# Full wwPDB EM Validation Report ⓘ

Apr 5, 2026 – 08:04 PM UTC

| | | |
|---|---|---|
| PDB ID | : | 9HEO / pdb_00009heo |
| EMDB ID | : | EMD-52085 |
| Title | : | Open-state RyR1 in 0.05% POPC micelles, in complex with a nanobody and FKBP |
| Authors | : | Li, C.; Efremov, R.G. |
| Deposited on | : | 2024-11-14 |
| Resolution | : | 3.40 Å(reported) |

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

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

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

---

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

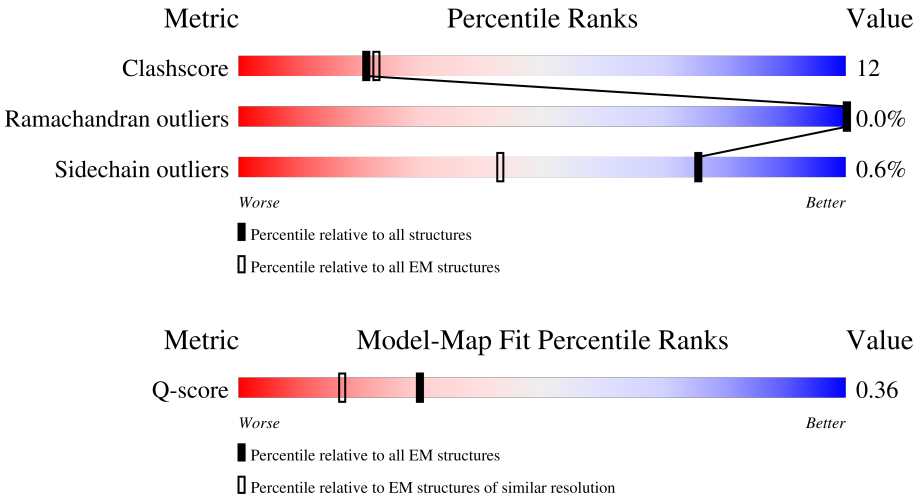
| | | |
|---|---|---|
| EMDB validation analysis | : | 0.0.1.dev132 |
| Mogul | : | 2022.3.0, CSD as543be (2022) |
| MolProbity | : | 4-5-2 with Phenix2.0 |
| Buster-report | : | wwPDB partial adaption of 1.1.7 (2018) |
| Percentile statistics | : | 20250101.v01 (using entries in the PDB archive January 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) | : | 2.49 |

# 1 Overall quality at a glance

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

The reported resolution of this entry is 3.40 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.







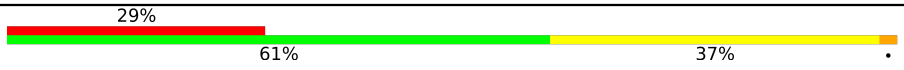
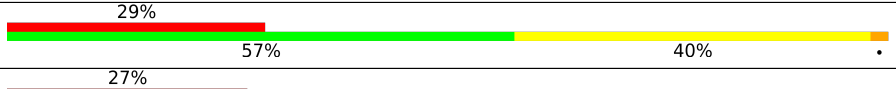
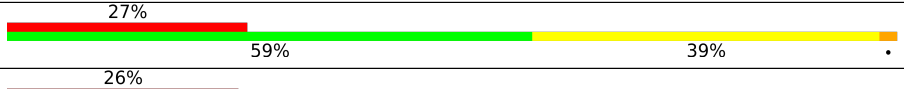
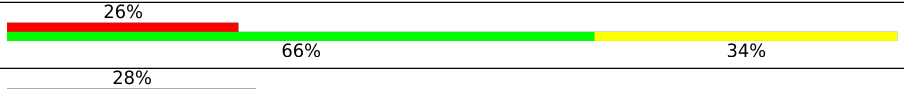
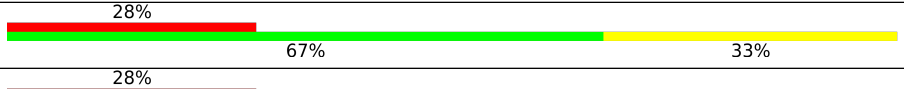
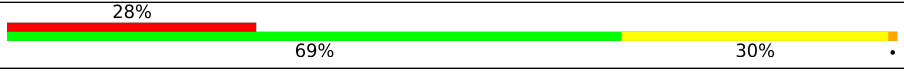
| Metric | Whole archive (#Entries) | EM structures (#Entries) | Similar EM resolution (#Entries, resolution range(Å)) |
|---|---|---|---|
| Clashscore | 229148 | 23984 | - |
| Ramachandran outliers | 224038 | 23583 | - |
| Sidechain outliers | 223484 | 23102 | - |
| Q-score | - | 25397 | 14717 ( 2.90 - 3.90 ) |

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

| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 1 | A | 5027 | 63% 23% 14% |
| 1 | C | 5027 | 63% 23% 14% |
| 1 | G | 5027 | 63% 23% 14% |
| 1 | J | 5027 | 63% 23% 14% |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Length | Quality of chain |
|---|---|---|---|
| 2 | B | 126 |   |
| 2 | D | 126 |   |
| 2 | H | 126 |   |
| 2 | K | 126 |   |
| 3 | E | 107 |   |
| 3 | F | 107 |   |
| 3 | I | 107 |   |
| 3 | L | 107 |   |

# 2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 146783 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 Ryanodine receptor 1.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 1 | A | 4327 | Total | C | N | O | S | 1 | 0 |
| | | | 34225 | 21798 | 5895 | 6303 | 229 | | |
| 1 | C | 4327 | Total | C | N | O | S | 1 | 0 |
| | | | 34225 | 21798 | 5895 | 6303 | 229 | | |
| 1 | G | 4327 | Total | C | N | O | S | 1 | 0 |
| | | | 34225 | 21798 | 5895 | 6303 | 229 | | |
| 1 | J | 4327 | Total | C | N | O | S | 1 | 0 |
| | | | 34224 | 21797 | 5895 | 6303 | 229 | | |

- Molecule 2 is a protein called Nanobody 9657.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 2 | B | 126 | Total | C | N | O | S | 0 | 0 |
| | | | 961 | 594 | 167 | 195 | 5 | | |
| 2 | D | 126 | Total | C | N | O | S | 0 | 0 |
| | | | 961 | 594 | 167 | 195 | 5 | | |
| 2 | H | 126 | Total | C | N | O | S | 0 | 0 |
| | | | 961 | 594 | 167 | 195 | 5 | | |
| 2 | K | 126 | Total | C | N | O | S | 0 | 0 |
| | | | 961 | 594 | 167 | 195 | 5 | | |

- Molecule 3 is a protein called Peptidyl-prolyl cis-trans isomerase FKBP1B.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 3 | E | 107 | Total | C | N | O | S | 0 | 0 |
| | | | 818 | 516 | 144 | 154 | 4 | | |
| 3 | F | 107 | Total | C | N | O | S | 0 | 0 |
| | | | 818 | 516 | 144 | 154 | 4 | | |
| 3 | I | 107 | Total | C | N | O | S | 0 | 0 |
| | | | 818 | 516 | 144 | 154 | 4 | | |
| 3 | L | 107 | Total | C | N | O | S | 0 | 0 |
| | | | 818 | 516 | 144 | 154 | 4 | | |

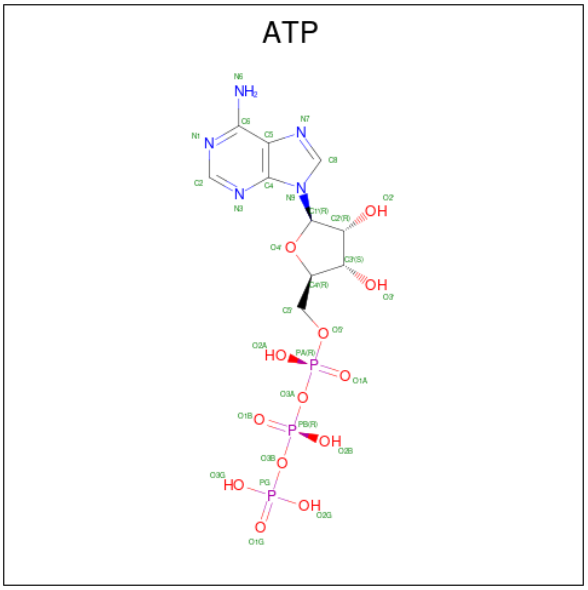
There are 4 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| E | 100 | ASP | GLY | conflict | UNP Q8HYX6 |
| F | 100 | ASP | GLY | conflict | UNP Q8HYX6 |
| I | 100 | ASP | GLY | conflict | UNP Q8HYX6 |
| L | 100 | ASP | GLY | conflict | UNP Q8HYX6 |

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms | AltConf |
|---|---|---|---|---|
| 4 | A | 1 | Total Zn<br>1 1 | 0 |
| 4 | C | 1 | Total Zn<br>1 1 | 0 |
| 4 | G | 1 | Total Zn<br>1 1 | 0 |
| 4 | J | 1 | Total Zn<br>1 1 | 0 |

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



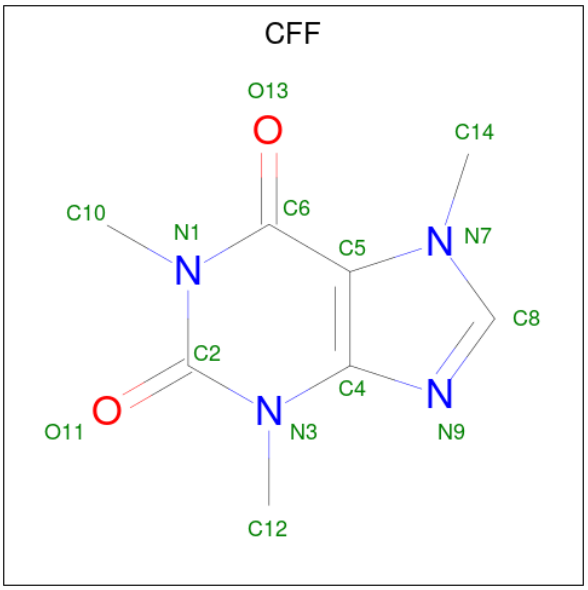

| Mol | Chain | Residues | Atoms | AltConf |
|---|---|---|---|---|
| 5 | A | 1 | Total C N O P<br>31 10 5 13 3 | 0 |
| 5 | C | 1 | Total C N O P<br>31 10 5 13 3 | 0 |
| 5 | G | 1 | Total C N O P<br>31 10 5 13 3 | 0 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Residues | Atoms | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|
| 5 | J | 1 | Total | C | N | O | P | 0 |
| | | | 31 | 10 | 5 | 13 | 3 | |

- Molecule 6 is CAFFEINE (CCD ID: CFF) (formula: $C_8H_{10}N_4O_2$) (labeled as "Ligand of Interest" by depositor).




| Mol | Chain | Residues | Atoms | | | | AltConf |
|---|---|---|---|---|---|---|---|
| 6 | A | 1 | Total | C | N | O | 0 |
| | | | 14 | 8 | 4 | 2 | |
| 6 | C | 1 | Total | C | N | O | 0 |
| | | | 14 | 8 | 4 | 2 | |
| 6 | G | 1 | Total | C | N | O | 0 |
| | | | 14 | 8 | 4 | 2 | |
| 6 | J | 1 | Total | C | N | O | 0 |
| | | | 14 | 8 | 4 | 2 | |

- Molecule 7 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

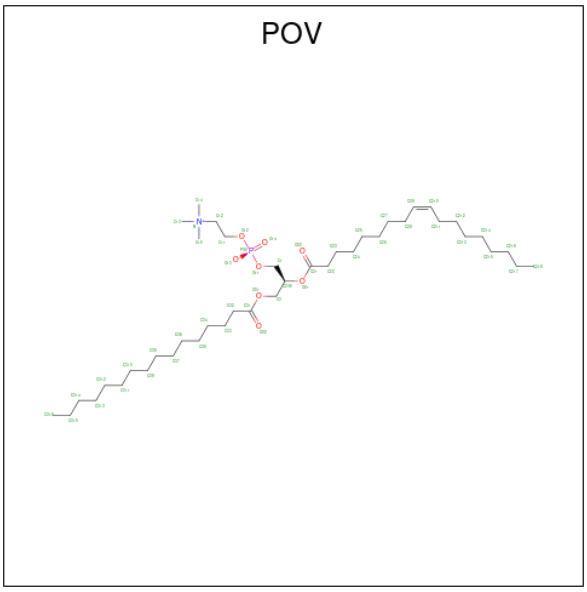
| Mol | Chain | Residues | Atoms | | AltConf |
|---|---|---|---|---|---|
| 7 | A | 1 | Total | Ca | 0 |
| | | | 1 | 1 | |
| 7 | C | 1 | Total | Ca | 0 |
| | | | 1 | 1 | |
| 7 | G | 1 | Total | Ca | 0 |
| | | | 1 | 1 | |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Residues | Atoms | AltConf |
|---|---|---|---|---|
| 7 | J | 1 | Total Ca<br>1 1 | 0 |

- Molecule 8 is (2S)-3-(hexadecanoyloxy)-2-[(9Z)-octadec-9-enoyloxy]propyl 2-(trimethylammonio)ethyl phosphate (CCD ID: POV) (formula: $C_{42}H_{82}NO_8P$) (labeled as "Ligand of Interest" by depositor).




| Mol | Chain | Residues | Atoms | AltConf |
|---|---|---|---|---|
| 8 | A | 1 | Total C N O P<br>49 39 1 8 1 | 0 |
| 8 | A | 1 | Total C N O P<br>47 37 1 8 1 | 0 |
| 8 | A | 1 | Total C N O P<br>50 40 1 8 1 | 0 |
| 8 | A | 1 | Total C N O P<br>46 36 1 8 1 | 0 |
| 8 | A | 1 | Total C N O P<br>20 11 1 7 1 | 0 |
| 8 | A | 1 | Total C N O P<br>20 11 1 7 1 | 0 |
| 8 | A | 1 | Total C N O P<br>20 12 1 6 1 | 0 |
| 8 | A | 1 | Total C N O P<br>35 25 1 8 1 | 0 |
| 8 | A | 1 | Total C N O P<br>28 18 1 8 1 | 0 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Residues | Atoms | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|
| 8 | A | 1 | Total | C | N | O | P | 0 |
| | | | 24 | 15 | 1 | 7 | 1 | |
| 8 | A | 1 | Total | C | N | O | P | 0 |
| | | | 34 | 24 | 1 | 8 | 1 | |
| 8 | A | 1 | Total | C | N | O | P | 0 |
| | | | 52 | 42 | 1 | 8 | 1 | |
| 8 | A | 1 | Total | C | N | O | P | 0 |
| | | | 47 | 37 | 1 | 8 | 1 | |
| 8 | A | 1 | Total | C | N | O | P | 0 |
| | | | 41 | 31 | 1 | 8 | 1 | |
| 8 | A | 1 | Total | C | N | O | P | 0 |
| | | | 31 | 21 | 1 | 8 | 1 | |
| 8 | A | 1 | Total | C | N | O | P | 0 |
| | | | 40 | 30 | 1 | 8 | 1 | |
| 8 | A | 1 | Total | C | N | O | P | 0 |
| | | | 48 | 38 | 1 | 8 | 1 | |
| 8 | A | 1 | Total | C | | | | 0 |
| | | | 13 | 13 | | | | |
| 8 | C | 1 | Total | C | N | O | P | 0 |
| | | | 40 | 30 | 1 | 8 | 1 | |
| 8 | C | 1 | Total | C | N | O | P | 0 |
| | | | 48 | 38 | 1 | 8 | 1 | |
| 8 | C | 1 | Total | C | | | | 0 |
| | | | 13 | 13 | | | | |
| 8 | C | 1 | Total | C | N | O | P | 0 |
| | | | 49 | 39 | 1 | 8 | 1 | |
| 8 | C | 1 | Total | C | N | O | P | 0 |
| | | | 47 | 37 | 1 | 8 | 1 | |
| 8 | C | 1 | Total | C | N | O | P | 0 |
| | | | 50 | 40 | 1 | 8 | 1 | |
| 8 | C | 1 | Total | C | N | O | P | 0 |
| | | | 46 | 36 | 1 | 8 | 1 | |
| 8 | C | 1 | Total | C | N | O | P | 0 |
| | | | 20 | 11 | 1 | 7 | 1 | |
| 8 | C | 1 | Total | C | N | O | P | 0 |
| | | | 20 | 11 | 1 | 7 | 1 | |
| 8 | C | 1 | Total | C | N | O | P | 0 |
| | | | 20 | 12 | 1 | 6 | 1 | |
| 8 | C | 1 | Total | C | N | O | P | 0 |
| | | | 35 | 25 | 1 | 8 | 1 | |
| 8 | C | 1 | Total | C | N | O | P | 0 |
| | | | 28 | 18 | 1 | 8 | 1 | |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Residues | Atoms | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|
| 8 | C | 1 | Total | C | N | O | P | 0 |
| | | | 24 | 15 | 1 | 7 | 1 | |
| 8 | C | 1 | Total | C | N | O | P | 0 |
| | | | 34 | 24 | 1 | 8 | 1 | |
| 8 | C | 1 | Total | C | N | O | P | 0 |
| | | | 52 | 42 | 1 | 8 | 1 | |
| 8 | C | 1 | Total | C | N | O | P | 0 |
| | | | 47 | 37 | 1 | 8 | 1 | |
| 8 | C | 1 | Total | C | N | O | P | 0 |
| | | | 41 | 31 | 1 | 8 | 1 | |
| 8 | C | 1 | Total | C | N | O | P | 0 |
| | | | 31 | 21 | 1 | 8 | 1 | |
| 8 | G | 1 | Total | C | N | O | P | 0 |
| | | | 40 | 30 | 1 | 8 | 1 | |
| 8 | G | 1 | Total | C | N | O | P | 0 |
| | | | 48 | 38 | 1 | 8 | 1 | |
| 8 | G | 1 | Total | C | | | | 0 |
| | | | 13 | 13 | | | | |
| 8 | G | 1 | Total | C | N | O | P | 0 |
| | | | 49 | 39 | 1 | 8 | 1 | |
| 8 | G | 1 | Total | C | N | O | P | 0 |
| | | | 47 | 37 | 1 | 8 | 1 | |
| 8 | G | 1 | Total | C | N | O | P | 0 |
| | | | 50 | 40 | 1 | 8 | 1 | |
| 8 | G | 1 | Total | C | N | O | P | 0 |
| | | | 46 | 36 | 1 | 8 | 1 | |
| 8 | G | 1 | Total | C | N | O | P | 0 |
| | | | 20 | 11 | 1 | 7 | 1 | |
| 8 | G | 1 | Total | C | N | O | P | 0 |
| | | | 20 | 11 | 1 | 7 | 1 | |
| 8 | G | 1 | Total | C | N | O | P | 0 |
| | | | 20 | 12 | 1 | 6 | 1 | |
| 8 | G | 1 | Total | C | N | O | P | 0 |
| | | | 35 | 25 | 1 | 8 | 1 | |
| 8 | G | 1 | Total | C | N | O | P | 0 |
| | | | 28 | 18 | 1 | 8 | 1 | |
| 8 | G | 1 | Total | C | N | O | P | 0 |
| | | | 24 | 15 | 1 | 7 | 1 | |
| 8 | G | 1 | Total | C | N | O | P | 0 |
| | | | 34 | 24 | 1 | 8 | 1 | |
| 8 | G | 1 | Total | C | N | O | P | 0 |
| | | | 52 | 42 | 1 | 8 | 1 | |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Residues | Atoms | | | | | AltConf |
|---|---|---|---|---|---|---|---|---|
| 8 | G | 1 | Total | C | N | O | P | 0 |
| | | | 47 | 37 | 1 | 8 | 1 | |
| 8 | G | 1 | Total | C | N | O | P | 0 |
| | | | 41 | 31 | 1 | 8 | 1 | |
| 8 | G | 1 | Total | C | N | O | P | 0 |
| | | | 31 | 21 | 1 | 8 | 1 | |
| 8 | J | 1 | Total | C | N | O | P | 0 |
| | | | 52 | 42 | 1 | 8 | 1 | |
| 8 | J | 1 | Total | C | N | O | P | 0 |
| | | | 47 | 37 | 1 | 8 | 1 | |
| 8 | J | 1 | Total | C | N | O | P | 0 |
| | | | 41 | 31 | 1 | 8 | 1 | |
| 8 | J | 1 | Total | C | N | O | P | 0 |
| | | | 31 | 21 | 1 | 8 | 1 | |
| 8 | J | 1 | Total | C | N | O | P | 0 |
| | | | 40 | 30 | 1 | 8 | 1 | |
| 8 | J | 1 | Total | C | N | O | P | 0 |
| | | | 48 | 38 | 1 | 8 | 1 | |
| 8 | J | 1 | Total | C | | | | 0 |
| | | | 13 | 13 | | | | |
| 8 | J | 1 | Total | C | N | O | P | 0 |
| | | | 49 | 39 | 1 | 8 | 1 | |
| 8 | J | 1 | Total | C | N | O | P | 0 |
| | | | 47 | 37 | 1 | 8 | 1 | |
| 8 | J | 1 | Total | C | N | O | P | 0 |
| | | | 50 | 40 | 1 | 8 | 1 | |
| 8 | J | 1 | Total | C | N | O | P | 0 |
| | | | 46 | 36 | 1 | 8 | 1 | |
| 8 | J | 1 | Total | C | N | O | P | 0 |
| | | | 20 | 11 | 1 | 7 | 1 | |
| 8 | J | 1 | Total | C | N | O | P | 0 |
| | | | 20 | 11 | 1 | 7 | 1 | |
| 8 | J | 1 | Total | C | N | O | P | 0 |
| | | | 20 | 12 | 1 | 6 | 1 | |
| 8 | J | 1 | Total | C | N | O | P | 0 |
| | | | 35 | 25 | 1 | 8 | 1 | |
| 8 | J | 1 | Total | C | N | O | P | 0 |
| | | | 28 | 18 | 1 | 8 | 1 | |
| 8 | J | 1 | Total | C | N | O | P | 0 |
| | | | 24 | 15 | 1 | 7 | 1 | |
| 8 | J | 1 | Total | C | N | O | P | 0 |
| | | | 34 | 24 | 1 | 8 | 1 | |

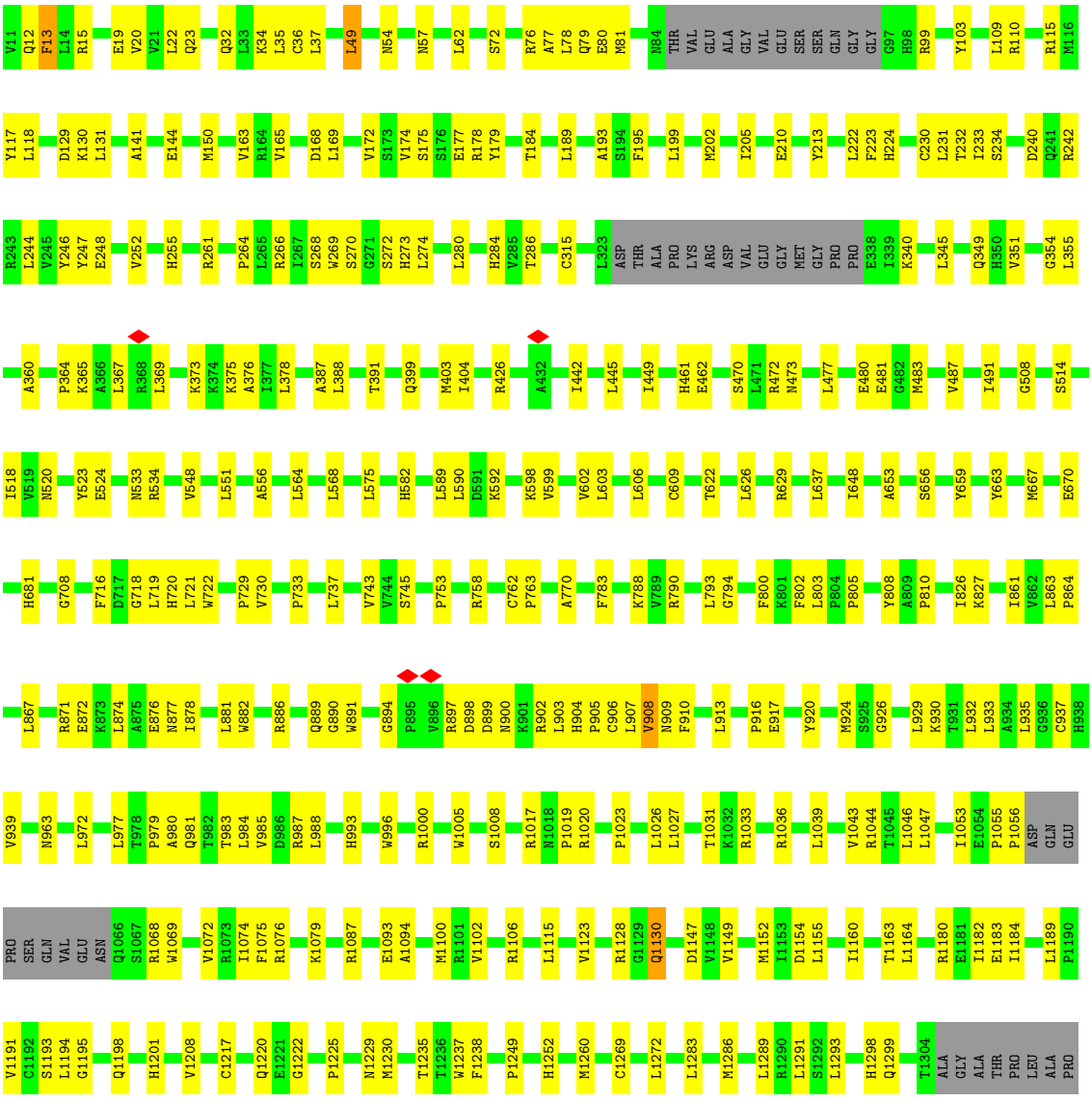
# 3 Residue-property plots (i)

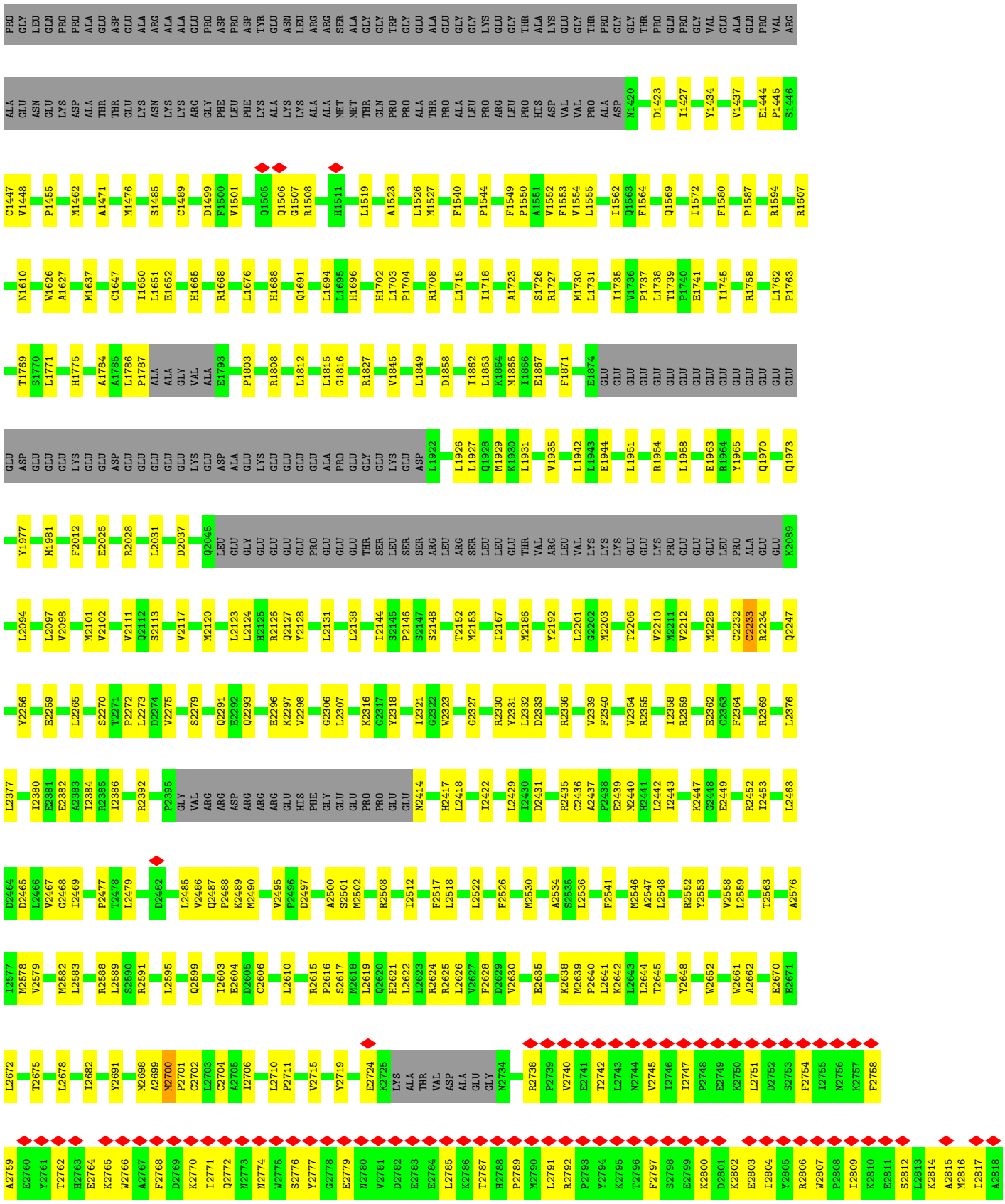
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

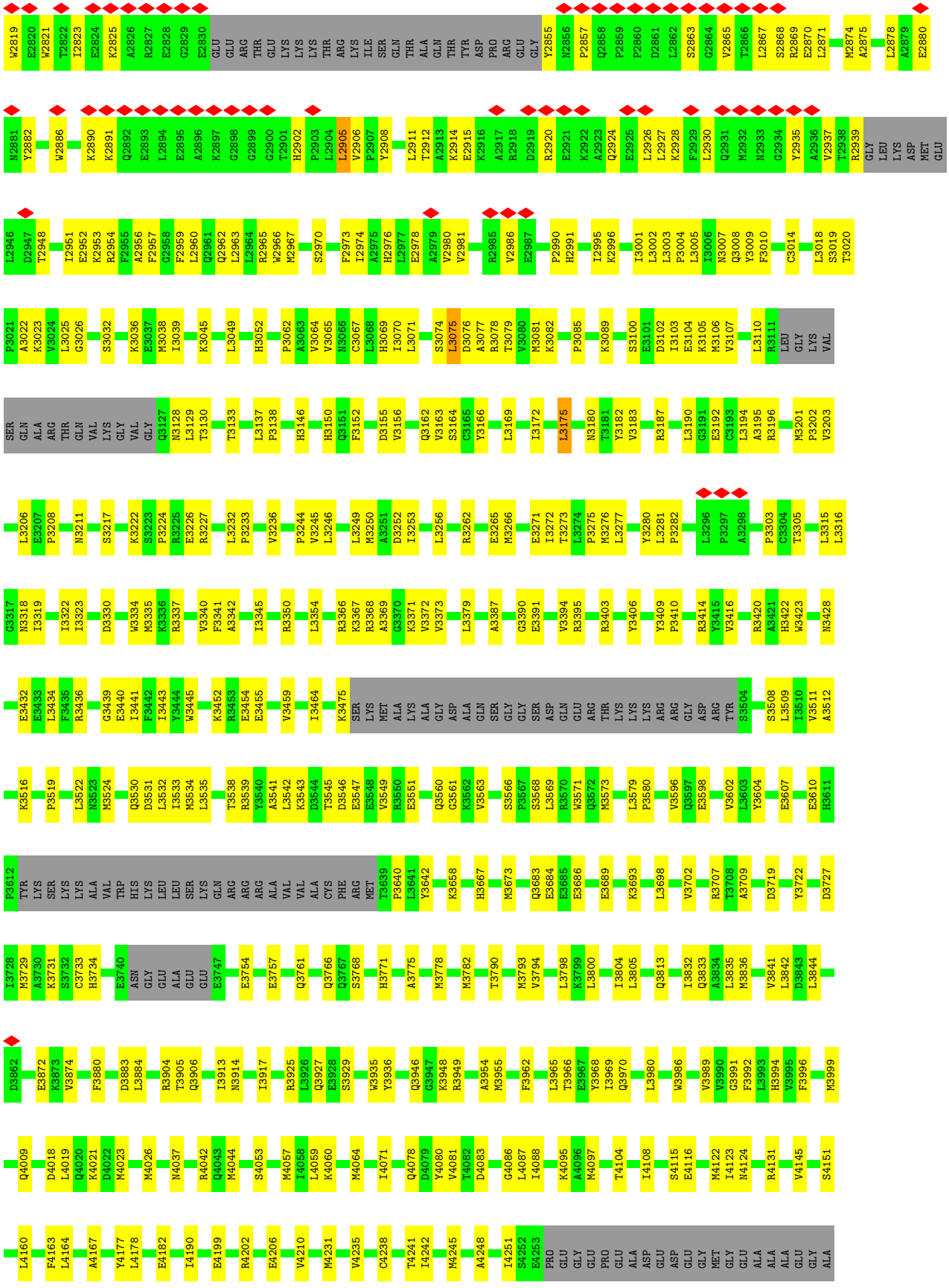
- Molecule 1: Ryanodine receptor 1

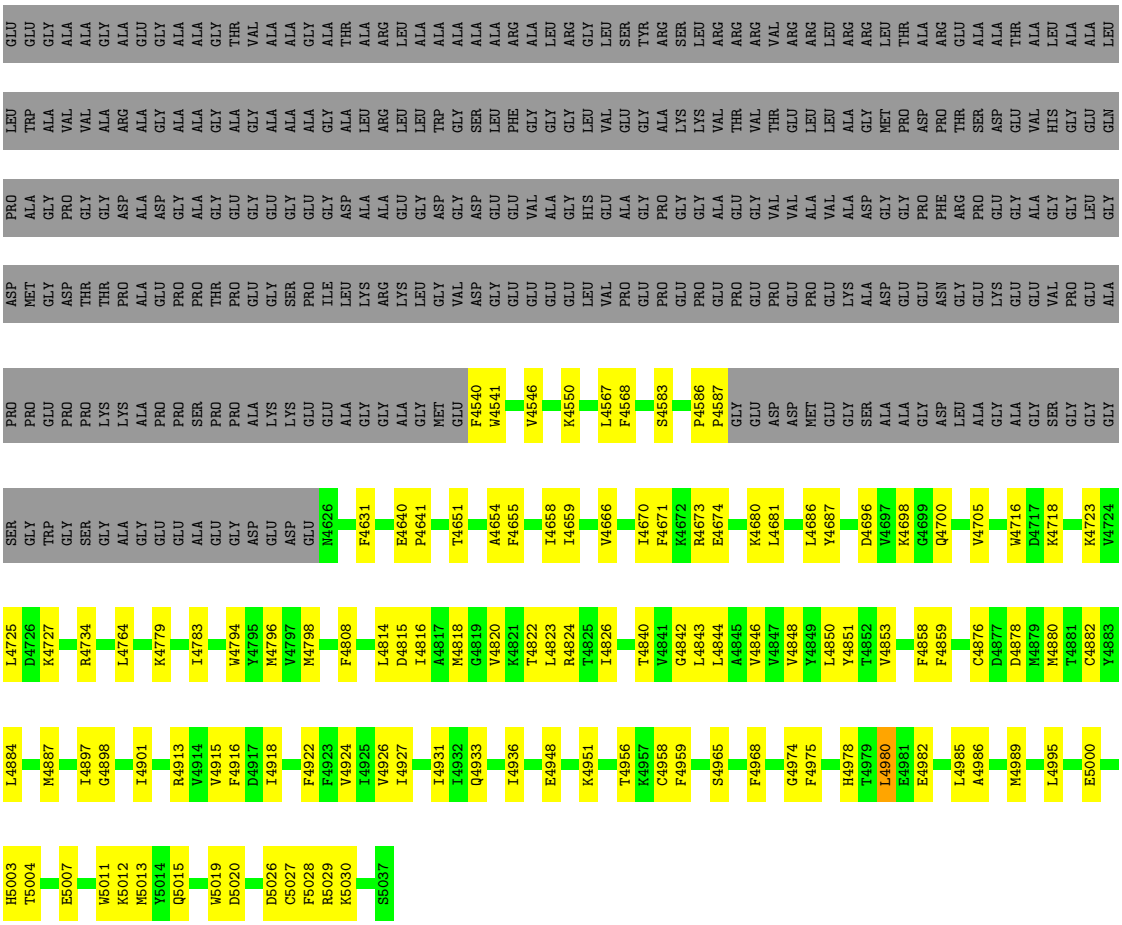
Chain A:




PRO GLY LEU GLN PRO PRO ALA GLU ASP GLU ALA ARG ALA ALA GLU PRO ASP PRO ASP TYR GLU ASN LEU ARG ARG SER ALA GLY GLY TRP GLY GLU ALA GLU GLY GLY LYS GLU GLY THR ALA LYS GLU GLY THR PRO GLY GLY THR PRO GLN PRO GLY VAL GLU ALA GLN PRO VAL ARG
ALA GLU ASN GLU LYS ASP ALA THR THR GLU LYS ASN LYS LYS ARG GLY PHE LEU PHE LYS ALA LYS LEU ALA ALA MET MET THR GLN PRO PRO ALA THR PRO ALA LEU PRO ARG LEU PRO HIS ASP VAL VAL PRO ALA ASP N1420 D1423 I1427 Y1434 V1437 E1444 P1445 S1446
C1447 V1448 P1455 M1462 A1471 M1476 S1485 C1489 D1499 F1500 V1501 Q1505 Q1506 G1507 R1508 H1511 L1519 A1523 L1526 M1527 F1540 P1544 F1549 P1550 A1551 V1552 F1553 V1554 L1555 I1562 Q1563 F1564 Q1569 I1572 F1580 P1587 R1594 R1607
N1610 W1626 A1627 M1637 C1647 I1650 L1651 E1652 H1665 R1668 L1676 H1688 Q1691 L1694 L1695 H1696 H1702 L1703 P1704 R1708 L1715 I1718 A1723 S1726 R1727 M1730 L1731 I1735 V1736 P1737 L1738 T1739 P1740 E1741 I1745 R1758 L1762 P1763
T1769 S1770 L1771 H1775 A1784 A1785 L1786 P1787 ALA ALA GLY VAL ALA E1793 P1803 R1808 L1812 L1815 G1816 R1827 V1845 L1849 D1858 I1862 L1863 K1864 M1865 I1866 E1867 F1871 E1874 GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU
GLU ASP GLU GLU LYS GLU GLU ASP GLU GLU GLU GLU LYS GLU ASP ALA GLU LYS GLU GLU GLU GLU ALA ALA PRO GLU GLY GLU GLU LYS GLU L1922 L1926 L1927 Q1928 M1929 K1930 L1931 V1935 L1942 L1943 E1944 L1951 R1954 L1958 E1963 R1964 Y1965 Q1970 Q1973
Y1977 M1981 F2012 E2025 R2028 L2031 D2037 Q2045 LEU LEU GLU GLY GLU GLU GLU GLU PRO GLU GLU GLU THR SER LEU SER SER ARG LEU ARG SER LEU LEU GLU THR VAL ARG LEU VAL LYS LYS LYS GLU GLU LYS PRO GLU GLU GLU LEU PRO ALA GLU GLU K2089
L2094 L2097 V2098 M2101 V2102 V2111 Q2112 S2113 V2117 M2120 L2123 L2124 H2125 R2126 Q2127 Y2128 L2131 L2138 I2144 S2145 P2146 S2147 S2148 T2152 M2153 I2167 M2186 Y2192 L2201 G2202 M2203 T2206 V2210 M2211 V2212 M2228 C2232 C2233 R2234 Q2247
Y2256 E2259 L2265 S2270 T2271 P2272 L2273 D2274 V2275 S2279 Q2291 E2292 Q2293 E2296 K2297 V2298 G2306 L2307 K2316 G2317 Y2318 I2321 G2322 W2323 G2327 R2330 Y2331 L2332 D2333 R2336 V2339 F2340 V2354 R2355 I2358 R2359 E2362 C2363 F2364 R2369 L2376
L2377 I2380 E2381 E2382 A2383 I2384 R2385 I2386 R2392 P2395 GLY VAL ARG ARG ASP ARG ARG ARG GLU HIS PHE GLY GLU GLU PRO PRO GLU GLU N2414 H2417 L2418 I2422 L2429 I2430 D2431 R2435 C2436 A2437 P2438 E2439 M2440 H2441 L2442 I2443 K2447 G2448 E2449 R2452 I2453 L2463
D2464 D2465 L2466 V2467 G2468 I2469 P2477 T2478 L2479 D2482 L2485 V2486 Q2487 P2488 K2489 M2490 V2495 P2496 D2497 A2500 S2501 M2502 R2508 I2512 F2517 L2518 L2522 F2526 M2530 A2534 S2535 L2536 F2541 M2546 A2547 L2548 R2552 Y2553 V2558 L2559 T2563 A2576
I2577 M2578 V2579 M2582 L2583 R2588 L2589 S2590 R2591 L2595 Q2599 I2603 E2604 D2605 C2606 L2610 R2615 P2616 S2617 M2618 L2619 Q2620 H2621 L2622 L2623 R2624 R2625 L2626 V2627 F2628 D2629 V2630 E2635 K2638 M2639 P2640 L2641 K2642 L2643 L2644 T2645 Y2648 W2652 W2661 A2662 E2670 E2671
L2672 T2675 L2678 I2682 Y2691 M2698 A2699 M2700 P2701 C2702 L2703 C2704 A2705 I2706 L2710 P2711 V2715 Y2719 E2724 K2725 LYS ALA THR VAL ASP ALA GLU GLY W2734 R2738 P2739 V2740 E2741 T2742 L2743 N2744 V2745 I2746 I2747 P2748 E2749 K2750 L2751 D2752 S2753 F2754 I2755 N2756 K2757 F2758
A2759 E2760 Y2761 T2762 H2763 E2764 K2765 W2766 A2767 F2768 D2769 K2770 I2771 Q2772 N2773 N2774 W2775 S2776 Y2777 G2778 E2779 N2780 V2781 D2782 E2783 E2784 L2785 K2786 T2787 H2788 P2789 M2790 L2791 R2792 P2793 Y2794 K2795 T2796 F2797 S2798 E2799 K2800 D2801 K2802 E2803 I2804 Y2805 R2806 W2807 P2808 I2809 K2810 E2811 S2812 L2813 K2814 A2815 M2816 I2817 A2818

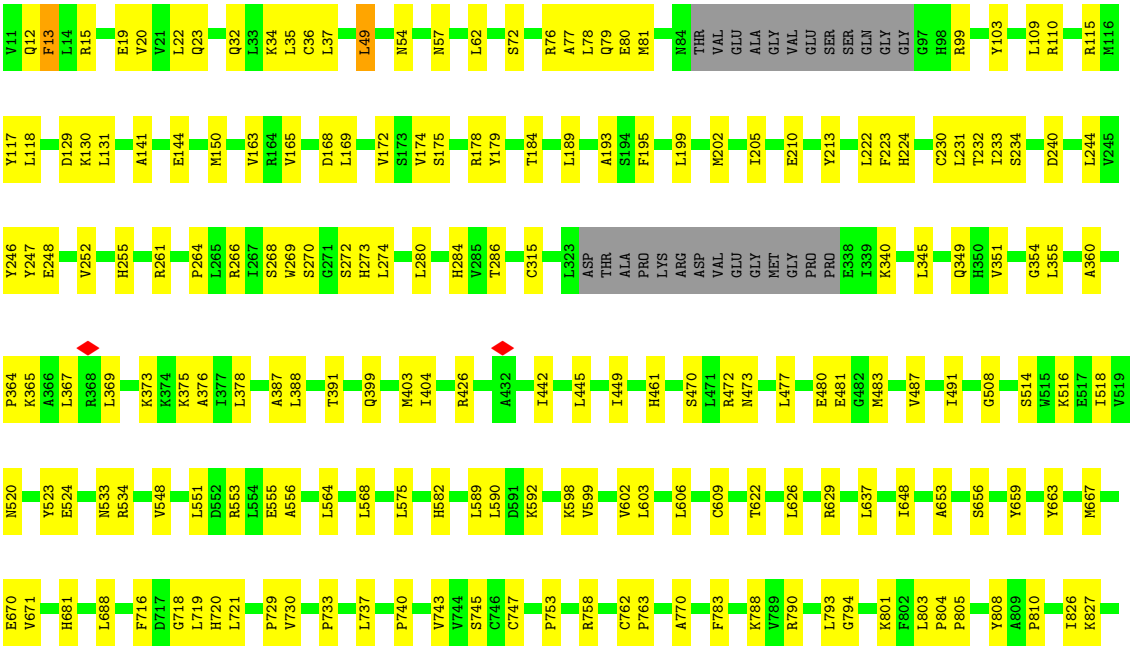

W2819 E2820 W2821 T2822 I2823 E2824 K2825 A2826 R2827 E2828 G2829 E2830 GLU GLU ARG THR GLU LYS LYS LYS THR ARG LYS ILE SER GLN THR ALA GLN THR TYR ASP PRO ARG GLU GLY Y2855 N2856 P2857 Q2858 P2859 P2860 D2861 L2862 S2863 G2864 V2865 T2866 L2867 S2868 R2869 E2870 L2871 M2874 A2875 L2878 A2879 E2880
N2881 Y2882 W2886 K2890 K2891 Q2892 E2893 L2894 E2895 A2896 K2897 G2898 G2899 G2900 T2901 H2902 P2903 L2904 L2905 V2906 P2907 Y2908 L2911 T2912 A2913 K2914 E2915 K2916 A2917 R2918 D2919 R2920 E2921 K2922 A2923 Q2924 E2925 L2926 L2927 K2928 F2929 L2930 Q2931 M2932 N2933 G2934 Y2935 A2936 V2937 T2938 R2939 GLY LEU LYS ASP MET GLU
L2946 D2947 T2948 I2951 E2952 K2953 R2954 F2955 A2956 F2957 G2958 F2959 L2960 Q2961 Q2962 L2963 L2964 R2965 W2966 M2967 S2970 F2973 T2974 A2975 H2976 L2977 E2978 A2979 V2980 V2981 R2985 V2986 E2987 P2990 H2991 I2995 K2996 I3001 L3002 L3003 P3004 L3005 I3006 N3007 Q3008 Y3009 F3010 C3014 L3018 S3019 T3020
P3021 A3022 K3023 V3024 L3025 G3026 S3032 K3036 E3037 M3038 I3039 K3045 L3049 H3052 P3062 A3063 V3064 V3065 N3066 C3067 L3068 H3069 I3070 L3071 S3074 L3075 D3076 A3077 R3078 T3079 V3080 M3081 K3082 P3085 K3089 S3100 E3101 D3102 I3103 E3104 K3105 M3106 V3107 L3110 R3111 LEU GLY LYS VAL
SER GLN ALA ARG THR GLN VAL LYS GLY VAL GLY Q3127 N3128 L3129 T3130 T3133 L3137 P3138 H3146 H3150 Q3151 F3152 D3155 V3156 Q3162 V3163 S3164 C3165 Y3166 L3169 I3172 L3175 N3180 T3181 Y3182 V3183 R3187 L3190 G3191 E3192 C3193 L3194 A3195 R3196 M3201 P3202 V3203
L3206 E3207 P3208 N3211 S3217 K3222 S3223 P3224 R3225 E3226 R3227 L3232 P3233 V3236 P3244 V3245 L3246 L3249 M3250 A3251 D3252 I3253 L3256 R3262 E3265 M3266 E3271 I3272 T3273 L3274 P3275 M3276 L3277 Y3280 L3281 P3282 L3296 P3297 A3298 P3303 C3304 T3305 L3315 L3316
G3317 N3318 I3319 I3322 I3323 D3330 W3334 M3335 K3336 R3337 V3340 F3341 A3342 I3345 R3350 L3354 R3366 K3367 R3368 A3369 G3370 K3371 V3372 V3373 L3379 A3387 G3390 E3391 V3394 R3395 R3403 Y3406 Y3409 P3410 R3414 Y3415 V3416 R3420 A3421 H3422 W3423 N3428
E3432 E3433 L3434 F3435 R3436 G3439 E3440 I3441 F3442 I3443 Y3444 W3445 K3452 R3453 E3454 E3455 V3459 I3464 K3475 SER LYS MET ALA LYS ALA GLY ASP ALA GLN SER GLY GLY SER ASP GLN GLU ARG THR LYS LYS LYS ARG ARG GLY ASP ARG TYR S3504 S3508 L3509 T3510 V3511 A3512
K3516 P3519 L3522 N3523 M3524 Q3530 D3531 L3532 I3533 M3534 L3535 T3538 R3539 Y3540 A3541 L3542 K3543 D3544 T3545 D3546 E3547 E3548 V3549 R3550 E3551 Q3560 G3561 K3562 V3563 S3566 P3567 S3568 L3569 R3570 W3571 Q3572 M3573 L3579 P3580 V3596 Q3597 E3598 V3602 L3603 Y3604 E3607 E3610 H3611
P3612 TYR LYS SER LYS LYS ALA VAL TRP HIS LYS LEU LEU SER LYS GLN ARG ARG ARG ALA VAL VAL ALA CYS PHE ARG MET T3639 P3640 L3641 Y3642 K3658 H3667 M3673 Q3683 E3684 E3685 E3686 E3689 K3693 L3698 V3702 R3707 T3708 A3709 D3719 Y3722 D3727
I3728 M3729 A3730 K3731 S3732 C3733 H3734 E3740 ASN GLY GLU ALA GLU GLU E3747 E3754 E3757 Q3761 Q3766 Q3767 S3768 H3771 A3775 M3778 M3782 T3790 M3793 V3794 L3798 K3799 L3800 I3804 L3805 Q3813 I3832 Q3833 A3834 L3835 M3836 V3841 L3842 D3843 L3844
D3862 E3872 K3873 V3874 F3880 D3883 L3884 R3904 T3905 Q3906 I3913 N3914 I3917 R3925 L3926 Q3927 E3928 S3929 W3935 Y3936 Q3946 G3947 K3948 R3949 A3954 M3955 F3962 L3965 T3966 E3967 Y3968 I3969 Q3970 L3980 W3986 V3989 V3990 G3991 F3992 L3993 H3994 V3995 F3996 M3999
Q4009 D4018 L4019 Q4020 K4021 D4022 M4023 M4026 N4037 R4042 Q4043 M4044 S4053 M4057 I4058 L4059 K4060 M4064 I4071 Q4078 D4079 Y4080 V4081 T4082 D4083 G4086 L4087 I4088 K4095 A4096 M4097 T4104 I4108 S4115 E4116 M4122 I4123 N4124 R4131 V4145 S4151
L4160 F4163 L4164 A4167 Y4177 L4178 E4182 I4190 E4199 R4202 E4206 V4210 M4231 V4235 C4238 T4241 I4242 M4245 A4248 I4251 S4252 E4253 PRO GLU GLY GLU PRO GLU ALA ASP GLU ASP GLU GLY MET GLY GLU ALA ALA ALA GLU GLY ALA

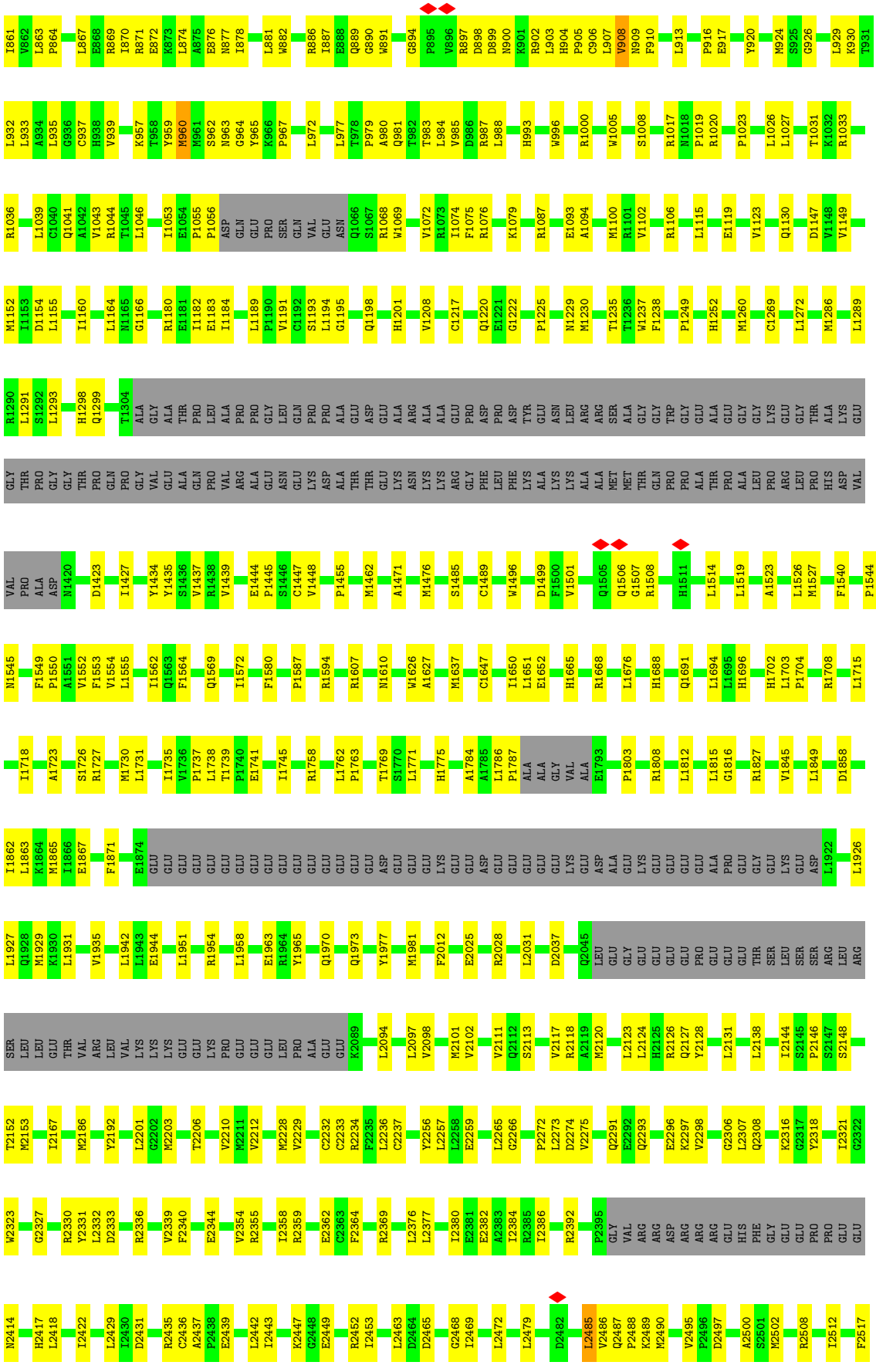


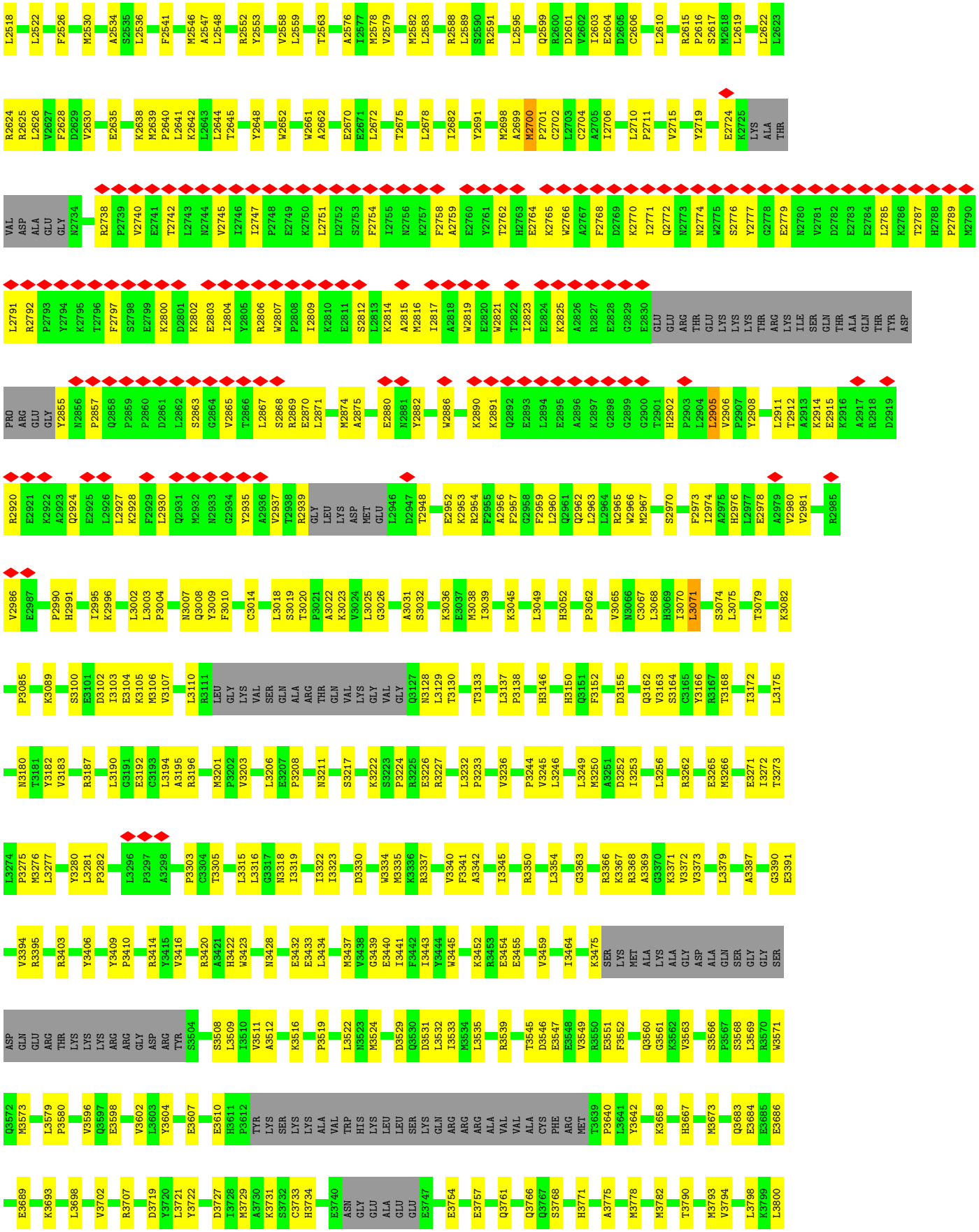
• Molecule 1: Ryanodine receptor 1

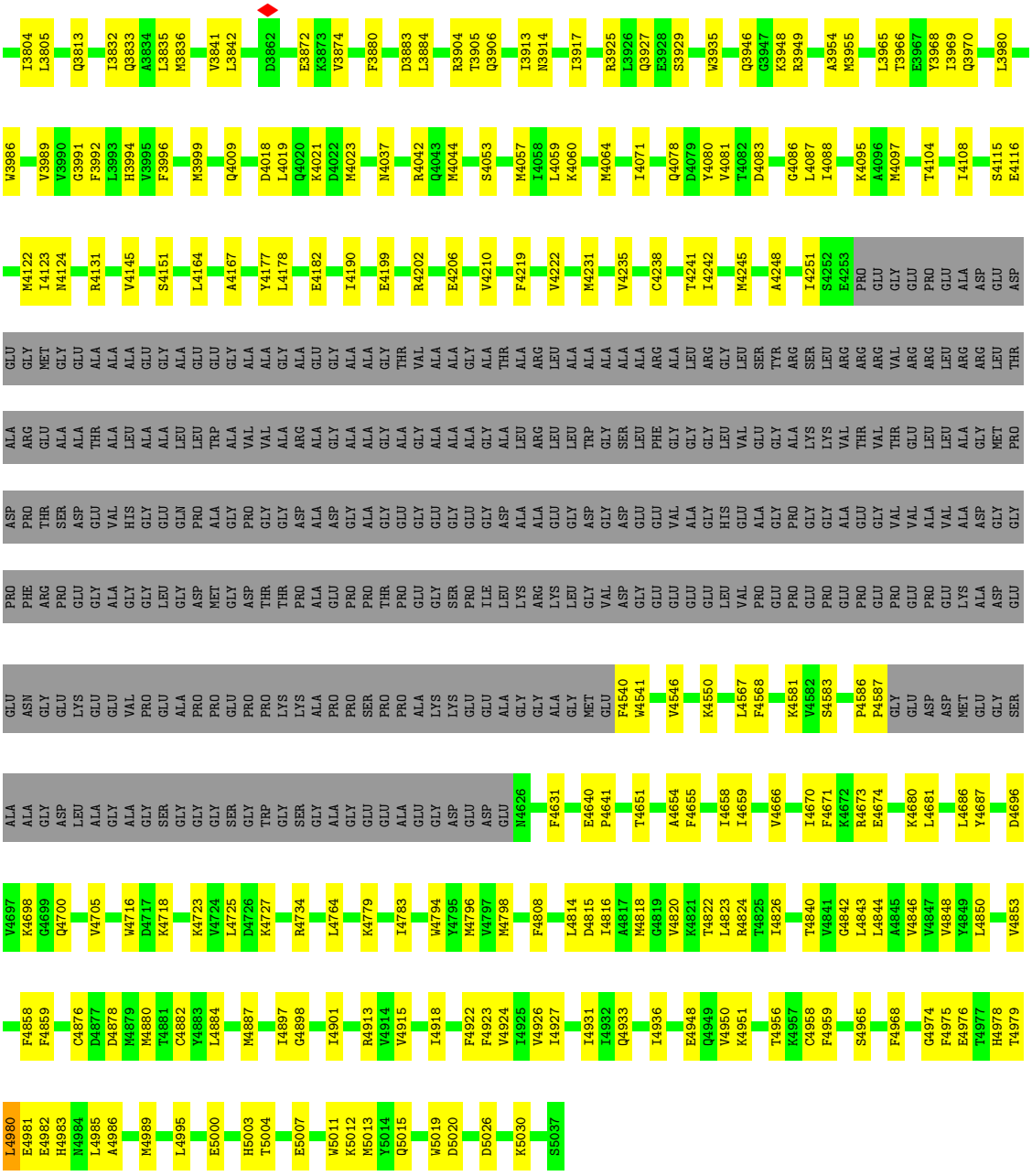
Chain C:





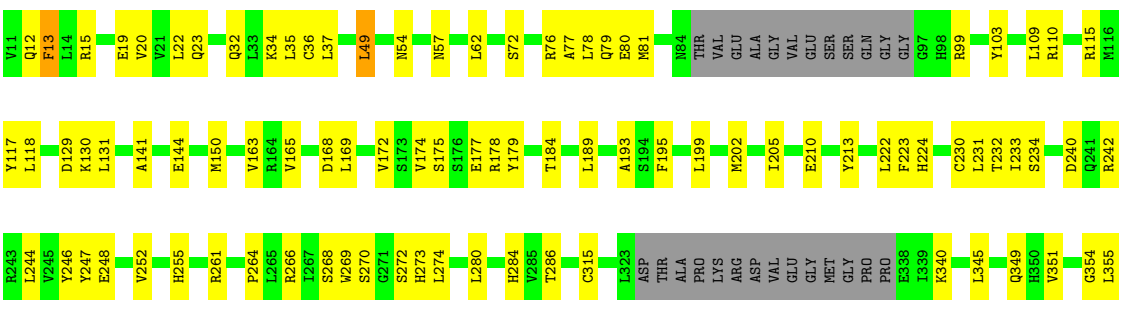


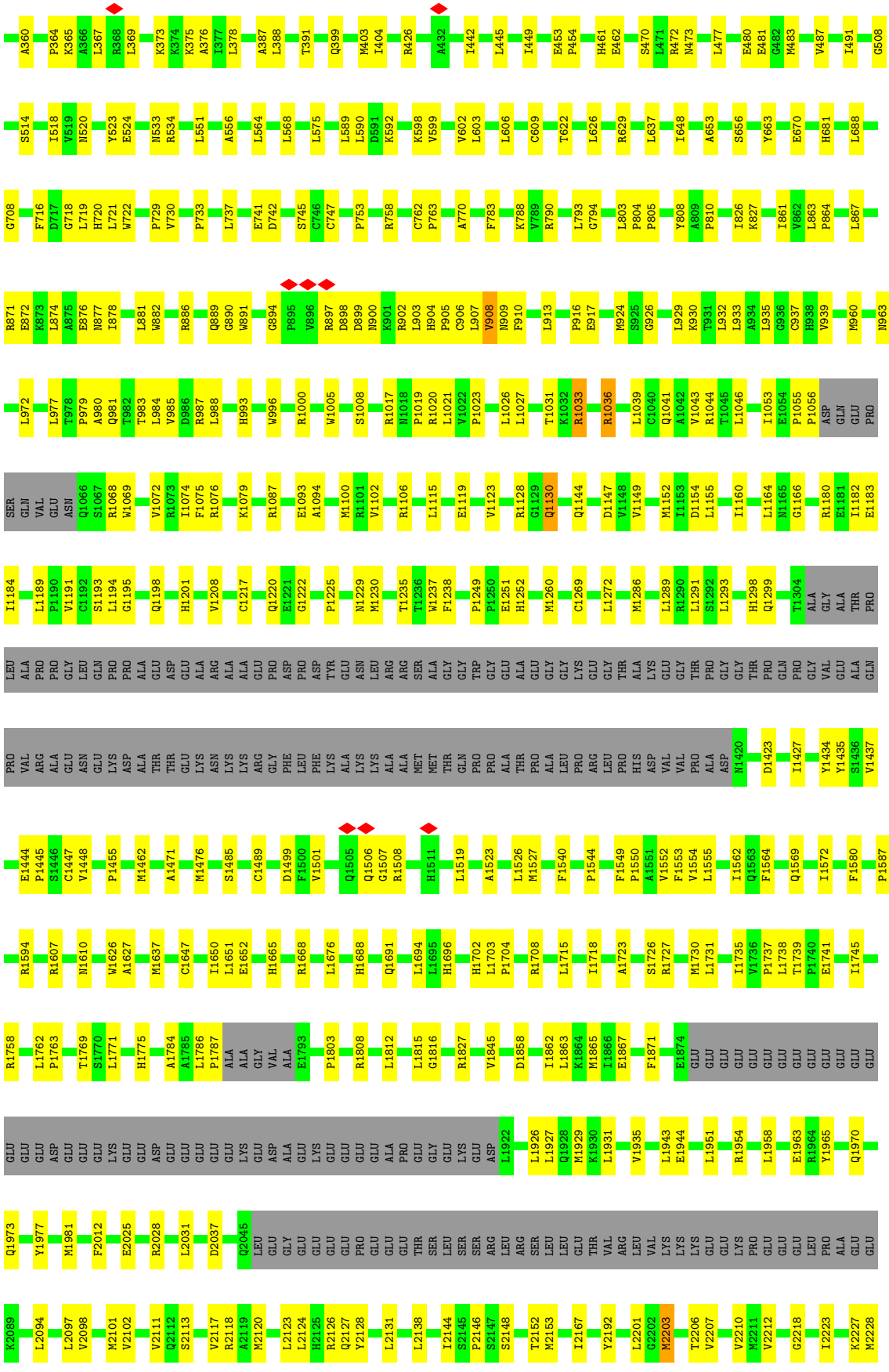


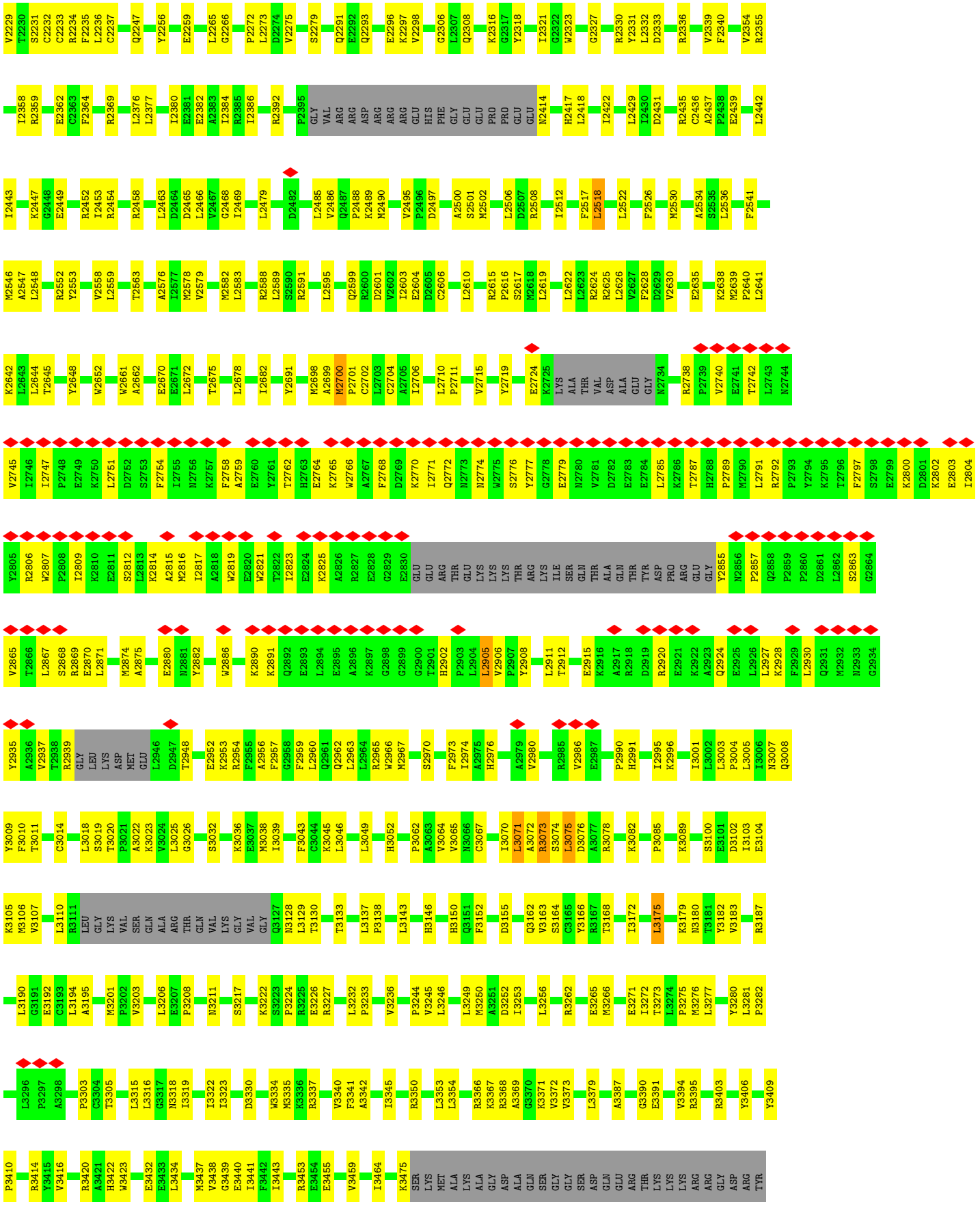
• Molecule 1: Ryanodine receptor 1

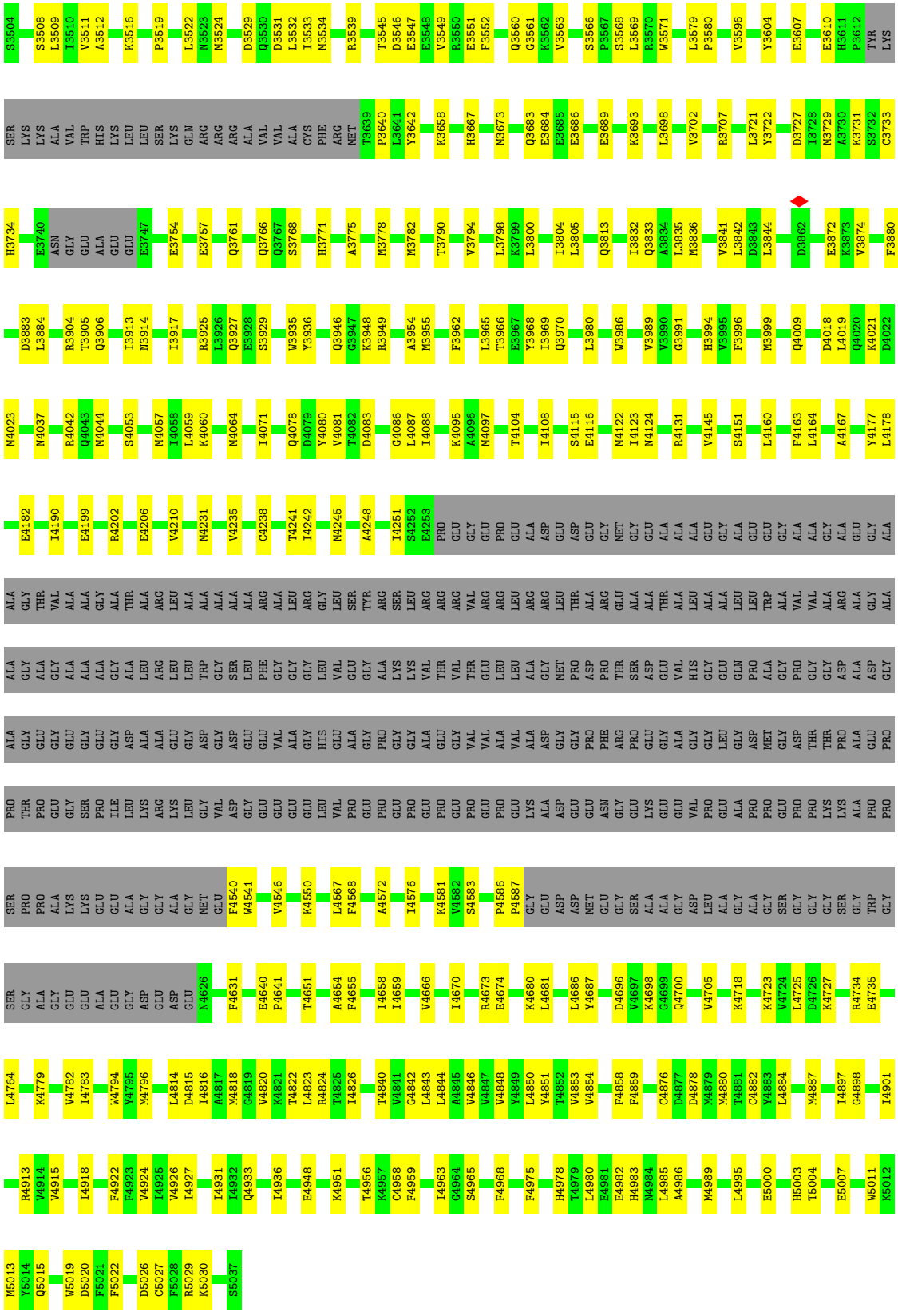
Chain G:




A360 P364 K365 A366 L367 R368 L369 K373 K374 K375 A376 I377 L378 A387 L388 T391 Q399 M403 I404 R426 A432 I442 L445 L449 E453 P454 H461 E462 S470 L471 R472 N473 L477 E480 E481 G482 M483 V487 I491 G508
S514 I518 V519 N520 Y523 E524 N533 R534 L551 A556 L564 L568 L575 L589 L590 D591 K592 K598 K599 V602 L603 L606 C609 T622 L626 R629 L637 I648 A653 S656 Y663 E670 H681 L688
G708 F716 D717 G718 L719 H720 L721 W722 P729 V730 P733 L737 E741 D742 S745 C746 C747 P753 R758 C762 P763 A770 F783 K788 V789 R790 L793 G794 L803 P804 P805 Y808 A809 P810 I826 K827 I861 V862 L863 P864 L867
R871 E872 K873 L874 A875 E876 N877 I878 L881 W882 R886 Q889 G890 W891 G894 P895 V896 R897 D898 D899 N900 K901 R902 L903 P904 P905 C906 L907 V908 N909 F910 L913 P916 E917 N924 S925 G926 L929 K930 T931 L932 L933 A934 L935 G936 C937 H938 V939 N960 N963
L972 L977 T978 P979 A980 Q981 T982 T983 L984 V985 D986 R987 L988 H993 W996 R1000 W1005 S1008 R1017 N1018 P1019 R1020 L1021 V1022 P1023 L1026 L1027 T1031 K1032 R1033 R1036 L1039 C1040 Q1041 A1042 A1043 R1044 T1045 L1046 I1053 E1054 P1055 P1056 ASP GLN GLU PRO
SER GLN VAL GLU ASN Q1066 S1067 R1068 W1069 V1072 R1073 I1074 F1075 R1076 K1079 R1087 E1093 A1094 M1100 R1101 V1102 R1106 L1115 E1119 V1123 R1128 G1129 Q1130 Q1144 D1147 V1148 V1149 M1152 I1153 D1154 L1155 I1160 L1164 N1165 G1166 R1180 E1181 I1182 E1183
I1184 L1189 P1190 V1191 C1192 S1193 L1194 G1195 Q1198 H1201 V1208 C1217 Q1220 E1221 G1222 P1225 N1229 M1230 T1235 T1236 W1237 F1238 P1249 P1250 E1251 H1252 M1260 C1269 L1272 M1286 L1289 R1290 L1291 S1292 L1293 H1298 Q1299 T1304 ALA GLY ALA THR PRO
LEU ALA PRO PRO GLY LEU GLN PRO PRO ALA GLU GLU ASP GLU ALA ARG ALA ALA GLU PRO ASP PRO ASP TYR GLU ASN LEU ARG ARG SER ALA GLY GLY GLY TRP GLY GLU ALA GLU GLY GLY LYS GLU GLU GLY THR ALA LYS GLU GLY THR PRO GLY GLY THR PRO GLN PRO GLY VAL GLU ALA GLN
PRO VAL ARG ALA GLU ASN GLU LYS ASP ALA THR THR GLU LYS ASN LYS LYS ARG GLY PHE LEU PHE LYS ALA LYS LYS ALA ALA MET MET THR GLN PRO PRO ALA THR PRO ALA LEU PRO ARG LEU PRO HIS ASP VAL VAL PRO ALA ASP N1420 D1423 I1427 Y1434 Y1435 S1436 V1437
E1444 P1445 S1446 C1447 V1448 P1455 M1462 A1471 M1476 S1485 C1489 D1499 F1500 V1501 Q1505 Q1506 G1507 R1508 H1511 L1519 A1523 L1526 M1527 F1540 P1544 F1549 P1550 A1551 V1552 F1553 V1554 L1555 I1562 Q1563 F1564 Q1569 I1572 F1580 P1587
R1594 R1607 N1610 W1626 A1627 M1637 C1647 I1650 L1651 E1652 H1665 R1668 L1676 H1688 Q1691 L1694 L1695 H1696 H1702 L1703 P1704 R1708 L1715 I1718 A1723 S1726 R1727 M1730 L1731 I1735 V1736 P1737 L1738 T1739 P1740 E1741 I1745
R1758 L1762 P1763 T1769 S1770 L1771 H1775 A1784 A1785 L1786 P1787 ALA ALA GLY VAL ALA E1793 P1803 R1808 L1812 L1815 L1816 R1827 V1845 D1858 I1862 I1863 K1864 M1865 I1866 E1867 F1871 E1874 GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU
GLU GLU GLU ASP GLU GLU GLU GLU ASP GLU GLU GLU GLU GLU LYS GLU GLU GLU ALA PRO GLU GLY GLU GLU GLU ASP L1922 L1926 L1927 Q1928 M1929 K1930 L1931 V1935 L1943 E1944 L1951 R1954 L1958 E1963 R1964 Y1965 Q1970
Q1973 Y1977 M1981 F2012 E2025 R2028 L2031 D2037 Q2045 LEU GLU GLU GLY GLU GLU GLU GLU PRO GLU GLU GLU THR SER LEU SER SER ARG LEU ARG ARG SER LEU LEU LEU GLU THR VAL ARG LEU LEU VAL LYS LYS LYS GLU GLU LYS PRO GLU GLU GLU LEU PRO ALA GLU GLU
K2089 L2094 L2097 V2098 M2101 V2102 V2111 Q2112 S2113 V2117 R2118 A2119 M2120 L2123 L2124 H2125 R2126 Q2127 V2128 L2131 L2138 I2144 S2145 P2146 S2147 S2148 T2152 M2153 I2167 Y2192 L2201 G2202 M2203 T2206 V2207 V2210 M2211 V2212 G2218 I2223 K2227 M2228

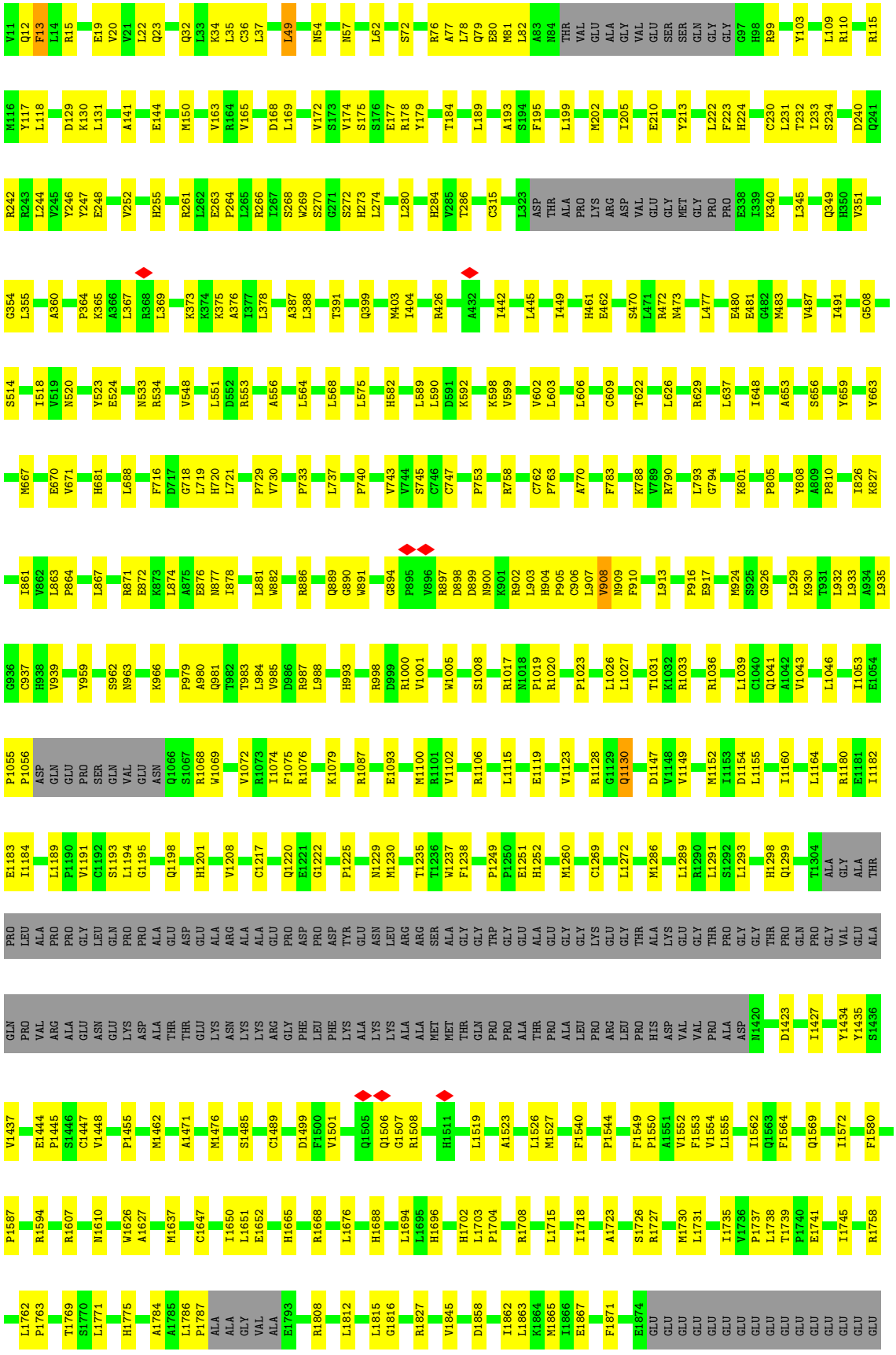


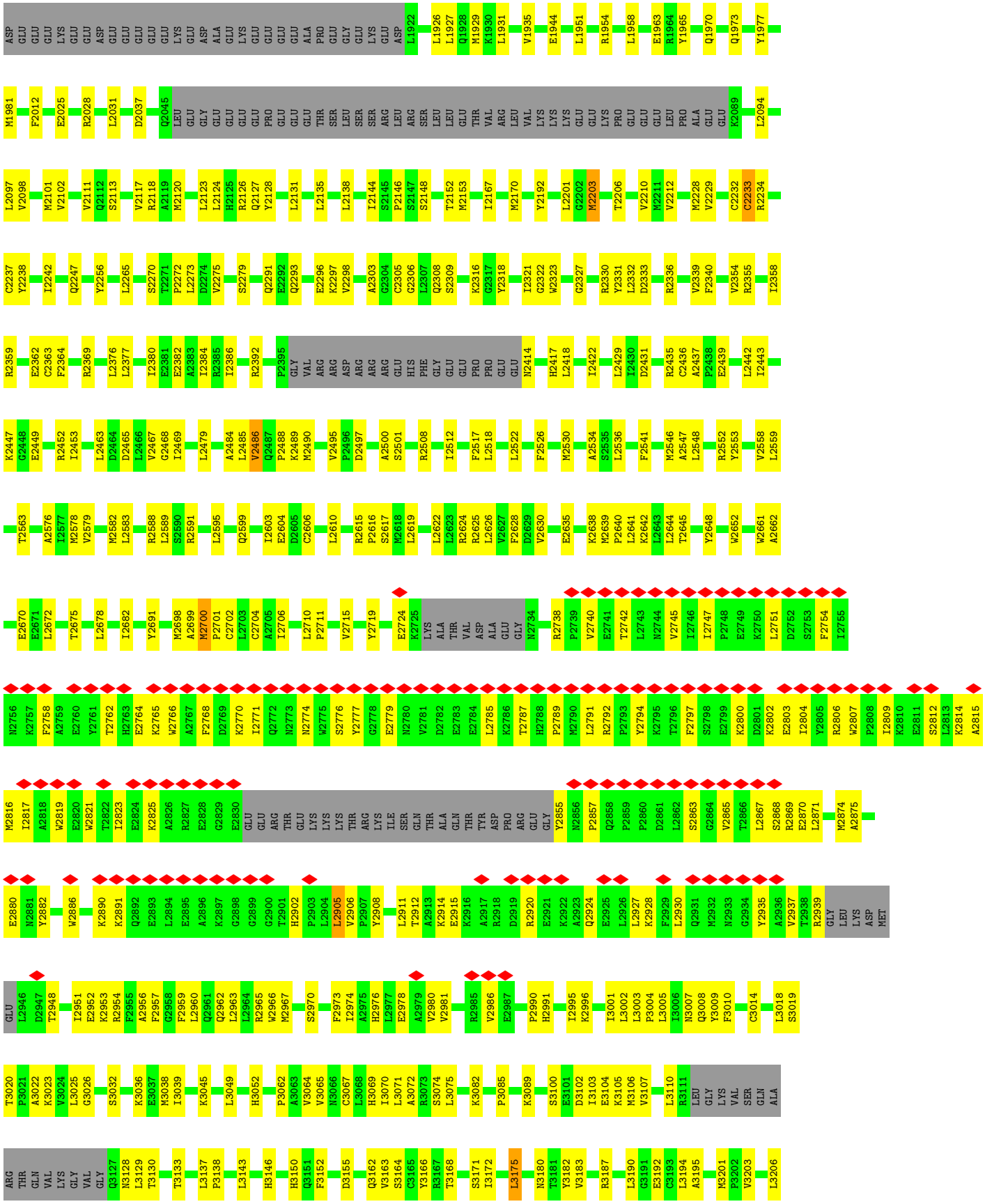


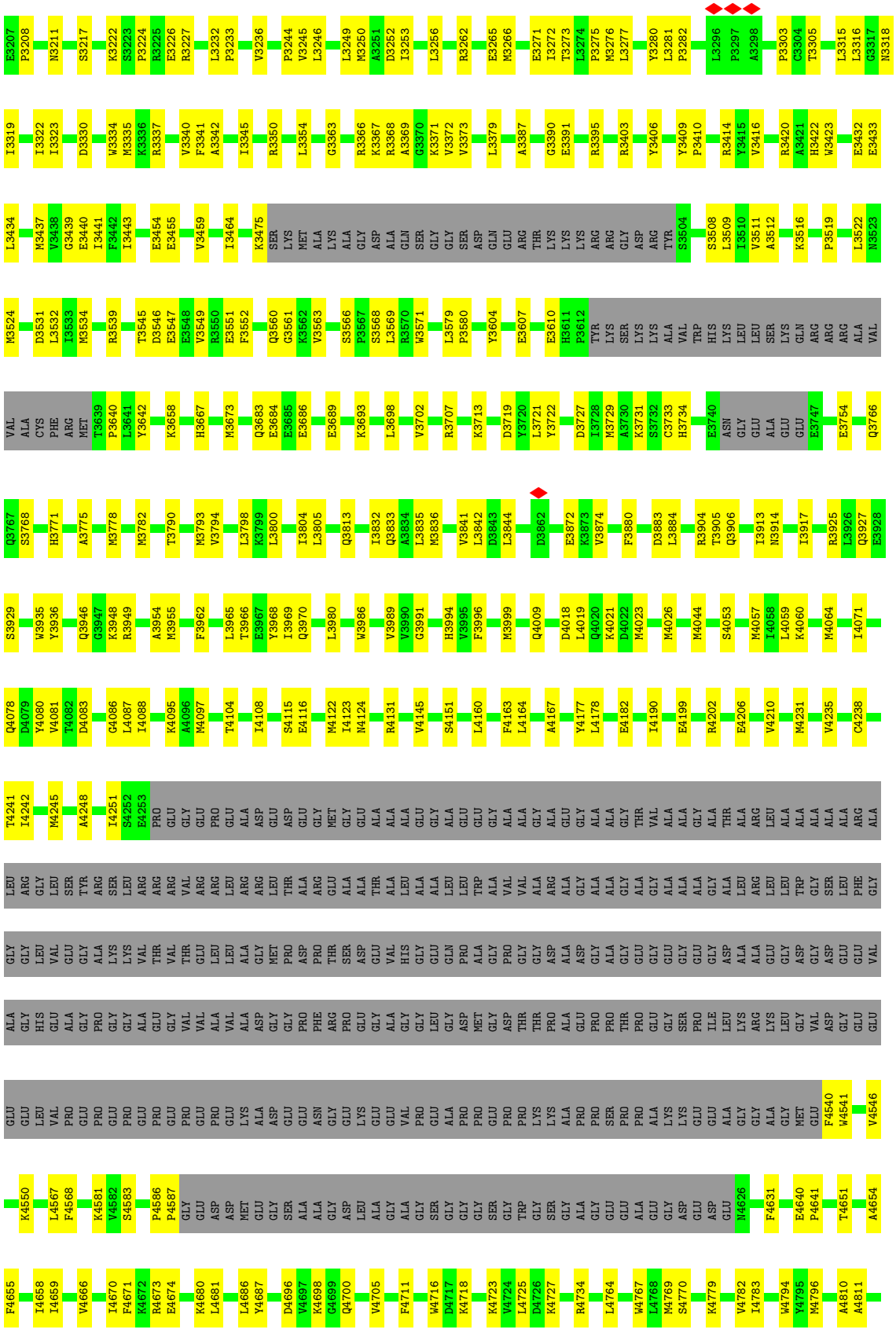
• Molecule 1: Ryanodine receptor 1

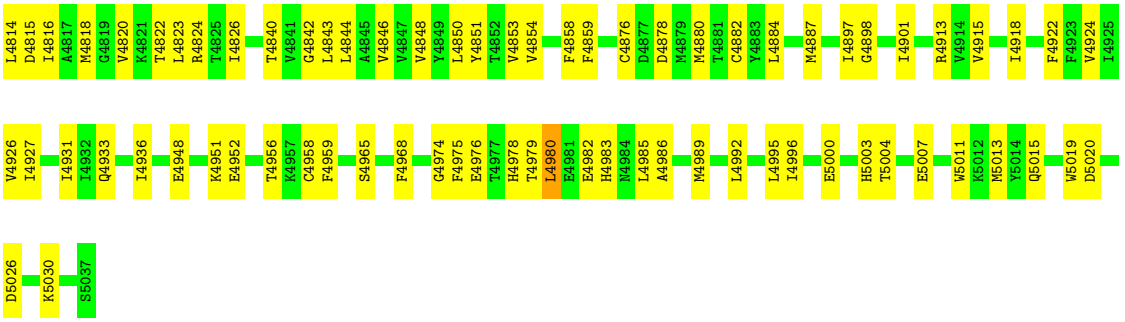
Chain J:




V11 Q12 F13 L14 R15 E19 V20 V21 L22 Q23 Q32 L33 K34 L35 C36 L37 L49 N54 N57 L62 S72 R76 A77 L78 Q79 E80 M81 L82 A83 N84 THR VAL GLU ALA GLY VAL GLU SER SER GLN GLY GLY G97 H98 R99 Y103 L109 R110 R115
M116 Y117 L118 D129 K130 L131 A141 E144 M150 V163 R164 V165 D168 L169 V172 S173 V174 S175 S176 E177 R178 Y179 T184 L189 A193 S194 F195 L199 M202 I205 E210 Y213 L222 F223 H224 C230 L231 T232 I233 S234 D240 Q241
R242 R243 L244 V245 Y246 Y247 E248 V252 H255 R261 L262 E263 P264 L265 R266 I267 S268 W269 S270 Q271 S272 H273 L274 L280 H284 V285 T286 C315 L323 ASP THR ALA PRO LYS ARG ASP VAL GLU GLY MET GLY PRO PRO E338 I339 K340 L345 Q349 H350 V351
G354 L355 A360 P364 K365 A366 L367 R368 L369 K373 K374 K375 A376 I377 L378 A387 L388 T391 Q399 M403 I404 R426 A432 I442 L445 I449 H461 E462 S470 L471 R472 N473 L477 E480 E481 G482 M483 V487 I491 G508
S514 I518 V519 N520 Y523 E524 N533 R534 V548 L551 D552 R553 A556 L564 L568 L575 H582 L589 L590 D591 K592 K598 V599 V602 L603 L606 C609 T622 L626 R629 L637 I648 A653 S656 Y659 Y663
M667 E670 V671 H681 L688 F716 D717 G718 L719 H720 L721 P729 V730 P733 L737 P740 V743 V744 S745 G746 C747 P753 R758 C762 P763 A770 F783 K788 V789 R790 L793 G794 K801 P805 Y808 A809 P810 I826 K827
I861 V862 L863 P864 L867 R871 E872 K873 L874 A875 E876 N877 I878 L881 W882 R886 Q889 G890 W891 G894 P895 V896 R897 D898 D899 N900 K901 R902 L903 H904 P905 C906 L907 V908 N909 F910 L913 P916 E917 M924 S925 G926 L929 K930 T931 L932 L933 A934 L935
G936 C937 H938 V939 Y959 S962 N963 K966 P979 A980 Q981 T982 T983 L984 V985 D986 R987 L988 H993 R998 D999 R1000 V1001 W1005 S1008 R1017 N1018 P1019 R1020 P1023 L1026 L1027 T1031 K1032 R1033 R1036 L1039 C1040 Q1041 A1042 V1043 L1046 I1053 E1054
P1055 P1056 ASP GLN GLU PRO SER GLN VAL GLU ASN Q1066 S1067 R1068 W1069 V1072 R1073 I1074 F1075 R1076 K1079 R1087 E1093 M1100 R1101 V1102 R1106 L1115 E1119 V1123 R1128 G1129 Q1130 D1147 V1148 V1149 M1152 I1153 D1154 L1155 I1160 L1164 R1180 E1181 I1182
E1183 I1184 L1189 P1190 V1191 C1192 S1193 L1194 G1195 Q1198 H1201 V1208 C1217 Q1220 E1221 G1222 P1225 N1229 M1230 T1235 T1236 W1237 F1238 P1249 P1250 E1251 H1252 M1260 C1269 L1272 M1286 L1289 R1290 L1291 S1292 L1293 H1298 Q1299 T1304 ALA GLY ALA THR
PRO LEU ALA PRO PRO GLY LEU GLN PRO PRO ALA GLU ASP GLU ALA ARG ALA ALA GLU PRO ASP PRO ASP TYR GLU ASN LEU ARG ALA ALA ARG SER ALA GLY GLY TRP GLY GLU ALA GLU GLY GLY LYS GLU GLY THR ALA LYS GLU GLY THR PRO GLY GLY THR PRO GLN PRO GLY V1437 E1444 P1445 S1446 C1447 V1448 P1455 M1462 A1471 M1476 S1485 C1489 D1499 F1500 V1501 Q1505 Q1506 G1507 R1508 M1511 L1519 A1523 L1526 M1527 F1540 P1544 F1549 P1550 A1551 V1552 F1553 V1554 L1555 I1562 Q1563 F1564 Q1569 I1572 F1580
GLN PRO VAL ARG ALA GLU ASN GLU LYS ASP ALA THR THR GLU LYS ASN LYS LYS ARG GLY PHE LEU PHE LYS ALA LYS LYS ALA ALA MET MET THR GLN PRO PRO ALA THR PRO ALA LEU PRO ARG LEU PRO HIS ASP VAL VAL PRO ALA ASP N1420 D1423 I1427 Y1434 Y1435 S1436
P1587 R1594 R1607 N1610 W1626 A1627 M1637 C1647 I1650 L1651 E1652 H1665 R1668 L1676 H1688 L1694 L1695 H1696 H1702 L1703 P1704 R1708 L1715 I1718 A1723 S1726 R1727 M1730 L1731 I1735 V1736 P1737 L1738 T1739 P1740 E1741 I1745 R1758
L1762 P1763 T1769 S1770 L1771 H1775 A1784 A1785 L1786 P1787 ALA ALA GLY VAL ALA E1793 R1808 L1812 L1815 G1816 R1827 V1845 D1858 I1862 L1863 K1864 M1865 I1866 E1867 F1871 E1874 GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU GLU



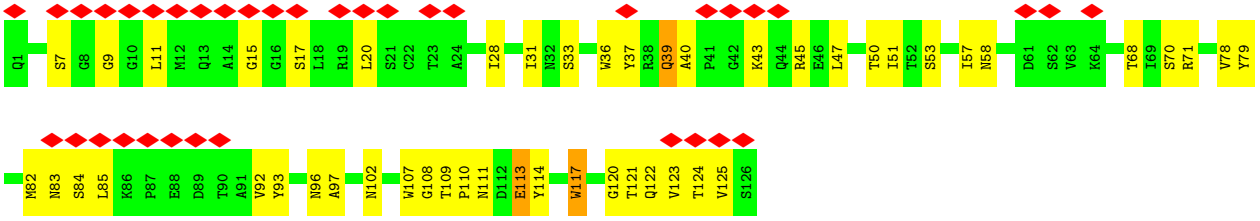





• Molecule 2: Nanobody 9657

Chain B:

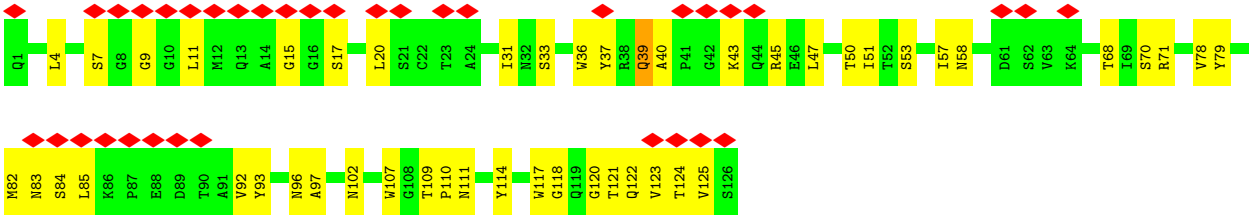



• Molecule 2: Nanobody 9657

Chain D:

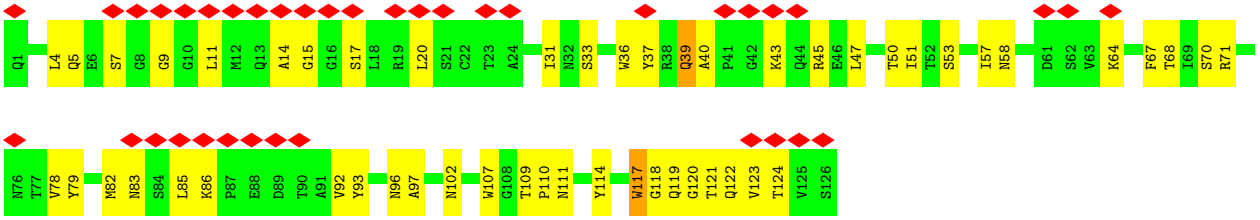



• Molecule 2: Nanobody 9657

Chain H:

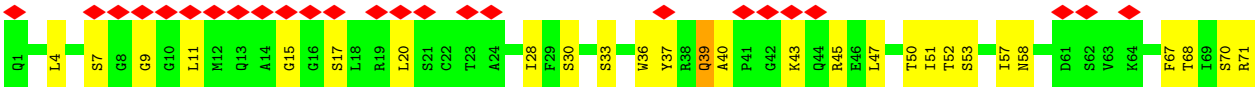


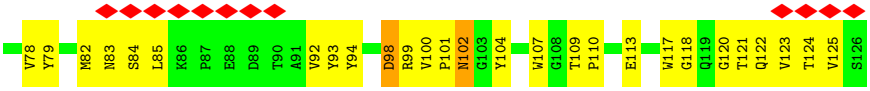




• Molecule 2: Nanobody 9657

Chain K:



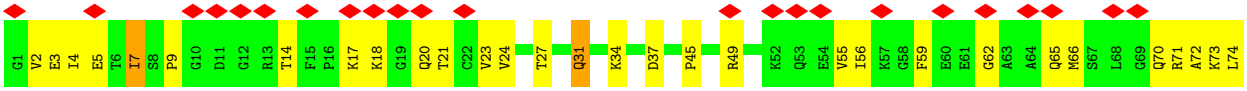



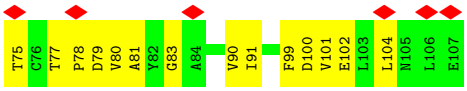



• Molecule 3: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain E:



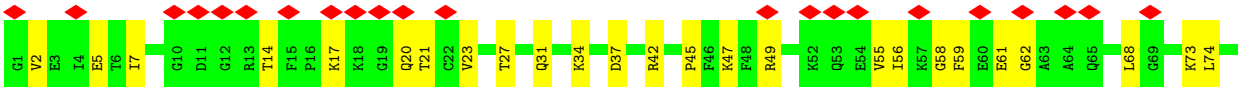



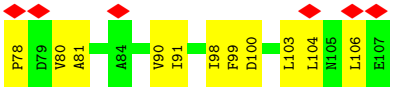




• Molecule 3: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain F:



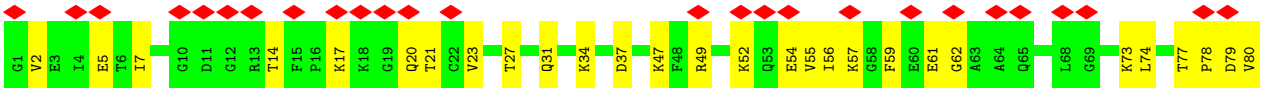



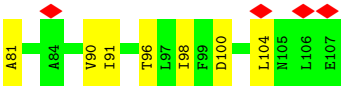




• Molecule 3: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain I:



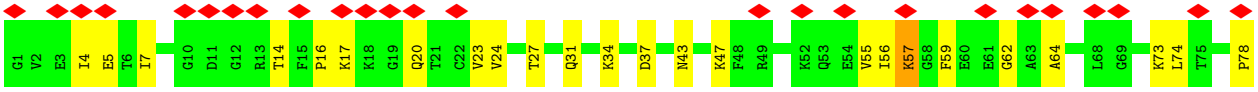



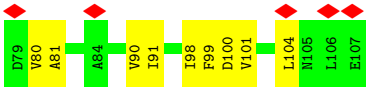




• Molecule 3: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain L:



# 4 Experimental information (i)

| Property | Value | Source |
|---|---|---|
| EM reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, Not provided | |
| Number of particles used | 279776 | Depositor |
| Resolution determination method | FSC 0.143 CUT-OFF | Depositor |
| CTF correction method | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope | JEOL CRYO ARM 300 | Depositor |
| Voltage (kV) | 300 | Depositor |
| Electron dose ($e^-/Å^2$) | 60 | Depositor |
| Minimum defocus (nm) | 1500 | Depositor |
| Maximum defocus (nm) | 2500 | Depositor |
| Magnification | Not provided | |
| Image detector | GATAN K3 (6k x 4k) | Depositor |
| Maximum map value | 5.280 | Depositor |
| Minimum map value | -0.106 | Depositor |
| Average map value | 0.043 | Depositor |
| Map value standard deviation | 0.121 | Depositor |
| Recommended contour level | 0.3 | Depositor |
| Map size (Å) | 479.136, 479.136, 479.136 | wwPDB |
| Map dimensions | 336, 336, 336 | wwPDB |
| Map angles (°) | 90.0, 90.0, 90.0 | wwPDB |
| Pixel spacing (Å) | 1.426, 1.426, 1.426 | Depositor |

# 5 Model quality

## 5.1 Standard geometry

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

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

| Mol | Chain | Bond lengths | | Bond angles | |
|---|---|---|---|---|---|
| | | RMSZ | #$\|Z\|$ >5 | RMSZ | #$\|Z\|$ >5 |
| 1 | A | 0.26 | 0/35002 | 0.49 | 3/47442 (0.0%) |
| 1 | C | 0.27 | 0/35002 | 0.50 | 1/47442 (0.0%) |
| 1 | G | 0.28 | 0/35002 | 0.51 | 2/47442 (0.0%) |
| 1 | J | 0.26 | 0/34999 | 0.49 | 2/47436 (0.0%) |
| 2 | B | 0.38 | 0/981 | 0.66 | 1/1333 (0.1%) |
| 2 | D | 0.35 | 0/981 | 0.65 | 1/1333 (0.1%) |
| 2 | H | 0.48 | 0/981 | 0.72 | 1/1333 (0.1%) |
| 2 | K | 0.52 | 0/981 | 0.74 | 1/1333 (0.1%) |
| 3 | E | 0.59 | 0/834 | 0.93 | 3/1123 (0.3%) |
| 3 | F | 0.57 | 0/834 | 0.87 | 0/1123 |
| 3 | I | 0.63 | 0/834 | 0.93 | 0/1123 |
| 3 | L | 0.66 | 0/834 | 0.90 | 0/1123 |
| All | All | 0.28 | 0/147265 | 0.52 | 15/199586 (0.0%) |

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

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|---|---|---|---|
| 1 | A | 0 | 1 |
| 1 | G | 0 | 2 |
| All | All | 0 | 3 |

There are no bond length outliers.

