O3-C30-C31 | 2.61 | 120.11 | 111.91 |
| 82 | QB | 502 | PEE | O3-C30-C31 | 2.61 | 120.10 | 111.91 |
| 82 | C1 | 609 | PEE | O3-C30-C31 | 2.59 | 120.04 | 111.91 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 83 | Qc | 403 | HEM | CHA-C1A-NA | 2.59 | 128.61 | 123.85 |
| 82 | QC | 404 | PEE | O3-C30-C31 | 2.59 | 120.02 | 111.91 |
| 83 | QC | 403 | HEM | C1C-CHC-C4B | -2.59 | 120.48 | 126.06 |
| 75 | AK | 401 | ADP | C4-N9-C8 | 2.55 | 108.49 | 105.73 |
| 83 | Qc | 403 | HEM | C4C-NC-C1C | 2.54 | 107.84 | 105.35 |
| 83 | QC | 403 | HEM | CHA-C1A-NA | 2.53 | 128.50 | 123.85 |
| 79 | C1 | 603 | HEA | C4D-C3D-C2D | -2.50 | 103.25 | 106.90 |
| 79 | C1 | 602 | HEA | CMB-C2B-C1B | -2.49 | 121.24 | 125.04 |
| 82 | N1 | 401 | PEE | O3-C30-C31 | 2.48 | 119.69 | 111.91 |
| 83 | Qc | 402 | HEM | C4C-NC-C1C | 2.47 | 107.77 | 105.35 |
| 83 | Qc | 402 | HEM | CAA-CBA-CGA | -2.46 | 108.32 | 113.60 |
| 79 | C1 | 603 | HEA | CMB-C2B-C1B | -2.45 | 121.31 | 125.04 |
| 82 | N3 | 201 | PEE | O3-C30-C31 | 2.43 | 119.53 | 111.91 |
| 83 | QC | 402 | HEM | C4C-NC-C1C | 2.43 | 107.73 | 105.35 |
| 82 | Qh | 101 | PEE | O3-C30-C31 | 2.43 | 119.52 | 111.91 |
| 84 | QD | 401 | HEC | O1A-CGA-CBA | -2.42 | 115.30 | 123.08 |
| 83 | QC | 403 | HEM | CHD-C1D-ND | 2.42 | 127.04 | 124.42 |
| 82 | N5 | 701 | PEE | O3-C30-C31 | 2.41 | 119.48 | 111.91 |
| 82 | QC | 401 | PEE | O3-C30-C31 | 2.40 | 119.45 | 111.91 |
| 83 | QC | 403 | HEM | C4A-CHB-C1B | -2.40 | 120.65 | 126.34 |
| 83 | QC | 402 | HEM | CAA-CBA-CGA | -2.39 | 108.46 | 113.60 |
| 79 | C1 | 603 | HEA | C1B-C2B-C3B | -2.37 | 103.96 | 106.80 |
| 79 | C1 | 603 | HEA | OMA-CMA-C3A | -2.37 | 120.33 | 125.69 |
| 82 | QB | 503 | PEE | O3-C30-C31 | 2.36 | 119.33 | 111.91 |
| 83 | QC | 403 | HEM | C2A-C1A-NA | -2.36 | 107.50 | 110.15 |
| 83 | Qc | 402 | HEM | CHB-C1B-C2B | -2.35 | 120.20 | 126.73 |
| 74 | AB | 201 | ZMP | C15-C14-C13 | -2.34 | 108.46 | 112.36 |
| 79 | C1 | 602 | HEA | C27-C19-C18 | -2.32 | 117.72 | 123.68 |
| 83 | QC | 402 | HEM | CHB-C1B-C2B | -2.32 | 120.29 | 126.73 |
| 77 | AL | 205 | PLX | C8-C7-C6 | -2.31 | 108.03 | 113.38 |
| 84 | Qd | 402 | HEC | O2A-CGA-O1A | 2.31 | 129.06 | 123.30 |
| 79 | C1 | 602 | HEA | CHC-C4B-NB | -2.30 | 121.53 | 124.37 |
| 79 | C1 | 603 | HEA | CMB-C2B-C3B | 2.30 | 134.73 | 130.34 |
| 79 | C1 | 602 | HEA | C1B-C2B-C3B | -2.29 | 104.06 | 106.80 |
| 79 | C1 | 602 | HEA | OMA-CMA-C3A | -2.29 | 120.50 | 125.69 |
| 84 | QD | 401 | HEC | O2A-CGA-O1A | 2.29 | 129.00 | 123.30 |
| 79 | C1 | 602 | HEA | CMB-C2B-C3B | 2.28 | 134.69 | 130.34 |
| 83 | Qc | 403 | HEM | CHB-C1B-C2B | -2.28 | 120.39 | 126.73 |
| 83 | Qc | 402 | HEM | CAD-CBD-CGD | -2.28 | 108.70 | 113.60 |
| 79 | C1 | 603 | HEA | C27-C19-C18 | -2.26 | 117.88 | 123.68 |
| 77 | QI | 301 | PLX | O3-P1-O2 | -2.26 | 101.08 | 112.24 |
| 79 | C1 | 603 | HEA | CHC-C4B-NB | -2.25 | 121.59 | 124.37 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 77 | B5 | 201 | PLX | O3-P1-O2 | -2.25 | 101.11 | 112.24 |
| 77 | AM | 201 | PLX | O3-P1-O2 | -2.24 | 101.17 | 112.24 |
| 79 | C1 | 603 | HEA | C26-C15-C16 | 2.24 | 119.03 | 115.27 |
| 83 | Qc | 402 | HEM | C4A-NA-C1A | 2.23 | 107.53 | 105.35 |
| 83 | Qc | 403 | HEM | C1C-CHC-C4B | -2.22 | 121.26 | 126.06 |
| 77 | QE | 301 | PLX | O3-P1-O2 | -2.21 | 101.30 | 112.24 |
| 83 | QC | 402 | HEM | C1C-CHC-C4B | -2.21 | 121.30 | 126.06 |
| 84 | Qd | 402 | HEC | O1A-CGA-CBA | -2.20 | 116.01 | 123.08 |
| 79 | C1 | 602 | HEA | C4D-C3D-C2D | -2.20 | 103.69 | 106.90 |
| 77 | AM | 203 | PLX | O3-P1-O2 | -2.20 | 101.38 | 112.24 |
| 83 | Qc | 402 | HEM | C1C-CHC-C4B | -2.19 | 121.33 | 126.06 |
| 83 | Qc | 403 | HEM | C4A-NA-C1A | 2.18 | 107.49 | 105.35 |
| 83 | QC | 403 | HEM | CAA-CBA-CGA | -2.18 | 108.91 | 113.60 |
| 79 | C1 | 602 | HEA | C26-C15-C16 | 2.18 | 118.93 | 115.27 |
| 77 | AL | 205 | PLX | O3-P1-O2 | -2.17 | 101.51 | 112.24 |
| 77 | CB | 201 | PLX | O3-P1-O2 | -2.17 | 101.51 | 112.24 |
| 79 | C1 | 603 | HEA | O1D-CGD-CBD | -2.17 | 116.11 | 123.08 |
| 77 | C2 | 301 | PLX | O3-P1-O2 | -2.17 | 101.53 | 112.24 |
| 84 | QD | 401 | HEC | CHC-C4B-NB | 2.17 | 127.04 | 124.37 |
| 84 | QD | 401 | HEC | CMD-C2D-C1D | -2.16 | 121.75 | 125.04 |
| 83 | Qc | 403 | HEM | C4A-CHB-C1B | -2.16 | 121.22 | 126.34 |
| 77 | N4 | 501 | PLX | O3-P1-O2 | -2.16 | 101.56 | 112.24 |
| 79 | C1 | 603 | HEA | CMC-C2C-C1C | 2.15 | 128.65 | 125.37 |
| 77 | N4 | 501 | PLX | C2-C1-N1 | -2.15 | 108.61 | 115.78 |
| 83 | QC | 403 | HEM | CHB-C1B-C2B | -2.14 | 120.78 | 126.73 |
| 83 | QC | 403 | HEM | C4C-CHD-C1D | -2.13 | 121.46 | 126.06 |
| 84 | QD | 401 | HEC | CBD-CAD-C3D | 2.12 | 118.51 | 112.63 |
| 74 | AB | 201 | ZMP | C14-C13-N1 | 2.11 | 119.97 | 116.42 |
| 83 | QC | 402 | HEM | C4A-NA-C1A | 2.11 | 107.41 | 105.35 |
| 82 | S8 | 303 | PEE | C17-C18-C19 | -2.10 | 108.60 | 124.73 |
| 75 | AK | 401 | ADP | C3'-C2'-C1' | 2.10 | 105.41 | 101.43 |
| 79 | C1 | 602 | HEA | CMD-C2D-C1D | 2.10 | 128.23 | 125.04 |
| 82 | N1 | 401 | PEE | C20-C19-C18 | -2.09 | 109.11 | 126.37 |
| 75 | AK | 401 | ADP | C6-C5-N7 | 2.08 | 135.90 | 132.02 |
| 83 | Qc | 402 | HEM | C4A-CHB-C1B | -2.06 | 121.44 | 126.34 |
| 83 | QC | 402 | HEM | C4A-CHB-C1B | -2.06 | 121.45 | 126.34 |
| 82 | Qc | 401 | PEE | C17-C18-C19 | -2.06 | 108.92 | 124.73 |
| 82 | N3 | 201 | PEE | C37-C38-C39 | -2.05 | 108.98 | 124.73 |
| 82 | Qd | 403 | PEE | C37-C38-C39 | -2.05 | 109.03 | 124.73 |
| 82 | S8 | 303 | PEE | C37-C38-C39 | -2.04 | 109.03 | 124.73 |
| 82 | QC | 401 | PEE | C37-C38-C39 | -2.04 | 109.05 | 124.73 |
| 79 | C1 | 602 | HEA | O1D-CGD-CBD | -2.04 | 116.52 | 123.08 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 82 | N3 | 201 | PEE | C40-C39-C38 | -2.04 | 109.07 | 124.73 |
| 82 | Qd | 403 | PEE | C20-C19-C18 | -2.04 | 109.10 | 124.73 |
| 82 | QE | 302 | PEE | C40-C39-C38 | -2.03 | 109.11 | 124.73 |
| 82 | Qh | 103 | PEE | C17-C18-C19 | -2.03 | 109.12 | 124.73 |
| 84 | QD | 401 | HEC | C1D-ND-C4D | 2.03 | 107.17 | 105.07 |
| 82 | Qh | 103 | PEE | C20-C19-C18 | -2.02 | 109.20 | 124.73 |
| 82 | QE | 302 | PEE | C2-O2-C10 | -2.02 | 112.81 | 117.79 |
| 82 | N3 | 201 | PEE | C17-C18-C19 | -2.02 | 109.20 | 124.73 |
| 82 | S2 | 501 | PEE | C37-C38-C39 | -2.02 | 109.22 | 124.73 |
| 82 | C1 | 609 | PEE | C20-C19-C18 | -2.02 | 109.25 | 124.73 |
| 79 | C1 | 602 | HEA | CMC-C2C-C1C | 2.01 | 128.43 | 125.37 |
| 82 | Qh | 101 | PEE | C37-C38-C39 | -2.01 | 109.29 | 124.73 |
| 82 | QB | 503 | PEE | C37-C38-C39 | -2.01 | 109.30 | 124.73 |
| 83 | QC | 402 | HEM | CAD-CBD-CGD | -2.01 | 109.29 | 113.60 |
| 82 | Qc | 401 | PEE | C20-C19-C18 | -2.00 | 109.35 | 124.73 |
| 79 | C1 | 602 | HEA | O1A-CGA-CBA | -2.00 | 116.64 | 123.08 |
| 79 | C1 | 603 | HEA | C2A-C1A-NA | 2.00 | 112.27 | 110.32 |
| 84 | QD | 401 | HEC | CMC-C2C-C3C | 2.00 | 129.93 | 125.61 |

All (2) chirality outliers are listed below:

| Mol | Chain | Res | Type | Atom |
|---|---|---|---|---|
| 84 | QD | 401 | HEC | NA |
| 84 | Qd | 402 | HEC | NA |