All (15) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | A | 3436 | ARG | N-CA-C | 7.07 | 118.99 | 111.28 |
| 1 | A | 1499 | ASP | N-CA-C | -5.49 | 106.75 | 113.50 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 1 | J | 1499 | ASP | N-CA-C | -5.41 | 106.85 | 113.50 |
| 1 | G | 1499 | ASP | N-CA-C | -5.35 | 106.92 | 113.50 |
| 1 | C | 967 | PRO | N-CA-CB | -5.32 | 98.29 | 102.28 |
| 3 | E | 7 | ILE | N-CA-C | -5.26 | 106.67 | 111.67 |
| 1 | A | 1499 | ASP | CA-CB-CG | 5.22 | 117.82 | 112.60 |
| 3 | E | 83 | GLY | N-CA-C | 5.16 | 116.42 | 111.67 |
| 1 | G | 1499 | ASP | CA-CB-CG | 5.14 | 117.75 | 112.60 |
| 1 | J | 1499 | ASP | CA-CB-CG | 5.13 | 117.73 | 112.60 |
| 2 | K | 39 | GLN | CA-CB-CG | 5.10 | 124.30 | 114.10 |
| 2 | H | 39 | GLN | CA-CB-CG | 5.08 | 124.27 | 114.10 |
| 2 | B | 39 | GLN | CA-CB-CG | 5.08 | 124.27 | 114.10 |
| 2 | D | 39 | GLN | CA-CB-CG | 5.08 | 124.25 | 114.10 |
| 3 | E | 31 | GLN | CA-CB-CG | 5.01 | 124.11 | 114.10 |

There are no chirality outliers.

All (3) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group |
|---|---|---|---|---|
| 1 | A | 5029 | ARG | Sidechain |
| 1 | G | 1033 | ARG | Sidechain |
| 1 | G | 5029 | ARG | Sidechain |

## 5.2 Too-close contacts (i)

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 1 | A | 34225 | 0 | 33636 | 808 | 0 |
| 1 | C | 34225 | 0 | 33636 | 822 | 0 |
| 1 | G | 34225 | 0 | 33636 | 809 | 0 |
| 1 | J | 34224 | 0 | 33634 | 809 | 0 |
| 2 | B | 961 | 0 | 905 | 33 | 0 |
| 2 | D | 961 | 0 | 905 | 32 | 0 |
| 2 | H | 961 | 0 | 905 | 31 | 0 |
| 2 | K | 961 | 0 | 905 | 35 | 0 |
| 3 | E | 818 | 0 | 824 | 32 | 0 |
| 3 | F | 818 | 0 | 824 | 25 | 0 |
| 3 | I | 818 | 0 | 824 | 22 | 0 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|---|---|---|---|---|---|---|
| 3 | L | 818 | 0 | 824 | 24 | 0 |
| 4 | A | 1 | 0 | 0 | 0 | 0 |
| 4 | C | 1 | 0 | 0 | 0 | 0 |
| 4 | G | 1 | 0 | 0 | 0 | 0 |
| 4 | J | 1 | 0 | 0 | 0 | 0 |
| 5 | A | 31 | 0 | 12 | 1 | 0 |
| 5 | C | 31 | 0 | 12 | 2 | 0 |
| 5 | G | 31 | 0 | 12 | 1 | 0 |
| 5 | J | 31 | 0 | 12 | 2 | 0 |
| 6 | A | 14 | 0 | 10 | 0 | 0 |
| 6 | C | 14 | 0 | 10 | 0 | 0 |
| 6 | G | 14 | 0 | 10 | 0 | 0 |
| 6 | J | 14 | 0 | 10 | 0 | 0 |
| 7 | A | 1 | 0 | 0 | 0 | 0 |
| 7 | C | 1 | 0 | 0 | 0 | 0 |
| 7 | G | 1 | 0 | 0 | 0 | 0 |
| 7 | J | 1 | 0 | 0 | 0 | 0 |
| 8 | A | 645 | 0 | 873 | 39 | 0 |
| 8 | C | 645 | 0 | 873 | 42 | 0 |
| 8 | G | 645 | 0 | 873 | 37 | 0 |
| 8 | J | 645 | 0 | 873 | 43 | 0 |
| All | All | 146783 | 0 | 145038 | 3476 | 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 12.

All (3476) 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) |
|---|---|---|---|
| 1:G:3539:ARG:HH12 | 1:G:3552:PHE:HB2 | 1.24 | 1.00 |
| 1:C:3539:ARG:HH12 | 1:C:3552:PHE:HB2 | 1.24 | 1.00 |
| 1:J:3539:ARG:HH12 | 1:J:3552:PHE:HB2 | 1.24 | 0.99 |
| 1:C:3315:LEU:HD22 | 1:C:3345:ILE:HG12 | 1.51 | 0.91 |
| 1:G:3315:LEU:HD22 | 1:G:3345:ILE:HG12 | 1.51 | 0.91 |
| 1:J:3315:LEU:HD22 | 1:J:3345:ILE:HG12 | 1.51 | 0.90 |
| 1:A:3315:LEU:HD22 | 1:A:3345:ILE:HG12 | 1.51 | 0.90 |
| 1:C:3018:LEU:HD13 | 1:C:3074:SER:HA | 1.56 | 0.86 |
| 1:G:2962:GLN:HG3 | 1:G:2965:ARG:HH21 | 1.41 | 0.86 |
| 1:G:897:ARG:HB2 | 1:G:900:ASN:HD22 | 1.42 | 0.85 |
| 1:A:1299:GLN:HG2 | 3:F:31:GLN:HE22 | 1.41 | 0.85 |
| 1:C:4087:LEU:HB2 | 1:C:4122:MET:HG3 | 1.58 | 0.85 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:2962:GLN:HG3 | 1:C:2965:ARG:HH21 | 1.41 | 0.85 |
| 1:J:2962:GLN:HG3 | 1:J:2965:ARG:HH21 | 1.41 | 0.85 |
| 1:A:4087:LEU:HB2 | 1:A:4122:MET:HG3 | 1.58 | 0.84 |
| 1:C:897:ARG:HB2 | 1:C:900:ASN:HD22 | 1.42 | 0.84 |
| 1:G:4081:VAL:HG12 | 1:G:4088:ILE:HB | 1.60 | 0.84 |
| 1:A:897:ARG:HB2 | 1:A:900:ASN:HD22 | 1.42 | 0.84 |
| 1:G:4087:LEU:HB2 | 1:G:4122:MET:HG3 | 1.58 | 0.84 |
| 1:J:4081:VAL:HG12 | 1:J:4088:ILE:HB | 1.60 | 0.84 |
| 1:A:2962:GLN:HG3 | 1:A:2965:ARG:HH21 | 1.41 | 0.84 |
| 1:J:897:ARG:HB2 | 1:J:900:ASN:HD22 | 1.42 | 0.84 |
| 1:J:1299:GLN:HG2 | 3:L:31:GLN:HE22 | 1.43 | 0.84 |
| 1:C:1299:GLN:HG2 | 3:E:31:GLN:HE22 | 1.43 | 0.83 |
| 1:C:4081:VAL:HG12 | 1:C:4088:ILE:HB | 1.60 | 0.83 |
| 1:C:4541:TRP:HZ3 | 1:C:4764:LEU:H | 1.26 | 0.83 |
| 1:G:1299:GLN:HG2 | 3:I:31:GLN:HE22 | 1.43 | 0.83 |
| 1:J:4087:LEU:HB2 | 1:J:4122:MET:HG3 | 1.58 | 0.83 |
| 3:E:5:GLU:HB3 | 3:E:73:LYS:HB2 | 1.59 | 0.82 |
| 1:A:4541:TRP:HZ3 | 1:A:4764:LEU:H | 1.26 | 0.82 |
| 1:A:4081:VAL:HG12 | 1:A:4088:ILE:HB | 1.60 | 0.82 |
| 1:G:3011:THR:HA | 1:G:3073:ARG:NH1 | 1.95 | 0.81 |
| 1:G:4541:TRP:HZ3 | 1:G:4764:LEU:H | 1.26 | 0.81 |
| 2:H:64:LYS:HG2 | 2:H:86:LYS:HZ2 | 1.46 | 0.81 |
| 1:J:2376:LEU:HB2 | 1:J:2465:ASP:HB3 | 1.61 | 0.80 |
| 3:I:5:GLU:HB3 | 3:I:73:LYS:HB3 | 1.63 | 0.80 |
| 1:C:2272:PRO:HA | 1:C:2275:VAL:HG23 | 1.64 | 0.80 |
| 1:J:4541:TRP:HZ3 | 1:J:4764:LEU:H | 1.26 | 0.80 |
| 1:A:1043:VAL:HA | 1:A:1046:LEU:HD12 | 1.63 | 0.80 |
| 1:C:908:VAL:HA | 1:C:963:ASN:HA | 1.62 | 0.79 |
| 3:I:78:PRO:HA | 3:I:81:ALA:HB3 | 1.65 | 0.79 |
| 1:G:2218:GLY:HA2 | 1:G:2223:ILE:HA | 1.64 | 0.79 |
| 1:A:3082:LYS:HD3 | 1:A:3155:ASP:HB2 | 1.65 | 0.79 |
| 1:A:3201:MET:HE3 | 1:A:3202:PRO:HD2 | 1.65 | 0.79 |
| 1:C:2700:MET:HE1 | 1:C:3004:PRO:HB2 | 1.64 | 0.79 |
| 1:G:2700:MET:HE1 | 1:G:3004:PRO:HB2 | 1.64 | 0.79 |
| 1:A:2700:MET:HE1 | 1:A:3004:PRO:HB2 | 1.64 | 0.78 |
| 1:C:1043:VAL:HA | 1:C:1046:LEU:HD12 | 1.63 | 0.78 |
| 1:J:2700:MET:HE1 | 1:J:3004:PRO:HB2 | 1.64 | 0.78 |
| 1:G:2700:MET:HG3 | 1:G:2701:PRO:HD3 | 1.66 | 0.78 |
| 1:J:2700:MET:HG3 | 1:J:2701:PRO:HD3 | 1.67 | 0.77 |
| 1:C:988:LEU:HB2 | 1:C:1039:LEU:HD21 | 1.65 | 0.77 |
| 1:J:575:LEU:HD12 | 1:J:609:CYS:HB3 | 1.67 | 0.77 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:2700:MET:HG3 | 1:A:2701:PRO:HD3 | 1.67 | 0.77 |
| 1:G:1043:VAL:HA | 1:G:1046:LEU:HD12 | 1.63 | 0.77 |
| 1:J:1043:VAL:HA | 1:J:1046:LEU:HD12 | 1.66 | 0.76 |
| 1:J:988:LEU:HB2 | 1:J:1039:LEU:HD21 | 1.68 | 0.76 |
| 1:G:3082:LYS:HD3 | 1:G:3155:ASP:HB2 | 1.68 | 0.76 |
| 1:J:2965:ARG:HH12 | 1:J:2966:TRP:HE3 | 1.31 | 0.76 |
| 1:C:575:LEU:HD12 | 1:C:609:CYS:HB3 | 1.67 | 0.76 |
| 1:C:2700:MET:HG3 | 1:C:2701:PRO:HD3 | 1.67 | 0.76 |
| 1:A:2965:ARG:HH12 | 1:A:2966:TRP:HE3 | 1.31 | 0.76 |
| 1:A:575:LEU:HD12 | 1:A:609:CYS:HB3 | 1.67 | 0.75 |
| 1:C:2965:ARG:HH12 | 1:C:2966:TRP:HE3 | 1.31 | 0.75 |
| 1:G:2218:GLY:CA | 1:G:2223:ILE:HA | 2.16 | 0.75 |
| 1:G:2965:ARG:HH12 | 1:G:2966:TRP:HE3 | 1.31 | 0.75 |
| 1:G:575:LEU:HD12 | 1:G:609:CYS:HB3 | 1.67 | 0.75 |
| 1:A:1286:MET:HE1 | 1:A:1553:PHE:HB3 | 1.69 | 0.74 |
| 1:G:1286:MET:HE1 | 1:G:1553:PHE:HB3 | 1.69 | 0.74 |
| 1:C:1286:MET:HE1 | 1:C:1553:PHE:HB3 | 1.69 | 0.74 |
| 1:C:3194:LEU:HD13 | 1:C:3276:MET:SD | 2.28 | 0.74 |
| 1:G:2628:PHE:HD2 | 1:G:2906:VAL:HG13 | 1.53 | 0.74 |
| 1:G:3072:ALA:HA | 1:G:3075:LEU:HD23 | 1.68 | 0.74 |
| 1:G:2376:LEU:HB2 | 1:G:2465:ASP:HB3 | 1.70 | 0.74 |
| 2:D:58:ASN:HD22 | 2:D:102:ASN:HA | 1.53 | 0.73 |
| 1:A:3195:ALA:HB2 | 1:A:3275:PRO:HB3 | 1.70 | 0.73 |
| 1:J:1286:MET:HE1 | 1:J:1553:PHE:HB3 | 1.69 | 0.73 |
| 1:C:2628:PHE:HD2 | 1:C:2906:VAL:HG13 | 1.53 | 0.73 |
| 1:C:3036:LYS:HD2 | 1:C:3079:THR:HG21 | 1.71 | 0.73 |
| 2:K:58:ASN:HD22 | 2:K:102:ASN:HA | 1.53 | 0.73 |
| 1:G:3194:LEU:HD13 | 1:G:3276:MET:SD | 2.29 | 0.73 |
| 1:C:77:ALA:HA | 1:G:3935:TRP:NE1 | 2.04 | 0.73 |
| 1:J:908:VAL:HG13 | 1:J:910:PHE:H | 1.54 | 0.73 |
| 1:J:2628:PHE:HD2 | 1:J:2906:VAL:HG13 | 1.53 | 0.73 |
| 1:J:3194:LEU:HD13 | 1:J:3276:MET:SD | 2.28 | 0.73 |
| 1:A:77:ALA:HA | 1:C:3935:TRP:NE1 | 2.04 | 0.73 |
| 1:A:3277:LEU:HG | 1:A:3315:LEU:HD12 | 1.71 | 0.73 |
| 2:B:58:ASN:HD22 | 2:B:102:ASN:HA | 1.53 | 0.73 |
| 1:C:908:VAL:HG13 | 1:C:910:PHE:H | 1.54 | 0.73 |
| 1:A:908:VAL:HG13 | 1:A:910:PHE:H | 1.54 | 0.73 |
| 1:A:3935:TRP:NE1 | 1:J:77:ALA:HA | 2.04 | 0.73 |
| 1:G:908:VAL:HG13 | 1:G:910:PHE:H | 1.54 | 0.73 |
| 1:J:3277:LEU:HG | 1:J:3315:LEU:HD12 | 1.71 | 0.73 |
| 1:C:3277:LEU:HG | 1:C:3315:LEU:HD12 | 1.71 | 0.72 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:H:58:ASN:HD22 | 2:H:102:ASN:HA | 1.53 | 0.72 |
| 1:A:3194:LEU:HD13 | 1:A:3276:MET:SD | 2.29 | 0.72 |
| 1:G:4824:ARG:HG3 | 8:G:5113:POV:H15 | 1.71 | 0.72 |
| 1:J:4810:ALA:CA | 1:J:4811:ALA:N | 2.53 | 0.72 |
| 1:G:77:ALA:HA | 1:J:3935:TRP:NE1 | 2.04 | 0.72 |
| 1:G:3277:LEU:HG | 1:G:3315:LEU:HD12 | 1.71 | 0.72 |
| 3:L:74:LEU:HB2 | 3:L:99:PHE:HB2 | 1.71 | 0.72 |
| 1:A:1506:GLN:HB2 | 1:C:2774:ASN:HD22 | 1.55 | 0.71 |
| 1:A:2628:PHE:HD2 | 1:A:2906:VAL:HG13 | 1.53 | 0.71 |
| 1:A:266:ARG:HD3 | 1:A:268:SER:H | 1.55 | 0.71 |
| 1:G:1506:GLN:HB2 | 1:J:2774:ASN:HD22 | 1.56 | 0.71 |
| 1:J:908:VAL:HA | 1:J:963:ASN:HA | 1.71 | 0.71 |
| 1:J:2771:ILE:HG22 | 1:J:2776:SER:HA | 1.72 | 0.71 |
| 1:J:3195:ALA:HB2 | 1:J:3275:PRO:HB3 | 1.73 | 0.71 |
| 3:E:59:PHE:HA | 3:E:74:LEU:HD21 | 1.73 | 0.71 |
| 1:G:988:LEU:HB2 | 1:G:1039:LEU:HD21 | 1.72 | 0.71 |
| 1:G:908:VAL:HA | 1:G:963:ASN:HA | 1.72 | 0.71 |
| 1:G:3195:ALA:HB2 | 1:G:3275:PRO:HB3 | 1.73 | 0.71 |
| 1:A:2774:ASN:HD22 | 1:J:1506:GLN:HB2 | 1.55 | 0.71 |
| 1:C:266:ARG:HD3 | 1:C:268:SER:H | 1.55 | 0.71 |
| 1:G:2771:ILE:HG22 | 1:G:2776:SER:HA | 1.72 | 0.71 |
| 1:J:266:ARG:HD3 | 1:J:268:SER:H | 1.55 | 0.71 |
| 1:A:4887:MET:HE2 | 8:A:5107:POV:H21B | 1.72 | 0.70 |
| 1:G:2233:CYS:O | 1:G:2237:CYS:N | 2.24 | 0.70 |
| 8:A:5114:POV:H12A | 8:A:5115:POV:H1 | 1.73 | 0.70 |
| 1:J:1738:LEU:HB3 | 1:J:2146:PRO:HD3 | 1.73 | 0.70 |
| 8:J:5101:POV:H312 | 8:J:5102:POV:H213 | 1.74 | 0.70 |
| 1:C:1506:GLN:HB2 | 1:G:2774:ASN:HD22 | 1.55 | 0.70 |
| 1:C:1738:LEU:HB3 | 1:C:2146:PRO:HD3 | 1.73 | 0.70 |
| 1:C:2771:ILE:HG22 | 1:C:2776:SER:HA | 1.72 | 0.70 |
| 1:J:3996:PHE:HE2 | 1:J:4023:MET:HG3 | 1.56 | 0.70 |
| 1:A:3996:PHE:HE2 | 1:A:4023:MET:HG3 | 1.56 | 0.70 |
| 1:C:3195:ALA:HB2 | 1:C:3275:PRO:HB3 | 1.74 | 0.70 |
| 1:G:266:ARG:HD3 | 1:G:268:SER:H | 1.55 | 0.70 |
| 1:A:1738:LEU:HB3 | 1:A:2146:PRO:HD3 | 1.73 | 0.70 |
| 1:A:2771:ILE:HG22 | 1:A:2776:SER:HA | 1.72 | 0.70 |
| 1:G:1738:LEU:HB3 | 1:G:2146:PRO:HD3 | 1.73 | 0.70 |
| 1:J:4887:MET:HE2 | 8:J:5114:POV:H21B | 1.72 | 0.70 |
| 1:C:4887:MET:HE2 | 8:C:5110:POV:H21B | 1.72 | 0.70 |
| 1:C:3110:LEU:HD13 | 1:C:3183:VAL:HG12 | 1.74 | 0.69 |
| 1:G:2265:LEU:HD11 | 1:G:2327:GLY:HA2 | 1.74 | 0.69 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:G:2233:CYS:O | 1:G:2234:ARG:C | 2.33 | 0.69 |
| 1:A:3110:LEU:HD13 | 1:A:3183:VAL:HG12 | 1.75 | 0.69 |
| 1:G:4887:MET:HE2 | 8:G:5110:POV:H21B | 1.72 | 0.69 |
| 1:J:2792:ARG:HE | 1:J:2797:PHE:HD1 | 1.40 | 0.69 |
| 1:C:3539:ARG:NH1 | 1:C:3549:VAL:HA | 2.08 | 0.69 |
| 1:C:2265:LEU:HD11 | 1:C:2327:GLY:HA2 | 1.74 | 0.69 |
| 1:G:3996:PHE:HE2 | 1:G:4023:MET:HG3 | 1.56 | 0.69 |
| 1:J:2265:LEU:HD11 | 1:J:2327:GLY:HA2 | 1.74 | 0.69 |
| 1:G:210:GLU:HB3 | 1:G:213:TYR:HD2 | 1.58 | 0.69 |
| 1:G:3539:ARG:NH1 | 1:G:3549:VAL:HA | 2.08 | 0.69 |
| 1:J:3282:PRO:HG3 | 1:J:3345:ILE:HD13 | 1.75 | 0.69 |
| 1:C:210:GLU:HB3 | 1:C:213:TYR:HD2 | 1.58 | 0.69 |
| 3:F:74:LEU:HB3 | 3:F:99:PHE:HB2 | 1.75 | 0.69 |
| 1:J:210:GLU:HB3 | 1:J:213:TYR:HD2 | 1.58 | 0.69 |
| 1:C:2233:CYS:HA | 1:C:2236:LEU:HB2 | 1.72 | 0.68 |
| 1:J:3539:ARG:NH1 | 1:J:3549:VAL:HA | 2.08 | 0.68 |
| 1:A:886:ARG:HE | 1:A:891:TRP:HB2 | 1.59 | 0.68 |
| 1:A:210:GLU:HB3 | 1:A:213:TYR:HD2 | 1.58 | 0.68 |
| 1:A:3282:PRO:HG3 | 1:A:3345:ILE:HD13 | 1.75 | 0.68 |
| 1:G:4567:LEU:HD13 | 1:G:4815:ASP:HB3 | 1.75 | 0.68 |
| 1:J:3018:LEU:HD13 | 1:J:3074:SER:HA | 1.75 | 0.68 |
| 1:A:2495:VAL:HG22 | 1:A:2497:ASP:H | 1.58 | 0.68 |
| 1:C:1147:ASP:HB3 | 1:C:1164:LEU:HD11 | 1.76 | 0.68 |
| 1:C:2233:CYS:O | 1:C:2234:ARG:C | 2.37 | 0.68 |
| 1:C:3996:PHE:HE2 | 1:C:4023:MET:HG3 | 1.56 | 0.68 |
| 1:J:1147:ASP:HB3 | 1:J:1164:LEU:HD11 | 1.76 | 0.68 |
| 1:J:2495:VAL:HG22 | 1:J:2497:ASP:H | 1.58 | 0.68 |
| 1:A:2265:LEU:HD11 | 1:A:2327:GLY:HA2 | 1.74 | 0.68 |
| 1:A:3018:LEU:HD13 | 1:A:3074:SER:HA | 1.76 | 0.68 |
| 1:A:5026:ASP:HA | 1:A:5030:LYS:HD3 | 1.75 | 0.68 |
| 1:G:1147:ASP:HB3 | 1:G:1164:LEU:HD11 | 1.76 | 0.68 |
| 1:G:2792:ARG:HE | 1:G:2797:PHE:HD1 | 1.40 | 0.68 |
| 1:J:3110:LEU:HD13 | 1:J:3183:VAL:HG12 | 1.75 | 0.68 |
| 3:L:78:PRO:HA | 3:L:81:ALA:HB3 | 1.75 | 0.68 |
| 8:A:5116:POV:H311 | 8:A:5117:POV:H21C | 1.76 | 0.68 |
| 1:G:2306:GLY:HA2 | 1:G:2323:TRP:CZ3 | 2.29 | 0.68 |
| 1:A:4567:LEU:HD13 | 1:A:4815:ASP:HB3 | 1.75 | 0.68 |
| 1:G:2495:VAL:HG22 | 1:G:2497:ASP:H | 1.58 | 0.68 |
| 1:J:4567:LEU:HD13 | 1:J:4815:ASP:HB3 | 1.75 | 0.68 |
| 1:A:1147:ASP:HB3 | 1:A:1164:LEU:HD11 | 1.76 | 0.67 |
| 1:C:886:ARG:HE | 1:C:891:TRP:HB2 | 1.59 | 0.67 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:269:TRP:HE3 | 1:C:272:SER:HB3 | 1.59 | 0.67 |
| 1:G:2102:VAL:HG13 | 1:G:2120:MET:HE2 | 1.77 | 0.67 |
| 1:A:2812:SER:HB2 | 1:A:2882:TYR:HE1 | 1.59 | 0.67 |
| 1:C:2495:VAL:HG22 | 1:C:2497:ASP:H | 1.58 | 0.67 |
| 8:C:5119:POV:H311 | 8:C:5120:POV:H21C | 1.75 | 0.67 |
| 1:G:3282:PRO:HG3 | 1:G:3345:ILE:HD13 | 1.75 | 0.67 |
| 2:K:30:SER:HA | 2:K:99:ARG:HA | 1.76 | 0.67 |
| 1:C:2233:CYS:SG | 1:C:2275:VAL:HG22 | 2.33 | 0.67 |
| 1:C:4567:LEU:HD13 | 1:C:4815:ASP:HB3 | 1.75 | 0.67 |
| 1:J:2102:VAL:HG13 | 1:J:2120:MET:HE2 | 1.77 | 0.67 |
| 1:G:2812:SER:HB2 | 1:G:2882:TYR:HE1 | 1.59 | 0.67 |
| 1:J:886:ARG:HE | 1:J:891:TRP:HB2 | 1.59 | 0.67 |
| 1:J:4884:LEU:HD22 | 8:J:5114:POV:H24A | 1.77 | 0.67 |
| 3:L:23:VAL:HG13 | 3:L:47:LYS:HG2 | 1.77 | 0.67 |
| 3:F:56:ILE:HG22 | 3:F:59:PHE:HB2 | 1.76 | 0.67 |
| 1:A:2102:VAL:HG13 | 1:A:2120:MET:HE2 | 1.77 | 0.67 |
| 1:J:719:LEU:HD11 | 3:L:7:ILE:HA | 1.75 | 0.67 |
| 1:J:2812:SER:HB2 | 1:J:2882:TYR:HE1 | 1.59 | 0.67 |
| 1:C:2376:LEU:HB2 | 1:C:2465:ASP:HB3 | 1.75 | 0.67 |
| 1:J:3539:ARG:NH1 | 1:J:3552:PHE:HB2 | 2.04 | 0.67 |
| 1:C:3282:PRO:HG3 | 1:C:3345:ILE:HD13 | 1.75 | 0.67 |
| 1:G:269:TRP:HE3 | 1:G:272:SER:HB3 | 1.59 | 0.67 |
| 1:A:4884:LEU:HD22 | 8:A:5107:POV:H24A | 1.77 | 0.67 |
| 1:G:3110:LEU:HD13 | 1:G:3183:VAL:HG12 | 1.74 | 0.67 |
| 1:C:2102:VAL:HG13 | 1:C:2120:MET:HE2 | 1.77 | 0.66 |
| 8:C:5113:POV:H14A | 8:C:5114:POV:H14A | 1.76 | 0.66 |
| 3:F:78:PRO:HA | 3:F:81:ALA:HB3 | 1.76 | 0.66 |
| 1:A:2792:ARG:HE | 1:A:2797:PHE:HD1 | 1.40 | 0.66 |
| 1:C:2902:HIS:HB3 | 1:C:2905:LEU:HB2 | 1.77 | 0.66 |
| 1:C:4884:LEU:HD22 | 8:C:5110:POV:H24A | 1.77 | 0.66 |
| 1:A:269:TRP:HE3 | 1:A:272:SER:HB3 | 1.60 | 0.66 |
| 1:C:2812:SER:HB2 | 1:C:2882:TYR:HE1 | 1.59 | 0.66 |
| 1:A:3935:TRP:HE1 | 1:J:80:GLU:HB3 | 1.61 | 0.66 |
| 1:C:2792:ARG:HE | 1:C:2797:PHE:HD1 | 1.40 | 0.66 |
| 3:I:57:LYS:HE3 | 3:I:80:VAL:HG12 | 1.77 | 0.66 |
| 3:E:2:VAL:HG23 | 3:E:80:VAL:HG21 | 1.77 | 0.66 |
| 1:C:2186:MET:HE2 | 1:C:2234:ARG:HG2 | 1.75 | 0.66 |
| 1:A:2902:HIS:HB3 | 1:A:2905:LEU:HB2 | 1.77 | 0.66 |
| 1:J:269:TRP:HE3 | 1:J:272:SER:HB3 | 1.59 | 0.66 |
| 8:J:5117:POV:H13A | 8:J:5118:POV:H14A | 1.77 | 0.66 |
| 1:C:2233:CYS:O | 1:C:2237:CYS:N | 2.27 | 0.65 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:1100:MET:HB3 | 1:A:1194:LEU:HD23 | 1.79 | 0.65 |
| 1:C:1100:MET:HB3 | 1:C:1194:LEU:HD23 | 1.79 | 0.65 |
| 1:C:4794:TRP:HE1 | 8:C:5115:POV:H37A | 1.62 | 0.65 |
| 1:C:2306:GLY:HA2 | 1:C:2323:TRP:CZ3 | 2.31 | 0.65 |
| 1:A:2098:VAL:HA | 1:A:2101:MET:HE3 | 1.79 | 0.65 |
| 1:G:4884:LEU:HD22 | 8:G:5110:POV:H24A | 1.77 | 0.65 |
| 2:D:82:MET:HE2 | 2:D:82:MET:HA | 1.79 | 0.65 |
| 1:G:886:ARG:HE | 1:G:891:TRP:HB2 | 1.59 | 0.65 |
| 1:G:2715:VAL:HG12 | 1:G:2954:ARG:HA | 1.79 | 0.65 |
| 1:J:2098:VAL:HA | 1:J:2101:MET:HE3 | 1.79 | 0.65 |
| 1:C:1293:LEU:HD11 | 1:C:1594:ARG:HD3 | 1.79 | 0.65 |
| 1:G:1293:LEU:HD11 | 1:G:1594:ARG:HD3 | 1.79 | 0.65 |
| 1:G:5026:ASP:HA | 1:G:5030:LYS:HD3 | 1.78 | 0.65 |
| 1:J:2902:HIS:HB3 | 1:J:2905:LEU:HB2 | 1.77 | 0.65 |
| 1:C:2098:VAL:HA | 1:C:2101:MET:HE3 | 1.79 | 0.65 |
| 1:C:2792:ARG:HB2 | 1:C:2797:PHE:HB2 | 1.79 | 0.65 |
| 1:G:2233:CYS:SG | 1:G:2275:VAL:HG22 | 2.36 | 0.65 |
| 1:G:3010:PHE:HE1 | 1:G:3074:SER:HB2 | 1.61 | 0.65 |
| 1:A:2792:ARG:HB2 | 1:A:2797:PHE:HB2 | 1.79 | 0.65 |
| 1:A:4794:TRP:HE1 | 8:A:5112:POV:H37A | 1.62 | 0.65 |
| 1:G:1100:MET:HB3 | 1:G:1194:LEU:HD23 | 1.79 | 0.65 |
| 1:G:2098:VAL:HA | 1:G:2101:MET:HE3 | 1.79 | 0.65 |
| 1:J:1445:PRO:HB2 | 1:J:1501:VAL:HA | 1.79 | 0.65 |
| 1:C:3539:ARG:NH1 | 1:C:3552:PHE:HB2 | 2.05 | 0.64 |
| 1:G:1445:PRO:HB2 | 1:G:1501:VAL:HA | 1.79 | 0.64 |
| 1:G:1973:GLN:HE22 | 1:G:3640:PRO:HB3 | 1.62 | 0.64 |
| 2:H:17:SER:HA | 2:H:83:ASN:HA | 1.79 | 0.64 |
| 1:J:1100:MET:HB3 | 1:J:1194:LEU:HD23 | 1.79 | 0.64 |
| 1:A:240:ASP:HB3 | 1:A:244:LEU:HD23 | 1.80 | 0.64 |
| 1:A:1447:CYS:HB2 | 1:A:1555:LEU:HB3 | 1.80 | 0.64 |
| 1:G:3539:ARG:NH1 | 1:G:3552:PHE:HB2 | 2.05 | 0.64 |
| 1:J:1447:CYS:HB2 | 1:J:1555:LEU:HB3 | 1.79 | 0.64 |
| 1:J:3082:LYS:HD3 | 1:J:3155:ASP:HB2 | 1.79 | 0.64 |
| 1:A:1973:GLN:HE22 | 1:A:3640:PRO:HB3 | 1.62 | 0.64 |
| 1:G:2902:HIS:HB3 | 1:G:2905:LEU:HB2 | 1.77 | 0.64 |
| 1:J:4794:TRP:HE1 | 8:J:5119:POV:H37A | 1.62 | 0.64 |
| 1:C:719:LEU:HD11 | 3:E:7:ILE:HA | 1.79 | 0.64 |
| 1:G:2792:ARG:HB2 | 1:G:2797:PHE:HB2 | 1.79 | 0.64 |
| 1:G:4794:TRP:HE1 | 8:G:5115:POV:H37A | 1.62 | 0.64 |
| 1:J:2792:ARG:HB2 | 1:J:2797:PHE:HB2 | 1.79 | 0.64 |
| 1:J:4810:ALA:CA | 1:J:4810:ALA:O | 2.46 | 0.64 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:82:MET:HE2 | 2:B:82:MET:HA | 1.79 | 0.64 |
| 1:C:1973:GLN:HE22 | 1:C:3640:PRO:HB3 | 1.62 | 0.64 |
| 1:C:2715:VAL:HG12 | 1:C:2954:ARG:HA | 1.79 | 0.64 |
| 3:E:77:THR:HG22 | 3:E:80:VAL:HG22 | 1.79 | 0.64 |
| 1:G:3103:ILE:HA | 1:G:3106:MET:HG2 | 1.79 | 0.64 |
| 1:J:1973:GLN:HE22 | 1:J:3640:PRO:HB3 | 1.62 | 0.64 |
| 1:J:3103:ILE:HA | 1:J:3106:MET:HG2 | 1.79 | 0.64 |
| 1:C:4824:ARG:HG3 | 8:C:5113:POV:H13 | 1.80 | 0.64 |
| 3:E:66:MET:HB2 | 3:E:70:GLN:OE1 | 1.98 | 0.64 |
| 8:G:5119:POV:H311 | 8:G:5120:POV:H21C | 1.79 | 0.64 |
| 1:A:1445:PRO:HB2 | 1:A:1501:VAL:HA | 1.79 | 0.64 |
| 2:K:82:MET:HE2 | 2:K:82:MET:HA | 1.79 | 0.64 |
| 1:A:1293:LEU:HD11 | 1:A:1594:ARG:HD3 | 1.79 | 0.63 |
| 1:C:2485:LEU:H | 1:C:2485:LEU:HD13 | 1.61 | 0.63 |
| 1:J:3072:ALA:HA | 1:J:3075:LEU:HD23 | 1.80 | 0.63 |
| 1:A:2340:PHE:HB2 | 1:A:2435:ARG:HG3 | 1.80 | 0.63 |
| 1:A:3103:ILE:HA | 1:A:3106:MET:HG2 | 1.79 | 0.63 |
| 8:A:5112:POV:H31B | 8:J:5102:POV:H210 | 1.79 | 0.63 |
| 1:J:240:ASP:HB3 | 1:J:244:LEU:HD23 | 1.80 | 0.63 |
| 1:A:2715:VAL:HG12 | 1:A:2954:ARG:HA | 1.79 | 0.63 |
| 1:C:1447:CYS:HB2 | 1:C:1555:LEU:HB3 | 1.80 | 0.63 |
| 1:C:3162:GLN:HE22 | 1:C:3217:SER:HA | 1.64 | 0.63 |
| 1:G:2340:PHE:HB2 | 1:G:2435:ARG:HG3 | 1.80 | 0.63 |
| 1:J:1293:LEU:HD11 | 1:J:1594:ARG:HD3 | 1.79 | 0.63 |
| 1:J:4810:ALA:O | 1:J:4811:ALA:N | 2.31 | 0.63 |
| 1:G:1447:CYS:HB2 | 1:G:1555:LEU:HB3 | 1.79 | 0.63 |
| 1:G:1527:MET:HB2 | 1:G:1540:PHE:HB2 | 1.80 | 0.63 |
| 1:C:240:ASP:HB3 | 1:C:244:LEU:HD23 | 1.80 | 0.63 |
| 1:C:3103:ILE:HA | 1:C:3106:MET:HG2 | 1.79 | 0.63 |
| 1:A:4680:LYS:HB3 | 1:A:4686:LEU:HD22 | 1.81 | 0.63 |
| 1:C:2624:ARG:HH21 | 1:C:2625:ARG:HH12 | 1.47 | 0.63 |
| 1:C:3082:LYS:HD3 | 1:C:3155:ASP:HB2 | 1.79 | 0.63 |
| 1:G:3162:GLN:HE22 | 1:G:3217:SER:HA | 1.64 | 0.63 |
| 1:J:2340:PHE:HB2 | 1:J:2435:ARG:HG3 | 1.80 | 0.63 |
| 1:G:4587:PRO:HG3 | 1:G:4631:PHE:HB3 | 1.80 | 0.63 |
| 3:E:62:GLY:HA3 | 3:E:74:LEU:HD13 | 1.80 | 0.62 |
| 3:F:5:GLU:HB2 | 3:F:73:LYS:HB2 | 1.80 | 0.62 |
| 1:J:3172:ILE:HD11 | 1:J:3190:LEU:HB3 | 1.80 | 0.62 |
| 1:C:1527:MET:HB2 | 1:C:1540:PHE:HB2 | 1.80 | 0.62 |
| 1:C:2340:PHE:HB2 | 1:C:2435:ARG:HG3 | 1.80 | 0.62 |
| 1:C:4918:ILE:HG21 | 8:G:5111:POV:H21F | 1.81 | 0.62 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:J:4680:LYS:HB3 | 1:J:4686:LEU:HD22 | 1.81 | 0.62 |
| 1:G:2548:LEU:HB3 | 1:G:2552:ARG:HH21 | 1.64 | 0.62 |
| 1:G:2624:ARG:HH21 | 1:G:2625:ARG:HH12 | 1.47 | 0.62 |
| 1:J:2548:LEU:HB3 | 1:J:2552:ARG:HH21 | 1.64 | 0.62 |
| 1:J:2715:VAL:HG12 | 1:J:2954:ARG:HA | 1.79 | 0.62 |
| 1:J:3162:GLN:HE22 | 1:J:3217:SER:HA | 1.64 | 0.62 |
| 1:C:3416:VAL:HG23 | 1:C:3423:TRP:HZ3 | 1.65 | 0.62 |
| 1:G:240:ASP:HB3 | 1:G:244:LEU:HD23 | 1.80 | 0.62 |
| 1:G:3416:VAL:HG23 | 1:G:3423:TRP:HZ3 | 1.65 | 0.62 |
| 1:A:4918:ILE:HG21 | 8:C:5111:POV:H21F | 1.82 | 0.62 |
| 3:E:7:ILE:HD11 | 3:E:73:LYS:HG3 | 1.81 | 0.62 |
| 1:J:4567:LEU:HD21 | 1:J:4816:ILE:HG22 | 1.82 | 0.62 |
| 1:A:1527:MET:HB2 | 1:A:1540:PHE:HB2 | 1.80 | 0.62 |
| 1:A:3162:GLN:HE22 | 1:A:3217:SER:HA | 1.64 | 0.62 |
| 1:C:80:GLU:HB3 | 1:G:3935:TRP:HE1 | 1.64 | 0.62 |
| 3:F:59:PHE:HA | 3:F:74:LEU:HD21 | 1.80 | 0.62 |
| 1:G:2742:THR:HA | 1:G:2745:VAL:HB | 1.82 | 0.62 |
| 1:G:3172:ILE:HD11 | 1:G:3190:LEU:HB3 | 1.81 | 0.62 |
| 1:A:3416:VAL:HG23 | 1:A:3423:TRP:HZ3 | 1.65 | 0.62 |
| 1:G:2624:ARG:HG2 | 1:G:2906:VAL:HG11 | 1.82 | 0.62 |
| 1:G:4567:LEU:HD21 | 1:G:4816:ILE:HG22 | 1.82 | 0.62 |
| 1:J:2624:ARG:HH21 | 1:J:2625:ARG:HH12 | 1.47 | 0.62 |
| 1:J:3969:ILE:HD13 | 1:J:3980:LEU:HD12 | 1.82 | 0.62 |
| 8:J:5121:POV:H12A | 8:J:5122:POV:H1 | 1.81 | 0.62 |
| 8:A:5108:POV:H21F | 1:J:4918:ILE:HG21 | 1.82 | 0.62 |
| 1:C:1230:MET:HG2 | 1:C:1827:ARG:HB2 | 1.82 | 0.62 |
| 1:C:2710:LEU:HD12 | 1:C:2711:PRO:HD2 | 1.82 | 0.62 |
| 1:G:248:GLU:HG2 | 1:G:373:LYS:HB3 | 1.82 | 0.62 |
| 1:G:2559:LEU:HG | 1:G:2603:ILE:HD13 | 1.82 | 0.62 |
| 1:G:4680:LYS:HB3 | 1:G:4686:LEU:HD22 | 1.81 | 0.62 |
| 1:J:2710:LEU:HD12 | 1:J:2711:PRO:HD2 | 1.82 | 0.62 |
| 1:J:5026:ASP:HA | 1:J:5030:LYS:HD3 | 1.82 | 0.62 |
| 1:C:248:GLU:HG2 | 1:C:373:LYS:HB3 | 1.82 | 0.62 |
| 1:J:1230:MET:HG2 | 1:J:1827:ARG:HB2 | 1.82 | 0.62 |
| 1:A:2742:THR:HA | 1:A:2745:VAL:HB | 1.82 | 0.62 |
| 1:C:210:GLU:HB2 | 1:C:273:HIS:HB3 | 1.81 | 0.62 |
| 1:C:4567:LEU:HD21 | 1:C:4816:ILE:HG22 | 1.81 | 0.62 |
| 1:C:4848:VAL:HG11 | 1:C:4887:MET:HG2 | 1.82 | 0.62 |
| 1:G:4880:MET:HG3 | 8:G:5110:POV:H27 | 1.82 | 0.62 |
| 1:J:2742:THR:HA | 1:J:2745:VAL:HB | 1.82 | 0.62 |
| 1:A:1552:VAL:HG11 | 1:A:1562:ILE:HD13 | 1.82 | 0.61 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:2710:LEU:HD12 | 1:A:2711:PRO:HD2 | 1.82 | 0.61 |
| 1:A:248:GLU:HG2 | 1:A:373:LYS:HB3 | 1.82 | 0.61 |
| 1:A:4848:VAL:HG11 | 1:A:4887:MET:HG2 | 1.82 | 0.61 |
| 1:C:1552:VAL:HG11 | 1:C:1562:ILE:HD13 | 1.82 | 0.61 |
| 1:C:2742:THR:HA | 1:C:2745:VAL:HB | 1.82 | 0.61 |
| 1:C:3768:SER:HA | 1:C:3771:HIS:CD2 | 2.36 | 0.61 |
| 1:C:4680:LYS:HB3 | 1:C:4686:LEU:HD22 | 1.81 | 0.61 |
| 3:E:78:PRO:HA | 3:E:81:ALA:HB3 | 1.81 | 0.61 |
| 1:G:1230:MET:HG2 | 1:G:1827:ARG:HB2 | 1.82 | 0.61 |
| 1:G:2710:LEU:HD12 | 1:G:2711:PRO:HD2 | 1.82 | 0.61 |
| 1:A:2624:ARG:HH21 | 1:A:2625:ARG:HH12 | 1.47 | 0.61 |
| 1:C:2548:LEU:HB3 | 1:C:2552:ARG:HH21 | 1.64 | 0.61 |
| 1:C:2559:LEU:HG | 1:C:2603:ILE:HD13 | 1.82 | 0.61 |
| 1:G:80:GLU:HB3 | 1:J:3935:TRP:HE1 | 1.64 | 0.61 |
| 1:A:2548:LEU:HB3 | 1:A:2552:ARG:HH21 | 1.64 | 0.61 |
| 1:G:3768:SER:HA | 1:G:3771:HIS:CD2 | 2.36 | 0.61 |
| 1:J:1000:ARG:HB3 | 1:J:1005:TRP:HB2 | 1.81 | 0.61 |
| 1:J:2306:GLY:HA2 | 1:J:2323:TRP:CZ3 | 2.35 | 0.61 |
| 1:A:1230:MET:HG2 | 1:A:1827:ARG:HB2 | 1.82 | 0.61 |
| 1:A:4880:MET:HG3 | 8:A:5107:POV:H27 | 1.82 | 0.61 |
| 8:C:5117:POV:H12A | 8:C:5118:POV:H1 | 1.82 | 0.61 |
| 1:G:4918:ILE:HG21 | 8:J:5115:POV:H21F | 1.82 | 0.61 |
| 1:J:1527:MET:HB2 | 1:J:1540:PHE:HB2 | 1.80 | 0.61 |
| 1:J:2624:ARG:HG2 | 1:J:2906:VAL:HG11 | 1.82 | 0.61 |
| 1:A:210:GLU:HB2 | 1:A:273:HIS:HB3 | 1.81 | 0.61 |
| 1:C:5026:ASP:HA | 1:C:5030:LYS:HD3 | 1.82 | 0.61 |
| 3:F:68:LEU:HD21 | 3:F:106:LEU:HD12 | 1.83 | 0.61 |
| 1:J:210:GLU:HB2 | 1:J:273:HIS:HB3 | 1.81 | 0.61 |
| 1:J:3768:SER:HA | 1:J:3771:HIS:CD2 | 2.36 | 0.61 |
| 1:A:4567:LEU:HD21 | 1:A:4816:ILE:HG22 | 1.82 | 0.61 |
| 1:C:3387:ALA:O | 1:C:3391:GLU:HB2 | 2.01 | 0.61 |
| 1:C:4878:ASP:HB3 | 8:G:5101:POV:H14 | 1.82 | 0.61 |
| 1:G:985:VAL:HG22 | 1:G:1043:VAL:HG21 | 1.83 | 0.61 |
| 1:J:3416:VAL:HG23 | 1:J:3423:TRP:HZ3 | 1.65 | 0.61 |
| 1:J:4848:VAL:HG11 | 1:J:4887:MET:HG2 | 1.82 | 0.61 |
| 1:A:2785:LEU:HD13 | 1:A:2789:PRO:HA | 1.83 | 0.61 |
| 1:C:2624:ARG:HG2 | 1:C:2906:VAL:HG11 | 1.82 | 0.61 |
| 1:G:210:GLU:HB2 | 1:G:273:HIS:HB3 | 1.81 | 0.61 |
| 1:A:80:GLU:HB3 | 1:C:3935:TRP:HE1 | 1.64 | 0.61 |
| 1:G:3969:ILE:HD13 | 1:G:3980:LEU:HD12 | 1.82 | 0.61 |
| 1:A:3969:ILE:HD13 | 1:A:3980:LEU:HD12 | 1.82 | 0.61 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:G:4901:ILE:HD12 | 1:G:4913:ARG:HH22 | 1.66 | 0.61 |
| 1:J:248:GLU:HG2 | 1:J:373:LYS:HB3 | 1.82 | 0.61 |
| 1:J:2340:PHE:HD2 | 1:J:2435:ARG:HE | 1.48 | 0.61 |
| 1:A:3531:ASP:HA | 1:A:3534:MET:HE2 | 1.83 | 0.60 |
| 1:A:3768:SER:HA | 1:A:3771:HIS:CD2 | 2.36 | 0.60 |
| 1:A:4083:ASP:HB2 | 1:A:4122:MET:HE2 | 1.83 | 0.60 |
| 1:C:2340:PHE:HD2 | 1:C:2435:ARG:HE | 1.48 | 0.60 |
| 1:C:4083:ASP:HB2 | 1:C:4122:MET:HE2 | 1.84 | 0.60 |
| 1:C:4880:MET:HG3 | 8:C:5110:POV:H27 | 1.82 | 0.60 |
| 1:G:719:LEU:HD11 | 3:I:7:ILE:HA | 1.83 | 0.60 |
| 1:G:1552:VAL:HG11 | 1:G:1562:ILE:HD13 | 1.82 | 0.60 |
| 1:J:985:VAL:HG22 | 1:J:1043:VAL:HG21 | 1.83 | 0.60 |
| 1:J:2785:LEU:HD13 | 1:J:2789:PRO:HA | 1.83 | 0.60 |
| 1:J:4059:LEU:HD13 | 1:J:4167:ALA:HB2 | 1.83 | 0.60 |
| 1:A:3835:LEU:HD22 | 1:A:3880:PHE:HZ | 1.67 | 0.60 |
| 1:G:2635:GLU:HA | 1:G:2638:LYS:HD3 | 1.84 | 0.60 |
| 1:A:719:LEU:HD11 | 3:F:7:ILE:HA | 1.82 | 0.60 |
| 1:A:1737:PRO:HD3 | 1:A:1771:LEU:HG | 1.84 | 0.60 |
| 1:A:4241:THR:HG22 | 1:A:4245:MET:HE3 | 1.83 | 0.60 |
| 1:C:2273:LEU:HD23 | 1:C:2330:ARG:HG3 | 1.82 | 0.60 |
| 1:C:2635:GLU:HA | 1:C:2638:LYS:HD3 | 1.84 | 0.60 |
| 1:C:2869:ARG:HH21 | 1:C:2948:THR:H | 1.48 | 0.60 |
| 1:G:3387:ALA:O | 1:G:3391:GLU:HB2 | 2.01 | 0.60 |
| 1:J:1552:VAL:HG11 | 1:J:1562:ILE:HD13 | 1.82 | 0.60 |
| 1:J:3835:LEU:HD22 | 1:J:3880:PHE:HZ | 1.67 | 0.60 |
| 1:J:4880:MET:HG3 | 8:J:5114:POV:H27 | 1.82 | 0.60 |
| 1:J:2869:ARG:HH21 | 1:J:2948:THR:H | 1.48 | 0.60 |
| 1:J:3273:THR:HA | 1:J:3276:MET:HG2 | 1.84 | 0.60 |
| 1:A:355:LEU:HB3 | 1:A:378:LEU:HB3 | 1.83 | 0.60 |
| 8:A:5120:POV:H14 | 1:J:4878:ASP:HB3 | 1.82 | 0.60 |
| 1:C:1607:ARG:HH22 | 1:C:1610:ASN:HD21 | 1.49 | 0.60 |
| 1:C:4241:THR:HG22 | 1:C:4245:MET:HE3 | 1.84 | 0.60 |
| 1:G:2340:PHE:HD2 | 1:G:2435:ARG:HE | 1.48 | 0.60 |
| 1:J:4824:ARG:HG3 | 8:J:5117:POV:H15 | 1.82 | 0.60 |
| 1:J:4901:ILE:HD12 | 1:J:4913:ARG:HH22 | 1.66 | 0.60 |
| 1:A:2186:MET:HE2 | 1:A:2234:ARG:HG2 | 1.83 | 0.60 |
| 1:A:2719:TYR:HB2 | 1:A:2953:LYS:HG3 | 1.84 | 0.60 |
| 1:A:3387:ALA:O | 1:A:3391:GLU:HB2 | 2.01 | 0.60 |
| 1:A:4878:ASP:HB3 | 8:C:5101:POV:H14 | 1.82 | 0.60 |
| 8:G:5117:POV:H12A | 8:G:5118:POV:H1 | 1.81 | 0.60 |
| 1:A:1033:ARG:HE | 1:A:1036:ARG:HD2 | 1.66 | 0.60 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:3273:THR:HA | 1:A:3276:MET:HG2 | 1.84 | 0.60 |
| 1:C:3969:ILE:HD13 | 1:C:3980:LEU:HD12 | 1.82 | 0.60 |
| 3:E:74:LEU:HB3 | 3:E:99:PHE:HB2 | 1.83 | 0.60 |
| 1:G:4059:LEU:HD13 | 1:G:4167:ALA:HB2 | 1.83 | 0.60 |
| 1:J:4083:ASP:HB2 | 1:J:4122:MET:HE2 | 1.83 | 0.60 |
| 1:A:2340:PHE:HD2 | 1:A:2435:ARG:HE | 1.48 | 0.60 |
| 1:A:2624:ARG:HG2 | 1:A:2906:VAL:HG11 | 1.82 | 0.60 |
| 1:A:2635:GLU:HA | 1:A:2638:LYS:HD3 | 1.84 | 0.60 |
| 1:C:3835:LEU:HD22 | 1:C:3880:PHE:HZ | 1.67 | 0.60 |
| 1:G:3316:LEU:HD13 | 1:G:3345:ILE:HG23 | 1.84 | 0.60 |
| 1:G:4848:VAL:HG11 | 1:G:4887:MET:HG2 | 1.82 | 0.60 |
| 1:G:4878:ASP:HB3 | 8:J:5105:POV:H14 | 1.82 | 0.60 |
| 1:J:3363:GLY:HA2 | 1:J:3437:MET:HE2 | 1.83 | 0.60 |
| 1:A:4901:ILE:HD12 | 1:A:4913:ARG:HH22 | 1.66 | 0.60 |
| 1:C:109:LEU:HD13 | 1:C:118:LEU:HD23 | 1.84 | 0.60 |
| 1:G:3273:THR:HA | 1:G:3276:MET:HG2 | 1.84 | 0.60 |
| 1:J:355:LEU:HB3 | 1:J:378:LEU:HB3 | 1.83 | 0.60 |
| 1:J:2740:VAL:HG12 | 1:J:2742:THR:H | 1.67 | 0.60 |
| 1:A:109:LEU:HD13 | 1:A:118:LEU:HD23 | 1.84 | 0.59 |
| 1:A:1607:ARG:HH22 | 1:A:1610:ASN:HD21 | 1.49 | 0.59 |
| 1:G:3070:ILE:HG23 | 1:G:3073:ARG:HD2 | 1.84 | 0.59 |
| 1:A:2762:THR:HG21 | 1:A:2809:ILE:HG21 | 1.84 | 0.59 |
| 1:C:2740:VAL:HG12 | 1:C:2742:THR:H | 1.67 | 0.59 |
| 1:C:3172:ILE:HD11 | 1:C:3190:LEU:HB3 | 1.85 | 0.59 |
| 1:G:109:LEU:HD13 | 1:G:118:LEU:HD23 | 1.84 | 0.59 |
| 1:J:109:LEU:HD13 | 1:J:118:LEU:HD23 | 1.84 | 0.59 |
| 1:J:2635:GLU:HA | 1:J:2638:LYS:HD3 | 1.84 | 0.59 |
| 1:A:920:TYR:HH | 2:B:107:TRP:CD1 | 2.21 | 0.59 |
| 1:G:1863:LEU:HB3 | 1:G:1871:PHE:HB3 | 1.84 | 0.59 |
| 1:G:2762:THR:HG21 | 1:G:2809:ILE:HG21 | 1.84 | 0.59 |
| 1:G:3684:GLU:HA | 1:G:3693:LYS:HE2 | 1.84 | 0.59 |
| 1:G:3835:LEU:HD22 | 1:G:3880:PHE:HZ | 1.67 | 0.59 |
| 1:G:4083:ASP:HB2 | 1:G:4122:MET:HE2 | 1.83 | 0.59 |
| 1:J:2719:TYR:HB2 | 1:J:2953:LYS:HG3 | 1.84 | 0.59 |
| 1:A:935:LEU:HD22 | 1:A:988:LEU:HD23 | 1.85 | 0.59 |
| 1:G:2869:ARG:HH21 | 1:G:2948:THR:H | 1.48 | 0.59 |
| 1:J:3387:ALA:O | 1:J:3391:GLU:HB2 | 2.01 | 0.59 |
| 1:A:2869:ARG:HH21 | 1:A:2948:THR:H | 1.48 | 0.59 |
| 1:C:1737:PRO:HD3 | 1:C:1771:LEU:HG | 1.84 | 0.59 |
| 1:C:4901:ILE:HD12 | 1:C:4913:ARG:HH22 | 1.66 | 0.59 |
| 1:G:5000:GLU:HA | 1:G:5003:HIS:ND1 | 2.18 | 0.59 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:J:1737:PRO:HD3 | 1:J:1771:LEU:HG | 1.83 | 0.59 |
| 1:A:3316:LEU:HD13 | 1:A:3345:ILE:HG23 | 1.84 | 0.59 |
| 1:C:3206:LEU:HG | 1:C:3246:LEU:HB3 | 1.85 | 0.59 |
| 1:C:4926:VAL:HG13 | 1:G:4933:GLN:HG2 | 1.85 | 0.59 |
| 1:C:4948:GLU:HA | 1:C:4951:LYS:HE2 | 1.84 | 0.59 |
| 1:G:2785:LEU:HD13 | 1:G:2789:PRO:HA | 1.83 | 0.59 |
| 1:G:4241:THR:HG22 | 1:G:4245:MET:HE3 | 1.84 | 0.59 |
| 1:J:3316:LEU:HD13 | 1:J:3345:ILE:HG23 | 1.84 | 0.59 |
| 1:C:355:LEU:HB3 | 1:C:378:LEU:HB3 | 1.83 | 0.59 |
| 1:G:355:LEU:HB3 | 1:G:378:LEU:HB3 | 1.83 | 0.59 |
| 1:G:2740:VAL:HG12 | 1:G:2742:THR:H | 1.67 | 0.59 |
| 1:A:4059:LEU:HD13 | 1:A:4167:ALA:HB2 | 1.83 | 0.59 |
| 1:G:4926:VAL:HG13 | 1:J:4933:GLN:HG2 | 1.85 | 0.59 |
| 1:J:3684:GLU:HA | 1:J:3693:LYS:HE2 | 1.84 | 0.59 |
| 1:A:144:GLU:HB2 | 1:A:175:SER:HB3 | 1.85 | 0.59 |
| 2:B:9:GLY:HA3 | 2:B:123:VAL:HG22 | 1.85 | 0.59 |
| 1:C:1863:LEU:HB3 | 1:C:1871:PHE:HB3 | 1.84 | 0.59 |
| 1:C:2762:THR:HG21 | 1:C:2809:ILE:HG21 | 1.84 | 0.59 |
| 1:C:3273:THR:HA | 1:C:3276:MET:HG2 | 1.84 | 0.59 |
| 1:G:3379:LEU:HD21 | 1:G:3390:GLY:HA3 | 1.85 | 0.59 |
| 1:J:935:LEU:HD22 | 1:J:988:LEU:HD23 | 1.85 | 0.59 |
| 1:J:3206:LEU:HG | 1:J:3246:LEU:HB3 | 1.85 | 0.59 |
| 1:A:3206:LEU:HG | 1:A:3246:LEU:HB3 | 1.85 | 0.59 |
| 1:C:2719:TYR:HB2 | 1:C:2953:LYS:HG3 | 1.84 | 0.59 |
| 1:C:2785:LEU:HD13 | 1:C:2789:PRO:HA | 1.83 | 0.59 |
| 1:J:2762:THR:HG21 | 1:J:2809:ILE:HG21 | 1.84 | 0.59 |
| 1:A:900:ASN:HD21 | 1:A:903:LEU:HD12 | 1.68 | 0.58 |
| 1:A:3729:MET:HE1 | 1:A:3778:MET:HE1 | 1.85 | 0.58 |
| 1:C:360:ALA:HB3 | 1:C:375:LYS:HB3 | 1.85 | 0.58 |
| 1:J:5000:GLU:HA | 1:J:5003:HIS:ND1 | 2.18 | 0.58 |
| 1:A:1863:LEU:HB3 | 1:A:1871:PHE:HB3 | 1.84 | 0.58 |
| 1:C:3363:GLY:HA2 | 1:C:3437:MET:HE2 | 1.83 | 0.58 |
| 1:G:3206:LEU:HG | 1:G:3246:LEU:HB3 | 1.85 | 0.58 |
| 1:J:3379:LEU:HD21 | 1:J:3390:GLY:HA3 | 1.85 | 0.58 |
| 1:J:4241:THR:HG22 | 1:J:4245:MET:HE3 | 1.84 | 0.58 |
| 1:G:360:ALA:HB3 | 1:G:375:LYS:HB3 | 1.84 | 0.58 |
| 1:G:1607:ARG:HH22 | 1:G:1610:ASN:HD21 | 1.49 | 0.58 |
| 1:J:2803:GLU:HA | 1:J:2806:ARG:HG2 | 1.85 | 0.58 |
| 1:A:2740:VAL:HG12 | 1:A:2742:THR:H | 1.67 | 0.58 |
| 1:A:4926:VAL:HG13 | 1:C:4933:GLN:HG2 | 1.85 | 0.58 |
| 1:C:2488:PRO:HG2 | 1:C:2546:MET:SD | 2.43 | 0.58 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:2803:GLU:HA | 1:C:2806:ARG:HG2 | 1.85 | 0.58 |
| 1:C:4059:LEU:HD13 | 1:C:4167:ALA:HB2 | 1.83 | 0.58 |
| 1:J:2791:LEU:HB3 | 1:J:2855:TYR:HE2 | 1.68 | 0.58 |
| 1:A:5000:GLU:HA | 1:A:5003:HIS:ND1 | 2.18 | 0.58 |
| 1:G:2522:LEU:HD23 | 1:G:2578:MET:HE1 | 1.84 | 0.58 |
| 2:H:9:GLY:HA3 | 2:H:123:VAL:HG22 | 1.85 | 0.58 |
| 1:J:908:VAL:HG22 | 1:J:909:ASN:H | 1.69 | 0.58 |
| 1:A:916:PRO:HB3 | 2:B:53:SER:HB3 | 1.86 | 0.58 |
| 1:A:3684:GLU:HA | 1:A:3693:LYS:HE2 | 1.84 | 0.58 |
| 1:C:935:LEU:HD22 | 1:C:988:LEU:HD23 | 1.85 | 0.58 |
| 1:C:5000:GLU:HA | 1:C:5003:HIS:ND1 | 2.18 | 0.58 |
| 1:G:144:GLU:HB2 | 1:G:175:SER:HB3 | 1.85 | 0.58 |
| 1:G:1737:PRO:HD3 | 1:G:1771:LEU:HG | 1.84 | 0.58 |
| 1:G:2719:TYR:HB2 | 1:G:2953:LYS:HG3 | 1.84 | 0.58 |
| 1:J:144:GLU:HB2 | 1:J:175:SER:HB3 | 1.85 | 0.58 |
| 1:J:1863:LEU:HB3 | 1:J:1871:PHE:HB3 | 1.84 | 0.58 |
| 2:K:9:GLY:HA3 | 2:K:123:VAL:HG22 | 1.85 | 0.58 |
| 1:A:908:VAL:HG22 | 1:A:909:ASN:H | 1.69 | 0.58 |
| 1:A:988:LEU:HB2 | 1:A:1039:LEU:HD21 | 1.84 | 0.58 |
| 1:A:2131:LEU:HD23 | 1:A:3667:HIS:HD2 | 1.69 | 0.58 |
| 1:A:2307:LEU:HD11 | 1:A:2362:GLU:HG2 | 1.84 | 0.58 |
| 3:F:62:GLY:HA3 | 3:F:74:LEU:HD13 | 1.85 | 0.58 |
| 1:A:2747:ILE:HG13 | 1:A:2814:LYS:HG2 | 1.86 | 0.58 |
| 1:C:1155:LEU:HD22 | 1:C:1184:ILE:HG12 | 1.86 | 0.58 |
| 1:C:2747:ILE:HG13 | 1:C:2814:LYS:HG2 | 1.86 | 0.58 |
| 1:C:3379:LEU:HD21 | 1:C:3390:GLY:HA3 | 1.85 | 0.58 |
| 1:G:900:ASN:HD21 | 1:G:903:LEU:HD12 | 1.68 | 0.58 |
| 1:J:1155:LEU:HD22 | 1:J:1184:ILE:HG12 | 1.86 | 0.58 |
| 1:J:1607:ARG:HH22 | 1:J:1610:ASN:HD21 | 1.49 | 0.58 |
| 1:A:2803:GLU:HA | 1:A:2806:ARG:HG2 | 1.85 | 0.58 |
| 1:C:720:HIS:HA | 1:C:730:VAL:HG12 | 1.85 | 0.58 |
| 1:C:3187:ARG:HA | 1:C:3190:LEU:HD12 | 1.86 | 0.58 |
| 1:G:213:TYR:HD1 | 1:G:340:LYS:HB2 | 1.69 | 0.58 |
| 1:G:908:VAL:HG22 | 1:G:909:ASN:H | 1.69 | 0.58 |
| 1:G:935:LEU:HD22 | 1:G:988:LEU:HD23 | 1.85 | 0.58 |
| 1:G:2791:LEU:HB3 | 1:G:2855:TYR:HE2 | 1.69 | 0.58 |
| 1:G:2803:GLU:HA | 1:G:2806:ARG:HG2 | 1.85 | 0.58 |
| 1:C:3316:LEU:HD13 | 1:C:3345:ILE:HG23 | 1.84 | 0.58 |
| 1:G:1155:LEU:HD22 | 1:G:1184:ILE:HG12 | 1.86 | 0.58 |
| 1:A:720:HIS:HA | 1:A:730:VAL:HG12 | 1.85 | 0.57 |
| 1:A:3414:ARG:HE | 1:A:3475:LYS:HB3 | 1.69 | 0.57 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:2131:LEU:HD23 | 1:C:3667:HIS:HD2 | 1.69 | 0.57 |
| 1:C:3106:MET:HE1 | 1:C:3129:LEU:HA | 1.86 | 0.57 |
| 1:C:4673:ARG:HH12 | 1:C:4698:LYS:HB3 | 1.69 | 0.57 |
| 1:G:720:HIS:HA | 1:G:730:VAL:HG12 | 1.85 | 0.57 |
| 1:A:360:ALA:HB3 | 1:A:375:LYS:HB3 | 1.85 | 0.57 |
| 1:C:144:GLU:HB2 | 1:C:175:SER:HB3 | 1.85 | 0.57 |
| 1:J:720:HIS:HA | 1:J:730:VAL:HG12 | 1.85 | 0.57 |
| 1:J:2747:ILE:HG13 | 1:J:2814:LYS:HG2 | 1.86 | 0.57 |
| 1:A:871:ARG:HA | 1:A:874:LEU:HD12 | 1.86 | 0.57 |
| 1:A:4587:PRO:HG3 | 1:A:4631:PHE:HB3 | 1.84 | 0.57 |
| 1:C:3684:GLU:HA | 1:C:3693:LYS:HE2 | 1.85 | 0.57 |
| 1:C:3729:MET:HE1 | 1:C:3778:MET:HE1 | 1.85 | 0.57 |
| 1:G:2974:ILE:HD13 | 1:G:3049:LEU:HD12 | 1.87 | 0.57 |
| 1:G:3414:ARG:HE | 1:G:3475:LYS:HB3 | 1.69 | 0.57 |
| 1:G:3729:MET:HE1 | 1:G:3778:MET:HE1 | 1.85 | 0.57 |
| 1:J:360:ALA:HB3 | 1:J:375:LYS:HB3 | 1.84 | 0.57 |
| 1:J:2131:LEU:HD23 | 1:J:3667:HIS:HD2 | 1.69 | 0.57 |
| 1:J:3989:VAL:HB | 1:J:4023:MET:HE1 | 1.86 | 0.57 |
| 1:J:4587:PRO:HG3 | 1:J:4631:PHE:HB3 | 1.85 | 0.57 |
| 2:K:71:ARG:HA | 2:K:78:VAL:HA | 1.87 | 0.57 |
| 1:C:900:ASN:HD21 | 1:C:903:LEU:HD12 | 1.68 | 0.57 |
| 1:G:2506:LEU:HD11 | 1:G:2517:PHE:HZ | 1.69 | 0.57 |
| 1:A:3379:LEU:HD21 | 1:A:3390:GLY:HA3 | 1.85 | 0.57 |
| 1:C:3354:LEU:HD11 | 1:C:3434:LEU:HD22 | 1.87 | 0.57 |
| 1:C:3414:ARG:HE | 1:C:3475:LYS:HB3 | 1.69 | 0.57 |
| 1:A:213:TYR:HD1 | 1:A:340:LYS:HB2 | 1.69 | 0.57 |
| 1:A:4673:ARG:HH12 | 1:A:4698:LYS:HB3 | 1.69 | 0.57 |
| 1:A:4933:GLN:HG2 | 1:J:4926:VAL:HG13 | 1.86 | 0.57 |
| 1:C:2439:GLU:HB2 | 1:C:2442:LEU:HG | 1.87 | 0.57 |
| 1:G:3989:VAL:HB | 1:G:4023:MET:HE1 | 1.86 | 0.57 |
| 1:J:2974:ILE:HD13 | 1:J:3049:LEU:HD12 | 1.87 | 0.57 |
| 1:A:2559:LEU:HG | 1:A:2603:ILE:HD13 | 1.87 | 0.57 |
| 2:B:71:ARG:HA | 2:B:78:VAL:HA | 1.87 | 0.57 |
| 1:C:2754:PHE:CG | 1:C:2825:LYS:HE2 | 2.40 | 0.57 |
| 1:C:3003:LEU:HB3 | 1:C:3004:PRO:HD3 | 1.87 | 0.57 |
| 1:G:916:PRO:HB3 | 2:H:53:SER:HB3 | 1.87 | 0.57 |
| 1:G:2754:PHE:CG | 1:G:2825:LYS:HE2 | 2.40 | 0.57 |
| 1:G:2779:GLU:HG3 | 1:G:2792:ARG:HG2 | 1.87 | 0.57 |
| 1:G:2960:LEU:HD13 | 1:G:3039:ILE:HD13 | 1.87 | 0.57 |
| 1:G:4959:PHE:HB3 | 1:G:4985:LEU:HD21 | 1.87 | 0.57 |
| 1:J:3414:ARG:HE | 1:J:3475:LYS:HB3 | 1.69 | 0.57 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:2779:GLU:HG3 | 1:A:2792:ARG:HG2 | 1.87 | 0.57 |
| 1:G:2377:LEU:HD21 | 1:G:2468:GLY:HA3 | 1.87 | 0.57 |
| 1:G:2604:GLU:HB2 | 1:G:2639:MET:HG3 | 1.87 | 0.57 |
| 1:J:2604:GLU:HB2 | 1:J:2639:MET:HG3 | 1.87 | 0.57 |
| 1:J:2754:PHE:CG | 1:J:2825:LYS:HE2 | 2.40 | 0.57 |
| 1:A:1155:LEU:HD22 | 1:A:1184:ILE:HG12 | 1.86 | 0.57 |
| 1:C:871:ARG:HA | 1:C:874:LEU:HD12 | 1.86 | 0.57 |
| 1:C:3433:GLU:O | 1:C:3437:MET:HG2 | 2.04 | 0.57 |
| 1:G:1102:VAL:HG11 | 1:G:1149:VAL:HG21 | 1.86 | 0.57 |
| 1:G:2144:ILE:HD13 | 1:G:2152:THR:HG21 | 1.87 | 0.57 |
| 3:I:56:ILE:HG22 | 3:I:59:PHE:HB2 | 1.87 | 0.57 |
| 1:A:2144:ILE:HD13 | 1:A:2152:THR:HG21 | 1.87 | 0.57 |
| 1:A:2791:LEU:HB3 | 1:A:2855:TYR:HE2 | 1.68 | 0.57 |
| 1:C:908:VAL:HG22 | 1:C:909:ASN:H | 1.69 | 0.57 |
| 1:C:2960:LEU:HD13 | 1:C:3039:ILE:HD13 | 1.87 | 0.57 |
| 2:D:71:ARG:HA | 2:D:78:VAL:HA | 1.87 | 0.57 |
| 1:G:1033:ARG:HA | 1:G:1036:ARG:HD2 | 1.86 | 0.57 |
| 1:J:900:ASN:HD21 | 1:J:903:LEU:HD12 | 1.68 | 0.57 |
| 1:J:2377:LEU:HG | 1:J:2465:ASP:HA | 1.87 | 0.57 |
| 1:J:3729:MET:HE1 | 1:J:3778:MET:HE1 | 1.85 | 0.57 |
| 1:A:3003:LEU:HB3 | 1:A:3004:PRO:HD3 | 1.87 | 0.56 |
| 1:C:4546:VAL:HG22 | 1:C:4550:LYS:HE3 | 1.87 | 0.56 |
| 1:G:2747:ILE:HG13 | 1:G:2814:LYS:HG2 | 1.86 | 0.56 |
| 1:G:3003:LEU:HB3 | 1:G:3004:PRO:HD3 | 1.87 | 0.56 |
| 2:H:71:ARG:HA | 2:H:78:VAL:HA | 1.87 | 0.56 |
| 1:J:213:TYR:HD1 | 1:J:340:LYS:HB2 | 1.69 | 0.56 |
| 1:J:2875:ALA:HB2 | 1:J:2927:LEU:HD13 | 1.87 | 0.56 |
| 1:J:2908:TYR:HA | 1:J:2911:LEU:HG | 1.87 | 0.56 |
| 1:J:4978:HIS:HA | 1:J:4982:GLU:HB3 | 1.86 | 0.56 |
| 8:A:5116:POV:H32A | 8:A:5117:POV:H27A | 1.87 | 0.56 |
| 1:C:905:PRO:HB2 | 1:C:963:ASN:HD21 | 1.69 | 0.56 |
| 1:C:920:TYR:HH | 2:D:107:TRP:CD1 | 2.22 | 0.56 |
| 1:G:3106:MET:HE1 | 1:G:3129:LEU:HA | 1.86 | 0.56 |
| 1:G:4546:VAL:HG22 | 1:G:4550:LYS:HE3 | 1.87 | 0.56 |
| 1:G:4673:ARG:HH12 | 1:G:4698:LYS:HB3 | 1.69 | 0.56 |
| 1:J:3003:LEU:HB3 | 1:J:3004:PRO:HD3 | 1.87 | 0.56 |
| 1:J:4673:ARG:HH12 | 1:J:4698:LYS:HB3 | 1.69 | 0.56 |
| 1:A:1102:VAL:HG11 | 1:A:1149:VAL:HG21 | 1.87 | 0.56 |
| 1:A:2439:GLU:HB2 | 1:A:2442:LEU:HG | 1.87 | 0.56 |
| 1:A:2974:ILE:HD13 | 1:A:3049:LEU:HD12 | 1.87 | 0.56 |
| 1:C:213:TYR:HD1 | 1:C:340:LYS:HB2 | 1.69 | 0.56 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:1694:LEU:HB3 | 1:C:1715:LEU:HD12 | 1.87 | 0.56 |
| 1:C:2974:ILE:HD13 | 1:C:3049:LEU:HD12 | 1.87 | 0.56 |
| 1:C:3531:ASP:O | 1:C:3535:LEU:HG | 2.05 | 0.56 |
| 2:D:9:GLY:HA3 | 2:D:123:VAL:HG22 | 1.85 | 0.56 |
| 3:F:68:LEU:HA | 3:F:103:LEU:HD23 | 1.87 | 0.56 |
| 1:G:803:LEU:HD12 | 1:G:804:PRO:HD2 | 1.87 | 0.56 |
| 1:J:1102:VAL:HG11 | 1:J:1149:VAL:HG21 | 1.87 | 0.56 |
| 1:J:2439:GLU:HB2 | 1:J:2442:LEU:HG | 1.87 | 0.56 |
| 1:J:2559:LEU:HG | 1:J:2603:ILE:HD13 | 1.87 | 0.56 |
| 1:J:2779:GLU:HG3 | 1:J:2792:ARG:HG2 | 1.87 | 0.56 |
| 1:J:3106:MET:HE1 | 1:J:3129:LEU:HA | 1.86 | 0.56 |
| 1:A:3106:MET:HE1 | 1:A:3129:LEU:HA | 1.86 | 0.56 |
| 1:C:916:PRO:HB3 | 2:D:53:SER:HB3 | 1.88 | 0.56 |
| 1:G:2131:LEU:HD23 | 1:G:3667:HIS:HD2 | 1.69 | 0.56 |
| 1:G:3354:LEU:HD11 | 1:G:3434:LEU:HD22 | 1.87 | 0.56 |
| 1:J:924:MET:HA | 2:K:107:TRP:CH2 | 2.40 | 0.56 |
| 1:J:2960:LEU:HD13 | 1:J:3039:ILE:HD13 | 1.87 | 0.56 |
| 1:J:3433:GLU:O | 1:J:3437:MET:HG2 | 2.04 | 0.56 |
| 3:L:7:ILE:HD11 | 3:L:73:LYS:HG3 | 1.86 | 0.56 |
| 1:A:1299:GLN:HG2 | 3:F:31:GLN:NE2 | 2.15 | 0.56 |
| 1:C:2144:ILE:HD13 | 1:C:2152:THR:HG21 | 1.87 | 0.56 |
| 1:C:3989:VAL:HB | 1:C:4023:MET:HE1 | 1.86 | 0.56 |
| 1:G:2908:TYR:HA | 1:G:2911:LEU:HG | 1.87 | 0.56 |
| 1:J:871:ARG:HA | 1:J:874:LEU:HD12 | 1.87 | 0.56 |
| 1:A:3989:VAL:HB | 1:A:4023:MET:HE1 | 1.86 | 0.56 |
| 1:J:4546:VAL:HG22 | 1:J:4550:LYS:HE3 | 1.87 | 0.56 |
| 1:A:3354:LEU:HD11 | 1:A:3434:LEU:HD22 | 1.87 | 0.56 |
| 1:C:2779:GLU:HG3 | 1:C:2792:ARG:HG2 | 1.87 | 0.56 |
| 1:C:2791:LEU:HB3 | 1:C:2855:TYR:HE2 | 1.68 | 0.56 |
| 1:C:3842:LEU:HB2 | 1:C:3929:SER:HB2 | 1.88 | 0.56 |
| 2:D:17:SER:HA | 2:D:83:ASN:HA | 1.88 | 0.56 |
| 1:J:1694:LEU:HB3 | 1:J:1715:LEU:HD12 | 1.87 | 0.56 |
| 1:J:2144:ILE:HD13 | 1:J:2152:THR:HG21 | 1.87 | 0.56 |
| 1:A:1694:LEU:HB3 | 1:A:1715:LEU:HD12 | 1.87 | 0.56 |
| 1:A:2960:LEU:HD13 | 1:A:3039:ILE:HD13 | 1.87 | 0.56 |
| 1:A:3733:CYS:HA | 1:A:3766:GLN:HB3 | 1.88 | 0.56 |
| 1:C:1763:PRO:HG3 | 1:C:2094:LEU:HD22 | 1.88 | 0.56 |
| 1:C:3733:CYS:HA | 1:C:3766:GLN:HB3 | 1.88 | 0.56 |
| 1:C:4978:HIS:HA | 1:C:4982:GLU:HB3 | 1.86 | 0.56 |
| 2:D:11:LEU:HD13 | 2:D:124:THR:OG1 | 2.06 | 0.56 |
| 1:J:3369:ALA:O | 1:J:3373:VAL:HG23 | 2.06 | 0.56 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:2298:VAL:HG23 | 1:A:2331:TYR:HD1 | 1.71 | 0.56 |
| 1:C:2536:LEU:HD13 | 1:C:2541:PHE:HB3 | 1.88 | 0.56 |
| 1:G:131:LEU:HD11 | 1:G:195:PHE:H | 1.71 | 0.56 |
| 1:G:790:ARG:HA | 1:G:1626:TRP:O | 2.06 | 0.56 |
| 1:G:2875:ALA:HB2 | 1:G:2927:LEU:HD13 | 1.87 | 0.56 |
| 1:G:3369:ALA:O | 1:G:3373:VAL:HG23 | 2.06 | 0.56 |
| 1:J:790:ARG:HA | 1:J:1626:TRP:O | 2.06 | 0.56 |
| 1:A:790:ARG:HA | 1:A:1626:TRP:O | 2.06 | 0.56 |
| 1:A:2754:PHE:CG | 1:A:2825:LYS:HE2 | 2.40 | 0.56 |
| 1:A:3369:ALA:O | 1:A:3373:VAL:HG23 | 2.06 | 0.56 |
| 2:B:11:LEU:HD13 | 2:B:124:THR:OG1 | 2.06 | 0.56 |
| 1:C:131:LEU:HD11 | 1:C:195:PHE:H | 1.71 | 0.56 |
| 1:G:3805:LEU:HD11 | 1:G:3813:GLN:HG3 | 1.88 | 0.56 |
| 1:J:1763:PRO:HG3 | 1:J:2094:LEU:HD22 | 1.88 | 0.56 |
| 1:J:3354:LEU:HD11 | 1:J:3434:LEU:HD22 | 1.86 | 0.56 |
| 1:A:2536:LEU:HD13 | 1:A:2541:PHE:HB3 | 1.88 | 0.55 |
| 1:A:3532:LEU:HD23 | 1:A:3535:LEU:HD12 | 1.89 | 0.55 |
| 1:A:4546:VAL:HG22 | 1:A:4550:LYS:HE3 | 1.87 | 0.55 |
| 1:C:1637:MET:HE3 | 1:C:1650:ILE:HG21 | 1.89 | 0.55 |
| 3:F:17:LYS:HG3 | 3:F:20:GLN:HE22 | 1.71 | 0.55 |
| 1:G:1694:LEU:HB3 | 1:G:1715:LEU:HD12 | 1.87 | 0.55 |
| 1:G:1763:PRO:HG3 | 1:G:2094:LEU:HD22 | 1.88 | 0.55 |
| 1:J:2233:CYS:O | 1:J:2237:CYS:N | 2.35 | 0.55 |
| 1:A:1763:PRO:HG3 | 1:A:2094:LEU:HD22 | 1.88 | 0.55 |
| 1:C:2604:GLU:HB2 | 1:C:2639:MET:HG3 | 1.87 | 0.55 |
| 1:C:2875:ALA:HB2 | 1:C:2927:LEU:HD13 | 1.87 | 0.55 |
| 1:C:3023:LYS:HE2 | 1:C:3025:LEU:HD21 | 1.89 | 0.55 |
| 3:E:17:LYS:HG3 | 3:E:20:GLN:HE22 | 1.71 | 0.55 |
| 1:G:826:ILE:HG22 | 1:G:827:LYS:HG3 | 1.89 | 0.55 |
| 2:H:11:LEU:HD13 | 2:H:124:THR:OG1 | 2.06 | 0.55 |
| 1:J:1299:GLN:HG2 | 3:L:31:GLN:NE2 | 2.18 | 0.55 |
| 1:A:826:ILE:HG22 | 1:A:827:LYS:HG3 | 1.88 | 0.55 |
| 1:A:2604:GLU:HB2 | 1:A:2639:MET:HG3 | 1.87 | 0.55 |
| 1:A:2908:TYR:HA | 1:A:2911:LEU:HG | 1.87 | 0.55 |
| 1:A:345:LEU:HB3 | 1:A:387:ALA:HB1 | 1.89 | 0.55 |
| 1:A:1637:MET:HE3 | 1:A:1650:ILE:HG21 | 1.89 | 0.55 |
| 1:C:1102:VAL:HG11 | 1:C:1149:VAL:HG21 | 1.87 | 0.55 |
| 3:E:4:ILE:HG13 | 3:E:65:GLN:HB3 | 1.87 | 0.55 |
| 1:G:22:LEU:HB2 | 1:G:37:LEU:HD22 | 1.89 | 0.55 |
| 1:J:826:ILE:HG22 | 1:J:827:LYS:HG3 | 1.89 | 0.55 |
| 1:J:2536:LEU:HD13 | 1:J:2541:PHE:HB3 | 1.88 | 0.55 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:J:3805:LEU:HD11 | 1:J:3813:GLN:HG3 | 1.88 | 0.55 |
| 1:J:4959:PHE:HB3 | 1:J:4985:LEU:HD21 | 1.87 | 0.55 |
| 8:J:5117:POV:H3A | 8:J:5119:POV:H24 | 1.88 | 0.55 |
| 1:C:826:ILE:HG22 | 1:C:827:LYS:HG3 | 1.89 | 0.55 |
| 1:G:871:ARG:HA | 1:G:874:LEU:HD12 | 1.87 | 0.55 |
| 1:G:1637:MET:HE3 | 1:G:1650:ILE:HG21 | 1.89 | 0.55 |
| 1:G:3800:LEU:O | 1:G:3804:ILE:HG12 | 2.06 | 0.55 |
| 1:A:3023:LYS:HE2 | 1:A:3025:LEU:HD21 | 1.88 | 0.55 |
| 1:C:2298:VAL:HG23 | 1:C:2331:TYR:HD1 | 1.71 | 0.55 |
| 1:C:2355:ARG:HH12 | 1:C:2453:ILE:HD11 | 1.71 | 0.55 |
| 1:C:4959:PHE:HB3 | 1:C:4985:LEU:HD21 | 1.88 | 0.55 |
| 1:G:2536:LEU:HD13 | 1:G:2541:PHE:HB3 | 1.88 | 0.55 |
| 1:G:3733:CYS:HA | 1:G:3766:GLN:HB3 | 1.88 | 0.55 |
| 1:J:1076:ARG:HB3 | 1:J:1191:VAL:HG23 | 1.88 | 0.55 |
| 3:L:17:LYS:HG3 | 3:L:20:GLN:HE22 | 1.71 | 0.55 |
| 1:C:2908:TYR:HA | 1:C:2911:LEU:HG | 1.87 | 0.55 |
| 1:J:4087:LEU:HD22 | 1:J:4124:ASN:HA | 1.89 | 0.55 |
| 2:B:93:TYR:O | 2:B:120:GLY:HA2 | 2.07 | 0.55 |
| 1:G:2439:GLU:HB2 | 1:G:2442:LEU:HG | 1.87 | 0.55 |
| 3:I:17:LYS:HG3 | 3:I:20:GLN:HE22 | 1.71 | 0.55 |
| 1:J:653:ALA:HB3 | 1:J:656:SER:HB2 | 1.89 | 0.55 |
| 1:J:1637:MET:HE3 | 1:J:1650:ILE:HG21 | 1.89 | 0.55 |
| 1:J:2355:ARG:HH12 | 1:J:2453:ILE:HD11 | 1.71 | 0.55 |
| 2:K:11:LEU:HD13 | 2:K:124:THR:OG1 | 2.06 | 0.55 |
| 1:A:2233:CYS:SG | 1:A:2270:SER:HB3 | 2.47 | 0.55 |
| 1:A:2355:ARG:HH12 | 1:A:2453:ILE:HD11 | 1.71 | 0.55 |
| 2:D:93:TYR:O | 2:D:120:GLY:HA2 | 2.07 | 0.55 |
| 1:G:1020:ARG:HB3 | 1:G:1031:THR:HG21 | 1.89 | 0.55 |
| 1:G:3052:HIS:HE1 | 1:G:3128:ASN:HB3 | 1.72 | 0.55 |
| 1:J:3842:LEU:HB2 | 1:J:3929:SER:HB2 | 1.88 | 0.55 |
| 1:A:653:ALA:HB3 | 1:A:656:SER:HB2 | 1.89 | 0.55 |
| 1:A:2875:ALA:HB2 | 1:A:2927:LEU:HD13 | 1.87 | 0.55 |
| 1:C:222:LEU:HB3 | 1:C:388:LEU:HD23 | 1.88 | 0.55 |
| 1:C:247:TYR:OH | 1:C:376:ALA:HA | 2.07 | 0.55 |
| 1:C:3369:ALA:O | 1:C:3373:VAL:HG23 | 2.06 | 0.55 |
| 1:J:3052:HIS:HE1 | 1:J:3128:ASN:HB3 | 1.72 | 0.55 |
| 1:J:3250:MET:HA | 1:J:3253:ILE:HG22 | 1.89 | 0.55 |
| 1:J:3800:LEU:O | 1:J:3804:ILE:HG12 | 2.06 | 0.55 |
| 2:K:93:TYR:O | 2:K:120:GLY:HA2 | 2.07 | 0.55 |
| 1:A:3800:LEU:O | 1:A:3804:ILE:HG12 | 2.06 | 0.54 |
| 1:A:3842:LEU:HD21 | 1:A:3954:ALA:HB2 | 1.90 | 0.54 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:G:247:TYR:OH | 1:G:376:ALA:HA | 2.07 | 0.54 |
| 1:G:2355:ARG:HH12 | 1:G:2453:ILE:HD11 | 1.71 | 0.54 |
| 1:J:131:LEU:HD11 | 1:J:195:PHE:H | 1.71 | 0.54 |
| 1:J:247:TYR:OH | 1:J:376:ALA:HA | 2.07 | 0.54 |
| 1:J:2298:VAL:HG23 | 1:J:2331:TYR:HD1 | 1.71 | 0.54 |
| 1:J:2362:GLU:HG3 | 1:J:2369:ARG:HH12 | 1.72 | 0.54 |
| 3:L:5:GLU:HB2 | 3:L:73:LYS:HB2 | 1.88 | 0.54 |
| 1:A:924:MET:HA | 2:B:107:TRP:CH2 | 2.41 | 0.54 |
| 1:A:1076:ARG:HB3 | 1:A:1191:VAL:HG23 | 1.88 | 0.54 |
| 1:A:3052:HIS:CE1 | 1:A:3128:ASN:HB3 | 2.43 | 0.54 |
| 1:A:3842:LEU:HB2 | 1:A:3929:SER:HB2 | 1.88 | 0.54 |
| 1:G:222:LEU:HB3 | 1:G:388:LEU:HD23 | 1.88 | 0.54 |
| 1:G:3842:LEU:HB2 | 1:G:3929:SER:HB2 | 1.88 | 0.54 |
| 1:A:131:LEU:HD11 | 1:A:195:PHE:H | 1.71 | 0.54 |
| 1:C:653:ALA:HB3 | 1:C:656:SER:HB2 | 1.89 | 0.54 |
| 1:C:3800:LEU:O | 1:C:3804:ILE:HG12 | 2.06 | 0.54 |
| 1:J:22:LEU:HB2 | 1:J:37:LEU:HD22 | 1.89 | 0.54 |
| 1:J:345:LEU:HB3 | 1:J:387:ALA:HB1 | 1.89 | 0.54 |
| 1:A:222:LEU:HB3 | 1:A:388:LEU:HD23 | 1.88 | 0.54 |
| 1:A:3805:LEU:HD11 | 1:A:3813:GLN:HG3 | 1.88 | 0.54 |
| 2:B:17:SER:HA | 2:B:83:ASN:HA | 1.88 | 0.54 |
| 1:C:3052:HIS:CE1 | 1:C:3128:ASN:HB3 | 2.43 | 0.54 |
| 1:C:3805:LEU:HD11 | 1:C:3813:GLN:HG3 | 1.88 | 0.54 |
| 1:C:3842:LEU:HD21 | 1:C:3954:ALA:HB2 | 1.90 | 0.54 |
| 1:G:3904:ARG:HG2 | 1:G:3905:THR:HG23 | 1.90 | 0.54 |
| 1:J:222:LEU:HB3 | 1:J:388:LEU:HD23 | 1.88 | 0.54 |
| 1:J:3733:CYS:HA | 1:J:3766:GLN:HB3 | 1.88 | 0.54 |
| 2:K:17:SER:HA | 2:K:83:ASN:HA | 1.88 | 0.54 |
| 1:A:3904:ARG:HG2 | 1:A:3905:THR:HG23 | 1.90 | 0.54 |
| 1:A:4959:PHE:HB3 | 1:A:4985:LEU:HD21 | 1.89 | 0.54 |
| 1:C:788:LYS:HE2 | 1:C:1627:ALA:HB1 | 1.89 | 0.54 |
| 1:G:2298:VAL:HG23 | 1:G:2331:TYR:HD1 | 1.71 | 0.54 |
| 1:G:4859:PHE:HB3 | 1:G:4913:ARG:HE | 1.72 | 0.54 |
| 2:H:93:TYR:O | 2:H:120:GLY:HA2 | 2.07 | 0.54 |
| 1:J:670:GLU:HB3 | 1:J:788:LYS:HB3 | 1.89 | 0.54 |
| 1:J:3023:LYS:HE2 | 1:J:3025:LEU:HD21 | 1.89 | 0.54 |
| 2:K:4:LEU:HB2 | 2:K:118:GLY:HA2 | 1.89 | 0.54 |
| 1:A:863:LEU:HD22 | 1:A:867:LEU:HD13 | 1.89 | 0.54 |
| 1:A:3052:HIS:HE1 | 1:A:3128:ASN:HB3 | 1.72 | 0.54 |
| 1:A:4918:ILE:HD12 | 8:C:5111:POV:H215 | 1.90 | 0.54 |
| 1:A:4948:GLU:HA | 1:A:4951:LYS:HE2 | 1.90 | 0.54 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:670:GLU:HB3 | 1:C:788:LYS:HB3 | 1.89 | 0.54 |
| 1:C:790:ARG:HA | 1:C:1626:TRP:O | 2.06 | 0.54 |
| 1:C:2362:GLU:HG3 | 1:C:2369:ARG:HH12 | 1.71 | 0.54 |
| 8:C:5120:POV:H26 | 8:G:5109:POV:H35A | 1.90 | 0.54 |
| 1:G:1076:ARG:HB3 | 1:G:1191:VAL:HG23 | 1.88 | 0.54 |
| 1:G:3842:LEU:HD21 | 1:G:3954:ALA:HB2 | 1.90 | 0.54 |
| 1:J:863:LEU:HD22 | 1:J:867:LEU:HD13 | 1.89 | 0.54 |
| 1:A:22:LEU:HB2 | 1:A:37:LEU:HD22 | 1.89 | 0.54 |
| 1:A:2362:GLU:HG3 | 1:A:2369:ARG:HH12 | 1.72 | 0.54 |
| 1:A:3250:MET:HA | 1:A:3253:ILE:HG22 | 1.89 | 0.54 |
| 1:C:3250:MET:HA | 1:C:3253:ILE:HG22 | 1.89 | 0.54 |
| 1:G:653:ALA:HB3 | 1:G:656:SER:HB2 | 1.89 | 0.54 |
| 1:G:3011:THR:HA | 1:G:3073:ARG:HH11 | 1.70 | 0.54 |
| 1:G:4087:LEU:HD22 | 1:G:4124:ASN:HA | 1.89 | 0.54 |
| 1:J:3842:LEU:HD21 | 1:J:3954:ALA:HB2 | 1.90 | 0.54 |
| 1:A:2233:CYS:O | 1:A:2234:ARG:C | 2.50 | 0.54 |
| 1:A:2306:GLY:HA2 | 1:A:2323:TRP:CZ3 | 2.42 | 0.54 |
| 1:A:3102:ASP:HA | 1:A:3105:LYS:HE2 | 1.90 | 0.54 |
| 8:A:5109:POV:H15B | 8:A:5111:POV:H12A | 1.90 | 0.54 |
| 1:C:22:LEU:HB2 | 1:C:37:LEU:HD22 | 1.89 | 0.54 |
| 1:C:3052:HIS:HE1 | 1:C:3128:ASN:HB3 | 1.72 | 0.54 |
| 1:C:4859:PHE:HB3 | 1:C:4913:ARG:HE | 1.72 | 0.54 |
| 8:C:5112:POV:H15B | 8:C:5114:POV:H12A | 1.90 | 0.54 |
| 1:C:345:LEU:HB3 | 1:C:387:ALA:HB1 | 1.89 | 0.54 |
| 1:C:1023:PRO:HD2 | 1:C:1026:LEU:HD12 | 1.90 | 0.54 |
| 1:C:1076:ARG:HB3 | 1:C:1191:VAL:HG23 | 1.88 | 0.54 |
| 1:C:1784:ALA:HA | 3:E:55:VAL:HA | 1.89 | 0.54 |
| 1:C:3904:ARG:HG2 | 1:C:3905:THR:HG23 | 1.90 | 0.54 |
| 8:C:5112:POV:H1 | 8:C:5113:POV:O13 | 2.07 | 0.54 |
| 1:G:2488:PRO:HG2 | 1:G:2546:MET:SD | 2.47 | 0.54 |
| 2:H:31:ILE:HG22 | 2:H:97:ALA:HB1 | 1.90 | 0.54 |
| 1:J:788:LYS:HE2 | 1:J:1627:ALA:HB1 | 1.89 | 0.54 |
| 1:J:1476:MET:HB2 | 1:J:1485:SER:HB3 | 1.90 | 0.54 |
| 3:L:56:ILE:HG22 | 3:L:59:PHE:HB2 | 1.90 | 0.54 |
| 1:A:247:TYR:OH | 1:A:376:ALA:HA | 2.07 | 0.54 |
| 1:A:4087:LEU:HD22 | 1:A:4124:ASN:HA | 1.89 | 0.54 |
| 1:G:863:LEU:HD22 | 1:G:867:LEU:HD13 | 1.89 | 0.54 |
| 1:G:2362:GLU:HG3 | 1:G:2369:ARG:HH12 | 1.71 | 0.54 |
| 1:J:2583:LEU:HD12 | 1:J:2622:LEU:HD22 | 1.90 | 0.54 |
| 1:J:3104:GLU:O | 1:J:3107:VAL:HG22 | 2.08 | 0.54 |
| 1:J:4859:PHE:HB3 | 1:J:4913:ARG:HE | 1.72 | 0.54 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:3104:GLU:O | 1:C:3107:VAL:HG22 | 2.08 | 0.53 |
| 1:G:3023:LYS:HE2 | 1:G:3025:LEU:HD21 | 1.89 | 0.53 |
| 2:H:4:LEU:HB2 | 2:H:118:GLY:HA2 | 1.90 | 0.53 |
| 1:J:2479:LEU:HB2 | 1:J:2541:PHE:HZ | 1.74 | 0.53 |
| 1:A:2512:ILE:HG21 | 1:A:2518:LEU:HG | 1.90 | 0.53 |
| 1:C:3539:ARG:HD3 | 1:C:3549:VAL:HG12 | 1.91 | 0.53 |
| 1:G:345:LEU:HB3 | 1:G:387:ALA:HB1 | 1.89 | 0.53 |
| 1:G:788:LYS:HE2 | 1:G:1627:ALA:HB1 | 1.89 | 0.53 |
| 1:G:1476:MET:HB2 | 1:G:1485:SER:HB3 | 1.90 | 0.53 |
| 1:G:2766:TRP:O | 1:G:2770:LYS:HG2 | 2.09 | 0.53 |
| 1:G:3250:MET:HA | 1:G:3253:ILE:HG22 | 1.89 | 0.53 |
| 1:J:3052:HIS:CE1 | 1:J:3128:ASN:HB3 | 2.43 | 0.53 |
| 1:A:788:LYS:HE2 | 1:A:1627:ALA:HB1 | 1.89 | 0.53 |
| 1:C:246:TYR:HB3 | 1:C:373:LYS:HB2 | 1.91 | 0.53 |
| 1:C:2583:LEU:HD12 | 1:C:2622:LEU:HD22 | 1.90 | 0.53 |
| 1:G:2583:LEU:HD12 | 1:G:2622:LEU:HD22 | 1.90 | 0.53 |
| 1:G:3434:LEU:O | 1:G:3438:VAL:HG12 | 2.08 | 0.53 |
| 1:G:4060:LYS:O | 1:G:4064:MET:HG2 | 2.09 | 0.53 |
| 1:J:520:ASN:O | 1:J:524:GLU:HG2 | 2.09 | 0.53 |
| 1:J:2522:LEU:HD23 | 1:J:2578:MET:HE1 | 1.91 | 0.53 |
| 1:J:3904:ARG:HG2 | 1:J:3905:THR:HG23 | 1.90 | 0.53 |
| 1:A:246:TYR:HB3 | 1:A:373:LYS:HB2 | 1.91 | 0.53 |
| 1:A:520:ASN:O | 1:A:524:GLU:HG2 | 2.09 | 0.53 |
| 1:A:2766:TRP:O | 1:A:2770:LYS:HG2 | 2.09 | 0.53 |
| 1:C:1476:MET:HB2 | 1:C:1485:SER:HB3 | 1.91 | 0.53 |
| 1:C:4918:ILE:HD12 | 8:G:5111:POV:H215 | 1.90 | 0.53 |
| 1:G:246:TYR:HB3 | 1:G:373:LYS:HB2 | 1.91 | 0.53 |
| 1:G:1784:ALA:HA | 3:I:55:VAL:HA | 1.89 | 0.53 |
| 1:G:4948:GLU:HA | 1:G:4951:LYS:HE2 | 1.89 | 0.53 |
| 1:J:246:TYR:HB3 | 1:J:373:LYS:HB2 | 1.91 | 0.53 |
| 1:J:4060:LYS:O | 1:J:4064:MET:HG2 | 2.09 | 0.53 |
| 1:A:1476:MET:HB2 | 1:A:1485:SER:HB3 | 1.90 | 0.53 |
| 1:A:2522:LEU:HD23 | 1:A:2578:MET:HE1 | 1.91 | 0.53 |
| 1:A:2583:LEU:HD12 | 1:A:2622:LEU:HD22 | 1.90 | 0.53 |
| 1:C:737:LEU:HD12 | 3:E:71:ARG:HH12 | 1.74 | 0.53 |
| 1:C:1033:ARG:HE | 1:C:1036:ARG:HD2 | 1.73 | 0.53 |
| 1:G:2306:GLY:HA2 | 1:G:2323:TRP:HZ3 | 1.74 | 0.53 |
| 1:J:4948:GLU:HA | 1:J:4951:LYS:HE2 | 1.89 | 0.53 |
| 1:A:2644:LEU:HD13 | 1:A:2678:LEU:HD21 | 1.91 | 0.53 |
| 1:C:863:LEU:HD22 | 1:C:867:LEU:HD13 | 1.89 | 0.53 |
| 1:C:3102:ASP:HA | 1:C:3105:LYS:HE2 | 1.90 | 0.53 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:G:670:GLU:HB3 | 1:G:788:LYS:HB3 | 1.89 | 0.53 |
| 1:G:3052:HIS:CE1 | 1:G:3128:ASN:HB3 | 2.43 | 0.53 |
| 1:G:4586:PRO:O | 1:G:4587:PRO:C | 2.51 | 0.53 |
| 1:G:4655:PHE:HD1 | 1:G:4796:MET:HE1 | 1.74 | 0.53 |
| 1:J:3102:ASP:HA | 1:J:3105:LYS:HE2 | 1.90 | 0.53 |
| 2:K:70:SER:O | 2:K:79:TYR:HB2 | 2.09 | 0.53 |
| 1:C:4655:PHE:HD1 | 1:C:4796:MET:HE1 | 1.73 | 0.53 |
| 1:G:2479:LEU:HB2 | 1:G:2541:PHE:HZ | 1.74 | 0.53 |
| 1:J:2644:LEU:HD13 | 1:J:2678:LEU:HD21 | 1.91 | 0.53 |
| 3:L:57:LYS:HE3 | 3:L:80:VAL:HG12 | 1.91 | 0.53 |
| 1:A:670:GLU:HB3 | 1:A:788:LYS:HB3 | 1.89 | 0.53 |
| 1:C:3519:PRO:HA | 1:C:3522:LEU:HB2 | 1.91 | 0.53 |
| 1:G:110:ARG:HD3 | 1:G:115:ARG:HH21 | 1.74 | 0.53 |
| 1:G:520:ASN:O | 1:G:524:GLU:HG2 | 2.09 | 0.53 |
| 1:G:1023:PRO:HD2 | 1:G:1026:LEU:HD12 | 1.90 | 0.53 |
| 1:J:916:PRO:HB3 | 2:K:53:SER:HB3 | 1.90 | 0.53 |
| 1:J:1737:PRO:HB2 | 1:J:1739:THR:HG23 | 1.91 | 0.53 |
| 1:J:2534:ALA:HB1 | 1:J:2588:ARG:HE | 1.74 | 0.53 |
| 1:J:3187:ARG:HA | 1:J:3190:LEU:HD12 | 1.91 | 0.53 |
| 1:A:1023:PRO:HD2 | 1:A:1026:LEU:HD12 | 1.90 | 0.53 |
| 1:A:3172:ILE:HD11 | 1:A:3190:LEU:HB3 | 1.90 | 0.53 |
| 1:C:520:ASN:O | 1:C:524:GLU:HG2 | 2.09 | 0.53 |
| 2:D:70:SER:O | 2:D:79:TYR:HB2 | 2.09 | 0.53 |
| 1:G:1737:PRO:HB2 | 1:G:1739:THR:HG23 | 1.91 | 0.53 |
| 1:G:3104:GLU:O | 1:G:3107:VAL:HG22 | 2.08 | 0.53 |
| 8:G:5112:POV:H15B | 8:G:5114:POV:H12A | 1.90 | 0.53 |
| 1:J:1784:ALA:HA | 3:L:55:VAL:HA | 1.90 | 0.53 |
| 1:A:4859:PHE:HB3 | 1:A:4913:ARG:HE | 1.72 | 0.53 |
| 8:A:5108:POV:H215 | 1:J:4918:ILE:HD12 | 1.91 | 0.53 |
| 2:B:96:ASN:OD1 | 2:B:117:TRP:HA | 2.09 | 0.53 |
| 1:C:2952:GLU:HA | 1:C:2957:PHE:HD2 | 1.74 | 0.53 |
| 1:J:2630:VAL:HG12 | 1:J:2682:ILE:HD11 | 1.91 | 0.53 |
| 1:J:2870:GLU:HG3 | 1:J:2939:ARG:HG2 | 1.91 | 0.53 |
| 1:J:3539:ARG:HD3 | 1:J:3549:VAL:HG12 | 1.91 | 0.53 |
| 1:J:4655:PHE:HD1 | 1:J:4796:MET:HE1 | 1.73 | 0.53 |
| 8:J:5116:POV:H15B | 8:J:5118:POV:H12A | 1.90 | 0.53 |
| 1:A:3104:GLU:O | 1:A:3107:VAL:HG22 | 2.08 | 0.52 |
| 1:A:3519:PRO:HA | 1:A:3522:LEU:HB2 | 1.91 | 0.52 |
| 1:A:4053:SER:O | 1:A:4057:MET:HG2 | 2.09 | 0.52 |
| 1:A:4568:PHE:HD1 | 8:A:5121:POV:H26 | 1.74 | 0.52 |
| 1:C:1299:GLN:HG2 | 3:E:31:GLN:NE2 | 2.18 | 0.52 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:4087:LEU:HD22 | 1:C:4124:ASN:HA | 1.89 | 0.52 |
| 1:G:2534:ALA:HB1 | 1:G:2588:ARG:HE | 1.74 | 0.52 |
| 1:G:2595:LEU:HD22 | 1:G:2599:GLN:HB3 | 1.92 | 0.52 |
| 1:G:2630:VAL:HG12 | 1:G:2682:ILE:HD11 | 1.91 | 0.52 |
| 1:G:2802:LYS:O | 1:G:2806:ARG:HB3 | 2.10 | 0.52 |
| 1:G:2870:GLU:HG3 | 1:G:2939:ARG:HG2 | 1.91 | 0.52 |
| 1:G:3187:ARG:HA | 1:G:3190:LEU:HD12 | 1.90 | 0.52 |
| 1:J:1023:PRO:HD2 | 1:J:1026:LEU:HD12 | 1.90 | 0.52 |
| 1:J:1758:ARG:HH12 | 1:J:2037:ASP:HA | 1.74 | 0.52 |
| 1:A:899:ASP:HB2 | 2:B:102:ASN:HB3 | 1.90 | 0.52 |
| 1:A:3798:LEU:HB3 | 1:A:3883:ASP:OD1 | 2.10 | 0.52 |
| 1:A:4060:LYS:O | 1:A:4064:MET:HG2 | 2.09 | 0.52 |
| 2:B:58:ASN:ND2 | 2:B:102:ASN:HA | 2.23 | 0.52 |
| 1:C:110:ARG:HD3 | 1:C:115:ARG:HH21 | 1.74 | 0.52 |
| 1:C:1703:LEU:HD12 | 1:C:1704:PRO:HD2 | 1.91 | 0.52 |
| 1:C:2364:PHE:HD1 | 1:C:2429:LEU:HD21 | 1.75 | 0.52 |
| 1:C:4053:SER:O | 1:C:4057:MET:HG2 | 2.09 | 0.52 |
| 1:G:1758:ARG:HH12 | 1:G:2037:ASP:HA | 1.74 | 0.52 |
| 1:G:2644:LEU:HD13 | 1:G:2678:LEU:HD21 | 1.91 | 0.52 |
| 1:G:3539:ARG:HD3 | 1:G:3549:VAL:HG12 | 1.91 | 0.52 |
| 1:J:1703:LEU:HD12 | 1:J:1704:PRO:HD2 | 1.92 | 0.52 |
| 1:J:2233:CYS:O | 1:J:2234:ARG:C | 2.51 | 0.52 |
| 1:J:2595:LEU:HD22 | 1:J:2599:GLN:HB3 | 1.92 | 0.52 |
| 1:J:3519:PRO:HA | 1:J:3522:LEU:HB2 | 1.91 | 0.52 |
| 1:A:1703:LEU:HD12 | 1:A:1704:PRO:HD2 | 1.91 | 0.52 |
| 1:A:2479:LEU:HB2 | 1:A:2541:PHE:HZ | 1.74 | 0.52 |
| 1:A:2952:GLU:HA | 1:A:2957:PHE:HD2 | 1.74 | 0.52 |
| 1:C:2386:ILE:HG23 | 1:C:2392:ARG:HB3 | 1.92 | 0.52 |
| 1:C:2874:MET:HE3 | 1:C:2927:LEU:HD11 | 1.92 | 0.52 |
| 1:G:1180:ARG:H | 1:G:1180:ARG:HD2 | 1.75 | 0.52 |
| 1:G:1703:LEU:HD12 | 1:G:1704:PRO:HD2 | 1.92 | 0.52 |
| 1:G:3368:ARG:O | 1:G:3372:VAL:HG23 | 2.10 | 0.52 |
| 1:J:110:ARG:HD3 | 1:J:115:ARG:HH21 | 1.74 | 0.52 |
| 1:J:3798:LEU:HB3 | 1:J:3883:ASP:OD1 | 2.10 | 0.52 |
| 1:A:985:VAL:HG13 | 1:A:1039:LEU:HG | 1.91 | 0.52 |
| 1:A:1180:ARG:H | 1:A:1180:ARG:HD2 | 1.75 | 0.52 |
| 1:A:2802:LYS:O | 1:A:2806:ARG:HB3 | 2.10 | 0.52 |
| 1:A:4655:PHE:HD1 | 1:A:4796:MET:HE1 | 1.73 | 0.52 |
| 2:B:70:SER:O | 2:B:79:TYR:HB2 | 2.09 | 0.52 |
| 1:C:2766:TRP:O | 1:C:2770:LYS:HG2 | 2.09 | 0.52 |
| 1:C:3798:LEU:HB3 | 1:C:3883:ASP:OD1 | 2.10 | 0.52 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:G:3519:PRO:HA | 1:G:3522:LEU:HB2 | 1.91 | 0.52 |
| 1:J:2766:TRP:O | 1:J:2770:LYS:HG2 | 2.09 | 0.52 |
| 1:J:2967:MET:HE2 | 1:J:3045:LYS:HD3 | 1.92 | 0.52 |
| 1:A:2874:MET:HE3 | 1:A:2927:LEU:HD11 | 1.92 | 0.52 |
| 2:B:31:ILE:HG22 | 2:B:97:ALA:HB1 | 1.90 | 0.52 |
| 1:C:957:LYS:HA | 1:C:959:TYR:CZ | 2.44 | 0.52 |
| 1:C:2257:LEU:HD13 | 1:C:2275:VAL:HB | 1.92 | 0.52 |
| 1:G:924:MET:HA | 2:H:107:TRP:CH2 | 2.45 | 0.52 |
| 1:G:3965:LEU:HD23 | 1:G:3968:TYR:HD2 | 1.74 | 0.52 |
| 1:J:1180:ARG:H | 1:J:1180:ARG:HD2 | 1.75 | 0.52 |
| 1:J:3698:LEU:O | 1:J:3702:VAL:HG23 | 2.10 | 0.52 |
| 1:A:996:TRP:HB2 | 2:B:114:TYR:HE1 | 1.74 | 0.52 |
| 1:A:2377:LEU:HD23 | 1:A:2469:ILE:HG13 | 1.92 | 0.52 |
| 1:A:2630:VAL:HG12 | 1:A:2682:ILE:HD11 | 1.92 | 0.52 |
| 1:A:3698:LEU:O | 1:A:3702:VAL:HG23 | 2.10 | 0.52 |
| 1:A:5004:THR:HG22 | 1:A:5007:GLU:HG3 | 1.92 | 0.52 |
| 1:C:255:HIS:CD2 | 1:C:480:GLU:HG2 | 2.45 | 0.52 |
| 1:C:733:PRO:HG3 | 1:C:762:CYS:HB2 | 1.92 | 0.52 |
| 1:C:2306:GLY:HA2 | 1:C:2323:TRP:HZ3 | 1.74 | 0.52 |
| 1:C:3368:ARG:O | 1:C:3372:VAL:HG23 | 2.10 | 0.52 |
| 1:C:3607:GLU:HA | 1:C:3610:GLU:HG2 | 1.92 | 0.52 |
| 1:G:2952:GLU:HA | 1:G:2957:PHE:HD2 | 1.74 | 0.52 |
| 1:G:3076:ASP:HB2 | 1:G:3146:HIS:HE1 | 1.74 | 0.52 |
| 1:A:110:ARG:HD3 | 1:A:115:ARG:HH21 | 1.74 | 0.52 |
| 1:A:255:HIS:CD2 | 1:A:480:GLU:HG2 | 2.45 | 0.52 |
| 1:C:2479:LEU:HB2 | 1:C:2541:PHE:HZ | 1.74 | 0.52 |
| 1:C:2522:LEU:HD23 | 1:C:2578:MET:HE1 | 1.91 | 0.52 |
| 1:C:4115:SER:HB2 | 1:C:4123:ILE:HG21 | 1.92 | 0.52 |
| 1:G:2386:ILE:HG23 | 1:G:2392:ARG:HB3 | 1.92 | 0.52 |
| 1:J:2874:MET:HE3 | 1:J:2927:LEU:HD11 | 1.92 | 0.52 |
| 1:A:1758:ARG:HH12 | 1:A:2037:ASP:HA | 1.74 | 0.52 |
| 1:A:2595:LEU:HD22 | 1:A:2599:GLN:HB3 | 1.91 | 0.52 |
| 1:C:1180:ARG:H | 1:C:1180:ARG:HD2 | 1.75 | 0.52 |
| 1:C:1858:ASP:O | 1:C:1862:ILE:HG13 | 2.10 | 0.52 |
| 1:C:2489:LYS:H | 1:C:2489:LYS:HD2 | 1.75 | 0.52 |
| 1:C:2630:VAL:HG12 | 1:C:2682:ILE:HD11 | 1.91 | 0.52 |
| 1:G:1299:GLN:HG2 | 3:I:31:GLN:NE2 | 2.18 | 0.52 |
| 1:G:3102:ASP:HA | 1:G:3105:LYS:HE2 | 1.90 | 0.52 |
| 1:G:4918:ILE:HD12 | 8:J:5115:POV:H215 | 1.90 | 0.52 |
| 2:H:70:SER:O | 2:H:79:TYR:HB2 | 2.09 | 0.52 |
| 1:J:255:HIS:CD2 | 1:J:480:GLU:HG2 | 2.45 | 0.52 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:J:1858:ASP:O | 1:J:1862:ILE:HG13 | 2.10 | 0.52 |
| 1:J:3607:GLU:HA | 1:J:3610:GLU:HG2 | 1.92 | 0.52 |
| 1:A:1691:GLN:HE21 | 3:F:42:ARG:HG2 | 1.75 | 0.52 |
| 1:A:2967:MET:HE2 | 1:A:3045:LYS:HD3 | 1.92 | 0.52 |
| 1:C:2595:LEU:HD22 | 1:C:2599:GLN:HB3 | 1.91 | 0.52 |
| 1:C:4568:PHE:HD1 | 8:C:5102:POV:H26 | 1.75 | 0.52 |
| 8:C:5119:POV:H31B | 8:C:5120:POV:H312 | 1.91 | 0.52 |
| 2:D:31:ILE:HG22 | 2:D:97:ALA:HB1 | 1.90 | 0.52 |
| 1:G:733:PRO:HG3 | 1:G:762:CYS:HB2 | 1.92 | 0.52 |
| 1:J:2485:LEU:H | 1:J:2485:LEU:HD22 | 1.75 | 0.52 |
| 1:C:2377:LEU:HD23 | 1:C:2469:ILE:HG13 | 1.92 | 0.52 |
| 1:C:2802:LYS:O | 1:C:2806:ARG:HB3 | 2.10 | 0.52 |
| 1:C:4060:LYS:O | 1:C:4064:MET:HG2 | 2.09 | 0.52 |
| 2:D:58:ASN:ND2 | 2:D:102:ASN:HA | 2.23 | 0.52 |
| 1:G:255:HIS:CD2 | 1:G:480:GLU:HG2 | 2.45 | 0.52 |
| 1:G:3798:LEU:HB3 | 1:G:3883:ASP:OD1 | 2.10 | 0.52 |
| 1:G:4053:SER:O | 1:G:4057:MET:HG2 | 2.09 | 0.52 |
| 1:J:2952:GLU:HA | 1:J:2957:PHE:HD2 | 1.75 | 0.52 |
| 1:A:758:ARG:HA | 1:A:763:PRO:HA | 1.92 | 0.51 |
| 1:A:2534:ALA:HB1 | 1:A:2588:ARG:HE | 1.74 | 0.51 |
| 1:C:908:VAL:CA | 1:C:963:ASN:HA | 2.35 | 0.51 |
| 1:C:1445:PRO:HG2 | 1:C:1501:VAL:HG21 | 1.92 | 0.51 |
| 1:C:1737:PRO:HB2 | 1:C:1739:THR:HG23 | 1.91 | 0.51 |
| 1:C:1758:ARG:HH12 | 1:C:2037:ASP:HA | 1.74 | 0.51 |
| 1:C:2563:THR:HG22 | 1:C:2606:CYS:HA | 1.92 | 0.51 |
| 1:C:2644:LEU:HD13 | 1:C:2678:LEU:HD21 | 1.91 | 0.51 |
| 1:C:3965:LEU:HD23 | 1:C:3968:TYR:HD2 | 1.74 | 0.51 |
| 1:C:5004:THR:HG22 | 1:C:5007:GLU:HG3 | 1.92 | 0.51 |
| 1:G:2970:SER:HA | 1:G:2973:PHE:CD2 | 2.45 | 0.51 |
| 1:J:2377:LEU:HD23 | 1:J:2469:ILE:HG13 | 1.92 | 0.51 |
| 1:J:3368:ARG:O | 1:J:3372:VAL:HG23 | 2.10 | 0.51 |
| 1:J:4053:SER:O | 1:J:4057:MET:HG2 | 2.09 | 0.51 |
| 8:J:5117:POV:H11A | 8:J:5118:POV:H12 | 1.92 | 0.51 |
| 1:A:2364:PHE:HD1 | 1:A:2429:LEU:HD21 | 1.74 | 0.51 |
| 1:A:2870:GLU:HG3 | 1:A:2939:ARG:HG2 | 1.91 | 0.51 |
| 1:C:2870:GLU:HG3 | 1:C:2939:ARG:HG2 | 1.91 | 0.51 |
| 1:C:3256:LEU:HD22 | 1:C:3266:MET:HE3 | 1.92 | 0.51 |
| 3:E:59:PHE:HA | 3:E:74:LEU:CD2 | 2.39 | 0.51 |
| 1:G:2364:PHE:HD1 | 1:G:2429:LEU:HD21 | 1.75 | 0.51 |
| 1:J:3531:ASP:O | 1:J:3534:MET:HG2 | 2.11 | 0.51 |
| 1:C:622:THR:HG23 | 1:C:626:LEU:HD22 | 1.93 | 0.51 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:758:ARG:HA | 1:C:763:PRO:HA | 1.92 | 0.51 |
| 1:C:3579:LEU:HD12 | 1:C:3580:PRO:HD2 | 1.93 | 0.51 |
| 1:C:3698:LEU:O | 1:C:3702:VAL:HG23 | 2.10 | 0.51 |
| 1:G:4568:PHE:HD1 | 8:G:5102:POV:H26 | 1.75 | 0.51 |
| 1:G:4654:ALA:O | 1:G:4658:ILE:HG13 | 2.11 | 0.51 |
| 1:J:758:ARG:HA | 1:J:763:PRO:HA | 1.93 | 0.51 |
| 1:J:3010:PHE:O | 1:J:3014:CYS:HB3 | 2.11 | 0.51 |
| 1:J:4568:PHE:HD1 | 8:J:5106:POV:H26 | 1.75 | 0.51 |
| 1:J:4586:PRO:O | 1:J:4587:PRO:C | 2.53 | 0.51 |
| 1:A:551:LEU:HB3 | 1:A:589:LEU:HD21 | 1.93 | 0.51 |
| 1:A:3010:PHE:O | 1:A:3014:CYS:HB3 | 2.11 | 0.51 |
| 1:A:4115:SER:HB2 | 1:A:4123:ILE:HG21 | 1.92 | 0.51 |
| 1:C:2967:MET:HE2 | 1:C:3045:LYS:HD3 | 1.92 | 0.51 |
| 1:G:150:MET:HB3 | 1:G:169:LEU:HD23 | 1.92 | 0.51 |
| 1:G:622:THR:HG23 | 1:G:626:LEU:HD22 | 1.93 | 0.51 |
| 1:G:637:LEU:HD21 | 1:G:1696:HIS:CD2 | 2.46 | 0.51 |
| 1:G:3256:LEU:HD22 | 1:G:3266:MET:HE3 | 1.92 | 0.51 |
| 1:G:3698:LEU:O | 1:G:3702:VAL:HG23 | 2.10 | 0.51 |
| 1:J:2802:LYS:O | 1:J:2806:ARG:HB3 | 2.10 | 0.51 |
| 1:J:4654:ALA:O | 1:J:4658:ILE:HG13 | 2.11 | 0.51 |
| 1:A:3368:ARG:O | 1:A:3372:VAL:HG23 | 2.10 | 0.51 |
| 1:A:3598:GLU:O | 1:A:3602:VAL:HG23 | 2.10 | 0.51 |
| 1:C:150:MET:HB3 | 1:C:169:LEU:HD23 | 1.92 | 0.51 |
| 1:C:2970:SER:HA | 1:C:2973:PHE:CD2 | 2.45 | 0.51 |
| 1:C:4202:ARG:O | 1:C:4206:GLU:HG2 | 2.11 | 0.51 |
| 1:C:4976:GLU:O | 1:C:4980:LEU:HB2 | 2.10 | 0.51 |
| 1:G:758:ARG:HA | 1:G:763:PRO:HA | 1.93 | 0.51 |
| 1:G:913:LEU:HB3 | 1:G:917:GLU:HB2 | 1.93 | 0.51 |
| 1:G:2874:MET:HE3 | 1:G:2927:LEU:HD11 | 1.92 | 0.51 |
| 1:G:2967:MET:HE2 | 1:G:3045:LYS:HD3 | 1.91 | 0.51 |
| 1:G:4115:SER:HB2 | 1:G:4123:ILE:HG21 | 1.92 | 0.51 |
| 1:J:551:LEU:HB3 | 1:J:589:LEU:HD21 | 1.93 | 0.51 |
| 1:J:3318:ASN:O | 1:J:3322:ILE:HG23 | 2.11 | 0.51 |
| 1:A:3318:ASN:O | 1:A:3322:ILE:HG23 | 2.11 | 0.51 |
| 1:A:4654:ALA:O | 1:A:4658:ILE:HG13 | 2.11 | 0.51 |
| 1:C:399:GLN:O | 1:C:403:MET:HG2 | 2.11 | 0.51 |
| 1:C:3010:PHE:O | 1:C:3014:CYS:HB3 | 2.11 | 0.51 |
| 1:G:984:LEU:HD23 | 1:G:987:ARG:HH21 | 1.76 | 0.51 |
| 1:G:2362:GLU:HA | 1:G:2369:ARG:HH22 | 1.76 | 0.51 |
| 1:G:3010:PHE:O | 1:G:3014:CYS:HB3 | 2.11 | 0.51 |
| 1:G:4202:ARG:O | 1:G:4206:GLU:HG2 | 2.11 | 0.51 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:J:3965:LEU:HD23 | 1:J:3968:TYR:HD2 | 1.74 | 0.51 |
| 1:J:4202:ARG:O | 1:J:4206:GLU:HG2 | 2.11 | 0.51 |
| 1:A:733:PRO:HG3 | 1:A:762:CYS:HB2 | 1.92 | 0.51 |
| 1:A:805:PRO:HB2 | 1:A:808:TYR:CD1 | 2.46 | 0.51 |
| 1:A:1737:PRO:HB2 | 1:A:1739:THR:HG23 | 1.91 | 0.51 |
| 1:A:1858:ASP:O | 1:A:1862:ILE:HG13 | 2.10 | 0.51 |
| 1:A:2563:THR:HG22 | 1:A:2606:CYS:HA | 1.92 | 0.51 |
| 1:C:637:LEU:HD21 | 1:C:1696:HIS:CD2 | 2.46 | 0.51 |
| 1:C:1299:GLN:O | 1:C:1544:PRO:HB3 | 2.11 | 0.51 |
| 1:G:1858:ASP:O | 1:G:1862:ILE:HG13 | 2.10 | 0.51 |
| 1:J:2364:PHE:HD1 | 1:J:2429:LEU:HD21 | 1.74 | 0.51 |
| 1:J:3256:LEU:HD22 | 1:J:3266:MET:HE3 | 1.92 | 0.51 |
| 1:A:1208:VAL:HG12 | 1:A:1225:PRO:HG2 | 1.93 | 0.51 |
| 1:A:1771:LEU:HD22 | 1:A:2153:MET:HE3 | 1.93 | 0.51 |
| 1:C:1208:VAL:HG12 | 1:C:1225:PRO:HG2 | 1.93 | 0.51 |
| 1:C:3318:ASN:O | 1:C:3322:ILE:HG23 | 2.11 | 0.51 |
| 2:D:39:GLN:HA | 2:D:45:ARG:HA | 1.93 | 0.51 |
| 1:G:3579:LEU:HD12 | 1:G:3580:PRO:HD2 | 1.93 | 0.51 |
| 3:I:78:PRO:HD3 | 3:I:96:THR:HA | 1.93 | 0.51 |
| 1:J:622:THR:HG23 | 1:J:626:LEU:HD22 | 1.93 | 0.51 |
| 1:J:2970:SER:HA | 1:J:2973:PHE:CD2 | 2.45 | 0.51 |
| 1:J:3211:ASN:HD22 | 1:J:3236:VAL:HG23 | 1.76 | 0.51 |
| 1:J:4115:SER:HB2 | 1:J:4123:ILE:HG21 | 1.92 | 0.51 |
| 1:J:5004:THR:HG22 | 1:J:5007:GLU:HG3 | 1.92 | 0.51 |
| 1:A:637:LEU:HD21 | 1:A:1696:HIS:CD2 | 2.46 | 0.51 |
| 1:A:2970:SER:HA | 1:A:2973:PHE:CD2 | 2.45 | 0.51 |
| 1:A:3211:ASN:HD22 | 1:A:3236:VAL:HG23 | 1.76 | 0.51 |
| 1:A:3256:LEU:HD22 | 1:A:3266:MET:HE3 | 1.92 | 0.51 |
| 1:A:4202:ARG:O | 1:A:4206:GLU:HG2 | 2.11 | 0.51 |
| 2:B:39:GLN:HA | 2:B:45:ARG:HA | 1.93 | 0.51 |
| 1:C:551:LEU:HB3 | 1:C:589:LEU:HD21 | 1.93 | 0.51 |
| 1:C:2418:LEU:O | 1:C:2422:ILE:HG12 | 2.11 | 0.51 |
| 1:C:3598:GLU:O | 1:C:3602:VAL:HG23 | 2.10 | 0.51 |
| 1:C:4666:VAL:O | 1:C:4670:ILE:HG12 | 2.11 | 0.51 |
| 1:G:461:HIS:CE1 | 1:G:3707:ARG:HG3 | 2.46 | 0.51 |
| 1:G:1299:GLN:O | 1:G:1544:PRO:HB3 | 2.11 | 0.51 |
| 1:G:3318:ASN:O | 1:G:3322:ILE:HG23 | 2.11 | 0.51 |
| 1:G:3999:MET:HA | 1:G:3999:MET:HE3 | 1.93 | 0.51 |
| 2:H:33:SER:HB2 | 2:H:50:THR:HB | 1.93 | 0.51 |
| 1:J:637:LEU:HD21 | 1:J:1696:HIS:CD2 | 2.46 | 0.51 |
| 1:J:3999:MET:HA | 1:J:3999:MET:HE3 | 1.93 | 0.51 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:B:20:LEU:HB3 | 2:B:36:TRP:CH2 | 2.46 | 0.51 |
| 1:C:913:LEU:HB3 | 1:C:917:GLU:HB2 | 1.93 | 0.51 |
| 1:C:984:LEU:HD23 | 1:C:987:ARG:HH21 | 1.76 | 0.51 |
| 1:G:2377:LEU:HD23 | 1:G:2469:ILE:HG13 | 1.92 | 0.51 |
| 1:G:2418:LEU:O | 1:G:2422:ILE:HG12 | 2.11 | 0.51 |
| 1:G:4666:VAL:O | 1:G:4670:ILE:HG12 | 2.11 | 0.51 |
| 2:H:20:LEU:HB3 | 2:H:36:TRP:CH2 | 2.46 | 0.51 |
| 1:J:733:PRO:HG3 | 1:J:762:CYS:HB2 | 1.92 | 0.51 |
| 1:J:2512:ILE:HA | 1:J:2517:PHE:HE2 | 1.76 | 0.51 |
| 2:K:58:ASN:ND2 | 2:K:102:ASN:HA | 2.23 | 0.51 |
| 1:A:399:GLN:O | 1:A:403:MET:HG2 | 2.11 | 0.50 |
| 1:A:622:THR:HG23 | 1:A:626:LEU:HD22 | 1.93 | 0.50 |
| 1:A:2512:ILE:HA | 1:A:2517:PHE:HE2 | 1.76 | 0.50 |
| 1:A:3533:ILE:HD13 | 1:A:3596:VAL:HG13 | 1.91 | 0.50 |
| 1:A:3607:GLU:HA | 1:A:3610:GLU:HG2 | 1.92 | 0.50 |
| 1:C:4670:ILE:O | 1:C:4674:GLU:HG3 | 2.11 | 0.50 |
| 1:G:1771:LEU:HD22 | 1:G:2153:MET:HE3 | 1.93 | 0.50 |
| 2:H:39:GLN:HA | 2:H:45:ARG:HA | 1.93 | 0.50 |
| 1:J:2386:ILE:HG23 | 1:J:2392:ARG:HB3 | 1.92 | 0.50 |
| 1:J:4976:GLU:O | 1:J:4980:LEU:HB2 | 2.10 | 0.50 |
| 2:K:33:SER:HB2 | 2:K:50:THR:HB | 1.93 | 0.50 |
| 1:A:461:HIS:CE1 | 1:A:3707:ARG:HG3 | 2.47 | 0.50 |
| 1:A:984:LEU:HD23 | 1:A:987:ARG:HH21 | 1.76 | 0.50 |
| 1:C:648:ILE:HD11 | 1:C:793:LEU:HD13 | 1.93 | 0.50 |
| 1:C:720:HIS:HB3 | 1:C:729:PRO:HA | 1.94 | 0.50 |
| 1:G:399:GLN:O | 1:G:403:MET:HG2 | 2.11 | 0.50 |
| 1:G:2563:THR:HG22 | 1:G:2606:CYS:HA | 1.92 | 0.50 |
| 1:G:2911:LEU:HD13 | 1:G:2915:GLU:HB2 | 1.94 | 0.50 |
| 1:G:4670:ILE:O | 1:G:4674:GLU:HG3 | 2.11 | 0.50 |
| 1:J:1115:LEU:HD21 | 1:J:1191:VAL:HG13 | 1.94 | 0.50 |
| 1:J:2563:THR:HG22 | 1:J:2606:CYS:HA | 1.92 | 0.50 |
| 1:A:1000:ARG:HB3 | 1:A:1005:TRP:HB2 | 1.94 | 0.50 |
| 1:C:2362:GLU:HA | 1:C:2369:ARG:HH22 | 1.76 | 0.50 |
| 1:G:551:LEU:HB3 | 1:G:589:LEU:HD21 | 1.93 | 0.50 |
| 1:G:648:ILE:HD11 | 1:G:793:LEU:HD13 | 1.93 | 0.50 |
| 1:G:899:ASP:HB2 | 2:H:102:ASN:HB3 | 1.93 | 0.50 |
| 1:G:5004:THR:HG22 | 1:G:5007:GLU:HG3 | 1.92 | 0.50 |
| 2:H:40:ALA:HB3 | 2:H:43:LYS:HB2 | 1.93 | 0.50 |
| 1:J:864:PRO:HG3 | 1:J:939:VAL:HG21 | 1.94 | 0.50 |
| 2:K:39:GLN:HA | 2:K:45:ARG:HA | 1.93 | 0.50 |
| 1:A:913:LEU:HB3 | 1:A:917:GLU:HB2 | 1.93 | 0.50 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:1087:ARG:NH2 | 1:A:1222:GLY:HA3 | 2.27 | 0.50 |
| 1:A:1115:LEU:HD21 | 1:A:1191:VAL:HG13 | 1.94 | 0.50 |
| 1:A:1784:ALA:HA | 3:F:55:VAL:HA | 1.93 | 0.50 |
| 1:A:3906:GLN:HE21 | 1:A:3913:ILE:H | 1.60 | 0.50 |
| 1:C:2479:LEU:HA | 1:C:2485:LEU:HA | 1.92 | 0.50 |
| 1:C:2911:LEU:HD13 | 1:C:2915:GLU:HB2 | 1.94 | 0.50 |
| 1:C:3546:ASP:O | 1:C:3549:VAL:HG22 | 2.12 | 0.50 |
| 1:G:720:HIS:HB3 | 1:G:729:PRO:HA | 1.94 | 0.50 |
| 1:J:150:MET:HB3 | 1:J:169:LEU:HD23 | 1.92 | 0.50 |
| 1:J:984:LEU:HD23 | 1:J:987:ARG:HH21 | 1.76 | 0.50 |
| 1:J:1087:ARG:NH2 | 1:J:1222:GLY:HA3 | 2.27 | 0.50 |
| 1:A:3965:LEU:HD23 | 1:A:3968:TYR:HD2 | 1.74 | 0.50 |
| 1:A:4723:LYS:O | 1:A:4727:LYS:HG2 | 2.12 | 0.50 |
| 2:B:33:SER:HB2 | 2:B:50:THR:HB | 1.93 | 0.50 |
| 1:C:20:VAL:HG11 | 1:C:202:MET:SD | 2.52 | 0.50 |
| 1:C:461:HIS:CE1 | 1:C:3707:ARG:HG3 | 2.46 | 0.50 |
| 1:C:2485:LEU:HD23 | 1:C:2487:GLN:HG3 | 1.93 | 0.50 |
| 1:C:2534:ALA:HB1 | 1:C:2588:ARG:HE | 1.74 | 0.50 |
| 1:C:2678:LEU:O | 1:C:2682:ILE:HG12 | 2.11 | 0.50 |
| 1:C:3999:MET:HA | 1:C:3999:MET:HE3 | 1.93 | 0.50 |
| 1:C:4723:LYS:O | 1:C:4727:LYS:HG2 | 2.12 | 0.50 |
| 2:D:20:LEU:HB3 | 2:D:36:TRP:CH2 | 2.47 | 0.50 |
| 1:J:224:HIS:HD2 | 1:J:231:LEU:HB2 | 1.76 | 0.50 |
| 1:J:2911:LEU:HD13 | 1:J:2915:GLU:HB2 | 1.93 | 0.50 |
| 1:J:4723:LYS:O | 1:J:4727:LYS:HG2 | 2.12 | 0.50 |
| 1:A:720:HIS:HB3 | 1:A:729:PRO:HA | 1.94 | 0.50 |
| 1:A:1691:GLN:NE2 | 3:F:42:ARG:HG2 | 2.26 | 0.50 |
| 1:A:2678:LEU:O | 1:A:2682:ILE:HG12 | 2.11 | 0.50 |
| 1:A:2911:LEU:HD13 | 1:A:2915:GLU:HB2 | 1.93 | 0.50 |
| 1:A:3579:LEU:HD12 | 1:A:3580:PRO:HD2 | 1.93 | 0.50 |
| 1:A:4586:PRO:O | 1:A:4587:PRO:C | 2.53 | 0.50 |
| 1:C:671:VAL:H | 1:C:740:PRO:HG3 | 1.76 | 0.50 |
| 1:C:864:PRO:HG3 | 1:C:939:VAL:HG21 | 1.94 | 0.50 |
| 1:C:1115:LEU:HD21 | 1:C:1191:VAL:HG13 | 1.94 | 0.50 |
| 1:C:2512:ILE:HA | 1:C:2517:PHE:HE2 | 1.76 | 0.50 |
| 1:C:3007:ASN:OD1 | 1:C:3070:ILE:HG13 | 2.11 | 0.50 |
| 2:D:40:ALA:HB3 | 2:D:43:LYS:HB2 | 1.93 | 0.50 |
| 1:G:224:HIS:HD2 | 1:G:231:LEU:HB2 | 1.76 | 0.50 |
| 2:H:58:ASN:ND2 | 2:H:102:ASN:HA | 2.23 | 0.50 |
| 1:J:248:GLU:HG2 | 1:J:373:LYS:HE2 | 1.93 | 0.50 |
| 1:J:2418:LEU:O | 1:J:2422:ILE:HG12 | 2.11 | 0.50 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:2386:ILE:HG23 | 1:A:2392:ARG:HB3 | 1.92 | 0.50 |
| 1:C:1771:LEU:HD22 | 1:C:2153:MET:HE3 | 1.93 | 0.50 |
| 1:C:2447:LYS:HG3 | 1:C:2449:GLU:HG2 | 1.94 | 0.50 |
| 1:G:864:PRO:HG3 | 1:G:939:VAL:HG21 | 1.94 | 0.50 |
| 8:G:5113:POV:H13A | 8:G:5114:POV:H14A | 1.93 | 0.50 |
| 1:J:399:GLN:O | 1:J:403:MET:HG2 | 2.11 | 0.50 |
| 1:J:461:HIS:CE1 | 1:J:3707:ARG:HG3 | 2.47 | 0.50 |
| 1:J:913:LEU:HB3 | 1:J:917:GLU:HB2 | 1.93 | 0.50 |
| 1:J:2678:LEU:O | 1:J:2682:ILE:HG12 | 2.11 | 0.50 |
| 1:J:4670:ILE:O | 1:J:4674:GLU:HG3 | 2.12 | 0.50 |
| 3:L:74:LEU:HD22 | 3:L:101:VAL:HG21 | 1.94 | 0.50 |
| 1:A:224:HIS:HD2 | 1:A:231:LEU:HB2 | 1.76 | 0.50 |
| 1:A:2418:LEU:O | 1:A:2422:ILE:HG12 | 2.11 | 0.50 |
| 2:B:40:ALA:HB3 | 2:B:43:LYS:HB2 | 1.93 | 0.50 |
| 1:C:224:HIS:HD2 | 1:C:231:LEU:HB2 | 1.76 | 0.50 |
| 1:C:2615:ARG:HG2 | 1:C:2617:SER:H | 1.76 | 0.50 |
| 2:D:33:SER:HB2 | 2:D:50:THR:HB | 1.93 | 0.50 |
| 1:G:1115:LEU:HD21 | 1:G:1191:VAL:HG13 | 1.94 | 0.50 |
| 1:G:1208:VAL:HG12 | 1:G:1225:PRO:HG2 | 1.93 | 0.50 |
| 1:G:4145:VAL:HG22 | 1:G:4178:LEU:HD13 | 1.94 | 0.50 |
| 1:G:4723:LYS:O | 1:G:4727:LYS:HG2 | 2.12 | 0.50 |
| 1:J:1208:VAL:HG12 | 1:J:1225:PRO:HG2 | 1.93 | 0.50 |
| 1:J:1249:PRO:HG2 | 1:J:1252:HIS:HB2 | 1.94 | 0.50 |
| 1:J:1694:LEU:HD11 | 1:J:1718:ILE:HD11 | 1.94 | 0.50 |
| 1:J:3579:LEU:HD12 | 1:J:3580:PRO:HD2 | 1.93 | 0.50 |
| 1:J:3906:GLN:HE21 | 1:J:3913:ILE:H | 1.60 | 0.50 |
| 1:A:20:VAL:HG11 | 1:A:202:MET:SD | 2.52 | 0.50 |
| 1:A:648:ILE:HD11 | 1:A:793:LEU:HD13 | 1.93 | 0.50 |
| 1:A:2536:LEU:HD12 | 1:A:2547:ALA:HB2 | 1.94 | 0.50 |
| 1:A:3224:PRO:HA | 1:A:3227:ARG:HD2 | 1.94 | 0.50 |
| 1:A:3315:LEU:O | 1:A:3319:ILE:HG13 | 2.12 | 0.50 |
| 1:A:3604:TYR:O | 1:A:3607:GLU:HG3 | 2.11 | 0.50 |
| 1:C:3062:PRO:HA | 1:C:3065:VAL:HG22 | 1.94 | 0.50 |
| 1:C:3224:PRO:HA | 1:C:3227:ARG:HD2 | 1.94 | 0.50 |
| 1:C:3604:TYR:O | 1:C:3607:GLU:HG3 | 2.12 | 0.50 |
| 3:F:21:THR:HG23 | 3:F:49:ARG:HH11 | 1.77 | 0.50 |
| 1:G:2751:LEU:HB2 | 1:G:2754:PHE:HE2 | 1.77 | 0.50 |
| 1:G:3062:PRO:HA | 1:G:3065:VAL:HG22 | 1.94 | 0.50 |
| 1:J:720:HIS:HB3 | 1:J:729:PRO:HA | 1.94 | 0.50 |
| 1:J:899:ASP:HA | 1:J:904:HIS:HA | 1.94 | 0.50 |
| 2:K:20:LEU:HB3 | 2:K:36:TRP:CH2 | 2.46 | 0.50 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:864:PRO:HG3 | 1:A:939:VAL:HG21 | 1.94 | 0.49 |
| 1:A:1100:MET:HA | 1:A:1193:SER:O | 2.12 | 0.49 |
| 1:A:1299:GLN:O | 1:A:1544:PRO:HB3 | 2.11 | 0.49 |
| 1:A:2362:GLU:HA | 1:A:2369:ARG:HH22 | 1.76 | 0.49 |
| 1:A:2447:LYS:HG3 | 1:A:2449:GLU:HG2 | 1.94 | 0.49 |
| 1:A:2615:ARG:HG2 | 1:A:2617:SER:H | 1.76 | 0.49 |
| 1:A:2751:LEU:HB2 | 1:A:2754:PHE:HE2 | 1.77 | 0.49 |
| 1:C:172:VAL:HA | 1:C:179:TYR:HA | 1.94 | 0.49 |
| 1:C:248:GLU:HG2 | 1:C:373:LYS:HE2 | 1.93 | 0.49 |
| 1:C:483:MET:HA | 1:C:483:MET:HE3 | 1.94 | 0.49 |
| 1:C:1000:ARG:HB3 | 1:C:1005:TRP:HB2 | 1.94 | 0.49 |
| 1:C:1100:MET:HA | 1:C:1193:SER:O | 2.12 | 0.49 |
| 1:G:20:VAL:HG11 | 1:G:202:MET:SD | 2.52 | 0.49 |
| 1:G:1249:PRO:HG2 | 1:G:1252:HIS:HB2 | 1.94 | 0.49 |
| 1:G:2447:LYS:HG3 | 1:G:2449:GLU:HG2 | 1.94 | 0.49 |
| 1:G:3211:ASN:HD22 | 1:G:3236:VAL:HG23 | 1.76 | 0.49 |
| 1:G:3437:MET:HA | 1:G:3437:MET:HE3 | 1.94 | 0.49 |
| 1:G:3546:ASP:O | 1:G:3549:VAL:HG22 | 2.12 | 0.49 |
| 1:J:483:MET:HA | 1:J:483:MET:HE3 | 1.94 | 0.49 |
| 1:J:2228:MET:HE3 | 1:J:2232:CYS:SG | 2.51 | 0.49 |
| 1:J:2536:LEU:HD12 | 1:J:2547:ALA:HB2 | 1.94 | 0.49 |
| 1:J:2751:LEU:HB2 | 1:J:2754:PHE:HE2 | 1.77 | 0.49 |
| 1:A:1694:LEU:HD11 | 1:A:1718:ILE:HD11 | 1.94 | 0.49 |
| 1:A:4670:ILE:O | 1:A:4674:GLU:HG3 | 2.12 | 0.49 |
| 1:C:3010:PHE:HE1 | 1:C:3074:SER:HB2 | 1.77 | 0.49 |
| 1:C:4654:ALA:O | 1:C:4658:ILE:HG13 | 2.11 | 0.49 |
| 1:G:1000:ARG:HB3 | 1:G:1005:TRP:HB2 | 1.94 | 0.49 |
| 1:G:2678:LEU:O | 1:G:2682:ILE:HG12 | 2.11 | 0.49 |
| 1:G:4978:HIS:HA | 1:G:4982:GLU:HB3 | 1.95 | 0.49 |
| 1:J:2362:GLU:HA | 1:J:2369:ARG:HH22 | 1.76 | 0.49 |
| 1:J:2615:ARG:HG2 | 1:J:2617:SER:H | 1.76 | 0.49 |
| 1:J:3315:LEU:O | 1:J:3319:ILE:HG13 | 2.12 | 0.49 |
| 1:A:1762:LEU:HD13 | 1:A:1863:LEU:HD13 | 1.93 | 0.49 |
| 1:A:3532:LEU:HD11 | 1:A:3560:GLN:HG2 | 1.94 | 0.49 |
| 1:A:3996:PHE:CE2 | 1:A:4023:MET:HG3 | 2.43 | 0.49 |
| 1:C:805:PRO:HB2 | 1:C:808:TYR:CD1 | 2.47 | 0.49 |
| 1:C:2751:LEU:HB2 | 1:C:2754:PHE:HE2 | 1.77 | 0.49 |
| 1:C:3130:THR:HA | 1:C:3133:THR:HG22 | 1.95 | 0.49 |
| 1:C:3211:ASN:HD22 | 1:C:3236:VAL:HG23 | 1.76 | 0.49 |
| 1:G:248:GLU:HG2 | 1:G:373:LYS:HE2 | 1.93 | 0.49 |
| 1:G:794:GLY:HA3 | 1:G:810:PRO:HB3 | 1.94 | 0.49 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:G:1087:ARG:NH2 | 1:G:1222:GLY:HA3 | 2.27 | 0.49 |
| 1:G:3996:PHE:CE2 | 1:G:4023:MET:HG3 | 2.43 | 0.49 |
| 1:J:1762:LEU:HD13 | 1:J:1863:LEU:HD13 | 1.93 | 0.49 |
| 1:J:3130:THR:HA | 1:J:3133:THR:HG22 | 1.95 | 0.49 |
| 1:J:3927:GLN:HE21 | 1:J:3991:GLY:HA3 | 1.77 | 0.49 |
| 2:K:40:ALA:HB3 | 2:K:43:LYS:HB2 | 1.93 | 0.49 |
| 1:A:150:MET:HB3 | 1:A:169:LEU:HD23 | 1.92 | 0.49 |
| 1:A:894:GLY:H | 1:A:903:LEU:HB3 | 1.78 | 0.49 |
| 1:A:4145:VAL:HG22 | 1:A:4178:LEU:HD13 | 1.94 | 0.49 |
| 1:C:794:GLY:HA3 | 1:C:810:PRO:HB3 | 1.94 | 0.49 |
| 1:C:899:ASP:HA | 1:C:904:HIS:HA | 1.94 | 0.49 |
| 1:G:483:MET:HA | 1:G:483:MET:HE3 | 1.94 | 0.49 |
| 1:G:1694:LEU:HD11 | 1:G:1718:ILE:HD11 | 1.94 | 0.49 |
| 1:G:2012:PHE:CE2 | 1:G:2028:ARG:HB2 | 2.47 | 0.49 |
| 1:G:3224:PRO:HA | 1:G:3227:ARG:HD2 | 1.94 | 0.49 |
| 1:G:3280:TYR:HD1 | 1:G:3281:LEU:HD12 | 1.78 | 0.49 |
| 1:G:3607:GLU:HA | 1:G:3610:GLU:HG2 | 1.92 | 0.49 |
| 1:G:4182:GLU:HB2 | 1:G:4983:HIS:HE2 | 1.77 | 0.49 |
| 1:G:4583:SER:HB3 | 1:G:4631:PHE:HE1 | 1.78 | 0.49 |
| 1:J:805:PRO:HB2 | 1:J:808:TYR:CD1 | 2.47 | 0.49 |
| 1:J:1771:LEU:HD22 | 1:J:2153:MET:HE3 | 1.93 | 0.49 |
| 1:A:487:VAL:O | 1:A:491:ILE:HG13 | 2.13 | 0.49 |
| 1:A:4843:LEU:HD22 | 1:C:4823:LEU:HD22 | 1.95 | 0.49 |
| 1:C:487:VAL:O | 1:C:491:ILE:HG13 | 2.13 | 0.49 |
| 1:C:1087:ARG:NH2 | 1:C:1222:GLY:HA3 | 2.27 | 0.49 |
| 1:C:2536:LEU:HD12 | 1:C:2547:ALA:HB2 | 1.94 | 0.49 |
| 1:C:2754:PHE:CD2 | 1:C:2825:LYS:HE2 | 2.48 | 0.49 |
| 1:G:1100:MET:HA | 1:G:1193:SER:O | 2.12 | 0.49 |
| 1:G:1762:LEU:HD13 | 1:G:1863:LEU:HD13 | 1.93 | 0.49 |
| 1:G:2233:CYS:O | 1:G:2236:LEU:N | 2.45 | 0.49 |
| 1:G:3032:SER:O | 1:G:3036:LYS:HG3 | 2.13 | 0.49 |
| 3:I:21:THR:HG23 | 3:I:49:ARG:HH11 | 1.77 | 0.49 |
| 1:J:894:GLY:H | 1:J:903:LEU:HB3 | 1.78 | 0.49 |
| 1:J:3546:ASP:O | 1:J:3549:VAL:HG22 | 2.12 | 0.49 |
| 1:J:4583:SER:HB3 | 1:J:4631:PHE:HE1 | 1.78 | 0.49 |
| 1:A:483:MET:HA | 1:A:483:MET:HE3 | 1.93 | 0.49 |
| 1:A:996:TRP:NE1 | 2:B:113:GLU:HB3 | 2.28 | 0.49 |
| 1:A:2012:PHE:CE2 | 1:A:2028:ARG:HB2 | 2.47 | 0.49 |
| 1:A:2376:LEU:HB2 | 1:A:2465:ASP:HB3 | 1.93 | 0.49 |
| 1:A:3062:PRO:HA | 1:A:3065:VAL:HG22 | 1.94 | 0.49 |
| 1:A:3280:TYR:HD1 | 1:A:3281:LEU:HD12 | 1.78 | 0.49 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:3546:ASP:O | 1:A:3549:VAL:HG22 | 2.12 | 0.49 |
| 1:A:3999:MET:HE3 | 1:A:3999:MET:HA | 1.93 | 0.49 |
| 1:A:4666:VAL:O | 1:A:4670:ILE:HG12 | 2.11 | 0.49 |
| 1:C:1694:LEU:HD11 | 1:C:1718:ILE:HD11 | 1.94 | 0.49 |
| 1:C:3018:LEU:HD11 | 1:C:3150:HIS:CE1 | 2.48 | 0.49 |
| 1:C:3330:ASP:HA | 1:C:3403:ARG:HH12 | 1.78 | 0.49 |
| 1:C:3350:ARG:NE | 1:C:3350:ARG:HA | 2.28 | 0.49 |
| 1:C:3547:GLU:O | 1:C:3551:GLU:HG2 | 2.13 | 0.49 |
| 1:G:2489:LYS:H | 1:G:2489:LYS:HD2 | 1.78 | 0.49 |
| 1:G:2754:PHE:CD2 | 1:G:2825:LYS:HE2 | 2.48 | 0.49 |
| 1:G:3547:GLU:O | 1:G:3551:GLU:HG2 | 2.13 | 0.49 |
| 1:J:648:ILE:HD11 | 1:J:793:LEU:HD13 | 1.93 | 0.49 |
| 1:A:172:VAL:HA | 1:A:179:TYR:HA | 1.94 | 0.49 |
| 1:A:2273:LEU:HD23 | 1:A:2330:ARG:HG3 | 1.94 | 0.49 |
| 2:B:108:GLY:H | 2:B:111:ASN:HD22 | 1.61 | 0.49 |
| 1:C:3906:GLN:HE21 | 1:C:3913:ILE:H | 1.60 | 0.49 |
| 1:C:4583:SER:HB3 | 1:C:4631:PHE:HE1 | 1.78 | 0.49 |
| 1:G:899:ASP:HA | 1:G:904:HIS:HA | 1.93 | 0.49 |
| 1:G:3010:PHE:CE1 | 1:G:3074:SER:HB2 | 2.45 | 0.49 |
| 1:G:3222:LYS:HB3 | 1:G:3226:GLU:HB3 | 1.95 | 0.49 |
| 1:G:3350:ARG:NE | 1:G:3350:ARG:HA | 2.28 | 0.49 |
| 1:G:3775:ALA:HA | 1:G:3778:MET:HE2 | 1.94 | 0.49 |
| 1:J:20:VAL:HG11 | 1:J:202:MET:SD | 2.52 | 0.49 |
| 1:J:3350:ARG:NE | 1:J:3350:ARG:HA | 2.28 | 0.49 |
| 1:J:4666:VAL:O | 1:J:4670:ILE:HG12 | 2.11 | 0.49 |
| 1:A:899:ASP:HA | 1:A:904:HIS:HA | 1.93 | 0.49 |
| 1:A:1423:ASP:O | 1:A:1427:ILE:HG23 | 2.13 | 0.49 |
| 1:A:3130:THR:HA | 1:A:3133:THR:HG22 | 1.95 | 0.49 |
| 1:A:3547:GLU:O | 1:A:3551:GLU:HG2 | 2.13 | 0.49 |
| 1:A:3927:GLN:HE21 | 1:A:3991:GLY:HA3 | 1.77 | 0.49 |
| 1:C:2012:PHE:CE2 | 1:C:2028:ARG:HB2 | 2.47 | 0.49 |
| 1:C:3529:ASP:O | 1:C:3533:ILE:HG12 | 2.13 | 0.49 |
| 1:C:4843:LEU:HD22 | 1:G:4823:LEU:HD22 | 1.95 | 0.49 |
| 1:G:172:VAL:HA | 1:G:179:TYR:HA | 1.95 | 0.49 |
| 1:G:3532:LEU:HD11 | 1:G:3560:GLN:HG2 | 1.94 | 0.49 |
| 1:G:3927:GLN:HE21 | 1:G:3991:GLY:HA3 | 1.77 | 0.49 |
| 1:J:1000:ARG:HA | 1:J:1000:ARG:HE | 1.77 | 0.49 |
| 1:J:1423:ASP:O | 1:J:1427:ILE:HG23 | 2.13 | 0.49 |
| 1:J:2447:LYS:HG3 | 1:J:2449:GLU:HG2 | 1.94 | 0.49 |
| 1:J:2803:GLU:O | 1:J:2807:TRP:HB2 | 2.13 | 0.49 |
| 1:J:3075:LEU:HD21 | 1:J:3143:LEU:HD13 | 1.95 | 0.49 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:J:3224:PRO:HA | 1:J:3227:ARG:HD2 | 1.94 | 0.49 |
| 1:J:4145:VAL:HG22 | 1:J:4178:LEU:HD13 | 1.94 | 0.49 |
| 1:A:248:GLU:HG2 | 1:A:373:LYS:HE2 | 1.93 | 0.49 |
| 1:A:716:PHE:HA | 1:A:721:LEU:HA | 1.95 | 0.49 |
| 1:A:1072:VAL:HG12 | 1:A:1195:GLY:HA2 | 1.95 | 0.49 |
| 1:C:894:GLY:H | 1:C:903:LEU:HB3 | 1.78 | 0.49 |
| 1:C:3367:LYS:O | 1:C:3371:LYS:HG2 | 2.13 | 0.49 |
| 1:C:3445:TRP:CE2 | 1:C:3452:LYS:HG2 | 2.48 | 0.49 |
| 1:C:4145:VAL:HG22 | 1:C:4178:LEU:HD13 | 1.94 | 0.49 |
| 1:G:1423:ASP:O | 1:G:1427:ILE:HG23 | 2.13 | 0.49 |
| 1:G:2536:LEU:HD12 | 1:G:2547:ALA:HB2 | 1.94 | 0.49 |
| 1:G:3168:THR:O | 1:G:3172:ILE:HG22 | 2.13 | 0.49 |
| 1:J:1100:MET:HA | 1:J:1193:SER:O | 2.12 | 0.49 |
| 1:J:2754:PHE:CD2 | 1:J:2825:LYS:HE2 | 2.48 | 0.49 |
| 1:J:3062:PRO:HA | 1:J:3065:VAL:HG22 | 1.94 | 0.49 |
| 1:J:3547:GLU:O | 1:J:3551:GLU:HG2 | 2.13 | 0.49 |
| 2:K:15:GLY:HA2 | 2:K:84:SER:HA | 1.95 | 0.49 |
| 1:A:3018:LEU:HD11 | 1:A:3150:HIS:CE1 | 2.48 | 0.49 |
| 1:A:3107:VAL:HA | 1:A:3175:LEU:HD11 | 1.95 | 0.49 |
| 1:A:3350:ARG:HA | 1:A:3350:ARG:NE | 2.28 | 0.49 |
| 8:A:5122:POV:H214 | 8:J:5114:POV:H21H | 1.95 | 0.49 |
| 1:C:603:LEU:HD23 | 1:C:606:LEU:HD12 | 1.95 | 0.49 |
| 1:C:1762:LEU:HD13 | 1:C:1863:LEU:HD13 | 1.93 | 0.49 |
| 1:C:2927:LEU:HA | 1:C:2930:LEU:HD12 | 1.95 | 0.49 |
| 1:G:2764:GLU:HB3 | 1:G:2857:PRO:HD3 | 1.95 | 0.49 |
| 1:G:2920:ARG:O | 1:G:2924:GLN:HG2 | 2.13 | 0.49 |
| 1:G:3018:LEU:HD11 | 1:G:3150:HIS:CE1 | 2.48 | 0.49 |
| 1:G:3130:THR:HA | 1:G:3133:THR:HG22 | 1.95 | 0.49 |
| 1:G:3330:ASP:HA | 1:G:3403:ARG:HH12 | 1.78 | 0.49 |
| 1:G:4843:LEU:HD22 | 1:J:4823:LEU:HD22 | 1.94 | 0.49 |
| 1:J:477:LEU:O | 1:J:481:GLU:HG2 | 2.13 | 0.49 |
| 1:J:1093:GLU:HB3 | 1:J:1201:HIS:HB3 | 1.95 | 0.49 |
| 1:J:1299:GLN:O | 1:J:1544:PRO:HB3 | 2.11 | 0.49 |
| 1:J:2012:PHE:CE2 | 1:J:2028:ARG:HB2 | 2.47 | 0.49 |
| 1:J:2920:ARG:O | 1:J:2924:GLN:HG2 | 2.13 | 0.49 |
| 1:J:3032:SER:O | 1:J:3036:LYS:HG3 | 2.13 | 0.49 |
| 1:A:3222:LYS:HB3 | 1:A:3226:GLU:HB3 | 1.95 | 0.48 |
| 1:A:4241:THR:HB | 1:A:4989:MET:HE1 | 1.95 | 0.48 |
| 1:C:3107:VAL:HA | 1:C:3175:LEU:HD11 | 1.95 | 0.48 |
| 1:C:3927:GLN:HE21 | 1:C:3991:GLY:HA3 | 1.77 | 0.48 |
| 1:C:4995:LEU:HD22 | 1:C:5003:HIS:HD2 | 1.78 | 0.48 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:G:487:VAL:O | 1:G:491:ILE:HG13 | 2.13 | 0.48 |
| 1:G:603:LEU:HD23 | 1:G:606:LEU:HD12 | 1.95 | 0.48 |
| 1:G:2615:ARG:HG2 | 1:G:2617:SER:H | 1.76 | 0.48 |
| 1:G:2927:LEU:HA | 1:G:2930:LEU:HD12 | 1.94 | 0.48 |
| 1:J:1072:VAL:HG12 | 1:J:1195:GLY:HA2 | 1.95 | 0.48 |
| 1:J:2355:ARG:O | 1:J:2359:ARG:HG2 | 2.13 | 0.48 |
| 1:J:3010:PHE:HE1 | 1:J:3074:SER:HB2 | 1.78 | 0.48 |
| 1:J:3222:LYS:HB3 | 1:J:3226:GLU:HB3 | 1.95 | 0.48 |
| 1:J:3280:TYR:HD1 | 1:J:3281:LEU:HD12 | 1.78 | 0.48 |
| 1:J:3775:ALA:HA | 1:J:3778:MET:HE2 | 1.94 | 0.48 |
| 1:J:4151:SER:HB3 | 1:J:4164:LEU:HD21 | 1.95 | 0.48 |
| 2:K:82:MET:HG3 | 2:K:85:LEU:HD23 | 1.95 | 0.48 |
| 1:A:477:LEU:O | 1:A:481:GLU:HG2 | 2.13 | 0.48 |
| 1:A:2754:PHE:CD2 | 1:A:2825:LYS:HE2 | 2.48 | 0.48 |
| 1:A:2803:GLU:O | 1:A:2807:TRP:HB2 | 2.13 | 0.48 |
| 1:A:3914:ASN:HB3 | 1:A:3917:ILE:HG12 | 1.96 | 0.48 |
| 1:A:4583:SER:HB3 | 1:A:4631:PHE:HE1 | 1.78 | 0.48 |
| 1:C:899:ASP:HB2 | 2:D:102:ASN:HB3 | 1.95 | 0.48 |
| 1:C:2616:PRO:HA | 1:C:2619:LEU:HD12 | 1.95 | 0.48 |
| 1:C:2764:GLU:HB3 | 1:C:2857:PRO:HD3 | 1.95 | 0.48 |
| 1:C:3532:LEU:HD11 | 1:C:3560:GLN:HG2 | 1.94 | 0.48 |
| 3:E:21:THR:HG23 | 3:E:49:ARG:HH11 | 1.77 | 0.48 |
| 1:G:894:GLY:H | 1:G:903:LEU:HB3 | 1.78 | 0.48 |
| 1:G:3914:ASN:HB3 | 1:G:3917:ILE:HG12 | 1.95 | 0.48 |
| 1:J:899:ASP:HB2 | 2:K:102:ASN:HB3 | 1.94 | 0.48 |
| 1:J:2449:GLU:HA | 1:J:2452:ARG:HE | 1.78 | 0.48 |
| 1:J:3367:LYS:O | 1:J:3371:LYS:HG2 | 2.13 | 0.48 |
| 1:J:4241:THR:HB | 1:J:4989:MET:HE1 | 1.95 | 0.48 |
| 1:A:681:HIS:O | 1:A:783:PHE:HA | 2.13 | 0.48 |
| 1:A:3032:SER:O | 1:A:3036:LYS:HG3 | 2.13 | 0.48 |
| 1:A:3445:TRP:CE2 | 1:A:3452:LYS:HG2 | 2.48 | 0.48 |
| 1:C:3222:LYS:HB3 | 1:C:3226:GLU:HB3 | 1.95 | 0.48 |
| 1:C:3315:LEU:O | 1:C:3319:ILE:HG13 | 2.12 | 0.48 |
| 1:C:3539:ARG:HH12 | 1:C:3552:PHE:CB | 2.12 | 0.48 |
| 1:G:35:LEU:HD13 | 1:G:49:LEU:HB2 | 1.95 | 0.48 |
| 1:G:2803:GLU:O | 1:G:2807:TRP:HB2 | 2.13 | 0.48 |
| 1:G:4968:PHE:HD2 | 1:G:4975:PHE:HD1 | 1.62 | 0.48 |
| 1:J:172:VAL:HA | 1:J:179:TYR:HA | 1.95 | 0.48 |
| 1:J:487:VAL:O | 1:J:491:ILE:HG13 | 2.13 | 0.48 |
| 1:J:2616:PRO:HA | 1:J:2619:LEU:HD12 | 1.95 | 0.48 |
| 1:J:4238:CYS:O | 1:J:4242:ILE:HG13 | 2.14 | 0.48 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:J:4767:TRP:HA | 1:J:4770:SER:HB3 | 1.95 | 0.48 |
| 1:A:794:GLY:HA3 | 1:A:810:PRO:HB3 | 1.94 | 0.48 |
| 2:B:15:GLY:HA2 | 2:B:84:SER:HA | 1.95 | 0.48 |
| 1:C:477:LEU:O | 1:C:481:GLU:HG2 | 2.13 | 0.48 |
| 1:C:881:LEU:HD11 | 1:C:1041:GLN:HG2 | 1.95 | 0.48 |
| 1:C:1072:VAL:HG12 | 1:C:1195:GLY:HA2 | 1.95 | 0.48 |
| 1:C:1249:PRO:HG2 | 1:C:1252:HIS:HB2 | 1.94 | 0.48 |
| 1:C:1423:ASP:O | 1:C:1427:ILE:HG23 | 2.13 | 0.48 |
| 1:C:1741:GLU:O | 1:C:1745:ILE:HG13 | 2.13 | 0.48 |
| 1:C:2803:GLU:O | 1:C:2807:TRP:HB2 | 2.13 | 0.48 |
| 1:C:3775:ALA:HA | 1:C:3778:MET:HE2 | 1.94 | 0.48 |
| 2:D:15:GLY:HA2 | 2:D:84:SER:HA | 1.95 | 0.48 |
| 1:G:2616:PRO:HA | 1:G:2619:LEU:HD12 | 1.95 | 0.48 |
| 1:G:3337:ARG:HA | 1:G:3340:VAL:HG12 | 1.95 | 0.48 |
| 1:G:4238:CYS:O | 1:G:4242:ILE:HG13 | 2.14 | 0.48 |
| 1:J:78:LEU:HD21 | 1:J:174:VAL:HG11 | 1.96 | 0.48 |
| 1:J:906:CYS:SG | 1:J:907:LEU:HD22 | 2.54 | 0.48 |
| 1:J:1434:TYR:CE2 | 1:J:1519:LEU:HG | 2.48 | 0.48 |
| 1:J:1926:LEU:HA | 1:J:1929:MET:HE3 | 1.96 | 0.48 |
| 1:J:2764:GLU:HB3 | 1:J:2857:PRO:HD3 | 1.95 | 0.48 |
| 1:J:2927:LEU:HA | 1:J:2930:LEU:HD12 | 1.94 | 0.48 |
| 1:J:3337:ARG:HA | 1:J:3340:VAL:HG12 | 1.96 | 0.48 |
| 1:J:3422:HIS:HD1 | 1:J:3423:TRP:CD1 | 2.32 | 0.48 |
| 1:A:906:CYS:SG | 1:A:907:LEU:HD22 | 2.54 | 0.48 |
| 1:A:2616:PRO:HA | 1:A:2619:LEU:HD12 | 1.95 | 0.48 |
| 1:A:2927:LEU:HA | 1:A:2930:LEU:HD12 | 1.95 | 0.48 |
| 8:A:5107:POV:H21H | 8:C:5103:POV:H214 | 1.95 | 0.48 |
| 8:A:5118:POV:H25 | 8:A:5118:POV:H32A | 1.96 | 0.48 |
| 2:B:82:MET:HG3 | 2:B:85:LEU:HD23 | 1.95 | 0.48 |
| 1:C:78:LEU:HD21 | 1:C:174:VAL:HG11 | 1.96 | 0.48 |
| 1:C:681:HIS:O | 1:C:783:PHE:HA | 2.13 | 0.48 |
| 1:C:1093:GLU:HB3 | 1:C:1201:HIS:HB3 | 1.95 | 0.48 |
| 1:C:3280:TYR:HD1 | 1:C:3281:LEU:HD12 | 1.78 | 0.48 |
| 1:C:3337:ARG:HA | 1:C:3340:VAL:HG12 | 1.96 | 0.48 |
| 1:C:3914:ASN:HB3 | 1:C:3917:ILE:HG12 | 1.96 | 0.48 |
| 1:G:2218:GLY:HA3 | 1:G:2223:ILE:HA | 1.94 | 0.48 |
| 1:G:3315:LEU:O | 1:G:3319:ILE:HG13 | 2.12 | 0.48 |
| 1:G:3906:GLN:HE21 | 1:G:3913:ILE:H | 1.60 | 0.48 |
| 1:J:794:GLY:HA3 | 1:J:810:PRO:HB3 | 1.94 | 0.48 |
| 1:J:1033:ARG:HE | 1:J:1036:ARG:HD2 | 1.79 | 0.48 |
| 1:J:2148:SER:O | 1:J:2152:THR:HG23 | 2.14 | 0.48 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:J:3330:ASP:HA | 1:J:3403:ARG:HH12 | 1.78 | 0.48 |
| 8:J:5103:POV:H25 | 8:J:5103:POV:H32A | 1.96 | 0.48 |
| 1:A:445:LEU:O | 1:A:449:ILE:HG13 | 2.14 | 0.48 |
| 1:A:603:LEU:HD23 | 1:A:606:LEU:HD12 | 1.95 | 0.48 |
| 1:A:1093:GLU:HB3 | 1:A:1201:HIS:HB3 | 1.95 | 0.48 |
| 1:A:2449:GLU:HA | 1:A:2452:ARG:HE | 1.78 | 0.48 |
| 1:A:3330:ASP:HA | 1:A:3403:ARG:HH12 | 1.78 | 0.48 |
| 1:A:3422:HIS:HD1 | 1:A:3423:TRP:CD1 | 2.32 | 0.48 |
| 1:A:4824:ARG:HG3 | 8:A:5110:POV:H15 | 1.96 | 0.48 |
| 1:C:3032:SER:O | 1:C:3036:LYS:HG3 | 2.13 | 0.48 |
| 1:C:4241:THR:HB | 1:C:4989:MET:HE1 | 1.95 | 0.48 |
| 1:G:681:HIS:O | 1:G:783:PHE:HA | 2.14 | 0.48 |
| 1:G:1041:GLN:HA | 1:G:1044:ARG:HG2 | 1.95 | 0.48 |
| 1:G:1434:TYR:CE2 | 1:G:1519:LEU:HG | 2.48 | 0.48 |
| 1:G:2148:SER:O | 1:G:2152:THR:HG23 | 2.14 | 0.48 |
| 1:G:2273:LEU:HD23 | 1:G:2330:ARG:HG3 | 1.94 | 0.48 |
| 1:G:2449:GLU:HA | 1:G:2452:ARG:HE | 1.78 | 0.48 |
| 1:G:2648:TYR:CE2 | 1:G:2675:THR:HG23 | 2.49 | 0.48 |
| 1:G:3007:ASN:HB2 | 1:G:3067:CYS:SG | 2.54 | 0.48 |
| 1:G:4080:TYR:HE1 | 1:G:4095:LYS:HG3 | 1.79 | 0.48 |
| 1:J:716:PHE:HA | 1:J:721:LEU:HA | 1.95 | 0.48 |
| 1:J:1741:GLU:O | 1:J:1745:ILE:HG13 | 2.13 | 0.48 |
| 1:J:2273:LEU:HD23 | 1:J:2330:ARG:HG3 | 1.94 | 0.48 |
| 1:A:274:LEU:HD13 | 1:A:280:LEU:HD22 | 1.96 | 0.48 |
| 1:A:1019:PRO:HD2 | 1:A:1020:ARG:NH1 | 2.29 | 0.48 |
| 1:A:2920:ARG:O | 1:A:2924:GLN:HG2 | 2.13 | 0.48 |
| 1:A:3367:LYS:O | 1:A:3371:LYS:HG2 | 2.13 | 0.48 |
| 1:A:3538:THR:O | 1:A:3542:LEU:HG | 2.13 | 0.48 |
| 1:C:445:LEU:O | 1:C:449:ILE:HG13 | 2.14 | 0.48 |
| 1:C:1815:LEU:HG | 1:C:1865:MET:HE1 | 1.96 | 0.48 |
| 1:C:2307:LEU:HD21 | 1:C:2362:GLU:HG2 | 1.95 | 0.48 |
| 1:C:3168:THR:O | 1:C:3172:ILE:HG22 | 2.13 | 0.48 |
| 2:D:82:MET:HG3 | 2:D:85:LEU:HD23 | 1.95 | 0.48 |
| 1:G:445:LEU:O | 1:G:449:ILE:HG13 | 2.14 | 0.48 |
| 1:G:2229:VAL:HA | 1:G:2232:CYS:SG | 2.54 | 0.48 |
| 1:G:3166:TYR:HE1 | 1:G:3203:VAL:HG11 | 1.79 | 0.48 |
| 1:G:3529:ASP:O | 1:G:3533:ILE:HG12 | 2.13 | 0.48 |
| 1:G:3841:VAL:HG11 | 1:G:3925:ARG:HG2 | 1.96 | 0.48 |
| 1:G:4151:SER:HB3 | 1:G:4164:LEU:HD21 | 1.95 | 0.48 |
| 1:G:4898:GLY:HA2 | 1:G:4901:ILE:HG12 | 1.96 | 0.48 |
| 1:G:5027:CYS:SG | 1:G:5030:LYS:HG3 | 2.53 | 0.48 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:J:35:LEU:HD13 | 1:J:49:LEU:HB2 | 1.95 | 0.48 |
| 1:J:874:LEU:O | 1:J:878:ILE:HG12 | 2.14 | 0.48 |
| 1:J:1152:MET:HE1 | 1:J:1217:CYS:HB2 | 1.96 | 0.48 |
| 1:J:2247:GLN:HG3 | 1:J:2279:SER:HA | 1.95 | 0.48 |
| 1:J:3107:VAL:HA | 1:J:3175:LEU:HD11 | 1.95 | 0.48 |
| 1:J:3914:ASN:HB3 | 1:J:3917:ILE:HG12 | 1.96 | 0.48 |
| 1:A:78:LEU:HD21 | 1:A:174:VAL:HG11 | 1.96 | 0.48 |
| 1:A:1249:PRO:HG2 | 1:A:1252:HIS:HB2 | 1.94 | 0.48 |
| 1:A:1741:GLU:O | 1:A:1745:ILE:HG13 | 2.13 | 0.48 |
| 1:A:2648:TYR:CE2 | 1:A:2675:THR:HG23 | 2.49 | 0.48 |
| 1:A:3007:ASN:HB2 | 1:A:3067:CYS:SG | 2.54 | 0.48 |
| 1:A:4823:LEU:HD22 | 1:J:4843:LEU:HD22 | 1.95 | 0.48 |
| 1:C:35:LEU:HD13 | 1:C:49:LEU:HB2 | 1.95 | 0.48 |
| 1:C:426:ARG:HE | 1:C:508:GLY:HA2 | 1.79 | 0.48 |
| 1:C:993:HIS:CE1 | 1:C:1027:LEU:HD11 | 2.49 | 0.48 |
| 8:C:5121:POV:H32A | 8:C:5121:POV:H25 | 1.96 | 0.48 |
| 1:G:716:PHE:HA | 1:G:721:LEU:HA | 1.95 | 0.48 |
| 1:G:1019:PRO:HD2 | 1:G:1020:ARG:NH1 | 2.29 | 0.48 |
| 1:G:3422:HIS:HD1 | 1:G:3423:TRP:CD1 | 2.32 | 0.48 |
| 1:G:3927:GLN:NE2 | 1:G:3991:GLY:HA3 | 2.29 | 0.48 |
| 1:G:4241:THR:HB | 1:G:4989:MET:HE1 | 1.95 | 0.48 |
| 8:G:5110:POV:H21H | 8:J:5107:POV:H214 | 1.95 | 0.48 |
| 1:J:1815:LEU:HG | 1:J:1865:MET:HE1 | 1.96 | 0.48 |
| 1:J:3107:VAL:HG11 | 1:J:3171:SER:HB2 | 1.95 | 0.48 |
| 1:A:977:LEU:HD13 | 1:A:1044:ARG:HB3 | 1.96 | 0.48 |
| 1:A:1434:TYR:CE2 | 1:A:1519:LEU:HG | 2.48 | 0.48 |
| 1:A:1926:LEU:HA | 1:A:1929:MET:HE3 | 1.96 | 0.48 |
| 1:A:2764:GLU:HB3 | 1:A:2857:PRO:HD3 | 1.95 | 0.48 |
| 1:A:3019:SER:HB2 | 1:A:3026:GLY:H | 1.79 | 0.48 |
| 1:A:4080:TYR:HE1 | 1:A:4095:LYS:HG3 | 1.79 | 0.48 |
| 1:A:4238:CYS:O | 1:A:4242:ILE:HG13 | 2.14 | 0.48 |
| 1:C:274:LEU:HD13 | 1:C:280:LEU:HD22 | 1.96 | 0.48 |
| 1:C:3432:GLU:HB3 | 1:C:3524:MET:SD | 2.54 | 0.48 |
| 3:E:71:ARG:HG2 | 3:E:102:GLU:HG2 | 1.94 | 0.48 |
| 1:G:1072:VAL:HG12 | 1:G:1195:GLY:HA2 | 1.95 | 0.48 |
| 1:G:1815:LEU:HG | 1:G:1865:MET:HE1 | 1.96 | 0.48 |
| 1:G:2355:ARG:O | 1:G:2359:ARG:HG2 | 2.13 | 0.48 |
| 1:G:2500:ALA:HB2 | 1:G:2553:TYR:HD1 | 1.79 | 0.48 |
| 1:J:349:GLN:HE21 | 1:J:354:GLY:HA2 | 1.79 | 0.48 |
| 1:J:2500:ALA:HB2 | 1:J:2553:TYR:HD1 | 1.79 | 0.48 |
| 1:J:3166:TYR:HE1 | 1:J:3203:VAL:HG11 | 1.79 | 0.48 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:J:3363:GLY:HA2 | 1:J:3437:MET:CE | 2.44 | 0.48 |
| 1:A:1815:LEU:HG | 1:A:1865:MET:HE1 | 1.96 | 0.48 |
| 1:A:2247:GLN:HG3 | 1:A:2279:SER:HA | 1.95 | 0.48 |
| 1:A:2377:LEU:HG | 1:A:2465:ASP:HA | 1.95 | 0.48 |
| 1:A:3432:GLU:HB3 | 1:A:3524:MET:SD | 2.54 | 0.48 |
| 1:A:3775:ALA:HA | 1:A:3778:MET:HE2 | 1.94 | 0.48 |
| 1:A:4116:GLU:HG2 | 1:A:4131:ARG:HH22 | 1.79 | 0.48 |
| 1:C:887:ILE:HD11 | 1:C:964:GLY:HA2 | 1.96 | 0.48 |
| 1:C:1434:TYR:CE2 | 1:C:1519:LEU:HG | 2.48 | 0.48 |
| 1:C:2920:ARG:O | 1:C:2924:GLN:HG2 | 2.13 | 0.48 |
| 1:C:4231:MET:HA | 1:C:4231:MET:HE3 | 1.96 | 0.48 |
| 8:C:5116:POV:H11A | 8:C:5117:POV:H14A | 1.96 | 0.48 |
| 3:F:23:VAL:HG22 | 3:F:47:LYS:HG2 | 1.96 | 0.48 |
| 3:F:90:VAL:HG12 | 3:F:91:ILE:HG13 | 1.96 | 0.48 |
| 1:G:960:MET:N | 1:G:960:MET:SD | 2.87 | 0.48 |
| 1:G:1220:GLN:O | 1:J:3522:LEU:HD23 | 2.14 | 0.48 |
| 1:G:2449:GLU:O | 1:G:2453:ILE:HG12 | 2.14 | 0.48 |
| 1:G:3367:LYS:O | 1:G:3371:LYS:HG2 | 2.13 | 0.48 |
| 1:J:445:LEU:O | 1:J:449:ILE:HG13 | 2.14 | 0.48 |
| 1:J:603:LEU:HD23 | 1:J:606:LEU:HD12 | 1.95 | 0.48 |
| 1:J:681:HIS:O | 1:J:783:PHE:HA | 2.13 | 0.48 |
| 1:J:1291:LEU:HB2 | 1:J:1550:PRO:HD2 | 1.96 | 0.48 |
| 1:J:2449:GLU:O | 1:J:2453:ILE:HG12 | 2.14 | 0.48 |
| 1:A:4673:ARG:NH1 | 1:A:4698:LYS:HE2 | 2.29 | 0.47 |
| 1:C:906:CYS:SG | 1:C:907:LEU:HD22 | 2.53 | 0.47 |
| 1:C:1019:PRO:HD2 | 1:C:1020:ARG:NH1 | 2.29 | 0.47 |
| 1:C:1152:MET:HE1 | 1:C:1217:CYS:HB2 | 1.96 | 0.47 |
| 1:C:1220:GLN:O | 1:G:3522:LEU:HD23 | 2.14 | 0.47 |
| 1:C:2449:GLU:HA | 1:C:2452:ARG:HE | 1.79 | 0.47 |
| 1:C:2449:GLU:O | 1:C:2453:ILE:HG12 | 2.14 | 0.47 |
| 1:G:62:LEU:HB2 | 1:G:261:ARG:HH21 | 1.79 | 0.47 |
| 1:G:426:ARG:HE | 1:G:508:GLY:HA2 | 1.79 | 0.47 |
| 1:G:2431:ASP:O | 1:G:2435:ARG:HB3 | 2.14 | 0.47 |
| 1:G:2506:LEU:HD11 | 1:G:2517:PHE:CZ | 2.48 | 0.47 |
| 1:G:4673:ARG:NH1 | 1:G:4698:LYS:HE2 | 2.29 | 0.47 |
| 1:G:4956:THR:O | 1:G:4965:SER:N | 2.46 | 0.47 |
| 1:J:274:LEU:HD13 | 1:J:280:LEU:HD22 | 1.96 | 0.47 |
| 1:J:2414:ASN:HB2 | 1:J:2417:HIS:CE1 | 2.49 | 0.47 |
| 1:J:3018:LEU:HD11 | 1:J:3150:HIS:CE1 | 2.48 | 0.47 |
| 1:J:3841:VAL:HG11 | 1:J:3925:ARG:HG2 | 1.96 | 0.47 |
| 1:J:4995:LEU:HD22 | 1:J:5003:HIS:HD2 | 1.79 | 0.47 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:35:LEU:HD22 | 1:A:49:LEU:HD23 | 1.97 | 0.47 |
| 1:A:1152:MET:HE1 | 1:A:1217:CYS:HB2 | 1.96 | 0.47 |
| 1:A:1291:LEU:HB2 | 1:A:1550:PRO:HD2 | 1.96 | 0.47 |
| 1:A:2355:ARG:O | 1:A:2359:ARG:HG2 | 2.13 | 0.47 |
| 1:A:2777:TYR:HB2 | 1:A:2791:LEU:HB2 | 1.96 | 0.47 |
| 1:A:3337:ARG:HA | 1:A:3340:VAL:HG12 | 1.96 | 0.47 |
| 1:A:4151:SER:HB3 | 1:A:4164:LEU:HD21 | 1.95 | 0.47 |
| 1:C:184:THR:HG22 | 1:C:189:LEU:HD13 | 1.96 | 0.47 |
| 1:C:924:MET:HA | 2:D:107:TRP:CH2 | 2.49 | 0.47 |
| 1:C:2702:CYS:O | 1:C:2706:ILE:HG13 | 2.14 | 0.47 |
| 1:C:2970:SER:O | 1:C:2974:ILE:HG23 | 2.15 | 0.47 |
| 8:G:5116:POV:H11A | 8:G:5117:POV:H14A | 1.96 | 0.47 |
| 1:J:1019:PRO:HD2 | 1:J:1020:ARG:NH1 | 2.29 | 0.47 |
| 1:J:1455:PRO:HB3 | 1:J:1549:PHE:HE1 | 1.79 | 0.47 |
| 1:J:2354:VAL:HG11 | 1:J:2453:ILE:HD12 | 1.95 | 0.47 |
| 1:J:2648:TYR:CE2 | 1:J:2675:THR:HG23 | 2.49 | 0.47 |
| 1:J:4901:ILE:HD12 | 1:J:4913:ARG:NH2 | 2.29 | 0.47 |
| 8:J:5120:POV:H11A | 8:J:5121:POV:H14A | 1.96 | 0.47 |
| 1:A:993:HIS:CE1 | 1:A:1027:LEU:HD11 | 2.49 | 0.47 |
| 1:A:1220:GLN:O | 1:C:3522:LEU:HD23 | 2.14 | 0.47 |
| 1:A:1951:LEU:HA | 1:A:1954:ARG:HD2 | 1.96 | 0.47 |
| 1:C:2648:TYR:CE2 | 1:C:2675:THR:HG23 | 2.49 | 0.47 |
| 1:C:3019:SER:HB2 | 1:C:3026:GLY:H | 1.79 | 0.47 |
| 1:C:3422:HIS:HD1 | 1:C:3423:TRP:CD1 | 2.32 | 0.47 |
| 1:C:4238:CYS:O | 1:C:4242:ILE:HG13 | 2.14 | 0.47 |
| 8:C:5110:POV:H21H | 8:G:5103:POV:H214 | 1.95 | 0.47 |
| 2:D:37:TYR:CZ | 2:D:47:LEU:HD13 | 2.49 | 0.47 |
| 1:G:906:CYS:SG | 1:G:907:LEU:HD22 | 2.54 | 0.47 |
| 1:G:1093:GLU:HB3 | 1:G:1201:HIS:HB3 | 1.95 | 0.47 |
| 1:G:1926:LEU:HA | 1:G:1929:MET:HE3 | 1.96 | 0.47 |
| 1:G:4231:MET:HA | 1:G:4231:MET:HE3 | 1.96 | 0.47 |
| 1:J:2431:ASP:O | 1:J:2435:ARG:HB3 | 2.14 | 0.47 |
| 1:A:3010:PHE:HE2 | 1:A:3071:LEU:HD13 | 1.79 | 0.47 |
| 1:A:3927:GLN:NE2 | 1:A:3991:GLY:HA3 | 2.29 | 0.47 |
| 8:A:5106:POV:H33A | 8:J:5101:POV:H32 | 1.96 | 0.47 |
| 1:C:349:GLN:HE21 | 1:C:354:GLY:HA2 | 1.79 | 0.47 |
| 1:C:1291:LEU:HB2 | 1:C:1550:PRO:HD2 | 1.96 | 0.47 |
| 1:C:2354:VAL:HG11 | 1:C:2453:ILE:HD12 | 1.95 | 0.47 |
| 1:C:2911:LEU:HB3 | 1:C:2915:GLU:HG3 | 1.97 | 0.47 |
| 1:C:4116:GLU:HG2 | 1:C:4131:ARG:HH22 | 1.79 | 0.47 |
| 1:C:4901:ILE:HD12 | 1:C:4913:ARG:NH2 | 2.29 | 0.47 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:G:1291:LEU:HB2 | 1:G:1550:PRO:HD2 | 1.96 | 0.47 |
| 1:G:1927:LEU:HD22 | 1:G:2101:MET:HG3 | 1.96 | 0.47 |
| 1:G:1951:LEU:HA | 1:G:1954:ARG:HD2 | 1.96 | 0.47 |
| 1:G:2485:LEU:O | 1:G:2486:VAL:C | 2.57 | 0.47 |
| 1:G:3107:VAL:HA | 1:G:3175:LEU:HD11 | 1.95 | 0.47 |
| 1:G:4116:GLU:HG2 | 1:G:4131:ARG:HH22 | 1.79 | 0.47 |
| 1:J:932:LEU:HB3 | 1:J:937:CYS:HB2 | 1.97 | 0.47 |
| 1:J:993:HIS:CE1 | 1:J:1027:LEU:HD11 | 2.49 | 0.47 |
| 1:J:2777:TYR:HB2 | 1:J:2791:LEU:HB2 | 1.97 | 0.47 |
| 1:J:3010:PHE:HE2 | 1:J:3071:LEU:HD13 | 1.79 | 0.47 |
| 1:J:4080:TYR:HE1 | 1:J:4095:LYS:HG3 | 1.79 | 0.47 |
| 1:J:4673:ARG:NH1 | 1:J:4698:LYS:HE2 | 2.29 | 0.47 |
| 1:J:4769:MET:HA | 1:J:4769:MET:HE3 | 1.96 | 0.47 |
| 1:A:874:LEU:O | 1:A:878:ILE:HG12 | 2.14 | 0.47 |
| 1:A:1808:ARG:O | 1:A:1812:LEU:HD23 | 2.15 | 0.47 |
| 1:A:3020:THR:HG22 | 1:A:3022:ALA:H | 1.80 | 0.47 |
| 1:A:4995:LEU:HD22 | 1:A:5003:HIS:HD2 | 1.79 | 0.47 |
| 1:C:716:PHE:HA | 1:C:721:LEU:HA | 1.95 | 0.47 |
| 1:C:2355:ARG:O | 1:C:2359:ARG:HG2 | 2.13 | 0.47 |
| 1:C:3146:HIS:CE1 | 1:C:3150:HIS:HE1 | 2.33 | 0.47 |
| 1:C:3927:GLN:NE2 | 1:C:3991:GLY:HA3 | 2.29 | 0.47 |
| 1:C:4151:SER:HB3 | 1:C:4164:LEU:HD21 | 1.95 | 0.47 |
| 1:C:4898:GLY:HA2 | 1:C:4901:ILE:HG12 | 1.96 | 0.47 |
| 1:G:477:LEU:O | 1:G:481:GLU:HG2 | 2.13 | 0.47 |
| 1:G:1000:ARG:HA | 1:G:1000:ARG:HE | 1.80 | 0.47 |
| 1:G:1735:ILE:HD11 | 1:G:2201:LEU:HD11 | 1.97 | 0.47 |
| 1:G:2414:ASN:HB2 | 1:G:2417:HIS:CE1 | 2.49 | 0.47 |
| 1:G:2764:GLU:HG2 | 1:G:2855:TYR:HD1 | 1.79 | 0.47 |
| 1:G:3432:GLU:HB3 | 1:G:3524:MET:SD | 2.54 | 0.47 |
| 1:G:4779:LYS:O | 1:G:4783:ILE:HG23 | 2.15 | 0.47 |
| 1:A:1455:PRO:HB3 | 1:A:1549:PHE:HE1 | 1.80 | 0.47 |
| 1:A:2500:ALA:HB2 | 1:A:2553:TYR:HD1 | 1.79 | 0.47 |
| 1:G:874:LEU:O | 1:G:878:ILE:HG12 | 2.14 | 0.47 |
| 1:G:1152:MET:HE1 | 1:G:1217:CYS:HB2 | 1.96 | 0.47 |
| 1:G:2777:TYR:HB2 | 1:G:2791:LEU:HB2 | 1.96 | 0.47 |
| 1:G:3019:SER:HB2 | 1:G:3026:GLY:H | 1.79 | 0.47 |
| 1:G:3754:GLU:HB2 | 1:G:4718:LYS:HG3 | 1.97 | 0.47 |
| 1:G:4995:LEU:HD22 | 1:G:5003:HIS:HD2 | 1.79 | 0.47 |
| 1:J:2764:GLU:HG2 | 1:J:2855:TYR:HD1 | 1.79 | 0.47 |
| 1:J:3432:GLU:HB3 | 1:J:3524:MET:SD | 2.54 | 0.47 |
| 1:J:3927:GLN:NE2 | 1:J:3991:GLY:HA3 | 2.29 | 0.47 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:72:SER:H | 1:A:99:ARG:HH21 | 1.63 | 0.47 |
| 1:A:932:LEU:HB3 | 1:A:937:CYS:HB2 | 1.97 | 0.47 |
| 1:A:2148:SER:O | 1:A:2152:THR:HG23 | 2.14 | 0.47 |
| 1:A:2354:VAL:HG11 | 1:A:2453:ILE:HD12 | 1.95 | 0.47 |
| 1:A:2764:GLU:HG2 | 1:A:2855:TYR:HD1 | 1.80 | 0.47 |
| 1:A:3146:HIS:CE1 | 1:A:3150:HIS:HE1 | 2.33 | 0.47 |
| 1:A:4901:ILE:HD12 | 1:A:4913:ARG:NH2 | 2.29 | 0.47 |
| 1:A:5013:MET:HE1 | 1:A:5020:ASP:HB3 | 1.96 | 0.47 |
| 1:C:35:LEU:HD22 | 1:C:49:LEU:HD23 | 1.97 | 0.47 |
| 1:C:72:SER:H | 1:C:99:ARG:HH21 | 1.63 | 0.47 |
| 1:C:637:LEU:HD23 | 1:C:637:LEU:HA | 1.76 | 0.47 |
| 1:C:932:LEU:HB3 | 1:C:937:CYS:HB2 | 1.97 | 0.47 |
| 1:C:996:TRP:HB2 | 2:D:114:TYR:HE1 | 1.79 | 0.47 |
| 1:C:1735:ILE:HD11 | 1:C:2201:LEU:HD11 | 1.97 | 0.47 |
| 1:C:1951:LEU:HA | 1:C:1954:ARG:HD2 | 1.96 | 0.47 |
| 1:C:2148:SER:O | 1:C:2152:THR:HG23 | 2.14 | 0.47 |
| 1:C:2321:ILE:HG12 | 1:C:2323:TRP:HB3 | 1.97 | 0.47 |
| 1:C:2431:ASP:O | 1:C:2435:ARG:HB3 | 2.14 | 0.47 |
| 1:C:2777:TYR:HB2 | 1:C:2791:LEU:HB2 | 1.97 | 0.47 |
| 1:C:3007:ASN:HB2 | 1:C:3067:CYS:SG | 2.54 | 0.47 |
| 1:C:3166:TYR:HE1 | 1:C:3203:VAL:HG11 | 1.79 | 0.47 |
| 1:C:3363:GLY:HA2 | 1:C:3437:MET:CE | 2.44 | 0.47 |
| 8:C:5119:POV:H32 | 8:G:5109:POV:H33A | 1.96 | 0.47 |
| 1:G:184:THR:HG22 | 1:G:189:LEU:HD13 | 1.96 | 0.47 |
| 1:G:233:ILE:HG23 | 1:G:234:SER:H | 1.80 | 0.47 |
| 1:G:932:LEU:HB3 | 1:G:937:CYS:HB2 | 1.97 | 0.47 |
| 1:G:2321:ILE:HG12 | 1:G:2323:TRP:HB3 | 1.97 | 0.47 |
| 1:G:2354:VAL:HG11 | 1:G:2453:ILE:HD12 | 1.95 | 0.47 |
| 1:G:3020:THR:HG22 | 1:G:3022:ALA:H | 1.80 | 0.47 |