All (1306) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 71 | 6A | 101 | PC1 | C11-O13-P-O14 |
| 71 | 7B | 101 | PC1 | C1-O11-P-O12 |
| 71 | 7B | 101 | PC1 | C1-O11-P-O14 |
| 71 | 7B | 101 | PC1 | O13-C11-C12-N |
| 71 | AL | 206 | PC1 | C11-O13-P-O14 |
| 71 | AL | 206 | PC1 | C1-O11-P-O12 |
| 71 | AL | 206 | PC1 | C1-O11-P-O14 |
| 71 | AL | 206 | PC1 | C1-O11-P-O13 |
| 71 | C1 | 606 | PC1 | C11-O13-P-O12 |
| 71 | C1 | 606 | PC1 | C11-O13-P-O14 |
| 71 | C1 | 607 | PC1 | O13-C11-C12-N |
| 71 | C3 | 301 | PC1 | C1-O11-P-O14 |
| 71 | C3 | 301 | PC1 | O13-C11-C12-N |
| 71 | C3 | 302 | PC1 | C11-O13-P-O11 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 71 | N5 | 704 | PC1 | C11-O13-P-O12 |
| 71 | N5 | 704 | PC1 | C11-O13-P-O14 |
| 71 | N5 | 704 | PC1 | C11-O13-P-O11 |
| 71 | N6 | 201 | PC1 | C11-O13-P-O12 |
| 71 | N6 | 201 | PC1 | C11-O13-P-O11 |
| 71 | QC | 407 | PC1 | C11-O13-P-O14 |
| 71 | QC | 407 | PC1 | O13-C11-C12-N |
| 71 | QH | 102 | PC1 | C1-O11-P-O12 |
| 71 | Qj | 101 | PC1 | C1-O11-P-O14 |
| 71 | Qj | 101 | PC1 | C1-O11-P-O13 |
| 72 | 6A | 102 | CDL | CA2-OA2-PA1-OA3 |
| 72 | 6A | 102 | CDL | CA3-OA5-PA1-OA3 |
| 72 | 6A | 102 | CDL | CB2-OB2-PB2-OB3 |
| 72 | 6A | 102 | CDL | CB2-OB2-PB2-OB4 |
| 72 | 6A | 102 | CDL | CB2-OB2-PB2-OB5 |
| 72 | 6A | 102 | CDL | CB3-OB5-PB2-OB3 |
| 72 | A8 | 301 | CDL | CA2-OA2-PA1-OA3 |
| 72 | A8 | 301 | CDL | CA2-OA2-PA1-OA4 |
| 72 | A8 | 301 | CDL | CA2-OA2-PA1-OA5 |
| 72 | A8 | 301 | CDL | CB3-OB5-PB2-OB3 |
| 72 | AL | 201 | CDL | CA2-OA2-PA1-OA3 |
| 72 | AL | 201 | CDL | CA3-OA5-PA1-OA2 |
| 72 | AL | 201 | CDL | CA3-OA5-PA1-OA4 |
| 72 | AL | 201 | CDL | CB3-OB5-PB2-OB4 |
| 72 | AL | 203 | CDL | CA2-OA2-PA1-OA4 |
| 72 | AL | 203 | CDL | CB2-OB2-PB2-OB3 |
| 72 | AL | 203 | CDL | CB2-OB2-PB2-OB4 |
| 72 | AL | 203 | CDL | CB2-OB2-PB2-OB5 |
| 72 | AL | 203 | CDL | CB3-OB5-PB2-OB3 |
| 72 | AL | 204 | CDL | CA3-OA5-PA1-OA4 |
| 72 | AL | 204 | CDL | CB2-OB2-PB2-OB3 |
| 72 | AL | 204 | CDL | CB2-OB2-PB2-OB4 |
| 72 | AL | 204 | CDL | CB2-OB2-PB2-OB5 |
| 72 | AL | 204 | CDL | OB5-CB3-CB4-OB6 |
| 72 | AM | 202 | CDL | CB3-OB5-PB2-OB4 |
| 72 | B5 | 202 | CDL | CB2-OB2-PB2-OB3 |
| 72 | B5 | 202 | CDL | CB2-OB2-PB2-OB4 |
| 72 | B5 | 202 | CDL | CB2-OB2-PB2-OB5 |
| 72 | CB | 203 | CDL | CA3-OA5-PA1-OA2 |
| 72 | CB | 203 | CDL | CB2-OB2-PB2-OB4 |
| 72 | CB | 203 | CDL | CB3-OB5-PB2-OB3 |
| 72 | N2 | 401 | CDL | CA3-OA5-PA1-OA2 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 72 | N2 | 401 | CDL | CA3-OA5-PA1-OA3 |
| 72 | N2 | 401 | CDL | CA3-OA5-PA1-OA4 |
| 72 | N5 | 702 | CDL | CA3-OA5-PA1-OA3 |
| 72 | N5 | 702 | CDL | CB2-OB2-PB2-OB3 |
| 72 | N5 | 702 | CDL | CB2-OB2-PB2-OB5 |
| 72 | N5 | 702 | CDL | CB3-OB5-PB2-OB2 |
| 72 | N5 | 702 | CDL | CB3-OB5-PB2-OB3 |
| 72 | N5 | 702 | CDL | CB3-OB5-PB2-OB4 |
| 72 | N5 | 703 | CDL | CA2-OA2-PA1-OA3 |
| 72 | QB | 501 | CDL | CA2-OA2-PA1-OA3 |
| 72 | QB | 501 | CDL | CB2-OB2-PB2-OB4 |
| 72 | QB | 501 | CDL | CB3-OB5-PB2-OB3 |
| 72 | QC | 406 | CDL | CA2-OA2-PA1-OA3 |
| 72 | QC | 406 | CDL | CA2-OA2-PA1-OA4 |
| 72 | QC | 406 | CDL | CA2-OA2-PA1-OA5 |
| 72 | QC | 406 | CDL | CB2-OB2-PB2-OB3 |
| 72 | QC | 406 | CDL | CB2-OB2-PB2-OB5 |
| 72 | QC | 406 | CDL | CB3-OB5-PB2-OB4 |
| 72 | QC | 408 | CDL | CA3-OA5-PA1-OA3 |
| 72 | QC | 408 | CDL | CA3-OA5-PA1-OA4 |
| 72 | QC | 408 | CDL | CB3-OB5-PB2-OB4 |
| 72 | QH | 101 | CDL | CB2-OB2-PB2-OB3 |
| 72 | QH | 101 | CDL | CB2-OB2-PB2-OB4 |
| 72 | QH | 101 | CDL | CB2-OB2-PB2-OB5 |
| 72 | Qb | 501 | CDL | CA2-OA2-PA1-OA4 |
| 72 | Qb | 501 | CDL | CA3-OA5-PA1-OA4 |
| 72 | Qb | 501 | CDL | CB2-OB2-PB2-OB3 |
| 72 | Qb | 501 | CDL | CB2-OB2-PB2-OB4 |
| 72 | Qb | 501 | CDL | CB2-OB2-PB2-OB5 |
| 72 | Qb | 501 | CDL | CB3-OB5-PB2-OB3 |
| 72 | Qd | 401 | CDL | CA2-OA2-PA1-OA4 |
| 72 | Qd | 401 | CDL | CA3-OA5-PA1-OA3 |
| 72 | Qd | 401 | CDL | OB5-CB3-CB4-OB6 |
| 72 | Qh | 102 | CDL | CA2-OA2-PA1-OA3 |
| 72 | Qh | 102 | CDL | CA3-OA5-PA1-OA3 |
| 73 | A9 | 401 | NDP | C5D-O5D-PN-O1N |
| 74 | AB | 201 | ZMP | S1-C11-C12-N1 |
| 74 | AB | 201 | ZMP | C9-C10-S1-C11 |
| 74 | AB | 201 | ZMP | C7-C8-C9-C10 |
| 74 | AC | 201 | ZMP | C17-C18-C21-O5 |
| 74 | AC | 201 | ZMP | C9-C10-S1-C11 |
| 74 | AC | 201 | ZMP | O1-C10-C9-C8 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 75 | AK | 401 | ADP | C3'-C4'-C5'-O5' |
| 76 | AL | 202 | 3PE | C1-O11-P-O12 |
| 76 | AL | 202 | 3PE | C11-O13-P-O14 |
| 76 | AL | 202 | 3PE | O13-C11-C12-N |
| 76 | C1 | 601 | 3PE | C11-O13-P-O12 |
| 76 | C1 | 601 | 3PE | O13-C11-C12-N |
| 76 | C1 | 608 | 3PE | O13-C11-C12-N |
| 76 | CA | 101 | 3PE | C1-O11-P-O12 |
| 76 | CB | 202 | 3PE | C1-O11-P-O12 |
| 76 | CB | 202 | 3PE | C1-O11-P-O14 |
| 76 | CB | 202 | 3PE | C11-O13-P-O14 |
| 76 | CB | 202 | 3PE | O13-C11-C12-N |
| 76 | N4 | 502 | 3PE | C1-O11-P-O12 |
| 76 | N4 | 502 | 3PE | C1-O11-P-O13 |
| 76 | N4 | 502 | 3PE | C1-O11-P-O14 |
| 76 | N4 | 502 | 3PE | C11-O13-P-O12 |
| 76 | N4 | 502 | 3PE | C11-O13-P-O14 |
| 76 | N4 | 502 | 3PE | O13-C11-C12-N |
| 76 | QE | 303 | 3PE | C11-O13-P-O12 |
| 76 | S7 | 302 | 3PE | C1-O11-P-O12 |
| 76 | S7 | 302 | 3PE | C11-O13-P-O12 |
| 76 | S7 | 302 | 3PE | O13-C11-C12-N |
| 77 | AL | 205 | PLX | C3-C4-O6-C6 |
| 77 | AL | 205 | PLX | C2-O1-P1-O4 |
| 77 | AL | 205 | PLX | C2-O1-P1-O3 |
| 77 | AL | 205 | PLX | C25-C24-O8-C5 |
| 77 | AM | 201 | PLX | O7-C6-C7-C8 |
| 77 | AM | 201 | PLX | C3-O4-P1-O1 |
| 77 | AM | 201 | PLX | C3-O4-P1-O2 |
| 77 | AM | 201 | PLX | C3-O4-P1-O3 |
| 77 | AM | 201 | PLX | N1-C1-C2-O1 |
| 77 | AM | 201 | PLX | O9-C24-O8-C5 |
| 77 | AM | 201 | PLX | O9-C24-C25-C26 |
| 77 | AM | 203 | PLX | O7-C6-O6-C4 |
| 77 | AM | 203 | PLX | C3-O4-P1-O2 |
| 77 | AM | 203 | PLX | C3-O4-P1-O3 |
| 77 | AM | 203 | PLX | O9-C24-O8-C5 |
| 77 | B5 | 201 | PLX | O7-C6-O6-C4 |
| 77 | B5 | 201 | PLX | C3-O4-P1-O1 |
| 77 | B5 | 201 | PLX | C3-O4-P1-O2 |
| 77 | B5 | 201 | PLX | C3-O4-P1-O3 |
| 77 | B5 | 201 | PLX | C2-O1-P1-O2 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 77 | B5 | 201 | PLX | C2-O1-P1-O3 |
| 77 | C2 | 301 | PLX | O7-C6-C7-C8 |
| 77 | C2 | 301 | PLX | N1-C1-C2-O1 |
| 77 | C2 | 301 | PLX | O9-C24-O8-C5 |
| 77 | C2 | 301 | PLX | O9-C24-C25-C26 |
| 77 | CB | 201 | PLX | O7-C6-C7-C8 |
| 77 | CB | 201 | PLX | O7-C6-O6-C4 |
| 77 | CB | 201 | PLX | C2-O1-P1-O2 |
| 77 | CB | 201 | PLX | C2-O1-P1-O3 |
| 77 | N4 | 501 | PLX | O7-C6-O6-C4 |
| 77 | N4 | 501 | PLX | C2-O1-P1-O4 |
| 77 | N4 | 501 | PLX | C25-C24-O8-C5 |
| 77 | QE | 301 | PLX | O7-C6-C7-C8 |
| 77 | QE | 301 | PLX | O7-C6-O6-C4 |
| 77 | QE | 301 | PLX | C2-O1-P1-O2 |
| 77 | QE | 301 | PLX | C2-O1-P1-O3 |
| 77 | QE | 301 | PLX | O9-C24-C25-C26 |
| 77 | QI | 301 | PLX | C2-O1-P1-O2 |
| 77 | QI | 301 | PLX | C2-O1-P1-O3 |
| 77 | QI | 301 | PLX | O9-C24-O8-C5 |
| 78 | B5 | 203 | 6F6 | C1-O11-P-O12 |
| 78 | B5 | 203 | 6F6 | C1-O11-P-O13 |
| 78 | QJ | 101 | 6F6 | C1-O11-P-O12 |
| 78 | QJ | 101 | 6F6 | C1-O11-P-O14 |
| 78 | QJ | 101 | 6F6 | C1-O11-P-O13 |
| 78 | QJ | 101 | 6F6 | O13-C11-C12-N |
| 79 | C1 | 602 | HEA | C1A-C2A-CAA-CBA |
| 79 | C1 | 602 | HEA | C3A-C2A-CAA-CBA |
| 79 | C1 | 602 | HEA | C2A-C3A-CMA-OMA |
| 79 | C1 | 602 | HEA | C4A-C3A-CMA-OMA |
| 79 | C1 | 603 | HEA | C3A-C2A-CAA-CBA |
| 79 | C1 | 603 | HEA | C2A-C3A-CMA-OMA |
| 79 | C1 | 603 | HEA | C4A-C3A-CMA-OMA |
| 79 | C1 | 603 | HEA | C17-C18-C19-C27 |
| 79 | C1 | 603 | HEA | C19-C20-C21-C22 |
| 82 | C1 | 609 | PEE | C4-O4P-P-O3P |
| 82 | C1 | 609 | PEE | C4-O4P-P-O2P |
| 82 | N1 | 401 | PEE | C1-O3P-P-O1P |
| 82 | N3 | 201 | PEE | C17-C18-C19-C20 |
| 82 | N3 | 201 | PEE | O2-C2-C3-O3 |
| 82 | N3 | 201 | PEE | C1-O3P-P-O1P |
| 82 | N3 | 201 | PEE | C4-O4P-P-O3P |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 82 | N3 | 201 | PEE | C4-O4P-P-O2P |
| 82 | N3 | 201 | PEE | C4-O4P-P-O1P |
| 82 | N5 | 701 | PEE | C4-O4P-P-O2P |
| 82 | N5 | 701 | PEE | O4P-C4-C5-N |
| 82 | QB | 502 | PEE | C11-C10-O2-C2 |
| 82 | QB | 502 | PEE | O4-C10-O2-C2 |
| 82 | QB | 502 | PEE | C4-O4P-P-O2P |
| 82 | QB | 503 | PEE | C1-O3P-P-O2P |
| 82 | QB | 503 | PEE | C1-O3P-P-O1P |
| 82 | QB | 503 | PEE | C1-O3P-P-O4P |
| 82 | QB | 503 | PEE | C4-O4P-P-O2P |
| 82 | QB | 503 | PEE | C37-C38-C39-C40 |
| 82 | QC | 401 | PEE | C11-C10-O2-C2 |
| 82 | QC | 401 | PEE | O4-C10-O2-C2 |
| 82 | QC | 401 | PEE | O4P-C4-C5-N |
| 82 | QC | 404 | PEE | C4-O4P-P-O2P |
| 82 | QC | 404 | PEE | C4-O4P-P-O1P |
| 82 | QE | 302 | PEE | C1-O3P-P-O2P |
| 82 | QE | 302 | PEE | C1-O3P-P-O1P |
| 82 | QE | 302 | PEE | C1-O3P-P-O4P |
| 82 | Qd | 403 | PEE | C1-O3P-P-O2P |
| 82 | Qd | 403 | PEE | C1-O3P-P-O1P |
| 82 | Qd | 403 | PEE | C1-O3P-P-O4P |
| 82 | Qd | 403 | PEE | O4P-C4-C5-N |
| 82 | Qh | 101 | PEE | C1-O3P-P-O4P |
| 82 | Qh | 101 | PEE | C4-O4P-P-O2P |
| 82 | Qh | 101 | PEE | O4P-C4-C5-N |
| 82 | Qh | 103 | PEE | C1-O3P-P-O2P |
| 82 | Qh | 103 | PEE | C1-O3P-P-O1P |
| 82 | Qh | 103 | PEE | C37-C38-C39-C40 |
| 82 | S2 | 501 | PEE | C1-O3P-P-O2P |
| 82 | S2 | 501 | PEE | O4P-C4-C5-N |
| 82 | S8 | 303 | PEE | O4P-C4-C5-N |
| 83 | QC | 402 | HEM | C2B-C3B-CAB-CBB |
| 83 | QC | 402 | HEM | C4B-C3B-CAB-CBB |
| 83 | QC | 403 | HEM | C2B-C3B-CAB-CBB |
| 83 | QC | 403 | HEM | C4B-C3B-CAB-CBB |
| 83 | QC | 403 | HEM | C2C-C3C-CAC-CBC |
| 83 | Qc | 402 | HEM | C2B-C3B-CAB-CBB |
| 83 | Qc | 402 | HEM | C4B-C3B-CAB-CBB |
| 83 | Qc | 403 | HEM | C2B-C3B-CAB-CBB |
| 83 | Qc | 403 | HEM | C4B-C3B-CAB-CBB |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 83 | Qc | 403 | HEM | C2C-C3C-CAC-CBC |
| 83 | Qc | 403 | HEM | C4C-C3C-CAC-CBC |
| 87 | V1 | 502 | FMN | C3'-C4'-C5'-O5' |
| 87 | V1 | 502 | FMN | O4'-C4'-C5'-O5' |
| 87 | V1 | 502 | FMN | C5'-O5'-P-O1P |
| 87 | V1 | 502 | FMN | C5'-O5'-P-O2P |
| 87 | V1 | 502 | FMN | C5'-O5'-P-O3P |
| 82 | Qc | 401 | PEE | O5-C30-O3-C3 |
| 82 | N1 | 401 | PEE | O5-C30-O3-C3 |
| 82 | QB | 502 | PEE | O5-C30-O3-C3 |
| 82 | Qc | 401 | PEE | C31-C30-O3-C3 |
| 79 | C1 | 602 | HEA | C27-C19-C20-C21 |
| 82 | N1 | 401 | PEE | C31-C30-O3-C3 |
| 82 | QB | 502 | PEE | C31-C30-O3-C3 |
| 82 | Qd | 403 | PEE | C31-C30-O3-C3 |
| 82 | QB | 503 | PEE | C17-C18-C19-C20 |
| 82 | QC | 401 | PEE | C17-C18-C19-C20 |
| 82 | S8 | 303 | PEE | C37-C38-C39-C40 |
| 79 | C1 | 603 | HEA | C1A-C2A-CAA-CBA |
| 79 | C1 | 602 | HEA | C17-C18-C19-C27 |
| 79 | C1 | 602 | HEA | C17-C18-C19-C20 |
| 79 | C1 | 603 | HEA | C17-C18-C19-C20 |
| 72 | QC | 408 | CDL | O1-C1-CB2-OB2 |
| 82 | N1 | 401 | PEE | C11-C10-O2-C2 |
| 82 | S8 | 303 | PEE | C11-C10-O2-C2 |
| 82 | Qd | 403 | PEE | O5-C30-O3-C3 |
| 74 | AC | 201 | ZMP | C3-C4-C5-C6 |
| 82 | C1 | 609 | PEE | C11-C12-C13-C14 |
| 82 | S2 | 501 | PEE | C2-C1-O3P-P |
| 83 | QC | 402 | HEM | C3D-CAD-CBD-CGD |
| 79 | C1 | 602 | HEA | C19-C20-C21-C22 |
| 82 | Qc | 401 | PEE | C17-C18-C19-C20 |
| 72 | Qb | 501 | CDL | CA2-C1-CB2-OB2 |
| 82 | N1 | 401 | PEE | O4-C10-O2-C2 |
| 82 | S8 | 303 | PEE | O4-C10-O2-C2 |
| 82 | QE | 302 | PEE | C33-C34-C35-C36 |
| 82 | S8 | 303 | PEE | C31-C30-O3-C3 |
| 77 | QE | 301 | PLX | O4-C3-C4-O6 |
| 72 | Qb | 501 | CDL | O1-C1-CB2-OB2 |
| 78 | B5 | 203 | 6F6 | C31-C32-C33-C34 |
| 71 | 7B | 101 | PC1 | O21-C2-C3-O31 |
| 72 | 6A | 102 | CDL | OB6-CB4-CB6-OB8 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 77 | CB | 201 | PLX | O6-C4-C5-O8 |
| 72 | AL | 201 | CDL | CA5-C11-C12-C13 |
| 72 | CB | 203 | CDL | CB7-C71-C72-C73 |
| 82 | QB | 503 | PEE | C30-C31-C32-C33 |
| 82 | QC | 401 | PEE | C30-C31-C32-C33 |
| 82 | Qd | 403 | PEE | C10-C11-C12-C13 |
| 82 | QC | 401 | PEE | C37-C38-C39-C40 |
| 72 | AL | 201 | CDL | CA7-C31-C32-C33 |
| 72 | AL | 203 | CDL | CB7-C71-C72-C73 |
| 72 | QC | 408 | CDL | CB7-C71-C72-C73 |
| 78 | B5 | 203 | 6F6 | C21-C22-C23-C24 |
| 82 | QC | 404 | PEE | C10-C11-C12-C13 |
| 82 | QE | 302 | PEE | C10-C11-C12-C13 |
| 82 | N3 | 201 | PEE | C11-C12-C13-C14 |
| 82 | Qc | 401 | PEE | C11-C12-C13-C14 |
| 78 | B5 | 203 | 6F6 | C11-C12-N-C15 |
| 82 | Qh | 103 | PEE | C10-C11-C12-C13 |
| 74 | AC | 201 | ZMP | C14-C15-N2-C16 |
| 82 | S8 | 303 | PEE | O5-C30-O3-C3 |
| 76 | AL | 202 | 3PE | C31-C32-C33-C34 |
| 72 | CB | 203 | CDL | O1-C1-CA2-OA2 |
| 82 | QB | 503 | PEE | C10-C11-C12-C13 |
| 82 | Qh | 101 | PEE | C14-C15-C16-C17 |
| 82 | Qh | 103 | PEE | C17-C18-C19-C20 |
| 82 | Qh | 101 | PEE | C11-C10-O2-C2 |
| 77 | AL | 205 | PLX | C9-C10-C11-C12 |
| 71 | 6A | 101 | PC1 | C11-O13-P-O11 |
| 71 | 7B | 101 | PC1 | C1-O11-P-O13 |
| 71 | AL | 206 | PC1 | C11-O13-P-O11 |
| 71 | C1 | 606 | PC1 | C11-O13-P-O11 |
| 71 | QH | 102 | PC1 | C1-O11-P-O13 |
| 71 | Qb | 502 | PC1 | C11-O13-P-O11 |
| 72 | 6A | 102 | CDL | CA2-OA2-PA1-OA5 |
| 72 | AL | 201 | CDL | CA2-OA2-PA1-OA5 |
| 72 | AL | 201 | CDL | CB2-OB2-PB2-OB5 |
| 72 | AL | 201 | CDL | CB3-OB5-PB2-OB2 |
| 72 | AL | 203 | CDL | CA2-OA2-PA1-OA5 |
| 72 | AL | 203 | CDL | CB3-OB5-PB2-OB2 |
| 72 | AL | 204 | CDL | CA2-OA2-PA1-OA5 |
| 72 | AM | 202 | CDL | CB3-OB5-PB2-OB2 |
| 72 | B5 | 202 | CDL | CA3-OA5-PA1-OA2 |
| 72 | CB | 203 | CDL | CB2-OB2-PB2-OB5 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 72 | N2 | 401 | CDL | CA2-OA2-PA1-OA5 |
| 72 | N2 | 401 | CDL | CB2-OB2-PB2-OB5 |
| 72 | N5 | 702 | CDL | CA2-OA2-PA1-OA5 |
| 72 | N5 | 702 | CDL | CA3-OA5-PA1-OA2 |
| 72 | QB | 501 | CDL | CA2-OA2-PA1-OA5 |
| 72 | QB | 501 | CDL | CA3-OA5-PA1-OA2 |
| 72 | QB | 501 | CDL | CB2-OB2-PB2-OB5 |
| 72 | QC | 406 | CDL | CA3-OA5-PA1-OA2 |
| 72 | QC | 406 | CDL | CB3-OB5-PB2-OB2 |
| 72 | QC | 408 | CDL | CA3-OA5-PA1-OA2 |
| 72 | QC | 408 | CDL | CB3-OB5-PB2-OB2 |
| 72 | QH | 101 | CDL | CA2-OA2-PA1-OA5 |
| 72 | Qb | 501 | CDL | CA2-OA2-PA1-OA5 |
| 72 | Qb | 501 | CDL | CA3-OA5-PA1-OA2 |
| 72 | Qd | 401 | CDL | CA2-OA2-PA1-OA5 |
| 72 | Qd | 401 | CDL | CB3-OB5-PB2-OB2 |
| 72 | Qh | 102 | CDL | CA2-OA2-PA1-OA5 |
| 72 | Qh | 102 | CDL | CA3-OA5-PA1-OA2 |
| 72 | Qh | 102 | CDL | CB2-OB2-PB2-OB5 |
| 72 | Qh | 102 | CDL | CB3-OB5-PB2-OB2 |
| 76 | AL | 202 | 3PE | C1-O11-P-O13 |
| 76 | C1 | 608 | 3PE | C1-O11-P-O13 |
| 76 | CA | 101 | 3PE | C1-O11-P-O13 |
| 76 | CB | 202 | 3PE | C1-O11-P-O13 |
| 76 | CB | 202 | 3PE | C11-O13-P-O11 |
| 76 | N4 | 502 | 3PE | C11-O13-P-O11 |
| 76 | QE | 303 | 3PE | C1-O11-P-O13 |
| 77 | AL | 205 | PLX | C3-O4-P1-O1 |
| 77 | AM | 203 | PLX | C3-O4-P1-O1 |
| 77 | B5 | 201 | PLX | C2-O1-P1-O4 |
| 77 | C2 | 301 | PLX | C2-O1-P1-O4 |
| 77 | CB | 201 | PLX | C3-O4-P1-O1 |
| 77 | CB | 201 | PLX | C2-O1-P1-O4 |
| 77 | QE | 301 | PLX | C2-O1-P1-O4 |
| 77 | QI | 301 | PLX | C2-O1-P1-O4 |
| 78 | Qc | 404 | 6F6 | C11-O13-P-O11 |
| 82 | C1 | 609 | PEE | C1-O3P-P-O4P |
| 82 | N3 | 201 | PEE | C1-O3P-P-O4P |
| 82 | N5 | 701 | PEE | C4-O4P-P-O3P |
| 82 | QB | 502 | PEE | C4-O4P-P-O3P |
| 82 | QC | 401 | PEE | C4-O4P-P-O3P |
| 82 | QC | 404 | PEE | C4-O4P-P-O3P |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 82 | Qh | 101 | PEE | C4-O4P-P-O3P |
| 82 | Qh | 103 | PEE | C1-O3P-P-O4P |
| 82 | S2 | 501 | PEE | C1-O3P-P-O4P |
| 82 | S2 | 501 | PEE | C4-O4P-P-O3P |
| 71 | AL | 206 | PC1 | C29-C2A-C2B-C2C |
| 72 | CB | 203 | CDL | CB2-C1-CA2-OA2 |
| 82 | Qh | 101 | PEE | O4-C10-O2-C2 |
| 71 | C1 | 607 | PC1 | C11-C12-N-C13 |
| 71 | C1 | 607 | PC1 | C11-C12-N-C14 |
| 71 | C1 | 607 | PC1 | C11-C12-N-C15 |
| 78 | B5 | 203 | 6F6 | C11-C12-N-C14 |
| 78 | QJ | 101 | 6F6 | C11-C12-N-C13 |
| 78 | QJ | 101 | 6F6 | C11-C12-N-C14 |
| 78 | Qc | 404 | 6F6 | C11-C12-N-C14 |
| 71 | AL | 206 | PC1 | C36-C37-C38-C39 |
| 82 | Qh | 101 | PEE | C30-C31-C32-C33 |
| 77 | AM | 201 | PLX | O6-C6-C7-C8 |
| 77 | CB | 201 | PLX | O6-C6-C7-C8 |
| 77 | CB | 201 | PLX | O8-C24-C25-C26 |
| 77 | QE | 301 | PLX | O6-C6-C7-C8 |
| 77 | AL | 205 | PLX | C30-C31-C32-C33 |
| 82 | C1 | 609 | PEE | C12-C13-C14-C15 |
| 82 | QB | 503 | PEE | C33-C34-C35-C36 |
| 82 | QB | 503 | PEE | C42-C43-C44-C45 |
| 76 | C1 | 608 | 3PE | C2B-C2C-C2D-C2E |
| 77 | AL | 205 | PLX | C14-C15-C16-C17 |
| 82 | Qh | 101 | PEE | C11-C12-C13-C14 |
| 82 | S8 | 303 | PEE | C13-C14-C15-C16 |
| 82 | QC | 401 | PEE | C11-C12-C13-C14 |
| 72 | N5 | 702 | CDL | C58-C59-C60-C61 |
| 76 | S7 | 302 | 3PE | C3B-C3C-C3D-C3E |
| 82 | Qh | 103 | PEE | C12-C13-C14-C15 |
| 77 | AM | 201 | PLX | C10-C11-C12-C13 |
| 82 | N5 | 701 | PEE | C11-C12-C13-C14 |
| 82 | Qd | 403 | PEE | C40-C41-C42-C43 |
| 72 | AM | 202 | CDL | O1-C1-CA2-OA2 |
| 83 | Qc | 402 | HEM | C3D-CAD-CBD-CGD |
| 72 | AL | 203 | CDL | C36-C37-C38-C39 |
| 72 | AL | 204 | CDL | C35-C36-C37-C38 |
| 77 | AL | 205 | PLX | C12-C13-C14-C15 |
| 82 | Qd | 403 | PEE | C20-C21-C22-C23 |
| 82 | Qd | 403 | PEE | C12-C13-C14-C15 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 72 | AL | 201 | CDL | CB7-C71-C72-C73 |
| 82 | Qd | 403 | PEE | C30-C31-C32-C33 |
| 82 | N1 | 401 | PEE | C12-C13-C14-C15 |
| 82 | Qd | 403 | PEE | C11-C12-C13-C14 |
| 82 | Qc | 401 | PEE | C22-C23-C24-C25 |
| 72 | AL | 203 | CDL | C58-C59-C60-C61 |
| 82 | QE | 302 | PEE | C32-C33-C34-C35 |
| 82 | Qd | 403 | PEE | C31-C32-C33-C34 |
| 77 | CB | 201 | PLX | C7-C8-C9-C10 |
| 77 | QE | 301 | PLX | C28-C29-C30-C31 |
| 82 | C1 | 609 | PEE | C40-C41-C42-C43 |
| 82 | N3 | 201 | PEE | C22-C23-C24-C25 |
| 71 | QC | 405 | PC1 | C28-C29-C2A-C2B |
| 72 | CB | 203 | CDL | C59-C60-C61-C62 |
| 77 | AM | 201 | PLX | C26-C27-C28-C29 |
| 77 | CB | 201 | PLX | C19-C20-C21-C22 |
| 82 | Qc | 401 | PEE | C31-C32-C33-C34 |
| 82 | S2 | 501 | PEE | C14-C15-C16-C17 |
| 82 | Qh | 101 | PEE | C19-C20-C21-C22 |
| 82 | Qh | 101 | PEE | C15-C16-C17-C18 |
| 82 | S2 | 501 | PEE | C35-C36-C37-C38 |
| 71 | QC | 405 | PC1 | C21-C22-C23-C24 |
| 72 | 6A | 102 | CDL | CB7-C71-C72-C73 |
| 72 | QC | 406 | CDL | CB5-C51-C52-C53 |
| 82 | N1 | 401 | PEE | C30-C31-C32-C33 |
| 71 | Qb | 502 | PC1 | C22-C23-C24-C25 |
| 74 | AC | 201 | ZMP | C2-C3-C4-C5 |
| 77 | AM | 203 | PLX | C34-C35-C36-C37 |
| 82 | QC | 401 | PEE | C33-C34-C35-C36 |
| 71 | N5 | 704 | PC1 | C11-C12-N-C15 |
| 78 | QJ | 101 | 6F6 | C11-C12-N-C15 |
| 78 | Qc | 404 | 6F6 | C11-C12-N-C13 |
| 78 | Qc | 404 | 6F6 | C11-C12-N-C15 |
| 71 | 6A | 101 | PC1 | C33-C34-C35-C36 |
| 72 | A8 | 301 | CDL | C55-C56-C57-C58 |
| 82 | QB | 503 | PEE | C22-C23-C24-C25 |
| 82 | QC | 401 | PEE | C42-C43-C44-C45 |
| 82 | S2 | 501 | PEE | C40-C41-C42-C43 |
| 82 | QE | 302 | PEE | O4P-C4-C5-N |
| 76 | CA | 101 | 3PE | C2B-C2C-C2D-C2E |
| 77 | B5 | 201 | PLX | C13-C14-C15-C16 |
| 77 | QE | 301 | PLX | C11-C10-C9-C8 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 82 | N3 | 201 | PEE | C30-C31-C32-C33 |
| 71 | C3 | 301 | PC1 | C39-C3A-C3B-C3C |
| 77 | N4 | 501 | PLX | C11-C10-C9-C8 |
| 82 | N5 | 701 | PEE | C33-C34-C35-C36 |
| 82 | S2 | 501 | PEE | C43-C44-C45-C46 |
| 82 | S8 | 303 | PEE | C21-C22-C23-C24 |
| 71 | N6 | 201 | PC1 | C23-C24-C25-C26 |
| 77 | QI | 301 | PLX | C7-C8-C9-C10 |
| 82 | C1 | 609 | PEE | C42-C43-C44-C45 |
| 82 | N3 | 201 | PEE | C33-C34-C35-C36 |
| 72 | A8 | 301 | CDL | C33-C34-C35-C36 |
| 77 | CB | 201 | PLX | C34-C35-C36-C37 |
| 77 | QE | 301 | PLX | C16-C17-C18-C19 |
| 71 | AL | 206 | PC1 | C3A-C3B-C3C-C3D |
| 77 | C2 | 301 | PLX | C12-C13-C14-C15 |
| 82 | C1 | 609 | PEE | C32-C33-C34-C35 |
| 72 | CB | 203 | CDL | C16-C17-C18-C19 |
| 77 | B5 | 201 | PLX | C17-C18-C19-C20 |
| 82 | Qc | 401 | PEE | C11-C10-O2-C2 |
| 77 | AL | 205 | PLX | O9-C24-C25-C26 |
| 77 | B5 | 201 | PLX | O9-C24-C25-C26 |
| 77 | CB | 201 | PLX | O9-C24-C25-C26 |
| 72 | CB | 203 | CDL | C38-C39-C40-C41 |
| 72 | N5 | 702 | CDL | C16-C17-C18-C19 |
| 76 | C1 | 608 | 3PE | C32-C33-C34-C35 |
| 82 | C1 | 609 | PEE | C19-C20-C21-C22 |
| 82 | C1 | 609 | PEE | C39-C40-C41-C42 |
| 82 | QE | 302 | PEE | C35-C36-C37-C38 |
| 82 | QB | 502 | PEE | C12-C13-C14-C15 |
| 77 | N4 | 501 | PLX | C32-C33-C34-C35 |
| 77 | QI | 301 | PLX | C34-C35-C36-C37 |
| 82 | N3 | 201 | PEE | C34-C35-C36-C37 |
| 77 | C2 | 301 | PLX | C25-C26-C27-C28 |
| 78 | B5 | 203 | 6F6 | C38-C39-C3A-C3B |
| 79 | C1 | 603 | HEA | C13-C14-C15-C16 |
| 82 | S8 | 303 | PEE | C12-C13-C14-C15 |
| 71 | QC | 405 | PC1 | C11-C12-N-C13 |
| 71 | Qj | 101 | PC1 | C11-C12-N-C15 |
| 71 | 7B | 101 | PC1 | C21-C22-C23-C24 |
| 82 | S2 | 501 | PEE | C31-C30-O3-C3 |
| 83 | Qc | 403 | HEM | C2A-CAA-CBA-CGA |
| 71 | C3 | 302 | PC1 | C2B-C2C-C2D-C2E |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 77 | AL | 205 | PLX | C26-C27-C28-C29 |
| 82 | N5 | 701 | PEE | C12-C13-C14-C15 |
| 82 | Qh | 101 | PEE | C10-C11-C12-C13 |
| 72 | B5 | 202 | CDL | C35-C36-C37-C38 |
| 77 | C2 | 301 | PLX | C11-C12-C13-C14 |
| 82 | S2 | 501 | PEE | C33-C34-C35-C36 |
| 82 | Qc | 401 | PEE | O4-C10-O2-C2 |
| 72 | QH | 101 | CDL | CA7-C31-C32-C33 |
| 72 | Qb | 501 | CDL | CA7-C31-C32-C33 |
| 71 | Qj | 101 | PC1 | C3C-C3D-C3E-C3F |
| 72 | N2 | 401 | CDL | C31-C32-C33-C34 |
| 74 | AC | 201 | ZMP | C6-C7-C8-C9 |
| 74 | AC | 201 | ZMP | C22-C23-C24-C25 |
| 71 | Qj | 101 | PC1 | C21-C22-C23-C24 |
| 82 | Qc | 401 | PEE | C30-C31-C32-C33 |
| 71 | 7B | 101 | PC1 | C22-C23-C24-C25 |
| 76 | C1 | 601 | 3PE | C2D-C2E-C2F-C2G |
| 82 | C1 | 609 | PEE | C21-C22-C23-C24 |
| 82 | S8 | 303 | PEE | C33-C34-C35-C36 |
| 77 | CB | 201 | PLX | C16-C17-C18-C19 |
| 82 | C1 | 609 | PEE | C41-C42-C43-C44 |
| 82 | QB | 503 | PEE | C41-C42-C43-C44 |
| 82 | QB | 503 | PEE | C11-C10-O2-C2 |
| 71 | QH | 102 | PC1 | O11-C1-C2-O21 |
| 77 | QI | 301 | PLX | O4-C3-C4-O6 |
| 72 | N2 | 401 | CDL | C12-C13-C14-C15 |
| 83 | QC | 403 | HEM | C4C-C3C-CAC-CBC |
| 82 | Qd | 403 | PEE | C22-C23-C24-C25 |
| 72 | N5 | 702 | CDL | O1-C1-CA2-OA2 |
| 77 | AL | 205 | PLX | O6-C4-C5-O8 |
| 82 | QB | 502 | PEE | O2-C2-C3-O3 |
| 82 | Qh | 101 | PEE | O2-C2-C3-O3 |
| 72 | QC | 406 | CDL | C14-C15-C16-C17 |
| 82 | C1 | 609 | PEE | C33-C34-C35-C36 |
| 78 | B5 | 203 | 6F6 | C11-C12-N-C13 |
| 71 | C1 | 607 | PC1 | C2C-C2D-C2E-C2F |
| 82 | QC | 401 | PEE | C31-C32-C33-C34 |
| 82 | N3 | 201 | PEE | C35-C36-C37-C38 |
| 82 | Qh | 101 | PEE | C35-C36-C37-C38 |
| 78 | QJ | 101 | 6F6 | C31-C32-C33-C34 |
| 77 | QI | 301 | PLX | C26-C27-C28-C29 |
| 75 | AK | 401 | ADP | O4'-C4'-C5'-O5' |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 77 | AM | 203 | PLX | C7-C8-C9-C10 |
| 74 | AC | 201 | ZMP | C4-C5-C6-C7 |
| 82 | N3 | 201 | PEE | C10-C11-C12-C13 |
| 77 | N4 | 501 | PLX | C27-C28-C29-C30 |
| 82 | S2 | 501 | PEE | O5-C30-O3-C3 |
| 82 | QB | 503 | PEE | O4-C10-O2-C2 |
| 82 | QE | 302 | PEE | C16-C17-C18-C19 |
| 71 | C3 | 301 | PC1 | C1-O11-P-O13 |
| 71 | QC | 407 | PC1 | C11-O13-P-O11 |
| 71 | Qj | 101 | PC1 | C11-O13-P-O11 |
| 72 | AL | 204 | CDL | CA3-OA5-PA1-OA2 |
| 72 | CB | 203 | CDL | CB3-OB5-PB2-OB2 |
| 72 | N5 | 703 | CDL | CA2-OA2-PA1-OA5 |
| 72 | QB | 501 | CDL | CB3-OB5-PB2-OB2 |
| 76 | C1 | 601 | 3PE | C11-O13-P-O11 |
| 74 | AB | 201 | ZMP | C3-C4-C5-C6 |
| 76 | N4 | 502 | 3PE | C2-C1-O11-P |
| 72 | AL | 204 | CDL | OB5-CB3-CB4-CB6 |
| 72 | Qb | 501 | CDL | OB5-CB3-CB4-CB6 |
| 77 | QE | 301 | PLX | O4-C3-C4-C5 |
| 76 | S7 | 302 | 3PE | C3A-C3B-C3C-C3D |
| 71 | C3 | 301 | PC1 | C3A-C3B-C3C-C3D |
| 72 | AL | 204 | CDL | C52-C53-C54-C55 |
| 72 | B5 | 202 | CDL | C83-C84-C85-C86 |
| 77 | CB | 201 | PLX | C32-C33-C34-C35 |
| 82 | Qc | 401 | PEE | C32-C33-C34-C35 |
| 82 | Qc | 401 | PEE | C33-C34-C35-C36 |
| 71 | C1 | 606 | PC1 | C29-C2A-C2B-C2C |
| 72 | Qd | 401 | CDL | C73-C74-C75-C76 |
| 77 | B5 | 201 | PLX | C30-C31-C32-C33 |
| 82 | QE | 302 | PEE | C21-C22-C23-C24 |
| 71 | N5 | 704 | PC1 | C11-C12-N-C14 |
| 71 | Qb | 502 | PC1 | C1-C2-C3-O31 |
| 72 | A8 | 301 | CDL | CB3-CB4-CB6-OB8 |
| 72 | QB | 501 | CDL | CB3-CB4-CB6-OB8 |
| 72 | Qb | 501 | CDL | CB3-CB4-CB6-OB8 |
| 72 | Qd | 401 | CDL | CA3-CA4-CA6-OA8 |
| 76 | C1 | 601 | 3PE | C1-C2-C3-O31 |
| 77 | B5 | 201 | PLX | C3-C4-C5-O8 |
| 77 | N4 | 501 | PLX | C3-C4-C5-O8 |
| 82 | QC | 401 | PEE | C1-C2-C3-O3 |
| 82 | QE | 302 | PEE | C1-C2-C3-O3 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 82 | Qc | 401 | PEE | C1-C2-C3-O3 |
| 82 | Qh | 101 | PEE | C17-C18-C19-C20 |
| 71 | C1 | 607 | PC1 | C36-C37-C38-C39 |
| 71 | C3 | 302 | PC1 | C29-C2A-C2B-C2C |
| 78 | Qc | 404 | 6F6 | C39-C3A-C3B-C4 |
| 82 | QC | 401 | PEE | C24-C25-C26-C27 |
| 82 | QE | 302 | PEE | C12-C13-C14-C15 |
| 78 | B5 | 203 | 6F6 | C29-C2A-C2B-C2C |
| 78 | QJ | 101 | 6F6 | C2F-C2G-C2H-C2I |
| 77 | AM | 203 | PLX | O8-C24-C25-C26 |
| 77 | C2 | 301 | PLX | O6-C6-C7-C8 |
| 77 | C2 | 301 | PLX | O8-C24-C25-C26 |
| 74 | AB | 201 | ZMP | O3-C16-C17-O4 |
| 72 | AL | 201 | CDL | C17-C18-C19-C20 |
| 82 | Qh | 103 | PEE | C41-C42-C43-C44 |
| 77 | QI | 301 | PLX | C27-C28-C29-C30 |
| 82 | C1 | 609 | PEE | C35-C36-C37-C38 |
| 82 | N1 | 401 | PEE | C35-C36-C37-C38 |
| 82 | Qc | 401 | PEE | C15-C16-C17-C18 |
| 82 | Qd | 403 | PEE | C15-C16-C17-C18 |
| 82 | Qh | 103 | PEE | C19-C20-C21-C22 |
| 82 | S8 | 303 | PEE | C35-C36-C37-C38 |
| 71 | Qj | 101 | PC1 | C24-C25-C26-C27 |
| 72 | QC | 406 | CDL | C75-C76-C77-C78 |
| 77 | C2 | 301 | PLX | C16-C17-C18-C19 |
| 82 | Qh | 103 | PEE | C20-C21-C22-C23 |
| 74 | AB | 201 | ZMP | C22-C23-C24-C25 |
| 77 | QE | 301 | PLX | C29-C30-C31-C32 |
| 82 | S8 | 303 | PEE | C3-C2-O2-C10 |
| 72 | AL | 204 | CDL | C53-C54-C55-C56 |
| 72 | CB | 203 | CDL | C80-C81-C82-C83 |
| 82 | N1 | 401 | PEE | C14-C15-C16-C17 |
| 82 | QC | 404 | PEE | C16-C17-C18-C19 |
| 82 | QC | 404 | PEE | C21-C22-C23-C24 |
| 82 | Qh | 101 | PEE | C37-C38-C39-C40 |
| 71 | N5 | 704 | PC1 | C11-C12-N-C13 |
| 71 | QC | 405 | PC1 | C11-C12-N-C14 |
| 71 | Qj | 101 | PC1 | C11-C12-N-C14 |
| 82 | QC | 404 | PEE | C33-C34-C35-C36 |
| 77 | AM | 203 | PLX | C36-C37-C38-C39 |
| 82 | QE | 302 | PEE | C40-C41-C42-C43 |
| 82 | Qc | 401 | PEE | C19-C20-C21-C22 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 71 | 6A | 101 | PC1 | O21-C2-C3-O31 |
| 77 | AM | 201 | PLX | O6-C4-C5-O8 |
| 77 | AM | 203 | PLX | O6-C4-C5-O8 |
| 72 | CB | 203 | CDL | C72-C73-C74-C75 |
| 71 | 7B | 101 | PC1 | C25-C26-C27-C28 |
| 82 | QB | 503 | PEE | C21-C22-C23-C24 |
| 82 | S2 | 501 | PEE | C16-C17-C18-C19 |
| 78 | Qc | 404 | 6F6 | O31-C31-C32-C33 |
| 72 | B5 | 202 | CDL | C21-C22-C23-C24 |
| 72 | N2 | 401 | CDL | C73-C74-C75-C76 |
| 77 | AM | 203 | PLX | C18-C19-C20-C21 |
| 77 | AM | 203 | PLX | C14-C15-C16-C17 |
| 82 | N3 | 201 | PEE | C31-C32-C33-C34 |
| 82 | Qc | 401 | PEE | C12-C13-C14-C15 |
| 82 | N1 | 401 | PEE | C32-C33-C34-C35 |
| 82 | QE | 302 | PEE | C11-C12-C13-C14 |
| 72 | N5 | 703 | CDL | CA7-C31-C32-C33 |
| 82 | S8 | 303 | PEE | C11-C12-C13-C14 |
| 72 | CB | 203 | CDL | OB5-CB3-CB4-CB6 |
| 72 | QC | 408 | CDL | OA5-CA3-CA4-CA6 |
| 72 | Qd | 401 | CDL | OB5-CB3-CB4-CB6 |
| 77 | AM | 203 | PLX | O4-C3-C4-C5 |
| 77 | QI | 301 | PLX | O4-C3-C4-C5 |
| 82 | Qc | 401 | PEE | O3P-C1-C2-C3 |
| 82 | Qc | 401 | PEE | C35-C36-C37-C38 |
| 82 | S2 | 501 | PEE | C32-C33-C34-C35 |
| 71 | Qj | 101 | PC1 | C23-C24-C25-C26 |
| 82 | S2 | 501 | PEE | C20-C21-C22-C23 |
| 72 | QB | 501 | CDL | CA5-C11-C12-C13 |
| 82 | Qc | 401 | PEE | C10-C11-C12-C13 |
| 72 | AL | 201 | CDL | C21-C22-C23-C24 |
| 82 | N5 | 701 | PEE | C39-C40-C41-C42 |
| 72 | QC | 406 | CDL | C16-C17-C18-C19 |
| 82 | Qh | 103 | PEE | C31-C32-C33-C34 |
| 82 | S2 | 501 | PEE | C41-C42-C43-C44 |
| 71 | Qb | 502 | PC1 | C21-C22-C23-C24 |
| 72 | N5 | 703 | CDL | C17-C18-C19-C20 |
| 82 | QE | 302 | PEE | C22-C23-C24-C25 |
| 72 | N5 | 703 | CDL | CA4-CA3-OA5-PA1 |
| 72 | QH | 101 | CDL | CB4-CB3-OB5-PB2 |
| 72 | Qh | 102 | CDL | C1-CA2-OA2-PA1 |
| 72 | AL | 201 | CDL | C13-C14-C15-C16 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 72 | N5 | 703 | CDL | C43-C44-C45-C46 |
| 71 | 6A | 101 | PC1 | C1-C2-C3-O31 |
| 72 | 6A | 102 | CDL | CB3-CB4-CB6-OB8 |
| 72 | N2 | 401 | CDL | CA3-CA4-CA6-OA8 |
| 76 | C1 | 608 | 3PE | C1-C2-C3-O31 |
| 77 | AL | 205 | PLX | C3-C4-C5-O8 |
| 77 | CB | 201 | PLX | C3-C4-C5-O8 |
| 82 | C1 | 609 | PEE | C1-C2-C3-O3 |
| 82 | N3 | 201 | PEE | C1-C2-C3-O3 |
| 82 | Qh | 101 | PEE | C1-C2-C3-O3 |
| 72 | A8 | 301 | CDL | C19-C20-C21-C22 |
| 76 | C1 | 601 | 3PE | C29-C2A-C2B-C2C |
| 82 | N1 | 401 | PEE | C33-C34-C35-C36 |
| 82 | QC | 404 | PEE | C11-C12-C13-C14 |
| 82 | C1 | 609 | PEE | C37-C38-C39-C40 |
| 82 | N5 | 701 | PEE | C24-C25-C26-C27 |
| 72 | Qd | 401 | CDL | C51-C52-C53-C54 |
| 77 | N4 | 501 | PLX | C12-C13-C14-C15 |
| 74 | AB | 201 | ZMP | N2-C16-C17-C18 |
| 79 | C1 | 603 | HEA | C27-C19-C20-C21 |
| 82 | S2 | 501 | PEE | C11-C12-C13-C14 |
| 72 | A8 | 301 | CDL | C56-C57-C58-C59 |
| 82 | S8 | 303 | PEE | C22-C23-C24-C25 |
| 76 | S7 | 302 | 3PE | C11-O13-P-O11 |
| 77 | B5 | 201 | PLX | C3-C4-O6-C6 |
| 77 | B5 | 201 | PLX | C5-C4-O6-C6 |
| 77 | C2 | 301 | PLX | C3-C4-O6-C6 |
| 77 | C2 | 301 | PLX | C5-C4-O6-C6 |
| 77 | CB | 201 | PLX | C3-C4-O6-C6 |
| 77 | CB | 201 | PLX | C5-C4-O6-C6 |
| 77 | N4 | 501 | PLX | C5-C4-O6-C6 |
| 82 | N1 | 401 | PEE | C1-O3P-P-O4P |
| 82 | QB | 503 | PEE | C4-O4P-P-O3P |
| 71 | QC | 405 | PC1 | O11-C1-C2-O21 |
| 72 | AL | 201 | CDL | OB5-CB3-CB4-OB6 |
| 72 | AL | 203 | CDL | OB5-CB3-CB4-OB6 |
| 72 | QB | 501 | CDL | OA5-CA3-CA4-OA6 |
| 72 | QC | 408 | CDL | OA5-CA3-CA4-OA6 |
| 72 | Qb | 501 | CDL | OB5-CB3-CB4-OB6 |
| 76 | AL | 202 | 3PE | O11-C1-C2-O21 |
| 82 | C1 | 609 | PEE | O3P-C1-C2-O2 |
| 82 | Qh | 101 | PEE | O3P-C1-C2-O2 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 72 | N5 | 703 | CDL | C52-C53-C54-C55 |
| 76 | S7 | 302 | 3PE | C21-C22-C23-C24 |
| 72 | N5 | 703 | CDL | C31-C32-C33-C34 |
| 82 | S2 | 501 | PEE | C13-C14-C15-C16 |
| 72 | N5 | 703 | CDL | C32-C31-CA7-OA8 |
| 82 | S8 | 303 | PEE | C32-C33-C34-C35 |
| 77 | QE | 301 | PLX | C12-C13-C14-C15 |
| 72 | A8 | 301 | CDL | OB6-CB4-CB6-OB8 |
| 72 | Qb | 501 | CDL | OB6-CB4-CB6-OB8 |
| 76 | C1 | 601 | 3PE | O21-C2-C3-O31 |
| 77 | B5 | 201 | PLX | O6-C4-C5-O8 |
| 82 | C1 | 609 | PEE | O2-C2-C3-O3 |
| 82 | QC | 401 | PEE | O2-C2-C3-O3 |
| 72 | N2 | 401 | CDL | C32-C33-C34-C35 |
| 72 | AM | 202 | CDL | CB2-C1-CA2-OA2 |
| 72 | QC | 408 | CDL | CA2-C1-CB2-OB2 |
| 79 | C1 | 602 | HEA | C15-C16-C17-C18 |
| 72 | A8 | 301 | CDL | C23-C24-C25-C26 |
| 76 | CA | 101 | 3PE | C24-C25-C26-C27 |
| 77 | QI | 301 | PLX | C11-C10-C9-C8 |
| 71 | C3 | 301 | PC1 | C3B-C3C-C3D-C3E |
| 72 | 6A | 102 | CDL | C1-CB2-OB2-PB2 |
| 72 | A8 | 301 | CDL | C1-CA2-OA2-PA1 |
| 72 | AL | 203 | CDL | C1-CB2-OB2-PB2 |
| 72 | CB | 203 | CDL | CB4-CB3-OB5-PB2 |
| 72 | QC | 408 | CDL | CA4-CA3-OA5-PA1 |
| 72 | QC | 408 | CDL | C1-CB2-OB2-PB2 |
| 72 | Qd | 401 | CDL | C1-CA2-OA2-PA1 |
| 72 | Qh | 102 | CDL | CA4-CA3-OA5-PA1 |
| 76 | QE | 303 | 3PE | C2-C1-O11-P |
| 82 | S8 | 303 | PEE | C2-C1-O3P-P |
| 71 | QC | 405 | PC1 | C3B-C3C-C3D-C3E |
| 71 | C3 | 301 | PC1 | O21-C21-C22-C23 |
| 82 | S2 | 501 | PEE | C18-C19-C20-C21 |
| 74 | AB | 201 | ZMP | O1-C10-S1-C11 |
| 74 | AC | 201 | ZMP | O1-C10-S1-C11 |
| 77 | CB | 201 | PLX | C33-C34-C35-C36 |
| 71 | C1 | 606 | PC1 | C31-C32-C33-C34 |
| 74 | AC | 201 | ZMP | S1-C10-C9-C8 |
| 82 | Qh | 101 | PEE | C38-C39-C40-C41 |
| 72 | 6A | 102 | CDL | OB5-CB3-CB4-CB6 |
| 72 | AL | 201 | CDL | OB5-CB3-CB4-CB6 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 72 | Qh | 102 | CDL | OB5-CB3-CB4-CB6 |
| 76 | AL | 202 | 3PE | O11-C1-C2-C3 |
| 76 | C1 | 608 | 3PE | O11-C1-C2-C3 |
| 77 | N4 | 501 | PLX | O4-C3-C4-C5 |
| 82 | N1 | 401 | PEE | O3P-C1-C2-C3 |
| 82 | N5 | 701 | PEE | O3P-C1-C2-C3 |
| 82 | QB | 502 | PEE | O3P-C1-C2-C3 |
| 74 | AB | 201 | ZMP | C1-C2-C3-C4 |
| 82 | Qh | 101 | PEE | C34-C35-C36-C37 |
| 72 | AL | 201 | CDL | C52-C53-C54-C55 |
| 72 | N2 | 401 | CDL | C13-C14-C15-C16 |
| 82 | S8 | 303 | PEE | C14-C15-C16-C17 |
| 82 | QC | 404 | PEE | C20-C21-C22-C23 |
| 77 | C2 | 301 | PLX | C26-C27-C28-C29 |
| 72 | AL | 201 | CDL | C62-C63-C64-C65 |
| 82 | N1 | 401 | PEE | C3-C2-O2-C10 |
| 71 | C1 | 606 | PC1 | C27-C28-C29-C2A |
| 82 | Qh | 103 | PEE | C21-C22-C23-C24 |
| 71 | C1 | 607 | PC1 | C24-C25-C26-C27 |
| 82 | Qh | 103 | PEE | C23-C24-C25-C26 |
| 71 | 7B | 101 | PC1 | C1-C2-C3-O31 |
| 78 | Qc | 404 | 6F6 | C1-C2-C3-O31 |
| 82 | QB | 502 | PEE | C1-C2-C3-O3 |
| 82 | QB | 503 | PEE | C1-C2-C3-O3 |
| 82 | Qc | 401 | PEE | C2-C1-O3P-P |
| 71 | Qj | 101 | PC1 | O11-C1-C2-O21 |
| 72 | 6A | 102 | CDL | OA5-CA3-CA4-OA6 |
| 72 | 6A | 102 | CDL | OB5-CB3-CB4-OB6 |
| 72 | CB | 203 | CDL | OB5-CB3-CB4-OB6 |
| 76 | C1 | 608 | 3PE | O11-C1-C2-O21 |
| 77 | AM | 201 | PLX | O4-C3-C4-O6 |
| 77 | AM | 203 | PLX | O4-C3-C4-O6 |
| 77 | CB | 201 | PLX | O4-C3-C4-O6 |
| 82 | N5 | 701 | PEE | O3P-C1-C2-O2 |
| 72 | QB | 501 | CDL | C72-C71-CB7-OB8 |
| 76 | CA | 101 | 3PE | C37-C38-C39-C3A |
| 76 | C1 | 601 | 3PE | C3C-C3D-C3E-C3F |
| 72 | CB | 203 | CDL | CA5-C11-C12-C13 |
| 72 | AL | 203 | CDL | C71-C72-C73-C74 |
| 82 | S8 | 303 | PEE | C34-C35-C36-C37 |
| 72 | N5 | 703 | CDL | C36-C37-C38-C39 |
| 72 | QB | 501 | CDL | OB6-CB4-CB6-OB8 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 72 | QH | 101 | CDL | OA6-CA4-CA6-OA8 |
| 72 | Qh | 102 | CDL | OA6-CA4-CA6-OA8 |
| 82 | QB | 503 | PEE | O2-C2-C3-O3 |
| 82 | Qd | 403 | PEE | O2-C2-C3-O3 |
| 72 | B5 | 202 | CDL | C53-C54-C55-C56 |
| 71 | QH | 102 | PC1 | C23-C24-C25-C26 |
| 71 | QC | 405 | PC1 | C11-C12-N-C15 |
| 73 | A9 | 401 | NDP | C5D-O5D-PN-O3 |
| 82 | QB | 503 | PEE | C32-C33-C34-C35 |
| 82 | S2 | 501 | PEE | C39-C40-C41-C42 |
| 71 | N6 | 201 | PC1 | C35-C36-C37-C38 |
| 77 | N4 | 501 | PLX | C9-C10-C11-C12 |
| 72 | A8 | 301 | CDL | C22-C23-C24-C25 |
| 76 | CA | 101 | 3PE | C25-C26-C27-C28 |
| 82 | N5 | 701 | PEE | C22-C23-C24-C25 |
| 72 | N2 | 401 | CDL | C52-C51-CB5-OB6 |
| 82 | Qc | 401 | PEE | C13-C14-C15-C16 |
| 72 | B5 | 202 | CDL | C17-C18-C19-C20 |
| 82 | N1 | 401 | PEE | C10-C11-C12-C13 |
| 71 | QC | 407 | PC1 | C1-O11-P-O13 |
| 71 | Qb | 502 | PC1 | C1-O11-P-O13 |
| 72 | 6A | 102 | CDL | CA3-OA5-PA1-OA2 |
| 72 | N5 | 703 | CDL | CA3-OA5-PA1-OA2 |
| 77 | AM | 203 | PLX | C2-O1-P1-O4 |
| 82 | S2 | 501 | PEE | C34-C35-C36-C37 |
| 72 | AL | 204 | CDL | C82-C83-C84-C85 |
| 72 | N2 | 401 | CDL | C1-CA2-OA2-PA1 |
| 72 | QC | 408 | CDL | C1-CA2-OA2-PA1 |
| 72 | Qd | 401 | CDL | CA4-CA3-OA5-PA1 |
| 77 | B5 | 201 | PLX | C33-C34-C35-C36 |
| 71 | 6A | 101 | PC1 | C11-O13-P-O12 |
| 71 | AL | 206 | PC1 | C11-O13-P-O12 |
| 71 | AL | 206 | PC1 | C11-C12-N-C14 |
| 71 | C3 | 301 | PC1 | C1-O11-P-O12 |
| 71 | C3 | 302 | PC1 | C11-O13-P-O12 |
| 71 | N6 | 201 | PC1 | C11-O13-P-O14 |
| 71 | Qb | 502 | PC1 | C11-O13-P-O12 |
| 71 | Qb | 502 | PC1 | C11-O13-P-O14 |
| 71 | Qj | 101 | PC1 | C11-O13-P-O12 |
| 71 | Qj | 101 | PC1 | C11-O13-P-O14 |
| 72 | 6A | 102 | CDL | CA2-OA2-PA1-OA4 |
| 72 | A8 | 301 | CDL | CB3-OB5-PB2-OB4 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 72 | AL | 201 | CDL | CA2-OA2-PA1-OA4 |
| 72 | AL | 201 | CDL | CA3-OA5-PA1-OA3 |
| 72 | AL | 201 | CDL | CB2-OB2-PB2-OB3 |
| 72 | AL | 201 | CDL | CB2-OB2-PB2-OB4 |
| 72 | AL | 203 | CDL | CB3-OB5-PB2-OB4 |
| 72 | AL | 204 | CDL | CA2-OA2-PA1-OA3 |
| 72 | AL | 204 | CDL | CA3-OA5-PA1-OA3 |
| 72 | B5 | 202 | CDL | CA3-OA5-PA1-OA3 |
| 72 | CB | 203 | CDL | CA3-OA5-PA1-OA4 |
| 72 | CB | 203 | CDL | CB2-OB2-PB2-OB3 |
| 72 | CB | 203 | CDL | CB3-OB5-PB2-OB4 |
| 72 | N2 | 401 | CDL | CA2-OA2-PA1-OA3 |
| 72 | N2 | 401 | CDL | CA2-OA2-PA1-OA4 |
| 72 | N2 | 401 | CDL | CB2-OB2-PB2-OB3 |
| 72 | N5 | 702 | CDL | CA2-OA2-PA1-OA3 |
| 72 | N5 | 702 | CDL | CA3-OA5-PA1-OA4 |
| 72 | N5 | 703 | CDL | CA2-OA2-PA1-OA4 |
| 72 | QB | 501 | CDL | CA2-OA2-PA1-OA4 |
| 72 | QB | 501 | CDL | CA3-OA5-PA1-OA4 |
| 72 | QB | 501 | CDL | CB3-OB5-PB2-OB4 |
| 72 | QC | 406 | CDL | CA3-OA5-PA1-OA3 |
| 72 | QC | 406 | CDL | CA3-OA5-PA1-OA4 |
| 72 | QC | 408 | CDL | CB3-OB5-PB2-OB3 |
| 72 | QH | 101 | CDL | CA2-OA2-PA1-OA3 |
| 72 | Qb | 501 | CDL | CA3-OA5-PA1-OA3 |
| 72 | Qd | 401 | CDL | CA2-OA2-PA1-OA3 |
| 72 | Qd | 401 | CDL | CB3-OB5-PB2-OB3 |
| 72 | Qd | 401 | CDL | CB3-OB5-PB2-OB4 |
| 72 | Qh | 102 | CDL | CA2-OA2-PA1-OA4 |
| 72 | Qh | 102 | CDL | CA3-OA5-PA1-OA4 |
| 72 | Qh | 102 | CDL | CB2-OB2-PB2-OB3 |
| 72 | Qh | 102 | CDL | CB2-OB2-PB2-OB4 |
| 72 | Qh | 102 | CDL | CB3-OB5-PB2-OB3 |
| 73 | A9 | 401 | NDP | C5D-O5D-PN-O2N |
| 76 | C1 | 601 | 3PE | C11-O13-P-O14 |
| 76 | C1 | 608 | 3PE | C1-O11-P-O14 |
| 76 | CB | 202 | 3PE | C11-O13-P-O12 |
| 76 | QE | 303 | 3PE | C1-O11-P-O14 |
| 76 | S7 | 302 | 3PE | C11-O13-P-O14 |
| 77 | AL | 205 | PLX | C3-O4-P1-O2 |
| 77 | AL | 205 | PLX | C3-O4-P1-O3 |
| 77 | AL | 205 | PLX | C2-O1-P1-O2 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 77 | C2 | 301 | PLX | C2-O1-P1-O2 |
| 77 | C2 | 301 | PLX | C2-O1-P1-O3 |
| 77 | CB | 201 | PLX | C3-O4-P1-O3 |
| 78 | Qc | 404 | 6F6 | C11-O13-P-O14 |
| 82 | C1 | 609 | PEE | C1-O3P-P-O2P |
| 82 | C1 | 609 | PEE | C4-O4P-P-O1P |
| 82 | N1 | 401 | PEE | C1-O3P-P-O2P |
| 82 | N3 | 201 | PEE | C1-O3P-P-O2P |
| 82 | N5 | 701 | PEE | C4-O4P-P-O1P |
| 82 | QB | 502 | PEE | C4-O4P-P-O1P |
| 82 | QB | 503 | PEE | C4-O4P-P-O1P |
| 82 | QC | 401 | PEE | C4-O4P-P-O2P |
| 82 | Qh | 101 | PEE | C4-O4P-P-O1P |
| 82 | S2 | 501 | PEE | C1-O3P-P-O1P |
| 82 | S2 | 501 | PEE | C4-O4P-P-O2P |
| 82 | S2 | 501 | PEE | C4-O4P-P-O1P |
| 82 | S8 | 303 | PEE | C1-O3P-P-O2P |
| 72 | 6A | 102 | CDL | CB5-C51-C52-C53 |
| 72 | 6A | 102 | CDL | OA5-CA3-CA4-CA6 |
| 72 | AL | 203 | CDL | OB5-CB3-CB4-CB6 |
| 77 | AM | 201 | PLX | O4-C3-C4-C5 |
| 82 | Qh | 101 | PEE | O3P-C1-C2-C3 |
| 77 | CB | 201 | PLX | C26-C27-C28-C29 |
| 77 | QI | 301 | PLX | C30-C31-C32-C33 |
| 78 | B5 | 203 | 6F6 | C22-C23-C24-C25 |
| 82 | S8 | 303 | PEE | C17-C18-C19-C20 |
| 82 | Qc | 401 | PEE | C14-C15-C16-C17 |
| 76 | AL | 202 | 3PE | C12-C11-O13-P |
| 77 | AL | 205 | PLX | C1-C2-O1-P1 |
| 77 | B5 | 201 | PLX | C1-C2-O1-P1 |
| 77 | CB | 201 | PLX | C1-C2-O1-P1 |
| 78 | Qc | 404 | 6F6 | C12-C11-O13-P |
| 82 | N3 | 201 | PEE | C5-C4-O4P-P |
| 71 | 6A | 101 | PC1 | C21-C22-C23-C24 |
| 72 | QC | 408 | CDL | CA7-C31-C32-C33 |
| 77 | C2 | 301 | PLX | C7-C8-C9-C10 |
| 72 | N5 | 703 | CDL | OA5-CA3-CA4-OA6 |
| 72 | Qh | 102 | CDL | CA7-C31-C32-C33 |
| 77 | N4 | 501 | PLX | O4-C3-C4-O6 |
| 78 | QJ | 101 | 6F6 | O11-C1-C2-O21 |
| 82 | N1 | 401 | PEE | O3P-C1-C2-O2 |
| 82 | QB | 502 | PEE | O3P-C1-C2-O2 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 82 | Qc | 401 | PEE | O3P-C1-C2-O2 |
| 72 | AL | 201 | CDL | C58-C59-C60-C61 |
| 82 | S2 | 501 | PEE | C38-C39-C40-C41 |
| 72 | QC | 406 | CDL | C36-C37-C38-C39 |
| 72 | N5 | 702 | CDL | C72-C73-C74-C75 |
| 74 | AB | 201 | ZMP | C1-C22-C23-C24 |
| 71 | Qj | 101 | PC1 | C11-C12-N-C13 |
| 72 | QC | 406 | CDL | C72-C71-CB7-OB8 |
| 72 | Qh | 102 | CDL | C52-C51-CB5-OB6 |
| 71 | 6A | 101 | PC1 | O13-C11-C12-N |
| 71 | C3 | 302 | PC1 | O13-C11-C12-N |
| 71 | QC | 405 | PC1 | O13-C11-C12-N |
| 72 | Qh | 102 | CDL | CA3-CA4-CA6-OA8 |
| 74 | AC | 201 | ZMP | C2-C1-C22-C23 |
| 77 | AL | 205 | PLX | N1-C1-C2-O1 |
| 77 | AM | 201 | PLX | C3-C4-C5-O8 |
| 77 | AM | 203 | PLX | C3-C4-C5-O8 |
| 77 | B5 | 201 | PLX | N1-C1-C2-O1 |
| 77 | N4 | 501 | PLX | N1-C1-C2-O1 |
| 77 | QE | 301 | PLX | N1-C1-C2-O1 |
| 78 | Qc | 404 | 6F6 | O13-C11-C12-N |
| 82 | QC | 401 | PEE | C12-C13-C14-C15 |
| 72 | Qd | 401 | CDL | OA6-CA4-CA6-OA8 |
| 72 | Qh | 102 | CDL | OB6-CB4-CB6-OB8 |
| 76 | C1 | 608 | 3PE | O21-C2-C3-O31 |
| 77 | N4 | 501 | PLX | O6-C4-C5-O8 |
| 82 | QE | 302 | PEE | O2-C2-C3-O3 |
| 82 | Qc | 401 | PEE | O2-C2-C3-O3 |
| 77 | AM | 203 | PLX | C26-C27-C28-C29 |
| 72 | B5 | 202 | CDL | C59-C60-C61-C62 |
| 82 | QC | 401 | PEE | C20-C21-C22-C23 |
| 82 | Qd | 403 | PEE | C14-C15-C16-C17 |
| 82 | Qh | 101 | PEE | C12-C13-C14-C15 |
| 72 | AL | 203 | CDL | CA4-CA3-OA5-PA1 |
| 74 | AB | 201 | ZMP | C2-C3-C4-C5 |
| 82 | Qh | 103 | PEE | C24-C25-C26-C27 |
| 77 | AM | 201 | PLX | O8-C24-C25-C26 |
| 72 | 6A | 102 | CDL | C16-C17-C18-C19 |
| 72 | CB | 203 | CDL | C53-C54-C55-C56 |
| 74 | AC | 201 | ZMP | O3-C16-C17-O4 |
| 77 | N4 | 501 | PLX | O9-C24-C25-C26 |
| 71 | N5 | 704 | PC1 | C3A-C3B-C3C-C3D |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 82 | QC | 404 | PEE | C14-C15-C16-C17 |
| 71 | AL | 206 | PC1 | C11-C12-N-C15 |
| 71 | N5 | 704 | PC1 | C33-C34-C35-C36 |
| 82 | N3 | 201 | PEE | C12-C13-C14-C15 |
| 72 | AL | 203 | CDL | C13-C14-C15-C16 |
| 74 | AC | 201 | ZMP | C22-C1-C2-C3 |
| 72 | CB | 203 | CDL | C74-C75-C76-C77 |
| 82 | Qc | 401 | PEE | C20-C21-C22-C23 |
| 74 | AB | 201 | ZMP | C19-C18-C21-O5 |
| 82 | QC | 401 | PEE | C34-C35-C36-C37 |
| 71 | C1 | 607 | PC1 | C29-C2A-C2B-C2C |
| 71 | C3 | 302 | PC1 | O31-C31-C32-C33 |
| 71 | Qj | 101 | PC1 | O11-C1-C2-C3 |
| 72 | A8 | 301 | CDL | OB5-CB3-CB4-CB6 |
| 82 | C1 | 609 | PEE | O3P-C1-C2-C3 |
| 79 | C1 | 602 | HEA | C11-C12-C13-C14 |
| 71 | QC | 405 | PC1 | C32-C33-C34-C35 |
| 72 | CB | 203 | CDL | C22-C23-C24-C25 |
| 82 | Qh | 103 | PEE | C16-C17-C18-C19 |
| 72 | AL | 204 | CDL | CB4-CB3-OB5-PB2 |
| 71 | Qj | 101 | PC1 | C22-C23-C24-C25 |
| 72 | Qh | 102 | CDL | OB5-CB3-CB4-OB6 |
| 77 | B5 | 201 | PLX | O4-C3-C4-O6 |
| 82 | S2 | 501 | PEE | C17-C18-C19-C20 |
| 72 | AL | 201 | CDL | C34-C35-C36-C37 |
| 77 | AL | 205 | PLX | C28-C29-C30-C31 |
| 82 | QB | 503 | PEE | C34-C35-C36-C37 |
| 82 | Qh | 101 | PEE | O2-C10-C11-C12 |
| 72 | AL | 201 | CDL | C55-C56-C57-C58 |
| 77 | B5 | 201 | PLX | C11-C10-C9-C8 |
| 82 | C1 | 609 | PEE | O2-C10-C11-C12 |
| 72 | AL | 203 | CDL | C40-C41-C42-C43 |
| 71 | Qb | 502 | PC1 | O21-C2-C3-O31 |
| 72 | N2 | 401 | CDL | OA6-CA4-CA6-OA8 |
| 72 | N5 | 703 | CDL | OB6-CB4-CB6-OB8 |
| 71 | 6A | 101 | PC1 | C1-O11-P-O13 |
| 71 | 7B | 101 | PC1 | C11-O13-P-O11 |
| 71 | C1 | 607 | PC1 | C11-O13-P-O11 |
| 71 | C3 | 302 | PC1 | C1-O11-P-O13 |
| 71 | QC | 405 | PC1 | C11-O13-P-O11 |
| 72 | 6A | 102 | CDL | CB3-OB5-PB2-OB2 |
| 72 | A8 | 301 | CDL | CB3-OB5-PB2-OB2 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 72 | AM | 202 | CDL | CA2-OA2-PA1-OA5 |
| 72 | AM | 202 | CDL | CB2-OB2-PB2-OB5 |
| 72 | Qd | 401 | CDL | CA3-OA5-PA1-OA2 |
| 76 | CA | 101 | 3PE | C11-O13-P-O11 |
| 77 | AM | 201 | PLX | C2-O1-P1-O4 |
| 77 | C2 | 301 | PLX | C3-O4-P1-O1 |
| 82 | QC | 401 | PEE | C1-O3P-P-O4P |
| 82 | Qc | 401 | PEE | C1-O3P-P-O4P |
| 77 | QI | 301 | PLX | C29-C30-C31-C32 |
| 72 | N5 | 703 | CDL | CB3-CB4-CB6-OB8 |
| 77 | QI | 301 | PLX | C3-C4-C5-O8 |
| 77 | AM | 203 | PLX | C2-C1-N1-C1A |
| 72 | Qh | 102 | CDL | CB7-C71-C72-C73 |
| 77 | AM | 201 | PLX | C4-C3-O4-P1 |
| 87 | V1 | 502 | FMN | C4'-C5'-O5'-P |
| 77 | AL | 205 | PLX | C27-C28-C29-C30 |
| 77 | QE | 301 | PLX | C25-C26-C27-C28 |
| 78 | B5 | 203 | 6F6 | C25-C26-C27-C28 |
| 72 | B5 | 202 | CDL | C37-C38-C39-C40 |
| 82 | C1 | 609 | PEE | C14-C15-C16-C17 |
| 82 | S8 | 303 | PEE | C15-C16-C17-C18 |
| 77 | CB | 201 | PLX | C11-C10-C9-C8 |
| 79 | C1 | 602 | HEA | CAD-CBD-CGD-O2D |
| 72 | AL | 204 | CDL | C13-C14-C15-C16 |
| 77 | QI | 301 | PLX | C12-C13-C14-C15 |
| 71 | 6A | 101 | PC1 | O31-C31-C32-C33 |
| 72 | B5 | 202 | CDL | C80-C81-C82-C83 |
| 72 | QC | 406 | CDL | C18-C19-C20-C21 |
| 78 | QJ | 101 | 6F6 | O11-C1-C2-C3 |
| 73 | A9 | 401 | NDP | O4D-C1D-N1N-C6N |
| 72 | QB | 501 | CDL | C53-C54-C55-C56 |
| 72 | A8 | 301 | CDL | OB5-CB3-CB4-OB6 |
| 72 | CB | 203 | CDL | C19-C20-C21-C22 |
| 76 | S7 | 302 | 3PE | O31-C31-C32-C33 |
| 74 | AC | 201 | ZMP | C5-C6-C7-C8 |
| 82 | QE | 302 | PEE | C34-C35-C36-C37 |
| 74 | AB | 201 | ZMP | O3-C16-C17-C18 |
| 83 | QC | 403 | HEM | CAA-CBA-CGA-O1A |
| 71 | N5 | 704 | PC1 | C2E-C2F-C2G-C2H |
| 83 | QC | 402 | HEM | CAD-CBD-CGD-O1D |
| 83 | Qc | 402 | HEM | CAA-CBA-CGA-O2A |
| 83 | Qc | 403 | HEM | CAD-CBD-CGD-O1D |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 77 | B5 | 201 | PLX | O6-C6-C7-C8 |
| 77 | N4 | 501 | PLX | O8-C24-C25-C26 |
| 78 | Qc | 404 | 6F6 | C2-C1-O11-P |
| 71 | 7B | 101 | PC1 | C2D-C2E-C2F-C2G |
| 83 | QC | 402 | HEM | CAA-CBA-CGA-O1A |
| 72 | 6A | 102 | CDL | C21-C22-C23-C24 |
| 72 | AL | 204 | CDL | C72-C73-C74-C75 |
| 72 | CB | 203 | CDL | C36-C37-C38-C39 |
| 82 | QC | 401 | PEE | C35-C36-C37-C38 |
| 72 | QC | 406 | CDL | C35-C36-C37-C38 |
| 72 | A8 | 301 | CDL | C74-C75-C76-C77 |
| 78 | QJ | 101 | 6F6 | C26-C27-C28-C29 |
| 83 | QC | 403 | HEM | CAA-CBA-CGA-O2A |
| 82 | S2 | 501 | PEE | C21-C22-C23-C24 |
| 71 | QC | 407 | PC1 | C27-C28-C29-C2A |
| 71 | C3 | 301 | PC1 | C1-C2-C3-O31 |
| 72 | N5 | 702 | CDL | CA3-CA4-CA6-OA8 |
| 76 | N4 | 502 | 3PE | C1-C2-C3-O31 |
| 82 | Qd | 403 | PEE | C1-C2-C3-O3 |
| 83 | Qc | 402 | HEM | CAA-CBA-CGA-O1A |
| 72 | CB | 203 | CDL | C84-C85-C86-C87 |
| 74 | AB | 201 | ZMP | C20-C18-C21-O5 |
| 74 | AC | 201 | ZMP | C20-C18-C21-O5 |
| 71 | C3 | 301 | PC1 | C32-C33-C34-C35 |
| 77 | AL | 205 | PLX | C15-C16-C17-C18 |
| 77 | QE | 301 | PLX | C7-C8-C9-C10 |
| 82 | Qd | 403 | PEE | C21-C22-C23-C24 |
| 71 | C3 | 301 | PC1 | C27-C28-C29-C2A |
| 72 | QC | 406 | CDL | C17-C18-C19-C20 |
| 71 | Qb | 502 | PC1 | C3-C2-O21-C21 |
| 71 | Qj | 101 | PC1 | C3-C2-O21-C21 |
| 72 | Qb | 501 | CDL | CA3-CA4-OA6-CA5 |
| 72 | Qd | 401 | CDL | CA3-CA4-OA6-CA5 |
| 76 | C1 | 608 | 3PE | C3-C2-O21-C21 |
| 71 | AL | 206 | PC1 | C11-C12-N-C13 |
| 83 | Qc | 403 | HEM | CAA-CBA-CGA-O1A |
| 78 | QJ | 101 | 6F6 | C11-O13-P-O11 |
| 79 | C1 | 603 | HEA | CAD-CBD-CGD-O1D |
| 82 | QC | 401 | PEE | C40-C41-C42-C43 |
| 77 | C2 | 301 | PLX | C6-C7-C8-C9 |
| 72 | AL | 204 | CDL | OA5-CA3-CA4-CA6 |
| 72 | Qh | 102 | CDL | OA5-CA3-CA4-CA6 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 77 | B5 | 201 | PLX | O4-C3-C4-C5 |
| 77 | CB | 201 | PLX | O4-C3-C4-C5 |
| 76 | S7 | 302 | 3PE | C25-C26-C27-C28 |
| 83 | Qc | 403 | HEM | CAD-CBD-CGD-O2D |
| 72 | QC | 406 | CDL | C13-C14-C15-C16 |
| 76 | S7 | 302 | 3PE | C2A-C2B-C2C-C2D |
| 72 | AL | 201 | CDL | CB5-C51-C52-C53 |
| 83 | QC | 402 | HEM | CAD-CBD-CGD-O2D |
| 83 | Qc | 402 | HEM | CAD-CBD-CGD-O1D |
| 82 | QC | 401 | PEE | C14-C15-C16-C17 |
| 74 | AB | 201 | ZMP | C12-C11-S1-C10 |
| 72 | N5 | 702 | CDL | OA6-CA4-CA6-OA8 |
| 76 | N4 | 502 | 3PE | O21-C2-C3-O31 |
| 77 | QE | 301 | PLX | O6-C4-C5-O8 |
| 82 | S2 | 501 | PEE | O2-C2-C3-O3 |
| 76 | C1 | 601 | 3PE | O21-C21-C22-C23 |
| 77 | QI | 301 | PLX | C36-C37-C38-C39 |
| 83 | Qc | 402 | HEM | CAD-CBD-CGD-O2D |
| 82 | S2 | 501 | PEE | C37-C38-C39-C40 |
| 82 | C1 | 609 | PEE | C38-C39-C40-C41 |
| 72 | AL | 201 | CDL | C35-C36-C37-C38 |
| 82 | QB | 503 | PEE | C43-C44-C45-C46 |
| 83 | QC | 402 | HEM | CAA-CBA-CGA-O2A |
| 83 | Qc | 403 | HEM | CAA-CBA-CGA-O2A |
| 71 | QH | 102 | PC1 | O21-C21-C22-C23 |
| 72 | N5 | 703 | CDL | C12-C11-CA5-OA6 |
| 77 | QE | 301 | PLX | C3-C4-C5-O8 |
| 82 | Qh | 103 | PEE | C30-C31-C32-C33 |
| 84 | QD | 401 | HEC | CAD-CBD-CGD-O2D |
| 77 | QI | 301 | PLX | C6-C7-C8-C9 |
| 71 | Qb | 502 | PC1 | C32-C33-C34-C35 |
| 78 | Qc | 404 | 6F6 | O32-C31-C32-C33 |
| 82 | C1 | 609 | PEE | C20-C21-C22-C23 |
| 72 | QC | 406 | CDL | C12-C13-C14-C15 |
| 77 | C2 | 301 | PLX | C15-C16-C17-C18 |
| 82 | Qd | 403 | PEE | C33-C34-C35-C36 |
| 72 | N5 | 702 | CDL | C14-C15-C16-C17 |
| 72 | AL | 204 | CDL | OA5-CA3-CA4-OA6 |
| 72 | Qh | 102 | CDL | OA5-CA3-CA4-OA6 |
| 76 | N4 | 502 | 3PE | O11-C1-C2-O21 |
| 77 | QI | 301 | PLX | C15-C16-C17-C18 |
| 82 | QC | 401 | PEE | C32-C33-C34-C35 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 79 | C1 | 602 | HEA | CAD-CBD-CGD-O1D |
| 71 | 7B | 101 | PC1 | C26-C27-C28-C29 |
| 82 | QB | 503 | PEE | C14-C15-C16-C17 |
| 71 | QC | 405 | PC1 | O11-C1-C2-C3 |
| 72 | QB | 501 | CDL | OA5-CA3-CA4-CA6 |
| 72 | N5 | 703 | CDL | C1-CB2-OB2-PB2 |
| 72 | N5 | 702 | CDL | C71-C72-C73-C74 |
| 71 | C1 | 606 | PC1 | C33-C34-C35-C36 |
| 79 | C1 | 603 | HEA | CAD-CBD-CGD-O2D |
| 82 | S8 | 303 | PEE | C16-C17-C18-C19 |
| 74 | AC | 201 | ZMP | N2-C16-C17-O4 |
| 78 | QJ | 101 | 6F6 | C38-C39-C3A-C3B |
| 82 | N3 | 201 | PEE | C32-C33-C34-C35 |
| 74 | AC | 201 | ZMP | C19-C18-C21-O5 |
| 71 | C3 | 301 | PC1 | C38-C39-C3A-C3B |
| 72 | N5 | 703 | CDL | C32-C31-CA7-OA9 |
| 77 | CB | 201 | PLX | C31-C32-C33-C34 |
| 82 | QE | 302 | PEE | C18-C19-C20-C21 |
| 71 | C3 | 301 | PC1 | C3-C2-O21-C21 |
| 72 | QB | 501 | CDL | CA6-CA4-OA6-CA5 |
| 72 | QH | 101 | CDL | CA6-CA4-OA6-CA5 |
| 72 | Qh | 102 | CDL | CB6-CB4-OB6-CB5 |
| 76 | S7 | 302 | 3PE | C1-C2-O21-C21 |
| 82 | QB | 502 | PEE | C30-C31-C32-C33 |
| 72 | B5 | 202 | CDL | C72-C73-C74-C75 |
| 72 | A8 | 301 | CDL | C38-C39-C40-C41 |
| 82 | QC | 401 | PEE | C41-C42-C43-C44 |
| 84 | QD | 401 | HEC | CAD-CBD-CGD-O1D |
| 72 | QB | 501 | CDL | C74-C75-C76-C77 |
| 71 | C1 | 606 | PC1 | O21-C21-C22-C23 |
| 72 | A8 | 301 | CDL | C32-C31-CA7-OA8 |
| 72 | A8 | 301 | CDL | C72-C71-CB7-OB8 |
| 82 | N3 | 201 | PEE | O3-C30-C31-C32 |
| 72 | N5 | 702 | CDL | C12-C11-CA5-OA6 |
| 72 | 6A | 102 | CDL | C13-C14-C15-C16 |
| 82 | N1 | 401 | PEE | C16-C17-C18-C19 |
| 82 | QE | 302 | PEE | C15-C16-C17-C18 |
| 76 | C1 | 608 | 3PE | C2-C1-O11-P |
| 77 | CB | 201 | PLX | C7-C6-O6-C4 |
| 71 | 6A | 101 | PC1 | O11-C1-C2-O21 |
| 82 | N1 | 401 | PEE | C37-C38-C39-C40 |
| 72 | 6A | 102 | CDL | C52-C51-CB5-OB6 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 72 | N2 | 401 | CDL | C32-C31-CA7-OA8 |
| 72 | QH | 101 | CDL | C52-C51-CB5-OB6 |
| 77 | AM | 203 | PLX | C2-C1-N1-C1B |
| 77 | QI | 301 | PLX | C32-C33-C34-C35 |
| 72 | N5 | 703 | CDL | C33-C34-C35-C36 |
| 72 | CB | 203 | CDL | C12-C13-C14-C15 |
| 72 | AM | 202 | CDL | C72-C71-CB7-OB8 |
| 78 | QJ | 101 | 6F6 | O21-C21-C22-C23 |
| 71 | C3 | 301 | PC1 | C28-C29-C2A-C2B |
| 77 | AM | 203 | PLX | C11-C12-C13-C14 |
| 71 | AL | 206 | PC1 | O21-C21-C22-C23 |
| 71 | Qj | 101 | PC1 | O21-C21-C22-C23 |
| 76 | C1 | 608 | 3PE | C34-C35-C36-C37 |
| 71 | QH | 102 | PC1 | O11-C1-C2-C3 |
| 71 | C3 | 302 | PC1 | O21-C21-C22-C23 |
| 72 | AL | 201 | CDL | C52-C51-CB5-OB6 |
| 72 | QC | 406 | CDL | C32-C31-CA7-OA8 |
| 72 | QC | 408 | CDL | C72-C71-CB7-OB8 |
| 72 | 6A | 102 | CDL | C17-C18-C19-C20 |
| 72 | CB | 203 | CDL | OB6-CB4-CB6-OB8 |
| 72 | AL | 204 | CDL | CB7-C71-C72-C73 |
| 71 | C3 | 301 | PC1 | O22-C21-C22-C23 |
| 82 | N3 | 201 | PEE | C36-C37-C38-C39 |
| 82 | Qd | 403 | PEE | C16-C17-C18-C19 |
| 71 | 7B | 101 | PC1 | O31-C31-C32-C33 |
| 71 | QC | 405 | PC1 | O31-C31-C32-C33 |
| 72 | CB | 203 | CDL | C32-C31-CA7-OA8 |
| 77 | N4 | 501 | PLX | C16-C17-C18-C19 |
| 73 | A9 | 401 | NDP | C2B-O2B-P2B-O2X |
| 77 | AM | 203 | PLX | O7-C6-C7-C8 |
| 72 | AL | 204 | CDL | C11-CA5-OA6-CA4 |
| 72 | Qh | 102 | CDL | C12-C11-CA5-OA6 |
| 82 | Qd | 403 | PEE | O3-C30-C31-C32 |
| 79 | C1 | 603 | HEA | C26-C15-C16-C17 |
| 72 | AL | 204 | CDL | CA7-C31-C32-C33 |
| 72 | QC | 406 | CDL | CB4-CB3-OB5-PB2 |
| 71 | N5 | 704 | PC1 | O21-C21-C22-C23 |
| 76 | QE | 303 | 3PE | O31-C31-C32-C33 |
| 82 | Qh | 103 | PEE | C11-C12-C13-C14 |
| 72 | AL | 203 | CDL | C37-C38-C39-C40 |
| 73 | A9 | 401 | NDP | O4B-C4B-C5B-O5B |
| 82 | QC | 401 | PEE | O3-C30-C31-C32 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 71 | QC | 405 | PC1 | C39-C3A-C3B-C3C |
| 72 | A8 | 301 | CDL | C72-C71-CB7-OB9 |
| 78 | QJ | 101 | 6F6 | O22-C21-C22-C23 |
| 72 | QC | 408 | CDL | C31-C32-C33-C34 |
| 77 | AM | 203 | PLX | C2-C1-N1-C1C |
| 72 | AL | 204 | CDL | C36-C37-C38-C39 |
| 77 | B5 | 201 | PLX | C34-C35-C36-C37 |
| 72 | AL | 203 | CDL | C21-C22-C23-C24 |
| 76 | CA | 101 | 3PE | C39-C3A-C3B-C3C |
| 72 | N2 | 401 | CDL | C32-C31-CA7-OA9 |
| 72 | N5 | 702 | CDL | C12-C11-CA5-OA7 |
| 72 | 6A | 102 | CDL | C15-C16-C17-C18 |
| 77 | C2 | 301 | PLX | C9-C10-C11-C12 |
| 71 | AL | 206 | PC1 | O22-C21-C22-C23 |
| 71 | C1 | 606 | PC1 | O22-C21-C22-C23 |
| 71 | C3 | 302 | PC1 | O22-C21-C22-C23 |
| 72 | Qh | 102 | CDL | C12-C11-CA5-OA7 |
| 72 | N2 | 401 | CDL | C72-C71-CB7-OB8 |
| 78 | QJ | 101 | 6F6 | C27-C28-C29-C2A |
| 71 | QC | 405 | PC1 | C33-C34-C35-C36 |
| 71 | QC | 407 | PC1 | O31-C31-C32-C33 |
| 71 | 7B | 101 | PC1 | C2-C1-O11-P |
| 72 | AL | 204 | CDL | CA4-CA3-OA5-PA1 |
| 76 | CA | 101 | 3PE | C2-C1-O11-P |
| 71 | Qj | 101 | PC1 | O22-C21-C22-C23 |
| 72 | A8 | 301 | CDL | C32-C31-CA7-OA9 |
| 82 | QE | 302 | PEE | C31-C32-C33-C34 |
| 72 | CB | 203 | CDL | C56-C57-C58-C59 |
| 71 | 7B | 101 | PC1 | C11-O13-P-O14 |
| 71 | C1 | 607 | PC1 | C11-O13-P-O14 |
| 71 | QC | 405 | PC1 | C11-O13-P-O14 |
| 71 | QC | 407 | PC1 | C11-O13-P-O12 |
| 72 | AM | 202 | CDL | CA2-OA2-PA1-OA3 |
| 72 | N5 | 703 | CDL | CA3-OA5-PA1-OA4 |
| 72 | Qb | 501 | CDL | CB3-OB5-PB2-OB4 |
| 76 | C1 | 601 | 3PE | C1-O11-P-O14 |
| 76 | QE | 303 | 3PE | C11-O13-P-O14 |
| 76 | S7 | 302 | 3PE | C1-O11-P-O14 |
| 78 | QJ | 101 | 6F6 | C11-O13-P-O12 |
| 82 | Qd | 403 | PEE | C4-O4P-P-O1P |
| 77 | AM | 203 | PLX | C25-C26-C27-C28 |
| 72 | CB | 203 | CDL | C32-C31-CA7-OA9 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 82 | QC | 404 | PEE | C12-C13-C14-C15 |
| 71 | 7B | 101 | PC1 | O32-C31-C32-C33 |
| 72 | AM | 202 | CDL | C72-C71-CB7-OB9 |
| 76 | S7 | 302 | 3PE | C26-C27-C28-C29 |
| 72 | 6A | 102 | CDL | C18-C19-C20-C21 |
| 82 | N3 | 201 | PEE | C40-C41-C42-C43 |
| 76 | N4 | 502 | 3PE | C31-C32-C33-C34 |
| 72 | AL | 201 | CDL | C52-C51-CB5-OB7 |
| 72 | AL | 204 | CDL | C33-C34-C35-C36 |
| 71 | N6 | 201 | PC1 | O31-C31-C32-C33 |
| 72 | B5 | 202 | CDL | C12-C11-CA5-OA6 |
| 71 | C3 | 301 | PC1 | C3D-C3E-C3F-C3G |
| 72 | N2 | 401 | CDL | C72-C71-CB7-OB9 |
| 71 | 6A | 101 | PC1 | C34-C35-C36-C37 |
| 71 | 6A | 101 | PC1 | C12-C11-O13-P |
| 71 | AL | 206 | PC1 | C12-C11-O13-P |
| 71 | C3 | 301 | PC1 | C1-C2-O21-C21 |
| 71 | QC | 407 | PC1 | C12-C11-O13-P |
| 72 | QB | 501 | CDL | CA3-CA4-OA6-CA5 |
| 72 | QH | 101 | CDL | CA3-CA4-OA6-CA5 |
| 72 | Qh | 102 | CDL | CB3-CB4-OB6-CB5 |
| 76 | S7 | 302 | 3PE | C3-C2-O21-C21 |
| 77 | AM | 201 | PLX | C1-C2-O1-P1 |
| 77 | AM | 201 | PLX | C25-C24-O8-C5 |
| 77 | AM | 203 | PLX | C1-C2-O1-P1 |
| 72 | 6A | 102 | CDL | C52-C51-CB5-OB7 |
| 72 | QH | 101 | CDL | C52-C51-CB5-OB7 |
| 72 | N2 | 401 | CDL | C12-C11-CA5-OA6 |
| 82 | N3 | 201 | PEE | O2-C10-C11-C12 |
| 82 | N5 | 701 | PEE | O2-C10-C11-C12 |
| 71 | 6A | 101 | PC1 | C28-C29-C2A-C2B |
| 79 | C1 | 602 | HEA | CAA-CBA-CGA-O1A |
| 72 | N2 | 401 | CDL | C12-C11-CA5-OA7 |
| 72 | QC | 408 | CDL | C72-C71-CB7-OB9 |
| 82 | Qd | 403 | PEE | O5-C30-C31-C32 |
| 71 | C1 | 606 | PC1 | C2E-C2F-C2G-C2H |
| 71 | QH | 102 | PC1 | C38-C39-C3A-C3B |
| 72 | N2 | 401 | CDL | C37-C38-C39-C40 |
| 76 | AL | 202 | 3PE | C2A-C2B-C2C-C2D |
| 71 | QC | 407 | PC1 | C11-C12-N-C15 |
| 71 | C1 | 606 | PC1 | O31-C31-C32-C33 |
| 76 | CA | 101 | 3PE | O31-C31-C32-C33 |

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| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 71 | N5 | 704 | PC1 | O22-C21-C22-C23 |
| 71 | QH | 102 | PC1 | C39-C3A-C3B-C3C |
| 82 | QC | 404 | PEE | O2-C10-C11-C12 |
| 71 | QH | 102 | PC1 | C22-C23-C24-C25 |
| 76 | AL | 202 | 3PE | C32-C33-C34-C35 |
| 71 | 6A | 101 | PC1 | C2-C1-O11-P |
| 72 | AL | 203 | CDL | C52-C51-CB5-OB7 |
| 82 | QC | 401 | PEE | O5-C30-C31-C32 |
| 72 | N2 | 401 | CDL | C74-C75-C76-C77 |
| 72 | A8 | 301 | CDL | C52-C51-CB5-OB6 |
| 72 | AL | 203 | CDL | C52-C51-CB5-OB6 |
| 76 | CB | 202 | 3PE | O31-C31-C32-C33 |
| 82 | Qc | 401 | PEE | C18-C19-C20-C21 |
| 82 | S2 | 501 | PEE | C31-C32-C33-C34 |
| 72 | B5 | 202 | CDL | C36-C37-C38-C39 |
| 72 | N5 | 703 | CDL | C12-C13-C14-C15 |
| 72 | QB | 501 | CDL | C13-C14-C15-C16 |
| 82 | N5 | 701 | PEE | C14-C15-C16-C17 |
| 71 | QC | 407 | PC1 | O32-C31-C32-C33 |
| 84 | Qd | 402 | HEC | CAA-CBA-CGA-O2A |
| 72 | B5 | 202 | CDL | C77-C78-C79-C80 |
| 78 | Qc | 404 | 6F6 | C24-C25-C26-C27 |
| 76 | QE | 303 | 3PE | C24-C25-C26-C27 |
| 71 | QC | 405 | PC1 | O32-C31-C32-C33 |
| 76 | CA | 101 | 3PE | C33-C34-C35-C36 |
| 71 | Qb | 502 | PC1 | O31-C31-C32-C33 |
| 74 | AB | 201 | ZMP | C11-C12-N1-C13 |
| 72 | N5 | 702 | CDL | C33-C34-C35-C36 |
| 82 | N5 | 701 | PEE | O4-C10-C11-C12 |
| 72 | N5 | 702 | CDL | C17-C18-C19-C20 |
| 82 | Qh | 101 | PEE | C32-C33-C34-C35 |
| 72 | 6A | 102 | CDL | C32-C31-CA7-OA8 |

There are no ring outliers.

78 monomers are involved in 256 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 82 | Qh | 101 | PEE | 5 | 0 |
| 83 | QC | 402 | HEM | 4 | 0 |
| 82 | Qd | 403 | PEE | 4 | 0 |
| 85 | QE | 304 | FES | 2 | 0 |
| 79 | C1 | 602 | HEA | 7 | 0 |

*Continued on next page...*

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 72 | QC | 406 | CDL | 6 | 0 |
| 77 | AM | 201 | PLX | 5 | 0 |
| 72 | Qb | 501 | CDL | 2 | 0 |
| 79 | C1 | 603 | HEA | 16 | 0 |
| 77 | B5 | 201 | PLX | 5 | 0 |
| 82 | QE | 302 | PEE | 5 | 0 |
| 76 | N4 | 502 | 3PE | 4 | 0 |
| 83 | Qc | 403 | HEM | 5 | 0 |
| 77 | QE | 301 | PLX | 6 | 0 |
| 72 | AL | 204 | CDL | 4 | 0 |
| 72 | AM | 202 | CDL | 1 | 0 |
| 72 | N5 | 703 | CDL | 3 | 0 |
| 75 | AK | 401 | ADP | 4 | 0 |
| 86 | S8 | 302 | SF4 | 2 | 0 |
| 86 | V1 | 501 | SF4 | 1 | 0 |
| 82 | QB | 503 | PEE | 1 | 0 |
| 72 | AL | 203 | CDL | 1 | 0 |
| 76 | CB | 202 | 3PE | 2 | 0 |
| 77 | QI | 301 | PLX | 5 | 0 |
| 71 | 7B | 101 | PC1 | 4 | 0 |
| 82 | C1 | 609 | PEE | 3 | 0 |
| 72 | Qh | 102 | CDL | 3 | 0 |
| 71 | QH | 102 | PC1 | 5 | 0 |
| 72 | QH | 101 | CDL | 3 | 0 |
| 72 | AL | 201 | CDL | 2 | 0 |
| 71 | C3 | 301 | PC1 | 6 | 0 |
| 71 | Qb | 502 | PC1 | 1 | 0 |
| 72 | N5 | 702 | CDL | 12 | 0 |
| 83 | Qc | 402 | HEM | 2 | 0 |
| 71 | QC | 405 | PC1 | 3 | 0 |
| 72 | CB | 203 | CDL | 11 | 0 |
| 77 | N4 | 501 | PLX | 1 | 0 |
| 74 | AB | 201 | ZMP | 1 | 0 |
| 76 | QE | 303 | 3PE | 3 | 0 |
| 82 | N5 | 701 | PEE | 5 | 0 |
| 76 | C1 | 601 | 3PE | 2 | 0 |
| 72 | A8 | 301 | CDL | 4 | 0 |
| 76 | S7 | 302 | 3PE | 4 | 0 |
| 82 | S2 | 501 | PEE | 3 | 0 |
| 74 | AC | 201 | ZMP | 4 | 0 |
| 82 | QC | 404 | PEE | 2 | 0 |
| 82 | QC | 401 | PEE | 1 | 0 |

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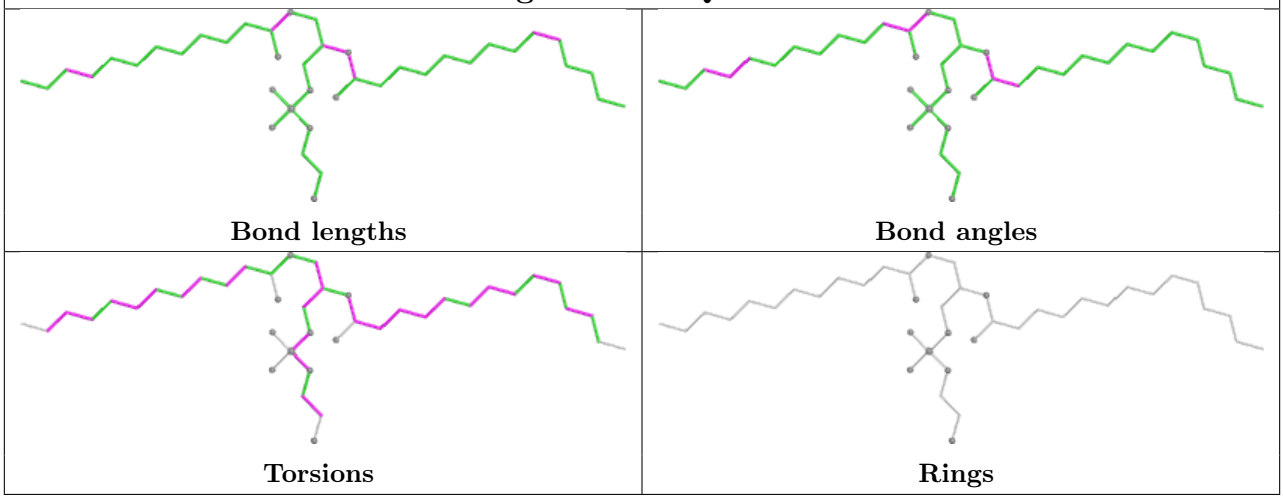
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 76 | CA | 101 | 3PE | 2 | 0 |
| 71 | C3 | 302 | PC1 | 2 | 0 |
| 87 | V1 | 502 | FMN | 1 | 0 |
| 72 | QC | 408 | CDL | 4 | 0 |
| 83 | QC | 403 | HEM | 6 | 0 |
| 72 | Qd | 401 | CDL | 6 | 0 |
| 82 | N1 | 401 | PEE | 1 | 0 |
| 77 | AL | 205 | PLX | 5 | 0 |
| 71 | C1 | 606 | PC1 | 3 | 0 |
| 71 | QC | 407 | PC1 | 3 | 0 |
| 72 | B5 | 202 | CDL | 3 | 0 |
| 85 | Qe | 301 | FES | 1 | 0 |
| 86 | S7 | 301 | SF4 | 1 | 0 |
| 71 | N5 | 704 | PC1 | 1 | 0 |
| 77 | CB | 201 | PLX | 4 | 0 |
| 78 | Qc | 404 | 6F6 | 1 | 0 |
| 71 | 6A | 101 | PC1 | 16 | 0 |
| 71 | AL | 206 | PC1 | 2 | 0 |
| 84 | Qd | 402 | HEC | 3 | 0 |
| 82 | QB | 502 | PEE | 1 | 0 |
| 72 | 6A | 102 | CDL | 4 | 0 |
| 77 | C2 | 301 | PLX | 1 | 0 |
| 82 | Qh | 103 | PEE | 3 | 0 |
| 76 | AL | 202 | 3PE | 2 | 0 |
| 77 | AM | 203 | PLX | 5 | 0 |
| 82 | S8 | 303 | PEE | 1 | 0 |
| 82 | N3 | 201 | PEE | 2 | 0 |
| 71 | C1 | 607 | PC1 | 1 | 0 |
| 84 | QD | 401 | HEC | 2 | 0 |
| 73 | A9 | 401 | NDP | 2 | 0 |
| 72 | N2 | 401 | CDL | 2 | 0 |

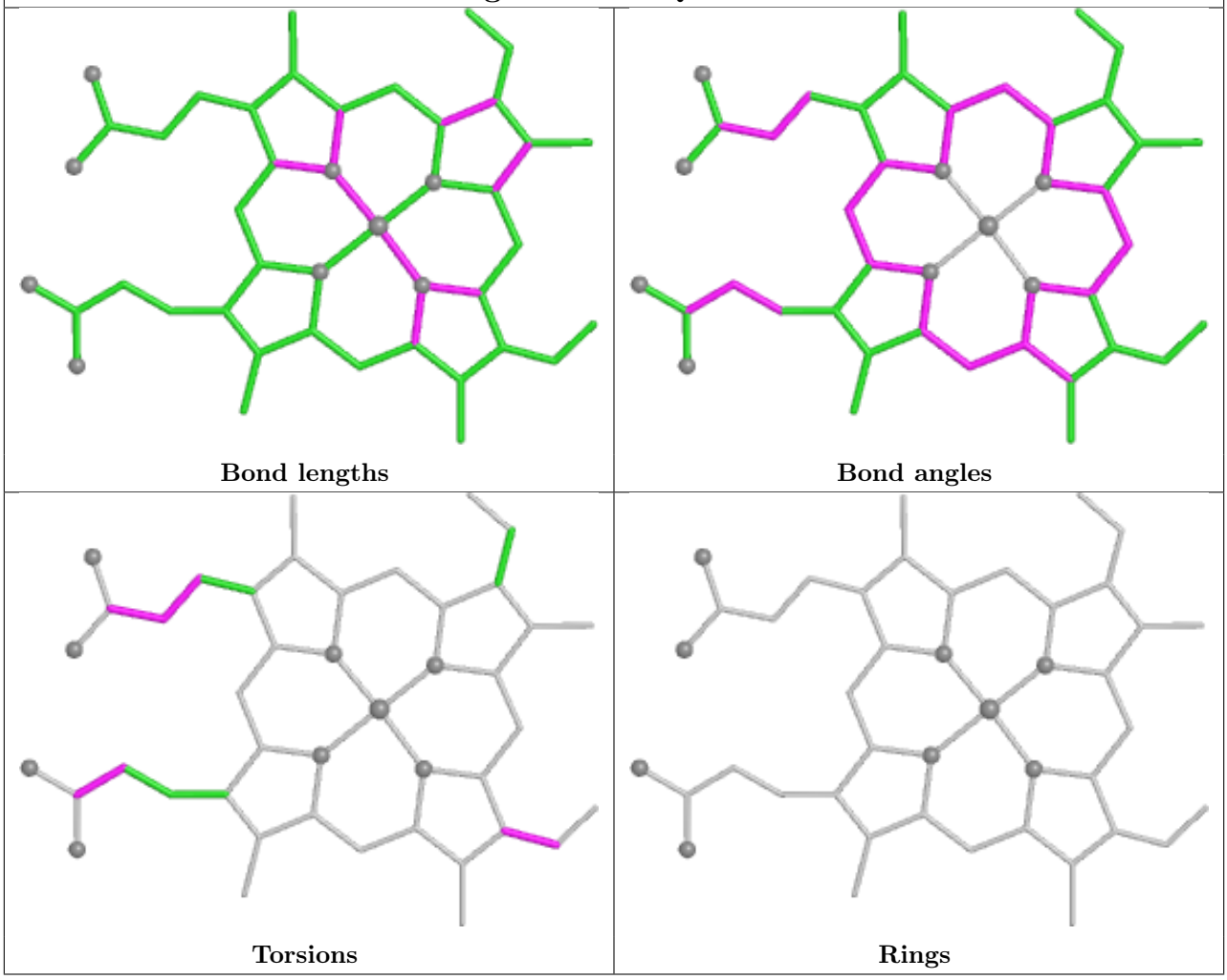
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