| 8:G:5121:POV:H25 | 8:G:5121:POV:H32A | 1.96 | 0.47 |
| 2:H:111:ASN:HA | 2:H:114:TYR:CD2 | 2.50 | 0.47 |
| 3:I:90:VAL:HG12 | 3:I:91:ILE:HG13 | 1.96 | 0.47 |
| 1:J:35:LEU:HD22 | 1:J:49:LEU:HD23 | 1.97 | 0.47 |
| 1:J:426:ARG:HE | 1:J:508:GLY:HA2 | 1.79 | 0.47 |
| 1:J:2485:LEU:O | 1:J:2486:VAL:C | 2.58 | 0.47 |
| 1:J:2702:CYS:O | 1:J:2706:ILE:HG13 | 2.14 | 0.47 |
| 1:J:2911:LEU:HB3 | 1:J:2915:GLU:HG3 | 1.97 | 0.47 |
| 1:J:3019:SER:HB2 | 1:J:3026:GLY:H | 1.79 | 0.47 |
| 1:J:3146:HIS:CE1 | 1:J:3150:HIS:HE1 | 2.33 | 0.47 |
| 1:J:3754:GLU:HB2 | 1:J:4718:LYS:HG3 | 1.97 | 0.47 |
| 1:J:4116:GLU:HG2 | 1:J:4131:ARG:HH22 | 1.79 | 0.47 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:J:4898:GLY:HA2 | 1:J:4901:ILE:HG12 | 1.96 | 0.47 |
| 1:A:35:LEU:HD13 | 1:A:49:LEU:HB2 | 1.95 | 0.47 |
| 1:A:62:LEU:HB2 | 1:A:261:ARG:HH21 | 1.79 | 0.47 |
| 1:A:233:ILE:HG23 | 1:A:234:SER:H | 1.80 | 0.47 |
| 1:A:404:ILE:HG23 | 1:A:483:MET:SD | 2.55 | 0.47 |
| 1:A:2414:ASN:HB2 | 1:A:2417:HIS:CE1 | 2.49 | 0.47 |
| 1:A:2702:CYS:O | 1:A:2706:ILE:HG13 | 2.14 | 0.47 |
| 1:A:2911:LEU:HB3 | 1:A:2915:GLU:HG3 | 1.97 | 0.47 |
| 1:A:3935:TRP:HE1 | 1:J:77:ALA:HA | 1.80 | 0.47 |
| 1:A:3948:LYS:HE2 | 1:A:4009:GLN:HG2 | 1.97 | 0.47 |
| 1:A:5027:CYS:SG | 1:A:5030:LYS:HG3 | 2.55 | 0.47 |
| 2:B:92:VAL:HA | 2:B:122:GLN:HA | 1.97 | 0.47 |
| 1:C:2764:GLU:HG2 | 1:C:2855:TYR:HD1 | 1.79 | 0.47 |
| 1:C:3841:VAL:HG11 | 1:C:3925:ARG:HG2 | 1.96 | 0.47 |
| 1:G:78:LEU:HD21 | 1:G:174:VAL:HG11 | 1.96 | 0.47 |
| 1:G:349:GLN:HE21 | 1:G:354:GLY:HA2 | 1.79 | 0.47 |
| 1:G:805:PRO:HB2 | 1:G:808:TYR:CD1 | 2.50 | 0.47 |
| 1:G:1455:PRO:HB3 | 1:G:1549:PHE:HE1 | 1.79 | 0.47 |
| 1:G:1786:LEU:HD12 | 1:G:1787:PRO:HD2 | 1.97 | 0.47 |
| 1:G:2702:CYS:O | 1:G:2706:ILE:HG13 | 2.14 | 0.47 |
| 1:G:2970:SER:O | 1:G:2974:ILE:HG23 | 2.15 | 0.47 |
| 1:G:4818:MET:HB3 | 8:G:5115:POV:H13A | 1.97 | 0.47 |
| 2:H:37:TYR:CZ | 2:H:47:LEU:HD13 | 2.49 | 0.47 |
| 1:J:233:ILE:HG23 | 1:J:234:SER:H | 1.80 | 0.47 |
| 1:J:908:VAL:HG23 | 1:J:962:SER:O | 2.15 | 0.47 |
| 1:J:2321:ILE:HG12 | 1:J:2323:TRP:HB3 | 1.97 | 0.47 |
| 1:A:1735:ILE:HD11 | 1:A:2201:LEU:HD11 | 1.97 | 0.47 |
| 1:A:2228:MET:HE3 | 1:A:2232:CYS:SG | 2.55 | 0.47 |
| 1:A:2321:ILE:HG12 | 1:A:2323:TRP:HB3 | 1.97 | 0.47 |
| 1:A:3252:ASP:O | 1:A:3256:LEU:HG | 2.15 | 0.47 |
| 2:B:37:TYR:CZ | 2:B:47:LEU:HD13 | 2.49 | 0.47 |
| 1:C:62:LEU:HB2 | 1:C:261:ARG:HH21 | 1.79 | 0.47 |
| 1:C:960:MET:N | 1:C:960:MET:SD | 2.88 | 0.47 |
| 1:C:977:LEU:HD13 | 1:C:1044:ARG:HB3 | 1.96 | 0.47 |
| 1:C:3252:ASP:O | 1:C:3256:LEU:HG | 2.15 | 0.47 |
| 2:D:92:VAL:HA | 2:D:122:GLN:HA | 1.97 | 0.47 |
| 3:E:90:VAL:HG12 | 3:E:91:ILE:HG13 | 1.96 | 0.47 |
| 1:G:54:ASN:HB3 | 1:G:57:ASN:HB2 | 1.96 | 0.47 |
| 1:G:274:LEU:HD13 | 1:G:280:LEU:HD22 | 1.96 | 0.47 |
| 1:G:993:HIS:CE1 | 1:G:1027:LEU:HD11 | 2.49 | 0.47 |
| 1:G:3252:ASP:O | 1:G:3256:LEU:HG | 2.15 | 0.47 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:J:54:ASN:HB3 | 1:J:57:ASN:HB2 | 1.96 | 0.47 |
| 1:J:1735:ILE:HD11 | 1:J:2201:LEU:HD11 | 1.97 | 0.47 |
| 1:J:3007:ASN:HB2 | 1:J:3067:CYS:SG | 2.54 | 0.47 |
| 3:L:98:ILE:HD13 | 3:L:98:ILE:HG21 | 1.65 | 0.47 |
| 1:A:184:THR:HG22 | 1:A:189:LEU:HD13 | 1.96 | 0.47 |
| 1:A:426:ARG:HE | 1:A:508:GLY:HA2 | 1.79 | 0.47 |
| 1:A:2306:GLY:HA2 | 1:A:2323:TRP:HZ3 | 1.78 | 0.47 |
| 1:A:3075:LEU:HG | 1:A:3076:ASP:N | 2.30 | 0.47 |
| 1:A:3841:VAL:HG11 | 1:A:3925:ARG:HG2 | 1.96 | 0.47 |
| 1:A:4655:PHE:O | 1:A:4659:ILE:HG12 | 2.15 | 0.47 |
| 1:C:168:ASP:HB3 | 1:C:199:LEU:HG | 1.96 | 0.47 |
| 1:C:2414:ASN:HB2 | 1:C:2417:HIS:CE1 | 2.49 | 0.47 |
| 1:C:4673:ARG:NH1 | 1:C:4698:LYS:HE2 | 2.29 | 0.47 |
| 1:G:2247:GLN:HG3 | 1:G:2279:SER:HA | 1.95 | 0.47 |
| 1:G:2991:HIS:O | 1:G:2995:ILE:HG13 | 2.15 | 0.47 |
| 1:G:3043:PHE:CD2 | 1:G:3075:LEU:HD13 | 2.51 | 0.47 |
| 1:J:592:LYS:HG2 | 1:J:1580:PHE:CD1 | 2.50 | 0.47 |
| 1:J:4779:LYS:O | 1:J:4783:ILE:HG23 | 2.15 | 0.47 |
| 2:K:92:VAL:HA | 2:K:122:GLN:HA | 1.97 | 0.47 |
| 1:A:2124:LEU:HD23 | 1:A:2124:LEU:HA | 1.79 | 0.46 |
| 1:A:3244:PRO:HD2 | 1:A:3249:LEU:HD21 | 1.97 | 0.46 |
| 1:A:3522:LEU:HD23 | 1:J:1220:GLN:O | 2.14 | 0.46 |
| 1:A:4779:LYS:O | 1:A:4783:ILE:HG23 | 2.15 | 0.46 |
| 1:C:184:THR:HA | 1:C:189:LEU:HD22 | 1.97 | 0.46 |
| 1:C:233:ILE:HG23 | 1:C:234:SER:H | 1.80 | 0.46 |
| 1:C:592:LYS:HG2 | 1:C:1580:PHE:CD1 | 2.51 | 0.46 |
| 1:C:1926:LEU:HA | 1:C:1929:MET:HE3 | 1.96 | 0.46 |
| 1:C:3244:PRO:HD2 | 1:C:3249:LEU:HD21 | 1.97 | 0.46 |
| 1:C:4779:LYS:O | 1:C:4783:ILE:HG23 | 2.15 | 0.46 |
| 1:G:977:LEU:HD13 | 1:G:1044:ARG:HB3 | 1.96 | 0.46 |
| 1:G:1741:GLU:O | 1:G:1745:ILE:HG13 | 2.13 | 0.46 |
| 1:G:5013:MET:HE1 | 1:G:5020:ASP:HB3 | 1.96 | 0.46 |
| 2:H:92:VAL:HA | 2:H:122:GLN:HA | 1.97 | 0.46 |
| 3:I:23:VAL:HG12 | 3:I:104:LEU:HD21 | 1.97 | 0.46 |
| 1:J:62:LEU:HB2 | 1:J:261:ARG:HH21 | 1.79 | 0.46 |
| 1:J:364:PRO:HA | 1:J:367:LEU:HG | 1.97 | 0.46 |
| 1:J:1927:LEU:HD22 | 1:J:2101:MET:HG3 | 1.96 | 0.46 |
| 1:J:3020:THR:HG22 | 1:J:3022:ALA:H | 1.80 | 0.46 |
| 1:J:3948:LYS:HE2 | 1:J:4009:GLN:HG2 | 1.97 | 0.46 |
| 1:A:2431:ASP:O | 1:A:2435:ARG:HB3 | 2.14 | 0.46 |
| 1:A:2891:LYS:HD3 | 1:A:2905:LEU:HD11 | 1.97 | 0.46 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 8:A:5113:POV:H11A | 8:A:5114:POV:H14A | 1.96 | 0.46 |
| 1:C:2113:SER:O | 1:C:2117:VAL:HG23 | 2.16 | 0.46 |
| 3:E:77:THR:OG1 | 3:E:78:PRO:HD2 | 2.15 | 0.46 |
| 3:F:23:VAL:HG12 | 3:F:104:LEU:HD21 | 1.98 | 0.46 |
| 1:G:4901:ILE:HD12 | 1:G:4913:ARG:NH2 | 2.29 | 0.46 |
| 1:A:1927:LEU:HD22 | 1:A:2101:MET:HG3 | 1.97 | 0.46 |
| 1:A:2113:SER:O | 1:A:2117:VAL:HG23 | 2.16 | 0.46 |
| 1:A:2526:PHE:HD2 | 1:A:2558:VAL:HG13 | 1.81 | 0.46 |
| 1:A:3081:MET:HG3 | 1:A:3156:VAL:HG22 | 1.97 | 0.46 |
| 8:A:5116:POV:H32 | 8:C:5109:POV:H33A | 1.96 | 0.46 |
| 1:C:1501:VAL:HG23 | 1:C:1514:LEU:HD13 | 1.97 | 0.46 |
| 1:C:2500:ALA:HB2 | 1:C:2553:TYR:HD1 | 1.79 | 0.46 |
| 1:C:4080:TYR:HE1 | 1:C:4095:LYS:HG3 | 1.79 | 0.46 |
| 1:G:2113:SER:O | 1:G:2117:VAL:HG23 | 2.16 | 0.46 |
| 1:G:2526:PHE:HD2 | 1:G:2558:VAL:HG13 | 1.81 | 0.46 |
| 1:J:998:ARG:HA | 1:J:1001:VAL:HG22 | 1.97 | 0.46 |
| 1:J:2758:PHE:O | 1:J:2762:THR:HG23 | 2.16 | 0.46 |
| 1:J:3996:PHE:CE2 | 1:J:4023:MET:HG3 | 2.43 | 0.46 |
| 2:K:37:TYR:CZ | 2:K:47:LEU:HD13 | 2.49 | 0.46 |
| 2:K:67:PHE:H | 2:K:82:MET:CE | 2.28 | 0.46 |
| 3:L:23:VAL:HG12 | 3:L:104:LEU:HD21 | 1.98 | 0.46 |
| 1:A:2449:GLU:O | 1:A:2453:ILE:HG12 | 2.14 | 0.46 |
| 1:A:4086:GLY:C | 1:A:4087:LEU:HD23 | 2.40 | 0.46 |
| 8:A:5108:POV:H29 | 1:J:4922:PHE:CE2 | 2.51 | 0.46 |
| 1:C:54:ASN:HB3 | 1:C:57:ASN:HB2 | 1.96 | 0.46 |
| 1:C:1808:ARG:O | 1:C:1812:LEU:HD23 | 2.15 | 0.46 |
| 1:C:1927:LEU:HD22 | 1:C:2101:MET:HG3 | 1.96 | 0.46 |
| 1:C:3948:LYS:HE2 | 1:C:4009:GLN:HG2 | 1.97 | 0.46 |
| 1:C:4958:CYS:HA | 5:C:5105:ATP:N7 | 2.31 | 0.46 |
| 1:G:592:LYS:HG2 | 1:G:1580:PHE:CD1 | 2.51 | 0.46 |
| 1:G:1808:ARG:O | 1:G:1812:LEU:HD23 | 2.15 | 0.46 |
| 1:G:3007:ASN:OD1 | 1:G:3070:ILE:HG13 | 2.15 | 0.46 |
| 1:G:3146:HIS:CE1 | 1:G:3150:HIS:HE1 | 2.33 | 0.46 |
| 1:J:81:MET:HG3 | 1:J:82:LEU:N | 2.30 | 0.46 |
| 1:J:2970:SER:O | 1:J:2974:ILE:HG23 | 2.15 | 0.46 |
| 1:J:2991:HIS:O | 1:J:2995:ILE:HG13 | 2.15 | 0.46 |
| 1:J:4245:MET:HE2 | 1:J:4245:MET:HB3 | 1.81 | 0.46 |
| 1:J:4655:PHE:O | 1:J:4659:ILE:HG12 | 2.15 | 0.46 |
| 1:A:178:ARG:HB2 | 1:A:193:ALA:HB1 | 1.98 | 0.46 |
| 1:A:364:PRO:HA | 1:A:367:LEU:HG | 1.97 | 0.46 |
| 1:A:2765:LYS:HA | 1:A:2768:PHE:HB3 | 1.97 | 0.46 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:3566:SER:HB3 | 1:A:3569:LEU:HB2 | 1.98 | 0.46 |
| 1:A:3754:GLU:HB2 | 1:A:4718:LYS:HG3 | 1.97 | 0.46 |
| 1:C:365:LYS:HE3 | 1:C:365:LYS:HB3 | 1.82 | 0.46 |
| 1:C:404:ILE:HG23 | 1:C:483:MET:SD | 2.55 | 0.46 |
| 1:C:874:LEU:O | 1:C:878:ILE:HG12 | 2.14 | 0.46 |
| 1:C:3100:SER:OG | 1:C:3164:SER:HB2 | 2.16 | 0.46 |
| 1:C:4820:VAL:HG23 | 1:C:4823:LEU:HB2 | 1.98 | 0.46 |
| 1:C:5013:MET:HE1 | 1:C:5020:ASP:HB3 | 1.96 | 0.46 |
| 1:G:35:LEU:HD22 | 1:G:49:LEU:HD23 | 1.97 | 0.46 |
| 1:G:168:ASP:HB3 | 1:G:199:LEU:HG | 1.96 | 0.46 |
| 1:G:404:ILE:HG23 | 1:G:483:MET:SD | 2.55 | 0.46 |
| 1:G:2911:LEU:HB3 | 1:G:2915:GLU:HG3 | 1.97 | 0.46 |
| 1:G:4086:GLY:C | 1:G:4087:LEU:HD23 | 2.40 | 0.46 |
| 8:G:5119:POV:H32 | 8:J:5113:POV:H33A | 1.96 | 0.46 |
| 1:J:22:LEU:HB2 | 1:J:37:LEU:CD2 | 2.46 | 0.46 |
| 1:J:1951:LEU:HA | 1:J:1954:ARG:HD2 | 1.96 | 0.46 |
| 1:J:2113:SER:O | 1:J:2117:VAL:HG23 | 2.16 | 0.46 |
| 1:J:2867:LEU:HG | 1:J:2868:SER:H | 1.81 | 0.46 |
| 3:L:90:VAL:HG12 | 3:L:91:ILE:HG13 | 1.96 | 0.46 |
| 1:A:349:GLN:HE21 | 1:A:354:GLY:HA2 | 1.79 | 0.46 |
| 1:A:1786:LEU:HD12 | 1:A:1787:PRO:HD2 | 1.97 | 0.46 |
| 1:A:2970:SER:O | 1:A:2974:ILE:HG23 | 2.15 | 0.46 |
| 1:A:4104:THR:O | 1:A:4108:ILE:HG13 | 2.16 | 0.46 |
| 1:A:4898:GLY:HA2 | 1:A:4901:ILE:HG12 | 1.96 | 0.46 |
| 1:C:178:ARG:HB2 | 1:C:193:ALA:HB1 | 1.98 | 0.46 |
| 1:C:1455:PRO:HB3 | 1:C:1549:PHE:HE1 | 1.80 | 0.46 |
| 1:C:2758:PHE:O | 1:C:2762:THR:HG23 | 2.16 | 0.46 |
| 1:C:2817:ILE:HB | 1:C:2823:ILE:HG22 | 1.98 | 0.46 |
| 1:C:3722:TYR:OH | 1:C:3782:MET:HG3 | 2.16 | 0.46 |
| 1:C:4104:THR:O | 1:C:4108:ILE:HG13 | 2.16 | 0.46 |
| 1:C:4818:MET:HB3 | 8:C:5115:POV:H13A | 1.97 | 0.46 |
| 1:G:178:ARG:HB2 | 1:G:193:ALA:HB1 | 1.98 | 0.46 |
| 1:G:2231:SER:HA | 1:G:2234:ARG:HD2 | 1.96 | 0.46 |
| 1:G:2316:LYS:HE3 | 1:G:2318:TYR:HE1 | 1.81 | 0.46 |
| 1:G:2817:ILE:HB | 1:G:2823:ILE:HG22 | 1.98 | 0.46 |
| 1:G:3100:SER:OG | 1:G:3164:SER:HB2 | 2.16 | 0.46 |
| 1:G:3406:TYR:HE2 | 1:G:3455:GLU:HG3 | 1.81 | 0.46 |
| 1:J:404:ILE:HG23 | 1:J:483:MET:SD | 2.55 | 0.46 |
| 1:J:2891:LYS:HD3 | 1:J:2905:LEU:HD11 | 1.97 | 0.46 |
| 1:J:2960:LEU:HB2 | 1:J:3038:MET:HE1 | 1.98 | 0.46 |
| 1:J:4816:ILE:O | 1:J:4820:VAL:HG22 | 2.16 | 0.46 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 2:K:98:ASP:OD1 | 2:K:98:ASP:N | 2.48 | 0.46 |
| 1:A:168:ASP:HB3 | 1:A:199:LEU:HG | 1.96 | 0.46 |
| 1:A:592:LYS:HG2 | 1:A:1580:PHE:CD1 | 2.50 | 0.46 |
| 1:A:2758:PHE:O | 1:A:2762:THR:HG23 | 2.16 | 0.46 |
| 1:A:3166:TYR:HE1 | 1:A:3203:VAL:HG11 | 1.79 | 0.46 |
| 1:C:77:ALA:HA | 1:G:3935:TRP:HE1 | 1.80 | 0.46 |
| 1:C:172:VAL:HB | 1:C:179:TYR:CD2 | 2.51 | 0.46 |
| 1:C:867:LEU:HD12 | 1:C:929:LEU:HD12 | 1.98 | 0.46 |
| 1:C:1786:LEU:HD12 | 1:C:1787:PRO:HD2 | 1.97 | 0.46 |
| 1:C:2206:THR:O | 1:C:2210:VAL:HG23 | 2.16 | 0.46 |
| 1:C:2816:MET:SD | 1:C:2937:VAL:HG21 | 2.56 | 0.46 |
| 1:C:2991:HIS:O | 1:C:2995:ILE:HG13 | 2.15 | 0.46 |
| 1:C:3319:ILE:O | 1:C:3323:ILE:HG13 | 2.16 | 0.46 |
| 1:C:3566:SER:HB3 | 1:C:3569:LEU:HB2 | 1.98 | 0.46 |
| 1:C:3996:PHE:CE2 | 1:C:4023:MET:HG3 | 2.43 | 0.46 |
| 1:G:172:VAL:HB | 1:G:179:TYR:CD2 | 2.51 | 0.46 |
| 1:G:184:THR:HA | 1:G:189:LEU:HD22 | 1.97 | 0.46 |
| 1:G:3137:LEU:HB3 | 1:G:3138:PRO:HD3 | 1.97 | 0.46 |
| 1:G:3722:TYR:OH | 1:G:3782:MET:HG3 | 2.16 | 0.46 |
| 1:G:4581:LYS:HB2 | 1:G:4581:LYS:HE2 | 1.65 | 0.46 |
| 1:G:4816:ILE:O | 1:G:4820:VAL:HG22 | 2.16 | 0.46 |
| 1:G:4963:ILE:HG13 | 1:G:5030:LYS:HD2 | 1.98 | 0.46 |
| 1:J:172:VAL:HB | 1:J:179:TYR:CD2 | 2.51 | 0.46 |
| 1:J:184:THR:HG22 | 1:J:189:LEU:HD13 | 1.96 | 0.46 |
| 1:J:2293:GLN:HA | 1:J:2296:GLU:HB3 | 1.98 | 0.46 |
| 1:J:2333:ASP:HA | 1:J:2336:ARG:HE | 1.81 | 0.46 |
| 1:J:3604:TYR:O | 1:J:3607:GLU:HG3 | 2.15 | 0.46 |
| 1:J:4231:MET:HE3 | 1:J:4231:MET:HA | 1.96 | 0.46 |
| 1:J:4818:MET:HB3 | 8:J:5119:POV:H13A | 1.97 | 0.46 |
| 1:A:22:LEU:HB2 | 1:A:37:LEU:CD2 | 2.46 | 0.46 |
| 1:A:54:ASN:HB3 | 1:A:57:ASN:HB2 | 1.96 | 0.46 |
| 1:A:663:TYR:CE1 | 1:A:745:SER:HB3 | 2.51 | 0.46 |
| 1:A:2333:ASP:HA | 1:A:2336:ARG:HE | 1.81 | 0.46 |
| 1:A:2867:LEU:HG | 1:A:2868:SER:H | 1.81 | 0.46 |
| 1:A:3319:ILE:O | 1:A:3323:ILE:HG13 | 2.16 | 0.46 |
| 1:A:3416:VAL:O | 1:A:3420:ARG:HB2 | 2.16 | 0.46 |
| 1:A:4986:ALA:O | 1:A:4989:MET:N | 2.49 | 0.46 |
| 8:A:5107:POV:H21C | 8:A:5107:POV:H31D | 1.98 | 0.46 |
| 1:C:663:TYR:CE1 | 1:C:745:SER:HB3 | 2.51 | 0.46 |
| 1:C:3020:THR:HG22 | 1:C:3022:ALA:H | 1.80 | 0.46 |
| 1:C:4182:GLU:OE2 | 1:C:4982:GLU:HG3 | 2.15 | 0.46 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:4655:PHE:O | 1:C:4659:ILE:HG12 | 2.15 | 0.46 |
| 1:G:22:LEU:HB2 | 1:G:37:LEU:CD2 | 2.46 | 0.46 |
| 1:G:72:SER:H | 1:G:99:ARG:HH21 | 1.63 | 0.46 |
| 1:G:470:SER:HA | 1:G:473:ASN:ND2 | 2.31 | 0.46 |
| 1:G:905:PRO:HB2 | 1:G:963:ASN:HD21 | 1.80 | 0.46 |
| 1:G:3150:HIS:HB3 | 1:G:3152:PHE:CD2 | 2.51 | 0.46 |
| 1:G:3244:PRO:HD2 | 1:G:3249:LEU:HD21 | 1.97 | 0.46 |
| 1:G:4655:PHE:O | 1:G:4659:ILE:HG12 | 2.15 | 0.46 |
| 1:J:1786:LEU:HD12 | 1:J:1787:PRO:HD2 | 1.97 | 0.46 |
| 1:J:3244:PRO:HD2 | 1:J:3249:LEU:HD21 | 1.97 | 0.46 |
| 1:A:981:GLN:O | 1:A:985:VAL:HG23 | 2.16 | 0.46 |
| 1:A:3150:HIS:HB3 | 1:A:3152:PHE:CD2 | 2.51 | 0.46 |
| 1:A:3271:GLU:HG2 | 1:A:3334:TRP:CD1 | 2.51 | 0.46 |
| 1:A:3722:TYR:OH | 1:A:3782:MET:HG3 | 2.16 | 0.46 |
| 1:A:4231:MET:HA | 1:A:4231:MET:HE3 | 1.96 | 0.46 |
| 1:C:4986:ALA:O | 1:C:4989:MET:N | 2.49 | 0.46 |
| 1:G:2206:THR:O | 1:G:2210:VAL:HG23 | 2.16 | 0.46 |
| 1:G:3319:ILE:O | 1:G:3323:ILE:HG13 | 2.16 | 0.46 |
| 1:G:4696:ASP:O | 1:G:4700:GLN:HG2 | 2.16 | 0.46 |
| 1:J:72:SER:H | 1:J:99:ARG:HH21 | 1.63 | 0.46 |
| 1:J:76:ARG:O | 1:J:79:GLN:HG3 | 2.16 | 0.46 |
| 1:J:2816:MET:SD | 1:J:2937:VAL:HG21 | 2.56 | 0.46 |
| 1:J:3539:ARG:HH12 | 1:J:3552:PHE:CB | 2.12 | 0.46 |
| 1:J:3566:SER:HB3 | 1:J:3569:LEU:HB2 | 1.98 | 0.46 |
| 1:J:4820:VAL:HG23 | 1:J:4823:LEU:HB2 | 1.98 | 0.46 |
| 1:J:4858:PHE:HE1 | 8:J:5101:POV:H2 | 1.81 | 0.46 |
| 2:K:94:TYR:HB3 | 2:K:117:TRP:HD1 | 1.80 | 0.46 |
| 3:L:16:PRO:HG2 | 3:L:64:ALA:HA | 1.97 | 0.46 |
| 1:A:3201:MET:HG3 | 1:A:3203:VAL:HG12 | 1.97 | 0.46 |
| 1:A:4922:PHE:CE2 | 8:C:5111:POV:H29 | 2.51 | 0.46 |
| 1:A:5013:MET:HE3 | 1:A:5013:MET:HB3 | 1.77 | 0.46 |
| 1:C:979:PRO:O | 1:C:983:THR:HG23 | 2.16 | 0.46 |
| 1:C:1965:TYR:CE2 | 1:C:2031:LEU:HD12 | 2.51 | 0.46 |
| 1:C:2582:MET:SD | 1:C:2610:LEU:HD21 | 2.56 | 0.46 |
| 1:G:637:LEU:HD23 | 1:G:637:LEU:HA | 1.76 | 0.46 |
| 1:G:1569:GLN:H | 1:G:1572:ILE:HB | 1.81 | 0.46 |
| 1:G:2333:ASP:HA | 1:G:2336:ARG:HE | 1.81 | 0.46 |
| 1:J:168:ASP:HB3 | 1:J:199:LEU:HG | 1.97 | 0.46 |
| 1:J:979:PRO:O | 1:J:983:THR:HG23 | 2.16 | 0.46 |
| 1:J:3100:SER:OG | 1:J:3164:SER:HB2 | 2.16 | 0.46 |
| 1:J:3150:HIS:HB3 | 1:J:3152:PHE:CD2 | 2.51 | 0.46 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:J:3271:GLU:HG2 | 1:J:3334:TRP:CD1 | 2.51 | 0.46 |
| 1:J:3319:ILE:O | 1:J:3323:ILE:HG13 | 2.16 | 0.46 |
| 1:J:4086:GLY:C | 1:J:4087:LEU:HD23 | 2.40 | 0.46 |
| 1:J:4986:ALA:O | 1:J:4989:MET:N | 2.49 | 0.46 |
| 1:J:5013:MET:HE1 | 1:J:5020:ASP:HB3 | 1.96 | 0.46 |
| 2:K:7:SER:O | 2:K:121:THR:HG21 | 2.16 | 0.46 |
| 1:A:902:ARG:H | 1:A:904:HIS:CE1 | 2.34 | 0.45 |
| 1:A:1651:LEU:HD23 | 1:A:1702:HIS:HB2 | 1.98 | 0.45 |
| 1:A:2293:GLN:HA | 1:A:2296:GLU:HB3 | 1.98 | 0.45 |
| 1:A:2582:MET:SD | 1:A:2610:LEU:HD21 | 2.56 | 0.45 |
| 1:A:2816:MET:SD | 1:A:2937:VAL:HG21 | 2.56 | 0.45 |
| 1:A:2991:HIS:O | 1:A:2995:ILE:HG13 | 2.15 | 0.45 |
| 8:A:5110:POV:H13A | 8:A:5111:POV:H14A | 1.98 | 0.45 |
| 1:C:76:ARG:O | 1:C:79:GLN:HG3 | 2.16 | 0.45 |
| 1:C:887:ILE:HG12 | 1:C:960:MET:HE1 | 1.98 | 0.45 |
| 1:C:981:GLN:O | 1:C:985:VAL:HG23 | 2.16 | 0.45 |
| 1:C:2316:LYS:HE3 | 1:C:2318:TYR:HE1 | 1.81 | 0.45 |
| 1:C:2865:VAL:HG13 | 1:C:2928:LYS:HD2 | 1.98 | 0.45 |
| 1:C:2867:LEU:HG | 1:C:2868:SER:H | 1.81 | 0.45 |
| 1:C:3342:ALA:O | 1:C:3345:ILE:HG22 | 2.16 | 0.45 |
| 1:C:4086:GLY:C | 1:C:4087:LEU:HD23 | 2.40 | 0.45 |
| 1:C:4922:PHE:CE2 | 8:G:5111:POV:H29 | 2.50 | 0.45 |
| 3:E:23:VAL:HG12 | 3:E:104:LEU:HD21 | 1.97 | 0.45 |
| 1:G:663:TYR:CE1 | 1:G:745:SER:HB3 | 2.51 | 0.45 |
| 1:G:897:ARG:NH1 | 1:G:898:ASP:H | 2.14 | 0.45 |
| 1:G:2758:PHE:O | 1:G:2762:THR:HG23 | 2.16 | 0.45 |
| 1:G:3948:LYS:HE2 | 1:G:4009:GLN:HG2 | 1.97 | 0.45 |
| 1:J:178:ARG:HB2 | 1:J:193:ALA:HB1 | 1.98 | 0.45 |
| 1:J:867:LEU:HD12 | 1:J:929:LEU:HD12 | 1.98 | 0.45 |
| 1:J:1155:LEU:HA | 1:J:1155:LEU:HD23 | 1.85 | 0.45 |
| 1:J:2124:LEU:HD23 | 1:J:2124:LEU:HA | 1.79 | 0.45 |
| 1:J:2206:THR:O | 1:J:2210:VAL:HG23 | 2.16 | 0.45 |
| 1:J:2526:PHE:HD2 | 1:J:2558:VAL:HG13 | 1.81 | 0.45 |
| 1:J:4104:THR:O | 1:J:4108:ILE:HG13 | 2.16 | 0.45 |
| 1:J:4980:LEU:HD13 | 1:J:4980:LEU:HA | 1.83 | 0.45 |
| 1:A:2768:PHE:HA | 1:A:2771:ILE:HG12 | 1.98 | 0.45 |
| 1:A:3010:PHE:HE1 | 1:A:3074:SER:HB2 | 1.82 | 0.45 |
| 1:A:3137:LEU:HB3 | 1:A:3138:PRO:HD3 | 1.97 | 0.45 |
| 2:B:51:ILE:HG22 | 2:B:57:ILE:HA | 1.99 | 0.45 |
| 1:C:667:MET:SD | 1:C:743:VAL:HG22 | 2.56 | 0.45 |
| 1:C:1737:PRO:HG2 | 1:C:1769:THR:HG22 | 1.98 | 0.45 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:2526:PHE:CD2 | 1:C:2558:VAL:HG13 | 2.52 | 0.45 |
| 1:C:2891:LYS:HD3 | 1:C:2905:LEU:HD11 | 1.97 | 0.45 |
| 1:C:3150:HIS:HB3 | 1:C:3152:PHE:CD2 | 2.51 | 0.45 |
| 1:C:3754:GLU:HB2 | 1:C:4718:LYS:HG3 | 1.97 | 0.45 |
| 1:C:4190:ILE:HD12 | 1:C:4190:ILE:H | 1.81 | 0.45 |
| 1:C:4222:VAL:HG11 | 1:C:4950:VAL:HA | 1.98 | 0.45 |
| 1:C:4816:ILE:O | 1:C:4820:VAL:HG22 | 2.16 | 0.45 |
| 1:G:364:PRO:HA | 1:G:367:LEU:HG | 1.97 | 0.45 |
| 1:G:629:ARG:HB2 | 3:I:34:LYS:HD3 | 1.98 | 0.45 |
| 1:G:3271:GLU:HG2 | 1:G:3334:TRP:CD1 | 2.51 | 0.45 |
| 1:G:3566:SER:HB3 | 1:G:3569:LEU:HB2 | 1.98 | 0.45 |
| 2:H:96:ASN:OD1 | 2:H:117:TRP:HA | 2.16 | 0.45 |
| 1:J:1808:ARG:O | 1:J:1812:LEU:HD23 | 2.15 | 0.45 |
| 1:J:3180:ASN:HD22 | 1:J:3182:TYR:HD2 | 1.64 | 0.45 |
| 1:J:3252:ASP:O | 1:J:3256:LEU:HG | 2.15 | 0.45 |
| 1:J:3532:LEU:HD11 | 1:J:3560:GLN:HG2 | 1.98 | 0.45 |
| 1:J:4696:ASP:O | 1:J:4700:GLN:HG2 | 2.17 | 0.45 |
| 1:A:1965:TYR:CE2 | 1:A:2031:LEU:HD12 | 2.52 | 0.45 |
| 1:A:2591:ARG:HG2 | 1:A:2591:ARG:HH11 | 1.81 | 0.45 |
| 1:A:2817:ILE:HB | 1:A:2823:ILE:HG22 | 1.98 | 0.45 |
| 1:A:2960:LEU:HB2 | 1:A:3038:MET:HE1 | 1.98 | 0.45 |
| 1:A:3100:SER:OG | 1:A:3164:SER:HB2 | 2.16 | 0.45 |
| 1:A:3180:ASN:HD22 | 1:A:3182:TYR:HD2 | 1.64 | 0.45 |
| 8:A:5116:POV:H211 | 8:A:5117:POV:H31B | 1.98 | 0.45 |
| 1:C:224:HIS:CD2 | 1:C:231:LEU:HB2 | 2.51 | 0.45 |
| 1:C:3319:ILE:HA | 1:C:3322:ILE:HG12 | 1.99 | 0.45 |
| 1:G:224:HIS:CD2 | 1:G:231:LEU:HB2 | 2.51 | 0.45 |
| 1:G:1237:TRP:CH2 | 1:G:1652:GLU:HG3 | 2.52 | 0.45 |
| 1:G:2816:MET:SD | 1:G:2937:VAL:HG21 | 2.56 | 0.45 |
| 1:G:3531:ASP:O | 1:G:3534:MET:HG2 | 2.16 | 0.45 |
| 1:G:4922:PHE:CE2 | 8:J:5115:POV:H29 | 2.51 | 0.45 |
| 1:G:4986:ALA:O | 1:G:4989:MET:N | 2.49 | 0.45 |
| 1:J:365:LYS:HE3 | 1:J:365:LYS:HB3 | 1.82 | 0.45 |
| 1:J:1269:CYS:HA | 1:J:1564:PHE:O | 2.17 | 0.45 |
| 1:J:3416:VAL:O | 1:J:3420:ARG:HB2 | 2.16 | 0.45 |
| 1:J:4182:GLU:OE2 | 1:J:4982:GLU:HG3 | 2.16 | 0.45 |
| 1:A:4696:ASP:O | 1:A:4700:GLN:HG2 | 2.16 | 0.45 |
| 1:C:2526:PHE:HD2 | 1:C:2558:VAL:HG13 | 1.81 | 0.45 |
| 1:C:2765:LYS:HA | 1:C:2768:PHE:HB3 | 1.97 | 0.45 |
| 1:C:2768:PHE:HA | 1:C:2771:ILE:HG12 | 1.98 | 0.45 |
| 1:C:3416:VAL:O | 1:C:3420:ARG:HB2 | 2.16 | 0.45 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:4858:PHE:HE1 | 8:C:5119:POV:H2 | 1.81 | 0.45 |
| 1:G:76:ARG:O | 1:G:79:GLN:HG3 | 2.16 | 0.45 |
| 1:G:979:PRO:O | 1:G:983:THR:HG23 | 2.16 | 0.45 |
| 1:G:1944:GLU:HB2 | 1:G:2123:LEU:HD11 | 1.99 | 0.45 |
| 1:G:2526:PHE:CD2 | 1:G:2558:VAL:HG13 | 2.51 | 0.45 |
| 1:G:2582:MET:SD | 1:G:2610:LEU:HD21 | 2.56 | 0.45 |
| 1:G:4725:LEU:HD11 | 1:G:4734:ARG:HG3 | 1.99 | 0.45 |
| 8:G:5110:POV:H31D | 8:G:5110:POV:H21C | 1.98 | 0.45 |
| 2:H:7:SER:O | 2:H:121:THR:HG21 | 2.16 | 0.45 |
| 1:J:470:SER:HA | 1:J:473:ASN:ND2 | 2.31 | 0.45 |
| 1:J:897:ARG:CZ | 1:J:898:ASP:H | 2.30 | 0.45 |
| 1:J:1020:ARG:HB3 | 1:J:1031:THR:HG21 | 1.99 | 0.45 |
| 1:J:2591:ARG:HG2 | 1:J:2591:ARG:HH11 | 1.82 | 0.45 |
| 1:J:4026:MET:HE3 | 1:J:4026:MET:HB3 | 1.87 | 0.45 |
| 1:A:172:VAL:HB | 1:A:179:TYR:CD2 | 2.51 | 0.45 |
| 1:A:224:HIS:CD2 | 1:A:231:LEU:HB2 | 2.51 | 0.45 |
| 1:A:897:ARG:CZ | 1:A:898:ASP:H | 2.30 | 0.45 |
| 1:A:4820:VAL:HG23 | 1:A:4823:LEU:HB2 | 1.98 | 0.45 |
| 1:C:78:LEU:O | 1:C:81:MET:HG3 | 2.17 | 0.45 |
| 1:C:470:SER:HA | 1:C:473:ASN:ND2 | 2.31 | 0.45 |
| 1:C:803:LEU:HD12 | 1:C:804:PRO:HD2 | 1.99 | 0.45 |
| 1:C:882:TRP:CZ3 | 1:C:886:ARG:HD3 | 2.52 | 0.45 |
| 1:C:1235:THR:HG21 | 1:C:1607:ARG:HH21 | 1.82 | 0.45 |
| 1:C:2333:ASP:HA | 1:C:2336:ARG:HE | 1.81 | 0.45 |
| 1:C:2960:LEU:HB2 | 1:C:3038:MET:HE1 | 1.98 | 0.45 |
| 1:C:3508:SER:HB3 | 1:C:3511:VAL:HG22 | 1.99 | 0.45 |
| 1:C:4581:LYS:HE2 | 1:C:4581:LYS:HB2 | 1.66 | 0.45 |
| 2:D:7:SER:O | 2:D:121:THR:HG21 | 2.16 | 0.45 |
| 1:G:882:TRP:CZ3 | 1:G:886:ARG:HD3 | 2.52 | 0.45 |
| 1:G:1269:CYS:HA | 1:G:1564:PHE:O | 2.17 | 0.45 |
| 1:G:2765:LYS:HA | 1:G:2768:PHE:HB3 | 1.97 | 0.45 |
| 1:G:2768:PHE:HA | 1:G:2771:ILE:HG12 | 1.98 | 0.45 |
| 1:G:3342:ALA:O | 1:G:3345:ILE:HG22 | 2.16 | 0.45 |
| 1:G:3508:SER:HB3 | 1:G:3511:VAL:HG22 | 1.99 | 0.45 |
| 1:G:4814:LEU:O | 1:G:4818:MET:HG2 | 2.17 | 0.45 |
| 1:J:1569:GLN:H | 1:J:1572:ILE:HB | 1.81 | 0.45 |
| 1:A:1569:GLN:H | 1:A:1572:ILE:HB | 1.81 | 0.45 |
| 1:A:2530:MET:HB3 | 1:A:2589:LEU:HD11 | 1.98 | 0.45 |
| 1:A:2963:LEU:O | 1:A:2967:MET:HB2 | 2.17 | 0.45 |
| 1:A:4026:MET:HE3 | 1:A:4026:MET:HB3 | 1.87 | 0.45 |
| 1:A:4245:MET:HE2 | 1:A:4245:MET:HB3 | 1.81 | 0.45 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 8:A:5116:POV:H36 | 8:A:5116:POV:H39A | 1.79 | 0.45 |
| 1:C:22:LEU:HB2 | 1:C:37:LEU:CD2 | 2.46 | 0.45 |
| 1:C:902:ARG:H | 1:C:904:HIS:CE1 | 2.34 | 0.45 |
| 1:C:996:TRP:HB2 | 2:D:114:TYR:CE1 | 2.52 | 0.45 |
| 1:C:1269:CYS:HA | 1:C:1564:PHE:O | 2.17 | 0.45 |
| 1:C:1569:GLN:H | 1:C:1572:ILE:HB | 1.81 | 0.45 |
| 1:C:2963:LEU:O | 1:C:2967:MET:HB2 | 2.17 | 0.45 |
| 1:C:3137:LEU:HB3 | 1:C:3138:PRO:HD3 | 1.98 | 0.45 |
| 1:C:3271:GLU:HG2 | 1:C:3334:TRP:CD1 | 2.51 | 0.45 |
| 1:C:5011:TRP:O | 1:C:5015:GLN:HG2 | 2.17 | 0.45 |
| 8:C:5110:POV:H21C | 8:C:5110:POV:H31D | 1.98 | 0.45 |
| 1:G:867:LEU:HD12 | 1:G:929:LEU:HD12 | 1.98 | 0.45 |
| 1:G:1651:LEU:HD23 | 1:G:1702:HIS:HB2 | 1.98 | 0.45 |
| 1:G:1737:PRO:HG2 | 1:G:1769:THR:HG22 | 1.98 | 0.45 |
| 1:G:2454:ARG:HD2 | 1:G:2458:ARG:HH21 | 1.81 | 0.45 |
| 1:G:2591:ARG:HG2 | 1:G:2591:ARG:HH11 | 1.82 | 0.45 |
| 1:G:2865:VAL:HG13 | 1:G:2928:LYS:HD2 | 1.98 | 0.45 |
| 1:G:3319:ILE:HA | 1:G:3322:ILE:HG12 | 1.99 | 0.45 |
| 1:G:4640:GLU:HB2 | 1:G:4641:PRO:HD3 | 1.99 | 0.45 |
| 1:G:5011:TRP:O | 1:G:5015:GLN:HG2 | 2.17 | 0.45 |
| 3:I:98:ILE:HD13 | 3:I:98:ILE:HG21 | 1.65 | 0.45 |
| 1:J:184:THR:HA | 1:J:189:LEU:HD22 | 1.97 | 0.45 |
| 1:J:667:MET:SD | 1:J:743:VAL:HG22 | 2.57 | 0.45 |
| 1:J:1237:TRP:CH2 | 1:J:1652:GLU:HG3 | 2.52 | 0.45 |
| 1:J:1965:TYR:CE2 | 1:J:2031:LEU:HD12 | 2.52 | 0.45 |
| 1:J:2817:ILE:HB | 1:J:2823:ILE:HG22 | 1.98 | 0.45 |
| 1:J:3342:ALA:O | 1:J:3345:ILE:HG22 | 2.16 | 0.45 |
| 1:J:3722:TYR:OH | 1:J:3782:MET:HG3 | 2.16 | 0.45 |
| 8:J:5114:POV:H21C | 8:J:5114:POV:H31D | 1.98 | 0.45 |
| 1:A:184:THR:HA | 1:A:189:LEU:HD22 | 1.98 | 0.45 |
| 1:A:629:ARG:HB2 | 3:F:34:LYS:HD3 | 1.98 | 0.45 |
| 1:A:979:PRO:O | 1:A:983:THR:HG23 | 2.16 | 0.45 |
| 1:A:2463:LEU:O | 1:A:2467:VAL:HG12 | 2.17 | 0.45 |
| 1:A:2526:PHE:CD2 | 1:A:2558:VAL:HG13 | 2.52 | 0.45 |
| 1:C:364:PRO:HA | 1:C:367:LEU:HG | 1.98 | 0.45 |
| 1:C:1496:TRP:HB3 | 1:C:1499:ASP:OD1 | 2.16 | 0.45 |
| 1:C:1931:LEU:HD22 | 1:C:1935:VAL:HG11 | 1.99 | 0.45 |
| 1:C:2591:ARG:HH11 | 1:C:2591:ARG:HG2 | 1.82 | 0.45 |
| 1:C:4725:LEU:HD11 | 1:C:4734:ARG:HG3 | 1.99 | 0.45 |
| 1:C:4968:PHE:HD2 | 1:C:4975:PHE:HD1 | 1.64 | 0.45 |
| 1:G:1272:LEU:HG | 1:G:1289:LEU:HD11 | 1.99 | 0.45 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:G:2891:LYS:HD3 | 1:G:2905:LEU:HD11 | 1.97 | 0.45 |
| 1:G:4820:VAL:HG23 | 1:G:4823:LEU:HB2 | 1.97 | 0.45 |
| 1:G:4858:PHE:HE1 | 8:G:5119:POV:H2 | 1.82 | 0.45 |
| 3:I:77:THR:C | 3:I:79:ASP:H | 2.25 | 0.45 |
| 1:J:224:HIS:CD2 | 1:J:231:LEU:HB2 | 2.51 | 0.45 |
| 1:J:908:VAL:CA | 1:J:963:ASN:HA | 2.42 | 0.45 |
| 1:J:1723:ALA:HB1 | 1:J:1775:HIS:ND1 | 2.32 | 0.45 |
| 1:J:2526:PHE:CD2 | 1:J:2558:VAL:HG13 | 2.52 | 0.45 |
| 1:J:2765:LYS:HA | 1:J:2768:PHE:HB3 | 1.97 | 0.45 |
| 1:J:4968:PHE:HD2 | 1:J:4975:PHE:HD1 | 1.64 | 0.45 |
| 1:A:76:ARG:O | 1:A:79:GLN:HG3 | 2.16 | 0.45 |
| 1:A:470:SER:HA | 1:A:473:ASN:ND2 | 2.31 | 0.45 |
| 1:A:2624:ARG:NH2 | 1:A:2625:ARG:HH12 | 2.14 | 0.45 |
| 1:C:1237:TRP:CH2 | 1:C:1652:GLU:HG3 | 2.52 | 0.45 |
| 1:C:2102:VAL:HG11 | 1:C:2124:LEU:HG | 1.99 | 0.45 |
| 1:C:2229:VAL:HA | 1:C:2232:CYS:SG | 2.55 | 0.45 |
| 1:C:4983:HIS:O | 5:C:5105:ATP:N6 | 2.50 | 0.45 |
| 1:G:4104:THR:O | 1:G:4108:ILE:HG13 | 2.16 | 0.45 |
| 1:G:4190:ILE:H | 1:G:4190:ILE:HD12 | 1.81 | 0.45 |
| 1:J:981:GLN:O | 1:J:985:VAL:HG23 | 2.16 | 0.45 |
| 1:J:2512:ILE:HA | 1:J:2517:PHE:CE2 | 2.52 | 0.45 |
| 1:J:2530:MET:HB3 | 1:J:2589:LEU:HD11 | 1.98 | 0.45 |
| 1:J:3137:LEU:HB3 | 1:J:3138:PRO:HD3 | 1.97 | 0.45 |
| 1:J:3568:SER:HA | 1:J:3571:TRP:NE1 | 2.32 | 0.45 |
| 1:J:4640:GLU:HB2 | 1:J:4641:PRO:HD3 | 1.99 | 0.45 |
| 1:J:4794:TRP:NE1 | 8:J:5119:POV:H37A | 2.30 | 0.45 |
| 8:J:5116:POV:H1 | 8:J:5117:POV:O13 | 2.17 | 0.45 |
| 1:A:897:ARG:NH1 | 1:A:898:ASP:H | 2.14 | 0.45 |
| 1:A:1020:ARG:HB3 | 1:A:1031:THR:HG21 | 1.99 | 0.45 |
| 1:A:3342:ALA:O | 1:A:3345:ILE:HG22 | 2.16 | 0.45 |
| 1:A:4818:MET:HB3 | 8:A:5112:POV:H13A | 1.97 | 0.45 |
| 1:A:4968:PHE:HD2 | 1:A:4975:PHE:HD1 | 1.65 | 0.45 |
| 2:B:92:VAL:HG22 | 2:B:122:GLN:HB2 | 1.99 | 0.45 |
| 1:C:13:PHE:HE1 | 1:C:15:ARG:HH21 | 1.65 | 0.45 |
| 1:G:897:ARG:CZ | 1:G:898:ASP:H | 2.30 | 0.45 |
| 1:G:902:ARG:H | 1:G:904:HIS:CE1 | 2.34 | 0.45 |
| 1:G:2960:LEU:HB2 | 1:G:3038:MET:HE1 | 1.98 | 0.45 |
| 1:G:3416:VAL:O | 1:G:3420:ARG:HB2 | 2.16 | 0.45 |
| 3:I:77:THR:C | 3:I:79:ASP:N | 2.74 | 0.45 |
| 1:J:598:LYS:HE3 | 1:J:598:LYS:HB3 | 1.80 | 0.45 |
| 1:J:747:CYS:SG | 1:J:805:PRO:HG2 | 2.56 | 0.45 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:J:882:TRP:CZ3 | 1:J:886:ARG:HD3 | 2.52 | 0.45 |
| 1:J:2316:LYS:HE3 | 1:J:2318:TYR:HE1 | 1.81 | 0.45 |
| 1:J:2624:ARG:NH2 | 1:J:2625:ARG:HH12 | 2.14 | 0.45 |
| 1:J:2764:GLU:HG2 | 1:J:2855:TYR:CD1 | 2.52 | 0.45 |
| 1:J:4190:ILE:H | 1:J:4190:ILE:HD12 | 1.81 | 0.45 |
| 1:A:1237:TRP:CH2 | 1:A:1652:GLU:HG3 | 2.52 | 0.45 |
| 1:A:1738:LEU:HD11 | 1:A:1963:GLU:HB2 | 1.99 | 0.45 |
| 1:A:1944:GLU:HB2 | 1:A:2123:LEU:HD11 | 1.99 | 0.45 |
| 1:A:4816:ILE:O | 1:A:4820:VAL:HG22 | 2.16 | 0.45 |
| 1:C:2764:GLU:HG2 | 1:C:2855:TYR:CD1 | 2.52 | 0.45 |
| 1:C:4897:ILE:HG13 | 1:C:4901:ILE:HG23 | 1.99 | 0.45 |
| 3:E:56:ILE:HG12 | 3:E:81:ALA:HA | 1.98 | 0.45 |
| 3:F:45:PRO:O | 3:F:47:LYS:HE2 | 2.17 | 0.45 |
| 1:G:3335:MET:HA | 1:G:3335:MET:HE3 | 1.99 | 0.45 |
| 1:G:3440:GLU:HG3 | 1:G:3443:ILE:HD11 | 2.00 | 0.45 |
| 1:J:663:TYR:CE1 | 1:J:745:SER:HB3 | 2.51 | 0.45 |
| 1:J:3440:GLU:HG3 | 1:J:3443:ILE:HD11 | 1.99 | 0.45 |
| 1:J:4814:LEU:O | 1:J:4818:MET:HG2 | 2.17 | 0.45 |
| 1:J:4897:ILE:HG13 | 1:J:4901:ILE:HG23 | 1.99 | 0.45 |
| 1:A:13:PHE:HE1 | 1:A:15:ARG:HH21 | 1.65 | 0.44 |
| 1:A:1703:LEU:HD23 | 1:A:1708:ARG:HG2 | 1.99 | 0.44 |
| 1:A:2764:GLU:HG2 | 1:A:2855:TYR:CD1 | 2.52 | 0.44 |
| 1:A:2863:SER:HA | 1:A:2928:LYS:HB2 | 1.99 | 0.44 |
| 1:A:4814:LEU:O | 1:A:4818:MET:HG2 | 2.17 | 0.44 |
| 2:B:7:SER:O | 2:B:121:THR:HG21 | 2.16 | 0.44 |
| 1:C:629:ARG:HB2 | 3:E:34:LYS:HD3 | 1.98 | 0.44 |
| 1:C:1427:ILE:HD12 | 1:C:1587:PRO:HB3 | 1.99 | 0.44 |
| 1:C:1651:LEU:HD23 | 1:C:1702:HIS:HB2 | 1.98 | 0.44 |
| 1:C:4696:ASP:O | 1:C:4700:GLN:HG2 | 2.16 | 0.44 |
| 1:C:4840:THR:HA | 1:G:4823:LEU:HD21 | 1.99 | 0.44 |
| 1:C:4956:THR:O | 1:C:4965:SER:N | 2.48 | 0.44 |
| 1:G:2293:GLN:HA | 1:G:2296:GLU:HB3 | 1.98 | 0.44 |
| 1:J:902:ARG:H | 1:J:904:HIS:CE1 | 2.34 | 0.44 |
| 1:J:1272:LEU:HG | 1:J:1289:LEU:HD11 | 1.99 | 0.44 |
| 1:J:2488:PRO:HG2 | 1:J:2546:MET:SD | 2.57 | 0.44 |
| 1:J:2865:VAL:HG13 | 1:J:2928:LYS:HD2 | 1.98 | 0.44 |
| 1:J:2963:LEU:O | 1:J:2967:MET:HB2 | 2.17 | 0.44 |
| 1:J:4844:LEU:HD11 | 1:J:4924:VAL:HG13 | 1.99 | 0.44 |
| 1:A:867:LEU:HD12 | 1:A:929:LEU:HD12 | 1.98 | 0.44 |
| 1:A:1723:ALA:HB1 | 1:A:1775:HIS:ND1 | 2.32 | 0.44 |
| 1:A:2102:VAL:HG11 | 1:A:2124:LEU:HG | 1.99 | 0.44 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:3335:MET:HA | 1:A:3335:MET:HE3 | 1.98 | 0.44 |
| 1:A:3440:GLU:HG3 | 1:A:3443:ILE:HD11 | 1.99 | 0.44 |
| 1:A:3955:MET:HB2 | 1:A:4019:LEU:HD22 | 1.99 | 0.44 |
| 1:C:1944:GLU:HB2 | 1:C:2123:LEU:HD11 | 1.99 | 0.44 |
| 1:C:2863:SER:HA | 1:C:2928:LYS:HB2 | 2.00 | 0.44 |
| 1:C:3512:ALA:O | 1:C:3516:LYS:HG2 | 2.17 | 0.44 |
| 1:C:4814:LEU:O | 1:C:4818:MET:HG2 | 2.17 | 0.44 |
| 8:C:5110:POV:H3A | 8:C:5110:POV:H23A | 1.99 | 0.44 |
| 1:G:2102:VAL:HG11 | 1:G:2124:LEU:HG | 1.99 | 0.44 |
| 1:G:2512:ILE:HD13 | 1:G:2517:PHE:CE2 | 2.52 | 0.44 |
| 1:G:3010:PHE:HB3 | 1:G:3070:ILE:HG22 | 1.99 | 0.44 |
| 1:J:2463:LEU:O | 1:J:2467:VAL:HG12 | 2.17 | 0.44 |
| 1:J:2582:MET:SD | 1:J:2610:LEU:HD21 | 2.56 | 0.44 |
| 1:J:3508:SER:HB3 | 1:J:3511:VAL:HG22 | 1.99 | 0.44 |
| 1:J:4983:HIS:O | 5:J:5109:ATP:N6 | 2.51 | 0.44 |
| 1:J:5011:TRP:O | 1:J:5015:GLN:HG2 | 2.17 | 0.44 |
| 1:A:1235:THR:HG21 | 1:A:1607:ARG:HH21 | 1.82 | 0.44 |
| 1:A:1931:LEU:HD22 | 1:A:1935:VAL:HG11 | 1.99 | 0.44 |
| 1:A:2206:THR:O | 1:A:2210:VAL:HG23 | 2.16 | 0.44 |
| 1:A:2816:MET:O | 1:A:2821:TRP:HB2 | 2.18 | 0.44 |
| 1:A:2865:VAL:HG13 | 1:A:2928:LYS:HD2 | 1.98 | 0.44 |
| 1:A:4640:GLU:HB2 | 1:A:4641:PRO:HD3 | 1.99 | 0.44 |
| 1:A:4958:CYS:HA | 5:A:5102:ATP:N7 | 2.31 | 0.44 |
| 8:A:5111:POV:H33 | 8:A:5112:POV:H35 | 2.00 | 0.44 |
| 1:C:897:ARG:CZ | 1:C:898:ASP:H | 2.30 | 0.44 |
| 1:C:1703:LEU:HD23 | 1:C:1708:ARG:HG2 | 1.99 | 0.44 |
| 1:C:1723:ALA:HB1 | 1:C:1775:HIS:ND1 | 2.32 | 0.44 |
| 1:C:2111:VAL:HG23 | 1:C:2117:VAL:HG22 | 2.00 | 0.44 |
| 1:C:2293:GLN:HA | 1:C:2296:GLU:HB3 | 1.98 | 0.44 |
| 1:C:3010:PHE:HE2 | 1:C:3071:LEU:HD13 | 1.83 | 0.44 |
| 1:G:981:GLN:O | 1:G:985:VAL:HG23 | 2.16 | 0.44 |
| 1:G:1965:TYR:CE2 | 1:G:2031:LEU:HD12 | 2.52 | 0.44 |
| 1:G:2530:MET:HB3 | 1:G:2589:LEU:HD11 | 1.98 | 0.44 |
| 1:G:3180:ASN:HD22 | 1:G:3182:TYR:HD2 | 1.64 | 0.44 |
| 1:G:3568:SER:HA | 1:G:3571:TRP:NE1 | 2.32 | 0.44 |
| 1:G:4681:LEU:HD21 | 1:G:4687:TYR:HD2 | 1.83 | 0.44 |
| 8:G:5110:POV:H3A | 8:G:5110:POV:H23A | 1.99 | 0.44 |
| 1:J:1703:LEU:HD23 | 1:J:1708:ARG:HG2 | 1.99 | 0.44 |
| 1:J:1737:PRO:HG2 | 1:J:1769:THR:HG22 | 1.98 | 0.44 |
| 1:J:2293:GLN:O | 1:J:2297:LYS:HG3 | 2.18 | 0.44 |
| 1:J:2626:LEU:HD21 | 1:J:2640:PRO:HB3 | 2.00 | 0.44 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:J:3319:ILE:HA | 1:J:3322:ILE:HG12 | 1.99 | 0.44 |
| 1:J:4681:LEU:HD21 | 1:J:4687:TYR:HD2 | 1.83 | 0.44 |
| 2:K:92:VAL:HG22 | 2:K:122:GLN:HB2 | 1.99 | 0.44 |
| 1:A:1269:CYS:HA | 1:A:1564:PHE:O | 2.17 | 0.44 |
| 1:A:2488:PRO:HG2 | 1:A:2546:MET:SD | 2.57 | 0.44 |
| 1:A:3196:ARG:HD3 | 1:A:3196:ARG:HA | 1.79 | 0.44 |
| 1:A:4844:LEU:HD11 | 1:A:4924:VAL:HG13 | 1.99 | 0.44 |
| 1:A:4858:PHE:HE1 | 8:A:5116:POV:H2 | 1.81 | 0.44 |
| 1:C:1867:GLU:HG2 | 1:C:2097:LEU:HD11 | 2.00 | 0.44 |
| 1:C:2626:LEU:HD21 | 1:C:2640:PRO:HB3 | 2.00 | 0.44 |
| 1:C:3010:PHE:HB3 | 1:C:3070:ILE:HG22 | 1.99 | 0.44 |
| 1:C:3068:LEU:HA | 1:C:3071:LEU:HB2 | 1.98 | 0.44 |
| 1:C:3232:LEU:HD13 | 1:C:3233:PRO:HD2 | 2.00 | 0.44 |
| 1:C:3731:LYS:HD3 | 1:C:3734:HIS:CE1 | 2.53 | 0.44 |
| 1:C:4844:LEU:HD11 | 1:C:4924:VAL:HG13 | 1.99 | 0.44 |
| 1:C:5013:MET:HE3 | 1:C:5013:MET:HB3 | 1.77 | 0.44 |
| 8:C:5114:POV:H33 | 8:C:5115:POV:H35 | 2.00 | 0.44 |
| 1:G:13:PHE:HE1 | 1:G:15:ARG:HH21 | 1.65 | 0.44 |
| 1:G:2463:LEU:HA | 1:G:2466:LEU:HD12 | 1.98 | 0.44 |
| 1:G:2816:MET:O | 1:G:2821:TRP:HB2 | 2.18 | 0.44 |
| 1:J:247:TYR:HH | 1:J:376:ALA:HA | 1.80 | 0.44 |
| 1:J:2886:TRP:CZ2 | 1:J:2890:LYS:HG2 | 2.53 | 0.44 |
| 1:J:3512:ALA:O | 1:J:3516:LYS:HG2 | 2.17 | 0.44 |
| 1:A:2233:CYS:SG | 1:A:2270:SER:CB | 3.05 | 0.44 |
| 1:A:2293:GLN:O | 1:A:2297:LYS:HG3 | 2.18 | 0.44 |
| 1:A:2512:ILE:HA | 1:A:2517:PHE:CE2 | 2.52 | 0.44 |
| 1:A:3075:LEU:HD23 | 1:A:3146:HIS:CE1 | 2.53 | 0.44 |
| 1:A:3232:LEU:HD13 | 1:A:3233:PRO:HD2 | 2.00 | 0.44 |
| 1:A:4681:LEU:HD21 | 1:A:4687:TYR:HD2 | 1.83 | 0.44 |
| 1:A:4823:LEU:HD21 | 1:J:4840:THR:HA | 1.99 | 0.44 |
| 1:C:3440:GLU:HG3 | 1:C:3443:ILE:HD11 | 1.99 | 0.44 |
| 1:C:4640:GLU:HB2 | 1:C:4641:PRO:HD3 | 1.99 | 0.44 |
| 2:D:51:ILE:HG22 | 2:D:57:ILE:HA | 1.98 | 0.44 |
| 2:D:92:VAL:HG22 | 2:D:122:GLN:HB2 | 1.99 | 0.44 |
| 1:G:232:THR:HG21 | 1:G:252:VAL:HG21 | 1.99 | 0.44 |
| 1:G:1427:ILE:HD12 | 1:G:1587:PRO:HB3 | 1.99 | 0.44 |
| 1:G:1665:HIS:CE1 | 1:G:1668:ARG:HH12 | 2.36 | 0.44 |
| 1:G:1867:GLU:HG2 | 1:G:2097:LEU:HD11 | 2.00 | 0.44 |
| 1:G:4794:TRP:NE1 | 8:G:5115:POV:H37A | 2.30 | 0.44 |
| 2:H:51:ILE:HG22 | 2:H:57:ILE:HA | 1.99 | 0.44 |
| 1:J:564:LEU:O | 1:J:568:LEU:HG | 2.18 | 0.44 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:J:926:GLY:O | 1:J:930:LYS:HG3 | 2.18 | 0.44 |
| 1:J:1235:THR:HG21 | 1:J:1607:ARG:HH21 | 1.82 | 0.44 |
| 1:J:2309:SER:HB2 | 1:J:2322:GLY:H | 1.82 | 0.44 |
| 1:J:2768:PHE:HA | 1:J:2771:ILE:HG12 | 1.98 | 0.44 |
| 1:J:4725:LEU:HD11 | 1:J:4734:ARG:HG3 | 1.99 | 0.44 |
| 2:K:52:THR:HG22 | 2:K:101:PRO:HB2 | 2.00 | 0.44 |
| 1:A:210:GLU:HB3 | 1:A:213:TYR:CD2 | 2.47 | 0.44 |
| 1:A:1074:ILE:O | 1:A:1238:PHE:HA | 2.18 | 0.44 |
| 1:A:1427:ILE:HD12 | 1:A:1587:PRO:HB3 | 1.99 | 0.44 |
| 1:A:2316:LYS:HE3 | 1:A:2318:TYR:HE1 | 1.81 | 0.44 |
| 1:A:3163:VAL:O | 1:A:3166:TYR:HB2 | 2.18 | 0.44 |
| 1:A:3319:ILE:HA | 1:A:3322:ILE:HG12 | 1.99 | 0.44 |
| 1:A:3439:GLY:O | 1:A:3443:ILE:HG23 | 2.18 | 0.44 |
| 1:A:4080:TYR:CE1 | 1:A:4095:LYS:HG3 | 2.53 | 0.44 |
| 1:A:4190:ILE:H | 1:A:4190:ILE:HD12 | 1.81 | 0.44 |
| 1:A:4725:LEU:HD11 | 1:A:4734:ARG:HG3 | 1.99 | 0.44 |
| 1:A:4927:ILE:HD11 | 1:C:4936:ILE:HD12 | 2.00 | 0.44 |
| 1:A:4936:ILE:HD12 | 1:J:4927:ILE:HD11 | 2.00 | 0.44 |
| 1:C:564:LEU:O | 1:C:568:LEU:HG | 2.18 | 0.44 |
| 1:C:897:ARG:NH1 | 1:C:898:ASP:H | 2.14 | 0.44 |
| 1:C:1020:ARG:HB3 | 1:C:1031:THR:HG21 | 1.98 | 0.44 |
| 1:C:1272:LEU:HG | 1:C:1289:LEU:HD11 | 1.99 | 0.44 |
| 1:C:2530:MET:HB3 | 1:C:2589:LEU:HD11 | 1.98 | 0.44 |
| 1:C:3533:ILE:HD13 | 1:C:3596:VAL:HG13 | 2.00 | 0.44 |
| 1:G:753:PRO:HB2 | 1:G:770:ALA:H | 1.83 | 0.44 |
| 1:G:877:ASN:O | 1:G:881:LEU:HG | 2.18 | 0.44 |
| 1:G:2886:TRP:CZ2 | 1:G:2890:LYS:HG2 | 2.53 | 0.44 |
| 1:G:4844:LEU:HD11 | 1:G:4924:VAL:HG13 | 1.99 | 0.44 |
| 1:J:462:GLU:H | 1:J:462:GLU:HG3 | 1.62 | 0.44 |
| 1:J:877:ASN:O | 1:J:881:LEU:HG | 2.18 | 0.44 |
| 1:J:1079:LYS:HA | 1:J:1189:LEU:HD11 | 2.00 | 0.44 |
| 1:J:1651:LEU:HD23 | 1:J:1702:HIS:HB2 | 1.98 | 0.44 |
| 1:J:2306:GLY:HA2 | 1:J:2323:TRP:CE3 | 2.52 | 0.44 |
| 1:J:3335:MET:HA | 1:J:3335:MET:HE3 | 1.98 | 0.44 |
| 1:J:4651:THR:HG23 | 8:J:5112:POV:H29 | 1.99 | 0.44 |
| 1:A:2886:TRP:CZ2 | 1:A:2890:LYS:HG2 | 2.53 | 0.44 |
| 1:A:3568:SER:HA | 1:A:3571:TRP:NE1 | 2.32 | 0.44 |
| 1:A:5011:TRP:O | 1:A:5015:GLN:HG2 | 2.17 | 0.44 |
| 1:C:926:GLY:O | 1:C:930:LYS:HG3 | 2.18 | 0.44 |
| 1:C:2980:VAL:HB | 1:C:2986:VAL:HG21 | 2.00 | 0.44 |
| 1:C:3166:TYR:OH | 1:C:3203:VAL:HG21 | 2.18 | 0.44 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:3335:MET:HA | 1:C:3335:MET:HE3 | 1.99 | 0.44 |
| 1:C:3439:GLY:O | 1:C:3443:ILE:HG23 | 2.18 | 0.44 |
| 1:C:4915:VAL:HG21 | 8:C:5122:POV:H36A | 2.00 | 0.44 |
| 1:C:4927:ILE:HD11 | 1:G:4936:ILE:HD12 | 2.00 | 0.44 |
| 1:G:1074:ILE:O | 1:G:1238:PHE:HA | 2.18 | 0.44 |
| 1:G:1723:ALA:HB1 | 1:G:1775:HIS:ND1 | 2.32 | 0.44 |
| 1:G:2382:GLU:O | 1:G:2386:ILE:HG12 | 2.18 | 0.44 |
| 1:G:2963:LEU:O | 1:G:2967:MET:HB2 | 2.17 | 0.44 |
| 1:G:3512:ALA:O | 1:G:3516:LYS:HG2 | 2.17 | 0.44 |
| 1:J:1944:GLU:HB2 | 1:J:2123:LEU:HD11 | 1.99 | 0.44 |
| 2:K:51:ILE:HG22 | 2:K:57:ILE:HA | 1.99 | 0.44 |
| 1:A:2382:GLU:O | 1:A:2386:ILE:HG12 | 2.18 | 0.44 |
| 1:A:2626:LEU:HD21 | 1:A:2640:PRO:HB3 | 2.00 | 0.44 |
| 1:A:3272:ILE:C | 1:A:3275:PRO:HD2 | 2.43 | 0.44 |
| 1:A:3508:SER:HB3 | 1:A:3511:VAL:HG22 | 1.99 | 0.44 |
| 1:A:4078:GLN:O | 1:A:4081:VAL:HG22 | 2.18 | 0.44 |
| 1:A:4651:THR:HG23 | 8:A:5105:POV:H29 | 1.99 | 0.44 |
| 1:A:4842:GLY:HA3 | 8:C:5103:POV:H21E | 2.00 | 0.44 |
| 1:C:1119:GLU:H | 1:C:1119:GLU:HG3 | 1.63 | 0.44 |
| 1:C:1471:ALA:HA | 1:C:1489:CYS:O | 2.18 | 0.44 |
| 1:C:2228:MET:HE3 | 1:C:2232:CYS:SG | 2.57 | 0.44 |
| 1:C:2502:MET:HE2 | 1:C:2502:MET:HB3 | 1.86 | 0.44 |
| 1:C:2886:TRP:CZ2 | 1:C:2890:LYS:HG2 | 2.53 | 0.44 |
| 1:C:3180:ASN:HD22 | 1:C:3182:TYR:HD2 | 1.64 | 0.44 |
| 1:C:3935:TRP:HZ3 | 1:C:3994:HIS:HE1 | 1.66 | 0.44 |
| 1:C:4080:TYR:CE1 | 1:C:4095:LYS:HG3 | 2.53 | 0.44 |
| 1:C:4995:LEU:HD22 | 1:C:5003:HIS:CD2 | 2.53 | 0.44 |
| 1:G:564:LEU:O | 1:G:568:LEU:HG | 2.18 | 0.44 |
| 1:G:1180:ARG:HD2 | 1:G:1180:ARG:N | 2.33 | 0.44 |
| 1:G:2867:LEU:HG | 1:G:2868:SER:H | 1.81 | 0.44 |
| 1:G:3272:ILE:C | 1:G:3275:PRO:HD2 | 2.43 | 0.44 |
| 1:G:4078:GLN:O | 1:G:4081:VAL:HG22 | 2.18 | 0.44 |
| 8:G:5117:POV:H11 | 8:G:5117:POV:H14B | 1.79 | 0.44 |
| 1:J:629:ARG:HB2 | 3:L:34:LYS:HD3 | 1.98 | 0.44 |
| 1:J:2816:MET:O | 1:J:2821:TRP:HB2 | 2.18 | 0.44 |
| 1:J:2914:LYS:H | 1:J:2914:LYS:HG3 | 1.68 | 0.44 |
| 1:J:3689:GLU:CD | 1:J:3689:GLU:H | 2.26 | 0.44 |
| 1:A:1527:MET:HE2 | 1:A:1527:MET:HB3 | 1.83 | 0.44 |
| 1:C:877:ASN:O | 1:C:881:LEU:HG | 2.18 | 0.44 |
| 1:C:2025:GLU:HA | 1:C:2028:ARG:HG2 | 2.00 | 0.44 |
| 1:C:2272:PRO:HA | 1:C:2275:VAL:CG2 | 2.42 | 0.44 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:2512:ILE:HA | 1:C:2517:PHE:CE2 | 2.52 | 0.44 |
| 1:C:3163:VAL:O | 1:C:3166:TYR:HB2 | 2.18 | 0.44 |
| 1:C:3955:MET:HB2 | 1:C:4019:LEU:HD22 | 1.99 | 0.44 |
| 1:G:365:LYS:O | 1:G:369:LEU:HG | 2.18 | 0.44 |
| 1:G:972:LEU:HD13 | 1:G:1044:ARG:NE | 2.33 | 0.44 |
| 1:G:1815:LEU:HD22 | 1:G:1845:VAL:HG21 | 2.00 | 0.44 |
| 1:G:1931:LEU:HD22 | 1:G:1935:VAL:HG11 | 1.99 | 0.44 |
| 1:G:2293:GLN:O | 1:G:2297:LYS:HG3 | 2.18 | 0.44 |
| 1:G:2626:LEU:HD21 | 1:G:2640:PRO:HB3 | 2.00 | 0.44 |
| 1:G:2956:ALA:O | 1:G:2960:LEU:HG | 2.18 | 0.44 |
| 1:G:3232:LEU:HD13 | 1:G:3233:PRO:HD2 | 2.00 | 0.44 |
| 1:G:3414:ARG:HH21 | 1:G:3475:LYS:HB2 | 1.83 | 0.44 |
| 1:G:3439:GLY:O | 1:G:3443:ILE:HG23 | 2.18 | 0.44 |
| 1:J:3272:ILE:C | 1:J:3275:PRO:HD2 | 2.43 | 0.44 |
| 1:A:232:THR:HG21 | 1:A:252:VAL:HG21 | 1.99 | 0.43 |
| 1:A:365:LYS:HE3 | 1:A:365:LYS:HB3 | 1.82 | 0.43 |
| 1:A:365:LYS:O | 1:A:369:LEU:HG | 2.18 | 0.43 |
| 1:A:637:LEU:HD23 | 1:A:637:LEU:HA | 1.76 | 0.43 |
| 1:A:877:ASN:O | 1:A:881:LEU:HG | 2.18 | 0.43 |
| 1:A:2956:ALA:O | 1:A:2960:LEU:HG | 2.18 | 0.43 |
| 1:A:3409:TYR:HB2 | 1:A:3509:LEU:HD21 | 2.00 | 0.43 |
| 1:A:4915:VAL:HG21 | 8:A:5119:POV:H36A | 2.00 | 0.43 |
| 1:C:2126:ARG:HG2 | 1:C:2127:GLN:NE2 | 2.33 | 0.43 |
| 1:C:2382:GLU:O | 1:C:2386:ILE:HG12 | 2.18 | 0.43 |
| 1:C:2588:ARG:HA | 1:C:2591:ARG:HH11 | 1.83 | 0.43 |
| 1:C:2816:MET:O | 1:C:2821:TRP:HB2 | 2.18 | 0.43 |
| 1:C:3272:ILE:C | 1:C:3275:PRO:HD2 | 2.43 | 0.43 |
| 1:G:908:VAL:CA | 1:G:963:ASN:HA | 2.43 | 0.43 |
| 1:G:1471:ALA:HA | 1:G:1489:CYS:O | 2.18 | 0.43 |
| 1:G:2502:MET:HE2 | 1:G:2502:MET:HB3 | 1.86 | 0.43 |
| 1:G:2764:GLU:HG2 | 1:G:2855:TYR:CD1 | 2.52 | 0.43 |
| 1:G:4080:TYR:CE1 | 1:G:4095:LYS:HG3 | 2.53 | 0.43 |
| 8:G:5114:POV:H33 | 8:G:5115:POV:H35 | 2.00 | 0.43 |
| 3:I:62:GLY:HA3 | 3:I:74:LEU:HD13 | 2.00 | 0.43 |
| 1:J:232:THR:HG21 | 1:J:252:VAL:HG21 | 1.99 | 0.43 |
| 1:J:753:PRO:HB2 | 1:J:770:ALA:H | 1.83 | 0.43 |
| 1:J:881:LEU:HD21 | 1:J:1041:GLN:HG2 | 2.00 | 0.43 |
| 1:J:3731:LYS:HD3 | 1:J:3734:HIS:CE1 | 2.53 | 0.43 |
| 8:J:5118:POV:H33 | 8:J:5119:POV:H35 | 2.00 | 0.43 |
| 2:K:28:ILE:H | 2:K:28:ILE:HG13 | 1.62 | 0.43 |
| 1:A:564:LEU:O | 1:A:568:LEU:HG | 2.18 | 0.43 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:882:TRP:CZ2 | 1:A:905:PRO:HD3 | 2.53 | 0.43 |
| 1:A:1471:ALA:HA | 1:A:1489:CYS:O | 2.18 | 0.43 |
| 1:A:1815:LEU:HD22 | 1:A:1845:VAL:HG21 | 2.00 | 0.43 |
| 1:A:2502:MET:HE2 | 1:A:2502:MET:HB3 | 1.86 | 0.43 |
| 1:A:3512:ALA:O | 1:A:3516:LYS:HG2 | 2.17 | 0.43 |
| 1:A:3689:GLU:H | 1:A:3689:GLU:CD | 2.26 | 0.43 |
| 1:C:1180:ARG:HD2 | 1:C:1180:ARG:N | 2.33 | 0.43 |
| 1:C:2339:VAL:HG21 | 1:C:2436:CYS:SG | 2.58 | 0.43 |
| 1:G:2126:ARG:HG2 | 1:G:2127:GLN:NE2 | 2.33 | 0.43 |
| 1:G:3166:TYR:OH | 1:G:3203:VAL:HG21 | 2.18 | 0.43 |
| 1:G:3731:LYS:HD3 | 1:G:3734:HIS:CE1 | 2.53 | 0.43 |
| 1:G:3935:TRP:HZ3 | 1:G:3994:HIS:HE1 | 1.66 | 0.43 |
| 1:G:3955:MET:HB2 | 1:G:4019:LEU:HD22 | 1.99 | 0.43 |
| 2:H:15:GLY:H | 2:H:85:LEU:H | 1.66 | 0.43 |
| 2:H:92:VAL:HG22 | 2:H:122:GLN:HB2 | 1.99 | 0.43 |
| 1:J:13:PHE:HE1 | 1:J:15:ARG:HH21 | 1.65 | 0.43 |
| 1:J:867:LEU:O | 1:J:871:ARG:HB3 | 2.19 | 0.43 |
| 1:J:1676:LEU:HD12 | 1:J:2167:ILE:HD12 | 2.00 | 0.43 |
| 1:J:1738:LEU:HD11 | 1:J:1963:GLU:HB2 | 1.99 | 0.43 |
| 1:J:2724:GLU:HB2 | 1:J:2738:ARG:HH22 | 1.84 | 0.43 |
| 1:J:2863:SER:HA | 1:J:2928:LYS:HB2 | 2.00 | 0.43 |
| 1:J:4995:LEU:HD22 | 1:J:5003:HIS:CD2 | 2.53 | 0.43 |
| 1:A:882:TRP:CZ3 | 1:A:886:ARG:HD3 | 2.52 | 0.43 |
| 1:A:1665:HIS:CE1 | 1:A:1668:ARG:HH12 | 2.36 | 0.43 |
| 1:A:1737:PRO:HG2 | 1:A:1769:THR:HG22 | 1.98 | 0.43 |
| 1:A:4822:THR:O | 1:A:4826:ILE:HG13 | 2.19 | 0.43 |
| 1:A:4897:ILE:HG13 | 1:A:4901:ILE:HG23 | 1.99 | 0.43 |
| 8:A:5107:POV:H3A | 8:A:5107:POV:H23A | 1.99 | 0.43 |
| 8:A:5122:POV:H21E | 1:J:4842:GLY:HA3 | 2.00 | 0.43 |
| 1:C:365:LYS:O | 1:C:369:LEU:HG | 2.18 | 0.43 |
| 1:C:1815:LEU:HD22 | 1:C:1845:VAL:HG21 | 2.00 | 0.43 |
| 1:C:2293:GLN:O | 1:C:2297:LYS:HG3 | 2.18 | 0.43 |
| 1:C:2490:MET:HA | 1:C:2490:MET:HE3 | 2.01 | 0.43 |
| 1:C:3568:SER:HA | 1:C:3571:TRP:NE1 | 2.32 | 0.43 |
| 1:C:4078:GLN:O | 1:C:4081:VAL:HG22 | 2.18 | 0.43 |
| 1:C:4850:LEU:O | 1:C:4853:VAL:HG22 | 2.18 | 0.43 |
| 1:G:1115:LEU:HG | 1:G:1123:VAL:HG11 | 2.00 | 0.43 |
| 1:G:1235:THR:HG21 | 1:G:1607:ARG:HH21 | 1.82 | 0.43 |
| 1:G:2025:GLU:HA | 1:G:2028:ARG:HG2 | 2.00 | 0.43 |
| 1:G:2339:VAL:HG21 | 1:G:2436:CYS:SG | 2.58 | 0.43 |
| 1:G:2490:MET:HA | 1:G:2490:MET:HE3 | 2.01 | 0.43 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:G:2559:LEU:O | 1:G:2563:THR:HG23 | 2.19 | 0.43 |
| 1:G:2863:SER:HA | 1:G:2928:LYS:HB2 | 2.00 | 0.43 |
| 1:G:3163:VAL:O | 1:G:3166:TYR:HB2 | 2.18 | 0.43 |
| 1:G:4850:LEU:O | 1:G:4853:VAL:HG22 | 2.19 | 0.43 |
| 1:J:882:TRP:CZ2 | 1:J:905:PRO:HD3 | 2.53 | 0.43 |
| 1:J:1427:ILE:HD12 | 1:J:1587:PRO:HB3 | 1.99 | 0.43 |
| 1:J:1815:LEU:HD22 | 1:J:1845:VAL:HG21 | 2.00 | 0.43 |
| 1:J:3163:VAL:O | 1:J:3166:TYR:HB2 | 2.18 | 0.43 |
| 1:A:1079:LYS:HA | 1:A:1189:LEU:HD11 | 2.00 | 0.43 |
| 1:A:2124:LEU:HD22 | 1:A:2128:TYR:HE1 | 1.84 | 0.43 |
| 1:A:4840:THR:HA | 1:C:4823:LEU:HD21 | 1.99 | 0.43 |
| 1:C:315:CYS:SG | 1:C:351:VAL:HG22 | 2.59 | 0.43 |
| 1:C:1444:GLU:HG3 | 1:C:1508:ARG:HH21 | 1.84 | 0.43 |
| 1:C:2259:GLU:H | 1:C:2259:GLU:HG2 | 1.68 | 0.43 |
| 1:C:3414:ARG:HH21 | 1:C:3475:LYS:HB2 | 1.83 | 0.43 |
| 1:C:3833:GLN:HA | 1:C:3836:MET:HE3 | 2.01 | 0.43 |
| 1:C:4822:THR:O | 1:C:4826:ILE:HG13 | 2.19 | 0.43 |
| 8:C:5119:POV:H39A | 8:C:5119:POV:H36 | 1.79 | 0.43 |
| 3:E:45:PRO:HB3 | 3:E:104:LEU:HD21 | 2.00 | 0.43 |
| 1:G:926:GLY:O | 1:G:930:LYS:HG3 | 2.18 | 0.43 |
| 1:G:2980:VAL:HB | 1:G:2986:VAL:HG21 | 2.00 | 0.43 |
| 1:G:3409:TYR:HB2 | 1:G:3509:LEU:HD21 | 2.00 | 0.43 |
| 1:G:3833:GLN:HA | 1:G:3836:MET:HE3 | 2.01 | 0.43 |
| 1:G:4651:THR:HG23 | 8:G:5108:POV:H29 | 1.99 | 0.43 |
| 2:H:14:ALA:HA | 2:H:85:LEU:HB2 | 2.00 | 0.43 |
| 1:J:897:ARG:NH1 | 1:J:898:ASP:H | 2.14 | 0.43 |
| 1:J:3955:MET:HB2 | 1:J:4019:LEU:HD22 | 1.99 | 0.43 |
| 1:J:4078:GLN:O | 1:J:4081:VAL:HG22 | 2.18 | 0.43 |
| 1:J:4958:CYS:HA | 5:J:5109:ATP:N7 | 2.32 | 0.43 |
| 1:A:753:PRO:HB2 | 1:A:770:ALA:H | 1.83 | 0.43 |
| 1:A:1027:LEU:HD23 | 1:A:1027:LEU:HA | 1.90 | 0.43 |
| 1:A:1272:LEU:HG | 1:A:1289:LEU:HD11 | 1.99 | 0.43 |
| 1:A:1816:GLY:HA2 | 1:A:1865:MET:HE3 | 2.01 | 0.43 |
| 1:A:2126:ARG:HG2 | 1:A:2127:GLN:NE2 | 2.33 | 0.43 |
| 1:A:2914:LYS:H | 1:A:2914:LYS:HG3 | 1.68 | 0.43 |
| 1:A:3833:GLN:HA | 1:A:3836:MET:HE3 | 2.01 | 0.43 |
| 1:C:129:ASP:OD1 | 1:C:131:LEU:HG | 2.19 | 0.43 |
| 1:C:210:GLU:HB3 | 1:C:213:TYR:CD2 | 2.47 | 0.43 |
| 1:C:1738:LEU:HD11 | 1:C:1963:GLU:HB2 | 1.99 | 0.43 |
| 1:C:2439:GLU:O | 1:C:2443:ILE:HG12 | 2.19 | 0.43 |
| 1:C:4037:ASN:HB3 | 1:C:4042:ARG:HH21 | 1.83 | 0.43 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:4586:PRO:O | 1:C:4587:PRO:C | 2.60 | 0.43 |
| 1:G:1444:GLU:HG3 | 1:G:1508:ARG:HH21 | 1.84 | 0.43 |
| 1:G:3003:LEU:HG | 1:G:3067:CYS:SG | 2.58 | 0.43 |
| 1:G:3533:ILE:HD13 | 1:G:3596:VAL:HG13 | 2.00 | 0.43 |
| 1:G:4541:TRP:N | 1:G:4541:TRP:CD1 | 2.87 | 0.43 |
| 1:J:12:GLN:O | 1:J:165:VAL:HG13 | 2.18 | 0.43 |
| 1:J:315:CYS:SG | 1:J:351:VAL:HG22 | 2.59 | 0.43 |
| 1:J:1074:ILE:O | 1:J:1238:PHE:HA | 2.18 | 0.43 |
| 1:J:1665:HIS:CE1 | 1:J:1668:ARG:HH12 | 2.36 | 0.43 |
| 1:J:2102:VAL:HG11 | 1:J:2124:LEU:HG | 1.99 | 0.43 |
| 1:J:2439:GLU:O | 1:J:2443:ILE:HG12 | 2.19 | 0.43 |
| 1:J:3103:ILE:O | 1:J:3107:VAL:HG13 | 2.19 | 0.43 |
| 1:J:3232:LEU:HD13 | 1:J:3233:PRO:HD2 | 2.00 | 0.43 |
| 1:J:3409:TYR:HB2 | 1:J:3509:LEU:HD21 | 2.00 | 0.43 |
| 1:J:3833:GLN:HA | 1:J:3836:MET:HE3 | 2.01 | 0.43 |
| 1:J:4897:ILE:HG23 | 1:J:4901:ILE:HD13 | 2.01 | 0.43 |
| 3:L:57:LYS:HG3 | 3:L:80:VAL:HB | 2.00 | 0.43 |
| 1:A:442:ILE:HD11 | 1:A:514:SER:HB2 | 2.01 | 0.43 |
| 1:A:972:LEU:HD13 | 1:A:1044:ARG:NE | 2.33 | 0.43 |
| 1:A:2588:ARG:HA | 1:A:2591:ARG:NH1 | 2.34 | 0.43 |
| 1:A:2980:VAL:HB | 1:A:2986:VAL:HG21 | 2.00 | 0.43 |
| 1:C:2691:TYR:CD1 | 1:C:2996:LYS:HB3 | 2.54 | 0.43 |
| 1:C:3345:ILE:HD12 | 1:C:3345:ILE:HA | 1.90 | 0.43 |
| 1:C:4235:VAL:HG11 | 1:C:5019:TRP:CH2 | 2.54 | 0.43 |
| 1:C:4923:PHE:CZ | 8:G:5113:POV:H22A | 2.54 | 0.43 |
| 1:G:315:CYS:SG | 1:G:351:VAL:HG22 | 2.59 | 0.43 |
| 1:G:907:LEU:HD23 | 1:G:913:LEU:HD23 | 2.01 | 0.43 |
| 1:G:1055:PRO:HA | 1:G:1056:PRO:HD2 | 1.85 | 0.43 |
| 1:G:2124:LEU:HD22 | 1:G:2128:TYR:HE1 | 1.84 | 0.43 |
| 1:G:2228:MET:HE3 | 1:G:2232:CYS:SG | 2.59 | 0.43 |
| 1:G:2439:GLU:O | 1:G:2443:ILE:HG12 | 2.19 | 0.43 |
| 1:G:3075:LEU:HD21 | 1:G:3143:LEU:HD13 | 2.00 | 0.43 |
| 1:G:4822:THR:O | 1:G:4826:ILE:HG13 | 2.19 | 0.43 |
| 1:J:1180:ARG:HD2 | 1:J:1180:ARG:N | 2.33 | 0.43 |
| 1:J:1471:ALA:HA | 1:J:1489:CYS:O | 2.18 | 0.43 |
| 1:J:1931:LEU:HD22 | 1:J:1935:VAL:HG11 | 1.99 | 0.43 |
| 1:J:2124:LEU:HD22 | 1:J:2128:TYR:HE1 | 1.84 | 0.43 |
| 1:J:2305:CYS:HA | 1:J:2308:GLN:HE21 | 1.83 | 0.43 |
| 8:J:5114:POV:H3A | 8:J:5114:POV:H23A | 1.99 | 0.43 |
| 3:L:62:GLY:HA3 | 3:L:74:LEU:HD21 | 2.01 | 0.43 |
| 1:A:2025:GLU:HA | 1:A:2028:ARG:HG2 | 2.00 | 0.43 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:2339:VAL:HG21 | 1:A:2436:CYS:SG | 2.58 | 0.43 |
| 1:A:2490:MET:HA | 1:A:2490:MET:HE3 | 2.01 | 0.43 |
| 1:A:2691:TYR:CD1 | 1:A:2996:LYS:HB3 | 2.54 | 0.43 |
| 1:A:3103:ILE:O | 1:A:3107:VAL:HG13 | 2.19 | 0.43 |
| 1:A:3345:ILE:HD12 | 1:A:3345:ILE:HA | 1.90 | 0.43 |
| 1:A:3530:GLN:O | 1:A:3533:ILE:HB | 2.19 | 0.43 |
| 1:A:4968:PHE:O | 1:A:4974:GLY:HA3 | 2.19 | 0.43 |
| 2:B:109:THR:N | 2:B:110:PRO:HD2 | 2.34 | 0.43 |
| 1:C:1079:LYS:HA | 1:C:1189:LEU:HD11 | 2.00 | 0.43 |
| 1:C:1115:LEU:HG | 1:C:1123:VAL:HG11 | 2.00 | 0.43 |
| 1:C:2124:LEU:HD22 | 1:C:2128:TYR:HE1 | 1.84 | 0.43 |
| 1:C:4651:THR:HG23 | 8:C:5108:POV:H29 | 1.99 | 0.43 |
| 1:C:4897:ILE:HG23 | 1:C:4901:ILE:HD13 | 2.01 | 0.43 |
| 1:G:2770:LYS:HD3 | 1:G:2787:THR:HB | 2.01 | 0.43 |
| 1:G:4995:LEU:HD22 | 1:G:5003:HIS:CD2 | 2.53 | 0.43 |
| 1:J:365:LYS:O | 1:J:369:LEU:HG | 2.18 | 0.43 |
| 1:J:1119:GLU:H | 1:J:1119:GLU:HG3 | 1.63 | 0.43 |
| 1:J:1437:VAL:HG11 | 1:J:1552:VAL:HG21 | 2.00 | 0.43 |
| 1:J:1816:GLY:HA2 | 1:J:1865:MET:HE3 | 2.01 | 0.43 |
| 1:J:1970:GLN:HG3 | 1:J:3642:TYR:HA | 2.00 | 0.43 |
| 1:J:2126:ARG:HG2 | 1:J:2127:GLN:NE2 | 2.33 | 0.43 |
| 1:J:2479:LEU:HA | 1:J:2484:ALA:O | 2.18 | 0.43 |
| 1:J:2559:LEU:O | 1:J:2563:THR:HG23 | 2.18 | 0.43 |
| 1:J:3414:ARG:HH21 | 1:J:3475:LYS:HB2 | 1.83 | 0.43 |
| 1:J:4235:VAL:HG11 | 1:J:5019:TRP:CH2 | 2.54 | 0.43 |
| 1:J:4850:LEU:O | 1:J:4853:VAL:HG22 | 2.18 | 0.43 |
| 1:J:4915:VAL:HG21 | 8:J:5104:POV:H36A | 2.00 | 0.43 |
| 1:A:315:CYS:SG | 1:A:351:VAL:HG22 | 2.58 | 0.43 |
| 1:A:1286:MET:HE3 | 1:A:1286:MET:HB3 | 1.90 | 0.43 |
| 1:A:1867:GLU:HG2 | 1:A:2097:LEU:HD11 | 2.00 | 0.43 |
| 1:A:3166:TYR:OH | 1:A:3203:VAL:HG21 | 2.18 | 0.43 |
| 1:A:3731:LYS:HD3 | 1:A:3734:HIS:CE1 | 2.53 | 0.43 |
| 1:A:4995:LEU:HD22 | 1:A:5003:HIS:CD2 | 2.53 | 0.43 |
| 1:C:753:PRO:HB2 | 1:C:770:ALA:H | 1.83 | 0.43 |
| 1:C:2559:LEU:O | 1:C:2563:THR:HG23 | 2.19 | 0.43 |
| 1:C:2626:LEU:HD23 | 1:C:2626:LEU:HA | 1.79 | 0.43 |
| 1:C:3003:LEU:HG | 1:C:3067:CYS:SG | 2.58 | 0.43 |
| 1:G:12:GLN:O | 1:G:165:VAL:HG13 | 2.18 | 0.43 |
| 1:G:1298:HIS:HB2 | 1:G:1523:ALA:HA | 2.01 | 0.43 |
| 1:G:1448:VAL:HG22 | 1:G:1554:VAL:HG12 | 2.01 | 0.43 |
| 1:G:2724:GLU:HB2 | 1:G:2738:ARG:HH22 | 1.84 | 0.43 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:G:4927:ILE:HD11 | 1:J:4936:ILE:HD12 | 2.01 | 0.43 |
| 8:G:5110:POV:H21E | 8:J:5106:POV:H311 | 2.01 | 0.43 |
| 1:J:1867:GLU:HG2 | 1:J:2097:LEU:HD11 | 2.00 | 0.43 |
| 1:J:2698:MET:O | 1:J:2701:PRO:HD2 | 2.19 | 0.43 |
| 1:J:3166:TYR:OH | 1:J:3203:VAL:HG21 | 2.18 | 0.43 |
| 1:J:4822:THR:O | 1:J:4826:ILE:HG13 | 2.19 | 0.43 |
| 1:J:4876:CYS:HA | 1:J:4882:CYS:HB2 | 2.01 | 0.43 |
| 1:A:551:LEU:HD13 | 1:A:589:LEU:HD11 | 2.01 | 0.43 |
| 1:A:1437:VAL:HG11 | 1:A:1552:VAL:HG21 | 2.00 | 0.43 |
| 1:A:2111:VAL:HG23 | 1:A:2117:VAL:HG22 | 2.00 | 0.43 |
| 1:A:2724:GLU:HB2 | 1:A:2738:ARG:HH22 | 1.84 | 0.43 |
| 1:A:2962:GLN:CG | 1:A:2965:ARG:HH21 | 2.23 | 0.43 |
| 1:A:3003:LEU:HG | 1:A:3067:CYS:SG | 2.58 | 0.43 |
| 1:A:3414:ARG:HH21 | 1:A:3475:LYS:HB2 | 1.83 | 0.43 |
| 1:A:4037:ASN:HB3 | 1:A:4042:ARG:HH21 | 1.83 | 0.43 |
| 1:C:972:LEU:HD13 | 1:C:1044:ARG:NE | 2.33 | 0.43 |
| 1:C:1527:MET:HE2 | 1:C:1527:MET:HB3 | 1.83 | 0.43 |
| 1:C:1665:HIS:CE1 | 1:C:1668:ARG:HH12 | 2.36 | 0.43 |
| 1:C:1676:LEU:HD12 | 1:C:2167:ILE:HD12 | 2.00 | 0.43 |
| 1:C:3531:ASP:OD2 | 1:C:3561:GLY:HA3 | 2.19 | 0.43 |
| 1:C:4681:LEU:HD21 | 1:C:4687:TYR:HD2 | 1.83 | 0.43 |
| 1:G:867:LEU:O | 1:G:871:ARG:HB3 | 2.19 | 0.43 |
| 1:G:1703:LEU:HD23 | 1:G:1708:ARG:HG2 | 1.99 | 0.43 |
| 1:G:2740:VAL:HG11 | 1:G:2815:ALA:HB2 | 2.01 | 0.43 |
| 1:G:3395:ARG:HG2 | 1:G:3453:ARG:HH12 | 1.84 | 0.43 |
| 1:G:4840:THR:HA | 1:J:4823:LEU:HD21 | 2.00 | 0.43 |
| 1:J:1100:MET:SD | 1:J:1198:GLN:HB3 | 2.59 | 0.43 |
| 1:J:2800:LYS:O | 1:J:2804:ILE:HG12 | 2.19 | 0.43 |
| 1:A:12:GLN:O | 1:A:165:VAL:HG13 | 2.18 | 0.43 |
| 1:A:78:LEU:O | 1:A:81:MET:HG3 | 2.18 | 0.43 |
| 1:A:667:MET:SD | 1:A:743:VAL:HG22 | 2.59 | 0.43 |
| 1:A:926:GLY:O | 1:A:930:LYS:HG3 | 2.18 | 0.43 |
| 1:A:1115:LEU:HG | 1:A:1123:VAL:HG11 | 2.00 | 0.43 |
| 1:A:3727:ASP:O | 1:A:3731:LYS:HG2 | 2.19 | 0.43 |
| 1:A:4235:VAL:HG11 | 1:A:5019:TRP:CH2 | 2.54 | 0.43 |
| 1:A:4897:ILE:HG23 | 1:A:4901:ILE:HD13 | 2.01 | 0.43 |
| 1:C:117:TYR:CG | 1:C:141:ALA:HB2 | 2.54 | 0.43 |
| 1:C:719:LEU:H | 1:C:737:LEU:HD23 | 1.84 | 0.43 |
| 1:C:747:CYS:SG | 1:C:805:PRO:HG2 | 2.58 | 0.43 |
| 1:C:937:CYS:HB3 | 1:C:1053:ILE:HG23 | 2.01 | 0.43 |
| 1:C:1074:ILE:O | 1:C:1238:PHE:HA | 2.18 | 0.43 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:1970:GLN:HG3 | 1:C:3642:TYR:HA | 2.00 | 0.43 |
| 1:C:2724:GLU:HB2 | 1:C:2738:ARG:HH22 | 1.84 | 0.43 |
| 1:C:3986:TRP:HA | 1:C:3989:VAL:HG22 | 2.01 | 0.43 |
| 1:C:4794:TRP:NE1 | 8:C:5115:POV:H37A | 2.30 | 0.43 |
| 1:C:4968:PHE:O | 1:C:4974:GLY:HA3 | 2.19 | 0.43 |
| 1:G:78:LEU:O | 1:G:81:MET:HG3 | 2.18 | 0.43 |
| 1:G:719:LEU:H | 1:G:737:LEU:HD23 | 1.84 | 0.43 |
| 1:G:1676:LEU:HD12 | 1:G:2167:ILE:HD12 | 2.00 | 0.43 |
| 1:G:2111:VAL:HG23 | 1:G:2117:VAL:HG22 | 2.00 | 0.43 |
| 1:G:2588:ARG:HA | 1:G:2591:ARG:NH1 | 2.34 | 0.43 |
| 1:G:2588:ARG:HA | 1:G:2591:ARG:HH11 | 1.83 | 0.43 |
| 1:G:2626:LEU:HD23 | 1:G:2626:LEU:HA | 1.78 | 0.43 |
| 1:G:3604:TYR:O | 1:G:3607:GLU:HG3 | 2.19 | 0.43 |
| 1:G:3689:GLU:H | 1:G:3689:GLU:CD | 2.26 | 0.43 |
| 1:G:4897:ILE:HG23 | 1:G:4901:ILE:HD13 | 2.01 | 0.43 |
| 2:H:67:PHE:CD1 | 2:H:82:MET:HE1 | 2.54 | 0.43 |
| 3:I:52:LYS:HB2 | 3:I:54:GLU:HG3 | 2.01 | 0.43 |
| 1:J:688:LEU:HD23 | 1:J:688:LEU:HA | 1.89 | 0.43 |
| 1:J:1160:ILE:HG13 | 1:J:1182:ILE:HD13 | 2.01 | 0.43 |
| 1:J:2382:GLU:O | 1:J:2386:ILE:HG12 | 2.18 | 0.43 |
| 1:J:2588:ARG:HA | 1:J:2591:ARG:NH1 | 2.34 | 0.43 |
| 1:J:2770:LYS:HD3 | 1:J:2787:THR:HB | 2.01 | 0.43 |
| 1:J:2956:ALA:O | 1:J:2960:LEU:HG | 2.18 | 0.43 |
| 8:J:5101:POV:H13A | 8:J:5101:POV:H11A | 1.90 | 0.43 |
| 1:A:980:ALA:O | 1:A:984:LEU:HG | 2.19 | 0.42 |
| 1:A:1970:GLN:HG3 | 1:A:3642:TYR:HA | 2.00 | 0.42 |
| 1:A:3187:ARG:HA | 1:A:3190:LEU:HD12 | 2.01 | 0.42 |
| 1:A:3192:GLU:HA | 1:A:3341:PHE:HZ | 1.84 | 0.42 |
| 1:A:3986:TRP:HA | 1:A:3989:VAL:HG22 | 2.01 | 0.42 |
| 1:A:4541:TRP:N | 1:A:4541:TRP:CD1 | 2.87 | 0.42 |
| 1:A:4850:LEU:O | 1:A:4853:VAL:HG22 | 2.18 | 0.42 |
| 1:C:12:GLN:O | 1:C:165:VAL:HG13 | 2.18 | 0.42 |
| 1:C:232:THR:HG21 | 1:C:252:VAL:HG21 | 1.99 | 0.42 |
| 1:C:882:TRP:CZ2 | 1:C:905:PRO:HD3 | 2.53 | 0.42 |
| 1:C:985:VAL:HG13 | 1:C:1039:LEU:HG | 2.01 | 0.42 |
| 1:C:1100:MET:SD | 1:C:1198:GLN:HB3 | 2.59 | 0.42 |
| 1:C:1448:VAL:HG22 | 1:C:1554:VAL:HG12 | 2.01 | 0.42 |
| 1:C:3689:GLU:CD | 1:C:3689:GLU:H | 2.26 | 0.42 |
| 1:C:3872:GLU:HG2 | 1:C:3874:VAL:H | 1.84 | 0.42 |
| 8:C:5112:POV:H1A | 8:C:5114:POV:H1A | 2.00 | 0.42 |
| 1:G:210:GLU:HB3 | 1:G:213:TYR:CD2 | 2.46 | 0.42 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:G:1079:LYS:HA | 1:G:1189:LEU:HD11 | 2.00 | 0.42 |
| 1:G:1943:LEU:HD23 | 1:G:1943:LEU:HA | 1.87 | 0.42 |
| 1:G:2624:ARG:NH2 | 1:G:2625:ARG:HH12 | 2.14 | 0.42 |
| 1:G:2800:LYS:O | 1:G:2804:ILE:HG12 | 2.19 | 0.42 |
| 1:J:551:LEU:HD13 | 1:J:589:LEU:HD11 | 2.01 | 0.42 |
| 1:J:801:LYS:HE2 | 1:J:801:LYS:HB2 | 1.84 | 0.42 |
| 1:J:1087:ARG:HG2 | 1:J:1154:ASP:HA | 2.01 | 0.42 |
| 1:J:2111:VAL:HG23 | 1:J:2117:VAL:HG22 | 2.00 | 0.42 |
| 1:J:2203:MET:H | 1:J:2203:MET:HG2 | 1.54 | 0.42 |
| 1:J:2339:VAL:HG21 | 1:J:2436:CYS:SG | 2.59 | 0.42 |
| 1:J:2437:ALA:HB3 | 1:J:2508:ARG:HG2 | 2.02 | 0.42 |
| 1:J:2490:MET:HE3 | 1:J:2490:MET:HA | 2.01 | 0.42 |
| 1:J:2939:ARG:H | 1:J:2939:ARG:HG3 | 1.66 | 0.42 |
| 1:J:2959:PHE:HE2 | 1:J:3009:TYR:CE2 | 2.37 | 0.42 |
| 1:A:1087:ARG:HG2 | 1:A:1154:ASP:HA | 2.01 | 0.42 |
| 1:A:2358:ILE:HB | 1:J:195:PHE:CE2 | 2.54 | 0.42 |
| 1:A:2559:LEU:O | 1:A:2563:THR:HG23 | 2.19 | 0.42 |
| 1:A:3935:TRP:HZ3 | 1:A:3994:HIS:HE1 | 1.66 | 0.42 |
| 1:A:4071:ILE:HD13 | 1:A:4097:MET:SD | 2.59 | 0.42 |
| 8:A:5109:POV:H1A | 8:A:5111:POV:H1A | 2.00 | 0.42 |
| 1:C:470:SER:HA | 1:C:473:ASN:HD21 | 1.84 | 0.42 |
| 1:C:867:LEU:O | 1:C:871:ARG:HB3 | 2.19 | 0.42 |
| 1:C:908:VAL:HG23 | 1:C:962:SER:O | 2.19 | 0.42 |
| 1:C:1087:ARG:HG2 | 1:C:1154:ASP:HA | 2.01 | 0.42 |
| 1:C:2624:ARG:NH2 | 1:C:2625:ARG:HH12 | 2.14 | 0.42 |
| 1:C:2914:LYS:H | 1:C:2914:LYS:HG3 | 1.68 | 0.42 |
| 1:C:4842:GLY:HA3 | 8:G:5103:POV:H21E | 2.00 | 0.42 |
| 1:G:882:TRP:CZ2 | 1:G:905:PRO:HD3 | 2.53 | 0.42 |
| 1:G:1160:ILE:HG13 | 1:G:1182:ILE:HD13 | 2.01 | 0.42 |
| 1:G:2959:PHE:HE2 | 1:G:3009:TYR:CE2 | 2.37 | 0.42 |
| 1:G:3078:ARG:HD2 | 1:G:3152:PHE:CD2 | 2.53 | 0.42 |
| 1:G:3303:PRO:O | 1:G:3305:THR:HG22 | 2.20 | 0.42 |
| 1:J:284:HIS:HE1 | 1:J:286:THR:HB | 1.84 | 0.42 |
| 1:J:980:ALA:O | 1:J:984:LEU:HG | 2.19 | 0.42 |
| 1:J:2588:ARG:HA | 1:J:2591:ARG:HH11 | 1.83 | 0.42 |
| 1:J:2980:VAL:HB | 1:J:2986:VAL:HG21 | 2.00 | 0.42 |
| 1:J:3003:LEU:HG | 1:J:3067:CYS:SG | 2.58 | 0.42 |
| 1:J:3727:ASP:O | 1:J:3731:LYS:HG2 | 2.19 | 0.42 |
| 8:J:5121:POV:H14B | 8:J:5121:POV:H11 | 1.79 | 0.42 |
| 1:A:523:TYR:HD2 | 1:A:556:ALA:HB3 | 1.85 | 0.42 |
| 1:A:626:LEU:HD23 | 1:A:1688:HIS:CD2 | 2.55 | 0.42 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:872:GLU:O | 1:A:876:GLU:HG2 | 2.19 | 0.42 |
| 1:A:2815:ALA:O | 1:A:2819:TRP:HD1 | 2.03 | 0.42 |
| 1:A:3531:ASP:OD2 | 1:A:3561:GLY:HA3 | 2.19 | 0.42 |
| 2:B:45:ARG:HD3 | 2:B:117:TRP:CZ2 | 2.54 | 0.42 |
| 1:C:872:GLU:O | 1:C:876:GLU:HG2 | 2.19 | 0.42 |
| 1:C:1160:ILE:HG13 | 1:C:1182:ILE:HD13 | 2.01 | 0.42 |
| 1:C:1437:VAL:HG11 | 1:C:1552:VAL:HG21 | 2.00 | 0.42 |
| 1:C:1816:GLY:HA2 | 1:C:1865:MET:HE3 | 2.01 | 0.42 |
| 1:C:2740:VAL:HG11 | 1:C:2815:ALA:HB2 | 2.01 | 0.42 |
| 1:C:2880:GLU:HB2 | 1:C:2908:TYR:CZ | 2.55 | 0.42 |
| 1:C:2959:PHE:HE2 | 1:C:3009:TYR:CE2 | 2.37 | 0.42 |
| 1:C:3103:ILE:O | 1:C:3107:VAL:HG13 | 2.19 | 0.42 |
| 2:D:111:ASN:HA | 2:D:114:TYR:CD2 | 2.55 | 0.42 |
| 3:F:2:VAL:HG23 | 3:F:80:VAL:HG21 | 2.01 | 0.42 |
| 1:G:284:HIS:HE1 | 1:G:286:THR:HB | 1.84 | 0.42 |
| 1:G:514:SER:O | 1:G:518:ILE:HG13 | 2.19 | 0.42 |
| 1:G:1816:GLY:HA2 | 1:G:1865:MET:HE3 | 2.01 | 0.42 |
| 1:G:3206:LEU:HD12 | 1:G:3206:LEU:HA | 1.85 | 0.42 |
| 1:G:3727:ASP:O | 1:G:3731:LYS:HG2 | 2.19 | 0.42 |
| 1:G:4842:GLY:HA3 | 8:J:5107:POV:H21E | 2.00 | 0.42 |
| 1:G:4897:ILE:HG13 | 1:G:4901:ILE:HG23 | 1.99 | 0.42 |
| 3:I:27:THR:HB | 3:I:100:ASP:HB3 | 2.01 | 0.42 |
| 1:J:1298:HIS:HB2 | 1:J:1523:ALA:HA | 2.01 | 0.42 |
| 1:J:2740:VAL:HG11 | 1:J:2815:ALA:HB2 | 2.01 | 0.42 |
| 1:J:2815:ALA:O | 1:J:2819:TRP:HD1 | 2.03 | 0.42 |
| 2:K:45:ARG:H | 2:K:45:ARG:HG2 | 1.52 | 0.42 |
| 1:A:129:ASP:OD1 | 1:A:131:LEU:HG | 2.19 | 0.42 |
| 1:A:1100:MET:SD | 1:A:1198:GLN:HB3 | 2.59 | 0.42 |
| 1:A:1160:ILE:HG13 | 1:A:1182:ILE:HD13 | 2.01 | 0.42 |
| 1:A:2588:ARG:HA | 1:A:2591:ARG:HH11 | 1.83 | 0.42 |
| 1:A:2675:THR:HB | 1:A:2710:LEU:HD13 | 2.02 | 0.42 |
| 1:A:2770:LYS:HD3 | 1:A:2787:THR:HB | 2.01 | 0.42 |
| 1:A:2871:LEU:HA | 1:A:2874:MET:HE2 | 2.01 | 0.42 |
| 1:A:3872:GLU:HG2 | 1:A:3874:VAL:H | 1.85 | 0.42 |
| 1:C:889:GLN:HG2 | 1:C:890:GLY:H | 1.85 | 0.42 |
| 1:C:2332:LEU:O | 1:C:2336:ARG:HG3 | 2.19 | 0.42 |
| 1:C:3002:LEU:HD23 | 1:C:3002:LEU:HA | 1.86 | 0.42 |
| 1:C:3018:LEU:HD11 | 1:C:3150:HIS:NE2 | 2.35 | 0.42 |
| 1:C:3036:LYS:CD | 1:C:3079:THR:HG21 | 2.47 | 0.42 |
| 1:C:3366:ARG:HA | 1:C:3441:ILE:HD11 | 2.01 | 0.42 |
| 1:C:4980:LEU:HD13 | 1:C:4980:LEU:HA | 1.82 | 0.42 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:G:1229:ASN:HB2 | 1:G:1827:ARG:HG3 | 2.01 | 0.42 |
| 1:G:1738:LEU:HD11 | 1:G:1963:GLU:HB2 | 1.99 | 0.42 |
| 1:G:2203:MET:H | 1:G:2203:MET:HG2 | 1.54 | 0.42 |
| 1:G:2437:ALA:HB3 | 1:G:2508:ARG:HG2 | 2.02 | 0.42 |
| 1:G:2512:ILE:HG21 | 1:G:2518:LEU:HG | 2.00 | 0.42 |
| 1:G:2675:THR:HB | 1:G:2710:LEU:HD13 | 2.02 | 0.42 |
| 1:G:2691:TYR:CD1 | 1:G:2996:LYS:HB3 | 2.54 | 0.42 |
| 1:G:2815:ALA:O | 1:G:2819:TRP:HD1 | 2.03 | 0.42 |
| 1:G:4177:TYR:CE1 | 1:G:4199:GLU:HG2 | 2.55 | 0.42 |
| 1:J:442:ILE:HD11 | 1:J:514:SER:HB2 | 2.01 | 0.42 |
| 1:J:2025:GLU:HA | 1:J:2028:ARG:HG2 | 2.00 | 0.42 |
| 1:J:2489:LYS:H | 1:J:2489:LYS:HD2 | 1.84 | 0.42 |
| 1:J:3002:LEU:HD23 | 1:J:3002:LEU:HA | 1.86 | 0.42 |
| 1:J:3778:MET:O | 1:J:3782:MET:HG2 | 2.20 | 0.42 |
| 1:A:103:TYR:CE1 | 1:A:163:VAL:HG22 | 2.55 | 0.42 |
| 1:A:622:THR:HA | 1:A:626:LEU:HD13 | 2.01 | 0.42 |
| 1:A:907:LEU:HD23 | 1:A:913:LEU:HD23 | 2.01 | 0.42 |
| 1:A:1229:ASN:HB2 | 1:A:1827:ARG:HG3 | 2.01 | 0.42 |
| 1:A:1676:LEU:HD12 | 1:A:2167:ILE:HD12 | 2.00 | 0.42 |
| 1:A:2698:MET:O | 1:A:2701:PRO:HD2 | 2.19 | 0.42 |
| 1:A:2800:LYS:O | 1:A:2804:ILE:HG12 | 2.19 | 0.42 |
| 2:B:28:ILE:H | 2:B:28:ILE:HG13 | 1.62 | 0.42 |
| 1:C:514:SER:O | 1:C:518:ILE:HG13 | 2.20 | 0.42 |
| 1:C:964:GLY:O | 1:C:965:TYR:C | 2.61 | 0.42 |
| 1:C:2588:ARG:HA | 1:C:2591:ARG:NH1 | 2.34 | 0.42 |
| 1:C:3031:ALA:HB3 | 1:C:3036:LYS:HZ3 | 1.85 | 0.42 |
| 1:C:3196:ARG:HD3 | 1:C:3196:ARG:HA | 1.76 | 0.42 |
| 1:C:3790:THR:HA | 1:C:3794:VAL:HG11 | 2.01 | 0.42 |
| 1:C:4210:VAL:HG21 | 1:C:4245:MET:HE2 | 2.01 | 0.42 |
| 1:C:4846:VAL:O | 1:C:4850:LEU:HG | 2.20 | 0.42 |
| 1:C:4975:PHE:CZ | 1:C:4979:THR:HG21 | 2.54 | 0.42 |
| 1:G:551:LEU:HD13 | 1:G:589:LEU:HD11 | 2.01 | 0.42 |
| 1:G:980:ALA:O | 1:G:984:LEU:HG | 2.19 | 0.42 |
| 1:G:1155:LEU:HD23 | 1:G:1155:LEU:HA | 1.85 | 0.42 |
| 1:G:3778:MET:O | 1:G:3782:MET:HG2 | 2.20 | 0.42 |
| 1:J:514:SER:O | 1:J:518:ILE:HG13 | 2.20 | 0.42 |
| 1:J:523:TYR:HD2 | 1:J:556:ALA:HB3 | 1.85 | 0.42 |
| 1:J:622:THR:HA | 1:J:626:LEU:HD13 | 2.01 | 0.42 |
| 1:J:719:LEU:H | 1:J:737:LEU:HD23 | 1.84 | 0.42 |
| 1:J:2691:TYR:CD1 | 1:J:2996:LYS:HB3 | 2.54 | 0.42 |
| 1:J:3439:GLY:O | 1:J:3443:ILE:HG23 | 2.18 | 0.42 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:J:3531:ASP:OD2 | 1:J:3561:GLY:HA3 | 2.19 | 0.42 |
| 1:J:3935:TRP:HZ3 | 1:J:3994:HIS:HE1 | 1.66 | 0.42 |
| 1:J:4541:TRP:N | 1:J:4541:TRP:CD1 | 2.87 | 0.42 |
| 1:A:937:CYS:HB3 | 1:A:1053:ILE:HG23 | 2.01 | 0.42 |
| 1:A:1448:VAL:HG22 | 1:A:1554:VAL:HG12 | 2.01 | 0.42 |
| 1:A:2128:TYR:CD2 | 1:A:3673:MET:HB2 | 2.55 | 0.42 |
| 1:A:2272:PRO:HA | 1:A:2275:VAL:HG23 | 2.02 | 0.42 |
| 1:A:2489:LYS:H | 1:A:2489:LYS:HD2 | 1.84 | 0.42 |
| 1:A:2704:CYS:HB3 | 1:A:3008:GLN:HG2 | 2.02 | 0.42 |
| 1:A:2959:PHE:HE2 | 1:A:3009:TYR:CE2 | 2.37 | 0.42 |
| 1:A:4177:TYR:CE1 | 1:A:4199:GLU:HG2 | 2.55 | 0.42 |
| 1:C:1260:MET:HE2 | 1:C:1269:CYS:SG | 2.60 | 0.42 |
| 1:C:1298:HIS:HB2 | 1:C:1523:ALA:HA | 2.01 | 0.42 |
| 1:C:2377:LEU:HD21 | 1:C:2468:GLY:HA3 | 2.01 | 0.42 |
| 1:C:2675:THR:HB | 1:C:2710:LEU:HD13 | 2.02 | 0.42 |
| 1:C:2698:MET:O | 1:C:2701:PRO:HD2 | 2.19 | 0.42 |
| 1:C:2770:LYS:HD3 | 1:C:2787:THR:HB | 2.01 | 0.42 |
| 1:C:2800:LYS:O | 1:C:2804:ILE:HG12 | 2.19 | 0.42 |
| 1:C:2815:ALA:O | 1:C:2819:TRP:HD1 | 2.03 | 0.42 |
| 1:C:2956:ALA:O | 1:C:2960:LEU:HG | 2.18 | 0.42 |
| 1:C:3303:PRO:O | 1:C:3305:THR:HG22 | 2.20 | 0.42 |
| 1:C:3727:ASP:O | 1:C:3731:LYS:HG2 | 2.19 | 0.42 |
| 1:C:3835:LEU:HD22 | 1:C:3880:PHE:CZ | 2.51 | 0.42 |
| 1:G:103:TYR:CE1 | 1:G:163:VAL:HG22 | 2.55 | 0.42 |
| 1:G:129:ASP:OD1 | 1:G:131:LEU:HG | 2.19 | 0.42 |
| 1:G:195:PHE:CE2 | 1:J:2358:ILE:HB | 2.55 | 0.42 |
| 1:G:470:SER:HA | 1:G:473:ASN:HD21 | 1.85 | 0.42 |
| 1:G:937:CYS:HB3 | 1:G:1053:ILE:HG23 | 2.02 | 0.42 |
| 1:G:1100:MET:SD | 1:G:1198:GLN:HB3 | 2.59 | 0.42 |
| 1:G:1437:VAL:HG11 | 1:G:1552:VAL:HG21 | 2.00 | 0.42 |
| 1:G:2698:MET:O | 1:G:2701:PRO:HD2 | 2.19 | 0.42 |
| 1:G:3103:ILE:O | 1:G:3107:VAL:HG13 | 2.19 | 0.42 |
| 1:G:4037:ASN:HB3 | 1:G:4042:ARG:HH21 | 1.83 | 0.42 |
| 1:G:4210:VAL:HG21 | 1:G:4245:MET:HE2 | 2.01 | 0.42 |
| 1:J:907:LEU:HD23 | 1:J:913:LEU:HD23 | 2.01 | 0.42 |
| 1:J:1958:LEU:HD23 | 1:J:2138:LEU:HD21 | 2.02 | 0.42 |
| 1:J:2576:ALA:HA | 1:J:2579:VAL:HG22 | 2.01 | 0.42 |
| 1:J:3018:LEU:HD11 | 1:J:3150:HIS:NE2 | 2.35 | 0.42 |
| 1:J:4080:TYR:CE1 | 1:J:4095:LYS:HG3 | 2.53 | 0.42 |
| 1:J:4177:TYR:CE1 | 1:J:4199:GLU:HG2 | 2.55 | 0.42 |
| 1:J:4968:PHE:O | 1:J:4974:GLY:HA3 | 2.19 | 0.42 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:470:SER:HA | 1:A:473:ASN:HD21 | 1.84 | 0.42 |
| 1:A:718:GLY:HA3 | 1:A:737:LEU:HA | 2.02 | 0.42 |
| 1:A:867:LEU:O | 1:A:871:ARG:HB3 | 2.19 | 0.42 |
| 1:A:1260:MET:HE2 | 1:A:1269:CYS:SG | 2.60 | 0.42 |
| 1:A:1444:GLU:HG3 | 1:A:1508:ARG:HH21 | 1.84 | 0.42 |
| 1:A:1462:MET:HA | 1:A:1462:MET:HE3 | 2.02 | 0.42 |
| 1:A:2138:LEU:HB3 | 1:A:3658:LYS:HE2 | 2.02 | 0.42 |
| 1:A:2437:ALA:HB3 | 1:A:2508:ARG:HG2 | 2.01 | 0.42 |
| 1:A:2880:GLU:HB2 | 1:A:2908:TYR:CZ | 2.55 | 0.42 |
| 1:A:3778:MET:O | 1:A:3782:MET:HG2 | 2.20 | 0.42 |
| 1:A:4210:VAL:HG21 | 1:A:4245:MET:HE2 | 2.01 | 0.42 |
| 1:A:4876:CYS:HA | 1:A:4882:CYS:HB2 | 2.01 | 0.42 |
| 1:C:103:TYR:CE1 | 1:C:163:VAL:HG22 | 2.55 | 0.42 |
| 1:C:551:LEU:HD13 | 1:C:589:LEU:HD11 | 2.01 | 0.42 |
| 1:C:598:LYS:HE3 | 1:C:598:LYS:HB3 | 1.80 | 0.42 |
| 1:C:801:LYS:HE2 | 1:C:801:LYS:HB2 | 1.84 | 0.42 |
| 1:C:1094:ALA:HA | 1:C:1100:MET:HE1 | 2.02 | 0.42 |
| 1:C:2437:ALA:HB3 | 1:C:2508:ARG:HG2 | 2.02 | 0.42 |
| 1:C:4177:TYR:CE1 | 1:C:4199:GLU:HG2 | 2.55 | 0.42 |
| 1:C:4541:TRP:N | 1:C:4541:TRP:CD1 | 2.87 | 0.42 |
| 8:C:5110:POV:H21E | 8:G:5102:POV:H311 | 2.01 | 0.42 |
| 8:C:5120:POV:H29 | 8:C:5120:POV:H34A | 2.01 | 0.42 |
| 1:G:1958:LEU:HD23 | 1:G:2138:LEU:HD21 | 2.02 | 0.42 |
| 1:G:3366:ARG:HA | 1:G:3441:ILE:HD11 | 2.01 | 0.42 |
| 1:J:178:ARG:HG2 | 1:J:195:PHE:CE1 | 2.55 | 0.42 |
| 1:J:1286:MET:HE3 | 1:J:1286:MET:HB3 | 1.90 | 0.42 |
| 1:J:2704:CYS:HB3 | 1:J:3008:GLN:HG2 | 2.02 | 0.42 |
| 1:J:3986:TRP:HA | 1:J:3989:VAL:HG22 | 2.01 | 0.42 |
| 1:A:223:PHE:HA | 1:A:230:CYS:HA | 2.02 | 0.42 |
| 1:A:3169:LEU:O | 1:A:3172:ILE:HG22 | 2.19 | 0.42 |
| 1:A:3539:ARG:HE | 1:A:3549:VAL:HA | 1.84 | 0.42 |
| 1:A:3798:LEU:HD21 | 1:A:3884:LEU:HD13 | 2.02 | 0.42 |
| 1:C:568:LEU:HD12 | 1:C:602:VAL:HG13 | 2.02 | 0.42 |
| 1:C:626:LEU:HD23 | 1:C:1688:HIS:CD2 | 2.55 | 0.42 |
| 1:C:980:ALA:O | 1:C:984:LEU:HG | 2.19 | 0.42 |
| 1:C:1000:ARG:HA | 1:C:1000:ARG:HE | 1.85 | 0.42 |
| 1:C:3192:GLU:HA | 1:C:3341:PHE:HZ | 1.85 | 0.42 |
| 1:C:3409:TYR:HB2 | 1:C:3509:LEU:HD21 | 2.00 | 0.42 |
| 1:C:3966:THR:O | 1:C:3970:GLN:N | 2.53 | 0.42 |
| 1:C:4979:THR:O | 1:C:4980:LEU:HD22 | 2.20 | 0.42 |
| 1:G:117:TYR:CG | 1:G:141:ALA:HB2 | 2.54 | 0.42 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:G:626:LEU:HD23 | 1:G:1688:HIS:CD2 | 2.55 | 0.42 |
| 1:G:1087:ARG:HG2 | 1:G:1154:ASP:HA | 2.01 | 0.42 |
| 1:G:3192:GLU:HA | 1:G:3341:PHE:HZ | 1.85 | 0.42 |
| 1:G:4071:ILE:HD13 | 1:G:4097:MET:SD | 2.59 | 0.42 |
| 1:G:4235:VAL:HG11 | 1:G:5019:TRP:CH2 | 2.54 | 0.42 |
| 8:G:5112:POV:H1A | 8:G:5114:POV:H1A | 2.00 | 0.42 |
| 1:J:470:SER:HA | 1:J:473:ASN:HD21 | 1.84 | 0.42 |
| 1:J:718:GLY:HA3 | 1:J:737:LEU:HA | 2.02 | 0.42 |
| 1:J:1229:ASN:HB2 | 1:J:1827:ARG:HG3 | 2.01 | 0.42 |
| 1:J:3406:TYR:HE2 | 1:J:3455:GLU:HG3 | 1.85 | 0.42 |
| 1:A:178:ARG:HG2 | 1:A:195:PHE:CE1 | 2.55 | 0.42 |
| 1:A:514:SER:O | 1:A:518:ILE:HG13 | 2.20 | 0.42 |
| 1:A:1526:LEU:HD12 | 1:A:1526:LEU:HA | 1.91 | 0.42 |
| 1:A:2976:HIS:CE1 | 1:A:2995:ILE:HD11 | 2.55 | 0.42 |
| 1:A:3018:LEU:HD11 | 1:A:3150:HIS:NE2 | 2.35 | 0.42 |
| 1:A:3406:TYR:HE2 | 1:A:3455:GLU:HG3 | 1.85 | 0.42 |
| 1:A:4846:VAL:O | 1:A:4850:LEU:HG | 2.20 | 0.42 |
| 1:C:516:LYS:HZ3 | 1:C:555:GLU:HG3 | 1.85 | 0.42 |
| 1:C:2512:ILE:HG21 | 1:C:2518:LEU:HG | 2.02 | 0.42 |
| 1:C:3406:TYR:HE2 | 1:C:3455:GLU:HG3 | 1.85 | 0.42 |
| 1:C:4876:CYS:HA | 1:C:4882:CYS:HB2 | 2.01 | 0.42 |
| 1:G:365:LYS:HB3 | 1:G:365:LYS:HE3 | 1.82 | 0.42 |
| 1:G:568:LEU:HD12 | 1:G:602:VAL:HG13 | 2.02 | 0.42 |
| 1:G:3410:PRO:O | 1:G:3414:ARG:HG2 | 2.20 | 0.42 |
| 1:G:3531:ASP:OD2 | 1:G:3561:GLY:HA3 | 2.19 | 0.42 |
| 1:G:3986:TRP:HA | 1:G:3989:VAL:HG22 | 2.01 | 0.42 |
| 1:G:4876:CYS:HA | 1:G:4882:CYS:HB2 | 2.01 | 0.42 |
| 1:G:4915:VAL:HG21 | 8:G:5122:POV:H36A | 2.01 | 0.42 |
| 1:J:117:TYR:CG | 1:J:141:ALA:HB2 | 2.54 | 0.42 |
| 1:J:626:LEU:HD23 | 1:J:1688:HIS:CD2 | 2.55 | 0.42 |
| 1:J:2128:TYR:CD2 | 1:J:3673:MET:HB2 | 2.55 | 0.42 |
| 1:J:2170:MET:HE2 | 1:J:2170:MET:HB2 | 1.83 | 0.42 |
| 1:J:2238:TYR:O | 1:J:2242:ILE:HG12 | 2.20 | 0.42 |
| 1:J:2332:LEU:O | 1:J:2336:ARG:HG3 | 2.19 | 0.42 |
| 1:J:2670:GLU:CD | 1:J:2912:THR:HA | 2.45 | 0.42 |
| 1:J:3303:PRO:O | 1:J:3305:THR:HG22 | 2.20 | 0.42 |
| 1:J:4071:ILE:HD13 | 1:J:4097:MET:SD | 2.59 | 0.42 |
| 8:J:5116:POV:H1A | 8:J:5118:POV:H1A | 2.00 | 0.42 |
| 1:A:264:PRO:HG2 | 1:A:270:SER:HA | 2.02 | 0.42 |
| 1:A:1298:HIS:HB2 | 1:A:1523:ALA:HA | 2.01 | 0.42 |
| 1:A:2576:ALA:HA | 1:A:2579:VAL:HG22 | 2.01 | 0.42 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:3303:PRO:O | 1:A:3305:THR:HG22 | 2.20 | 0.42 |
| 1:A:3719:ASP:H | 1:A:3793:MET:HE2 | 1.85 | 0.42 |
| 8:A:5107:POV:H21E | 8:C:5102:POV:H311 | 2.01 | 0.42 |
| 8:A:5116:POV:H13A | 8:A:5116:POV:H11A | 1.90 | 0.42 |
| 1:C:284:HIS:HE1 | 1:C:286:THR:HB | 1.84 | 0.42 |
| 1:C:1462:MET:HE3 | 1:C:1462:MET:HA | 2.02 | 0.42 |
| 1:C:2128:TYR:CD2 | 1:C:3673:MET:HB2 | 2.55 | 0.42 |
| 1:C:2672:LEU:HD22 | 1:C:2710:LEU:HD12 | 2.02 | 0.42 |
| 1:C:2825:LYS:HD2 | 1:C:2825:LYS:HA | 1.87 | 0.42 |
| 1:C:3391:GLU:HA | 1:C:3394:VAL:HG22 | 2.02 | 0.42 |
| 1:C:3778:MET:O | 1:C:3782:MET:HG2 | 2.20 | 0.42 |
| 1:C:4071:ILE:HD13 | 1:C:4097:MET:SD | 2.59 | 0.42 |
| 1:C:4219:PHE:HA | 1:C:4950:VAL:HG11 | 2.02 | 0.42 |
| 2:D:109:THR:N | 2:D:110:PRO:HD2 | 2.35 | 0.42 |
| 3:E:3:GLU:HG2 | 3:E:75:THR:HB | 2.02 | 0.42 |
| 1:G:77:ALA:HA | 1:J:3935:TRP:HE1 | 1.80 | 0.42 |
| 1:G:590:LEU:HG | 1:G:599:VAL:HG11 | 2.02 | 0.42 |
| 1:G:2128:TYR:CD2 | 1:G:3673:MET:HB2 | 2.55 | 0.42 |
| 1:G:2272:PRO:HA | 1:G:2275:VAL:HG23 | 2.02 | 0.42 |
| 1:J:861:ILE:HG21 | 1:J:933:LEU:HB2 | 2.02 | 0.42 |
| 1:J:937:CYS:HB3 | 1:J:1053:ILE:HG23 | 2.01 | 0.42 |
| 1:J:1444:GLU:HG3 | 1:J:1508:ARG:HH21 | 1.84 | 0.42 |
| 1:J:1448:VAL:HG22 | 1:J:1554:VAL:HG12 | 2.01 | 0.42 |
| 1:J:2675:THR:HB | 1:J:2710:LEU:HD13 | 2.02 | 0.42 |
| 1:J:2976:HIS:CE1 | 1:J:2995:ILE:HD11 | 2.55 | 0.42 |
| 1:J:3410:PRO:O | 1:J:3414:ARG:HG2 | 2.20 | 0.42 |
| 1:J:3790:THR:HA | 1:J:3794:VAL:HG11 | 2.01 | 0.42 |
| 1:J:4248:ALA:HA | 1:J:4251:ILE:HG12 | 2.02 | 0.42 |
| 1:J:4581:LYS:HB2 | 1:J:4581:LYS:HE2 | 1.66 | 0.42 |
| 1:J:4979:THR:O | 1:J:4980:LEU:HD22 | 2.20 | 0.42 |
| 1:A:32:GLN:HB3 | 1:A:34:LYS:HE2 | 2.02 | 0.41 |
| 1:A:117:TYR:CG | 1:A:141:ALA:HB2 | 2.54 | 0.41 |
| 1:A:551:LEU:HD11 | 1:A:564:LEU:HD22 | 2.02 | 0.41 |
| 1:A:800:PHE:HB3 | 1:A:802:PHE:O | 2.20 | 0.41 |
| 1:A:1180:ARG:HD2 | 1:A:1180:ARG:N | 2.33 | 0.41 |
| 1:A:2672:LEU:HD22 | 1:A:2710:LEU:HD12 | 2.02 | 0.41 |
| 1:A:2762:THR:HA | 1:A:2765:LYS:HE3 | 2.02 | 0.41 |
| 1:A:3395:ARG:HB3 | 1:A:3454:GLU:OE2 | 2.20 | 0.41 |
| 1:A:3459:VAL:HG22 | 1:A:3464:ILE:HB | 2.02 | 0.41 |
| 1:A:4927:ILE:O | 1:A:4931:ILE:HG13 | 2.20 | 0.41 |
| 1:A:4980:LEU:HD13 | 1:A:4980:LEU:HA | 1.88 | 0.41 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 8:A:5121:POV:H311 | 8:J:5114:POV:H21E | 2.01 | 0.41 |
| 1:C:223:PHE:HE2 | 1:C:391:THR:HB | 1.85 | 0.41 |
| 1:C:553:ARG:HA | 1:C:553:ARG:HD2 | 1.87 | 0.41 |
| 1:C:907:LEU:HD23 | 1:C:913:LEU:HD23 | 2.01 | 0.41 |
| 1:C:2212:VAL:HG22 | 1:C:2256:TYR:CZ | 2.55 | 0.41 |
| 1:C:2229:VAL:O | 1:C:2232:CYS:HB2 | 2.20 | 0.41 |
| 1:C:3459:VAL:HG22 | 1:C:3464:ILE:HB | 2.02 | 0.41 |
| 8:C:5116:POV:H11A | 8:C:5116:POV:H15A | 1.91 | 0.41 |
| 3:F:58:GLY:HA2 | 3:F:61:GLU:OE2 | 2.20 | 0.41 |
| 1:G:442:ILE:HD11 | 1:G:514:SER:HB2 | 2.01 | 0.41 |
| 1:G:861:ILE:HG21 | 1:G:933:LEU:HB2 | 2.02 | 0.41 |
| 1:G:889:GLN:HG2 | 1:G:890:GLY:H | 1.85 | 0.41 |
| 1:G:1260:MET:HE2 | 1:G:1269:CYS:SG | 2.60 | 0.41 |
| 1:G:1291:LEU:HD12 | 1:G:1550:PRO:HG2 | 2.02 | 0.41 |
| 1:G:1970:GLN:HG3 | 1:G:3642:TYR:HA | 2.01 | 0.41 |
| 1:G:2332:LEU:O | 1:G:2336:ARG:HG3 | 2.19 | 0.41 |
| 1:G:2880:GLU:HB2 | 1:G:2908:TYR:CZ | 2.55 | 0.41 |
| 1:G:3018:LEU:HD11 | 1:G:3150:HIS:NE2 | 2.35 | 0.41 |
| 3:I:2:VAL:HG23 | 3:I:80:VAL:HG21 | 2.01 | 0.41 |
| 1:J:264:PRO:HG2 | 1:J:270:SER:HA | 2.02 | 0.41 |
| 1:J:1462:MET:HA | 1:J:1462:MET:HE3 | 2.02 | 0.41 |
| 1:J:2377:LEU:HD21 | 1:J:2468:GLY:HA3 | 2.01 | 0.41 |
| 1:J:3201:MET:HG3 | 1:J:3203:VAL:HG12 | 2.02 | 0.41 |
| 1:A:659:TYR:HB2 | 1:A:1017:ARG:HH12 | 1.86 | 0.41 |
| 1:A:2332:LEU:O | 1:A:2336:ARG:HG3 | 2.19 | 0.41 |
| 1:A:2502:MET:H | 1:A:2502:MET:HG2 | 1.71 | 0.41 |
| 1:A:2740:VAL:HG11 | 1:A:2815:ALA:HB2 | 2.01 | 0.41 |
| 1:A:3946:GLN:HA | 1:A:3949:ARG:HE | 1.85 | 0.41 |
| 1:C:223:PHE:HA | 1:C:230:CYS:HA | 2.02 | 0.41 |
| 1:C:902:ARG:HG2 | 1:C:903:LEU:HD23 | 2.01 | 0.41 |
| 1:C:1229:ASN:HB2 | 1:C:1827:ARG:HG3 | 2.01 | 0.41 |
| 1:C:2871:LEU:HA | 1:C:2874:MET:HE2 | 2.01 | 0.41 |
| 3:E:27:THR:HB | 3:E:100:ASP:HB3 | 2.01 | 0.41 |
| 3:F:27:THR:HB | 3:F:100:ASP:HB3 | 2.01 | 0.41 |
| 1:G:688:LEU:HD23 | 1:G:688:LEU:HA | 1.89 | 0.41 |
| 1:G:2212:VAL:HG22 | 1:G:2256:TYR:CZ | 2.55 | 0.41 |
| 1:G:3208:PRO:HD2 | 1:G:3245:VAL:HG23 | 2.03 | 0.41 |
| 1:G:3966:THR:O | 1:G:3970:GLN:N | 2.53 | 0.41 |
| 1:J:129:ASP:OD1 | 1:J:131:LEU:HG | 2.19 | 0.41 |
| 1:J:872:GLU:O | 1:J:876:GLU:HG2 | 2.19 | 0.41 |
| 1:J:902:ARG:HG2 | 1:J:903:LEU:HD23 | 2.02 | 0.41 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:J:1115:LEU:HG | 1:J:1123:VAL:HG11 | 2.00 | 0.41 |
| 1:J:1260:MET:HE2 | 1:J:1269:CYS:SG | 2.60 | 0.41 |
| 1:J:2229:VAL:HA | 1:J:2232:CYS:SG | 2.61 | 0.41 |
| 1:J:4210:VAL:HG21 | 1:J:4245:MET:HE2 | 2.01 | 0.41 |
| 2:K:109:THR:N | 2:K:110:PRO:HD2 | 2.35 | 0.41 |
| 1:A:598:LYS:HE3 | 1:A:598:LYS:HB3 | 1.80 | 0.41 |
| 1:A:2431:ASP:HB2 | 1:A:2501:SER:HB2 | 2.02 | 0.41 |
| 1:A:2439:GLU:O | 1:A:2443:ILE:HG12 | 2.19 | 0.41 |
| 1:A:3835:LEU:HD22 | 1:A:3880:PHE:CZ | 2.51 | 0.41 |
| 1:A:3935:TRP:HZ3 | 1:A:3994:HIS:CE1 | 2.38 | 0.41 |
| 1:C:3545:THR:O | 1:C:3549:VAL:HG13 | 2.20 | 0.41 |
| 1:C:3832:ILE:HG22 | 1:C:3836:MET:HE2 | 2.02 | 0.41 |
| 1:C:3935:TRP:HZ3 | 1:C:3994:HIS:CE1 | 2.38 | 0.41 |
| 1:G:223:PHE:HA | 1:G:230:CYS:HA | 2.02 | 0.41 |
| 1:G:264:PRO:HG2 | 1:G:270:SER:HA | 2.02 | 0.41 |
| 1:G:462:GLU:H | 1:G:462:GLU:HG3 | 1.62 | 0.41 |
| 1:G:872:GLU:O | 1:G:876:GLU:HG2 | 2.19 | 0.41 |
| 1:G:2576:ALA:HA | 1:G:2579:VAL:HG22 | 2.01 | 0.41 |
| 1:G:2628:PHE:CD2 | 1:G:2906:VAL:HG13 | 2.44 | 0.41 |
| 1:G:2758:PHE:O | 1:G:2758:PHE:HD1 | 2.04 | 0.41 |
| 1:G:2871:LEU:HA | 1:G:2874:MET:HE2 | 2.01 | 0.41 |
| 1:G:2976:HIS:CD2 | 1:G:2990:PRO:HD2 | 2.55 | 0.41 |
| 1:G:3545:THR:O | 1:G:3549:VAL:HG13 | 2.21 | 0.41 |
| 1:G:4231:MET:HE2 | 1:G:5022:PHE:CD1 | 2.55 | 0.41 |
| 1:G:4958:CYS:HA | 5:G:5105:ATP:N7 | 2.35 | 0.41 |
| 1:J:103:TYR:CE1 | 1:J:163:VAL:HG22 | 2.55 | 0.41 |
| 1:J:590:LEU:HG | 1:J:599:VAL:HG11 | 2.02 | 0.41 |
| 1:J:1291:LEU:HD12 | 1:J:1550:PRO:HG2 | 2.03 | 0.41 |
| 1:J:2138:LEU:HB3 | 1:J:3658:LYS:HE2 | 2.02 | 0.41 |
| 1:J:2431:ASP:HB2 | 1:J:2501:SER:HB2 | 2.02 | 0.41 |
| 1:J:2512:ILE:HG21 | 1:J:2518:LEU:HG | 2.02 | 0.41 |
| 1:J:2672:LEU:HD22 | 1:J:2710:LEU:HD12 | 2.02 | 0.41 |
| 1:J:2880:GLU:HB2 | 1:J:2908:TYR:CZ | 2.55 | 0.41 |
| 1:J:3395:ARG:HB3 | 1:J:3454:GLU:OE2 | 2.20 | 0.41 |
| 1:J:3832:ILE:HD13 | 1:J:3835:LEU:HD12 | 2.03 | 0.41 |
| 1:A:23:GLN:HG2 | 1:A:36:CYS:HB3 | 2.03 | 0.41 |
| 1:A:284:HIS:HE1 | 1:A:286:THR:HB | 1.84 | 0.41 |
| 1:A:462:GLU:H | 1:A:462:GLU:HG3 | 1.62 | 0.41 |
| 1:A:719:LEU:H | 1:A:737:LEU:HD23 | 1.84 | 0.41 |
| 1:A:3410:PRO:O | 1:A:3414:ARG:HG2 | 2.20 | 0.41 |
| 1:A:3966:THR:O | 1:A:3970:GLN:N | 2.53 | 0.41 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:19:GLU:HB3 | 1:C:205:ILE:HD12 | 2.03 | 0.41 |
| 1:C:23:GLN:HG2 | 1:C:36:CYS:HB3 | 2.03 | 0.41 |
| 1:C:472:ARG:NH2 | 1:C:534:ARG:H | 2.19 | 0.41 |
| 1:C:590:LEU:HG | 1:C:599:VAL:HG11 | 2.02 | 0.41 |
| 1:C:861:ILE:HG21 | 1:C:933:LEU:HB2 | 2.02 | 0.41 |
| 1:C:1055:PRO:HA | 1:C:1056:PRO:HD2 | 1.85 | 0.41 |
| 1:C:2576:ALA:HA | 1:C:2579:VAL:HG22 | 2.01 | 0.41 |
| 1:C:2641:LEU:HD21 | 1:C:2699:ALA:HA | 2.02 | 0.41 |
| 1:C:2652:TRP:CD1 | 1:C:2652:TRP:C | 2.99 | 0.41 |
| 1:C:2976:HIS:CD2 | 1:C:2990:PRO:HD2 | 2.55 | 0.41 |
| 1:C:3719:ASP:H | 1:C:3793:MET:HE2 | 1.85 | 0.41 |
| 8:C:5113:POV:H3A | 8:C:5115:POV:H24 | 2.03 | 0.41 |
| 3:E:2:VAL:HG13 | 3:E:74:LEU:HD12 | 2.01 | 0.41 |
| 1:G:32:GLN:HB3 | 1:G:34:LYS:HE2 | 2.02 | 0.41 |
| 1:G:178:ARG:HG2 | 1:G:195:PHE:CE1 | 2.55 | 0.41 |
| 1:G:622:THR:HA | 1:G:626:LEU:HD13 | 2.01 | 0.41 |
| 1:G:1106:ARG:HH21 | 1:G:1183:GLU:HG3 | 1.86 | 0.41 |
| 1:G:1251:GLU:H | 1:G:1251:GLU:HG3 | 1.71 | 0.41 |
| 1:G:2118:ARG:HG3 | 1:G:3721:LEU:HD22 | 2.02 | 0.41 |
| 1:G:2291:GLN:HB3 | 1:G:2293:GLN:OE1 | 2.21 | 0.41 |
| 1:G:3798:LEU:HD21 | 1:G:3884:LEU:HD13 | 2.02 | 0.41 |
| 1:G:4927:ILE:O | 1:G:4931:ILE:HG13 | 2.20 | 0.41 |
| 1:J:49:LEU:HG | 1:J:189:LEU:HB2 | 2.03 | 0.41 |
| 1:J:76:ARG:HD3 | 1:J:79:GLN:HE21 | 1.86 | 0.41 |
| 1:J:568:LEU:HD12 | 1:J:602:VAL:HG13 | 2.02 | 0.41 |
| 1:J:882:TRP:CD1 | 2:K:104:TYR:HE1 | 2.38 | 0.41 |
| 1:J:889:GLN:HG2 | 1:J:890:GLY:H | 1.85 | 0.41 |
| 1:J:1075:PHE:CE1 | 1:J:1194:LEU:HD12 | 2.55 | 0.41 |
| 1:J:2233:CYS:SG | 1:J:2270:SER:HB3 | 2.60 | 0.41 |
| 1:J:2272:PRO:HA | 1:J:2275:VAL:HG23 | 2.02 | 0.41 |
| 1:J:2291:GLN:HB3 | 1:J:2293:GLN:OE1 | 2.21 | 0.41 |
| 1:J:2306:GLY:HA2 | 1:J:2323:TRP:HZ3 | 1.83 | 0.41 |
| 1:J:2624:ARG:HD2 | 1:J:2911:LEU:HD23 | 2.03 | 0.41 |
| 1:J:2871:LEU:HA | 1:J:2874:MET:HE2 | 2.01 | 0.41 |
| 1:J:3192:GLU:HA | 1:J:3341:PHE:HZ | 1.85 | 0.41 |
| 1:J:3208:PRO:HD2 | 1:J:3245:VAL:HG23 | 2.03 | 0.41 |
| 8:J:5101:POV:H36 | 8:J:5101:POV:H39A | 1.79 | 0.41 |
| 2:K:109:THR:O | 2:K:113:GLU:HG2 | 2.20 | 0.41 |
| 1:A:195:PHE:CE2 | 1:C:2358:ILE:HB | 2.55 | 0.41 |
| 1:A:223:PHE:HE2 | 1:A:391:THR:HB | 1.85 | 0.41 |
| 1:A:861:ILE:HG21 | 1:A:933:LEU:HB2 | 2.02 | 0.41 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:1008:SER:HB2 | 1:A:1017:ARG:CZ | 2.51 | 0.41 |
| 1:A:1055:PRO:HA | 1:A:1056:PRO:HD2 | 1.85 | 0.41 |
| 1:A:1106:ARG:HH21 | 1:A:1183:GLU:HG3 | 1.85 | 0.41 |
| 1:A:2291:GLN:HB3 | 1:A:2293:GLN:OE1 | 2.21 | 0.41 |
| 1:A:2377:LEU:HD21 | 1:A:2468:GLY:HA3 | 2.02 | 0.41 |
| 1:A:2652:TRP:CD1 | 1:A:2652:TRP:C | 2.99 | 0.41 |
| 1:C:178:ARG:HG2 | 1:C:195:PHE:CE1 | 2.55 | 0.41 |
| 1:C:3798:LEU:HD21 | 1:C:3884:LEU:HD13 | 2.02 | 0.41 |
| 2:D:4:LEU:HB2 | 2:D:118:GLY:HA2 | 2.02 | 0.41 |
| 3:E:9:PRO:HA | 3:E:70:GLN:HG2 | 2.02 | 0.41 |
| 1:G:453:GLU:HA | 1:G:454:PRO:HD3 | 1.94 | 0.41 |
| 1:G:598:LYS:HB3 | 1:G:598:LYS:HE3 | 1.80 | 0.41 |
| 1:G:2124:LEU:HD23 | 1:G:2124:LEU:HA | 1.78 | 0.41 |
| 1:G:2641:LEU:HD21 | 1:G:2699:ALA:HA | 2.02 | 0.41 |
| 1:G:2976:HIS:CE1 | 1:G:2995:ILE:HD11 | 2.55 | 0.41 |
| 1:G:3832:ILE:HD13 | 1:G:3835:LEU:HD12 | 2.03 | 0.41 |
| 1:J:551:LEU:HD11 | 1:J:564:LEU:HD22 | 2.02 | 0.41 |
| 1:J:1055:PRO:HA | 1:J:1056:PRO:HD2 | 1.85 | 0.41 |
| 1:J:1106:ARG:HH21 | 1:J:1183:GLU:HG3 | 1.86 | 0.41 |
| 1:J:2976:HIS:CD2 | 1:J:2990:PRO:HD2 | 2.55 | 0.41 |
| 1:J:3007:ASN:OD1 | 1:J:3070:ILE:HG13 | 2.21 | 0.41 |
| 1:J:4956:THR:O | 1:J:4965:SER:N | 2.50 | 0.41 |
| 8:J:5101:POV:H211 | 8:J:5102:POV:H31B | 2.02 | 0.41 |
| 3:L:27:THR:HB | 3:L:100:ASP:HB3 | 2.01 | 0.41 |
| 1:A:19:GLU:HB3 | 1:A:205:ILE:HD12 | 2.03 | 0.41 |
| 1:A:233:ILE:HD11 | 1:A:242:ARG:O | 2.21 | 0.41 |
| 1:A:1691:GLN:OE1 | 1:A:1803:PRO:HD2 | 2.21 | 0.41 |
| 1:A:2641:LEU:HD21 | 1:A:2699:ALA:HA | 2.02 | 0.41 |
| 1:A:3003:LEU:HD21 | 1:A:3064:VAL:HA | 2.03 | 0.41 |
| 1:A:3007:ASN:OD1 | 1:A:3070:ILE:HG13 | 2.21 | 0.41 |
| 1:A:3366:ARG:HA | 1:A:3441:ILE:HD11 | 2.01 | 0.41 |
| 1:A:3539:ARG:NE | 1:A:3549:VAL:HA | 2.36 | 0.41 |
| 1:A:3790:THR:HA | 1:A:3794:VAL:HG11 | 2.01 | 0.41 |
| 1:C:718:GLY:HA3 | 1:C:737:LEU:HA | 2.02 | 0.41 |
| 1:C:891:TRP:HA | 1:C:902:ARG:HG3 | 2.03 | 0.41 |
| 1:C:1439:VAL:HA | 1:C:1562:ILE:HG13 | 2.03 | 0.41 |
| 1:C:2479:LEU:HD12 | 1:C:2485:LEU:HB3 | 2.02 | 0.41 |
| 1:C:2601:ASP:O | 1:C:2604:GLU:HG2 | 2.20 | 0.41 |
| 1:C:2670:GLU:CD | 1:C:2912:THR:HA | 2.45 | 0.41 |
| 1:C:2825:LYS:NZ | 1:C:2935:TYR:HB3 | 2.36 | 0.41 |
| 1:C:3395:ARG:HB3 | 1:C:3454:GLU:OE2 | 2.20 | 0.41 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:5012:LYS:HE3 | 1:C:5012:LYS:HB3 | 1.92 | 0.41 |
| 1:G:78:LEU:HA | 1:G:81:MET:HG3 | 2.03 | 0.41 |
| 1:G:718:GLY:HA3 | 1:G:737:LEU:HA | 2.02 | 0.41 |
| 1:G:996:TRP:HB2 | 2:H:114:TYR:HE1 | 1.85 | 0.41 |
| 1:G:1027:LEU:HD23 | 1:G:1027:LEU:HA | 1.90 | 0.41 |
| 1:G:1075:PHE:CE1 | 1:G:1194:LEU:HD12 | 2.55 | 0.41 |
| 1:G:1435:TYR:HE2 | 1:G:1564:PHE:HD1 | 1.68 | 0.41 |
| 1:G:1977:TYR:O | 1:G:1981:MET:HG2 | 2.20 | 0.41 |
| 1:G:2138:LEU:HB3 | 1:G:3658:LYS:HE2 | 2.02 | 0.41 |
| 1:G:3353:LEU:HD23 | 1:G:3353:LEU:HA | 1.92 | 0.41 |
| 1:G:3790:THR:HA | 1:G:3794:VAL:HG11 | 2.02 | 0.41 |
| 8:G:5119:POV:H39A | 8:G:5119:POV:H36 | 1.79 | 0.41 |
| 1:J:1068:ARG:HG3 | 1:J:1069:TRP:CD2 | 2.56 | 0.41 |
| 1:J:1435:TYR:HE2 | 1:J:1564:PHE:HD1 | 1.68 | 0.41 |
| 1:J:1977:TYR:O | 1:J:1981:MET:HG2 | 2.20 | 0.41 |
| 1:J:2118:ARG:HG3 | 1:J:3721:LEU:HD22 | 2.02 | 0.41 |
| 1:J:2447:LYS:HA | 1:J:2447:LYS:HD2 | 1.92 | 0.41 |
| 1:J:3003:LEU:HD21 | 1:J:3064:VAL:HA | 2.03 | 0.41 |
| 1:J:3345:ILE:HD12 | 1:J:3345:ILE:HA | 1.90 | 0.41 |
| 1:J:3719:ASP:H | 1:J:3793:MET:HE2 | 1.85 | 0.41 |
| 1:J:3966:THR:O | 1:J:3970:GLN:N | 2.53 | 0.41 |
| 1:J:4044:MET:HE3 | 1:J:4044:MET:HB2 | 1.93 | 0.41 |
| 1:A:130:LYS:HD2 | 1:A:130:LYS:H | 1.86 | 0.41 |
| 1:A:889:GLN:HG2 | 1:A:890:GLY:H | 1.85 | 0.41 |
| 1:A:1075:PHE:CE1 | 1:A:1194:LEU:HD12 | 2.55 | 0.41 |
| 1:A:1155:LEU:HD23 | 1:A:1155:LEU:HA | 1.85 | 0.41 |
| 1:A:1283:LEU:HD23 | 1:A:1283:LEU:HA | 1.93 | 0.41 |
| 1:A:2624:ARG:HD2 | 1:A:2911:LEU:HD23 | 2.03 | 0.41 |
| 1:A:3545:THR:O | 1:A:3549:VAL:HG13 | 2.20 | 0.41 |
| 1:A:4671:PHE:HE1 | 1:A:4716:TRP:HD1 | 1.69 | 0.41 |
| 1:A:4978:HIS:HA | 1:A:4982:GLU:HB3 | 2.02 | 0.41 |
| 1:A:5012:LYS:HE3 | 1:A:5012:LYS:HB3 | 1.92 | 0.41 |
| 1:C:195:PHE:CE2 | 1:G:2358:ILE:HB | 2.55 | 0.41 |
| 1:C:442:ILE:HD11 | 1:C:514:SER:HB2 | 2.01 | 0.41 |
| 1:C:1691:GLN:OE1 | 1:C:1803:PRO:HD2 | 2.21 | 0.41 |
| 1:C:2118:ARG:HG3 | 1:C:3721:LEU:HD22 | 2.02 | 0.41 |
| 1:C:2431:ASP:O | 1:C:2435:ARG:CB | 2.69 | 0.41 |
| 1:C:2976:HIS:CE1 | 1:C:2995:ILE:HD11 | 2.55 | 0.41 |
| 1:C:3010:PHE:CE1 | 1:C:3074:SER:HB2 | 2.55 | 0.41 |
| 1:C:3085:PRO:O | 1:C:3089:LYS:HG3 | 2.21 | 0.41 |
| 1:C:3410:PRO:O | 1:C:3414:ARG:HG2 | 2.20 | 0.41 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:4798:MET:HE1 | 1:C:4808:PHE:HD1 | 1.86 | 0.41 |
| 1:G:891:TRP:HA | 1:G:902:ARG:HG3 | 2.03 | 0.41 |
| 1:G:1068:ARG:HG3 | 1:G:1069:TRP:CD2 | 2.56 | 0.41 |
| 1:G:1094:ALA:HA | 1:G:1100:MET:HE1 | 2.02 | 0.41 |
| 1:G:2700:MET:HE2 | 1:G:2700:MET:HB2 | 1.95 | 0.41 |
| 1:G:3201:MET:HG3 | 1:G:3203:VAL:HG12 | 2.02 | 0.41 |
| 1:G:3391:GLU:HA | 1:G:3394:VAL:HG22 | 2.02 | 0.41 |
| 1:G:3410:PRO:HD3 | 1:G:3509:LEU:HD21 | 2.03 | 0.41 |
| 1:G:4245:MET:HE2 | 1:G:4245:MET:HB3 | 1.81 | 0.41 |
| 1:G:4248:ALA:HA | 1:G:4251:ILE:HG12 | 2.02 | 0.41 |
| 2:H:109:THR:N | 2:H:110:PRO:HD2 | 2.36 | 0.41 |
| 1:J:130:LYS:H | 1:J:130:LYS:HD2 | 1.86 | 0.41 |
| 1:J:233:ILE:HD11 | 1:J:242:ARG:O | 2.21 | 0.41 |
| 1:J:553:ARG:HA | 1:J:553:ARG:HD2 | 1.87 | 0.41 |
| 1:J:1008:SER:HB2 | 1:J:1017:ARG:CZ | 2.51 | 0.41 |
| 1:J:2641:LEU:HD21 | 1:J:2699:ALA:HA | 2.02 | 0.41 |
| 1:J:2825:LYS:NZ | 1:J:2935:TYR:HB3 | 2.36 | 0.41 |
| 1:J:3545:THR:O | 1:J:3549:VAL:HG13 | 2.20 | 0.41 |
| 1:A:1094:ALA:HA | 1:A:1100:MET:HE1 | 2.02 | 0.41 |
| 1:A:1958:LEU:HD23 | 1:A:2138:LEU:HD21 | 2.02 | 0.41 |
| 1:A:2380:ILE:O | 1:A:2384:ILE:HG13 | 2.21 | 0.41 |
| 1:A:2485:LEU:O | 1:A:2487:GLN:N | 2.53 | 0.41 |
| 1:A:2670:GLU:CD | 1:A:2912:THR:HA | 2.45 | 0.41 |
| 1:A:2700:MET:HE2 | 1:A:2700:MET:HB2 | 1.95 | 0.41 |
| 1:A:2825:LYS:NZ | 1:A:2935:TYR:HB3 | 2.36 | 0.41 |
| 1:A:3085:PRO:O | 1:A:3089:LYS:HG3 | 2.21 | 0.41 |
| 8:A:5121:POV:H13B | 8:A:5121:POV:H11A | 1.94 | 0.41 |
| 1:C:622:THR:HA | 1:C:626:LEU:HD13 | 2.01 | 0.41 |
| 1:C:1008:SER:HB2 | 1:C:1017:ARG:CZ | 2.51 | 0.41 |
| 1:C:1041:GLN:HA | 1:C:1044:ARG:HG2 | 2.03 | 0.41 |
| 1:C:1526:LEU:HD12 | 1:C:1526:LEU:HA | 1.91 | 0.41 |
| 1:C:1726:SER:O | 1:C:1730:MET:HG2 | 2.21 | 0.41 |
| 1:C:1727:ARG:O | 1:C:1731:LEU:HG | 2.21 | 0.41 |
| 1:C:2380:ILE:O | 1:C:2384:ILE:HG13 | 2.21 | 0.41 |
| 1:C:2762:THR:HA | 1:C:2765:LYS:HE3 | 2.02 | 0.41 |
| 1:C:4248:ALA:HA | 1:C:4251:ILE:HG12 | 2.03 | 0.41 |
| 2:D:85:LEU:HD13 | 2:D:125:VAL:HG22 | 2.03 | 0.41 |
| 3:E:4:ILE:HG23 | 3:E:72:ALA:HB1 | 2.03 | 0.41 |
| 1:G:1166:GLY:HA2 | 1:G:1217:CYS:SG | 2.61 | 0.41 |
| 1:G:2431:ASP:HB2 | 1:G:2501:SER:HB2 | 2.02 | 0.41 |
| 1:G:2601:ASP:O | 1:G:2604:GLU:HG2 | 2.21 | 0.41 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:G:2661:TRP:CD1 | 1:G:2662:ALA:H | 2.39 | 0.41 |
| 1:G:2672:LEU:HD22 | 1:G:2710:LEU:HD12 | 2.02 | 0.41 |
| 3:I:56:ILE:HD12 | 3:I:56:ILE:HA | 1.98 | 0.41 |
| 1:J:19:GLU:HB3 | 1:J:205:ILE:HD12 | 2.03 | 0.41 |
| 1:J:223:PHE:HE2 | 1:J:391:THR:HB | 1.85 | 0.41 |
| 1:J:548:VAL:HG11 | 1:J:582:HIS:HD2 | 1.86 | 0.41 |
| 1:J:659:TYR:HB2 | 1:J:1017:ARG:HH12 | 1.86 | 0.41 |
| 1:J:2758:PHE:O | 1:J:2758:PHE:HD1 | 2.04 | 0.41 |
| 1:J:4846:VAL:O | 1:J:4850:LEU:HG | 2.20 | 0.41 |
| 1:A:49:LEU:HG | 1:A:189:LEU:HB2 | 2.02 | 0.41 |
| 1:A:76:ARG:HD3 | 1:A:79:GLN:HE21 | 1.86 | 0.41 |
| 1:A:472:ARG:NH2 | 1:A:534:ARG:H | 2.19 | 0.41 |
| 1:A:568:LEU:HD12 | 1:A:602:VAL:HG13 | 2.02 | 0.41 |
| 1:A:590:LEU:HG | 1:A:599:VAL:HG11 | 2.03 | 0.41 |
| 1:A:908:VAL:HA | 1:A:963:ASN:HA | 2.03 | 0.41 |
| 1:A:1291:LEU:HD12 | 1:A:1550:PRO:HG2 | 2.02 | 0.41 |
| 1:A:1726:SER:O | 1:A:1730:MET:HG2 | 2.21 | 0.41 |
| 1:A:2359:ARG:HH22 | 1:J:177:GLU:HB3 | 1.86 | 0.41 |
| 1:A:2431:ASP:O | 1:A:2435:ARG:CB | 2.69 | 0.41 |
| 1:A:3065:VAL:O | 1:A:3069:HIS:HD2 | 2.04 | 0.41 |
| 1:A:3410:PRO:HD3 | 1:A:3509:LEU:HD21 | 2.03 | 0.41 |
| 1:A:4798:MET:HE1 | 1:A:4808:PHE:HD1 | 1.86 | 0.41 |
| 1:A:4918:ILE:HG13 | 8:C:5111:POV:H217 | 2.02 | 0.41 |
| 1:C:523:TYR:HD2 | 1:C:556:ALA:HB3 | 1.85 | 0.41 |
| 1:C:1166:GLY:HA2 | 1:C:1217:CYS:SG | 2.61 | 0.41 |
| 1:C:2447:LYS:HA | 1:C:2447:LYS:HD2 | 1.92 | 0.41 |
| 1:C:2758:PHE:O | 1:C:2758:PHE:HD1 | 2.04 | 0.41 |
| 1:C:3018:LEU:HD12 | 1:C:3018:LEU:HA | 1.86 | 0.41 |
| 1:C:3208:PRO:HD2 | 1:C:3245:VAL:HG23 | 2.03 | 0.41 |
| 1:C:3428:ASN:O | 1:C:3432:GLU:HG2 | 2.21 | 0.41 |
| 1:C:3757:GLU:O | 1:C:3761:GLN:HG3 | 2.21 | 0.41 |
| 1:C:4918:ILE:HG13 | 8:G:5111:POV:H217 | 2.02 | 0.41 |
| 8:C:5117:POV:H14B | 8:C:5117:POV:H11 | 1.79 | 0.41 |
| 3:F:98:ILE:HG21 | 3:F:98:ILE:HD13 | 1.65 | 0.41 |
| 1:G:19:GLU:HB3 | 1:G:205:ILE:HD12 | 2.03 | 0.41 |
| 1:G:130:LYS:H | 1:G:130:LYS:HD2 | 1.86 | 0.41 |
| 1:G:223:PHE:HE2 | 1:G:391:THR:HB | 1.85 | 0.41 |
| 1:G:523:TYR:HD2 | 1:G:556:ALA:HB3 | 1.85 | 0.41 |
| 1:G:1008:SER:HB2 | 1:G:1017:ARG:CZ | 2.51 | 0.41 |
| 1:G:1119:GLU:H | 1:G:1119:GLU:HG3 | 1.63 | 0.41 |
| 1:G:1462:MET:HA | 1:G:1462:MET:HE3 | 2.02 | 0.41 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:G:1526:LEU:HD12 | 1:G:1526:LEU:HA | 1.91 | 0.41 |
| 1:G:1726:SER:O | 1:G:1730:MET:HG2 | 2.21 | 0.41 |
| 1:G:2207:VAL:HG11 | 1:G:2235:PHE:CD1 | 2.56 | 0.41 |
| 1:G:2227:LYS:HE2 | 1:G:2227:LYS:HB2 | 1.94 | 0.41 |
| 1:G:2259:GLU:H | 1:G:2259:GLU:HG2 | 1.68 | 0.41 |
| 1:G:2670:GLU:CD | 1:G:2912:THR:HA | 2.45 | 0.41 |
| 1:G:2759:ALA:HB1 | 1:G:2806:ARG:HB2 | 2.03 | 0.41 |
| 1:G:2825:LYS:NZ | 1:G:2935:TYR:HB3 | 2.36 | 0.41 |
| 1:G:3001:ILE:O | 1:G:3005:LEU:HB2 | 2.21 | 0.41 |
| 1:G:3085:PRO:O | 1:G:3089:LYS:HG3 | 2.21 | 0.41 |
| 1:G:3832:ILE:HG22 | 1:G:3836:MET:HE2 | 2.02 | 0.41 |
| 1:G:3962:PHE:O | 1:G:3966:THR:HG23 | 2.21 | 0.41 |
| 1:G:4182:GLU:OE2 | 1:G:4982:GLU:HG3 | 2.21 | 0.41 |
| 1:G:4846:VAL:O | 1:G:4850:LEU:HG | 2.20 | 0.41 |
| 1:G:4918:ILE:HG13 | 8:J:5115:POV:H217 | 2.03 | 0.41 |
| 2:H:5:GLN:HA | 2:H:119:GLN:NE2 | 2.36 | 0.41 |
| 1:J:891:TRP:HA | 1:J:902:ARG:HG3 | 2.03 | 0.41 |
| 1:J:959:TYR:HE1 | 1:J:966:LYS:H | 1.69 | 0.41 |
| 1:J:1128:ARG:HB2 | 1:J:1130:GLN:HE22 | 1.86 | 0.41 |
| 1:J:2212:VAL:HG22 | 1:J:2256:TYR:CZ | 2.55 | 0.41 |
| 1:J:2661:TRP:CD1 | 1:J:2662:ALA:H | 2.39 | 0.41 |
| 1:J:2762:THR:HA | 1:J:2765:LYS:HE3 | 2.02 | 0.41 |
| 1:J:2978:GLU:O | 1:J:2981:VAL:HG12 | 2.21 | 0.41 |
| 1:J:3001:ILE:O | 1:J:3005:LEU:HB2 | 2.21 | 0.41 |
| 1:J:3168:THR:O | 1:J:3172:ILE:HG22 | 2.21 | 0.41 |
| 1:J:3410:PRO:HD3 | 1:J:3509:LEU:HD21 | 2.03 | 0.41 |
| 1:J:3832:ILE:HG22 | 1:J:3836:MET:HE2 | 2.02 | 0.41 |
| 1:J:3872:GLU:HG2 | 1:J:3874:VAL:H | 1.85 | 0.41 |
| 8:J:5112:POV:H311 | 8:J:5112:POV:H38 | 1.99 | 0.41 |
| 2:K:85:LEU:HD13 | 2:K:125:VAL:HG22 | 2.03 | 0.41 |
| 1:A:803:LEU:HD23 | 1:A:803:LEU:H | 1.86 | 0.41 |
| 1:A:1043:VAL:O | 1:A:1047:LEU:HG | 2.21 | 0.41 |
| 1:A:1727:ARG:O | 1:A:1731:LEU:HG | 2.21 | 0.41 |
| 1:A:1849:LEU:HD12 | 1:A:1942:LEU:HD11 | 2.03 | 0.41 |
| 1:A:2212:VAL:HG22 | 1:A:2256:TYR:CZ | 2.55 | 0.41 |
| 1:A:2259:GLU:H | 1:A:2259:GLU:HG2 | 1.68 | 0.41 |
| 1:A:2978:GLU:O | 1:A:2981:VAL:HG12 | 2.21 | 0.41 |
| 1:A:3077:ALA:O | 1:A:3079:THR:HG23 | 2.21 | 0.41 |
| 1:A:3208:PRO:HD2 | 1:A:3245:VAL:HG23 | 2.03 | 0.41 |
| 1:A:3262:ARG:HB2 | 1:A:3265:GLU:HB2 | 2.03 | 0.41 |
| 1:C:551:LEU:HD11 | 1:C:564:LEU:HD22 | 2.02 | 0.41 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:2138:LEU:HB3 | 1:C:3658:LYS:HE2 | 2.02 | 0.41 |
| 1:C:2265:LEU:HD13 | 1:C:2266:GLY:N | 2.36 | 0.41 |
| 1:C:2642:LYS:HA | 1:C:2645:THR:HG22 | 2.02 | 0.41 |
| 1:C:2759:ALA:HB1 | 1:C:2806:ARG:HB2 | 2.02 | 0.41 |
| 1:C:3989:VAL:HA | 1:C:3992:PHE:HB2 | 2.03 | 0.41 |
| 8:C:5113:POV:H11A | 8:C:5114:POV:H12 | 2.03 | 0.41 |
| 1:G:472:ARG:NH2 | 1:G:534:ARG:H | 2.19 | 0.41 |
| 1:G:1691:GLN:OE1 | 1:G:1803:PRO:HD2 | 2.21 | 0.41 |
| 1:G:2642:LYS:HA | 1:G:2645:THR:HG22 | 2.02 | 0.41 |
| 1:G:3003:LEU:HD21 | 1:G:3064:VAL:HA | 2.03 | 0.41 |
| 1:G:3946:GLN:HA | 1:G:3949:ARG:HE | 1.85 | 0.41 |
| 1:J:671:VAL:H | 1:J:740:PRO:HG3 | 1.85 | 0.41 |
| 1:J:2642:LYS:HA | 1:J:2645:THR:HG22 | 2.02 | 0.41 |
| 1:J:3065:VAL:O | 1:J:3069:HIS:HD2 | 2.04 | 0.41 |
| 1:J:3366:ARG:HA | 1:J:3441:ILE:HD11 | 2.01 | 0.41 |
| 1:J:3683:GLN:HA | 1:J:3686:GLU:HG2 | 2.02 | 0.41 |
| 1:J:3798:LEU:HD21 | 1:J:3884:LEU:HD13 | 2.02 | 0.41 |
| 1:J:4671:PHE:HE1 | 1:J:4716:TRP:HD1 | 1.69 | 0.41 |
| 1:A:891:TRP:HA | 1:A:902:ARG:HG3 | 2.03 | 0.40 |
| 1:A:902:ARG:HG2 | 1:A:903:LEU:HD23 | 2.02 | 0.40 |
| 1:A:1128:ARG:HB2 | 1:A:1130:GLN:HE22 | 1.86 | 0.40 |
| 1:A:2477:PRO:HB3 | 1:A:2487:GLN:HA | 2.03 | 0.40 |
| 1:A:2976:HIS:CD2 | 1:A:2990:PRO:HD2 | 2.55 | 0.40 |
| 1:A:3391:GLU:HA | 1:A:3394:VAL:HG22 | 2.02 | 0.40 |
| 1:A:3757:GLU:O | 1:A:3761:GLN:HG3 | 2.21 | 0.40 |
| 1:A:3832:ILE:HD13 | 1:A:3835:LEU:HD12 | 2.03 | 0.40 |
| 1:A:4018:ASP:O | 1:A:4021:LYS:HG2 | 2.21 | 0.40 |
| 1:A:4182:GLU:CD | 1:A:5028:PHE:HB2 | 2.46 | 0.40 |
| 1:A:4248:ALA:HA | 1:A:4251:ILE:HG12 | 2.02 | 0.40 |
| 1:C:32:GLN:HB3 | 1:C:34:LYS:HE2 | 2.02 | 0.40 |
| 1:C:76:ARG:HD3 | 1:C:79:GLN:HE21 | 1.86 | 0.40 |
| 1:C:3201:MET:HG3 | 1:C:3203:VAL:HG12 | 2.02 | 0.40 |
| 1:C:3946:GLN:HA | 1:C:3949:ARG:HE | 1.85 | 0.40 |
| 1:G:1000:ARG:HB2 | 1:G:1021:LEU:HD11 | 2.02 | 0.40 |
| 1:G:1128:ARG:HB2 | 1:G:1130:GLN:HE22 | 1.86 | 0.40 |
| 1:G:2265:LEU:HD13 | 1:G:2266:GLY:N | 2.37 | 0.40 |
| 1:G:2704:CYS:HB3 | 1:G:3008:GLN:HG2 | 2.02 | 0.40 |
| 1:G:2768:PHE:O | 1:G:2772:GLN:HG2 | 2.21 | 0.40 |
| 1:G:3262:ARG:HB2 | 1:G:3265:GLU:HB2 | 2.03 | 0.40 |
| 1:G:3757:GLU:O | 1:G:3761:GLN:HG3 | 2.21 | 0.40 |
| 1:G:3872:GLU:HG2 | 1:G:3874:VAL:H | 1.85 | 0.40 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:J:23:GLN:HG2 | 1:J:36:CYS:HB3 | 2.03 | 0.40 |
| 1:J:637:LEU:HD23 | 1:J:637:LEU:HA | 1.76 | 0.40 |
| 1:J:2380:ILE:O | 1:J:2384:ILE:HG13 | 2.21 | 0.40 |
| 1:J:2951:ILE:H | 1:J:2951:ILE:HD12 | 1.87 | 0.40 |
| 1:J:3010:PHE:CE1 | 1:J:3074:SER:HB2 | 2.56 | 0.40 |
| 1:J:3844:LEU:HD21 | 1:J:3936:TYR:HB2 | 2.03 | 0.40 |
| 1:J:4160:LEU:HD12 | 1:J:4163:PHE:HD2 | 1.87 | 0.40 |
| 1:J:4975:PHE:CZ | 1:J:4979:THR:HG21 | 2.55 | 0.40 |
| 1:A:548:VAL:HG11 | 1:A:582:HIS:HD2 | 1.86 | 0.40 |
| 1:A:1506:GLN:HG3 | 1:A:1507:GLY:H | 1.87 | 0.40 |
| 1:A:3001:ILE:O | 1:A:3005:LEU:HB2 | 2.21 | 0.40 |
| 1:A:3002:LEU:HD23 | 1:A:3002:LEU:HA | 1.86 | 0.40 |
| 1:A:3563:VAL:HG21 | 1:A:3573:MET:HG3 | 2.03 | 0.40 |
| 1:A:4956:THR:O | 1:A:4965:SER:N | 2.51 | 0.40 |
| 8:A:5105:POV:H35 | 8:A:5105:POV:H32 | 1.87 | 0.40 |
| 1:C:130:LYS:H | 1:C:130:LYS:HD2 | 1.86 | 0.40 |
| 1:C:264:PRO:HG2 | 1:C:270:SER:HA | 2.02 | 0.40 |
| 1:C:659:TYR:HB2 | 1:C:1017:ARG:HH12 | 1.86 | 0.40 |
| 1:C:869:ARG:HD2 | 1:C:870:ILE:HD11 | 2.04 | 0.40 |
| 1:C:1068:ARG:HG3 | 1:C:1069:TRP:CD2 | 2.56 | 0.40 |
| 1:C:1291:LEU:HD12 | 1:C:1550:PRO:HG2 | 2.02 | 0.40 |
| 1:C:1849:LEU:HD12 | 1:C:1942:LEU:HD11 | 2.04 | 0.40 |
| 1:C:1958:LEU:HD23 | 1:C:2138:LEU:HD21 | 2.02 | 0.40 |
| 1:C:1977:TYR:O | 1:C:1981:MET:HG2 | 2.21 | 0.40 |
| 1:C:2661:TRP:CD1 | 1:C:2662:ALA:H | 2.39 | 0.40 |
| 1:C:2704:CYS:HB3 | 1:C:3008:GLN:HG2 | 2.02 | 0.40 |
| 1:C:2768:PHE:O | 1:C:2772:GLN:HG2 | 2.21 | 0.40 |
| 1:C:2978:GLU:O | 1:C:2981:VAL:HG12 | 2.21 | 0.40 |
| 1:C:3262:ARG:HB2 | 1:C:3265:GLU:HB2 | 2.03 | 0.40 |
| 1:C:3563:VAL:HG21 | 1:C:3573:MET:HG3 | 2.04 | 0.40 |
| 1:C:3832:ILE:HD13 | 1:C:3835:LEU:HD12 | 2.03 | 0.40 |
| 1:C:4018:ASP:O | 1:C:4021:LYS:HG2 | 2.22 | 0.40 |
| 2:D:96:ASN:OD1 | 2:D:117:TRP:HA | 2.21 | 0.40 |
| 1:G:747:CYS:SG | 1:G:805:PRO:HG2 | 2.61 | 0.40 |
| 1:G:1727:ARG:O | 1:G:1731:LEU:HG | 2.21 | 0.40 |
| 1:G:2380:ILE:O | 1:G:2384:ILE:HG13 | 2.21 | 0.40 |
| 1:G:2624:ARG:HD2 | 1:G:2911:LEU:HD23 | 2.03 | 0.40 |
| 1:G:3046:LEU:HD12 | 1:G:3071:LEU:HG | 2.02 | 0.40 |
| 1:G:3459:VAL:HG22 | 1:G:3464:ILE:HB | 2.02 | 0.40 |
| 1:G:3683:GLN:HA | 1:G:3686:GLU:HG2 | 2.02 | 0.40 |
| 1:G:3844:LEU:HD21 | 1:G:3936:TYR:HB2 | 2.03 | 0.40 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:J:263:GLU:HA | 1:J:264:PRO:HD3 | 1.97 | 0.40 |
| 1:J:1251:GLU:H | 1:J:1251:GLU:HG3 | 1.71 | 0.40 |
| 1:J:1526:LEU:HD12 | 1:J:1526:LEU:HA | 1.91 | 0.40 |
| 1:J:2303:ALA:HB2 | 1:J:2363:CYS:SG | 2.61 | 0.40 |
| 1:J:3072:ALA:HA | 1:J:3075:LEU:CD2 | 2.49 | 0.40 |
| 1:J:3459:VAL:HG22 | 1:J:3464:ILE:HB | 2.02 | 0.40 |
| 1:J:3563:VAL:HG12 | 1:J:3569:LEU:HB3 | 2.03 | 0.40 |
| 3:L:24:VAL:HG21 | 3:L:101:VAL:HG13 | 2.03 | 0.40 |
| 1:A:177:GLU:HB3 | 1:C:2359:ARG:HH22 | 1.86 | 0.40 |
| 1:A:2621:HIS:CE1 | 1:A:2624:ARG:HH22 | 2.39 | 0.40 |
| 1:A:2642:LYS:HA | 1:A:2645:THR:HG22 | 2.02 | 0.40 |
| 1:A:3428:ASN:O | 1:A:3432:GLU:HG2 | 2.21 | 0.40 |
| 1:A:3541:ALA:O | 1:A:3543:LYS:HD2 | 2.20 | 0.40 |
| 1:A:3563:VAL:HG12 | 1:A:3569:LEU:HB3 | 2.02 | 0.40 |
| 1:A:3832:ILE:HG22 | 1:A:3836:MET:HE2 | 2.02 | 0.40 |
| 1:A:3844:LEU:HD21 | 1:A:3936:TYR:HB2 | 2.03 | 0.40 |
| 1:A:4794:TRP:NE1 | 8:A:5112:POV:H37A | 2.30 | 0.40 |
| 1:A:4851:TYR:HD1 | 1:A:4916:PHE:CE1 | 2.40 | 0.40 |
| 1:C:4927:ILE:O | 1:C:4931:ILE:HG13 | 2.20 | 0.40 |
| 3:E:18:LYS:HA | 3:E:18:LYS:HD2 | 1.99 | 0.40 |
| 3:E:24:VAL:HG21 | 3:E:101:VAL:HG13 | 2.03 | 0.40 |
| 1:G:23:GLN:HG2 | 1:G:36:CYS:HB3 | 2.03 | 0.40 |
| 1:G:49:LEU:HG | 1:G:189:LEU:HB2 | 2.02 | 0.40 |
| 1:G:708:GLY:HA3 | 1:G:722:TRP:HB3 | 2.04 | 0.40 |
| 1:G:902:ARG:HG2 | 1:G:903:LEU:HD23 | 2.02 | 0.40 |
| 1:G:2377:LEU:HG | 1:G:2465:ASP:HA | 2.02 | 0.40 |
| 1:G:2431:ASP:O | 1:G:2435:ARG:CB | 2.69 | 0.40 |
| 1:G:2762:THR:HA | 1:G:2765:LYS:HE3 | 2.02 | 0.40 |
| 1:G:3563:VAL:HG12 | 1:G:3569:LEU:HB3 | 2.03 | 0.40 |
| 1:G:4160:LEU:HD12 | 1:G:4163:PHE:HD2 | 1.87 | 0.40 |
| 1:J:223:PHE:HA | 1:J:230:CYS:HA | 2.02 | 0.40 |
| 1:J:1726:SER:O | 1:J:1730:MET:HG2 | 2.21 | 0.40 |
| 1:J:2431:ASP:O | 1:J:2435:ARG:CB | 2.69 | 0.40 |
| 1:J:2652:TRP:CD1 | 1:J:2652:TRP:C | 2.99 | 0.40 |
| 1:J:3085:PRO:O | 1:J:3089:LYS:HG3 | 2.21 | 0.40 |
| 1:J:3262:ARG:HB2 | 1:J:3265:GLU:HB2 | 2.03 | 0.40 |
| 1:J:4927:ILE:O | 1:J:4931:ILE:HG13 | 2.20 | 0.40 |
| 3:L:74:LEU:HD13 | 3:L:101:VAL:CG2 | 2.51 | 0.40 |
| 1:A:78:LEU:HA | 1:A:81:MET:HG3 | 2.02 | 0.40 |
| 1:A:708:GLY:HA3 | 1:A:722:TRP:HB3 | 2.04 | 0.40 |
| 1:A:1068:ARG:HG3 | 1:A:1069:TRP:CD2 | 2.56 | 0.40 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:A:1977:TYR:O | 1:A:1981:MET:HG2 | 2.20 | 0.40 |
| 1:A:2661:TRP:CD1 | 1:A:2662:ALA:H | 2.39 | 0.40 |
| 1:A:2758:PHE:O | 1:A:2758:PHE:HD1 | 2.04 | 0.40 |
| 1:A:2759:ALA:HB1 | 1:A:2806:ARG:HB2 | 2.03 | 0.40 |
| 1:A:2951:ILE:H | 1:A:2951:ILE:HD12 | 1.87 | 0.40 |
| 1:A:3989:VAL:HA | 1:A:3992:PHE:HB2 | 2.03 | 0.40 |
| 1:A:4160:LEU:HD12 | 1:A:4163:PHE:HD2 | 1.87 | 0.40 |
| 2:B:85:LEU:HD13 | 2:B:125:VAL:HG22 | 2.03 | 0.40 |
| 1:C:178:ARG:HG2 | 1:C:195:PHE:CD1 | 2.56 | 0.40 |
| 1:C:1106:ARG:HH21 | 1:C:1183:GLU:HG3 | 1.85 | 0.40 |
| 1:C:1506:GLN:HG3 | 1:C:1507:GLY:H | 1.87 | 0.40 |
| 1:C:2291:GLN:HB3 | 1:C:2293:GLN:OE1 | 2.21 | 0.40 |
| 1:C:3683:GLN:HA | 1:C:3686:GLU:HG2 | 2.02 | 0.40 |
| 1:G:177:GLU:HB3 | 1:J:2359:ARG:HH22 | 1.87 | 0.40 |
| 1:G:233:ILE:HD11 | 1:G:242:ARG:O | 2.21 | 0.40 |
| 1:G:1144:GLN:HG2 | 1:G:1147:ASP:CG | 2.46 | 0.40 |
| 1:G:3179:LYS:HE3 | 1:G:3179:LYS:HB3 | 1.93 | 0.40 |
| 1:G:4018:ASP:O | 1:G:4021:LYS:HG2 | 2.22 | 0.40 |
| 1:G:4735:GLU:H | 1:G:4735:GLU:HG3 | 1.74 | 0.40 |
| 1:G:4779:LYS:HA | 1:G:4782:VAL:HG22 | 2.04 | 0.40 |
| 1:G:4851:TYR:HA | 1:G:4854:VAL:HG22 | 2.04 | 0.40 |
| 1:J:233:ILE:HG23 | 1:J:234:SER:N | 2.37 | 0.40 |
| 1:J:472:ARG:NH2 | 1:J:534:ARG:H | 2.19 | 0.40 |
| 1:J:2794:TYR:HD1 | 1:J:2802:LYS:HE2 | 1.86 | 0.40 |
| 1:J:3713:LYS:HE3 | 1:J:3713:LYS:HB2 | 1.90 | 0.40 |
| 1:J:3946:GLN:HA | 1:J:3949:ARG:HE | 1.85 | 0.40 |
| 1:J:3962:PHE:O | 1:J:3966:THR:HG23 | 2.21 | 0.40 |
| 1:J:4018:ASP:O | 1:J:4021:LYS:HG2 | 2.21 | 0.40 |
| 1:J:4779:LYS:HA | 1:J:4782:VAL:HG22 | 2.04 | 0.40 |
| 1:J:4851:TYR:HA | 1:J:4854:VAL:HG22 | 2.04 | 0.40 |
| 1:J:4992:LEU:O | 1:J:4996:ILE:HG13 | 2.22 | 0.40 |
| 3:L:4:ILE:HD11 | 3:L:62:GLY:HA2 | 2.03 | 0.40 |
| 1:A:178:ARG:HG2 | 1:A:195:PHE:CD1 | 2.56 | 0.40 |
| 1:A:2440:MET:HA | 1:A:2440:MET:HE2 | 2.04 | 0.40 |
| 1:A:2768:PHE:O | 1:A:2772:GLN:HG2 | 2.21 | 0.40 |
| 1:A:2878:LEU:HD21 | 1:A:2926:LEU:HD22 | 2.04 | 0.40 |
| 1:A:3683:GLN:HA | 1:A:3686:GLU:HG2 | 2.02 | 0.40 |
| 1:A:3709:ALA:HB2 | 1:A:3782:MET:SD | 2.62 | 0.40 |
| 1:A:3962:PHE:O | 1:A:3966:THR:HG23 | 2.21 | 0.40 |
| 1:C:49:LEU:HG | 1:C:189:LEU:HB2 | 2.03 | 0.40 |
| 1:C:548:VAL:HG11 | 1:C:582:HIS:HD2 | 1.86 | 0.40 |