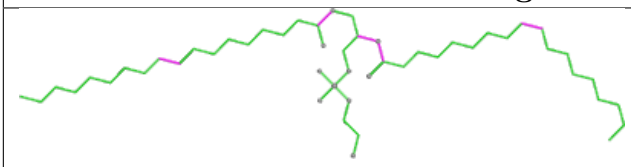
**Ligand PEE Qh 101**



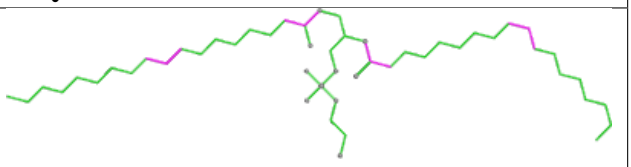

**Ligand HEM QC 402**



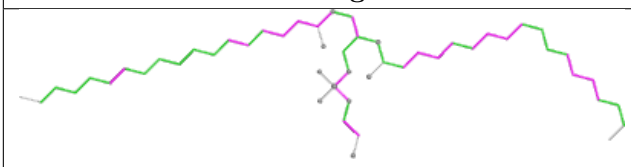
## Ligand PEE Qd 403



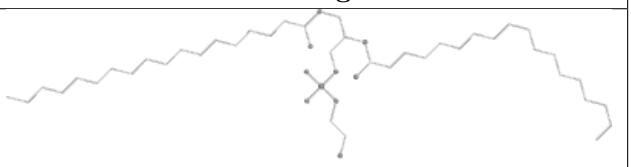
Bond lengths



Bond angles

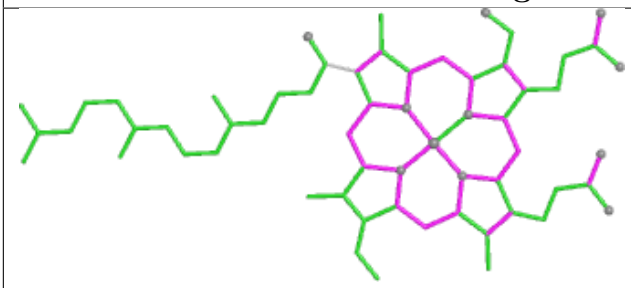


Torsions

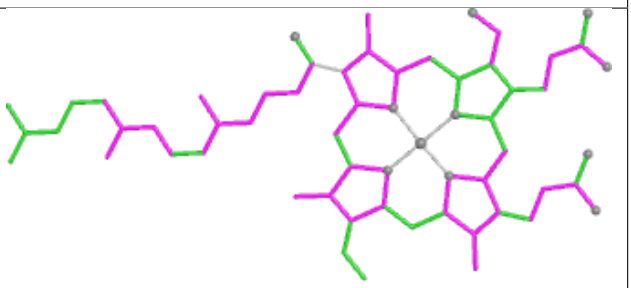


Rings

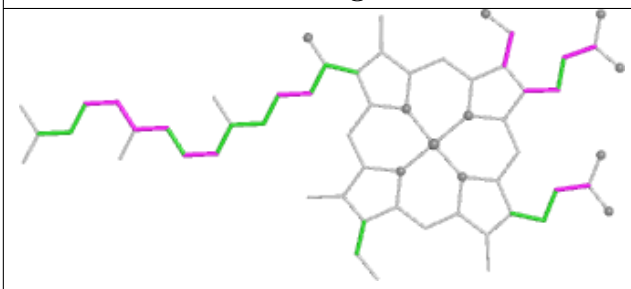
## Ligand HEA C1 602



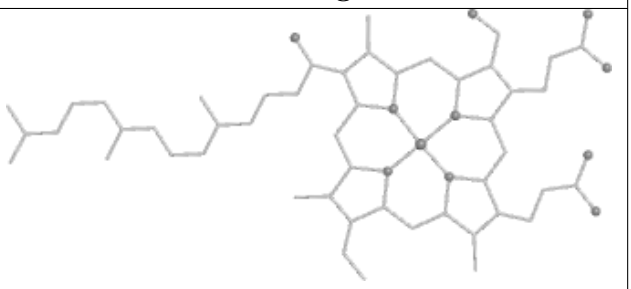
Bond lengths



Bond angles

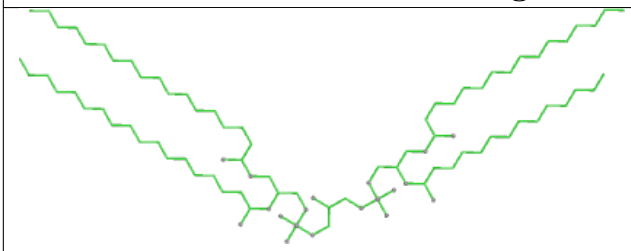


Torsions

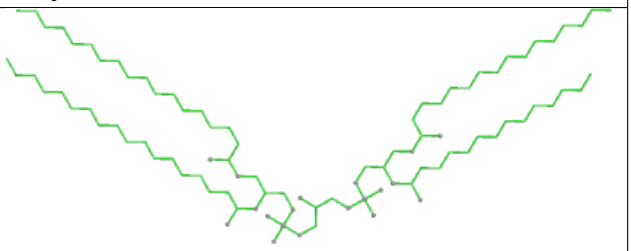


Rings

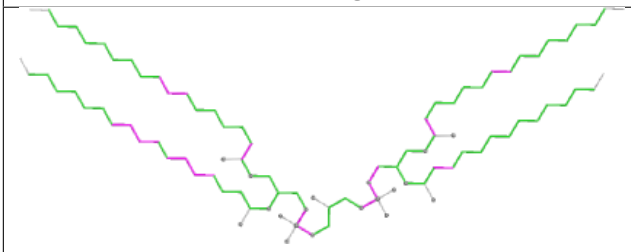
## Ligand CDL QC 406



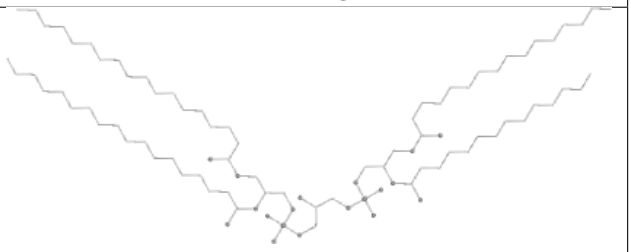
Bond lengths



Bond angles

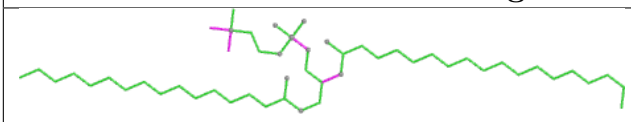


Torsions

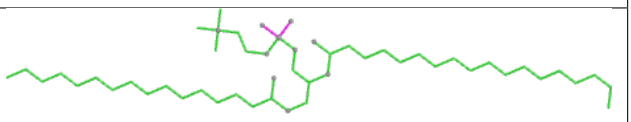


Rings

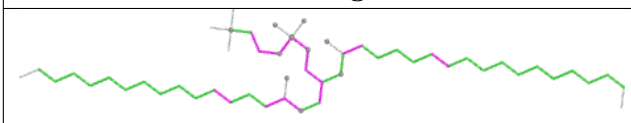
## Ligand PLX AM 201



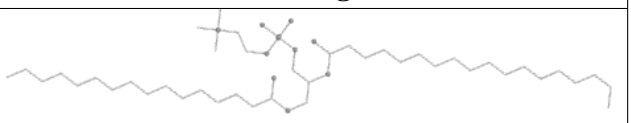
Bond lengths



Bond angles

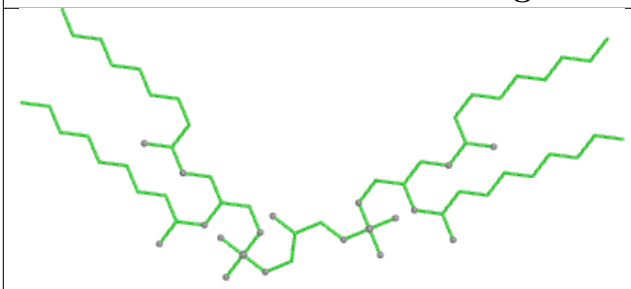


Torsions

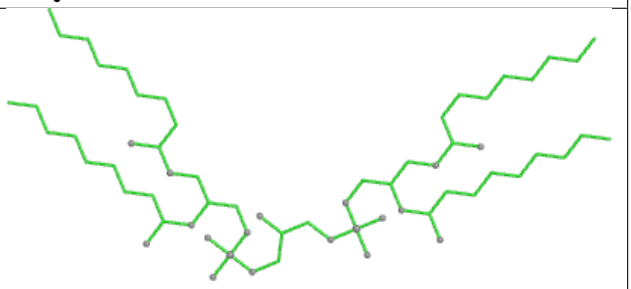


Rings

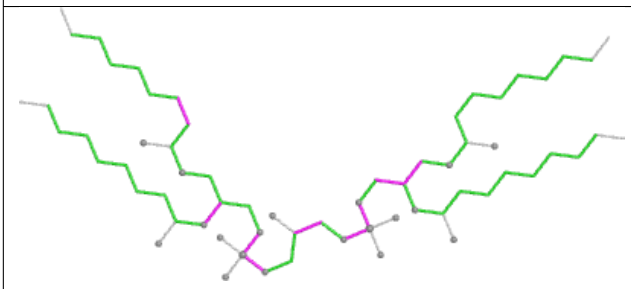
## Ligand CDL Qb 501



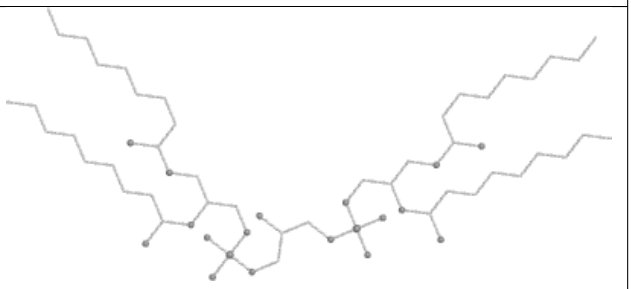
Bond lengths



Bond angles

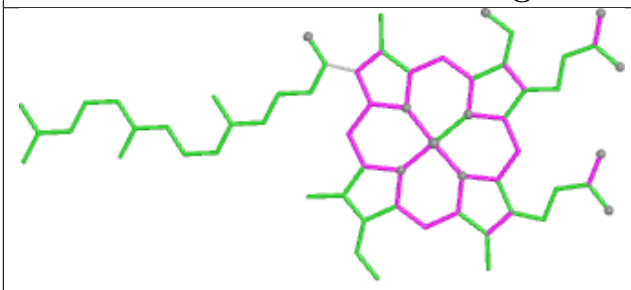


Torsions

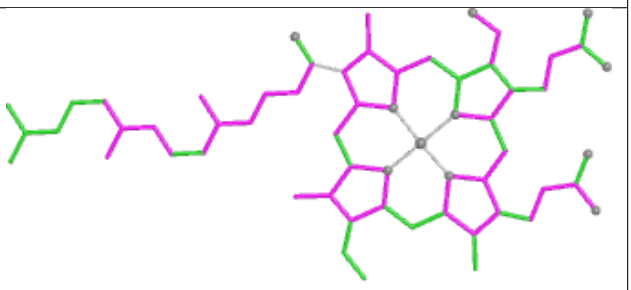


Rings

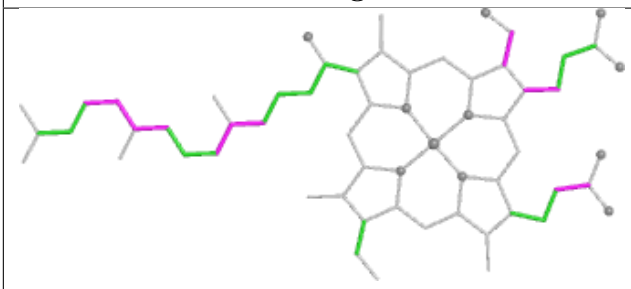
## Ligand HEA C1 603



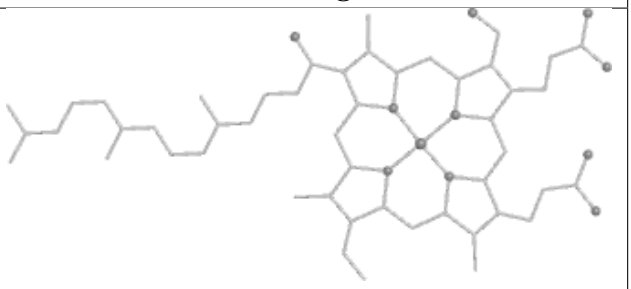
Bond lengths



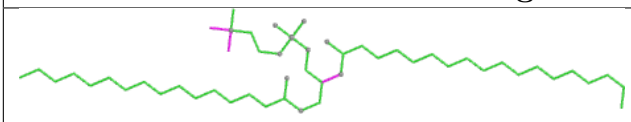
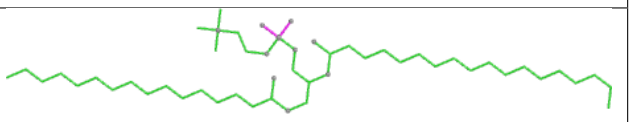
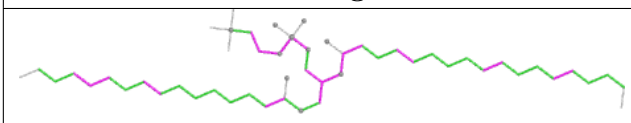
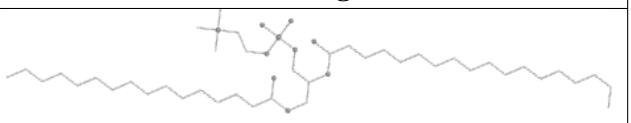
Bond angles

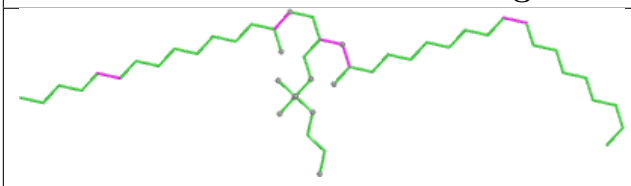
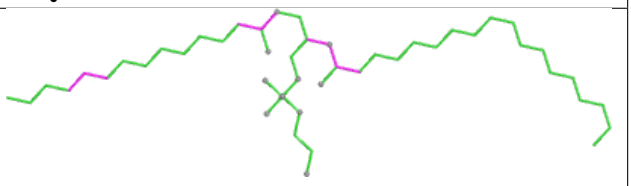
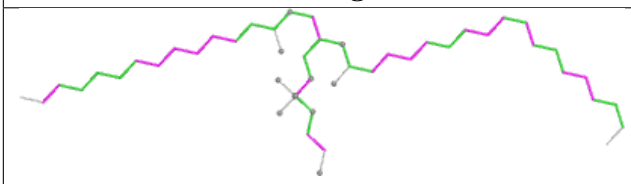
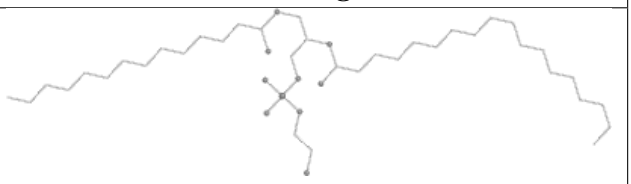


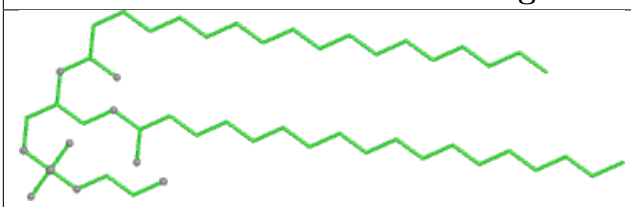
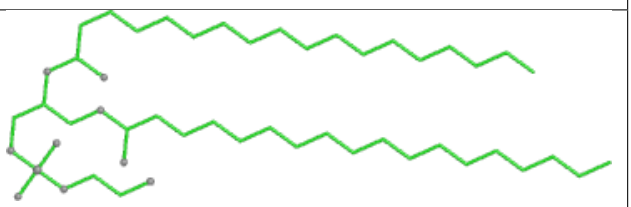
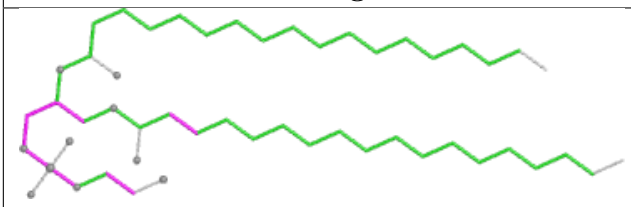
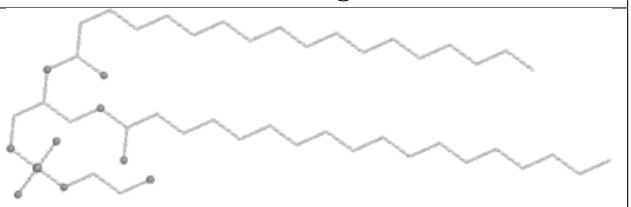
Torsions



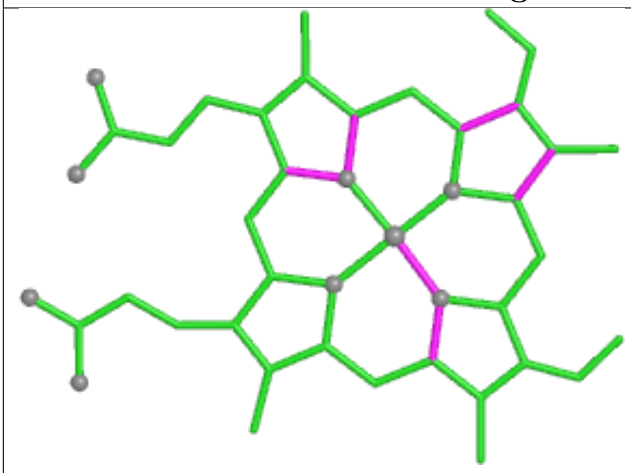
Rings

| Ligand PLX B5 201 | |
|---|---|
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

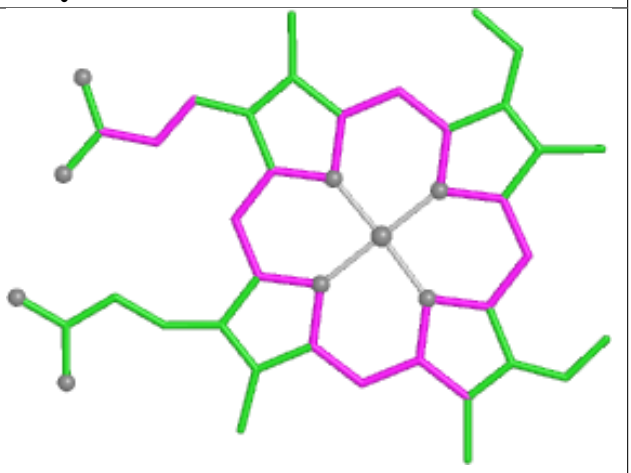
| Ligand PEE QE 302 | |
|---|---|
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

| Ligand 3PE N4 502 | |
|---|---|
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

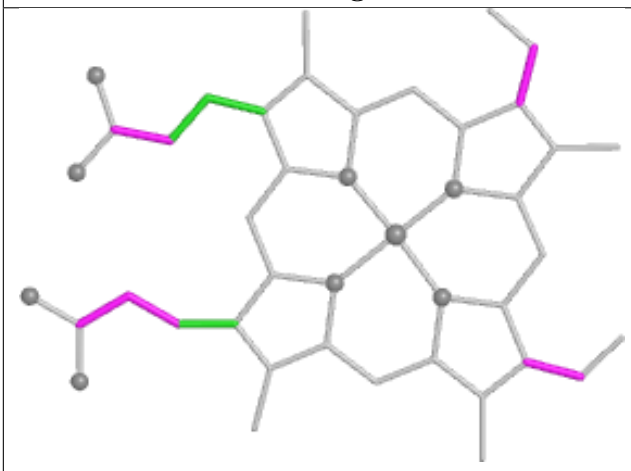
## Ligand HEM Qc 403



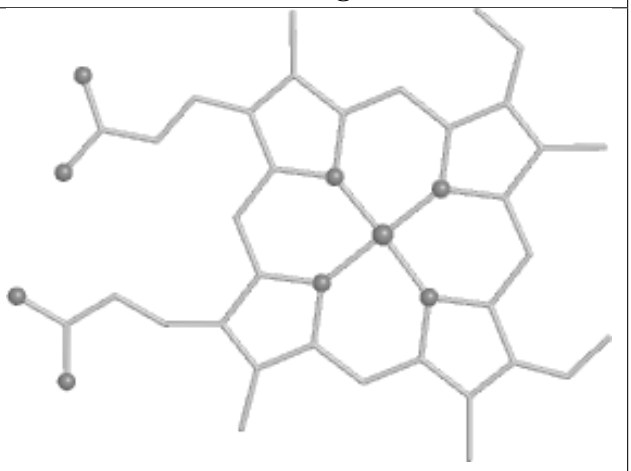
Bond lengths



Bond angles

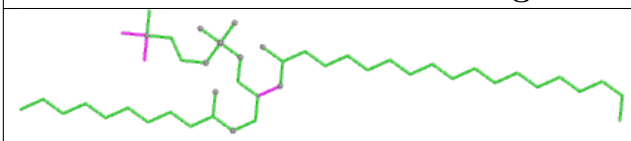


Torsions

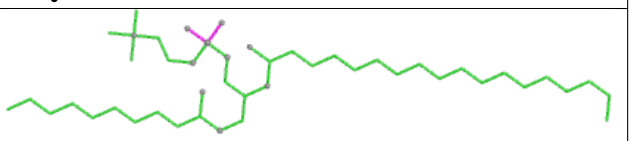


Rings

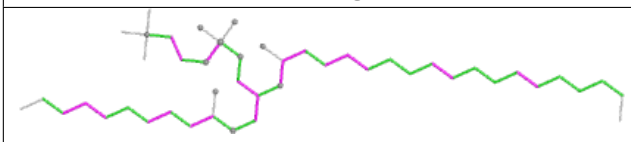
## Ligand PLX QE 301



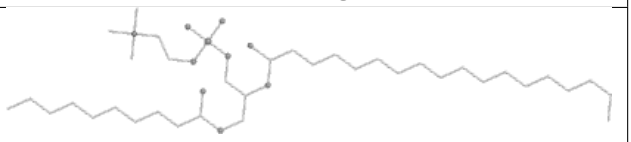
Bond lengths



Bond angles

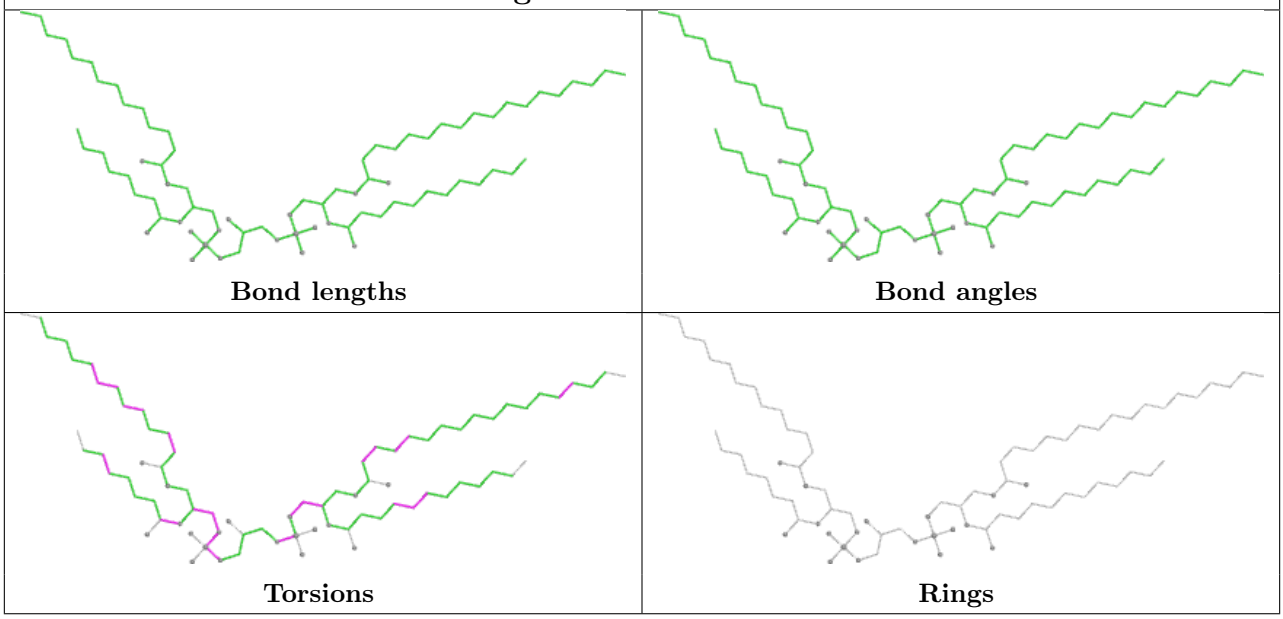


Torsions

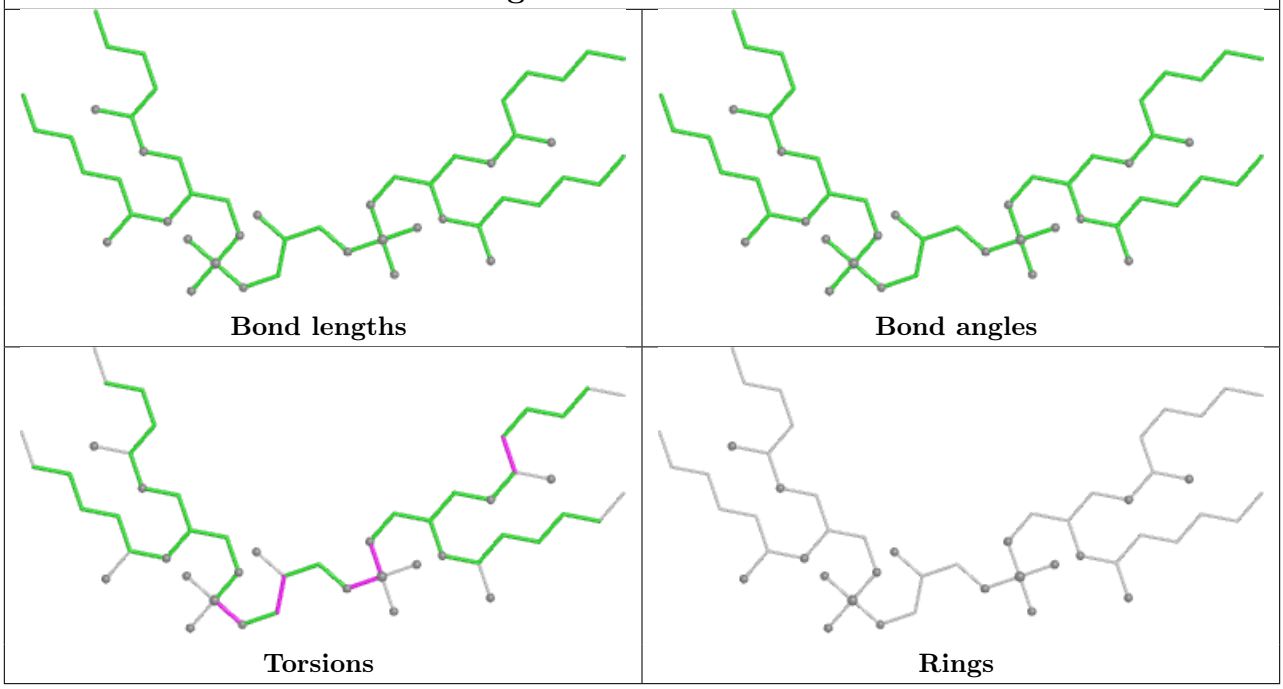


Rings

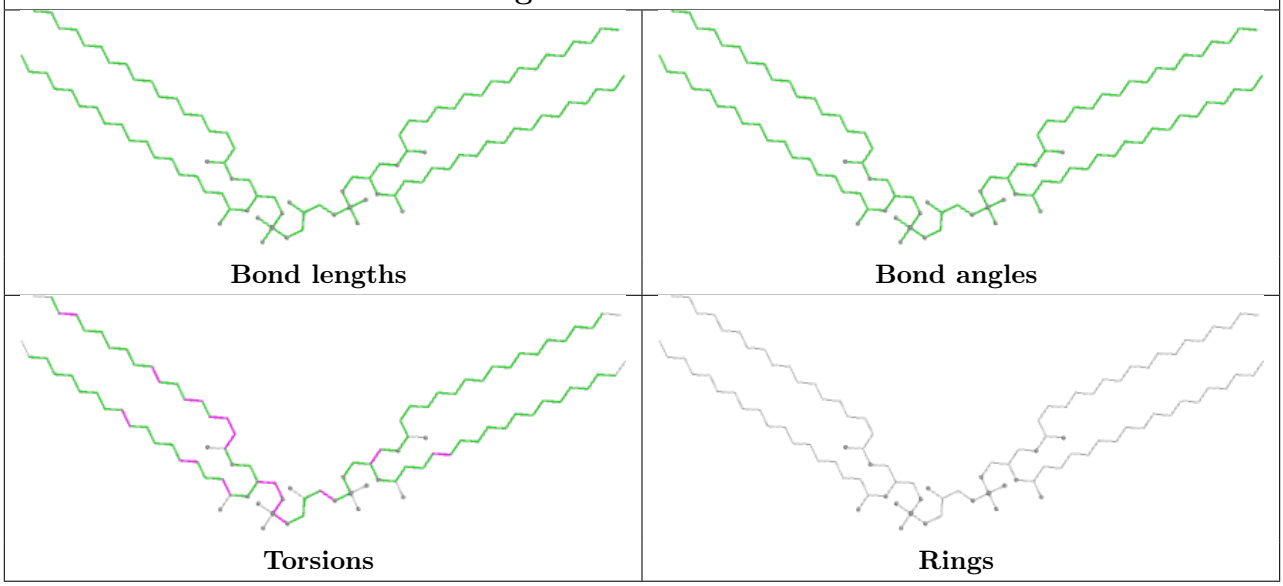
## Ligand CDL AL 204



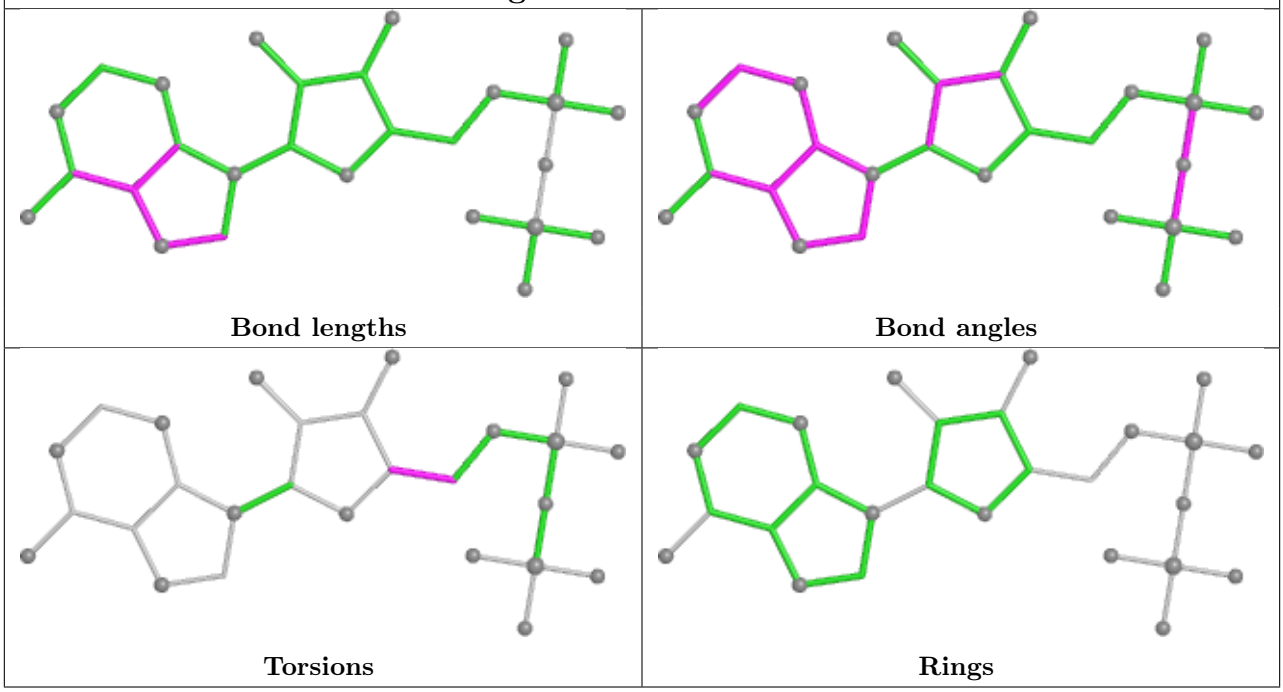

## Ligand CDL AM 202



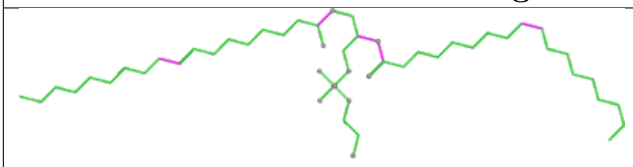
## Ligand CDL N5 703



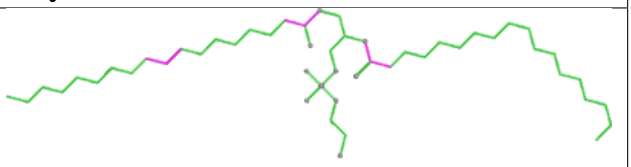

## Ligand ADP AK 401



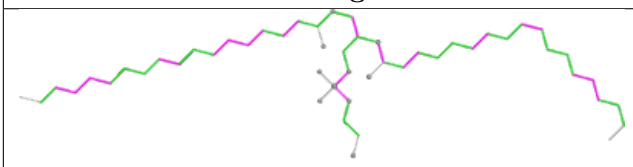
## Ligand PEE QB 503



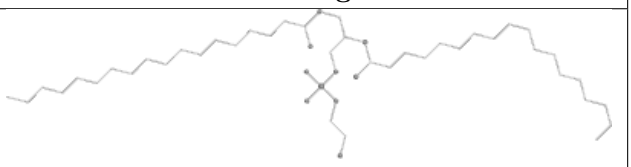
Bond lengths



Bond angles

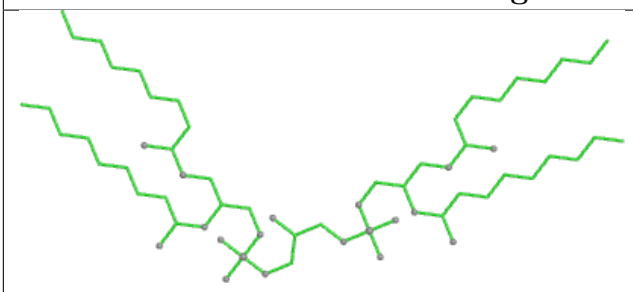


Torsions

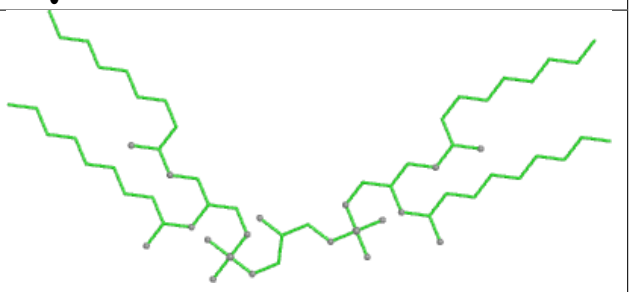


Rings

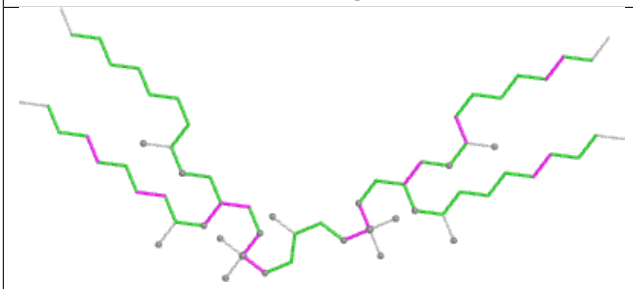
## Ligand CDL QB 501



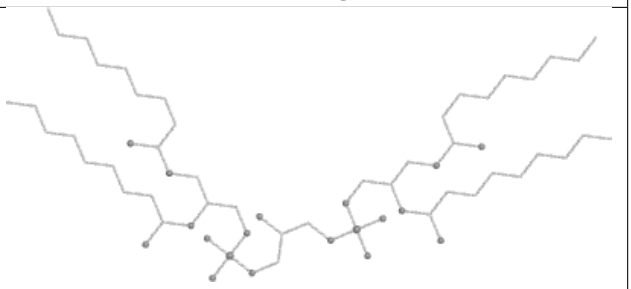
Bond lengths



Bond angles

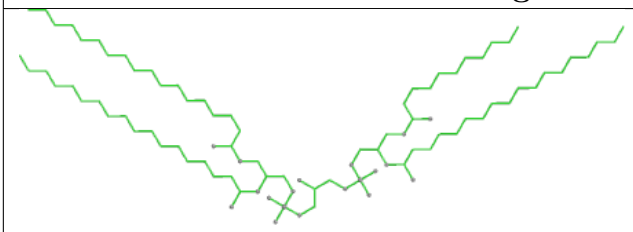


Torsions

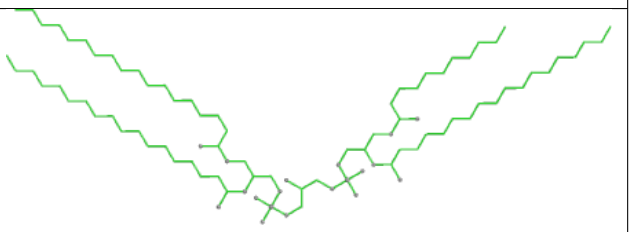


Rings

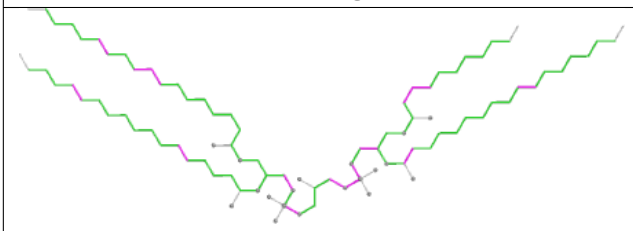
## Ligand CDL AL 203



Bond lengths



Bond angles



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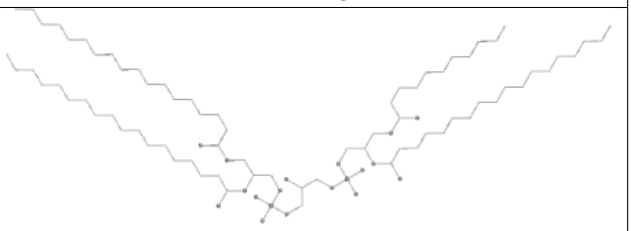
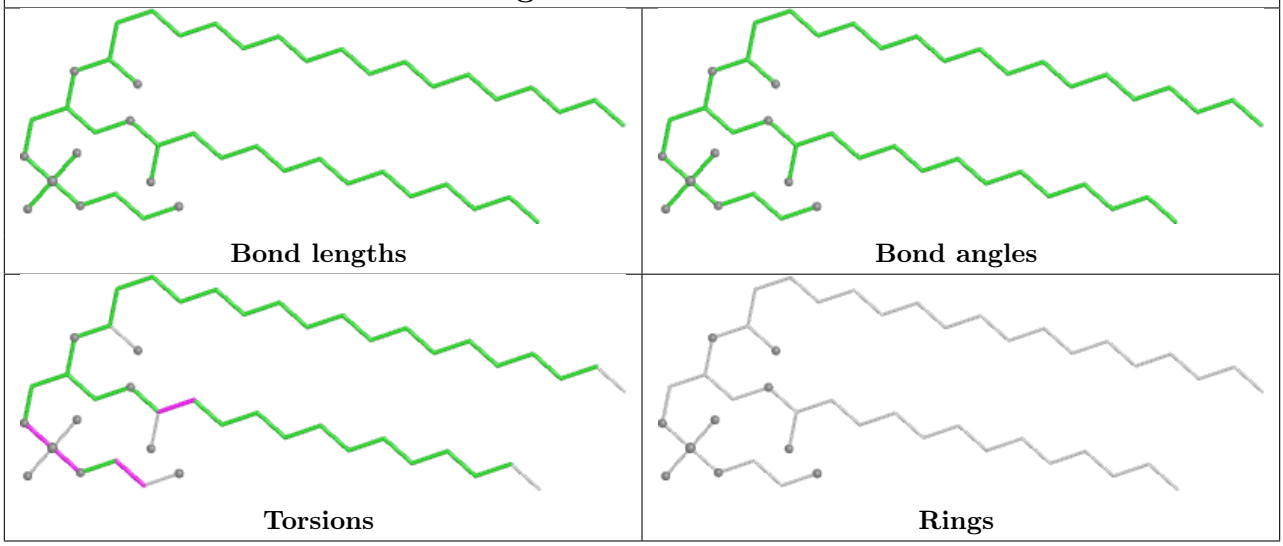
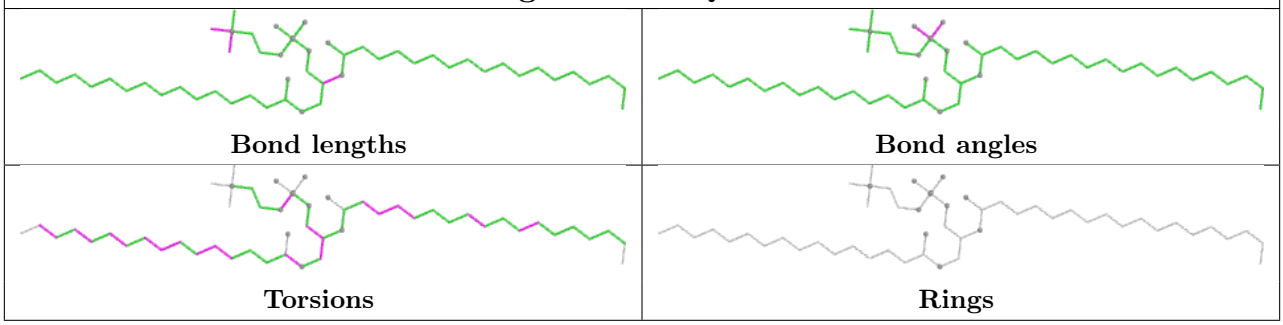


Rings

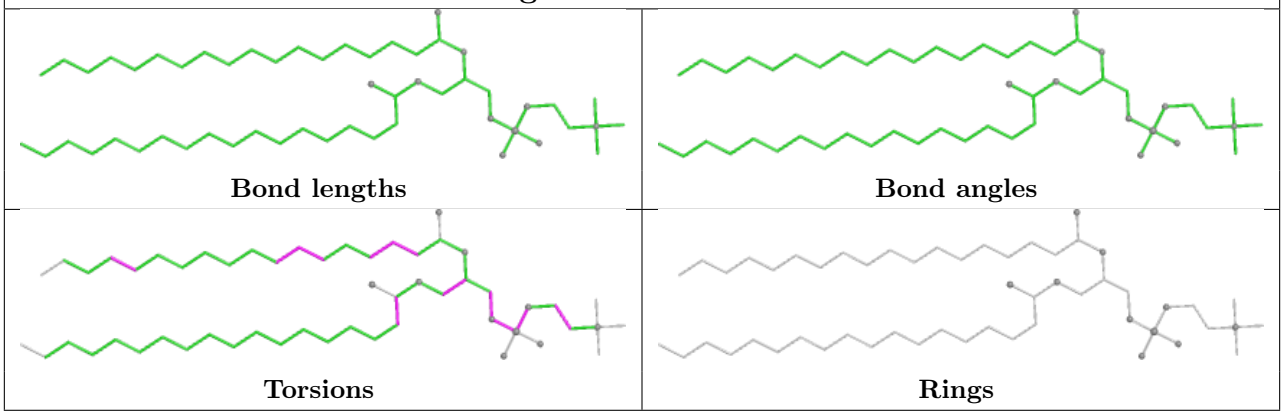
## Ligand 3PE CB 202



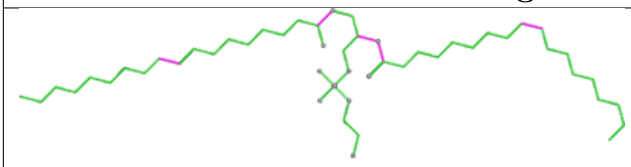

## Ligand PLX QI 301



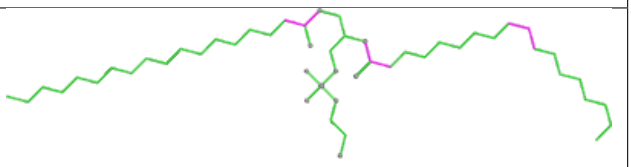

## Ligand PC1 7B 101



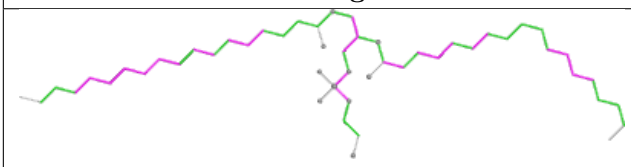
## Ligand PEE C1 609



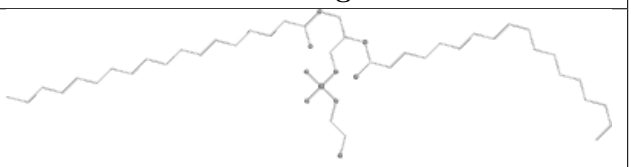
Bond lengths



Bond angles

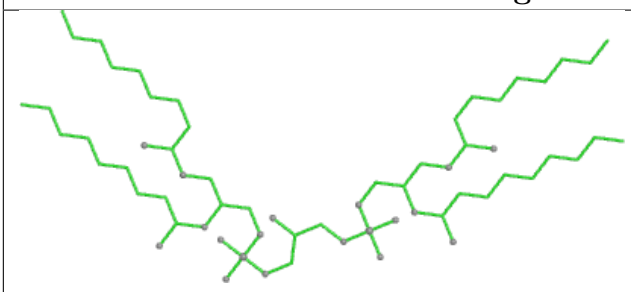


Torsions

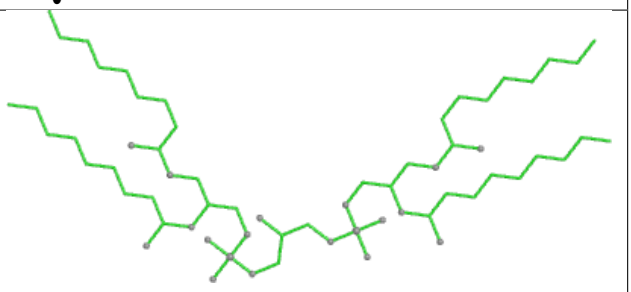


Rings

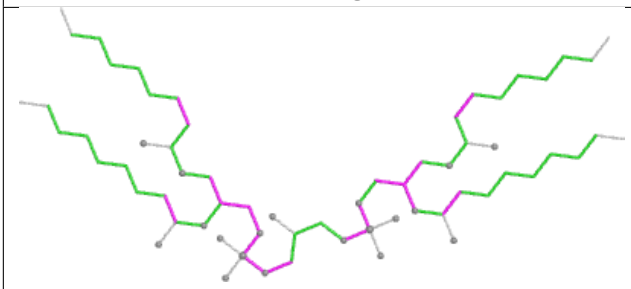
## Ligand CDL Qh 102



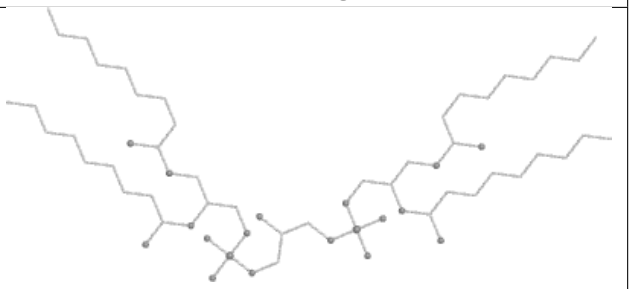
Bond lengths



Bond angles

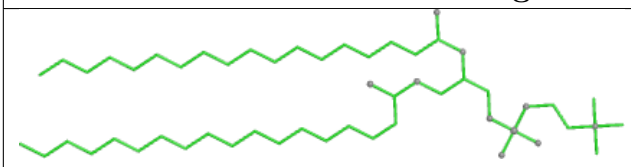


Torsions

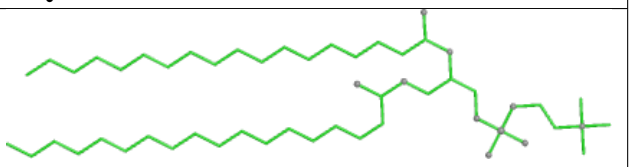


Rings

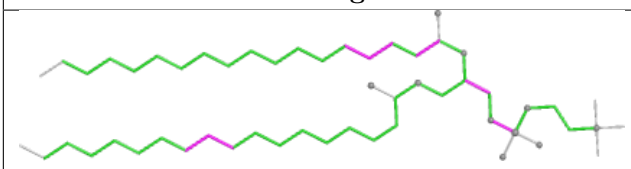
## Ligand PC1 QH 102



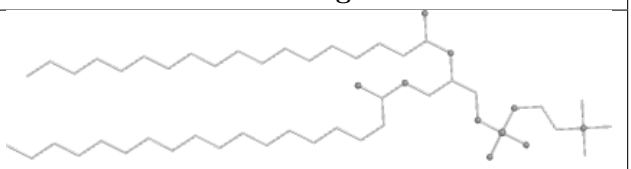
Bond lengths



Bond angles

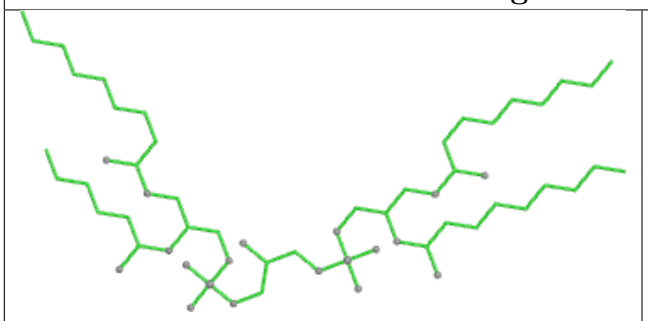


Torsions

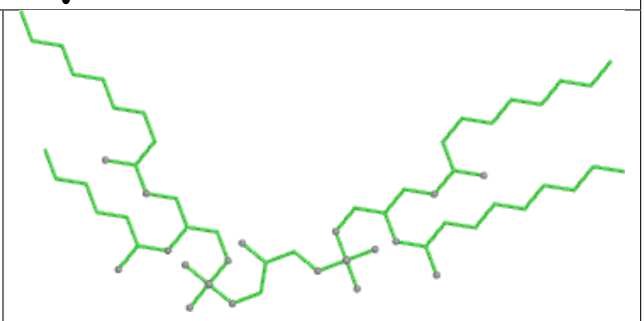


Rings

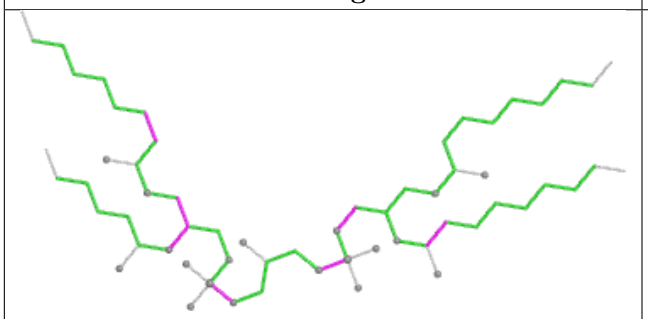
## Ligand CDL QH 101



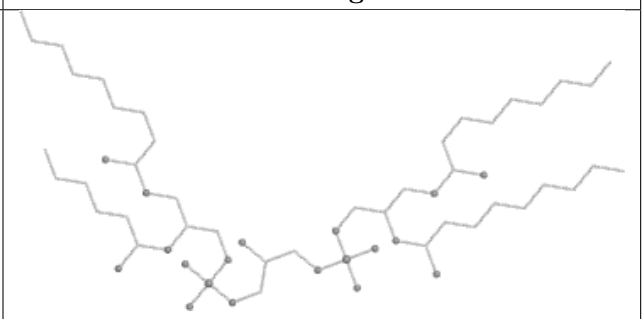
Bond lengths



Bond angles

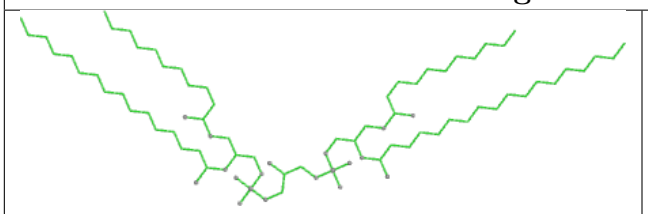


Torsions

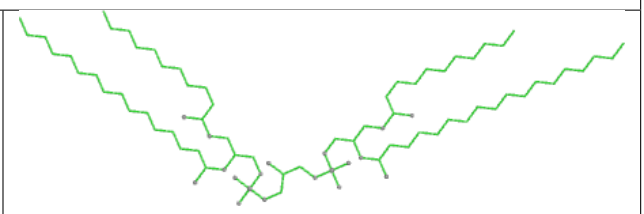


Rings

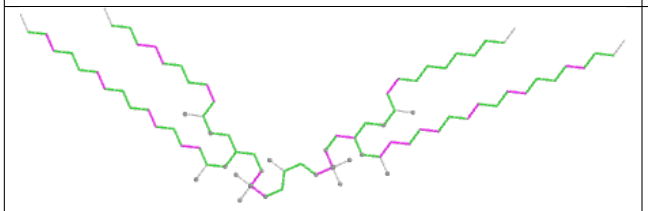
## Ligand CDL AL 201



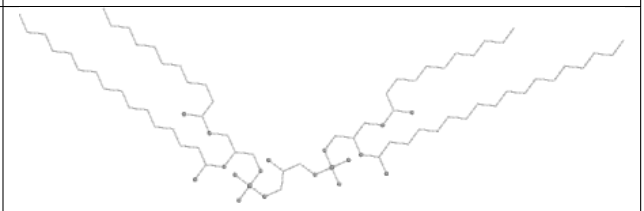
Bond lengths



Bond angles

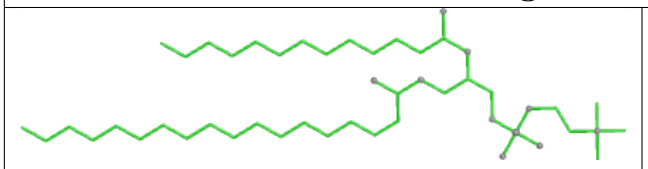


Torsions

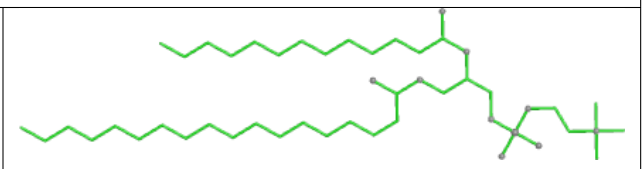


Rings

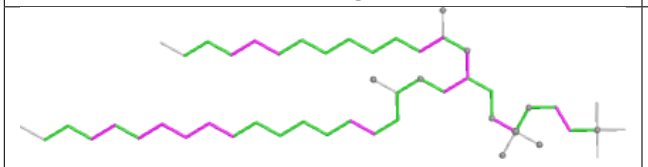
## Ligand PC1 C3 301



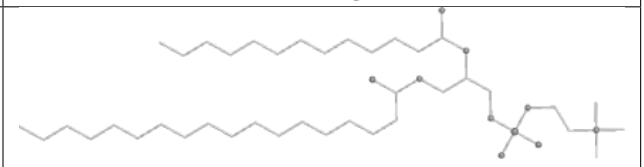
Bond lengths



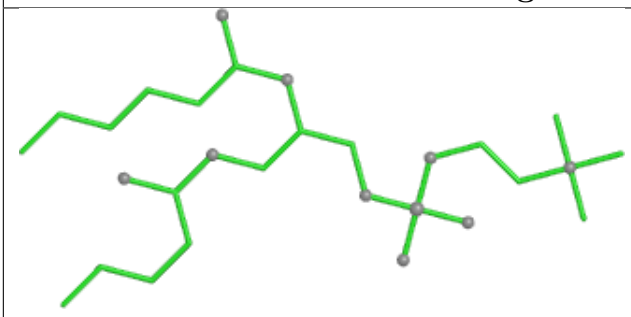
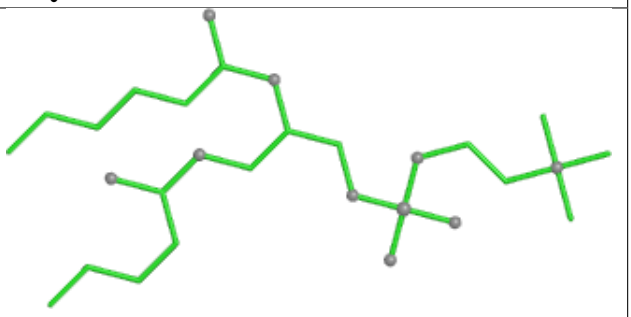
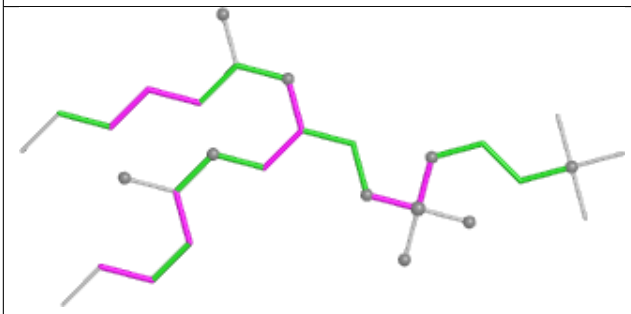
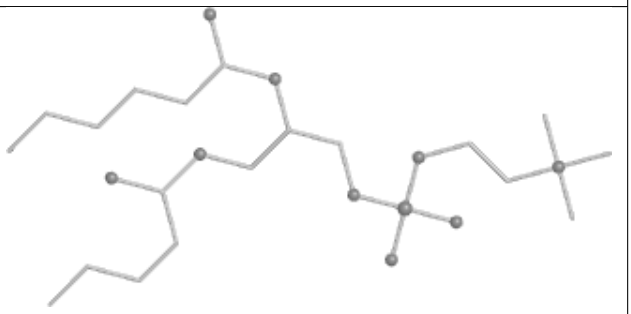
Bond angles

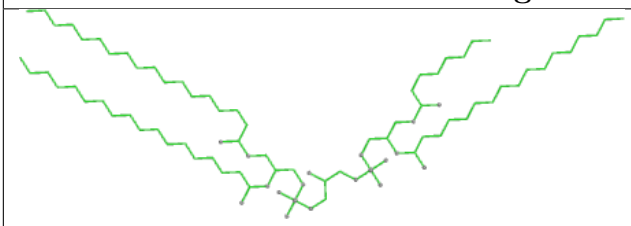
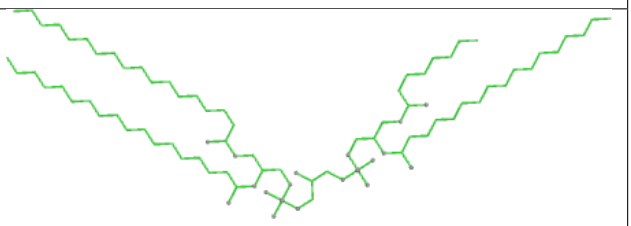
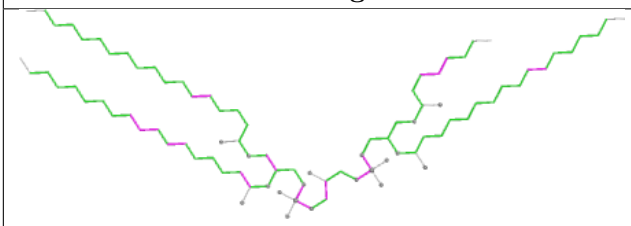
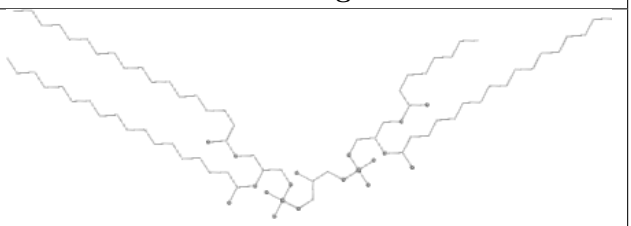


Torsions

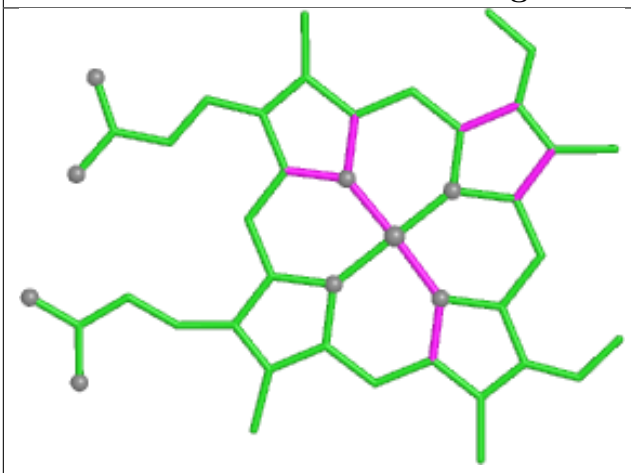


Rings

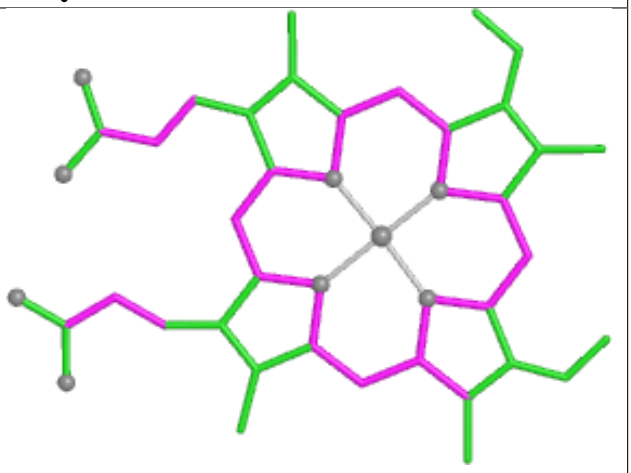
| Ligand PC1 Qb 502 | |
|---|---|
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

| Ligand CDL N5 702 | |
|---|---|
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

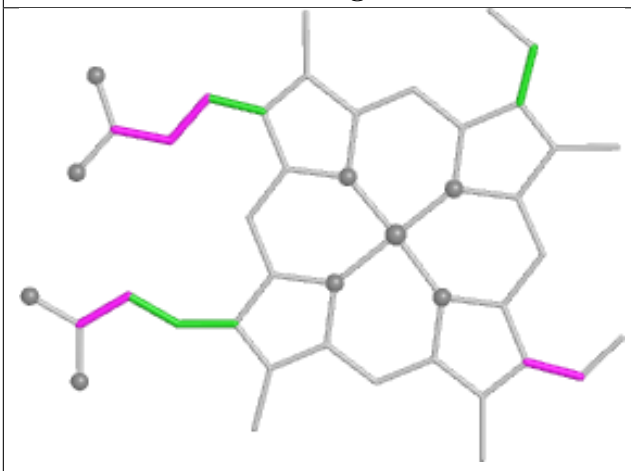
## Ligand HEM Qc 402



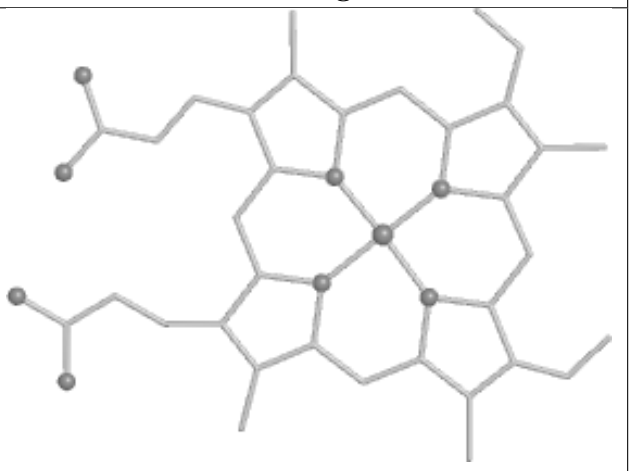
Bond lengths



Bond angles

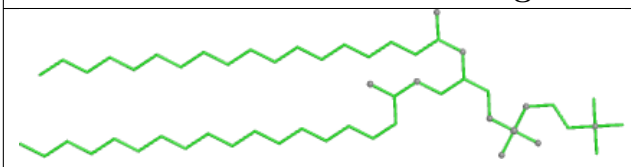


Torsions



Rings

## Ligand PC1 QC 405



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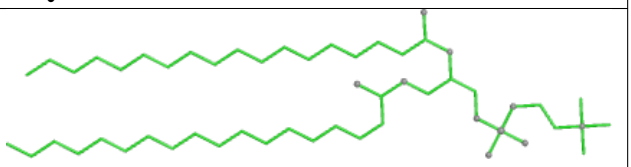
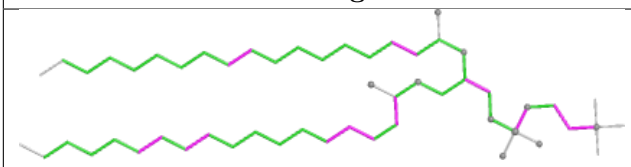


Bond angles



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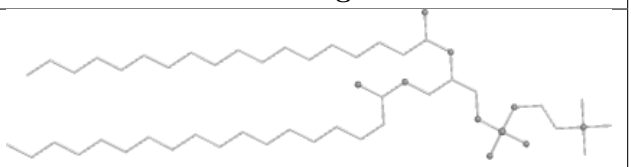
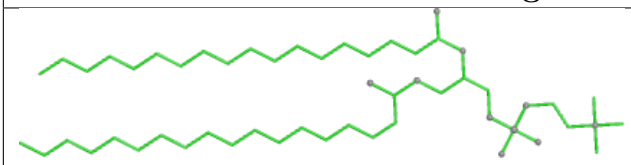
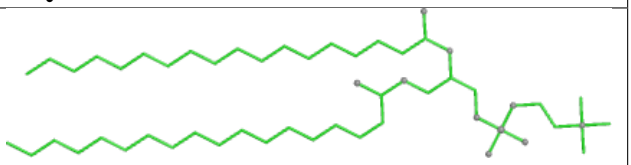


Rings

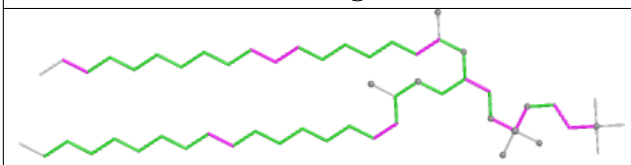
## Ligand 6F6 QJ 101



Bond lengths



Bond angles



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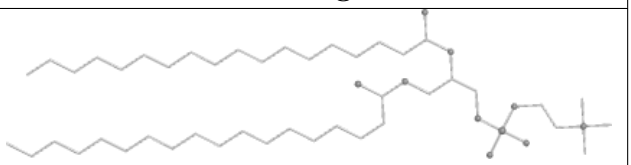
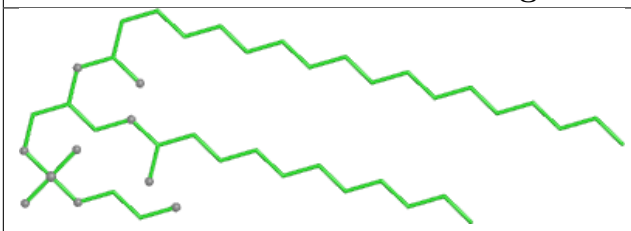


Rings

## Ligand 3PE C1 608



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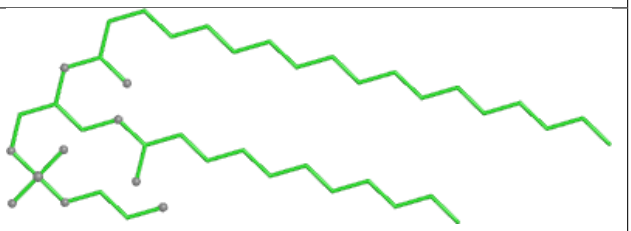
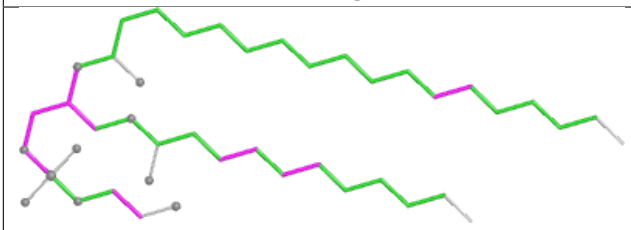


Bond angles



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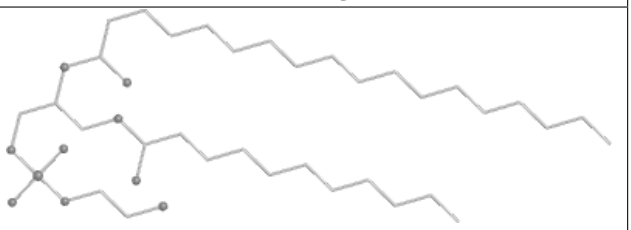
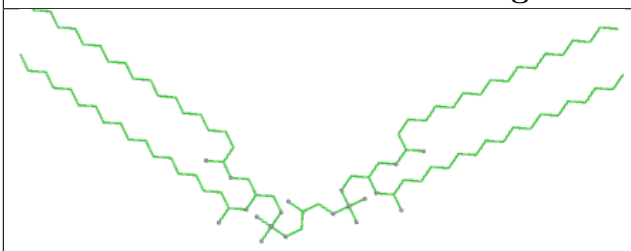
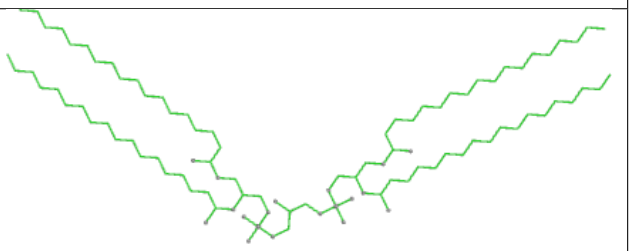


Rings

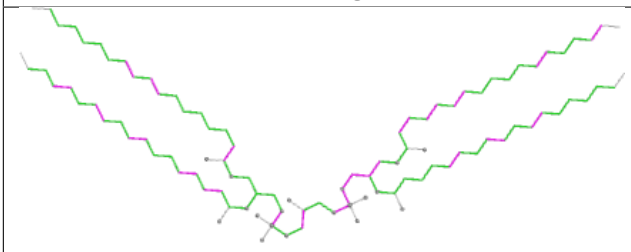
## Ligand CDL CB 203



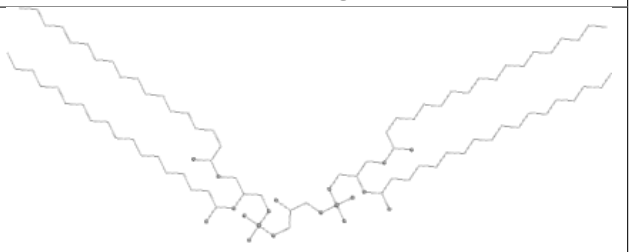
Bond lengths



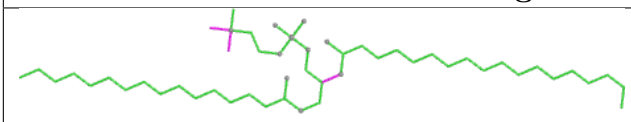
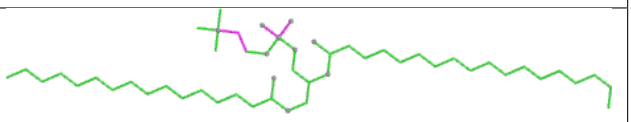
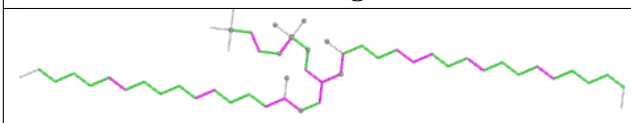
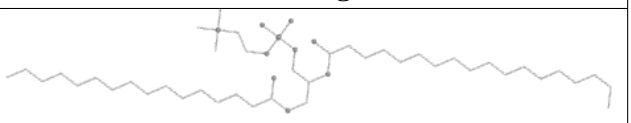
Bond angles

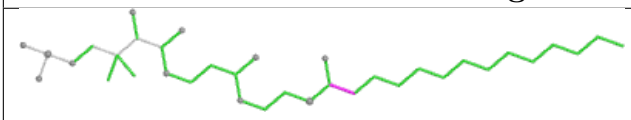
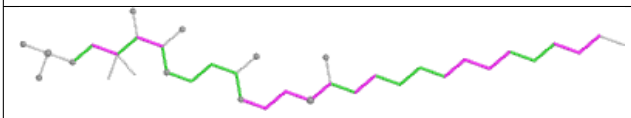
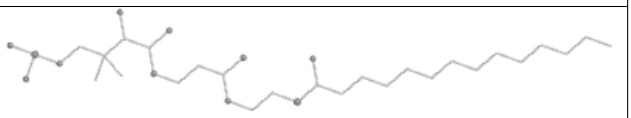


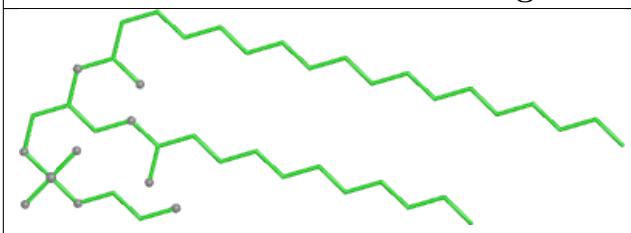
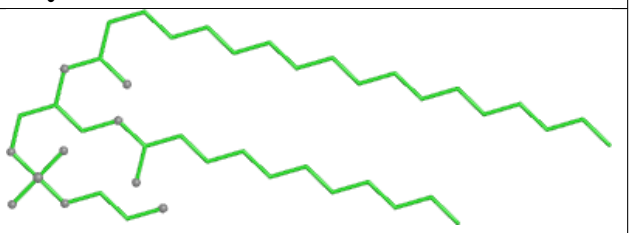
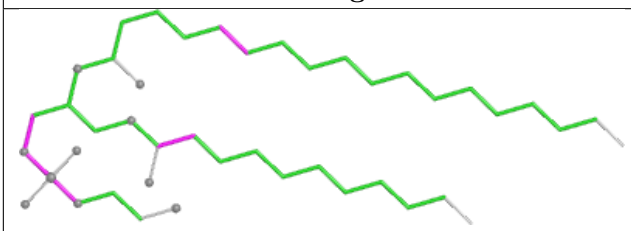
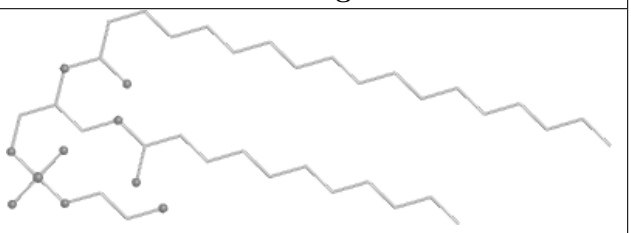
Torsions



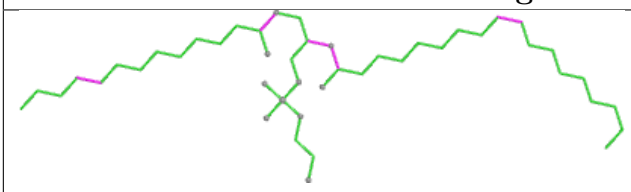
Rings

| Ligand PLX N4 501 | |
|---|---|
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

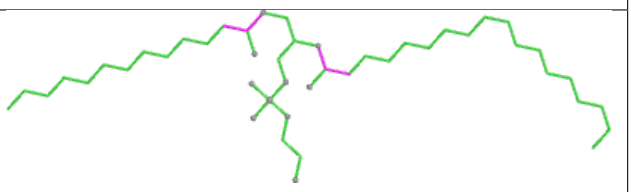
| Ligand ZMP AB 201 | |
|---|---|
|  Bond lengths | Bond angles |
|  Torsions |  Rings |

| Ligand 3PE QE 303 | |
|---|---|
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

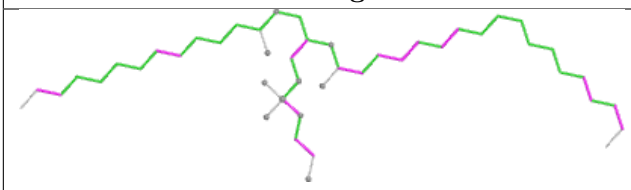
## Ligand PEE N5 701



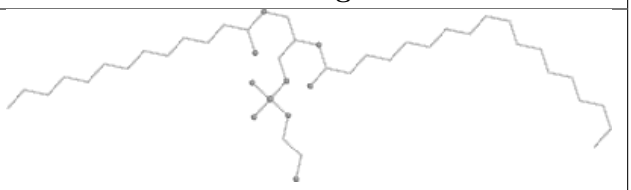
Bond lengths



Bond angles

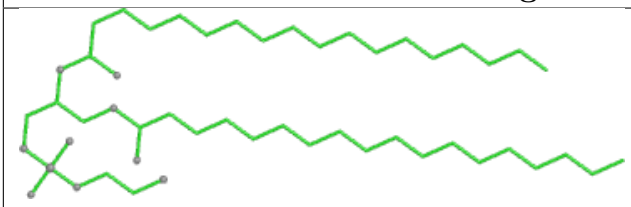


Torsions

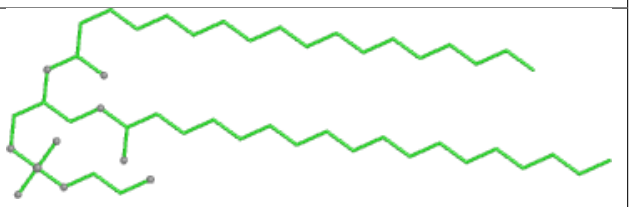


Rings

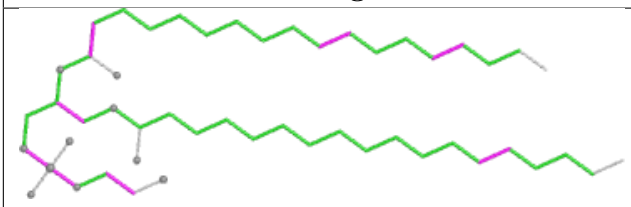
## Ligand 3PE C1 601



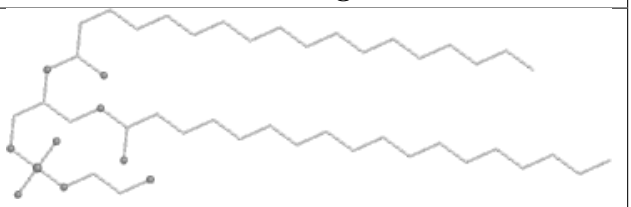
Bond lengths



Bond angles

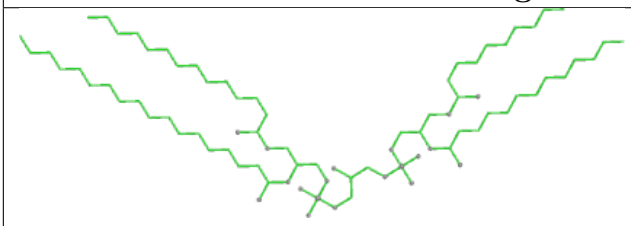


Torsions

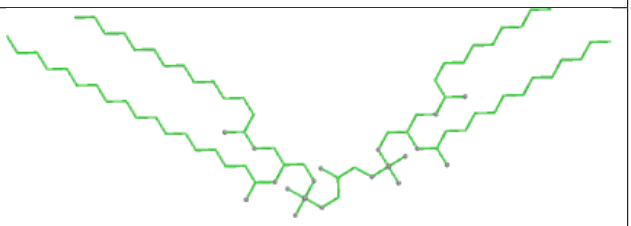


Rings

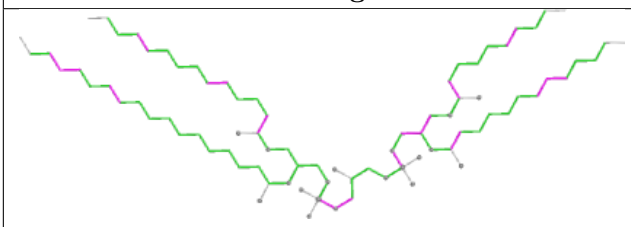
## Ligand CDL A8 301



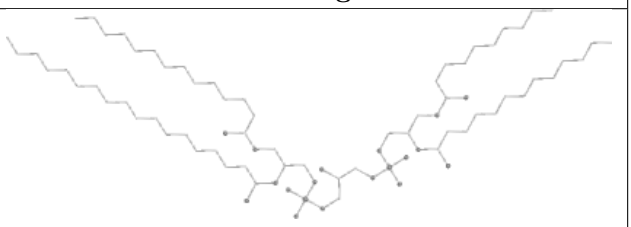
Bond lengths



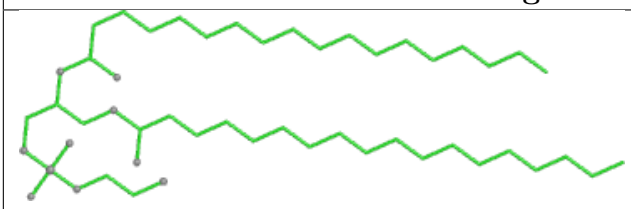
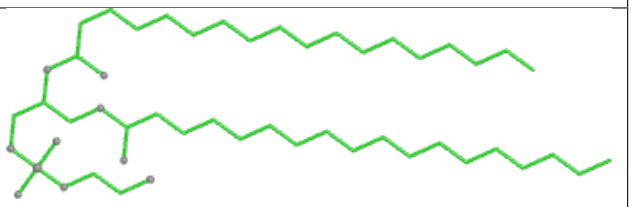
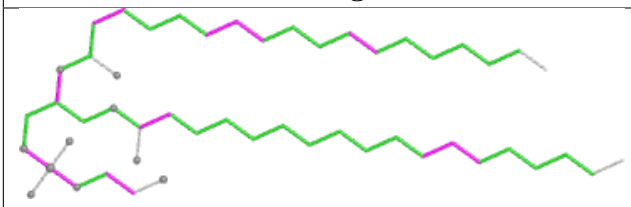
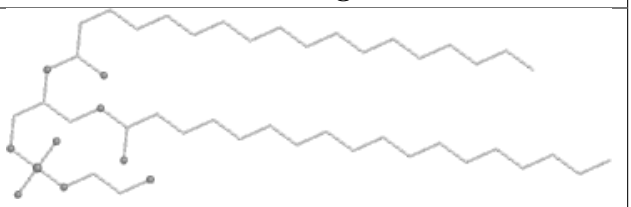
Bond angles

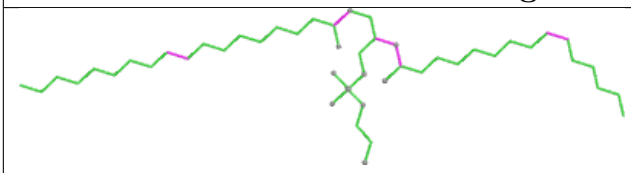
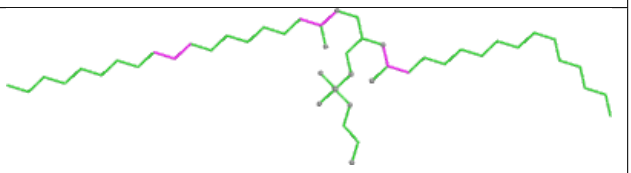
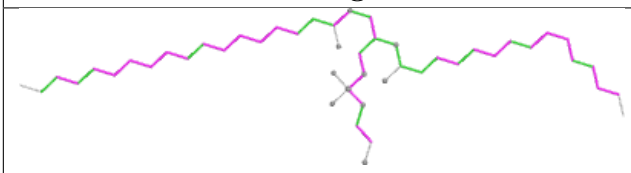
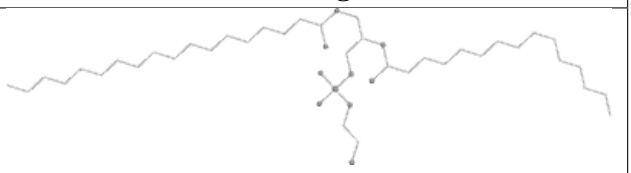