*Continued on next page...*

*Continued from previous page...*

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|---|---|---|---|
| 1:C:688:LEU:HD23 | 1:C:688:LEU:HA | 1.89 | 0.40 |
| 1:C:1075:PHE:CE1 | 1:C:1194:LEU:HD12 | 2.56 | 0.40 |
| 1:C:1299:GLN:OE1 | 1:C:1545:ASN:HB2 | 2.22 | 0.40 |
| 1:C:1435:TYR:HE2 | 1:C:1564:PHE:HD1 | 1.68 | 0.40 |
| 1:C:2340:PHE:HE1 | 1:C:2344:GLU:N | 2.20 | 0.40 |
| 1:C:2472:LEU:HD12 | 1:C:2472:LEU:HA | 1.92 | 0.40 |
| 1:C:3906:GLN:NE2 | 1:C:3913:ILE:H | 2.19 | 0.40 |
| 1:C:4671:PHE:HE1 | 1:C:4716:TRP:HD1 | 1.69 | 0.40 |
| 1:G:1506:GLN:HG3 | 1:G:1507:GLY:H | 1.87 | 0.40 |
| 1:G:2652:TRP:CD1 | 1:G:2652:TRP:C | 2.99 | 0.40 |
| 1:G:3014:CYS:HB3 | 1:G:3073:ARG:HD3 | 2.03 | 0.40 |
| 1:G:3835:LEU:HD22 | 1:G:3880:PHE:CZ | 2.51 | 0.40 |
| 1:G:4572:ALA:O | 1:G:4576:ILE:HG13 | 2.22 | 0.40 |
| 1:J:32:GLN:HB3 | 1:J:34:LYS:HE2 | 2.02 | 0.40 |
| 1:J:1506:GLN:HG3 | 1:J:1507:GLY:H | 1.87 | 0.40 |
| 1:J:1727:ARG:O | 1:J:1731:LEU:HG | 2.21 | 0.40 |
| 1:J:3935:TRP:HZ3 | 1:J:3994:HIS:CE1 | 2.38 | 0.40 |
| 1:J:4711:PHE:CD1 | 1:J:4711:PHE:C | 3.00 | 0.40 |
| 1:J:4952:GLU:O | 1:J:4956:THR:HG23 | 2.21 | 0.40 |
| 8:J:5113:POV:H13B | 8:J:5113:POV:H11A | 1.95 | 0.40 |

There are no symmetry-related clashes.

## 5.3 Torsion angles (i)

### 5.3.1 Protein backbone (i)

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

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

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|---|---|---|---|---|---|---|---|
| 1 | A | 4292/5027 (85%) | 4162 (97%) | 128 (3%) | 2 (0%) | 100 | 100 |
| 1 | C | 4292/5027 (85%) | 4162 (97%) | 129 (3%) | 1 (0%) | 100 | 100 |
| 1 | G | 4292/5027 (85%) | 4164 (97%) | 127 (3%) | 1 (0%) | 100 | 100 |
| 1 | J | 4290/5027 (85%) | 4161 (97%) | 127 (3%) | 2 (0%) | 100 | 100 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|---|---|---|---|---|---|---|---|
| 2 | B | 124/126 (98%) | 112 (90%) | 12 (10%) | 0 | 100 | 100 |
| 2 | D | 124/126 (98%) | 111 (90%) | 13 (10%) | 0 | 100 | 100 |
| 2 | H | 124/126 (98%) | 112 (90%) | 12 (10%) | 0 | 100 | 100 |
| 2 | K | 124/126 (98%) | 109 (88%) | 14 (11%) | 1 (1%) | 16 | 44 |
| 3 | E | 105/107 (98%) | 100 (95%) | 5 (5%) | 0 | 100 | 100 |
| 3 | F | 105/107 (98%) | 99 (94%) | 6 (6%) | 0 | 100 | 100 |
| 3 | I | 105/107 (98%) | 101 (96%) | 4 (4%) | 0 | 100 | 100 |
| 3 | L | 105/107 (98%) | 100 (95%) | 5 (5%) | 0 | 100 | 100 |
| All | All | 18082/21040 (86%) | 17493 (97%) | 582 (3%) | 7 (0%) | 100 | 100 |

All (7) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 908 | VAL |
| 1 | C | 908 | VAL |
| 1 | G | 908 | VAL |
| 1 | J | 908 | VAL |
| 2 | K | 102 | ASN |
| 1 | A | 2486 | VAL |
| 1 | J | 2486 | VAL |

### 5.3.2 Protein sidechains (i)

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

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

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles | |
|---|---|---|---|---|---|---|
| 1 | A | 3688/4270 (86%) | 3670 (100%) | 18 (0%) | 81 | 81 |
| 1 | C | 3688/4270 (86%) | 3666 (99%) | 22 (1%) | 78 | 80 |
| 1 | G | 3688/4270 (86%) | 3666 (99%) | 22 (1%) | 78 | 80 |
| 1 | J | 3688/4270 (86%) | 3673 (100%) | 15 (0%) | 84 | 83 |
| 2 | B | 103/104 (99%) | 100 (97%) | 3 (3%) | 37 | 60 |
| 2 | D | 103/104 (99%) | 102 (99%) | 1 (1%) | 68 | 75 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Analysed | Rotameric | Outliers | Percentiles |
|---|---|---|---|---|---|
| 2 | H | 103/104 (99%) | 101 (98%) | 2 (2%) | 50 66 |
| 2 | K | 103/104 (99%) | 100 (97%) | 3 (3%) | 37 60 |
| 3 | E | 88/88 (100%) | 85 (97%) | 3 (3%) | 32 57 |
| 3 | F | 88/88 (100%) | 86 (98%) | 2 (2%) | 44 63 |
| 3 | I | 88/88 (100%) | 84 (96%) | 4 (4%) | 24 51 |
| 3 | L | 88/88 (100%) | 84 (96%) | 4 (4%) | 24 51 |
| All | All | 15516/17848 (87%) | 15417 (99%) | 99 (1%) | 76 80 |

All (99) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 13 | PHE |
| 1 | A | 49 | LEU |
| 1 | A | 533 | ASN |
| 1 | A | 1130 | GLN |
| 1 | A | 1163 | THR |
| 1 | A | 1647 | CYS |
| 1 | A | 2192 | TYR |
| 1 | A | 2203 | MET |
| 1 | A | 2233 | CYS |
| 1 | A | 2700 | MET |
| 1 | A | 2905 | LEU |
| 1 | A | 3075 | LEU |
| 1 | A | 3078 | ARG |
| 1 | A | 3175 | LEU |
| 1 | A | 4044 | MET |
| 1 | A | 4540 | PHE |
| 1 | A | 4705 | VAL |
| 1 | A | 4980 | LEU |
| 2 | B | 68 | THR |
| 2 | B | 113 | GLU |
| 2 | B | 117 | TRP |
| 1 | C | 13 | PHE |
| 1 | C | 49 | LEU |
| 1 | C | 533 | ASN |
| 1 | C | 960 | MET |
| 1 | C | 1130 | GLN |
| 1 | C | 1647 | CYS |
| 1 | C | 2192 | TYR |
| 1 | C | 2203 | MET |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | C | 2274 | ASP |
| 1 | C | 2308 | GLN |
| 1 | C | 2463 | LEU |
| 1 | C | 2485 | LEU |
| 1 | C | 2486 | VAL |
| 1 | C | 2700 | MET |
| 1 | C | 2905 | LEU |
| 1 | C | 3071 | LEU |
| 1 | C | 3075 | LEU |
| 1 | C | 4044 | MET |
| 1 | C | 4540 | PHE |
| 1 | C | 4705 | VAL |
| 1 | C | 4980 | LEU |
| 1 | C | 4981 | GLU |
| 2 | D | 68 | THR |
| 3 | E | 14 | THR |
| 3 | E | 37 | ASP |
| 3 | E | 79 | ASP |
| 3 | F | 14 | THR |
| 3 | F | 37 | ASP |
| 1 | G | 13 | PHE |
| 1 | G | 49 | LEU |
| 1 | G | 533 | ASN |
| 1 | G | 741 | GLU |
| 1 | G | 742 | ASP |
| 1 | G | 1036 | ARG |
| 1 | G | 1130 | GLN |
| 1 | G | 1647 | CYS |
| 1 | G | 2192 | TYR |
| 1 | G | 2203 | MET |
| 1 | G | 2308 | GLN |
| 1 | G | 2518 | LEU |
| 1 | G | 2700 | MET |
| 1 | G | 2905 | LEU |
| 1 | G | 3071 | LEU |
| 1 | G | 3073 | ARG |
| 1 | G | 3075 | LEU |
| 1 | G | 3175 | LEU |
| 1 | G | 4044 | MET |
| 1 | G | 4540 | PHE |
| 1 | G | 4705 | VAL |
| 1 | G | 4980 | LEU |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | H | 68 | THR |
| 2 | H | 117 | TRP |
| 3 | I | 14 | THR |
| 3 | I | 37 | ASP |
| 3 | I | 47 | LYS |
| 3 | I | 61 | GLU |
| 1 | J | 13 | PHE |
| 1 | J | 49 | LEU |
| 1 | J | 533 | ASN |
| 1 | J | 1130 | GLN |
| 1 | J | 1647 | CYS |
| 1 | J | 2135 | LEU |
| 1 | J | 2192 | TYR |
| 1 | J | 2203 | MET |
| 1 | J | 2233 | CYS |
| 1 | J | 2700 | MET |
| 1 | J | 2905 | LEU |
| 1 | J | 3175 | LEU |
| 1 | J | 4540 | PHE |
| 1 | J | 4705 | VAL |
| 1 | J | 4980 | LEU |
| 2 | K | 68 | THR |
| 2 | K | 98 | ASP |
| 2 | K | 100 | VAL |
| 3 | L | 14 | THR |
| 3 | L | 37 | ASP |
| 3 | L | 43 | ASN |
| 3 | L | 57 | LYS |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (230) such sidechains are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 151 | HIS |
| 1 | A | 412 | ASN |
| 1 | A | 461 | HIS |
| 1 | A | 465 | GLN |
| 1 | A | 473 | ASN |
| 1 | A | 533 | ASN |
| 1 | A | 582 | HIS |
| 1 | A | 636 | ASN |
| 1 | A | 720 | HIS |
| 1 | A | 735 | GLN |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 838 | HIS |
| 1 | A | 921 | ASN |
| 1 | A | 949 | ASN |
| 1 | A | 1084 | GLN |
| 1 | A | 1127 | HIS |
| 1 | A | 1198 | GLN |
| 1 | A | 1459 | GLN |
| 1 | A | 1541 | GLN |
| 1 | A | 1569 | GLN |
| 1 | A | 1571 | ASN |
| 1 | A | 1660 | GLN |
| 1 | A | 1665 | HIS |
| 1 | A | 1693 | GLN |
| 1 | A | 1719 | HIS |
| 1 | A | 1776 | HIS |
| 1 | A | 1973 | GLN |
| 1 | A | 2007 | ASN |
| 1 | A | 2204 | HIS |
| 1 | A | 2283 | ASN |
| 1 | A | 2284 | ASN |
| 1 | A | 2599 | GLN |
| 1 | A | 2774 | ASN |
| 1 | A | 2856 | ASN |
| 1 | A | 2924 | GLN |
| 1 | A | 3052 | HIS |
| 1 | A | 3066 | ASN |
| 1 | A | 3146 | HIS |
| 1 | A | 3150 | HIS |
| 1 | A | 3326 | ASN |
| 1 | A | 3456 | GLN |
| 1 | A | 3611 | HIS |
| 1 | A | 3667 | HIS |
| 1 | A | 3734 | HIS |
| 1 | A | 3869 | GLN |
| 1 | A | 3882 | GLN |
| 1 | A | 3927 | GLN |
| 1 | A | 4020 | GLN |
| 1 | A | 4204 | GLN |
| 1 | A | 4650 | HIS |
| 1 | A | 4700 | GLN |
| 1 | A | 4857 | ASN |
| 2 | B | 1 | GLN |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 2 | B | 3 | GLN |
| 2 | B | 111 | ASN |
| 2 | B | 119 | GLN |
| 1 | C | 151 | HIS |
| 1 | C | 412 | ASN |
| 1 | C | 461 | HIS |
| 1 | C | 465 | GLN |
| 1 | C | 473 | ASN |
| 1 | C | 533 | ASN |
| 1 | C | 582 | HIS |
| 1 | C | 636 | ASN |
| 1 | C | 838 | HIS |
| 1 | C | 921 | ASN |
| 1 | C | 963 | ASN |
| 1 | C | 1041 | GLN |
| 1 | C | 1084 | GLN |
| 1 | C | 1127 | HIS |
| 1 | C | 1198 | GLN |
| 1 | C | 1459 | GLN |
| 1 | C | 1541 | GLN |
| 1 | C | 1569 | GLN |
| 1 | C | 1571 | ASN |
| 1 | C | 1610 | ASN |
| 1 | C | 1660 | GLN |
| 1 | C | 1665 | HIS |
| 1 | C | 1693 | GLN |
| 1 | C | 1719 | HIS |
| 1 | C | 1776 | HIS |
| 1 | C | 1825 | HIS |
| 1 | C | 1837 | GLN |
| 1 | C | 1973 | GLN |
| 1 | C | 2007 | ASN |
| 1 | C | 2283 | ASN |
| 1 | C | 2284 | ASN |
| 1 | C | 2599 | GLN |
| 1 | C | 2774 | ASN |
| 1 | C | 2856 | ASN |
| 1 | C | 2924 | GLN |
| 1 | C | 2933 | ASN |
| 1 | C | 2961 | GLN |
| 1 | C | 3052 | HIS |
| 1 | C | 3066 | ASN |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | C | 3150 | HIS |
| 1 | C | 3326 | ASN |
| 1 | C | 3456 | GLN |
| 1 | C | 3611 | HIS |
| 1 | C | 3667 | HIS |
| 1 | C | 3869 | GLN |
| 1 | C | 3927 | GLN |
| 1 | C | 3978 | GLN |
| 1 | C | 4020 | GLN |
| 1 | C | 4204 | GLN |
| 1 | C | 4650 | HIS |
| 1 | C | 4700 | GLN |
| 1 | C | 4707 | ASN |
| 1 | C | 4857 | ASN |
| 2 | D | 3 | GLN |
| 2 | D | 119 | GLN |
| 3 | E | 31 | GLN |
| 3 | E | 43 | ASN |
| 3 | F | 31 | GLN |
| 3 | F | 43 | ASN |
| 1 | G | 151 | HIS |
| 1 | G | 412 | ASN |
| 1 | G | 461 | HIS |
| 1 | G | 465 | GLN |
| 1 | G | 473 | ASN |
| 1 | G | 533 | ASN |
| 1 | G | 582 | HIS |
| 1 | G | 636 | ASN |
| 1 | G | 720 | HIS |
| 1 | G | 838 | HIS |
| 1 | G | 921 | ASN |
| 1 | G | 963 | ASN |
| 1 | G | 1041 | GLN |
| 1 | G | 1084 | GLN |
| 1 | G | 1127 | HIS |
| 1 | G | 1459 | GLN |
| 1 | G | 1541 | GLN |
| 1 | G | 1569 | GLN |
| 1 | G | 1610 | ASN |
| 1 | G | 1660 | GLN |
| 1 | G | 1665 | HIS |
| 1 | G | 1693 | GLN |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | G | 1719 | HIS |
| 1 | G | 1776 | HIS |
| 1 | G | 1825 | HIS |
| 1 | G | 1837 | GLN |
| 1 | G | 1973 | GLN |
| 1 | G | 2007 | ASN |
| 1 | G | 2204 | HIS |
| 1 | G | 2283 | ASN |
| 1 | G | 2284 | ASN |
| 1 | G | 2599 | GLN |
| 1 | G | 2774 | ASN |
| 1 | G | 2856 | ASN |
| 1 | G | 2924 | GLN |
| 1 | G | 2933 | ASN |
| 1 | G | 2961 | GLN |
| 1 | G | 3052 | HIS |
| 1 | G | 3066 | ASN |
| 1 | G | 3146 | HIS |
| 1 | G | 3150 | HIS |
| 1 | G | 3326 | ASN |
| 1 | G | 3449 | HIS |
| 1 | G | 3456 | GLN |
| 1 | G | 3611 | HIS |
| 1 | G | 3667 | HIS |
| 1 | G | 3734 | HIS |
| 1 | G | 3869 | GLN |
| 1 | G | 3927 | GLN |
| 1 | G | 4020 | GLN |
| 1 | G | 4204 | GLN |
| 1 | G | 4650 | HIS |
| 1 | G | 4700 | GLN |
| 1 | G | 4857 | ASN |
| 2 | H | 3 | GLN |
| 2 | H | 102 | ASN |
| 2 | H | 119 | GLN |
| 3 | I | 31 | GLN |
| 3 | I | 65 | GLN |
| 1 | J | 98 | HIS |
| 1 | J | 151 | HIS |
| 1 | J | 412 | ASN |
| 1 | J | 461 | HIS |
| 1 | J | 465 | GLN |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | J | 473 | ASN |
| 1 | J | 533 | ASN |
| 1 | J | 636 | ASN |
| 1 | J | 720 | HIS |
| 1 | J | 838 | HIS |
| 1 | J | 921 | ASN |
| 1 | J | 1041 | GLN |
| 1 | J | 1084 | GLN |
| 1 | J | 1127 | HIS |
| 1 | J | 1198 | GLN |
| 1 | J | 1459 | GLN |
| 1 | J | 1541 | GLN |
| 1 | J | 1569 | GLN |
| 1 | J | 1571 | ASN |
| 1 | J | 1610 | ASN |
| 1 | J | 1660 | GLN |
| 1 | J | 1665 | HIS |
| 1 | J | 1693 | GLN |
| 1 | J | 1719 | HIS |
| 1 | J | 1776 | HIS |
| 1 | J | 1825 | HIS |
| 1 | J | 1837 | GLN |
| 1 | J | 1973 | GLN |
| 1 | J | 2007 | ASN |
| 1 | J | 2204 | HIS |
| 1 | J | 2283 | ASN |
| 1 | J | 2284 | ASN |
| 1 | J | 2308 | GLN |
| 1 | J | 2599 | GLN |
| 1 | J | 2621 | HIS |
| 1 | J | 2774 | ASN |
| 1 | J | 2856 | ASN |
| 1 | J | 2881 | ASN |
| 1 | J | 2924 | GLN |
| 1 | J | 3052 | HIS |
| 1 | J | 3066 | ASN |
| 1 | J | 3150 | HIS |
| 1 | J | 3326 | ASN |
| 1 | J | 3456 | GLN |
| 1 | J | 3611 | HIS |
| 1 | J | 3667 | HIS |
| 1 | J | 3869 | GLN |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | J | 3927 | GLN |
| 1 | J | 4020 | GLN |
| 1 | J | 4204 | GLN |
| 1 | J | 4650 | HIS |
| 1 | J | 4700 | GLN |
| 1 | J | 4857 | ASN |
| 2 | K | 3 | GLN |
| 2 | K | 102 | ASN |
| 2 | K | 119 | GLN |
| 3 | L | 31 | GLN |

### 5.3.3 RNA

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry

Of 88 ligands modelled in this entry, 8 are monoatomic - leaving 80 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 | $\#\|Z\| > 2$ |
| 8 | POV | J | 5115 | - | 45,45,51 | 0.52 | 0 | 51,53,59 | 0.48 | 0 |
| 8 | POV | C | 5122 | - | 30,30,51 | 0.75 | 1 (3%) | 34,37,59 | 0.60 | 0 |
| 8 | POV | C | 5116 | - | 27,27,51 | 0.66 | 0 | 33,35,59 | 0.60 | 0 |
| 8 | POV | C | 5108 | - | 48,48,51 | 0.52 | 0 | 54,56,59 | 0.47 | 0 |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\|>2$ | Counts | RMSZ | $\#\|Z\|>2$ |
| 8 | POV | G | 5108 | - | 48,48,51 | 0.51 | 0 | 54,56,59 | 0.47 | 0 |
| 8 | POV | J | 5105 | - | 39,39,51 | 0.54 | 0 | 45,47,59 | 0.66 | 1 (2%) |
| 8 | POV | A | 5115 | - | 33,33,51 | 0.34 | 0 | 39,41,59 | 0.39 | 0 |
| 8 | POV | C | 5114 | - | 19,19,51 | 0.66 | 0 | 24,25,59 | 0.58 | 0 |
| 8 | POV | A | 5107 | - | 49,49,51 | 0.50 | 0 | 55,57,59 | 0.48 | 0 |
| 8 | POV | G | 5112 | - | 19,19,51 | 0.73 | 0 | 24,26,59 | 0.72 | 0 |
| 8 | POV | G | 5114 | - | 19,19,51 | 0.66 | 0 | 24,25,59 | 0.58 | 0 |
| 8 | POV | A | 5120 | - | 39,39,51 | 0.55 | 0 | 45,47,59 | 0.65 | 1 (2%) |
| 8 | POV | C | 5113 | - | 19,19,51 | 0.41 | 0 | 24,26,59 | 0.52 | 0 |
| 8 | POV | C | 5112 | - | 19,19,51 | 0.73 | 0 | 24,26,59 | 0.72 | 0 |
| 8 | POV | C | 5121 | - | 40,40,51 | 0.54 | 0 | 46,48,59 | 0.62 | 1 (2%) |
| 8 | POV | G | 5121 | - | 40,40,51 | 0.54 | 0 | 46,48,59 | 0.62 | 1 (2%) |
| 5 | ATP | A | 5102 | - | 32,33,33 | 0.53 | 0 | 48,52,52 | 0.59 | 0 |
| 8 | POV | J | 5113 | - | 46,46,51 | 0.52 | 0 | 52,54,59 | 0.49 | 0 |
| 8 | POV | A | 5109 | - | 19,19,51 | 0.73 | 0 | 24,26,59 | 0.72 | 0 |
| 8 | POV | G | 5111 | - | 45,45,51 | 0.52 | 0 | 51,53,59 | 0.48 | 0 |
| 8 | POV | C | 5115 | - | 34,34,51 | 0.60 | 0 | 40,42,59 | 0.56 | 0 |
| 8 | POV | J | 5102 | - | 46,46,51 | 0.31 | 0 | 52,54,59 | 0.29 | 0 |
| 8 | POV | A | 5122 | - | 12,12,51 | 0.22 | 0 | 11,11,59 | 0.23 | 0 |
| 8 | POV | A | 5116 | - | 51,51,51 | 0.50 | 0 | 57,59,59 | 0.47 | 0 |
| 6 | CFF | J | 5110 | - | 15,15,15 | 0.32 | 0 | 23,23,23 | 0.49 | 0 |
| 5 | ATP | J | 5109 | - | 32,33,33 | 0.53 | 0 | 48,52,52 | 0.59 | 0 |
| 5 | ATP | C | 5105 | - | 32,33,33 | 0.53 | 0 | 48,52,52 | 0.59 | 0 |
| 8 | POV | J | 5119 | - | 34,34,51 | 0.59 | 0 | 40,42,59 | 0.56 | 0 |
| 5 | ATP | G | 5105 | - | 32,33,33 | 0.53 | 0 | 48,52,52 | 0.59 | 0 |
| 8 | POV | J | 5104 | - | 30,30,51 | 0.75 | 1 (3%) | 34,37,59 | 0.60 | 0 |
| 8 | POV | C | 5118 | - | 33,33,51 | 0.61 | 0 | 39,41,59 | 0.54 | 0 |
| 8 | POV | C | 5102 | - | 47,47,51 | 0.51 | 0 | 53,55,59 | 0.48 | 0 |
| 8 | POV | J | 5120 | - | 27,27,51 | 0.66 | 0 | 33,35,59 | 0.60 | 0 |
| 8 | POV | A | 5106 | - | 46,46,51 | 0.53 | 0 | 52,54,59 | 0.49 | 0 |
| 8 | POV | G | 5115 | - | 34,34,51 | 0.60 | 0 | 40,42,59 | 0.56 | 0 |
| 8 | POV | A | 5117 | - | 46,46,51 | 0.32 | 0 | 52,54,59 | 0.31 | 0 |
| 8 | POV | G | 5120 | - | 46,46,51 | 0.31 | 0 | 52,54,59 | 0.34 | 0 |
| 6 | CFF | C | 5106 | - | 15,15,15 | 0.33 | 0 | 23,23,23 | 0.49 | 0 |
| 8 | POV | C | 5120 | - | 46,46,51 | 0.31 | 0 | 52,54,59 | 0.31 | 0 |
| 8 | POV | J | 5117 | - | 19,19,51 | 0.39 | 0 | 24,26,59 | 0.51 | 0 |
| 8 | POV | J | 5107 | - | 12,12,51 | 0.23 | 0 | 11,11,59 | 0.23 | 0 |
| 8 | POV | C | 5109 | - | 46,46,51 | 0.53 | 0 | 52,54,59 | 0.49 | 0 |
| 8 | POV | A | 5110 | - | 19,19,51 | 0.38 | 0 | 24,26,59 | 0.53 | 0 |
| 8 | POV | G | 5109 | - | 46,46,51 | 0.53 | 0 | 52,54,59 | 0.49 | 0 |
| 8 | POV | J | 5103 | - | 40,40,51 | 0.54 | 0 | 46,48,59 | 0.62 | 1 (2%) |
| 8 | POV | J | 5118 | - | 19,19,51 | 0.67 | 0 | 24,25,59 | 0.58 | 0 |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\|>2$ | Counts | RMSZ | $\#\|Z\|>2$ |
| 8 | POV | J | 5112 | - | 48,48,51 | 0.52 | 0 | 54,56,59 | 0.47 | 0 |
| 6 | CFF | A | 5103 | - | 15,15,15 | 0.32 | 0 | 23,23,23 | 0.49 | 0 |
| 8 | POV | A | 5105 | - | 48,48,51 | 0.52 | 0 | 54,56,59 | 0.47 | 0 |
| 8 | POV | G | 5102 | - | 47,47,51 | 0.51 | 0 | 53,55,59 | 0.48 | 0 |
| 8 | POV | C | 5119 | - | 51,51,51 | 0.50 | 0 | 57,59,59 | 0.47 | 0 |
| 8 | POV | G | 5116 | - | 27,27,51 | 0.66 | 0 | 33,35,59 | 0.60 | 0 |
| 8 | POV | A | 5108 | - | 45,45,51 | 0.52 | 0 | 51,53,59 | 0.48 | 0 |
| 8 | POV | A | 5111 | - | 19,19,51 | 0.66 | 0 | 24,25,59 | 0.58 | 0 |
| 8 | POV | J | 5106 | - | 47,47,51 | 0.51 | 0 | 53,55,59 | 0.48 | 0 |
| 8 | POV | J | 5122 | - | 33,33,51 | 0.61 | 0 | 39,41,59 | 0.54 | 0 |
| 8 | POV | A | 5113 | - | 27,27,51 | 0.66 | 0 | 33,35,59 | 0.60 | 0 |
| 8 | POV | A | 5112 | - | 34,34,51 | 0.60 | 0 | 40,42,59 | 0.56 | 0 |
| 8 | POV | A | 5114 | - | 23,23,51 | 0.67 | 0 | 28,30,59 | 0.68 | 0 |
| 8 | POV | G | 5122 | - | 30,30,51 | 0.74 | 1 (3%) | 34,37,59 | 0.60 | 0 |
| 8 | POV | G | 5113 | - | 19,19,51 | 0.39 | 0 | 24,26,59 | 0.52 | 0 |
| 8 | POV | C | 5117 | - | 23,23,51 | 0.67 | 0 | 28,30,59 | 0.68 | 0 |
| 8 | POV | G | 5119 | - | 51,51,51 | 0.49 | 0 | 57,59,59 | 0.47 | 0 |
| 8 | POV | A | 5121 | - | 47,47,51 | 0.51 | 0 | 53,55,59 | 0.48 | 0 |
| 8 | POV | J | 5114 | - | 49,49,51 | 0.50 | 0 | 55,57,59 | 0.48 | 0 |
| 8 | POV | G | 5117 | - | 23,23,51 | 0.66 | 0 | 28,30,59 | 0.68 | 0 |
| 8 | POV | G | 5101 | - | 39,39,51 | 0.54 | 0 | 45,47,59 | 0.66 | 1 (2%) |
| 6 | CFF | G | 5106 | - | 15,15,15 | 0.32 | 0 | 23,23,23 | 0.50 | 0 |
| 8 | POV | J | 5121 | - | 23,23,51 | 0.66 | 0 | 28,30,59 | 0.68 | 0 |
| 8 | POV | C | 5101 | - | 39,39,51 | 0.54 | 0 | 45,47,59 | 0.65 | 1 (2%) |
| 8 | POV | C | 5103 | - | 12,12,51 | 0.22 | 0 | 11,11,59 | 0.23 | 0 |
| 8 | POV | A | 5118 | - | 40,40,51 | 0.54 | 0 | 46,48,59 | 0.62 | 1 (2%) |
| 8 | POV | C | 5110 | - | 49,49,51 | 0.50 | 0 | 55,57,59 | 0.48 | 0 |
| 8 | POV | G | 5103 | - | 12,12,51 | 0.23 | 0 | 11,11,59 | 0.23 | 0 |
| 8 | POV | J | 5101 | - | 51,51,51 | 0.50 | 0 | 57,59,59 | 0.47 | 0 |
| 8 | POV | G | 5110 | - | 49,49,51 | 0.50 | 0 | 55,57,59 | 0.48 | 0 |
| 8 | POV | G | 5118 | - | 33,33,51 | 0.61 | 0 | 39,41,59 | 0.54 | 0 |
| 8 | POV | A | 5119 | - | 30,30,51 | 0.75 | 1 (3%) | 34,37,59 | 0.60 | 0 |
| 8 | POV | J | 5116 | - | 19,19,51 | 0.72 | 0 | 24,26,59 | 0.72 | 0 |
| 8 | POV | C | 5111 | - | 45,45,51 | 0.52 | 0 | 51,53,59 | 0.48 | 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 |
|---|---|---|---|---|---|---|---|
| 8 | POV | J | 5115 | - | - | 10/49/49/55 | - |
| 8 | POV | C | 5122 | - | - | 14/33/33/55 | - |
| 8 | POV | C | 5116 | - | - | 9/31/31/55 | - |
| 8 | POV | C | 5108 | - | - | 23/52/52/55 | - |
| 8 | POV | G | 5108 | - | - | 23/52/52/55 | - |
| 8 | POV | J | 5105 | - | - | 10/43/43/55 | - |
| 8 | POV | A | 5115 | - | - | 9/37/37/55 | - |
| 8 | POV | C | 5114 | - | - | 7/20/20/55 | - |
| 8 | POV | A | 5107 | - | - | 23/53/53/55 | - |
| 8 | POV | G | 5112 | - | - | 8/22/22/55 | - |
| 8 | POV | G | 5114 | - | - | 7/20/20/55 | - |
| 8 | POV | A | 5120 | - | - | 10/43/43/55 | - |
| 8 | POV | C | 5113 | - | - | 6/22/22/55 | - |
| 8 | POV | C | 5112 | - | - | 8/22/22/55 | - |
| 8 | POV | C | 5121 | - | - | 15/44/44/55 | - |
| 8 | POV | G | 5121 | - | - | 15/44/44/55 | - |
| 5 | ATP | A | 5102 | - | - | 3/22/38/38 | 0/3/3/3 |
| 8 | POV | J | 5113 | - | - | 11/50/50/55 | - |
| 8 | POV | A | 5109 | - | - | 8/22/22/55 | - |
| 8 | POV | G | 5111 | - | - | 10/49/49/55 | - |
| 8 | POV | C | 5115 | - | - | 10/38/38/55 | - |
| 8 | POV | J | 5102 | - | - | 3/50/50/55 | - |
| 8 | POV | A | 5122 | - | - | 1/10/10/55 | - |
| 8 | POV | A | 5116 | - | - | 15/55/55/55 | - |
| 6 | CFF | J | 5110 | - | - | - | 0/2/2/2 |
| 5 | ATP | J | 5109 | - | - | 3/22/38/38 | 0/3/3/3 |
| 5 | ATP | C | 5105 | - | - | 3/22/38/38 | 0/3/3/3 |
| 8 | POV | J | 5119 | - | - | 10/38/38/55 | - |
| 5 | ATP | G | 5105 | - | - | 3/22/38/38 | 0/3/3/3 |
| 8 | POV | J | 5104 | - | - | 14/33/33/55 | - |
| 8 | POV | C | 5118 | - | - | 9/37/37/55 | - |
| 8 | POV | C | 5102 | - | - | 12/51/51/55 | - |
| 8 | POV | J | 5120 | - | - | 9/31/31/55 | - |
| 8 | POV | A | 5106 | - | - | 11/50/50/55 | - |
| 8 | POV | G | 5115 | - | - | 10/38/38/55 | - |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 8 | POV | A | 5117 | - | - | 5/50/50/55 | - |
| 8 | POV | G | 5120 | - | - | 7/50/50/55 | - |
| 6 | CFF | C | 5106 | - | - | - | 0/2/2/2 |
| 8 | POV | C | 5120 | - | - | 5/50/50/55 | - |
| 8 | POV | J | 5117 | - | - | 9/22/22/55 | - |
| 8 | POV | J | 5107 | - | - | 1/10/10/55 | - |
| 8 | POV | C | 5109 | - | - | 11/50/50/55 | - |
| 8 | POV | A | 5110 | - | - | 6/22/22/55 | - |
| 8 | POV | G | 5109 | - | - | 11/50/50/55 | - |
| 8 | POV | J | 5103 | - | - | 15/44/44/55 | - |
| 8 | POV | J | 5118 | - | - | 7/20/20/55 | - |
| 8 | POV | J | 5112 | - | - | 23/52/52/55 | - |
| 6 | CFF | A | 5103 | - | - | - | 0/2/2/2 |
| 8 | POV | A | 5105 | - | - | 23/52/52/55 | - |
| 8 | POV | G | 5102 | - | - | 12/51/51/55 | - |
| 8 | POV | C | 5119 | - | - | 15/55/55/55 | - |
| 8 | POV | G | 5116 | - | - | 9/31/31/55 | - |
| 8 | POV | A | 5108 | - | - | 10/49/49/55 | - |
| 8 | POV | A | 5111 | - | - | 7/20/20/55 | - |
| 8 | POV | J | 5106 | - | - | 12/51/51/55 | - |
| 8 | POV | J | 5122 | - | - | 9/37/37/55 | - |
| 8 | POV | A | 5113 | - | - | 9/31/31/55 | - |
| 8 | POV | A | 5112 | - | - | 10/38/38/55 | - |
| 8 | POV | A | 5114 | - | - | 7/26/26/55 | - |
| 8 | POV | G | 5122 | - | - | 14/33/33/55 | - |
| 8 | POV | G | 5113 | - | - | 8/22/22/55 | - |
| 8 | POV | C | 5117 | - | - | 7/26/26/55 | - |
| 8 | POV | G | 5119 | - | - | 15/55/55/55 | - |
| 8 | POV | A | 5121 | - | - | 12/51/51/55 | - |
| 8 | POV | J | 5114 | - | - | 23/53/53/55 | - |
| 8 | POV | G | 5117 | - | - | 7/26/26/55 | - |
| 8 | POV | G | 5101 | - | - | 10/43/43/55 | - |
| 6 | CFF | G | 5106 | - | - | - | 0/2/2/2 |
| 8 | POV | J | 5121 | - | - | 7/26/26/55 | - |
| 8 | POV | C | 5101 | - | - | 10/43/43/55 | - |

*Continued on next page...*

*Continued from previous page...*

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 8 | POV | C | 5103 | - | - | 1/10/10/55 | - |
| 8 | POV | A | 5118 | - | - | 15/44/44/55 | - |
| 8 | POV | C | 5110 | - | - | 23/53/53/55 | - |
| 8 | POV | G | 5103 | - | - | 1/10/10/55 | - |
| 8 | POV | J | 5101 | - | - | 15/55/55/55 | - |
| 8 | POV | G | 5110 | - | - | 23/53/53/55 | - |
| 8 | POV | G | 5118 | - | - | 9/37/37/55 | - |
| 8 | POV | A | 5119 | - | - | 14/33/33/55 | - |
| 8 | POV | J | 5116 | - | - | 8/22/22/55 | - |
| 8 | POV | C | 5111 | - | - | 10/49/49/55 | - |

All (4) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 8 | A | 5119 | POV | O21-C2 | -2.70 | 1.43 | 1.46 |
| 8 | C | 5122 | POV | O21-C2 | -2.70 | 1.43 | 1.46 |
| 8 | J | 5104 | POV | O21-C2 | -2.70 | 1.43 | 1.46 |
| 8 | G | 5122 | POV | O21-C2 | -2.61 | 1.43 | 1.46 |

All (8) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 8 | C | 5101 | POV | C2-O21-C21 | 2.56 | 123.92 | 117.80 |
| 8 | G | 5101 | POV | C2-O21-C21 | 2.56 | 123.92 | 117.80 |
| 8 | J | 5105 | POV | C2-O21-C21 | 2.56 | 123.92 | 117.80 |
| 8 | A | 5120 | POV | C2-O21-C21 | 2.55 | 123.90 | 117.80 |
| 8 | C | 5121 | POV | C2-O21-C21 | 2.33 | 123.37 | 117.80 |
| 8 | J | 5103 | POV | C2-O21-C21 | 2.32 | 123.35 | 117.80 |
| 8 | G | 5121 | POV | C2-O21-C21 | 2.31 | 123.32 | 117.80 |
| 8 | A | 5118 | POV | C2-O21-C21 | 2.30 | 123.30 | 117.80 |

There are no chirality outliers.

All (797) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 8 | A | 5105 | POV | C1-O11-P-O12 |
| 8 | A | 5105 | POV | C1-O11-P-O14 |
| 8 | A | 5105 | POV | C11-O12-P-O11 |
| 8 | A | 5105 | POV | C11-O12-P-O14 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 8 | A | 5105 | POV | O12-C11-C12-N |
| 8 | A | 5106 | POV | C1-O11-P-O12 |
| 8 | A | 5106 | POV | C1-O11-P-O13 |
| 8 | A | 5106 | POV | C2-C1-O11-P |
| 8 | A | 5106 | POV | O12-C11-C12-N |
| 8 | A | 5107 | POV | C1-O11-P-O12 |
| 8 | A | 5107 | POV | C1-O11-P-O13 |
| 8 | A | 5107 | POV | C1-O11-P-O14 |
| 8 | A | 5107 | POV | C11-O12-P-O14 |
| 8 | A | 5108 | POV | C1-O11-P-O14 |
| 8 | A | 5109 | POV | C1-O11-P-O12 |
| 8 | A | 5109 | POV | C1-O11-P-O13 |
| 8 | A | 5109 | POV | C11-O12-P-O11 |
| 8 | A | 5109 | POV | C11-O12-P-O13 |
| 8 | A | 5109 | POV | C12-C11-O12-P |
| 8 | A | 5111 | POV | O12-C11-C12-N |
| 8 | A | 5112 | POV | C1-O11-P-O14 |
| 8 | A | 5112 | POV | C11-O12-P-O13 |
| 8 | A | 5113 | POV | C1-O11-P-O12 |
| 8 | A | 5113 | POV | C1-O11-P-O13 |
| 8 | A | 5113 | POV | C1-O11-P-O14 |
| 8 | A | 5113 | POV | C11-O12-P-O11 |
| 8 | A | 5114 | POV | C1-O11-P-O12 |
| 8 | A | 5114 | POV | O12-C11-C12-N |
| 8 | A | 5115 | POV | C11-O12-P-O14 |
| 8 | A | 5115 | POV | O22-C21-O21-C2 |
| 8 | A | 5116 | POV | C22-C21-O21-C2 |
| 8 | A | 5116 | POV | O22-C21-O21-C2 |
| 8 | A | 5117 | POV | O22-C21-O21-C2 |
| 8 | A | 5118 | POV | C1-O11-P-O12 |
| 8 | A | 5118 | POV | C1-O11-P-O13 |
| 8 | A | 5118 | POV | C1-O11-P-O14 |
| 8 | A | 5119 | POV | C1-O11-P-O12 |
| 8 | A | 5119 | POV | C1-O11-P-O13 |
| 8 | A | 5119 | POV | C11-O12-P-O11 |
| 8 | A | 5119 | POV | C11-O12-P-O14 |
| 8 | A | 5119 | POV | O22-C21-O21-C2 |
| 8 | A | 5120 | POV | C1-O11-P-O12 |
| 8 | A | 5120 | POV | C1-O11-P-O13 |
| 8 | A | 5120 | POV | C22-C21-O21-C2 |
| 8 | A | 5121 | POV | O12-C11-C12-N |
| 8 | A | 5121 | POV | C22-C21-O21-C2 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 8 | C | 5101 | POV | C1-O11-P-O12 |
| 8 | C | 5101 | POV | C1-O11-P-O13 |
| 8 | C | 5101 | POV | C22-C21-O21-C2 |
| 8 | C | 5102 | POV | O12-C11-C12-N |
| 8 | C | 5102 | POV | C22-C21-O21-C2 |
| 8 | C | 5108 | POV | C1-O11-P-O12 |
| 8 | C | 5108 | POV | C1-O11-P-O14 |
| 8 | C | 5108 | POV | C11-O12-P-O11 |
| 8 | C | 5108 | POV | C11-O12-P-O14 |
| 8 | C | 5108 | POV | O12-C11-C12-N |
| 8 | C | 5109 | POV | C1-O11-P-O12 |
| 8 | C | 5109 | POV | C1-O11-P-O13 |
| 8 | C | 5109 | POV | C2-C1-O11-P |
| 8 | C | 5109 | POV | O12-C11-C12-N |
| 8 | C | 5110 | POV | C1-O11-P-O12 |
| 8 | C | 5110 | POV | C1-O11-P-O13 |
| 8 | C | 5110 | POV | C1-O11-P-O14 |
| 8 | C | 5110 | POV | C11-O12-P-O14 |
| 8 | C | 5111 | POV | C1-O11-P-O14 |
| 8 | C | 5112 | POV | C1-O11-P-O12 |
| 8 | C | 5112 | POV | C1-O11-P-O13 |
| 8 | C | 5112 | POV | C11-O12-P-O11 |
| 8 | C | 5112 | POV | C11-O12-P-O13 |
| 8 | C | 5112 | POV | C12-C11-O12-P |
| 8 | C | 5113 | POV | C1-O11-P-O12 |
| 8 | C | 5113 | POV | C1-O11-P-O13 |
| 8 | C | 5113 | POV | C2-C1-O11-P |
| 8 | C | 5114 | POV | O12-C11-C12-N |
| 8 | C | 5115 | POV | C1-O11-P-O14 |
| 8 | C | 5115 | POV | C11-O12-P-O13 |
| 8 | C | 5116 | POV | C1-O11-P-O12 |
| 8 | C | 5116 | POV | C1-O11-P-O13 |
| 8 | C | 5116 | POV | C1-O11-P-O14 |
| 8 | C | 5116 | POV | C11-O12-P-O11 |
| 8 | C | 5117 | POV | C1-O11-P-O12 |
| 8 | C | 5117 | POV | O12-C11-C12-N |
| 8 | C | 5118 | POV | C1-O11-P-O14 |
| 8 | C | 5118 | POV | O22-C21-O21-C2 |
| 8 | C | 5119 | POV | C22-C21-O21-C2 |
| 8 | C | 5119 | POV | O22-C21-O21-C2 |
| 8 | C | 5120 | POV | C22-C21-O21-C2 |
| 8 | C | 5121 | POV | C1-O11-P-O12 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 8 | C | 5121 | POV | C1-O11-P-O13 |
| 8 | C | 5121 | POV | C1-O11-P-O14 |
| 8 | C | 5122 | POV | C1-O11-P-O12 |
| 8 | C | 5122 | POV | C1-O11-P-O13 |
| 8 | C | 5122 | POV | C11-O12-P-O11 |
| 8 | C | 5122 | POV | C11-O12-P-O14 |
| 8 | C | 5122 | POV | O22-C21-O21-C2 |
| 8 | G | 5101 | POV | C1-O11-P-O12 |
| 8 | G | 5101 | POV | C1-O11-P-O13 |
| 8 | G | 5101 | POV | C22-C21-O21-C2 |
| 8 | G | 5102 | POV | O12-C11-C12-N |
| 8 | G | 5102 | POV | C22-C21-O21-C2 |
| 8 | G | 5108 | POV | C1-O11-P-O12 |
| 8 | G | 5108 | POV | C1-O11-P-O14 |
| 8 | G | 5108 | POV | C11-O12-P-O11 |
| 8 | G | 5108 | POV | C11-O12-P-O14 |
| 8 | G | 5108 | POV | O12-C11-C12-N |
| 8 | G | 5109 | POV | C1-O11-P-O12 |
| 8 | G | 5109 | POV | C1-O11-P-O13 |
| 8 | G | 5109 | POV | C2-C1-O11-P |
| 8 | G | 5109 | POV | O12-C11-C12-N |
| 8 | G | 5110 | POV | C1-O11-P-O12 |
| 8 | G | 5110 | POV | C1-O11-P-O13 |
| 8 | G | 5110 | POV | C1-O11-P-O14 |
| 8 | G | 5110 | POV | C11-O12-P-O14 |
| 8 | G | 5111 | POV | C1-O11-P-O14 |
| 8 | G | 5112 | POV | C1-O11-P-O12 |
| 8 | G | 5112 | POV | C1-O11-P-O13 |
| 8 | G | 5112 | POV | C11-O12-P-O11 |
| 8 | G | 5112 | POV | C11-O12-P-O13 |
| 8 | G | 5112 | POV | C12-C11-O12-P |
| 8 | G | 5113 | POV | C1-O11-P-O14 |
| 8 | G | 5113 | POV | C2-C1-O11-P |
| 8 | G | 5113 | POV | O12-C11-C12-N |
| 8 | G | 5114 | POV | O12-C11-C12-N |
| 8 | G | 5115 | POV | C1-O11-P-O14 |
| 8 | G | 5115 | POV | C11-O12-P-O13 |
| 8 | G | 5116 | POV | C1-O11-P-O12 |
| 8 | G | 5116 | POV | C1-O11-P-O13 |
| 8 | G | 5116 | POV | C1-O11-P-O14 |
| 8 | G | 5116 | POV | C11-O12-P-O11 |
| 8 | G | 5117 | POV | C1-O11-P-O12 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 8 | G | 5117 | POV | O12-C11-C12-N |
| 8 | G | 5118 | POV | C1-O11-P-O14 |
| 8 | G | 5118 | POV | O22-C21-O21-C2 |
| 8 | G | 5119 | POV | C22-C21-O21-C2 |
| 8 | G | 5119 | POV | O22-C21-O21-C2 |
| 8 | G | 5120 | POV | C11-O12-P-O11 |
| 8 | G | 5120 | POV | C11-O12-P-O13 |
| 8 | G | 5121 | POV | C1-O11-P-O12 |
| 8 | G | 5121 | POV | C1-O11-P-O13 |
| 8 | G | 5121 | POV | C1-O11-P-O14 |
| 8 | G | 5122 | POV | C1-O11-P-O12 |
| 8 | G | 5122 | POV | C1-O11-P-O13 |
| 8 | G | 5122 | POV | C11-O12-P-O11 |
| 8 | G | 5122 | POV | C11-O12-P-O14 |
| 8 | G | 5122 | POV | O22-C21-O21-C2 |
| 8 | J | 5101 | POV | C22-C21-O21-C2 |
| 8 | J | 5101 | POV | O22-C21-O21-C2 |
| 8 | J | 5103 | POV | C1-O11-P-O12 |
| 8 | J | 5103 | POV | C1-O11-P-O13 |
| 8 | J | 5103 | POV | C1-O11-P-O14 |
| 8 | J | 5104 | POV | C1-O11-P-O12 |
| 8 | J | 5104 | POV | C1-O11-P-O13 |
| 8 | J | 5104 | POV | C11-O12-P-O11 |
| 8 | J | 5104 | POV | C11-O12-P-O14 |
| 8 | J | 5104 | POV | O22-C21-O21-C2 |
| 8 | J | 5105 | POV | C1-O11-P-O12 |
| 8 | J | 5105 | POV | C1-O11-P-O13 |
| 8 | J | 5105 | POV | C22-C21-O21-C2 |
| 8 | J | 5106 | POV | O12-C11-C12-N |
| 8 | J | 5106 | POV | C22-C21-O21-C2 |
| 8 | J | 5112 | POV | C1-O11-P-O12 |
| 8 | J | 5112 | POV | C1-O11-P-O14 |
| 8 | J | 5112 | POV | C11-O12-P-O11 |
| 8 | J | 5112 | POV | C11-O12-P-O14 |
| 8 | J | 5112 | POV | O12-C11-C12-N |
| 8 | J | 5113 | POV | C1-O11-P-O12 |
| 8 | J | 5113 | POV | C1-O11-P-O13 |
| 8 | J | 5113 | POV | C2-C1-O11-P |
| 8 | J | 5113 | POV | O12-C11-C12-N |
| 8 | J | 5114 | POV | C1-O11-P-O12 |
| 8 | J | 5114 | POV | C1-O11-P-O13 |
| 8 | J | 5114 | POV | C1-O11-P-O14 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 8 | J | 5114 | POV | C11-O12-P-O14 |
| 8 | J | 5115 | POV | C1-O11-P-O14 |
| 8 | J | 5116 | POV | C1-O11-P-O12 |
| 8 | J | 5116 | POV | C1-O11-P-O13 |
| 8 | J | 5116 | POV | C11-O12-P-O11 |
| 8 | J | 5116 | POV | C11-O12-P-O13 |
| 8 | J | 5116 | POV | C12-C11-O12-P |
| 8 | J | 5117 | POV | C1-O11-P-O12 |
| 8 | J | 5117 | POV | C1-O11-P-O13 |
| 8 | J | 5117 | POV | C2-C1-O11-P |
| 8 | J | 5118 | POV | O12-C11-C12-N |
| 8 | J | 5119 | POV | C1-O11-P-O14 |
| 8 | J | 5119 | POV | C11-O12-P-O13 |
| 8 | J | 5120 | POV | C1-O11-P-O12 |
| 8 | J | 5120 | POV | C1-O11-P-O13 |
| 8 | J | 5120 | POV | C1-O11-P-O14 |
| 8 | J | 5120 | POV | C11-O12-P-O11 |
| 8 | J | 5121 | POV | C1-O11-P-O12 |
| 8 | J | 5121 | POV | O12-C11-C12-N |
| 8 | J | 5122 | POV | C1-O11-P-O14 |
| 8 | J | 5122 | POV | O22-C21-O21-C2 |
| 8 | A | 5113 | POV | C32-C31-O31-C3 |
| 8 | C | 5116 | POV | C32-C31-O31-C3 |
| 8 | G | 5116 | POV | C32-C31-O31-C3 |
| 8 | J | 5120 | POV | C32-C31-O31-C3 |
| 8 | A | 5113 | POV | O32-C31-O31-C3 |
| 8 | C | 5116 | POV | O32-C31-O31-C3 |
| 8 | G | 5116 | POV | O32-C31-O31-C3 |
| 8 | J | 5120 | POV | O32-C31-O31-C3 |
| 8 | A | 5120 | POV | O22-C21-O21-C2 |
| 8 | A | 5121 | POV | O22-C21-O21-C2 |
| 8 | C | 5101 | POV | O22-C21-O21-C2 |
| 8 | C | 5102 | POV | O22-C21-O21-C2 |
| 8 | C | 5120 | POV | O22-C21-O21-C2 |
| 8 | G | 5101 | POV | O22-C21-O21-C2 |
| 8 | G | 5102 | POV | O22-C21-O21-C2 |
| 8 | J | 5102 | POV | O22-C21-O21-C2 |
| 8 | J | 5105 | POV | O22-C21-O21-C2 |
| 8 | J | 5106 | POV | O22-C21-O21-C2 |
| 8 | A | 5115 | POV | C22-C21-O21-C2 |
| 8 | A | 5117 | POV | C22-C21-O21-C2 |
| 8 | C | 5118 | POV | C22-C21-O21-C2 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 8 | G | 5118 | POV | C22-C21-O21-C2 |
| 8 | J | 5102 | POV | C22-C21-O21-C2 |
| 8 | J | 5122 | POV | C22-C21-O21-C2 |
| 8 | A | 5118 | POV | C32-C31-O31-C3 |
| 8 | C | 5121 | POV | C32-C31-O31-C3 |
| 8 | G | 5121 | POV | C32-C31-O31-C3 |
| 8 | J | 5103 | POV | C32-C31-O31-C3 |
| 8 | A | 5105 | POV | O32-C31-O31-C3 |
| 8 | C | 5108 | POV | O32-C31-O31-C3 |
| 8 | G | 5108 | POV | O32-C31-O31-C3 |
| 8 | J | 5112 | POV | O32-C31-O31-C3 |
| 8 | A | 5105 | POV | C32-C31-O31-C3 |
| 8 | A | 5107 | POV | C32-C31-O31-C3 |
| 8 | C | 5108 | POV | C32-C31-O31-C3 |
| 8 | C | 5110 | POV | C32-C31-O31-C3 |
| 8 | G | 5108 | POV | C32-C31-O31-C3 |
| 8 | G | 5110 | POV | C32-C31-O31-C3 |
| 8 | J | 5112 | POV | C32-C31-O31-C3 |
| 8 | J | 5114 | POV | C32-C31-O31-C3 |
| 8 | A | 5118 | POV | O32-C31-O31-C3 |
| 8 | C | 5121 | POV | O32-C31-O31-C3 |
| 8 | G | 5121 | POV | O32-C31-O31-C3 |
| 8 | J | 5103 | POV | O32-C31-O31-C3 |
| 8 | A | 5107 | POV | O32-C31-O31-C3 |
| 8 | C | 5110 | POV | O32-C31-O31-C3 |
| 8 | G | 5110 | POV | O32-C31-O31-C3 |
| 8 | J | 5114 | POV | O32-C31-O31-C3 |
| 8 | A | 5108 | POV | C32-C31-O31-C3 |
| 8 | C | 5111 | POV | C32-C31-O31-C3 |
| 8 | G | 5111 | POV | C32-C31-O31-C3 |
| 8 | J | 5115 | POV | C32-C31-O31-C3 |
| 8 | J | 5112 | POV | C311-C310-C39-C38 |
| 8 | A | 5105 | POV | C311-C310-C39-C38 |
| 8 | C | 5108 | POV | C311-C310-C39-C38 |
| 8 | G | 5108 | POV | C311-C310-C39-C38 |
| 8 | A | 5107 | POV | C31-C32-C33-C34 |
| 8 | C | 5110 | POV | C31-C32-C33-C34 |
| 8 | G | 5110 | POV | C31-C32-C33-C34 |
| 8 | J | 5114 | POV | C31-C32-C33-C34 |
| 8 | A | 5112 | POV | O11-C1-C2-O21 |
| 8 | C | 5115 | POV | O11-C1-C2-O21 |
| 8 | G | 5115 | POV | O11-C1-C2-O21 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 8 | J | 5119 | POV | O11-C1-C2-O21 |
| 8 | A | 5107 | POV | C22-C21-O21-C2 |
| 8 | C | 5110 | POV | C22-C21-O21-C2 |
| 8 | G | 5110 | POV | C22-C21-O21-C2 |
| 8 | J | 5114 | POV | C22-C21-O21-C2 |
| 8 | G | 5101 | POV | C31-C32-C33-C34 |
| 8 | A | 5108 | POV | O32-C31-O31-C3 |
| 8 | C | 5111 | POV | O32-C31-O31-C3 |
| 8 | G | 5111 | POV | O32-C31-O31-C3 |
| 8 | J | 5115 | POV | O32-C31-O31-C3 |
| 8 | A | 5117 | POV | C21-C22-C23-C24 |
| 8 | A | 5120 | POV | C31-C32-C33-C34 |
| 8 | C | 5101 | POV | C31-C32-C33-C34 |
| 8 | J | 5105 | POV | C31-C32-C33-C34 |
| 8 | J | 5101 | POV | C310-C311-C312-C313 |
| 8 | A | 5116 | POV | C310-C311-C312-C313 |
| 8 | C | 5119 | POV | C310-C311-C312-C313 |
| 8 | G | 5119 | POV | C310-C311-C312-C313 |
| 8 | A | 5107 | POV | O22-C21-O21-C2 |
| 8 | C | 5110 | POV | O22-C21-O21-C2 |
| 8 | G | 5110 | POV | O22-C21-O21-C2 |
| 8 | J | 5114 | POV | O22-C21-O21-C2 |
| 8 | G | 5113 | POV | C22-C21-O21-C2 |
| 8 | G | 5113 | POV | O22-C21-O21-C2 |
| 8 | A | 5120 | POV | C210-C211-C212-C213 |
| 8 | C | 5101 | POV | C210-C211-C212-C213 |
| 8 | G | 5101 | POV | C210-C211-C212-C213 |
| 8 | J | 5105 | POV | C210-C211-C212-C213 |
| 8 | A | 5118 | POV | C22-C21-O21-C2 |
| 8 | C | 5121 | POV | C22-C21-O21-C2 |
| 8 | G | 5121 | POV | C22-C21-O21-C2 |
| 8 | J | 5103 | POV | C22-C21-O21-C2 |
| 8 | A | 5112 | POV | C37-C38-C39-C310 |
| 8 | A | 5121 | POV | C34-C35-C36-C37 |
| 8 | C | 5102 | POV | C34-C35-C36-C37 |
| 8 | C | 5115 | POV | C37-C38-C39-C310 |
| 8 | G | 5102 | POV | C34-C35-C36-C37 |
| 8 | G | 5115 | POV | C37-C38-C39-C310 |
| 8 | G | 5120 | POV | C22-C23-C24-C25 |
| 8 | J | 5106 | POV | C34-C35-C36-C37 |
| 8 | J | 5119 | POV | C37-C38-C39-C310 |
| 8 | J | 5115 | POV | C32-C33-C34-C35 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 8 | A | 5108 | POV | C32-C33-C34-C35 |
| 8 | C | 5111 | POV | C32-C33-C34-C35 |
| 8 | G | 5111 | POV | C32-C33-C34-C35 |
| 8 | A | 5105 | POV | C35-C36-C37-C38 |
| 8 | A | 5116 | POV | C37-C38-C39-C310 |
| 8 | C | 5108 | POV | C35-C36-C37-C38 |
| 8 | C | 5119 | POV | C37-C38-C39-C310 |
| 8 | G | 5119 | POV | C37-C38-C39-C310 |
| 8 | J | 5101 | POV | C37-C38-C39-C310 |
| 8 | J | 5112 | POV | C35-C36-C37-C38 |
| 8 | A | 5118 | POV | O22-C21-O21-C2 |
| 8 | C | 5121 | POV | O22-C21-O21-C2 |
| 8 | G | 5121 | POV | O22-C21-O21-C2 |
| 8 | J | 5103 | POV | O22-C21-O21-C2 |
| 8 | G | 5108 | POV | C35-C36-C37-C38 |
| 8 | A | 5105 | POV | C311-C312-C313-C314 |
| 8 | C | 5108 | POV | C311-C312-C313-C314 |
| 8 | G | 5108 | POV | C311-C312-C313-C314 |
| 8 | J | 5112 | POV | C311-C312-C313-C314 |
| 8 | A | 5106 | POV | C22-C21-O21-C2 |
| 8 | A | 5110 | POV | C22-C21-O21-C2 |
| 8 | C | 5109 | POV | C22-C21-O21-C2 |
| 8 | C | 5113 | POV | C22-C21-O21-C2 |
| 8 | G | 5109 | POV | C22-C21-O21-C2 |
| 8 | G | 5120 | POV | C22-C21-O21-C2 |
| 8 | J | 5113 | POV | C22-C21-O21-C2 |
| 8 | J | 5117 | POV | C22-C21-O21-C2 |
| 8 | J | 5117 | POV | O22-C21-O21-C2 |
| 8 | G | 5119 | POV | C36-C37-C38-C39 |
| 8 | A | 5116 | POV | C311-C312-C313-C314 |
| 8 | C | 5119 | POV | C311-C312-C313-C314 |
| 8 | G | 5119 | POV | C311-C312-C313-C314 |
| 8 | J | 5101 | POV | C311-C312-C313-C314 |
| 8 | A | 5116 | POV | C36-C37-C38-C39 |
| 8 | C | 5119 | POV | C36-C37-C38-C39 |
| 8 | J | 5101 | POV | C36-C37-C38-C39 |
| 8 | G | 5118 | POV | C23-C24-C25-C26 |
| 8 | A | 5107 | POV | C24-C25-C26-C27 |
| 8 | C | 5110 | POV | C24-C25-C26-C27 |
| 8 | C | 5118 | POV | C23-C24-C25-C26 |
| 8 | J | 5114 | POV | C24-C25-C26-C27 |
| 8 | J | 5122 | POV | C23-C24-C25-C26 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 8 | G | 5110 | POV | C24-C25-C26-C27 |
| 8 | A | 5112 | POV | O11-C1-C2-C3 |
| 8 | C | 5115 | POV | O11-C1-C2-C3 |
| 8 | G | 5115 | POV | O11-C1-C2-C3 |
| 8 | J | 5119 | POV | O11-C1-C2-C3 |
| 8 | G | 5108 | POV | C37-C38-C39-C310 |
| 8 | J | 5112 | POV | C37-C38-C39-C310 |
| 8 | A | 5105 | POV | C37-C38-C39-C310 |
| 8 | C | 5108 | POV | C37-C38-C39-C310 |
| 8 | A | 5105 | POV | C21-C22-C23-C24 |
| 8 | C | 5108 | POV | C21-C22-C23-C24 |
| 8 | G | 5108 | POV | C21-C22-C23-C24 |
| 8 | J | 5112 | POV | C21-C22-C23-C24 |
| 8 | A | 5110 | POV | O22-C21-O21-C2 |
| 8 | G | 5120 | POV | O22-C21-O21-C2 |
| 8 | A | 5119 | POV | C35-C36-C37-C38 |
| 8 | C | 5122 | POV | C35-C36-C37-C38 |
| 8 | G | 5122 | POV | C35-C36-C37-C38 |
| 8 | J | 5104 | POV | C35-C36-C37-C38 |
| 8 | A | 5110 | POV | O21-C21-C22-C23 |
| 8 | G | 5109 | POV | O22-C21-O21-C2 |
| 8 | G | 5119 | POV | C311-C310-C39-C38 |
| 8 | A | 5116 | POV | C311-C310-C39-C38 |
| 8 | C | 5119 | POV | C311-C310-C39-C38 |
| 8 | J | 5101 | POV | C311-C310-C39-C38 |
| 8 | A | 5119 | POV | C32-C31-O31-C3 |
| 8 | C | 5122 | POV | C32-C31-O31-C3 |
| 8 | G | 5122 | POV | C32-C31-O31-C3 |
| 8 | J | 5104 | POV | C32-C31-O31-C3 |
| 8 | A | 5120 | POV | C1-C2-O21-C21 |
| 8 | C | 5101 | POV | C1-C2-O21-C21 |
| 8 | G | 5101 | POV | C1-C2-O21-C21 |
| 8 | J | 5105 | POV | C1-C2-O21-C21 |
| 8 | A | 5107 | POV | C210-C211-C212-C213 |
| 8 | C | 5110 | POV | C210-C211-C212-C213 |
| 8 | G | 5110 | POV | C210-C211-C212-C213 |
| 8 | J | 5114 | POV | C210-C211-C212-C213 |
| 8 | A | 5121 | POV | C25-C26-C27-C28 |
| 8 | C | 5102 | POV | C25-C26-C27-C28 |
| 8 | G | 5102 | POV | C25-C26-C27-C28 |
| 8 | J | 5106 | POV | C25-C26-C27-C28 |
| 8 | A | 5106 | POV | O22-C21-O21-C2 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 8 | A | 5107 | POV | O21-C2-C3-O31 |
| 8 | A | 5120 | POV | O21-C2-C3-O31 |
| 8 | C | 5101 | POV | O21-C2-C3-O31 |
| 8 | C | 5110 | POV | O21-C2-C3-O31 |
| 8 | G | 5101 | POV | O21-C2-C3-O31 |
| 8 | G | 5110 | POV | O21-C2-C3-O31 |
| 8 | J | 5105 | POV | O21-C2-C3-O31 |
| 8 | J | 5114 | POV | O21-C2-C3-O31 |
| 8 | C | 5109 | POV | O22-C21-O21-C2 |
| 8 | C | 5113 | POV | O22-C21-O21-C2 |
| 8 | J | 5113 | POV | O22-C21-O21-C2 |
| 8 | A | 5106 | POV | C32-C31-O31-C3 |
| 8 | A | 5111 | POV | C32-C31-O31-C3 |
| 8 | A | 5116 | POV | C32-C31-O31-C3 |
| 8 | C | 5109 | POV | C32-C31-O31-C3 |
| 8 | C | 5119 | POV | C32-C31-O31-C3 |
| 8 | G | 5109 | POV | C32-C31-O31-C3 |
| 8 | G | 5114 | POV | C32-C31-O31-C3 |
| 8 | G | 5119 | POV | C32-C31-O31-C3 |
| 8 | J | 5101 | POV | C32-C31-O31-C3 |
| 8 | J | 5113 | POV | C32-C31-O31-C3 |
| 8 | J | 5118 | POV | C32-C31-O31-C3 |
| 8 | A | 5109 | POV | C22-C21-O21-C2 |
| 8 | C | 5112 | POV | C22-C21-O21-C2 |
| 8 | G | 5112 | POV | C22-C21-O21-C2 |
| 8 | J | 5116 | POV | C22-C21-O21-C2 |
| 8 | A | 5105 | POV | C34-C35-C36-C37 |
| 8 | C | 5108 | POV | C34-C35-C36-C37 |
| 8 | G | 5108 | POV | C34-C35-C36-C37 |
| 8 | J | 5112 | POV | C34-C35-C36-C37 |
| 8 | C | 5114 | POV | C32-C31-O31-C3 |
| 8 | A | 5107 | POV | C35-C36-C37-C38 |
| 8 | C | 5110 | POV | C35-C36-C37-C38 |
| 8 | G | 5110 | POV | C35-C36-C37-C38 |
| 8 | J | 5114 | POV | C35-C36-C37-C38 |
| 8 | A | 5119 | POV | O11-C1-C2-C3 |
| 8 | A | 5121 | POV | O11-C1-C2-C3 |
| 8 | C | 5102 | POV | O11-C1-C2-C3 |
| 8 | C | 5122 | POV | O11-C1-C2-C3 |
| 8 | G | 5102 | POV | O11-C1-C2-C3 |
| 8 | G | 5122 | POV | O11-C1-C2-C3 |
| 8 | J | 5104 | POV | O11-C1-C2-C3 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 8 | J | 5106 | POV | O11-C1-C2-C3 |
| 8 | C | 5118 | POV | C21-C22-C23-C24 |
| 8 | G | 5118 | POV | C21-C22-C23-C24 |
| 8 | J | 5122 | POV | C21-C22-C23-C24 |
| 8 | A | 5119 | POV | O32-C31-O31-C3 |
| 8 | C | 5122 | POV | O32-C31-O31-C3 |
| 8 | G | 5122 | POV | O32-C31-O31-C3 |
| 8 | J | 5104 | POV | O32-C31-O31-C3 |
| 8 | A | 5121 | POV | O11-C1-C2-O21 |
| 8 | C | 5102 | POV | O11-C1-C2-O21 |
| 8 | G | 5102 | POV | O11-C1-C2-O21 |
| 8 | J | 5106 | POV | O11-C1-C2-O21 |
| 8 | A | 5114 | POV | C2-C1-O11-P |
| 8 | C | 5117 | POV | C2-C1-O11-P |
| 8 | G | 5117 | POV | C2-C1-O11-P |
| 8 | J | 5121 | POV | C2-C1-O11-P |
| 8 | G | 5116 | POV | C31-C32-C33-C34 |
| 8 | A | 5113 | POV | C31-C32-C33-C34 |
| 8 | C | 5116 | POV | C31-C32-C33-C34 |
| 8 | J | 5120 | POV | C31-C32-C33-C34 |
| 8 | C | 5119 | POV | C24-C25-C26-C27 |
| 8 | G | 5119 | POV | C24-C25-C26-C27 |
| 8 | J | 5101 | POV | C24-C25-C26-C27 |
| 8 | A | 5116 | POV | C24-C25-C26-C27 |
| 8 | A | 5105 | POV | O21-C21-C22-C23 |
| 8 | C | 5108 | POV | O21-C21-C22-C23 |
| 8 | G | 5108 | POV | O21-C21-C22-C23 |
| 8 | J | 5112 | POV | O21-C21-C22-C23 |
| 8 | A | 5106 | POV | O32-C31-O31-C3 |
| 8 | A | 5111 | POV | O32-C31-O31-C3 |
| 8 | C | 5109 | POV | O32-C31-O31-C3 |
| 8 | C | 5114 | POV | O32-C31-O31-C3 |
| 8 | G | 5109 | POV | O32-C31-O31-C3 |
| 8 | G | 5114 | POV | O32-C31-O31-C3 |
| 8 | J | 5113 | POV | O32-C31-O31-C3 |
| 8 | J | 5118 | POV | O32-C31-O31-C3 |
| 8 | A | 5110 | POV | C3-C2-O21-C21 |
| 8 | A | 5116 | POV | O32-C31-O31-C3 |
| 8 | G | 5119 | POV | O32-C31-O31-C3 |
| 8 | J | 5101 | POV | O32-C31-O31-C3 |
| 8 | C | 5120 | POV | C22-C23-C24-C25 |
| 8 | C | 5119 | POV | O32-C31-O31-C3 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 8 | A | 5109 | POV | O22-C21-O21-C2 |
| 8 | C | 5112 | POV | O22-C21-O21-C2 |
| 8 | G | 5112 | POV | O22-C21-O21-C2 |
| 8 | J | 5116 | POV | O22-C21-O21-C2 |
| 8 | A | 5119 | POV | O11-C1-C2-O21 |
| 8 | C | 5122 | POV | O11-C1-C2-O21 |
| 8 | G | 5122 | POV | O11-C1-C2-O21 |
| 8 | J | 5104 | POV | O11-C1-C2-O21 |
| 8 | A | 5106 | POV | C12-C11-O12-P |
| 8 | A | 5115 | POV | C12-C11-O12-P |
| 8 | C | 5109 | POV | C12-C11-O12-P |
| 8 | C | 5118 | POV | C12-C11-O12-P |
| 8 | G | 5109 | POV | C12-C11-O12-P |
| 8 | G | 5118 | POV | C12-C11-O12-P |
| 8 | J | 5113 | POV | C12-C11-O12-P |
| 8 | J | 5122 | POV | C12-C11-O12-P |
| 8 | A | 5105 | POV | C36-C37-C38-C39 |
| 8 | G | 5108 | POV | C36-C37-C38-C39 |
| 8 | J | 5112 | POV | C36-C37-C38-C39 |
| 8 | C | 5108 | POV | C36-C37-C38-C39 |
| 8 | A | 5107 | POV | O12-C11-C12-N |
| 8 | A | 5108 | POV | O12-C11-C12-N |
| 8 | A | 5109 | POV | O12-C11-C12-N |
| 8 | A | 5118 | POV | O12-C11-C12-N |
| 8 | A | 5119 | POV | O12-C11-C12-N |
| 8 | C | 5110 | POV | O12-C11-C12-N |
| 8 | C | 5111 | POV | O12-C11-C12-N |
| 8 | C | 5112 | POV | O12-C11-C12-N |
| 8 | C | 5113 | POV | O12-C11-C12-N |
| 8 | C | 5121 | POV | O12-C11-C12-N |
| 8 | C | 5122 | POV | O12-C11-C12-N |
| 8 | G | 5110 | POV | O12-C11-C12-N |
| 8 | G | 5111 | POV | O12-C11-C12-N |
| 8 | G | 5112 | POV | O12-C11-C12-N |
| 8 | G | 5121 | POV | O12-C11-C12-N |
| 8 | G | 5122 | POV | O12-C11-C12-N |
| 8 | J | 5102 | POV | O12-C11-C12-N |
| 8 | J | 5103 | POV | O12-C11-C12-N |
| 8 | J | 5104 | POV | O12-C11-C12-N |
| 8 | J | 5114 | POV | O12-C11-C12-N |
| 8 | J | 5115 | POV | O12-C11-C12-N |
| 8 | J | 5116 | POV | O12-C11-C12-N |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 8 | J | 5117 | POV | O12-C11-C12-N |
| 8 | A | 5115 | POV | C23-C24-C25-C26 |
| 8 | C | 5121 | POV | C26-C27-C28-C29 |
| 8 | A | 5118 | POV | C33-C34-C35-C36 |
| 8 | C | 5121 | POV | C33-C34-C35-C36 |
| 8 | G | 5121 | POV | C33-C34-C35-C36 |
| 8 | J | 5103 | POV | C33-C34-C35-C36 |
| 8 | A | 5118 | POV | C21-C22-C23-C24 |
| 8 | C | 5121 | POV | C21-C22-C23-C24 |
| 8 | J | 5103 | POV | C21-C22-C23-C24 |
| 8 | A | 5105 | POV | C2-C1-O11-P |
| 8 | C | 5108 | POV | C2-C1-O11-P |
| 8 | G | 5108 | POV | C2-C1-O11-P |
| 8 | J | 5112 | POV | C2-C1-O11-P |
| 8 | A | 5118 | POV | C26-C27-C28-C29 |
| 8 | G | 5121 | POV | C26-C27-C28-C29 |
| 8 | G | 5121 | POV | C21-C22-C23-C24 |
| 8 | A | 5120 | POV | C1-C2-C3-O31 |
| 8 | C | 5101 | POV | C1-C2-C3-O31 |
| 8 | G | 5101 | POV | C1-C2-C3-O31 |
| 8 | J | 5105 | POV | C1-C2-C3-O31 |
| 8 | J | 5103 | POV | C26-C27-C28-C29 |
| 8 | A | 5115 | POV | C27-C28-C29-C210 |
| 8 | C | 5109 | POV | C25-C26-C27-C28 |
| 8 | G | 5109 | POV | C25-C26-C27-C28 |
| 8 | A | 5106 | POV | C25-C26-C27-C28 |
| 8 | J | 5113 | POV | C25-C26-C27-C28 |
| 8 | A | 5105 | POV | C1-O11-P-O13 |
| 8 | A | 5110 | POV | C11-O12-P-O14 |
| 8 | A | 5111 | POV | C1-O11-P-O14 |
| 8 | A | 5111 | POV | C11-O12-P-O14 |
| 8 | A | 5112 | POV | C11-O12-P-O11 |
| 8 | A | 5112 | POV | C11-O12-P-O14 |
| 8 | A | 5113 | POV | C11-O12-P-O14 |
| 8 | A | 5114 | POV | C1-O11-P-O14 |
| 8 | A | 5115 | POV | C1-O11-P-O14 |
| 8 | A | 5116 | POV | C1-O11-P-O14 |
| 8 | A | 5118 | POV | C11-O12-P-O14 |
| 8 | C | 5108 | POV | C1-O11-P-O13 |
| 8 | C | 5114 | POV | C1-O11-P-O14 |
| 8 | C | 5114 | POV | C11-O12-P-O14 |
| 8 | C | 5115 | POV | C11-O12-P-O11 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 8 | C | 5115 | POV | C11-O12-P-O14 |
| 8 | C | 5116 | POV | C11-O12-P-O14 |
| 8 | C | 5117 | POV | C1-O11-P-O14 |
| 8 | C | 5118 | POV | C11-O12-P-O14 |
| 8 | C | 5119 | POV | C1-O11-P-O14 |
| 8 | C | 5121 | POV | C11-O12-P-O14 |
| 8 | G | 5108 | POV | C1-O11-P-O13 |
| 8 | G | 5114 | POV | C1-O11-P-O14 |
| 8 | G | 5114 | POV | C11-O12-P-O14 |
| 8 | G | 5115 | POV | C11-O12-P-O11 |
| 8 | G | 5115 | POV | C11-O12-P-O14 |
| 8 | G | 5116 | POV | C11-O12-P-O14 |
| 8 | G | 5117 | POV | C1-O11-P-O14 |
| 8 | G | 5118 | POV | C11-O12-P-O14 |
| 8 | G | 5119 | POV | C1-O11-P-O14 |
| 8 | G | 5120 | POV | C1-O11-P-O12 |
| 8 | G | 5120 | POV | C11-O12-P-O14 |
| 8 | G | 5121 | POV | C11-O12-P-O14 |
| 8 | J | 5101 | POV | C1-O11-P-O14 |
| 8 | J | 5103 | POV | C11-O12-P-O14 |
| 8 | J | 5112 | POV | C1-O11-P-O13 |
| 8 | J | 5118 | POV | C1-O11-P-O14 |
| 8 | J | 5118 | POV | C11-O12-P-O14 |
| 8 | J | 5119 | POV | C11-O12-P-O11 |
| 8 | J | 5119 | POV | C11-O12-P-O14 |
| 8 | J | 5120 | POV | C11-O12-P-O14 |
| 8 | J | 5121 | POV | C1-O11-P-O14 |
| 8 | J | 5122 | POV | C11-O12-P-O14 |
| 8 | A | 5107 | POV | C2-C1-O11-P |
| 8 | A | 5118 | POV | C2-C1-O11-P |
| 8 | C | 5110 | POV | C2-C1-O11-P |
| 8 | C | 5121 | POV | C2-C1-O11-P |
| 8 | G | 5110 | POV | C2-C1-O11-P |
| 8 | G | 5121 | POV | C2-C1-O11-P |
| 8 | J | 5103 | POV | C2-C1-O11-P |
| 8 | J | 5114 | POV | C2-C1-O11-P |
| 8 | A | 5107 | POV | C27-C28-C29-C210 |
| 8 | C | 5110 | POV | C27-C28-C29-C210 |
| 8 | G | 5110 | POV | C27-C28-C29-C210 |
| 8 | J | 5114 | POV | C27-C28-C29-C210 |
| 8 | A | 5118 | POV | C3-C2-O21-C21 |
| 8 | C | 5121 | POV | C3-C2-O21-C21 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 8 | G | 5121 | POV | C3-C2-O21-C21 |
| 8 | J | 5103 | POV | C3-C2-O21-C21 |
| 8 | J | 5117 | POV | C3-C2-O21-C21 |
| 8 | A | 5114 | POV | C11-C12-N-C14 |
| 8 | J | 5121 | POV | C11-C12-N-C14 |
| 8 | A | 5108 | POV | C29-C210-C211-C212 |
| 8 | A | 5117 | POV | C27-C28-C29-C210 |
| 8 | C | 5111 | POV | C29-C210-C211-C212 |
| 8 | C | 5120 | POV | C27-C28-C29-C210 |
| 8 | G | 5111 | POV | C29-C210-C211-C212 |
| 8 | J | 5115 | POV | C29-C210-C211-C212 |
| 8 | A | 5105 | POV | O11-C1-C2-O21 |
| 8 | C | 5108 | POV | O11-C1-C2-O21 |
| 8 | G | 5108 | POV | O11-C1-C2-O21 |
| 8 | J | 5112 | POV | O11-C1-C2-O21 |
| 8 | A | 5112 | POV | O21-C2-C3-O31 |
| 8 | C | 5115 | POV | O21-C2-C3-O31 |
| 8 | G | 5115 | POV | O21-C2-C3-O31 |
| 8 | J | 5119 | POV | O21-C2-C3-O31 |
| 8 | A | 5111 | POV | C1-C2-C3-O31 |
| 8 | C | 5114 | POV | C1-C2-C3-O31 |
| 8 | G | 5114 | POV | C1-C2-C3-O31 |
| 8 | J | 5118 | POV | C1-C2-C3-O31 |
| 8 | C | 5117 | POV | C11-C12-N-C14 |
| 8 | G | 5117 | POV | C11-C12-N-C14 |
| 8 | A | 5107 | POV | C37-C38-C39-C310 |
| 8 | C | 5110 | POV | C37-C38-C39-C310 |
| 8 | G | 5110 | POV | C37-C38-C39-C310 |
| 8 | J | 5114 | POV | C37-C38-C39-C310 |
| 8 | A | 5114 | POV | C11-C12-N-C15 |
| 8 | C | 5117 | POV | C11-C12-N-C15 |
| 8 | G | 5117 | POV | C11-C12-N-C15 |
| 8 | J | 5121 | POV | C11-C12-N-C15 |
| 8 | G | 5113 | POV | O21-C21-C22-C23 |
| 8 | A | 5117 | POV | C29-C210-C211-C212 |
| 5 | A | 5102 | ATP | O4'-C1'-N9-C8 |
| 5 | C | 5105 | ATP | O4'-C1'-N9-C8 |
| 5 | G | 5105 | ATP | O4'-C1'-N9-C8 |
| 5 | J | 5109 | ATP | O4'-C1'-N9-C8 |
| 5 | A | 5102 | ATP | O4'-C1'-N9-C4 |
| 5 | C | 5105 | ATP | O4'-C1'-N9-C4 |
| 5 | G | 5105 | ATP | O4'-C1'-N9-C4 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 5 | J | 5109 | ATP | O4'-C1'-N9-C4 |
| 8 | C | 5120 | POV | C2-C1-O11-P |
| 8 | C | 5110 | POV | C1-C2-C3-O31 |
| 8 | G | 5110 | POV | C1-C2-C3-O31 |
| 8 | J | 5114 | POV | C1-C2-C3-O31 |
| 8 | J | 5114 | POV | C310-C311-C312-C313 |
| 8 | C | 5110 | POV | C310-C311-C312-C313 |
| 8 | G | 5110 | POV | C310-C311-C312-C313 |
| 8 | A | 5107 | POV | C310-C311-C312-C313 |
| 8 | A | 5115 | POV | O31-C31-C32-C33 |
| 8 | J | 5117 | POV | O22-C21-C22-C23 |
| 8 | A | 5107 | POV | C1-C2-C3-O31 |
| 8 | A | 5118 | POV | C31-C32-C33-C34 |
| 8 | G | 5121 | POV | C31-C32-C33-C34 |
| 8 | J | 5103 | POV | C31-C32-C33-C34 |
| 8 | C | 5121 | POV | C31-C32-C33-C34 |
| 8 | C | 5118 | POV | C22-C23-C24-C25 |
| 8 | J | 5122 | POV | C22-C23-C24-C25 |
| 8 | G | 5118 | POV | C22-C23-C24-C25 |
| 8 | J | 5106 | POV | C35-C36-C37-C38 |
| 8 | C | 5102 | POV | C35-C36-C37-C38 |
| 8 | G | 5102 | POV | C35-C36-C37-C38 |
| 8 | C | 5118 | POV | C27-C28-C29-C210 |
| 8 | J | 5122 | POV | C27-C28-C29-C210 |
| 8 | A | 5121 | POV | C35-C36-C37-C38 |
| 8 | G | 5110 | POV | C25-C26-C27-C28 |
| 8 | C | 5110 | POV | C25-C26-C27-C28 |
| 8 | A | 5107 | POV | C25-C26-C27-C28 |
| 8 | J | 5114 | POV | C25-C26-C27-C28 |
| 8 | A | 5105 | POV | O11-C1-C2-C3 |
| 8 | C | 5108 | POV | O11-C1-C2-C3 |
| 8 | G | 5108 | POV | O11-C1-C2-C3 |
| 8 | J | 5112 | POV | O11-C1-C2-C3 |
| 8 | J | 5117 | POV | O21-C21-C22-C23 |
| 8 | G | 5118 | POV | C27-C28-C29-C210 |
| 8 | G | 5122 | POV | C311-C310-C39-C38 |
| 8 | A | 5121 | POV | C23-C24-C25-C26 |
| 8 | C | 5122 | POV | C311-C310-C39-C38 |
| 8 | G | 5102 | POV | C23-C24-C25-C26 |
| 8 | J | 5106 | POV | C23-C24-C25-C26 |
| 8 | C | 5102 | POV | C23-C24-C25-C26 |
| 8 | A | 5119 | POV | C311-C310-C39-C38 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 8 | J | 5104 | POV | C311-C310-C39-C38 |
| 8 | G | 5113 | POV | O22-C21-C22-C23 |
| 8 | A | 5119 | POV | C1-C2-O21-C21 |
| 8 | A | 5119 | POV | C3-C2-O21-C21 |
| 8 | C | 5122 | POV | C1-C2-O21-C21 |
| 8 | C | 5122 | POV | C3-C2-O21-C21 |
| 8 | G | 5122 | POV | C1-C2-O21-C21 |
| 8 | G | 5122 | POV | C3-C2-O21-C21 |
| 8 | J | 5104 | POV | C1-C2-O21-C21 |
| 8 | J | 5104 | POV | C3-C2-O21-C21 |
| 8 | A | 5108 | POV | C27-C28-C29-C210 |
| 8 | C | 5111 | POV | C27-C28-C29-C210 |
| 8 | G | 5111 | POV | C27-C28-C29-C210 |
| 8 | J | 5115 | POV | C27-C28-C29-C210 |
| 8 | G | 5113 | POV | C3-C2-O21-C21 |
| 8 | A | 5107 | POV | C29-C210-C211-C212 |
| 8 | A | 5120 | POV | C27-C28-C29-C210 |
| 8 | C | 5101 | POV | C27-C28-C29-C210 |
| 8 | C | 5110 | POV | C29-C210-C211-C212 |
| 8 | G | 5101 | POV | C27-C28-C29-C210 |
| 8 | G | 5110 | POV | C29-C210-C211-C212 |
| 8 | J | 5114 | POV | C29-C210-C211-C212 |
| 8 | J | 5105 | POV | C27-C28-C29-C210 |
| 8 | A | 5116 | POV | C39-C310-C311-C312 |
| 8 | C | 5119 | POV | C39-C310-C311-C312 |
| 8 | G | 5119 | POV | C39-C310-C311-C312 |
| 8 | J | 5101 | POV | C39-C310-C311-C312 |
| 8 | A | 5115 | POV | O32-C31-C32-C33 |
| 8 | A | 5105 | POV | C12-C11-O12-P |
| 8 | C | 5108 | POV | C12-C11-O12-P |
| 8 | G | 5108 | POV | C12-C11-O12-P |
| 8 | J | 5112 | POV | C12-C11-O12-P |
| 8 | A | 5116 | POV | C27-C28-C29-C210 |
| 8 | A | 5121 | POV | C27-C28-C29-C210 |
| 8 | C | 5102 | POV | C27-C28-C29-C210 |
| 8 | C | 5119 | POV | C27-C28-C29-C210 |
| 8 | G | 5102 | POV | C27-C28-C29-C210 |
| 8 | G | 5119 | POV | C27-C28-C29-C210 |
| 8 | J | 5101 | POV | C27-C28-C29-C210 |
| 8 | J | 5106 | POV | C27-C28-C29-C210 |
| 8 | A | 5105 | POV | O22-C21-C22-C23 |
| 8 | C | 5108 | POV | O22-C21-C22-C23 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 8 | G | 5108 | POV | O22-C21-C22-C23 |
| 8 | J | 5112 | POV | O22-C21-C22-C23 |
| 8 | A | 5116 | POV | O11-C1-C2-C3 |
| 8 | C | 5119 | POV | O11-C1-C2-C3 |
| 8 | G | 5119 | POV | O11-C1-C2-C3 |
| 8 | J | 5101 | POV | O11-C1-C2-C3 |
| 8 | A | 5107 | POV | O21-C21-C22-C23 |
| 8 | C | 5102 | POV | O21-C21-C22-C23 |
| 8 | C | 5110 | POV | O21-C21-C22-C23 |
| 8 | G | 5102 | POV | O21-C21-C22-C23 |
| 8 | G | 5110 | POV | O21-C21-C22-C23 |
| 8 | J | 5106 | POV | O21-C21-C22-C23 |
| 8 | J | 5114 | POV | O21-C21-C22-C23 |
| 8 | A | 5121 | POV | O21-C21-C22-C23 |
| 5 | J | 5109 | ATP | O4'-C4'-C5'-O5' |
| 8 | A | 5113 | POV | O12-C11-C12-N |
| 8 | C | 5116 | POV | O12-C11-C12-N |
| 8 | G | 5116 | POV | O12-C11-C12-N |
| 8 | J | 5120 | POV | O12-C11-C12-N |
| 8 | C | 5115 | POV | C36-C37-C38-C39 |
| 8 | G | 5115 | POV | C36-C37-C38-C39 |
| 8 | A | 5112 | POV | C36-C37-C38-C39 |
| 8 | J | 5119 | POV | C36-C37-C38-C39 |
| 8 | A | 5110 | POV | O22-C21-C22-C23 |
| 8 | A | 5116 | POV | C215-C216-C217-C218 |
| 8 | C | 5119 | POV | C215-C216-C217-C218 |
| 8 | J | 5101 | POV | C215-C216-C217-C218 |
| 8 | G | 5119 | POV | C215-C216-C217-C218 |
| 5 | A | 5102 | ATP | O4'-C4'-C5'-O5' |
| 5 | C | 5105 | ATP | O4'-C4'-C5'-O5' |
| 5 | G | 5105 | ATP | O4'-C4'-C5'-O5' |
| 8 | A | 5105 | POV | O31-C31-C32-C33 |
| 8 | C | 5108 | POV | O31-C31-C32-C33 |
| 8 | G | 5108 | POV | O31-C31-C32-C33 |
| 8 | J | 5112 | POV | O31-C31-C32-C33 |
| 8 | A | 5108 | POV | O11-C1-C2-C3 |
| 8 | C | 5111 | POV | O11-C1-C2-C3 |
| 8 | G | 5111 | POV | O11-C1-C2-C3 |
| 8 | J | 5115 | POV | O11-C1-C2-C3 |
| 8 | A | 5108 | POV | C214-C215-C216-C217 |
| 8 | J | 5115 | POV | C214-C215-C216-C217 |
| 8 | C | 5111 | POV | C214-C215-C216-C217 |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 8 | G | 5111 | POV | C214-C215-C216-C217 |
| 8 | A | 5122 | POV | C211-C212-C213-C214 |
| 8 | C | 5103 | POV | C211-C212-C213-C214 |
| 8 | G | 5103 | POV | C211-C212-C213-C214 |
| 8 | J | 5107 | POV | C211-C212-C213-C214 |
| 8 | A | 5108 | POV | O11-C1-C2-O21 |
| 8 | C | 5111 | POV | O11-C1-C2-O21 |
| 8 | G | 5111 | POV | O11-C1-C2-O21 |
| 8 | J | 5115 | POV | O11-C1-C2-O21 |
| 8 | J | 5121 | POV | C11-C12-N-C13 |
| 8 | C | 5108 | POV | O32-C31-C32-C33 |
| 8 | G | 5108 | POV | O32-C31-C32-C33 |
| 8 | J | 5112 | POV | O32-C31-C32-C33 |
| 8 | A | 5121 | POV | O22-C21-C22-C23 |
| 8 | C | 5102 | POV | O22-C21-C22-C23 |
| 8 | G | 5102 | POV | O22-C21-C22-C23 |
| 8 | J | 5106 | POV | O22-C21-C22-C23 |
| 8 | A | 5105 | POV | O32-C31-C32-C33 |
| 8 | C | 5110 | POV | O22-C21-C22-C23 |
| 8 | G | 5110 | POV | O22-C21-C22-C23 |
| 8 | J | 5114 | POV | O22-C21-C22-C23 |
| 8 | A | 5107 | POV | O22-C21-C22-C23 |
| 8 | A | 5114 | POV | C11-C12-N-C13 |
| 8 | C | 5117 | POV | C11-C12-N-C13 |
| 8 | G | 5117 | POV | C11-C12-N-C13 |
| 8 | J | 5119 | POV | C311-C310-C39-C38 |
| 8 | A | 5112 | POV | C311-C310-C39-C38 |
| 8 | C | 5115 | POV | C311-C310-C39-C38 |
| 8 | G | 5115 | POV | C311-C310-C39-C38 |
| 8 | A | 5106 | POV | O21-C21-C22-C23 |
| 8 | A | 5111 | POV | O31-C31-C32-C33 |
| 8 | C | 5114 | POV | O31-C31-C32-C33 |
| 8 | G | 5109 | POV | O21-C21-C22-C23 |
| 8 | G | 5114 | POV | O31-C31-C32-C33 |
| 8 | J | 5113 | POV | O21-C21-C22-C23 |
| 8 | J | 5118 | POV | O31-C31-C32-C33 |
| 8 | C | 5109 | POV | O21-C21-C22-C23 |

There are no ring outliers.

76 monomers are involved in 153 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 8 | J | 5115 | POV | 4 | 0 |
| 8 | C | 5122 | POV | 1 | 0 |
| 8 | C | 5116 | POV | 2 | 0 |
| 8 | C | 5108 | POV | 1 | 0 |
| 8 | G | 5108 | POV | 1 | 0 |
| 8 | J | 5105 | POV | 1 | 0 |
| 8 | A | 5115 | POV | 1 | 0 |
| 8 | C | 5114 | POV | 5 | 0 |
| 8 | A | 5107 | POV | 7 | 0 |
| 8 | G | 5112 | POV | 2 | 0 |
| 8 | G | 5114 | POV | 4 | 0 |
| 8 | A | 5120 | POV | 1 | 0 |
| 8 | C | 5113 | POV | 5 | 0 |
| 8 | C | 5112 | POV | 3 | 0 |
| 8 | C | 5121 | POV | 1 | 0 |
| 8 | G | 5121 | POV | 1 | 0 |
| 5 | A | 5102 | ATP | 1 | 0 |
| 8 | J | 5113 | POV | 2 | 0 |
| 8 | A | 5109 | POV | 2 | 0 |
| 8 | G | 5111 | POV | 4 | 0 |
| 8 | C | 5115 | POV | 5 | 0 |
| 8 | J | 5102 | POV | 3 | 0 |
| 8 | A | 5122 | POV | 2 | 0 |
| 8 | A | 5116 | POV | 7 | 0 |
| 5 | J | 5109 | ATP | 2 | 0 |
| 5 | C | 5105 | ATP | 2 | 0 |
| 8 | J | 5119 | POV | 5 | 0 |
| 5 | G | 5105 | ATP | 1 | 0 |
| 8 | J | 5104 | POV | 1 | 0 |
| 8 | C | 5118 | POV | 1 | 0 |
| 8 | C | 5102 | POV | 2 | 0 |
| 8 | J | 5120 | POV | 1 | 0 |
| 8 | A | 5106 | POV | 1 | 0 |
| 8 | G | 5115 | POV | 4 | 0 |
| 8 | A | 5117 | POV | 3 | 0 |
| 8 | G | 5120 | POV | 1 | 0 |
| 8 | C | 5120 | POV | 4 | 0 |
| 8 | J | 5117 | POV | 5 | 0 |
| 8 | J | 5107 | POV | 2 | 0 |
| 8 | C | 5109 | POV | 1 | 0 |
| 8 | A | 5110 | POV | 2 | 0 |
| 8 | G | 5109 | POV | 2 | 0 |
| 8 | J | 5103 | POV | 1 | 0 |

*Continued on next page...*

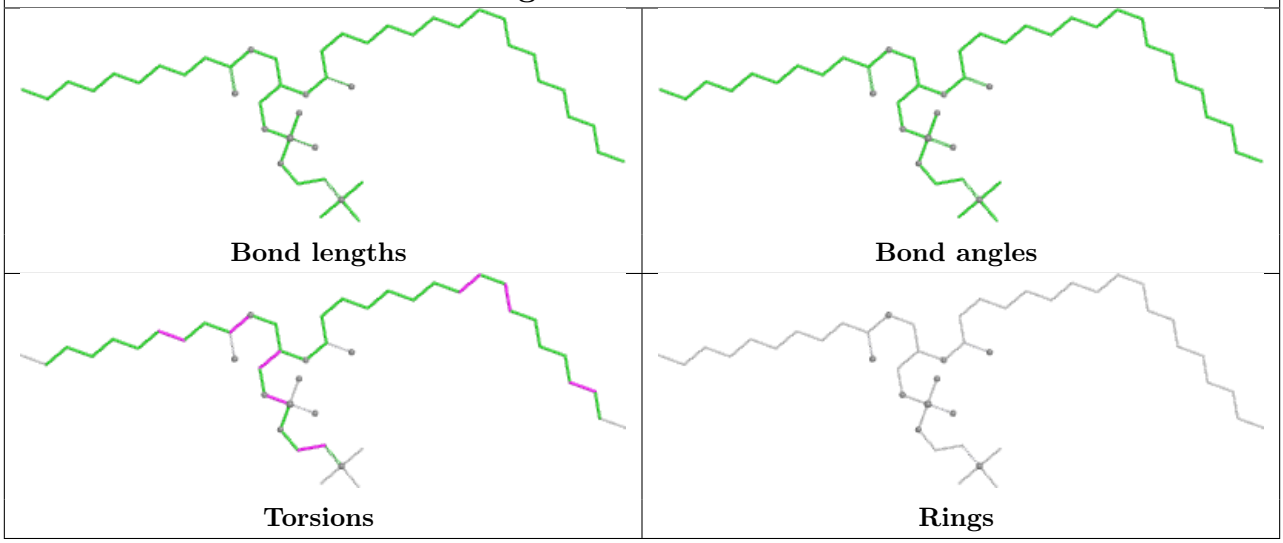
*Continued from previous page...*

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 8 | J | 5118 | POV | 5 | 0 |
| 8 | J | 5112 | POV | 2 | 0 |
| 8 | A | 5105 | POV | 2 | 0 |
| 8 | G | 5102 | POV | 2 | 0 |
| 8 | C | 5119 | POV | 5 | 0 |
| 8 | G | 5116 | POV | 1 | 0 |
| 8 | A | 5108 | POV | 3 | 0 |
| 8 | A | 5111 | POV | 4 | 0 |
| 8 | J | 5106 | POV | 2 | 0 |
| 8 | J | 5122 | POV | 1 | 0 |
| 8 | A | 5113 | POV | 1 | 0 |
| 8 | A | 5112 | POV | 5 | 0 |
| 8 | A | 5114 | POV | 2 | 0 |
| 8 | G | 5122 | POV | 1 | 0 |
| 8 | G | 5113 | POV | 3 | 0 |
| 8 | C | 5117 | POV | 3 | 0 |
| 8 | G | 5119 | POV | 4 | 0 |
| 8 | A | 5121 | POV | 3 | 0 |
| 8 | J | 5114 | POV | 7 | 0 |
| 8 | G | 5117 | POV | 3 | 0 |
| 8 | G | 5101 | POV | 1 | 0 |
| 8 | J | 5121 | POV | 3 | 0 |
| 8 | C | 5101 | POV | 1 | 0 |
| 8 | C | 5103 | POV | 2 | 0 |
| 8 | A | 5118 | POV | 1 | 0 |
| 8 | C | 5110 | POV | 7 | 0 |
| 8 | G | 5103 | POV | 2 | 0 |
| 8 | J | 5101 | POV | 6 | 0 |
| 8 | G | 5110 | POV | 7 | 0 |
| 8 | G | 5118 | POV | 1 | 0 |
| 8 | A | 5119 | POV | 1 | 0 |
| 8 | J | 5116 | POV | 3 | 0 |
| 8 | C | 5111 | POV | 4 | 0 |

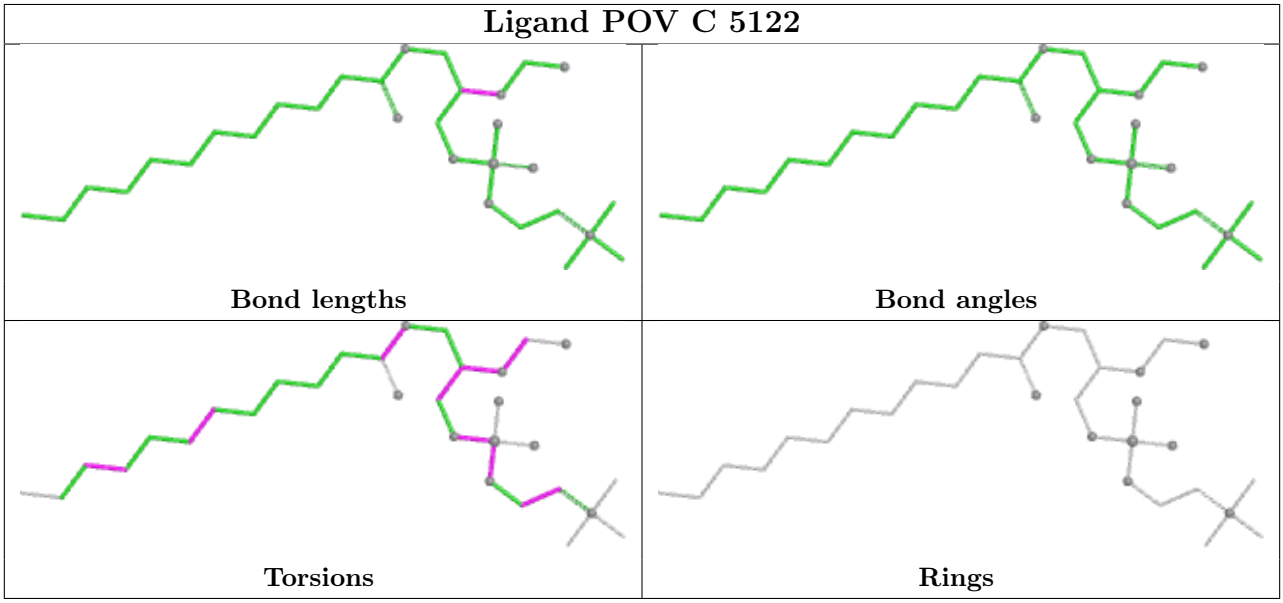
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

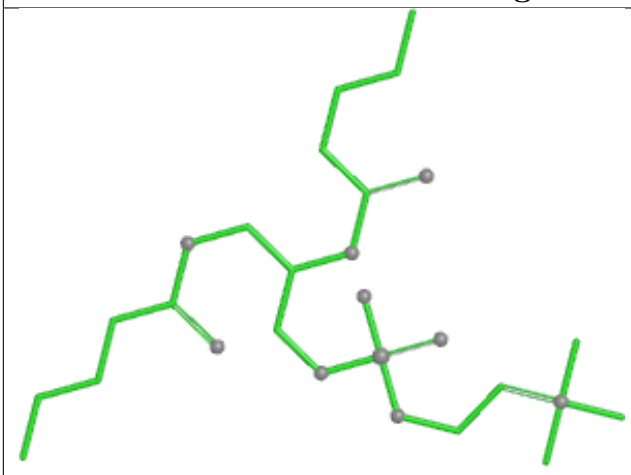
**Ligand POV J 5115**



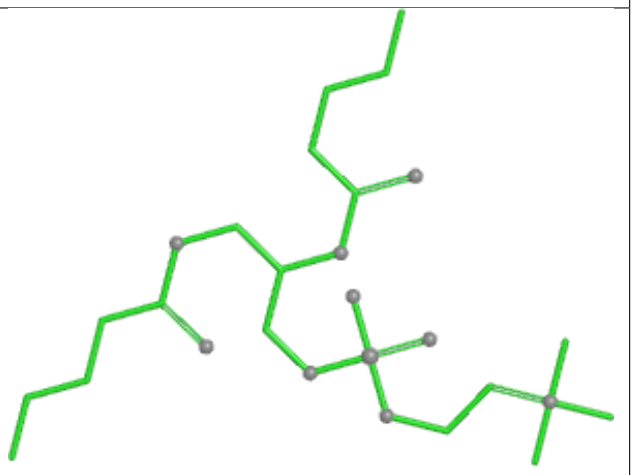

**Ligand POV C 5122**



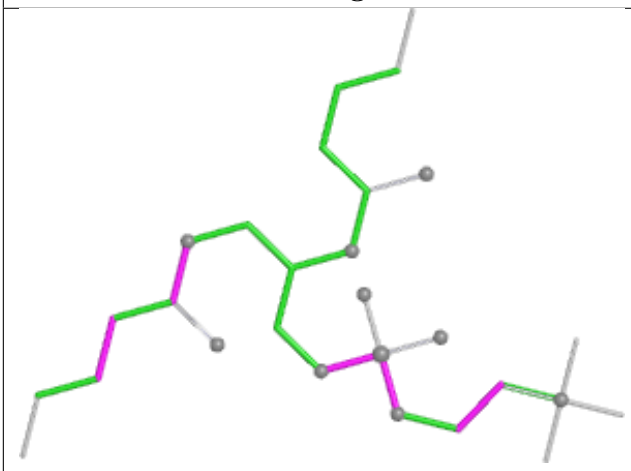
## Ligand POV C 5116



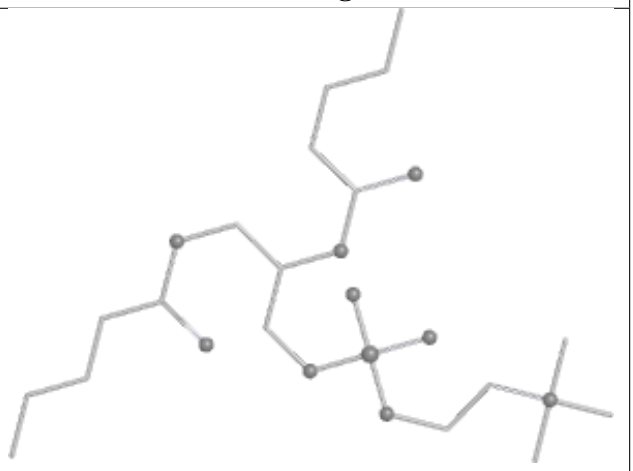
Bond lengths



Bond angles

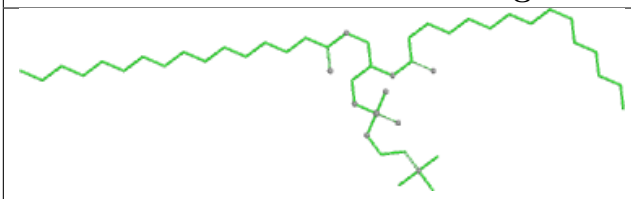


Torsions

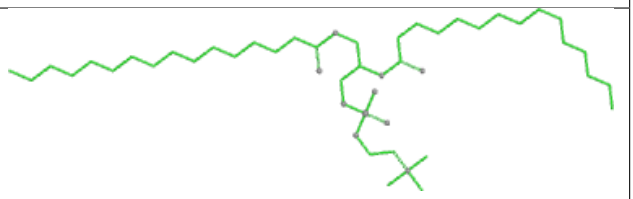


Rings

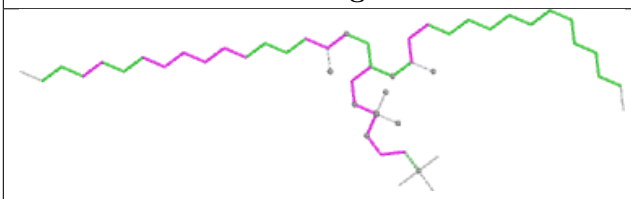
## Ligand POV C 5108



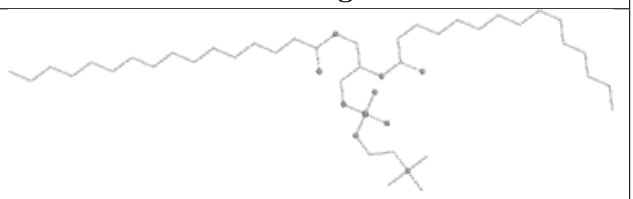
Bond lengths



Bond angles

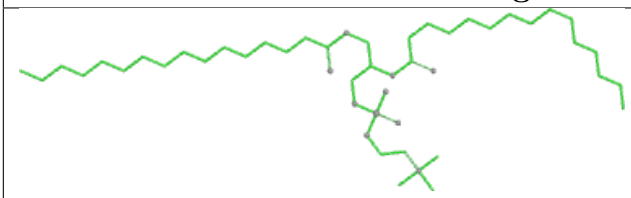


Torsions

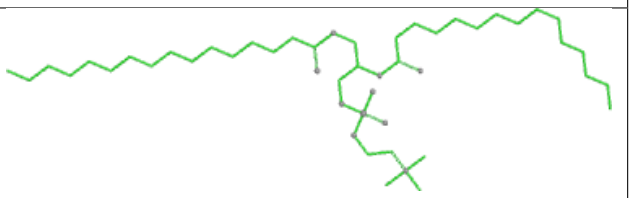


Rings

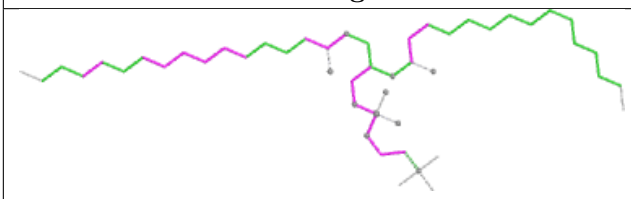
**Ligand POV G 5108**



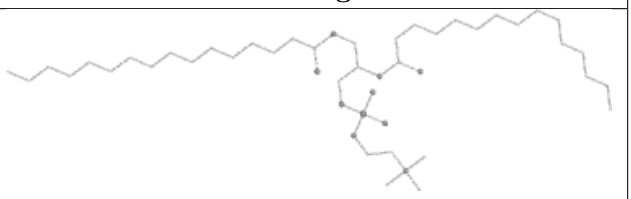
Bond lengths



Bond angles

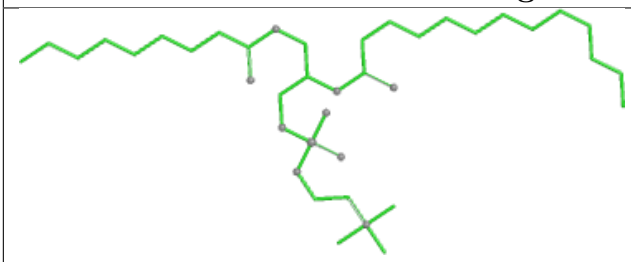


Torsions

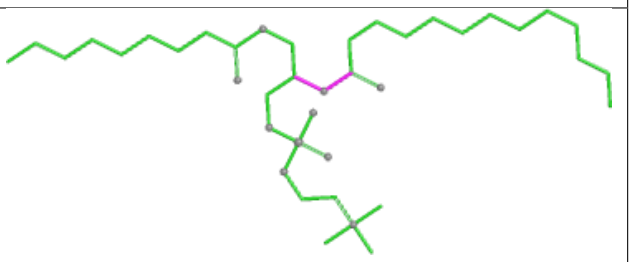


Rings

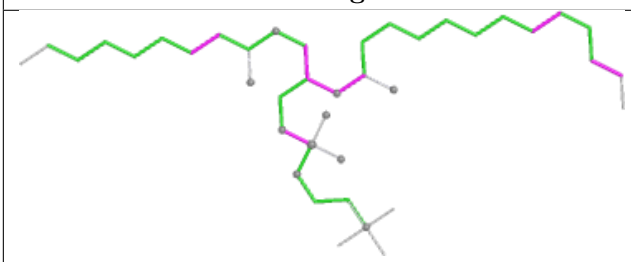
**Ligand POV J 5105**



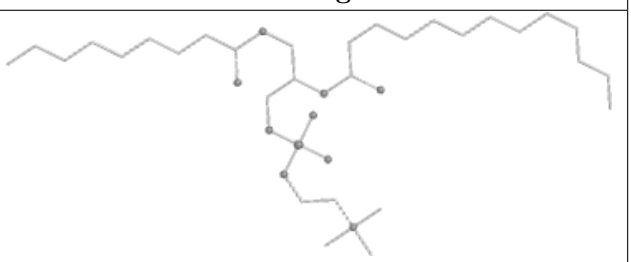
Bond lengths



Bond angles

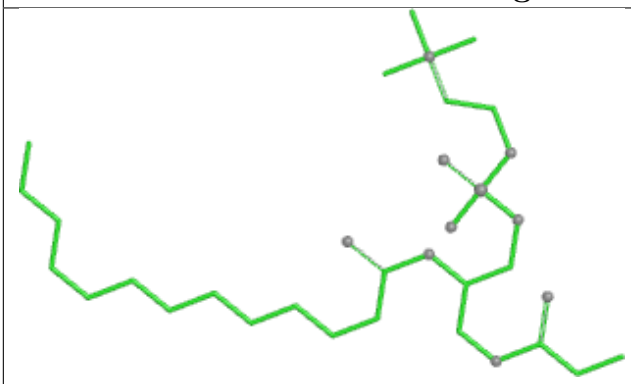


Torsions

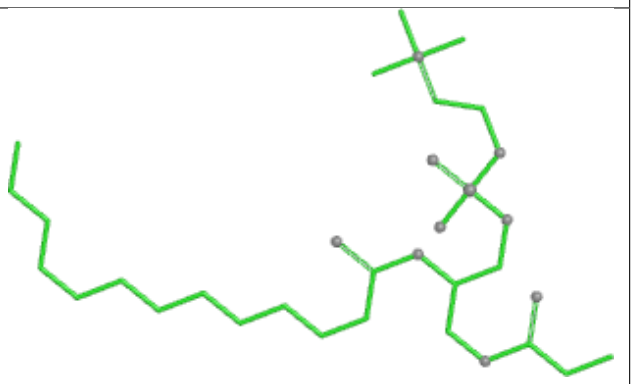


Rings

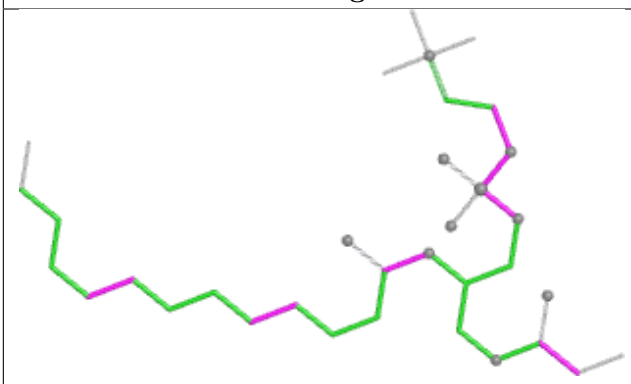
## Ligand POV A 5115



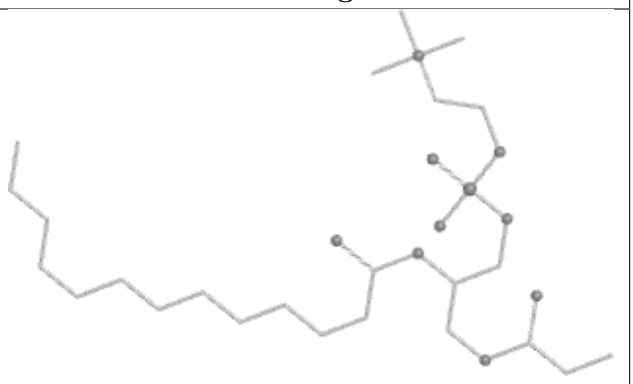
Bond lengths



Bond angles

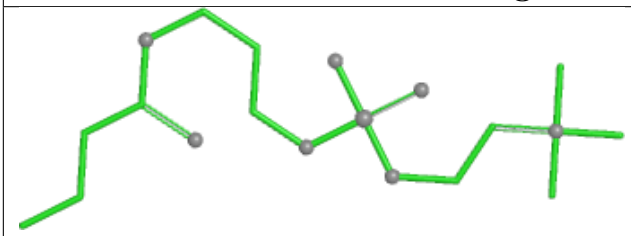


Torsions

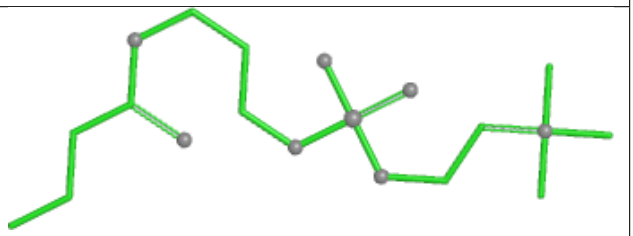


Rings

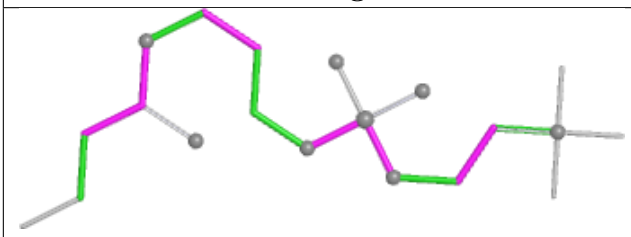
## Ligand POV C 5114



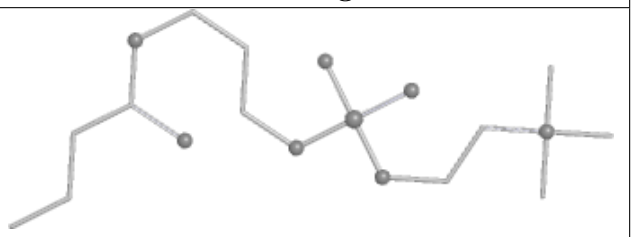
Bond lengths



Bond angles

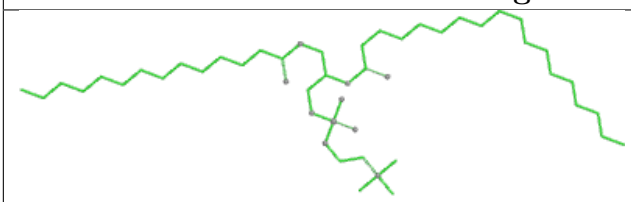


Torsions

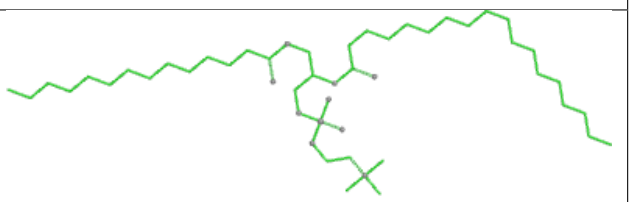


Rings

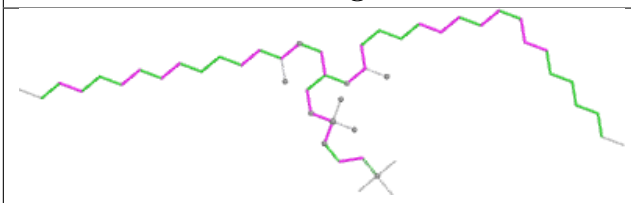
**Ligand POV A 5107**



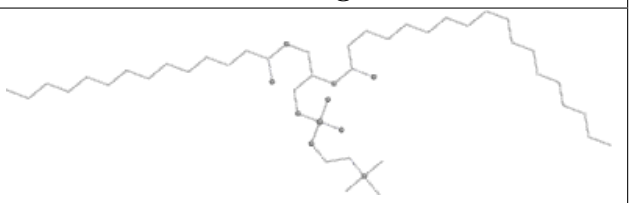
Bond lengths



Bond angles

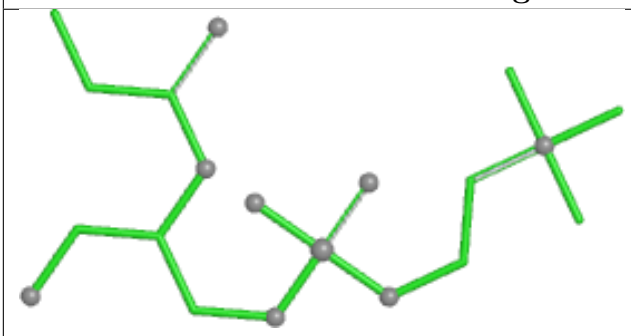


Torsions

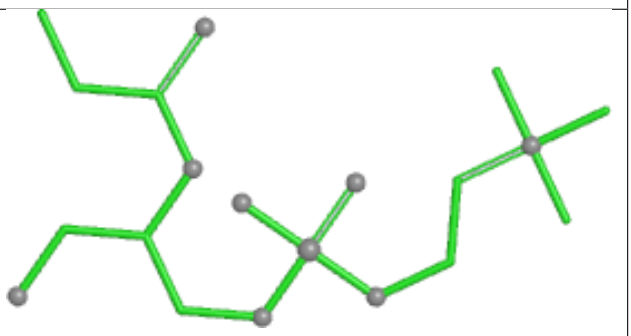


Rings

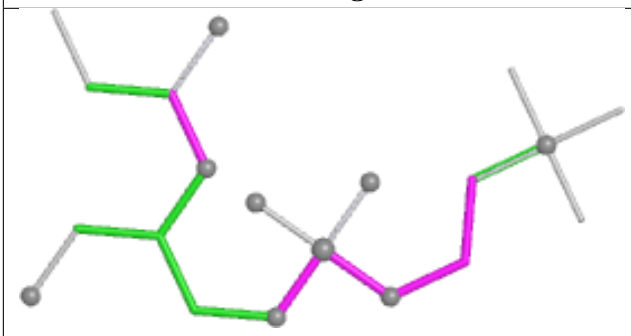
**Ligand POV G 5112**



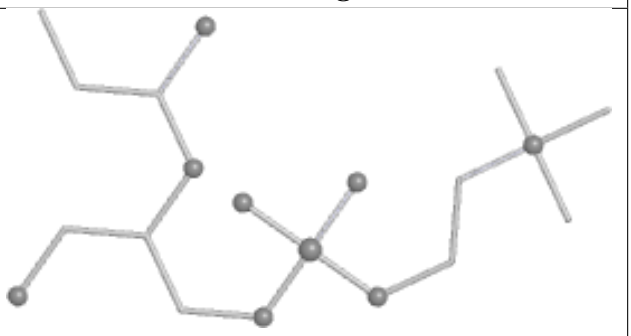
Bond lengths



Bond angles

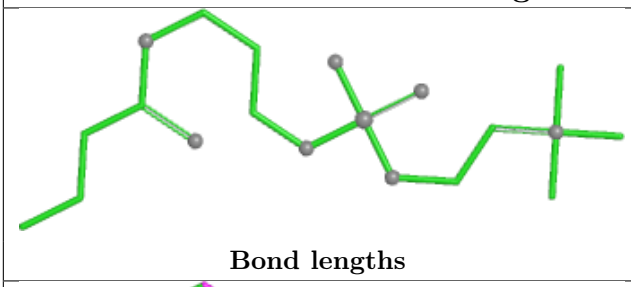


Torsions

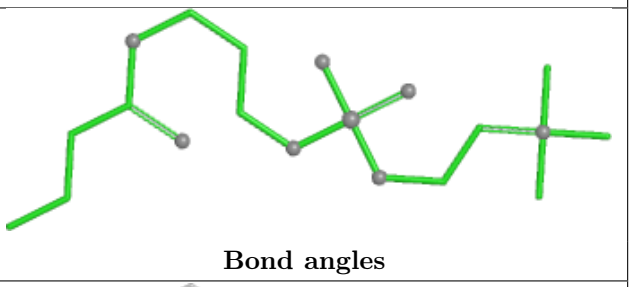


Rings

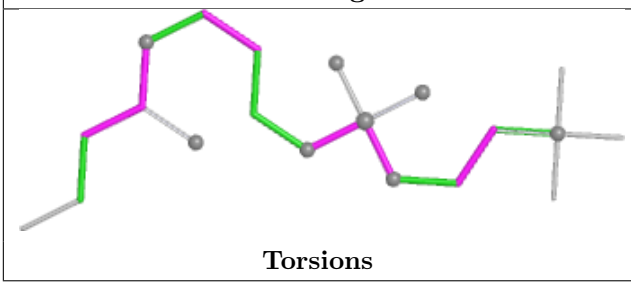
## Ligand POV G 5114



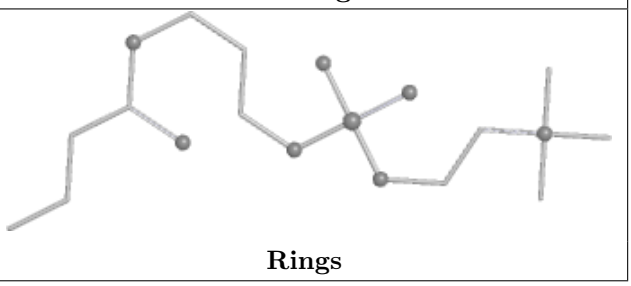
Bond lengths



Bond angles

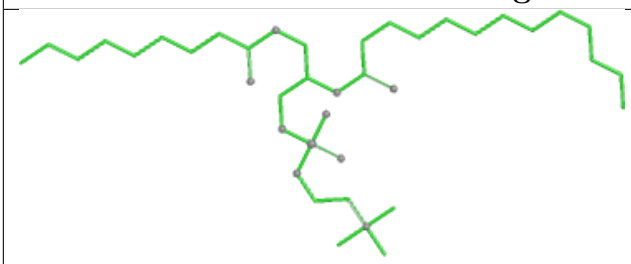


Torsions

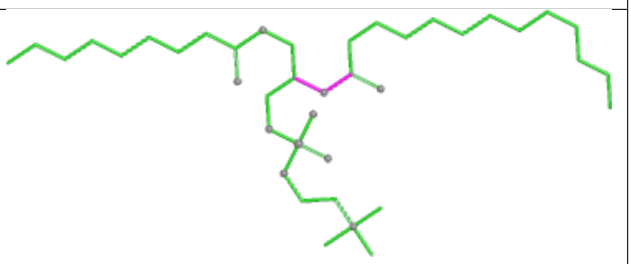


Rings

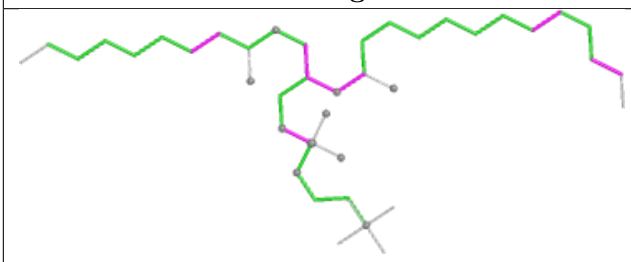
## Ligand POV A 5120



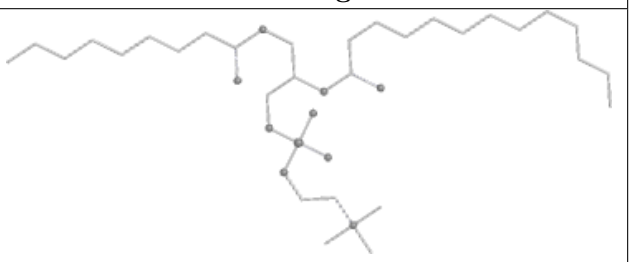
Bond lengths



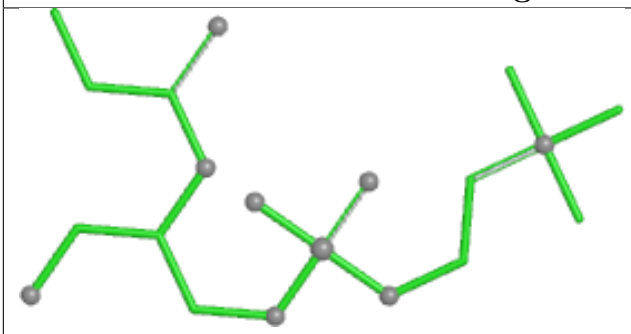
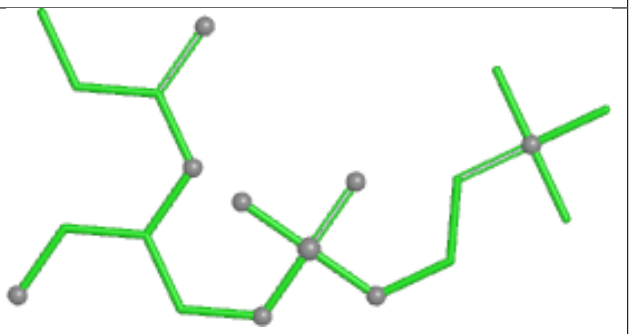
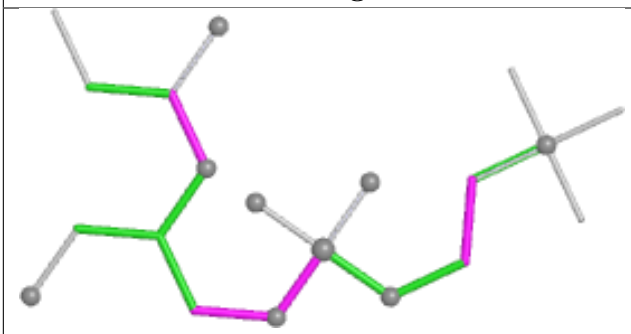
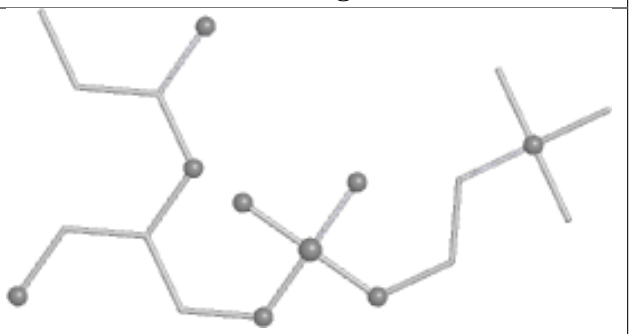
Bond angles