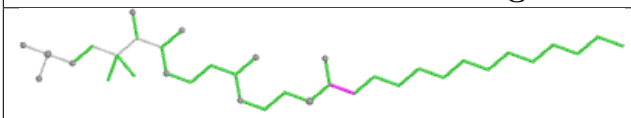
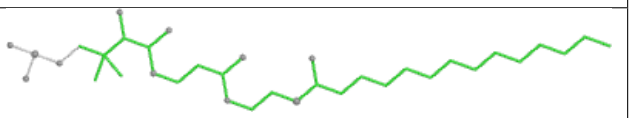
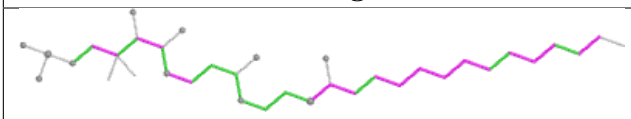
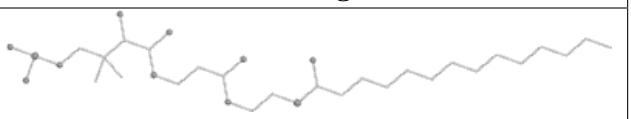
Torsions



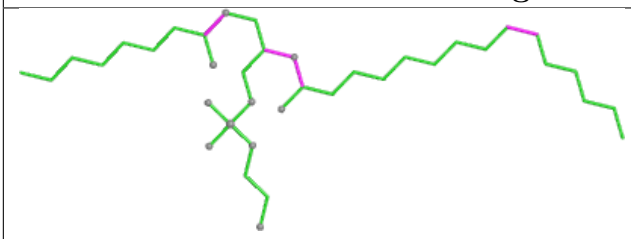
Rings

| Ligand 3PE S7 302 | |
|---|---|
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

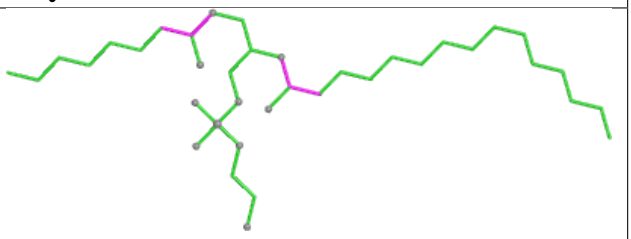
| Ligand PEE S2 501 | |
|---|---|
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

| Ligand ZMP AC 201 | |
|---|---|
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

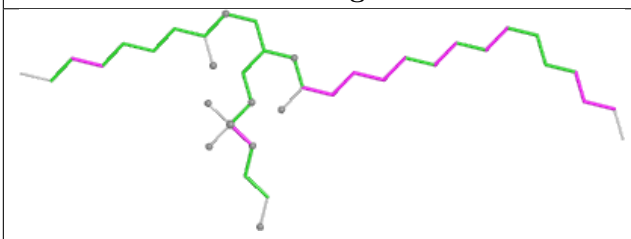
## Ligand PEE QC 404



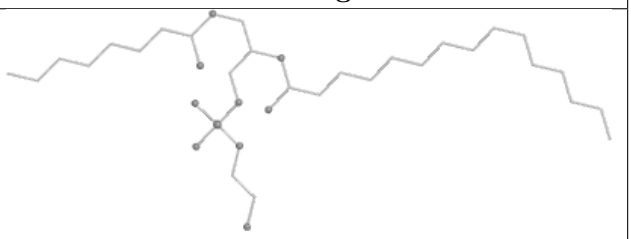
Bond lengths



Bond angles

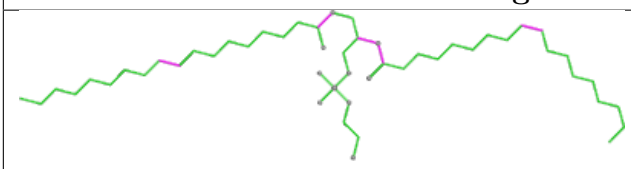


Torsions



Rings

## Ligand PEE QC 401



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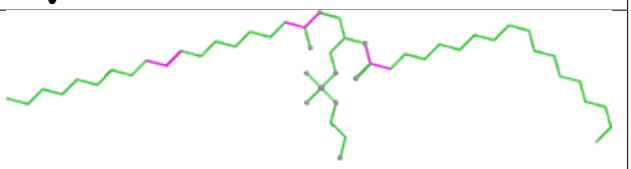
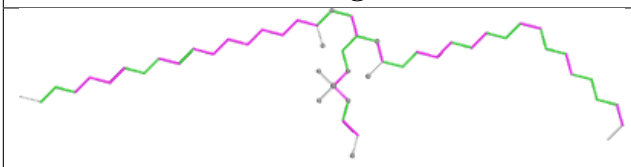


Bond angles



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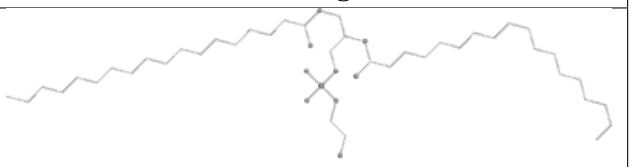
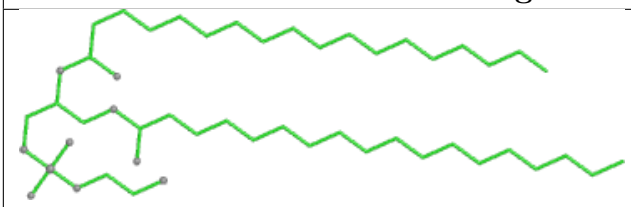
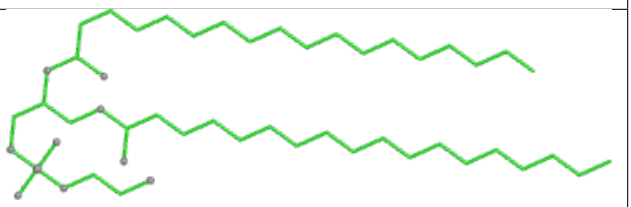


Rings

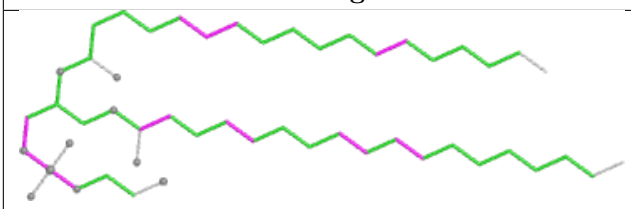
## Ligand 3PE CA 101



Bond lengths



Bond angles



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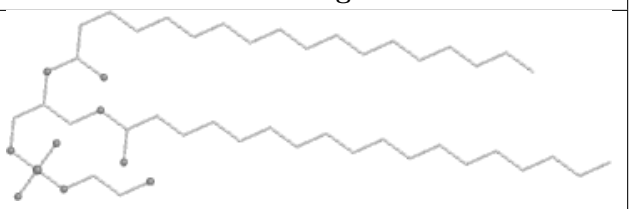
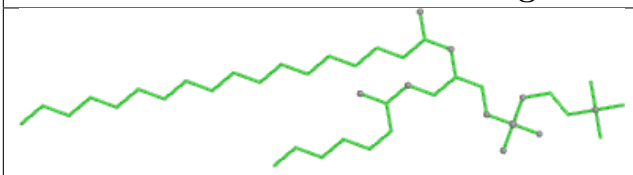
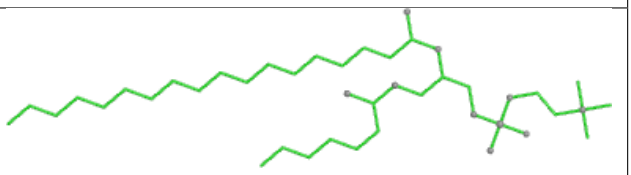


Rings

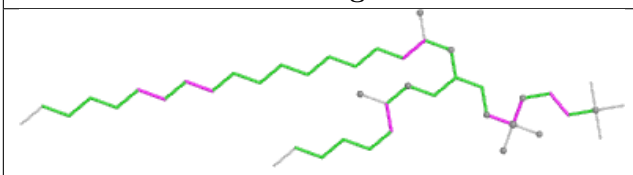
## Ligand PC1 C3 302



Bond lengths



Bond angles



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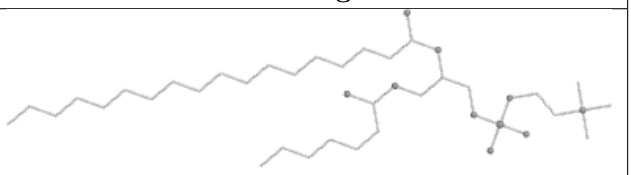
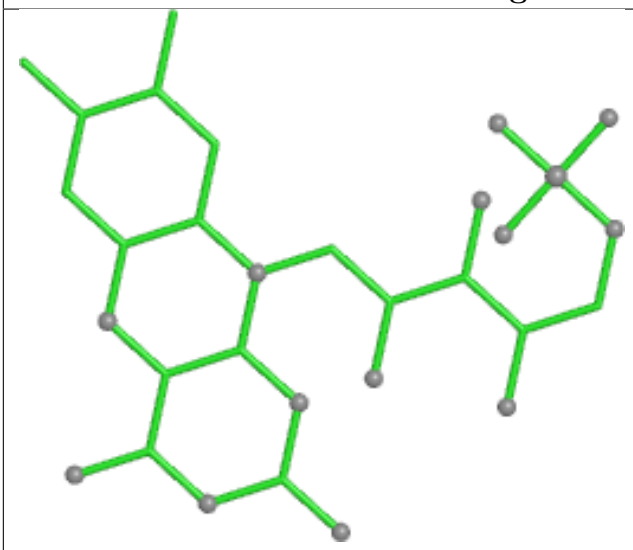


Rings

## Ligand FMN V1 502



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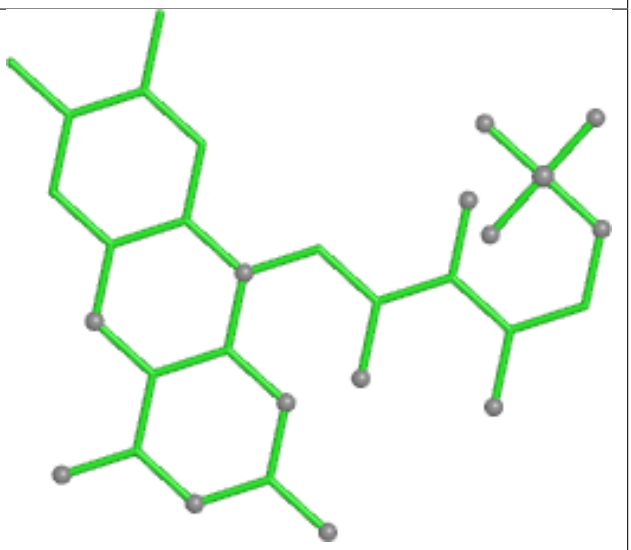
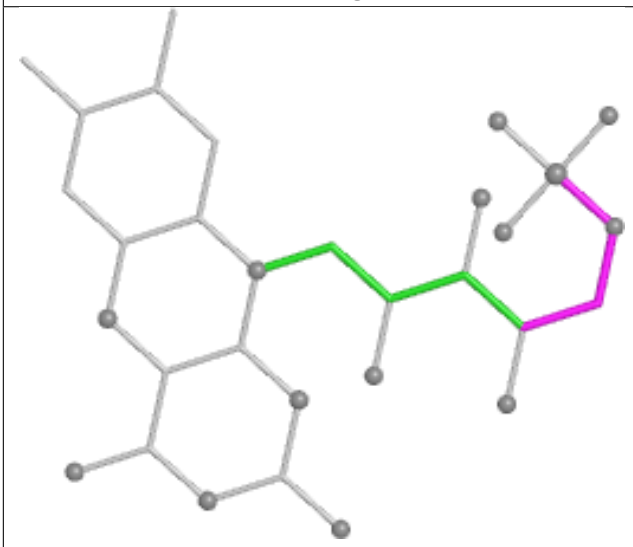


Bond angles



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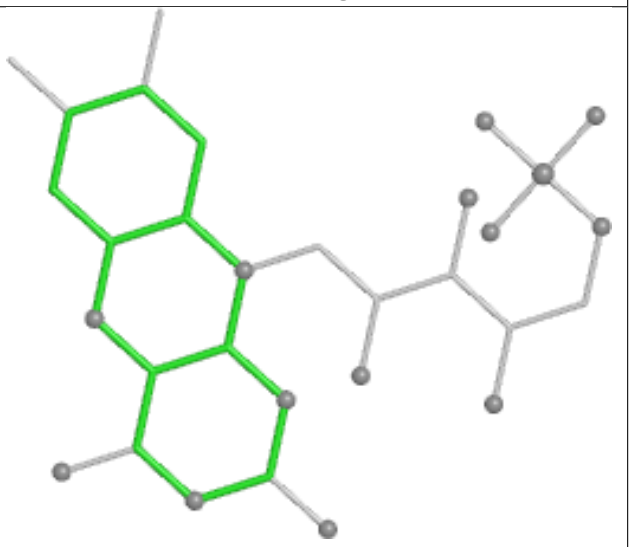
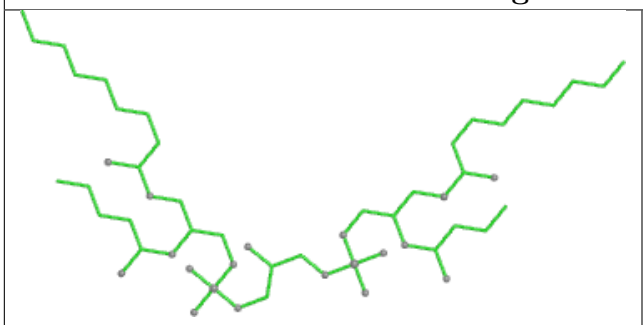
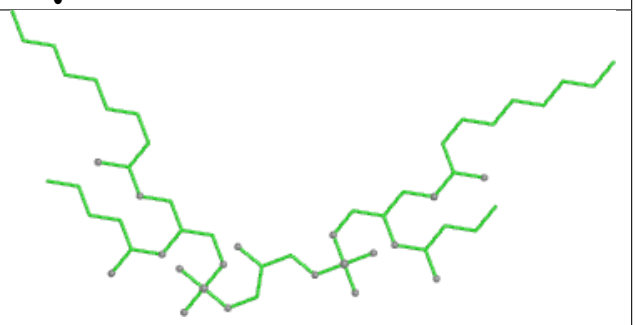
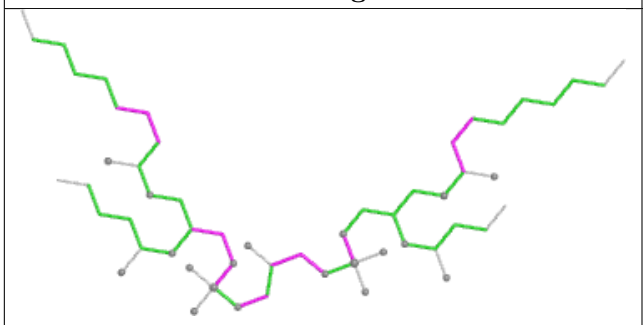
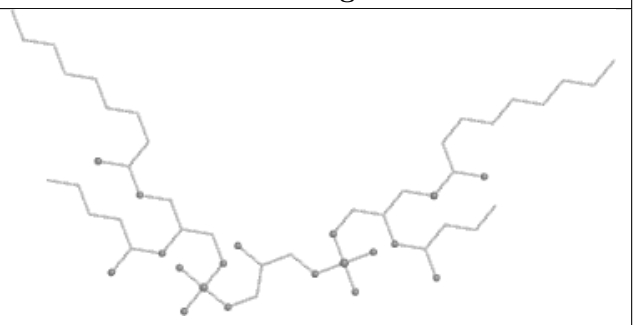
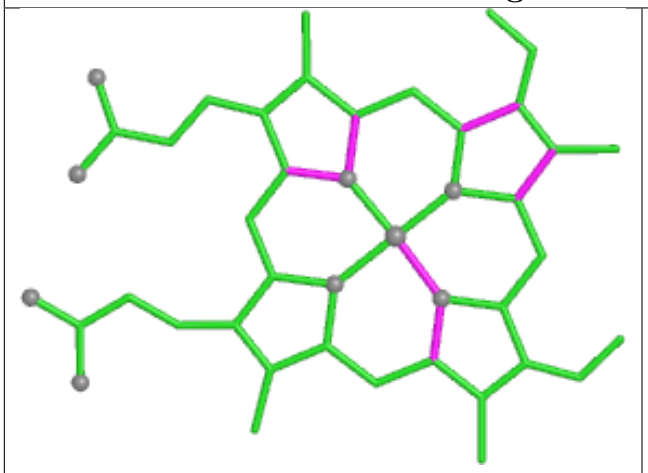


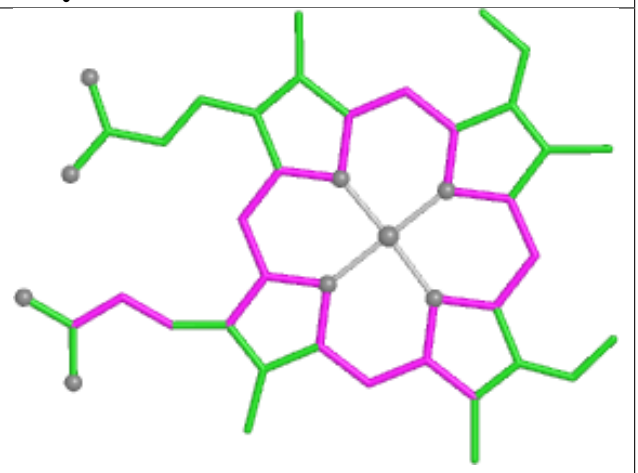
Rings

| Ligand CDL QC 408 | |
|---|---|
|  **Bond lengths** |  **Bond angles** |
|  **Torsions** |  **Rings** |

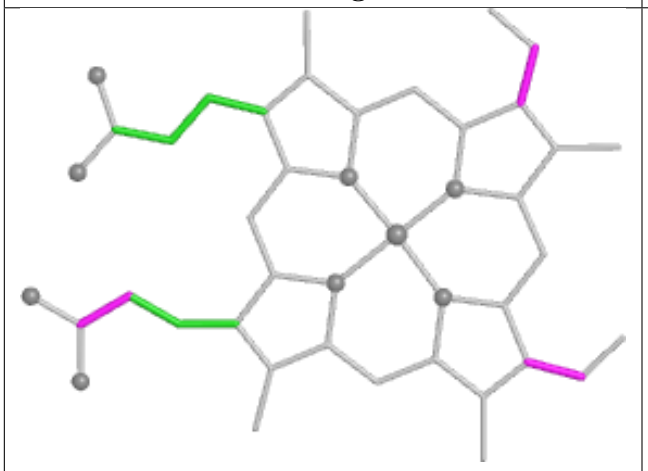
## Ligand HEM QC 403



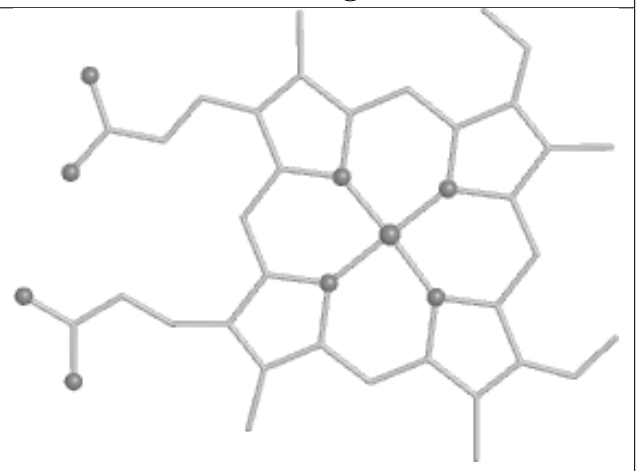
Bond lengths



Bond angles

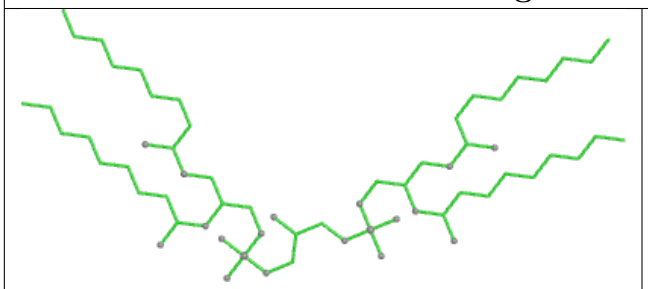


Torsions

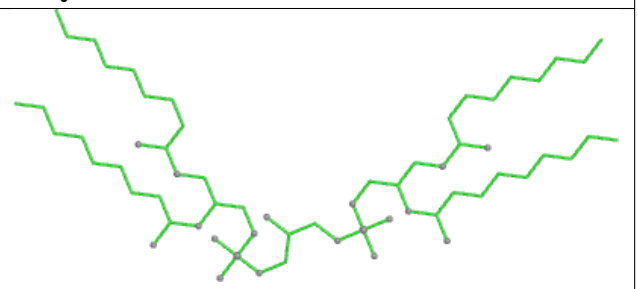


Rings

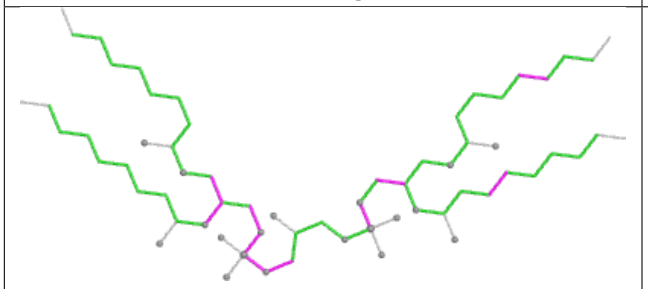
## Ligand CDL Qd 401



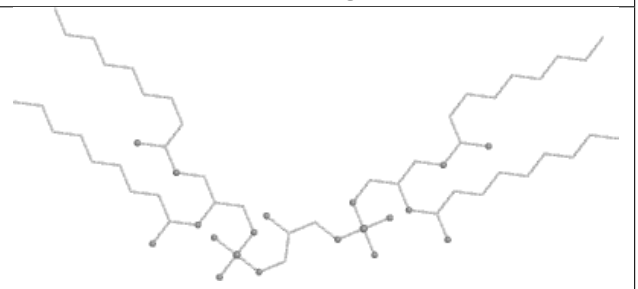
Bond lengths



Bond angles

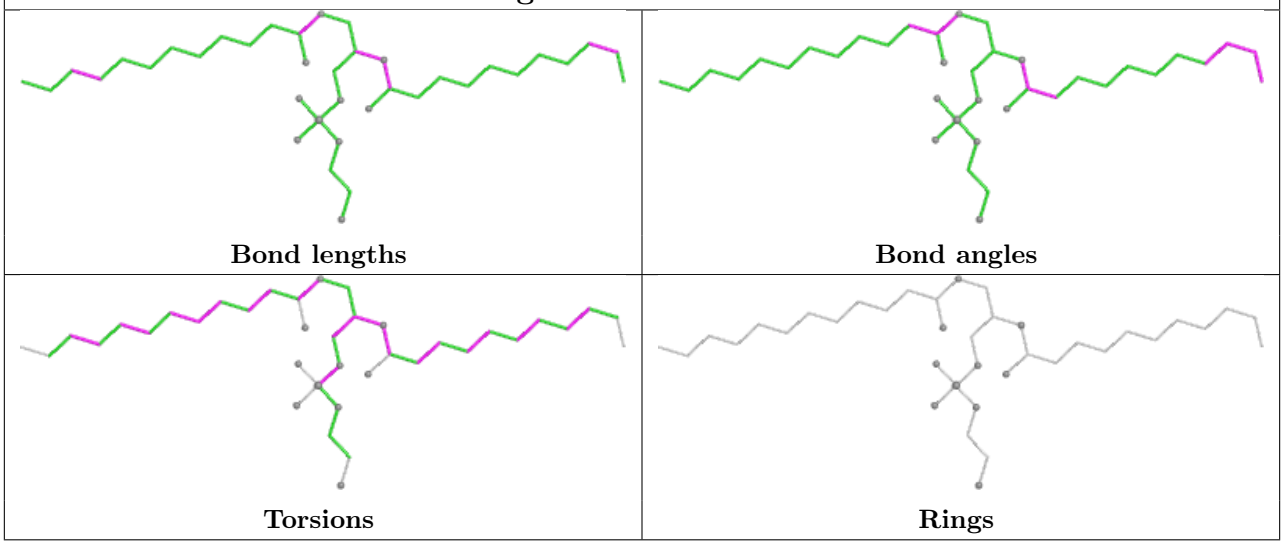


Torsions

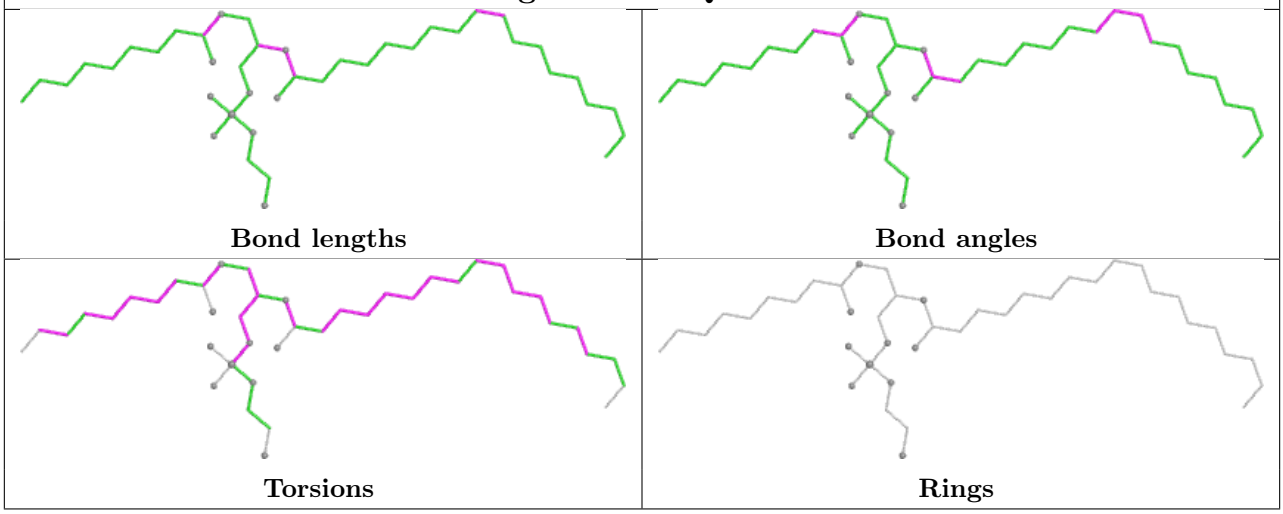


Rings

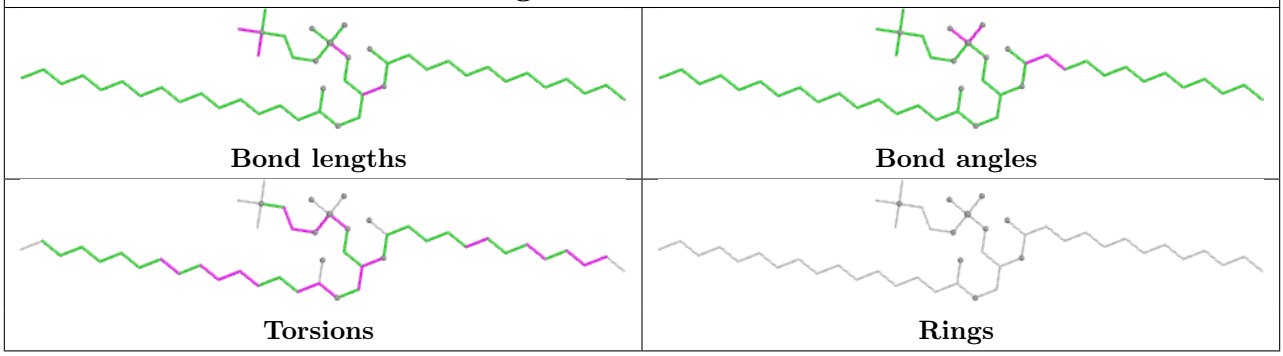
## Ligand PEE N1 401



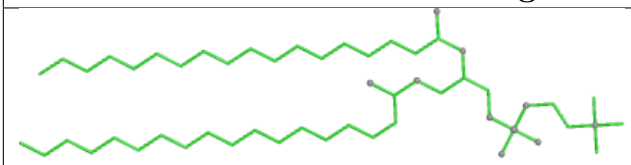

## Ligand PEE Qc 401



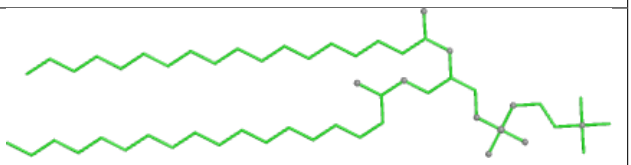

## Ligand PLX AL 205



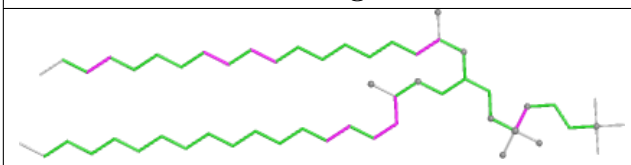
## Ligand PC1 C1 606



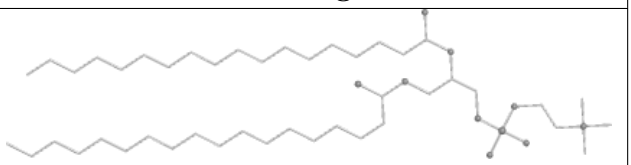
Bond lengths



Bond angles

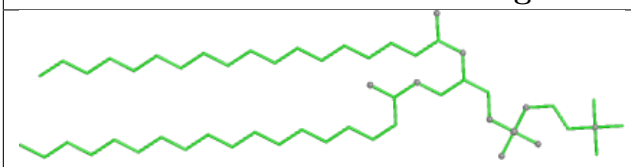


Torsions

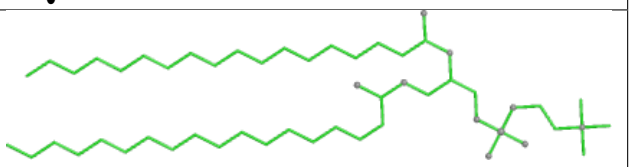


Rings

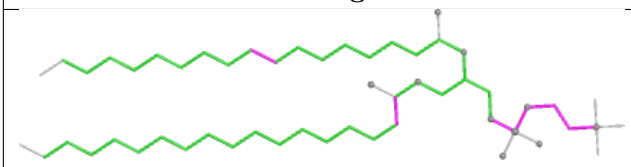
## Ligand PC1 QC 407



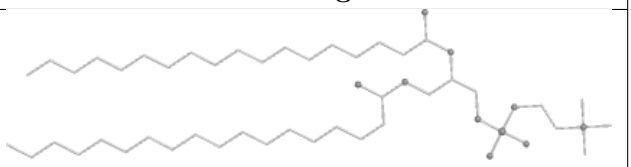
Bond lengths



Bond angles

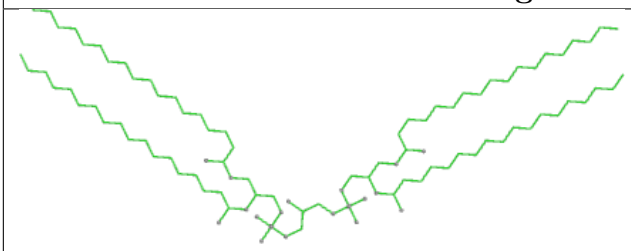


Torsions

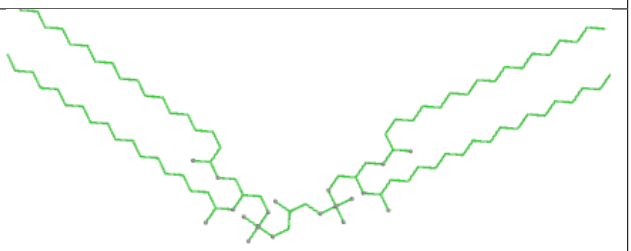


Rings

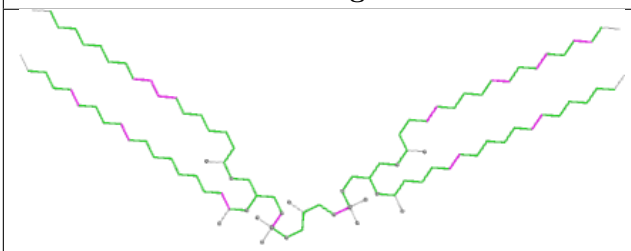
## Ligand CDL B5 202



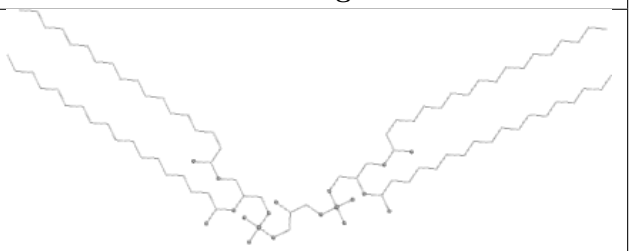
Bond lengths



Bond angles

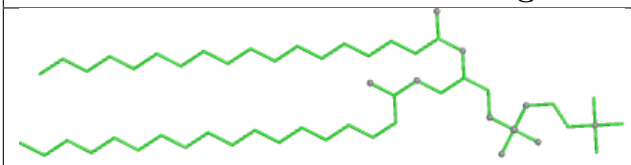


Torsions

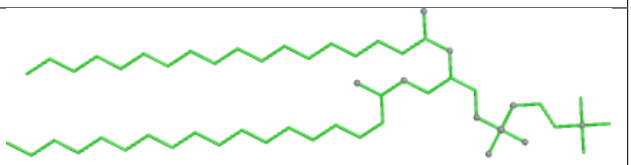


Rings

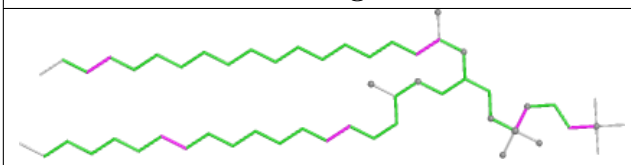
## Ligand PC1 N5 704



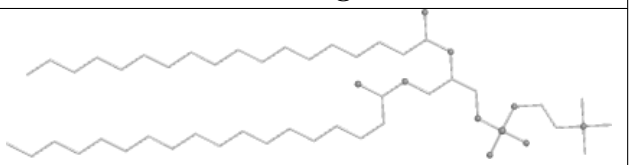
Bond lengths



Bond angles

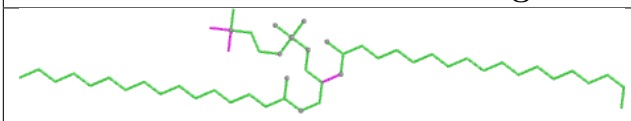


Torsions

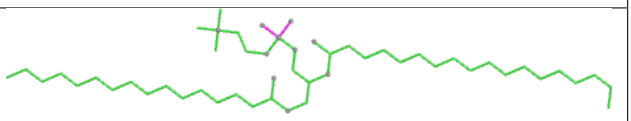


Rings

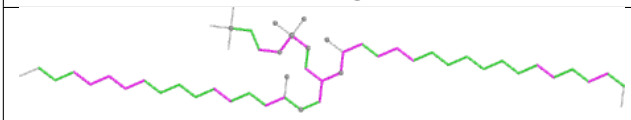
## Ligand PLX CB 201



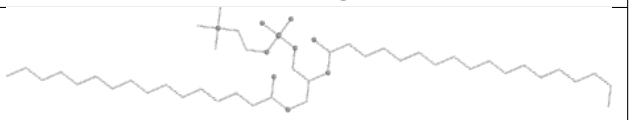
Bond lengths



Bond angles

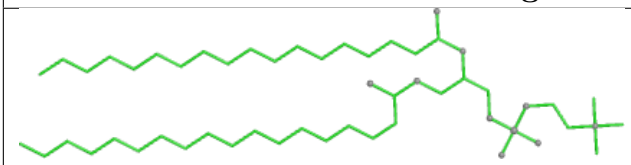


Torsions

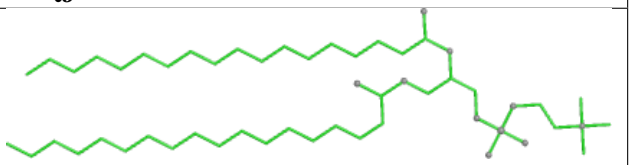


Rings

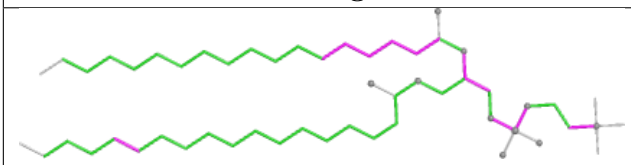
## Ligand PC1 Qj 101



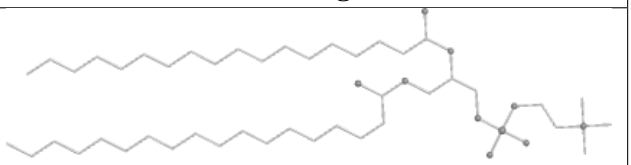
Bond lengths



Bond angles

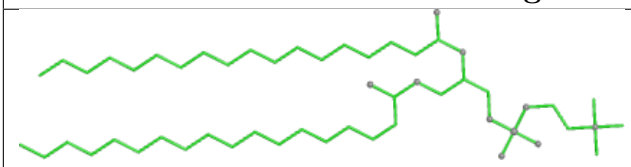


Torsions

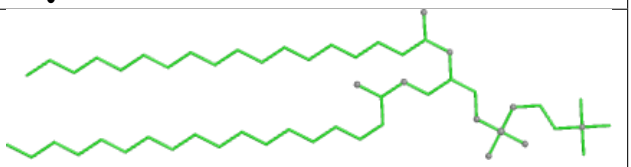


Rings

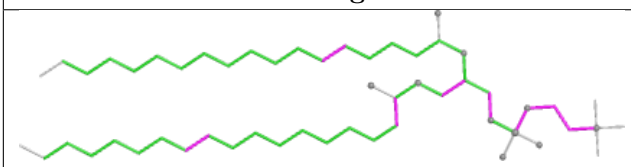
## Ligand 6F6 Qc 404



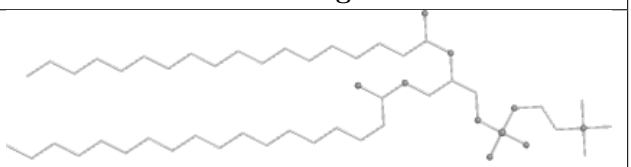
Bond lengths



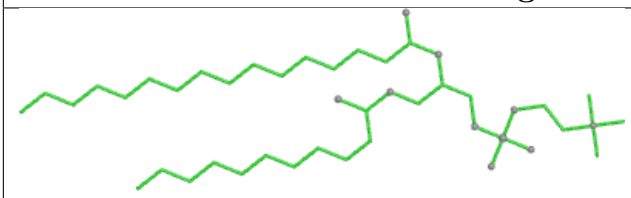
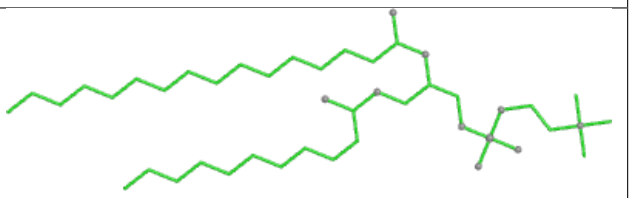
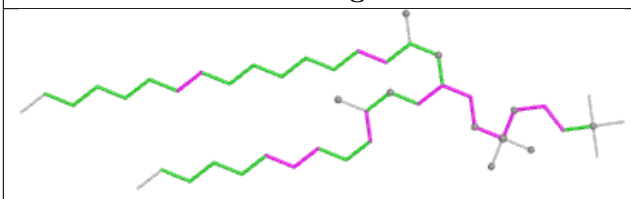
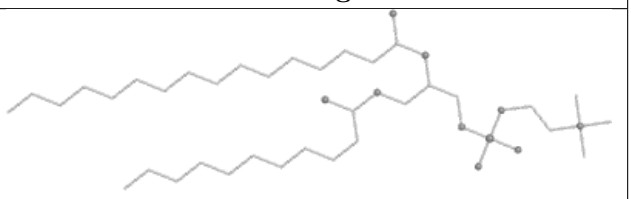
Bond angles