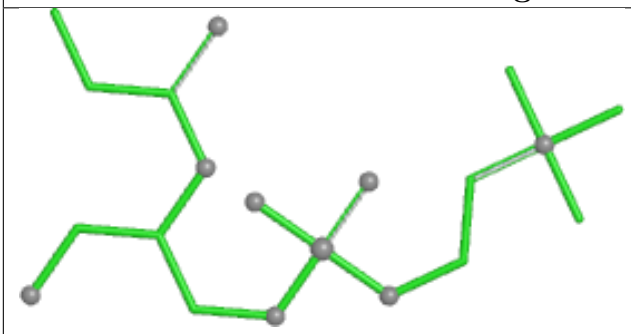
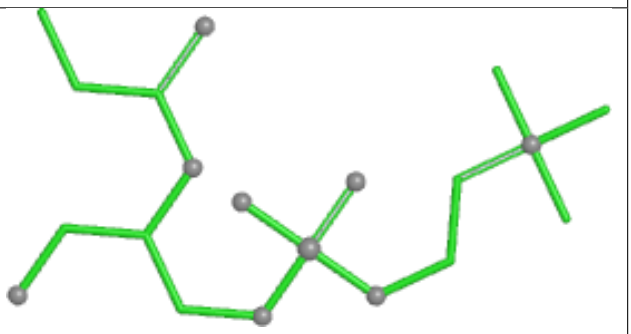
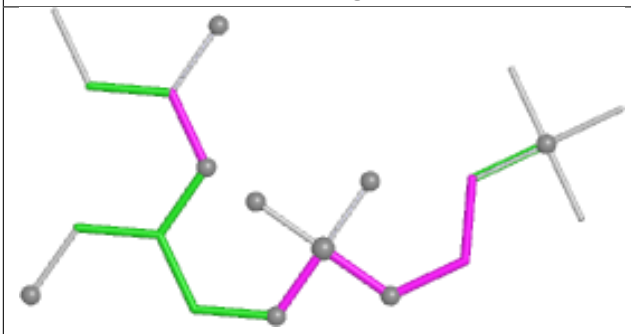
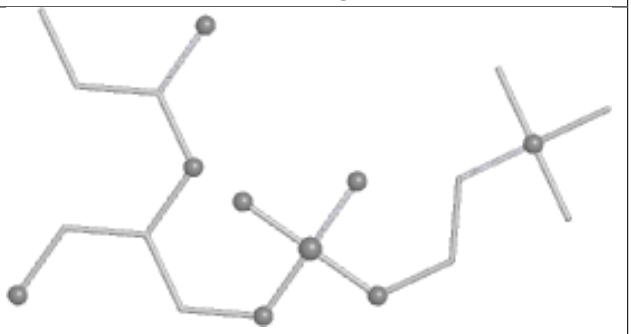


Torsions

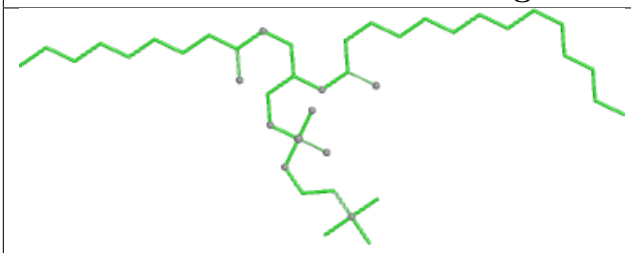


Rings

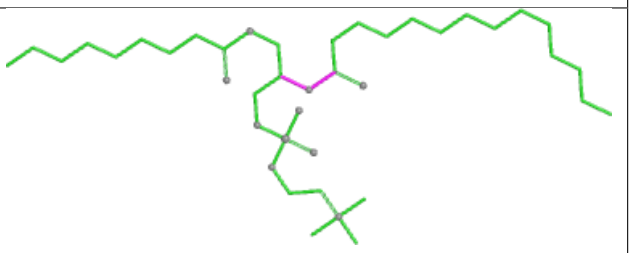
| Ligand POV C 5113 | |
|---|---|
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

| Ligand POV C 5112 | |
|---|---|
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

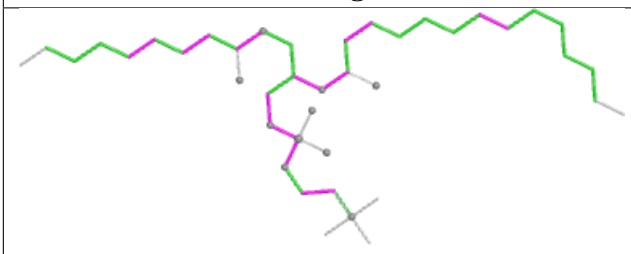
## Ligand POV C 5121



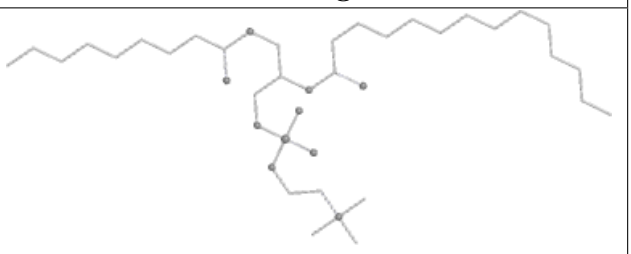
Bond lengths



Bond angles

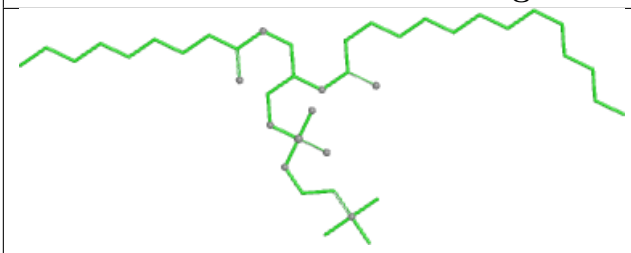


Torsions

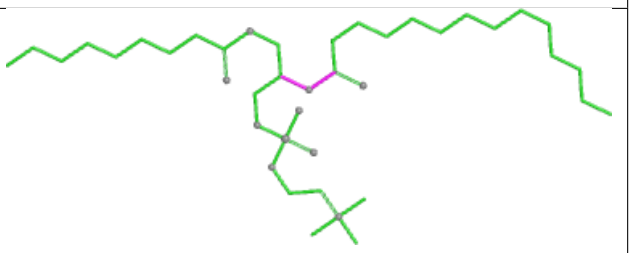


Rings

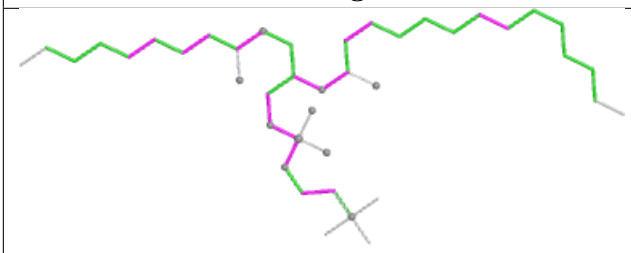
## Ligand POV G 5121



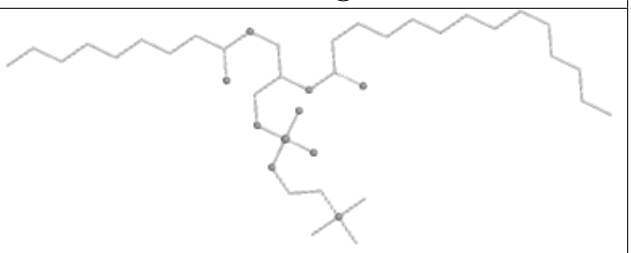
Bond lengths



Bond angles

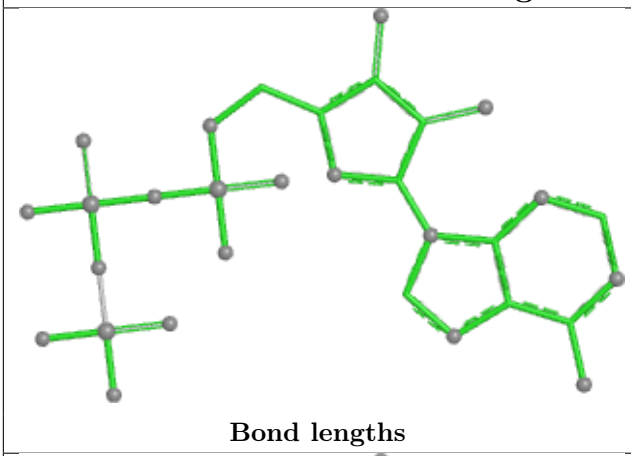


Torsions

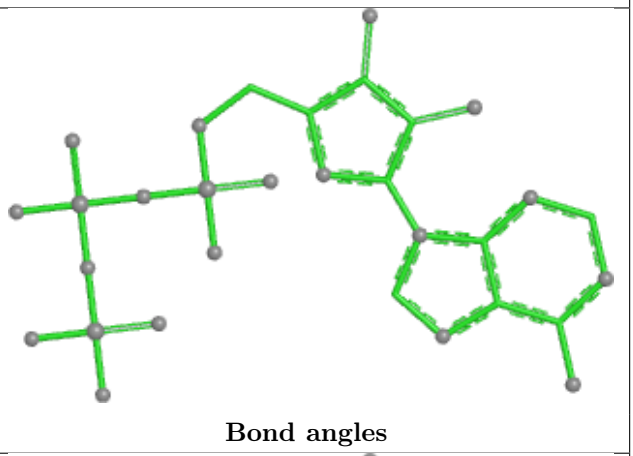


Rings

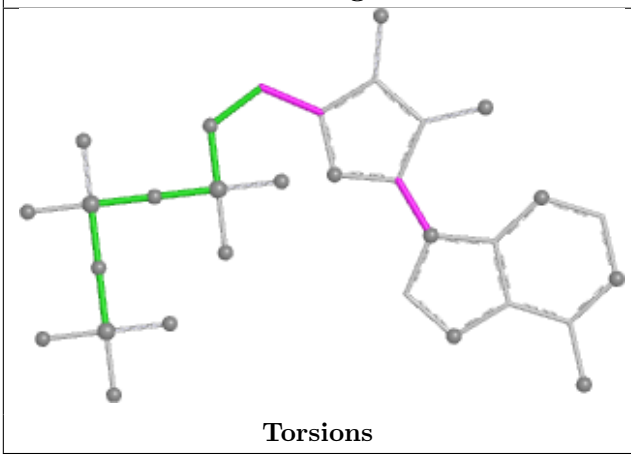
## Ligand ATP A 5102



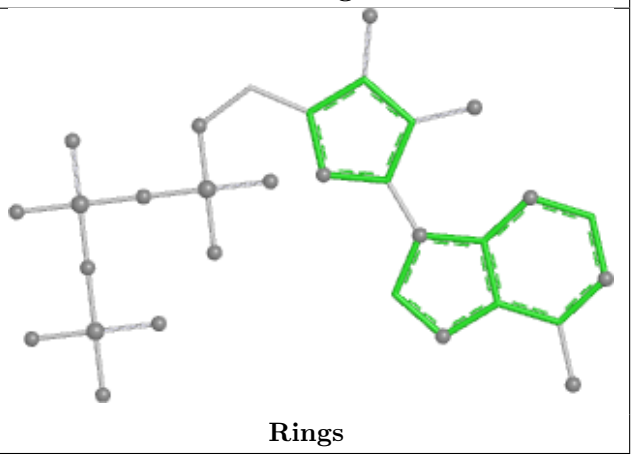
Bond lengths



Bond angles

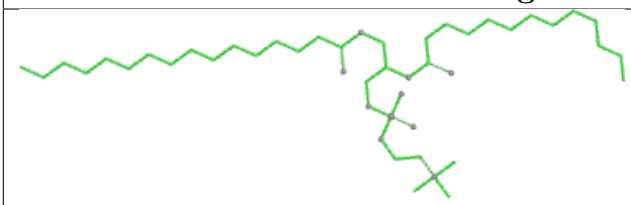


Torsions

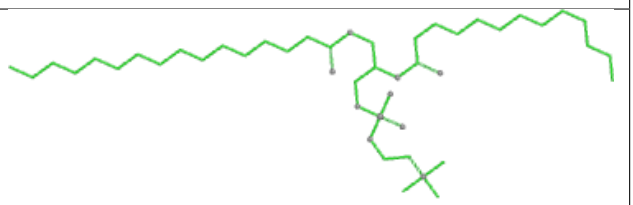


Rings

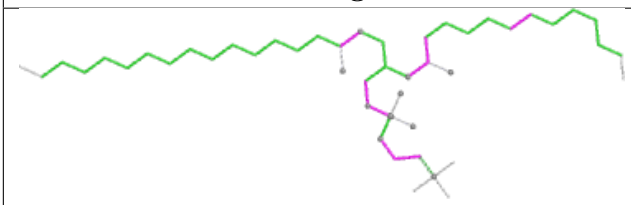
## Ligand POV J 5113



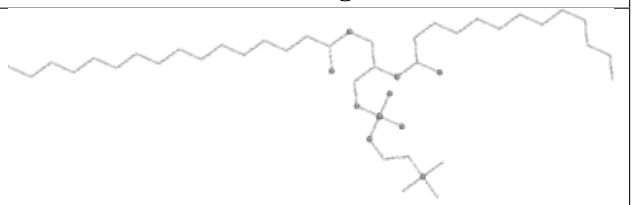
Bond lengths



Bond angles

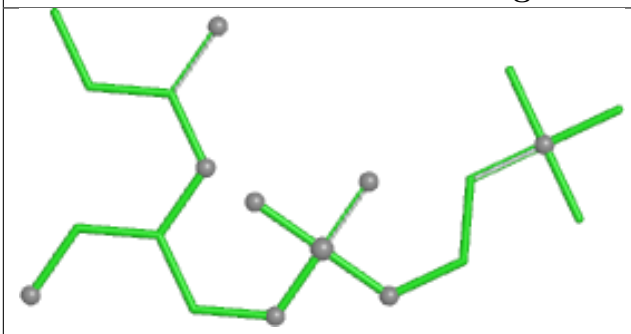


Torsions

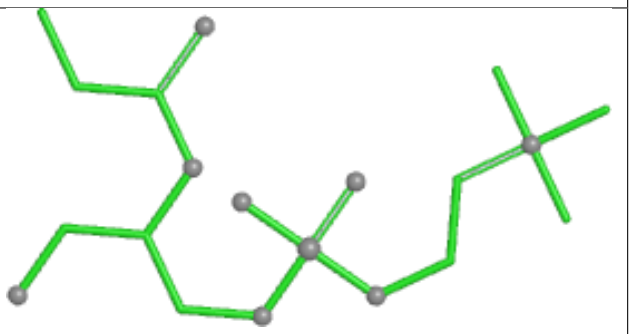


Rings

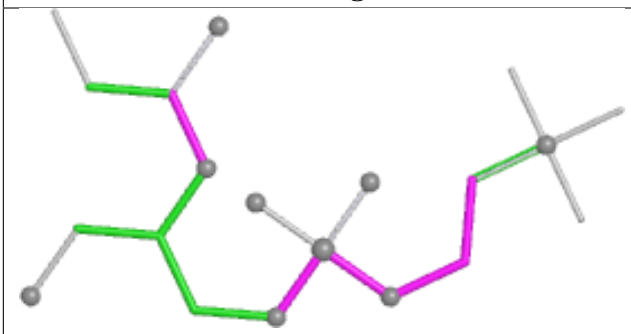
## Ligand POV A 5109



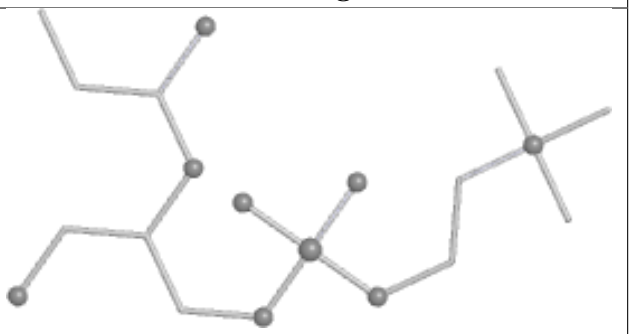
Bond lengths



Bond angles

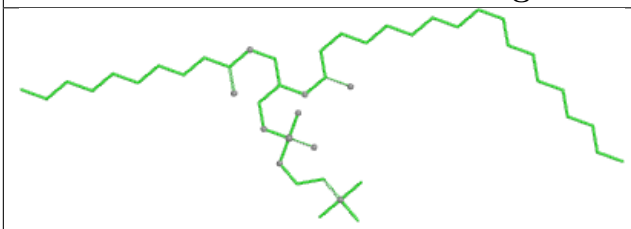


Torsions

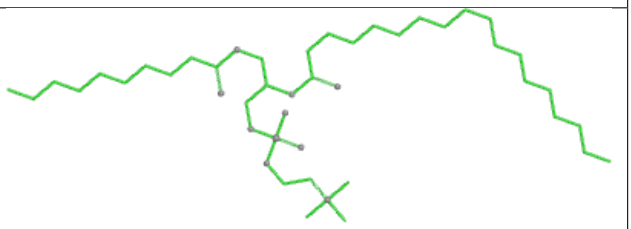


Rings

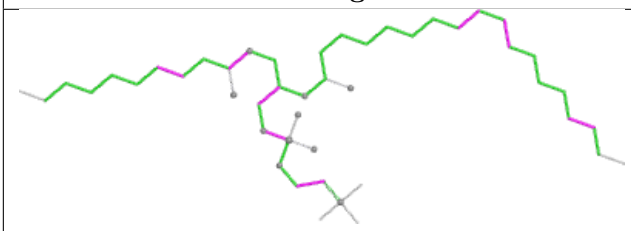
## Ligand POV G 5111



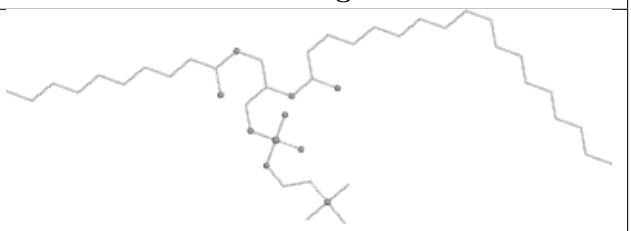
Bond lengths



Bond angles

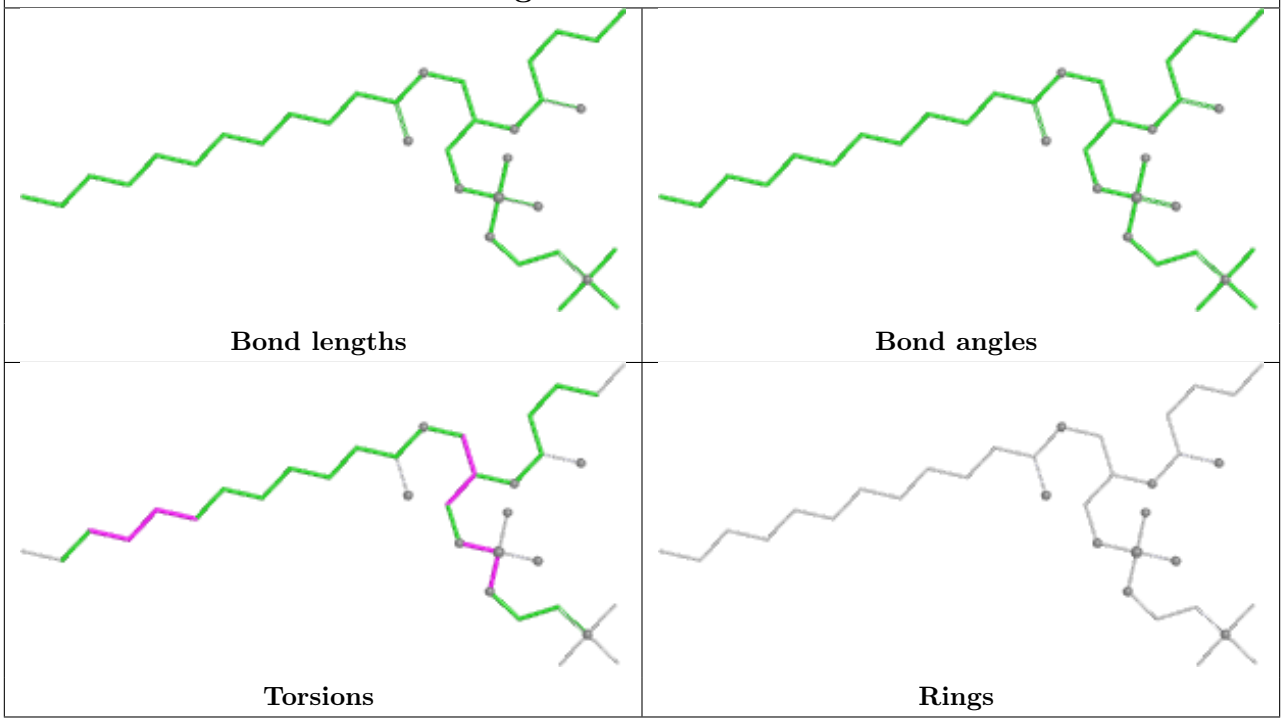


Torsions

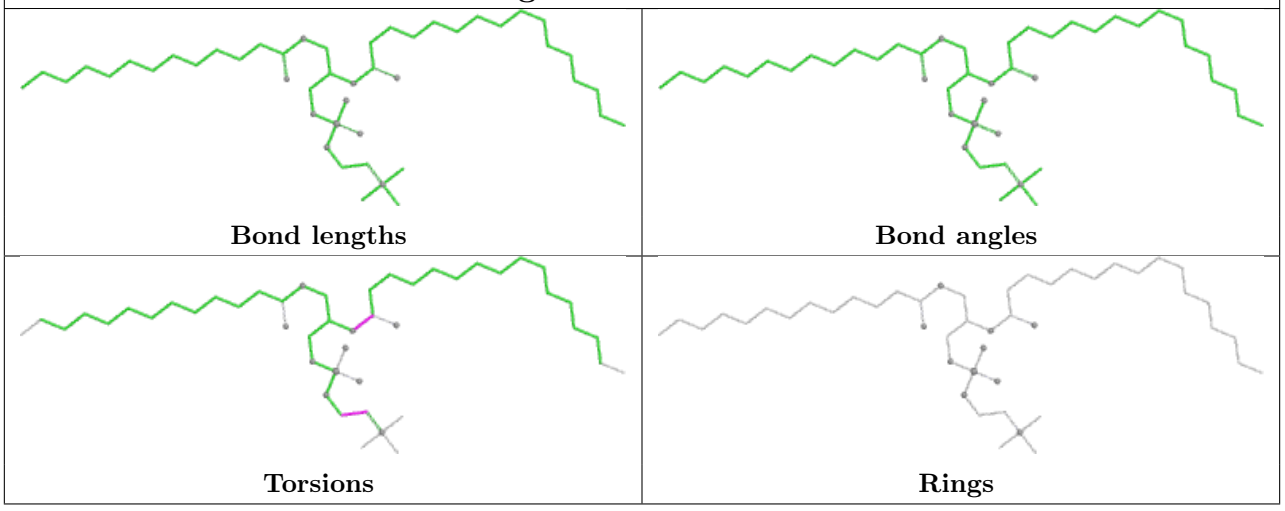


Rings

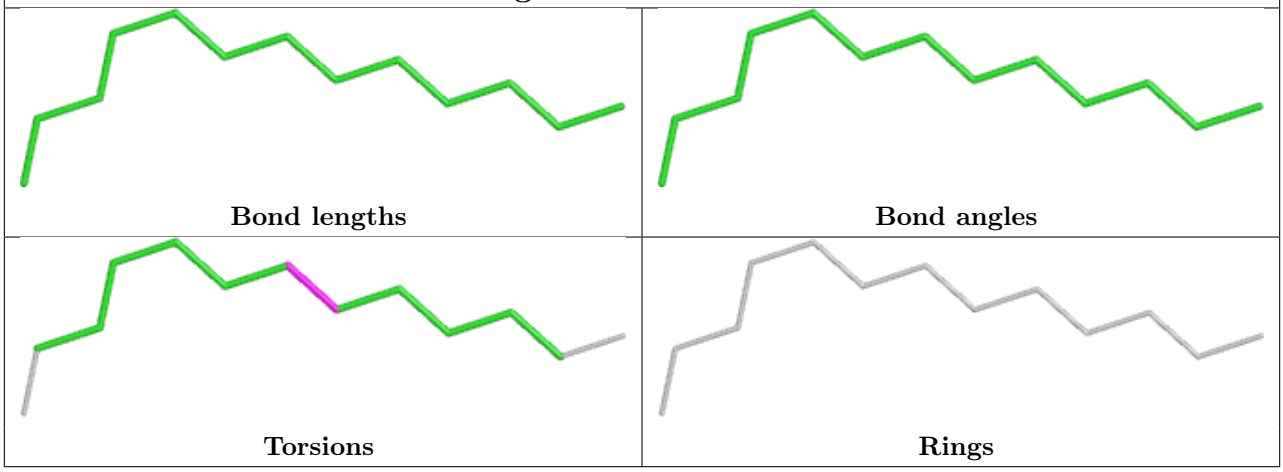
## Ligand POV C 5115



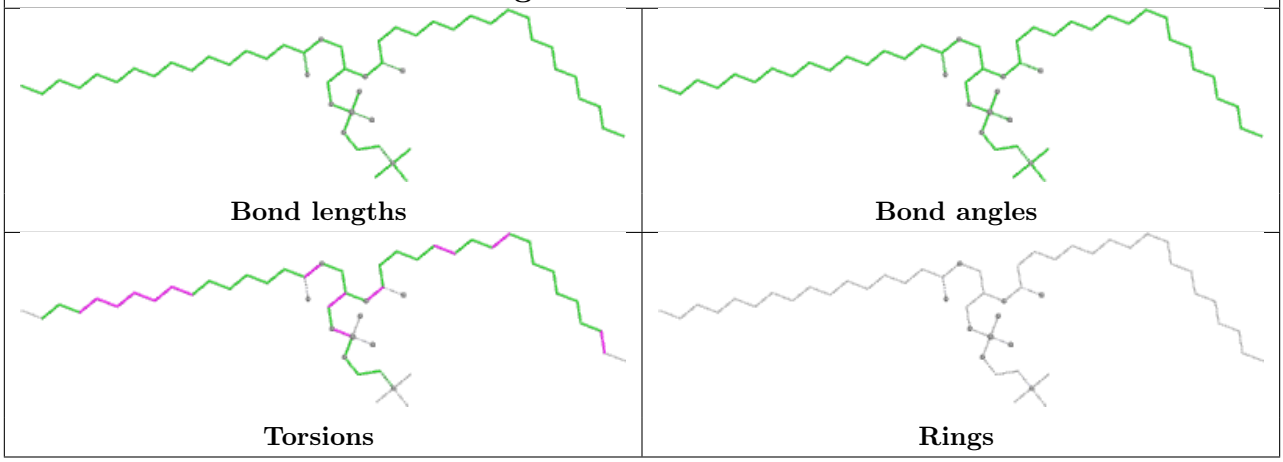

## Ligand POV J 5102



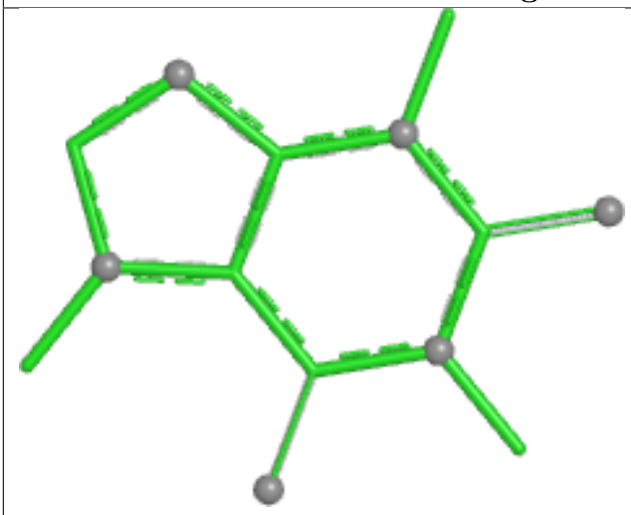
**Ligand POV A 5122**



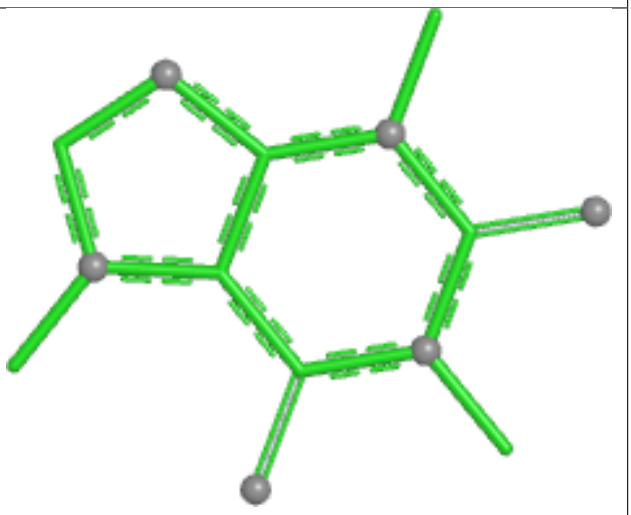

**Ligand POV A 5116**



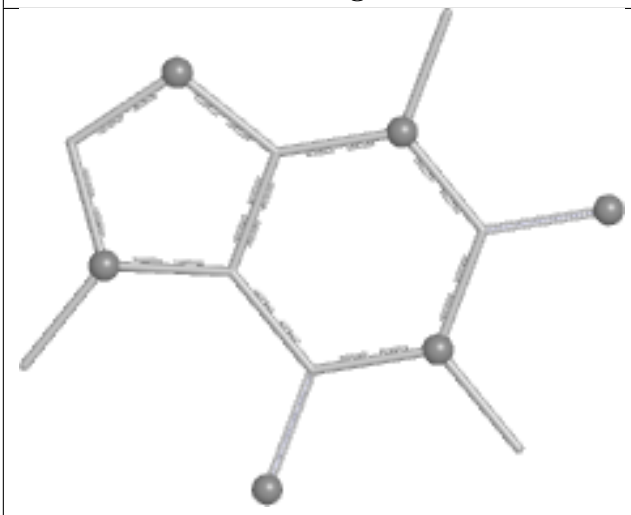
**Ligand CFF J 5110**



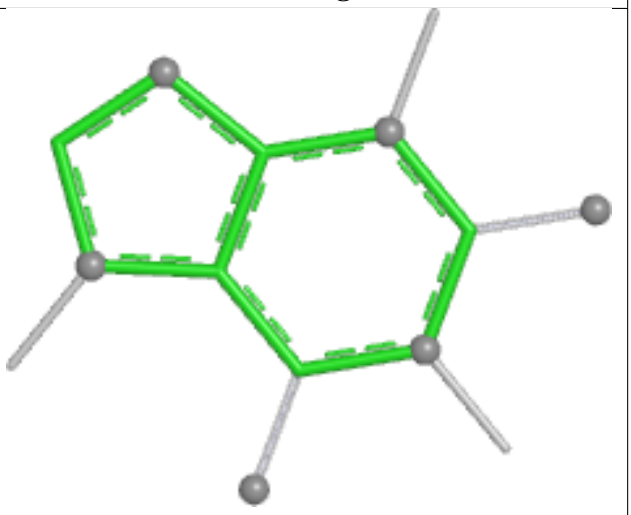
**Bond lengths**



**Bond angles**

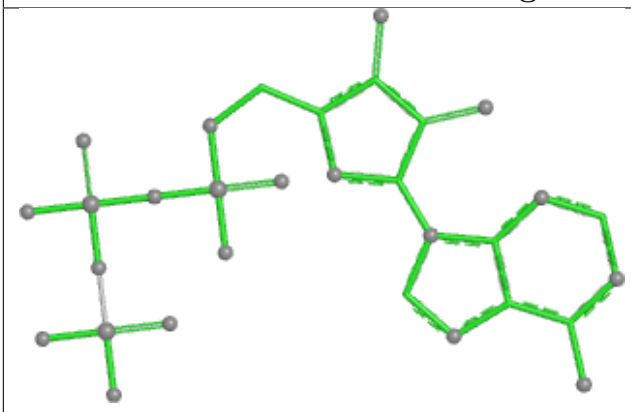


**Torsions**

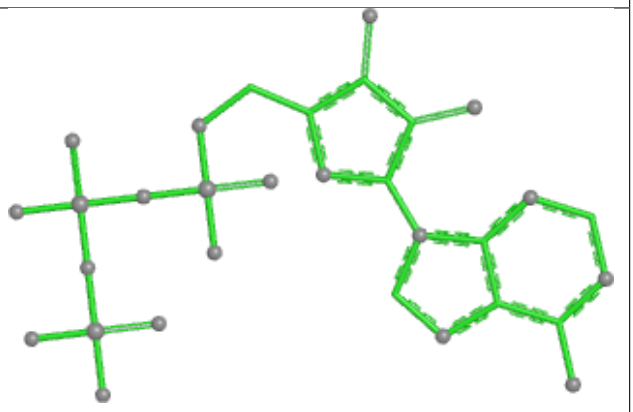


**Rings**

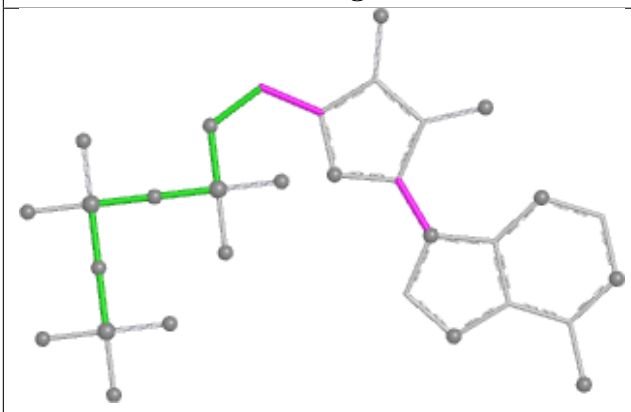
**Ligand ATP J 5109**



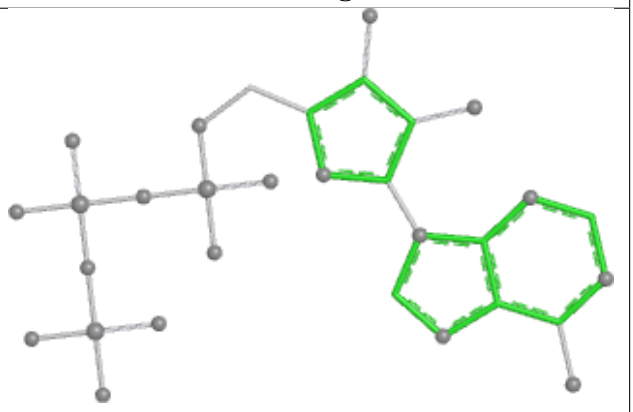
Bond lengths



Bond angles

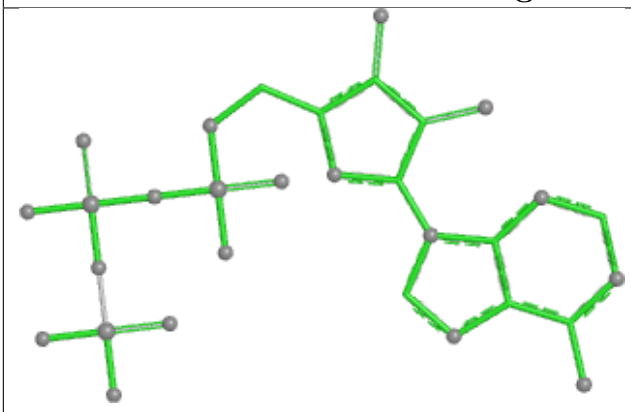


Torsions

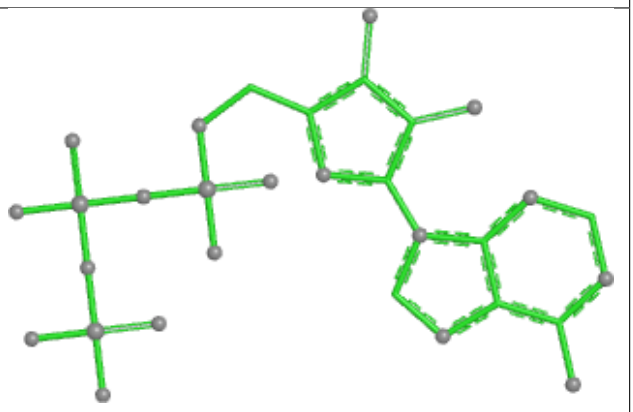


Rings

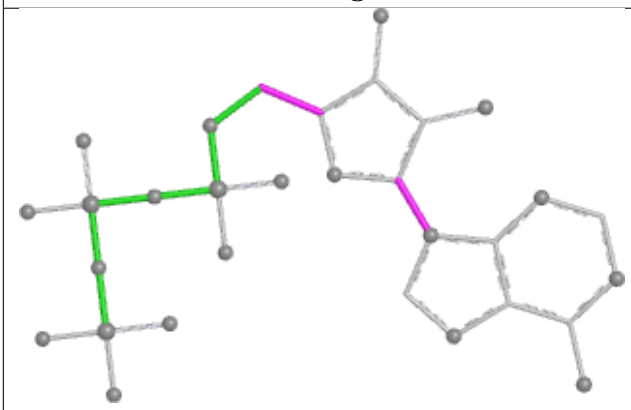
## Ligand ATP C 5105



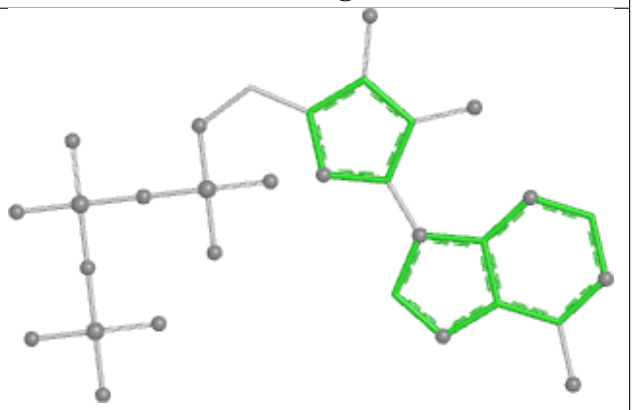
Bond lengths



Bond angles

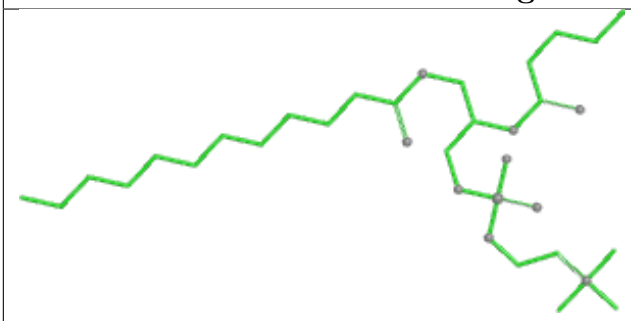


Torsions

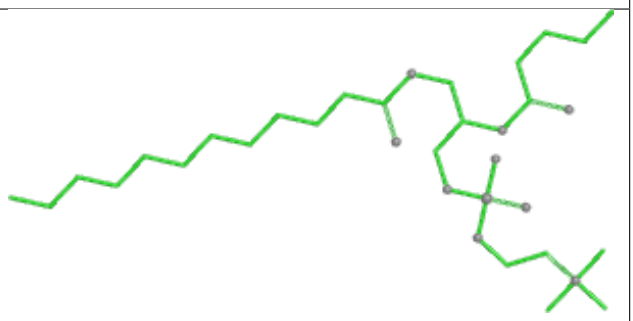


Rings

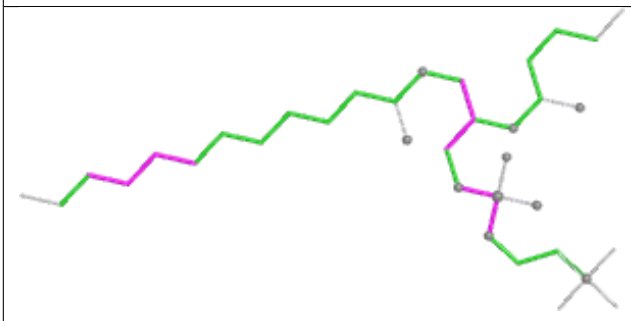
## Ligand POV J 5119



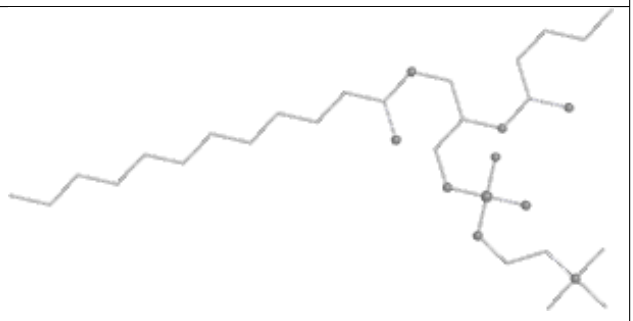
Bond lengths



Bond angles

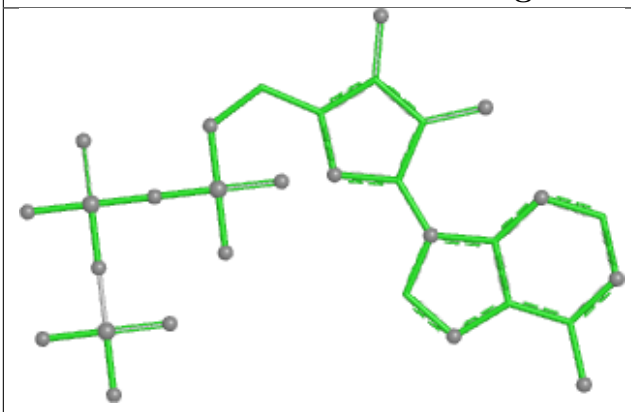


Torsions

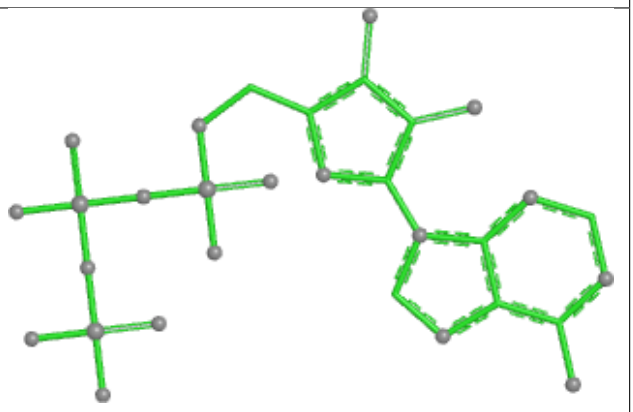


Rings

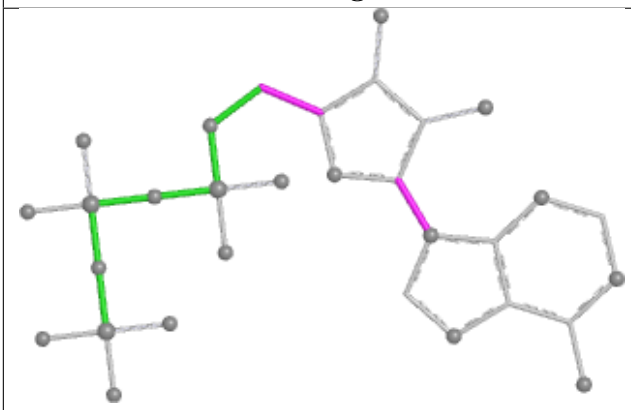
## Ligand ATP G 5105



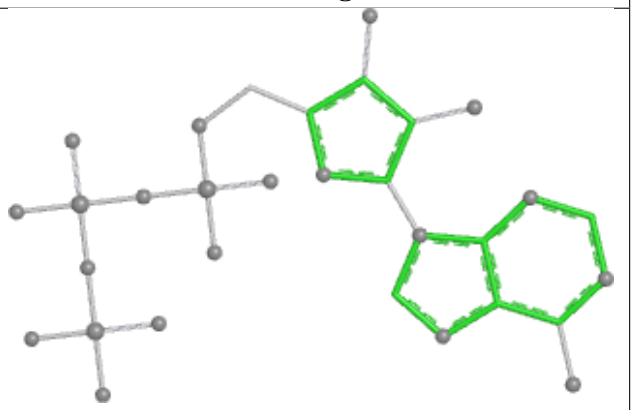
Bond lengths



Bond angles

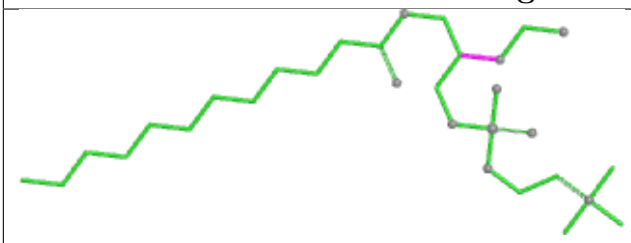


Torsions

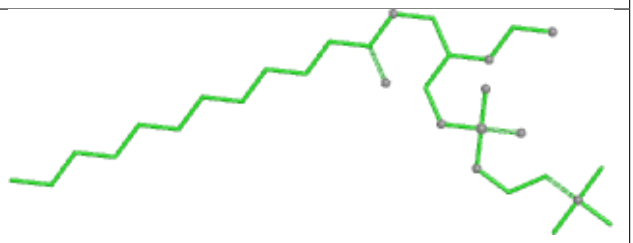


Rings

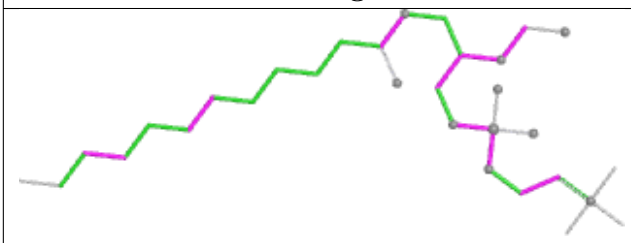
## Ligand POV J 5104



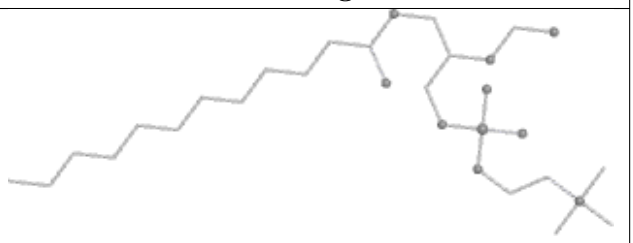
Bond lengths



Bond angles

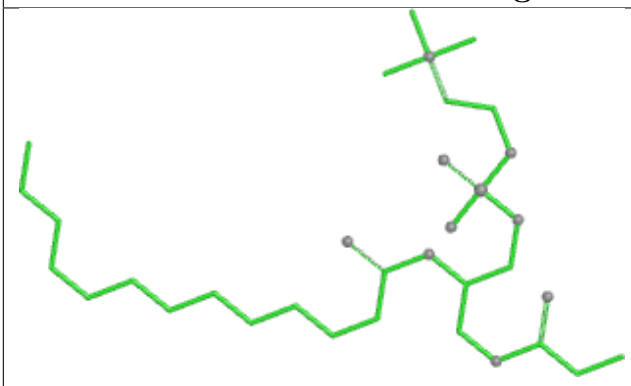


Torsions

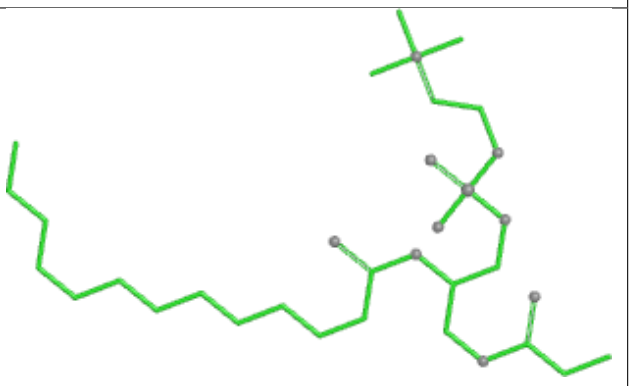


Rings

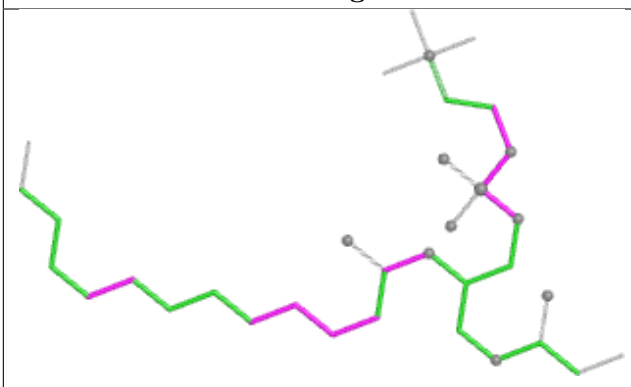
## Ligand POV C 5118



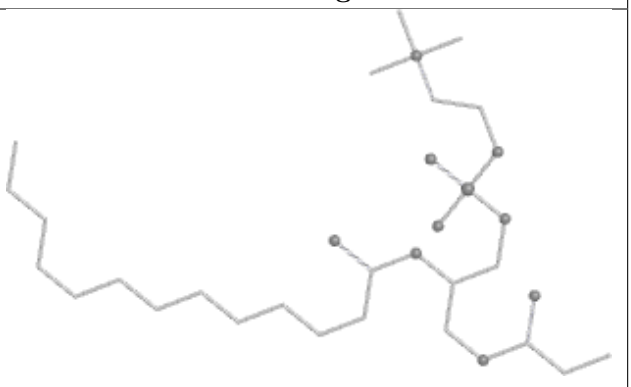
Bond lengths



Bond angles

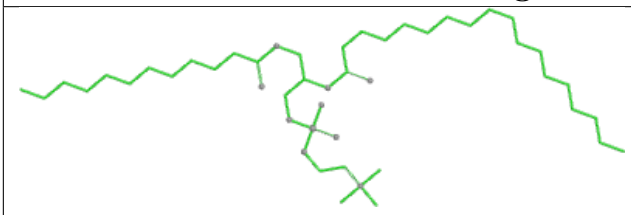


Torsions

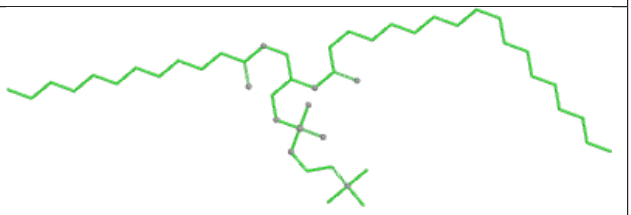


Rings

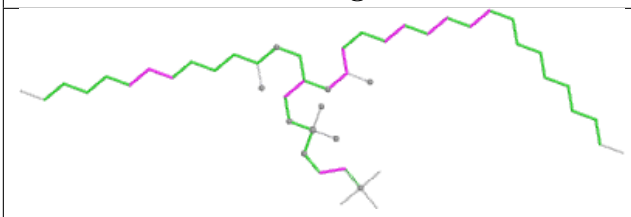
## Ligand POV C 5102



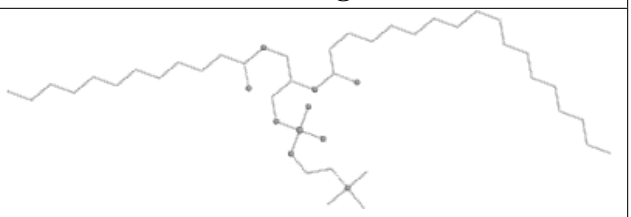
Bond lengths



Bond angles

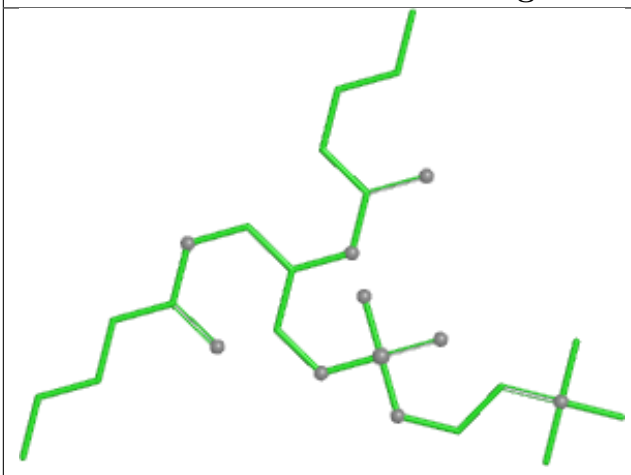


Torsions

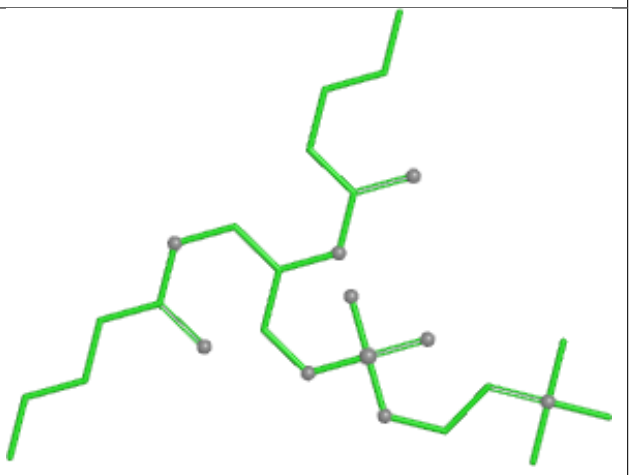


Rings

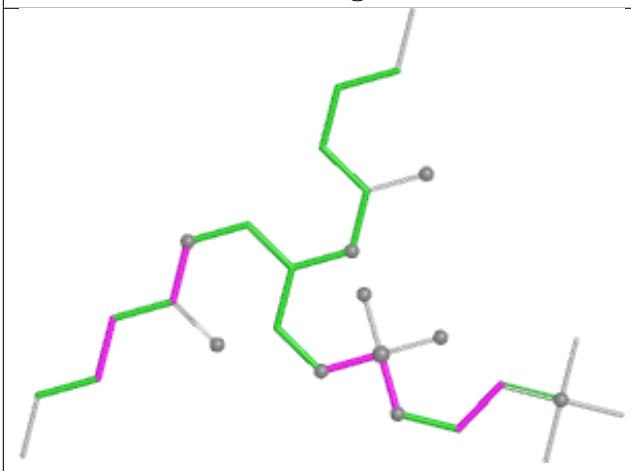
**Ligand POV J 5120**



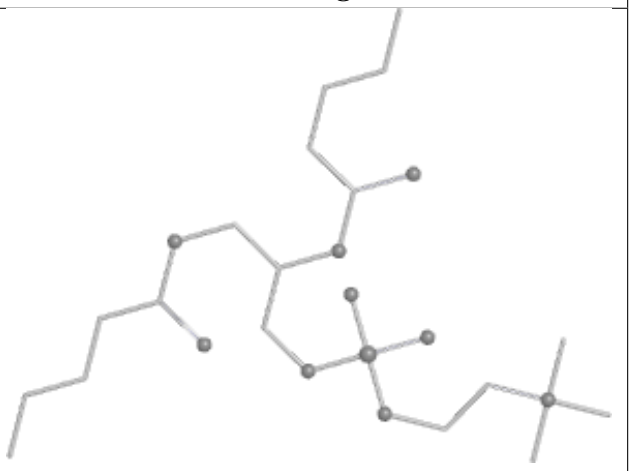
Bond lengths



Bond angles

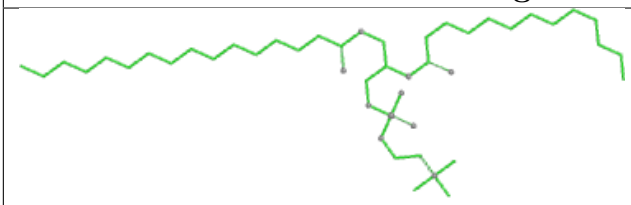


Torsions

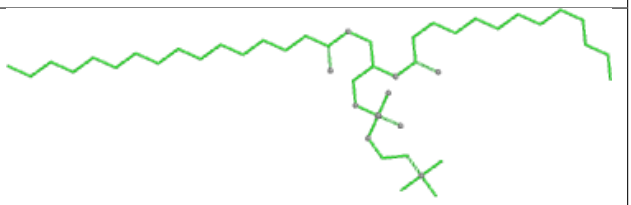


Rings

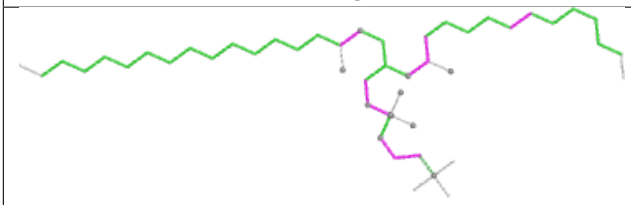
**Ligand POV A 5106**



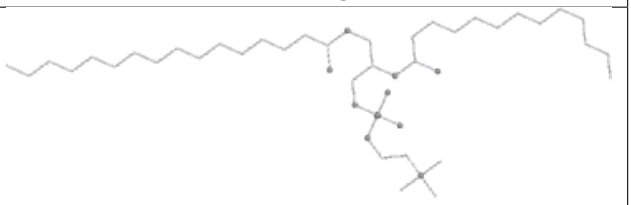
Bond lengths



Bond angles

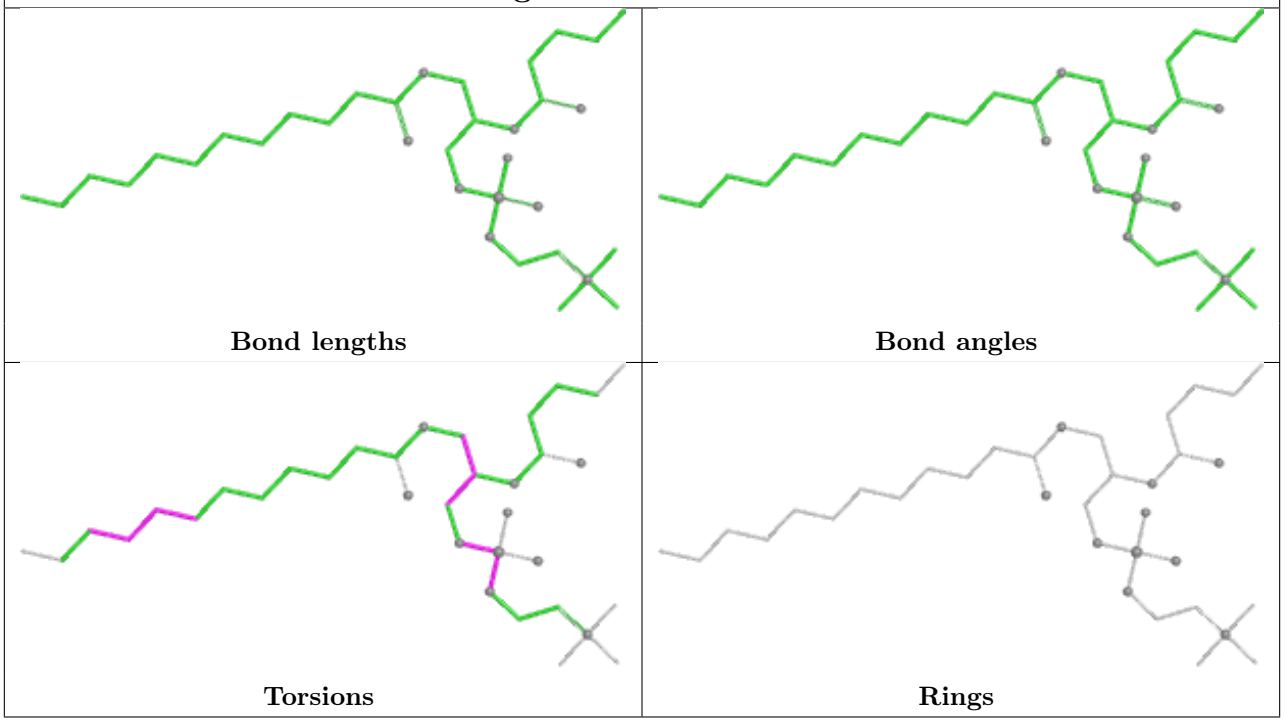


Torsions

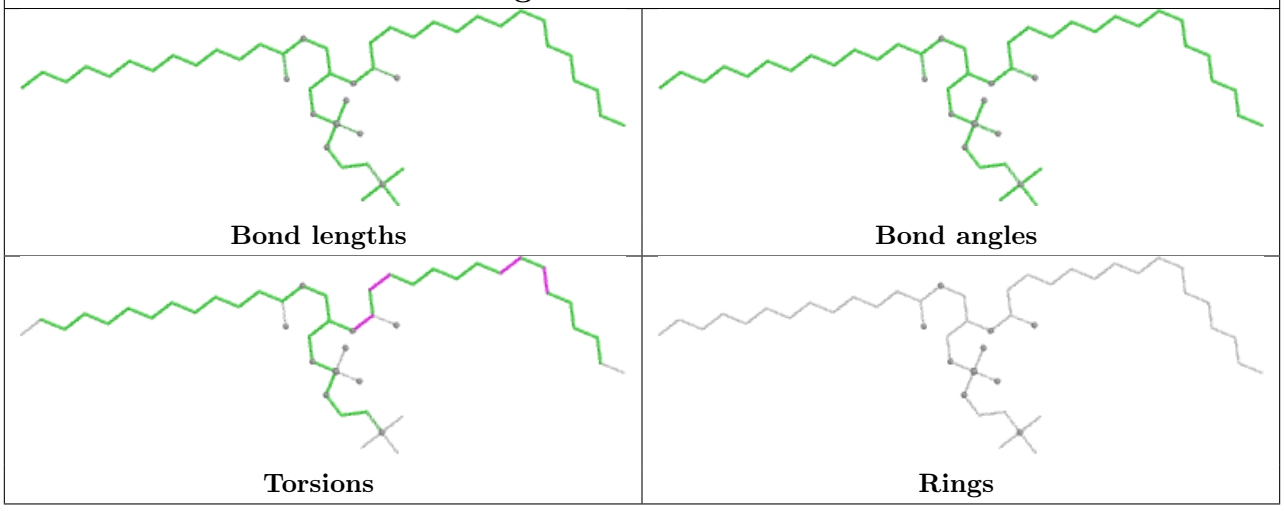


Rings

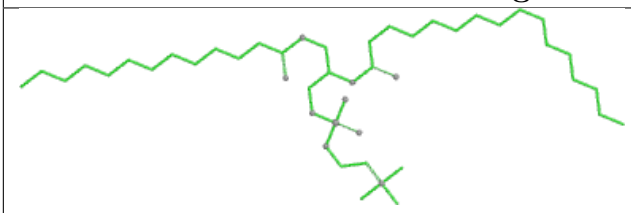
## Ligand POV G 5115



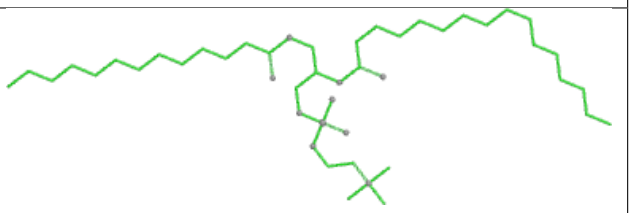

## Ligand POV A 5117



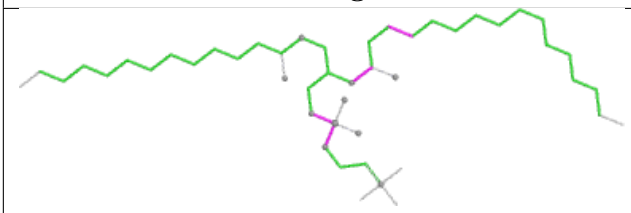
## Ligand POV G 5120



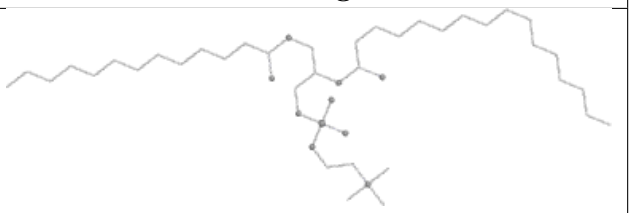
Bond lengths



Bond angles

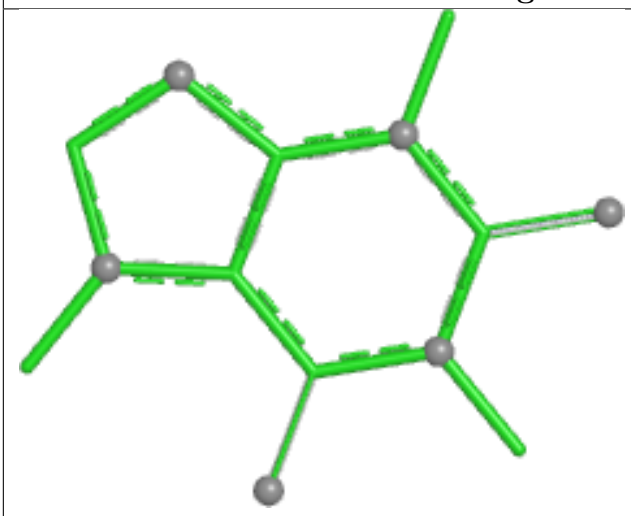


Torsions

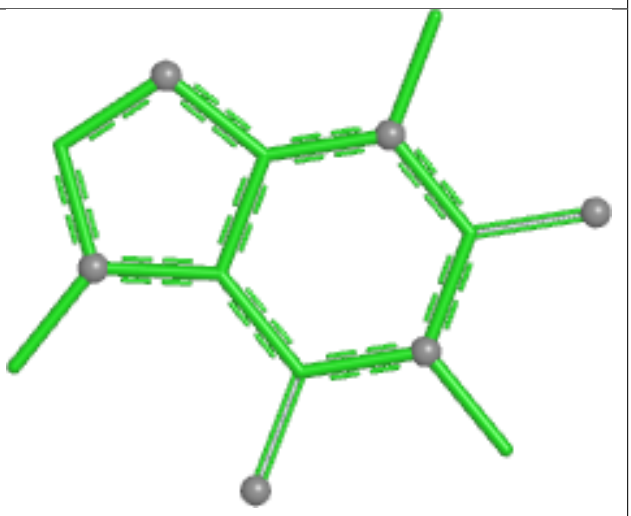


Rings

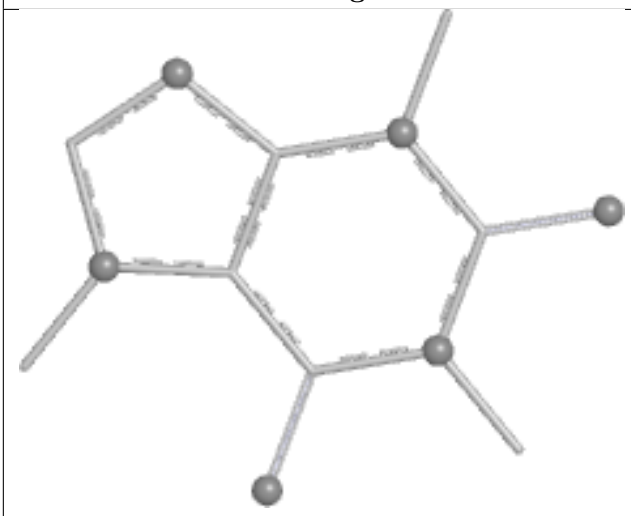
## Ligand CFF C 5106



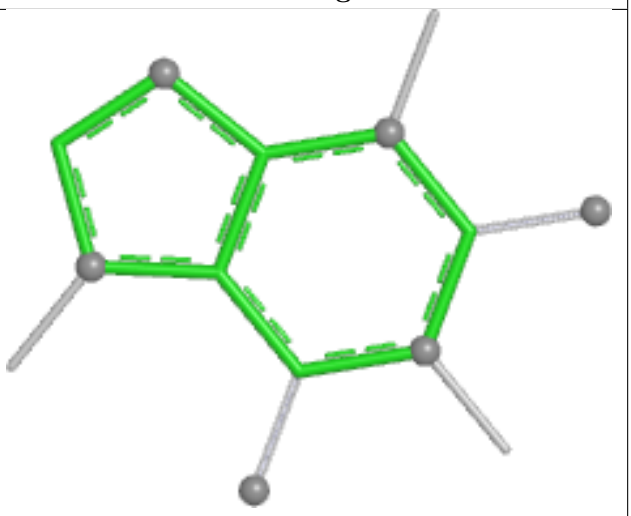
Bond lengths



Bond angles

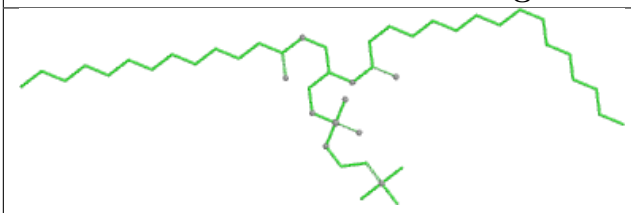


Torsions

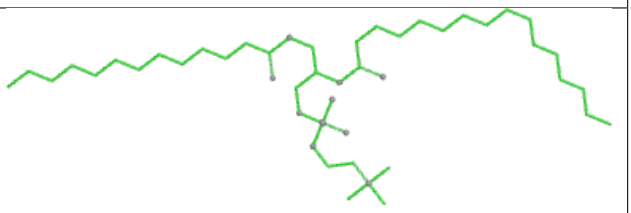


Rings

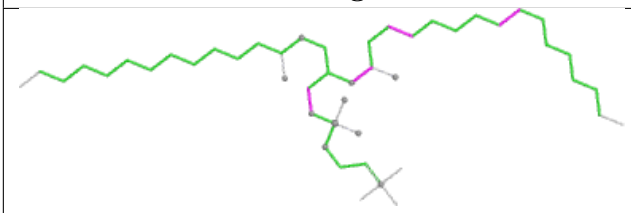
**Ligand POV C 5120**



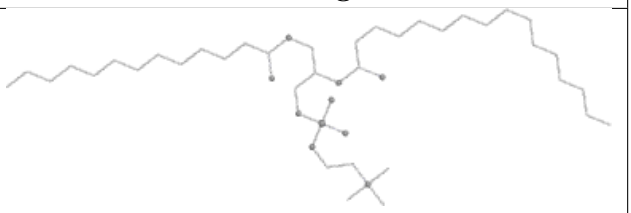
Bond lengths



Bond angles

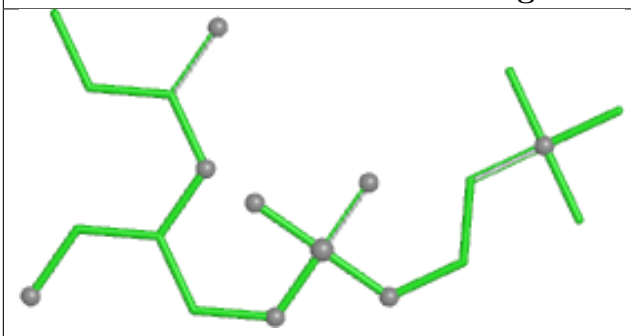


Torsions

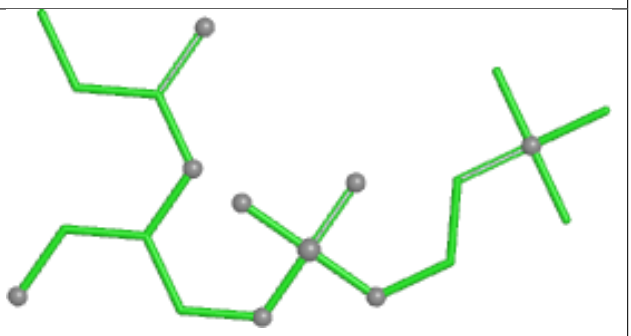


Rings

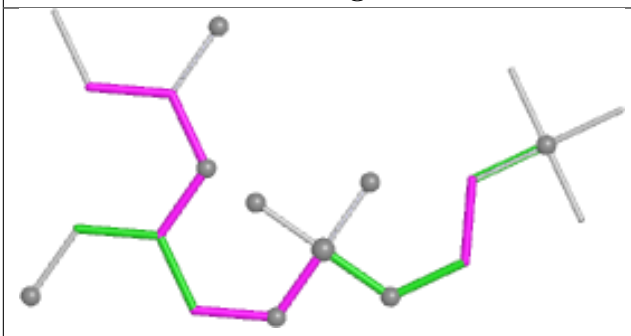
**Ligand POV J 5117**



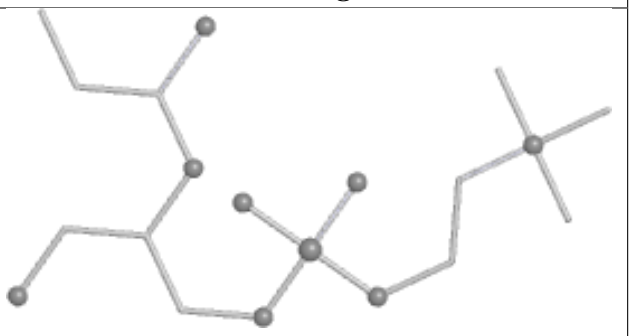
Bond lengths



Bond angles

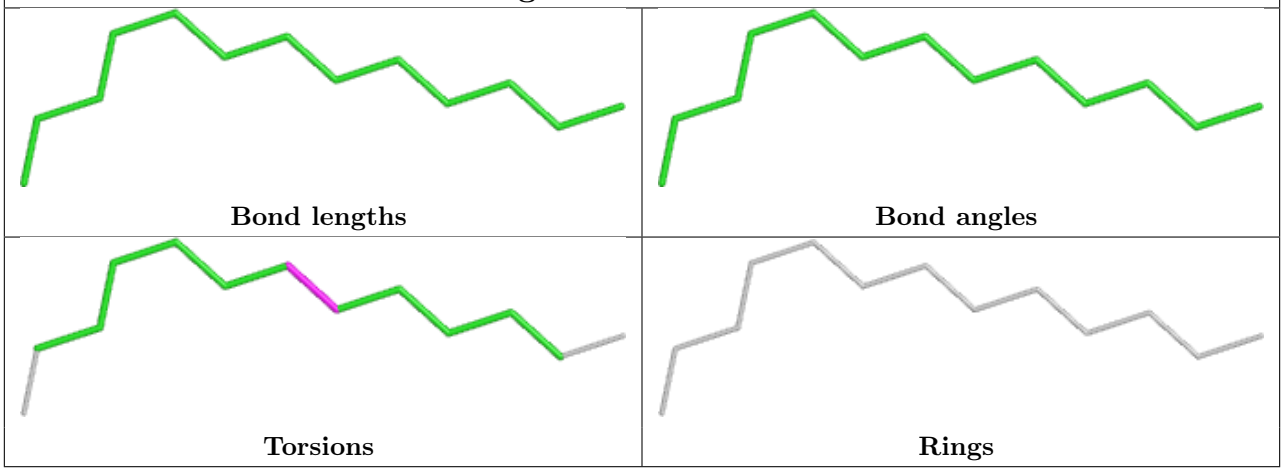


Torsions

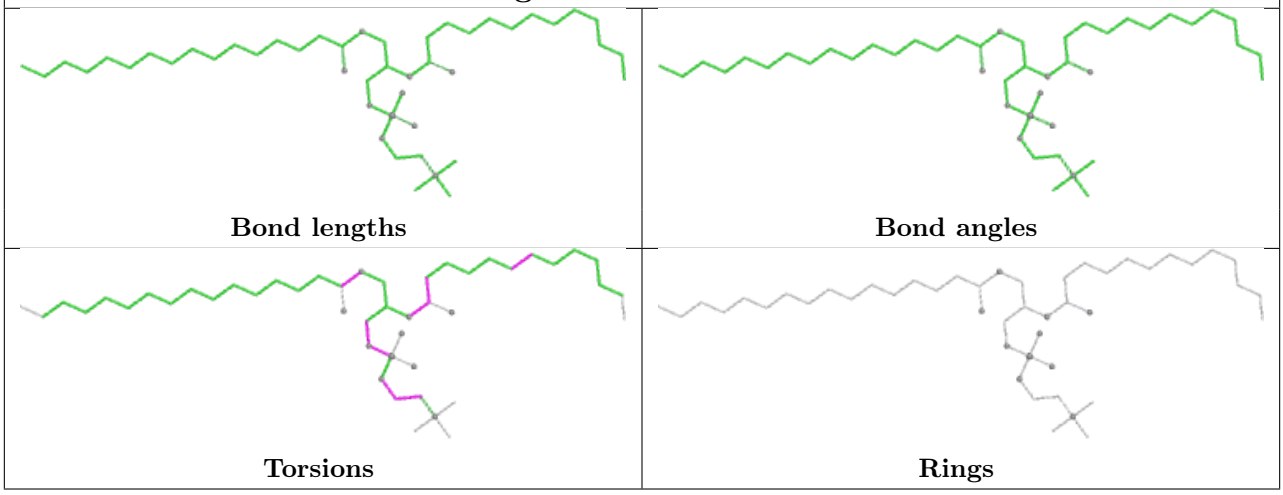


Rings

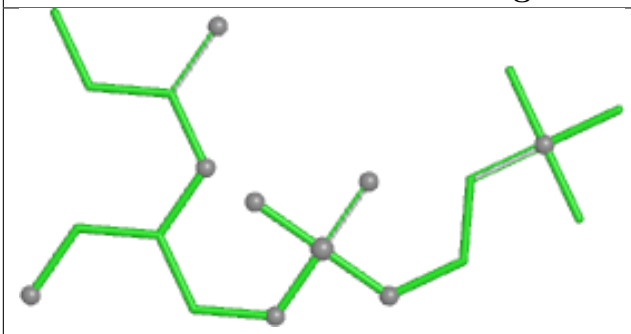
**Ligand POV J 5107**



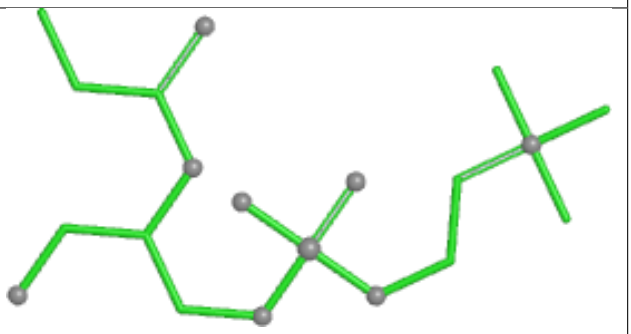

**Ligand POV C 5109**



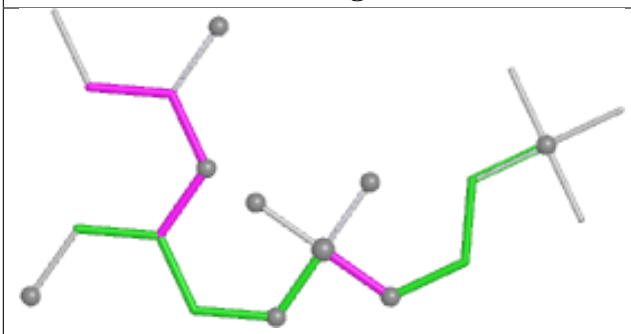
## Ligand POV A 5110



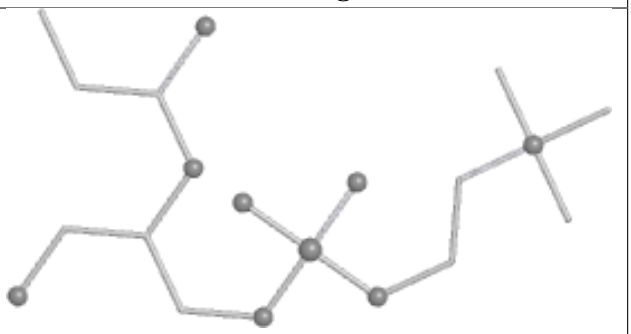
Bond lengths



Bond angles

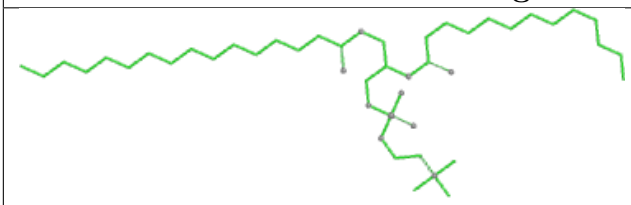


Torsions

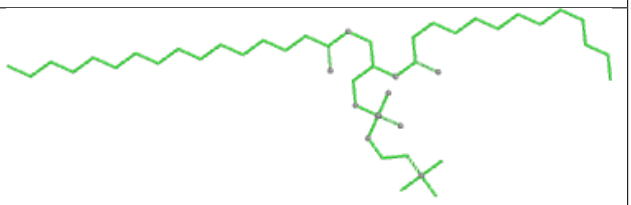


Rings

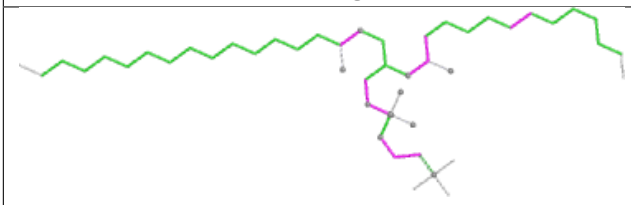
## Ligand POV G 5109



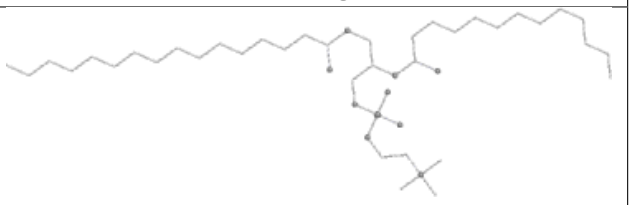
Bond lengths



Bond angles

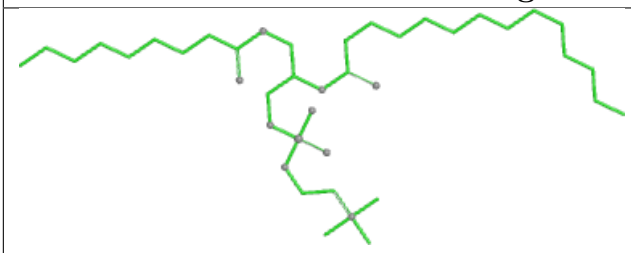


Torsions

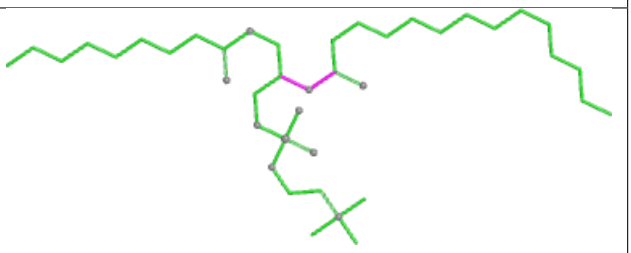


Rings

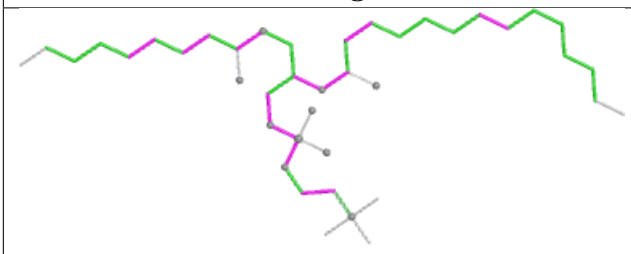
## Ligand POV J 5103



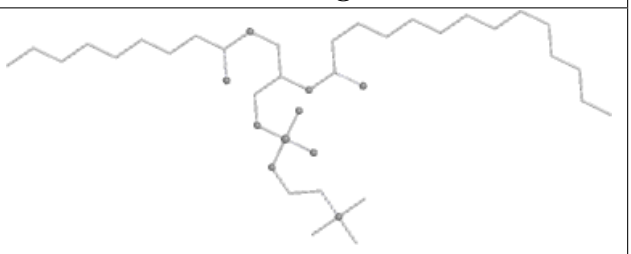
Bond lengths



Bond angles

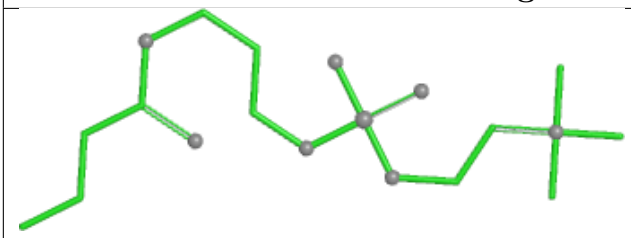


Torsions

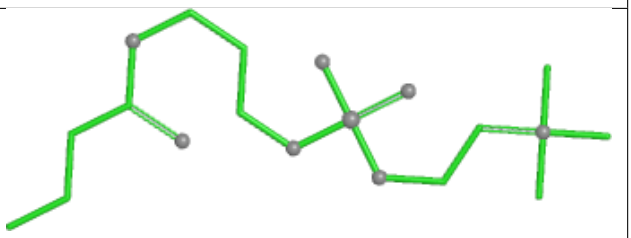


Rings

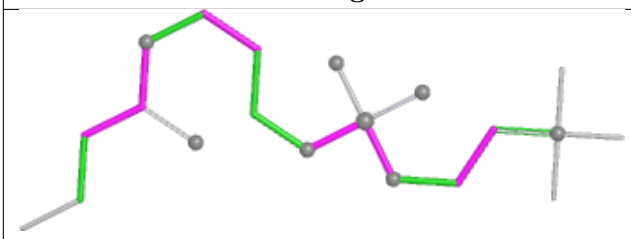
## Ligand POV J 5118



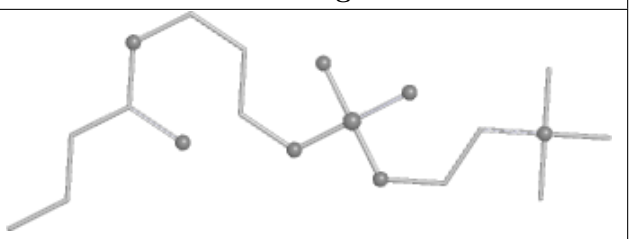
Bond lengths



Bond angles

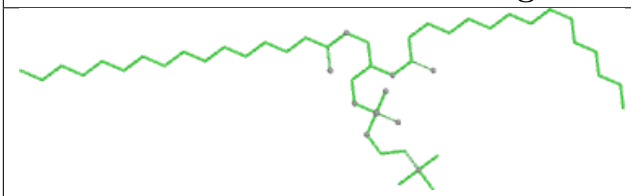


Torsions

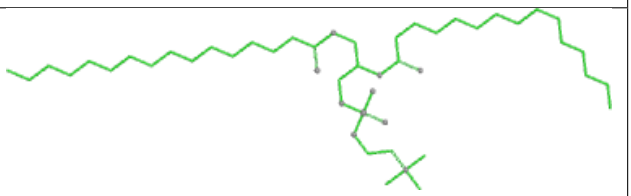


Rings

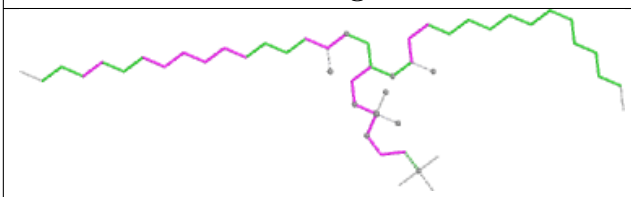
## Ligand POV J 5112



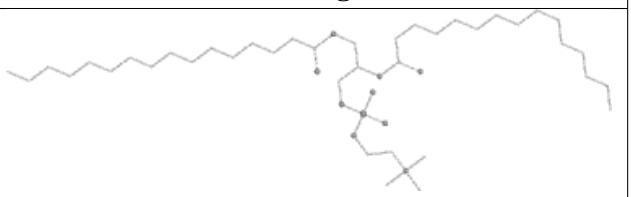
Bond lengths



Bond angles

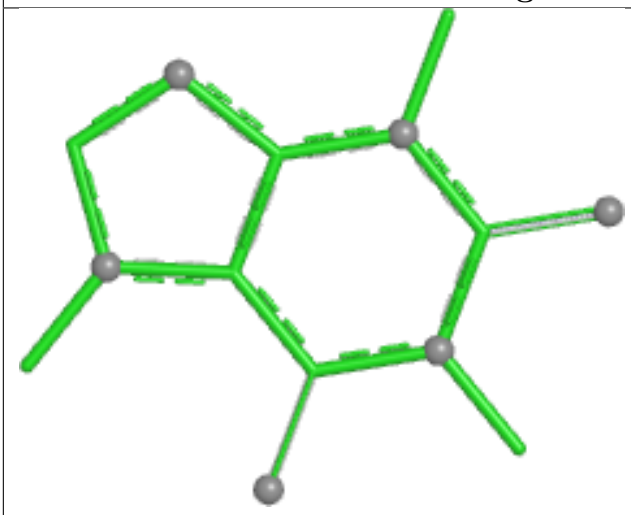


Torsions

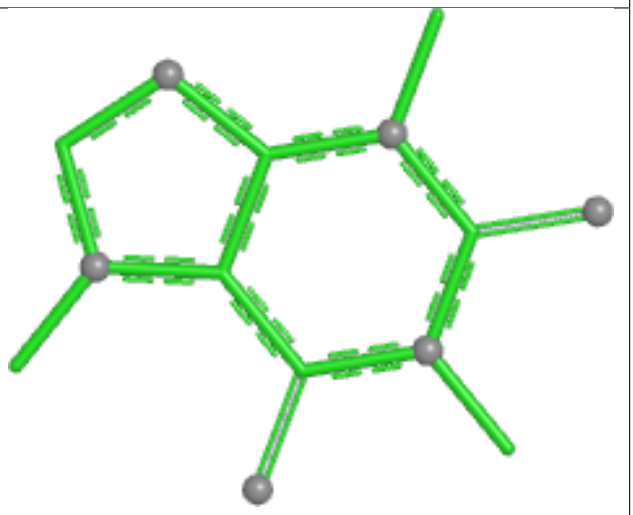


Rings

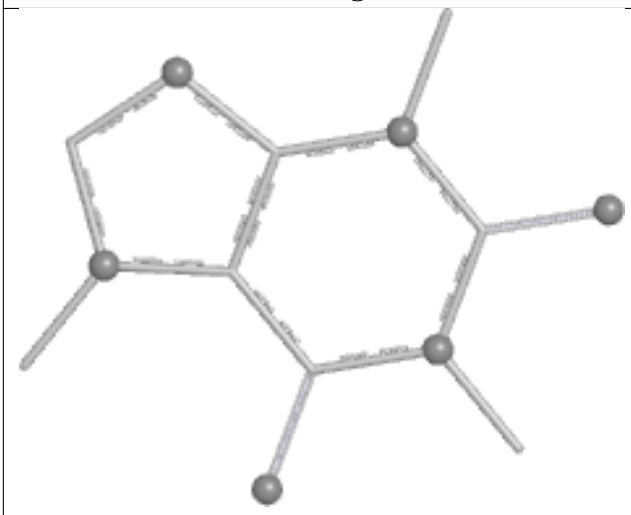
## Ligand CFF A 5103



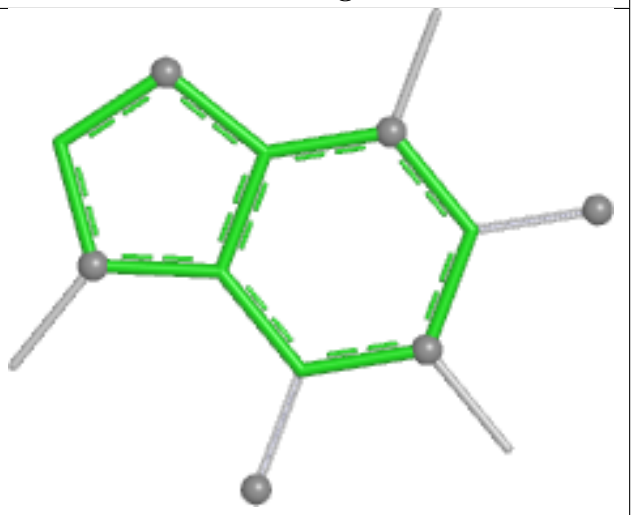
Bond lengths



Bond angles

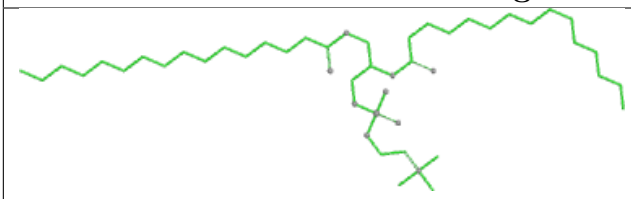


Torsions

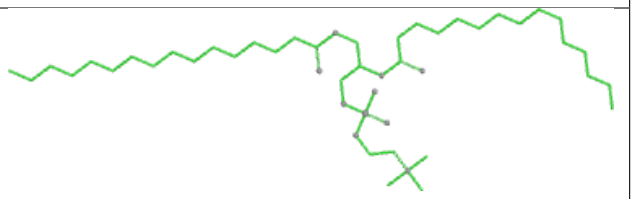


Rings

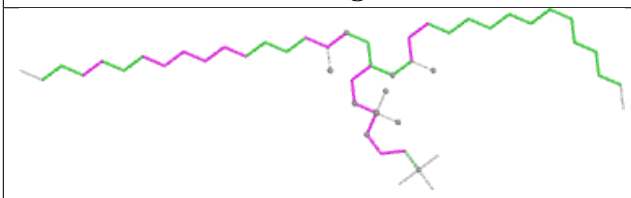
## Ligand POV A 5105



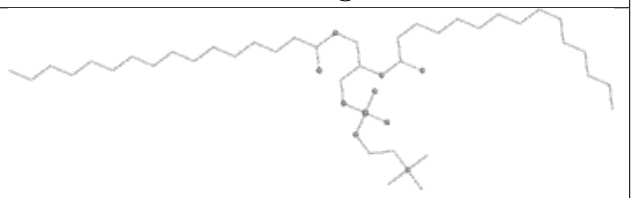
Bond lengths



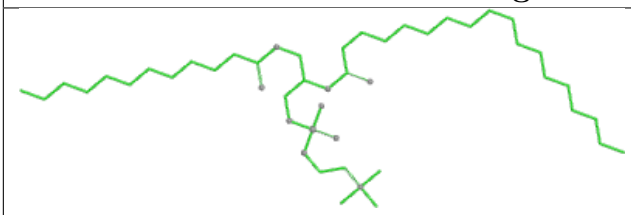
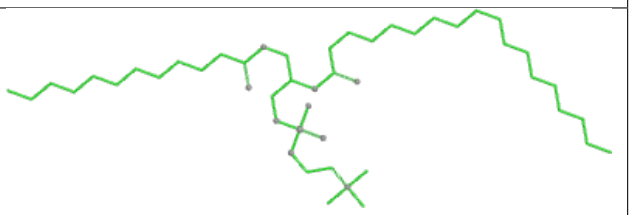
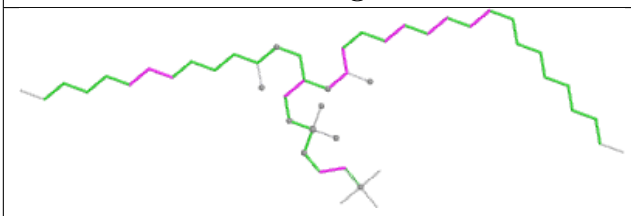
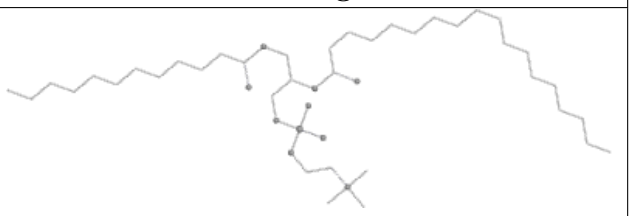
Bond angles

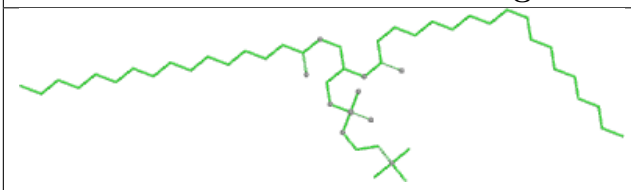
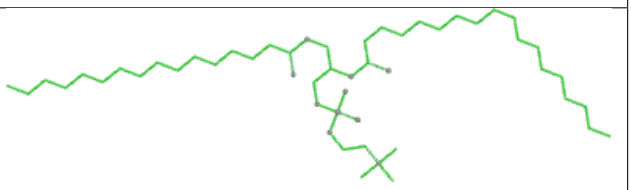
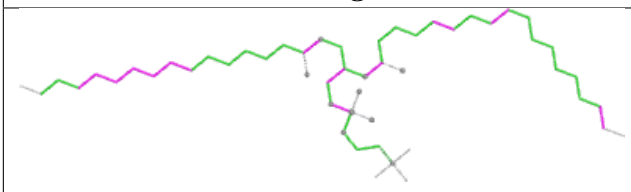
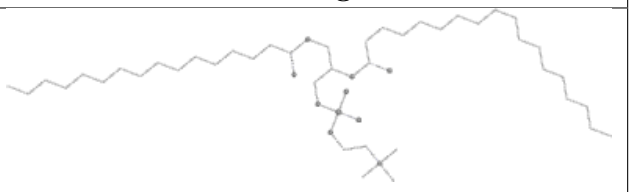


Torsions

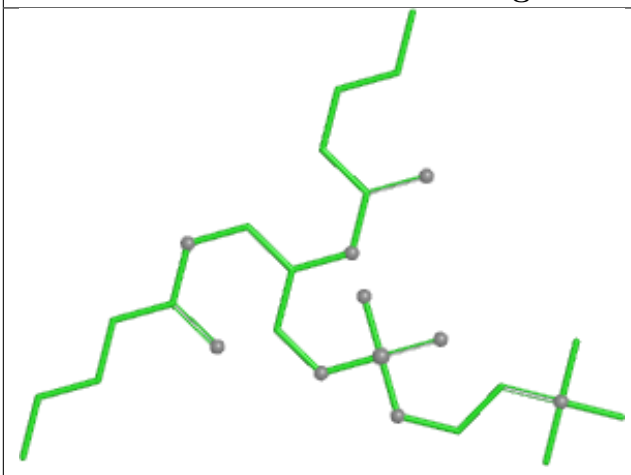


Rings

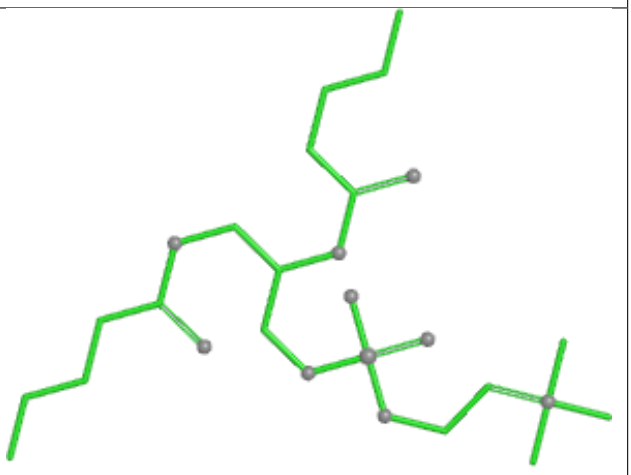
| Ligand POV G 5102 | |
|---|---|
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

| Ligand POV C 5119 | |
|---|---|
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