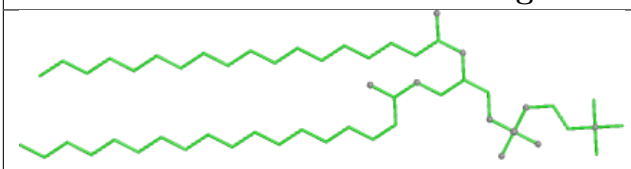
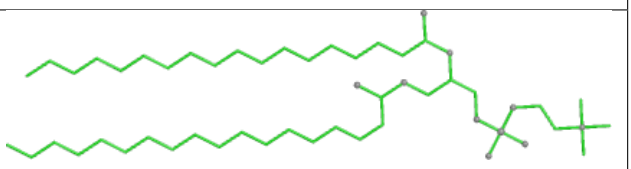
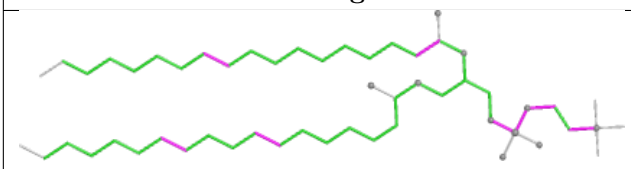
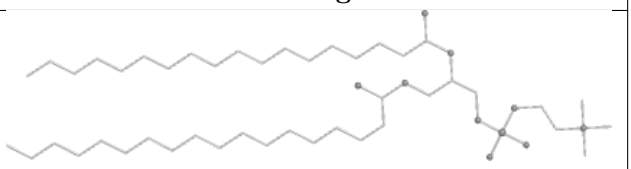


Torsions

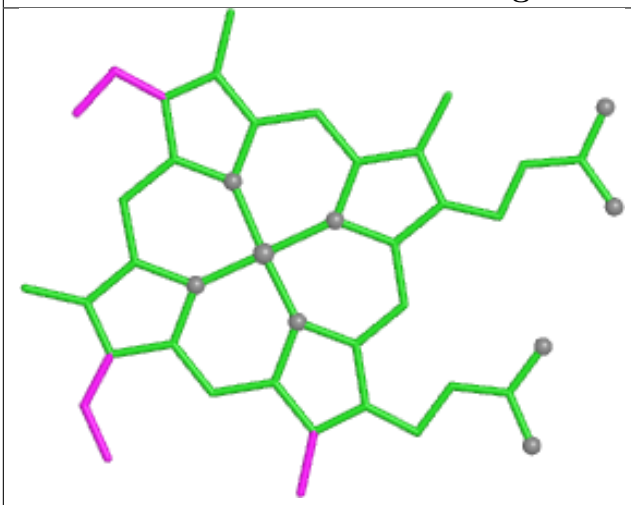


Rings

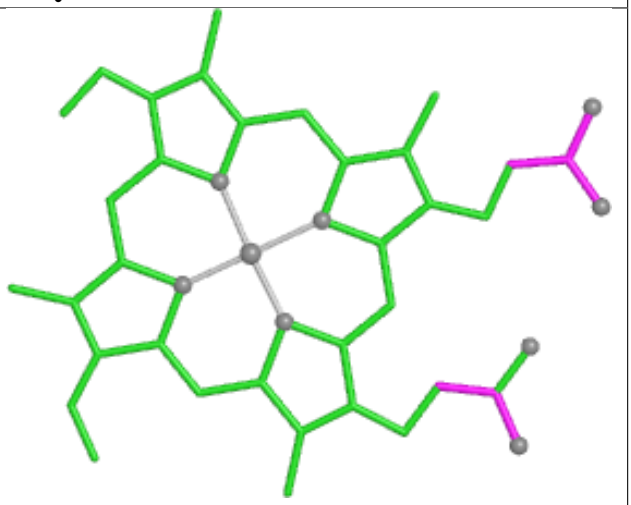
| Ligand PC1 6A 101 | |
|---|---|
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

| Ligand PC1 AL 206 | |
|---|---|
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

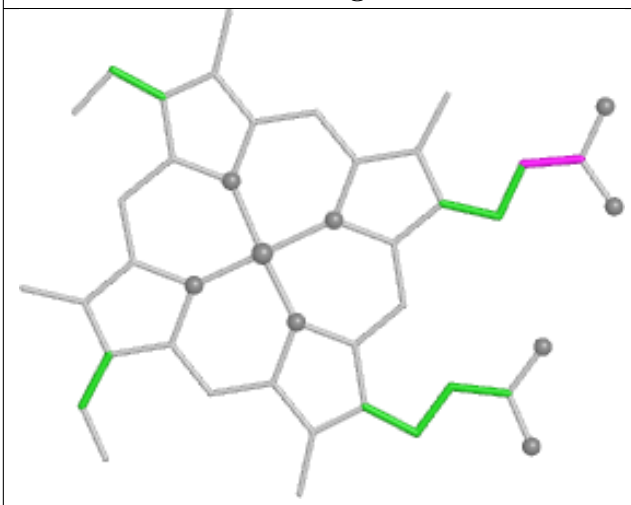
## Ligand HEC Qd 402



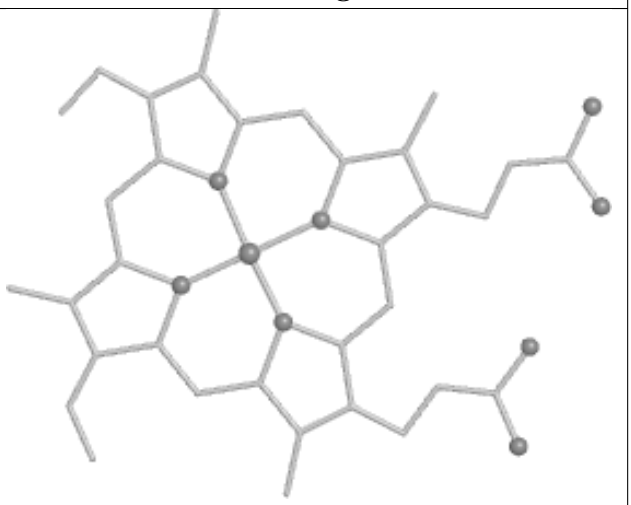
Bond lengths



Bond angles

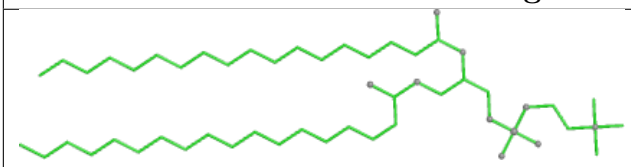


Torsions

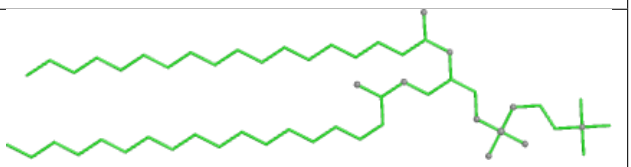


Rings

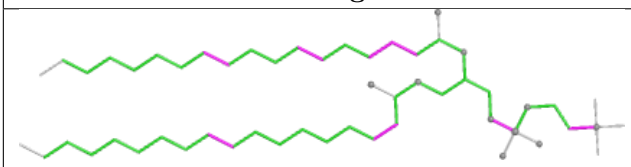
## Ligand 6F6 B5 203



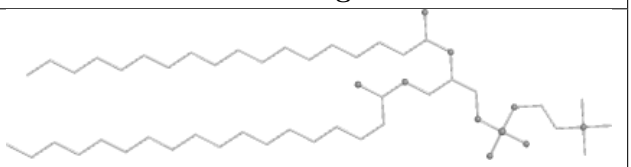
Bond lengths



Bond angles

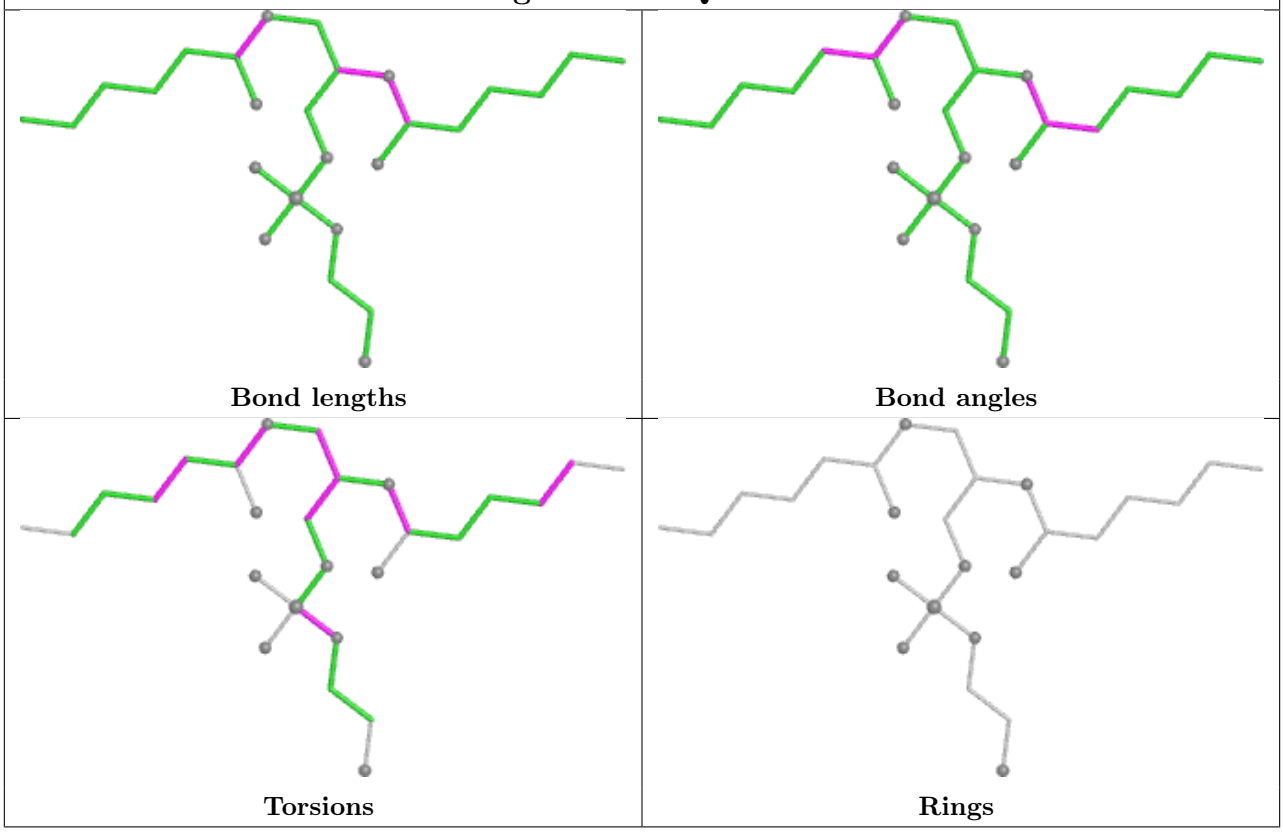


Torsions

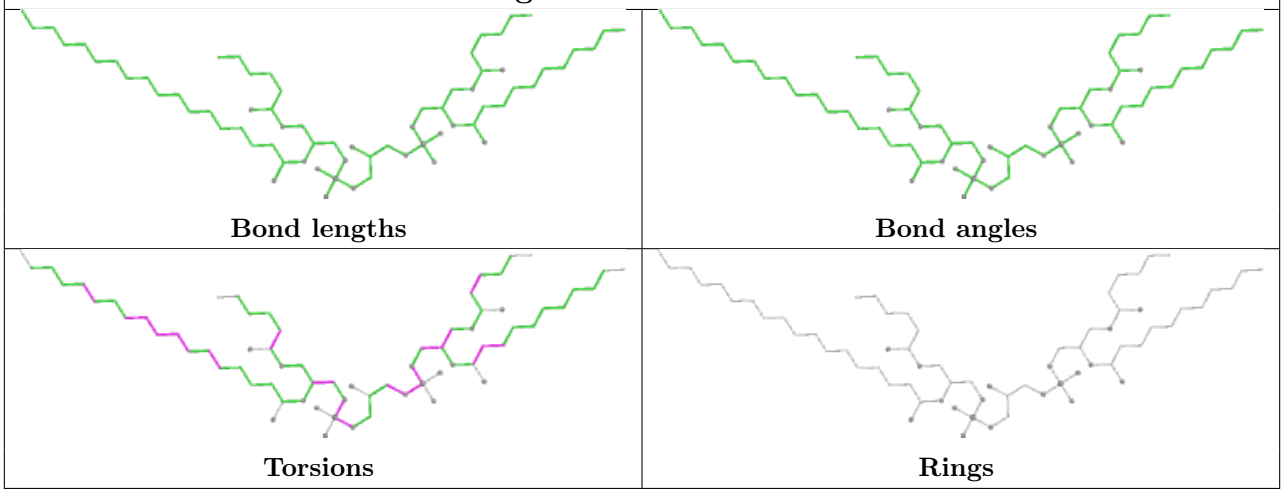


Rings

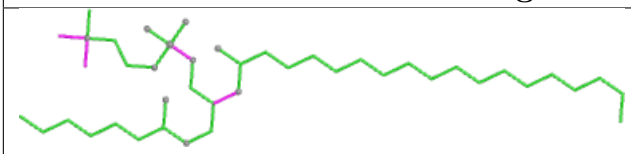
## Ligand PEE QB 502



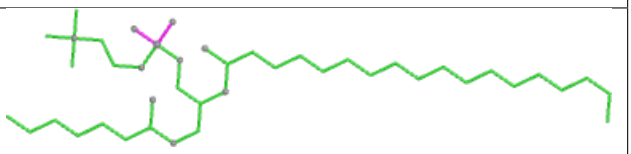

## Ligand CDL 6A 102



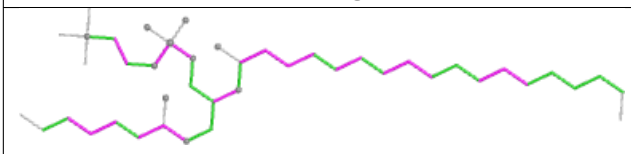
## Ligand PLX C2 301



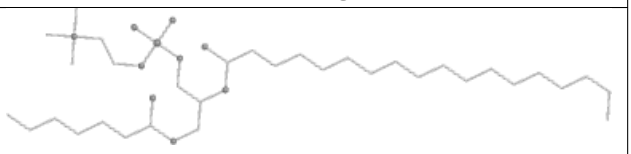
Bond lengths



Bond angles

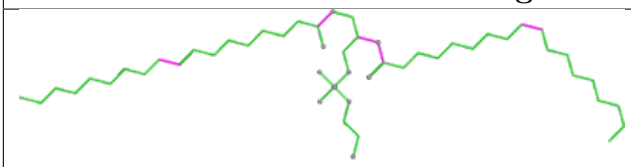


Torsions

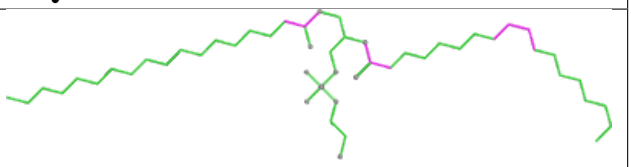


Rings

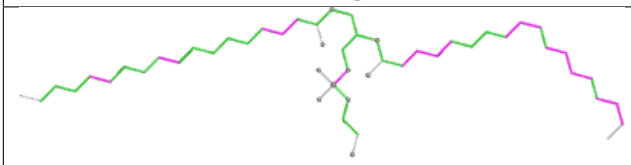
## Ligand PEE Qh 103



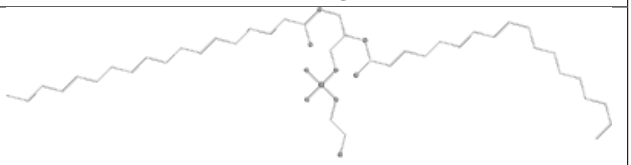
Bond lengths



Bond angles

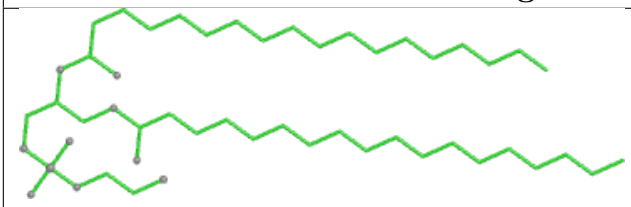


Torsions

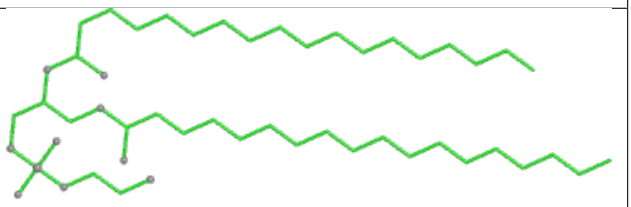


Rings

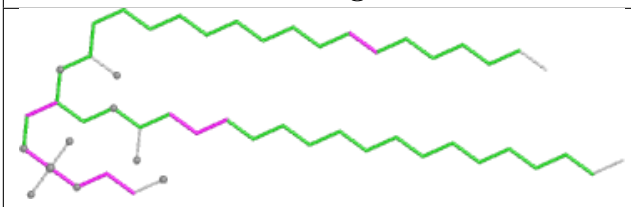
## Ligand 3PE AL 202



Bond lengths



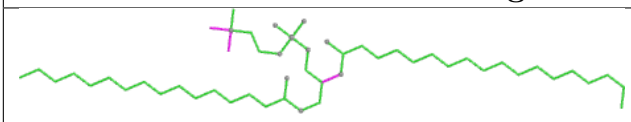
Bond angles



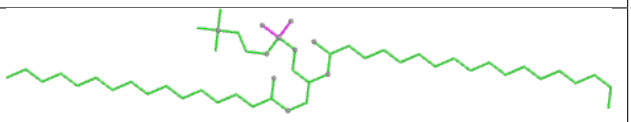
Torsions

Rings

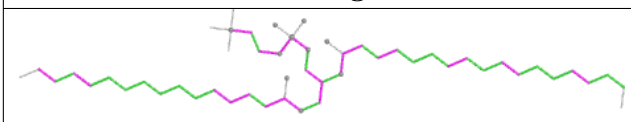
## Ligand PLX AM 203



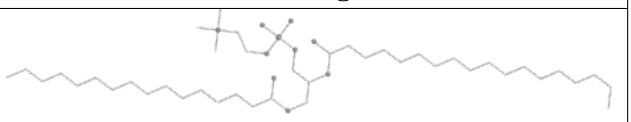
Bond lengths



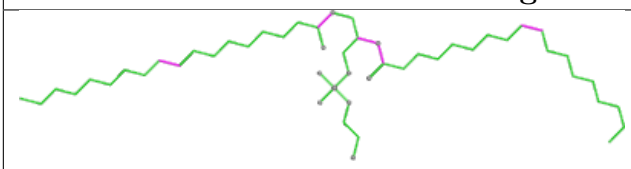
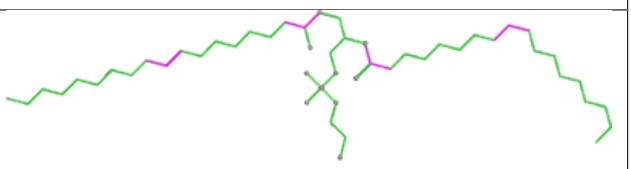
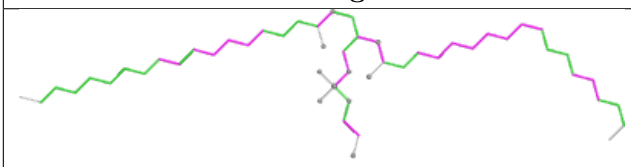
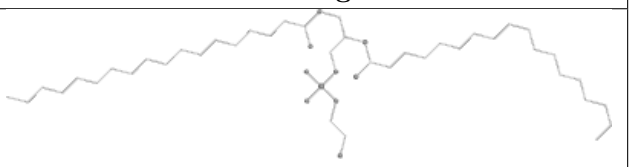
Bond angles

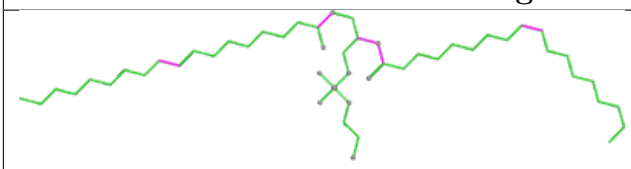
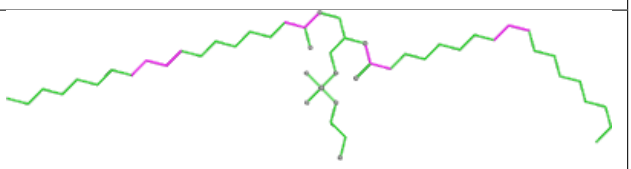
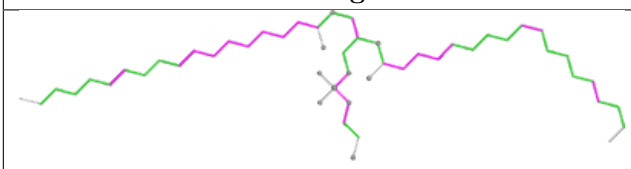
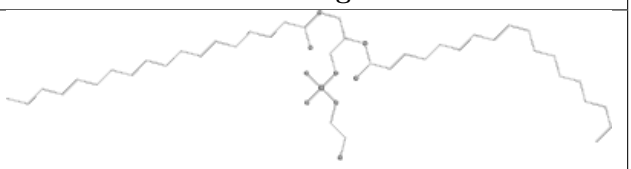


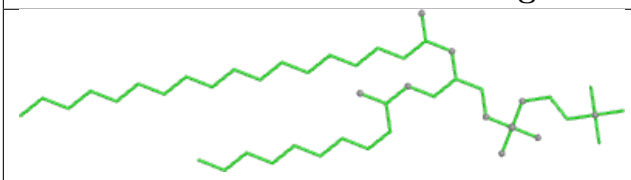
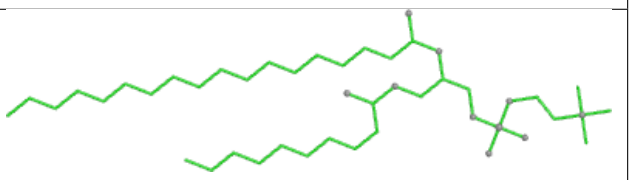
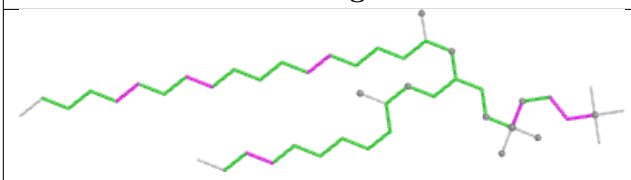
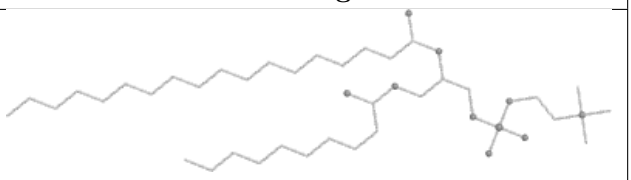
Torsions



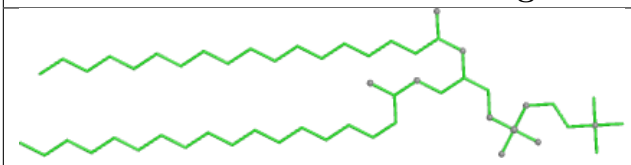
Rings

| Ligand PEE S8 303 | |
|---|---|
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

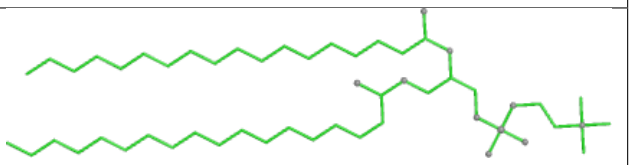
| Ligand PEE N3 201 | |
|---|---|
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

| Ligand PC1 C1 607 | |
|---|---|
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

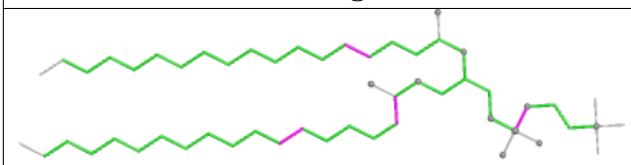
## Ligand PC1 N6 201



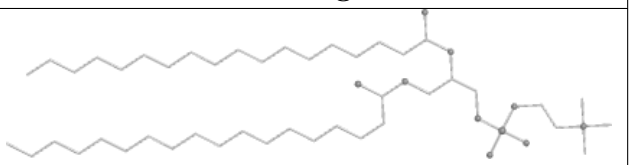
Bond lengths



Bond angles

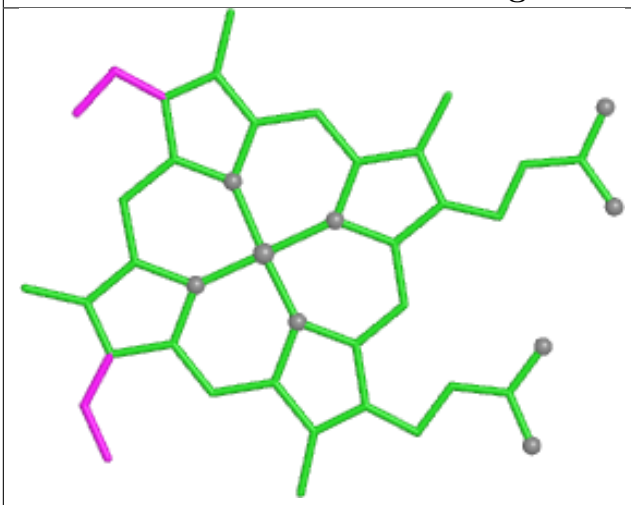


Torsions

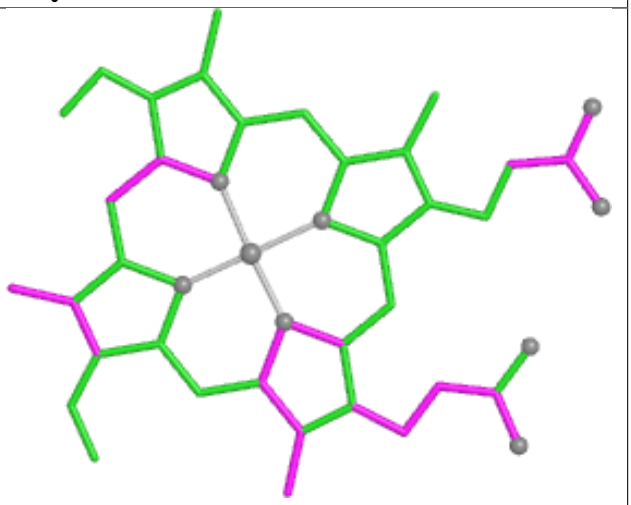


Rings

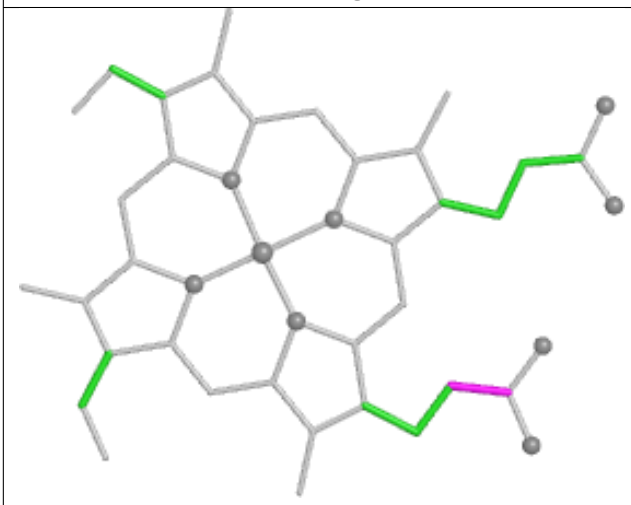
## Ligand HEC QD 401



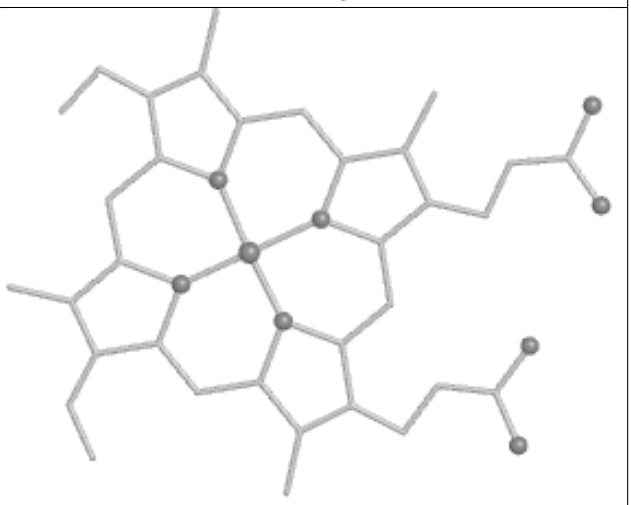
Bond lengths



Bond angles

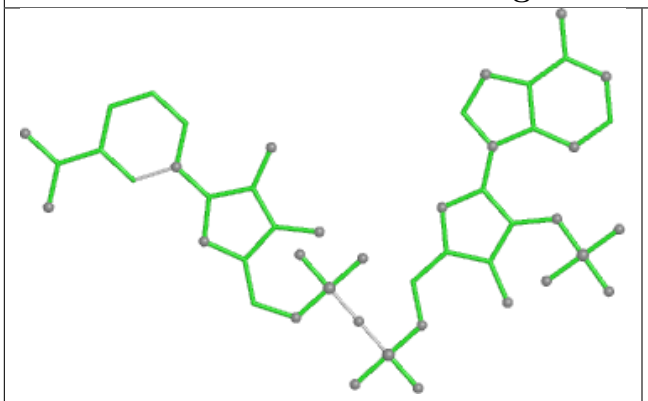


Torsions

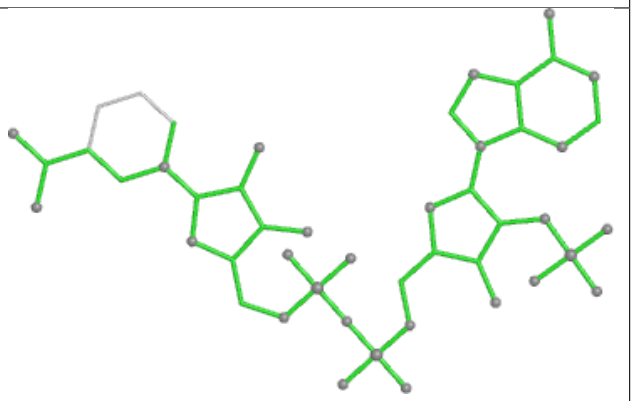


Rings

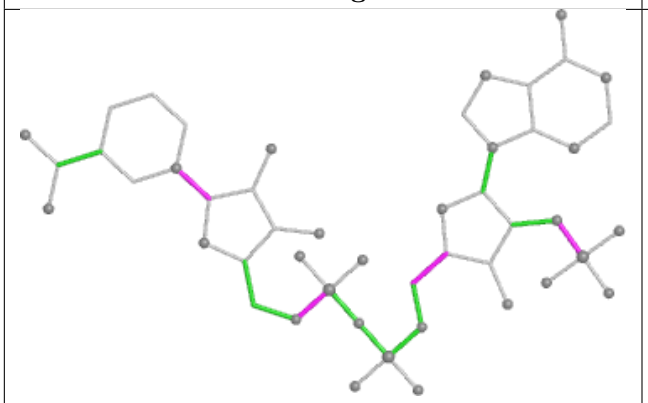
## Ligand NDP A9 401



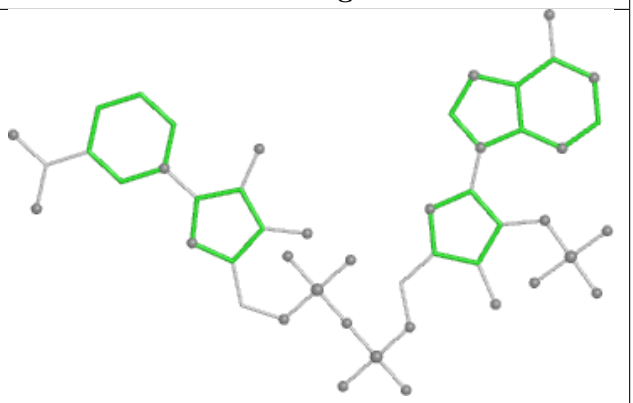
Bond lengths



Bond angles

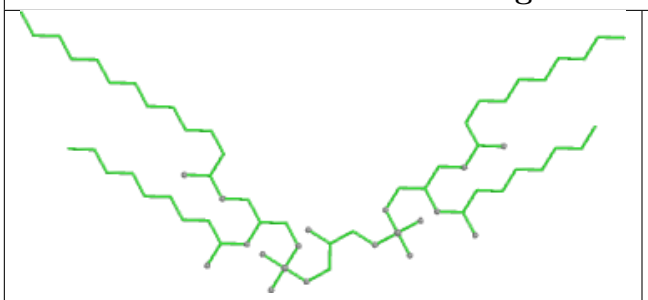


Torsions

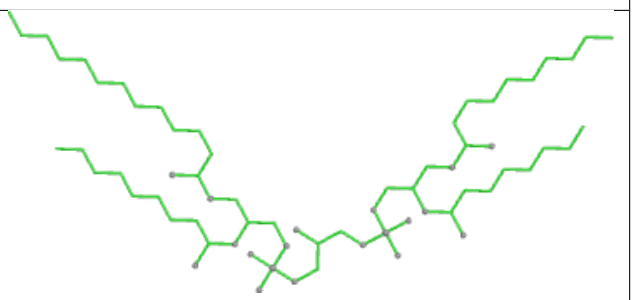


Rings

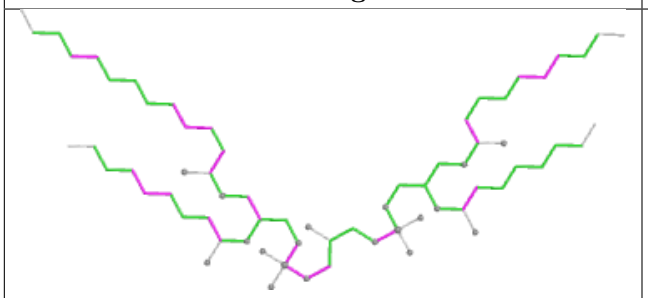
## Ligand CDL N2 401



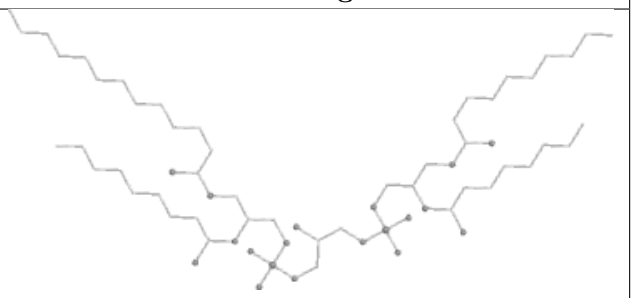
Bond lengths



Bond angles



Torsions



Rings

## 5.7 Other polymers (i)

There are no such residues in this entry.

## 5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

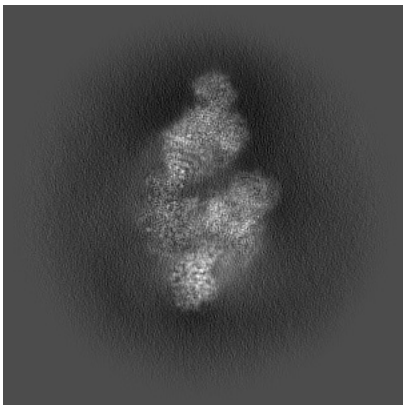
# 6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-60284. These allow visual inspection of the internal detail of the map and identification of artifacts.