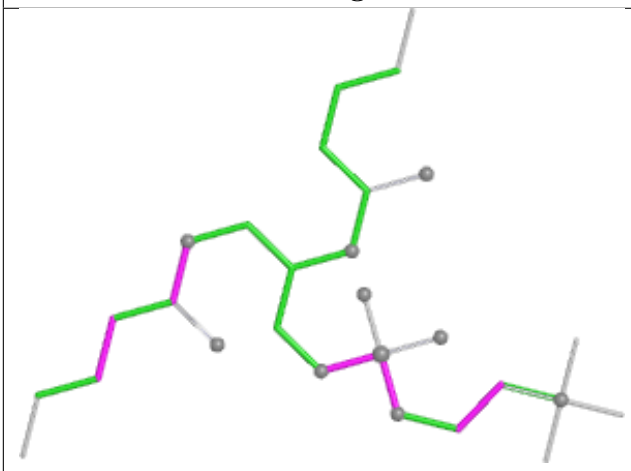
## Ligand POV G 5116



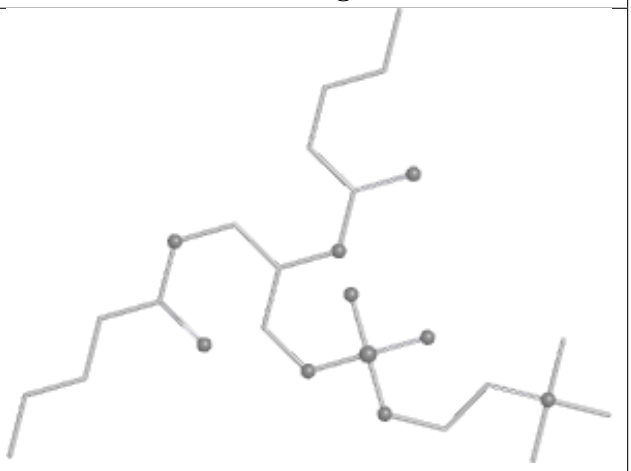
Bond lengths



Bond angles

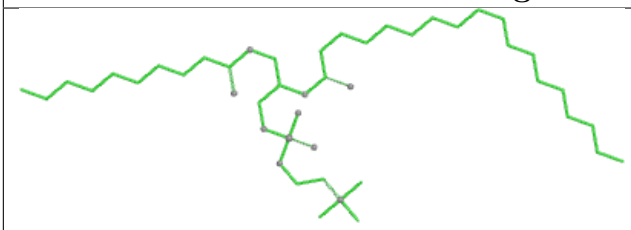


Torsions

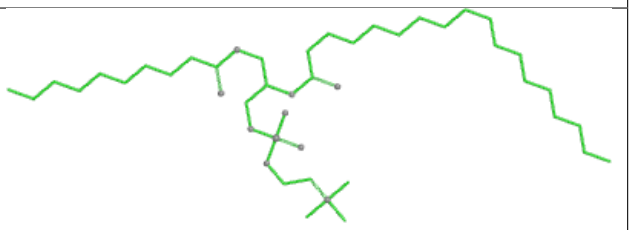


Rings

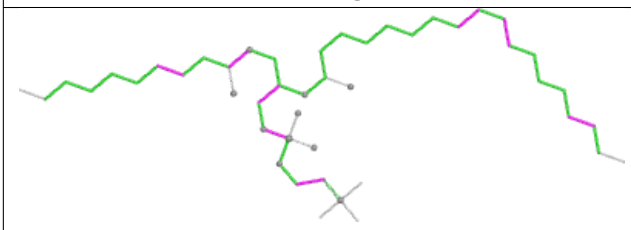
## Ligand POV A 5108



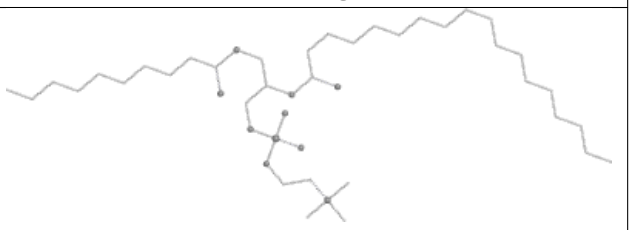
Bond lengths



Bond angles

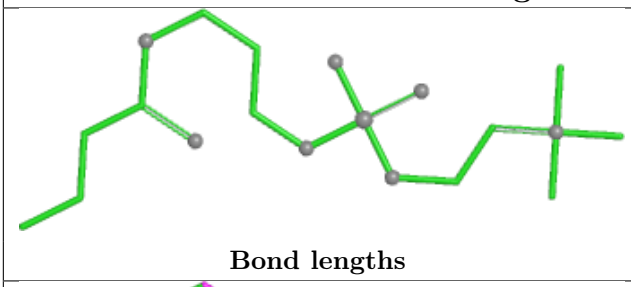


Torsions

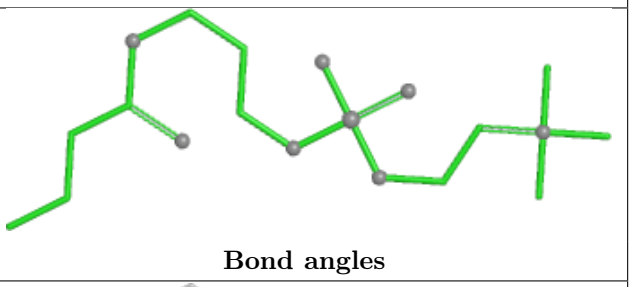


Rings

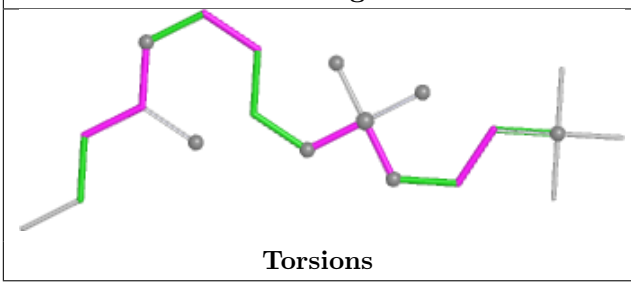
## Ligand POV A 5111



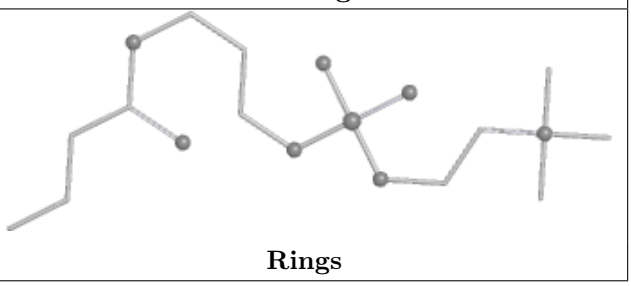
Bond lengths



Bond angles

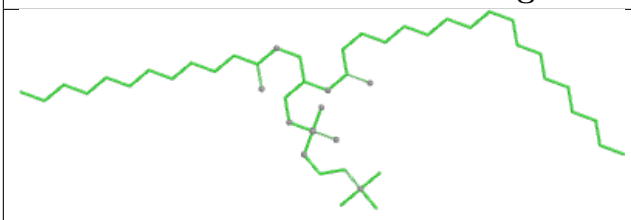


Torsions

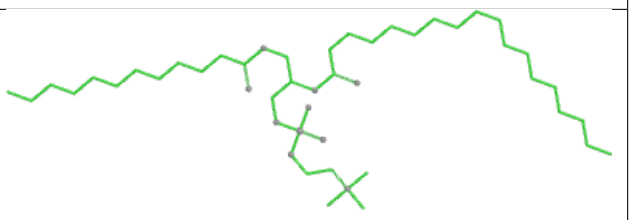


Rings

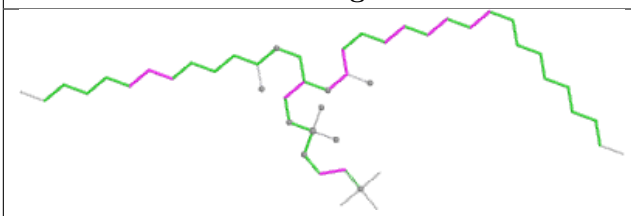
## Ligand POV J 5106



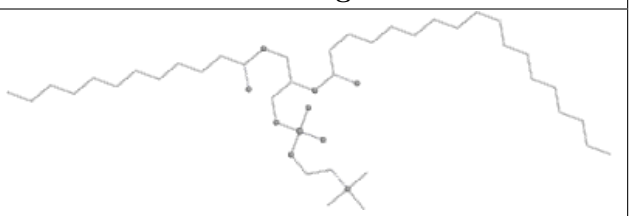
Bond lengths



Bond angles

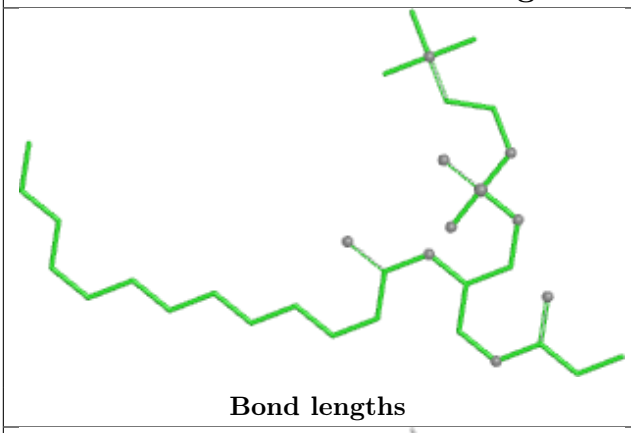


Torsions

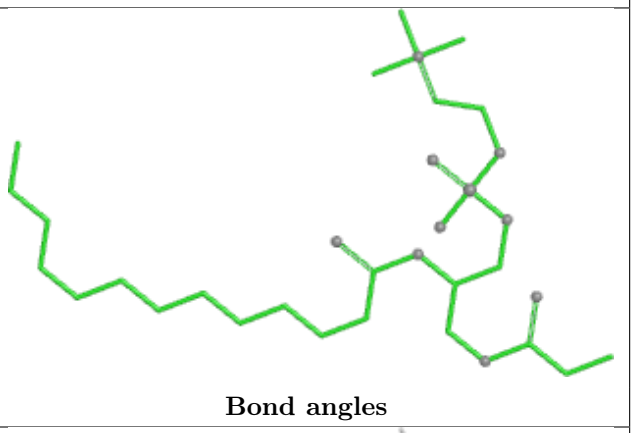


Rings

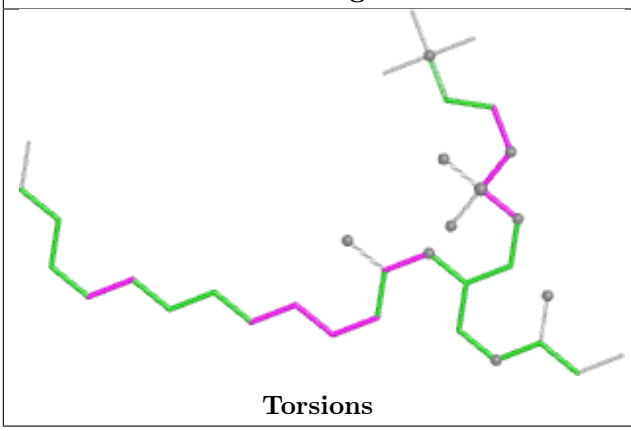
**Ligand POV J 5122**



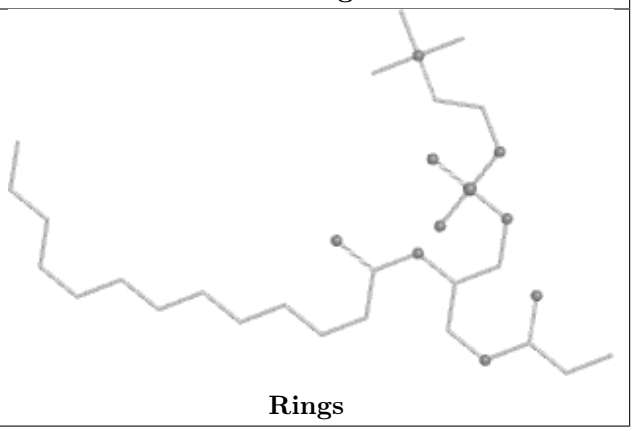
Bond lengths



Bond angles

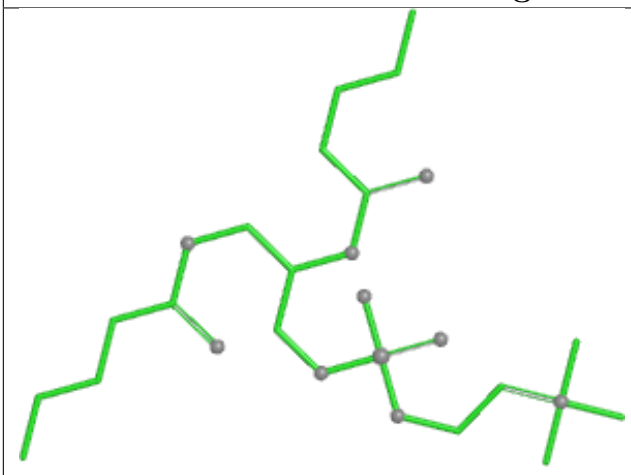


Torsions

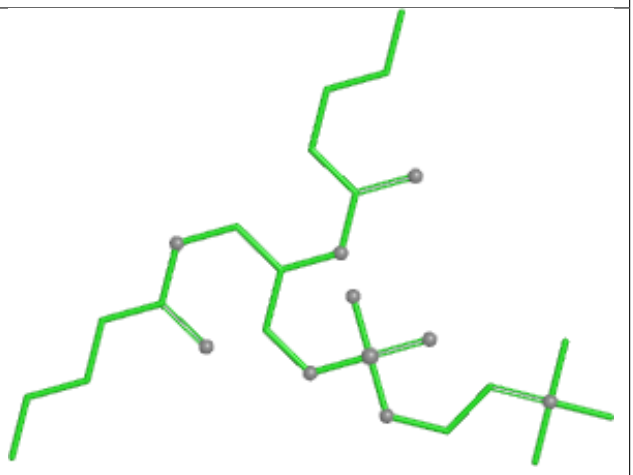


Rings

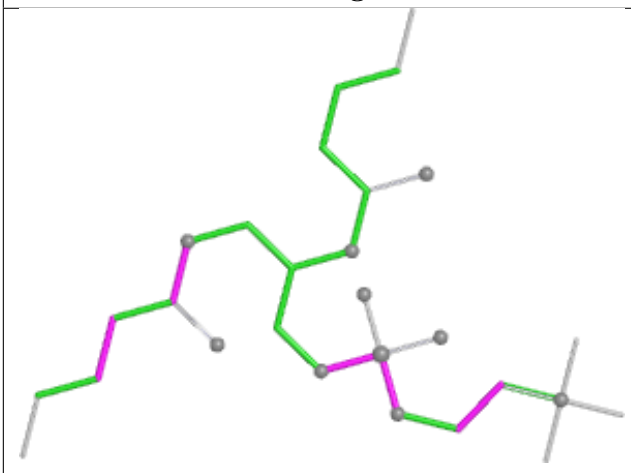
**Ligand POV A 5113**



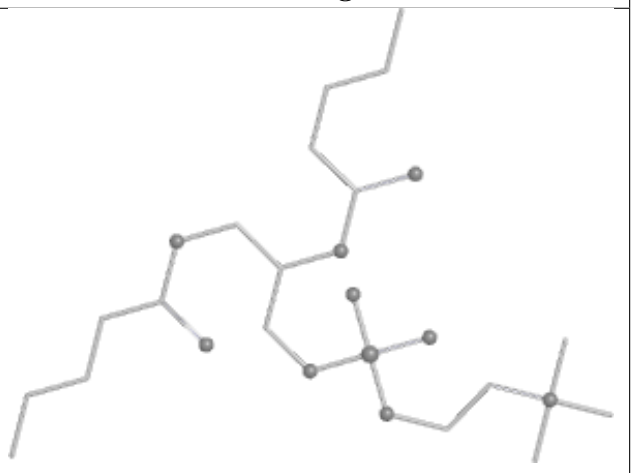
**Bond lengths**



**Bond angles**

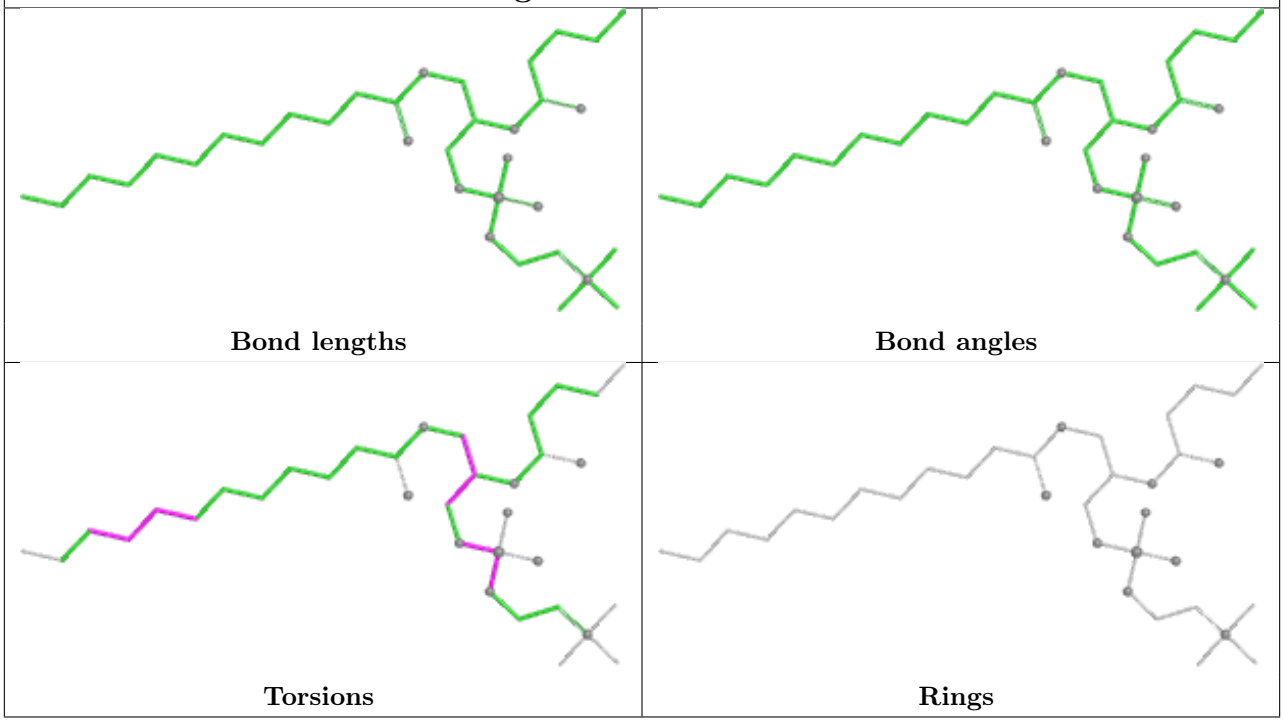


**Torsions**

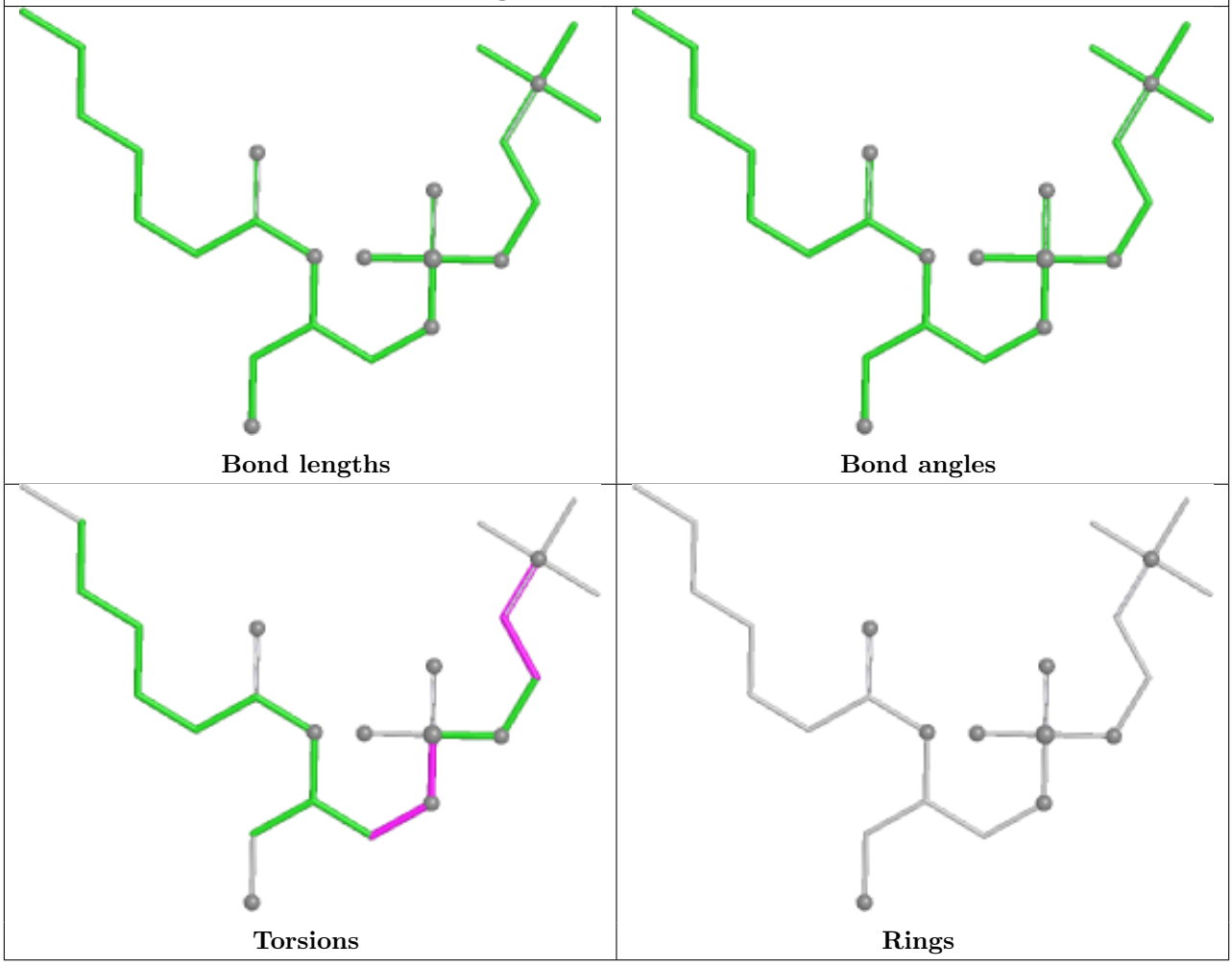


**Rings**

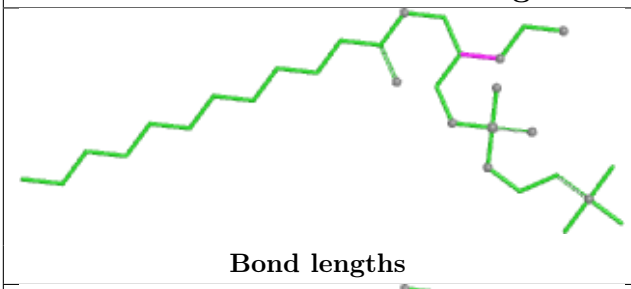
## Ligand POV A 5112



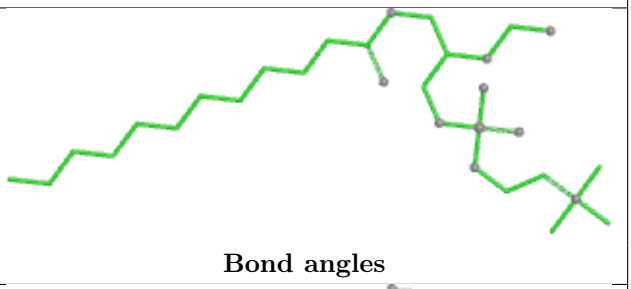

## Ligand POV A 5114



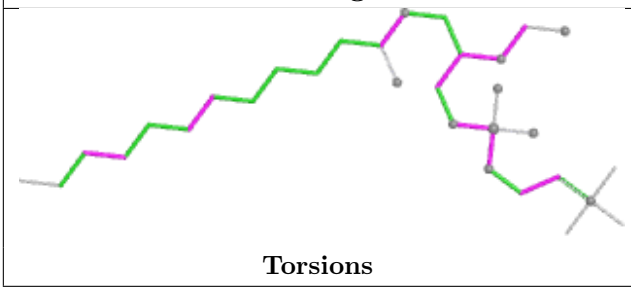
**Ligand POV G 5122**



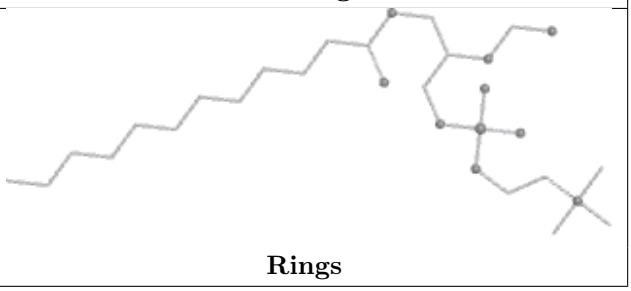
Bond lengths



Bond angles

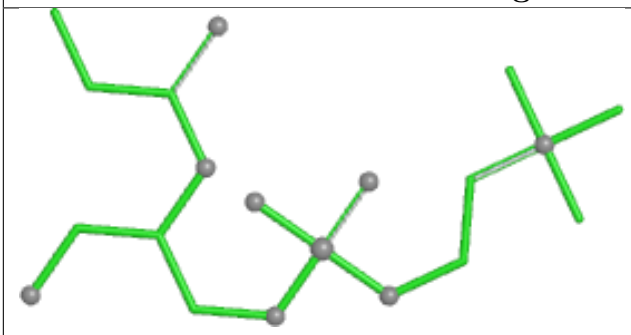


Torsions

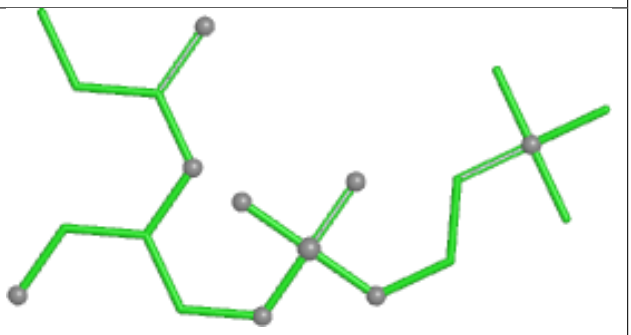


Rings

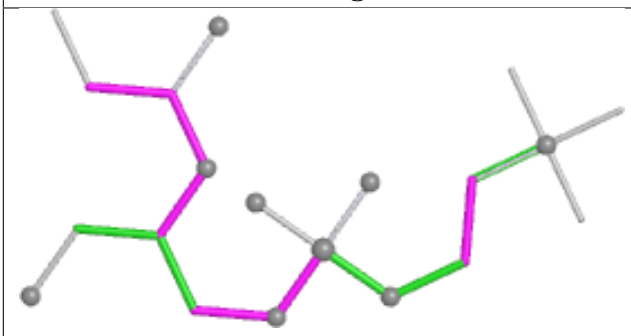
**Ligand POV G 5113**



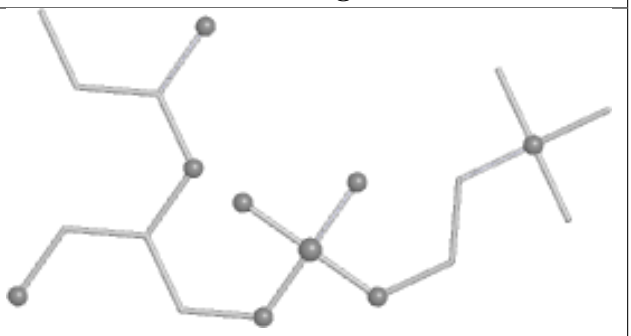
Bond lengths



Bond angles

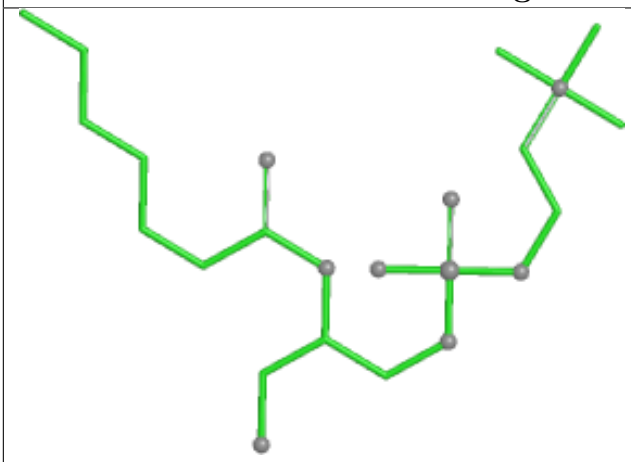


Torsions

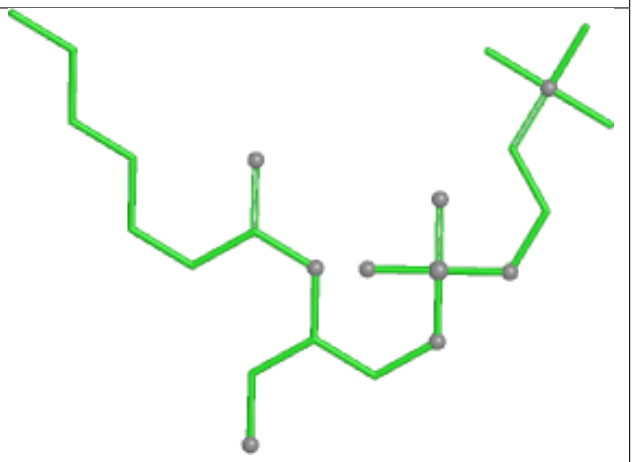


Rings

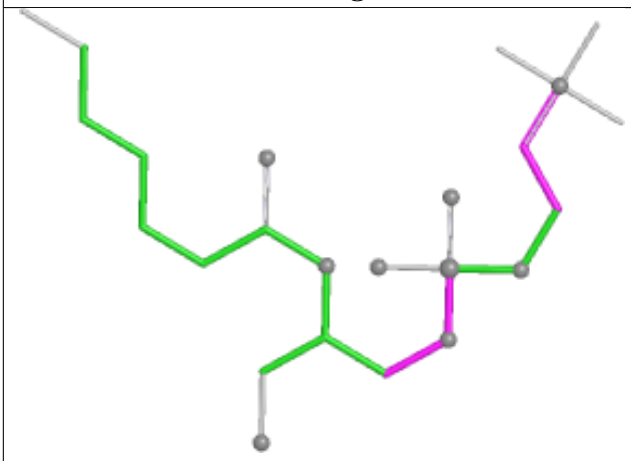
## Ligand POV C 5117



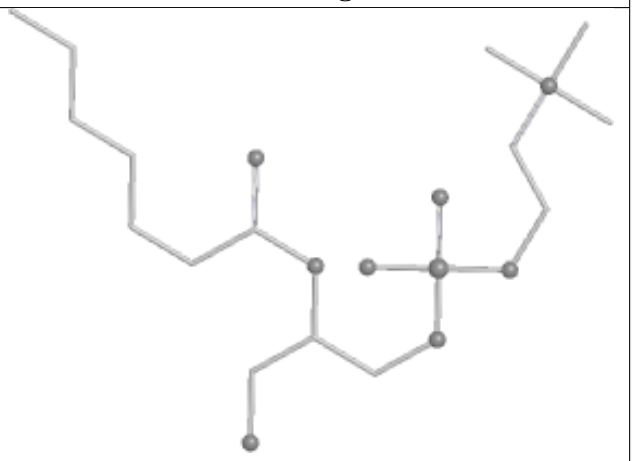
Bond lengths



Bond angles

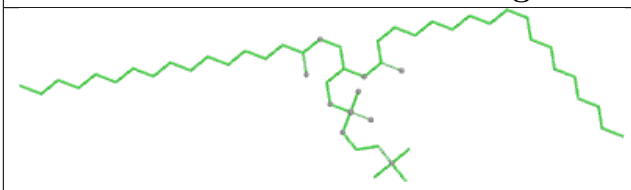


Torsions

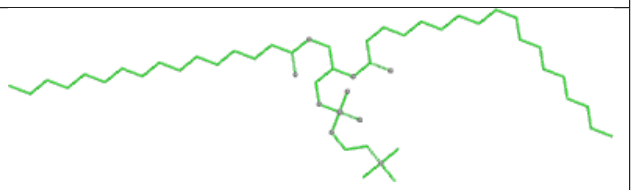


Rings

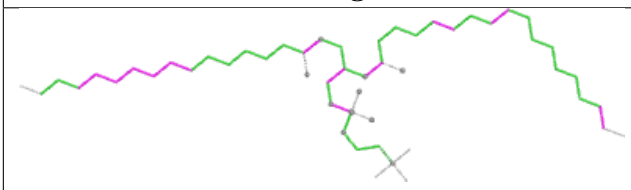
## Ligand POV G 5119



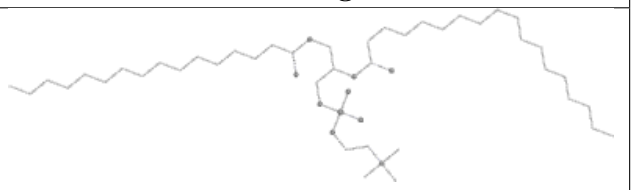
Bond lengths



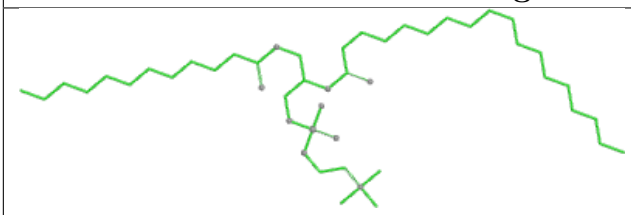
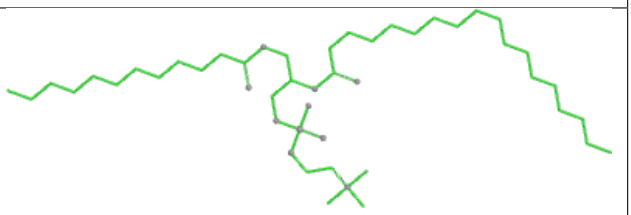
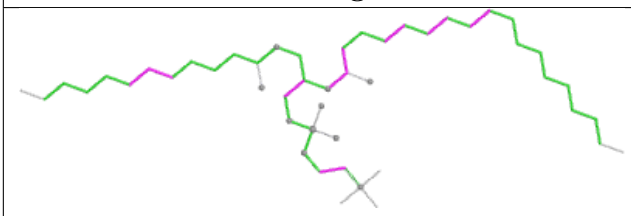
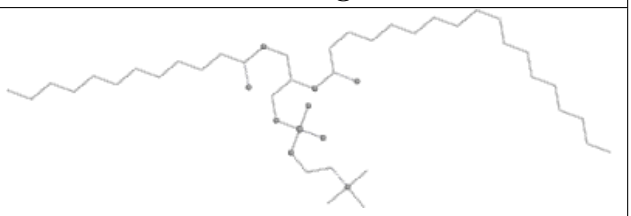
Bond angles

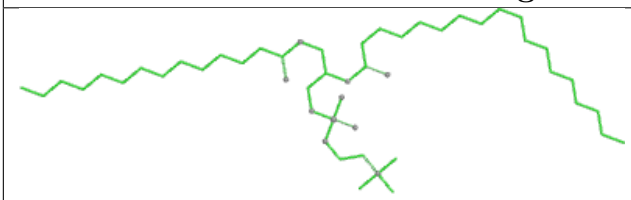
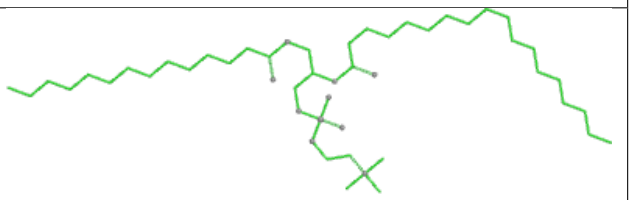
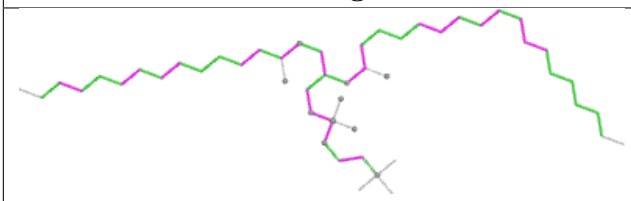
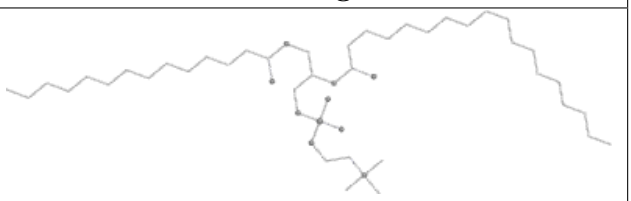


Torsions

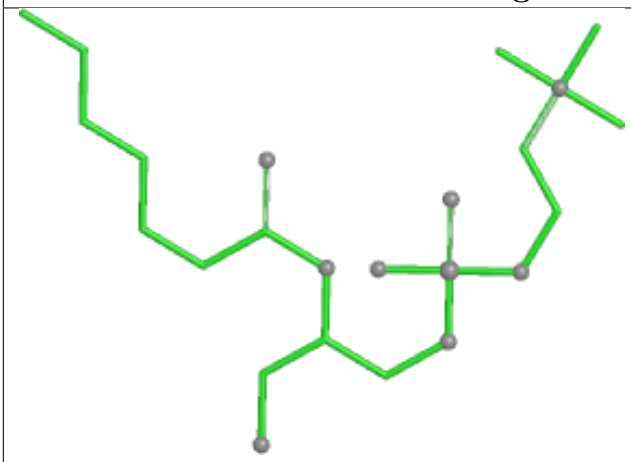


Rings

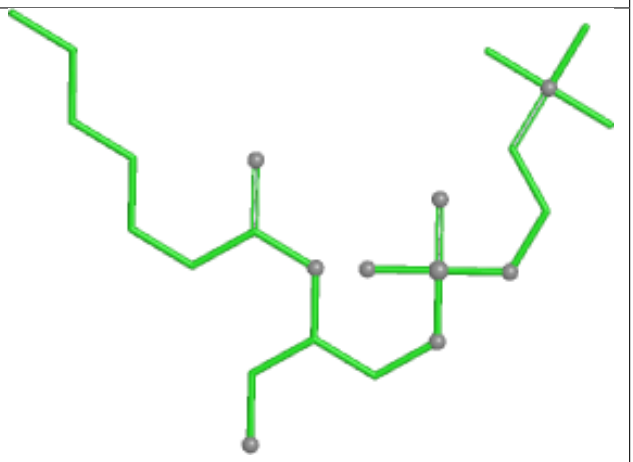
| Ligand POV A 5121 | |
|---|---|
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

| Ligand POV J 5114 | |
|---|---|
|  Bond lengths |  Bond angles |
|  Torsions |  Rings |

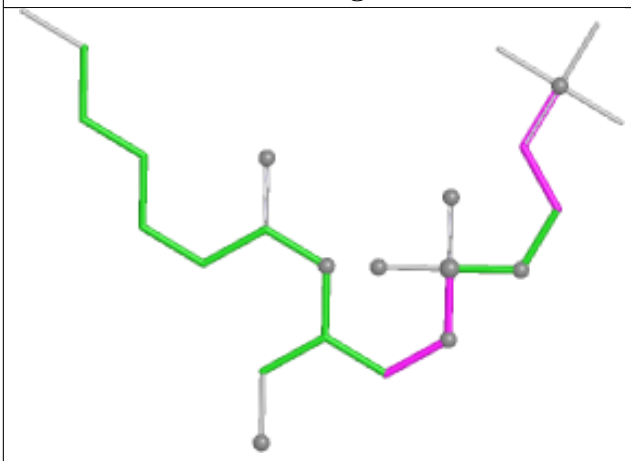
## Ligand POV G 5117



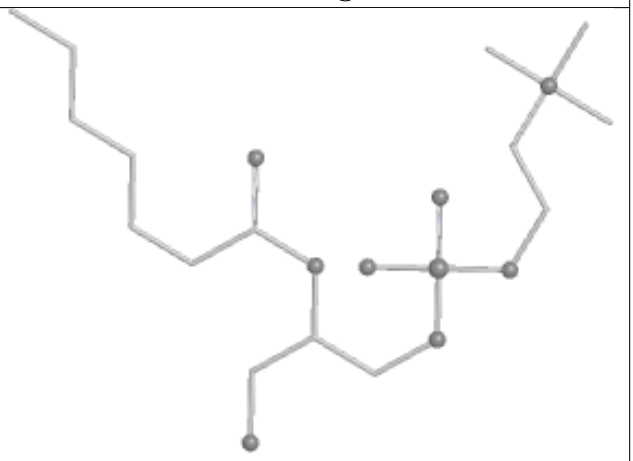
Bond lengths



Bond angles

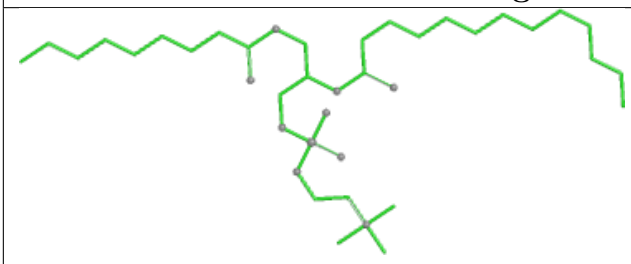


Torsions

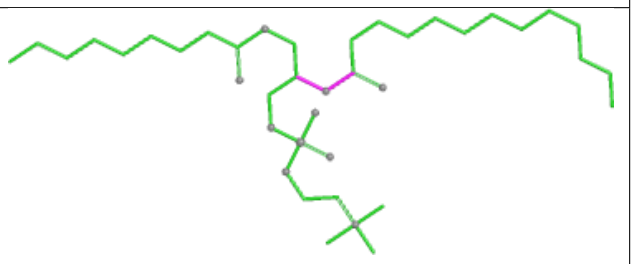


Rings

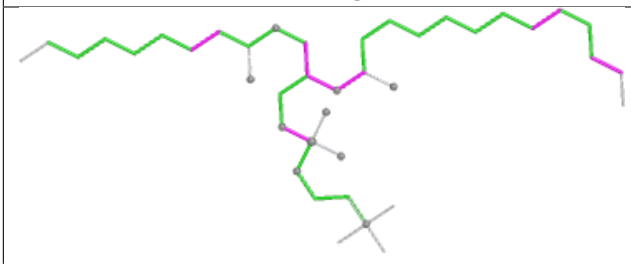
## Ligand POV G 5101



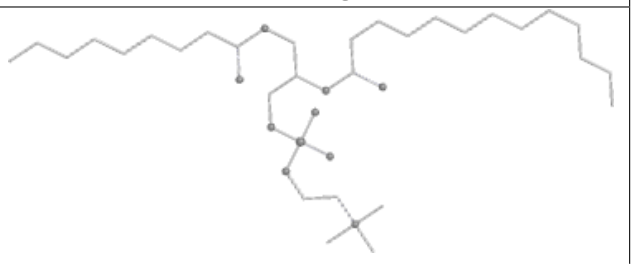
Bond lengths



Bond angles

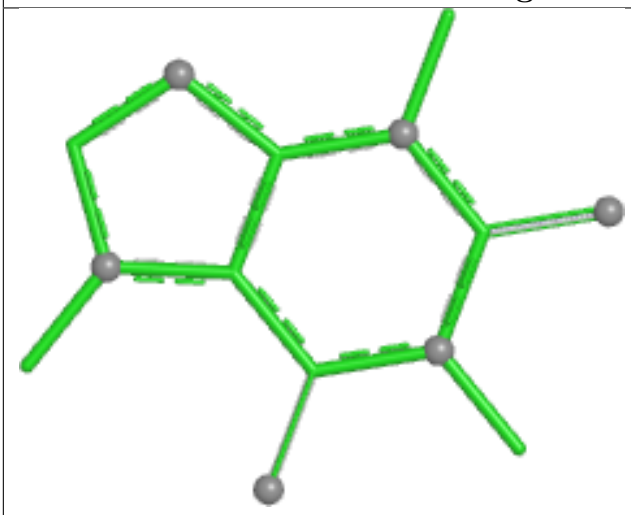


Torsions

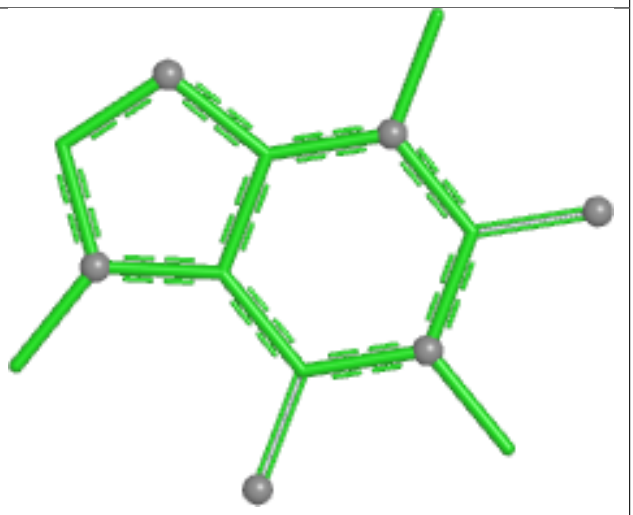


Rings

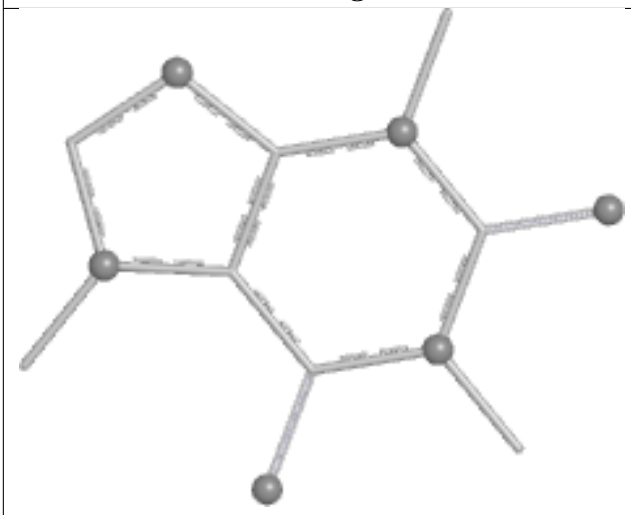
**Ligand CFF G 5106**



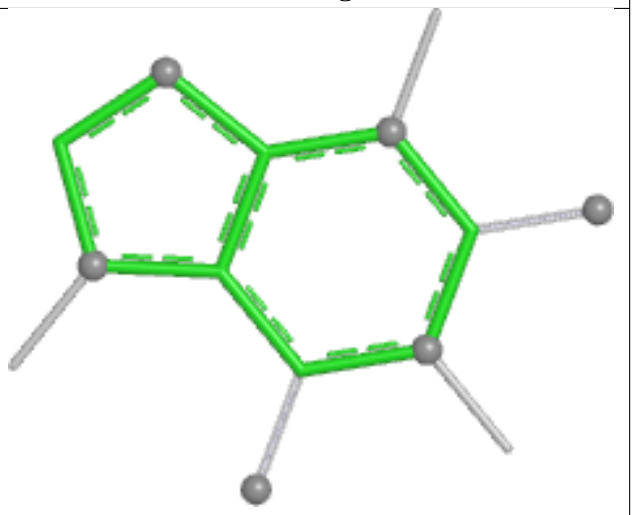
**Bond lengths**



**Bond angles**

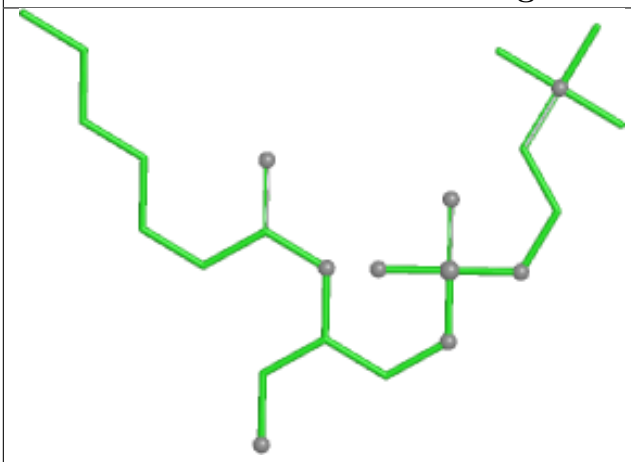


**Torsions**

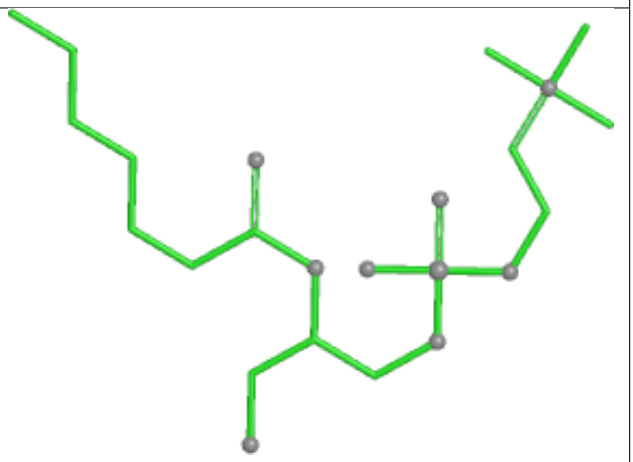


**Rings**

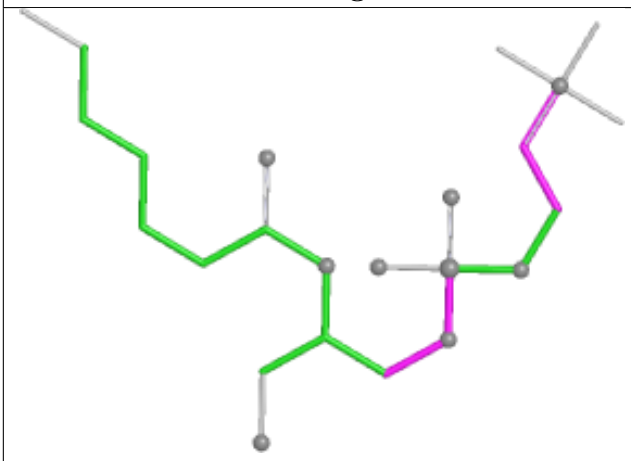
## Ligand POV J 5121



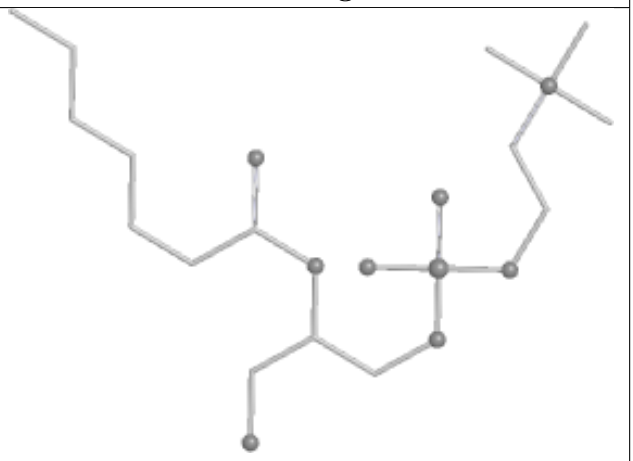
Bond lengths



Bond angles

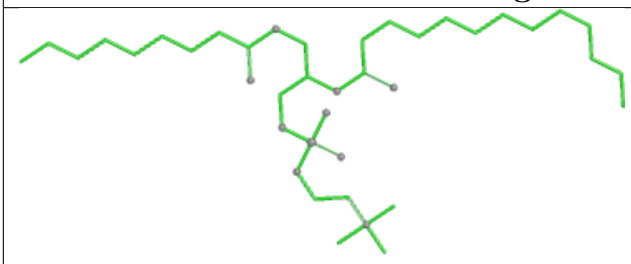


Torsions

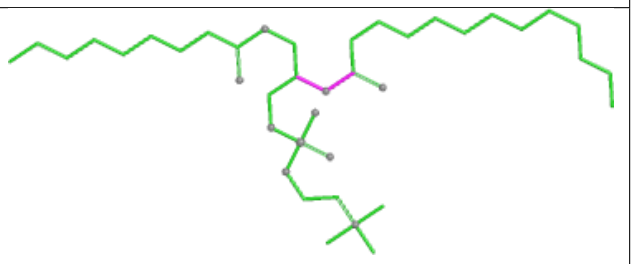


Rings

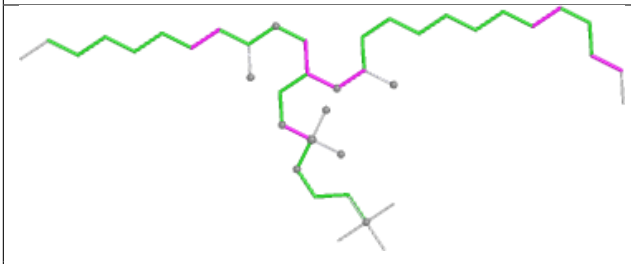
## Ligand POV C 5101



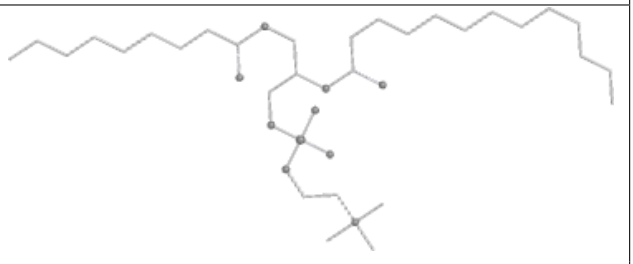
Bond lengths



Bond angles

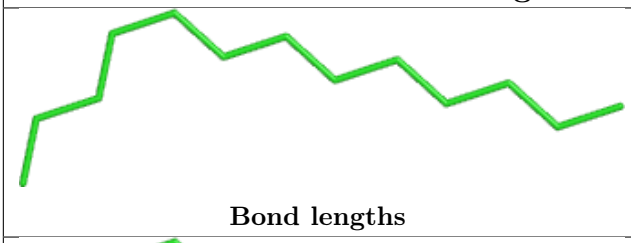


Torsions

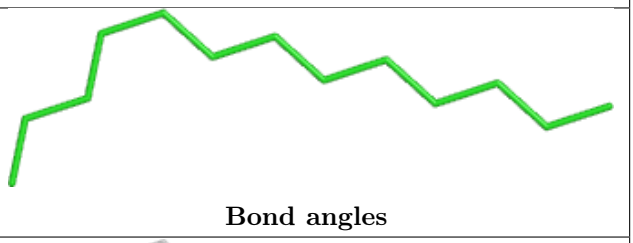


Rings

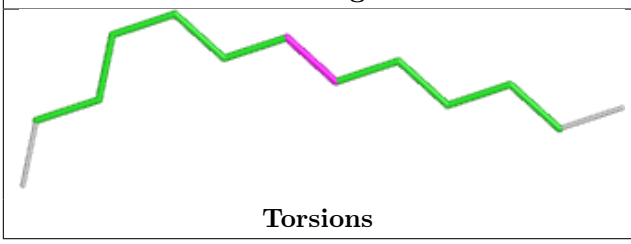
## Ligand POV C 5103



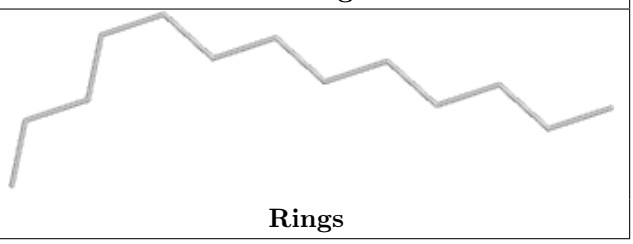
Bond lengths



Bond angles

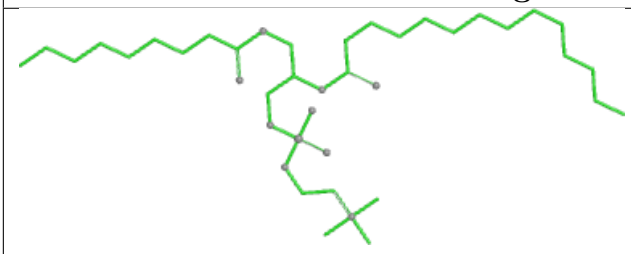


Torsions

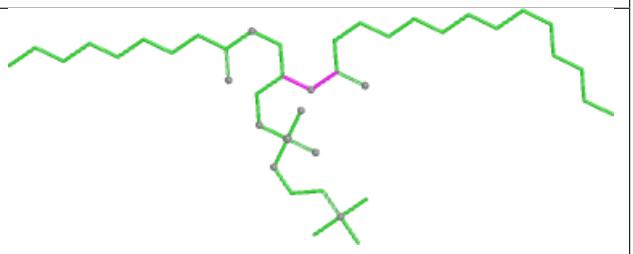


Rings

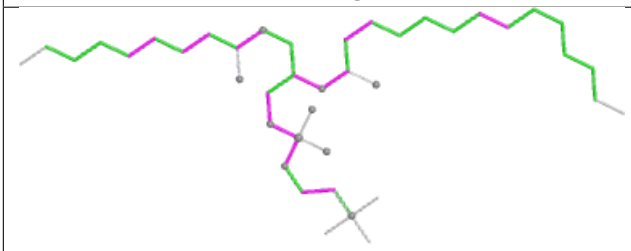
## Ligand POV A 5118



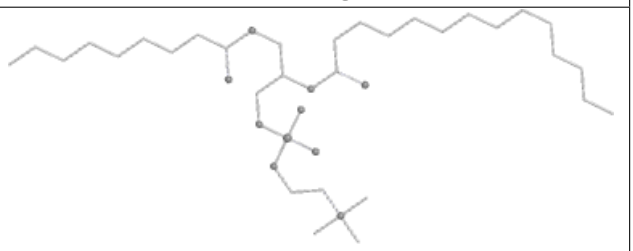
Bond lengths



Bond angles

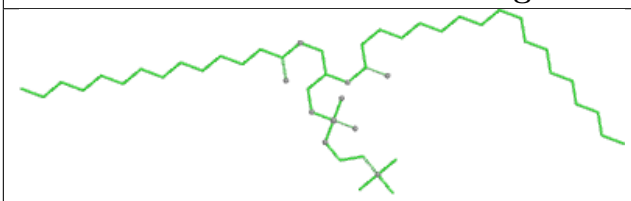


Torsions

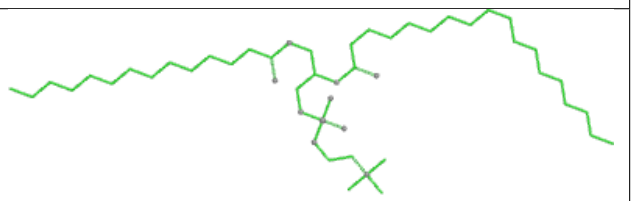


Rings

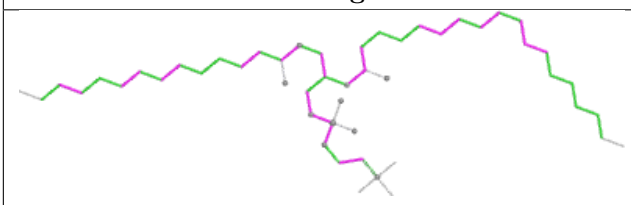
## Ligand POV C 5110



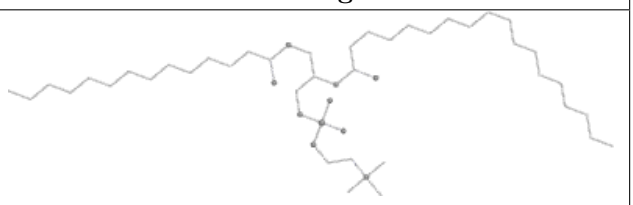
Bond lengths



Bond angles

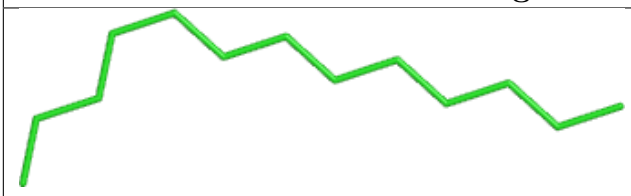


Torsions

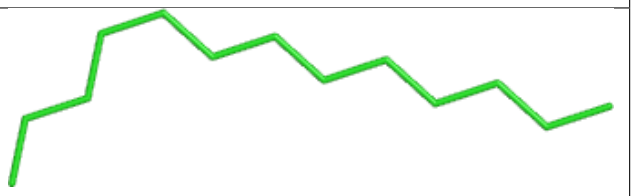


Rings

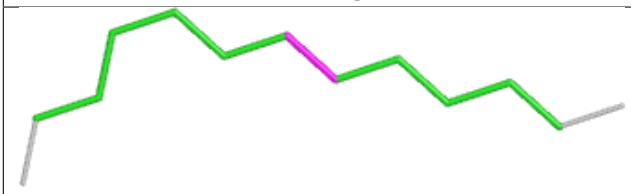
## Ligand POV G 5103



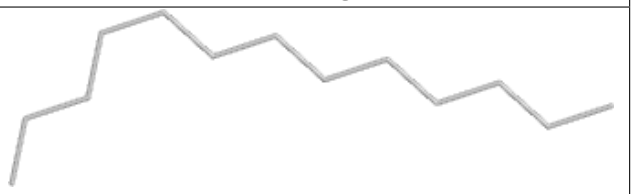
Bond lengths



Bond angles

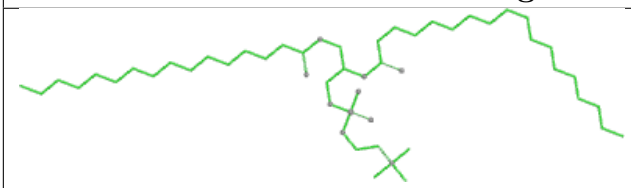


Torsions

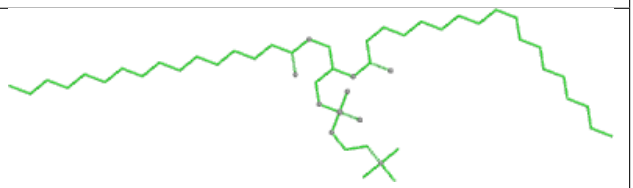


Rings

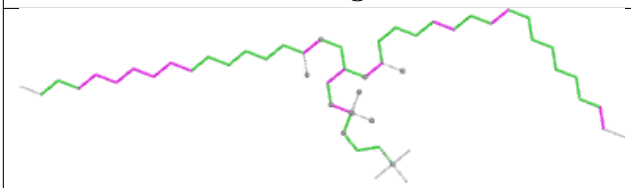
## Ligand POV J 5101



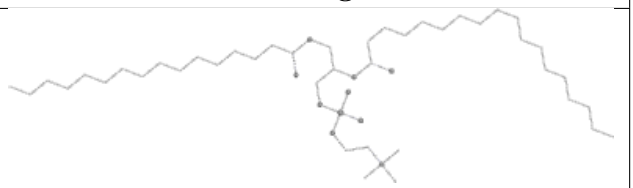
Bond lengths



Bond angles

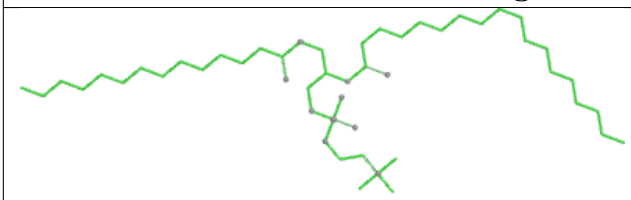


Torsions

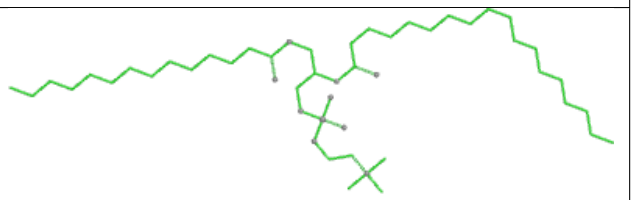


Rings

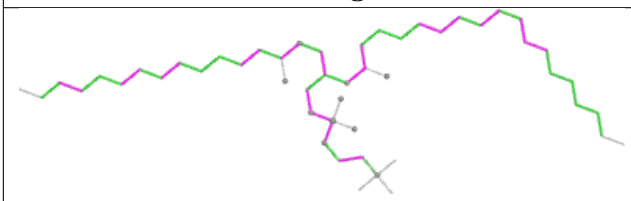
## Ligand POV G 5110



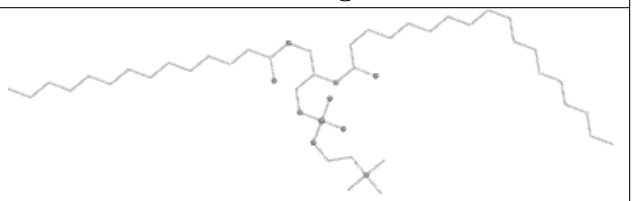
Bond lengths



Bond angles

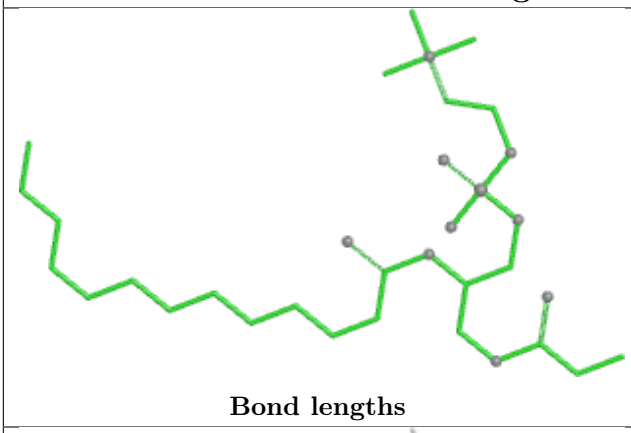


Torsions

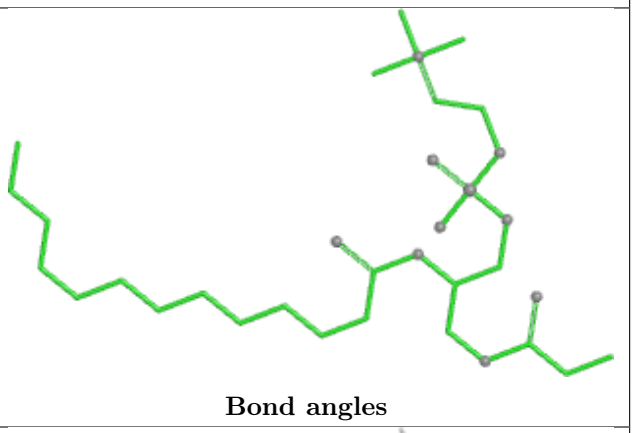


Rings

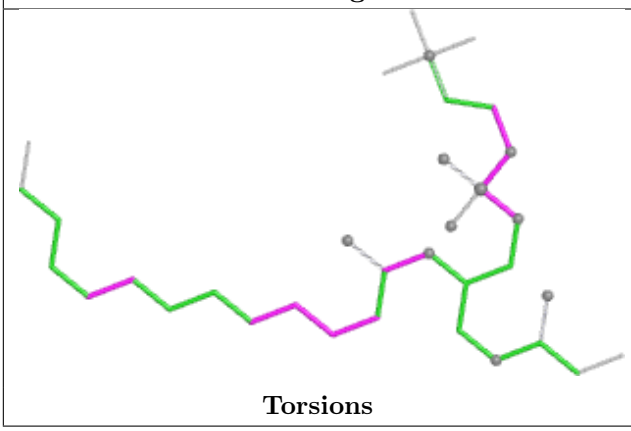
**Ligand POV G 5118**



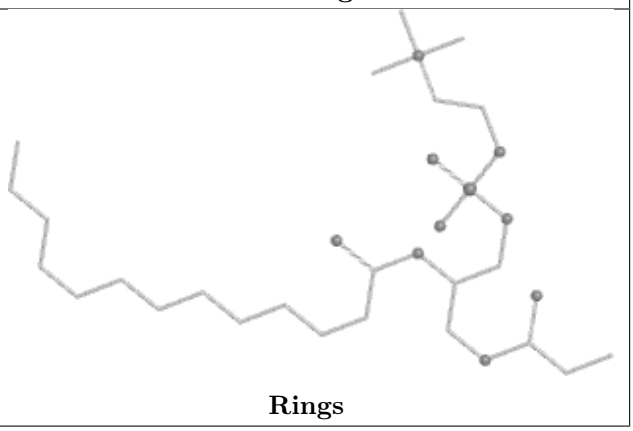
Bond lengths



Bond angles

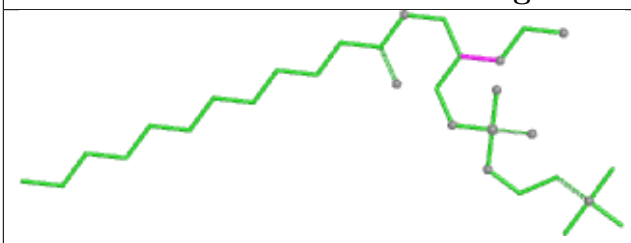


Torsions

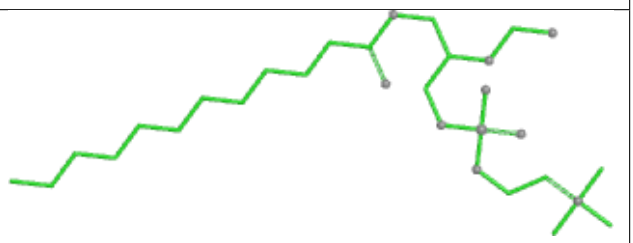


Rings

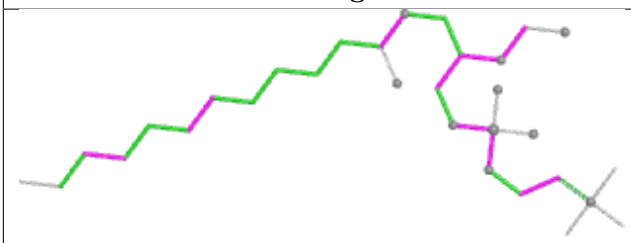
**Ligand POV A 5119**



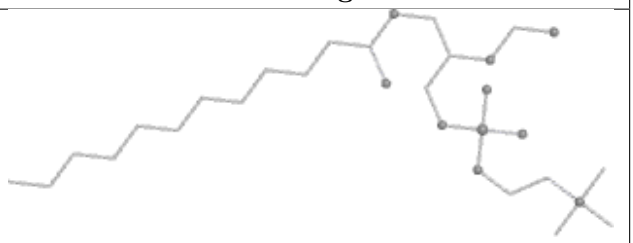
Bond lengths



Bond angles

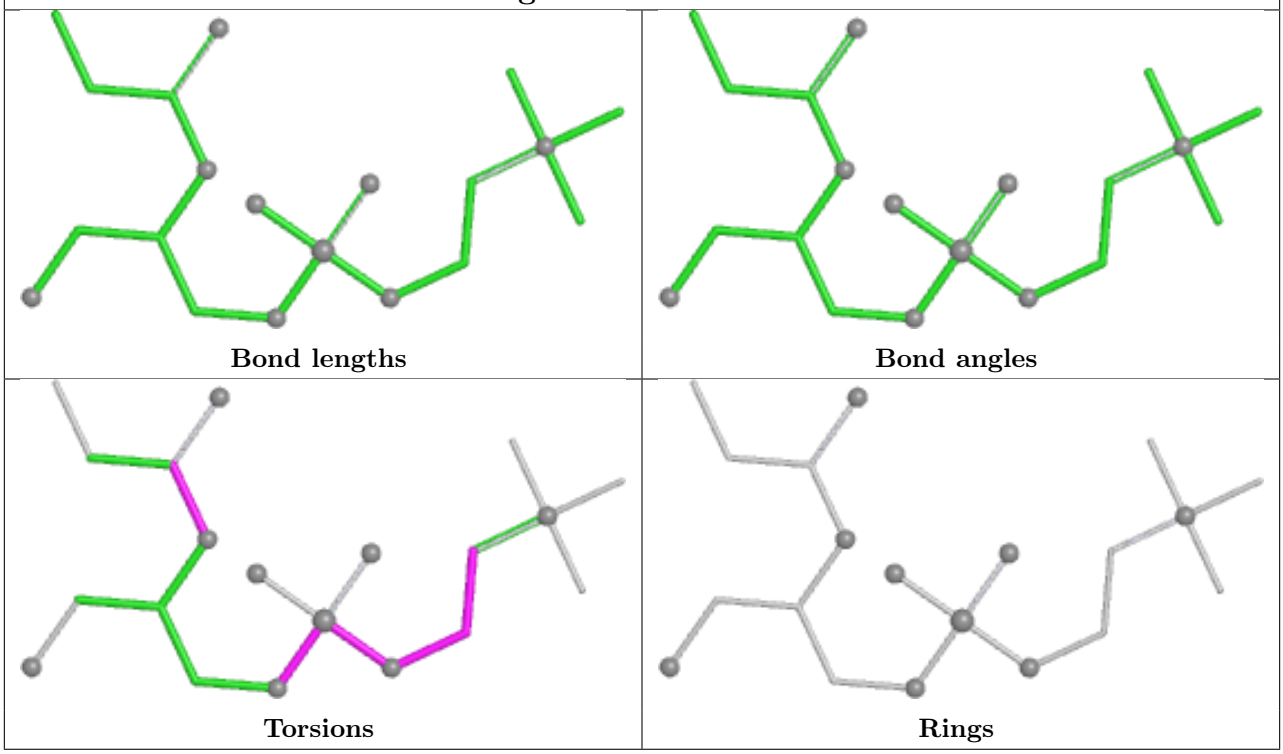


Torsions

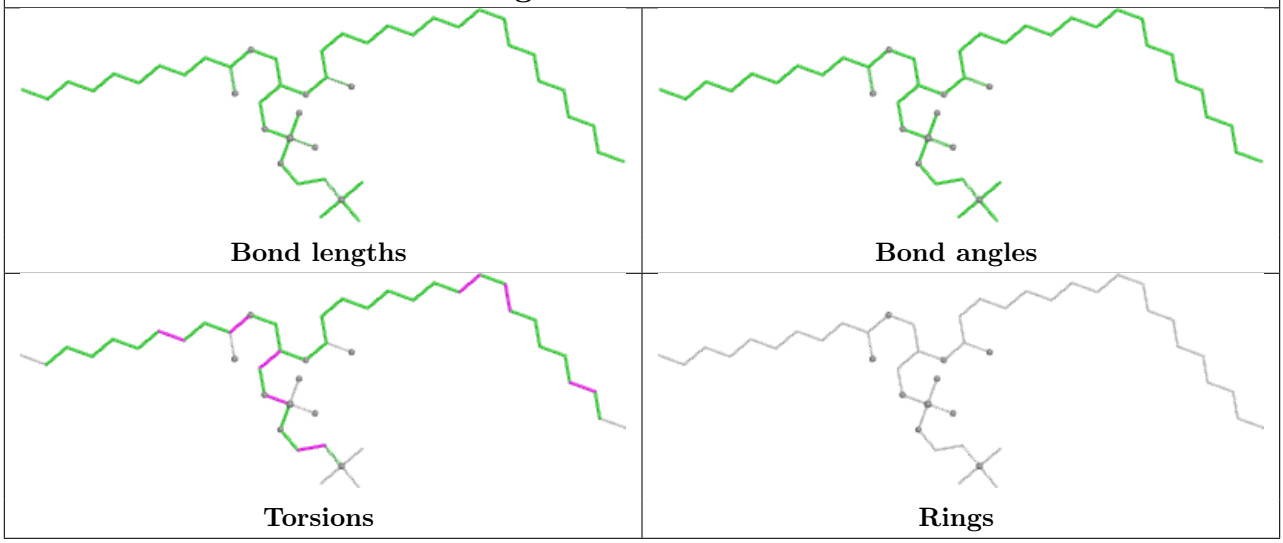


Rings

**Ligand POV J 5116**




**Ligand POV C 5111**




## 5.7 Other polymers (i)

There are no such residues in this entry.

## 5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

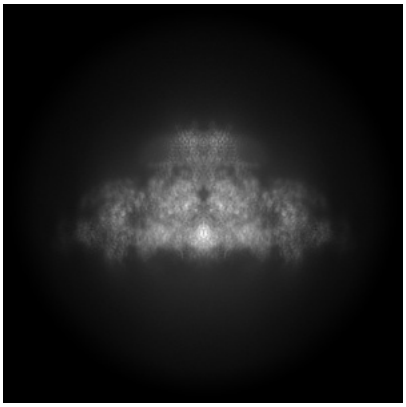
# 6 Map visualisation

This section contains visualisations of the EMDB entry EMD-52085. These allow visual inspection of the internal detail of the map and identification of artifacts.

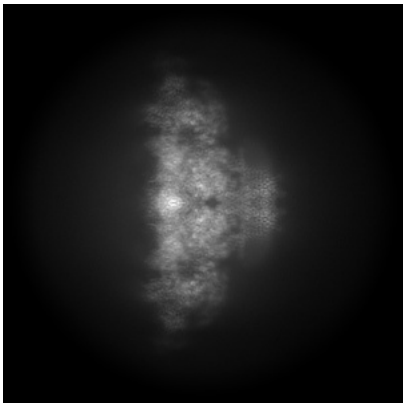
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

## 6.1 Orthogonal projections

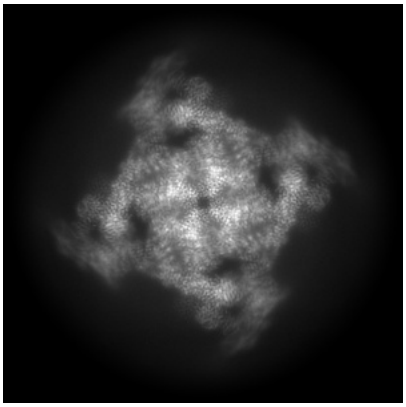
### 6.1.1 Primary map



X



Y

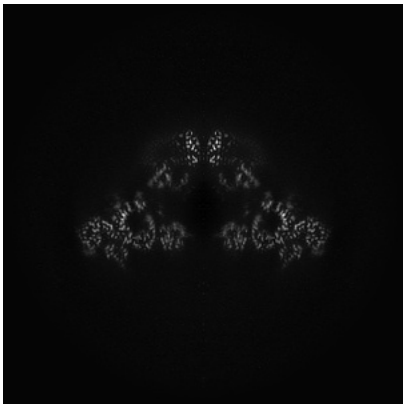


Z

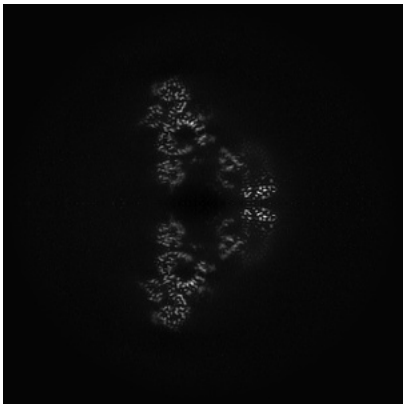
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices

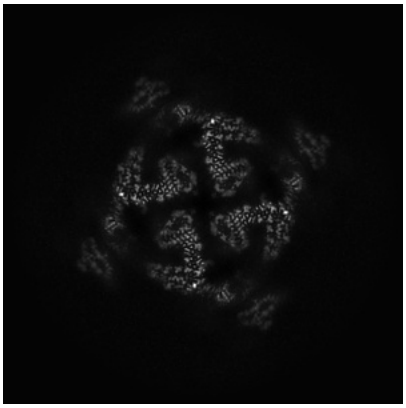
### 6.2.1 Primary map



X Index: 168



Y Index: 168



Z Index: 168

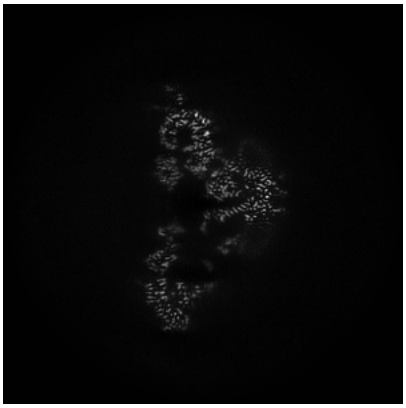
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices (i)

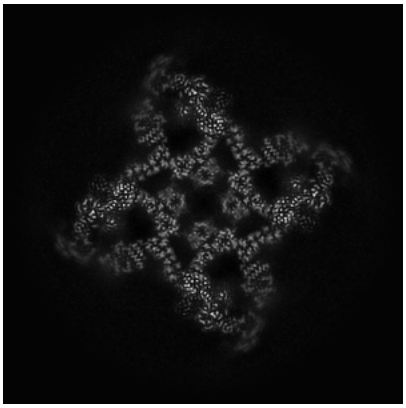
### 6.3.1 Primary map



X Index: 161



Y Index: 161

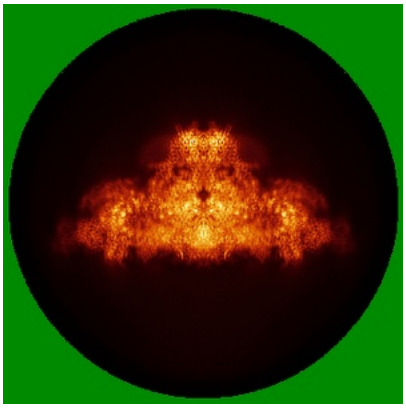


Z Index: 144

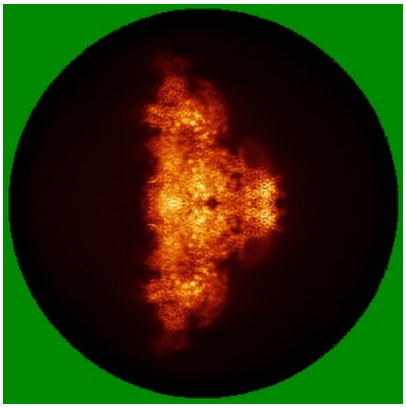
The images above show the largest variance slices of the map in three orthogonal directions.

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

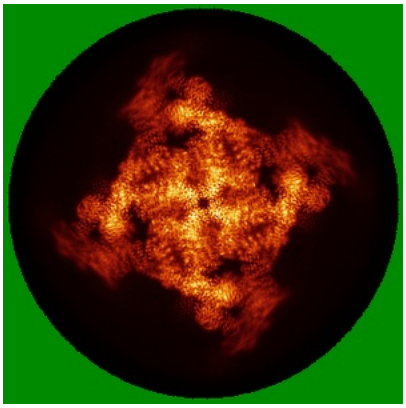
### 6.4.1 Primary map



X



Y

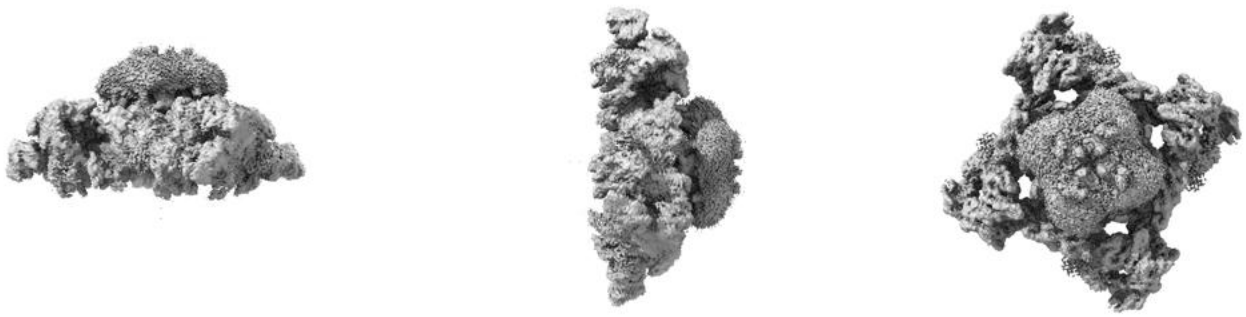


Z

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

## 6.5 Orthogonal surface views (i)

### 6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.3. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

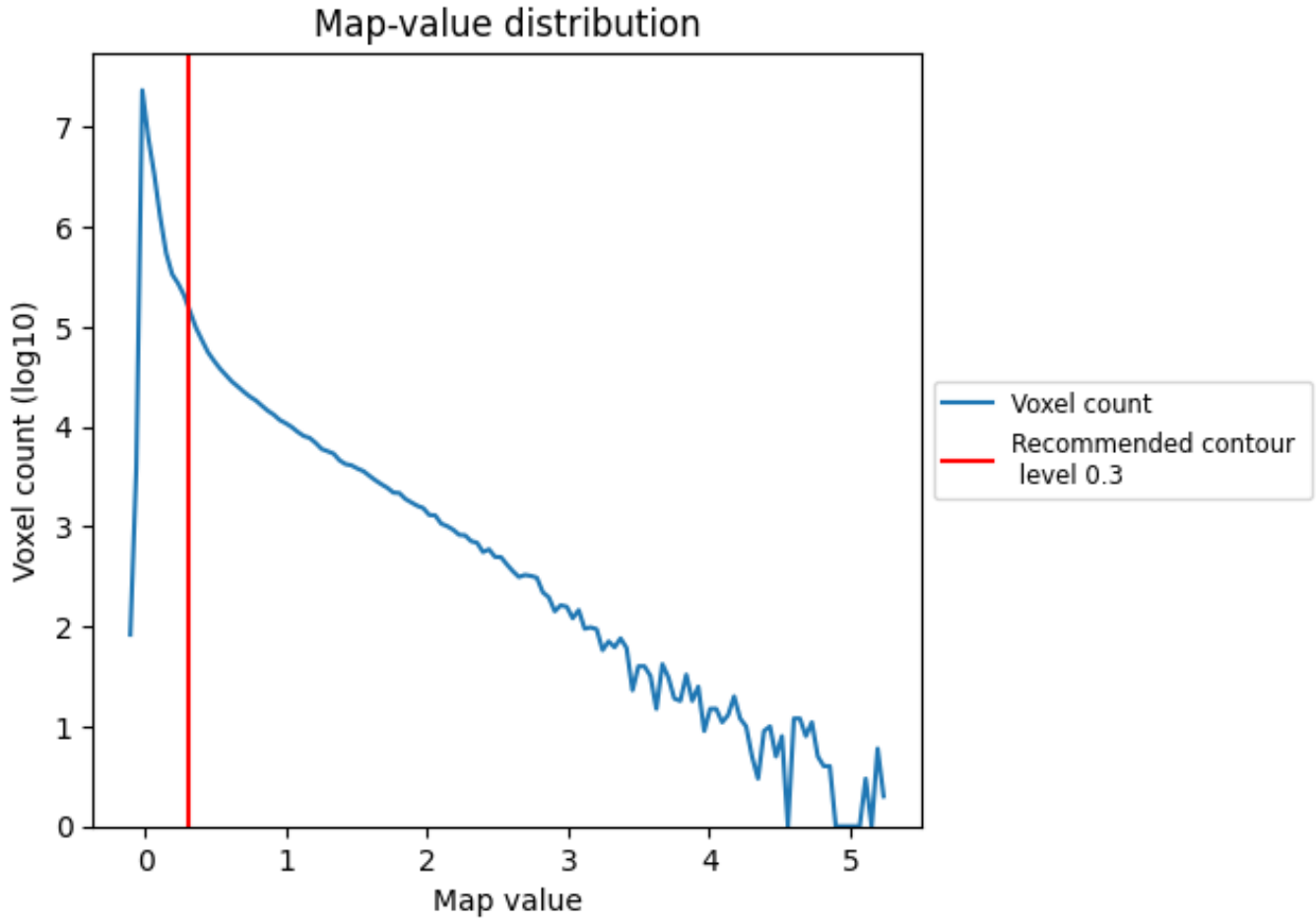
## 6.6 Mask visualisation (i)

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

# 7 Map analysis

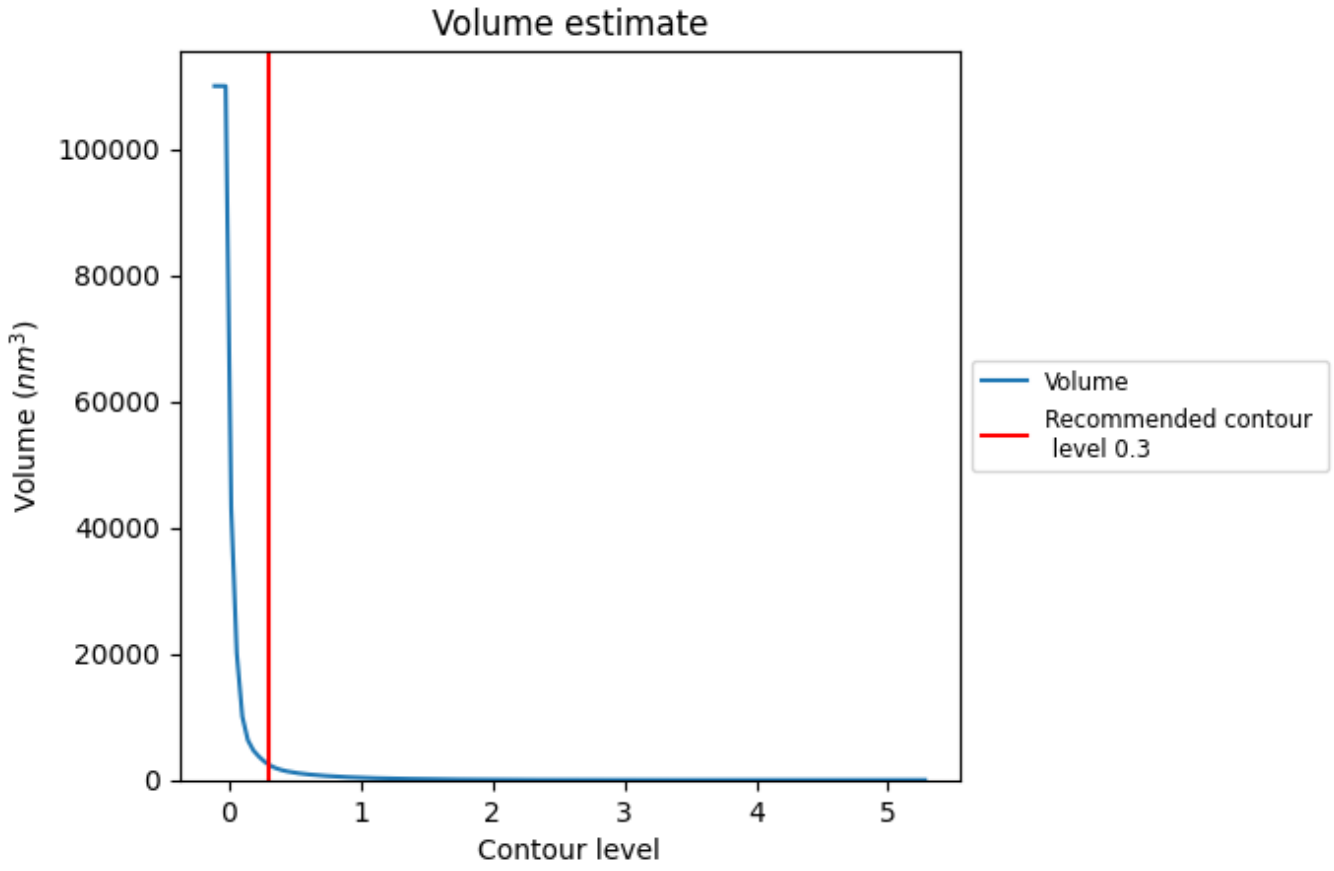
This section contains the results of statistical analysis of the map.

## 7.1 Map-value distribution




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

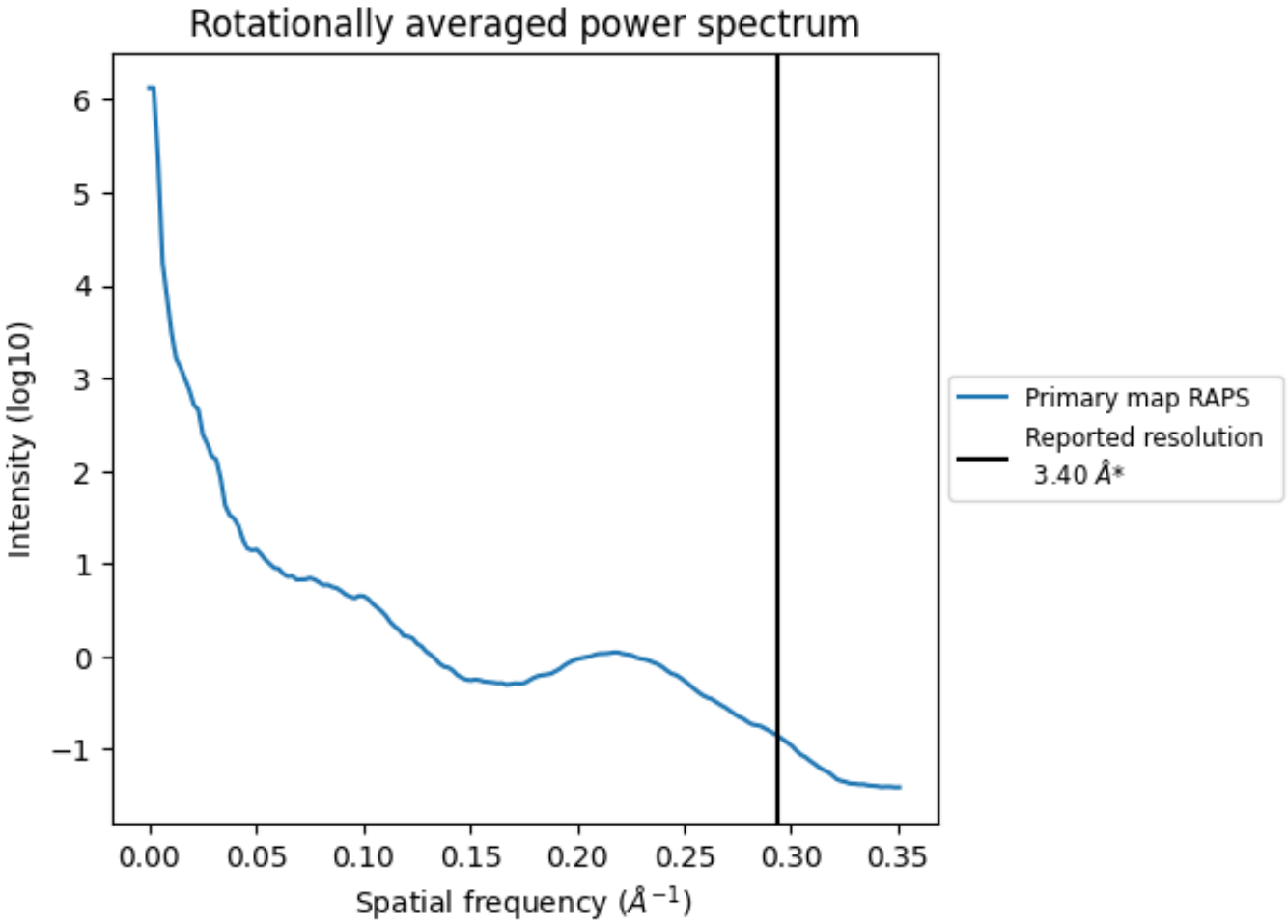
## 7.2 Volume estimate




The volume at the recommended contour level is 2518 $nm^3$; this corresponds to an approximate mass of 2275 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 0.294 Å$^{-1}$

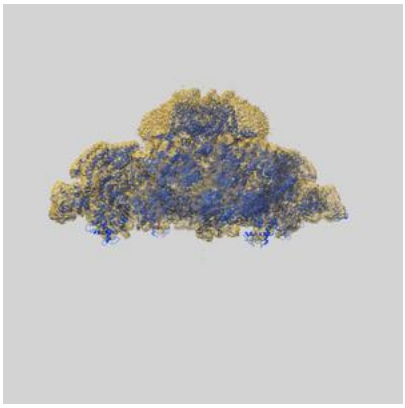
# 8 Fourier-Shell correlation (i)

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

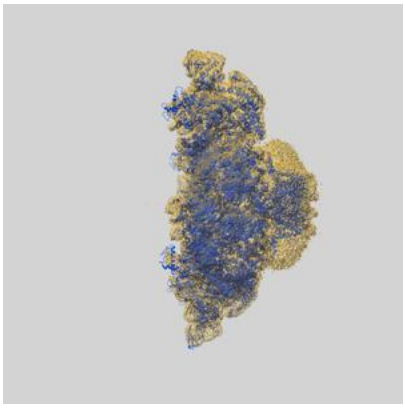
# 9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-52085 and PDB model 9HEO. Per-residue inclusion information can be found in section 3 on page 11.

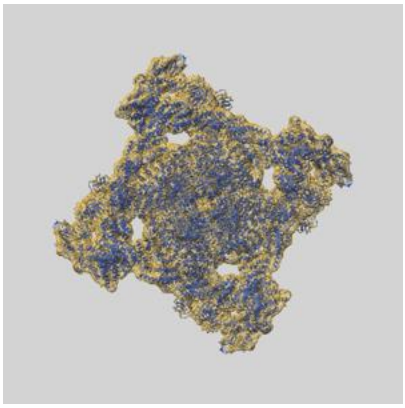
## 9.1 Map-model overlay



X



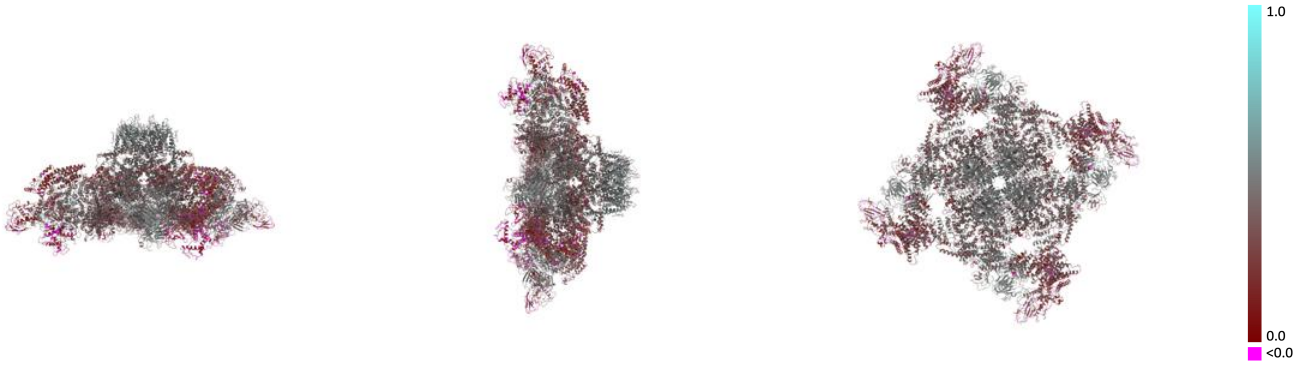
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.3 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.

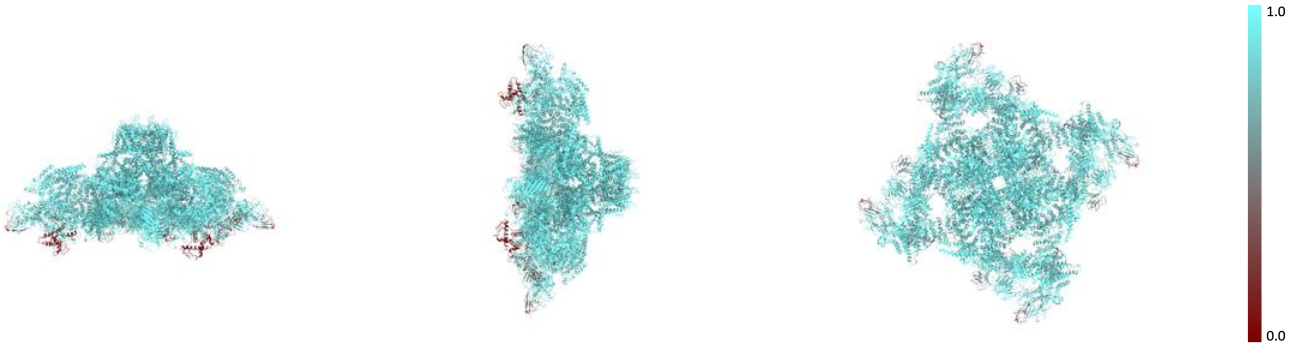
## 9.2 Q-score mapped to coordinate model (i)




X Y Z

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

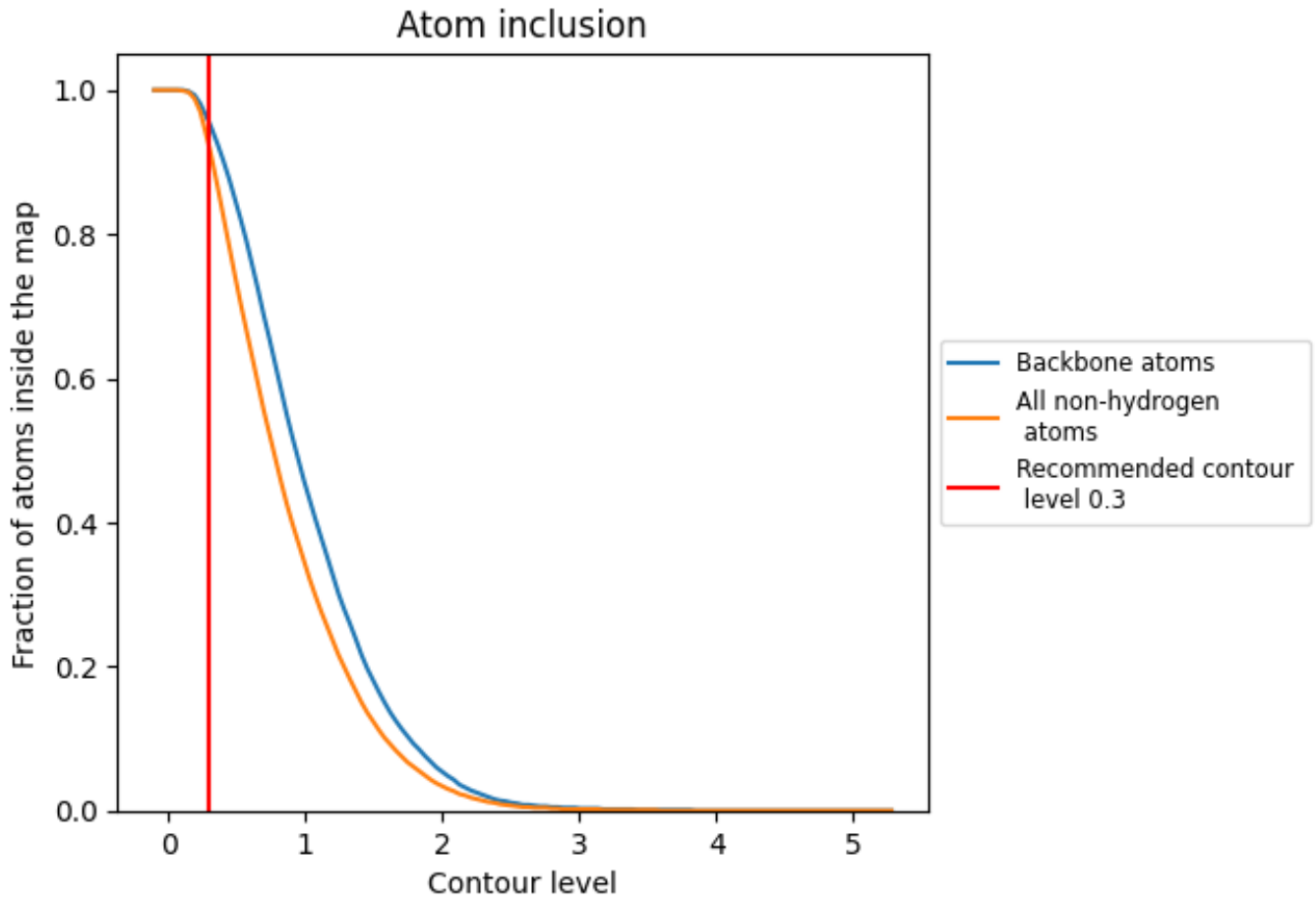
## 9.3 Atom inclusion mapped to coordinate model (i)




X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.3).

## 9.4 Atom inclusion (i)




At the recommended contour level, 95% of all backbone atoms, 92% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.3) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion | Q-score |
|---|---|---|
| All | 0.9180 | 0.3600 |
| A | 0.9340 | 0.3650 |
| B | 0.6020 | 0.1630 |
| C | 0.9340 | 0.3660 |
| D | 0.6020 | 0.1660 |
| E | 0.6010 | 0.3560 |
| F | 0.5980 | 0.3610 |
| G | 0.9340 | 0.3650 |
| H | 0.6160 | 0.1670 |
| I | 0.6080 | 0.3710 |
| J | 0.9340 | 0.3650 |
| K | 0.6030 | 0.1660 |
| L | 0.6080 | 0.3670 |