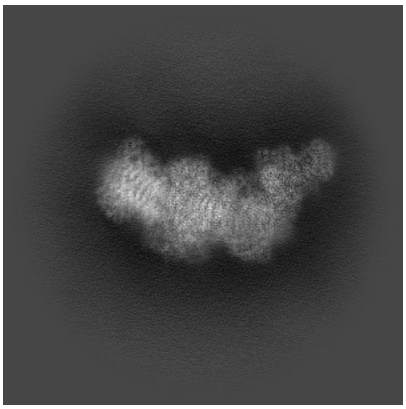
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

## 6.1 Orthogonal projections (i)

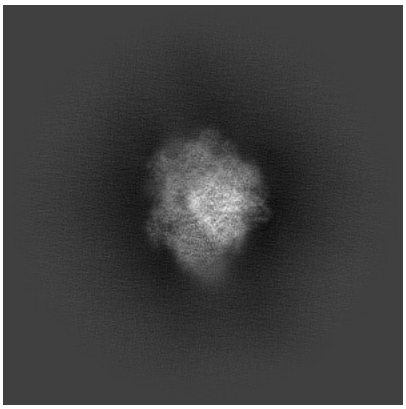
### 6.1.1 Primary map



X

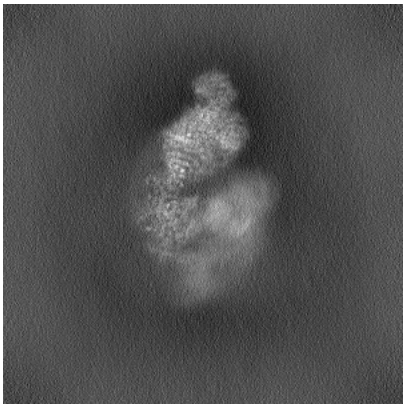


Y

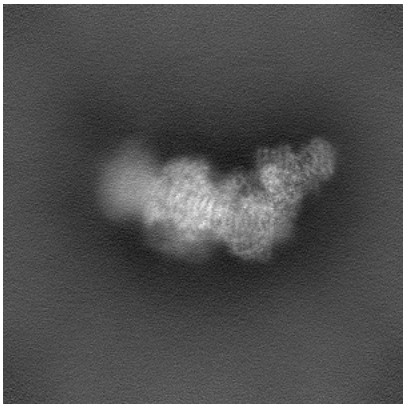


Z

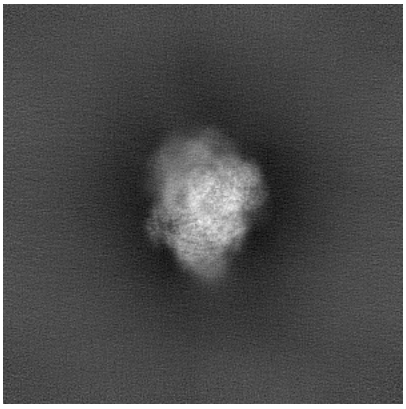
### 6.1.2 Raw map



X



Y

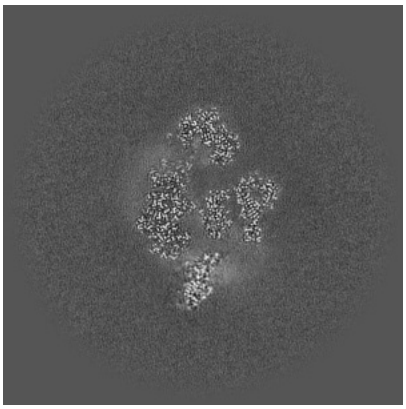


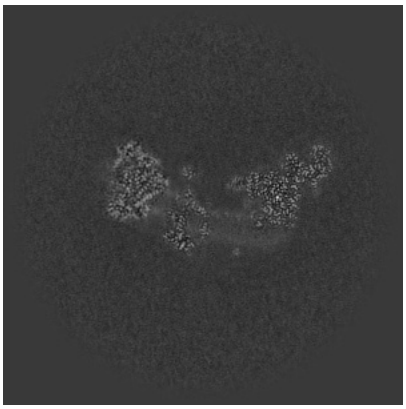
Z

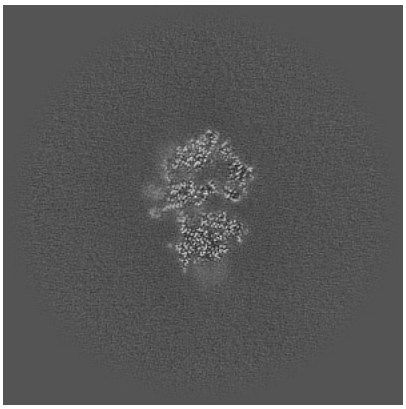
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices (i)

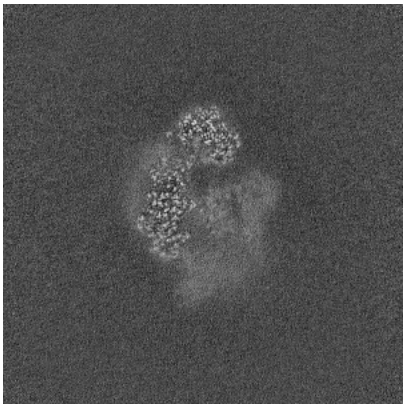
### 6.2.1 Primary map

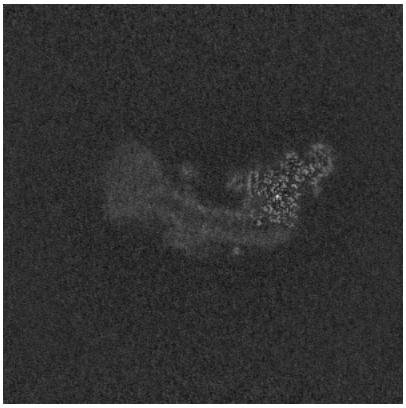

X Index: 240

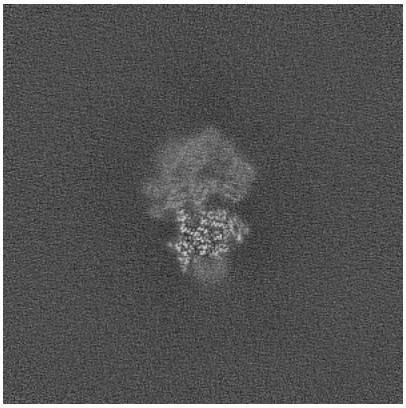

Y Index: 240


Z Index: 240

### 6.2.2 Raw map


X Index: 240

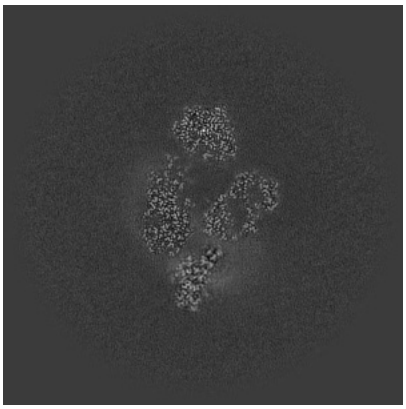

Y Index: 240

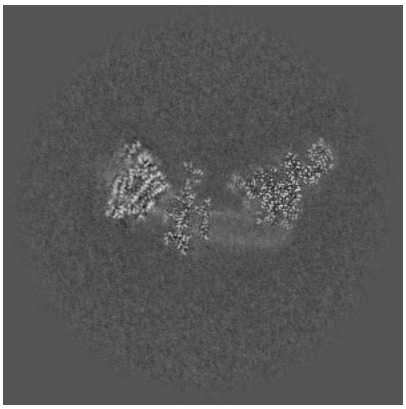

Z Index: 240

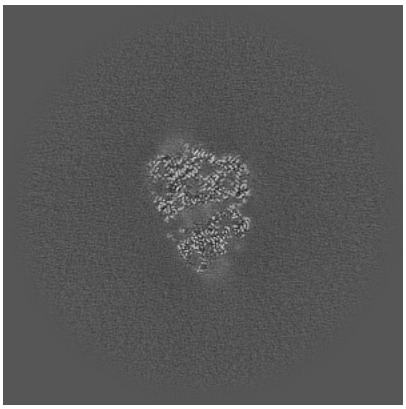
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices (i)

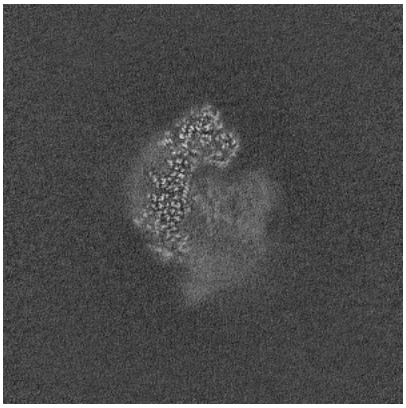
### 6.3.1 Primary map

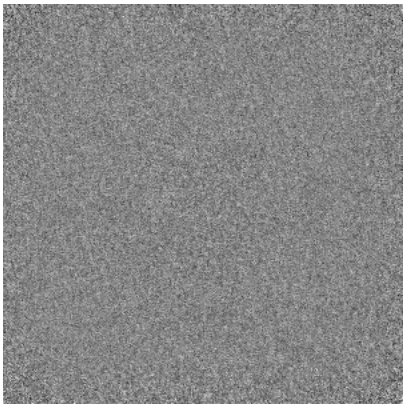

X Index: 248

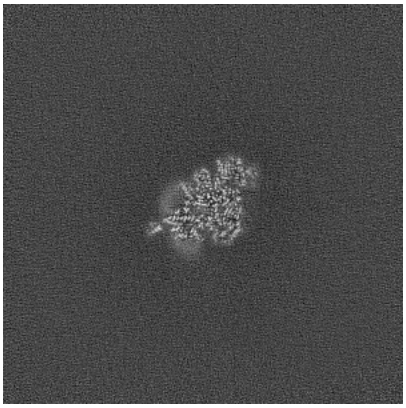

Y Index: 243


Z Index: 217

### 6.3.2 Raw map


X Index: 235

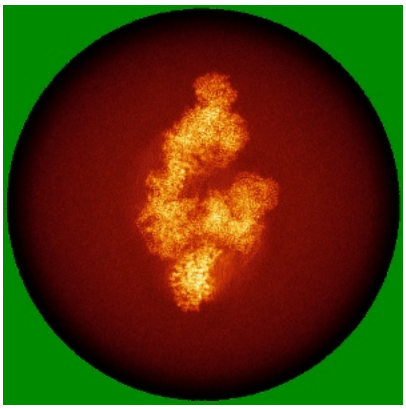

Y Index: 0

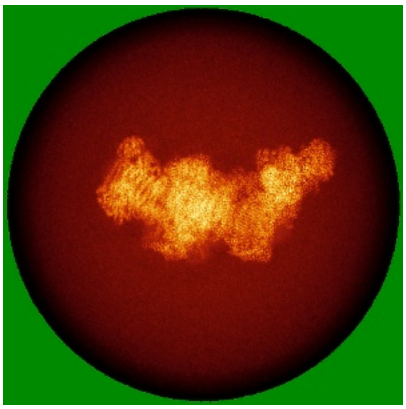

Z Index: 321

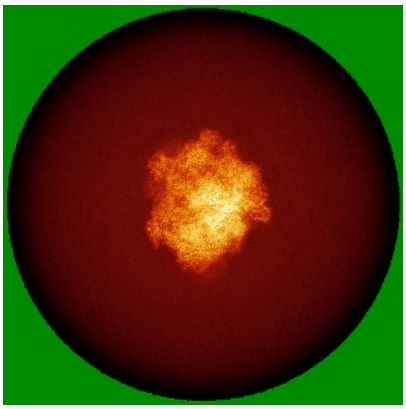
The images above show the largest variance slices of the map in three orthogonal directions.

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

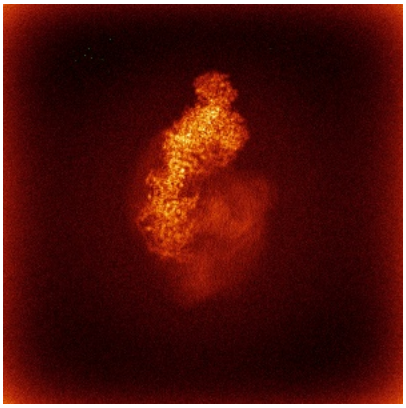
### 6.4.1 Primary map

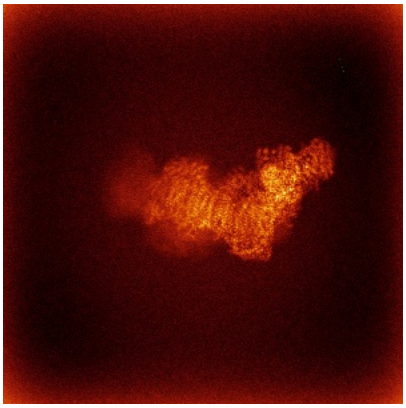

X

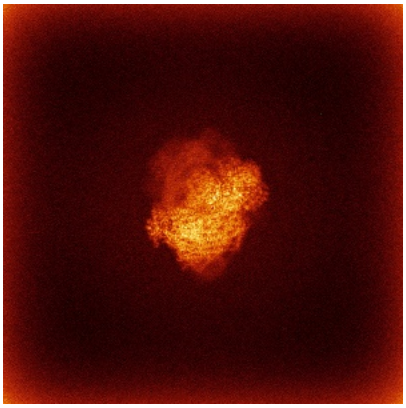

Y


Z

### 6.4.2 Raw map


X

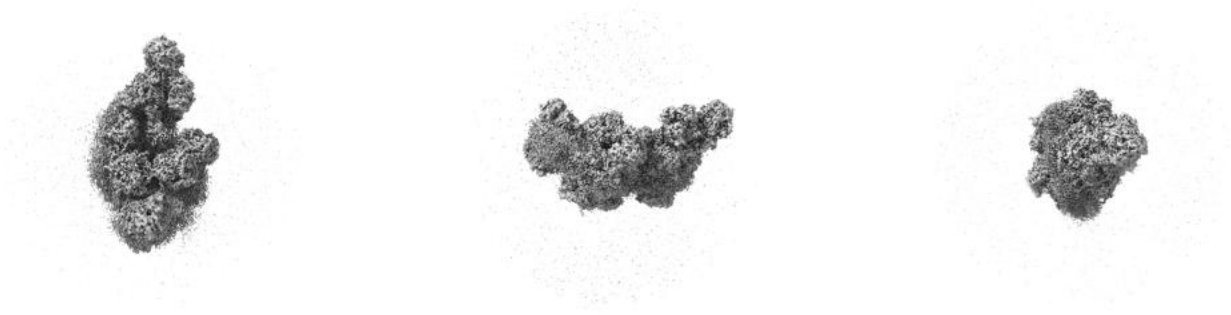

Y


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)

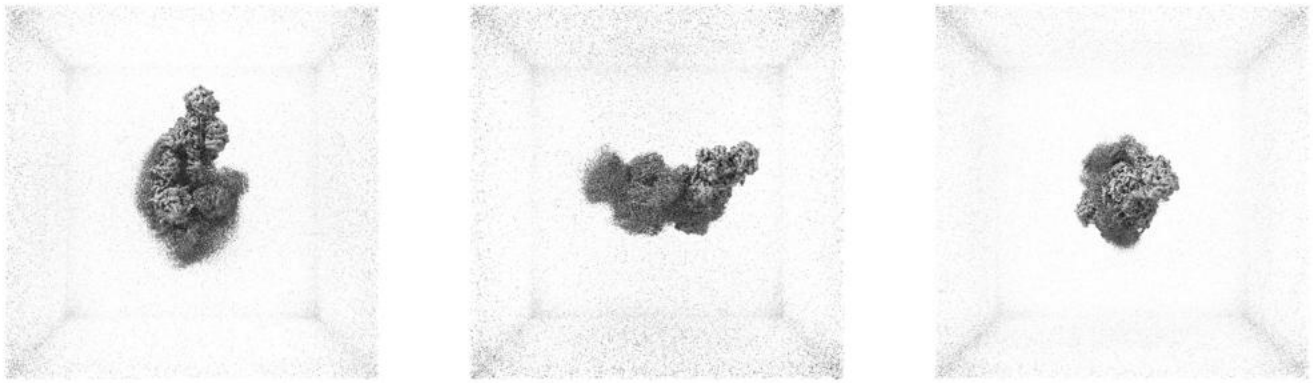
### 6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 4.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



X Y Z

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

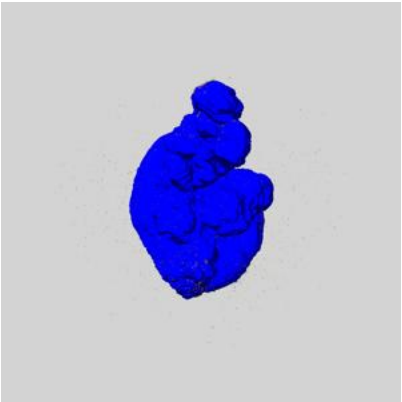
## 6.6 Mask visualisation (i)

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

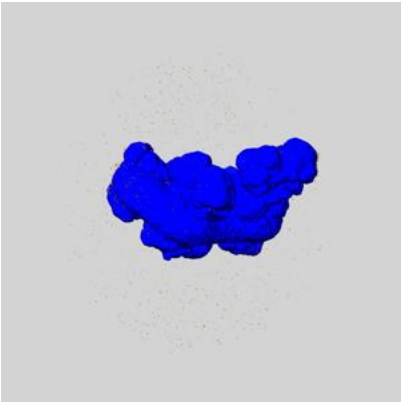
A mask typically either:

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

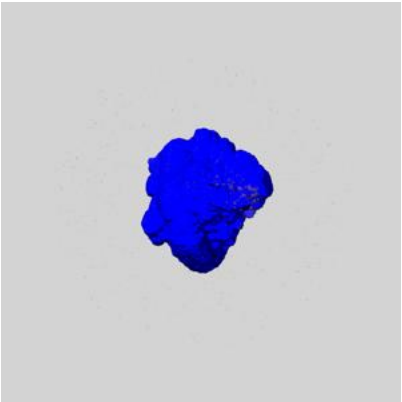
### 6.6.1 emd_60284_msk_1.map (i)



X



Y

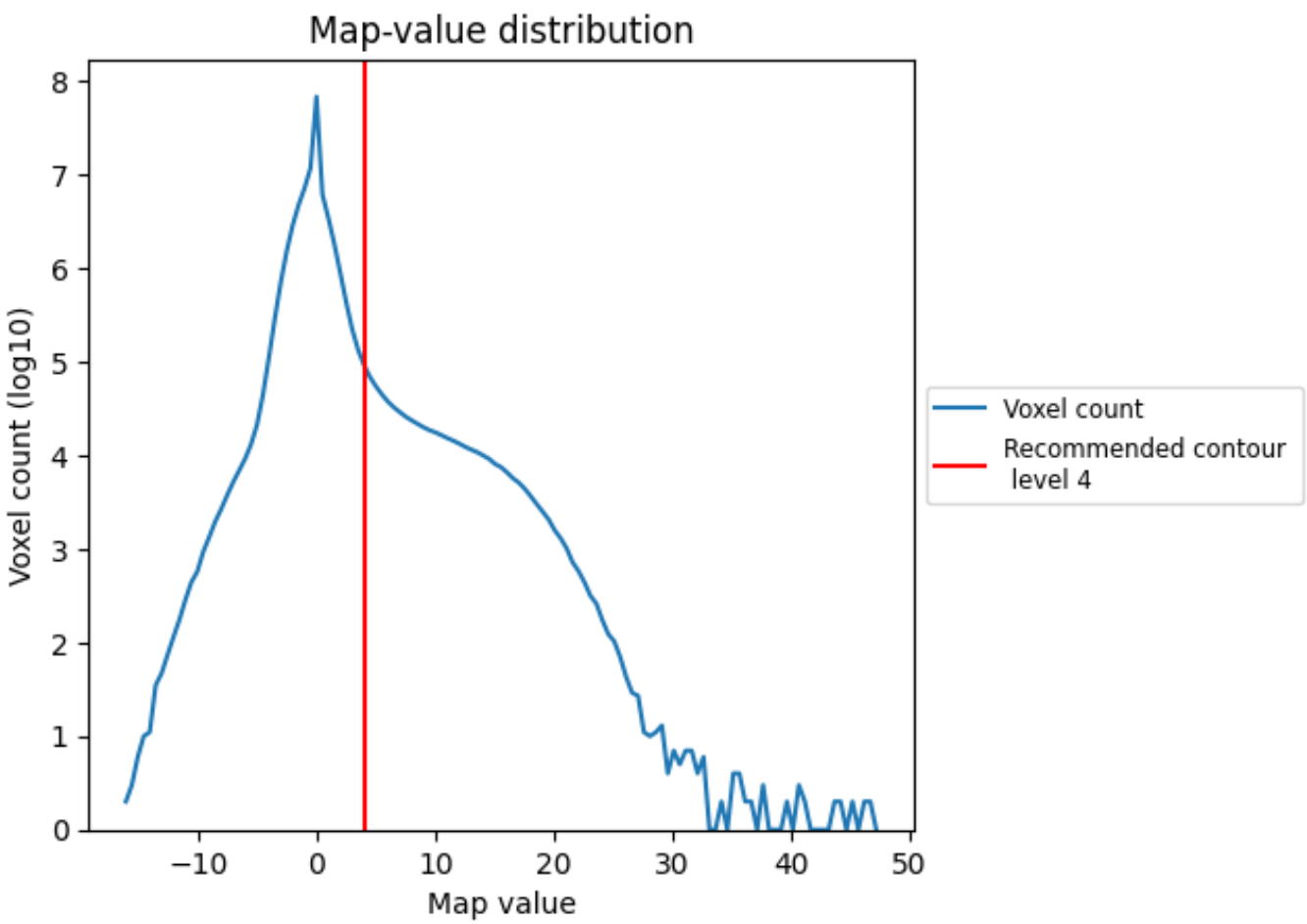


Z

# 7 Map analysis (i)

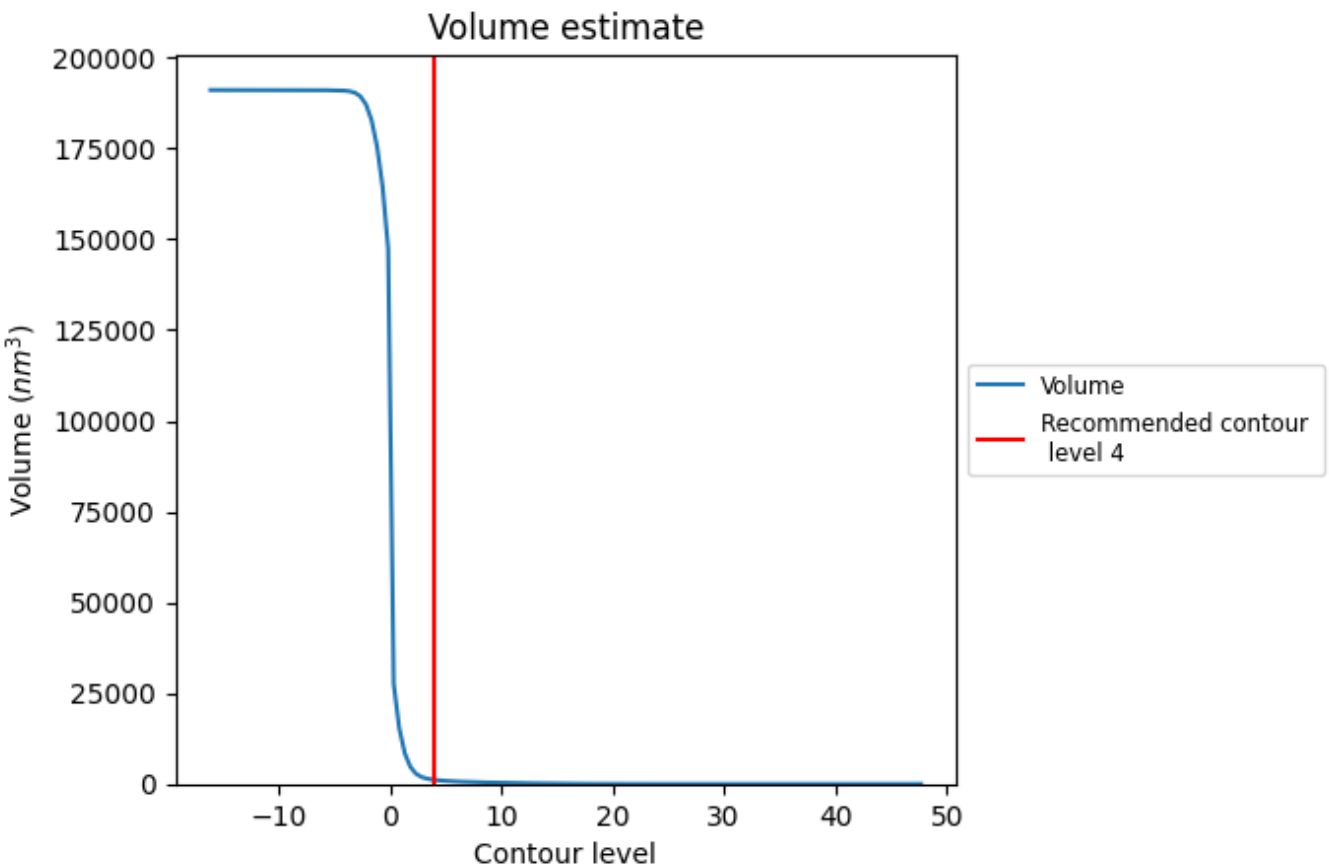
This section contains the results of statistical analysis of the map.

## 7.1 Map-value distribution (i)




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

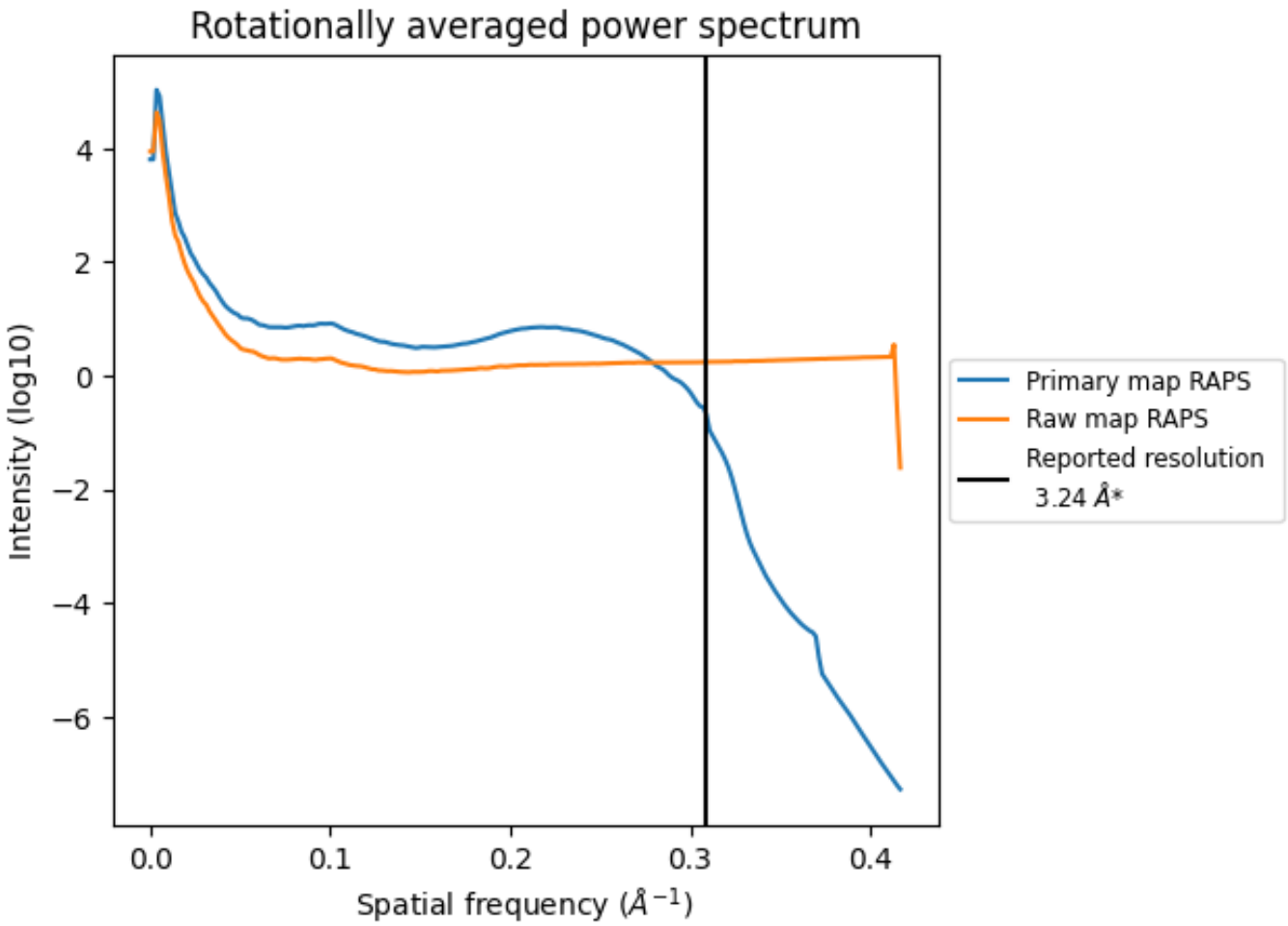
## 7.2 Volume estimate (i)




The volume at the recommended contour level is 1136 $nm^3$; this corresponds to an approximate mass of 1026 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)

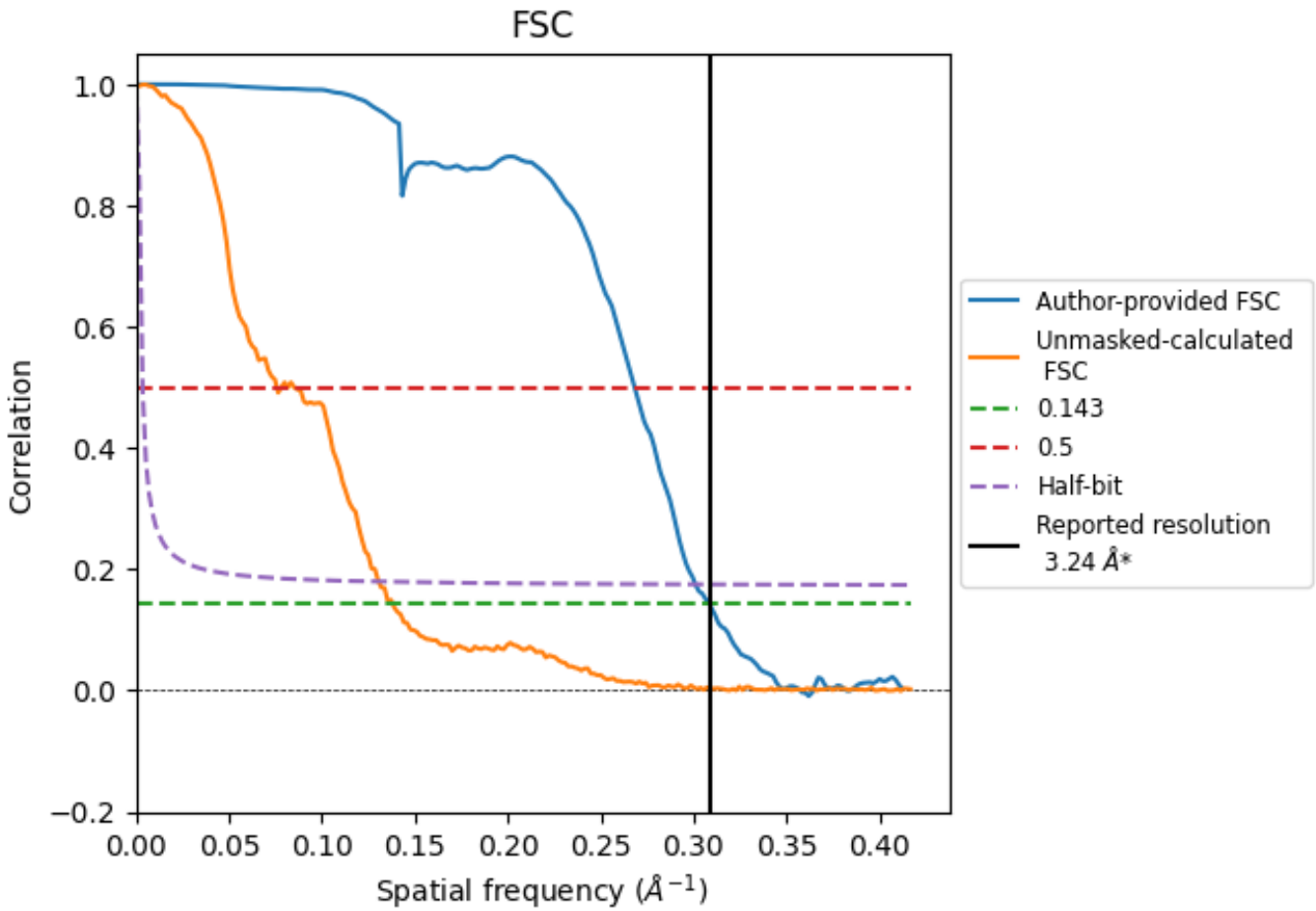



*Reported resolution corresponds to spatial frequency of 0.309 Å$^{-1}$

# 8 Fourier-Shell correlation (i)

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

## 8.1 FSC (i)




*Reported resolution corresponds to spatial frequency of 0.309 Å$^{-1}$

## 8.2 Resolution estimates (i)

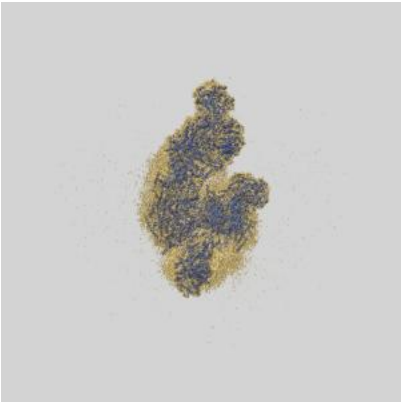
| Resolution estimate (Å) | Estimation criterion (FSC cut-off) | | |
|---|---|---|---|
| | 0.143 | 0.5 | Half-bit |
| Reported by author | 3.24 | - | - |
| Author-provided FSC curve | 3.24 | 3.72 | 3.32 |
| Unmasked-calculated* | 7.25 | 13.21 | 7.66 |

*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 7.25 differs from the reported value 3.24 by more than 10 %

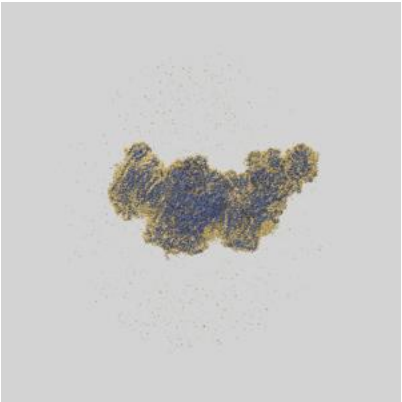
# 9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-60284 and PDB model 8ZO8. Per-residue inclusion information can be found in section 3 on page 31.

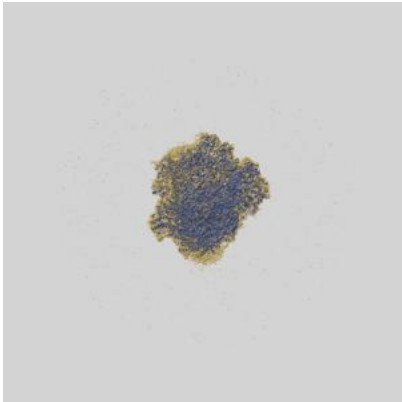
## 9.1 Map-model overlay (i)



X



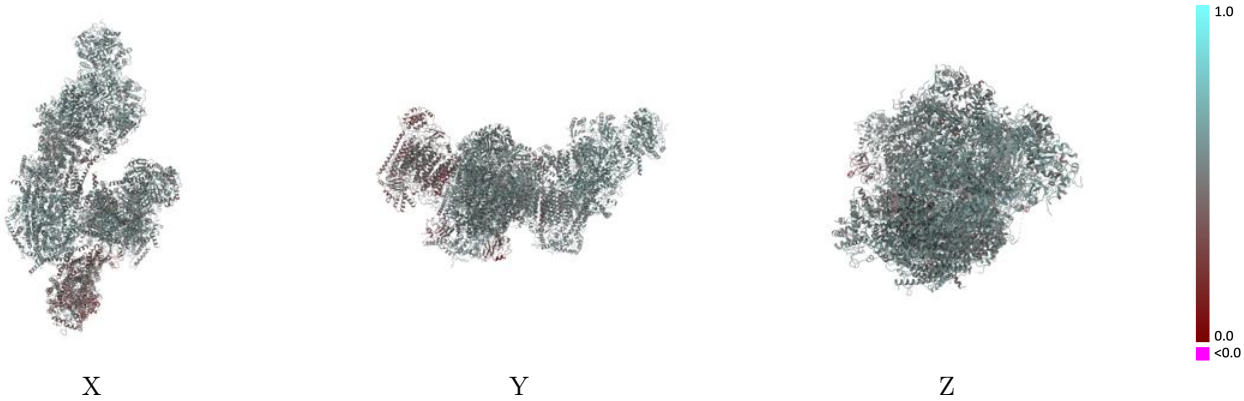
Y



Z

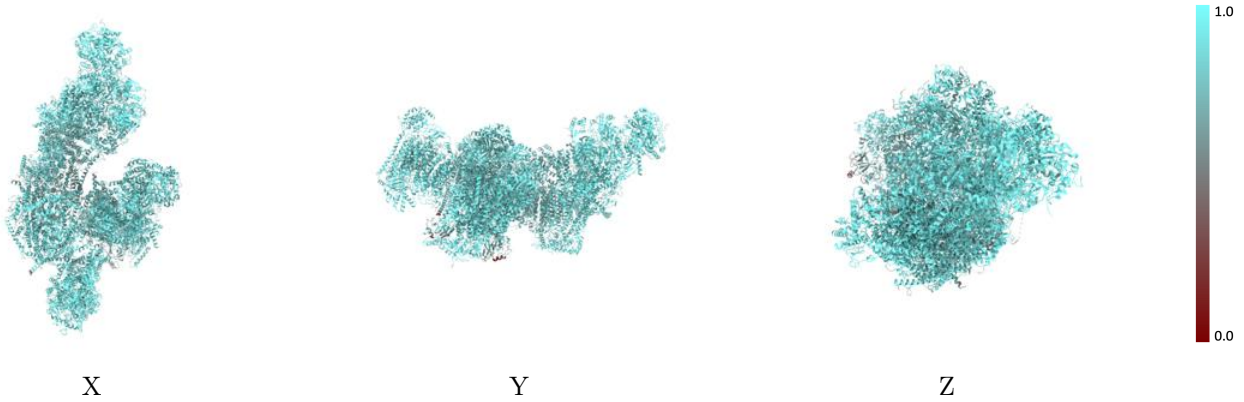
The images above show the 3D surface view of the map at the recommended contour level 4.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



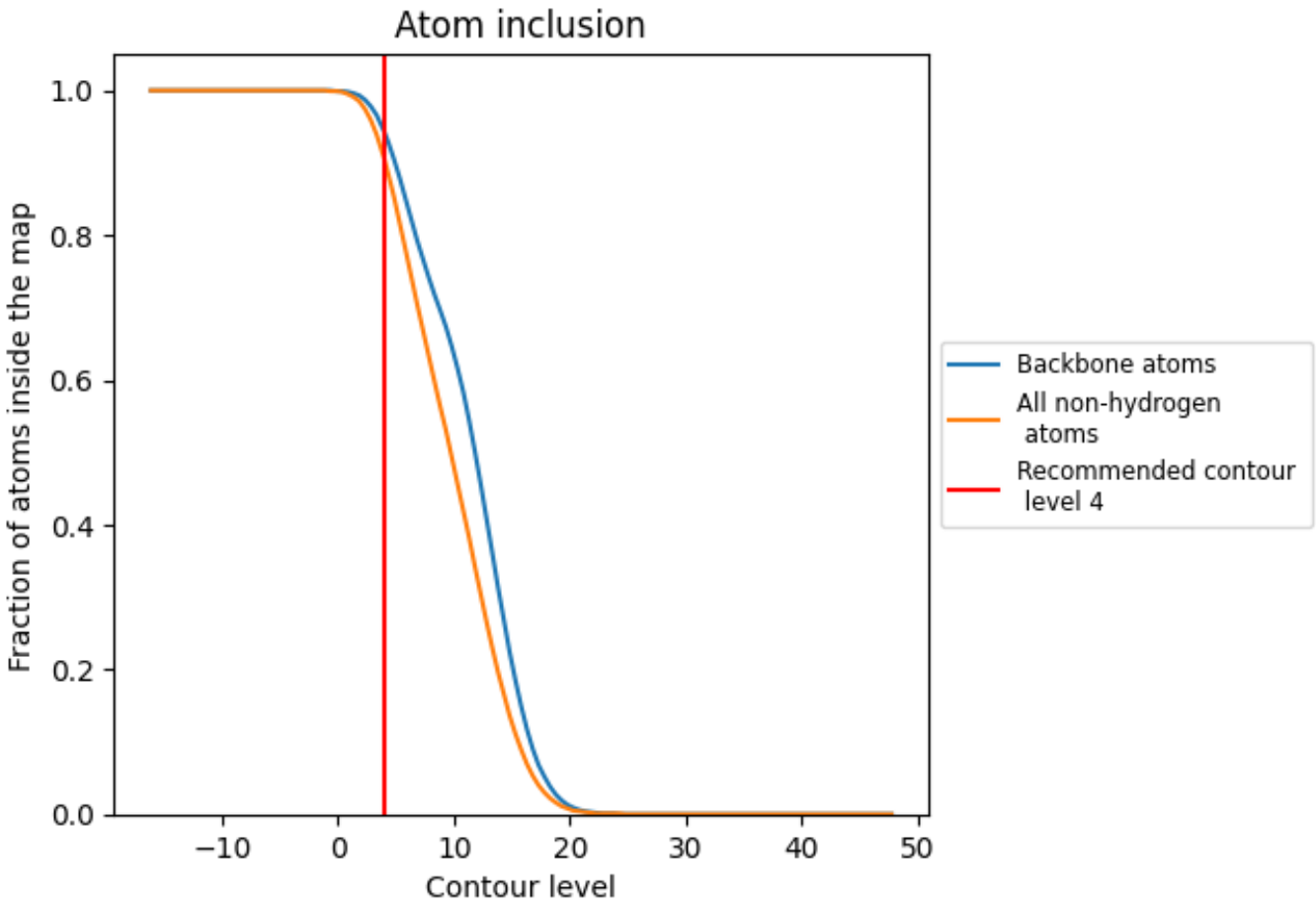

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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




The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (4).

## 9.4 Atom inclusion (i)




At the recommended contour level, 94% of all backbone atoms, 91% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (4) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion | Q-score |
|---|---|---|
| All | 0.9060 | 0.5230 |
| 4L | 0.8920 | 0.5330 |
| 5A | 0.8780 | 0.3720 |
| 5B | 0.9470 | 0.3950 |
| 6A | 0.9500 | 0.3820 |
| 6B | 0.9550 | 0.4030 |
| 6C | 0.8530 | 0.3780 |
| 7A | 0.9200 | 0.3970 |
| 7B | 0.8800 | 0.4190 |
| 7C | 0.9610 | 0.4060 |
| 8B | 0.9550 | 0.4040 |
| A1 | 0.9560 | 0.5430 |
| A2 | 0.9040 | 0.5270 |
| A3 | 0.9520 | 0.5390 |
| A5 | 0.9130 | 0.5320 |
| A6 | 0.9060 | 0.5390 |
| A7 | 0.8810 | 0.5380 |
| A8 | 0.9350 | 0.5470 |
| A9 | 0.9270 | 0.5480 |
| AB | 0.7680 | 0.4310 |
| AC | 0.9130 | 0.5590 |
| AK | 0.8350 | 0.5000 |
| AL | 0.8060 | 0.5060 |
| AM | 0.8860 | 0.5400 |
| AN | 0.9410 | 0.5390 |
| B1 | 0.8600 | 0.5310 |
| B2 | 0.9260 | 0.5520 |
| B3 | 0.8940 | 0.5380 |
| B4 | 0.8830 | 0.5500 |
| B5 | 0.9220 | 0.5710 |
| B6 | 0.8690 | 0.5350 |
| B7 | 0.9020 | 0.5510 |
| B8 | 0.9040 | 0.5610 |
| B9 | 0.9120 | 0.5620 |
| BK | 0.8910 | 0.5490 |

*Continued on next page...*

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| Chain | Atom inclusion | Q-score |
|---|---|---|
| BL | 0.8770 | 0.5430 |
| C1 | 0.9430 | 0.4490 |
| C2 | 0.9360 | 0.4280 |
| C3 | 0.9370 | 0.4070 |
| C4 | 0.9020 | 0.3950 |
| CA | 0.8680 | 0.5190 |
| CB | 0.9090 | 0.5530 |
| N1 | 0.9280 | 0.5420 |
| N2 | 0.9340 | 0.5510 |
| N3 | 0.9110 | 0.5370 |
| N4 | 0.9220 | 0.5690 |
| N5 | 0.9150 | 0.5680 |
| N6 | 0.8620 | 0.4940 |
| QA | 0.9000 | 0.5270 |
| QB | 0.9030 | 0.5350 |
| QC | 0.9190 | 0.5400 |
| QD | 0.9090 | 0.5310 |
| QE | 0.7200 | 0.4260 |
| QF | 0.8220 | 0.4780 |
| QG | 0.9140 | 0.5330 |
| QH | 0.9090 | 0.5250 |
| QI | 0.9090 | 0.5260 |
| QJ | 0.8890 | 0.4980 |
| QK | 0.7450 | 0.4870 |
| Qa | 0.8870 | 0.5260 |
| Qb | 0.9010 | 0.5300 |
| Qc | 0.9390 | 0.5360 |
| Qd | 0.9110 | 0.5390 |
| Qe | 0.6850 | 0.4040 |
| Qf | 0.8160 | 0.4670 |
| Qg | 0.8860 | 0.5230 |
| Qh | 0.8910 | 0.5260 |
| Qi | 0.9290 | 0.5290 |
| Qj | 0.8840 | 0.5140 |
| S1 | 0.9300 | 0.5560 |
| S2 | 0.9260 | 0.5650 |
| S3 | 0.9660 | 0.5800 |
| S4 | 0.9240 | 0.5630 |
| S5 | 0.9210 | 0.5370 |
| S6 | 0.9210 | 0.5560 |
| S7 | 0.9440 | 0.5670 |
| S8 | 0.9650 | 0.5740 |

*Continued on next page...*

*Continued from previous page...*

| Chain | Atom inclusion | Q-score |
|---|---|---|
| V1 | 0.9330 | 0.5460 |
| V2 | 0.9140 | 0.5410 |
| V3 | 0.9450 | 0.5440 |